44th SACI NATIONAL CONVENTION

Chemistry for sustainable development in Africa

STELLENBOSCH

ABSTRACT BOOK

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Message from the SACI president

Dear SACI-44 delegate – on behalf of the South African Chemical Institute (SACI) I would like to warmly welcome you to Stellenbosch University for the 44th SACI National Convention! We are looking forward to getting to know you better, on academic and social levels, and the exciting program for the Convention provides ample opportunities for this to occur!

In terms of thanks and acknowledgements, I would also like to firstly thank all the delegates who registered to take part in this National Convention, the first since SACI-43 which took place under the leadership of the North Section (Gauteng North of the Jukskei river, Limpopo and Mpumalanga) in December 2018 (and more than a pandemic away…) The program, organized by the individual SACI Divisions, enlists a wide array of local and international contributors and we look forward to engaging in the exciting science described in this abstract book - many thanks to the leadership of the SACI Divisions for their time and expertise in putting together their programs. I would also like to wholeheartedly acknowledge all the sponsors of the Convention for their valuable financial support – please visit their presentation booths and stands during the convention and meet up with their representatives. We also look forward to engaging with members of various learned societies including the ACS and RSC! I would also like to highlight that our SACI-44 event contributes to South Africa's participation in the important International Year of Basic Sciences for Sustainable Development (IYBSSD) – special acknowledgement to the Academy of Science of South Africa (ASSAf) and the Department of Science and Innovation (DSI) for including us in their IYBSSD plans.

Finally, I need to specifically thank the following people in terms of their invaluable part in the organization of SACI-44: Debbie Rorich and her organizational team, and Laila Smith, SACI secretary and general "go to" person… you guys "rock"! The Western Cape SACI Section, from which the Local Organizing Committee (LOC) is drawn, deserves specific acknowledgement – under the inspiring leadership of Profs Catharine Esterhuysen (Chair) and Delia Haynes (Co-chair), their hard work and exemplary volunteerism has meant that despite some serious time constraints, an awesome SACI-44 program has been arranged. Hat tips to all the others on the committee: Wade, Andre, Niki, Megan, Gareth, Edith and Peter, and in terms of a bitter-sweet moment, a fond farewell to our dear LOC colleague, Rehana Malgas-Enus, who passed away far too soon in September 2022.

Lastly, dear delegate, I wish you a wonderful, enriching SACI-44 Convention – please enjoy the university, the town, the science and of course the camaraderie of your fellow chemists!

Willem van Otterlo (SACI President)

Message from the chair of the organising committee

Dear SACI-44 delegate,

On behalf of the Organising Committee I am delighted to welcome you to Stellenbosch for this, the 44th National Convention of the South African Chemical Institute and flagship event in the South African celebration of the International Year of Basic Sciences for Sustainable Development. Thank you for participating – after all, it is your contribution that impacts the most on the success of a conference such as this! The SACI-44 programme showcases research from all aspects of Chemistry currently studied in South Africa, bringing together both young and experienced scientists through plenary, keynote and invited lectures as well is contributed orals, poster flash presentations and posters. In addition, we have some exciting special sessions on breaking barriers in science, advice on publishing and how we as members of a learned society like SACI can contribute to sustainable development in Africa through Chemistry. As the first face-to-face conference under the auspices of SACI since the COVID-19 pandemic we have specifically designed the programme to give delegates the opportunity to interact with old friends and make new contacts, so we encourage you to participate at every chance. I wish you a successful week of conferencing, and an enjoyable time in Stellenbosch!

Best wishes,

Catharine Esterhuysen

Previous SACI Conventions

Convention number	Host Section	Date	City	Chair
43	Northern Gauteng	3 - 7 Dec 2018	Pretoria	Dr Richard Mampa
42	KwaZulu-Natal	29 Nov - 4 Dec 2015	Durban	Prof Bice Martincigh
41	Eastern Cape	1 - 6 Dec 2013	East London	Prof Adebola Oyedeji
40	Gauteng	16 - 21 Jan 2011	Johannesburg	Prof James Darkwa
39	Western Cape	30 Nov - 5 Dec 2008	Stellenbosch	Prof Len Barbour
38	KwaZulu-Natal	3 - 8 Dec 2006	Durban	Prof Sreekanth Jonnalagadda
37	Northern Gauteng	4 - 9 July 2004	Pretoria	Prof Jan Boeyens
36	Eastern Cape	30 June - 5 July 2002	Port Elizabeth	Dr Chris Woolard
35	Transvaal	24 - 29 Sept 2000	Potchefstroom	Prof Ernst Breet
34	Natal	6 - 10 July 1998	Durban	Prof Trevor Letcher
33	Western Cape	29 Jan - 2 Feb 1996	Cape Town	Prof James Bull
32	Northern Transvaal	30 Jan - 3 Feb 1994	Halfway House	Dr Willie van Niekerk
31	Eastern Cape	24 - 27 July 1991	Grahamstown	Prof Trevor Letcher
30	Western Province	15 - 20 Jan 1989	Cape Town	Dr GML Cragg
29	Natal	6 - 10 July 1987	Durban	Prof Mike Laing
28	Western Province	30 Jan - 3 Feb 1984	Stellenbosch	Prof Ivan Green
27	Pretoria Section	25 July - 1 Aug 1980	Pretoria	Dr Jan Boeyens
26	Eastern Cape	1979 (3.5 days)	Port Elizabeth	Prof Andre Goosen
25	Northern Transvaal	31 Jan - 4 Feb 1977	Johannesburg	Dr VM Lovell
24	Natal	14 - 18 July 1975	Durban	Dr Terence MS Higgins

23	Western Province	28 Jan - 1 Feb 1974	Cape Town	Dr GML Cragg
22	Northern Transvaal	3 - 7 July 1972	Pretoria	Dr A Jordaan
21	Eastern Province	1 - 4 Feb 1971	Grahamstown	Dr DEA Rivett
20	Natal	10 - 14 July 1967	Durban	Mr MP Theunissen
19	Western Province	Feb 1966	Stellenbosch	Dr M Lamchen
18	Northern Transvaal	July 1964	Pretoria	Dr TL Webb
17	Eastern Province	15 - 19 July 1963	Port Elizabeth	Mr JM Tucker
16	Natal	July 1962	Pietermaritzburg	Prof Israelstam
15	Natal	17 - 21 July 1961	Durban	Mr JL du Toit
14	Western Province	8 - 12 Feb 1960	Cape Town	Prof LH Ahrens
13	Northern Transvaal	20 - 24 July 1959	Pretoria	Mr CC van der Merwe
12	Eastern Province	14 - 18 July 1958	Port Elizabeth	VA Morris
11	Natal	8 - 12 July 1957	Durban / Pietermaritzburg	Mr JE Worsdale
10	Transvaal	24 - 29 Sept 1956	Johannesburg	Dr SS Israelstam
9	Western Cape	6 - 10 Feb 1955	Cape Town	Dr Lamchen
8	Northern Transvaal	30 Aug - 4 Sept 1954	Pretoria	Dr AJ Petrick
7	Natal	6 - 10 July 1953	Durban	Dr GC Scully
6	Transvaal	30 June - 4 July 1952	Johannesburg	Dr SS Israelstam
5	Eastern Cape	1 - 6 October 1951	Port Elizabeth	Mr L-F Addis-Smith
4	Western Cape	September 1950	Cape Town	Mr AL Abbott
3	Natal	20 - 23 July 1949	Durban	Mr A Gregory
2	Northern Transvaal	June 1948 (4 days)	Pretoria	Dr ER Orchard
1	Transvaal	27 - 29 June 1947	Johannesburg	Mr CF Lindemann

Organising committee

Catharine Esterhuysen
Stellenbosch University
Conference Chair

Edith Antunes
University of the Western Cape
Social Progamme

Gareth Arnott
Stellenbosch University
Website/Marketing

Nikoletta Báthori
Cape Peninsula University of Technology
Programme Committee

André de Villiers
Stellenbosch University
Sponsorship & Bursaries

Delia Haynes
Stellenbosch University
Vice-chair & Programme Committee

Rehana Malgas-Enus
(1983-2022)
Stellenbosch University
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On-site Logistics

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Acknowledgements

A very sincere and heartfelt thank you to all our wonderful sponsors and affiliates – without you this conference would not have been possible!

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SACNASP South African Council for Natural Scientific Professions Integrity in science

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SACNASP South African Council for Natural Scientific Professions Integrity in science

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General information

Registration and information desk

The registration desk is located in the Konservatorium in Victoria Street (building 79 on the campus map). See the floor plan on the next page for the location of the registration desk. The registration desk will be open from 14h30 on Sunday 8 January 2023, and then from 08h00 every day of the conference.

WiFi

Eduroam is available across the Stellenbosch University campus. Conference WiFi details are as follows:

SSID: SACI2023
Password: Saci65@St3lli3s

Speaker information

Slides should be prepared in MS PowerPoint or PDF format in 16:9 or 4:3 slide size. The slides need to be loaded in the **speaker prep area** in the Konservatorium (see site map below). Talks should be loaded on a USB flash drive and handed to the technical support **preferably the day before**, but no later than 3 hours before your talk. The speaker prep area will be open during all breaks and 30 minutes before the first lecture and after the last lecture each day. Use of your own computer is not possible.

Poster presenter information

Posters should be prepared in A0 size portrait orientation. Poster sessions will be held in the Konservatorium and De Beers building on Monday 9 January, Tuesday 10 January and Thursday 12 January; please consult the abstract book to identify when and where your poster session is. The posters need to be put up by the morning tea break on the day of your poster session in the correct building and according to your abstract number. Materials to hang your poster will be provided. If you have an odd-numbered poster please be present at your poster for the first half of your poster session, whereas if your poster has an even number please be available at your poster in the second half of the session. Posters should be taken down after the poster session, by the morning tea break on the following day at the latest.

Airport transfers

Cape Town International Airport is approximately 40 kms from Stellenbosch (about a 40 minute drive). There are several car hire agencies at the airport. These are located in front of the Transport Plaza and Central Terminal building, and can be accessed via the pedestrian subways on either side of the terminal building. The e-hailing (Uber) pick-up point is clearly marked, and is at Level 1 Arrivals. An Uber from the airport to Stellenbosch will cost R250-R350.

Weather

Stellenbosch in January is usually warm and dry, with an average daily high of 26 °C, and an average daily low of 12 °C. It does sometimes get up to 40 °C however, so please bring sunscreen and a hat. That being said, evenings can be cooler than you might expect, so bring a light jersey or jacket as well. The sun will rise and set at approximately 05h45 and 20h00, respectively.

Contact information and emergency numbers

University of Stellenbosch Campus Security www.sun.ac.za/safety
Report incidents to the Control Room - Tel.: +27 (0)21 808 2333 (24h) WhatsApp 082 808 2333

Ambulance Stellenbosch Ambulance: 021 937 0500 Ambulance Western Cape: 10177 Netcare 911 ambulance: 082 911 ER24 ambulance: 084 124	**Police Emergency Number** Tel: 10111 / 021 808 5015 / 021 809 5000 **US Law Enforcement** Tel: 021 808 4666

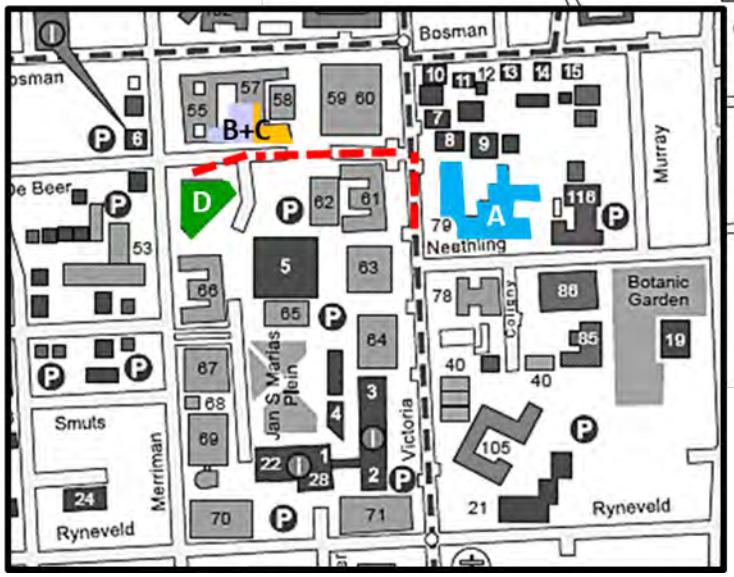
Venues and facilities

SACI-44 will be held in the Endler hall at the Konservatorium of Stellenbosch University, with parallel sessions in two of the Chemistry buildings, de Beers and First Year Chemistry (a three-minute walk). Please see the map on the next page, which shows the locations of these buildings.

Morning teas will be served directly after the plenary sessions in the mezzanine area outside the Endler auditorium. Lunch boxes should be collected at the same place, and can be enjoyed anywhere on campus; we encourage you to find a comfortable spot under a tree and have a picnic with old friends! Afternoon teas will also be served outside the Endler auditorium, but there will be an additional serving point in the quad of the De Beers building for those delegates attending parallel sessions in the 1st year building and De Beers. While drinking afternoon tea, please take the opportunity to look at the posters; snacks and drinks will also be available from the same serving points during the poster sessions later in the day.

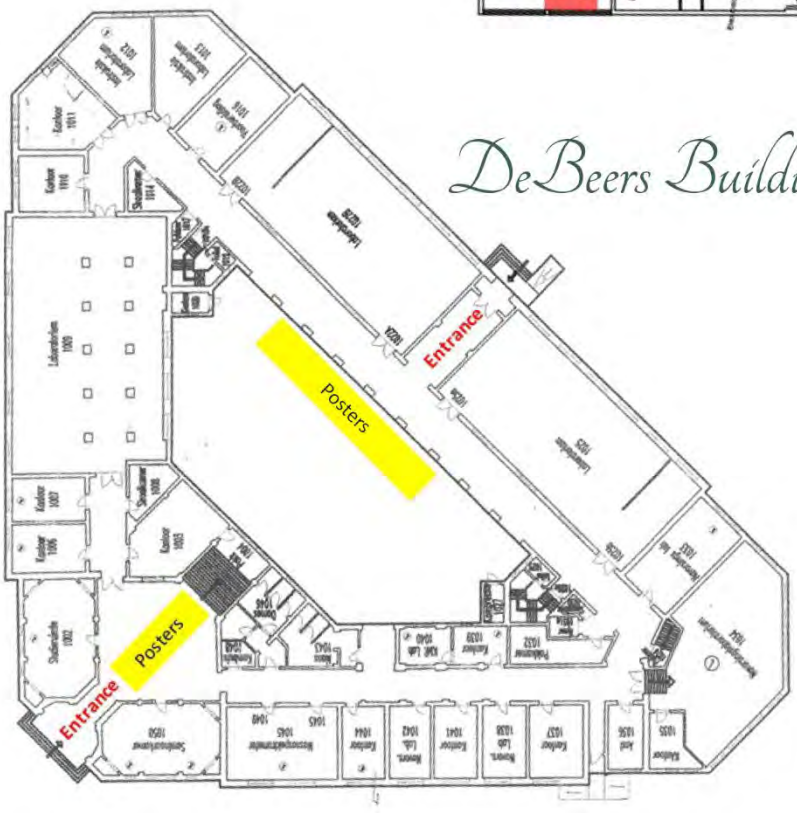
STELLENBOSCH CAMPUS MAP

A Endler Hall
B First Year Chemistry Neon (1015)
C First Year Chemistry Argon (2011)
D de Beers Building
- walking route



Endler Floor plan

DeBeers Building



Social program

Welcome cocktail function (Sunday 8th January; 7:30 pm)

The cocktail function will take place in the foyer at the Endler Conservatorium, Stellenbosch University at 7:30 pm. Dress code is casual.

Pub Quiz (Tuesday 10th January 2022; 6.30 pm)

There are two venues available for the pub quiz: Dorp Bar or the Aandklas Stellenbosch – both are within walking distance from the Endler Conservatorium. Following the quiz, the Dorp bar will have a DJ available, while the Aandklas venue will have karaoke after the quiz. Teams will consist of 6 people, and you will need to provide a name for your team. A board where you can sign up with your team's name and team members will be available in the Endler Conservatorium foyer at the registration desk. There will be a prize for the winning team at each venue.

Dorp Bar (DJ): 62 Andringa Street, Stellenbosch.
Aandklas (karaoke): 43a Bird Street, Stellenbosch
Pizza and a drink voucher will be provided and a cash bar will be available thereafter.

Excursions (Wednesday afternoon, 11th January 2022, 12:45pm)

Please make your way to the Endler Conservatorium for your lunch box and excursion, prior to departure for the excursions

Wine tasting

Wine tasting will take place at one of four wine farms. Lunch boxes will be available at the Endler Conservatorium and sufficient time will be provided before leaving for the wine tasting excursion. You will be given a wristband to wear on the day. Student helpers will guide you to the transport to one of the wine farms.

Hiking

The hike will take you through the Jonkershoek Valley. You will be given a wristband at registration and a packed lunch will be provided for you. Please bring a small backpack to carry your goods. Student helpers will guide you to your transport. Please be prepared for the January summer heat in Stellenbosch i.e. please ensure you have a hat, sunscreen, extra water and walking shoes.

Stellenbosch tour

The guide tour will start from the Endler Conservatorium. You will be given a wristband at registration and a packed lunch will be provided. Please be prepared for the January summer heat in Stellenbosch i.e. please ensure you have a hat, sunscreen, extra water, good shoes.

Conference dinner (Thursday evening 12th January 2022, 6:30pm)

The conference dinner will be held on the 12th of January at Allée Bleue Wine estate at 6:30 pm. Transport will be provided from the Endler Conservatorium to and from the dinner. Dress code is casual. We are looking forward to an evening of good food and dancing.

The locals recommend ...

Welcome to Stellenbosch, also known as the Gourmet capital of South Africa. Stellenbosch is a beautiful wine region surrounded by mountains and vineyards and the second oldest town in South Africa. To make your stay more pleasurable we have put together a list of places to visit, which includes restaurants, cafes, entertainment, arts, and culture. Please don't hesitate to contact us for further advice or information.

Recommended Restaurants and Cafés

Stellenbosch offers a wide selection of restaurants; we recommend you book your table in advance to avoid inconvenience.

Recommended restaurants

Name	Cuisine	Address	Phone
Java Bistro	Bistro style foods with an extensive wine list	8 Jan Katz Building, 31 Church St, Stellenbosch Central	021 887 6261
Craft Wheat & Hops	Craft beer, artisan bread, flammkuchen and tapas	16 Andringa St, Stellenbosch Central	021 882 8069
Rome in a Bite	Authentic Italian cuisine	7 Andringa St, Stellenbosch Central,	021 886 5123
Basic Bistro	Burgers, Pasta, Malay curry, steak and coffees	31 Church St, Stellenbosch Central	021 883 3629
Man'oushe	Lebanese cuisine	14 Andringa St, Stellenbosch Central	021 886 7545
Meraki	Coffee & baked pastries and authentic heart-warming meals	43 Church St, Stellenbosch Central	021 007 3999
Simply Greek	Greek cuisine	3 Plein St, Stellenbosch Central	072 830 0997
De Warenmarkt	Speciality meats, crepes, baked goods, craft beer, coffee, oysters, MCC & much more	20 Ryneveld St, Stellenbosch Central	021 883 2274
Col' Cacchio	Italian chain serving gourmet wood-fired pizzas	Shop 29-31 Simonsplein Centre, Plein St	021 886 7088
Ginos	Italian style restaurant	De Kelder, 63 Dorp St, Stellenbosch Central	021 887 9786
Vendettas Pizzeria	Traditional Italian pizzeria	15 Hamman St, Stellenbosch Central	081 321 0638
Asta	Italian restaurant	95 Dorp St, Stellenbosch Central	021 887 7300
Decameron	Italian restaurant	50 Plein St, Stellenbosch Central	021 883 3331
The Fat Butcher	Contemporary steakhouse	1 Van Riebeeck St, Stellenbosch Central	021 883 3857
De Vleispaleis	Grillroom and steakhouse	56 Dorp St, Stellenbosch Central	021 879 2356
Hussar Grill	South African steak house	Shop G3, Good Hope Building, 23 Plein St	021 882 8088
De Volkskombuis	Traditional South African fare	De Volkskombuis, Aan-de-Wagenweg, Krigeville	021 741 0980
Watami - Sushi & Asian Cuisine	Sushi & Asian cuisine	7 Beyers Street, Stellenbosch	021 886 5828
Genki	Japanese cuisine	Shop 2, De Wet Centre Courtyard, Church St, Stellenbosch Central	021 887 5699
Sushi Guru	Sushi & Asian cuisine	107 Dorp St, Stellenbosch Central	081 814 7407
Spek and Bone	Acclaimed tapas restaurant	84 Dorp St, Stellenbosch Central	082 569 8958
Post and Pepper	Exquisite small plates fine dining	c\o Plein and Bird St, Stellenbosch Central	021 203 5165
Punjab	North Indian cuisine	Stellenbosch square, Jamestown	021 880 0123
Casa cerveza	Beer house and bistro	c\o Dorp &, Mark St, Stellenbosch	021 023 0346
Hudson's Burger Joint	Gourmet Burgers	77 Dorp St, Stellenbosch Central	021 887 2052
Juvenate Eatery	Plant based menu	145 Dorp St, Stellenbosch Central	064 688 9375
La Coco C	Health-conscious eatery	43 Plein St, Stellenbosch Central	081 880 3093

Popular cafés

Name	Address	Phone
Häzz coffee shop	32 Ryneveld St, Stellenbosch Central	021 882 9976
Bootleggers	13 Ryneveld St, Stellenbosch	021 201 7448
Legado coffee	19 Andringa St or Dorp St, Stellenbosch Central	073 220 5481
Seattle Coffee Company	3b Plein St, Stellenbosch Central	021 180 3078
Schoon	c/o Bird & Church St, Stellenbosch Central,	087 159 5605
Deluxe coffee work	Ou Strandpad Rd, Stellenbosch Central	060 731 4088
Starbucks	c/o Dorp & Mill St, Stellenbosch	
Vida e caffè	c/o Ryneveld St & Plein St, Stellenbosch Central	

Local wine-bars

Name	Address	Phone
The Wine Glass	13 Ryneveld St, Stellenbosch Central	082 555 2332
Stellenbosch wine Bar	Church St, Stellenbosch Central	063 646 3207
Q-bar	De Wet Centre, Stellenbosch Central	021 888 4740
Simon Wine Bar	c/o Ryneveld Street &, Van Riebeeck St, Stellenbosch Central	021 883 2274
Bartinney Wine Bar	5 Bird St, Stellenbosch	076 348 5374
Bramptons Wine Studio	11 Church St, Stellenbosch Central	021 883 9097
Beyerskloof Wine Bar	19 Ryneveld St, Stellenbosch Central	081 846 7997

Trendy ice-cream parlours

Name	Address	Phone
Moro Stellenbosch	13 Andringa St, Stellenbosch Central	
Crème de Levain	15 Church St, Stellenbosch Central	021 886 5116
Kristen's kick Ass Ice-cream	c/o Bird & Church St, Stellenbosch Central	069 560 5785
Gelato Mania	18 Andringa St, Stellenbosch Central	060 710 6095
Gelato Lab	109 Dorp St, Stellenbosch,	021 300 5365
Crumbs and Cream	Neelsie student center	
Marcels	Eikestad Mall, Andringa Street, Stellenbosch	021 882 8133
Swirl'n Stellenbosch	Le Coutzenbourg Building, Church St, CBD	021 883 3423

Wine Estates

If you have access to a car there are restaurants on wine estates, with gourmet food and superb wines. Here are a few recommendations.

Delaire Graff

Cavalli

Lanzerac

Delaire Graff - delaire.co.za
Cavalli - cavalliestate.com
Lanzerac - lanzerac.co.za
Spier - spier.co.za
Babylonstoren - babylonstoren.com
Uva Mira - uvamira.com
Peter Falke - peterfalkewines.com
Ernie els - ernieelswines.com
Rust en Vrede - rustenvrede.com
Kleine Zalze Wine Estate - kleinezalze.co.za
Morgenhof - morgenhof.com

Night Life

Dorp (affectionately referred to as '**the Happy Oak'** by older students) on Andringa Street is one of the more relaxed watering holes in Stellenbosch, with good food, great people, and affordable prices.

Balboas (Andringa St) is slightly hidden away but has become a favourite for drinks following a long day. Thursdays offer live blues music to add to the atmosphere.

De Akker (Dorp Street) is one of the oldest bars in South Africa, but don't let that put you off, as it has a very relaxed bar atmosphere.

AandKlas is the place to experience the Stellenbosch local band scene with affordable food and drink.

Mystic Boer & Bohemia (Victoria Street) are for the more hippie-type folks with affordable food and drinks: definitely a must-see.

Catwalk if you find yourself in the mood for dancing. **Catwalk** caters to all music tastes, and you can even try your hand at "Sokkie".

Outdoor activities

People seeking nature and outdoor experiences, here are some places worth a visit…….

Jonkershoek Nature Reserve - Jonkershoek Rd, Stellenbosch
Jan Marais Nature Reserve - Marais Rd, Mostertsdrift, Stellenbosch
SU Botanical Garden - Neethling St &, Van Riebeeck St, Stellenbosch Central
Old Nectar Garden - Jonkershoek Rd, Stellenbosch
Rustenburg Garden - Rustenburg Rd, Idasvallei, Stellenbosch
Babylonstoren Garden - Klapmuts - Simondium Rd, Simondium

Arts and Culture

Stellenbosch is a historical town; the streets are lined with centuries-old oaks and historic Cape Dutch houses. The arts and culture are captivating, with the Rupert Museum displaying the finest collection of South African art. Other museums worth visiting are Stellenbosch University Museum and Babylonstoren wine museum. There is also a curated collection of art and sculpture all around the town in Stellenbosch – KEEP YOUR EYES OPEN!

Rupert Museum: Stellentia Rd, Stellenbosch Central Phone: 021 888 3344

Stellenbosch University museum: 52 Ryneveld St, Stellenbosch Central Phone: 021 808 3695

Village Museum: 18 Ryneveld St, Stellenbosch Central Phone: 021 887 2937

Babylonstoren wine museum: Klapmuts - Simondium Rd. Phone: 021 863 3852

Scientific Programme

The scientific programme begins on Sunday evening, with two SACI Gold Medal Lectures. The programme ends on Friday evening, with a third SACI Gold Medal Lecture.

Details regarding the social programme are given in the abstract book.

Special sessions

Publishing: Getting your article published – advice from the journals (Thursday morning)
Come join us for an informative session on publishing. Journal editors as well as reps from the various academic publishing houses will offer their advice and guidance through the publishing process.

Diversity and Inclusivity session: Breaking barriers in science (Thursday afternoon)
The chemistry community comprises people from diverse cultures with varied backgrounds and experiences. The South African Chemical Institute is committed to nurturing the values of diversity and inclusivity in the chemical sciences. SACI recognises that for the chemical sciences to prosper, we as a community need to actively 'br*eak barriers in science*'. Talking to this theme, in this session, we will hear from several speakers (chaired by SACI CDI), followed by a general discussion lead by questions from our community. As the leading professional chemistry body in the country, we have a responsibility to promote inclusivity and improve diversity.

Societies Round Table: The IYBSSD and you (Friday morning)
In celebration of the International Year of Basic Sciences for Sustainable Development, please join a panel discussion involving representatives from SACI, the ACS, RSC, Commonwealth Chemistry and the African Crystallographic Association on what members of learned societies can do to contribute to sustainable development in Africa and how we can work together as learned societies to make sustainable development happen.

Sunday

Endler	
from 14h30	registration
17h30 – 18h00	Opening Ceremony *Chairs: Catharine Esterhuysen & Willem van Otterlo*
18h00 – 18h45	**Gold Medal Lecture: Charles de Koning** My name is Bond. Covalent carbon-carbon, carbon-oxygen and carbon-nitrogen bonds
18h45 – 19h30	**Gold Medal Lecture: Fanie van Heerden** Marvellous meanderings with natural product chemistry
19h30 –	**Welcome function**

Monday (morning)

09h00 - 10h00: **Natalie Stingelin**
Establishing structure/property interrelations for functional polymer systems using thermal analysis
Chair: Peter Mallon

10h00-10h30: TEA and move to sessions

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	ANALYTICAL	**POLYMER**	**INORGANIC**	**ENVIRONMENTAL**
	Green Sample preparation *Chair: Mathew Nindi*	*Chair: Bert Klumperman*	**Incorporates the 19th Inorg/Carman conference** *Chair: Caren Billing*	**Chemicals of emerging concern in environmental media** *Chair: Jonathan Okonkwo*
10h30-11h10	**Charlotta Turner** Quantitative analysis of unknown compounds in complex samples – Challenges in extraction, chromatography and detection	**Christian Pester** Heterogeneous photoredox catalysis using polymer brush-functionalized glass beads	**Gregory Smith** Bioorganometallic strategies to target malaria	**Bice Martincigh** A week in the life of a wastewater treatment plant in Durban
11h10-11h30	**Petra van der Merwe** Comparison of GC-MS versus GC-ECD detection and derivatization methods for the analysis of haloacetic acids in drinking water	**Ruvimbo Chagwedera** Side reactions in the copolymerization of maleic anhydride and n-butyl vinyl ether	**Monsuru Temitope Kelani** Synthesis of n,n'-bipyridyl chiral-at-metal ruthenium complexes as catalysts for asymmetric hydrogenation of ketones	**Bulelwa Batayi** Per-and polyfluoroalkyl substances (PFASs) in source water and sediments from South Africa and estimated human exposure
11h30-11h50	**Njabulo Mdluli** Magnetic solid phase extraction based on Fe_3O_4@Al_2O_3 adsorbant for simultaneous preconcentration of selected metal ions in fuel oils followed by ICP-OES determination	**Lauren Ball** PLA-b-SMA as an amphiphilic diblock copolymer for encapsulation of lipophilic cargo	**Athi Welsh** Rationally designed trimetallic ruthenium(II) 2-arylbenzimidazole complexes for chemotherapy and photodynamic therapy	**Nondumiso Mofokeng** Source apportionment, transport and fate of pollutants in the paper recycling chain: an analytical exploration of the South African recycled paper chain
11h50-12h10	**Thrineshen Moodley** The LC-MS/MS method development and validation of novel anti-malarials for preclinical evaluation	**Ndivhuwo Shumbula** 3D wound healing scaffolds made of nanoparticles embedded within biodegradable polymers	**Andrew Swarts** Highly efficient transfer hydrogenation of alkenes with ammonia borane mediated by a simple Ni(II) catalyst system	**Babatunde Koiki** Sulphate radical enhanced photoelectrochemical degradation of sulfamethoxazole on a fluorine doped tin oxide – copper(I) oxide photoanode
12h10-12h40	**Patricia Forbes** Turning green – Sustainable approaches to environmental sample preparation	**Rueben Pfukwa** Poly(N-vinylpyrrolidone) in advanced polymers for biomedical applications	**Rob Luckay** Separation of base metal ions using inner- and outer-sphere chemistry	**Beatrice Opeolu** Emerging contaminants-the bittersweet cocktails in water systems

12h40 – 14h00 | LUNCH

Monday (afternoon)

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	ANALYTICAL	**POLYMER**	**INORGANIC**	**ENVIRONMENTAL**
	Green Sample preparation *Chair: André de Villiers*	*Chair: Peter Mallon*	**Incorporates the 19th Inorg/Carman conference** *Chair: Zeni Tshentu*	**Risk and environmental assessment** *Chair: Bice Martincigh*
14h00-14h30	**Hlanganani Tutu** Text mining for enhancing water quality data	**Gestél Kuyler** Novel terpolymers for detergent-free isolation of GPCRs	**Alice Brink** The Wonderland of Multinuclear Mn, Tc & Re Complexes in Small Molecule and Macromolecular Environments	**Tlou Chokwe** Neonicotinoids and insect growth regulators in honey: concentrations and exposure assessment under the framework of national residue monitoring program
14h30-14h50	**Thamani Gondo** Exploring the selectivity of carbon dioxide-ethanol-water ternary solvent mixtures in the extraction of antioxidative compounds from brown seaweed	**Dan Molefe** Heat stabilising flexible PVC with layered double hydroxide derivatives	**Mametsi Maseme** The chemistry of spin-coated Rhodium complexes supported on silanol-capped silicon wafers	**Jeanri Stevens** Obstacles to sustainable development in environmental commercial laboratories based in South Africa
14h50-15h10	**Samuel Mgiba** Analysis of organosulphur compounds in fuel oil samples using magnetic solid phase extraction based on Au-Fe_3O_4 adsorbent and GC-HR-ToFM	**David Sibanda** Controlling the Multiporous Structure of Carbon Nanofibers Using Solution Aging Properties of PAN/PBA Block Copolymers	**Malcolm Ndlovu** Synthesis of novel ferrocenyl-benzimidazole derivatives and their evaluation as antiplasmodial agents	**Karabo Mashiloane** Occurrence of per and polyflouroalkyl substances (PFASs) as contaminants of emerging concern (CEC) in tap water in South Africa
	15h10-15h40 | TEA			
15h40-16h00	**Walter Mahlangu** Quantitative analysis and health risk assessment of bisphenol A and its derivatives in selected canned food in South Africa, using a modified QuEChERS method coupled with gas chromatography-mass spectrometry	**Zahn Stanvliet** Responsivity analysis of smart nanoparticles using asymmetric flow field-flow fractionation	**Larnelle Garnie** Studying the growth of the digestive vacuole lumen in NF54 and Dd2 to aid in understanding the haem detoxification pathway in Plasmodium falciparum.	**Sihle Mngadi** Elemental composition and potential health risk of vegetable cultivated in residential area situated close to mine tailings
16h00-16h40	**Titus Msagati** Azole antifungal drugs in water and wastewater systems	**Róża Szweda** Stereocontrolled polymers with defined monomer sequence – how far are we from the structural precision of biomacromolecules?	**Katherine de Villiers (Raikes Medal)** The heme detoxification pathway as a target for antimalarial drug development	**Nonhlanhla Kalebaila** Managing chemicals within the environment – whose job is it anyway?

16h40-16h50 | move to poster flash sessions

16h50-17h20 | poster flash presentations

17h20-18h30 | POSTERS

This session is generously sponsored by Elsevier

ELSEVIER

Tuesday (morning)

09h00 - 10h00: **Tomislav Friščić**:
Exploring a Different Self-Assembly Space: Halogen Bonding to Carbon and Other Elements
Chair: Delia Haynes

10h00-10h30: TEA and move to sessions

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	ANALYTICAL	**ACS SESSION**	**GREEN**	**PHYSICAL**
				Incorporates the 19th Inorg/Carman conference
	Electrochemistry / General *Chair: Omotayo Arotiba*	**Drugs and devices for sustainable health** *Chair: Kevin Naidoo*	*Chair: Alufelwi Tshavhungwe*	**Development and understanding of materials** *Chair: Melanie Rademeyer*
10h30-11h10	**Priscilla Baker** Frontiers of modern day electro-analysis – to infinity and beyond!	10h30 **Opening** ACS President Angela Wilson, Christopher LaPrade and Charles de Koning	**Marcus Baumann** Flow Photochemistry as a Greener Approach for the Synthesis of Drugs and Drug-Like Scaffolds	**Christien Strydom** Thermal Analysis as a crucial step during research on thermal processing of coal fines, waste biomass and solid waste material.
11h10-11h30	**Babatope Ojo** Coupling piezo-polarization effect on Ti/BaZrTiO3 anode with sonoelectro-Fenton and sonoelectrochemical oxidation for the mineralization of aspirin in wastewater.	10h50 **Shoameng Wang** Induced protein degradation as a strategy for the development of new medicines	**Zodidi Obiechefu** Comparative assessment of the physicochemical characteristics of Nano-hydroxyapatite extracted from fish scales and eggshells	**Denis Moyo** Isothermal TGA investigation of the sublimation of fipronil at polymer processing temperatures
11h30-11h50	**Anzel Falch** Nanostructured electrocatalysts for water electrolysis	11h35 **Richard D. Cummings** Using Chemical Glycobiology to Decipher the Glyco-Code of Human Diseases	**Rosa Klein** Curriculum change in chemistry	**Vincent Nyamori** Enhanced performance by heteroatom-doped reduced graphene oxide-TiO2-based nanocomposites as photoanodes in dye-sensitised solar cells
11h50-12h10	**Danica Moodley** Construction of Functional Cobalt Phthalocyanine-Modified Electrodes for the Electrocatalytic Detection of Paraquat	12h20 **Gerrit van der Klashorst** The establishment of commercial manufacturing of API's in Africa	**Olamide Daramola** Encapsulation of Thiol-Co-Capped CdTe/CdSe/ZnSe Multi-Core-Shell QDs in Liposomes and Chitosan Nanoparticles; Comparative Bio-compatibility Studies Using Hela and Vero Cells	**Jean Lombard** Calcium oxalate precipitation kinetics in mixed solvent media.
12h10-12h40	**Krishna Bisetty** Smart Electrochemical Sensing of Xylitol using a Combined Machine learning and Simulation approach	(LUNCH at 12h55)	**Werner Van Zyl** Nanocellulose and bacterial cellulose as a multifunctional green material	**Vincent Smith** Solid-state Chemistry at Rhodes University in the Context of Sustainable Physical Chemistry

12h40 – 14h00 | LUNCH

Tuesday (afternoon)

	Endler ANALYTICAL	1st year Argon (2011) ACS SESSION	1st year Neon (1015) GREEN	de Beers 2003 PHYSICAL
				Incorporates the 19th Inorg/Carman conference
	Electrochemistry / General *Chair: Patricia Forbes*	**Drugs and devices for sustainable health** *Chair: Charles de Koning*	*Chair: Rosa Klein*	**Computational approaches to sustainability** *Chair: Vincent Nyamori*
14h00-14h30	**Luke Chimuka** Comparison of PSA to Moringa Oleifera seed protein as sorbent in QuEChERS: A Response Surface Methodology optimisation for extraction of some Endocrine Disrupting Chemicals in food	14h00 **Amanda Bryant-Friedrich** Creation of a nucleic acids' toolbox for the treatment and investigation of the etiology of disease	**Ettigounder (Samy) Ponnusamy** DOZN™2.0 - A Quantitative Green Chemistry Evaluator	**Thishana Singh** Theoretical Chemistry: A tool for sustainable chemistry in Africa
14h30-14h50	**Phathisanani Hloma** Smart electrochemical immunosensor for detection of aspartame in dietary products supported by in silico methods	14h45 **Kenneth Ozoemena** Developing electrochemical immunosensors for poverty-related diseases: tuberculosis, cholera, and cervical cancers	**James Dicks** Development of wholly biobased acid-terminated thermosetting polymers from castor oil, glycerol, and itaconic acid	**Okikiola Olaniyan** Ab initio study of the mechano-chemical coupling of Au(221) with chemisorbed oxygen atoms
14h50-15h10	**Lebogang Manamela** Evaluation of cellulose acetate supported MOF-5/crystalline nanocellulose nanocomposite as an adsorbent for methylene blue removal from water	15h20 **TEA (30 mins)**	**Pierre Mubiayi** Inorganic perovskites and nanocrystalline materials toward energy applications	**Gerhard Venter** Predicting transport properties of ionic liquids using molecular dynamics simulations including explicit polarization
		15h10-15h40 | TEA		
15h40-16h00	**Grace Ngubeni** Semiconducting Cu_2ZnSnS/Se_4 quaternary chalcogenides as alternative counter electrodes for DSSCs	**Computational and theoretical chemistry** 15h50 **Angela Wilson**	**Wesley Feldman** **(sponsored talk)** African laboratory growth and development	**Shane de Beer** Computational study probing sustainable applications of greenhouse gases
16h00-16h40	**David Benanou** Think green –.play green SBSE: the right enrichment technique	16h35 **Closing remarks** Kevin Naidoo	**Discussion**: Green chemistry for sustainable development in Africa	**Eric van Steen** Aerobic oxidation of methane to formaldehyde over platinum

16h40-16h50 | move to poster flash sessions
16h50-17h20 | poster flash presentations

17h20-18h30 | POSTERS

Pub Quiz night!

Wednesday (morning)

09h00 - 10h00: **Jan Weigand**
The element phosphorus - a challenge of the not too distant future
Chair: Catharine Esterhuysen

10h00-10h30: TEA and move to sessions

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	INORGANIC	**ENVIRO/ANALYTICAL**	**YOUNG CHEMISTS**	**ENVIRONMENTAL**
	Incorporates the 19th Inorg/Carman conference *Chair: Dave Billing*	*Chair: Lawrence Madikizela*	*Chair: Megan Matthews (Willem van Otterlo EXCO)*	**Remediation** *Chair: Rob Luckay*
10h30-11h10	**Nosipho Moloto** Semiconductor nanocrystals as effective HER electrocatalysts	10h50 **Tsepo Lebeko (20 mins)** Health Risks Assessment of Trace Metals in Ground Water Collected From Berlin, Eastern Cape, South Africa	**Kelly Chibale** From synthetic organic chemistry to translational medicine and scientific entrepreneurship	**Leslie Petrik** Chemical escapades: persistent organic pollutants in the marine environment
11h10-11h30	**Caren Billing** Solid oxide electrolytes: Dopant effects on structural and conductivity properties of bismuth oxides	**Silindile Ntombela** Mineral beneficiation from seawater: development and optimization of selective extraction techniques for essential minerals from seawater brine	**Discussion** With Prof Chibale	**Mandla Mabaso** Fe_3O_4@SiO_2@Zr(OH) nanocomposite for the removal of Pb^{2+} ions from aqueous solution.
11h30-11h50	**Sanam Maikoo** Biomolecular Interactions of Cytotoxic Ruthenium Compounds with Thiosemicarbazone or Benzothiazole Schiff Base Chelates	**Sandisiwe Zondo** Assessment of microwave assisted extraction efficiency for the determination of herbicides in soil and maize cob: cumulative and health risks assessment	**Luke Invernizzi** High throughput screening of South African medicinal plants in the search for novel anti-viral agents against SARS-CoV-2	**Ebrahiem Botha** The Effect of Slurry Wet Mixing Time, Thermal Treatment, and Method of Electrode Preparation on Membrane Capacitive Deionisation Performance
11h50-12h10	**Philani Mashazi** Unraveling biomimetic properties of nanomaterials for diagnostic applications	**Maria Mashigo** Phytoremediation potential, chemical profiling and biological properties of South African indigenous species	**Xueting Wei** Single-Crystal to Single-Crystal Dimensionality Transformation of Metallocycle to Coordination Polymer	**Agnes Pholosi** The Effect of Slurry Wet Mixing Time, Thermal Treatment, and Method of Electrode Preparation on Membrane Capacitive Deionisation Performance
12h10-12h40	**Peter Ajibade** Metal complexes of alkyl-aryl dithiocarbamates: Molecular structures and uses as precursors for semiconductor metal sulphide nanophotocatalysts and potential as anticancer agents	**Brenda Moodley** Analysis of selected pharmaceuticals in a wastewater treatment plant during Covid-19	**Tricia Naicker (Raikes Medal)** Tips for young chemists to thrive in academia - based on my experience	**Ntebogeng Mokgalaka-Fleischmann** Contaminants of Concern in South African Water Resources: The Establishment of a Knowledge Hub

12h40 LUNCH | EXCURSION

Thursday (morning)

09h00 - 10h00: **Erick M. Carreira**
Strategies and Tactics in Natural Products as an Engine for Discovery
Chair: Gareth Arnott

10h00-10h30: TEA and move to sessions

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	ANALYTICAL	**PUBLISHING**	**ORGANIC**	**PHYSICAL**
	Chromatography/MS *Chair: Luke Chimuka (Zeni Tshentu EXCO)*	*Chair: Thishana Singh*	*Chair: Wade Petersen*	**Incorporates the 19th Inorg/Carman conference** **Crystals as functional materials** *Chair: Vincent Smith*
10h30-11h10	**Ralf Zimmerman** Air pollution and health: Improvements in characterisation of the composition and toxicological impact of aerosol emissions and the polluted ambient air		**Daniel Rauh** Cancer meets Chemistry - Translational Research	**Melanie Rademeyer** Versatile organic-inorganic hybrid materials: structures and properties
11h10-11h30	**Samuel Makobe** Spatial and temporal variations in the presence, levels, and risk assessment of selected polycyclic aromatic hydrocarbons in sediments and water from Klip River, Johannesburg, South Africa	**Getting your article published – advice from the journals**	**Catherine Kaschula** Natural dietary compounds and cancer prevention: investigations into the anti-cancer mechanism of action of flavonols and polysulfanes	**Alan Eaby** Direct observation of rapid water uptake and release from a vapochromic single crystal
11h30-11h50	**Angeline van Biljon** Size exclusion and reverse phase high performance liquid chromatography as complementary tools to study wheat gluten protein		**Ross Robinson** Utilising anatase nano-seeds coupled with a visible-light antennae system () for effective photo-organic transformations	**Tracy Lau** Comparing the cooperative feedback reaction dynamics of imino-dithiin charge-transfer co-crystal compounds
11h50-12h10	**Khuliso Maphakela** Quantification and toxicity evaluation of steroid hormones in wastewater effluent		**Lloyd Chetty** Organic base-mediated carboxylation of (hetero)aromatic compounds using supercritical carbon dioxide ($scCO_2$)	**David Billing** Limits of lab XRD and average crystal structure concepts – when studying energy and related functional materials.
12h10-12h40	**Lawrence Madikizela (Raikes Medal)** Fate of pharmaceuticals in South African environment: Past, present and future research		**Vinesh Maharaj** South African plants as a panacea to health challenges: Insights on collaborative endeavors exploring this resource in search of treatments	**Patrice Kenfack Tsobnang** Structure–properties relationship in two hydrogen-bonded MOF based of $[Cr(ox)_3]^{3-}$ anions and cations built with 2-picolylamine and M = Co^{3+} or Cu^{2+}

12h40 – 14h00 | LUNCH

Thursday (afternoon)

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	ANALYTICAL	**SACI CDI**	**ORGANIC**	**MR USERS MEETING**
	Chair: Priscilla Baker	**Breaking barriers in science** *Chairs: Sadhna Mathura and Niki Báthori*	*Chair: Clint Veale*	*Chair: Denzil Beukes*
14h00-14h30	**Kwenga Sichilongo** Automated deconvolution, pre-processing and statistical evaluation of GC-MS data for untargeted/targeted metabolomics for mining metabolites in matrices of interest		**Mamoalosi Selepe** A search for bioactive compounds from natural sources	**Neil Ravenscroft** Using NMR spectroscopy to facilitate the development of vaccines against Group B Streptococcus disease
14h30-14h50	**Madelien Wooding** Human exposure to plasticisers from single-use plastic food contact materials	**Breaking barriers in science: Hosted by SACI CDI and IUPAC Global Women's Breakfast 2023**	**Mpelegeng Bvumbi** The photo-switchable polarity of conjugated cinnamic acid/chloroquinoline: Synthesis, isomerization, and antimalarial activities	**Discussion**
14h50-15h10	**Moloko Morethe** Quantification Of Per and Polyfluorinated Alkyl Substances in Wastewater Treatment Plants in South Africa		**Dino Berthold** Total Syntheses of 5,8'-Naphthylisoquinoline Alkaloids Employing Hartwig's Borylation/Methylation Strategy and a Novel Nickel/N,N-Ligand-catalyzed Atroposelective Cross-Coupling	**Kabelo Ramollo** Redox-switchable gold catalysis monitored by NMR and EPR spectroscopy
	15h10-15h40 | TEA			
15h40-16h00	**Kedibone Mashale** Gravimetric quantification of low-grade gold in mine tailings	*Chair: Margaret Blackie* **Breaking barriers in science: Engaging with questions from our community**	**Vladimir Azov** Stabilizing peptide nano-structures using non-canonical amino acids with donors and acceptors	**Izak Kotze** Conformational analysis and potential anticancer activity of [Pt(phen)(L1-κS)$_2$] studied by single crystal X-ray Diffraction and Variable Temperature 1H and ^{195}Pt NMR Spectroscopy
16h00-16h40	**Egmont Rohwer** A method for sampling skin volatile compounds and their analysis by GCxGC-TOFMS for TB related metabolic profiling.		**Winston Nxumalo** Reduction of α,β-alkynyl carbonyl compounds using $SnCl_2$ and computational investigation of the reaction mechanism	**Rainer Kerssebaum** Bruker NMR spectroscopy

16h40-16h50 | move to poster sessions
16h50-18h00 | POSTERS

18h00 | end of poster session, busses to conference dinner leave at 18h30

Friday (morning)

09h00 - 10h00: **Perdita Barran**
Sebum and Joy – non-invasive sampling for disease diagnosis
Chair: André de Villiers

10h00-10h30: TEA and move to sessions

	Endler	1st year Argon (2011)	1st year Neon (1015)	de Beers 2003
	ORGANIC	**SOCIETIES ROUND TABLE**	**EDUCATION**	**INDUSTRIAL**
	Chair: Catherine Kaschula	**The IYBSSD and you** *Chair: Catharine Esterhuysen*	*Chair: Margaret Blackie*	**Industrial challenges & transition into the sustainable future** *Chair: Suzanne Finney*
10h30-11h10	**Alison Hulme** Track and Trace by SRS: A New Tool for MedChem	**Panel discussion with representatives from SACI and other learned societies on the International Year of Basic Sciences for Sustainable Development and how we as scientists can contribute to sustainable development in Africa through Chemistry**	**Tom Holme** From Context to Systems Thinking in Chemistry Education	**Fahmida Smith** PGMs – A key enabler in addressing global challenges and unlocking societal benefits
11h10-11h30	**Aaron Bender** Development of Peripherally Restricted 5-HT2B Antagonists for Treatment of Pulmonary Arterial Hypertension		**Shawn Gouws** Digitalize learning via process simulation to understand process control	**Josiane Ayingeneye** Solvent-dependent extraction of steam-exploded sugarcane bagasse: Lignin and glucose yields, and structural and thermal properties of lignin
11h30-11h50	**Setshaba Khanye** Ferrocene: A versatile organometallic fragment in the design of novel therapeutic agents		**Marissa Rollnick** A review of the topic specific pck in available videos on the big idea, "What is chemical equilibrium?"	**Thembelihle Mehlo** Synthesis of Aluminium Fumarate Metal Organic Frameworks from Multi-Layered Food Packages Recycled Waste Materials
11h50-12h10	**Kimberleigh Govender** Synthesis of "Dual Warhead" β-Aryl Ethenesulfonyl Fluorides and One-Pot Reaction to β-Sultams		**Dudley Shallcross** The myriad positive impacts of the Virtual Learning Environment, from LabSims to Smart Worksheets (a 17 year journey)	**Shane Smith** Effect of magnetic fields on limescale: an experimental investigation
12h10-12h40	**Paul Watts** Can South Africa facilitate local API manufacturing: The vision of continuous flow chemistry?		**Kgadi Mathabathe** Towards infusing education for sustainable development imperatives in chemistry education: pedagogical considerations	**Cosmas Chiteme** South Africa's Journey towards a Hydrogen Economy: Lessons Learnt in Funding Innovations

12h40 – 14h00 | LUNCH

Friday (afternoon)

	Endler ORGANIC	1st year Argon (2011)	1st year Neon (1015) EDUCATION	de Beers 2003 INDUSTRIAL
	Chair: Winston Nxumalo		*Chair: Helen Drummond (Peter Mallon EXCO)*	**Industrial challenges & transition into the sustainable future** *Chair: Eric van Steen*
14h00-14h30	**Maya Makatini** Cyclic peptidomimetic inhibitors from natural templates targeting the Mycobacterium tuberculosis caseinolytic protease ClpP1P2 and ClpC1 ATPase		14h00 **Margaret Blackie (Education medal)** Connecting to Chemistry: Lessons from a Longitudinal Study	**Estee Moodley** Rand Refinery, our past, present, and future
14h30-14h50	**Sbonelo Hlengwa** Anti-HIV and cytotoxicity activity of diterpenoids from South African Euphorbia species		14h30 **Christine Mundy (Education medal)** Making chemistry meaningful (TEA at 15h00)	**Brandon Davoran** The importance of chemistry for e-mobility development: An African perspective
14h50-15h10	**Meghan Oddy** Visible-Light Mediated Triplet Energy Photosensitization for the Formation of Nitrogen-Containing Heterocycles			**Taella Thiart** Synthesis and evaluation of chelating collectors designed for improved sperrylite recovery
	15h10-15h40 | TEA			
15h40-16h00	**Bahne Stechmann** Sharing compounds within in pre-competitive international research infrastructure initiative for chemical biology and early drug discovery		**Ayodele Odularu** Student-centered approach via infographic to enhance chemistry learning among first year undergraduate students in South African universities	**Jan Rijn Zeevaart** The options Nuclear Medicine offers to Drug Researchers for translation of their Compounds into the Clinic
16h00-16h40	**Kerry McPhail** Structure and Function of Microbial Natural Product Macrocycles		**Rene Toerien (Education medal)** Partnerships to support science teaching at school level	**Cathy Dwyer** The role of chemistry in enabling South Africa's Just Energy Transition

16h40-16h50 | move to final session, Endler

16h50-17h35 | Gold Medal Lecture - **Fernando Albericio**: Peptides, Key Building Blocks for Drug Development
Chair: Willem van Otterlo

17h35-18h00 | Prizegiving and closing ceremony
Chairs: Catharine Esterhuysen & Delia Haynes

Travel home safely!

Poster flash presentations

Monday

Endler		de Beers 2003	
Margareta	Sandahl	Emile	Maggott
Tsholofelo	Sebokolodi	GH	Rakodi
Andrea	du Preez	Josef	Spath
Sandiso	Ngwenya	Sarah	Wright
Ursula	Ralepelle	Althea	Carstens
Redolf	Segodi		

Tuesday

Endler		de Beers 2003	
Sol	Nety	Matthew	Scheepers
Perceverence	Tenza	Gciniwe	Mathenjwa
Nonhlazeko	Nxumalo	Hlawulekani	Rikhotso
Seth	Rapoo	Mogammad Luqmaan	Samsodien
Mofeli Benedict	Leoma	Kgaugelo	Tapala
Pinky Ncomela	Mjwara	Luccile	Mbonzhe

Poster sessions

Please ensure you are at your poster during your allocated session. If you have an even-numbered poster, please be at your poster for the first 35 mins of the session. If you have an odd-numbered poster, please be at your poster for the second 35 minutes of the session.

Monday

Endler	de Beers 2003
PA1, PA2, PA3, PA4, PA5, PA6, PA7, PA8, PA9, PA10, PA11, PA12, PA13, PA14, PA15, PA16, PA17, PA18, PA19, PA21, PA22, PA26, PA31, PA32, PA36, PA38, PA39, PA40, PA44, PA47	PI1, PI2, PI3, PI4, PI5, PI6, PI7, PI8, PI9, PI10, PI11, PI13, PI14, PI15, PI16, PI17, PI18, PIND1, PIND2, PG1, PG2, PG3, PG4, PE1, PE2, PE3, PE4

Tuesday

Endler	de Beers 2003
PA20, PA23, PA24, PA25, PA27, PA28, PA29, PA30, PA33, PA35, PA37, PA41, PA42, PA43, PA45, PA46, PA48, PA34, PE6, PE7, PE8, PE10, PE11, PE12, PE13, PE14	PP11, PP12, PP13, PP14, PP15, PP16, PP17, PP18, PP19, PP20, PP21, PO1, PO3, PO4, PO5, PO6, PO7, PO8, PO9, PO10, PO11, PO12, PO13, PO14, PO15, PO16, PO17, PO18, PO19, PO20

Thursday

Endler	de Beers 2003
PO21, PO22, PO23, PO24, PO25, PO26, PO27, PO28, PO29, PO30, PO31, PO32, PO33, PO34, PO35, PO36, PO37, PM2, PM3, PM4, PM5, PM6, PM7	PI12, PI19, PI20, PI21, PI22, PI23, PI24, PI25, PI26, PI27, PI28, PI29, PI30, PI31, PI32, PI33, PI34, PI35, PP1, PP2, PP3, PP4, PP5, PP6, PP7, PP8, PP9, PP10, PED1

G1 My name is Bond. Covalent carbon-carbon, carbon-oxygen and carbon-nitrogen bonds

Charles B. de Koning[1]
[1]*School of Chemistry, University of the Witwatersrand Johannesburg, South Africa*
E-mail: Charles.deKoning@wits.ac.za

Our research group has conducted research over 30 years involving the synthesis of aromatic and heteroaromatic compounds. The first part of this presentation will show examples of the development of novel synthetic methodology conducted in our group. Included will be the discovery of a ceric ammonium sulfate (CAS) mediated xanthone forming reaction (Figure 1, eq. 1)[1-2] as well as a carbon-nitrogen aromatic ring forming reaction (Figure 1, eq. 2).[3-4]

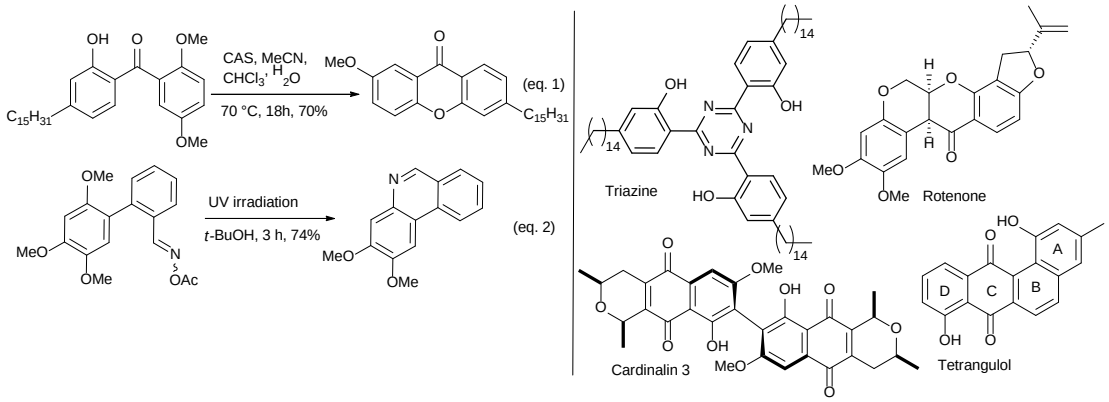


Figure 1: Aromatic and heteroaromatic natural products and derivatives

The second part of the presentation will focus on the total synthesis of natural products, including the synthesis of cardinalin 3,[5] rotenone,[6] and tetrangulol.[7] Finally, projects on the use of waste biomass for the synthesis of UV absorbers such as triaznes will be highlighted.[8] During the course of the presentation, attention will be directed to the assembly of new (covalent) Bonds as well as the drinking of martinis; shaken not stirred of course.

References

1. J. Dam, M. L. Bode, C. B. de Koning, *Journal of Organic Chemistry*, **2019**, *84*, 150 – 160.
2. F. Jagot, I. Minnie, A. Rahman, K. J. Ngwira, C. B. de Koning, *SynOpen*, **2022**, *06*, 58 – 66.
3. K.J. Ngwira, A.L. Rousseau, M.M. Johnson and C.B. de Koning, *European Journal of Organic Chemistry*, **2017**, 1479 – 1488.
4. S. Ntsimango, K.J. Ngwira, M.L. Bode, C.B. de Koning, *Beilstein Journal of Organic Chemistry*. **2021**, *17*, 2340 – 2347.
5. S. Govender, E. M. Mmutlane, W. A. L. van Otterlo, C. B. de Koning, *Organic & Biomolecular Chemistry*, **2007**, *5*, 2433 – 2440.
6. K. Hadje Georgiou, S. C. Pelly, C. B. de Koning, *Tetrahedron*, **2017**, *73*, 853 – 858.
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G2 Marvellous meanderings with natural product chemistry

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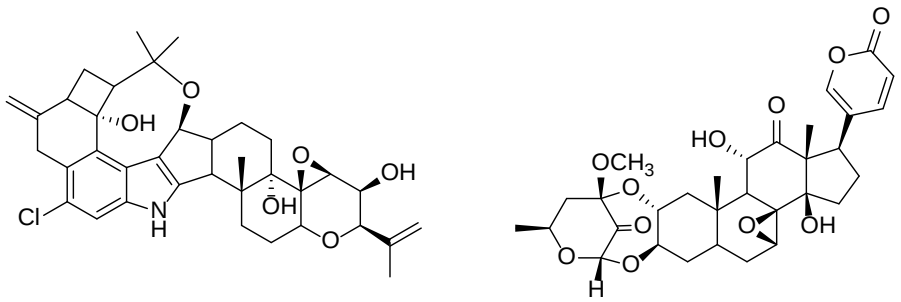
South Africa has a rich history of research in natural product chemistry, starting with identifying monofluoroacetate as the active principle in the poisonous plant *Dichapetalum cymosum* in 1943.[1] This was the first natural product isolated that contained fluorine. During the early parts of my career, I was part of a productive natural product research group that focused on mycotoxins and plant toxins. The structures of complex metabolites such as penitrem A (from *Penicillium crutosum*)[2] and tyledoside A (from T*ylecodon grandiflorus*)[3] were unravelled. Compounds isolated from plants have played a significant role in the pharmaceutical industry, and even today, some essential drugs still contain plant natural products such as morphine (pain killer), quinine (antimalarial), and vincristine (anti-cancer drug). These drugs were discovered in plants used by indigenous populations as medicinal plants (ethnopharmacology). The presentation will also deal with the results of my current research group on the phytochemical analysis of South African medicinal plants.



Penitrem A Tyledoside A

Figure 1

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G3 Peptides, Key Building Blocks for Drug Development

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Peptides have experienced a remarkable renaissance as therapeutic agents in recent years. They are situated between small molecules (<1000 Da) and proteins, two of the most extensive classes of well-established therapeutic agents. Peptides provide both the specificity and potency of larger protein biologics but with zero or low immunogenicity. Furthermore, they are smaller, more accessible and cheaper to manufacture using chemical methods, thus presumably combining the advantages of the two therapeutic approaches. While nature has been fine-tuning the bioactive chemical structure of these structures for thousands of years, peptide chemists and protein engineers have the exciting challenge of improving the intrinsically unfavorable pharmacokinetic properties of the majority of native peptides. The drawbacks of peptides as therapeutic agents are associated with their generally high conformational instability. In this presentation, we will review some examples of our research devoted to the synthesis of peptides with biological activity.

P1 Establishing structure/property interrelations for functional polymer systems using thermal analysis

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In recent years, immense efforts in the functional polymer field have led to unprecedented progress and to numerous new opportunities for polymers in, e.g., electronics, energy storage, energy harvesting, health care, and beyond. Despite these advances, many challenges still exist: predicting properties, identifying reliable processing protocols and, more fundamentally, gaining a complete understanding of the way structural features over all length scales affect functions in macromolecular matter, including electron/ion transport, charge generation, ferroelectric characteristics, and/or photophysical processes. Here we demonstrate how classical polymer science tools can be used to elucidate the structure development of functional polymers from the liquid phase, how such knowledge can be exploited to manipulate their phase transformations and solid-state order and, in turn, their performance. We provide examples how side-chain softening can influence mechanical and optoelectronic properties, and how vitrification can dominate the structure formation of ferroectric:semiconducting polymer blends. We moreover discuss how differential scanning calorimetry techniques, including fast calorimetry, can be used for the identification of thermodynamic transitions of “unusual” polymers, including hairy-rod polymers (used, e.g., in organic solar cells) or high-refractive index inorganic:organic hybrid materials. Generally, we will demonstrate how thermal analysis can be exploited to obtain important structural information of these new material classes and, in turn, how processing guidelines can be established towards materials of specific optical or electrical characteristics, towards improved materials design and new understanding of this next generation polymer systems.

P2 Exploring a Different Self-Assembly Space: Halogen Bonding to Carbon and Other Elements

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Halogen bonds (XB) are highly versatile interactions for the assembly of new functional, light-responsive materials.[1] In contrast to hydrogen bonds, which are largely limited to acceptor atoms of the 2nd period oxygen and nitrogen, and sometimes also sulfur, halogen bonds permit for a much broader diversity of acceptors. This provides new, unexplored opportunities for the design of materials. This lecture will highlight our team's explorations of this novel and inviting self-assembly space, ranging from light (carbon)[2] to heavy (antimony) acceptors.[3] We will show how the use of such interactions permits the assembly of complex materials from the simplest components, and also show how the use of azobenzene (azo) dyes as halogen-bonding building blocks permits the controlled development and design of light-matter interactions in crystalline solids – notably well-established phenomena such as dichroism,[4] pleochroism[2] and photo-mechanical motion. The use of azo dyes as halogen-bonding cocrystal components, however, also leads to the creation of dye-volatile cocrystals – materials that exhibit a previously not explored type of photoresponsive behavior: cold photo-carving (CBC) that enables shaping, cutting and embossing crystals using low-energy light and micrometer-scale resolution.[5]

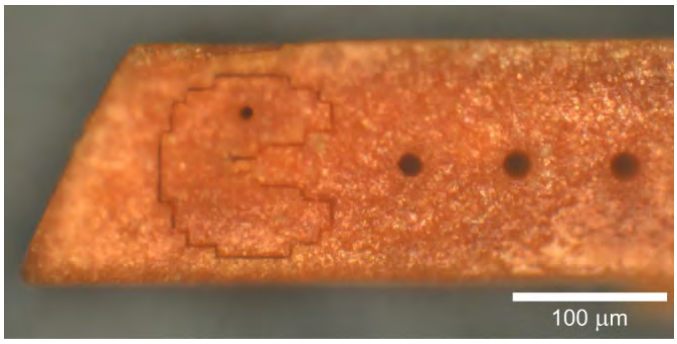

Figure 1: A Pac-Man figure drawn on a halogen-bonded dye-volatile cocrystal using cold photo-carving (CPC)

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P3 The element phosphorus - a challenge of the not too distant future

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The current depletion of available primary phosphorus resources is extremely worrying, which is why phosphate rock and elemental phosphorus are listed as critical raw materials worldwide (Figure 1). So far, the value chain from phosphate ores to basic chemicals does not correspond to the guiding principle of "green chemistry". In addition, the problem of phosphorus recovery through suitable large-scale recycling processes to recover valuable phosphorus compounds will become drastically more acute in the future. For these reasons, the development of new and innovative chemical methods in the value chain of the important element phosphorus is urgently needed. In our blueprint for a modern sustainable phosphorus chemistry, we investigate systematic and atom and energy efficient ways to either directly convert P_4 via our concept of "*oxidative onioation*" selectively into salts of versatile P(III) transfer reagents suitable for subsequent formation of P–O, P–N and P–C bonds or the deoxygenation of phosphoric acid and recycled phosphate resources to P_1 building blocks,[1] allowing "redox neutral" synthesis of a variety of valuable P(V) compounds. Both concepts represent versatile and chlorine-free approaches to value-added and highly relevant phosphorus containing chemicals.

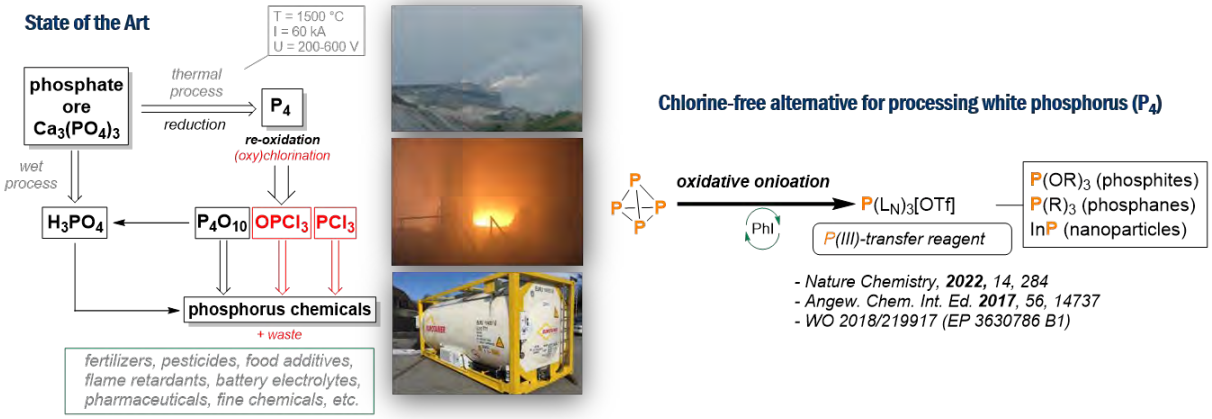

Figure 1: The element phosphorus - a challenge of the not too distant future.

Acknowledgements
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P4 From synthetic organic chemistry to translational medicine and scientific entrepreneurship

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As an undergraduate student at the University of Zambia (UNZA), I fell in love with organic chemistry. I was particularly inspired by the ability to recognize functional groups in a molecule, regardless of its size and complexity, and immediately starting to think about possible chemical reactions that could be performed. This was the planting of the seed for my synthetic organic chemistry career. Thanks to the excellent teaching of undergraduate organic chemistry at UNZA by the late Namboole Moses Munkombwe, I also realized that mechanistic rigor was foundational to the understanding of organic chemistry. This realization and my interest in modifying functional groups led me to choose the late Stuart Warren as my supervisor when I got the opportunity to study at the University of Cambridge (UK) for my PhD. My synthetic organic chemistry career started from here and was entrenched following my postdoctoral stints with Nick Greeves (University of Liverpool, UK) and K.C. Nicolaou (The Scripps Research Institute, USA). Moving to the University of Cape Town (UCT), I continued as a synthetic organic chemist while also reinventing myself as opportunities in translational medicine presented themselves. This necessitated the need to foster a culture of scientific entrepreneurship and develop the necessary infrastructure, technology platforms and skilled talent. In this presentation I will talk about my career, introduce the UCT Holistic Drug Discovery and Development Centre (H3D) with associated successes and challenges along with insights into scientific entrepreneurship in the chemical sciences.

P5 Strategies and Tactics in Natural Products as an Engine for Discovery

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The talk will include discussion and analysis of recent natural product targets that have been synthesized in the group. It will focus on target oriented synthesis as an engine for the generation of novel methods and approaches to bioactive agents. The methods involve novel, unexpected reactivity and unusual building blocks that are fully integrated to lead to efficient routes.

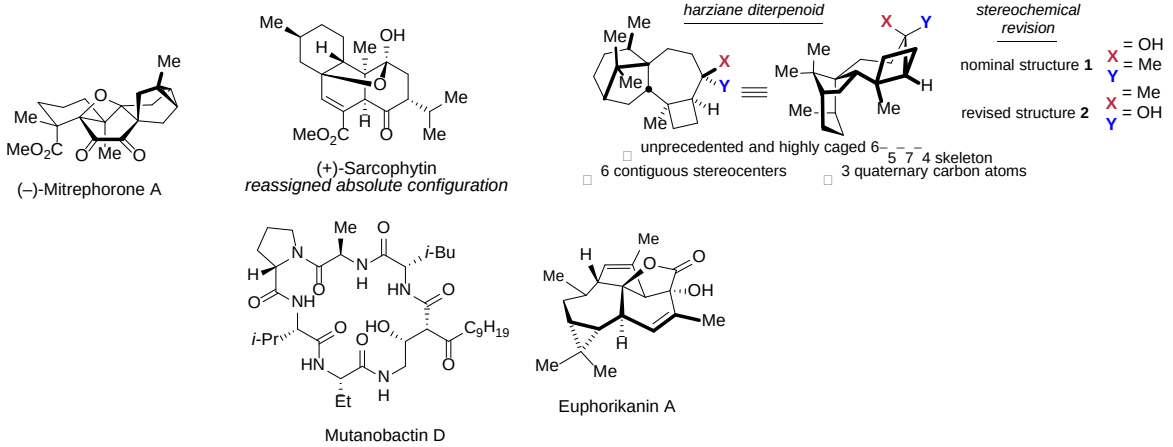

Figure 1

P6 Sebum and Joy – non-invasive sampling for disease diagnosis

Perdita E. Barran[1], Eleanor Sinclair[1], Caitlin Walton-Doyle[1], Joy Milne[1], Kat Hollywood[1], Depanjan Sarkar[1], Drupad Trivedi[1], Monty Silverdale[1,2],
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Our research program uses mass spectrometry (MS) to find biomarkers for Parkinson's disease to enable diagnosis[1-3]. We do this from endogenous compounds excreted with sebum and obtained from skin swabs. In lab, we can determine if an individual has PD with >95% accuracy[3]. Our unique research program has been initiated by Mrs. Joy Milne, a retired nurse from Perth who noticed a change in her husband's body odour 11 years before his clinical diagnosis of Parkinson's disease (PD). Joy noticed the same distinctive odour was associated with other PD sufferers and hence linked it to onset of the disease. We have also used metabolomics from sebum to reveal alterations in the regulation of lipid synthesis and the carnitine cycle as PD progresses[2]. Recently we demonstrated the equivalence of sebum to serum as a diagnostic biofluid[4]. Based on Joy's observation, with simple non-invasive sampling of skin from the upper back, we have developed a diagnostic platform that is able to classify PD from sebum samples with >95% accuracy. The focus of our work to date has been to detect and identify the compound(s) that encompass the unique odour of PD. We have now assessed the feasibility and quality of information provided by using sebum as a diagnostic biofluid via multiple mass spectrometry (MS) based analytical methods, and are now positioned to translate these methods, by incorporating clinical data to stratify PD diagnosis from prodromal to overt. This talk will discuss our methodological approach, recent findings and give a perspective on the use of sebum for non-invasive sampling.

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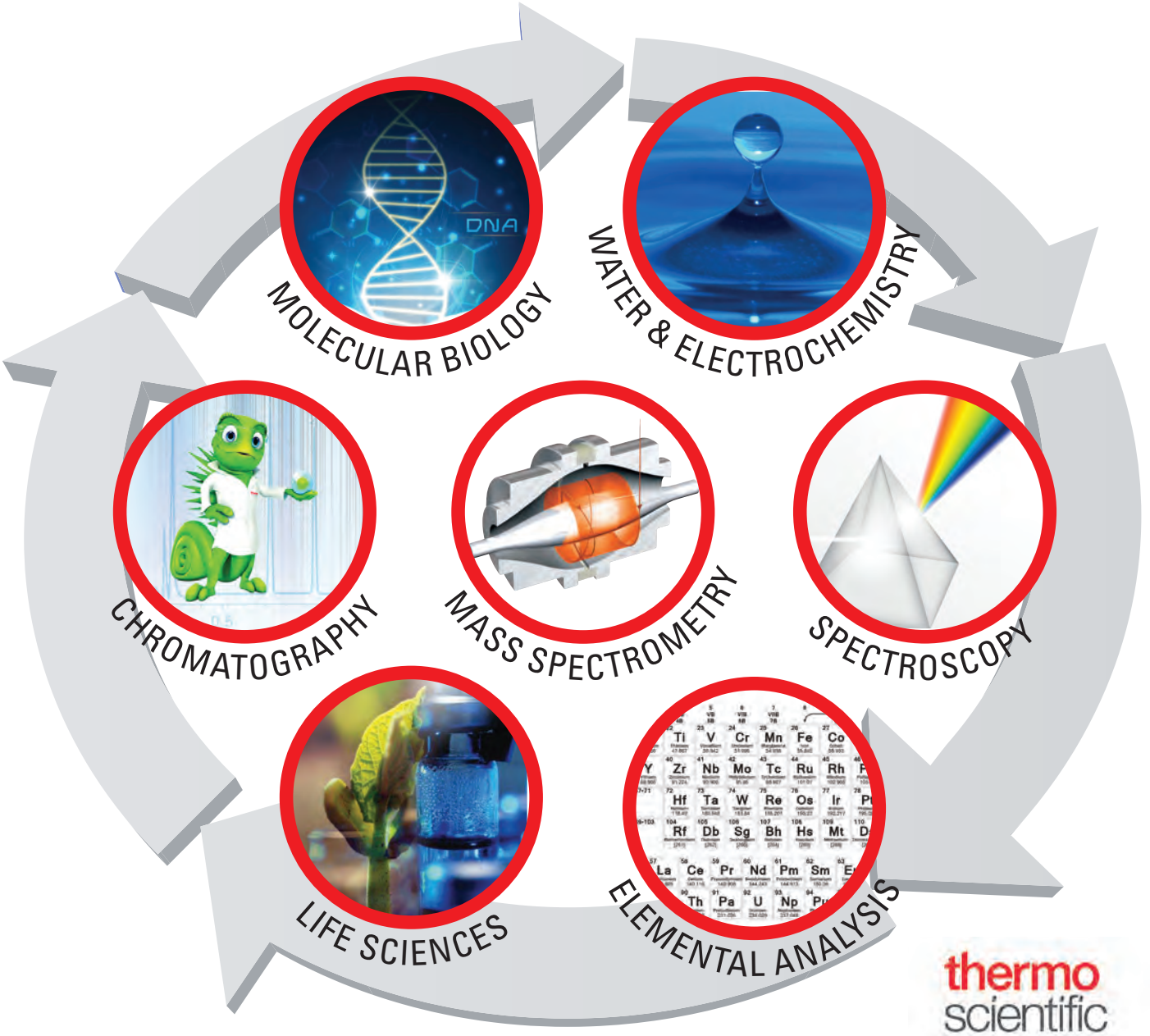

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K5 Azole antifungal drugs in water and wastewater systems

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The azole antifungals are among many of the contaminants of emerging concerns (CECs) that are present in the environment and posing risks to humans and ecosystem including the evolution of drug resistant fungi in the environment. We report, the occurrence of these drugs in the aquatic environments as well as the risk quotient (RQ) method to investigate the potential ecological and human health risks associated with their presence in the wastewater and/or drinking water. The azole antifungal drugs investigated included Clotrimazole, econazole, fluconazole, itraconazole, ketoconazole, miconazole posaconazole validation studies should be conducted for those drugs that seem to pose human health and ecological risks.

Acknowledgements
The University of South Africa for financial support to HA Assress and running costs for the project.

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K9 Frontiers of modern day electro-analysis – to infinity and beyond!

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Electrochemical sensors are tools capable of very sensitive, multi-element analysis, they are cost effective and remotely deployable for species evaluation and quantitative analysis. The integration of these sensors with microelectromechanical support systems may lead to the development of tools for real time problem solving in the environment and/or health domain with real world deployment capability. Examples of novel interfaces for sensor development from current research will be presented as examples of new sensors incorporating guest -host interactions of cucurbituril molecules and metal ligated Schiff base complexes for NO detection.

Current research is focused on the integrated application of analytical tools and technology to develop early warning systems for trace-level detection and quantification of critical contaminants. These systems are primarily electrochemically driven, but draw on a wide range of supporting analytical techniques and energy sources for feasible outcomes. This integrated approach to research is informed by the South African Research Infrastructure Roadmap (SARIR) that supports the National development Goals derived from global Sustainable Development Goals. Electrochemistry practitioners have responded with solutions to these challenges by proposing an integrated smart electrochemical systems strategy, that incorporates skills that are not historically associated with academic electrochemistry teaching and training. The new skills set is not necessarily prescriptive and varies in response to specific problems. However, the inclusion of micro-electronics, microfabrication and nano-micro scale materials design into the current academic research context, becomes mandatory to meet the demands for electrochemically driven devices that respond within a challenging analytical context and that meets the demand for integration with the internet of things (IoT). In turn the demand for multi-skilled electrochemistry artisans and professionals is ever increasing, notwithstanding the limitations imposed on the holistic development of expertise in this area.

K18

THINK GREEN…PLAY GREEN
SBSE: the Right Enrichment Technique

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Environmental investigations regarding analytical chemistry become during the last decade more intensive due to regulations, priority lists of emerging contaminants as well as the objective to characterize exhaustively the organic matter in different matrices. Even with the right sample prep, or because of the sample prep itself, a wide and complete vision of organic content remains impossible very easily. Furthermore, labor intensive sample prep techniques need hundreds of mL of solvent for the enrichment of only a few nanograms or less of micro pollutants when considering standard methods. For the last Twenty years we use the Stir Bar Sorptive Extraction link to GCMS or LCMS for the characterization of environmental matrices as well as for applying a “green philosophy” to dramatically reduce our consumption of solvent. At the beginning dedicated to off-flavors in tap water, SBSE was rapidly applied to waste water, sludge and even oil & gas effluent. In-situ derivatization technique were developed to extract polar compounds from water such as halophenols and aldehydes (formaldehyde, acetaldehyde); for non GC amenable molecules with multi polar sites, an on-liner derivatization technique was developed where the compounds desorbed from the stir bar were successively cryofocused and silylated automatically. Whatever the matrices considered, quantitation is possible and exhibit a very high sensitivity for off-flavor compounds with a limit of quantitation of 0,1 ppq with a single quad furthermore, very recently we applied this technique to sea water characterization for the quantitation of the European Union pollutants priority list. Creator since 2011 of the International SBSE Technical Meeting we have pushed this technique in multiple fields of activity that we will present you.

K22 Air pollution and health: Improvements in characterisation of the composition and toxicological impact of aerosol emissions and the polluted ambient air and

R. Zimmermann[1,2], J. Passig[1,2], R. Irsig[3], H. Czech[1,2], P. Martens[1], J. Schade[1,6], Sven Ehlert[3], T. Gröger[2], E. Zimmermann[1,2], J. Pantzke[1,2], S. Offer[1,2], Y. Rudich[4], A. Kiendler-Scharr[5], M. N. Delaval[2], S. Di Bucchianico[1,2], T. Adam[6]

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Air pollution with inhalable particle matter (PM) is known to be one most severe environmental health-risks worldwide (WHO, 2001). The investigation of the adverse effect mechanisms of aerosols (i.e. suspended, airborne particles) is a complex, multidisciplinary task with many scientific and technological challenges. The lecture starts with an introduction on the air pollution and health problem. In order to better understand the causes of the health effects, new methods and technologies for a more comprehensive characterisation of the chemical composition and physical properties of aerosols (i.e. particles and gases) need to be developed. Furthermore, improved biological assessment approaches for the adverse/toxic effects of aerosols are needed. In this lecture new approaches for both, the chemical and the toxicological characterisation of aerosols are presented, discussed and demonstrated by application examples. Firstly, a new method to directly assess the toxicological impact of aerosols is shown. In the last decade, air-liquid-interface (ALI) exposable biological lung models using human lung cell-cultures have been established. The ALI cell exposure approach is combined with state-of-the-art biological effect analysis. As an example, an ALI study elucidating the impact of atmospheric photochemical aging on aerosol particle-induced health effects is presented (aeroHEALTH, www.aeroHEALTH.eu). Fresh and photochemical aged gasoline car emissions (EURO 6 level) were tested, showing a significant toxification of the emissions by photochemical aging. This is highlighting the important influence of atmospheric chemistry for the adverse health-outcomes of air pollution and emissions. In the second part or the lecture, a new concept for an improved aerosol characterisation approach is presented. The new Single Particle Mass Spectrometric (SPMS) method based on bipolar laser mass spectrometry (Photonion GmbH) will be explained (Schade et al, Anal Chem. 2019). The aerosol is directly sampled from the air. The organic coating of the size-classified aerosol particles (laser velocimetry) is desorbed by an IR-laser pulse. A few µs later, the relevant toxicants (transition metals, PAH and soot) are ionized by a novel combined laser ionization scheme and are detected in the mass spectrometer. The SPMS technology has been applied for ambient aerosol analyses and combustion emission monitoring and is giving new insights into the mixing state of the air toxicants (PAH/metals/soot) and other compounds (e.g., nitrate, sulfate etc.). In the summary the desiderata for innovative aerosol and health research are discussed.

K25 A method for sampling skin volatile compounds and their analysis by GCxGC-TOFMS for TB related metabolic profiling.

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Tuberculosis (TB) is a leading infectious disease worldwide, especially in areas where immune-deficiencies abound. The development of drug resistant and multi-drug resistant strains are a great concern and effective screening techniques to detect the illness could go a long way to combat this scourge. It is known that volatile organic compounds (VOCs) indicative of TB can be found in the breath of infected patients[1] that can be used for diagnostic purposes. Our search for a simpler, more robust collection of diagnostic biomarkers for TB led us to polydimethylsiloxane (PDMS, silicone rubber) sampling of the human skin, that we had shown to reliably sample more than a thousand emanating VOCs in a study directed towards the understanding of profiles associated with attractiveness for blood-meal seeking female mosquitoes[2,3]. The sheer number of VOCs and the repeatability of their relative quantitative abundances led us to believe we would find reliable patterns of markers due to the metabolic profiles associated with infection by *Mycobacterium tuberculosis*. We will describe modifications to our PDMS sampling method to better eliminate artifacts resulting from the concentration of VOCs from surrounding air and the subsequent direct thermal desorption and analysis by comprehensively coupled two-dimensional gas chromatography and mass spectrometry (GCxGC-TOFMS). Infected patients (n=15) and uninfected controls (n=23) were sampled in duplicate and scrutinized using multivariate methods of data analysis, providing characteristic biomarker profiles for TB. Promising initial results bode well for the further development of a non-invasive, cheap and robust diagnostic tool for TB, that can be handled by untrained staff at point-of-care with access to a centralized GC-MS laboratory for reliable screening of patients. The risk of infecting on-site as well as laboratory staff is very low and drones could help bring an important diagnostic service to distant, off-grid communities.

Acknowledgements
Special acknowledgement goes to our late co-worker Prof Anton Stoltz for his enthusiastic support, planning and guidance in all clinical matters.

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I1 Turning green – Sustainable approaches to environmental sample preparation

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The preparation of samples prior to analysis can incur considerable environmental impacts. This is of concern particularly with respect to environmental samples, as they are analysed with the objective of protecting the environment. Recent advances have fortunately been made in sampling and sample preparation methods[1], which aim to address green chemistry concerns such as solvent and reagent use and energy consumption. Samplers which combine analyte pre-concentration with sampling are advantageous, and passive sampling approaches have the benefit of not requiring electricity. Microextraction techniques are important from a green chemistry perspective, as they significantly reduce solvent consumption. Therefore approaches including solid phase microextraction, dispersive liquid-liquid microextraction, single drop extraction and stir bar sorptive extraction have been applied in the preparation of environmental samples prior to analysis. Novel sorptive materials, including molecularly imprinted polymers, hold promise for more efficient sampling and extraction and may thereby improve analytical detection limits essential for monitoring pollutants at trace levels. There is a global movement within the chemistry community towards more sustainable laboratory practices[2], and practical means towards this goal with respect to sample preparation will be highlighted in this presentation. The provision of methods for environmental analysis which are facile, effective and green is challenging and requires both ongoing innovation and a holistic evaluation of the benefits as well as the trade-offs which are invariably incurred.

Acknowledgements
Funding provided by Rand Water is gratefully acknowledged.

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I4 Emerging contaminants- the bittersweet cocktails in water systems

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Emerging contaminants are chemicals of global environmental concerns in aquatic systems. They include polycyclic aromatic hydrocarbons, perfluorinated compounds, pharmaceuticals, nanomaterials and nano/microplastics. These compounds are present in household cleaning products, personal care products, industrial wastes liquids, semi/solids). They are therefore ubiquitous in environmental matrices due to these various applications. Their pathway into the environment is diverse – domestic, industrial, municipal pathways. Wastewater treatment plants (WWTPs) have also been found to be significant sources of emerging contaminants into the environment. This is because the WWTPs were not designed to remove these contaminants. Many of them are carcinogens and endocrine disruptors. Endocrine disrupting chemicals (EDCs) are substances that alter the function of the endocrine system. They are very significant at ultra-trace levels is due to their potential adverse effects on man and the biotic components of ecosystems. Although they occur at trace and ultra-trace levels in aquatic systems, they pose significant threats to human health and ecological systems. The need for environmental monitoring, risk assessment and pollution abatement therefore, become imperative. An overview of selected studies on emerging contaminants in the Western Cape will be presented. Instrumentations used included GC-FID, HPLC-MS-TOF, FTIR and microscopy (SEM and stereomicroscopy). Results obtained from field monitoring of selected emerging contaminants in water systems, their remediation and risk assessment will be presented. Most of the analytes studied were detected in environmental samples with significant human and ecological health risks. Some recommendations for policy decisions and social relevance will be provided.

Acknowledgements

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I5 Text mining for enhancing water quality data

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Text mining forms part of the broader field of Natural Language Processing (NLP), which in turn forms the intersection between linguistic studies and artificial language[1-2]. This study aimed to investigate the feasibility of implementing text mining on online platforms such as Twitter to enhance acquisition of water quality data. The approach used to achieve this involved: i) developing a framework and guidelines, based on coding to extract text on water quality from Twitter and (ii) collating the collected text data, transforming it to structured format and modelling it using machine learning techniques to yield insights into opinions and sentiments that are proxies to water quality.
The findings revealed that text data could be successfully processed, cleaned, transformed into structured form through vectorisation and modelled with respect to opinions and sentiments (Figure 1). These opinions and sentiments illustrated instances where users were satisfied, dissatisfied, trusted or distrusted their water quality. Word clusters, word clouds and networks were obtained that further revealed these and several other delineations.

Figure 1: Sentiment scores for water quality.

The success of this approach provides the possibility to extend it to other online platforms such as Facebook and WhatsApp. Further, real time capture and modelling of text can be explored that can be useful for decision making by regulatory agencies related to water quality.

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I8 Smart Electrochemical Sensing of Xylitol using a Combined Machine learning and Simulation approach

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The study makes use of Au nanoparticles (NPs) derived from *Callistemon viminalis* leaf extract coupled with multiwalled carbon nanotubes (MWCNTs) doped onto glassy carbon electrode (GCE) for the detection of xylitol in sugar free chewing gum. In comparison to the bare GCE, the modified GCE/MWCNT/AuNPs sensor showed about 45-fold better electrochemical response to xylitol. Under the optimal conditions, the designed sensor achieved a detection limit of 9.8×10^{-6} pM for concentrations ranging from 9.9×10^{-6} to 2.9×10^{-5} pM. The practicability was tested on sugar-free sample yielding recoveries of 97–100% with RSDs of 2.83–3.33%. Machine learning (ML) was used to predict changes in voltammetric signal with changing potential over time demonstrating the fundamental knowledge of the electrochemical reaction. The performance of the Artificial Neural Network (ANN) provides good accuracy and precision in predicting the intensity (I) along with repeated ANN runs, with a mean square error (MSE) of 0.007 (± 0.002) and a determination coefficient (R^2) of 0.9992 ± 0.0006. Additionally, the interaction of xylitol on the electrode surfaces were investigated using Monte Carlo adsorption studies and 1000 ps Molecular Dynamics simulations under NVT conditions. According to the frontier molecular orbitals obtained through Density Functional Theory calculations, the reactive sites of xylitol occur at the hydroxyl group on the second carbon. Using complementary measurement techniques, this new strategy exhibits a great potential for rapid detection of xylitol in food and dental products.

I11 Comparison of PSA to *Moringa Oleifera* seed protein as sorbent in QuEChERS: A Response Surface Methodology optimisation for extraction of some Endocrine Disrupting Chemicals in food

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This work aimed at optimising the QuEChERS method with PSA and then comparing it with *Moringa Oleifera* seed protein as clean-up sorbent for the extraction of endocrine disrupting chemicals. Response surface methodology approach was used in the optimisation. A design of experiment (DoE) was used to investigate the effect of the sample mass (0.5-3 g), centrifuge speed (3400-4000 rpm) and time (5-20 min), mass of $NaCl$ and $MgSO_4(1-3\ g)$, and solvent extraction volume (5-10 mL). The analysis was done using GC-ECD and GC x GC TOFMS. The PSA method which was later replaced with *Moringa Oleifera* seed protein presented optimal values of 3 g of sample, 150 mg PSA, 4000 rpm for 6 min centrifuge conditions, including 2 g NaCl and 2 g $\mathrm{MgSO_4}$ extracted in 10 mL methanol, respectively. *Moringa Oleifera* seed protein gave better selectivity and the detection limits ranged between 0.16 to 1.77 $\mu g\ kg^{-1}$ with RSD values $\leq 13.32\%$, respectively. Moreover, recoveries were between 76,2$\pm$0.85% to 105.2$\pm$2.24%. Application of the developed method in food samples detected some EDCs. This study has shown that *Moringa Oleifera* seed protein is a promising alternative to PSA in clean-up of food related samples using QuEChERS approach.

I16 Fate of pharmaceuticals in South African environment: Past, present and future research

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In recent years, large amounts of pharmaceuticals belonging to different therapeutic groups which include non-steroidal anti-inflammatory drugs (NSAIDs), antibiotics and antiretroviral drugs have been found present in South African water resources. The analytical approach for monitoring pharmaceuticals in South African environment mostly focused on solid-phase extraction (SPE) followed by liquid chromatographic analysis. In a most recent study, a suspect screening of 92 compounds with target monitoring of 21 pharmaceuticals in a river flowing through Soweto Township, Johannesburg, were performed with an analytical method which was based on SPE and ultra-high-performance liquid chromatography-quadrupole time-of-flight-mass spectrometry (UHPLC-QTOF-MS)[1]. In this case, 47 pharmaceuticals were detected, with 31 being found present for the first time in South African waters, while 7 were not recognized as South African medications. Acetaminophen had the highest concentration of 430 ng L^{-1}, while oxolinic acid with the highest hazard quotient of 48.6 indicated a risk of toxicity to aquatic organisms. The detection of a wide range of antibiotics in a stream flowing in Soweto suggested a release of these pharmaceuticals from wastewater treatment plants and dumpsites[2]. The fate of pharmaceuticals in South African environment is not yet well-understood. However, in recent years, different drugs have been found present in different South African environmental compartments such as aquatic plants, sediments and coastal waters[3]. In aquatic plants, the uptake through roots for both NSAIDs and antiretroviral drugs was observed to be followed by translocation into aerial tissues.

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I19 Automated deconvolution, pre-processing and statistical evaluation of GC-MS data for untargeted/targeted metabolomics for mining metabolites in matrices of interest

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Metabolomics has taken root in the family of "omics' which is an emerging multi-disciplinary area of global interest. It is the large-scale study of small molecules called metabolites within cells, biofluids, tissues or organisms. Some spin off benefits from metabolomics include agricultural research i.e. crop protection and engineering, in health care, medical diagnostics, biomarker mining and food/drug safety. The most commonly used analytical methods for metabolomics are NMR, LC-MS and GC-MS. These methods complimented by automated deconvolution, preprocessing and multivariate statistical data analysis. In my laboratory, we have utilized the Automated Mass Spectral Deconvolution and Identification System (AMDIS) to perform automated deconvolution of raw data acquired by GC-MS followed by pre-processing using Metab R^2. Other pre-processing freeware used are the GC–MS Assignment Validator and Integrator (GAVIN) script for Matlab[3] and MetAlign[4]. GAVIN is used to integrate results from multiple AMDIS files to produce a peak table of metabolites. MetAlign can perform format conversions automatically, baseline corrections, saturation and mass peak artifact filtering and many other data filtration functions. In addition, we explored cloud based metabolomics using Galaxy and the Workflow4metabolomics e-infrastructure for LC-MS, GC-MS and NMR data. In this lecture, metabolomics work flows that have so far been utilized in this laboratory for mining metabolites in honey[5] and human urine samples[6] will be discussed including their advantages and disadvantages.

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C1 Comparison of GC-MS versus GC-ECD detection and derivatization methods for the analysis of haloacetic acids in drinking water

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Water sustains all living organisms on earth, and due to the central role water plays, the United Nations have declared that "clean water and sanitation for all" is one of the sustainable development goals[1]. To achieve this, disinfection before consumption becomes crucial. Besides the desired effects, it has become known that disinfection leads to the formation of unwanted disinfection by-products (DBPs). To date over 600 DBPs have been discovered, which is of concern due to their carcinogenicity and other adverse health effects. One class of DBPs, namely the haloacetic acids (HAAs), are regulated in only very few countries. HAAs should, however, be routinely monitored in drinking water prior to distribution to ensure that it is safe. Multiple methods to quantify HAAs in water are reported in literature and many of these rely on GC-based analysis. However, due to the extreme volatility and polarity of the HAAs, derivatization before analysis is necessary. In the standard and most widely implemented method, the analytes are extracted by liquid-liquid extraction and then derivatized into the methyl ester by a simple Fischer esterification[2]. This requires harmful chemicals and harsh acidic conditions. To make the derivatization more environmentally friendly and safe, an esterification to the octyl ester was thus investigated. This alternate method uses less harmful chemicals and moreover, reaction times were reduced from over 2 hours to 30 minutes. The US EPA method uses Gas Chromatography-Electron Capture Detection (GC-ECD) to analyze the derivatized compounds, which is extremely selective for halogenated analytes and thus provides analytical sensitivity. The GC-ECD was compared to the more commonly used and easily accessible Gas Chromatography-Mass Spectrometric Detection (GC-MS). It was found that the GC-ECD remains superior in sensitivity; four out of nine derivatized analytes could be detected at 5 ppb and 10 ppb, whereas only one could be detected at 10 ppb with the GC-MS. This research has shown that the proposed derivatization method is superior, whereas the conventional detector is preferable with respect to sensitivity.

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C2 Magnetic Solid Phase Extraction Based on Fe_3O_4@Al_2O_3 Adsorbent for Simultaneous Preconcentration of Selected Metal Ions in Fuel Oils Followed By ICP-OES Determination

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Crude oil is a fossil fuel that occurs because of large quantities of living organisms compressed between the sedimentary rocks of the sea under intense heat and pressure[1]. This petroleum is then refined to produce crude oil derivatives such as gasoline, diesel, kerosene, just to name the few[2]. These fuel oils are energy sources that are vital in our everyday life[1-3]. However, crude oil and its derivatives contain metal ions, which are corrosion of refinery equipment, catalyst poisoning and severe air pollution[4]. Therefore, the study of metal ions in fuel oils remains a key, as this helps to create awareness on metal concentration levels for development of proper control measures. In this study, Fe_3O_4@Al_2O_3 nanoparticles were synthesised, characterized (FTIR, SEM-EDS, TEM and XRD) and applied as magnetic adsorbents for simultaneous preconcentration and extraction of 15 metal ions in selected petroleum samples prior to analysis using inductively coupled plasma-optical emission spectroscopy (ICP-OES). Various experimental parameters affecting the proposed magnetic solid phase extraction (m-SPE) method were investigated by using CONOSTAN oil analysis standard-custom bled containing Ag, Al, Cd, Co, Cr, Cu, Fe, Mn, Mo, Pb, Ti, V and Zn metal ions. Additionally, multivariate mathematical tools such as two level fractional factorial design (FrFD) and the central composite design (CCD) were used for the optimization. The optimization results showed that Fe_3O_4@Al_2O_3 adsorbent exhibited excellent performance of when 40 mg adsorbent mass, 35 minutes extraction time, 6.5 pH, 20 µg/L spike concentration and 1.0 mol/L eluent concentration were used. Under optimum conditions, the developed m-SPE displayed good accuracy (86-96%) for all metals with exception of Zn at 74%, precision (0.9-4.8%) and low method detection limits (0.114-0.62 µg/g). The proposed m-SPE method also reported preconcentration factors of 168, 166, 152, 165, 164, 150 and 150 for Co, Cr, Cu, Mn, Mo, Pb and V, respectively. Additionally, the enrichment factors were 30, 24, 11, 20, 26, 10 and 8 for Co, Cr, Cu, Mn, Mo, Pb and V, respectively, which were quite comparable with other literature reported SPE methods. The optimised and validated m-SPE method was then applied in real fuel oil samples.

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C3 LC-MS/MS method development and validation of novel anti-malarials for preclinical evaluation

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Malaria is one of the most widespread diseases in Africa[1], only further compounded by the advent of drug resistance. Therefore, there is a need to develop pharmacophores that may combat drug resistance. Our collaborators at the University of Kwazulu-Natal have developed quinoline-urea-benzathiozole hybrids (Figure 1) that have displayed antimicrobial activity *in vitro*[2]. The aim of our research is to study these drugs in a preclinical setting to further evaluate its pharmacokinetic, pharmacodynamic and anti-malarial activity *in vivo*. A LC-MS/MS method had to first be developed and validated for these parameters to be investigated and quantified. Extraction optimization studies were performed in blank plasma spiked with compounds I-IV (Figure 1) where protein precipitation, liquid-liquid extraction and solid phase extraction were investigated to determine the optimum analyte enrichment technique. Method validation was performed according to the European Medicines Agency guideline for bioanalytical validation. The accuracy, precision, matrix effects, specificity, stability, and dilution integrity validation parameters all fell within the acceptable statistical values stipulated by this validation guide. Therefore, this LC-MS/MS is suitable to use for the quantification of compounds I-IV in plasma.

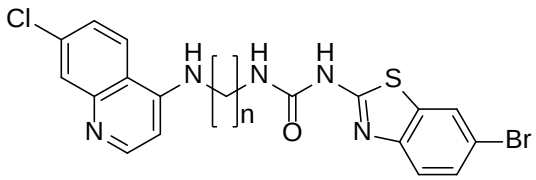

Figure 1: Structure of quinoline-urea-benzathiozole hybrids I-IV where n=2 (I), 3 (II), 4 (III), 6 (IV)

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C13 Exploring the selectivity of carbon dioxide-ethanol-water ternary solvent mixtures in the extraction of antioxidative compounds from brown seaweed

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Seaweed is considered one of the most promising food ingredients[1], with the potential to be processed into several other products. The growing need to reduce environmental burden has propelled the use of techniques utilizing non-toxic solvents. Among such explored techniques is supercritical fluid extraction (SFE), employing carbon dioxide (CO_2) with additional ethanol (EtOH) and water (H_2O) as cosolvents [2]. However, the developed extraction methods˝ ability to discriminate between matrix components and target analytes (selectivity), is still to be investigated. There is also a general limitation in the quantitative definition of selectivity, despite being one of the performance indicators used in extraction. This study aims to synthesize the theory of extraction selectivity and comprehensiveness, utilizing CO_2-EtOH-H_2O ternary mixtures in SFE, targeting antioxidative compounds in seaweed biomass against high molecular weight compounds being carbohydrates and proteins, as well as toxic metals. The approach also utilizes a validated supercritical fluid chromatography method[3], coupled with ultra-violet/visible (UV/VIS) detection techniques, gravimetry and multi-linear regression (MLR). The degree of selectivity here explains the extent to which the extraction of the target compound will be favoured over the matrix components, scaled from 0-1 (or 0-100%). This value shows the ratio of extractability of an individual target analyte over the sum of contributions of all solubilized interferences measured. The use of CO_2 with 5% ethanol as a cosolvent, held at 300 bar and 60°C, allowed for the highest extraction selectivity, favouring 70% selectivity degree towards β-carotene over measured interferences, followed by 48% towards tocopherols. In addition, these conditions also allowed for extracts free of toxic metals. The addition of water to EtOH cosolvent enhanced the extractability of phloroglucinol and fucoxanthin, while on other hand it resulted in lower extraction selectivity due to the co-extraction of carbohydrates and metals. Further, the extraction selectivity of target compounds was increased by carefully optimizing the extraction times in each fractionation step.

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C14 Analysis of organosulphur compounds in fuel oil samples using magnetic solid phase extraction based on Au-Fe_3O_4 adsorbent and GC-HR-ToFMS

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This study focused on the development of a magnetic solid phase extraction (m-SPE) method using Au-Fe_3O_4 as an adsorbent followed by GC-HR-ToFMS analysis for the determination of organosulphur compounds (OSCs) in fuel samples. The m-SPE using Au-Fe_3O_4 NPs was preferred because of the low toxicity of the adsorbent[1], high separation efficiency using external magnet[2] and greater extraction selectivity between sulphur and Au atom[3]. The Au-Fe_3O_4 NPs were characterized using XRD, UV-Vis, TEM, SEM and FTIR. This method was optimized using multivariate analysis based on a two level full factorial and central composite designs. The conditions which produced optimum efficiency were found to be 150 mg mass of sorbent, 100 µL eluent volume, 50 min extraction time and 6,5 pH of the sample. These optimum conditions showed a relatively low limit of detection in the range of 0.02 – 0.0416 µg/g and limit of quantification of 0.126 – 0.602 µg/g. Furthermore, a relative standard deviation of triplicates analysis was between 0.8 – 0.2 % with good linearity of 0.9816 – 0.9961. The percentage recovery for thiophene, 3-methylthiophene, benzothiophene and dibenzothiophene ranged from 88 to 104 % for the spiked samples. The optimized m-SPE method was then applied in real fuel oil samples. The concentration of thiophene, 3-methylthiophene, benzothiophene and dibenzothiophene in crude oil, gasoline, diesel and kerosene ranged from 0.3 – 4.09 µg/g, 1.06 – 1.65 µg/g, 0.02 – 3.06 µg/g and 1.01 – 5.02 µg/g respectively. The m-SPE, followed by GC-HR-ToFMS method proved to be efficient, rapid, inexpensive and an alternative method for OSCs analysis in fuel oils.

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C15 Quantitative analysis and health risk assessment of bisphenol A and its derivatives in selected canned food in South Africa, using a modified QuEChERS method coupled with gas chromatography-mass spectrometry

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Bisphenols (BPs) are a group of endocrine destructive chemicals, that are used as monomers for the synthesis of epoxy resin. Epoxy resin is used as an inner can coating[1]. Bisphenol A and its analoges can migrate from can coatings to food causing adverse health issues to human even when consumed in ppb[2]. The general aim of the study is to conduct qualitative and quantitative analysis of Bisphenol A and its common derivatives in canned foods locally produced in South Africa. Canned food locally produced in South Africa were purchased across Ga-Rankuwa supermarkets and convenient stores. Prior to extraction, food samples were first homogenized and spiked with analytical standards. Extraction of analytes was done using QuEChERS and acetonitrile as the solvent followed by derivatization using BSTFA. Analysis was carried out using GCMS. Bisphenol A and B were detected in the food samples with concentration range of 14 - 113 and 13 - 37 µg/Kg, respectively. However, these concentrations were all below the specific migration level of 600 µg/Kg. Bisphenol C, E and F were not detected in all tests. The mean estimated daily intake for bisphenol A and B were 0.12 and 0.043 µg/Kg body wt/day, respectively. A health risk assessment showed that the potential of non-carcinogenic effects due to a lifetime consumption of the studied canned foods was minimal with the Hazard Quotient values calculated for bisphenol A and B were all less than 1. However, the canned food still poses potential risks for babies and consumption of these food sources should be delayed or at least minimized. Generally, the detection of these bisphenols in the studied food samples has also highlighted the existence of bisphenols in food cans, their potential to migrate into the canned contents and ubiquity in canned food products.

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C25 Coupling piezo-polarization effect on Ti/$BaZrTiO_3$ anode with sonoelectro-Fenton and sonoelectrochemical oxidation for the mineralization of aspirin in wastewater

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We hereby present the sonoelectro-Fenton and sonoelectrochemical oxidation of aspirin in water on Ti/$BaZrTiO_3$ anode and carbon felt cathode. Piezo potential possessing $BaZrTiO_3$ can generate internal dipolar charges within the crystal lattice of its structure when agitated mechanically [1]. These surface localized charges can interact with hydroxyl ions and dissolved oxygen in an aqueous medium to generate hydroxyl and superoxide radicals, which are responsible for the non-selective breakdown of the target organic pollutant in water [2]. Hence $BaZrTiO_3$ was synthesized and immobilized on an etched titanium sheet to obtain Ti/$BaZrTiO_3$ anode. The Ti/$BaZrTiO_3$ anode was applied for sonoelectro-Fenton and sonoelectrochemical oxidation for the removal of aspirin in water. Degradation efficiencies of 96.36% and 69.43% were obtained at optimum operating conditions of 60 W ultrasound power, 10 $mAcm^{-1}$ applied current density for 120 min. The impressive performance was obtained during sonoelectro-Fenton processes can be attributed to the simultaneous oxidation taking place at the surfaces of both Ti/$BaZrTiO_3$ anode and carbon felt cathode. In addition, the presence of ultrasound irradiation in the reactor contributed immensely to the performance of the electrodes and the technique by continuously cleaning the electrode surfaces and improving the rate of electroregeneration of Fenton reagent (Fe^{2+}) on the cathode. The synergy developed during sonoelectro-Fenton technique, which stems from the in situ oxidative action occurring at the surfaces of both electrodes positions sonoelectro-Fenton oxidation technique as a reliable method for the treatment of pharmaceutical polluted water.

Acknowledgements

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C26 Nanostructured electrocatalysts for water electrolysis

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Water is considered as one of the "magic" molecules as its efficient electrocatalytic conversion can produce limitless renewable energy. [1] Water electrolysis produces hydrogen and oxygen, while the process can be driven by renewable sources such as wind or solar. The produced hydrogen can then be used for example as a fuel or as a reducing agent in chemical processes. We aim to provide a brief overview on different electrocatalysts which were evaluated for water electrolysis. Pt, Pd, and Al sputtered thin film (60 nm) electrocatalyst combinations (Figure 1a and b) were investigated towards SO_2 assisted water electrolysis. A Pt_3Pd_2 thin film (800 °C), and a ternary combination of $Pt_{40}Pd_{57}Al_3$ (900 °C, Figure 1c), were identified as potential contenders to compete with pure Pt that is currently being employed as the electrocatalyst of choice.[2] Reactive sputtering was employed to prepare various $Ir_{1-y}Ni_yO_x$ electrocatalyst combinations for catalysing the oxygen evolution reaction (OER). Combinations containing higher amounts of Ir ($Ir_{92}Ni_8O_x$, $Ir_{68}Ni_{32}O_x$ and $Ir_{62}Ni_{38}O_x$) exhibited the best overall electrochemical performance of the studied mixed metal oxide electrocatalysts. However, in terms of mass-specific activity (current per mass of noble metal), none of the mixed metal oxides could outperform Ni.[3] We also report on 2D metal oxide and metal organic framework (MOF) Ni-based nanostructured electrocatalysts containing Fe. Synthesised via a solvothermal method using 2,5-dihydroterephaltic acid (dhta) as the ligand, Ni/FeO performed the best for catalysing the OER, exhibiting an overpotential of 0.73 V at a current density of 50 mA.cm^{-2} (Figure 1d-g).

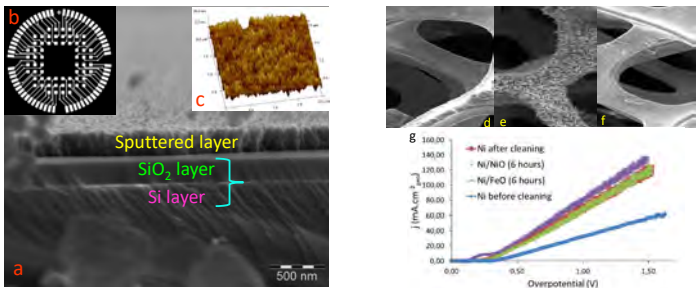

Figure 1: a) Sputtered thin film on a Si/SiO_2 wafer, b) high-throughput screening circuit pattern, c) AFM image of $Pt_{40}Pd_{57}Al_3$ (900°C). SEM images for: d) Ni foam after cleaning; e) Ni deposited on Ni foam; f) Fe deposited on Ni foam, and d) LSV plot exhibiting OER performance.

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C27 Construction of Functional Cobalt Phthalocyanine-Modified Electrodes for the Electrocatalytic Detection of Paraquat

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The rising levels of pollution in water bodies due to industrial and agricultural pollution demands the need for prompt and accurate analysis of water quality. In particular, heavy metal cations and pesticides, have detrimental health effects on aquatic, human and animal life forms. However, traditional methods involve the use laboratory-based instrumentation which are time-consuming and expensive to operate. In contrast, electrochemical sensors can provide no or minimal sample preparation and on-site time analysis. Literature trends illustrate that the selectivity and sensitivity of bare electrodes can be fine-tuned through the immobilization of conductive chemical modifiers such as metallophthalocyanines (MPcs) and their nanoconjugates[1]. This research study explores the use of a Au modified electrode (CoPc-cou-f-MWCNTs/3-HT/Au). It was fabricated via a sequential modification procedure entailing the formation of self-assembled monolayer (SAM) of the coumarin-substituted cobalt phthalocyanines, followed by the in-situ deposition of poly(3-hexylthiophene) ([3-HT]n) via electropolymerisation. Subsequently, the chemically modified electrode was used for the electrocatalytic detection of paraquat (PQ). Peak currents for PQ were linear in the range of 0.1 – 1 mM with a limit of detection (LOD) and limit of quantification (LOQ) of 1.77 x 10-4 M and 5.37 x 10-4 M, respectively. CoPc-cou-f-MWCNTs/3-HT/Au exhibited good sensitivity towards PQ in the presence of other pesticides assumed to be in a real water sample collected from the Durban lagoon.

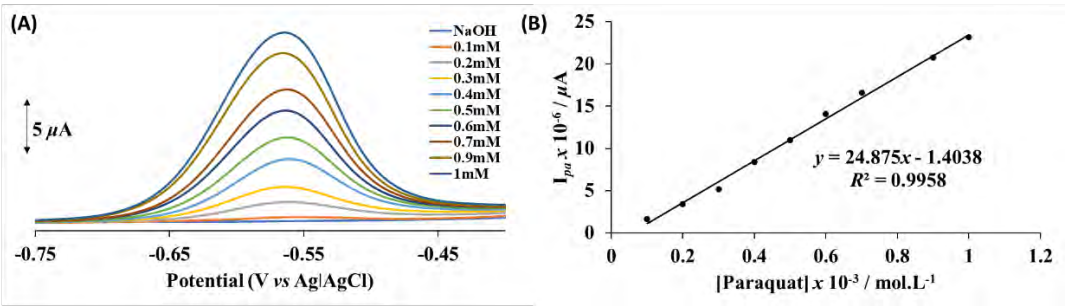

Figure 1: (A) DPV's recorded of PQ in 0.1 M NaOH using a CoPc-cou-f-MWCNTs/3-HT/Au modified electrode at increasing concentrations (0.1 – 1.0 mM), (B) Calibration curve of peak current response against PQ concentration

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C34 Smart electrochemical immunosensor for detection of aspartame in dietary products supported by *in silico* methods

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Aspartame (ASP) is one of the most widely used artificial sweeteners; therefore, there is a need to develop reliable and reproducible analytical methods for its detection. In this study, a novel detection of ASP using biosynthesized polyvinylpyrrolidone-capped silver nanoparticles (PVP-AgNPs) with functionalized multiwalled carbon nanotubes (fMWCNTs) and TIR2 antibodies doped onto glassy carbon electrodes (GCEs) is described. A variety of complementary analytical measurement techniques were employed for the separation and characterization of AgNPs capped with PVP. The electro-oxidation of ASP was observed by a well-defined oxidation peak potential at 1.4 V. The immunosensor sensor showed a linear dynamic range of 2.89–27.61 µM (R2 = 0.9170) based on differential pulse voltammetry, with limits of detection and quantification (S/N = 3) of 0.40 and 1.34 µM respectively. The chemical reactivity of ASP was confirmed by density functional theory (DFT) calculations. In addition, a coupled molecular docking and Monte Carlo (MC) simulations revealed a high binding affinity between ASP and the developed GCE/PVP-AgNPs/fMWCNTs/T1R2, electrode. Molecular dynamics (MD) simulations were used to examine the conformational profile of the docked structure. The immunosensor has been applied successfully to sensing of ASP in commercially available dietary products, which can be applied to newly developed electroactive sweeteners.

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C35 Evaluation of cellulose acetate supported MOF-5/crystalline nanocellulose nanocomposite as an adsorbent for methylene blue removal from water

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In this study, a novel, low-cost and efficient adsorbent was fabricated through a solvothermal method. The adsorbent consists of cellulose acetate (CA) substrate as a support membrane and MOF-5/crystalline nanocellulose embedded on it. The performance of the material was evaluated for the adsorptive removal of methylene blue (MB) from aqueous solution. Crystalline MOF-5/CNC nanocomposite was successfully supported on amorphous CA as demonstrated by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and Energy-dispersive X-ray (EDX)[1-2]. Figure 1 demonstrates the porosity and pore channels of the adsorbent. The adsorbent's point of zero charge (pH_{pzc}) was measured to be 7.0. The adsorption process of this material was characterized by a rapid increase in MB adsorption during the first hour with equilibrium being achieved 4 hours into the adsorption process. Adsorption efficiency was observed to increase with pH as at pH values beyond the pH_{pzc}, the material's surface charge is negative and it has a higher affinity to the cationic MB dye. The maximum adsorption capacity was determined to be 3.92 mg/g. The MB adsorption process was found to conform to a Freundlich isotherm model with a 1/n value of 0.672, suggesting a favorable adsorption process. The adsorption process favored a pseudo-second-order rate implying that adsorption occurs through chemisorption. This study has shown that CA-supported MOF-5/CNC is a promising adsorbent for the treatment of contaminated water.

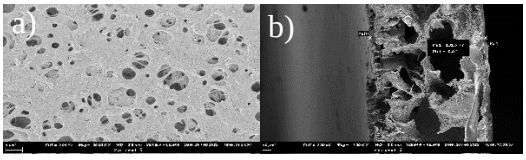

Figure 1: a) Surface and b) Cross-section SEM images of CA-supported MOF-5/CNC.

Acknowledgements
Supervisors: Dr N Nombona and Dr P Mdluli, University of Pretoria, Chemistry department, NRF, Lab colleagues

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C36 Semiconducting Cu_2ZnSnS/Se_4 quaternary chalcogenides as alternative counter electrodes for DSSCs

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Quaternary semiconductors are among the emerging *third generation* nanomaterials which are promising candidates for photovoltaic applications. The advancements to harvest solar radiation from the sun and convert it into electricity are needed to meet the increasing global demands for clean and renewable energy[1]. To contribute towards energy demands, the colloidal synthesis of quaternary nanomaterials enables the simple and low cost production of thin film photovoltaic (PV) solar cells. In this study, quaternary copper zinc tin sulfide/selenide (Cu_2ZnSnS/Se_4) abbreviated as CZTS/Se respectively. The as-synthesized CZTS and CZTSe nanocrystals are composed of earth-abundant elements, which have been reported to exhibit a bandgap within the range 1.0 – 1.5 eV[2-3]. Electrochemically, CZTSe exhibited the highest series resistance and charge transfer resistance smallest exchange current density and limiting diffusion current thereby making it the least favorable electrocatalyst. On the other hand, CZTS had the lowest series resistance and charge transfer resistance however had the largest exchange current density and limiting diffusion current thereby making it the best electrocatalyst. The DSSC using CZTSe-ITO only exhibited 1.01% and CZTS–ITO gave the best performance with the power conversion efficiency (PCE) of 3.62% while.

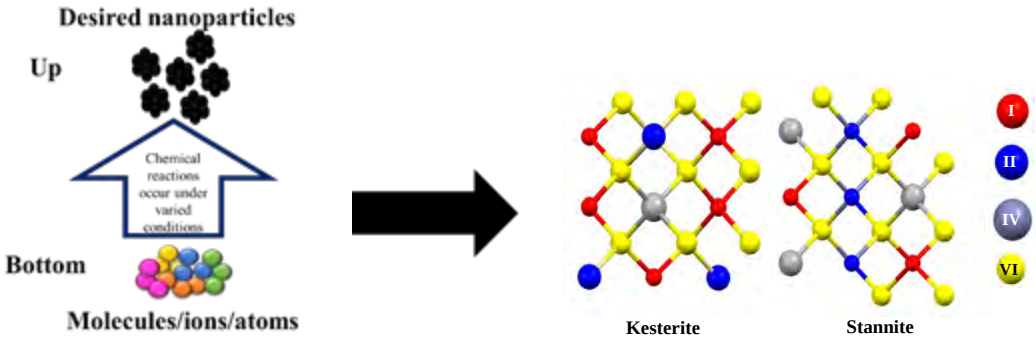

Figure 1: Synthesis of quaternary semiconducting nanomaterials using the bottom-up method.

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C51 Spatial and temporal variations in the presence, levels, and risk assessment of selected polycyclic aromatic hydrocarbons in sediments and water from Klip River, Johannesburg, South Africa

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in the environment and have been found to be carcinogenic, teratogenic, and mutagenic[1]. The aim of this study was to identify and quantify the levels of selected PAHs, including those in the USEPA priority list, in water and sediment samples collected from Klip River, Gauteng Province. Acid mine drainage, automobile exhaust, treated and untreated sewage discharge from industries near the river, municipal/industrial waste disposal, emissions, refuse burning, and coal combustion at the Klip River industrial complex are all potential sources of PAHs in the Klip River wetland system[2]. The levels of PAHs in water and sediment samples collected in low and high flow seasons were assessed by gas chromatographic-flame ionization detector (GC-FID) and -time of flight mass spectrometric detection (GC-TOF-MS). The total detected PAH concentration were in the range of 47- 98 mg/kg in sediment samples and 0.0210-0.0689 mg/L in water sampes. Furthermore, the evaluation of ecotoxicological effects of water and sediment samples were conducted using the zebrafish embryo development test (ZFET). Upon exposure and motoring of zebrafish embryos to water and sediment samples, every 24 h post fertilization (hpf), up to 96 (hpf), the major toxicological endpoints evaluated and observed included the primary endpoints, mortality, hatch rate and development. Specifically, the development was monitored by tracking the somite formation, heartbeat, blood circulation, pigmentation, spinal deformation, coagulation of embryos and non-detachment of a tail. High mortality (66-100%) and late hatching (33-66%) of the zebrafish have been observed in sediment samples as compared to the water samples due to high concentration of PAHs detected in sediments relative to water samples. Chemometrics was applied for determination of links between PAHs presence and environmental effects.

Acknowledgements
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C52 Size exclusion and reverse phase high performance liquid chromatography as complementary tools to study wheat gluten protein

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Wheat is considered unique amongst cereal crops due to its unique gluten proteins, which compose approximately 80-85% of the total grain protein. Gluten proteins characteristically fall into two groups based on their solubility in aqueous alcohol solutions; gliadin and glutenin. These proteins play a key role in determining the unique baking quality characteristics of wheat. The size distribution of glutenin polymers is a main determinant of the end-use quality of wheat. Size exclusion high-performance liquid chromatography (SE-HPLC) is a technique used to separate large molecules, such as proteins, based on their molecular size. SE-HPLC separates wheat proteins into high molecular weight glutenins (large polymeric proteins), low molecular weight glutenins (small polymeric proteins), gliadins (large monomeric proteins) and albumins/globulins (small monomeric proteins). This technique involves moderate interactions with a sample, thus permitting the high retention of biomolecular activity. Roughly 80% of the glutenin polymer can be solubilised with the detergent sodium dodecyl sulphate (SDS), and the residual polymers require sonication. The first SDS extraction helps to remove virtually all monomeric gliadins and some smaller polymeric glutenins. The second extraction, involving sonification, removes most of the remaining larger polymeric glutenins.
Reverse-phase high-performance liquid chromatography (RP-HPLC) fractionates proteins based on hydrophobicity rather than molecular mass and thus complements SE-HPLC. This technique depends on the surface hydrophobic binding of the protein from the mobile phase to the hydrophobic ligands that are attached to the stationary phase. The analysis of proteins and peptides is typically made up of an n-alkyl silica-based sorbent where solutes are eluted with increasing gradient concentrations of organic solvent. It is a sensitive technique with excellent reproducibility and resolution. RP-HPLC separates proteins into three main groups, each consisting of two or three protein types; a HMW group including the x- and y-type; a medium molecular weight group (S-poor group) containing the omega-bound (*ω5*- and *ω1,2*-type) gliadins; and a LMW group (S-rich group), consisting of LMW-GS and the *α*- and *γ*-type gliadins. This study reports on the use of SE-HPLC and RP-HPLC in the analysis of gluten protein of nine bread wheat cultivars under two levels of different intensities of heat stress and drought stress, with an optimal control. The two techniques were complementary, with SE-HPLC separating polymeric and monomeric protein peaks, and RP-HPLC separating a range of peaks including the gliadins, LMW glutenins and HMW glutenins. The two techniques looked at the gluten from different perspectives and highlighted different aspects of the response of gluten protein to abiotic stress.

C53 Quantification and toxicity evaluation of steroid hormones in wastewater effluent

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Steroid hormones are chemical messengers responsible for the regulation of several physiological processes in the human body[1]. These hormones have found wide pharmaceutical application (i.e. contraceptives and hormonal replacement) which has resulted in their introduction into the environment as constituents of wastewater effluent. Steroid hormones are classified as endocrine disrupting compounds and are associated with several health risks on their external exposure[2]. The aim of the study was to investigate the presence of steroid hormones in the wastewater effluent and further evaluate their toxicity and that of the effluent. The effluent was sampled from the discharge point of seven treatment plants in Ekurhuleni, Gauteng. Samples were filtered and extracted using solid phase extraction. Liquid chromatography-mass spectrometry was used for the quantitative and qualitative analysis of the sex steroid hormones. The zebrafish embryo assay was used to study the toxicity of the effluent and the hormones detected in the samples. Seven steroid hormones namely estrone, estriol, 17β-estradiol, 17α-ethinylestradiol, progesterone, testosterone and androstenedione, were detected in the effluent with a concentration range of <LOQ – 0.993 ng/mL. The effluent and hormones were found to be toxic towards the zebrafish embryos, indicated by the development of several end points including mortality, embryo coagulation, scoliosis, oedema, and delayed hatching.

Acknowledgements
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C60 Human exposure to plasticisers from single-use plastic food contact materials

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280 million tonnes of plastic are produced annually around the globe, of which half is single-use items such as straws, polyethylene terephthalate (PET) bottles, polypropylene (PP) food packaging and polystyrene (PS) take-away containers. Plasticisers are added to these plastic food contact materials (FCMs) to promote flexibility but have been found to leach into food and drink media. Plasticisers occur at trace concentrations, rendering their detection and regulation a challenge. The World Health Organisation confirms that these trace levels are sufficient to compromise human health, especially in the case of repetitive exposure through various exposure routes. [1-2] This study provides a simple detection and quantification method for extractable and leachable (EL) compounds that emerge from FCMs. Food contact materials were exposed to ambient conditions, elevated temperatures, UV/Vis radiation and microwaving to simulate various scenarios, such as leaving PET-bottled beverages in a car or in the sun, microwaving take-away food in PS or PP packaging, drinking hot beverages out of PS cups or drinking cooldrink out of PP cups. Detection and quantification of ELs migrating out of plastic FCMs using an in-house developed PDMS loop for sorptive extraction is reported for the first time. Sampling was followed by analyses with comprehensive gas chromatography – time of flight mass spectrometry (GC×GC-TOFMS) and ultra-performance liquid chromatography – ion-mobility spectrometry – high resolution mass spectrometry (UPLC-IMS-HRMS). These complimentary techniques enabled the detection of wide volatility range of ELs at trace levels. Diethyl phthalate, a known endocrine disrupting chemical (EDC), was detected in levels up to 167 µg per single-use food contact material. Other EDCs detected included several phthalates and plasticisers, as well as BPA. Toxic compounds released upon microwaving plastic FCMs included styrene, styrene oxide, benzonitrile and hydrogen azide. The high trapping power of an in-house developed PDMS sorptive sampler enabled extraction of a diversity of compound classes from the FCMs analysed. PDMS loops were desorbed directly in the GC inlet to optimise analysis time, prevent sensitivity loss and avoid the use of expensive cryogenics. LODs and LOQs for LC analysis ranged from 0.014 µg/L (Octabenzone) to 7.4 µg/L (Irganox 1076) and 0.042 µg/L (Octabenzone) to 22 µg/L (Irganox 1076), respectively. Extractable and leachable target compounds were detected in water stored in single-use FCMs in concentrations ranging from 0.019 to 25 µg/L.

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C61 Quantification Of Per and Polyfluorinated Alkyl Substances in Wastewater Treatment Plants in South Africa

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Per and polyfluorinated alkyl substances (PFASs) have been a cause for concern owing to their high resistance to degradation, bioaccumulation in biological systems and their impacts on human health and the environment[1]. Wastewater treatment plants (WWTPs) are identified as significant contributors of PFASs because municipal and industrial wastewater contain, among other contaminants, fluorochemicals[2]. WWTPs have also been recognized as secondary point sources of PFASs pollution to surface water and groundwater[3]. Monitoring and regulation of PFASs in water sources is still in its infancy in South Africa. Therefore, more data on PFASs is vital for informed decision on regulation. Wastewater influent and effluent samples (41) were collected from 14 WWTPs in South Africa using high-density polypropylene sample bottles. After spiking with a surrogate standard, solid phase extraction (SPE) was optimized and adopted for sample extraction, and samples analyzed using LC-MS/MS, after optimization. Of the 24 PFASs targeted in this study, at least 15 PFASs were detected in all samples. The highest concentrations were observed for PFOA, PFBS, FHEA, PFOS, FOET, PFHpS, PFHxA, PFHxS, 6:2 FTS and PFBA at 1063 ng/L, 1001 ng/L, 662 ng/L, 658 ng/L, 575 ng/L, 482 ng/L, 359 ng/L, 340ng/L, 298 ng/L and 279 ng/L, respectively. High levels of these PFASs in WWTPs effluent indicate that conventional WWTPs are not efficient in removing these PFASs. These results are alarmingly high as PFASs are likely to end up in rivers, drinking water treatment plants and eventually in tap water. The results obtained in this study are comparable to those from other parts of the world.

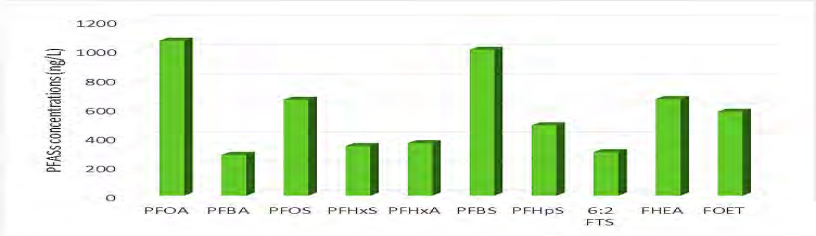

Figure 1: Highest concentrations of observed in wastewater samples

Acknowledgements
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C62 Gravimetric quantification of low-grade gold in mine tailings

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A large amount of land (>300 km) in the Gauteng region, is occupied by mine tailings, which still consist of valuable minerals such as gold and platinum group metals[1]. Currently, various tailings retreatment plants have been set up to recover the gold that was initially lost through methods with low efficiencies. This indicates the need for an industrial and analytical method that can be employed to quantify the gold with the highest accuracy and fewer uncertainties. Therefore, this study aims to quantify low-grade gold in mine tailings from the Ventersdorp Contact Reef of the Witwatersrand Basin using a gravimetric method. The tailings were characterized using X-Ray Diffraction for mineralogical analysis, and elemental and oxide content using alkaline fusion with ICP-OES analysis. A gold deportment test was carried out to quantify the amount of gold locked in various minerals and to determine how much gold is freely accessible. The characterization tests showed the presence of quartz (80%), talc (1%), gypsum (0.5%), calcite (0.3%), and pyrite (1%) which were also consistent with the pH (7-9) and the elemental composition. Fire assay using a lead flux with a lead oxide: carbon ratio of 11-12 and quantification using gravimetry, showed an improvement in the recovered gold, compared to a flux with a ratio of 8 for the specific matrix. The gravimetric method used showed to be accurate and also at an advantage as it is directly related to the mass physical unit, making traceability easier. Furthermore, a statistical study that investigated the uncertainties in the method used, showed significantly low or tolerable uncertainties, thus increasing the confidence in the method.

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C85 Mineral beneficiation from seawater: development and optimization of selective extraction techniques for essential minerals from seawater brine

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The world's demand for mineral salts is growing rapidly. This study therefore focuses on extracting mineral salts in seawater by developing a technique which is more selective, efficient, cheaper and environmentally friendly. These minerals includes Calcium, Magnesium and Lithium. The polymer inclusion membrane (PIMs) is one of the techniques that are being studied which consist of cellulose triacetate (CTA), trioctyl phosphine oxide (TOPO), thenoyltrifluoroacetone (TTA) and Nitrophenyl octyl ether (NPOE)[1-2]. The PIM prepared was used to separate the feed phase from the receiving phase. During the optimization of PIM, the main parameters were optimized which include composition of the membrane, pH effect, concentration of the receiver solution and extraction time. A feed solution containing ultrapure water was spiked with 15 ppm of the target compounds for optimization purposes. A 5 ml of 0.05 M HCl was prepared for the receiving phase. The optimum conditions were applied into real seawater samples. The extraction time was varied between 1 to 30 days to investigate the membrane uptake. The membrane showed to be more selective towards magnesium followed by calcium. However, lithium was detected at very low concentrations. The uptake has reached the equilibrium at day 13 as there was no major change until day 30. The final concentrations of the targeted analytes in the spiked samples were Ca (268 mg/L), Mg (180 mg/L) and Li (11 mg/L). Whereas, in real seawater samples the Ca obtained was (135 mg/L), Mg (231 mg/L) and Li (6 mg/L). The stability of the membrane is under investigation. Currently, the method is being up scaled for the extraction of magnesium, calcium and lithium from seawater brine. Furthermore, the membrane was tested before and after analysis using FTIR and showed no degradation because all the components were still present in the spectrum. Therefore, this is the evidence that PIMs are promising for mineral extraction in seawater.

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C86 Assessment of microwave assisted extraction efficiency for the determination of herbicides in soil and maize cob: cumulative and health risks assessment

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The effectiveness of microwave-assisted extraction (MAE) was used for the determination of herbicides (atrazine, 2,4-D, mesotrione and glyphosate) in soil and maize crop followed by gas chromatography with flame ionization detector. The parameters optimised were extraction time (2, 8 and 15 minutes) and extraction solvent volume (5, 12, and 25 mL) and extraction solvents (hexane: acetone (1:2 v/v), acetonitrile: acetone (1:2 v/v) and the mixture of methanol: ethyl acetate (1:1 v/v). The recoveries of herbicides in maize and soil were 80-98% and 85-101%. The analysis repeatability, represented as relative standard deviations were less than 20% for all herbicides. All the herbicides calibration curves showed a good correlation coefficient (R^2) ≥0.996, indicating good linearity. The limits of detection and quantification ranged between 0.1-0.29 µg L^{-1} and 1.0-2.9 µg L^{-1}. These findings showed that MAE method is more accurate and sensitive, thus can be accurately applied for the determination of the assessed herbicides in soil and maize cop. Herbicides concentrations obtained ranged from 2.7 – 20.4 µg L^{-1} in maize and 1.2 - 30.5 µg L^{-1} in soil samples. The concentrations obtained in maize were higher than the maximum residue limits suggesting that health effect may occur upon continuous consumption. The herbicides toxicity index further confirmed the possible high toxicity effect of the studied maize crop as it exceeded the threshold value of 1. However, the health risk index was lower than 100% limit and did not exceed the acceptable daily intake of the maize crop in both adult and children indicating no possible health effects.

Acknowledgements
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C87 Phytoremediation potential, chemical profiling and biological properties of South African indigenous species

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Coal-fired power stations generate large quantities of solid waste biproducts and fly ash (FA) is the predominant waste classified as a health hazard[1]. Phytoremediation is a green technology that utilize plants to rehabilitate polluted sites. Pot trials were conducted to assess the phytoremediation capacity of four indigenous species in fly ash. The grass (*Digitaria eriantha*) and three aromatic species (*Salvia africana*, *Mentha longifolia* and *Helichrsyum splendidum*) were selected for the study. Plants were grown in 100% FA, 70% FA (amended with garden soil), 50% FA and uncontaminated garden soil was used as the control. The grass adapted well in all FA treatments, and growth rate recorded after three months was similar to the controls. All the aromatic plants investigated adapted to FA, but a stunted growth was observed for plants growing in 100% FA. The restricted growth is be attributed to high pH (> 8.40) that limits availability of nutrients and natural compaction of FA particles that inhibits water infiltration[2]. Phytotoxicity was further manifested by the discolored leaves due to chlorosis, indicating inhibition of chlorophyll production due to nutrient deficiencies[3]. Growth rate for plants growing in 50% and 70% FA were similar to the control plants. The study suggests that, these plants can be cultivated in FA and improved growth can be achieved with organic amendments. The use of aromatic plants is a sustainable approach that is linked to economic benefits, as they produce essential oils (EO) that can be commercialized. The secondary metabolites produced by plants are influenced by environmental factors, resulting in varying chemical profiles and biological properties. Chemometric models revealed that *H. splendidum* sourced from different locations (Mpumalanga and Limpopo) differ in their chemical profiles. The specimens from Mpumalanga displayed better anti-oxidant and anti-inflammatory properties, suggesting that activity is linked to chemical composition. Thus, cultivation of plants in FA polluted sites can lead to the discovery of new phytochemicals.

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K28 From Context to Systems Thinking in Chemistry Education

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Chemistry, as the Central Science, affords many opportunities for educators to connect content being taught to connect to broader contexts. When these contexts are not consciously connected to each other, they pose the risk of appearing random to students. The concept of connecting chemistry content to larger Earth and societal systems presents an opportunity to move past individual context connections to a more wholistic and compelling narrative of the role of chemistry in addressing the most pressing concerns of humanities. This presentation will combine descriptions and efficacy evidence from the classroom with analysis of publications in the Journal of Chemical Education that leverage systems thinking. This approach holds the promise of engaging student interest in using science to address pressing needs of humankind while also motivating foundational chemistry content for the teaching and learning of chemistry.

K31 Partnerships to support science teaching at school level

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Quality education is the 4th UNESCO Sustainable Development Goal and 2022/23 was declared the International Year of Basic Sciences for Sustainable Development. This presentation continues a conversation on providing quality education in one of the basic sciences, namely Physical Sciences, when three important stakeholders, industry, tertiary education, and schools, combine efforts to better prepare learners for careers in science. Currently South Africa is struggling to deliver quality education in the basic sciences. Only 27% of Physical Sciences candidates in the 2021 National Senior Certificate were able to obtain more than 50% for the examination[1]. This provides a very small pool of individuals who can enter tertiary education in a science field. Furthermore, schools are closing their Physical Sciences departments. Since 2013, 269 South African high schools have ceased offering Physical Sciences,[1] with the lack of qualified teachers provided as one of the main reasons.

Universities are aware of the need for quality education as is evident from the numerous outreach programmes in South Africa. Most initiatives, however, focus on learners and not teachers and very few initiatives involve expert teachers sharing their knowledge with less experienced colleagues. Expertise in teaching involves deep content understanding and the ability to transform the content to make it understandable for learners. Developing teaching expertise takes time and requires access to quality resource materials and regular training opportunities which not only provides teachers with exam questions and worked solutions, but with insight into how to teach a topic, which sections learners struggle with, and why, what misconceptions learners may have for a topic, which content representations are the best to use and where the topic fits into the curriculum. These components form the basis of topic-specific pedagogical content knowledge (TSPCK)[2] and provides a useful framework for in-service teacher professional development. Three-way partnerships between industries, that provide real world teaching contexts, universities, that provide facilities and subject expertise, and expert teachers, who ensures that the support is aimed at the right level, will bring us one step closer to delivering quality education in the basic sciences in South Africa.

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I23 Towards infusing education for sustainable development imperatives in chemistry education: pedagogical considerations

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The emergence of Covid-19 served as a reminder that in our teaching we need to prepare students and learners for an uncertain future and constantly changing world of work. At the same time, it is in this era that we observed the utility of the 21st century skills such as collaboration, critical thinking, systems thinking etc. for solving wicked problems in a short space of time e.g., Covid-19 vaccine. This experience put a spotlight on the need to rethink and re-imagine our pedagogical approaches when preparing learners for the world of work regardless of contextual challenges.

We have an opportunity now more than ever before, in our classrooms be it at school or university level when teaching future chemists or chemistry educators to teach for sustainability by modelling and infusing sustainable development or the Sustainable Development Goals (SDGs) in our teaching. For students and learners in resource constrained school environments or overloaded curricula we can at least innovate our pedagogy of teaching particularly for topics that lend themselves to the teaching of sustainability issues. This can be done by adopting pedagogical approaches such as inquiry-based teaching, simulated context-based teaching, collaborative learning approaches and exposing students to contexts where they must solve real-life problems. I will present one case of how this was done in a university setting. I will also share a case study from a PhD project demonstrating how an online professional development intervention was used to develop high school chemistry teachers' pedagogical content knowledge about the teaching of the extraction of metals with infused elements of environmental sustainability. More examples of emerging pedagogical approaches we can use in support of Agenda 2030 and Education for Sustainable Development (ESD)[1-2] will be shared to stimulate discussion.

Acknowledgements
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I26 Connecting to chemistry: Lessons from a longitudinal study

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Beginning in 2015 we have been tracking chemistry and chemical engineering students through their undergraduate degrees (UKSA project) and on into whichever path they took next (GEEK project). We have covered six institutions across three countries – South Africa, England and the United States. With one exception all institutions in the study were research intensive universities. The research design was to interview 25 students from each program in the first year and then to follow 10 students from this group for the next seven years.
This paper is a summary of the findings thus far particularly with respect to chemistry. We have examined assessment, knowledge building, curriculum structure, study practices and identity formation. In this paper I look at the implications of the findings of this project for undergraduate education in South Africa. One of the key findings is the importance of the personal relationship the student experience with both the institution and the department of chemistry.

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I28 Making chemistry meaningful

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Meaningfulness in chemistry is the ultimate learning goal, evidenced by the long-term recall of information which has been synthesized and embedded in the minds of students.[1] Meaningful learning is defined as engaging three domains: thinking (cognitive), feeling (affective) and doing (psychomotor).[2] Cognitive demands can be supported by lowering language demands on second language students or by adjusting the level of difficulty. The affective domain can be engaged by embedding chemistry in real-life contexts. Finally, well-designed experiments and research projects allow the student to interact with chemistry in a tangible manner. There are endless ways to make chemistry meaningful. Research into the spontaneous dissemination of a self-made mini spectroscope into the general public, across vast distances and across various languages, was a prime example of meaningful learning and quality education inside and outside the laboratory. In another study, the simple scaffolding of the UN SDGs into a pre-existing practical on water pollution allowed students to engage with several SDGs, namely life below water and life on land. Students linked many UN SDGs to the practical, thinking of systems beyond the immediate pollution. This complex thinking was still evident in a survey two months after the practical. In a current study, meaningfulness drove the design of a novel laboratory practical on matter and separation by using the context of boot-legging alcohol (affective), which was extremely prevalent under the South African prohibition during the Covid-19 lockdown. In this practical, students are also prompted to think about the impacts of boot-legging on society, industry and the environment.

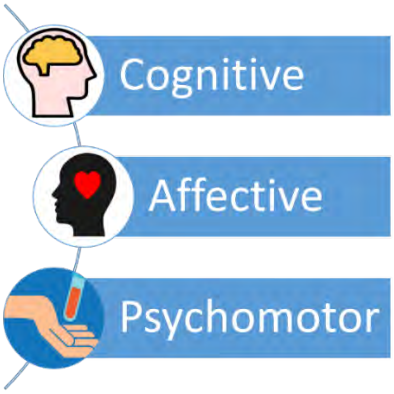

Figure 1: Three domains required for meaningful learning.

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C72 Digitalize learning via process simulation to understand process control

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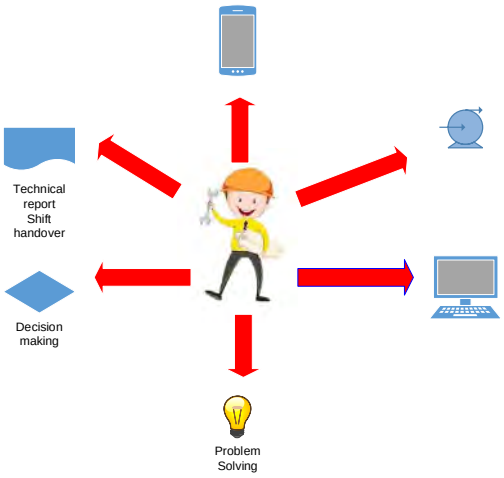
In recent years, a talent shortage has been one of the biggest threats facing chemical and petrochemical organisations. This, together with declining employment, looming retirements, and large demographic age gaps in the workforce has made us, together with industry, determine to tackle the problem and bridge the gap by developing a formal course between a low-skill operator level and that of the process engineer. The course needed to address the technical knowledge of introductory chemical and mechanical engineering principles, the chemistry involved in process chemistry, and mathematics. On the 'softer' side, modules such as Academic and Professional Skills and essential Computer Skills were introduced to develop an all-round chemical operator / technician. This paper describes the course materials in brief to provide insight into how this course has been developed and implemented. In this research presentation it will discuss how these students benefit from process simulations and how What-ifs can be used to pinpoint a potential problem. Once problem have been identified then through simulation, the students will then implement a corrective plan to successfully mitigate the risk. Feedback from student groups and industry partners on course content and relevance to today's industry needs confirms the relevance and value of the course.



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C73 A review of the topic specific PCK in available videos on the big idea, "What is chemical equilibrium?"

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The isolation caused by the recent COVID pandemic drove many teachers to online teaching and learning. As a result, many teachers gravitated towards the use of teaching videos, commonly selected from platforms such as YouTube. On such platforms, there is no check on lesson quality, and teachers work on primarily on instinct when selecting videos. To assist in this selection, it would be useful to have a defendable criterion for gauging the teaching quality of these lessons. One such criterion would be to judge the quality of the video's ability to display transformation of the content being taught on the video, known as PCK[1]. There is ample evidence that the quality of the teaching encapsulated in the video would be a central factor in determining the quality of the video, as many of the features such as representations, would be chosen by the creators of the video. While there is literature on guidelines for maximising student learning from videos[2], they are mostly geared at potential creators of videos, rather than assessing the teaching quality of existing videos on offer. Surprisingly, there is no specific literature analysing the PCK portrayed in the videos themselves. Thus, in this study we conduct an analysis of the PCK demonstrated in freely available videos on a specific topic, in this case chemical equilibrium. We ask the question, "What level of TSPCK is demonstrated in a collection of short freely available videos on the concept of dynamic chemical equilibrium?". To answer this question, we developed a rubric considering TSPCK and technical components. TSPCK considers five components for content knowledge transformation – Students' Prior Knowledge, Curricular Saliency, what is Difficult to Teach, Representations and Conceptual Teaching Strategies[3]. This study is a systematic review of internet videos, on "The meaning of dynamic chemical equilibrium", embracing the concepts of open and closed systems, reversible reactions, and conditions for a reversible reaction, particularly a closed system. Criteria for selection were that videos should be shorter than 10 minutes, in English, and at high school level. 12 videos from four countries were sourced and analysed using a validated rubric. The analysis scheme also considered technical criteria such as signalling, segmenting, and weeding. Findings indicated an imaginative use of representations, but surprisingly little use of sub-microscopic representations and only some videos actively involved the viewer. The rubric does offer a way forward for critiquing the videos and further investigation is now warranted.

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C74 The myriad positive impacts of the Virtual Learning Environment, from LabSims to Smart Worksheets (a 17 year journey)

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Introducing a virtual learning environment in support of practical teaching in Chemistry is not trivial. In this study we identify keys areas which are essential for successful implementation based on 17 years of experience of the Centre for Excellence in Teaching and Learning (CETL) called Bristol ChemLabS (2006 implementation) and compare and contrast these with a recent implementation in the Faculty of Natural Sciences at The University of the Western Cape in South Africa in 2020. There are strong similarities in both environments following implementation of a VLE. Raising of confidence of students in using instruments and carrying out techniques found in an undergraduate chemistry laboratory is clear, increasing students understanding of the theory behind techniques and their real appreciation of health and safety. For demonstrators, their role changes from one where they are giving instruction to one where they are discussing the development of the practical investigation with the students. For academics, the transformation in the practical ability of students, and long-term impacts on practical skills and final year projects that can be undertaken are noted. Recently, smart worksheets have been implemented, these e-enabled worksheets guide students through calculations, providing instant feedback and marking where appropriate. In their best examples, these smart worksheets represent all the knowledge an academic has in terms of areas where students struggle, their typical misconceptions and feedback and support that guides them to a complete and correct understanding. In this talk we focus on the implementation of smart worksheets in a second-year kinetics course and demonstrate the transformation of student cognition before and after implementation. Students who used the worksheets were extremely well prepared for workshops and saw their scores in assessment increase (statistically significant) compared with those who did not. Students using the smart worksheets did not make the common mistakes associated with this course. Analysis of surveys suggest that students enjoy working in this unbiased, neutral environment that provides instant feedback and support. It can be accessed at any time and there is no restriction on the number of times that it can be used. Students feel well prepared for subsequent workshops and assessments.

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C81 Student-centered approach via infographic to enhance chemistry learning among first year undergraduate students in South African universities

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This study was aimed at integrating infographic with student-centered approach to enhance chemistry learning among first year students in South African universities. Abstract concepts, lack of access to laboratory instruments, technical language barrier, and large class size are some of the challenging factors affecting the effective application of student-centered approach to achieve its aims chemistry learning among first year undergraduate students in South African universities. Among these challenging factors, the study focused on abstract concepts, because among other factors it directly affects the cognition needed for Chemistry learning for excellent academic performance[1]. A study conducted in one of the South African universities reported less than 50% pass in chemistry among first year undergraduate students[1]. In line with this pass rate problem, the research question was, "how do first year undergraduate students learn chemistry effectively via infographic? "The methodology used to achieve the aim was a systematic review of the literature entailing a ten year (2011-2021) duration in response to the research question. Methodology further entailed a Google Scholar and Scopus databases' searches of the keywords. In conclusion, successful outcome in learning chemistry was achieved from the application of student via infographic. The implications of this study are improved graduation rates in chemistry students, successful twenty-first century competency and fulfilment of fourth 2030 United Nations sustainable development goal (SDG).

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K4 A week in the life of a wastewater treatment plant in Durban

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Wastewater treatment plants (WWTPs) form an integral part of sanitation and water management in order to ensure public health safety. A typical municipal WWTP treats water arising from domestic households, commercial enterprises, and industrial plants. The process steps at the plant entail collecting, treating and purifying wastewater before its release back into the environment. Wastewater was determined to be the source of a number of epidemics and, hence, WWTPs were originally designed to treat pathogens. However, the advent of industrialization and globalization has meant an improvement in general lifestyles that has also impacted on the compounds that accumulate in wastewater. Of particular concern are micropollutants (MPs) derived from metabolized or unmetabolized treatment drugs, electronic equipment (such as flame retardants), personal care products, and pesticides, among others. These compounds can now be easily detected at the ng L^{-1} level due to advances in analytical instrumentation. It has been ascertained that a number of these MPs have endocrine-disrupting properties and, in particular, antibiotics can give rise to antibiotic resistant genes in microorganisms. Their subsequent build-up in the environment poses numerous adverse health and environmental effects. Influent and effluent water from five WWTPs in the eThekwini municipality was monitored daily over a week for a wide range of MPs. This lecture will discuss the findings and removal rates of MPs of concern.

Figure 1

K8 Managing chemicals within the environment – whose job is it anyway?

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South Africa is a medium-sized country, with a total land area of about 1.2 million square kilometres and an estimated population of 59,62 million (Statistics South Africa, 2020). It is also a middle-income and an emerging market with a diverse economy, supported by an abundance of resources, extensive and modern infrastructure networks (Department of Mineral Resources, 2019). The South African chemicals industry is a key component of the country's industrial base, contributing 3.4 percent to the GDP and 22.8 percent to manufacturing[1]. Whilst the chemicals sector provides substantial opportunities for economic growth, it is one of the main contributors to environmental pollution and degradation[2]. Environmental pollution is one of the leading cause of the biggest challenge to our civilization: climate change. Furthermore, when these chemical pollutants are left unchecked, they can pose severe health and environmental risks. The transfer of chemical pollutants onto the water environment is of greatest concern, water is the lifeblood of the environment, economy and our well-being. Despite the existence of regulations, environmental chemical controls remains weak and inadequate. The main aim of this paper is to present a synopsis of the many factors that hamper the sound management of chemicals in South Africa. Furthermore, insights on the need for a shared responsibility to improve the governance of chemicals and related waste as means of significantly reducing the negative impacts on the environment and human health is discussed.

Acknowledgements
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K21 Chemical escapades: persistent organic pollutants in the marine environment

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Although carbon is a useful element, it can be highly problematic too. Forms of carbon such as diamonds, coal and oil drive economies, but ultimately CO_2 drives climate change, and in the form of soot or plastic, it pollutes the environment. Some synthetic forms of carbon are catalysed by hydrocarbon processing. Chemists delight in designing and discovering new forms and uses for carbon based organic compounds. Many synthetic carbon compounds are embodied in nearly all consumer goods, such as pharmaceuticals, pesticides, perfluorinated compounds, and personal care products which we use daily. But, carbon compounds do not magically disappear after use, reappearing in unexpected places. Being persistent, they take long periods to degrade. We found that many synthetic organic carbon compounds escape via sewage through wastewater treatment plants, polluting water resources and ultimately end up in the ocean, causing chronic toxicity to diverse marine biota – a slow death sentence. Moreover, these compounds contaminate our food chains and aquatic environment, thus are transported back to us via potable water and food consumption, incrementally damaging our health. The invisible nature of much carbon waste means that few understand that it is toxic, causing health issues such as cancer, endocrine disruption, birth defects, sterility, or feminisation. Chemists' unfortunate legacy is our ever increasing chemical footprint which impacts on our collective future.

I7 Neonicotinoids and insect growth regulators in honey: Concentrations and exposure assessment under the framework of national residue monitoring program

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Neonicotinoid insecticides are a class of pesticides that were introduced in the 1990s as replacement for organophosphate pesticides. Due to their high efficacy for insect control and ease of application, neonicotinoids have quickly become the most widely used insecticides in agriculture, veterinary, and residential environments. Despite their high efficacy, selectivity, and versatile application, there are growing concerns regarding toxicity of neonicotinoid not only to non-target organisms - especially pollinators such as honeybees and wild bees as well as other terrestrial and aquatic invertebrates- but also to vertebrates, including humans. Neonicotinoids toxic effects include mainly reproductive toxicology, neurotoxicity, hepatotoxicity/hepatocarcinogenicity, immunotoxicity, and genetic toxicity. Studies also showed that neonicotinoids can adversely affect the developing brain especially for children.
In this study, sample preparation for honey was based on the “dilute and shoot” principle, followed by analysis using an internally validated ultra-high-performance liquid chromatographic coupled to tandem mass spectrometric method. Estimated daily intake and acute and chronic hazard quotients were determined to measure human exposure and health risk to NEO and IGR as well as the risk posed to honeybee. NEO and IGR were detected in 50% and 21% of the 115 honey samples, respectively. The average concentration ranged 0.062-6.50 µg kg^{-1} and 0.479-1.644 µg kg^{-1} for NEO and IGR, respectively. While acetamiprid was the most detected (24.35%) NEO, imidacloprid presented the highest concentration (16.945 µg kg^{-1}) in a sample. IGR co-occurred at variable concentrations with NEO in honey samples. The estimated daily intakes (EDI) of NEO and IGR ranged from 9.35 × 10-7 to 4.93 × 10-6 mg kg^{-1} bwd^{-1}. The chronic hazard quotient (HQc) and acute hazard quotient (HQa) for NEO and IGR were considerably < 1, indicating negligible risk to human health and honeybee population.
In conclusion, an UHPLC-MS/MS method was validated for the simultaneous determination of neonicotinoids and insect growth regulators in honey. Overall, the result of the present study confirms the widespread occurrence of NEO and IGR in honey consumed in South Africa. The EDIs, HQc, and HQa indicate that exposure to all target NEO and IGR via honey consumption constitutes negligible human health risk; however, the consequences of multiple routes of exposure to NEO and IGR cannot be overemphasized.

I15 Contaminants of Concern in South African Water Resources: The Establishment of a Knowledge Hub

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Contaminants of emerging concern (CEC) have stimulated increasing concern due to their ubiquitous presence in the environment and harmful potential. Climate change, population growth and dwindling freshwater sources necessitates the protection of such resources. A report from the European Commission's Joint Research Centre estimates that there is a 75 - 90 % chance of wars being fought over water within the next century[1]. In South Africa, the challenge of water resource management is complex and exarcebated by the semi-arid nature of the country, poor service delivery, acid mine drainage, fertiliser runoff, amongst others. Historically, society's response to a problem is based on funding availability, current threat, and public outcry. Achieving this is largely dependent on the knowledge of the factors that are resulting in compromised water sources. These factors are constantly changing as novel pollutants are introduced into surface water sources. As we are in the information age, the interest in contaminants of emerging concern (CEC) is gaining ground. Whilst research is being conducted to identify pollutants in South African water sources, the research outputs and available information is not collated and presented to the science community and stakeholders in readily available formats and platforms. Current research outcomes need to be made known to regulators in order to develop environmental laws. By using 4IR technology, we were able to collate available data in literature and display these in a user-friendly online format with an interactive map, available to the public, regulatory bodies as well as researchers. The near real-time access to information about CEC in South African water freshwater sources will reduce duplication of research efforts, enhance collaboration in the discipline, and act as a CEC early warning system.

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I33 Analysis of selected pharmaceuticals in a wastewater treatment plant during Covid-19

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Covid-19 infections resulted in an increased use of pharmaceuticals including the use of controversial treatment such as ivermectin. Wastewater treatment plants (WWTP) are on the receiving end of this household and hospital waste and trends can be mapped from analysis of its water. This study looked at the analysis of selected pharmaceuticals in the Darvill Wastewater Treatment Plant in Pietermaritzburg, Durban. Pharmaceuticals such as sulfmethoxazole and its metabolite as well as nevirapine, 17α-ethinylestradiol and ivermectin, amongst others were investigated. WWTP samples were subjected to solid-phase extraction (SPE) and liquid chromatography-mass spectrometry (LC-MS) once a suitable method was developed and validated. Resulting concentrations of pharmaceuticals used to treat chronic ailments such as diabetes, hypertension, tuberculosis and HIV/AIDS showed consistent daily usage while pharmaceuticals used for the treatment of COVID-19 and influenza showed distinct seasonal trends. Trends also directly correlated with the total number of active COVID-19 cases experienced in South Africa during sampling periods.

C10 Per-and polyfluoroalkyl substances (PFASs) in source water and sediments from South Africa and estimated human exposure

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PFASs are a group of persistent organic pollutants, which have been used as industrial and consumer products. At high concentrations, the C8, (PFOA and PFOS) have been linked to cause adverse health effects[1]. Studies on human exposures routes such as dietary intake and indoor dust have been reported. However, information on human exposure in South Africa is still scarce. The objective of this study was to; (a) report the concentrations of 20 PFASs in water and sediment samples from Hartbeespoort (HBD) and Roodeplaat (RPD) Dams (b) estimate human exposure risks of PFAS. PFASs were extracted from water and sediment samples collected from the dams using SPE and alkaline method, respectively. After spiking with surrogate standards and analysis was conducted using LCMSMS. The human exposure risk was estimated using the ADD and DAD. Nine PFAS were detected in the water samples and 10 in the sediment samples. L-PFOS, PFOA and L-PFDS, L-PFNS, L-PFOS, L-PFHpS, were the most dominant in water and sediment samples, respectively. The concentrations of the detected PFASs in water and sediment samples ranged from 1.66-346.33 ng L^{-1} and 0.03-89.04 ng g^{-1} respectively. The L-PFOS and PFOA concentrations determined in this study in water samples were generally higher than the United States advisory health limits of 70 ng L^{-1}. The ADD of the $\Sigma PFAS_9$ detected ranged from 2.85 x10^{-5} mg $kg^{-1}day^{-1}$ to 1.37 x10^{-4} mg $kg^{-1}day^{-1}$ in HBD and 2.16 x10^{-5} mg $kg^{-1}day^{-1}$ to 1.04 x10^{-4} mg $kg^{-1}day^{-1}$ in RPD, for the different age groups. The DAD ranged from 3.21 x10^{-7} mg kg^{-1} day^{-1} to 1.82 x10^{-6} mg kg^{-1} day^{-1} and 3.15 x10^{-7} mg kg^{-1} day^{-1} to 1.24 x10^{-6} mg kg^{-1} day^{-1} mg $kg^{-1}day^{-1}$ in HBD and RPD, respectively. The hazard quotient values ∑PFAS (5.79-27.77) suggested a moderate to high exposure of the PFAS in the population and infants were the most exposed out of the age groups. Considering the health implications of PFASs, there is cause for concern, particularly for the most vulnerable in the population.

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C11 Source apportionment, transport and fate of pollutants in the paper recycling chain: An analytical exploration of the South African recycled paper chain

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Recycled paper is a valuable commodity which forms an intrinsic part of actualising a circular economy. The disadvantage of the circular economy is that unwanted, hazardous substances may be introduced in the subsequent product's life cycle. The current South African recycled paper chain includes the collection of recycled paper by informal waste collectors after post-consumer recycled paper has been disposed of and/or landfilled. The aim of this study was to identify and quantify organic pollutants present in the South African paper recycling chain as well as to apportion the sources and possible transport and fate of these pollutants. A mixed methodology study was conducted using quantitative and qualitative techniques. Thus far, 110 samples were collected and analysed from various points of the recycled paper chain in Cape Town, South Africa. The collected samples included magazines, newspapers, office paper, mixed waste and cardboard collected at retail, pre-consumer and post-consumer sites. Multi-residue analyses were performed using gas chromatography coupled with mass spectrometry after accelerated solvent extraction. The method detection limits ranged from 2.05 ηg/g for butylated hydroxytoluene to 6.34 ηg/g for benzophenone. The method quantification limits ranged from 6.83 ηg/g for butylated hydroxytoluene to 21.14 ηg/g for benzophenone. Preliminary findings indicated that the South African paper recycling stream contains pollutants associated with plastic-related pollutants. Dibutyl phthalate was the most prevalently detected pollutant in the samples with the highest value of 55.64 mg/kg found in post-consumer corrugated board. Organophosphorus pollutants, phenols and alkyl phenanthrenes were identified using the 2020 National Institute of Standards and Technology electron ionization mass spectral library database. Trends analysis indicated that the pollutants prevalent were likely from mingling of waste and unregulated use of additives containing organic pollutants.

C12 Sulphate radical enhanced photoelectrochemical degradation of Sulfamethoxazole on a fluorine doped tin oxide – copper(I) oxide photoanode

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We report a sulphate radical enhanced photoelectrochemical degradation of sulfamethoxazole on a solar light driven fluorine doped tin oxide - copper(I) oxide photoanode. Copper(I) oxide was prepared by a template-free method and dispersed onto the surface of a fluorine doped tin oxide glass to form the photoanode[1]. UV-Vis diffuse reflectance spectroscopy showed that the photoanode absorbed in the visible light region[2]. With sodium persulphate as the source of sulphate radical, photoelectrochemical degradation studies showed that sodium persulphate markedly enhanced the degradation of sulfamethoxazole. Studies on the effects of change in concentration of the persulphate and the absence of the persulphate on the photoelectrocatalytic degradation process were conducted. Overall, the extent of degradation and mineralisation of sulfamethoxazole in water was found to be 86% and 67% respectively with bias potential of 1.5 V for the sulphate radical enhanced process. Scavenger studies showed that the photogenerated holes and sulphate radicals were the primary active species in the abatement of sulfamethoxazole. The effectiveness of sulfamethoxazole removal in real matrices by the use of FTO-Cu_2O photoanode and sulphate radical was also confirmed.

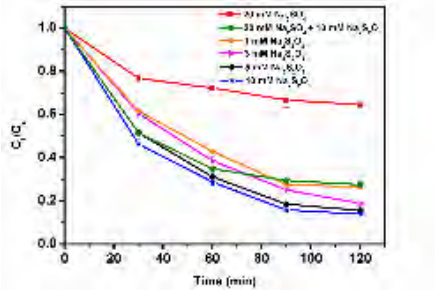

Figure1: Photoelectrocatalytic degradation plots of sulfamethoxazole

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C22 Obstacles to sustainable development in environmental commercial laboratories based in South Africa

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The journey from sample reception to analytical result is full of obstacles in a commercial laboratory. Some are easy to identify, and others can be quite hidden until they are large problems. Some articles can be found that list these main hindrances for laboratories, but seldom give an overview from start to finish.[1,2] Sustainable chemistry practices can be difficult to implement in an industry where historic approved and proven methods are at the order of the day. Focusing on every part of the journey of a sample through the laboratory, it is possible to identify, assess, and take action on almost all obstacles. Some key problem areas include client lack of knowledge, unknown content in samples, data management, cost and analytical limitations. Accreditation / conformity sets high expectations for the value of results and provides backing to the industry so rived with pitfalls. However, other aspects of sustainability such as safety, environmental impact and efficiency are becoming more important as we strive to achieve our global objectives towards a better future.

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C23 Occurrence of per and polyflouroalkyl substances as contaminants of emerging concern in tap water in South Africa

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Per- and polyflouroalkyl substance (PFASs) are a class of over 5000 man-made organic chemicals that have been manufactured and used worldwide since the 1950s [1]. These compounds are ubiquitous, bioaccummulative, persistent and toxic[2]. However, traditional water purification methods are not efficient in removing these compounds. As a result, these compounds have been detected in various environmental matrices including drinking water even at levels above national and international recommended limits[4]. Due to their adverse health implications to both humans and the environment, they have received a great deal of attention and have been classified as contaminants of emerging concern (CEC)[4]. Presently, there are few studies that have reported on concentrations of PFASs in tap water in South Africa. In this study, 21 PFAS compounds were targeted in 24 tap water samples in various provinces in South Africa. The samples were collected in high density polyethylene bottles, extracted using solid phase extraction (SPE) and analysed using liquid chromatography-tandem mass spectrometry (LC-MS/MS). The highest detected mean concentrations were PFBA (0.846-740 ng/L), 8:2 FTS (0.04-302.4ng/L), PFDS (1.17-247 ng/L), 6:2 FHET (0.037-253.1 ng/L), FHEA (0.03 -168.7 ng/L), PFHxA (2.46-170.3) and PFHxS (2.40-170.0 ng/L). These results revealed that some of the concentrations detected in the tap water samples in South Africa exceeded the established guidelines around the world such as in United States which has an advisory limit of 70 ng/L for PFOA and PFOS respectively3. Consequently, a number of South Africans may have been exposed to these chemicals through drinking water.

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C24 Elemental composition and potential health risk of vegetable cultivated in residential area situated close to mine tailings

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The presence of trace metals in areas surrounding abandoned gold mine tailings is a major environmental issue. This is because they have the potential to affect groundwater sources as well vegetation, thus posing human health effects. In this study, the elemental distribution of both toxic and essential elements in soils and leafy vegetables (*Brassica oleracea*) collected from eight different sites around abandoned gold mine dump were investigated. Nutritional value of vegetables to diet was determined to assess their value to human health. The results obtained revealed that the metal content in vegetables followed this descending order: Ca>Mg >;Ca >;Sb>; Pb>; Fe>; Mo >; Cr >; Se >;As >; V >; Ni >; Co >; Cd. Sites 7 and 8 were found to contain high concentrations of heavy and trace metals in both soil and vegetables. The bioaccumulation factor (BAF) revealed that the leafy vegetables tend to accumulate most metals even (toxic) during transfer and translocation process. Based on the recommended daily allowance (%RDA) the vegetables showed to contribute 152%, 84% and 75% towards RDA for Se, V and Ca, respectively for most adults and these play a role in human metabolic activities. Although the vegetables are grown in contaminated soil, it was found to be a good source of essential elements (Ca, Mg, Ni, Na, Fe) but with some traces of toxic metals such as Pb, As and Sb which may pose health impact if present at higher levels. Based on the health risk assessment, the vegetable grown in this region poses an adverse health hazard for human consumption due to As, Sb, Pb and Mo with high HRI >1.

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C48 $Fe_3O_4@SiO_{2@}$ Zr(OH) nanocomposite for the removal of Pb^{2+} ions from aqueous solution

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Water pollution by heavy metals is an increasing threat to the ecosystem and public health, mainly because they tend to persist and accumulate in the environment and their toxic effect cannot be undermined even at very trace concentrations. In this study, the MNP were synthesized via the co-precipitation method and coated with silica through the Stober route then followed by zirconium deposition onto MNP@SiO_2 to form MNP@SiO_2@Zr(OH). The synthesized materials were characterized using XRD, SEM, TEM and FTIR spectroscopy. Batch adsorption experiment for the removal of Pb^{2+} such as effect of solution pH, adsorbent dose and initial concentration were examined. The particle we observed to be spherical in shape with particle sizes of be 11.76 and 9.15 nm for MNP@SiO_2 and MNP@SiO_2@Zr(OH), respectively. FTIR showed functional groups of magnetite and confirm the silica coating and the deposition of zirconium. The optimum pH was found to be 6 for both materials and the adsorption capacity was found to be 90 mg/g and 121.73 mg/g for MNP@SiO_2 and MNP@SiO_2@Zr(OH), respectively. Zirconium deposition onto MNP@SiO_2 enhance the adsorption capacity for the removal of Pb^{2+} ions from aqueous solution due to the presence of a large hydroxyls group that can easily chelate with water and attract lead ions in aqueous solution.

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C49 The effect of slurry wet mixing time, thermal treatment, and method of electrode preparation on membrane capacitive deionisation performance

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Capacitive deionisation (CDI) electrodes with identical composition were prepared using three deposition methods: (1) slurry infiltration by calendering (SIC), (2) ink infiltration dropwise (IID), and (3) ink deposition by spray coating (IDSC). The SIC method clearly showed favourable establishment of an electrode with superior desalination capacity. Desalination results showed that electrodes produced from slurries mixed longer than 30 minutes displayed a significant reduction in the maximum salt adsorption capacity, due to the agglomeration of carbon black. The electrodes were thermally treated at 130, 250, and 350 °C. Polyvinylidene difluoride (PVDF) decomposition was observed when the electrodes were treated at temperatures higher than 180 °C. The electrodes treated at 350 °C showed contact angles of θ = 0°. The optimised electrodes showed a salt adsorption capacity value of 24.8 mg/g (130 °C). All CDI electrodes were analysed using specific surface area by N2 adsorption, contact angle measurements, conductivity by the four-point probe method and salt adsorption/desorption experiments. Selected reagents and CDI electrodes were characterised using thermogravimetric analysis coupled with mass spectrometry (TGA-MS) and differential scanning calorimetry (DSC), as well as scanning electron microscopy energy dispersive X-ray spectroscopy (SEM-EDS).

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C50 Efficient adsorption of 4- Nitrophenol using Cyclodextrin cross-linked magnetic nanocomposite

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In the present era of water resources scarcity, efficient treatment of wastewater is a major prerequisite especially for growing economy. Numerous approaches have been studied for the development of more effective adsorbents for removal of organic pollutants from wastewater[1-2]. The study aimed to develop a cyclodextrin-magnetite nano-biocomposite for the removal of 4-Nitrophenol from aqueous solution. The magnetic nanocomposite (Fe_3O_4-PCP) material was synthesized by co-precipitation method. Magnetite was coated with pine cone (NTP-NC) followed by crosslinking to beta cyclodextrin (β-CD) using 1,6-hexamethylene diisocyanate. Functional groups and magnetic properties of the composite were characterized using SEM, FTIR and VSM analysis. Batch adsorption studies were performed to optimize operating parameters such as solution pH, adsorbent dose, contact time, and initial concentration. Pseudo first, pseudo second, intraparticle diffusion, pore and film diffusion kinetic models were determined to investigate the mechanism of adsorption process. Structural characterization of magnetite coated pine cone and the magnetite coated pine crosslinked to cyclodextrin using 1,6-hexamethylene diisocyanate were confirmed by characterization techniques applied. Adsorption of 4-nitrophenol onto NTPNC-HMDI-CD was observed to be favoured at solution pH of 7 and adsorbent dose of 0.1 g at 2 hours contact time with adsorption capacity of 36.68 mg/g. Kinetic modelling showed that the experimental data better fitter pseudo second order. The adsorption of 4-Nitrophenol onto magnetite coated pine crosslinked cyclodextrin was controlled by chemisorption.

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C84 Health Risks Assessment of Trace Metals in Ground Water Collected From Berlin, Eastern Cape, South Africa

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In the recent years, draught caused shortages of water in most provinces and the most affected provinces were the Western Cape and Eastern Cape[1]. Most of Eastern Cape municipalities resorted to using ground water in order to make up for these water shortages, but there is less to no information regarding ground water quality in the province[1]. Pollution of water sources by trace metals is global problem, especially in developing countries like South Africa, as a result of anthropogenic activities such as agriculture, industrial activities, and poor waste management (landfill and effluent from wastewater treatment plant)[2]. Human health effects such as kidney dysfunction, vascular damage, skin lesions, birth defects, cancer and various disorders have been linked to exposure to some trace metals[3]. In this study the seasonal variations of the trace metal levels in some groundwater and soil sediments in East London (Berlin) was monitored, and the impact these metals have on the environment was assessed. The water samples collected from twenty-seven sampling sites were processed and eighteen trace metals were determined using Inductively Coupled Plasma - Optical Emission Spectrophotometer (ICP-OES). The test results of Ni, Cr, Pb and As in the water sources surrounding Berlin were in the range between (901.25-2638.11µg/L, 80.38-581.49µg/L,6.79-148.88µg/L and 14.86-37.45µg/L respectively. The observed levels exceeded the stipulated thresholds listed in WHO and SANS 241:2015. The concentrations of the other fourteen metals tested were within specifications, as per World Health Organization (WHO) and the South African National Standard 241 (SANS 241) standards for drinking water. The principal component analysis and Geographic Information System (GIS) suggested that natural and anthropogenic activities are sources of trace metal contamination in the groundwater samples. The carcinogenic risks (CR) values for Ni, Pb, As for adults in most sites were above the recommended values (1X10-4) by USEPA risks assessment guidelines. For Cr only one site's CR value was above specification. This indicates a high potential risk of cancer to adults if exposed to the water at these sites. For children and adults, the calculated sum of the carcinogenic risks through oral ingestion values was found to be in the order Ni>Pb>As>Cr.

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"Bringing data science and AI/ML tools to infectious disease research" Workshop 2022 – photo credit Tamara Krige

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K1 Quantitative analysis of unknown compounds in complex samples – Challenges in extraction, chromatography and detection

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Moving towards a more sustainable, circular bioeconomy, new challenges arise in terms of chemical analysis of complex plant-based materials. In a biorefinery, biomass is converted to chemicals, and the analysis of process streams as well as end products is a necessity. Often, the compounds of interest are unknown and/or commercial chemical standards are lacking. This poses a great challenge in analytical chemistry; and several examples will be discussed in this lecture including lignin analysis. Extraction is a sample preparation step that often introduces a large bias in the overall quantitative analytical method, especially for solid complex samples. One reason for this is that for analytes to be completely extracted from a solid sample, a relatively harsh method is needed, which inherently leads to degradation of the analytes. For instance, an elevated temperature is often needed to increase both speed and recovery in an extraction method. In our research we have shown that: (i) a relatively high temperature can be used if the extraction is fast enough so that the extraction time can be kept short in order to minimize degradation[1]; and (ii) liquid or supercritical carbon dioxide can be added to the extraction solvent to enhance diffusivity without increasing the temperature, which then leads to fast extractions with minimal bias[2]. Our research also shows that the solubility of the analyte in the extraction solvent is a key parameter for fast extractions[4]. In chromatography, comprehensiveness and selectivity are important qualities in the analysis of unknown compounds in complex samples. Clearly, supercritical fluid chromatography (SFC) is a technique that enables the separation of a wide polarity-range of compounds in a single run, as well as it offers high separation selectivity for individual compounds[5]. In combination with high-resolution mass spectrometry (HRMS) and charged aerosol detection (CAD), this is a powerful tool to address the challenge of quantitative analysis of unknown analytes in complex samples. One example that will be presented is the analysis of lignin monomers and oligomers by SFC-CAD and SFC-HRMS[5]. Strategies will be presented that enables both classification and quantification of analytes with limited availability of chemical standards.

Acknowledgements
The Swedish Research Council VR, the Swedish Research Council FORMAS, and Crafoord Foundation.

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K10 Flow Photochemistry as a Greener Approach for the Synthesis of Drugs and Drug-Like Scaffolds

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This talk will highlight recent studies geared at the greener preparation of drugs and their building blocks exploiting photochemical approaches as the key step. The use of light to drive chemical reactions is highly attractive as photons are traceless reagent equivalents whose energy can be tuned via their wavelength. The presented studies exploit modern continuous flow reactor technology to overcome challenges commonly encountered with chemical synthesis such as safety, efficiency, and standardization. Moreover, we demonstrate how both known photochemical reactions as well as novel transformations can be developed and exploited in flow mode. The ability to use light-driven reactions for the generation of drugs and their precursors in tandem with continuous processing is a very attractive approach to generate these species at low cost, at various scales and with minimal amounts of chemical waste which contributes to modern sustainable chemistry.

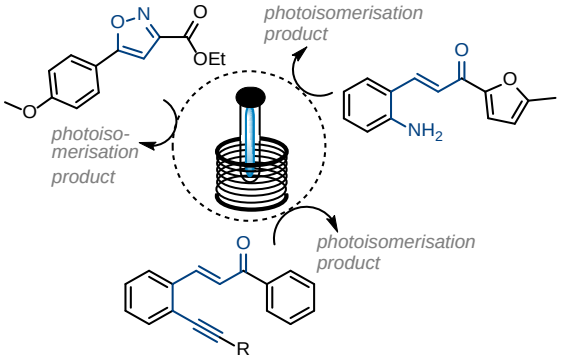

Figure 1: Representative photochemical flow transformations.

Acknowledgements
We gratefully acknowledge financial support by the School of Chemistry at UCD as well as Science Foundation Ireland and our industrial partners.

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I9 Nanocellulose and bacterial cellulose as a multifunctional green material

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Cellulose is regarded as the most abundant biopolymer and renewable material on earth and is known for its biodegradability, non-toxicity, and biocompatibility. We formed nanocrystalline cellulose (NCC) from synthetic materials isolated from cigarette filters[1] as well as natural materials isolated from melon seed shell.[2] We formed bacterial cellulose and composites from a dialysis-free Kombucha-based process.[3] The nanocellulose was used to both stabilise and reduce silver(I) to form silver nanoparticles (AgNPs)[4]; the composite NCC/AgNPs was investigated as a sensor in the detection of toxins[5,6] using surface-enhanced Raman scattering (SERS).[7] We additionally demonstrated for the first time the preparation of luminescent cellulose paper through the embedding of a tetranuclear Cu(I) cluster by performing a chemical reaction directly on Schweizer's reagent used as the inorganic solvent.[8] Finally, we used NCC as a component in a wearable strain sensor based on electroconductive hydrogel composites for human motion detection.[9]

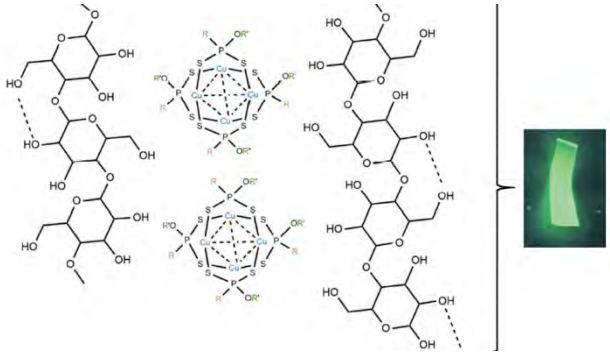

Figure 1: Luminescent cellulose/Cu_4L_4 paper formed from dithiophosphonic acid and a Cu(II) precursor.

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I12 DOZN™2.0 - A Quantitative Green Chemistry Evaluator

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MilliporeSigma (The life science business of Merck, KGaA, Darmstadt, Germany) developed and launched DOZN™2.0, a unique web-based greener alternative scoring matrix, also known as a quantitative green chemistry evaluator based on the 12 principles of green chemistry for customers to evaluate their relative greenness of their processes. The 12 principles of green chemistry provide a framework for learning about green chemistry and designing or improving materials, products, processes and systems. DOZN™2.0 scores products based on metrics for each principle and aggregates principle scores to derive a final aggregate score. The system calculates scores based on manufacturing inputs, GHS and SDS data which provide a green score for each substance. DOZN™2.0 is flexible enough to encompass the diverse portfolio of products ranging from chemistry to biology to material science-based products. The DOZN™2.0 system has also been verified and validated by a third party to ensure best practices are applied and also published. This new Greener Chemistry Initiative offer customers' an increased breadth of Greener Alternative products with confirmatory documentation to validate greener characteristics. Through DOZN™2.0 customers now have access to calculate the green scores of their own processes and products. This free, web-based tool provides users with even more data so that they are properly equipped to improve their sustainability. DOZN™2.0 keeps data privacy top of mind—allowing customers to score their processes/products in a safe and secure manner.

C28 Comparative assessment of the physicochemical characteristics of Nano-hydroxyapatite extracted from fish scales and eggshells

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The need for environmentally sustainable products has created a niche for bio-waste materials. This study comparatively assessed the physicochemical characteristics of nano-hydroxyapatite (nHAp) extracted from waste eggshells and fish scales. Alkaline hydrolysis followed by direct calcination, and milling were used to obtain nHAp from both fish scales and eggshells. The effect of the extraction process and bio-waste source on the physicochemical characteristics of the nHAp such as Ca/P ratio, functional groups, crystallinity and phase change, and surface morphology are presented in the study. The characterisation results showed a slight variation in the physicochemical characteristics of the extracted nHAp between eggshell (EnHAp) and fish scales (FnHAp and mFnHAp). The buffering characteristics of the nHAp extracted from eggshells was superior to those from fish scales. The salient point of the study showed that the characteristics of nHAp slightly differs based on the source of bio-waste and method of extraction. The study therefore serves as a baseline data for the extraction and use of nHAp from bio-waste.

C29 Curriculum Change in Chemistry: Developing graduates as agents of change for sustainable development

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Green Chemistry is a VALUES BASED approach to solving problems in chemistry guided by a set of PRINCIPLES which focus on safety and efficiency. The introduction of green chemistry into the undergraduate curriculum is therefore complicated by the difficulty of where to put it and how to teach it. The several members of the Green Chemistry Division of SACI come from every sub-discipline of chemistry, analytical, physical, organic and inorganic – as well as medicinal chemistry, nanotechnology, and theoretical chemistry. The wide interest in the application of Green Chemistry is an indicator that there are many options for how to include the *introduction* of green chemistry principles, and there are many opportunities throughout the undergraduate curriculum to teach the application of these principles. As a signer of the Green Chemistry Commitment[1] Rhodes University has incorporated the principles of Green Chemistry into each year of undergraduate, and into organic, general, and inorganic chemistry, as well as into nanotechnology. This presentation is a reflection of that process.

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C30 Encapsulation of Thiol-Co-Capped CdTe/CdSe/ZnSe Multi-Core-Shell QDs in Liposomes and Chitosan Nanoparticles; Comparative Bio-compatibility Studies Using Hela and Vero Cells.

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The common method used to reduce the toxicity posed to living cells by CdTe quantum dots (QDs) is through the synthesis of CdTe multi-core-shells nanoparticles[1]. This heterostructures can be in form of CdTe/CdSe/ZnSe or CdTe/CdSe/ZnS or CdTe/CdS/ZnS multi-core-shell QDs. However, it has recently been identified that the ZnSe or ZnS coating shell is insufficient to completely protect the highly toxic Cd metal from escaping into immediate solution[2]. This limits their use in biochemistry and with living systems. Liposomes and bi-polymers such as chitosan are known to be environmentally friendly compounds used as delivery systems for QDs and model drugs for drug delivery applications[3]. They are generally non-toxic and highly bio-compatible. In this study, multi-core-shell QDs were encapsulated in two different bio-compatible environments, namely liposome and chitosan nanoparticles (CNP) at 14 different formulations (F) for liposome and 12 different formulations for CNP. Cytotoxicity and florescence imaging studies using HeLa and Vero cells were used to investigate the improved bio-compatibility. Various characterization techniques were used to elucidate the properties and morphology of the nanocomposites. QD-liposome vesicles (LVs)-F12 and QD-CNP-F9 demonstrated the high loading efficiencies of 42 ± 6 % and 59 ± 5 % respectively. While the plain multi-core-shell QDs shows high toxicity, QD-LVs-F1 and F12; QD-CNP-F3 and QD-CNP-F9 depicted lower toxicity against the cells (IC_{50} > 0.5 mg/ml). The composites also retained most of their fluorescence properties and could easily be tracked in cells and visualized around the nucleus, indicating the successful internalization of the QDs composites in the cytosol.

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C37 Development of wholly biobased acid-terminated thermosetting polymers from castor oil, glycerol, and itaconic acid

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The incorporation of agri-resources, such as vegetable oils, as platform molecules for biobased polymers has been developed for several decades, yet usually require synthetic modifications to become suitable for free radical polymerisation. These synthesis strategies typically rely on petroleum derived and toxic reagents, diminishing their sustainability.[1-4] On the other hand, biotechnologically derived itaconic acid provides an opportunity for biobased reactive unsaturation on monomers for radical polymerisation.[5, 6] However, aside from unsaturated polyesters, robust examples of its efficient use in other biobased monomers remains underdeveloped.[7-10] Herein, the direct ring-opening anhydride esterification of itaconic anhydride with both castor oil and castor oil glycerides under mild conditions in a solvent-free system was demonstrated. Furthermore, employing stannous octoate as a catalyst and a catalyst-free pathway were investigated. The synthesis resulted in wholly biobased acid-terminated multifunctional monomers. The monomers were characterised by ATR-FTIR, ^{1}H NMR, ^{13}C NMR, and the green chemistry metrics (biobased carbon content, atom economy, process mass intensity) were calculated. The monomers were then polymerised using LED UV-curing at 365 nm. The resultant polymers' properties were investigated using ATR-FTIR, DMA, thermogravimetry, Soxhlet extraction, tensile testing, and flexural testing. This work presents some of the first examples of wholly biobased radical thermosetting polymers obtained with excellent green chemistry metrics and properties comparable to other analogous polymers in the literature.

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C38 Perovskites and nanocrystalline materials toward energy application

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Inorganic nanocrystals possess interesting properties researchers seek to overcome current technological challenges. Improving the performance of existing or new devices is the main aim set by scientist when studying nanoparticles. Inorganic perovskites and chalcogenide nanocrystals were prepared via classical colloidal method and microwave assisted method. Various parameters of synthesis including the time, temperature, precursor concentration, coordinating solvent and capping agent were investigated. Their properties were studied and optimized for effective application in photovoltaic devices. Several types of solar cell devices as well as perovskite cells were prepared from thin film of synthesized nanocrystals and the evidence of photovoltaic activity was shown. The performance of fabricated devices was influenced by the structure of deposited thin films, especially the absorbing layer made of synthesized nanocrystals.

C39 African Laboratory Growth and Development

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Africa is a continent with a wealth of resources, forming the basis of its industrial development. Laboratories are and have been developed to service both the established and growing industries, broadly categorized as agriculture, environmental testing, and mining. African laboratories play an important role in the continents economy, ensuring goods meet both import and export regulations, as well as serving a crucial role in protecting both people and the environment with the results produced. The laboratories are set up to focus on function, this may be metal determinations for mining extracts or NPK testing for soil analysis. The instrumentation and equipment selected for a laboratory setup is especially important to the success of the laboratory and the production of reliable results. The testing methods are closely linked to the instrumentation and selected based on factors such as industry acceptance and cost of analysis. The testing methods and procedures are continuously updated to improve both accuracy and precision. ISO/IEC 17025 is the international standard for testing and calibration laboratories. Laboratories need to implement measures to meet the requirements of the standard and undergo regular audits to ensure the results are reliable. Successful accreditation ultimately leads to international acceptance and recognition. Africa has and is growing in terms of its industrial output and the development of laboratory infrastructure has never been more important. Two examples of successful laboratory development projects will be discussed in detail, highlighting exactly how the laboratories serve their industry and local communities. These examples include an agricultural and environmental laboratory setup in Malawi and a series of water testing laboratories installed across Tanzania.

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K29 PGMs – A key enabler in addressing global challenges and unlocking societal benefits

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Platinum group metals - platinum, palladium, rhodium, ruthenium, iridium and osmium - offer unique characteristics to a diverse range of industries with a wide variety of existing and unexplored applications, addressing key global issues such as decarbonisation & the clean energy transition, medical technologies, food technologies, luxury & investment, etc.[1] This presentation focuses on the various opportunity areas PGMs enable.

Figure 1: Anglo American's Market Development Focus and Opportunities.[1]

References

1. Anglo American

K32 The role of chemistry in enabling South Africa's just energy transition

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In the context of science and technology, sustainability is a general term which comprises a number of interlinked imperatives including renewable energy, decarbonization, circularity and green chemicals. Globally, there is particular focus on reducing greenhouse gas emissions from the fossil fuel industry through a just energy transition, with the ultimate target being to reduce the rate of global warming to no more than 1.5^{o}C by 2050, in line with the Paris Agreement adopted by over 190 states at COP 21 in 2015.[1] In an unprecedented world-wide response, many companies and industries have committed to achieve step-wise emission reduction targets with the ultimate goal of achieving "net zero" by 2050.

The ability to deliver on these targets is highly dependent on development of new or improved technology, requiring a multi-disciplinary and collaborative approach between scientists and engineers across multiple elements of those fields, but also nationally and internationally. In order to drive localization efforts and address the need for skilled labour to enable industry's deployment of the various technologies, a concerted effort is required to ensure we build the required body of knowledge to enable the required energy transition. This includes managing risks but also exploiting opportunities which can accelerate transformation in a society which has multiple challenges and limited financial means. At the heart of much of this lies a mastery of Chemistry in its many forms. This presentation will explore the many ways in which furthering the understanding and application of chemistry in these new areas is critical to a successful energy transition and discuss ways in which we can address the very real constraints of time and money which require a new approach.

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I24 South Africa's journey towards a hydrogen economy: lessons learnt in funding innovations

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Following Cabinet approval of the Hydrogen and Fuel Cell Technologies (HFCT) research, development and innovation (RDI) Strategy in 2007 and the formal launch in 2008 of the 15-year Hydrogen South Africa (HySA) implementation programme, South Africa began its journey towards the development of the Hydrogen Economy. The implementation of the HySA programme and the country's endowment of platinum group metals (PGMs), which are key ingredients in the development of fuel cell technology and renewable or green hydrogen production, have positioned the country as a significant player in the global Hydrogen Economy. After 14 years of developing knowledge, technological and human capabilities, the country published its national Hydrogen Society Roadmap (HSRM) in February 2022, signaling the intention to leverage the Hydrogen Economy to reindustrialize and decarbonize key industrial sectors as part of the economic reconstruction and recovery plan. A presentation will be given to appreciate the journey, progress made in implementing the HSRM and the lessons learnt.

I27 Rand Refinery, our past, present, and future

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Rand Refinery was established one hundred years ago, in 1920, by the Chamber of Mines.[1] Currently we are one of the largest integrated smelter and refinery single-site complexes in the World.[1] Our primary products consist of gold and silver in that we produce a range of kilo bars, minted bars, and granules; having recently added 99.999% Ag to our product range.[1] Our smelter recovers Au, Ag, Pt and Pd from mine by products, PC scrap, carbonaceous material, and our own sweeps material.[1] The concentrates of which then feed our refinery. Our laboratory is equipped with state-of-the-art equipment and assaying capabilities that allow us to analyze and quantify all incoming deposits and out-going final products.[1] We are one of five internationally recognized LBMA referees which means that the laboratory is part of a technical adjudication in case of refiner disputes in assays, as well as the on-boarding of new refineries to the Good Delivery List.[1] Looking to the future of Rand Refinery, our Board has approved a pilot project that is based on the commercialization of our evaluation processes. This exciting project, named Project Volta, is already underway and we look forward to sharing more during the presentation.

Figure 1: An image of minted bars, produced at Rand Refinery.[1]

References

1. www.randrefinery.com

I29 The options nuclear medicine offers to drug researchers for translation of their compounds into the clinic

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The research and screening that precedes a successful drug is a very stringent and costly process. From 5000 to 10 000 new ideas (molecules), around 250 enter into clinical trials, of which ten will be fully tested and finally only one will come onto the market. A way to accelerate this process and to manage the cost lies in early *in vivo* evaluation of the lead drug candidates. This evaluation will highlight potential side effects and undesirable pharmacologic interactions, not noted during in vitro disease selectivity studies, that may lead to the agent to be withdrawn when tested in patients in phase II and III clinical trials. Molecular imaging (making use of ionizing radiation - radiotracers) has long been known with proven application in industry, agriculture and nuclear medicine. Radiopharmaceutical compounds are mainly used as diagnostic agents for the detection of various diseases in a real-time, non-invasive manner using PET or SPECT camera. In the same way radiotracers can also be used to follow and determine the biodistribution of a new compound. These preclinical animal studies can also be applied to humans because the drug is administered in microdoses (at least 100 times less than the toxicity level of the drug). South Africa has a global footprint in radioisotope production and supply and this has been the basis of a slow but sure increase in the use of nuclear imaging as a tool in drug development. The source of these radioisotopes in South Africa is i.a. the SAFARI-1 research reactor at Pelindaba which will start to wind down in 2030. An interministerial process for its replacement in the form of a Multi-Purpose Reactor (MPR) was started in 2019. Further to the improvement of molecular imaging in South Africa, the Nuclear Medicine Research Infrastructure initiative was established in 2018. NuMeRI is expected to increase the local capacity for collaborative development of targeted radiotherapeutic and diagnostic compounds. Both the NuMeRI and MPR initiatives will be illustrated and the opportunities for chemists within these spheres highlighted.

C75 The importance of chemistry for e-mobility development: An African perspective

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Electric vehicles are slowly reinforcing their place in the global market, with 6.75 million units sold in 2021, accounting for 8.3% of the global automotive market with expectations of this increasing to 33% by 2028.[1] South Africa and Kenya, however, only contributed approximately 1559 and 350 units to this total respectively. To accommodate the anticipated e-mobility growth in South Africa, and the rest of the continent, a sound understanding of the battery chemistry, developments and advances needs to be explored and integrated with additional principles, such as project and risk management, as summarised in Figure 1. The battery chemistry has a profound effect on cradle-to grave assessments from the initial mining value chain and beneficiation to exploring second-life applications which can increase battery utilisation before the need for recycling. Sound knowledge of the chemistry is also crucial in elucidating risks and providing a safe working environment, making risk-mitigation initiatives more transparent, improving manufacturing processes and providing opportunities for small start-ups to form, supporting the shift to a more electric powered mindset. Adopting new technologies and integrating electric mobility can not only enhance local efforts to advance electrochemistry research, but also support sustainable development schemes in Africa.

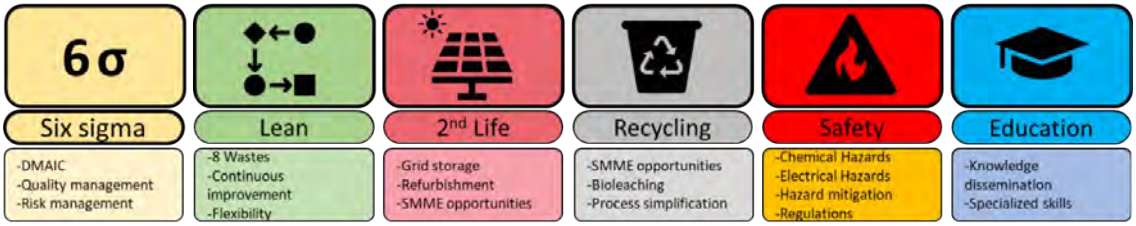

Figure 1: Basic overview of critical project management aspects required for e-mobility integration within the African context

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C76 Synthesis of aluminium fumarate metal organic frameworks from multi-layered food packages recycled waste materials

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Multi-layered food packages are commonly used packaging materials for perishable food products. The packages are made up of several laminated layers, including 75% paper, 5% aluminium and 20% low-density polyethylene polymer. The widespread use of the packaging material significantly contributes to large amounts of municipal solid waste. The hydropulping method is the extensively used method for recycling the multi-layered packages resulting in recycled paper material and PolyAl (i.e. polyethylene and aluminium) pellets. The aim of this study was to apply the chemical processing approach to produce high-value product from the multi-layered food packaging recycled waste materials. This work explores the extraction and use of aluminium as a low-cost feed stock from the PolyAl pellets for the synthesis of PolyAl-based metal organic framework (MOF) porous materials. PolyAl pellets were initially calcined in the presence of NaOH to recover sodium aluminate. The resultant sodium aluminate was thereafter treated with H_2O and H_2SO_4 respectively to obtain Al_2SO_4 powder. The PolyAl based Al_2SO_4 was then used for the synthesis of aluminium fumarate MOF. The obtained MOF materials were analyzed using XRD, SEM, FTIR, EDS and TGA. The textural properties were further studied using N_2 sorption isotherms to evaluate their potential for gas adsorption or capture capacity volumes.

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C77 Effect of magnetic fields on limescale: An experimental investigation

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Magnetic water treatment is often toted as a viable method to control limescale based crystalline growth[1], such as calcium carbonate, in an aqueous environment, but is also widely contested[2]. The viability of this technique was investigated by use of a dynamic scale loop, which allowed for high rate, reproducible experiments of crystalline growth in a flowthrough system. Rare earth magnets were used to generate high flux (965 mT) and high flux gradient (82.5 T/m) magnetic fields respectively. The results indicate that this method has little to no viability for inhibiting limescale based crystalline fouling in a practical environment.

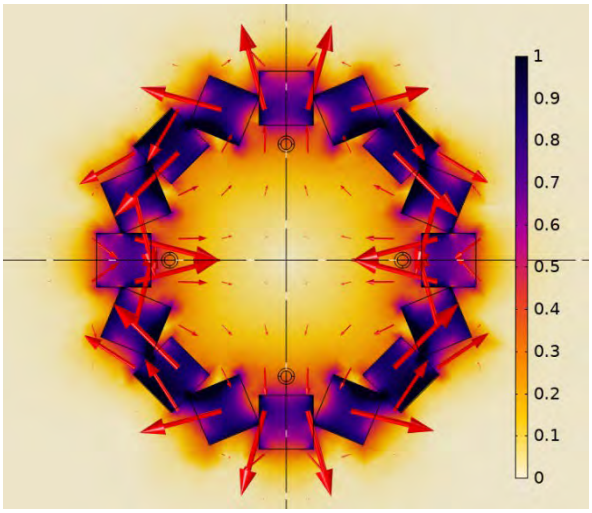

Figure 1: Simulated magnetic flux density of a permanent magnet-based quadrupole trap. The magnetic flux is indicated in Tesla as shown by the colour bar on the right.

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C82 Solvent-dependent extraction of steam-exploded sugarcane bagasse: Lignin and glucose yields, and structural and thermal properties of lignin

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The application area of lignins depends mainly on their structural, molecular, functional, and thermal properties. In this study, lignin was extracted from steam-exploded sugarcane bagasse which was obtained as residue from an industrial furfural plant. Three different organosolv extraction methods were employed in a systematic study, namely single-stage extraction at room-temperature (SSE), and multistage Soxhlet extraction at both room temperature (Soxh-RT) and 56.3-110.6°C (Soxh-Hot), with fifteen organic solvents of different polarities and solubility parameters. Furthermore, the resulting delignified solid residues were enzymatically hydrolysed to glucose monomers as a first step to the valorisation of the cellulose fraction. The study's core was to investigate the effect of the solvent properties on the extracted lignin and produced glucose yields. The structural and thermal properties of the extracted lignin were analysed by UV-Vis, FTIR, 2D NMR HSQC, ^{31}P NMR, and TGA analytics.

As expected, the time required to deplete the biomass of lignin (maximum extraction) was shorter using multistage extraction with hot solvent. Soxh-Hot method was 10 to 12 times and 2 to 4 times shorter than SSE and Soxh-RT methods, respectively.
Tetrahydrofuran showed the highest lignin yields in all extraction methods (20-24 %). The corresponding cellulose fraction gave rather low glucose yields of 0.20-0.24 g/g. On the other hand, 2-Methyltetrahydrofuran gave the overall highest glucose yields of 0.42g/g, closely followed by ethanol with 0.38 g/g and then toluene 0.26 g/g. The properties of the lignin obtained were found not to depend on the extraction conditions. However, a remarkable difference in these lignin properties was observed depending on the extracting solvent properties. For example, if the extraction was conducted with toluene, a total hydroxyl content of 1.6 mmol/g was obtained, while with ethanol, it was found to be 4.0 mmol/g. The solvent effect was highly pronounced on the spectroscopic, structural and thermal properties of the different lignins obtained, giving first indications of the potential application areas of these resulting extracted lignins.

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C83 Synthesis & evaluation of chelating collectors designed for improved Sperrylite recovery

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South Africa accounts for a large amount of the worlds Platinum group mineral (PGM) reserves. One such PGM is Sperrylite ($PtAs_2$) with typical extraction methods proving ineffective for this mineral.[1] Froth flotation is the process of treating the milled/crushed ores with amphiphilic collectors, that will slelectivly adsorb onto a mineral surface, rendering it hydrophobic. This hydrophobic character allows for complex attachment to air bubbles which are being passed through the pulp.[2] Chelating collectors show superior mineral and metal specificity through stronger hard- soft acid- base (HSAB) interactions. In this study a library of collectors was prepared, incorporating 2- to 5-carbon chains and a combination of trithiocarbonate (TTC) (**1**, **2**) and thiourea (TU) (**3**) donor groups. Collector efficacy was then evaluated by micro-flotation and microcalorimetry testing. TTC collectors **1** were readily prepared in high yield and purity, while TU collectors **3** were challenging to synthesize in good purity at large scale. The floatation abilities were dependent on the solubility and stability under flotation conditions. Studies demonstrated pH-dependent decomposition (hydrolysis) (Figure 2), accounting in part for poor flotation performance. Dialkyl TTCs (**2)** were found to be less soluble but more stable in aqueous solutions.

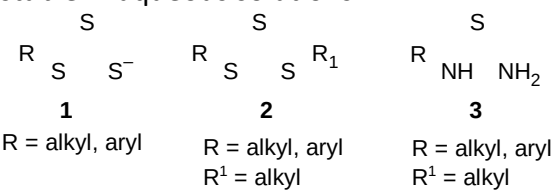

Figure 1: Collector families synthesized for improved Sperrylite recovery

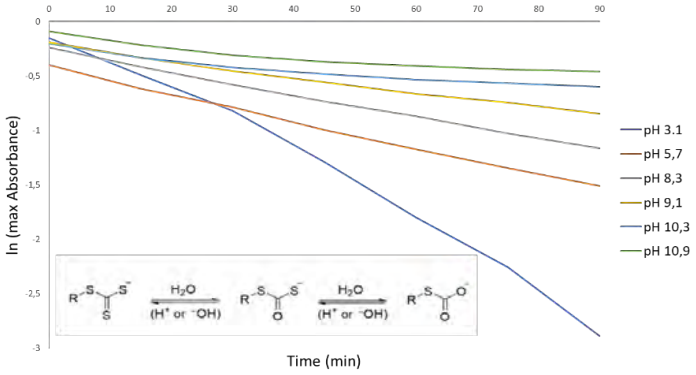

Figure 2: Decomposition plots of 0.1mM n-butyl TTC at various pH.

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K3 Bioorganometallic Strategies to Target Malaria

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Malaria is a parasitic disease that has an impact on millions of people globally. The pathogenic protozoan *Plasmodium*, which invades red blood cells, is the primary cause. Despite advancements in the fight against the disease, reports of rising drug resistance render the present generation of conventional chemotherapies useless. In order to combat resistance and find new chemicals with excellent antiplasmodial capabilities, ongoing research is crucial. Ferroquine, which incorporates ferrocene in the lateral side-chain of the conventional chemotherapeutic chloroquine and overcomes the resistance experienced by the parent compound, exemplifies the promising effects displayed by metal complexes in the treatment of malaria, especially in combating rising resistance. This has spurred work on creating new metal-containing systems with improved potencies to combat resistance.
This presentation will highlight some of our recent efforts in the design of bioorganometallic antiplasmodial complexes, some of which have demonstrated remarkable activity, notably against resistant forms of the *Plasmodium falciparum* parasite. Invariably, we have consistently demonstrated that the inclusion of sandwich (ferrocene) and half-sandwich organometallic complexes based on compounds containing platinum group metals can boost the activity. Studies on microsomal metabolic stability and putative mechanisms of action will also be discussed.

Acknowledgements
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K7 The heme detoxification pathway as a target for antimalarial drug development

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Together with human immunodeficiency virus (HIV) and tuberculosis (TB), malaria is one of the three most serious infectious diseases in the world. This is no less true on the African continent; according to the World Health Organisation, sub-Saharan Africa accounts for 95% of the world's malaria cases, and children under the age of five are most vulnerable.
The malaria parasite undergoes a complex lifecycle in both the *Anopheles* mosquito vector and the human host. In the latter, the parasite's residency in red blood cells (RBCs), the so-called blood cycle, is associated with common disease symptoms such as fever and chills. Whilst undergoing rapid asexual development, parasites digest host hemoglobin, which results in a build up of free heme in the digestive vacuole. Through a process of biocrystallization referred to as the heme detoxification process, parasites overcome the threat of toxic heme through the formation of hemozoin crystals (malaria pigment).[1] Quinoline antimalarials such as chloroquine have been shown to inhibit this process, however, this class of drugs has been severely compromised by resistance, highlighting the urgent need for new antimalarials. In this presentation I will highlight some early studies in heme speciation that led to our improved understanding of the hemozoin formation process. Thereafter, I will focus on our more recent contributions towards the rational design and development of new inhibitors that target the heme detoxification pathway.[1]

Acknowledgements
The late Professor Tim Egan, my supervisor, collaborator, mentor and friend. Tim stimulated my interest in this field of bioinorganic chemistry as a postgraduate student, and it was a great honor to work closely with him for almost two decades thereafter. He supported my nomination for the Raikes Medal, and this presentation is given in his memory.

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K20 Semiconductor Nanocrystals as Effective HER Electrocatalysts

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Hydrogen (H_2) although abundant on earth as an element, is almost exclusively found as part of another compound such as H_2O. As such, it must be separated into pure hydrogen (H_2) for use as fuel in fuel cell electric vehicles. Hydrogen can be produced from diverse resources, that include fossil fuels, biomass, and water electrolysis. As a result, the environmental impact and energy efficiency of hydrogen depends on how it is produced. Water splitting through electrolysis is considered as one of the cleanest production processes of H_2 as it produces oxygen and hydrogen; and when coupled with photovoltaics as a source of electricity for the electrolysis, it is regarded as renewable. The Hydrogen Evolution Reaction (HER) as commonly known, is an electrocatalytic process that is conducted with the use of platinum as a catalyst. The use of platinum while highly efficient is relatively expensive thus making the HER an economically unfavorable process compared to other production methods. The synthesis of non-noble metal nanocrystals as cheaper alternatives to Pt for HER electrocatalysts is highly desired. Herein, we report on the colloidal synthesis of metal chalcogenide and metal phosphide nanocrystals and their use as electrocatalysts for HER in acidic conditions. The electrocatalytic efficiency largely depends on the structural properties of the nanocrystals. For MoP for instance, the amorphous particles showed better efficiency than crystalline particles, while for $SnSe_2$, activated $SnSe_2$ was a better electrocatalyst compared to inactivated $SnSe_2$. Herein, we describe in detail, the synthesis, characterization and electrocatalytic properties of $MoSe_2$, $ReSe_2$ and $SnSe_2$ as well as MoP and WP.

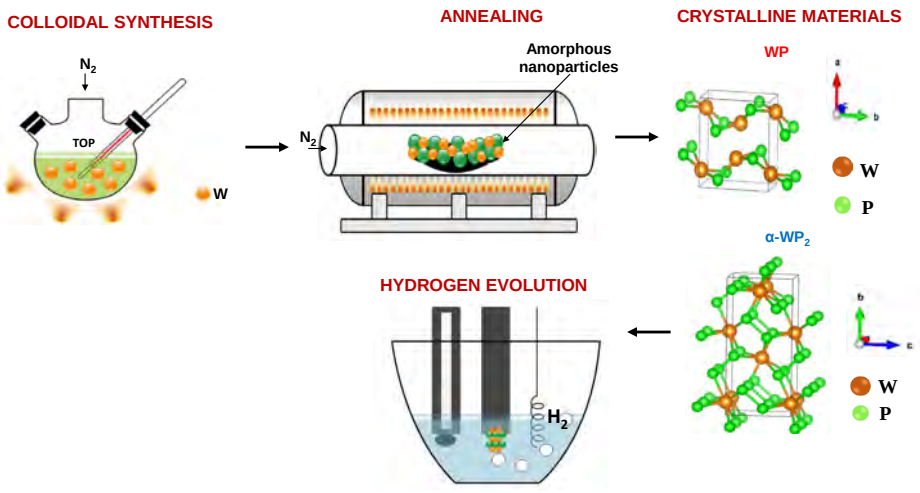

Figure 1: Tungsten phosphide electrocatalysts for HER.

I3 Separation of base metal ions using inner- and outer-sphere coordination chemistry

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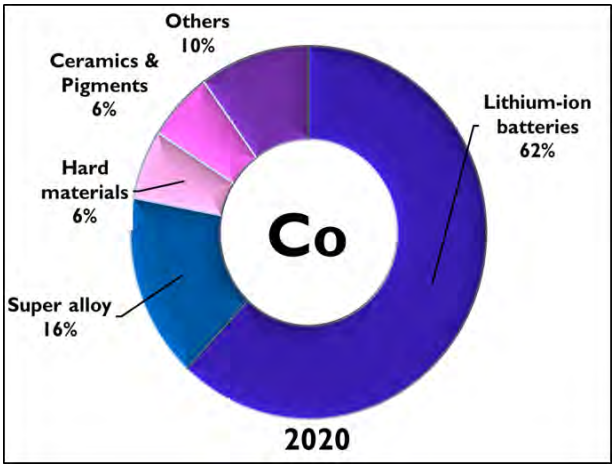
Nickel, cobalt and manganese have important uses in super alloys, hard materials, ceramics and pigments. Its most significant use by far is in Lithium Ion Batteries (LIB), where this has been its most important use since 2020.[1] Cobalt is rare and expensive and in the last two years its price increased by 450 %. Cobalt also forms the most energy dense material in LIB usage.



Inner coordination sphere involves the donor atoms directly coordinated to the metal ion, whereas outer coordination sphere involves coordination beyond the inner coordination sphere.[2] We have looked at several novel amic acid type ligands for the inner sphere coordination to cobalt(II) and these have shown high and selective coordination to cobalt(II) compared to nickel(II) and manganese(II). Similarly, tertiary amine amido type pro-ligands also show selective coordination to tetrachlorido cobaltate(II) compared to the non-existent nickelate(II) and manganate(II) analogues.[3] These ligands could also be used to recycle cobalt from important electronics, e.g. cell phone batteries and batteries used in other power tools. Such recycling is known as urban mining.

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I6 The Wonderland of Multinuclear Mn, Tc & Re Complexes in Small Molecule and Macromolecular Environments

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Drug design, particularly the development of target specific radiopharmaceuticals, is a world of wonder involving the selective receptor binding of a radioactive organometallic complex to a possible disease site and requires a multi-faceted approach of study. Simple manipulation of the organic ligand system bound to the metal centre can significantly alter parameters such as steric and electronic character, chirality, reactivity, biological and hydro/lipophilicity properties. Our research utilising the group 7 transition metal triad of manganese, technetium and rhenium for nuclear medical imaging and therapy, is supported by the observed interactions with proteins as elucidated via macromolecular crystallography, in a similar vein to fragment based drug discovery (FBDD). This perspective highlights the wonderland of opportunities when incorporating multiple metals (Re & Tc) into a single agent with dual (therapy & diagnostic) application. The multidiscipline approach to radiopharmaceutical development will include the interoperable harvesting of both small molecule and macromolecular structural data and describe kinetic reactivity studies highlighting how subtle changes can significantly affect chemical reactivity and hence the protein residue coordination.

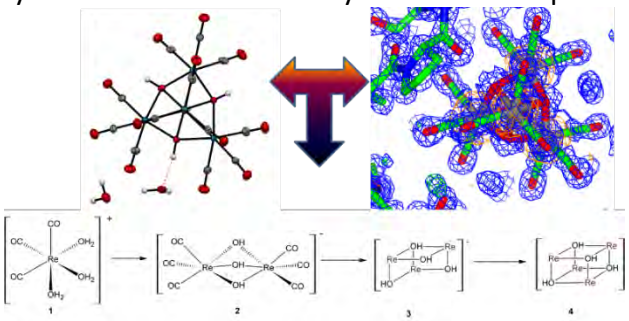

Figure 1: The structure and reaction kinetic usage of chemical and macromolecular data during the formation of tetranuclear rhenium clusters.

Acknowledgements
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I13 Metal Complexes of Alkyl-aryl Dithiocarbamates: Molecular Structures and uses as Precursors for Semiconductor Metal Sulphide Nanophotocatalysts and Potential as Anticancer Agents

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Dithiocarbamates are versatile ligands that are able to stabilize metal ions in different oxidation states with the partial double bond character of the thioureide moiety. Variation of the substituents attached to the nitrogen atom of dithiocarbamate moiety generates various intermolecular interactions, which can lead to different structural arrangement in the solid state. The presence of bulky substituents on the N atom obviates the supramolecular aggregation via secondary M-S interactions whereas smaller substituents encourage such aggregation that results in different properties and potential applications. Over the past decade, we have carried out the synthesis and structural studies of metal complexes of dithiocarbamates[1-8], evaluate their anticancer potentials and their use as single source precursors to prepared metal sulphide nanoparticles for the development of novel therapeutics agents and nanophotocatalysts [1-11]. Some of the compounds are highly potent and could serve as lead compounds for novel anticancer agents. The nanophotocatalysts are highly efficient for the photocatalytic degradation of organic dyes.

Acknowledgements
National Research Foundation and University of KwaZulu-Natal for financial support.

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C7 Synthesis of *n, n'* Bipyridyl Chiral-at-metal Ruthenium Complexes as Catalysts for Asymmetric Hydrogenation of Ketones

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Chiral drug molecules exhibit striking differences in their pharmacodynamic, pharmacokinetic and toxicological properties.[1] In 1992, the United States Food and Drug Administration (FDA) passed a policy that recommends the development of chiral racemic drugs into a single biologically active enantiopure drugs.[2] This policy guideline stems from life-threatening effects resulting from one of the two enantiomers of a racemic drug such as the thalidomide which later led to a phenomenon known as chiral switch. Chiral switch is a process in which a single enantiomerically pure drug molecule is developed from a racemic drug which was approved and marketed as a racemate after the discovery that one of the enantiomers is unsafe. Ibuprofen was the first of the non-steroidal anti-inflammatory drugs (NSAIDs) to undergo chiral switch to the single pharmacologically active enantiomer.[2] Catalytic asymmetric synthesis, thus provides a simple, concise and cheap methods of producing enantiomers.[3] Frequently, the conventional chiral catalysts applied in asymmetric synthesis are often obtained through the complexation of metal salts with expensive and sophisticated chiral ligands. Recently, the exploration of chiral-at-metal transition metal complexes usually derived from the coordination of simple achiral ligands with certain transition metal salts, provides an advantage of forming a plethora of complexes through cheap and diverse pool of achiral ligands available. Complexes described as "chiral-at-metal" are those often coordinated to simple and low-cost achiral ligands with the chirality residing exclusively at the metal center as opposed to the conventional chiral metal complexes where the chirality is strictly due to the ligand scaffold.[4] In this study, several *N*,*N*'-bipyridyl chiral-at-metal ruthenium complexes were synthesized, characterized, and applied as catalysts for the asymmetric hydrogenation of prochiral aromatic ketones via hydrogen transfer. The resulting chiral alcohols were obtained in high yield and enantioselectivity. To the best of our knowledge, these types of complexes have not been used till date for the catalytic asymmetric hydrogenation of ketones, based on literature. Hence, the *N*,*N*'-bipyridyl chiral-at-metal ruthenium complexes will be economically viable with respect to the more expensive conventional system of chiral metal catalysts.

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C8 Rationally designed trimetallic ruthenium(II) 2-arylbenzimidazole complexes for chemotherapy and photodynamic therapy

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Platinum(II) complexes have remained at the forefront of the treatment of various cancers. However, the evolution of resistance by cancers and the undesirable side effects associated with the use of these platinum-based drugs limit the scope of use of these metallodrugs. As a result, recent research in the development of novel metallodrugs has focused on alternate platinum-group metals, with ruthenium complexes being at the forefront. These studies, however, are limited to monometallic ruthenium complexes with polymetallic complexes seldom being the subject of investigation. In this presentation, the rational design and development of a series of trinuclear ruthenium(II) complexes based on the benzimidazole pharmacophore are described. The effects of various aryl moieties at the 2-positions, and varying the substituents on the 5-positions of the benzimidazole scaffold, the alteration of the dendritic core, and the effects of these nuance changes on the overall biological activity of the complexes are explored. A set of organoruthenium complexes developed as part of this study was also investigated as photodynamic therapy (PDT) agents with negligible short and long-term dark cytotoxicity and enhanced cytotoxicity upon light irradiation. This further highlights the versatility of the ruthenium(II) complexes in different treatment modalities for cancer, as we have shown how nuanced structural alterations may influence the overall biological activity and applications of these complexes in the treatment of cancer. Overall, the compounds developed in this study show very promising activity in breast cancer cell lines (MCF-7 and the triple-negative MDA-MB-231) and a cervical cancer cell line (HeLa). Most importantly, some of these complexes show activity that is either comparable or enhanced compared to clinically used cisplatin, and the PDT agents developed as part of this study show appreciable long-term phototoxicity suggesting that these compounds may minimize cancer recurrence.

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C9 Highly Efficient Transfer Hydrogenation of Alkenes with Ammonia Borane Mediated by a Simple Ni(II) Catalyst System

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The transition metal catalysed hydrogenation of unsaturated compounds containing π-systems remains an essential reaction in organic chemistry due to the valuable products resulting from it.[1] These reactions typically use dihydrogen (H_2) and have received particular attention in homogeneous Ni catalysed hydrogenations.[2] Typical drawbacks include high reaction temperatures, extended reaction times, high catalyst loadings and safety concerns. This resulted in research moving towards transfer hydrogenation (TH) reactions, which is a much safer method for the hydrogenation of unsaturated compounds.[3] The research efforts of the Swarts Research Group focus on the development of catalyst systems derived from earth-abundant metals. As part of our program, we have reported the TH of N-heteroaromatics[4] and nitriles[5] mediated by readily-available Ni(II)-based pre-catalyst with ammonia borane (AB) as hydrogen source. Extending the scope of our catalyst system, we describe the catalytic transfer hydrogenation of alkenes (aromatic, aliphatic and α,β-unsaturated) to their respective alkane products utilizing an ethylene diamine ligated Ni(II)-catalyst with AB as the source of H_2 (Figure 1). Using only 1 mol% of the pre-catalyst at ambient conditions provided excellent conversions and isolated yields of the respective alkane products, with TON values up to 3960. The chemoselective hydrogenation of α,β-unsaturated esters was also achieved. Mechanistic elucidation revealed that borane activates dihydrogen, leading to the proposal of a two-step process during the transfer hydrogenation of styrene.

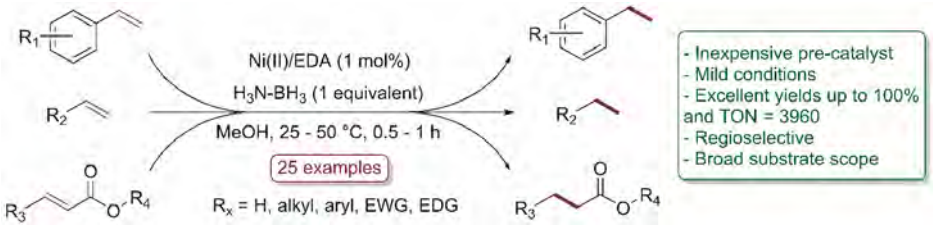

Figure 1: Efficient Ni(II)-catalyzed TH of alkenes.

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C19 The Chemistry of Spin-Coated Rhodium Complexes Supported on Silanol-Capped Silicon Wafers

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A flat (2-D) model limits unknown parameters for a well-defined catalyst to be mimicked to better understand fundamental chemical surface dynamics.[1,2] Catalytic sites are also optimally available for reactions and can be probed with surface techniques such as TEM and XPS. The aim of this paper was to spin-coat rhodium(I) complexes, [Rh(FcCOCHCOCH$_3$)(CO)$_2$] and [Rh(FcCOCHCOCH$_3$)(CO)(PPh$_3$)], on a 2-D silanol-capped silicon wafer support and to analyze the spontaneous chemistry that occurs at the surface. The observed chemistry on the surface was found to be different from that found in a homogeneous solution phase (Figure 1). Surface species formed were identified as the spin-coated precursor rhodium(I) complex and the rhodium(I) species that resulted from the β-diketonato displacement from the original rhodium complexes by surface silanol OH's to generate [wafer-(O)$_2$-Rh-(CO)$_2$] and [wafer-(O)$_2$-Rh-(CO)(PPh$_3$)] units. Several Rh(III) surface species resulting from the oxidative addition of surface Si-OH groups to surface-coordinated Rh(I) core atoms were also identified. Finally, the XPS determined binding energies of the Rh(I) and Rh(III) 3d$_{5/2}$ photoelectron lines were found to be functions of the Gordy scale R-group electronegativities and the electrochemically determined Rh(I) oxidation potentials.

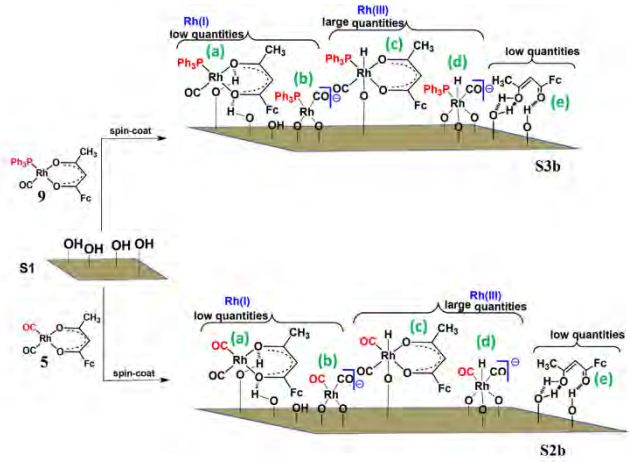

Figure 1: Various surface species formed when [Rh(FcCOCHCOCH$_3$)(CO)$_2$] and [Rh(FcCOCHCOCH$_3$)(CO)(PPh$_3$)] were spin-coated on hydroxylated silicon surface S1.

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C20 Synthesis of Novel Ferrocenyl-benzimidazole Derivatives and their Evaluation as Antiplasmodial Agents

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Malaria, a potentially deadly disease, is caused by plasmodium parasites.[1] Of the five malaria causing plasmodium parasites, *Plasmodium falciparum* poses the greatest threat to human health, accounting for majority of the global malaria deaths and developing resistance to existing frontline treatments.[2] With the resistance of *P. falciparum* in mind, alongside the need for multimodal drug compounds targeting malaria, a small library of four ferrocenyl benzimidazole conjugates was synthesised (Figure 1). The synthesised target compounds were fully characterised by ^{1}H and ^{13}C NMR, FTIR, and electrospray ionisation mass spectroscopy. To investigate their potential mode(s) of action, the compounds were evaluated against *Toxoplasma gondii*, which is commonly used as a model apicomplexan parasite due to the ease of handling the parasite in a laboratory setting compared to *P. falciparum*.[3] The ability of the compounds to generate reactive oxygen species (ROS) was evaluated and the most active compounds were found to produce ROS. Fluorescence microscopy images for one complex in the parasites were also obtained. In addition to cyclic voltammetry to evaluate their electrochemical behaviour, UV-vis and turbidimetric studies were also carried out to evaluate the stability and solubility of the synthesised compounds. Finally, the compounds were evaluated against chloroquine sensitive and chloroquine resistant strains of *P. falciparum*.

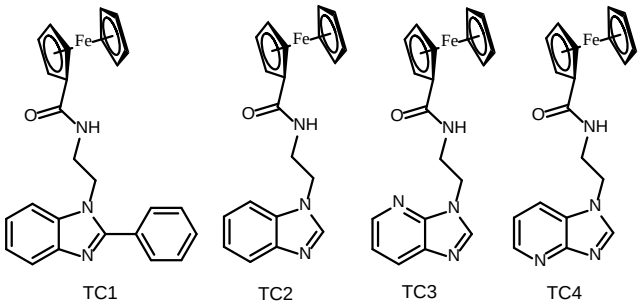

Figure 1: Synthesised target compounds

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C21 Studying the growth of the digestive vacuole lumen in NF54 and Dd2 to aid in understanding the haem detoxification pathway in *Plasmodium falciparum*

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Plasmodium falciparum (Pf) causes the deadliest form of malaria. Imperative to parasite survival is the haem detoxification pathway which results in haemozoin formation. Disruption of this pathway is an attractive target for antimalarials. Fully understanding the haem detoxification pathway by way of a mathematical model, would greatly aid in mode of action studies on various antimalarials and may inform rational drug design. Whilst numerous parameters are imperative for model development, in the current study, the parameters studied were the volume of the digestive vacuole (DV) lumen and rate of uptake into the DV. Previous studies have shown that macromolecules are taken up through endocytosis, pinocytosis and the formation of cytostomes.[1] Thus, red blood cells (RBCs) were pre-loaded with pHrodo™ dextran beads. With these, *Pf* trophozoites were incubated to allow reinvasion. Following incubation, parasites were visualized using a confocal microscope and parasite age was confirmed with flow cytometry. Image processing was done using ImageJ. The growth of the lumen in NF54 follows a Gompertz growth curve. In Dd2, the collapse of the DV lumen occurs earlier than NF54. Subtle differences suggest that different models are required for each strain. Whilst the rate of uptake of pHrodo™ follows a similar trend to the volume growth, the concentration remains constant. This may have important implications for protein, drug and other macromolecule concentrations.

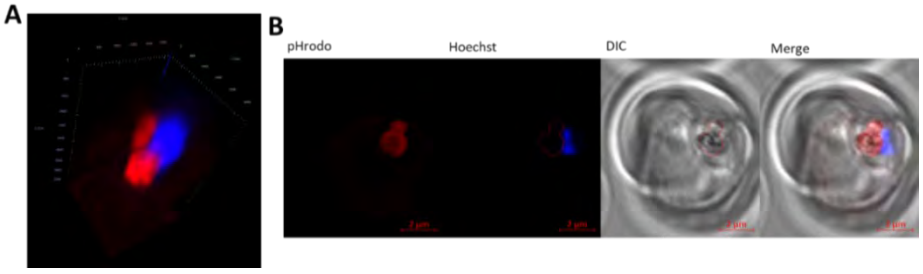

Figure 1: A. 3D rendering of confocal microscopy Z-stack images taken of a *Pf* parasite containing pHrodo dextran red and stained with Hoechst (nuclear stain). B. Single slice through *Pf* parasite shown in A.

Acknowledgements
A special acknowledgement goes to the late Professor Timothy John Egan, who's great mind is behind all this work.

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C43 Solid Oxide Electrolytes: Dopant Effects on Structural and Conductivity Properties of Bismuth Oxides

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Bismuth oxide is the highest known ceramic oxide conductor to date, with conductivities comparable to that for most molten salts[1]. This is mainly due to long Bi-O bond lengths and the number of vacant oxide sites in the face-centered cubic conducting phase. In each unit cell the six oxide ions are distributed between the 8c sites and 32f sites (see Figure 1). This enables relatively low activation energies for the thermally activated hopping of oxides into adjacent vacant sites. Unfortunately, the face-centered cubic conducting phase is only stable between 730 – 824 °C. To stabilise this phase to room temperature bismuth has to be substituted by other metals ions. In this work we firstly look at how the amount and type of substituent ions, as well as combinations thereof, affect the structure and phase stability of the material. Secondly, the oxide conductivity and the degradation thereof due to oxide ordering upon long term annealing at ~500 °C in the solid electrolytes were investigated. This work encompasses the application of a range of techniques to build a more fundamental understanding of these materials, including powder X-ray diffraction and total scattering, and Raman, X-ray absorption and electrochemical impedance spectroscopies. Results from these laboratory and synchrotron-based techniques provide good insight into the complexities of these materials.

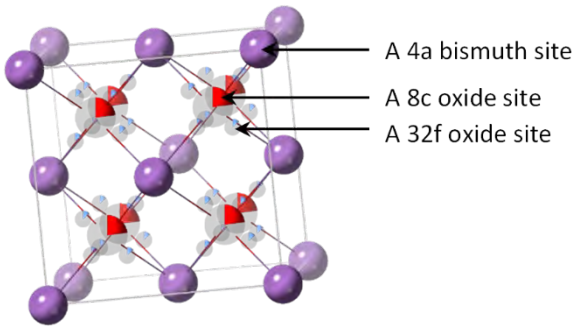

Figure 1: Unit cell of the face-centered cubic phase of Bi_2O_3 indicating the various sites.

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C44 Biomolecular Interactions of Cytotoxic Ruthenium Compounds with Thiosemicarbazone or Benzothiazole Schiff Base Chelates.

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Recent advances in the formulation of metal-based chemotherapeutics, see the utilization of biocompatible ligands which may can tailor the biodistribution patterns[1]. Herein, we illustrate the formation and characterization of new paramagnetic ruthenium compounds, *trans-P*-[RuCl(PPh_3)$_2$(pmt)]Cl (**1**) (Hpmt = 1-((pyridin-2-yl)methylene)thiosemicarbazide), *trans-P*-[RuCl(PPh_3)$_2$(tmc)]Cl (**2**) (Htmc = 1-((thiophen-2-yl)methylene)thiosemicarbazide) and a diamagnetic ruthenium complex, *cis-Cl, trans-P*-[$RuCl_2$(PPh_3)$_2$(btm)] (**3**) (btm = 2-((5-hydroxypentylimino)methyl)benzothiazole). Agarose gel electrophoresis experiments of the metal compounds illustrated dose-dependent binding to gDNA by **1** – **3**, while methylene blue competition assays suggested that **1** and **2**, were also DNA intercalators Assessment of the effects of the compounds on topoisomerase function indicated that 1 – 3 were capable of inhibiting topoisomerase I activity in terms of the ability to nick supercoiled plasmid DNA. The cytotoxic activities of the complexes were determined against a range of cancer cell lines vs. a non-tumorigenic control cell line and the complexes were, in general, more cytotoxic towards the cancer cells, displaying IC_{50} values in the low micromolar range. Time-dependent stability studies showed that in the presence of strong nucleophilic species (such as DMSO), the chloride co-ligands of **1** – **3** are rapidly substituted by the former as proven by the suppression of the substitution reactions in the presence of an excess amount of chloride ions. The metal complexes are stable in both DCM and an aqueous phosphate buffer containing 2% DMSO.

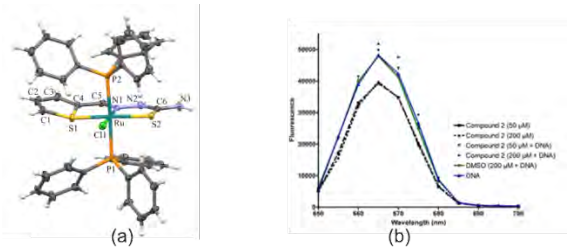

Figure 1: The ORTEP diagram of *trans-P*-[RuCl(PPh_3)$_2$(tmc)]Cl (**2**) (a), accompanied by its methylene blue competition assay (b).

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C45 Unraveling Biomimetic Properties of Nanomaterials for Diagnostic Applications

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Nanoscience brought about various interesting properties such as optical gold nanoparticles, excellent catalysts like palladium nanoparticles, magnetic iron oxide nanoparticles, and inert silica nanoparticles. A plethora of their properties are still being unraveled and explored. In various research, we have explored their potential as biomimetics due to their excellent reactive oxygen radical species generation for disease biomarker detection. A number of various nanomaterial have been investigated and their properties (mechanism of action) thoroughly investigated as potential enzyme substituents for colorimetric sensing. **Figure 1** shows a select few nanomaterials that were prepared and evaluated their biomimetic properties. The presentation will show the intricate procedures for preparing nanomaterials with the aim of enhanced catalytic effect for biomimetic evaluations and some of the recent nanomaterials which showed excellent enzymatic properties.

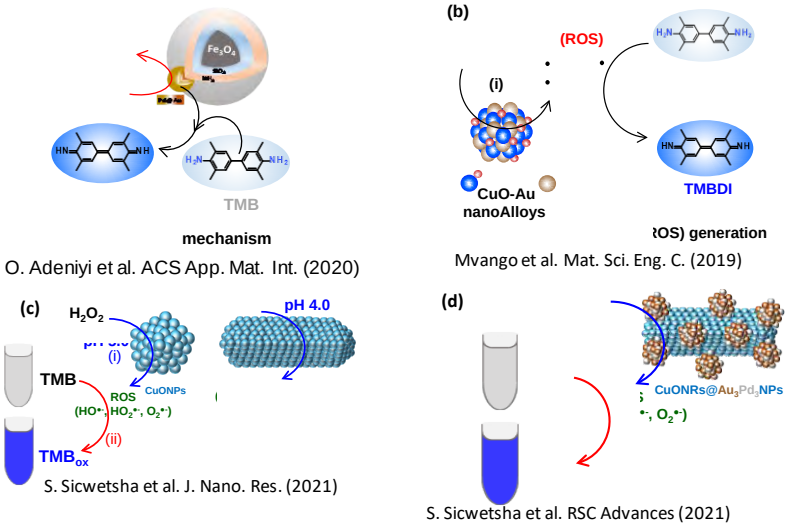

Figure 1: Nanoparticles (NPs) with enzyme-like catalysis (a) nanomagnetic particles[1], (b) CuO-Au nanoalloys[2], (c) spherical and rod-like CuONPs[3], and (d) CuO nanorods decorated with Au@PdNPs[4].

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K23 Cancer meets Chemistry - Translational Research

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The treatment of genetically defined cancer is experiencing a revolution. Over the last 15 years, the knowledge gained about the biochemical features of biomarkers and their predictive power has led to the development of targeted small-molecule molecules that have improved the quality of life and increased the survival of cancer patients. However, the occurrence of inevitable drug resistance limits these approaches and requires the constant development of next-generation precision medicines.[1-4] Against this background, we employ protein X-ray crystallography[5-6], structure-based design approaches[7-9], organic synthesis[10-13], as well as biochemical[14-16] and cellular compound screening[17-18] to understand the mechanisms of acquired resistance better and to develop next-generation inhibitors. We are also interested in devising means to bridge the innovation gap between academic research and practical application. We recently established the “Zentrum für integrierte Wirkstoffforschung” (ZIW) as well as the Drug Discovery Hub Dortmund (DDHD) to serve as incubators for the translation of basic academic research into pharmaceutical applications. Some of our current endeavors will be outlined during the talk.

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K27 Track and Trace by SRS: A new tool for MedChem

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A large proportion of the compounds which enter clinical trials never make it to patients. So there is an urgent need to enhance our understanding of the interplay between small molecules, either from nature or designed in the laboratory, and the intricate network of cellular machinery for which they are intended. Integrating advanced imaging techniques into the early stages of drug-discovery campaigns may help to improve pre-clinical modelling studies and reduce the high attrition rates of clinical drug candidates. Stimulated Raman scattering (SRS) microscopy is a new imaging technique which can be used to detect specific chemical bonds within either the small molecule, or the cell, to give high contrast, label-free imaging and to provide intracellular quantification of small molecules.[1-5] In this lecture, recent advances from our group will be discussed including: the design of synthetic Raman-active labels which exploit spectroscopically bioorthogonal functional groups; the use of both dual-colour SRS and multi-modal imaging to probe intracellular drug distribution and drug resistance mechanisms; and analysis of the quantitative data which SRS imaging provides to allow the kinetics of bioorthogonal reactions to be studied in the intracellular environment itself.

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K30 Structure and function of microbial natural product macrocycles

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Microorganisms are talented chemists that produce structurally diverse specialized metabolites (natural products) with ranging biological properties and largely unknown ecological roles.[1] These energetically expensive metabolites are thought to play critical roles in environmental adaption of the producing organisms, and have also served as molecular probes of cellular mechanisms of disease and as pharmaceutical lead compounds.[2] In collaborations that integrate microbiologists, synthetic chemists, chemical biologists and pharmacologists, we have characterized complex nonpolar macrocycles of polyketide, peptide or hybrid biogenesis from a variety of microbial consortia, including from living stromatolites that occur peritidally in the Eastern Cape of South Africa.[3,4] LCMS-based untargeted metabolomics approaches in tandem with collaborative phylogenetic and metagenomic sequencing were used to guide targeted chromatographic isolation of key natural product macrocycles at microgram scales for structure elucidation using NMR spectroscopy and chemical derivatization. Large lipophilic macrocycles with constrained conformational flexibility[5] may be evolutionarily optimized to access and bind proteins at or in membranes. Thus, in collaborative work to characterize cellular function we have focused on expanding the small class of natural product macrocycles known to disrupt cellular proteostasis by binding the Sec61 translocon to modulate protein biogenesis and secretion.[6,7]

Acknowledgements
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I17 South African plants as a panacea to health challenges: Insights on collaborative endeavors exploring this resource in search of treatments

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South Africa is endowed with one of the largest plant biodiversity's in the world, complemented by a rich heritage of traditional knowledge on the use of medicinal plants. Despite this tremendous wealth of resources, there is no block buster pharmaceutical that has emerged from the country on this resource. It is perhaps that the country has lacked new approaches to undertake research on these resources and research may have been too fragmented. Arguable, a collaborative endeavor is best suited to efficiently explore the country's resources in search of much needed medicine. As part of efforts towards the discovery and development of drugs we have established a consortium of local and international experts, whose mandate is to accelerate these efforts by tapping into the diverse, unique South African flora. This is being achieved by high-throughput conversion of an existing library of 10 000 plants which is linked to their traditional uses into an enhanced pre-fractionated natural product repository amenable for high-throughput screening against various diseases. The technologies and skills in modern methods is the basis of the research programme and is shared with partner institutes to start entrenching and developing new skills in modern natural product drug discovery techniques while also expanding the library. This will be the first of its kind for the continent which will provide the infrastructure and skills for African scientists to participate in modern day drug discovery programmes. The platform also includes hyphenated analytical technologies for the accelerated approach towards identifying the natural biologically active compounds. In search of much needed new medications, we recently investigated selected subsets samples from the library, and evaluated their potential against a variety of diseases such as malaria, HIV, cancer, COVID-19, microbial drug resistance and trypanosomiasis. The results have demonstrated the value in the new hyphenated approach with one lead now in preclinical studies within a short space of time.

I20 A search for bioactive compounds from natural sources

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Over the years, natural products have played an important role as sources of new drug leads.[1] Natural compounds offer unique characteristics that include structural complexity, chemo-diversity, and biochemical specificity.[2] When worked on in conjunction with other strategies including synthetic chemistry, the intricate frameworks of natural origin offer an indispensable source for drug discovery.[2] Despite the successes in the development of drugs based on natural scaffolds, the discovery of new drug leads from natural sources presents several challenges. The main challenge in natural products research lies in the efficient identification and isolation of new bioactive compounds from complex matrices.[3] Another barrier is that, often low quantities of material are obtained, which are insufficient for further development.[2] Several strategies have been employed to overcome some of the challenges. With advances in analytical and purification techniques, novel compounds can be targeted by employing various approaches.[3] Strategies that have been employed to provide more material for intensive bioactivity studies include directed biosynthesis, semisynthesis and total synthesis of the natural products.[2] Synthesis can also be employed for structural modification of natural compounds, to provide analogues with enhanced properties.[2] In this presentation, our recent work on isolation and synthesis of bioactive natural compounds will be discussed.

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I21 Reduction of α, β-alkynyl carbonyl compounds using $SnCl_2$ and computational investigation of the reaction mechanism

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Our research group has been synthesising novel heterocyclic compounds that are tested for their biological activities against diseases, such as TB and cancer. The design of some of the compounds was done computationally, where active sites of known enzymes were docked with heterocyclic compounds to determine the binding affinity, which can affect the enzyme activity. One compound that we were interested in synthesising was **2**, which we planned to prepare using the conditions as shown in Figure 1 below, which were meant to reduce the NO_2 only. Surprisingly, both the NO_2 and alkyne groups were reduced under these conditions. When doing literature search on the reduction of alkynes with $SnCl_2$, no reactions were reported. It is against this backdrop that we formulated a research project to understand the reaction mechanism for this reduction reaction. A number of reactions with different compounds containing α, β - alkynyl carbonyl moiety, were performed to better understand the versatility and limitations of the reaction (Scheme 2). $SnCl_2$ was able to reduce alkyne to alkane in the presence and absence of the NO_2 group, with yields ranging from 65 to 80 %. The reactions only worked when the alkyne was attached to a heterocyclic ring and a carbonyl group, but no reduction of the alkyne if one group was absent.

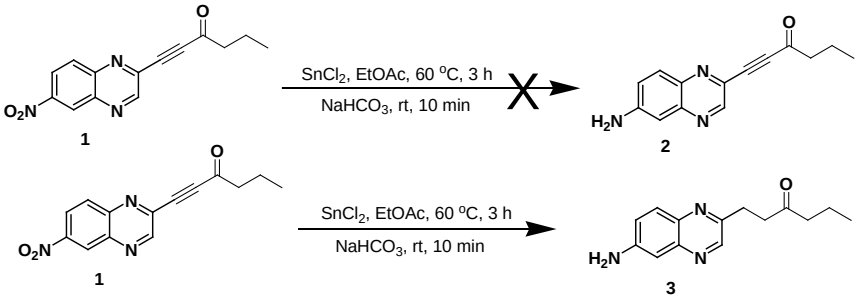

Figure 1

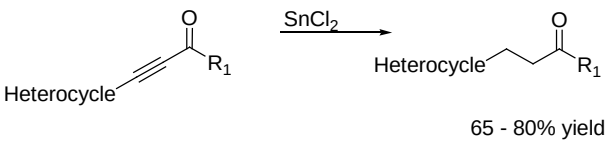

Figure 2

I22 Can South Africa facilitate local API manufacturing: The vision of continuous flow chemistry?

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Africa has a variety of formulation companies, however the active pharmaceutical ingredient (API) are generally imported. This results in increased drug costs, making medications unaffordable to many patients in Africa.[1] When micro reactor technology was introduced it was seen as a research and development tool, however it is now being used to produce large quantities of product. The driver being increased safety, higher yields and purity as well as reduced production cost. There is now a range of commercial reactors on the market, which means that most companies are investigating this technology to rapidly screen reactions utilising continuous flow, leading to the identification of reaction conditions that are suitable for use at a production level. [2-4] COVID-19 caused drug shortages around the world, demonstrating the need for local production capacity. To this effect, we are working on developing local drug manufacturing capacity in Africa using continuous flow technology, with the goal of lowering the cost of drugs, improving drug accessibility and ultimately improving Africa's health. A selection of cases studies will be presented.

Acknowledgements
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I25 Cyclic peptidomimetic inhibitors from natural templates targeting the *Mycobacterium* tuberculosis caseinolytic protease ClpP1P2 and ClpC1 ATPase

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In South Africa, tuberculosis (TB) caused by the mycobacterium tuberculosis agent is the leading cause of death with about 80% of the population currently infected. The majority of these infections are latent with about 1% developing into active TB each year.[1] Unfortunately the TB treatment is lengthy, not shorter than six months and has dangerous side effects.[2] Furthermore the world is also faced with antibiotic resistance leading to growing numbers of multidrug-resistant TB infections. The lack of new suitable lead compounds is now a major problem in the development of effective TB drugs.[3] In this study, novel selective peptidomimetics derived from natural sequences of lariatin A, lassomycin and acyldepsipeptides were synthesized using the solid phase peptide synthesis technique to inhibit the TB caseinolytic protease, thereby causing cell death of the mycobacterium. The developed peptidomimetics were characterized using Liquid Chromatography Mass Spectroscopy (LCMS), Nuclear Magnetic Resonance (NMR) spectroscopy and screened for antituberculosis activity. Pep_2_ NN (lassomycin derivative) was found to exhibit a Minimum Inhibitory Concentration (MIC_{99} = 9.87µg/ml) that is comparable to that of ethambutol for 7 days and an inhibitory effect (79%) on the ClpP Protease activity. Lariatin A (Pep TAA, Pep TA) and lassomycin (ring-2-NN, Tail-2-NN) peptidomimetics were observed to significantly inhibit the ClpP Protease activity (49-85%) while the majority of acyldepsipeptides derivatives were observed to activate the enzyme activity. These peptides contribute to a new class of TB drugs with a different mechanism of action from the current drugs which the mycobacterium is already resistant to.

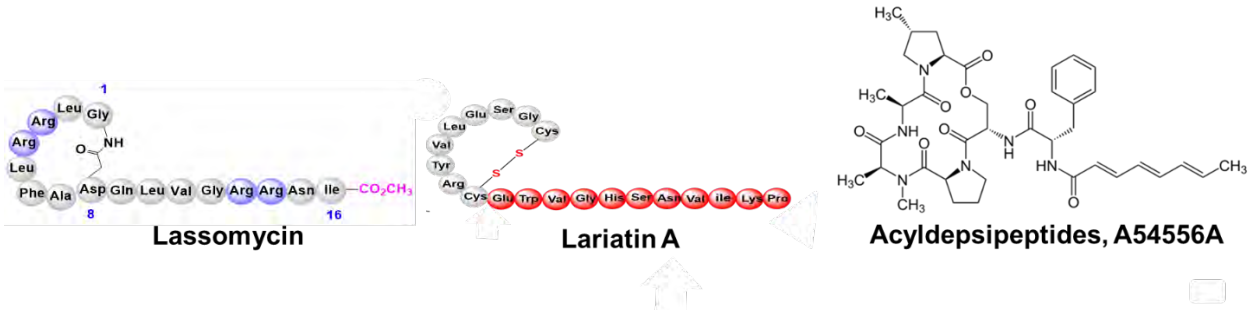

Figure 1: Structures of lassomycin, lariatin A and acyldepsipeptides

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C54 Natural dietary compounds and cancer prevention: investigations into the anti-cancer mechanism of action of flavonols and polysulfanes

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Cancer is a hyper-proliferative disease that affects all people regardless of race, with limited treatment options. Cancer prevention is thus an attractive intervention strategy. In this context, there are a number of natural chemopreventative agents, often available through the diet. These compounds include the flavonols from edible plants, and the polysulfanes from garlic. Both compound classes are cytotoxic to cancer cells. The flavonols are well known for their antioxidant activity however protein binding also plays an important role. The organosulfur compounds, which include ajoene, diallyl trisulfide and diallyl tetrasulfide, are proposed to act by *S*-thiolating cysteine residues on target proteins (Figure 1). Libraries of flavonols have been synthesised in order to uncover structure-activity aspects in the natural series, and to synthesise and study the mechanism of action of more active analogues. We have developed synthetic routes to the various polysulfanes,[1-2] which has enabled the study of their anti-cancer mechanism, as well as the synthesis of more potent analogues and mechanistic probes. By tracking the movement of a fluorescently tagged ajoene, we identified its location in the endoplasmic reticulum of breast cancer cells where it was found to interfere with protein folding and to activate the unfolded protein response.[3] In another experiment, we used a biotinylated ajoene probe to tag and pull-down the protein targets of ajoene. We have identified and validated a number of these targets, many of which contain reactive cysteines, important in cancer.

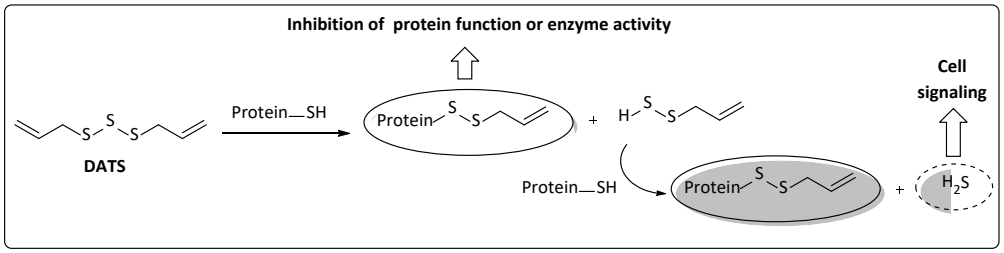

Figure 1: Hypothesis for the cytotoxic mechanism of action of organotrisulfides in cancer cells

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C55 Utilising anatase nano-seeds coupled with a visible-light antennae system for effective photo-organic transformations

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A Cu and Pd bi-metallic surface loading strategy with nitrogen functionalisation (Cu/Pd and N) on a sol-gel prepared metal oxide (titanium dioxide, Cu/Pd-N-TiO2) has afforded a novel method to attenuate the restriction of titanium dioxide's inherent ultraviolet light activation. The functionalisation strategy (Cu, Pd, and N) has provided the opportunity to facilitate the oxidation of a range of cyclic alcohols, which was subsequently extended to access a range of heterocyclic systems via a tandem oxidation type process (Figure 1). In-depth photo-physical studies using spectroscopic, microscopic and powder X-ray diffraction techniques were utilised to characterise defect-free nano-seeds of titanium dioxide (anatase). Trace surface loadings of nanomaterial copper (as copper oxide) and metallic palladium species were detected at 0.04 wt.% and 0.18 wt.%, respectively. These nanoparticles induced a red-shift in titanium dioxide's optical band gap towards the visible region (> 440 nm).

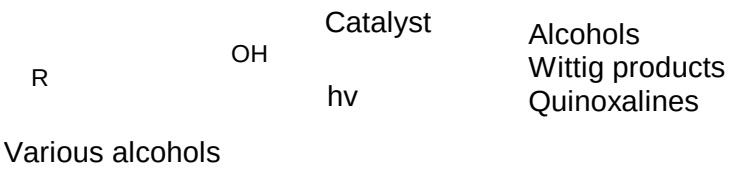

Figure 1: Access to a range of organic products via a simple oxidation process

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C63 The photo-switchable polarity of conjugated cinnamic acid/chloroquinoline: Synthesis, isomerization, and antimalarial activities.

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The resistance of malaria against known drugs warrants development of 'smarter' future drugs. New drug discovery strategies include synthesis of hybrid compounds as antimalarials. Herein, we show a simple and facile strategy for conjugating, a natural and biologically active molecule, cinnamic acid to a well-known anti-malarial compound, chloroquinoline, through different linkers. Apart from its known independent biological attributes[1-3], cinnamic acid can be used as a photoswitachable moiety, which further allows changes in hydrophobicity, thereby forming structurally related compounds (trans/cis - geometrical isomers) that differs in polarity. UHPLC-QTOF-MS analyses of the photo-isomers/products revealed the emergence the cis isomer which eluted before its synthesized trans counterpart suggesting a reduced polarity. This polarity change could be exploited as it can aid in synergistic pharmacological properties by covering a wider pharmacophoric space.

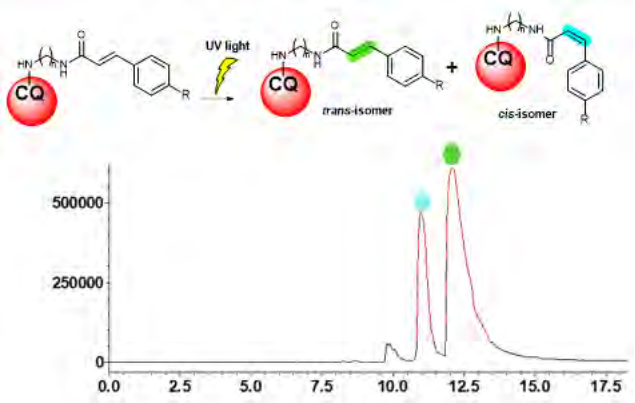

Figure 1: Schematic representation of analyzed isomerized compounds.

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C64 Total Syntheses of 5,8'-Naphthyl*iso*quinoline Alkaloids Employing Hartwig's Borylation/Methylation Strategy and a Novel Nickel/*N*,*N*-Ligand-catalyzed Atroposelective Cross-Coupling

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We have developed a new, reliable route to the northern naphthalene building blocks of naphthyl*iso*quinoline alkaloids[1-2] utilizing Hartwig's borylation/methylation strategy for the regioselective introduction of pinacolborane.[3-7] This approach then allows for the introduction of orthogonal protecting groups on this moiety, relevant for the synthesis of differently alkylated biaryl alkaloids. For the synthesis of the other cross-coupling precursors, we employed a modification of Bringmann's known approach to the dihydro*iso*quinoline compounds and a newly developed route for the naphthalene building blocks. Furthermore, we have found by serendipity and optimized a new Ni/*N*,*N*-ligand-catalyzed, atroposelective Negishi cross-coupling reaction making use of Lassaletta's ligand, that provides the desired naphthyl*iso*quinoline natural products in reasonable yields and consistently high optical purities. To demonstrate its value, this approach was utilized to synthesize the naturally-occuring Ancistrolikokine, Ancistroealaine A, *ent*-Ancistrotanzanine A and Ancistrolikokine E_3 naphthyl*iso*quinoline alkaloids, all of which are now available in appreciable amounts for detailed biochemical evaluation in terms of bioactivity and mode of actions studies (to be reported later). To the best of our knowledge, this method thus represents the first catalyst-controlled and therefore atroposelective cross-coupling directly providing different naphthyl*iso*quinoline alkaloids from their respective precursors.

Acknowledgements
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C65 Stabilizing peptide nano-structures using non-canonical amino acids with donors and acceptors

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Low molecular weight peptides can associate into nanostructured assemblies such as hydrogels or peptide nanotubes.[1] The self-assembly process is based on weak intermolecular interactions, such as hydrogen bonds, hydrophobic contacts, and π-stacking. In our project we aim to synthesize non-canonical amino acids[2,3] that should allow to strengthen π-stacking by adding the charge transfer (CT) component between the appended donor (D) and acceptor (A) moieties. CT interaction[4] between hydrophobic D/A units is expected particularly strong in aqueous medium; moreover, it can be switched on/off by oxidation of a donor counterpart or redaction of an acceptor counterpart. Reversibly oxidizable tetrathiafulvalene[5] (TTF) is used as a donor amino acid residue, whereas naphtalimide, naphthalene diimide, nitroarene, and TCNQ groups are used as molecular acceptors. The novel donor- and acceptor-modified amino acids were incorporated into known amphiphilic peptide sequences, and the fibre-based hydrogels of the resulting peptides were prepared and investigated. The gels will be tested as drug delivery systems with prolonged drug-release capability. The inherent fluorescent properties of arylenediimide derivatives may lead to a new generation of biomaterials capable of in vitro and in vivo sensing. Since the presence of redox-active groups in peptide sequence may enable the electron transport, future application of such redox-active nano-structured materials in organic electronics can be envisaged.

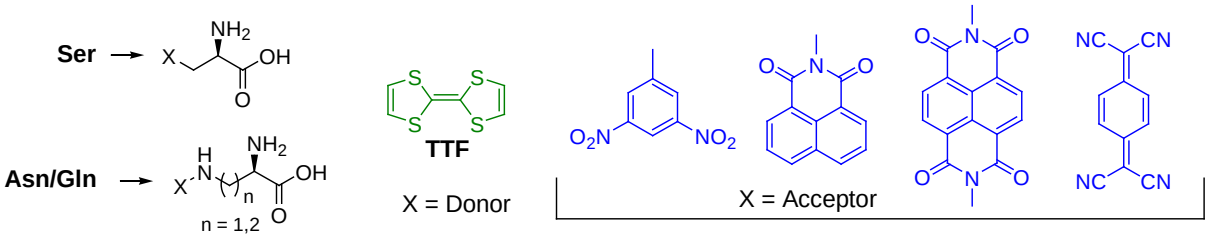

Figure 1: Structures of the donor- and acceptor-modified amino acids.

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C69 Development of Peripherally Restricted 5-HT$_{2B}$ Antagonists for Treatment of Pulmonary Arterial Hypertension

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Pulmonary arterial hypertension (PAH) is an often lethal condition characterized by extensive pulmonary vascular remodeling leading to lung microvasculature obstruction and right heart failure.[1] Many of the currently available therapeutics for the treatment of PAH are characterized by their high cost and the potential for adverse effects, and have not been shown to be disease modifying.[2] The serotonin 2B receptor (5-HT$_{2B}$) has been shown to be a driver of PAH disease progression; serotonergic drugs including fenfluramine are known to cause fatal drug-induced PAH in human subjects.[3] These agents, which are potent 5-HT$_{2B}$ agonists, have been discontinued from use. Selective 5-HT$_{2B}$ antagonists have subsequently shown utility for the treatment of PAH, but such compounds are often centrally active (can permeate the blood-brain barrier). Because 5-HT$_{2B}$ inhibition in the central nervous system is associated with a risk for suicidality in human subjects,[4] clinically useful 5-HT$_{2B}$ antagonists would need to be non-centrally penetrant. Reported here is a series of structurally novel 5-HT$_{2B}$ antagonists with high potency and selectivity for the 5-HT$_{2B}$ receptor subtype that are peripherally restricted and display favorable pharmacokinetic properties in rodents. An exemplary compound from this series, VU6047534, is highly efficacious in preclinical mouse models of PAH treatment and prevention.

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C70 Ferrocene: A versatile organometallic fragment in the design of novel therapeutic agents

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A significant number of FDA approved drugs are purely organic compounds. In recent years, the field of bioorganometallic chemistry has made significant strides in the context of drug discovery; it offers alternative therapeutic tools for treating diseases. In our case, the organometallic ferrocene is of particular interest considering its inherent attributes. A vast range of compounds containing organometallic ferrocene fragment have been shown to possess a broad spectrum of biological properties. Recent examples of ferrocene-based compounds reported in literature illustrate the journey of ferrocene towards the development of therapeutic agents intended for various ailments.[1,2] Ferroquine and ferrocifen are notable examples of ferrocene containing drugs, which have reached the clinical trials for treatment malaria and breast cancer, respectively. The presentation will share our recent work involving the synthesis of new ferrocene containing compounds in the quest of novel of antitumour and antiparasitic agents.[2,3]

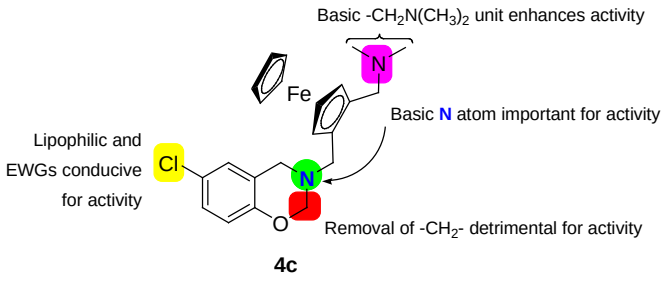

Figure 1: Preliminary SAR of ferrocenyl 1,3-benzoxazines.

Acknowledgements
The authors are gratefully indebted to Rhodes University (Sandisa Imbewu) and the National Research Foundation (NRF, South Africa) for financial support.

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C71 Synthesis of "Dual Warhead" β-Aryl Ethenesulfonyl Fluorides and One-Pot Reaction to β-Sultams

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Herein, we report an operationally simple, ligand and additive-free oxidative boron-Heck coupling that is compatible with the ethenesulfonyl fluoride group – an important fuctional group in click chemistry. The protocol proceeds at room temperature with chem and *E*-isomer selectivity and offers facile access to a wide range of β-aryl-/heteroaryl ethenesulfonyl fluoride, which are known to display two electrophilic sites towards *e.g.,* enzyme bound nucleophiles. Furthermore, we demonstrate a "one-pot click" reaction to directly access aryl substituted β-sultams – another group with potential as activity based reactive probe and as covalent enzyme inhibitor.

C78 Anti-HIV and cytotoxicity activity of diterpenoids from South African *Euphorbia* species

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South Africa has the largest HIV epidemic in the world and is ranked the 50th on the World Cancer Research Fund's list of countries with highest prevalence rates[1]. The current drugs against these diseases suffer from major setbacks such as drug resistance, making the search for new drugs a priority. Plants are an important source of novel pharmacologically active compounds. Southern Africa has a rich plant biodiversity and for most of the plants, the phytochemistry has not been investigated[2]. Plants of the *Euphorbia* genus are indigenous to South Africa and rich in structurally unique diterpenoids. Some of these diterpenoids have displayed potent anti-HIV and cytotoxic activities. The project aimed to identify bioactive diterpenoids from South African *Euphorbia* species, elucidate their structures and evaluate them for cytotoxicity and anti-HIV activities. Six *Euphorbias* were selected for investigation. The phytochemical investigation of *E. cooperi* led to the isolation of two new and two known phorbol diterpenoids, one new and one known norsesquiterpenoids as well as one triterpenoid. From *E. triangularis* one new and six known phorbol diterpenoids including two diterpenoids were identified. The extracts and compounds were evaluation cytotoxicity against three cancer cell lines: Hela, Vero and MCF7. Their anti-HIV activity was also evaluated against the HIV-1 (NL4.3 subtype B). Phorbol ester B showed the exceptional cytotoxicity activity with IC50 values of 32.07 and 53.17 µM, and strong anti-HIV activity with an IC50 value of 3.19 µM.

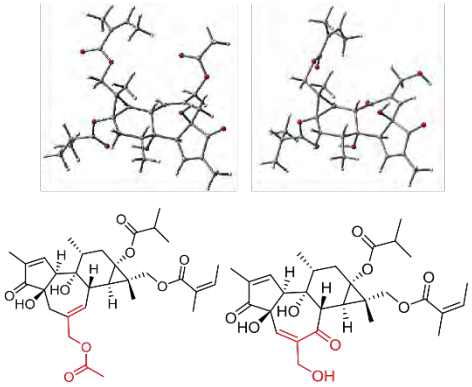

Figure 1: A pancake-bonded dithiadiazolyl dimer.

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C79 Visible-Light Mediated Triplet Energy Photosensitization for the Formation of Nitrogen-Containing Heterocycles

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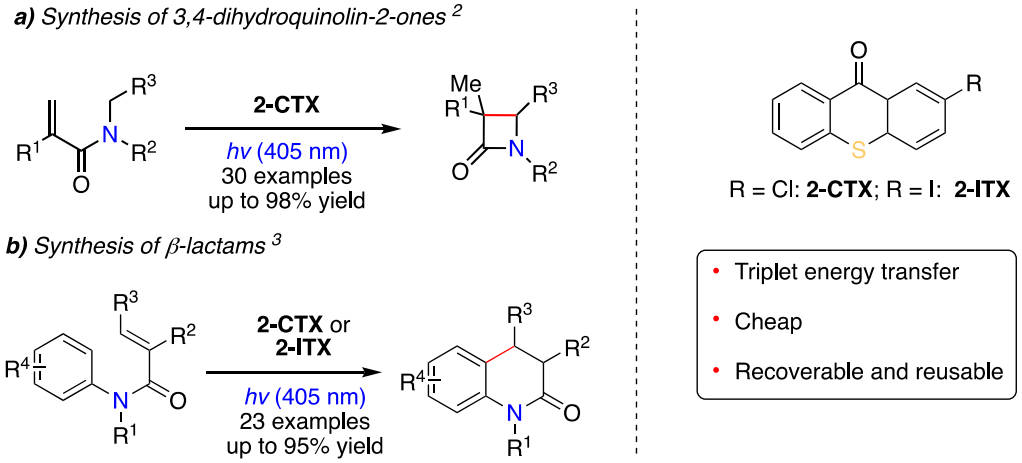
Visible-light mediated triplet energy transfer (TET)[1] has recently experienced a resurgence of interest and relies on the activation of organic molecules through photophysical processes. Unfortunately, the majority of TET processes involve the use of either rare and expensive metals or harsh UV light. This research focuses on the use of the 2-thioxanthone (**2-TX**) class of molecules to serves as metal-replacement alternatives for visible light mediated TET. In 2021, we demonstrated that 2-substituted thioxanthones (**2-TX**) could efficiently catalyse the synthesis of 3,4-dihydroquinolin-2-ones — a privileged medicinal chemistry scaffold via a formal C(sp^2)–H/C(sp^3)–H arylation (a)[2]. This was significant as up until our work, this chemistry had only been reported using iridium or platinum photocatalysts. More recently, we described the synthesis of β-lactams from simple acrylamide starting materials by visible-light mediated energy transfer using these powerful **2-TX** catalysts (b)[3]. The reaction proceeds through triplet sensitization of the C–C olefin moiety and features a C(sp^3)–H functionalization through a biradical carbon-to-carbon 1,5-hydrogen atom transfer. β-Lactams are amongst the most important compound classes in medicinal and biological chemistry – most famously in frontline penicillin antibiotics. Previous methods for the synthesis of these β-lactams typically requires harsh UV light, which limits the reaction scope and selectivities. This work hopes to promote the **2-TX** class of organic molecules as powerful alternatives for metal catalysis.



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C80 Sharing compounds within in pre-competitive international research infrastructure initiative for chemical biology and early drug discovery

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The quality of a screening collection is one of the most critical factors of success in drug discovery. Academic compound collections often predominantly consist of compounds that are commercially available, but compounds synthesized by academic chemists as well as natural products represent a rich, untapped source for novel chemical diversity. In order to make the invaluable chemistry accessible to a broader scientific community and to allow chemists to uncover novel bioactivities of their compounds, EU-OPENSCREEN offers chemists the opportunity to make their compounds available, in a regulated and transparent framework, to a wider community of biologists, who test these compounds in suitable bioassays. By doing so, chemists can expose their compounds to a broad range of different biological/drug targets to uncover the unknown bioactivities of their compounds, which would otherwise not be feasible in individual one-to-one-collaborations. Once a compound has been identified as an active hit compound, a research collaboration between the chemist (who submitted the compound) and the biologist (who developed the bioassay) can be initiated. The publicly funded international research infrastructure EU-OPENSCREEN (www.eu-openscreen.eu) aims to support projects in early drug discovery by democratizing access to technology platforms, expertise and compound collections and by creating a pre-competitive network of like-minded researchers. The 30 academic partner institutes offer complementary expertise and instrumentation to collaboratively develop novel chemical probes for the life sciences community. The primary screening data will be made available to the scientific community through its open-access European Chemical Biology Database (www.ecbd.eu). Training activities are also available, and in March 2023, EU-OPENSCREEN, H3D/UCT and Fraunhofer ITMP co-organise a practical workshop in pre-clinical drug discovery in Cape Town. Here, I will present this unique pre-competitive compound sharing model and explain the opportunities and benefits for South African chemists to make their compounds available to a broader scientific community.

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K11 Thermal Analysis as a crucial step during research on thermal processing of coal fines, waste biomass and solid waste material

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Various thermal analysis techniques are used as a first step to investigate the possibilities of utilization of waste coal, waste biomass and various other solid waste material in thermal conversion processes. Coal is unfortunately still crucial for the socio-economic development in South Africa. 77% of the energy needs are supplied by the utilization of coal, which resulted in 91% of electricity generated and production of 30% of South Africa's produced liquid fuels.[1] South Africa is the 6th largest coal producer in the world. 27% of the saleable coal is exported, making coal one of South Africa's largest export products. Coal fines, the waste product that forms during physical handling of coal, accounts for approximately 12% of the total South African mined coal. This amounts to a total of 38.8 Mt of fines that are currently discarded in slime dams contributing to acid mine drainage and various other environmental problems.[2] South Africa annually generates approximately 54.2 million tons of municipal, commercial, and industrial waste.[3] This waste consists mainly of organic material, with only ±10% recycled and ±90% landfilled. Waste biomass is produced from the agricultural, municipal, forestry and paper industries. 9.51 million tons of spent coffee grounds was discarded into landfill in 2017.[4] The first step in assessing whether a solid waste material may be utilized for combustion, pyrolysis or gasification purposes is usually thermogravimetry. Using thermogravimetry, various reactivity indices are determined and compared to required values. Kinetic models have been developed for coal conversion processes and these are applied to co-utilization of coal with waste biomass material. Examples from our research will be given and the importance of the various thermal analysis methods highlighted.

Acknowledgements
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K19 Aerobic oxidation of methane to formaldehyde over platinum

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The selective, aerobic oxidation of methane to oxygenates could provide an efficient route for the production of chemicals, but it remains a challenging route as the products are more reactive than the substrate, methane. It has been postulated that selective, activation of methane over metal surfaces can be achieved if methane interacts with adsorbed oxygen on a metal surface, whereas the direct interaction of methane with the metal surface would result in the formation of the total oxidation products CO or CO_2[1,2]. The interaction of the resulting oxygen-containing with the metal surface should not be too strong, so that the product may desorb from the surface. Group 10-11 metals are suitable candidates as the catalytically active metal for the selective oxidation of methane provided that the surface can be saturated with oxygen. The latter is not that simple as lateral interactions between adsorbed atomic oxygen on the surface typically prevents high coverages. This can be negated by co-feed water and generating surfaces which are covered with atomic oxygen, OH and adsorbed water and our DFT-calculations show that co-feeding of water is necessary to obtain a fully covered surface.[3] The aerobic oxidation of methane over Pt/TiO_2 in the presence of water results in the selective formation of formaldehyde with a selectivity of ca. 90%. The selectivity appears to be unaffected by the level of conversion (X_{CH4} < 3%) and this represents a significant step forward in the selective oxidation of methane. Furthermore, we show that the rate of oxidation of methane under these conditions is zero order with respect to methane and oxygen implying that the reaction is desorption limited with our DFT calculations suggesting the formation of the stable di-σ-hydroxy methoxy species under these conditions. The reaction is enhanced by the presence of liquid water, which is attributed to water facilitating the desorption via H-shuttling.

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K24 Versatile organic-inorganic hybrid materials: structures and properties

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An organic-inorganic hybrid material combines an organic- and inorganic component at the nano-scale, offering the opportunity to merge the properties of the components into a single material that typically retains the properties of the individual components. The components are selected in such a way as to impart specific properties to the hybrid material, to allow for the design of materials with desired properties. The organic component may template the inorganic sub-structure, and can impart optical and electronic properties to the material, while the inorganic component can provide hardness, magnetic properties and optical properties. Our research focusses on organic-inorganic hybrid materials formed through the combination of organic amines or amides and metal halides. These materials exhibit a variety of structural types, including halide-bridged polymers, metal organic frameworks and perovskites. Since the material properties also depend on the structure, and specifically the dimensionality of the inorganic substructure, engineering of the structure of an organic-inorganic hybrid is key to designing a material with specific properties. Thus, understanding structure-property relationships in these different types of hybrid materials is crucial. An overview of a number of families of organic-inorganic hybrid compounds studied in our research group will be presented, with structural trends highlighted. In addition, the relationship between structure and properties, including magnetism, fluorescence and band gap will be discussed. Both experimental and computational results will be presented.

I10 Solid-state Chemistry at Rhodes University in the Context of Sustainable Physical Chemistry

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Improving the efficiency with which chemical products and materials are used in order to meet human needs while reducing hazardous substances and waste – is a tenet of sustainable chemistry. Efforts to reduce, reuse and recycle include design, materials, processes, optimization and engagement.[1] It is within this context that we place solid-state chemistry research at Rhodes university. Our efforts have been specifically geared towards the preparation of new materials, the physicochemical derivatization of existing active pharmaceutical ingredients (APIs), the implementation of critical process parameters and developing industry-university projects.

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I13 Theoretical Chemistry: A tool for sustainable chemistry in Africa

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Currently the focus of many research groups is sustainable chemistry. Computational chemistry as a tool for sustainable chemistry is fast gaining popularity particularly in the pharmaceutical industry. In South Africa and in other African countries researchers are using theoretical chemistry to explain and compliment experimental results. Computational nutraceutics[1] is a new concept for predicting the molecular structure, spectroscopy, and chemical reactivity of nutraceuticals by means of computational chemistry and molecular modelling. The term nutraceutical is the result of combining the words 'nutrition' and 'pharmaceutical'. The structural and electronic properties (Figure 1a and b) of four pentacyclic triterpenoic acids: betulinic acid (BA), oleanolic acid (OA), ursolic acid (UA) and maslinic acid (MA) were investigated at the molecular level using conceptual density functional theory (DFT) and hence providing insights on the stability, reactivity and selectivity of these compounds as possible drug candidates. Simulated spectroscopic parameters: UV-vis and IR (Figure 1c) agree with experimental data. Calculated charge distribution, frontier molecular orbitals, electrostatic potential plots and global and local reactivity descriptors were used to predict the reactivity and the reactive sites on these molecules. Non-linear optical (NLO) properties, natural bond (NBO) and Fukui function analysis was also carried out. The study provides a theoretical understanding of the bioactivity.

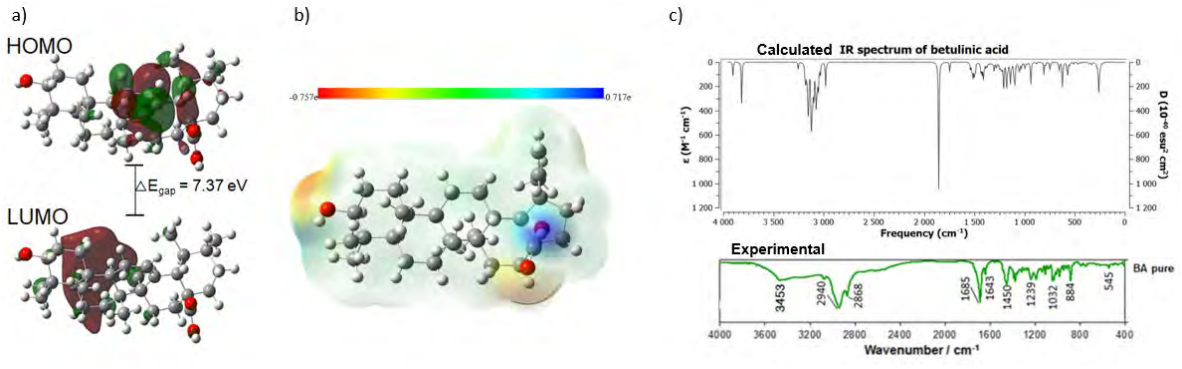

Figure 1: Betulinic acid a) frontier molecular orbitals, b) electrostatic potential plot, and c) calculated vs experimental IR spectrum.

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I18 Structure – properties relationship in two hydrogen-bonded MOF based of $[Cr(ox)_3]^{3-}$ anions and cations built with 2-picolylamine and M = Co^{3+} or Cu^{2+}

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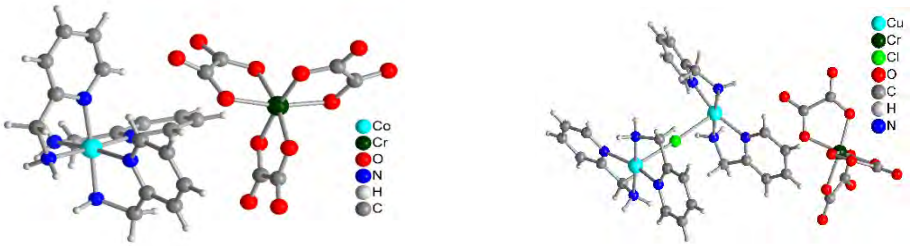
The compounds $[Co(amp)_3][Cr(C_2O_4)_3]\cdot 6H_2O$(I) and $[Cu_2(amp)_4Cl][Cr(ox)_3]\cdot 6H_2O$ (II) were synthetized by a self-assembly process of the ionic complexes $[Co(amp)_3]^{3+}$ and $[Cu_2(amp)_4Cl]^{3+}$with $[Cr(C_2O_4)^3]^{3-1}$. This results in supramolecular potentially porous architectures exhibiting channels filled with water clusters[1, 2]. The activated phases of I and II (I' and II' respectively), can readsorb the water molecules to regenerate I and II which are stable for many water adsorption and desorption cycles[2]. I' and II' exhibit water adsorption and desorption isotherms having a sigmoidal shape and resulting in the combination of a type I(b) profile followed by an S-shaped type V isotherm in the IUPAC classification. At 20 °C, a pronounced H1-type hysteresis loop with parallel and steep adsorption (at 0.25P/P_0) and desorption branches (at 0.17P/P_0) is observed for I' while for II', the steep water adsorption and desorption branches occurs at 0.1P/P_0. The water adsorption capacities of the two materials I' and II' are 17 and 12 wt% respectively. Temperature does not have a great effect on their water sorption properties, and they all exclude N_2 and CO_2 gases in the low pressure range. I' and II' are classified among the materials which can be used for automatic indoor control. The structure-property relationship in I' and II' is studied through single crystal X-ray diffraction analyses of I, II, I' and II' and situ powder X-Ray Diffraction (PXRD) measurements during the water sorption processes.



(a) (b)

Figure 1: Molecular metal complex building units of I (a) and II (b).

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C31 Isothermal TGA investigation of the sublimation of fipronil at polymer processing temperatures

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Most malaria vectors are endophilic; i.e., the mosquitoes rest indoors after taking a blood meal. Historically, transmission of malaria has been disrupted through killing endophilic malaria vectors using indoor residual spraying (IRS) with DDT. However, issues involving access to an adequate supply of DDT and the possible adverse effects of DDT on human health and the environment cannot be ignored. To remedy this problem an alternative to IRS which employs controlled release technology in the form of a tri-layer polyethylene film containing a phenylpyrazole insecticide (fipronil) in the middle layer was investigated. In preliminary studies, thermogravimetric analysis (TGA) of fipronil showed very little mass loss when heated to 140 °C, indicating the absence of a hydrate or a solvate. However, when heated beyond 150 °C a significant mass loss was observed even below the melting range of fipronil (195–203 °C). This could not be accounted for by the presence of volatile impurities in the substance. Furthermore, it was observed that fipronil crystals deposited on the die face of the extruder during the polymer conversion processes, suggesting that the fipronil was subliming.
This study investigated the propensity of fipronil to sublimate at elevated temperature. This led to a better understanding of the mass loss observed during manufacturing of fipronil-containing polymer films at temperatures between 180 and 210 °C. Knowledge of the chemical and physical properties of insecticides is essential for reliable environmental fate and risk assessments and the subsequent design of effective mitigation and remediation strategies

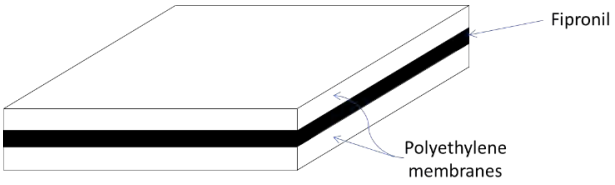

Figure 1: Polyethylene trilayer film with fipronil entrapped in the middle layer.

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C32 Enhanced performance by heteroatom-doped reduced graphene oxide-TiO_2-based nanocomposites as photoanodes in dye-sensitised solar cells

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The photoanode in a dye-sensitised solar cell (DSSC) plays a crucial role in achieving a high power conversion efficiency (PCE). It supports the sensitiser and acts as a transporter of photo-excited electrons from the sensitiser to the external circuit. These two functions are enhanced by a large surface area and a fast charge transport rate. This study compared the photoanode performance of boron- or nitrogen-doped reduced graphene oxide (B- or N-rGO) nanocomposites integrated with TiO_2 (Figure 1). N-rGO-TiO2 exhibited the lowest bandgap of 2.1 eV. It displayed good charge carrier separation ability and electron transfer, attributed to the Ti-O-N bonds and the suppression of electron-hole recombination, resulting in higher current density. Two sensitisers were investigated, i.e., eosin B and Sudan II. A higher light-harvesting efficiency was obtained from eosin B, indicating the presence of more dye molecules anchored onto the TiO_2. Photoanodes fabricated from N-rGO-TiO_2, and B-rGO-TiO_2 showed enhanced photo-exciton generation, higher short-circuit current densities, and significantly better PCEs than their undoped rGO-TiO_2 counterparts[1]. Therefore, heteroatom-doped, rGO-TiO_2-based nanocomposites have excellent potential to be used as photoanodes in DSSCs.

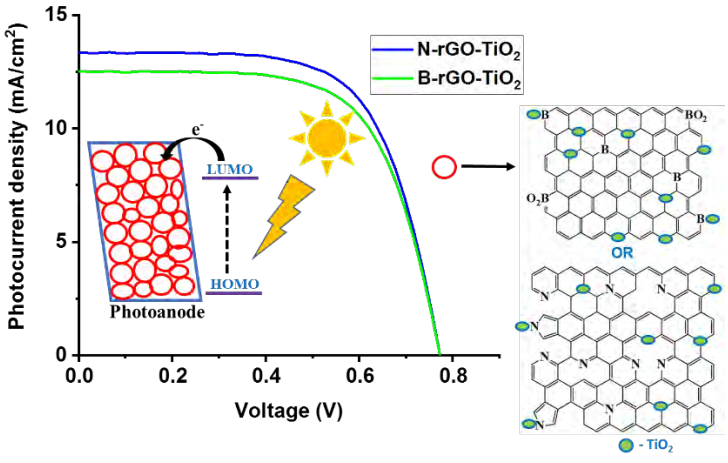

Figure 1: Nanocomposites of boron- or nitrogen-doped rGO integrated with TiO_2 as photoanodes in DSSCs

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C33 Calcium oxalate precipitation kinetics in mixed solvent media

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Calcium scaling, such as the formation of calcium oxalate, is a significant concern in industrial water systems.[1] Calcium oxalate crystals are also a major component of kidney stones.[2] An experimental and computational investigation was carried out to gain insight into the kinetics of calcium oxalate precipitation. Specifically, the rate of calcium oxalate precipitation in water,[3] water-ethanol and water-sucrose solutions was determined. It was found that calcium oxalate is not a binary salt, but instead forms zwitterionic metal chelate macromolecular structures that assemble rapidly in aqueous solutions. Furthermore, these structures have different solubilities and interactions with the solvent, depending on the polarity of the solvent medium. Mixtures of solvents lead to more complex solvent-solute interactions which may accelerate the precipitation, depending on the temperature and solvent ratios.

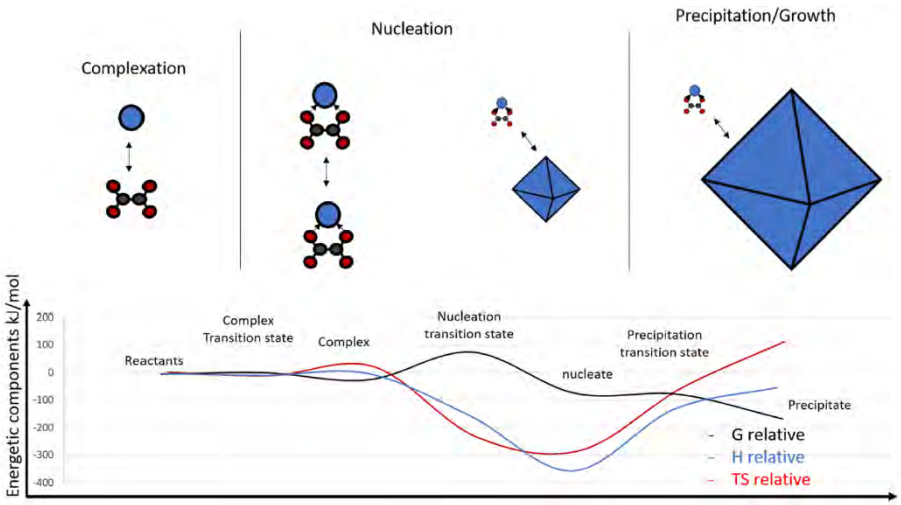

Figure 1: Reaction scheme of calcium oxalate precipitation in water as modelled with density functional theory.

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C40 Ab initio study of the mechano-chemical coupling of Au(221) with chemisorbed oxygen atoms

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Reactivity and /or selectivity of Gold with adsorbed O atoms (Au+O), a catalytically active material[1-3] and many other heterogeneous catalysts can be altered by applying strain to the active layers. Mechano-chemical coupling (ξ) is an essential quantity that can be employed to determine the direction of this alteration. This quantity can be measured using cantilever bending experiments during the potential scans of the cyclic voltammetry or by dynamic electro-chemomechanical analysis (DECMA). Recently, DECMA, combined with cantilever bending experiments, was employed to investigate ξ of oxygen electrosorption on Au.[4] It was revealed that ξ <0 at the initial stage of the experiment while a sign inversion is observed as more time is admitted. Not until this study, the sign inversion has not been rationalised. In this study, using density functional theory (DFT), we report an efficient method to calculate the ξ of gold with adsorbed O atoms by analysis of the surface charge density dependence of the surface stress. For an application, Au(221) with chemisorbed O atoms along its straight step was employed as our model (see Figure 1). Our calculations reveal that the sign of the ξ could be rationalised with the applied method and model. The value of the ξ lies within the range portrays by the experiment, and the sign can be used to rationalise the stability of O atoms on Au(221).

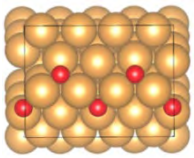

Figure 1: Top view of Au(221) surface with adsorbed O atoms. The O atoms formed a chain structure and are indicated in red, while the Au atoms are shown in gold color.

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C41 Predicting transport properties of ionic liquids using molecular dynamics simulations including explicit polarization

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Ionic liquids (ILs) are broadly defined as polyatomic organic or inorganic salts that are liquid at ambient temperature and consist purely of ions. Due to favourable properties such as low vapour pressure and high thermal and electrochemical stability, this class of liquids has received extensive attention as alternatives to carbonate-based electrolytes in next-generation batteries. To develop this application, further exploration is needed to understand the properties of IL electrolytes. In this presentation, the results of classical molecular dynamics (MD) simulations of ILs consisting of imidazolium and pyrrolidinium cations with symmetric and asymmetric fluorinated sulfonylimide anions (Fig. 1), will be presented. It has now become well-established that the electrostatic interaction is overestimated in the condensed phase when fixed-charge force fields (FFs) that are based on gas phase parameterization are used in IL simulations, leading to dynamics that are far too slow and consequently an overestimation of transport properties such as diffusion, viscosity and conductivity. This can be remedied by the introduction of explicit polarization; in this work, this was achieved using the Drude model that includes electronic polarization by introducing an auxiliary particle that is attached to each polarizable atom via a harmonic spring. In addition to commenting on the accuracy of the polarizable FF against experimental properties, we will provide some insight into the relationship between structure and fluidity. We will also share some strategies that can be used to improve the reliability of calculated transport properties from MD simulation, for these highly viscous liquids.

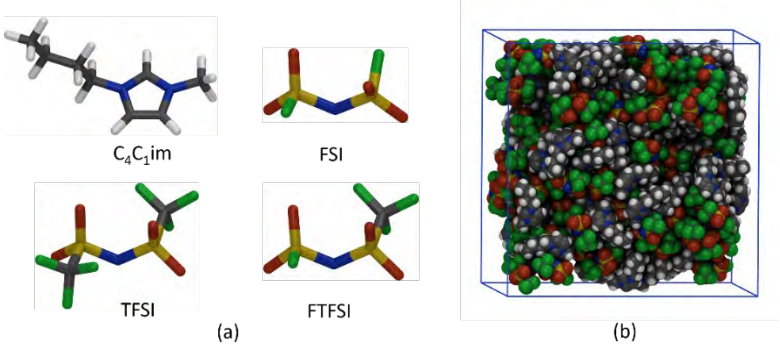

Figure 1: (a) The ionic liquid cation 1-butyl-3-methylimidazolium (C_4C_1im) and anions bis(fluorosulfonylimide) (FSI), bis(trifluoromethanesulfonyl) imide (TFSI), and (fluorosulfonyl)(trifluoromethanesulfonyl) imide (FTFSI), and (b) an MD simulation cell for [C_4C_1im][TFSI]

Acknowledgements
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C42 Computational study probing sustainable applications of greenhouse gases

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Climate change is a current environmental concern that is linked to the production and release of greenhouse gases. The amounts of these gases present in the atmosphere can be reduced by adsorbing them onto a variety of materials that are being developed for the purpose[1]. A previous study[2] has shown that a porous Cd-metallocycle (Figure 1) can adsorb CO_2 as well as C_2H_2. Although sorption and guest capture are interesting properties themselves, the question then arises as to how to treat the pollutants after capture. This study computationally investigates the viability of photocatalytic reactions between greenhouse gases adsorbed into the metallocycle below. To reduce the environmental impact we also consider the use of more abundant and less toxic metal centres while still retaining the functionality or even improving thereupon. DFT studies using the PBE function as implemented in CASTEP are used to determine favourable geometries of the host materials, while the adsorption properties are investigated using the Sorption Tools in Materials Studio. Finally, the reaction between CO_2 and C_2H_2 within the porous framework is modelled using Orca and Gaussian software to determine the requirements for them to undergo a photocatalytic reaction to form useful products.

Figure 1: The Cd-metallocycle used as a starting point for this investigation.

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C57 Direct Observation of Rapid Water Uptake and Release from a Vapochromic Single Crystal

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Establishing the conditions that govern hydration and dehydration is a critical aspect of materials science. The ongoing quest for versatile new materials for desiccation[1] and atmospheric water harvesting[2] requires fine tuning of several application-specific parameters, important among which are a balance between water release kinetics and the energetic cost of thermal regeneration.[3] **T1** is vapochromic crystal that readily and reversibly adsorbs atmospheric water into its 1 nm wide channels. The stark water-induced colour change (from yellow to red), triggered at 55% relative humidity (RH), allowed us to visually monitor the hydration state of the self-indicating crystals. Using a combination of theoretical methods, gravimetry and single-crystal X-ray diffraction (SCXRD), we have elucidated the mechanism of water uptake and release in **T1**, rationalised its vapochromic response and measured the sorption kinetics at varying RH. Additionally, the kinetics of dehydration (0% RH, 1 atm) were measured by optical microscopy (Figure 1) revealing Arrhenius behaviour. This work offers new insight into the processes that influence dehydration and establishes a new method for measuring the desorption kinetics of a channel hydrate. These results show that non- complementarity between the hydrophilic sites of a channel and a crystallographically commensurate water structure does not preclude the ready uptake of water, but that it may dramatically enhance the kinetics of dehydration. Using crystal engineering, complementary combinations of channel geometry and pore functionality can be incorporated into new materials, allowing for the target kinetics of water uptake and release to be systematically tuned.

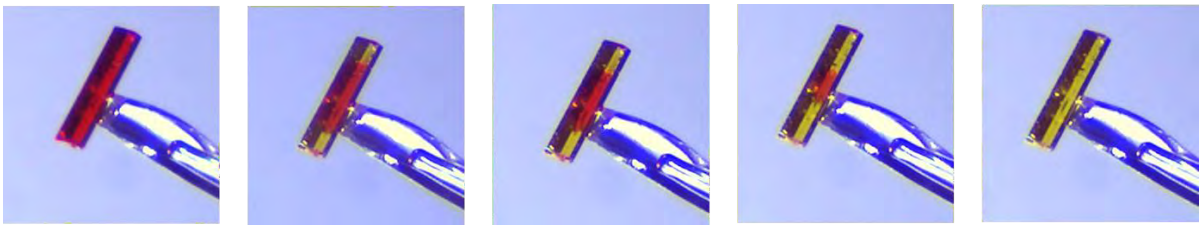

Figure 1: Time-lapse photomicrographs of an initially hydrous crystal of **T1** releasing included water at 0% RH.

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C58 Comparing the cooperative feedback reaction dynamics of imino-dithiin charge-transfer co-crystal compounds

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Reactions that occur in the solid-state can lead to products in higher yields, as well as allow regio- and stereospecific products due to the crystal environment.[1] Similar to polymorphs which can have very different properties such as melting points and colours, solid-state reactions within a crystal lead to changes in molecular structure, thus affecting the physical and chemical properties of the material.[2] Solid-state reactions can occur in crystals by undergoing topochemical and topotactic reactions, where the final product crystal structure is influenced by the arrangement of molecules in the starting crystal.[3] A single-crystal-to-single-crystal (SCSC) reaction occurs when a solid-state reaction in a crystal begins and ends as a single crystal, and is usually regarded as a topochemical reaction, while topotactic reactions lead to crystal integrity being lost.[3] Such reactions can be induced by conditions such as light and heat.[4,5] Charge-transfer (CT) co-crystals containing symmetrical imino-dithiins as the acceptors (A) and 9-bromoanthracene as the donor (D) underwent a solid-state Diels-Alder reaction, when heated, to produce a cycloadduct product (P). In these crystals, the A and D molecules are stacked in either a 1:1 or 2:1 ratio of D:A. These stacking patterns gave rise to products arranged as …P-P-P-P… or …D-P-D-P… respectively and the reaction proceeded topotactically. The mechanisms and solid-state products of these crystals can be contrasted with prior work done on a CT co-crystal of *bis-N*-cyclobutyliminodithiin-9-bromoanthracene with a 2:1 ratio of D:A which led to a …D-D-P-P-D-D… arrangement.[5]

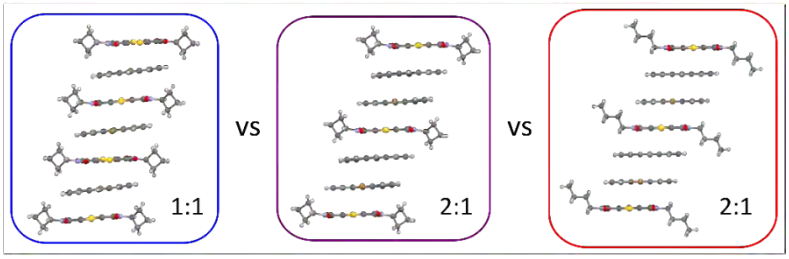

Figure 1

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C59 Limits of lab XRD and average crystal structure concepts – when studying energy and related functional materials

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In the century since the dawn of modern crystallography, single crystal and powder diffraction techniques have become standard go to methods in many fields, providing critical structural details that have great understanding and developments in these scientific disciplines. Instrument and computational advances have also made these characterization techniques and methodologies far more accessible to non-specialists, and it is now quite likely that many regular users are not familiar with the fundamentals and limiting assumptions on which these techniques are based. Sadly, this has resulted in instances where poor measurements and/or poor interpretation and analyses of the measurements, effectively undermine much of the remainder of the research presented. Most concerning are instances where the presented XRD traces do not support the structure model on which the paper rests. Much of this results from the inherent limitations of routine laboratory XRD measurements. In this presentation I will highlight some of these pitfalls with examples from literature as well as our own research into structure property relations in energy materials. On the flip side, synchrotron X-ray diffraction and scattering techniques make it possible to investigate the local structure and distribution of defects in great detail, thus affording a more nuanced understanding of structure and how this relates to bulk properties of materials. I will introduce this using simultaneous near and far field measurements done on the XPDF beamline at the NSLS-II on a number of our own samples. Focusing on studies in which we investigate the effect doping or atomic substitution has on the ionic conductivity of selected energy materials. I will also describe how the local structural defects introduced the doping that can be investigated via XAS methods, and how when coupled with the PDF results and suitable atomistic modelling, this can provide a more comprehensive understanding of the real structure of the materials under investigation.


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K2 Heterogeneous photoredox catalysis using polymer brush-functionalized glass beads

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Photoredox catalysis is a potent approach that provides user-friendly access to small and macromolecular molecules under mild reaction conditions and visible light irradiation. However, the photocatalysts' inherent visible light absorption means that catalyst residuals in final polymers product can lead to discoloration and their excited states can promote material degradation. Further, the high cost of common transition metal photocatalysts and complex synthetic pathways for organic alternatives makes their use on large scales economically prohibitive. This presentation introduces a heterogeneous photoredox catalysis platform based on fully organic fluorescein functionalized polymers grafted to micron-scale glass beads. These photocatalytic beads were used for light-mediated heterogeneous photoredox RAFT polymerizations. Monomer conversion is possible in excess of 90%, and the polymerization can be switched on and off by triggering the light source. Furthermore, good oxygen tolerance is possible. Recyclability of the heterogeneous catalyst was verified through sequential re-use of the particles for multiple polymerizations. Finally, through the covalent tether, final products are obtained free of catalyst impurities.

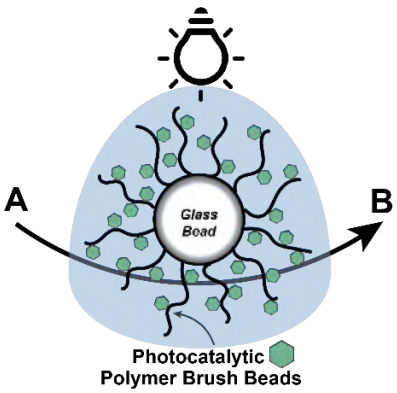

Figure 1: Photocatalytic polymer brushes tethered to glass supports for heterogeneous photocatalysis

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K6 Stereocontrolled polymers with defined monomer sequence – how far are we from the structural precision of biomacromolecules?

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In recent years, advances in polymer chemistry have enabled the synthesis of polymers with similar precision as observed in nature, represented by proteins and nucleic acids.[1] Sequence control is emerging as an invaluable tool for the fine regulation of polymer properties. In general, the functionalities of biological macromolecules derive from their secondary structure. Therefore, one of the directions to induce complex functions into abiotic macromolecules lies in the control of the folding of sequence-defined polymers. Here, I discuss the possibilities of using sequence and stereochemistry as tools to tune the functionalities of abiotic oligourethanes.[2] I present how structural properties of oligourethanes and folding can be examined and tuned by the sequence of monomers and stereocenters. I also discuss the recent advancements in the synthesis methods towards high-molar mas polyurethanes that could display features of "artificial proteins".[3]

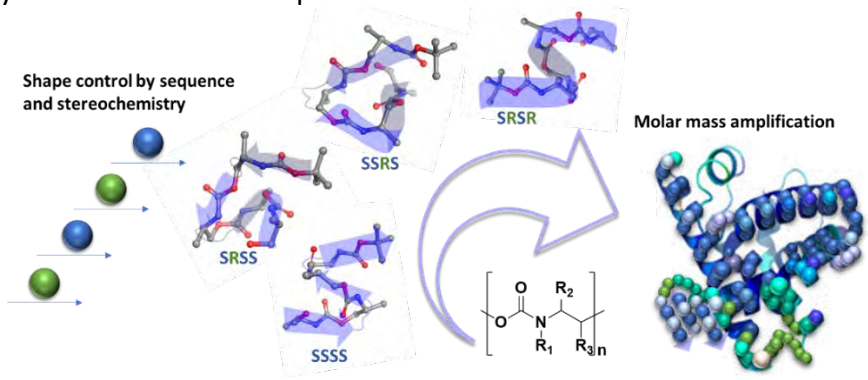

Figure 1: Sequence and stereocontrol are tools for tuning oligourethane conformations. Amplification of molar mass could lead to macromolecules with "artificial protein" features

Acknowledgements

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I2 Poly(*N*-vinylpyrrolidone) in advanced polymers for biomedical applications

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Pyrrolidone functional polymers have many important applications due to the properties of the pyrrolidone ring, i.e. biocompatibility, amphiphilicity, hydrogen bonding and metal coordination capacity. The preeminent example is poly(*N*-vinylpyrrolidone) (PVP), a water soluble and biocompatible polymer with many biomedical and industrial uses. PVP is readily synthesized via radical polymerization methods, including reversible deactivation radical polymerization (RDRP) techniques, producing well-defined polymers with predictable end-groups and molar masses, and low molar mass dispersity. Herein we will show our recent work on PVP based polymer materials.[1-3] The polymers are easily end-functionalised and incorporated into block copolymers for subsequent self-assembly into nanostructured materials for biomedical applications.

Acknowledgements
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I5 Novel terpolymers for detergent-free isolation of GPCRs

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G-protein-coupled receptors (GPCRs) are a family of membrane proteins (MPs) considered significant diagnostic and therapeutic targets due to their role in an array of physiological processes, including basic senses, e.g., vision, taste, smell as well as endocrine, neurological, reproductive, and cardiovascular functions.[1] Thus, it is imperative to gain an understanding of the structural diversity and functional significance of GPCRs. Compared to soluble proteins, MP research has been hampered by difficulties in effective extraction from the cell membrane. Previously, MP extraction was largely reliant on detergent-based methods, which commonly disrupted the functional and structural integrity of the MPs.[2] More recently, amphiphilic polymers have significantly improved MP extraction through the stabilization of MPs and annular phospholipids in nano-scale discs, enabling investigation in a native-like environment while retaining original physiological properties.[3] During this research, controlled polymerization allowed for the rational design of polymers with premeditated structural and chemical characteristics intended for MP isolation. Series of terpolymers emanating from the same alternating base copolymer, poly(styrene-*alt*-maleic anhydride) (SMAnh), with well-defined chemical characteristics and narrow molecular weight distributions, were synthesized. The water-soluble SMAnh derivative, poly(styrene-*alt*-maleic acid), was too hydrophilic for effective membrane solubilization. This problem was overcome by altering the polymer's hydrophobic/hydrophilic balance through partial modification of available comonomer moieties that resulted in incrementally increased hydrophobic character throughout the series. Different modifications produced three different terpolymer series with distinct charge variations, i.e., anionic, cationic, and zwitterionic derivatives. The resulting terpolymers will form part of a solubilizing polymer "toolkit". Variations in overall amphiphilicity and charge will allow for the systematic investigation of the polymers' abilities to solubilize phospholipid membranes and their effect on the isolated GPCRs. Ultimately providing new insights into GPCR structure and molecular mechanisms.

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C4 Side reactions in the copolymerization of maleic anhydride and n-butyl vinyl ether

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Chain transfer (CT) to polymer, either via intra and intermolecular processes, Figure 1, resulting in mid chain radical (MCR) formation is a well-known phenomenon in radical polymerization, particularly in the synthesis of polyacrylates.[1] Herein, we report some of the findings from our investigation into the occurrence of CT side reactions during the conventional radical copolymerization of maleic anhydride (MAnh) with *n*-butyl vinyl ether (*n*-BVE). Evidence of CT followed by *β*-scission was obtained via ^{1}H NMR spectroscopy which showed the appearance of vinylic signals in the region 5.7 ppm to 6.9 ppm. Further investigations via APT NMR experiments, examining the carbon multiplicities, also revealed branch formation. This work, for the first time, presents evidence of unsaturated product formation due to H abstraction and subsequent *β*-scission during radical copolymerization of MAnh and *n*-BVE.

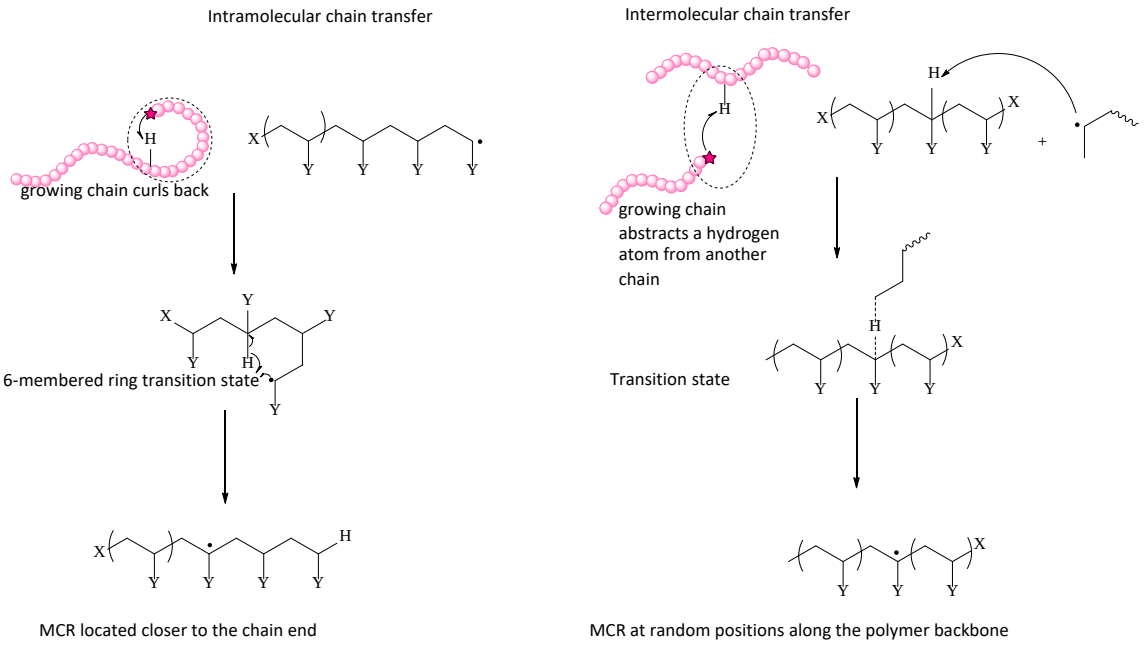

Figure 1: An illustration of intermolecular and intramolecular chain transfer.

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C5 PLA-*b*-SMA as an amphiphilic diblock copolymer for encapsulation of lipophilic cargo

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The physicochemical properties of active pharmaceutical ingredients (APIs) can limit the efficiency of drugs administered in bulk forms such as injectable formulations, capsules, suspensions, tablets, etc[1]. These limitations include solubility, bioavailability and a reduction in the APIs half-life and selectivity[1]. The therapeutic efficiency of APIs can be improved via encapsulation in polymeric nanoparticles (PNPs) constituting block copolymers with a hydrophobic and hydrophilic block. Encapsulation of lipophilic components in the PNP core is facilitated by the hydrophobic block, while the hydrophilic block forms the corona, helping to stabilize PNPs against aggregation in solution. Poly(lactic acid)-*b*-poly(styrene-*alt*-maleic acid) (PLA-*b*-SMA) is an attractive block copolymer for the synthesis of PNPs, as the hydrophobic PLA block is biodegradable and the hydrophilic SMA block provides opportunity for post-polymerisation functionalisation and helps prevent PNP aggregation. This study investigates the synthesis of the novel PLA-*b*-SMA block copolymer via sequential ring-opening polymerisation (ROP) and reversible addition-fragmentation chain transfer (RAFT) polymerisation. Monodisperse PLA-*b*-SMA nanospheres and nanocapsules are synthesized via nanoprecipitation and range in hydrodynamic diameter between 60 and 220 nm. Fluorescent PLA-*b*-SMA nanocapsules (NCs) are produced via encapsulation of the lipophilic dye DiI, and the uptake of these NCs assessed in a preliminary cell uptake study.

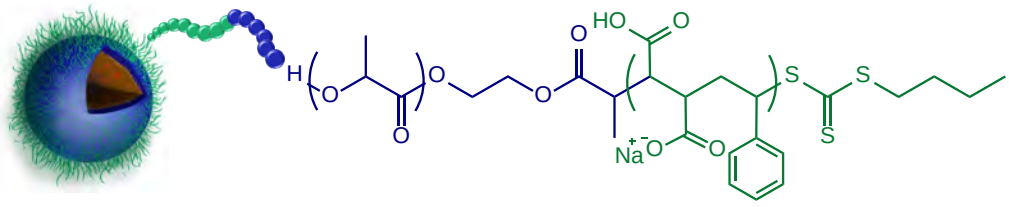

Figure 1: Fluorescent PLA-*b*-SMA NC (DiI in red, PLA in blue and SMA in green).

Acknowledgements
Authors gratefully acknowledge funding through BRICS multilateral project (South African National Research Foundation and National Council for Scientific and Technological Development). B.K. acknowledges support by South African Research Chair Initiative.

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C6 3D wound healing scaffolds made of nanoparticles embedded within biodegradable polymers

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Recent developments in advanced technology and nanotechnology have proven to be promising solutions in therapeutics, including wound care management[1,2]. Advanced wound dressings in the form of hydrocolloids, films, foams, hydrogels and scaffolds have been designed and used to solve health problems underlying wound care treatments[3,4]. These wound dressings are designed to meet ideal requirements which include the ability to maintain a balanced moist environment, adherence to the wound, allow the exchange of oxygen and prevent bacterial infection. The requirements ensure the acceleration of wound healing and reduce the complications that are associated with the process. Herein we showecase a facile way of fabricating bioactive nanomaterials to design an advanced wound dressing in the form of 3D scaffolds. The scaffolds were made of nanocomposites containing biocompatible and biodegradable polymers decorated with metal nanoparticles with fast and broad spectrum of antimicrobial activity against gram-(positive and negative) bacteria. Additionally, these NPs are also non-toxic to mammalian cells at regulated concentrations rendering them suitable for wound healing applications. The antimicrobial activity of the scaffolds was tested against *E. coli* and *S. aureus* bacterial strains. Cell proliferation and the cytotoxicity were evaluated using human dermal fibroblasts (HDF) cells. The scaffolds were found to posses exelent antimicrobial activity against E. Coli and S. aureus with minimal toxicity towards HDF cell. eminently, the scaffolds were found to improve the rate of proliferation of HDF cells.

Acknowledgements
The authors would like to acknowledge Wits University school of chemistry and Mintek AMD for providing resources and research facilities together with NRF for funding.

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C16 Heat stabilising flexible PVC with layered double hydroxide derivatives

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The layered double hydroxide ($[Mg_{0.667}\ Al_{0.333}\ (OH)_2](CO_3)_{\ 0.167}\cdot mH_2O$) (LDH) has found application as a heat stabiliser for PVC. Derivatives of this compound were synthesised using a hydrothermal method. Emulsion grade PVC was plasticised with 100 phr diisononyl phthalate and stabilised with 30 phr of the LDH filler additives. Heat stabilities were determined at 200 °C. The dynamic heat stability tests were performed on the plastisols using the torque rheometer method. Static heat stability was evaluated on the fused compounds. It was evaluated from discoloration profiles of strips exposed for various lengths of time to heat in a Metrastat oven. The time dependence of hydrogen chloride evolution was followed with a Metrohm Thermomat instrument. The conventional LDH provided the best dynamic heat stability. However, partial replacement of the magnesium with copper significantly delayed the release of volatile HCl. If instead the replacement was done using zinc, better colour retention was achieved.

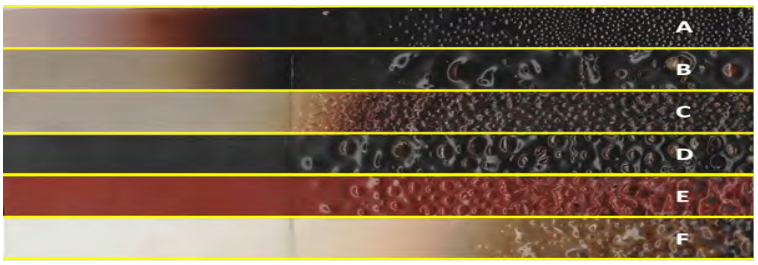

Figure 1: Metrastat sample appearances. (A) Neat PVC; (B) MgAl-LDH; (C) CaAl-LDH; (D) MgCuAl-LDH; (E) MgFeAL-LDH, and (F) MgZnAl-LDH

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C17 Controlling the Multiporous Structure of Carbon Nanofibers Using Solution Aging Properties of PAN/PBA Block Copolymers

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Both the physical properties and morphology of carbon nanofibers produced by electrospinning the precursor material(s) are dependent on various factors. Some of these factors are discussed in terms of electrospinning and phase segregation between the block of copolymers. A series of polyacrylonitrile-*block*-poly(butyl acrylate) (PAN-b-PBA) with varying block lengths, were prepared by controlled radical polymerization techniques (ATRP). These BCPs were then used as precursors to carbon nanofibers. Previous studies on nanostructured carbons using the well-reported PAN-b-PBA as carbon precursors and the PBA block serving as a sacrificial porogen have demonstrated how the size of the mesopores can be controlled by the length of the sacrificial block and the effect of phase segregation between the blocks has in mesopore connectivity[1,2]. In this study, multiporous (micro-, meso-, nanoporous) carbon nanofibers/films were synthesized by manipulating the block lengths and processing parameters of these materials, most notably that of the solution ageing of the electrospinning solution (Figure 1).

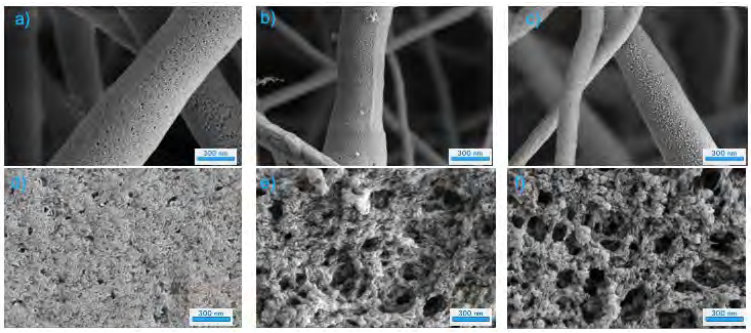

Figure 1: SEM images of PAN-b-PBA electrospun nanofibers (a-c) and films (d-f) at varying ageing times.

Acknowledgements
This research was financially supported by the Nation Research Foundation (NRF) of South Africa. The Stellenbosch University, Department of Chemistry and Polymer Sciences. We thank Ms. Elsa Malherbe for assistance with the NMR analysis (Stellenbosch University) and Central Analytical Facilities (CAF) – Stellenbosch University for assistance with the SEM analysis.

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C18 Responsivity analysis of smart nanoparticles using asymmetric flow field-flow fractionation

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Future research on advanced nanoparticles (NPs) for drug delivery systems (DDs) will be based on smart, biodegradable polymers. Amphiphilic block copolymers can self-assemble into NPs, particularly polymersomes, which are versatile carriers due to the possibility to tune their properties at the molecular level and their potential to encapsulate a range of bioactive compounds.[1] Smart polymersomes, in particular, exhibit a variety of characteristics that are essential for DDs as they are stimuli-responsive and can modify their structure or morphology in response to a given stimulus. A detailed understanding of self-assembly, responsive behaviour, and the influence of structural features are required to develop smart polymersomes for a given application. Asymmetric flow field-flow fractionation (AF4) is an emerging technology for the detailed separation and characterization of complex, fragile self-assemblies.[2] Firstly, this study aimed to better understand the responsiveness of tertiary amine methacrylate-based block copolymers (BCPs) in solution and how their composition influences their behaviour. By increasing the hydrophobicity of the BCP, the phase transition is pushed to lower pH (at constant temperature) or lower temperatures (at constant pH). Secondly, the responsiveness of tertiary amine methacrylate-based polymersomes was also investigated by studying how their characteristics change when subjected to different temperature and pH conditions. AF4 was used to collect essential information regarding the molar mass, shape and conformation properties when in different pH conditions. Coupled with a refractive index, static and dynamic light scattering detector it was possible to characterize the polymersomes' responsivity. It was observed that certain polymersomes demonstrated responsiveness at low temperatures and exhibited a shape-shifting behaviour. This response is reversible and is suppressed through cross-linking. This phenomenon is hypothesized to be caused by surface plasticization of the insoluble structure-directing block.

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K12 Induced protein degradation as a strategy for the development of new medicines

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In recent years, design of small molecules to induce protein degradation has become a powerful strategy for the discovery and development of new therapeutics for the treatment of human cancers and other human diseases. This approach offers a number of major advantages over traditional small molecule inhibitors. In this lecture, I will present our recent research in the discovery and development of small-molecule degraders, including targeting those traditional undruggable targets. I will discuss both promises and challenges in the development of small-molecule degraders as a new class of therapeutics.

K13 Using Chemical Glycobiology to Decipher the Glyco-Code of Human Diseases

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The plasma membranes of all cells are densely populated with glycoproteins and glycolipids expressing a myriad of complex glycans (oligosaccharides and polysaccharides) covalently linked to amino acids and to lipids. The functions of these glycans are being identified through chemical, biochemical, genetic, and physiologic approaches. Many human diseases involve alterations in these glycans or specific recognition of glycans by pathogens that have glycan-binding proteins to facilitate their adhesion. We use a variety of chemical and biological approaches to synthesize glycans and glycoconjugates to aid in deciphering the structures of glycans, the glycoproteins that carry them, and the functions of these glycans in diseases. The glycans on human white blood cells, e.g. neutrophils, express a key glycoprotein PSGL-1 that is required for interactions with endothelial and platelet-expressed P-selectin, which is expressed only under hypoxic or inflammatory conditions. Antibodies to P-selectin are now used as a novel immunotherapeutic drug (Adakveo®, marketed by Novartis) to reduce vaso-occlusive pain crises in patients with sickle cell disease (SCD). We have synthesized many novel glycosulfopeptides (GSPs), which are peptides with specific sulfated tyrosine residues adjacent to glycosylation amino acids; these represent the recognition determinant for P-selectin. Such novel GSPs can effectively block P-selectin engagement, suggesting a new type of therapeutic drug as an anti-inflammatory and a potential replacement for heparin without the risk of bleeding complications. Interestingly, these types of GSPs represent the functional domains of many G-protein-coupled receptors (GPCRs), and we have now shown, using a GSP-type glycan array approach, that modifications of sulfated tyrosine and glycosylation regulates binding by chemokines to such receptors. In other studies we have explored the glyco-code of the human and murine brain, as many disorders of glycosylation in humans are associated with cognitive defects. Our results demonstrate vast differences in the glycoproteomes of the brain in terms of N-glycosylated versus O-glycosylated glycoproteins, and alterations are seen in patients with Alzheimer's and in animals engineered to express mutations of glycosylation seen in patients with Schizophrenia (missense mutation (A391T) in *SLC39A8*, encoding a manganese-transporter). Thus, chemical glycobiology is a challenging but rewarding area of investigation and with many druggable pathways.

K14 The establishment of commercial manufacturing of API's in Africa

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We like to share with you the work we are doing at Chemical Process Technologies Pharma (CPT Pharma) on the establishment of commercial manufacturing of Active Pharmaceutical Ingredients (API) in the region. The commercial manufacturing of API's requires sustainable, cost competitive and high yielding synthesis processes to be able to compete with the current suppliers from over the world. This necessitates the development of new and more competitive manufacturing processes based on improved synthesis routes, lower raw material costs as well as improved isolation techniques. We will illustrate the translation of basic bench scale synthesis processes to commercial manufacturing processes with some examples. The development of a competitive commercial route starts with the selection of a preferred synthesis route based on the costing of raw materials and process conditions to identify the key cost drivers. This is followed by the adaption of the synthesis procedure to commercial and GMP acceptable reaction conditions. The improvements typically also require the selection of the isolation procedures of the intermediates and the final product to be practical under industrial conditions. The latter may impact the synthesis procedure, in particular the selection of solvents, to allow for effective isolation (e.g., crystallization). The development of GMP manufacturing processes also requires the development of analytical procedures that allow for the in-process monitoring of intermediates and final product as well as the understanding of impurities throughout the process. CPT Pharma cannot do this work alone and collaborates with universities and institutions such as Medicines-4-All and US Pharmacopeia to broaden the capacity and skills base. These organizations assist with the selection of improved competitive synthetic routes as well as the training of process chemists, analysts, and regulatory personnel.

K15 Creation of a nucleic acids' toolbox for the treatment and investigation of the etiology of disease

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Nucleic acids, as monomers, oligomers and conjugates, in their natural and modified states, have proven to be valuable tools in the expansion of our understanding of disease etiology and in the treatment of viral and bacterial infections as well as cancer. We have used the tools of synthetic organic chemistry, photochemistry and automated nucleic acid synthesis to create tools which have successfully been used in the identification of oxidative damage processes in DNA and RNA precipitated by oxidative stress. Recognizing the utility and versatility of our synthetic approaches to the creation of modified nucleic acids, we have expanded our work to the discovery of novel nucleosides and nucleotides as potential therapeutics. Oxidative stress, which results from the overproduction of free radicals such as reactive oxygen species (ROS), has been associated with many degenerative diseases, with evidence that RNA damage is significantly elevated in these disorders. Many post-transcriptional modifications of RNA have been reported to play an essential role in snRNA biogenesis and pre-mRNA splicing. Evidence suggest that the human spliceosomal machinery may be stabilized by the extensive modifications in U2 snRNA. In humans, this oligomer contains methylated guanosines, 2'*O*-methylated sugars, and pseudouridine. We have developed several tools to explore the role of post-transcriptional modifications in the modulation of oxidative damage in U2 snRNA. These tools act as radical precursors which allow for the site specific generation of radicals at predetermined locations in RNA monomers. Results from these studies indicate that the presence of pseudouridine in RNA has a significant impact on oxidative damage processes.Utilizing the same synthetic design as that utilized for radical precursors, we have synthesized 2'-C-acetyl and 2'-C-(1-hydroxyethyl) uridine as potential antivirals targeting RNA dependent RNA polymerase (RdRp). Drug design efforts were driven by the structure and conserved nature of the HCV NS5B RdRp active site across viral species, as compared to other HCV viral proteins, along with the fact that there is no human NS5B. Based on the successful utilization of Sofosbuvir, which is a 2'-modified uridine that acts as an NS5B inhibitor, we have pursued these compounds as non-obligate chain terminators of the synthesis of the viral RNA by the NS5B enzyme.

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K16 Developing electrochemical immunosensors for poverty-related diseases: tuberculosis, cholera, and cervical cancers

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Tuberculosis, cholera, and cervical cancers have long been recognized as some of the most health challenges in resource-limited countries in Sub-Saharan Africa, Asia, and Latin America. The proper management of these diseases requires affordable and reliable diagnostic techniques that allow for rapid detection. The traditional diagnostic methods such as the gold standard culture method, enzyme-linked immunosorbent assay (ELISA), radioimmunoassay, and polymerase chain reaction (PCR) are bulky, expensive, time-consuming for sample preparation and analysis, and require highly skilled personnel to operate them. On the other hand, electrochemical methods are not only sensitive, reliable, low-cost, and simple, but can easily be miniaturized for hand-held diagnostic devices for many diseases, which can be easily operated by non-experts. This presentation will describe some of our recent research activities[1-3] geared toward the development of future point-of-care, electrochemical-based immunosensors for efficient screening (i.e., for asymptomatic people) and diagnostic tests (i.e., for symptomatic people) of tuberculosis, Cholera, and cervical cancer.

Acknowledgements
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K26 Bruker NMR spectroscopy

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In 2019, Bruker announced the world's first 1.2 GHz NMR instrument (Figure 1) at the EUROISMAR conference and in 2022, at the Experimental Nuclear Magnetic Resonance Conference, Bruker demonstrated a unique single-story Ascend Evo 1.0 GHz NMR magnet (Figure 1), operating at 4.2 Kelvin, with a significantly reduced footprint, weight, and ceiling height requirement, together with a threefold reduction in liquid helium consumption. By investing more than any other company in R&D, constantly focusing on innovations using a fundamental approach to develop cutting edge applications, Bruker has been leading the world for over 60 years in MR software, coil, magnet, and electronic technology. This talk will focus on the latest developments in NMR technology and applications, together with helpful tips and tricks in getting the most out of data acquisition and processing.

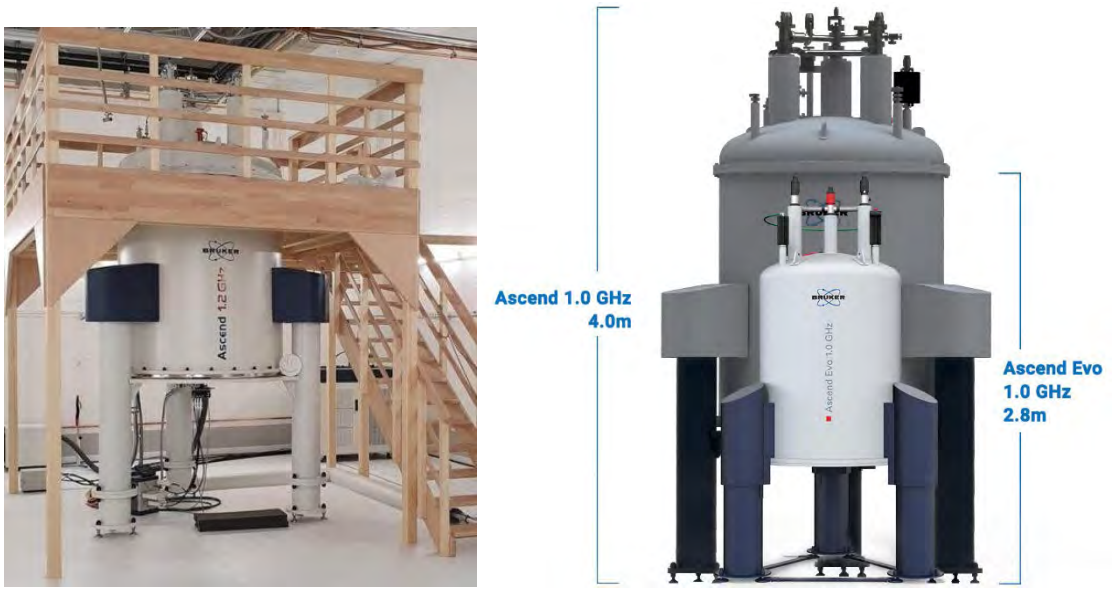

Figure 1: Latest NMR instruments operating at 1.2 GHz (left) and the new, unique compact Ascend Evo 1.0 GHz NMR magnet (right)

I14 Tips for young chemists to thrive in academia – based on my experience

Tricia Naicker[1]

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Taking place in the Young Chemists' session, my talk aims to inspire emerging academics and students; to provide advice and guidance for their future careers. I will share my experiences on how I have succeeded against the many challenges to find a rewarding career in the field of chemistry. Amongst other aspects, I will highlight the value of teamwork in one's career and the importance of mentors as essential components for personal, academic and professional achievement.

I23 Using NMR spectroscopy to facilitate the development of vaccines against Group B Streptococcus disease

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Group B Streptococcus (*Streptococcus agalactiae*) is a Gram-positive β-haemolytic bacterium and the leading cause of neonatal mortality by sepsis, pneumonia and meningitis particularly in LMICs (low and middle income countries).[1] To date, ten serotypes of Group B Streptococcus (GBS) have been recognized, each identified and differentiated by their sialic acid-containing capsular polysaccharide. Capsular polysaccharides are the virulence factor for bacterial pathogens and the target for vaccine development as polysaccharide-protein conjugates against the main GBS serotypes causing invasive disease (Ia, Ib, II, III, IV, and V).[2] Nuclear magnetic resonance (NMR) spectroscopy has been established as an extremely useful and robust method for tracking the manufacturing process of carbohydrate vaccines from polysaccharide antigen through to conjugate vaccines.[3] The 1D proton profiles of most of the GBS antigens have been published[4], however, the identity spectra were recorded at 298 K, resulting in broad peaks and overlap of the large water signal with diagnostic GBS signals in the anomeric region (see ^{1}H NMR overlay for GBS III). This study attempts to aid the development of GBS glycoconjugate vaccines by fully characterizing the repeating units of the six most common GBS serotypes by NMR recorded at 600 MHz and at a higher temperature of 343 K to create a database of reference GBS NMR spectra and chemical shift assignments. Full NMR characterization of the repeating unit of each serotype was achieved by use of an array of 1D and 2D NMR experiments. The 1D and 2D NMR spectra presented can be used for identity, integrity and purity testing of polysaccharide batches. They allow identification of each serotype by its diagnostic anomeric peaks, can confirm the structural integrity of the polysaccharide both before and after conjugation, and can detect the presence of impurities such as residuals. This constitutes a powerful reference resource for use in the development, preparation and control testing of future GBS glycoconjugate vaccines.

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C46 High throughput screening of South African medicinal plants in the search for novel anti-viral agents against SARS-CoV-2

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The COVID-19 pandemic continues to spread, prolonging international global health fears despite the numerous efforts undertaken to curb it. Although many anti-SARS-CoV-2 vaccines are available, the emergence of new variants remains a real threat which could undermine their efficacy[1]. Together with vaccines, complementary tools, like antiviral agents are required to combat the disease. Encouragingly, natural products have routinely served as a source of inspiration for drug development[2]. The current study aims at exploring South Africa's rich biodiversity in search of novel anti-viral agents against the SARS-CoV-2 virus. A dual approach was followed in which both medicinal plants and natural product compounds were selected and screened in in-vitro bioassays for any potential antiviral activity against the SARS-CoV-2 virus. A high-throughput fractionation technique was used in which twenty medicinal plants were extracted and fractionated using automated liquid handlers for an accelerated screening approach. Encouragingly, from the twenty plant species screened, 3 bioactive compounds were identified as potent SARS-CoV-2 inhibitors in-vitro, these, identified with the use of hyphenated analytical techniques like UPLC--HRMS, HPLC-UV/MS, NMR spectroscopy and X- ray crystallography. Additionally, the extract and active compounds of *Gunnera perpensa* L., a medicinal plant used by a South African traditional health practitioner for SARS-CoV-2 management, exhibited potent antiviral activity against SARS-CoV-2 in both enzyme and phenotypic screens. The identified active compounds, punicalagin and punicalin, presented remarkable activity (IC50 < 10 nM) in enzyme-based bioassays against the wuhan, beta, delta and omicron variants. Both compounds additionally exhibited activity in phenotypic screens (> 75% plaque reduction at 15 µg/ml) with no cytotoxicity observed. Our data validates the high-throughput fractionation screening methodology used and motivates the continued interrogation of plants in search of anti-SARS-CoV-2 agents.

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C47 Single-crystal to single-crystal dimensionality transformation of metallocycle to coordination polymer

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Dinuclear metallocycles are a type of metal-organic material that consists of two metal centres which are bridged by two exo-bidentate C-shaped ligands to form a discrete cyclic unit.[1,2] Although there are accounts of single-crystal to single-crystal transformation,[3, 4] owing to the mechanical strain during structural changes on the crystal lattice, single crystallinity is readily lost. However, the importance of single-crystal to single-crystal transformation is that it makes the detailed study of structure-property relationships a possibility.[5] A novel dinuclear metallocycle was found to undergo single-crystal to single-crystal transformation from a 0D metallocycle to a 1D coordination polymer. As the interstitial solvent molecules are released from the crystal structure, the ligand rearranges and recoordinates to nearby metal centres. This mechanism is irreversible and the resulting coordination polymer is stable up to 200 °C. This is the first dinuclear metallocycle that undergoes this type of transformation, which could be ascribed to the restrained coordination environment around the metal centre, the interstitial space created by the pendant group of the ligand, and the lack of intermolecular interactions stabilizing the overall structure.

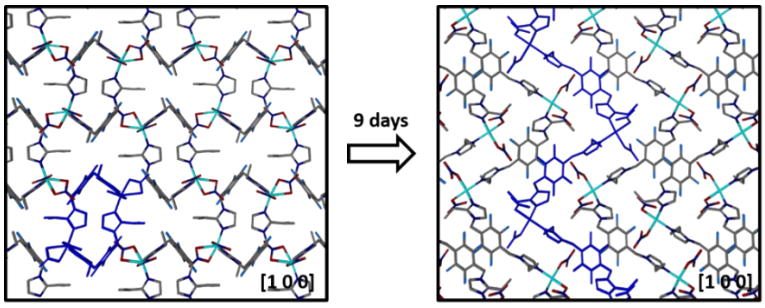

Figure 1: Single-crystal to single-crystal transformation of a metallocycle (left) to a coordination polymer (right).

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C67 Redox-switchable gold catalysis monitored by NMR and EPR spectroscopy

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Au(I) Fischer-type carbene complexes of the form [Au{C(NHR)Ar}Cl] {R = $(CH_2)_2CH_3$, $(CH_2)_2NMe_2$; Ar = o-furyl, p-N,N-dimethylaniline, and ferrocenyl} were synthesized by means of transmetallation from Group 6 transition metal carbene precursors[1] and subsequent modification of the carbene ligand. The complexes were employed as pre-catalysts for the intramolecular cyclisation of N(2-propyn-1-yl)-benzamide. As depicted in Scheme 1 below, a chemical oxidant additive is necessary to activate the Au(I) precatalyst. Many examples of gold-NHC complexes have been applied in these cyclisation reactions,[2–4] however, only one study of the utilization of a gold(I) Fischer carbene complex in the cyclisation of N(2-propyn-1-yl)-benzamide has been reported[5] to date. We herein report a comprehensive study of these catalytic reactions, which involves using NMR spectroscopy to quantify the %conversions and %yields, with EPR spectroscopy employed to identify the paramagnetic Au(II) species generated *in situ*.

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C68 Conformational analysis and potential anticancer activity of [Pt(phen)(L^1-κ*S*)$_2$] studied by single crystal X-ray Diffraction and Variable Temperature ^{1}H and ^{195}Pt NMR Spectroscopy

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The novel mixed-ligand [Pt(phen)(L^1-κ*S*)$_2$] complex was successfully synthesized, in which two N,N-diethyl-N'-1-naphthoylthioureato ligand (L^1)- coordinate in an unusual κ*S*-thio/amido mode. The structure was confirmed by single crystal X-ray diffraction which revealed two solvatomorphs, Form I and Form II. These crystals were obtained from tetrahydrofuran and methanol/water respectively showing interesting variation in the intramolecular π-stacking interactions between the naphthoyl moiety of the acylthioureato ligands and the 1,10-phenanthroline ligand. [Pt(phen)(L^1-κ*S*)$_2$] solvatomorphs exhibit a sandwich and half-sandwich π-stacking arrangements that adopt an anti-conformation above and below the square planar coordination plane. Variable temperature ^{1}H and ^{195}Pt NMR spectroscopy showed that these π-stacking arrangements persist in methanol solution especially at lower temperatures, where significant chemical shift shielding and asymmetry are observed indicating at least 3 conformers at -50 ºC. A preliminary study indicates that this new compound may have potential as a new anticancer agent since it is active against the A549 lung cancer cell-line with an IC_{50} value of 6.43 ± 0.94 µM.

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PA1 Computational modeling of a prototypical photocatalyst: a zeolite encapsulated TiO2-supported Cu5 cluster

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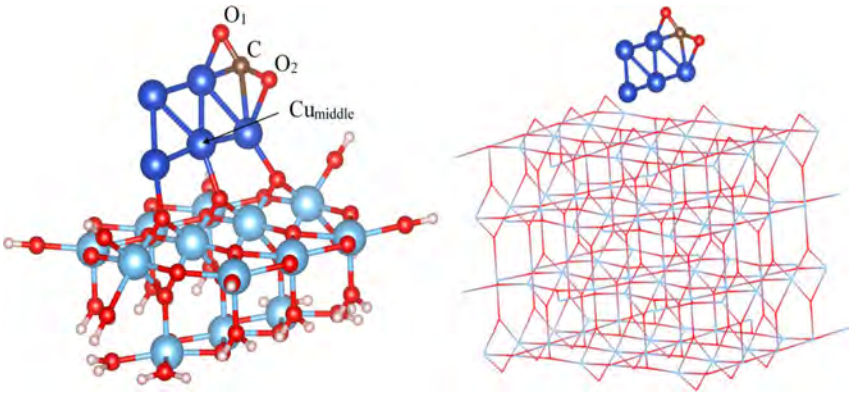
We performed a theoretical study on the modelling of the prototypical photocatalyst composed of titania-supported subnanometer sized copper clusters confined in zeolite cages. Firstly, a hydroxylated titanium dioxide nanoparticle was modelled inside a cage of zeolite Y. Its structure was optimized using DFT. Next, adsorption of a Cu5 cluster on a titania particle confined inside a zeolite was modelled, exploring different geometric orientations of the cluster, and using dispersion-corrected PBE-D3BJ functional in combination with two different basis sets, def2-SVP and def2-TZVPP. The copper cluster (Cu5) can attach to the TiO2 in three different geometries. The most stable geometry was selected to be used in the further study. The study also intends to investigate the CO2 reduction which will take place on the supported Cu5 particles encapsulated inside the zeolite cage. This part of the study will be also done using DFT to elucidate the reaction mechanism, energies of the intermediates and transition states, and the effectiveness of the photocatalyst.



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PA2 Investigation of selected toxic metals accumulation in vegetables grown by irrigation with water from Mokolo River and potential risks to human health

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The increase in environmental pollution has been reported to be one of the greatest threats globally[1]. Lephalale, which is situated in Limpopo Province is the mother of two power stations namely, the Matimba and Medupi power stations. These power stations generate electricity through the burning of coal from Grootegeluk coal mine, which contribute to pollution of the environment. The industrial activities in Lephalale could possibly contaminate vegetables being grown in the area with high levels of potentially toxic elements (PTEs) such as cadmium (Cd), lead (Pb), copper (Cu), mercury (Hg), nickel (Ni) and vanadium (V). The PTEs could accumulate in soil and be transferred to vegetables, which are subsequently transferred to human *via* the food chain [2]. The aim of this study is to investigate the levels of Cd, Pb, Cu, Ni, Hg and V in water and sediments collected from Mokolo River as well as in soil and vegetable samples collected from the farms in the vicinity of Mokolo River using inductively coupled plasma-mass spectrometry (ICP-MS). The methods for quantification of selected PTEs in water, sediments, soil, and vegetables were optimized, and the accuracy of the methods were confirmed using standard reference materials (SRMs) of each sample matrix. The preliminary results revealed high concentrations of selected PTEs in vegetables. The target health quotient (THQ) and hazard index (HI) were used to evaluate possible health risks to humans who consume these vegetables.

Acknowledgements

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PA3 The effect of different reactor geometries on silica-coated iron oxide nanoparticles synthesized in flow

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Magnetic solid-phase extraction (MSPE) has received significant attention as a sample preparation technique for the analysis of a wide variety of compounds due to numerous advantages compared to classical methods. MSPE is a modern, miniaturized, and automatable SPE technique based on the use of magnetic sorbents that exhibit excellent adsorption efficiency and simple separation from the matrix by applying an external magnetic field[1]. Magnetic nanoparticles (MNPs) are a type of magnetic sorbent commonly used for MSPE[2]. MNPs based on iron oxide are well known due to advantages such a simple synthetic process and unique physical properties[3]. Even though surface modification is required to stabilize the MNPs, it enhances its separation and extraction capabilities[4]. Silica is a popular coating material for iron oxide nanoparticles (IONPs) because of its porous structure, size-selective permeability, chemical stability, and biocompatibility. Additionally, it provides the possibility for further functionalisation[5]. Flow techniques for the synthesis of IONPs have been established[6], however due to the prohibitive costs of the equipment, flow techniques are not often implemented in research laboratories with limited resources. The use of open-source hardware and 3D-printed flow components are known to drastically reduce costs[7]. Therefore, a cost-effective, 3D-printed flow system was developed to synthesize silica-coated iron oxide nanoparticles. Two 3D-printed polypropylene devices with different channel geometries (T and coaxial) and diameters (1.0 – 2.0 mm) were investigated for the synthesis of bare IONPs. Furthermore, the devices were modified to include an additional inlet stream for the silica coating process. The synthesized NPs were characterized using transmission electron microscopy (TEM), Fourier transform infrared (FT-IR) spectroscopy, dynamic light scattering (DLS), zeta potential and a vibrating sample magnetometer (VSM).

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PA4 Method Development for the Determination of Multi-Contaminants in Chicken Liver Using Dispersive Liquid-Liquid Microextraction followed by LC-MS/MS

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A simple analytical method is developed for the simultaneous determination of pesticides, sulphonamides, fluoroquinolones, anthelmintic and aflatoxin B1 in chicken liver using dispersive liquid- liquid microextraction method combined with liquid chromatography high resolution mass spectrometry. Liquid phase microextraction is a family of sample preparation techniques, which utilises microliters volumes of organic solvent for the extraction of different samples. The performance of DLLME methods in aqueous samples is outstanding, however, applications in complex matrixes such as solid biological samples and application for multi-contaminants is limited and is still a challenge. In this work the first part was the selection of an appropriate dissolving solvent that enabled the dissolution of the analytes from the biological matrix (chicken livers). The method was adopted from D. Moema, et al[1]. Various parameters that affect extraction efficiency such as the type and volume of extraction solvent, the type and volume of disperser solvent and sample pH were optimised. Under optimised conditions, pH 7 was found to good optimum condition, acetonitrile as a disperser solvent, tetrachloroethane as the extracting solvent were used. The matrix-matched calibration curves showed good linearity in the range 0.05–50.0 µg/kg for aflatoxin B1 and 50- 500 µg kg-1 for pesticides, fluoroquinolone, sulphonamides, anthelmintics with correlation coefficients in excess of 0.9916 – 0.9967. The mean recoveries were in the range of 80.4 – 96.3 %, and the relative standard deviations (RSDs) were in the range of 1.53 –8.98 %.The limit of detection (LOD) and limits of quantifications (LOQ) was 0.02 µg kg-1 and 0.04 µg kg-1 respectively for aflatoxin-B1 and were in the range of 0.011 - 1.197 µg kg-1 and 0.150- 2.579 µg kg-1 and for pesticides, fluoroquinolone, sulphonamides, anthelmintics. The developed method is accurate and rapid and suitable for the simultaneous determination of mixed contaminants in chicken lever. The method was successfully applied to chicken liver samples collected from local supermarkets in Gauteng (South Africa).

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PA5 Development of a novel graphene-based passive air sampler for mercury monitoring

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Mercury poses a significant threat to human health due to its chemical properties and resulting ability to bioaccumulate and persist in the environment. In recognition of this, implementation of the Minamata Convention on mercury has been adopted since 2013, which focusses on the protection of human health and the environment from the effects of mercury globally. South Africa ratified the convention in 2019, thus efforts to monitor mercury within the South African environment have become more imperative to uphold the agreement. Challenges associated with achieving compliance with the convention filter down to the lack of monitoring and source data for mercury as well as the lack of cost-effective alternatives to established methods like active sampling. Current quantification of mercury releases in South Africa thus relies mainly on making use of inventories and emission factors. To fill this gap, more consistent and reliable monitoring data is required which can be supplemented by means of passive sampling for temporally averaged mercury concentrations in air. Herein, the development of a novel graphene-based material, a candidate for mercury sorption, and its subsequent characterization is presented. The sorbent is catalytically grown on a foam structured template through chemical vapor deposition using methane as a carbon source, followed by removal of the template and chemical modification to enhance mercury sorption by the carbonaceous material. These modifications reduce the surface of the material and introduce heteroatoms (specifically sulfur) into the graphene framework. Various sulfur sources were tested including sodium sulfide, thiourea, dimethyl sulfoxide and elemental sulfur. Characterization of the resulting materials was achieved through use of Raman spectroscopy, X-ray photoelectron spectroscopy, energy-dispersive X-ray spectroscopy and thermo-gravimetric analysis. Deployment of the materials as passive air samplers with subsequent analysis by cold vapor atomic absorption spectroscopy, showed sorption of approximately 0.54 ng Hg over a one month sampling period in ambient air. This was achieved within an established 0.0003 ng to 100 ng matrix-matched calibration range (R^2 = 0.9972). This shows promise for the use of this sorbent as a material for sampling airborne mercury.

Acknowledgements
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PA6 digestion Development of greener microwave -assisted hydrogen peroxide sample preparation method for spectrometric determination of REEs in fuel oil samples

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Rare Earth Elements (REEs) are at the center of the Fourth Industrial Revolution (4IR) as they are irreplaceable materials in modern technology[1]. These elements are introduced into fossil fuels (coal, crude-oil and natural gas) by natural processes[2]. Then the crude oil is refined to produce fuel oils (gasoline, diesel, kerosene, just to name the few) mainly used as energy sources[3-5]. Therefore, the study of REEs in fuel oils remains a key as this helps to create awareness on REEs concentration levels for development of proper removal/recovery strategies. In this study, microwave-assisted hydrogen peroxide digestion (MA-HPD) was applied for the mineralisation of selected fuel oils (crude oil, diesel, gasoline, and kerosene) prior to REEs determination using inductively coupled plasma-optical emission spectroscopy (ICP-OES). Two level fractional factorial design (FrFD) and the central composite design (CCD) were used to optimize the most influential parameters of the microwave system. The optimization results showed that efficient performance was exhibited when 150 mg sample mass, 60 minutes digestion time, 5M H_2O_2 concentration and 200 ℃ digestion temperature were used. The optimised MA-HPD displayed excellent accuracy (99-110%), precision (1.7-8.4%) and low method detection limits (0.002-0.542 µg/g). The optimised and validated MA-HPD method was then applied in real fuel oil samples and all the REEs were above 1 µg/g but below 10 µg/g.

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PA7 Absorption of antiretroviral drugs, abacavir, nevirapine, and efavirenz from water using exfoliated graphite: isotherm and kinetic studies

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Antiretroviral drugs are pharmaceutical compounds that are an evolving class of environmental pollutants. Several published studies have proven the presence of antiretroviral drugs in water[1, 2]. Detecting antiretroviral drugs in wastewater effluent samples shows that current wastewater treatment plant technologies do not entirely remove these compounds during treatment. Antiretroviral drugs can adversely affect aquatic life and human health upon unintentional consumption[2]. As a result, exploring and applying a new, improved, and cost-effective method to remove antiretroviral drugs in water is necessary. Graphite-based sorbents can adsorb various contaminants such as halogenated organic dyes and pharmaceuticals due to their large surface area and delocalized π-π electron system that can create a stable bonding with different contaminants[3]. In this work, the synthesized and characterized exfoliated graphite was used to absorb antiretroviral drugs from water. The exfoliated graphite characterization using the Fourier Transform Infrared Spectroscopy showed functional groups such as phenolic, alcoholic, and carboxylic between 1000 cm^{-1} and 1700 cm^{-1}. The X-ray diffraction pattern showed the characteristics of a hexagonal phase graphitic structure. The highest antiretroviral drugs removal from the water was achieved with a solution pH of 7, an adsorbent mass of 60 mg, and an adsorption time of 30 minutes. The kinetic model and adsorption isotherm studies showed that the experimental data fit well in pseudo-second-order kinetics and is well explained by Freundlich's adsorption isotherm. The maximum adsorption capacity of the exfoliated graphite for antiretroviral drugs ranges between 1.660-197.0, 1.660-232.5, and 1.650-237.7 mg/g for abacavir, nevirapine, and efavirenz, respectively.

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PA8 Quality analysis of borehole water from selected villages at Ga-Matlala area in the Limpopo province of South Africa

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More than 60 % of people in South Africa still rely on underground water for their household usage and many of them are living in rural areas[2]. Groundwater, accessed mainly through boreholes, continues to be in use although the quality thereof in many areas has not been established. Quality analysis of water involve among others, the determination of chemical and physical properties[1]. Thus, the aim of the study was to investigate the quality of borehole water in selected villages at Ga-Matlala area in the Limpopo Province of South Africa. Twenty-four borehole water samples were collected from selected villages in the Ga-Matlala area during the rainy and dry seasons of the year in 2021. Samples were analysed for determination of calcium and fluoride concentrations, total hardness and other properties using qualitative and quantitative analytical methods. The water samples were found to record fluoride concentrations ranging from 1.94 - 3.22 mg/L during rainy season, while lower concentrations were recorded in the dry season. Calcium concentrations ranged from 252.54 - 448.82 mg/L in the rainy season and 183.43 – 385.37 mg/L in the dry season, while for total hardness concentrations in the range 146.10 - 1136.49 mg/L and 177 - 1003 mg/L were recorded in the rainy and dry season, respectively. The results indicated that fluoride levels, calcium contents and hardness properties of borehole water from Ga-Matlala were mostly exceeding the maximum permissible levels set by WHO, posing a health risk to the communities.

Acknowledgements

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PA9 Sulphur added chlorinated carbon nanomaterials and their use as electrocatalysts for oxygen reduction reaction

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Herein, we report on the synthesis of chlorinated sulfur doped carbon nanotubes (SClCNTs) with excellent oxygen reduction reaction activity using the pyrolysis and thermal annealing methods. The morphology and quality of the materials produced was dependent on the synthesis method used. The pyrolysis of acetylene over a solution mixture of dichlorobenzene and thiophene resulted in the poisoning of the catalyst and inhibition of CNT growth. Thermal annealing of ClCNTs in the presence of sulfur at various temperatures (800 ^{o}C – 1000 ^{o}C) resulted in production of SClCNTs with increased density. Materials produced at 800 °C revealed formation of metal particles clustered at the surface of the SClCNTs, whilst those produced at 900 and 1000 °C appeared much cleaner, with evidence of well-defined cube-shaped metal nanoparticles decorated at their surface. XRD revealed the identity of the metal nanoparticles as pyrite (FeS_2). The formation of this pyrite nanoparticles was thought to have been initiated by the presence of defects on the walls of the ClCNTs because of chlorine incorporation. The formation of FeS_2 nanoparticles was explained using the vapor-liquid-solid process. The incorporation of sulfur into the lattice of ClCNTs was confirmed by Raman spectra analysis, which increased/enhanced the formation of defected nanocarbon. The ORR activity was greatly enhanced after addition of sulfur into the ClCNTs, the greatest enhancement was observed for materials produced at 900 and 1000 °C, annealing temperature.

PA10 Development of a modified QuEChERS molecularly imprinted solid phase extraction (QuEChERS-MISPE) technique for the analysis of DDT and its derivatives in farmed leafy vegetables

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Analysis of trace organic pollutants requires development of sensitive analytical techniques[1]. In the current study, a molecularly imprinted polymer (MIP) was synthesized using the target analytes as templates for creating cavities with an affinity for DDT and its derivatives. Batch adsorption and kinetic studies confirmed that the binding of the DDTs to the polymer exhibited the Langmuir isotherm and the pseudo-second order model which was an indication that adsorption followed a monolayer formation through chemisorption. The maximum adsorption capacity for the MIP was achieved in 120 min for both DDD (166.8 ng/g) and DDE (171.4 ng/g) while that for DDT (164.5 ng/g) was achieved at 230 min (Fig 1). The MIP was finally combined with the modified QuEChERS method to form a new hybrid technique, the QuEChERS-MISPE as an alternative method for analysis of pesticides. Toluene was used as the MIP eluting solvent while acetonitrile was the optimum acceptor solvent for QuEChERS. The hybrid technique was coupled with gas chromatography-mass spectrometry and applied in the analysis of DDTs in leafy vegetables from the Limpopo province.

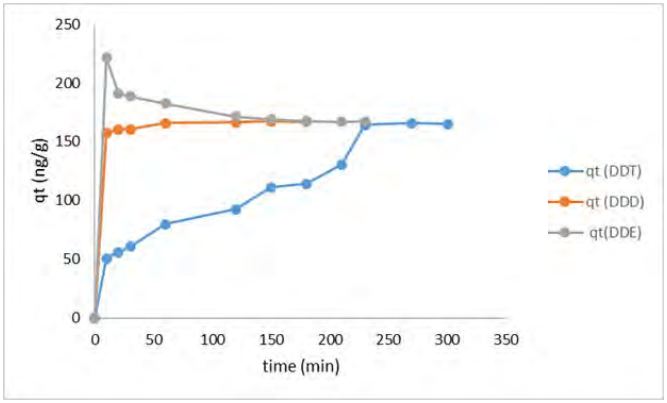

Figure1: Maximum adsorption capacity (n = 3)

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PA11 Elemental bioaccumulation and nutritional profiling of an indigenous South African mushroom species, Termitomyces umkowaani

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Wild-growing mushrooms of the genus *Termitomyces* are commonly consumed in certain parts of Africa and Asia. This genus grows only in symbiotic association with termites, and it is dependent on the latter for organic matter. The current study looked at *T. umkowaani's* nutritional profile (proteins, lipids, carbohydrates, and ash) and elemental bioaccumulation (the gradual uptake of a substance by a living organism). Samples were collected from six different locations (Cathedral peak, Nquthu, Seven Oaks, Umgeni valley-1, Umgeni valley-2 and uMshwathi). Analytical procedures (Kjeldahl, Soxhlet, and Incineration) were used to determine the nutritional profile of *T. umkowaani*. The results show that the stems and caps of *T. umkowaani* contain 17.6 % and 26.3 % protein, 3.2 % and 4.5 % lipids, 1.9 % and 4.8 % ash, 77.3 % and 64.6 % carbohydrates, respectively. Elemental analysis was carried out in both the mushroom and soil samples using Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES). The results shows that *T. umkowaani* bioaccumulate K, Mg, Na, and Zn in both the stems and caps. Potassium was found to be the most abundant element in this species from all sites with concentrations ranging from 3901 to 23508 mg kg^{-1}.

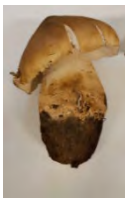

Figure 1: Physical structure of the mushroom, *Termitomyces umkowaani*

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PA12 Enhanced Visible light driven photoelectrocatalytic degradation of paracetamol at a ternary z-scheme Bi_2WO_6-CNP-TiO_2 NTA electrode

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In this study, a ternary z-scheme heterojunction of Bi_2WO_6 with carbon nanoparticles and TiO_2 nanotube arrays was used to remove paracetamol from water by photoelectrocatalysis. The materials and z-scheme electrode were characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), energy dispersive X-ray spectroscopy (EDS), EDS mapping, ultraviolet diffuse reflection spectroscopy (UV-DRS), photocurrent measurement, electrochemical impedance spectroscopy (EIS), uv-vis spectroscopy and total organic carbon measurement (TOC). The effects of parameters such as current density and pH were studied. At optimal conditions the electrode was applied for photoelectrocatalytic degradation of paracetamol, which gave a degradation efficiency of 84% within 180 min. The total organic carbon removal percentage obtained when using this electrode was 72%. Scavenger studies revealed that the holes played a crucial role during the photoelectrocatalytic degradation of paracetamol. The electrode showed high stability and reusability therefore suggesting that the z-scheme Bi_2WO_6-CNP-TiO_2 nanotube arrays electrode is an efficient photoanode for the degradation of pharmaceuticals in wastewater.[1-4]

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PA13 Synthesis and application of a multi-template molecularly imprinted polymer for the effective removal of pesticides in water: seasonal variation effect

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Pesticides are chemicals which are used to kill pests, rodents and weeds in order to protect crops and thus increase crop yields. However, they can end up in river water via leaching and surface run-off where they can have an adverse effect on humans and environment hence they need to be monitored[1,2]. A selective multi-template molecularly imprinted polymer (MIP) for simazine, atrazine, ametryn, propazine and terbuthylazine was synthesised and applied as a solid-phase extraction sorbent for selective extraction of these pesticides. The MIP was synthesized using 2-vinylpyridine as a functional monomer, ethylene glycol dimethacrylate as a crosslinker, 1, 1'-azobis (cyclohexanecarbonitrile) as an initiator, acetonitrile as a porogenic solvent and the five above mentioned pesticides as templates. The non-imprinted polymer (NIP) was synthesised similarly to the MIP with the exclusion of the templates. Characterization with thermogravimetric analysis indicated that the polymers were thermally stable up to 250 °C. FTIR results showed that the functional groups present in both polymers were similar and the MIP had a C-N stretch arising from the template. BET results showed the specific surface area of 362 m^2/g and pore volume of 1.16 cm^3/ g for MIP which were higher than NIP indicating high adsorption capability for MIP. SEM results showed that the synthesized polymers were amorphous. Solid-phase extraction cartridges packed with MIP (MIPSE) were used for the extraction of pesticides from water and eluted with methanol prior the quantitative analysis using liquid chromatography with photo diode array detector. The analytical method gave detection limits of 0.0133 to 0.0660 µg L^{-1} and quantification limits were 0.054 to 0.200 µg L^{-1}. The percentage recoveries obtained were between 89 – 107 %. The concentration of pesticides in the river water samples ranged from 0.08 – 6.1 µg/L. Overall, the analytical method for the analysis of pesticides in river samples proved to be quick, affordable, accurate, precise, sensitive, and selective.

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PA14 Multivariate optimization of norfloxacin monitoring in environmental water samples

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Antibiotics are emerging organic contaminants in environmental water samples. Their presence is of concern because of their ability to induce antibacterial resistance. Thus, there is a need to develop innovative, efficient, and green analytical methods to detect antibiotics such as norfloxacin in environmental water samples. A central composite design based on a passive sampling device composed of polymer inclusion membranes was applied to optimize the effect of pH, source solution concentration and receiver solution concentration on the preconcentration of norfloxacin in surface waters. The optimised parameters were found to be pH 8.5, 0.70 M NaCl for the receiver solution and 70 ppb for the source solution. The polymer inclusion membrane method gave detection and quantification limits ranging from 5 ppb to 300 ppm. Spiked river water samples resulted in recoveries ranging from 20 to 94% depending on the water matrix. Upon application, norfloxacin was detected in the studied rivers with a maximum preconcentration factor of 107.

Figure 1: Schematic illustration.

PA15 Phytochemical Screening, Antioxidant, Antimicrobial Activity and Anti-Stroke Properties of *Ricinus Cummunis* Extracts

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Stroke known as tumor disease worldwide[1] caused by death of brain cell affecting cerebral artery[2] medicinal plants Ricinus Cummins proved to treat or cure tumor disease cancer, debates etc. The aim of the current research is to investigate the invitro antistroke, antioxidant, antimicrobial and photochemical screening and evaluate cytotoxicity effect on LDH from PC12 cell line. Plants collected dried room temperature grand to powder extracted with (hexane, dichloromethane and methanol) three mobile phase BEA, CEF, EMW used for qualitative: antioxidant, photochemical, TLC profiling. Quantitative photochemical done by UV spectroscopy six bacteria strain used for antimicrobial quantitative MIC and qualitative bio autography MCFland was used as instruments to measure bacterial concentration. Methanol best extracts 13,09% yield primary (carbohydrates, etc.) and secondary (phenolic, etc.) metabolites showed positive and negative results antioxidant higher in methanol with yellow spots and highest R_f value, BEA:0,93haxane, CEF: 0,95 dichloromethane, EMW0,97mehanol: quantitative:more tannins in methanol:0,148 mg/ml more flavonoids dichloromethane: 3,3mg/ml MIC lower concentration observed at methanol in E.facalis bacillus A.baummanii E.coli staphylococcus Pseudomonas dichloromethane higher concentrations at dichloromethane in E.coli, Psedumonusl bio autography inhibition bend at staphylococcus hexane dichloromethane bacillus hexane. *Ricinus Cummins* methanol extracts can be considered to be antibiotic for bacteria since it can inhibit bacteria and more antioxidant can be recommended for human health linked with stroke further study due to follow.

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PA16 Spatial-Temporal Variations of Neonicotinoids in the Letaba River System (Limpopo Province, South Africa)

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Agricultural activities are one of the main contributors to the growth of the African economy, as it employs approximately 65% and provide important food sources [1]. As the world population increases, the need for good quality food also increases. Neonicotinoids are systematic agricultural insecticides used globally as crop protection mechanism in the agricultural sector. These compounds selectively control pests, by binding strongly to nicotinic acetylcholine receptors in the central nervous system. However, studies evaluating the uptake of neonicotinoids by crops reported that less than 20% of the active ingredient is absorbed by the crop while <2% gets absorbed by dust and 80% gets absorbed by the soil. In addition, climatic conditions and the physicochemical characteristics of neonicotinoids result in their translocation from the original source into water bodies [2]. This implies that they will persist in the environment [3]. These compounds have also been demonstrated to pose adverse health effects on humans and organisms, with their toxicity leading to possible mortality [2]. This study is aimed at evaluating the spatial and temporal distribution of neonicotinoids and their metabolites in water and sediment from the Letaba River Catchment and its tributaries. This water system is situated in the Limpopo Province, South Africa, in the vicinity of intense agricultural activities. Water and sediment samples will be collected seasonally and subjected to solid phase extraction (SPE) and microwave-assisted extraction (MAE), respectively. Targeted and non-target analysis will be carried out by GC-MS and LC-MS [2-3]. Chemometric methods will be used to evaluate the trends in distribution of neonicotinoids and the key contributing factors. This study is important in evaluating the effects of anthropogenic activities on water quality, spatio-temporal variations and advancing the information available on neonicotinoid profiles in South African water bodies.

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PA17 Fabrication of NH2-ZIF-8@Sugarcane Bagasse/Cellulose Acetate Membrane for Desalination of Brackish Water in Nwadzekudzeku Village, Limpopo Province

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Nwadzekudzeku village and other neighbouring villages under the greater Giyani municipality depend only on borehole water for drinking and domestic use. The water has a salty taste reflecting the presence of metal ions like Ca^{2+} and Mg^{2+} which are responsible for water hardness. This study aims to fabricate a cellulose acetate-based nanofiltration composite membranes that will be used to reject high concentrations of cations (Ca^{2+} and Mg^{2+}) and anions (Cl^- and F^-) found in borehole water in Nwadzekudzeku village, Limpopo Province. Furthermore, cellulose will be extracted from sugarcane bagasse to enhance the hydrophilic properties of the cellulose acetate polymeric membrane. Amine functionalized zeolitic imidazolate framework-8 (NH_2-ZIF-8) will be incorporated to enhance the selectivity of the composite membranes toward targeted cations and anions. The NH_2-ZIF-8@sugacane bagasse/cellulose acetate nanocomposite membrane will be synthesized via artificial polymerisation. Microscopic and spectroscopic techniques such as Fourier transform infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), powder X-ray diffraction (PXRD), and Brunauer-Emmett-Teller (BET) will be used to assess the properties of the composite and membranes. The dead-end cell will be used to investigate the performance of the resulting membrane in terms of the permeation flux, salt rejection, and flux recovery ratio. The analysis of cleaned water samples using the fabricated membrane will be done using the Ion chromatography (IC) for anions and flame atomic absorption spectrometry (FAAS) for cations.

PA18 Investigating the Impact of Desalination and Mainland Pollutants on Marine Life and Coastal Ecosystems of South Africa Using a Combination of passive samplers and Ecotoxicology Approaches

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Passive sampling is a technique used to accumulate and collect contaminants present in the environment over time. It has several advantages over traditional sampling which include detection of pollutants present in trace concentrations, accounting for temporal concentration fluctuance and passive sampling devices can be tailored to selectively sample a particular class of compounds. The present study aims to screen the presence and types of polar and non-polar organic pollutants in the mainland and coastal areas of South Africa using passive sampling techniques, and to evaluate the toxicity of the passive sampling extracts using various standardized bioassays. Polar organic chemical integrative (POCIS) and chemcatcher-like passive samplers were used to sample polar and non-polar organic pollutants, respectively. Sampling was carried out at three sites in the Hartbeespoort dam, located in the northwest province of south Africa and at five sites in the Durban harbour, located in the Province of KwaZulu Natal. The passive samplers were deployed for a duration of 10 and 14 days, respectively, after which they were retrieved. To extract the accumulated pollutants, methanol was used for the POCIS, and hexane was used for the chemcatcher-like samplers. To screen for the organic pollutants accumulated in the passive samplers, HPLC-MS and GC-MS were used for the polar and non-polar organic extracts, respectively. The preliminary screening results showed the presence of an array of chemical compounds. These include pharmaceuticals, illicit drugs, personal care products, pesticides, polycyclic aromatic hydrocarbons, and metabolites. Sources of these pollutants were identified as water treatment plants which dispose effluent near the sampling sites, sewer leaks and industrial activities near the sampling sites. The pesticides detected find uses in the agricultural industry, which implies that their sources could be agricultural run-off from the farming activities that take place in the area, especially crop farming which is prevalent in the Northwest province.

PA19 Development of quality control method and standards for the tuberous rhizomes of *Pelargonium sidoides* plant using liquid chromatography

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Natural products, also known as traditional medicine, have been utilised by mankind over many centuries to cure a variety of maladies[1]. Pharmaceutical medicines, which have systems in place for quantifying the active ingredients, this particular aspect of traditional medicine still require much work. *Pelargonium sidoides* is one of those species that has been used for ages to treat a variety of diseases[1,3]. Despite significant phytochemical and pharmacological research on various portions of the plant, there is still no analytical approach that allows for the quantification of chemicals in *Pelargonium* products on the market[2]. The goal of this study was to create a high-performance liquid chromatography (HPLC) separation method for quantifying some of the compounds contained in *Pelargonium sidoides* products. The isolated compounds were used to develop an HPLC separation and quantification method. Then, the developed HPLC separation method was validated. The developed quantitative HPLC separation method showed a good linearity between peak area and compound concentration, with coefficients of determination ranging from 0.9916 to 0.9998. The developed method was found to be accurate, with a percent relative standard deviation (%RSD) value ranging between 1.08 and 4.82.

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PA20 The Spatial Bio-Distribution Studies of Antiretroviral Drugs in Rodent Brain Tissues using Mass Spectrometric Techniques

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The quality of life in people living with human immunodeficiency virus (HIV) is further compromised due to neuropsychological impairments associated with central nervous system HIV cytotoxicity, this despite antiretroviral therapy controlling systemic viral loads. The high prevalence of HIV-associated neurocognitive disorders consequently contributes to morbidity and mortality of the disease; this complication includes those HIV positive patients that are on treatment with satisfactory immunological and virological status. The central nervous system (CNS) contributes to the prevalence of CNS-HIV since it acts as a compartment in which the virus can replicate independently from antiretroviral therapeutic agents (ARTs) in circulation due to the blood brain barrier limiting the entry of these agents into the CNS. Whilst HIV enters the CNS during the early stages of an infection, and damages neurons primarily by stimulating the production of cytokines that are toxic to neurons, leading to excitotoxicity cell death. The neuro-degenerative regions associated with HIV have been identified using Magnetic Resonance Imaging (MRI). Severe atrophy has been observed in the thalamus, globus pallidus, putamen, posterior limb of the internal capsule, corpus callosum, basal forebrain region, and the extreme tissue loss is in neocortex. Herein this research, aims to investigate the plasma/CNS penetration ratios, brain pharmacokinetics and brain spatial bio-distribution patterns of ARTs using Liquid Chromatography tandem mass spectrometry (LC-MS/MS) and Imaging Mass Spectrometry (MSI) techniques. Through animal experiments and mass spectrometric analysis, the CNS penetration of abacavir (ABC), emtricitabine (FTC), lamivudine (3TC), stavudine (d4T), zidovudine (AZT), nevirapine (NVP), rilpivirine (RPV), efavirenz (EFV) and elvitegravir (EVG) were found intense, whilst didanosine (ddI) and tenofovir (TFV) were investigated. With the benefit of mass spectrometric imaging technology; ABC, FTC, 3TC, d4T, AZT, NVP, RPV, EFV and EVG were found to localize at the brain sites that are reported to undergo tissue deficit during an HIV infection, whilst ddI and TFV data was not conclusive due to low concentration levels in the brain. These findings grant health practitioners and scientists an opportunity to offer ART regimens that have the ability to highly penetrate the CNS and halt the progression of neuro-developmental disorders associated with HIV in infected individuals. These findings also warrant further studies in improving and developing ARTs that are able to penetrate through biological membranes, specifically the BBB and localize at target sites known to be damaged during an HIV infection.

Acknowledgement
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PA21 Ionic Liquid Based Extraction Induced by Emulsion Breaking for ICP-OES Determination of Trace Metal Ions in Fuel Oil Samples

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Crude oil is a fossil fuel that occurs because of large quantities of living organisms compressed between the sedimentary rocks of the sea under intense heat and pressure[1]. This petroleum is then refined to produce crude oil derivatives such as gasoline, diesel, kerosene, just to name the few[2]. These fuel oils are energy sources that are vital in our everyday life[1-3]. However, crude oil and its derivatives contain metal ions, which have been proven problematic in different ways which include corrosion of refinery equipment, catalyst poisoning and severe air pollution[4]. Therefore, the study of metal ions in fuel oils remains a key, as this helps to create awareness on metal concentration levels for development of proper control measures. This study describes a cost-effective ionic liquid assisted extraction induced by emulsion breaking (ILA-EIEB) method was developed for preconcentration and extraction of As, Ba, Pb, Sb, Sn, Tb and Te in crude oil, kerosene, diesel and gasoline samples, prior to inductively coupled plasma-optical emission spectroscopy (ICP-OES) analysis. The optimum extraction conditions were achieved through the use of multivariate optimization strategies (two-level full factorial design and Box-Behnken design). The optimum conditions for ILA-EIEB were found to be 0.035% 1- Ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) concentration, 18% nitric acid, 15% Triton X-100 and 0.1 g sample mass. The emulsions were broken by heating at a controlled water bath at 80 ±2 °C for 30 ±4 minutes and an additional centrifugation step (15 minutes at 3 500 rpm) was required for a clear separation of the two phases. The optimum conditions were able to give good accuracy and precision of 80.1-101% and 1.9-4.7%, respectively. This method was also able to report very low MDL for Ba, Na, Ni and V, which were 0.107, 0.013, 3.494 and 0.560 µg/g, respectively. The overall metal concentration range was between 0.072 and 8.610 mg/kg, which were in line with other literature reports. Therefore, this study concludes that fuel oils around Johannesburg contain acceptable concentration levels of the investigated metal ions.

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PA22 Structural properties of nickel sulphide on lignin-derived carbon material and its electrochemical properties for supercapacitors applications

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Supercapacitors, as an important kind of energy storage device, has been of interest due to their high-power density, rapid charge/discharge, and long life[1], but they are disadvantaged by their low energy density, which can be improved by promoting the specific capacitance of electrode materials[2]. Therefore, the improvement of carbon-based materials as electrode materials has little effect hence there is a focus on the development of transitional metal sulphides such as nickel sulphide (NiS) as electrode materials. In this study, lignin was successfully extracted from black liqour using H_2SO_4 and used to prepare activated carbon. NiS nanoparticles and NiS/L-AC (L: Lignin, AC: activated carbon) are prepared by a power-controlled microwave. All materials were characterized by FTIR, TGA, BET, XRD and SEM and their electrochemical properties were assessed by cyclic voltammetry (CV) and galvanostatic charge-discharge measurements. The XRD pattern of NiS/L-AC (Figure 1a) showed sharp intense peaks of highly crystalline NiS NPs and broad peaks which are attributed to the amorphous and graphitic structure of carbon from L-AC. CV curves of NiS NPs, L-AC and NiS/L-AC (Figure 1b) at a scan rate of 100 mV s^{-1} have specific capacitance of 590.9, 197.8 and 701.7 F g^{-1} respectively.

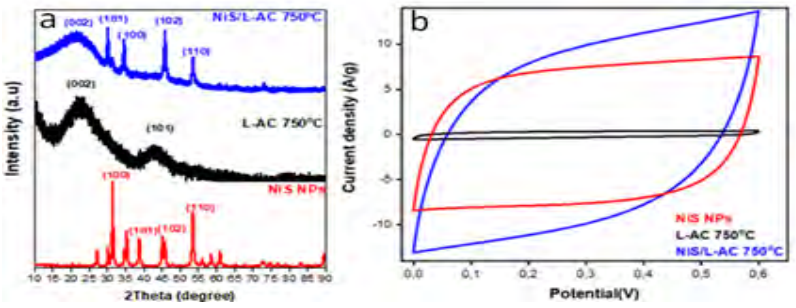

Figure 1: (a) XRD pattern and (b) CV curves of L-AC 750°C, NiS NPs and NiS/AC 750°C

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PA23 Synthesis and visible-light photocatalytic activity of $Fe_3O_4/TiO_2/Ag$ mesostructures

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Mesocrystals have been considered as efficient photocatalysts due to the effective charge transport[1]. They usually exhibit properties differing from single crystal counterparts. In this work, the synthesis of the photocatalyst $Fe_3O_4/TiO_2/Ag$, the characterization and photoactivity activity have been conducted. The synthesis was initiated by preparation of Fe_3O_4 particles using sol-gel method. The Fe_3O_4 particles were then coated with TiO_2, and then Ag nanoparticles were deposited onto of Fe_3O_4/TiO_2 by photo reduction method. The $Fe_3O_4/TiO_2/Ag$ was characterized by UV-visible, XRD, TEM, SEM-EDX methods. Photocatalytic activity of the $Fe_3O_4/TiO_2/Ag$ was carried out using Remazol Brilliant Blue R (RBBR) and the Reactive Blue 4 (RB 4) dye as a target molecule. The degradation of RBBR and RB 4 solution was performed under exposure to visible light under optimum conditions. UV-Vis spectra showed the presence of the visible peaks in the visible region of $Fe_3O_4/TiO_2/Ag$, this result shows that the photocatalyst was responsive to visible light. The target dye solutions can be well photodegraded at a pH of 7 for 120 min with the catalyst loading of 200 mg. The $Fe_3O_4/TiO_2/Ag$ has the highest ability to dye photo-degradation with degradation percentage of 91,12 % and 88,84 % for RBBR and RB 4 dye under visible irradiation, respectively. Pseudo first order kinetics were conducted to determine the rate constant of the different dyes. The rate constant was evaluated to be 0,0293 min^{-1} and 0.0178 min^{-1} for RBBR and RB 4 dye respectively.

Acknowledgements
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PA24 Solid state gelation of manganese sulphide with layered alginate-gelation beads for the direct degradation of complex micro-pollutants in water matrices

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The presence of micro-pollutants in water matrices has been a topic of interest in environmental studies. This is because of their potential effects on humans and natural ecosystem as a result of their chronic and acute toxicity. Additionally, their persistent nature, phenomena such as bioaccumulation or synergetic toxicity should is possible. For this reason, different methodologies (such as membrane processes, advanced oxidation processes and adsorption) have been used for the removal of these pollutants from waster systems. Among the abovementioned technologies, adsorption combined with advanced oxidation processes, deserves major attention. Therefore, this project aims at combining the adsorption nature of hydrogels and catalytic properties of manganese sulphide for removal of of micro-pollutants in complex water matrices this will be achieved by synthesizing alginate gelation beads coated with manganese sulfide. The characterization of the synthesized hydrogel beads will be carried out using Fourier-transform infrared spectroscopy (FTIR), Energy-dispersive X-ray spectroscopy (EDS), Brunauer–Emmett–Teller (BET), X-ray diffraction (XRD), Transmission electron microscopes (TEM), and Scanning electron microscope (SEM). The anticipated outcome of this study is to successfully synthesize an employable absorbent, rehabilitate contaminated water, and try to achieve maximum degradation of various PPCPs in water matrices.

PA25 Comprehensive metabolite profiling of *Viscum combreticola* Engl. through the UHPLC-q-TOF-MS and molecular networking approach

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A metabolomics profiling approach based on mass spectrometry is a powerful tool for fast and cost-effective chemical screening of natural products from plants.[1] However, the identification of compounds from the massive amount of LC-MS/MS data is still an enormous challenge without any prior knowledge.[2] *Viscum* is one of the well-known medicinal plants in various countries[3] and there is no doubt that the healing properties of these plants are due to their phytochemical richness. However, the phytochemical composition of African mistletoes is still scarce to date. Therefore, in this study, the UHPLC-q-TOF-MS profiling approach and classical molecular networking were used to investigate the phytochemical diversity of *Viscum combreticola* Engl. sampled from two different host plants. To gain insights into the substructural diversity of compounds in the *Viscum combreticola* Engl. samples from different hosts, co-occurring fragments or neutral losses called Mass2Motifs were extracted from the data set using MS2LDA. Computational tools employed in this study revealed that *Viscum combreticola* Engl. is a very phytochemically rich plant containing various compound classes, including, phenolic acids, flavonoids, triterpenes and fatty acids. A total of 123 secondary metabolites were putatively identified, where the majority of them were polyphenols. This heterogeneous profile of biochemical compounds might contribute to a wide variety of pharmacological activities of this plant.

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PA26 Synthetic ilmenite ($FeTiO_3$) nanoparticles as heterogeneous electro-Fenton catalyst for the degradation of tetracycline in wastewater

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Explorations into the potential application of dual metallic iron oxides, ($FeXO_3$), [where X is a transition metal] as heterogeneous electro-Fenton (HEF) catalysts have been of interest due to their enhanced catalytic activity. Due to their recalcitrant nature, pharmaceutical organic pollutants require robust advanced oxidation processes for their complete mineralization [1]. We thus present the synthesis and application of ilmenite ($FeTiO_3$) nanoparticles as catalyst for HEF degradation of tetracycline (a pharmaceutical pollutant) in water. $FeTiO_3$ nanoparticles are robust HEF catalyst due to the envisaged co-catalysis effect of the Ti hetero atom [2]. The ilmenite nanoparticles were characterised with scanning electron microscope, X-ray diffraction and Fourier transform IR prior to its immobilisation on a graphite felt (GF) cathode for HEF reactions. The effects of pH and catalyst loading on the HEF process were investigated. The extent of degradation was monitored with UV/Vis spectroscopy and total organic carbon (TOC) measurements. The HEF system was robust over a wide pH range. Tetracycline in synthetic and real wastewater matrices were degraded producing 61% and 40% TOC removal in 2 h respectively. The comparative studies for the catalytic efficiencies of ilmenite (Ti doped iron oxide) and commonly used HEF iron oxide catalysts, like magnetite, hematite and goethite showed that synthetic ilmenite is an effective HEF catalyst for the degradation of organic pollutants in water. A slight Ti co-catalysis effect was observed in ilmenite nanoparticles based on the comparative HEF degradation results catalysed by pristine iron oxide (hematite – Fe_2O_3) and ilmenite (iron titanium oxide) [3]. Our results show that ilmenite can be re-used up to 6 cycles without loss of activity and therefore it is an effective HEF catalyst for wastewater treatment.

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PA27 Extraction of rutin from *Moringa oleifera* leaves by pipette-tip micro-solid phase extraction using activated carbon nanospheres as sorbents

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Conventional methods of extraction have proven to make use of large amounts of reagents and solvents which generate large amount of waste and have long analysis times. This has led to the development of micro-extraction techniques that make use of a small volume of the extracting phase relative to the volume of the sample and thus implying high enrichment factors. Pipette tip micro solid phase extraction (PT-µSPE) is a new type of miniaturized solid phase extraction (SPE) that is simple, potable and a rapid sample pre-treatment method for proteins, peptides and drugs[1-2]. In this technique, a microscale amount of a sorbent is packed inside a pipette tip with the aim of reducing volume of solvents and samples. The choice of extraction sorbent in the PT-µSPE is important for the sample pre-treatment process and to achieve maximum extraction capacity of the target analyte[3-4]. Sorbents play a crucial role in sample pretreatment and enhance selectivity and specificity toward target analytes[5]. In this study, a PT-µSPE for the extraction of rutin was developed, with activated carbon nanospheres (CNSs) used as the sorbent. The activated carbon nanospheres were characterized using scanning electron microscopy (SEM), thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), and fourier transform infrared spectroscopy (FTIR) analysis. The results of this study showed the PT-µSPE was effective in the extraction of rutin at pH 2 with a standard concentration of 2 µg/mL. The results also revealed that the optimum mass of CNSs was 2 mg and 500 µL loading volume gave maximum recovery of rutin. It was also observed that propan-2-ol was the best elution solvent with 15 aspirating/dispensing cycles. These optimized parameters were applied in the extraction of rutin from *M. oleifera* leaves, and high enrichment factors were obtained. From these results, it can be noted that PT-µSPE is as efficient as any other modern extraction analytical technique with a distinct advantage of the use of sample sorbents on small samples.

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PA28 Comparison of ultra-sonication and microwave extraction followed by filtration or solid phase extraction clean-up for PAH determination from sediment and sludge: ecological risk assessment

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This study aimed at evaluating the concentrations, origin and ecological risk of polycyclic aromatic hydrocarbons (PAHs), a group of environmentally toxic and persistent chemicals in sediment and sludge samples[1]. This is a requirement by the South African government (The Department of Water and Sanitation) which has set national norms and standards for the assessment of waste for landfill disposal through the National Environmental Management: Waste Act, 2008 (NEMWA) license (Act No. 59 of 2008)[2]. The PAHs were determined using optimised ultrasonic extraction (UE) and microwave assisted extraction (MAE) methods, followed by filtration or filtration then clean-up with solid phase extraction (SPE). These results obtained indicated that both methods can be used for the extraction of PAHs with relative accuracy and sensitivity, shown by the recoveries which were determined to be 93.7% - 121% for UE-SPE and 79.7% – 122% for MAE-SPE. The LOD and LOQ were 0.0337 µg/kg - 1.21 µg/kg and 0.0800 µg/kg - 3.54 µg/kg for MAE, and 0.0192 µg/kg - 0.215 µg/kg & 0.0491 µg/kg - 0.642 µg/kg for UE respectively. However, higher concentrations were obtained with SPE cleaned samples (95.96 – 926.0 µg/kg) compared to filtered (F) samples (21.61 – 380.6 µg/kg), with pyrene showing dominance over all other PAHs. Although the concentrations obtained were high for these PAHs, they were still within the total acceptable concentration levels of 5.0 x 10^4 µg/kg as prescribed by the NENWA standards for sludge[2] and 3000 µg/kg for sediments accept for DahA in all sampling site accept for 14a. The type of clean-up method had strong influence on the concentrations obtained using both the optimised methods for the determination of PAHs in sediment and sludge samples. Our findings proved that the PAHs were a result of pyrolytic sources and all the investigated sampling sites were determined to be highly contaminated ([PAH] >1000 µg/kg) with TEQ and MEQ of DahA suggesting carcinogenic and mutagenic risk.

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PA29 Optimization and validation of ultrasonic assisted derivatization of naphthenic acids via central composite design for two-dimensional gas chromatography/ high resolution time of flight mass spectrometry analysis

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Naphthenic acids are petrochemically derived carboxylic acid mixtures, like other crude oil components, they vary greatly in size and structural conformation, generally they have a molecular weight of 200-700 g/mol and a structure defined by the isomer $C_nH_{2n+Z}O_2$. Where ***n*** denotes the carbon number, while the ***Z*** is a negative integer referring to the hydrogen deficiency due to ring formation. Because of their corrosive nature, which can damage oil distillation infrastructure, these chemicals must be monitored by the oil industry. The toxicity of oil sands process impacted water (OSPW), a by-product of oil sands extraction activities in Canada's oil sands, has been linked mostly to NAs[1-3]. The chromatographic separation of NAs mixtures into its components is quite challenging. In this study, we report the optimization and validation of ultrasonic assisted derivatization of naphthenic acids via central composite design with various derivatization reagents, namely pentafluorobenzyl bromide (PFBBr) and BF3/MeOH. The factors for derivatization signal yield optimization were molar ratio, temperature, time and sonic power. It was found that the pentafluorobenzyl derivatives have a characteristic fragment ion at *m/z* 181, that is indicative of the carboxylic and non-carboxylic acid components within mixtures. The hexane and methanol fractions of various crude and refined oil fractions were obtained using open column chromatography. When the NA oil extracts were spiked with 11 separate NA standards and detected in the methanol fraction, the efficacy of PFBBr and BF3/MeOH was validated.

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PA30 Investigation of sugars in honey for authentication and detection of adulterants using selected analytical techniques

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Over the last decades, food safety and authenticity have been a growing area of research due to the globalization of trade in food products and extensive growth in technology[1]. There has been an increasing interest in research relating to the authentication of honey as it is one of the most adulterated products. This study aims to address the issue of honey adulteration in South Africa by developing analytical techniques for the detection of sugar adulterants in honey products. Honey adulteration processes include adulterating with starch and mixing pure honey with low-grade honey and/or sugar syrups such as beet sugar syrup, inverted sugar syrup, agave syrup, inverted sugar syrup, and golden syrup. Different adulterants were investigated in the study by inspecting physicochemical parameters such as water content, ash content, pH, acidity, Lugol test, and Lund reaction. To achieve this study, crystals from the samples were removed and the aqueous solution of honey was obtained, the Lugol reagent and tannic acid were used for the Lugol and Lund test. In addition to the physicochemical parameters study, different techniques such as nuclear magnetic resonance (NMR) proton and carbon 13, and Fourier transform infrared (FT-IR) spectroscopy were used for the detection/investigation of different sugars (fructose, glucose, sucrose, and maltose) and possible added ingredients in honey. The obtained results showed that artificial honey does not contain albuminoids. Pure honey does not contain starch and the pH of pure honey decreased from 4.43 to 3.10 in the presence of inverted sugar syrup. The FT-IR spectra of adulterated honey showed a peak at 2361.4 cm^{-1} which is not present in commercial honey, NMR showed signals of different sugars present in honey. The reliability of the developed methods was confirmed by the analysis of sugar standards.

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PA31 Gold-dendrimer nanocomposite based electrochemical sensor for Dopamine

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Dopamine (DA) is a neurotransmitter that has important functions in the neurological, hormonal, and renal systems[1-3]. This study presents the development of an electrochemical sensor for DA by electrodepositing poly(propylene imine) (PPI) dendrimer and gold nanoparticles (AuNPs) onto a glassy carbon electrode (GCE). Electrochemical characterisation of the sensor was carried out by cyclic voltammetry and electrochemical impedance spectroscopy in ferri/ferrocyanide electrolyte. The nanocomposite electrode (GCE-PPI-AuNPs) showed improved electroactive surface area and electrochemical response over bare GCE. The sensor recorded a detection limit of 0.16 µM over a concentration range of 0.1 µM to 125 µM. The sensor was applied for DA detection in human serum samples and in the presence of interfering substances such as ascorbic acid and epinephrine.

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PA32 Perovskite in photoelectrocatalytic water treatment: $BiFeO_3$/GNPs nanoparticles photoanode for removal of Ciprofloxacin in water

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Towards the application of perovskite in photoelectrocatalytic oxidation of organic pollutants in water, bismuth ferrite ($BiFeO_3$) was prepared by facile hydrothermal method[1] and composited with graphite nanoparticles (GNPs) to form $BiFeO_3$/GNPs composite. The materials and photoanodes were characterised with XRD, FESEM, TEM and UV-DRS. Furthermore, the photoanodes were photoelectrochemically characterized for photocurrent response and charge transfer resistance. Results confirmed enhancement in the visible light absorbance, photocurrent density and charge transfer resistance over $BiFeO_3$ owing to the excellent electrical conductivity of graphite nanoparticle. The photoelectrocatalytic performance of $BiFeO_3$, GNPs and $BiFeO_3$/GNPs photoanodes were studied through the degradation of ciprofloxacin in aqueous solution. Degradation percentages of 48%, 50% and 78% were recorded for $BiFeO_3$, GNPs and $BiFeO_3$/GNPs after 4 h respectively [2]. In addition, the total organic carbon (TOC) removal analysis showed 30%, 38% and 56% for $BiFeO_3$, GNPs and $BiFeO_3$/GNPs respectively [1,3]. Degradation pattern, product studies and scavenger studies data, showed that the degradation of ciprofloxacin was activated by the hydroxyl and hole radicals, and it followed a direct oxidation of piperazine ring with other intermediate degradation products. This study showed the beneficial effect of doping $BiFeO_3$ with graphite nanoparticles and the synergy of electrochemical oxidation and photocatalysis in photoelectrocatalytic process performance.

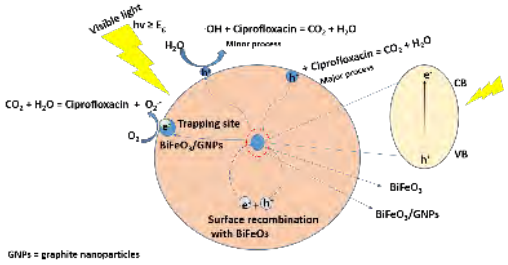

Figure 1: Schematic diagram of the proposed mechanism of PEC for BiFeO3 and BiFeO3/GNPs composite

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PA33 Comparison of analytical methods to characterize natural organic matter in water

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When treating water for drinking purposes, it is crucial to factor in the composition of natural organic matter (NOM) in the source water. NOM is responsible for the yellow-brown colour of water, it can incur an unpleasant taste or odour to water and contributes to bacterial regrowth and corrosion in water distribution networks[1]. Additionally, NOM in water may react with disinfectants to produce potential carcinogenic disinfection by-products[2]. Combining conventional and advanced analytical techniques may provide a robust tool for efficient NOM characterization, thereby guiding drinking water treatment. This study explores the use of a portable, cost-effective instrument (UV254Go!, Photonic Measurements, UK) that can be taken to the field and used to perform surrogate measurements of water samples, including dissolved organic carbon (DOC) and ultraviolet (UV) absorbance at 254 nm, to measure NOM concentration. The instrument results are compared to results obtained using conventional laboratory-based instruments. Source water was sampled at the intake of a water treatment plant, after flocculation and after rapid gravity sand filtration. The UV_{254} results obtained using the portable instrument revealed that this parameter is comparable to that obtained with a conventional UV-Vis spectrophotometer. The DOC concentration of the samples obtained with a conventional TOC analyzer, were within the range of 5.0 to 7.0 mg/L, which were comparable to results obtained with the portable instrument for samples after flocculation and sand filtration, respectively. However, DOC results obtained with the portable instrument for raw water samples were somewhat elevated and need further investigation. The UV254Go! instrument therefore shows potential as a convenient and cost effective means to determine NOM concentrations at water treatment plants and thereby assist in real-time optimization of the treatment process.

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PA34 Developing a mass spectrometry platform for identifying protein-ligand interaction

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The initial stages of drug discovery are increasingly reliant on development and improvement of analytical methods to investigate protein-protein and protein-ligand interactions[1]. Mass spectrometry (MS) has been recognized as providing a fast, sensitive, and high-throughput methodology for analysis of weak non-covalent protein-ligand complexes[2]. In this study, MS method was used to explore the binding affinity of carbonic anhydrase II (CA II) and its interactions with three different ligands, namely two sulfonamide inhibitors acetazolamide (AZA) and dorzolamide (Doz), and a non-steroidal anti-inflammatory drug (NSAID), ibuprofen (IBU). The interaction of these ligands was studied at buffer pH 5 and 7. The ligands concentration range from 50 µM-500 µM, while the protein concentration was kept at 10 µM. The physico-chemical parameters used to characterize and determine the binding affinity of protein-ligand interactions were, peak PDA, calculation of % binding and dissociation constant (KD). Consequently, the % binding for the interaction of CA II with these ligands at pH 5 was 10-97 % AZA, 67-99 % Doz and 79-120 % IBU and at pH 7 was 20-119 % AZA, 67-105 % Doz, and 42-94 % IBU, respectively. Moreover, the KD values showed high affinity binding for the interaction of CA II with AZA and Doz, whereas moderate binding for the interaction of CAII and IBU was observed. Accordingly, these parameters showed that Doz and AZA binds to CA II at pH 5. However, Doz had high affinity binding compared to AZA. More so, the interaction of CA II and IBU showed high affinity binding at pH 7. Overall, this research reveals that mass spectrometry represents an excellent tool for the study of protein-ligand interaction and determining the binding affinity of carbonic anhydrase to it inhibitors.

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PA35 Ball-milled biochar derived from sweet prickly pear for the removal of Bisphenol A (BPA) from wastewater

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The pollution of Bisphenol A (BPA) has attracted attention globally and it has emerged as one of the contaminants of emerging concern[1]. Researchers have demonstrated that BPA can cause endocrine system disruption and has a certain level of biological harm to organisms[2]. In this study, pristine biochar derived from the waste of sweet prickly pear was modified using a ball milling modification approach and was applied for the removal of BPA from wastewater. The modified biochar was characterized by BET, FTIR, and TGA-DSC to understand the physicochemical properties of the material. The BET results revealed that the ball-milled biochar possesses a higher surface area than the pristine biochar. FTIR results revealed the presence of C-H, C=O, C=H, and C-O functional groups in the biochar. From the TGA-DSC result, the material is thermally stable up to 550 ^{o}C. A full factorial 2^5 experimental design using Minitab 21 Statistical software was employed to optimize the adsorption experimental conditions. The F-value and P-values for the lack-of-Fit of the model show the acceptable and significance of the ANOVA model. The adsorption experiment was found to be fitted best to Freundlich than Langmuir isotherm with the values of $R^2 \geq 0.92$ for Langmuir and $R^2 \geq 0.95$ for Freundlich isotherm. A removal percentage of 86% and 78% were obtained for wastewater effluent and influent respectively.

Acknowledgements

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PA36 An electrochemical immunosensor for Alpha-fetoprotein cancer biomarker based on carbon black/palladium nanoparticles platform

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A novel label-free electrochemical immunosensor for the detection of alpha-fetoprotein (AFP), a cancer biomarker, is developed on a platform of carbon black nanoparticles (CBNPs) modified with palladium nanoparticles (PdNPs). The platform for the immunosensor was prepared by drop drying and electrodeposition method on a glassy carbon electrode (GCE). The high conductivity and sensitivity of the CBNPs together with the good biocompatibility, excellent catalytic tendency, and large surface area of the PdNPs generated good signal enhancement and gave a low detection limit for AFP biomarker detection. The alpha-fetoprotein immunosensor was examined using square wave voltammetry (SWV) and electrochemical impedance (EIS), respectively. Under optimal experimental conditions, the developed immunosensor had a wide linear detection range from 0.005 to 1000 ng mL^{-1}, with low detection limits of 0.0039 ng mL^{-1} and 0.0131 ng mL^{-1} for SWV and EIS respectively. The prepared immunosensor resulted in good stability, reproducibility, and selectivity toward interfering biomarkers.

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PA37 Synthesis and characterization of ternary quantum dots metal-organic frameworks composites as sensors for Bisphenol A

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Endocrine disrupting chemicals are chemicals compounds which altered the normal functioning of the endocrine glands in human body when inhaled or consumed1. Bisphenol A is one of the most dangerous endocrine disrupting chemicals and methods to accurately detect it is of paramount importance2. In this work metal-organic frameworks(MOFs) were synthesized using two major methods which are room temperature (RT) and hydrothermal (HT) synthesis followed by the synthesis of the quantum dots (QDs) using reflux methods. Secondly, the as-synthesized precursors of MOFs and QDs were complexed together to form a composite of metal-organic framework quantum dots (QDs@MOFs) which enhanced the fluorescence sensing ability and capability of the MOFs and QDs separately. The colour light emitting QDs@MOFs composites manifest excellent fluorescent properties in the solution of the bisphenol A with a significant quantum yield of above 70%. The composites exhibit high fluorescent stability, favourable sensitivity and outstanding selectivity for the analyte solution, and this fluorescence was quenched and/or enhanced depending on the composites used. Spectroscopic, electron microscope, and GC-MS were employed to characterize the composites before and after usage to determine the quantitative and qualitative detection of the analyte. Considerable advantages of the detection system such as rapid response time with a low detection limit of 0.12 µM over a broad range concentration of 5 – 1000 µM (R2 = 0.999) were recorded. Various properties of the sensors highlighted provides a promising method for rapid, selective, and sensitive detection of other small harmful substances.

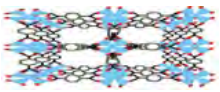

Figure 1: A pancake-bonded dithiadiazolyl dimer.

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PA38 Analysing the chemical composition of oligomeric products from the oxidative depolymerisation of lignin

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Technical lignins are very complex biopolymers, and the planet's most abundant renewable source of aromatic compounds. For the development of valuable products based on the renewable feedstock, it is important to understand its molecular structure. However, the chemical composition of technical lignins is still not well known as the lignin subunits are bonded irregularly. When lignin is depolymerised, a complex mixture of monomeric and oligomeric compounds is obtained.[1] While a significant number of monomers have been defined by advanced analytical methods, the majority of the depolymerisation products are ill-defined lignin oligomers.[2] The work presented here focuses on investigating the molecular structure of lignin-derived oligomers. A multidimensional analytical approach that is based on first fractionating the complex depolymerisation product according to hydrodynamic volume using preparative size exclusion chromatography (SEC), followed by chemical compositional analysis by reversed phase liquid chromatography (RP-LC) coupled to high-resolution multiple-stage tandem mass spectrometry was utilised. RP-LC elution orders, UV spectral information and high resolution, high-energy MS^E data were implemented to unravel the complexity of the lignin depolymerisation products.

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PA39 Determination of vitamin D metabolites in biological samples by supercritical fluid chromatography – tandem mass spectrometry

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Vitamin D deficiency is associated with osteoporosis, high blood pressure, obesity, type I and type II diabetes. To form physiologically active forms, Vitamin D is biologically activated by 25-hydroxylation in the liver and 1-hydroxylation in the kidney[1]. It is however unknown exactly how vitamin D is stored and metabolized in vivo. One hypothesis is that vitamin D is stored in fatty tissue as different forms of vitamin D esters. The status of vitamin D is clinically monitored by measurement of 25-hydroxycholecalciferol, the most abundant of the different vitamin D metabolites in plasma. Measurement of 1,25-dihydroxycholecalciferol, the biologically active form of vitamin D, is rarely performed. With regard to the potential storage form of vitamin D in their ester form, there were until now no available analytical methods, not even for research purposes. The lipophilic nature of vitamin D metabolites makes quantitative analysis in biological samples challenging due to their low abundance in comparison to other lipids in the sample, causing sensitivity problems in extraction and analysis. Moreover, current methods suffer from low selectivity both within the different vitamin D species and against other lipids[2]. There is a great need for quantitative selective and sensitive methods targeting vitamin D2 and D3 including their esterified and hydroxylated species. Supercritical fluid chromatography – tandem mass spectrometry (SFC-MS/MS) is an interesting approach[3]. In this presentation, separations of vitamin D including esterified and hydroxylated metabolites in a single step analysis will be presented. Method performance in terms of selectivity, sensitivity and detectability will be discussed[4-5].

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PA40 Electrochemical Detection of Nicotine at a Carbon Nanofiber-Poly(amidoamine) Dendrimer Modified Glassy Carbon Electrode

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Development of electrochemical sensors for important drugs such nicotine (an addictive drug) is important for the society. This study reports the electrochemical detection of nicotine at a carbon nanofiber/poly (amido- amine) dendrimer modified glassy carbon electrode. The carbon nanofiber (CNF) modified GCE was prepared by drop-coating followed by the electrodeposition of generation 4 poly (amidoamine) succinamic acid dendrimer (PAMAM) to form the sensor - CNF-PAMAM GCE. Characterization of prepared materials and modified electrodes was carried out using Fourier transmission infrared spectroscopy, field emission scanning electron microscopy, transmission electron microscopy, Raman spectroscopy, cyclic voltammetry, electrochemical impedance spectroscopy (EIS) and differential pulse voltammetry (DPV). The CNF-PAMAM composite was confirmed by microscopy. A marked reduction in charge transfer resistance and increase in current of the CNF-PAMAM GCE in comparison to the bare electrode showed a synergic improvement electrochemical response because of the CNF- PAMAM nanocomposite. The CNF-PAMAM demonstrated an enhanced performance in the oxidation of nicotine in comparison to the bare GCE by shifting the anodic potential E_{pa} of nicotine from 0.9 V to 0.8 V. The electrochemical sensor achieved a detection limit (LOD) of 0.02637 µM in the concentration range of 0.4815–15.41 µM of nicotine in 0.1 M PBS at pH 7.5. The sensor ability to determine nicotine in real samples was assessed in cigarettes obtaining recovery percentages of 88.00 and 97.42%. The sensor demonstrated selectivity toward nicotine in the presence of interferences. Finally, the method was validated by ultraviolet–visible spectroscopy analysis.

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PA41 Assessing biostimulant activity of Moringa Leaf Extract *obtained via* Pressurised Hot Water Extraction on broad bean *Vicia faba*

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M*oringa oleifera* leaf extract (MLE) is an excellent alternative to expensive inorganic fertilisers because it is equally or more effective than synthetic growth promotors.[1,2] Pressurised Hot Water Extraction (PHWE) is a green, environmentally friendly, faster, and more efficient extraction technique of essential compounds.[3] In this current study, greenhouse experiments were carried out to evaluate the effects of Moringa leaf extract on the growth and pod yield of the broad bean (*Vicia faba*). Moringa leaf powder was extracted at 25 °C, 50 °C, 100 °C and 150 °C by PHWE, and the extract was applied by foliar application every ten days over a three-month period. The PHWE extracts were compared to a control (tap water), a commercial biostimulant and a water-blended Moringa extract. Quantification of macronutrient contents such as Ca, K, P and Mg and micronutrient elements such as Fe, Ni, Zn, Mo, Co, Mn and Cu from the soil and broad bean biomass was determined using inductively coupled plasma-optical emission spectroscopy (ICP-OES). A Carbon, Hydrogen, Nitrogen and Sulphur (CHNS) analyser was used to establish the Carbon, Hydrogen, Nitrogen and Sulphur content in broad bean biomass. Plants treated with the PHWE Moringa extracts increased plant height, number of leaves, number of branches, root length, pod and seed weight compared to the control. It can be concluded that Moringa leaf extract obtained *via* PHWE can be used to enhance the growth and development of broad beans.

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PA42 Application of amine functionalized MWCNTs as SPE adsorbents of pesticides in orange fruits and water

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Preparation of an appropriate stationery phase in solid phase extraction (SPE) is very critical to imperatively accomplish good analyte recoveries. The unique physicochemical properties of carbon nanotubes (CNTs) have enticed a great attention[1,2]. In this work, multi-walled carbon nanotubes (MWCNTs) were functionalized with diverse amine compounds in an effort to enhance the analyte to adsorbent interactions during SPE applications. Functionalization of the MWCNTs was first adopted from the work of Mkhondo *et al* where a successful introduction of carboxylic groups was observed[3]. The resultant oxidised MWCNTs where amine functionalised with various amine compounds and the physicochemical properties of the resultant nanocomposites were studied using XRD, SEM, TEM, EDS, BET, TGA, and FTIR. Pesticides extracts obtained from orange fruits and water samples *via* SPE using the amine-MWCNTs as adsorbents were analysed by GC-MS. The effects of different amine compounds fabricated on the walls of MWCNTs are discussed. The enhanced analyte to adsorbent interactions as a result of the different amine compounds was also investigated.

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PA43 Synthesis Of Naphthalene Derivatives as Bifunctional Electrolyte Additives for Lithium-Ion Batteries

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High-energy-density lithium-ion batteries (LIBs) are in high demand for cell phones, computers, and many other applications. These technologies may be the most promising for electric vehicles and smart grids. Research has focused for decades on improving LIB energy density and safety. Due to safety restrictions, extensive research is needed to increase their safety and stability over many cycles without sacrificing performance. Most commercial batteries contain organic carbonates and $LiPF_6$ as electrolyte, which can burn or explode if damaged or heated, and therefore are not intrinsically safe. Zhang[1] has studied the influence of electrolyte additives on LIB performance by improving the solid-electrolyte interphase (SEI), increasing cycle life, and enhancing thermal stability compared to carbonate-based organic electrolytes. This study intends to produce naphthalene-based bifunctional organic electrolyte additives to improve the electrochemical and safety performance of lithium-ion power sources. In this work we computed the oxidation and reduction potentials, HOMO and LUMO energy levels, and conformational preferences of proposed naphthalene derivatives (NAP) using DFT with Becke's three-parameter hybrid approach and the Lee-Young-Parr correlation functional (B3LYP) and the 6-31G(d,p) basis set. The HOMO energy levels of NAP are higher and the LUMO energy levels are lower than those of EC, DC, and PC solvents, indicating that they can be oxidized/reduced on the cathode/anode before the standard electrolyte solvents, thereby facilitating the formation of SEI film due to easier electron transfer at the graphite anode. Other descriptors that help comprehend NAP characteristics were also studied, including dipole moment, which predicts solubility in carbonate electrolyte[2], bonding interaction with Li^+ ion,[3] electron affinity (EA), and ionization potential (I)[3].

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PA44 Electrochemical Sensing of Epinephrine on a Carbon Nanofibers and Gold Nanoparticles Modified Electrode

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Carbon nanofiber- gold nanoparticle electrochemical sensor was fabricated by drop coating carbon nanofiber followed by electrodeposition of gold nanoparticles on a glassy carbon electrode (GCE), for the detection of epinephrine (EP). The acid activated carbon nanofibers were characterized by Fourier transform infrared spectroscopy. Field emission scanning electron microscopy and transmission electron microscopy were used to study the morphological and structural properties of the nanomaterials. Cyclic voltammetry, electrochemical impedance spectroscopy (EIS) and square wave voltammetry were used for the electrochemical characterisation of the electrodes in each step of the construction of the electrochemical sensor. Compared to the bare GCE, the modified electrode showed an enhanced electrocatalytic effect. Square wave voltammetry was used for the quantitative determination of epinephrine. A well-defined anodic peak potential for epinephrine was observed at pH 6 in 0.1 M phosphate-buffered solution (PBS). The sensor was linear within epinephrine concentration range of 50 µM to 1 mM with a detection limit of 1.70 µM.

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PA45 The use of microalgae for the removal of nutrients and nonsteroidal anti-inflammatory drugs in wastewater samples from South Africa

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Only about 20% of wastewater globally is properly treated before being discharged into receiving water bodies[1]. As a result, high concentrations of non-steroidal anti-inflammatory drugs (NSAIDs), nitrates, and phosphates have been detected in many South African rivers and wastewater, causing serious health and environmental threats. Bioremediation of wastewater with microalgae is the most captivating idea that has the potential of reducing many organic and inorganic compounds in wastewater. Microalgae can bio-absorb pollutants like pharmaceuticals and they have the added advantage of removing excess nutrients such as phosphates and nitrates to the acceptable discharge limits[2-3]. Therefore, research into microalgae bioremediation is highly needed in emerging economies countries like South Africa as it presents a cheaper option for efficiently treating wastewater. This project aimed to assess microalgae's capacity to remove the commonly occurring NSAIDs and nutrients in South African water environments. The first objective of this study was to develop and validate the solid extraction (SPE) methods followed by liquid chromatography – photodiode array analysis (SPE-LC-PDA) for the effective extraction of selected pharmaceuticals in water matrices. The correlation coefficients (R^2) ranged from 0.975 to 0.999, suggesting strong positive linear relationships of the newly developed method. The SPE recoveries ranged from 80% – 119% in water. The LODs and LOQs obtained indicated good method sensitivity which enables trace levels to be detected and ranged from 0.004 – 0.020 µg/L and 0.015 – 0.068 µg/L, respectively. Based on the preliminary results, the developed method is fit for its intended purpose. The study's second objective is currently being undertaken where the capacity of microalgae to remove selected NSAIDs and nutrients in wastewater influents and effluents is assessed.

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PA46 A novel molecularly imprinted polymer for *N*-nitrosodimethylamine extraction from drinking water

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Nitrosamines are considered highly carcinogenic and genotoxic compounds, which are formed in water as a result of a range of factors but mainly due to chloramination or chlorination disinfection in the presence of ammonia or nitrite[1]. Computational simulations were employed to find a suitable template for *N*-nitrosodimethylamine (NDMA) which can be used in the synthesis of a molecularly imprinted polymer (MIP) that has microcavities to selectively extract NDMA from water samples and thereby aid in the pre-concentration of these analytes [2]. Dimethylformamide (DMF) was found to be a suitable template, which was subsequently used in the synthesis of an imprinted polymer MIP—DMF. Non-imprinted polymers used as a control and MIPs were successfully synthesized and characterized by Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), thermogravimetric analysis (TGA), and the Brunauer-Emmet-Teller (BET) method. The synthesised MIPs may be used as a selective sorbent in the solid-phase extraction of *N*-nitrosamines, specifically NDMA, from water to allow for their simultaneous extraction and pre-concentration prior to analysis.

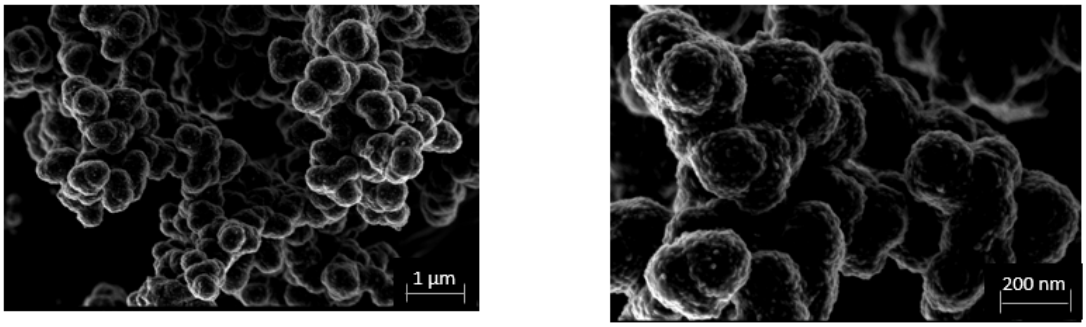

Figure 1: SEM micrographs of MIP—DMF, observed at different magnifications (20 000 X and 50 000 X) to study their morphologies (refer to 1 µm and 200 nm scale bars).

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PA47 Electro-Fenton/anodic oxidation treatment of Ciprofloxacin, Sulfamethoxazole and Tetracycline in water

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Global industrialisation, though a plausible index for economic expansion, has unfortunately led to a magnification in pollution owing to the discharge of waste or pollutants into the environment[1–3]. The goal of this study is to evaluate the efficiency of the titanium oxide (Ti_4O_7) electrode for potential application in electrochemical oxidation of complex organic pollutants in water. A degradation of a pharmaceutical cocktail that consists of sulfamethoxazole (SMX), ciprofloxacin (CIP) and tetracycline (TERT) organic pollutants was investigated using photo/electro-Fenton coupled to anodic oxidation. An organic pharmaceutical cocktail pollutant at 20 ppm was treated in an undivided cylinder where carbon felt (CF) was used as the cathode and Ti_4O_7 as anode, at a constant current density of 0.96 $mA.cm^{-2}$. The treatment of the pharmaceutical cocktail was monitored by UV-Vis, TOC, UPLC-MS. In UV-Vis, of the EF/AO and photo EF/AO processes, almost all the major peaks present in the initial spectrum (before degradation) disappeared. A high TOC removal of the pharmaceutical cocktail was recorded within 30 min. The concentrations of each of the pharmaceuticals present in the cocktail was detected using UPLC-MS where the concentration of SMX was no longer detected in the cocktail solution in 30 min and CIP and TERT were detected in trace amounts. Reaction pathways were proposed based on the data of high-resolution spectrometry and intermediate products were detected which were smaller than the parent molecule after 4 h treatment. The titanium oxide (Ti_4O_7) as an anode and carbon felt as a cathode electrode can be used to treat complex organic pollutants by EF/AO and photo EF/AO.

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PA48 The use of plant growth promoting rhizobacteria to enhance growth and biological activities in *Lessertia frutescens* under drought and salt stress

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Lessertia frutescens is a medicinal plant used in southern Africa to treat a diverse range of illnesses, including wounds, fever, and cancer[1]. Abiotic stressors, such as salinity and drought, are amongst the most harmful environmental conditions limiting the productivity of plant[2]. Previous studies have proven that abiotic stress has a negative impact on the physiology, morphology and phytochemistry of medicinal plants[3]. The aim of this study was to evaluate the effect of plant growth promoting rhizobacteria (PGPR) on plant growth, production of secondary metabolites and biological activities of *L. frutescens* growing under simulated salt and drought stress. The randomized block design pot trial was conducted under glasshouse conditions. The experiment consisted of control plants treated with a commercial growth promoting agent and nitrate solution, test plants inoculated with PGPR previously isolated from *L. frutescens* rhizobia and test plants subjected to different drought and salt stress levels and inoculated with PGPR. After 60 days, upon harvesting, plant growth and plant productivity parameters were determined. The inoculation of *L. frutescens* with PGPR yielded a significantly high biomass compared the controls. The antioxidant activity was estimated using FRAP and DPPH free radical scavenging assays. The total flavonoids and phenolics content were determined with colorimetric methods. An increase in plant biomass, phenolics content and decrease in antioxidants was noted with increasing salinity, whereas antioxidant activity and phenolics content increased with increasing drought. The findings of this study indicate that inoculating *L. frutescens* subjected to abiotic stress with rhizobacteria alleviates the impact of drought and salinity on *L. frutescens* plant growth and improves the efficacy of plant extracts, except for salinity which altered the antioxidant activity of plant extracts.

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PED1 Developing and evaluating systems thinking in first-year organic chemistry

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Powerful arguments have been made recently to advocate for the introduction of systems thinking in chemistry education in order to equip graduates to address sustainability challenges. The purpose of this poster is to present the systems thinking (ST) intervention that was designed and implemented in first-year organic chemistry and to present the evidence that suggests students were developing ST skills and a sustainable action perspective. Students learnt about the chemical principles and real-world implications of the system of Linear Alkylbenzene Sulfonate, an anionic surfactant commonly used in laundry detergents. The activities in the intervention incorporated concept maps and system-oriented concept mapping extensions (SOCMEs) as visualization tools to scaffold the development of ST skills. A mixed-methods research design was used to collect data from a sample of 18 students' perceptions, reflections, and demonstrations during and after the learning process. Findings from students' perceptions, reflections and demonstrations indicated that they were developing the ability to identify the concepts and relationships within the system, however, struggled to integrate the parts of the system to visualize the whole. During focus group interviews students acknowledged that they were used to thinking about chemistry topics in isolation and were not used to visualizing the real-world implications of chemistry. Evidence also suggested that students engaged deeply with the relevant topic of surfactants and gained an understanding of the system. The intervention enabled meaningful learning as students' moved between different levels of granularity to view the system as a whole and not just as a collection of parts. In conclusion, evidence suggested that meaningful progress was made towards developing systems thinking skills and a sustainable action perspective.

Acknowledgements
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PE1 The immobilization of selected bacterial isolates on glutaldehyde, activated amberlite resin, polyvinyl alcohol-sodium alginate for the optimization controlled degradation of automotive and marine waste oils

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The oil industry including insulating and lubricating oils, has been considered an energy source commodity thus incorporating it as an indispensable part of the global economy and environment. This is a direct consequence of its pivotal importance applied to the functioning of transformers in the power industry and lubricating engines in the transport industry. These oils over a prolonged period are prone to undergoing chemical reactions such as oxidation, nitration and sulfation that subsequently lead to its break down and thus decreasing its ability to function optimally. The inherent need for its immediate replacing is a direct consequence of a large accumulation of waste oil which is hazardous to both humans and the environment. The degradation of waste oils (transformer insulating oil, truck and ship engine lubricating oil) using selected bacterial isolates (Acinetobacter V2 and Paenibacillus D9), over an incubation period of 144 hrs has been investigated. The immobilisation of Acinetobacter V2 and Paenibacillus D9 bacterium isolates through supporting material viz. glutaldehyde, activated amberlite resin, polyvinyl alcohol-sodium alginate and chitosan-sodium alginate matrix beads was executed to render them more desirable and applicable to industrial processes. A profiling of the physical and chemical properties immobilised isolates are reported. Finally, to gain a better understanding of the susceptibility of hydrocarbon n-alkane analogues to degradation coupled with the selectivity of bacterium isolates, this study implemented degradation on a range of n-alkanes (C8-C36) by bacterial isolates V2, D9 and Hybrid systems (V2:D9, 1:1). After 144 hours of incubation, 80 % degradation was observed for all waste oils by both isolates, with D9 showing superior degradative capabilities than bacterial isolate V2. The data and observed trends show that developed immobilisation techniques achieved successful in immobilising bacterial isolate strains V2 and D9, with free cell degradation being most efficient (14.7 - 31.6 %) followed by PVA-SA (5.3 – 26.7 %) , CHI-SA (8.8 – 20.3 %) and AMB-GLU (2.2 – 7.0 %). The n-alkane analogues ranging from C8-C36 degraded at a rate proportionate to their individual chain length with larger chains requiring a longer degradation time. On the other hand, liquids alkanes in the range C8-C16 (22.1 – 38.1 %) proved to be more susceptible to degradation in comparison to the solid alkanes ranging C18-C36 (1.2 – 25.8 %). The hybrid system gained the greatest percentage degradation (6.9 – 38.7 %).

PE2 Transformation of engineered nanomaterials: pristine vs. Nano-enabled products during simulated usage and disposal

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In recent times we have witnessed the increase in nano-enabled products (NEPs) commercially available on the market[1-2]. It is common that these products are not explicitly labelled as nano-enabled. NEPs are often not assessed based on the safety of their use with no protocol for their disposal in place. NEPs could potentially pose threats to the environment as they are often disposed of via water sources and thus enters the aquatic environment via leaching and can undergo various transformations which may be toxic to ecosystems, living organisms and the environment at large[1]. Herein, several commercially available NEPs labelled to contain Ag, Ti and Au metal NPs, were selected. Engineered NPs (ENPs), comparable to those contained in the selected NEPs were synthesized. The simulated usage and disposal of the selected NEPs into water sources were monitored over several months. Various characterization techniques including ultraviolet-visible spectroscopy (UV-vis), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and High-Resolution Transmission Electron Microscopy (HR-TEM) were used to confirm the presence of NMs in the NEPs and to monitor the transformations undergone by these NMs in the NEPs during its simulated usage and disposal into water sources. Toxicity of the transformed NMs from NEPs and ENPs were assessed and monitored with lettuce seed dosing and plant dosing.

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PE3 Seasonal variation and temporospatial migration of emerging contaminants within drinking water treatment unit processes

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The contamination of surface water sources varies with the intensity of domestic, agricultural, or industrial activities, which depends on the region's level of urbanization[1]. Drinking water is often obtained from surface water sources for which quality varies seasonally and according to geographical location. Various treatment unit processes and technologies are applied to produce drinking water of acceptable quality from surface water sources[2]. In this study, the seasonal variations and temporospatial migration of emerging contaminants within different drinking water treatment unit processes were evaluated. The assessed unit processes comprise the pre-chlorination, coagulation, flocculation, sedimentation, filtration, and post chlorination. A total of nine (9) sampling points were identified and samples were collected after each unit process of the selected water treatment plant. Sampling was done from January to August 2022 covering autumn and winter seasons. The samples were quantified using high-pressure liquid chromatography-mass spectrometry. Assessed emerging contaminants of concern comprise Sulfamethoxazole, Carbamazepine, 1.7 Dimethylxanthine, Tramadol and Venlafaxine. Findings from this study confirmed the presence of carbamazepine having the highest median concentration (116 ng/L), followed by Venlafaxine (10 ng/L) during winter season and 1.7 Dimethylxanthine (642 ng/L) ≥ Sulfamethoxazole (114 ng/L) ≥ Tramadol (107 ng/L) during autumn season in the collected water matrices. Interestingly, certain contaminants of emerging concern i.e., Sulfamethoxazole, Tramadol, Venlafaxine, Carbamazepine, 1.7 Dimethylxanthine and Benzoylecgonine were present in raw water, and were not completely removed at the final water pumped to different points of use, hence denoting potential toxicological concerns. Henceforth, the obtained results show that conventional drinking water treatment plants do not completely remove some of the emerging contaminants, however the concentrations from the raw water are attenuated to some extend in the treatment. In light of the obtained results, it is imperative to optimize operational conditions for water treatment plants and devise prudent and pragmatic technologies for the removal of CEC from drinking water.

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PE4 Characterization and remediation of polychlorinated biphenyls sorbed onto suspended solids in the Blesbokspruit wetland

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The main objective of this study was to characterise PCBs sorption onto suspended solids from the Blesbokspruit wetland system. Sorbed and non-sorbed PCBs were extracted from samples collected in 2021 and 2022 using liquid-liquid extraction followed by a solid-phase extraction, then the PCBs quantified in them using a validated GC-MS method[1]. Important physicochemical measurements recorded including alkalinity, found to exceed acceptable levels on the two major sites (BSP and BGV) while the other parameters (EC and DO) were within tolerance levels according to the water quality guidelines of the DWS. The average (n=15) total concentrations of PCBs in the suspended phase were found to be 167.35 $ng.L^{-1}$ and 69.52 $ng.L^{-1}$ for PCB-52 and 61.62 $ng.L^{-1}$ and 21.67 $ng.L^{-1}$ for PCB-28 in the dissolved phase, in 2021 and 2022, respectively. From this study, and compared to the WHO water quality standard values, the Blesbokspruit is acceptable as a natural water body but certainly not as potable water. A GC-MS method was also developed and validated for quantifying the PCB-28 and PCB-52 congeners. The conclusion is that the wetland system needs to be rehabilitated, re-managed, and restored to obtain high water quality and ecologically healthy wetlands.

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PE6 Assessment of alfalfa (*Medicago sativa* L.) plants for effectiveness in phytoremediation and ecorestoration of fly ash deposits

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Fly ash (FA) is the bi-product of coal produced in the process of electricity generation. Disposal of coal FA can have negative consequences on the environment, including atmospheric pollution, soil and groundwater contamination, as well as converting valuable agricultural land to unproductive ash dumps. Phytoremediation involves the selection of suitable plant species for reclamation of polluted environments. Alfalfa (*Medicago sativa* L.) is a perennial legume with fast growth rates and therefore an excellent candidate for phytoremediation studies. Pot experiments were conducted to predict the field performance of alfalfa when planted in fly ash under natural conditions. Fly ash collected from Kriel Power Station was tested. The treatments included planting alfalfa in 100% fly ash, 70 % fly ash (ash mixed with sand) and uncontaminated soils collected from the vicinity of the Power Station served as controls. Gas-exchange studies were conducted on six-month old alfalfa plants, and the parameters measured included photosynthetic rates (A), stomatal conductance (Gs), leaf transpiration (E) and intrinsic water-use efficiency (WUEi). Alfafa plants grown in 70% and 100% fly ash recorded similar photosynthetic rates as plants grown in uncontaminated soil control. For example, the photosynthetic rates of control plants were found to be 19.37 $\mu molCO_2m^{-2}.s^{-1}$ compared to 16.83 $\mu molCO_2m^{-2}.s^{-1}$ for 100% FA with the lowest values being recorded by plants grown in 70% fly ash (13.07 $\mu molCO_2m^{-2}.s^{-1}$). The Gs value recorded for 100% fly ash plants was 0.48 $mmolHO_2m^{-1}.s^{-}$ compared to 0.47 $mmolHO_2m^{-1}.s^{-}$ for plants grown in 70% fly ash. These results indicate that even with 100% fly ash, there was increased supply of CO_2 to the leaf interior leading to improved accumulation of biomass for 100% fly ash plants. The WUEi value recorded for 100% fly ash plants was 37.71 $\mu molCO_2m^{-1}H_2O$, which was close to the control WUEi of 41.9 $\mu molCO_2m^{-1}H_2O$, thus indicating that carbon gain occurred with minimal loss of water. Establishing plants on dumpsites of fly ash poses a challenge. However, our results suggest that *Medicago sativa* grow well when planted in fly ash, and is a good candidate species for reclaiming fly ash-contaminated environments.

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PE7 Polymer-brush modified graphene oxide thin film nanocomposite membranes for enhanced heavy metal adsorption

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Heavy metal contamination of freshwater sources is a major concern due to its negative effects on human and aquatic health.[1,2] Herein, we report the synthesis of graphene oxide (GO) functionalized with poly (glutamic acid) polymer brushes for efficient Cobalt ion adsorption. Polymer brushes were grown on the surface of GO using surface-initiated polymerization (SIP). This technique involved the attachment of an initiator a-bromoisobutyryl bromide followed by the polymerization of poly (glutamic acid (PGLU) using atom transfer radical polymerization (ATRP). The synthesis of GO and its polymer derivatives was confirmed by Fourier Transmission Infrared (FTIR), Powder X-ray diffraction (XRD), Transmission electron microscopy (TEM), and Thermogravimetric analysis (TGA). Thin film nanocomposite (TFN) membranes were then fabricated by incorporation of poly (glutamic acid) polymer-brush modified nanosheets (GO-GLU) into the polyamide (PA) thin layer. The GO-GLU/TFN membranes were characterized and evaluated in comparison with bare TFC membranes by the SEM-EDS, contact angle, permeation measurements, Cobalt ion adsorption, and antifouling behavior. In this paper, the effect of polymerization on GO in the adsorption of Cobalt ions and membrane antifouling behavior is discussed.

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PE8 Development of a rapid and simple digestion method for determination of trace metals in sludge using an ultrasound assisted system prior ICP-OES analysis: A greener approach method

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The aim of this study was to develop, optimize and validate a rapid and simple method for extraction analysis of trace metals in sludge prior ICP-OES analysis. The factors (volume of acid and time) affecting the extraction method were optimised and the optimisation process was carried out using CRM (TCLP Metals in Soil – QC Certified Reference Material SQC005). This was conducted by comparing the traditional TCLP method with the modified method where an ultrasonic bath was used to accelerate the extraction of metals in sludge. The results of the CRM revealed that for elements such as; Ni, Cr, Mo, Be, Co, Pb, Cd, V their concentrations were found to be within the acceptable limit with recoveries ranging between 98-111%, implying that the method is accurate for the analysis of sludge samples. The optimal conditions for volume and time were 10 mL of acetic acid and 30 minutes, respectively. Under optimum conditions, the method demonstrated good linearity with a correlation coefficient greater than 0.999 for all twelve metals of interest. The limit of detection (LOD) was found to be between 0.001 to 0.002µg/L and the Limit of Quantification (LOQ) was between 0.5-1000 µg/L. The method was then applied to sludge samples from twenty-eight sites where sludge is disposed to assess the presence of trace metals and their disposal procedure where their concentrations were compared with NEMWA guidelines. The guidelines showed that only Ixopo sludge exceeded limits for Ni (class c), Cd (class b) and Pb (class b) and was classified as harmful. This implies that Ixopo sludge need to be disposed using strict limitation due to the nature of its harm to the environment On the other hand, Howick sludge and other sites were classified as non-harmful (class a) for all elements studied. Overall, the greener developed method will be beneficial since it uses less chemical usage and it is effective and efficient.

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PE10 Comparative study of the photodegradation of chloramphenicol under LED light irradiation using pristine and Ag doped TiO_2 and ZnO photocatalysts

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Unregulated discharge of antibiotics has become a global concern for water pollution, of which chloramphenicol known as emerging pollutant is the pollutant study herein[1-3]. This work describes a comparative study of the degradation of chloramphenicol (CAP) in aqueous solution using pristine and Ag-doped semiconductor photocatalysts obtained from TiO_2 and ZnO. Varying weight percentages (2.5, 5, and 7.5 wt. %) of Ag nanoparticles were doped on the semiconductor photocatalysts via the sol gel method and then calcined at 500℃ for 3h. The pristine and Ag-doped semiconductor photocatalysts were characterized using UV-Vis, diffuse reflectance spectroscopy (UV-DRS), photoluminescence spectroscopy (PL), Fourier transform infrared spectroscopy (FTIR), and Scanning electron microscopy (SEM). These techniques confirmed the successful synthesis of the pristine and Agdoped materials. The photocatalytic activities of all materials used for the degradation of CAP were carried out under LED visible light irradiation for 2h; and the effects of various operating parameters (such as doping agent Ag, catalyst loading, pH, and pollutant concentration) were also investigated. The result showed enhanced CAP degradation in Ag doped in comparison to the pristine materials was most suitable for CAP degradation, especially at low pollutant concentration. The effect of pH on the CAP degradation was very versatile, depending on the catalyst introduced in the solution. Lower loadings of the photocatalysts were usually more effective for CAP degradation and the degradation trend in TiO2 was 5 wt. % Ag doped > 7.5 wt. % Ag doped > 2.5 wt. % Ag doped > Pristine, while it was 2.5 wt. % Ag doped > 5 wt. % Ag doped > 7.5 wt. % Ag doped > Pristine in the ZnO.

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PE11 Analysis of per- and polyfluoroalkyl substances in drinking water treatment plants in some parts of South Africa

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Per- and polyfluoroalkyl substances (PFAS) are a diverse group of human-made chemicals used in a wide range of consumer and industrial products such as water-resistant fabrics and carpeting, cleaning products, paints, and fire-fighting foams[1]. They can migrate from these products into different environmental compartments with their concomitant health and environmental impacts. Therefore, their presence in the environment is not desirable, particularly in water sources. In the current study, water samples from drinking water treatment plants in some parts of South Africa were collected during dry and wet seasons to account for seasonal variations. Samples were subjected to solid phase extraction (SPE) and liquid chromatography-tandem mass spectrometry (LC-MS/MS) was used for analysis. PFASs were observed in all DWTPs. 6:2 FTS, 8:2 FOET, PFBA were the most dominant compounds with concentrations ranging from <LOQ-292 ng/L, 1.9 – 595.6 ng/L and 0.119 - 73.7 ng/L respectively. PFOS and PFOA were detected at concentrations ranging from 0.520–103.2 ng/L and 0.504–9.34 ng/L respectively. L-PFHxS, L-PFOS, PFOA, L-PFBS, L-PFDS, LPFHpS, FHEA, PFDoA, PFHxA, PFHxDA, PFNA, PFODA, PFPeA, PFUdA, 8-2 FTS, 4-2 FTS were also detected with concentration range of <LOD-675.1 ng/L. However, PFOS concentration was detected above the health advisory levels of 70 ng/L suggested by the United State Environmental Protection Agency (USEPA). Higher detection of PFASs was observed in dry season than in wet season. The presence of these PFASs in water systems is attributed to anthropogenic activities such as firefighting stations, airports, mining activities and manufacturing sectors where PFAS-containing products are in use. From the products, PFASs can leach into wastewater treatment plants and eventually rivers, groundwater and drinking water[1]. The detection of these compounds in the drinking water treatment is a cause for concern.

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PE12 Trace metals concentration in turf grass irrigated with sewage sludge and their environmental implications in Pietermaritzburg, South Africa

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Darvill Wastewater Treatment Works (DWWTW) uses land application to dispose of sewage sludge due to the lack of appropriate sewage sludge disposal methods, the sewage sludge is irrigated onto turf grass which is then used for commercial purposes.[1] This study was conducted to determine the concentrations of selected trace metals in the sewage sludge amended soil (DWWTW) and in the soil where turf grass has been planted (Dumabezwe sports field and Mqulela sports field). Environmental pollution indices were used to assess the extent of trace metal pollution in the environment, while statistical and inferential tools such as predictive correlation coefficient, principal component analysis, cluster analysis were used to analyse and quantify the data, and origin of the trace metals. [2] The trace metals concentration (mean ± SD, mg/kg) in the main site (DWWTW) were: Pb (263,2 – 771,7), Mo (10,03 ± 36,77), B (63,53– 287,9), Ba (38,09 – 332,8), Se (368,4 – 2116), Sb (18,68 – 141,6) and Cr (1550 – 3454) and V (10,32 -32,49), these values are higher than the results obtained from the control sports field (PMB sports field).The observed geo-accumulation factor, contamination factor and the pollution load index, indicated that the soils around DWWTW are heavily contaminated by Cr, Pb, V, Se, Zn, and Sb. The potential ecological risk index suggests that there is a high environmental risk of Cr and Zn pollution after effect in the soils. Low values of environmental pollution indices were obtained for soils in Dumabezwe sport field and Mqulela sport field and for which there are no evidences that trace metals cross-contamination occurred when turf grass is applied on standard soil. The cluster analysis and the enrichment factor confirmed that trace metals in the soil collected from around DWWTW originates from the anthropogenic activities which is the continuous application of sewage sludge in the environment.

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PE13 Photoelectrocatalytic degradation of sulfamethoxazole over S—Scheme $Co_3Se_4/BiVO_4$ heterojunction

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The pollution of the water environment by industrial effluents is an ongoing challenge due to the rate of industrialisation and globalisation. Photoelectrocatalysis (PEC), an electrochemical advanced oxidation process, has proven to be an effective method for removing organics from wastewater.[1,2] Thus we demonstrate the photoelectrochemical degradation of sulfamethoxazole (SMX) with a photoanode developed based on S—scheme heterojunction. The difference in the energy levels of the band gaps and conduction bands of $BiVO_4$ and Co_3Se_4 makes them suitable semiconductors for the fabrication of an S-scheme heterojunction. The $BiVo_4/Co_3Se_4$ composite is prepared by solvothermal method and characterized using X-ray diffraction (XRD), field emission-scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), Energy Dispersive X-Ray Analysis (EDX), Ultraviolet-Visible Diffuse Reflectance Spectroscopy (UV—DRS). The photoelectrochemical properties of the fabricated photoanode are studied using Electrochemical impedance spectroscopy (EIS), Mott—Schottky, and photocurrent response. The UV—DRS spectra show an improved band gap (1.88 eV) for the composite in comparison with pristine $BiVO_4$ (2.39 eV). The XRD patterns reveal the presence of monoclinic phases of $BiVO_4$ and Co_3Se_4 in the composite. This is further confirmed by the microscopic studies that show the surface coating of Co_3Se_4 on $BiVO_4$. The composite photoanode shows improved photocurrent density and low charge transfer resistance in comparison with the pristine semiconductors. This can be attributed to the effective charge carrier separation occasioned by the heterojunction created in the composite. This provides the composite with the capacity to effectively degrade SMX with improve efficiency. At optimum conditions, the SMX degradation efficiency reached 75% with a rate constant of 0.0115 min^{-1}. The holes majorly facilitate the degradation of SMX as revealed by the scavenger study. Comparative studies indicate that photoelectrocatalytic contributions supersede photocatalytic and electrocatalytic contributions.

Acknowledgements
T. L. Yusuf is grateful to the Faculty of Science, the University of Johannesburg, for a postdoctoral research fellowship award.

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PE14 Fabrication of Biochar Materials from Biowaste Coffee Grounds and Assessment of its Adsorbent Efficiency for Remediation of Water-Soluble Pharmaceuticals

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Water scarcity is a major problem that is made worse by the population increase, which result to rapid urbanization leading to climate change. Reclaimed water from the treated wastewater in wastewater treatment plants (WWTPs) seems to be a valuable alternative water resource to meet the demand of the ever-growing population. However, one challenge of promoting the use of reclaimed water is the safety concern owing to contamination of various pollutants present in reclaimed water. Contaminants of emerging concern (CECs), especially pharmaceuticals, have become a new issue gaining public attention. Furthermore, there have been several developments in the literature that support the circular bio-economy paradigm of using biochar as an adsorbent for removal micropollutant. Therefore, biowaste coffee grounds have been recognized as an effective and relatively low-cost adsorbent to complement conventional treatment techniques for removing emerging contaminants (ECs) from the waste stream through modification to useful biochar. The purpose of this study was to make biochar from biowaste coffee grounds through the pyrolysis process and investigate its potential capacity for the removal of pharmaceuticals from water. The biochar was prepared by pyrolysis process under argon gas conditions, and its adsorption capacity and removal efficiency for pharmaceuticals was evaluated. The as-prepared biochar shows a surface area of 232 $m^2 g^{-1}$. The removal of salicylic acid, diclofenac, and caffeine from water under optimised adsorption conditions show adsorption efficiencies of 71%, 96%, and 19%, respectively. The morphology, functional groups, crystallinity, and specific surface area were determined by SEM, FTIR, XRD, and BET techniques, respectively. Kinetic results reveal that the experimental data fit the pseudo-second-order model and the Temkin isotherm model. In conclusion, these results illustrate the potential of biochar produced from biowaste coffee grounds could play an important role in environmental pollution mitigation by enhancing removal of pharmaceuticals from conventional wastewater treatment effluent, thereby minimizing their potential risks in the environment.

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PG1 Catalytic oxidative transformation of phenols and 1-naphthols over heterogeneous bismuth-promoted noble metal catalysts supported on silica

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The catalytic oxidation of alkyl-substituted phenols and naphthols is an important goal in organic synthesis[1]. The products obtained such as quinones and binaphthones, serve as the elementary building blocks for several classes of complex molecules that play essential roles in biological systems[2]. In this study, the oxidation of trimethylhydroquinone and 4-methoxy-1-naphthol were carried out over silica-supported bimetallic Au-Bi, Ru-Bi and Au-Ru catalysts under different reaction conditions (Figure 1b). The microwave-assisted loading (MW) and deposition (DP) methods were used to synthesize the catalysts and characterization for their physicochemical properties was carried out with N_2 physisorption, XRD, SEM-EDX, TEM (Figure 1a) and XPS analysis. Trimethylhydroquinone, 2,3,5-trimethylphenol and 4-methoxy-1-naphthol were tested over the prepared catalysts for oxidation reactions in methanol and/or nitromethane at room temperature and under reflux using hydrogen peroxide as an oxidant. In the oxidation of trimethylhydroquinone **(1)** [Figure 1b] in $MeNO_2$ at r.t and 96°C over DP- and MW-Au-Ru catalysts, 100% conversion of the substrate was achieved with 100% yields for trimethyl-1,4-benzoquinone obtained. However, no reaction was observed when MW-Au-Bi and MW-Ru-Bi catalysts were used under the same reaction conditions. When 4-methoxy-1-naphthol **(3)** was used as a substrate over MW-Au-Ru catalyst at under reflux, yielded 96% (Conversion: 96%) and 52% (Conversion: 99%) for binaphthone in MeOH and $MeNO_2$, respectively. The selectivity of this reaction depends on the solvent, temperature and catalyst used.

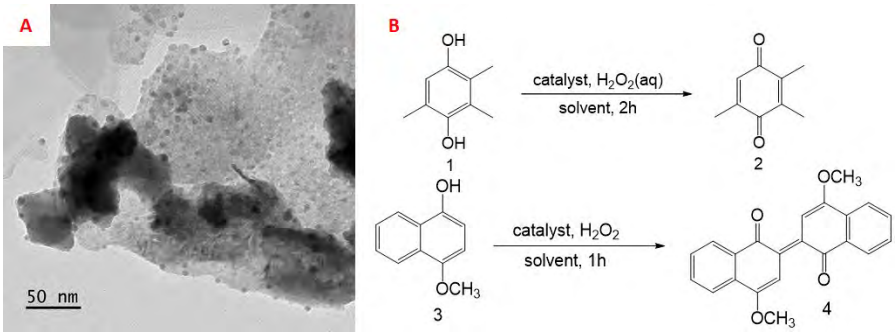

Figure 1: TEM image of DP-Au-Ru/SiO_2 (a) and oxidation of phenols and naphthols on silica supported noble metal catalysts (b)

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PG2 Application of TOPSIS in ranking of analytical procedures for the determination of mifepristone in water

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The study presents the application of multi-criteria decision analysis (MCDA) to select analytical procedures that are more environmentally benign. TOPSIS, known as Technique for Order of Preference by Similarity to Ideal Solution, is an example of a MCDA tools useful for decision making for ranking or selecting best alternative based on multiple criteria[1]. In this study, 13 analytical procedures for the determination of mifepristone in water samples were selected as input alternatives to TOPSIS analysis. The input data consisting of these alternatives was described by assessment criteria based on 12 principles of green analytical chemistry (GAC). The weights for each criterion were assigned equally based on the objective mean weighting (MW). The ranking placed solid phase extraction with micellar electrokinetic chromatography (SPE-MEKC) high as the most preferable analytical technique, while solid phase extraction coupled to ultra-high performance liquid chromatography tandem mass spectrometry (SPE-UHPLC-MS/MS) was placed last in the ranking. TOPSIS ranking results were also compared with generally accepted green metrics tools, i.e., NEMI, Eco-Scale and AGREE. The results show that AGREE metric tool correlated with TOPSIS, while no correlation was observed with NEMI and Eco-scale metric tools. The results show that TOPSIS is a very promising MCDA tool and can be successfully incorporated into green analytical chemistry to select the most preferable analytical procedure with respect to greenness assessment.

Acknowledgement
The authors acknowledge financial support from Chemistry Department and Institute for Nanotechnology and Water Sustainability, University of South Africa (Unisa)

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PG3 Efficient and selective oxidative transformation of aminophenols on titanium oxide supported bimetallic Ru-Au and Ru-Pd nanocatalysts

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Selective synthesis of aminoquinones and phenoxazinones from oxidation reactions of aminophenols plays an important role in fine organic synthesis. The products obtained from these reactions are vital molecules used in pharmaceutical and medicinal industries due to their biological activeness[1]. This work is focused on the selective oxidation of 2-aminophenols on titania supported Ru-Au and Ru-Pd catalysts that were prepared by microwave-polyol assisted methods. The physicochemical properties of the catalysts were determined by XRD, XPS, SEM, SEM-EDX, and TEM. The SEM and TEM micrographs of 1%Ru-1%Pd/TiO_2 catalyst showed the presence of metal NPs homogenously dispersed on the support surface (Figure 1a and b), and their identity was further confirmed by EDX analysis. The catalysts were tested for the oxidation of 2-aminophenol in different solvents with hydrogen peroxide as an oxidant at room temperature and under reflux (Figure 1b). It was observed that the catalysts' activities and selectivities highly depend on the type of solvent and catalyst, as well as temperature used. A yield of 94% 2-amino-3*H*-phenoxazin-3-one (APX) was obtained when using Ru-Pd catalyst in methanol at room temperature in comparison to 54% obtained on Ru-Au under the same reaction conditions. However, Ru-Au showed a significant catalytic activity when methanol was replaced with nitromethane, where a yield of 68% for APX was obtained. Low catalytic activities were obtained for both Ru-Pd and Ru-Au catalysts in acetonitrile under the same reaction conditions. In addition, monometallic catalysts possessed lower catalytic activities in comparison to Ru-Pd catalyst.

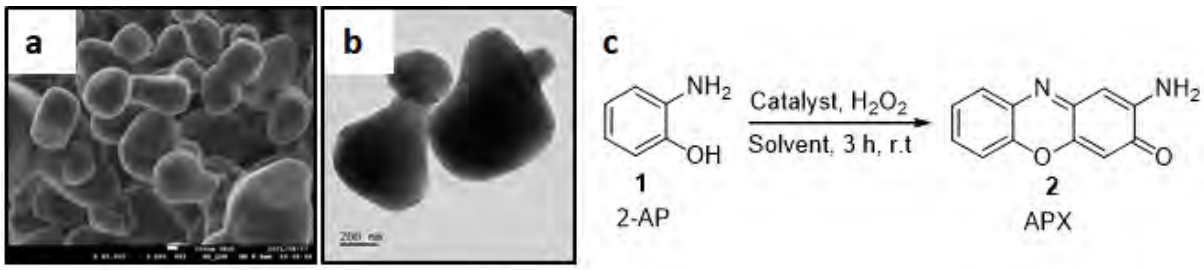

Figure 1: (a) SEM and TEM micrographs of 1%Ru-1%Pd/TiO_2 catalyst (a and b), and (c) reaction scheme for the oxidation of 2-aminophenols over noble metal catalysts in different solvents at room temperature and under reflux

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PG4 Graphene-Silver and Zinc Oxide Nanocomposites synthesized using mixed *Malus domestica* and *Solanum lycopersicum* extracts

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This study reports on the novel and simple green method involving the use of apple (*Malus domestica*) and tomato (*Solanum lycopersicum*) extracts in the synthesis of electroactive layers of silver nanoparticles|graphene oxide (AgNPs|GO) and zinc oxide nanoparticles|graphene oxide (ZnONPs|GO). The surface morphology of the green synthesized nanocomposites were studied using High-Resolution Transmission Electron Microscopy (HRTEM), High-Resolution Scanning Electron Microscopy (HRSEM) while the elemental analysis were studied using Fourier Transform Infrared Spectroscopy (FTIR), Raman spectroscopy and X-Ray diffraction (XRD) and their optical properties where further characterised using Ultraviolet Spectroscopy (UV-vis). The electrochemical studies of these nanocomposites was achieved using cyclic voltammetry (CV) where an increase in electron conductivity of the AgNPs|GO and ZnONPs|GO nanocomposite was observed an indication of their suitability as platforms towards sensor development. Comparatively, the silver nanoparticulate based platforms were observed to have superior electrochemical properties as opposed to the zinc oxide based platform.

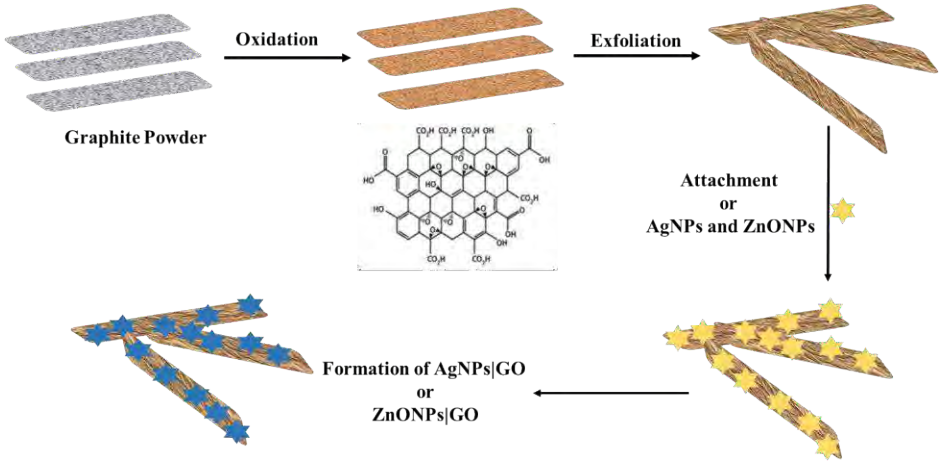

Figure 1: A representation of the green method for the synthesis of AgNPs/GO and ZnONPs/GO nanocomposites using a mixture of Malus domestica and Solanum lycopersicum extracts

PIND1 Characterization of PEM electrolyser oxidative evolution reaction catalysts

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Currently, the main source of hydrogen comes from carbon-based fuels. This defeats the objectives of green and renewable energy, where non-renewable carbon-based fuels are used, as well as contributing to the CO_2 emission. Hydrogen is the most efficient carrier. Hydrogen could be produced from various sources such as fossil fuels, such as natural gas (grey hydrogen) or by preventing the release of CO_2 emissions into the atmosphere but rather capture and store safely in underground tanks (blue hydrogen) and then there is green hydrogen. Green hydrogen is mainly produced from water electrolysers and utilizing renewable energy sources as power source to split water. This research paper will cover aspects of the characterization of OER (oxidative evolution reaction) catalysts to reduce the Iridium loading and to find alternative elements to ensure good reproducibility and hydrogen production through proton exchange membrane (PEM) Electrolyser. Various metal mixtures have been synthesized as Ir:Ru, Ir:Au and Ir:Ti. Characterization involves XRD, XRF, electrochemical techniques, and electrolysis to investigate long term efficiency and hydrogen production.

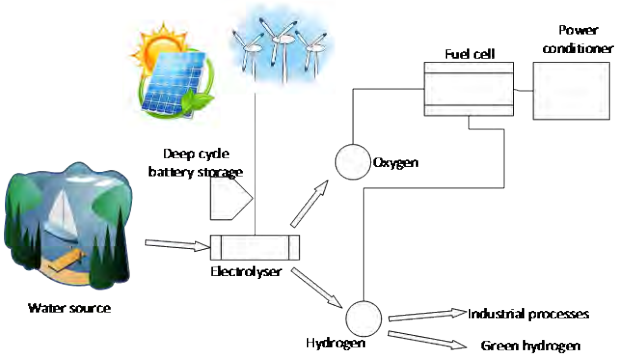

Figure 1

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PIND2 TiO_2–catalysed C–^{18}F bond formation from a ditosylated aromatic substrate and [$^{18}F^-$]fluoride: A model reaction

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Positron emission tomography (PET) is a nuclear medicine non-invasive imaging technology that provides real-time images of the biodistribution of a radioactive compound in vivo.[1] Information obtained from PET imaging may assist in disease diagnosis (eg: cancer, infection), monitoring patient therapeutic response and helping to validate drug targets.[2] Fluorine-18 (β^+ emission abundance = 96.7%, half-life = 109.8 min) is by far the most utilized positron emitting radionuclide in PET imaging, and generally gets incorporated into a targeting molecule through carbon–fluorine bond formation.[1,3] Currently, the challenge is to develop more efficient nucleophilic substitution reactions to form C–^{18}F bonds while overcoming inherent problems such as (a) the weak nucleophilic property of the fluoride ion in [^{18}F]fluoride/[^{18}O]water, and (b) the poor reactivity and selectivity towards the [$^{18}F^-$]fluoride ion of activated substrates such as electron-rich alkenes, aromatic and heteroatomic derivatives.[4] Herein, we report an S_NAr [^{18}F]radiofluorination reaction catalysed by TiO_2 in the presence of a reference aromatic ditosylated compound, methyl 2,6-bis(tosyloxy)benzoate, and [$^{18}F^-$]fluoride/[^{18}O]water to form an Csp^2—^{18}F (Ar–^{18}F) bond (**Figure 1**).[5] Application of this reaction will permit investigation of known aromatic fluorinated anticancer drugs by synthesizing their [^{18}F]radiolabelled analogues to develop radiotracers for diagnostic PET imaging purposes.

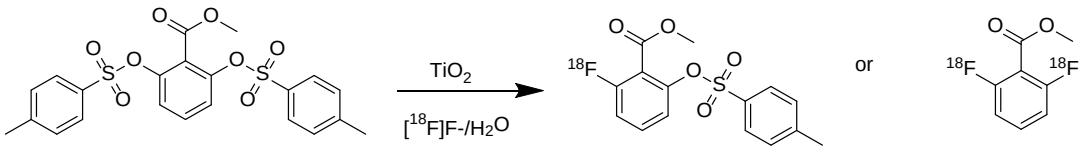

Figure 1: Proposed TiO_2-catalyzed formation of an Ar–^{18}F bond from a ditosylated model substrate.

Acknowledgements
NTP for project funding; PET Labs for provision of [^{18}F]fluoride/[^{18}O]water

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PI1 Towards Development of Ru-based Anti-cancer Drugs: Redox-mediated Interactions of Diruthenium Complexes with Small Biological Molecules

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Binuclear ruthenium complexes have emerged as propitious anticancer metallodrugs, owing to their stable topologies, adopting paddlewheel structural motifs, and have the ability to interact with biological small molecules.[1] As such, novel diruthenium, Ru_2^{5+} complexes bearing one equatorial anilinopyridinate (ap) and axial dansyl imidazole (DsIm) ligands $[Ru_2(O_2CCH_3)_3(Xap)(DsIm)_y]Cl$ where X = 2-F or 4-F and y = 1 or 2 were synthesised and characterised as to their spectroscopic and electrochemical properties. The UV-Vis spectra of the complexes displayed three major bands owing to metal to ligand charge transfer[2] while cyclic voltammograms revealed that the Ru_2^{5+} containing both anilinopyridinate and dansyl imidazole ligands were easier to reduce to Ru_2^{4+} compared to their respective precursors, bearing only the anilinopyridinate ligand. Paramagneticity of these Ru_2^{5+} complexes is confirmed by the 3 unpaired electrons determined *via* the Evans method.[3] Magnetic susceptibility measurements reveal magnetic moments of 3.28-3.30 μ_B. Upon reduction of these Ru_2^{5+} complexes by the glutathione (GSH) redox co-factor through binding (where K = 10^7-10^{10} M^{-1}), diamagnetic Ru_2^{4+} complexes are formed. Through an MTT assay screening, anti-cancer inhibition of the Ru_2^{5+} complexes against MCF-7 breast cancer cells is observed *in-vitro*. The bis-dansyl imidazole complex, having the lowest binding constant, shows superior anti-proliferative activity.

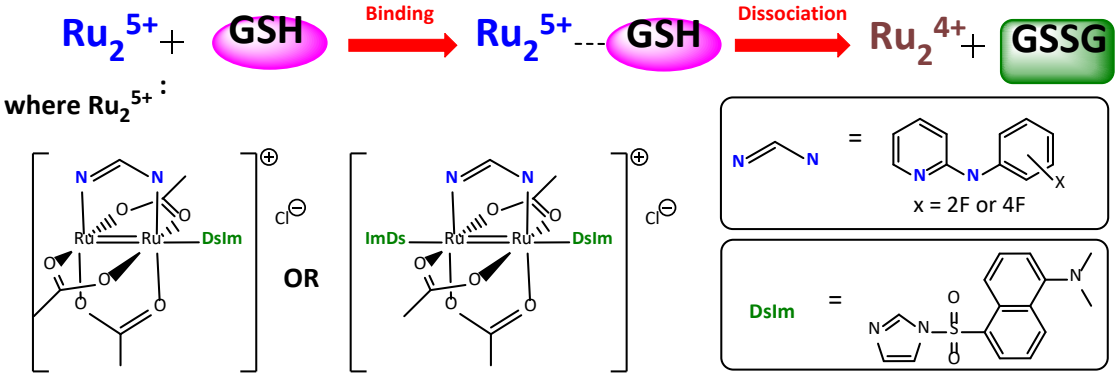

Figure 1: The proposed interactions of the Ru^{5+} complexes with GSH

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PI2 Biphasic hydroformylation and hydroaminomethylation catalysed by novel pyridyl-triazole rhodium complexes

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Amines are an important class of compounds that are widely used to prepare pharmaceuticals, dyes, and surfactants among other fine and bulk chemicals.[1,2] The syntheses of amines are generally performed via substitution reactions, which often result in low yields. Additionally, these processes generate toxic by-products due to the use of alkyl halides, resulting in the production of large amounts of waste.[1] This can be addressed using one-pot catalytic processes, such as the hydroaminomethylation (HAM) reaction, which allows for the synthesis of amines from widely available and affordable alkenes. A challenge of homogeneous catalytic processes, such as HAM, is the difficulty in recovering the expensive rhodium catalyst after the reaction. One solution is the use of aqueous biphasic systems, which have been successfully employed in HAM by various research groups. In this work, we developed a new aqueous biphasic system for the hydroformylation and HAM of olefins using novel water-soluble diimine Rh(I) complexes. Pyridyl-triazole ligands were synthesised from affordable starting materials via simple reaction procedures and were modified via the incorporation of a polyethylene glycol (PEG) tether to enhance their solubility in water. The complexes were successfully employed as precatalysts in the aqueous biphasic hydroformylation and HAM of 1-octene as a model substrate. Additionally, the recyclability of these complexes was investigated to evaluate their potential as environmentally friendly catalysts.

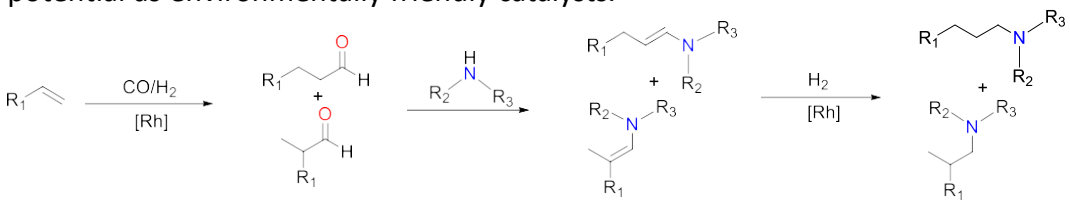

Figure 1: General reaction scheme for HAM of olefins.

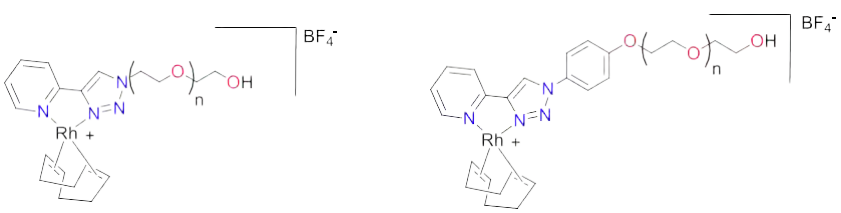

Figure 2: Structures of new pyridyl-triazole rhodium complexes (n = 1 or 2).

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PI3 Cationic Dirhodium(II,II) acetato-bipyridyl Chelate Complexes: Synthesis and Application as Catalytic Precursors for the Hydroformylation of 1-octene

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Heteroleptic dirhodium(II,II) complexes offer means of fine tuning key physicochemical properties for applications in various fields of research.[1] To this end, the synthesis of three dirhodium(II,II) acetato-bipyridyl complexes containing acetate (**1**-**3**) and hexafluorophosphate (**4**-**6**) counter ions is herein described. Each rhodium atom is chelated by a substituted bipyridyl ligand and bridged by the acetate ligands, shown in Figure 1. The acetate complexes were isolated through modification of reported methods[1] and obtained in excellent yields. Diffusion correlation spectroscopic (DOSY) analysis was employed for distinguishing acetyl proton signals. Anion exchange reactions of complexes **1**-**3** with ammonium hexafluorophosphate afforded complexes **4**-**6** in good yields.[2] Electronic effects imparted by the substituents on the bipyridyl ligands to the complexes (**1**-**6**) were evaluated by cyclic voltammetry. The synthesized complexes were evaluated as catalytic precursors in the hydroformylation of 1-octene and compared to $Rh_2(OAc)_4$ compound previously reported.[3] Expected conversion of the 1-octene substrate was observed for all tested compounds (**1**-**6**) under optimized conditions. Acetate counter ion involvement through rhodium axial binding were correlated to the chemo- and regioselectivity observed for catalyst precursors **1**-**3**. Furthermore, the electronic effects and influence of the substituent bound to the bipyridyl moiety on the activity, regio- and chemoselectivity is described. Post-reaction precipitation of the methoxy bearing compound (**6**) lead to a simplistic method of catalyst recyclability.

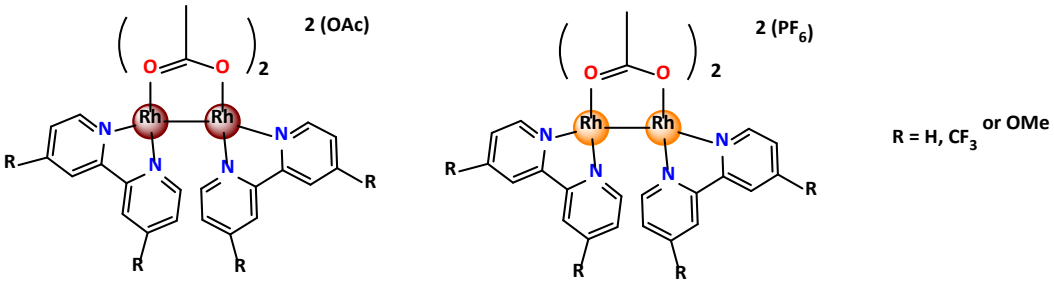

Figure 1: Structures of synthesized complexes containing OAc and PF_6 counter ions.

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PI4 Design and Synthesis of Hexose-Platinum Conjugates

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Cisplatin and other platinum drugs are an essential part of combination chemotherapy to treat cancer. The compounds bind to and crosslink DNA, thus initiating apoptotic pathways in cancer cells. While many patients exhibit high initial responsiveness to treatment, numerous side effects lessen the therapeutic value of these metallodrugs. When cancer cells grow at a high rate, they have an increased energy demand compared to non-cancerous cells; with that they need to facilitate an increased cellular uptake of energy sources, namely glucose, fructose, and galactose. Accordingly, many cancer cells overexpress hexose transporters, integral membrane proteins responsible for the transport of hexoses across cellular membranes. To focus the uptake of platinum drugs on fast-growing cells and by that to reduce deleterious side effects due to the interaction of the drugs with biomolecules other than DNA in cancer cells, hexose platinum conjugates that are potential substrates of hexose transporters are being synthesized. The conjugates consist of three domains, namely a transporter substrate, a spacer, and a chelant for platinum. A convergent synthetic approach makes it possible to independently vary these domains and to systematically study substrate-transporter and drug-DNA interactions. Several drug candidates have been synthesized and characterized.

Acknowledgements
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PI5 Ferrocenyl Aminoquinoline-benzimidazole Molecular Hybrids as Antiplasmodial Agents

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Malaria, one of the most striking infectious diseases, is caused by several *Plasmodia* species. *Plasmodium falciparum*, in particular, is the most virulent strain and responsible for the greatest number of malaria-related deaths globally. Quinoline antimalarials have proven to be a vital part of the chemotherapeutic armory against this disease. However, despite the various treatment regimens available, the increasing threat of drug resistance has prompted investigations into alternative approaches toward antimalarial drug design. To circumvent this rising resistance, the molecular hybridization of biologically important pharmacophores, such as the quinoline and benzimidazole scaffolds, has proven to be a fruitful avenue within drug discovery, with quinoline-based hybrid compounds shown to be a promising new class of antiplasmodial agents.[1] Additionally, metal incorporation, which is exemplified by the antimalarial drug candidate, Ferroquine (FQ), has also been extensively explored.[2] Despite its structural and biological similarities with chloroquine, FQ has demonstrated remarkable activity, notably against resistant forms of the *Plasmodium* parasite. The incorporation of the ferrocene moiety was shown to impose an additional mechanism of action and thus the potency of FQ is attributed to its dual action mechanism.[3] This presentation will highlight the concepts of both molecular hybridization and metal incorporation used to design of a series of bioorganometallic ferrocenyl aminoquinoline-benzimidazole hybrids.[4] The investigation into their *in vitro* antiplasmodial activity, as well as putative mechanistic studies will also be discussed.

Acknowledgements
Financial support from the University of Cape Town and the National Research Foundation of South Africa.

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PI6 Cationic Decoration of Single Walled Carbon Nanotubes (SWCNTs) with Cationic Porphyrins for the Potential Treatment of Cancer

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In sub-Saharan Africa, with about 1 billion people, cancer is a public health concern. The disease is one of the top three causes of premature mortality (i.e., between the ages of 30 and 69) in almost every member state responsible for 1 in 7 premature deaths overall and 1 in 4 fatalities from non-communicable diseases. The purpose of this study was to decorate SWCNTs with cationic porphyrins for optimization as photodynamic cancer agents [1]. SWCNTs have shown an interesting potential as photothermal agents in the treatment of cancer. In this study, two different cationic porphyrins: 5,10,15,20 tetrakis amino porphyrin and 5,10,15,20 tetrakis pyridyl porphyrin were synthesized using a combination of the Alder Longo and Lindsey methods to obtain optimised results[2]. Due to their and to increase biocompatibility, the SWCNTs were functionalized with polymer carboxylic acid functional group. The SWCNTs-porphyrins conjugates were synthesized, and the electronic properties were determined by various methods (UV-Vis, PL, FTIR), and the morphology (SEM, /HRTEMTEM) of the materials analysed. The TEM micrographs show and verify that the porphyrins form aggregated poly-disperse nano-crystalline structures of both TAP and TPyP. Microanalyses confirms the elemental composition of the nanoconjugates. The nanoconjugates displayed intriguing properties with high potential to be used as photodynamic agents.

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PI7 Electrochemical Water Oxidation Catalyzed by *N*-(pyrazol-1-ylmethyl) pyridine-ligated Mn(I) Complexes

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Society depends on fossil fuels for energy production, but the combustion of hydrocarbons produces CO_2, a known greenhouse gas, as a waste product.[1] Therefore the development of sustainable energy production based on carbon-neutral sources is of continuing interest.[1,2] Artificial photosynthesis, which converts renewable energy sources to chemical fuels, is a promising alternative to the use of fossil fuels.[3-5] Electrolysis of water by the electrochemical hydrogen evolution reactions (HER) is a more valuable and proficient method to produce H_2 because it is of low cost and pollution free. The key point of electrochemical water splitting to produce hydrogen is that its kinetics is slow. To enhance the H_2 production, the HER kinetics need to be faster and for that an efficient electrocatalyst is required which must be earth-abundant and cost-effective. In the last decade, there has been increased interest in molecular catalysts for electrocatalytic water oxidation that are based on first-row transition metals. In particular, manganese catalysts are of interest and have shown potential in the development of efficient electrocatalytic water oxidation catalysts[6], however, there is still a lack of electrochemically driven water oxidation processes employing manganese complexes. Herein, we report on the synthesis, characterization and electrochemical water oxidation of pyrazolyl-pyridine ligated manganese complexes with different substituents. We envisaged that this characteristic offers the potential to fine-tune the metal's electrophilicity, hence modulating the reactivity of these complexes.

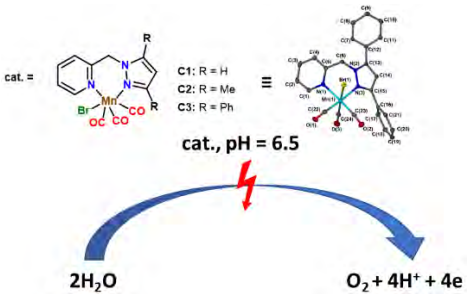

Figure 1: Electrochemical water oxidation using Mn(I) complexes

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PI8 A Copper-decorated Porphyrin-containing Porous Organic Polymer as Catalyst Precursor in Oxidation Reactions

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The manufacturing of high-end fine chemicals from fossil fuel reserves such as natural gas and coal has become a major concern due to the negative effect it has on the environment. There is a need to shift our attention to renewable resources such as biomass valorization. Lignin is a source of biomass and has shown great potential as a renewable resource towards value-added products. Although a fair number of examples have been reported in the literature, lignin remains under-explored and further research is required to fully understand the valorization of lignin.[1–4] In this presentation, the synthesis and characterization of a porous organic polymer containing porphyrin units within the polymer backbone are discussed. Subsequently, we employed the copper-coated POP as catalyst precursor in oxidation reactions. Herein, we discuss the optimization of various parameters for both activity and selectivity. Our results have shown that a range of biomass derived substrates were converted to the corresponding aldehydes and carboxylic acids. In addition to this, the copper-decorated POP exhibited excellent recyclability for up to five subsequent runs with minimal loss in activity.

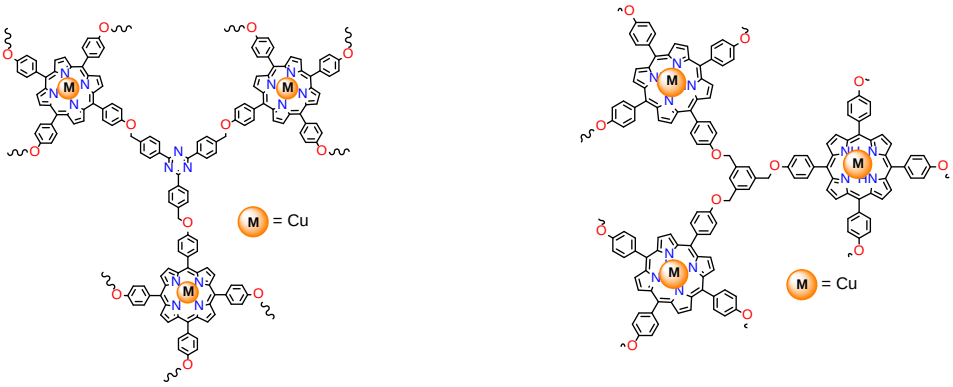

Figure 1: Porous organic polymer containing porphyrin moieties.

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PI9 Improving the Stability of $CsSnBr_3$ Perovskite Nanocrystals by Ag Doping for High-performance Photovoltaics

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Inorganic tin-halide perovskites, $ASnX_3$ (A = Cs^+ and X = Br^-, I^- or Cl^-), have captured broad interest as promising alternatives to lead-halide perovskites in photovoltaics because of tin's reduced toxicity compared to lead.[1] Sn-based perovskite have similar optoelectronic properties as their lead-based counterparts but also feature narrower band gaps, which make them more suited for photovoltaic applications.[1–3] However, their poor stability impedes their overall performance. The poor stability arises from the rapid oxidation of Sn^{2+} into its most stable Sn^{4+} state when exposed to ambient conditions.[1-3] Studies have been conducted to overcome the poor stability of the tin-based perovskite materials and doping the lattice of inorganic perovskites with specific atoms was reported to be a relatively effective strategy for solving this issue while providing additional tunable electrical and optical properties.[3,4] In this work, monovalent silver cations (Ag^+) were doped into the lattice of $CsSnBr_3$ perovskite nanocrystals via the colloidal hot injection method. The effect of the Ag^+ cations on the structure (X-ray diffraction), morphology (Transmission electron microscopy), and optical (photoluminescence spectroscopy) properties of the $CsSnBr_3$ perovskite nanocrystals. Our findings showed that the incorporation of Ag^+ cations into the $CsSnBr_3$ does not destroy their lattice and their cubic morphology was preserved. Notably, all the Ag-doped nanocrystals present better air stability than the pure perovskite nanocrystals.

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PI10 Synthesis of Ferrocenyl-benzimidazole Derivatives

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With the constant threat of malaria infections in high-risk areas as well as growing resistance of the parasite to available antimalarial drugs, the development of new therapeutic agents is a necessity.[1] Researchers have suggested developing new drugs combining different known active pharmacophores in an attempt to discover new compounds with better antiplasmodial activity. [2] One such drug is ferroquine, a derivative of prophylactic and therapeutic drug called chloroquine. Ferroquine, a hybrid of the active antimalarial chloroquine and a ferrocenyl group, has been extensively studied and was found to have better efficacy than its parent drug chloroquine against resistant strains.[3] The strategy of conjugating metals to known pharmacopores is a strategy that continues to be studied. In this presentation, the design and synthesis of hybrid complexes of benzimidazole and ferrocene (Figure 1) complexes will be discussed. These complexes contain a ferrocene moiety, a potent organometallic known to induce improved biological and anticancer properties when hybridized with certain organic scaffolds.[4] Benzimidazole derivatives are a class of compounds which have also been widely studied and have shown antimalarial properties.[5-7] The ferrocenyl-benzimidazole complexes were synthesized and characterized using typical analytical techniques. Their stability, chemical reactivity and antiplasmodial activity will be studied at a later stage.

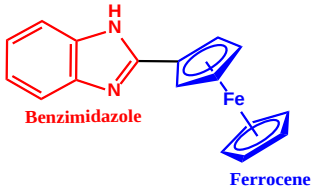

Figure 1: Ferrocenyl benzimidazole derivative.

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PI11 Synthesis and Characterization of Dipyrromethenes as Possible Probes for the Quantification of Bilirubin Pigments

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2,2'-Dipyrromethenes (dipyrrins) are a class of basic, generally planar, fully conjugated and vibrantly colored compounds comprising two pyrrole rings joined by a methyne bridge (Fig 1a).[1] Dipyrrins (and transition metal complexes thereof) have garnered research interest due to their predictable coordination chemistry and favorable fluorescent properties.[1] These properties are what make them an attractive option to be explored as fluorescent probes for the quantification of bilirubin pigments (Fig 1b). The quantification of bilirubin pigments is challenging for several reasons, one of which is the stability of suitable probes.[2] We thus aim to screen a series of metal-ligand complexes as possible probes for the reliable quantification of bilirubin pigments, starting with a selection of metal-dipyrrins complexes. This *preliminary* work reports on the successful synthesis and spectroscopic characterization of selected *meso*-substituted dipyrrin precursors, dipyrromethanes, (5-phenyl dipyrromethane; 5-(4-hydroxyphenyl) dipyrromethane; 5-(4-nitrophenyl) dipyrromethane;), dipyrrin ligands (5-(4-hydroxyphenyl) dipyrromethene; 5-(4-nitrophenyl) dipyrromethene); and metal-dipyrrin complexes (tris[5-(4-hydroxyphenyl)-4,6-dipyrrinato]Co(III)). Ligands and complexes were synthesized using methods adapted from Dolphin *et al.*,[1] and characterized by spectroscopy (NMR, UV-Vis, LCMS, IR), melting point analysis and crystallography (Fig 1c).

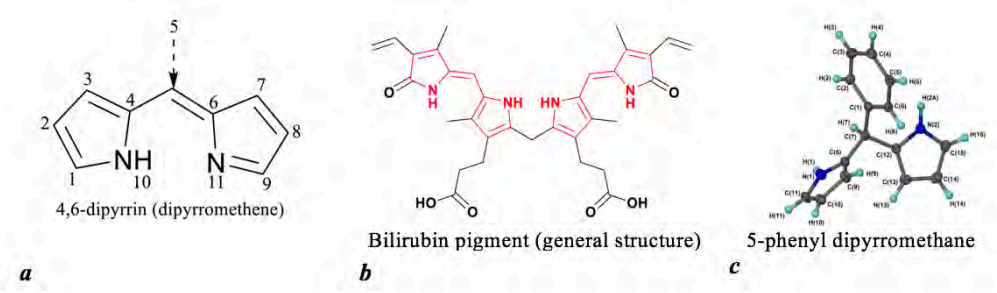

Figure 1: (a) general structure of dipyrromethene ligands (dipyrrins) *meso*-position; (b) general structure of bilirubin pigments; (c) crystal structure of 5-phenyl dipyrromethane from this work

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PI12 A Zinc-Based 3D Mixed Ligand Metal-Organic-Framework with Stepwise CO_2 Adsorption at Low Temperature

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The need to replace the current energy generation from burning fossil fuels that pollute the environment and the need to mitigate rising CO_2 levels in the atmosphere has spurred an interest in green technology.[1] Hydrogen is a potential fuel because of its huge energy content, clean combustion, and zero CO_2 emission.[2] However, the hydrogen fuel cells system is not applicable without safe and sufficient storage materials. Metal-organic frameworks (MOFs)[3] are potential physisorption candidates for hydrogen storage owing to their unique structures.[4,5] MOFs are organic-inorganic hybrid materials composed of metal ions and organic ligands.[6] We report the synthesis, crystal structure, and gas (CO_2, H_2, and N_2) sorption studies of a mixed-ligand 3-D MOF, namely, $\{[Zn_2(OBZ)_2L1]\cdot 3DMF\}_n$ (**1**), where L1 = *N*, *N*'–bis–(3-pyridylmethy)–biphenyl di-imide, OBZ = 4,4'-oxybis(benzoic acid), and DMF = *N, N*'-dimethylformamide. **1** has a solvent-accessible volume of 31.5% and maintains crystallinity with activation at high temperatures. CO_2 sorption capacity of 1 was investigated at 195 K, 273 K, 283 K and 298 K and it was found that **1** adsorbs 120 $cm^3\ g^{-1}$ (STP) at $P/P°$= 0.90, 15.1 $cm^3\ g^{-1}$ (STP) at 0.030 $P/P°$, 15.1 $cm^3\ g^{-1}$ (STP) at 0.030 $P/P°$ and 8.55 $cm^3\ g^{-1}$ (STP) at 0.017 $P/P°$, respectively. At 195 K, **1** displays a reversible type-IV isotherm with stepwise CO_2 adsorption. The hysteresis could be indicative of a structural transformation during sorption. H_2 sorption experiments at 77 K show that the MOF adsorbs approximately 3.00 $cm^3\ g^{-1}$ (STP) H_2 at 1.98 $P/P°$, displaying a reversible type-I behaviour with some degree of hysteresis. The MOF also adsorbs 11.99 $cm^3\ g^{-1}$ (STP) N_2 at 1.02 $P/P°$ and displays a reversible type-II sorption isotherm.

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PI13 Synthesis, Spectroscopic Characterization and Crystal Structures of Lead(II) Dithiocarbamates: Structural and Photocatalytic Studies of PbS Nanophotocatalysts from the Complexes

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We report the preparation and characterization of lead(II) dithiocarbamate complexes and their use as single-source precursors for the photocatalytic degradation of organic dyes. Lead(II) dithiocarbamate complexes were prepared and characterized using spectroscopic techniques and some by single crystal X-ray crystallography.[1, 2] The infrared spectra studies confirmed bidentate coordination of the dithiocarbamato anions to the lead(II) ions to form four coordinate tetrahedral complexes. The single crystal structures of bis(4-methylpiperidine-1-carbodithioato)-lead(II) and bis(4-benzylpiperidine-1-carbodithioato)-lead(II) revealed mononuclear lead(II) compounds in which each lead(II) ion coordinates two dithiocarbamato anions in a distorted tetrahedral geometry.[1] The lead(II) dithiocarbamate complexes were thermolyzed at 180℃ in different capping agents to study the influence of the precursor and capping agents on the structural and optical properties of the PbS nanoparticles. Powder X-ray diffraction patterns of the PbS nanoparticles are indexed to the face-centered cubic phase of PbS. High-resolution transmission electron microscopy micrographs revealed varying shapes from quasi-spherical to cubic shapes with particle sizes in the range of 14-130 nm. The optical studies revealed that the PbS nanoparticles are quantum confined as the calculated energy band gaps show a blue shift relative to the bulk. The as-prepared PbS nanoparticles were used as nano photocatalysts to degrade methylene blue, rhodamine B, and phenol. The photodegradation efficiencies of 47-75% for methylene blue, 30-45% for rhodamine B, and 11-32 % for phenol were obtained. The photocatalytic studies show a correlation between degradation efficiency and morphological properties of the as-prepared lead sulphide nanoparticles. The effect of pH on the degradation of the organic dyes by the as-prepared nanoparticles was investigated, and it was found that the degradation efficiency increases with an increase in pH. The PbS nanoparticles were found to be recyclable up to four cycles of photocatalytic reaction with good stability.

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PI14 Hydroformylation of 1-octene using Phosphine-based Dirhodium(II) Adducts as Catalysts

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Precursor dirhodium(II) complexes, $[Rh_2(OAc)_4]$ and $[Rh_2(TfOAc)_4]$ (**C1** and **C2**) were reacted with either triphenylphosphine or triphenyl phosphite towards the preparation of a series of phosphine $[Rh_2(OAc)_4(PPh_3)]$, $[Rh_2(TfOAc)_4(P(OPh)_3)]$ (**C3** and **C4**) and phosphite $[Rh_2(OAc)_4(PPh_3)]$, $[Rh_2(TfOAc)_4(P(OPh)_3)]$ (**C5** and **C6**) adducts.[1,2] These complexes were fully characterised as to their spectroscopic and electrochemical properties. Catalytic activity of the complexes in the hydroformylation of 1-octene was evaluated under 50 bar syngas (H_2/CO) pressure at 95 ^oC. Product distribution favours the formation of aldehydes and iso-octenes as major products, without formation of any alcohol products. Complexes **C1** and **C2** show complete conversion and selectivity towards aldehydes and favour the formation of branched aldehydes.[3,4] The regioselectivity of products catalysed by the triphenylphosphine (**C3** and **C4**) and triphenyl phosphite (**C5** and **C6**) adducts is towards the formation of linear aldehydes to a 1.86 *n/iso* ratio, while retaining the conversion and activity like **C1** and **C2**. Mercury-drop tests indicate that the trifluoroacetate complexes (**C2**, **C4** and **C6**) acts as homogeneous catalysts while the acetate derivatives (**C1**, **C3** and **C5**) are active in a combination of homogeneous and heterogeneous catalysis.[5]

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PI15 Synthesis and Characterization of Iron Oxide Nanoparticles for Potential Application in Photothermal Therapy and Magnetic Hyperthermia

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Conventional cancer treatment techniques such as chemotherapy and radiation therapy are highly invasive and may result in harsh side-effects such as anaemia, hair loss and fertility problems[1]. Minimally invasive treatment techniques such as photothermal therapy and magnetic hyperthermia possess improved efficacy and selectivity[2,3]. Herein, we report facile synthesis of iron oxide nanoparticles and their characterization for potential application in photothermal therapy and magnetic hyperthermia. Iron oxide nanoparticles were synthesized by a co-precipitation method in which a weak base was used to precipitate iron(II) and iron(III) salts in solution in a 1:1 mole ratio. The reactions were carried out at different temperatures and precursor concentrations to evaluate the influence of temperature and precursor concentration on the spectroscopic and morphological properties of the nanoparticles. TEM analysis revealed various shapes including quasi-spherical and rod-like iron oxide nanoparticles. Powder X-ray diffraction patterns confirmed that the iron oxides nanoparticles are in magnetite (Fe_3O_4) crystalline phase. The mean particle sizes and the particle size range of the iron oxide nanoparticles increased with increasing precursor concentration, with average particle sizes ranging between 8.9 and 10.1 nm and band gaps from 3.21 to 4.75 eV. The particle sizes varied directly with reaction temperature, from 9.4 to 33.8 nm while the length of the obtained iron oxide nanorod is 125 nm. The band gaps also increased from 4.31 to 4.76 eV with increasing temperature.

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PI16 Synthesis and Characterization of Nickel Catalysts for the Hydrogenolysis of Erythritol

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The global community is tasked with coordinating and co-operating to find innovative solutions for clean energy from renewable energy sources. This urgency stems from the detrimental effects traditional means of harnessing energy from fossil deposits, such as coal, have on the environment and climate. Sugar alcohols, such as erythritol, are profusely oxygenated compounds that present an opportunity for tailored and selective deoxygenation to useful platform chemicals, such as butanediols, through the scission of C-C and C-O bond hydrogenolysis reactions.[1] Catalysts for hydrogenolysis reactions must have the ability to activate hydrogen, one of the key reactants, which is activated over a metal surface. Hydrogenolysis catalysts consisting of a base metal (Ni, Co, Cu etc.) promoted or mixed by a noble metal (Pt, Pd, Rh, Ru, etc.) supported on stabilized supports (alumina, ceria, etc.) are critical for the hydrogenolysis of erythritol to useful chemicals. Ni-W/Al_2O_3 catalysts were synthesized *via* wet impregnation, co-precipitation and sol-gel methods.[2] Catalysts were calcined and characterized by ICP-OES, PXRD, N_2 physisorption, Raman spectroscopy, TPR and SEM and TEM. The catalysts will be tested in a high-pressure autoclave for the hydrogenolysis of erythritol.

Acknowledgements
I would like to acknowledgement grant funding from the DSI-NRF Research Development Grants for New Generation of Academics Programme (nGAP) Scholars and Walter Sisulu University.

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PI17 Development of New Antimalarial Ferrocenyl-Artesunate Complexes

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The use of artemisinin-based combination therapy has quickly become the main intervention in the fight against malaria but rising resistance has led to the need for new treatments.[1] In this presentation, the preparation of four novel ferrocenyl-artesunate complexes with varying ester and amide linkers and their characterisation using a variety of techniques will be discussed. The complexes' stability and solubility in organic-aqueous mixtures were also determined using UV-vis spectroscopy, HPLC and turbidimetric assays. The complexes were tested for their ability to inhibit the growth *P. falciparum* and *T. gondii*. For the search of drugs with alternative mechanisms of action, *Toxoplasma gondii* is an important model for Apicomplexa parasites.[2,3] Thus, *T. gondii* was used to determine the potential mechanism of action (MoA) for the ferrocenyl-artesunate derivatives prepared. The three complexes tested against *T. gondii* were able to inhibit the growth with EC_{50} values ranging from 0.596 to 1.18 µM. Immunofluorescence assays were used to monitor physiological changes and revealed an unusual and novel mode of death of the parasite. CellROX stained cells counted using flow cytometry were used to assess the presence of reactive oxygen species (ROS) and the relationship between the EC_{50} values and ROS production was determined.

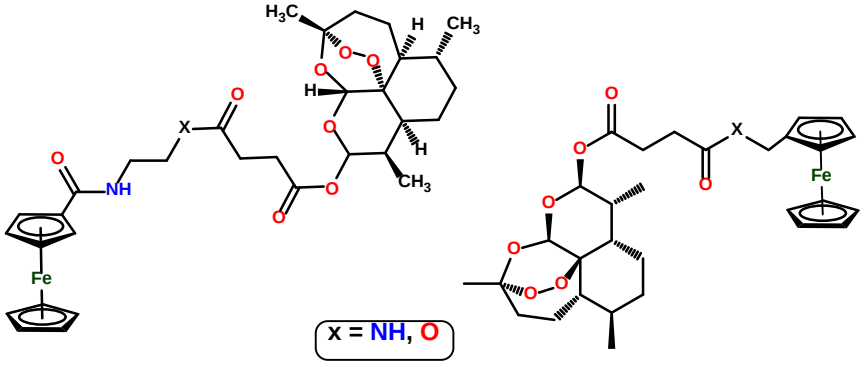

Figure 1: Structures of synthesized ferrocenyl-artesunate complexes.

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PI18 Synthesis, Characterization and Bioactivity Studies of Novel Salen-based Ruthenium Complexes

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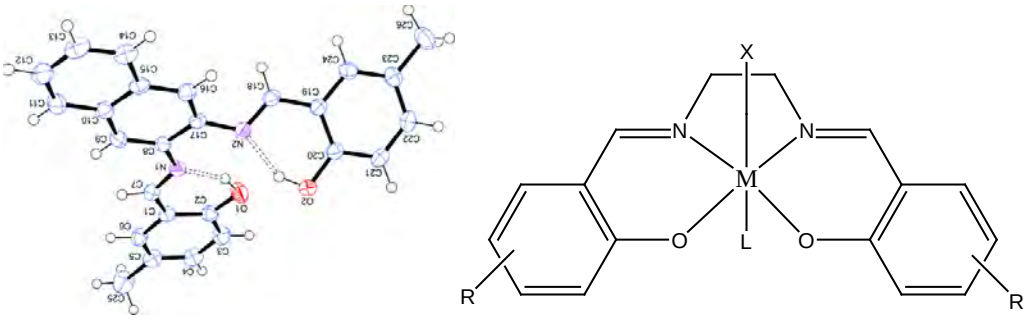
The reported success and shortcomings of platinum based drugs, such as Cisplatin, has been a driving force towards the further development of metallodrugs. Research has shown ruthenium complexes to be feasible alternatives to Pt(II) anticancer drugs because they have a similar kinetic spectrum of ligand substitution in aqueous medium; a key property for anticancer activity.[1] In this work a series of novel salen based ligands (Figure 1a) have been synthesized and characterized using a range of spectroscopic techniques in addition to X-ray crystallography. Additionally, the corresponding ruthenium complexes (Fig. 1b) have been synthesized and fully characterized. DNA binding studies using spectroscopic titrations, for both ligands and complexes have been conducted, in order to understand their possible interaction with CT-DNA. The results obtained predict that both ligands and complexes interact with DNA, possibly via an intercalative mode; and this might be the possible mode of action for these complexes. However, additional work is required to determine the possible mode of action; which may include the ability of the synthesized compounds to induce apoptosis and produce reactive oxygen species. Bioactivity studies of the synthesized compounds against cancer cells as well as anti-malarial and anti-tuberculosis activity studies are planned. Lastly, structure-activity relationships will be explored using density functional theory and molecular docking methods.



(a) (b)

Figure 1: The class of salen ligands (a) and coordination complexes (b) under investigation
M = Ru (III); X = Cl; L = Phosphine ligand; R = alkyl or aromatic groups

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PI19 A Comparative Study of Calcined and Uncalcined VOx/MgO Catalysts Prepared via Solution Combustion Synthesis

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VMgO catalysts are considered as good candidates for the oxidative dehydrogenation of long-chain alkanes such as n-octane[1]. The method of preparation of these catalysts is critical as it influences the phases of magnesium vanadates formed[2]. Solution combustion synthesis using glycine as a fuel was chosen for the preparation of the material based on the superior structural and morphological properties of the catalysts reported previously[3]. The effects of calcination and calcination temperature on the structural and morphological characteristics of vanadia based material is reported [4].The aim of the present work was to compare the effect of calcined and uncalcined VOx/MgO catalysts prepared via solution combustion synthesis on the structural and morphological properties of the material. These catalysts may be applied in the oxidative dehydrogenation of *n*-octane. The catalysts were prepared via solution combustion synthesis. Ammonium metavanadate was first dissolved separately, which was followed by addition of stoichiometric amounts of glycine and magnesium nitrate hexahydrate in distilled water. Solutions were then introduced into a muffle furnace heated at 400 ◦C for 1 h, which was kept constant for a further 2 h. The formed powders were then ground and calcined at 500 ◦C for 6 h. The diffraction patterns showed peaks attributed to MgO as periclase. Several reflections on the calcined samples indicated the presence of magnesium orthovanadate ($Mg_3(VO_4)_2$) and magnesium pyrovanadate ($Mg_2V_2O_7$) phases. The surface areas and crystallite sizes of the catalysts varied, which indicated that they are different in textural properties. The surface areas ranged from 5.19 to 78.81 m^2g^{-1}. Also, the porosity was relatively higher on the uncalcined catalysts which indicated a positive effect on the porosity as a result of treating MgO under vacuum. Thermal analysis indicated that calcined VOx/MgO catalysts demonstrated a lower mass loss compared to the uncalcined catalysts. Scanning Electron Microscopy will share information on the structural morphology of the supports and catalysts, while Transmission Electron Microscopy will be used to determine structural morphology, shape and size of the material.

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PI20 Spectral Analysis and Antibacterial Activities of Oxovanadium(IV) and Zinc(II) Coordination Compounds

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Herein, four mixed ligand metal complexes of [VO(sfz)(eh-dtc)] (**1**), [VO(sfz)(ea-dtc)] (**2**), [Zn(sfz)(eh-dtc)], (**3**) and [Zn(sfz)(ea-dtc)] (**4**) (where ligands: sfz (L_1) is sulfadiazine. (sfz; L_1), eh-dtc (L_{21}) is ammonium hydrazine hydrate, and ea-dtc (L_{22}), is sodium hydrazine hydrate) were synthesized using one pot synthesis[1]. Ligands and metal complexes were successfully characterized with FT-IR, melting point (MP), molar conductivity, NMR (^{1}H NMR and ^{13}C NMR) and UV-Vis techniques[1,2]. Antibacterial activities of studied compounds against gram positive and gram negative bacteria showed that ammonium based mixed oxovanadium(IV) and zinc(II) complexes were more active (higher zone of inhibition (ZOI)) than sodium based mixed oxovanadium(IV) and zinc(II) complexes, except in gram positive PA01. Progressively for antibacterial activities, minimum inhibition concentration (MIC) results confirmed ammonium based compounds as best active MIC inhibition, while sodium based compounds as moderate MIC inhibition[2]. The significance of this study is in support of the third 2030 Sustainable Development Goals (SDG) and to control prevalent bacterial disease.

Acknowledgements
Authors appreciate South African Chemical Institute (SACI) and Govan Mbeki Research and Development Centre (GMRDC) for the financial assistance.

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PI21 Synthesis, Characterization and Anticancer Potentials of Palladium(II) and Organoruthenium(II) Dithiocarbamate Complexes

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The development of potent therapeutic agents against cancer have been an active area of research in the past decades [1]. The success of metal-based drugs, such as *cis*platin and its analogues as therapeutic agent for cancer has renewed interest in the development of other metallodrug candidates [2-3]. This is necessary to address inherent problems associated with the current cancer drugs such as non-specificity, toxic side effects and emergence of drug resistance [4]. In this study, we report the synthesis of dithiocarbamate ligands and their corresponding homoleptic Pd(II) and heteroleptic organoruthenium(II) dithiocarbamate complexes. Their anticancer potential were evaluated against cervical, breast adenocarcinoma, epithelial colorectal adenocarcinoma and lung cancer lines. Each Pd(II) is coordinated to two chelating dithiocarbamato anions while the organoruthenium(II) complex form a classic three-legged piano-stool arrangement with a pseudo-tetrahedral geometry. Two of the Pd(II) complexes are very potent against three cancer cell lines and are more active than the corresponding dithiocarbamate ligands whereas the anticancer potency of two dithiocarbamate ligands are higher than the corresponding Pd(II) complexes. The organoruthenium(II) complexes are potently cytotoxic against two cancer cell lines, HeLa and MRC5-SV2, models of cervical and lung cancer, respectively, and in some instances better than standard platinum-based anticancer drug (*cis*platin) highlighting the anti-cancer prospect of the compounds.

Acknowledgements
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PI22 Synthesis and Characterization of Ferrocenyl Tetrahydrofuran/Tetrahydropyran Oxalato Platinum (II) Complexes

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Platinum II metallodrugs (cisplatin, carboplatin, and oxaliplatin) have been hailed for their high success in clinics; however they are compromised mainly by drug resistance and side effects.[1] Incorporating bioactive pharmacophores into metal centres has emerged as an excellent strategy to enhance their bioactivities and modulate the toxicities. We are interested in oxygen-heterocycles, tetrahydrofurans (THFs) and tetrahydropyrans (THPs), the common scaffolds in natural products and bioactive compounds.[2,3] In this work, we report the synthesis and characterization of platinum II complex bearing ferrocenyl THF/THP and oxalato ligand. Ferrocene-conjugated heterocyclic compounds also play crucial role in medicinal chemistry, and therefore we hypothesize that the complex will exhibit synergistic effects. The steps involved in synthesizing of platinum complexes are shown in the Scheme below. To prepare the ligands of choice (THF **10** and THP **5/6**), the key intermediate (homoallylic alcohol **2**) was synthesized in good yields (a: 80%, b: 93%). A series of steps were subjected to the homoallylic alcohols including dihydroxylation, tin-mediated sulfonylation, mesylation, azidation, and Staudinger reduction to prepare the amino THFs (a: 85%, b:78%). While the key steps in synthesizing THPs includes allylation, Grubbs-metathesis, and alkene-amination; this is a short route to obtaining THPs and gives much better yields. Platinum complexes were synthesized *via* Dhara's synthetic approach where K_2PtCl_4 is first converted to PtI_4^{2-} before coordinating the amine ligands, to take advantage of the *trans* effect of the iodo ligand. S-methylbenzylamine was used as a model ligand for the synthesis of platinum complexes, and intermediate **11** was obtained in good yields (80%), while final complex **12** was obtained in 40% yields. All the synthesized compounds were characterized by IR and NMR (1D & 2D).

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PI23 The electronic effect of the cyclo schiff base *N*-donor monodentate ligand systems on the inert *fac*-$[re(co)_3]^+$ synthon

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Chelators (ligands) take an intergral part in the development of late transition metal complexes mostly for nuclear imaging, cancer therapeutic, photodynamic therapy (PDT) and more. Therefore, due to the ideal nuclear properties of the two radionuclides of rhenium, ^{186}Re ($t_{1/2}$ = 90 h; Emax = 1.07 MeV) and ^{188}Re ($t_{1/2}$ = 17 h; Emax = 2.12 MeV), complexes of this metal are high-energy beta emitters that find growing applications mentioned above. Furthermore, the tricarbonyl synthon of this metal, *fac*-$[Re(OH_2)_3(CO)_3]^+$ is versatile and can accommodate a wide range of ligand systems (bidentate and monodentate) through a [2 + 1] mixed ligand model to saturate the metal coordination sphere.[1-3] Herein, synthesis, single-crystal X-ray diffraction of a cyclo-schiff base pyrazole monodentate ligand and density functional calculations of the corresponding Re(I) tricarbonyl complexes are presented.

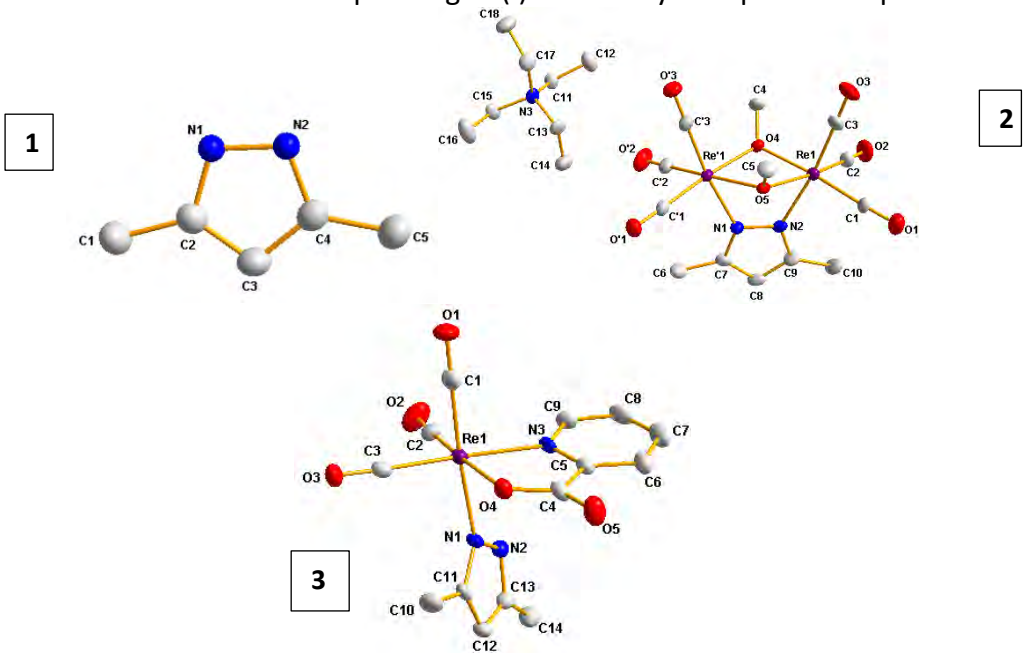

Figure 1: Solid state crystal structures of chelator **1** and Re(I) complexes **2** and **3**

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PI24 Cu_2ZnSnS_4 Reinforced on Hollow Carbon Spheres for Application in Dye Sensitized Solar Cells

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Dye-sensitized solar cells (DSSCs) have enticed significant attention owing to their low fabrication cost, easy fabrication process, and excellent performance under diffuse light conditions[1]. Platinum is generally used in DSSCs as a counter-electrode catalyst due to its favourable catalytic activity toward electrolytes such as iodide/triiodide (I^-/I^-_3) redox couple. Irrespective of the attractive properties, platinum is expensive, and it tends to form platinum (IV) iodide in iodide/triiodide electrolyte hence its advantages become limited[2-3]. In pursuit of finding alternative counter electrode catalysts that may achieve comparable electrocatalytic activities as the commonly used platinum catalysts in DSSCs, Copper Zinc tin sulfide (Cu_2ZnSnS_4) nanocrystals have been reported as competent electrocatalytic material. Agglomeration of nanomaterials is known to be one of the factors responsible for the reduction in catalytic activity[4]. The incorporation of a support was used to decrease the metal agglomeration. Herein, we report on the synthesis of hollow carbon spheres (HCS) using SiO_2 as the sacrificial template and resorcinol as the carbon source. Cu_2ZnSnS_4 nanocrystals with 25%, 50%, and 75% percentage loading were supported on the hollow carbon spheres. The three materials were characterized using UV-vis spectroscopy, Raman spectroscopy, TEM, SEM, and PXRD. The morphology of the nanocrystals displayed an irregular spherical shape. Additionally, the nanocrystals were polydispersed and had extreme agglomeration. The TEM images of the hollow carbon spheres exhibited homogeneously shaped carbon spheres interlinked with each other at the surfaces of the spheres. The PXRD sizes of the Cu_2ZnSnS_4@HCSs displayed an increase in size with percentage loading. Loading of Cu_2ZnSnS_4 on HCS reduced the aggregation of the nanocrystals and increased their electrocatalytic activities significantly.

Acknowledgement
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PI25 The Synthesis of a Potential Antimalarial Drug and the Study of its Uptake into a Polymer Drug Delivery System

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Resistance to currently available antimalarial drugs is responsible for the increase in malaria-related mortality, prevalently in sub-Saharan Africa. Artemisinin-based combination therapy (ACT) is one of the leading treatments in the fight against malaria.[1] Some therapeutic agents are linked to toxicity and poor intrinsic characteristics such as low water solubility and stability. Poor water solubility can hinder the delivery of highly efficacious therapeutic compounds. Delivering drugs at a controlled rate and targeted delivery are becoming increasingly attractive and have been researched extensively.[2] Nanoparticles have been widely researched due to their potential to improve the stability and solubility of encapsulated or conjugated drugs, promote the transport across membranes and prolong circulation times within the body to increase safety and efficacy.[3,4] A novel metallocene complex containing ferrocene was synthesized and characterized using various techniques with the potential for antimalarial activity due to the presence of the artesunate moiety attached. The polymer drug delivery system that was synthesized are micelle nano-drug carriers composed of poly(ethylene glycol) (PEG) and poly(lactic acid) (PLA) to form the amphiphilic block copolymer PEG-*b*-PLA. Due to the nature of the block copolymer, under aqueous conditions self-assembly will occur where the hydrophobic block will form the core and the hydrophilic block will form the corona of the micelle. The process of self-assembly was monitored and the micelles were visualized using various techniques.

Acknowledgements
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PI26 Lanthanoid Upconversion Nanoparticles: Design and Nanochemistry

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Upconversion nanoparticles (UCNPs) are luminescent contrast agents containing rare earth metals doped into its crystalline structure[1]. The doping of rare earth metals leads to the generation of unique optical properties by the nanoparticles upon excitation, where they are able to convert low energy light in the near-infrared region into higher energy ultra-violet light[1]. Due to their unique properties, such as tunable multi-colour emissions; photo stability; deep tissue penetration and low in vitro and in vivo toxicity, the nanoparticles have attracted a great deal of attention from researchers for applications in biological imaging, therapeutics and photovoltaics[2]. The luminescent properties of upconversion nanoparticles depend on the composition of the crystalline structure of the nanoparticles and its dopants[2]. By altering the composition of the nanoparticles the luminescent properties change. It is shown that by altering the composition of the $NaYF_4$:Yb/Er upconversion nanoparticle the luminescent properties produced different results. This was done by synthesizing three different UCNPs, namely $NaYF_4$:Yb/Er; $NaYF_4$:Yb/Ho and $NaScF_4$:Yb/Er, utilising a microwave solvothermal method. The UCNPs were confirmed through standard reference XRD patterns with the sizes ranging between 10 nm to 200 nm. The UCNPs were characterised using solid state NMR which showed broad powder like patterns for the ^{23}Na NMR spectra. The signals were distributed between 7 and –25 ppm, with maximum intensities at –18.4 ppm and a shoulder at -13.4 ppm. In the steady state fluorescence spectra, the NaYF:Yb/Er and $NaScF_4$:Yb/Er nanoparticles showed three strong emission bands in the spectra corresponding to the green and red emission bands. An additional strong emission band was observed for the NaScF nanoparticle centred at λ_{em} = 810 nm. The emissions observed for the $NaYF_4$:Yb/Ho samples showed four emission bands at slightly different wavelengths correlating to green, red and NIR emission bands.

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PI27 Synthesis of Ferrocenyl Conjugates of Sulfa Drugs and Study as Antimicrobials

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As humans have spread across the globe, so have infectious diseases. Tuberculosis (TB) and malaria are the major causes of mortality and morbidity in tropical and subtropical areas of the world. According to the World Health Organisation (WHO), TB is a communicable disease that is a major cause of ill health and the second leading cause of death from a single infectious agent, ranking above HIV/AIDS[1,2]. Approximately 10 million people developed TB in 2019 and more than 1.2 million died[2]. Furthermore, 241 million cases of malaria and 627 000 deaths were reported by the WHO in 2020[3]. The fight against malaria is based on artemisinin-based combined therapy (ACT). Even though this type of treatment is highly effective, similar to TB, antimicrobial resistance is a growing problem. Although most pharmaceuticals are purely organic compounds, the incorporation of metals into current drug therapies propound a vast potential for generating promising metal-based candidates with distinctive chemistry and biological activity of clinical significance[4]. A metal-based derivative of chloroquine, ferroquine, has shown promising biological activity as it can overcome the resistance shown by its parent compound[5]. Based on the promising biological activity displayed by many ferrocenyl complexes, this study aims to use the concept of derivatizing known drugs to design and synthesize a series of ferrocenyl conjugates of sulfa drugs. In this presentation, we will discuss the synthesis and characterisation of organometallic complexes that incorporate ferrocene into selected sulfonamides drugs and their ability as potential antimicrobial agents.

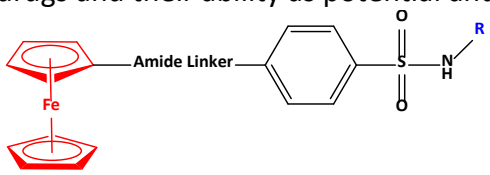

Figure 1: General structure of the target complexes

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PI28 Hydrogenolysis of Xylitol to Diols and Mono-alcohols over Nickel Catalysts supported on Sulfated-zirconia

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Replacing fossil-based feedstocks with biomass-derived resources to produce renewable fuels and chemicals addresses challenges facing chemical industries.[1] In this context, xylitol is one key platform intermediate to be explored. It can be hydrogenated into a variety of important chemicals, such as ethylene and propylene glycol which are used as monomers in the synthesis of polyester fibers, antifreezes and coolants and butanediols used for manufacturing plastics and solvents.[2,3] Other products formed are mono-alcohols such as ethanol and propanols as well as C2-C5 alkanes, common hydrocarbons found in petroleum and natural gas. This process can be achieved using bifunctional catalysts which contain both acid and metal sites.[4] Acid sites come from a solid support such as alumina, silica and sulfated-zirconia, while the metal sites are facilitated by a supported metal, such as Pt, Pd, Cu and Ni.[3,4] Bifunctional catalysts were synthesized using sol-gel method for the sulfated-zirconia support and wet impregnation to load Ni. The prepared catalysts were characterized using different techniques such as x-ray diffraction (XRD), inductively coupled plasma optical emission spectroscopy (ICP-OES), N_2 physisorption, scanning electron microscopy (SEM), transmission electron microscopy (TEM), temperature programmed reduction (TPR) and temperature programmed desorption (TPD). Catalytic testing was carried out in an autoclave at 50 bar H_2 pressure and 200 °C using 15 wt% xylitol as the feed.

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PI29 Synthesis, Characterization and Anticancer Studies of Half-sandwich Os(II) Complexes with Water-soluble P-donor Ligands

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Cancer research has taken an approach towards addressing the resistance and minimising undesirable side effects currently observed with metallodrugs in clinical use. This has resulted in fewer metal complexes entering the pre-clinical trials based on their general toxicity, inactivity and delays caused by formulation in bulkier complexes. However, some osmium complexes suffer the fate of being side-lined based on the inactivity or poor selectivity of their ruthenium analogues, regardless of some literature showing osmium complexes exhibiting superior potency against their ruthenium analogues.[1] The chemistry of the 1,3,5-triaza-7-phosphaadamantane (PTA) ligand has been pioneered and greatly developed by the research group of Dyson.[2] It has been reported that PTA ligands effect selectivity in some ruthenium complexes,[3] however, most osmium analogues of these ruthenium complexes have not been evaluated. It is anticipated that the Os-Br complexes are less labile as compared to their Ru-Cl analogues, hence different reactivity is also expected.[4] This study reports the synthesis, crystal structures, density functional theory and a preliminary anticancer study of Os-PTA complexes with the p-cymene, triphenylphosphane and bromine as ancillary ligands. A Hirshfeld surface analysis of these complexes reveals various types of interactions which may be exploited to actuate complex-protein/DNA interactions.

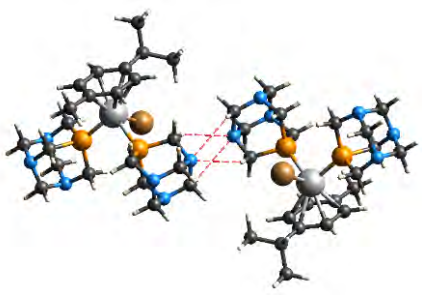

Figure 1: Hirshfeld surface analysis showing interactions of the PTA ligands.

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PI30 Coupling of CO_2 and Propylene Oxide using Ionic Functionalized Cr and Co Transition Metal Complexes as Catalysts

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Carbon dioxide is among gases that contribute to the greenhouse effect. Statista reports[1] that South Africa alone contribute nearly 452 million metric tons of CO_2 annually and this has raised much concern. Reducing the concentration of CO_2 by developing processes that utilize it as a feedstock to produce value added products has attracted much attention from both academia and industry[2]. A process currently of interest is the coupling of CO_2 with epoxides to produce biodegradable products such as co-polymer, which can potentially be used in place of non-biodegradable plastics, and cyclic products, used as solvents in Li-ion batteries. Transition metal complexes have been reported as active catalysts for the transformation of CO_2 in this process which is typically homogeneous. It is however very difficult to separate the catalyst system from the reaction products in homogeneous catalytic processes. Recent catalyst developments for the coupling process have focused on the preparation of transition metal complexes that have ionic functionalities incorporated as part of the ligands structure. The incorporation of these ionic functionalities has been shown to result in catalysts that do not require the use of a co-catalyst which is usually required as a nucleophile to facilitate ring opening of the epoxide[3]. In addition, the ionic functionality may also facilitate development of a biphasic process utilizing an ionic liquid as one of the solvents in the catalytic process which would allow catalyst recovery/recycling. The preparation of ionic functionalized metal complexes and their evaluation as catalysts will be presented with the focus specifically on the influence of the nature of the transition metal and ionic functionalities on catalyst performance.

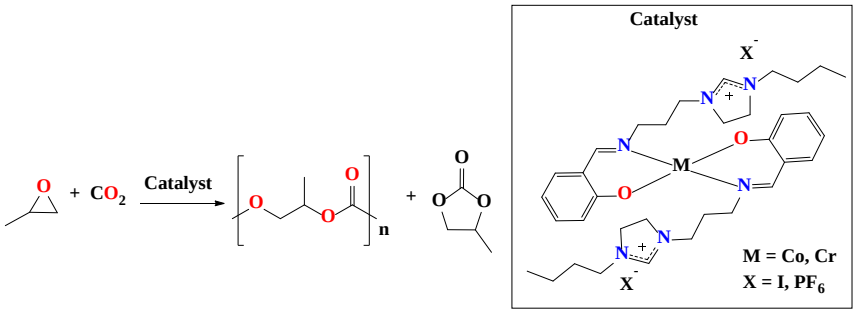

Figure 1: Catalytic coupling of CO_2 and propylene oxide using ionic functionalized catalysts

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PI31 Synthesis of Novel Artesunate Organometallic PGM Complexes for use as Potential Cancer Therapeutics

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Cancer is one of the leading causes of deaths worldwide and this is due to the fast rate at which cancer cells divide and grow. A current treatment for cancer, chemotherapy, which uses Platinum complexes like cisplatin or carboplatin, has proven to be very detrimental to the overall health of the patients due to the severe toxicity of these complexes on normal cells[1]. Combined with the toxicity of these complexes, drug resistance has also become a major issue which increases the need for research into new effective and less toxic anticancer drugs[2]. Artemisinin, one of the most effective antimalaria drugs, has shown great potential towards cancer treatment, with one of its derivatives, artesunate, being an all-around bioactive compound for further drug development[3]. Our target in the cancer cells is the endoplasmic reticulum (ER), since cancer cells exist under heightened levels of ER stress making it possible to tip the balance to apoptosis in the cancer cells by using ER stress inducing agents, while causing minimal effect to the normal cells[4]. In this poster presentation, the synthesis and characterisation of organometallic complexes (Figure 1) that contains an artemisinin moiety will be discussed. They were designed for possible use as anticancer drugs, where the hope is that the complexes are not cytotoxic to healthy cells and result in ER stress leading to the death of cancer cells. These complexes will be synthesised using di(2-pyriyl) methanone, artesunate and different metal dimers. The stability and chemical reactivity of these complexes will be studied, and a potential mode of action will also be explored.

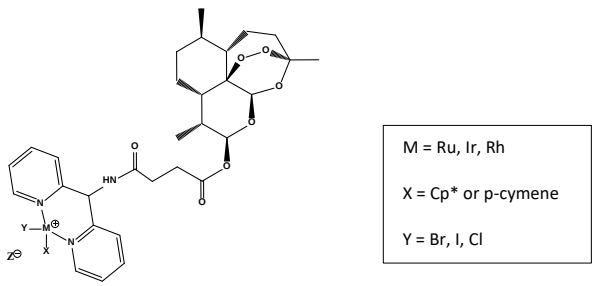

Figure 1: Target complexes.

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PI32 Investigation of cationic mononuclear palladacycles as anticancer agents

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In 2020, breast cancer surpassed lung cancer as the most diagnosed cancer worldwide, and while much progress has been made in the treatment of breast cancer, it still remains the leading cause of cancer related deaths among women.[1] Triple negative breast cancer (TNBC) is of particular concern since it cannot be targeted with hormonal or immunogenic therapies, therefore relying on rather toxic Pt-based therapies like carboplatin and oxaliplatin. Over the last two decades, Pd-based chemotherapeutics have shown significant promise as potent but less toxic alternatives for the treatment of TNBCs.[2] Our research group has a longstanding interest in binuclear palladacycles,[3,4] but an unanticipated detour resulted in the synthesis and characterization of two series of cationic mononuclear palladacycles (MC- and TMC-series). Contrary to our studies on binuclear palladacycles, the mononuclear complexes did not undergo solvation in the presence of DMSO. This talk outlines the main results of a preliminary investigation into the cytotoxicity of the compounds against two breast cancer cell lines and a non-cancerous cell line to assess the general toxicity. While all the complexes tested were more active that cisplatin, three complexes were identified that showed selectivity towards a TNBC cell line, MDA-MB-231, while remaining significantly less toxic towards a non-cancerous breast tissue cell line, MCF- 12A. These findings were supplemented by DNA and BSA binding studies to illuminate the mode of action of these complexes and revealed these types of complexes as highly promising anti- cancer agents.

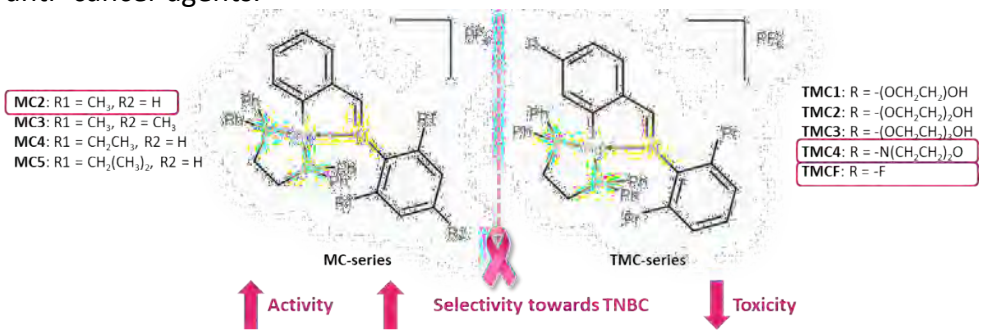

Figure 1: A summary of the complexes investigated

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PI33 Expanding the Versatility of Aminoquinoline Organometallic Complexes as Anticancer and Antibacterial Agents

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Despite the numerous research breakthroughs in prevention and treatment, cancer prevails as one of the most prevalent human diseases worldwide. The undesirable side-effects coupled with the manifestation of chemo-drug resistance has rendered many clinical chemotherapeutic drugs ineffective.[1] Concurrently, the rise of antimicrobial resistance presents a serious threat to public health by negatively affecting the cure and prevention of many persistent diseases.[1] Therefore, there is a paramount need for the design and development of novel anticancer and antimicrobial treatment modalities with superior efficacy. The aminoquinoline motif is a well-recognized scaffold within malaria research and included into chloroquine, the famed antimalarial drug. Since its discovery it has been repurposed for various other medical applications.[2] Due to its remarkable versatility and pharmacological activity the aminoquinoline structure has been incorporated into numerous clinical drugs and forms a well-founded scaffold upon which to develop favourable drug agents.[2] The incorporation of transition metals into traditional organic scaffolds has seen many notable advances in medicine. Organometallic compounds boast significant biological activity which makes them popular in rational drug design.[4] This presentation will highlight the synthesis of novel Re(I), Ru(II) and Ir(III) organometallic complexes bearing aminoquinoline Schiff base ligands. The significant antibacterial and anticancer activity of the tested complexes, explored through various avenues namely, chemotherapy and photodynamic therapy, will also be outlined. Furthermore, the photophysical properties of certain complexes will be presented, demonstrating their potential to act as photosensitisers for photo-induced anticancer and antibacterial therapies.

Acknowledgements
Financial support from The Oppenheimer Memorial Trust (OMT Ref. 22183/01), the University of Cape Town and the National Research Fund of South Africa is gratefully acknowledged.

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PI34 The Incorporation of Thiazyl Radicals into Metal-organic Compounds

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Several stable thiazyl radicals are known. Two of these, methylbenzodithiazolyl (MBDTA) and phenyl-1,2,3,5-dithiadiazolyl (PhDTDA) (Figure 1), have been well-studied. we have investigated the reaction of these radicals with metalloporphyrins, as well as their inclusion in metal-organic frameworks. The attempted reaction of thiazyl radicals with a series of metalloporphyrins reveals that thiazyl radicals appear to coordinate exclusively to cobalt porphyrins. Both UV-vis and EPR titrations were carried out to confirm this. The inclusion of PhDTDA radical into pillared-layer coordination polymers *-[Co_2(bpeb)(obc)$_2$]* (where bpeb = 1,4-bis[2-(4-pyridyl) ethenyl] benzene and obc= 4,4'-oxybisbenzoate)[1] via gas phase diffusion was a success. Single crystal X-ray diffraction analysis (SC-XRD), powder X-ray diffraction (PXRD), thermal gravimetric analysis (TGA), Fourier transform infrared (FTIR), solid state-UV-visible studies all confirmed the inclusion of the radical in the framework. XRD and TGA studies indicated that the radical in *[Co_2(bpeb)(obc)$_2$]* PhDTDA MOF exists in its monomeric form.

MBDTA PhDTDA

Figure 1: Structural representation of MBDTA and PhDTDA radical[2]

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PI35 Bipyridine Adducts of Zn(II) and Ni(II) Bis(*N*-methyl-*N*-phenyl dithiocarbamate): Synthesis, Characterization, and Biological Applications

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Substituted bipyridine adducts of Zn(II) and Ni(II) bis (*N*-methyl-*N*-phenyl dithiocarbamate) have been synthesized by the reaction of the dithiocarbamate complexes with Lewis bases of 4,4'-bipyridine (BP), 4,4'-dimethyl-2,2-bipyridine (DMeB), 4,4'-dimethoxy-2,2'-bipyridine (DMxB), 4,4'-ditertbutyl-2,2'-bipyridine (DTB). The resulting adducts were characterized using elemental analysis, various spectroscopic techniques and X-ray single crystallography. The spectroscopic data suggest octahedral coordination around the metal center due to the formation of a new M-N bond with the nitrogen of the Lewis bases. Single crystal data obtained for **[Zn(L)$_2$(BP)]** and **[Zn(L)$_2$(DMeB)]** adducts showed five and six coordinate geometry respectively around the Zn center. All adducts were tested for cytotoxicity, antioxidant, and anti-inflammatory properties and the compounds showed good activities in all biological properties compared to the standard.

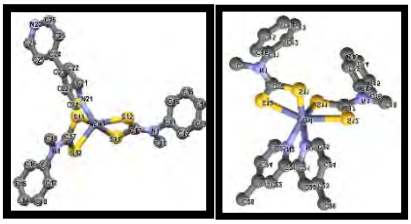

Figure 1: The molecular structure of [Zn(L)$_2$(BP)] and [Zn(L)$_2$DMeB] adducts with displacement ellipsoids drawn to 50% probability level

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PO1 Using the in vitro Parameter Lipophilic Metabolism Efficiency (LipMetE) to improve in vivo half-life prediction.

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Half-life is a key parameter in pharmacokinetics and drug optimization, as it is used to predict dose, peak-to-trough ratio, and dosing regimen. Prediction of in vivo half-life from in vitro data remains challenging, slowing the drug discovery optimization process. Recently, Cecere, G. et al. have described a method to predict half-life that may offer improved prediction using in vitro parameters. In rat and human, this method uses the in vitro parameters LogD, intrinsic clearance (CLint) and fraction unbound in rat and human liver microsomes (fu,mic). By querying our database, we identified 788 compounds for which we have rat CLint, fu, and in vivo clearance (CLp). We selected 96 compounds from our dataset and followed the method described in Cecere's manuscript to validate their finding. The data of this study is presented in this poster.

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PO3 Synthesis of 3-substituted 5-trifluoromethyl-1,2,4-oxadiazole derivatives as anti-malarial and anti-microbial agents

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Oxadiazoles are heterocyclic compounds of the azole family. The stability of the oxadiazole ring in aqueous medium is one of the most important characteristics that justify the interest in developing bioactive molecules which contain this motif. Another important aspect of oxadiazoles is their capability to act as hydrogen-bond acceptors due to the electron pairs on the heteroatoms. These electrons are also available for ligand binding.[1,2] The search for new medicinal compounds is a challenging task as there is a threat to parasite control that is caused by the resistance of parasites to most of the drugs in use. This ongoing problem is a motivation to continue searching for new, more effective, and low-cost compounds which can be used as anti-malarial drugs. Compounds containing a 3-substituted 5-trifluoromethyl-1,2,4-oxadiazole moiety were prepared through *O*-acylation of amidoximes using trifluoroacetic anhydride followed by dehydration and cyclisation of the *O*-acylamidoxime intermediates. Some of the synthesized compounds and their precursors showed mild to moderate activity with IC_{50} values of 2.7–8.0 µM against the wild-type drug sensitive strain (Nf54) of *Plasmodium falciparum* parasites. Other compounds showed good activity against both *Staphylococcus aureus* and *Escherichia coli* pathogens.

Acknowledgements
Anti-plasmodial and anti-bacterial assays were performed at the Drug Discovery and Development Centre (H3-D), Chemistry Department, University of Cape Town. This institute is supported by the South African Medical Research Council with funds received from the South African National Department of Health, and the UK Medical Research Council with funds received from the UK Government's Newton Fund.

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PO4 Phytochemistry and activity of South African indigenous plants that are used in skincare

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One of the most popular plants to treat skin conditions is *Aloe vera* Linne., a member of the Asphodelaceae. The gel of the leaves from this plant is also known for biological activities such as wound healing, anti-inflammatory, anti-oxidant and anti-diabetic activity.[1,2] The leaf gel of several South African plants of the Asphodelaceae, such as *Aloe ferox* Mill., *Aloe candelabrum* A. Berger, *Bulbine frutescens* (L.) Willd, and *Bulbine natalensis* (Baker) are used for skin preparations. Much information is available on the bitter fractions of Aloe leaves, consisting of anthrone glycosides such as aloin. However, only the gel of *A. ferox* has been investigated.[3,4] This presentation will describe the analysis of the gels of the *Aloe* and *Bulbine* species mentioned above. The overall composition of the gels was investigated by NMR analysis of the freeze-dried material. The monosaccharide composition was determined by size-exclusion filtration, followed by LC-MS analysis. To determine the composition of the polysaccharides, the gel was hydrolysed with CF_3COOH and analysed by LC-MS. The anti-oxidant activities of the fresh gels will be reported.

Figure 1: Leaf of *A. ferox* showing the bitters and the gel.

Acknowledgements
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PO5 Expanding the scope of aryl-pyrimidinones as inhibitors of Kaposi's sarcoma associated herpes virus

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The overall aim of this study was to synthesis three novel analogues of a hit compound identified as being a potential anti-viral agent, active against Kaposi Sarcoma Associated Herpes Virus (KSHV); an oncovirus of growing concern in Sub-Saharan Africa.[1] This study aims to aid in the optimisation of the anti-KSHV activity of this class of compounds and elucidate the structural features underpinning this activity. Herein, we report on the successful synthesis and characterisation of the aryl-pyrimidinone hit compound itself, as well as one of its analogues. Also included, is the synthesis and characterisation of two precursor compounds that could ultimately be used in the synthesis of the remaining two analogues, initially set out to be synthesised. Analogue specific β-keto esters were synthesised via a lithium di-isopropyl amide (LDA) reaction with analogue specific benzoyl chlorides and ethyl acetate. These respective β-keto esters were then reacted with guanidine carbonate to form cyclised, aryl-pyrimidinone, compounds; via an imine formation reaction. The aryl-pyrimidinone compounds were then selectively brominated to yield the hit compound as well as a novel analogue. These compounds were characterised by ^{1}H NMR, ^{13}C {^{1}H} NMR and infrared spectroscopy. Also included, is a discussion on tautomerization that was observed to have occurred with the β-keto ester compounds, as well as a discussion on optimising the LDA reaction to improve reaction yields from 8% to 57%.

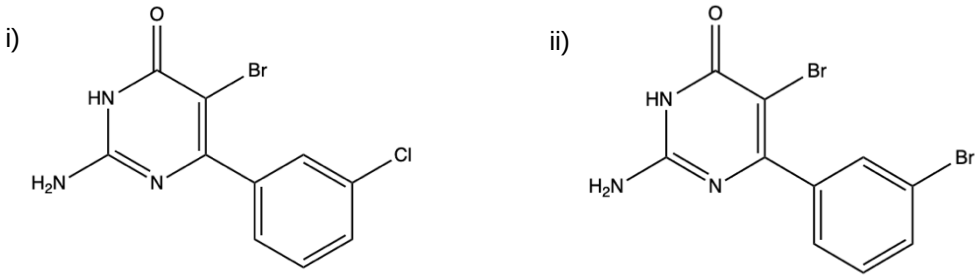

Figure 1: Showing i) the hit aryl-pyrimidinone compound and ii) its bromo analogue that have been successfully synthesised

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PO6 Synthesis and biological evaluation of novel β-lactam metallo β-Lactamase inhibitors

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β-Lactamases are enzymes that hydrolyse the β-Lactam antibiotics, thus deactivating them. There are two types of β-Lactamases, namely, serine β-Lactamases (SBLs) and metallo β-Lactamases (MBLs).[1] One of the strategies to overcome β-Lactamase-mediated resistance is to develop β-Lactamase inhibitors that deactivate the β-Lactamase enzymes and restore the efficacy of existing antibiotics. There are no commercially available MBL inhibitors (MBLIs), making the need to develop one crucial.[2] In this study, we present **12** novel potential MBLIs (via multi-step chemical synthesis), which have been shown to restore the complete efficacy of meropenem (≤ 2 mg/L) against NDM producing *Klebsiella pneumoniae in vitro*. These compounds contain a zinc metal chelator, conjugated to different commercially available β-Lactam antibiotics to assist with drug transport, lipophilicity, and pharmacokinetic/ pharmacodynamic properties. Biological evaluation of compounds **26b-c** have further highlighted the downstream application of these compounds since they are non-toxic at the selected doses. Time kill assays indicate that compounds **26b-c** exhibits sterilizing activity towards NDM producing *Klebsiella pneumoniae in vitro*, using minimal concentrations of meropenem. The overall findings of this study, the novel series of beta lactam MBLIs reported herein, are potent, efficacious, and safe therapeutic alternatives, that have the potential of becoming promising MBLIs in the near future.

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PO7 Molecular modelling and synthesis of small molecule viral inhibitors for SARS-COV 2

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SARS-CoV 2 is a highly infectious virus responsible for the deaths of 6.05 million people worldwide and continues to spread. The 3 chymotrypsin-like proteases (3CLPro), the main protease of SARS-CoV 2, offers an ideal target for small molecule viral inhibition. Small-molecule sulfone-containing irreversible protease inhibitors, utilizing aldehyde electrophilic warheads, have been explored *in-silico* (PDB IDs: 6M0K, 7BUY, 5REK, and 5REF) to find new motifs that can be utilized as drug candidates. At present, three potential libraries have been generated using molecular modelling, focusing on modifications of the R^1, R^2, and R^3 positions (Figure 1). Modifications to the R^1, R^2, and R^3 positions (Figure 1) were proposed to target the main protease binding site, involving Cys145 and His41 as key subunits for interactions in the binding pocket. In addition, the aryl-sulfonyl sub-structures were chosen due to their essential interactions with residues Glu166, Leu167, Pro168, and Gln192 within the binding pocket. So far, 18 compounds have been successfully synthesised for biological testing. Synthesis involving the R^3 position has progressed rapidly with the assistance of the high-yielding Suzuki-Miyaura reactions, offering upwards of 80% yield per reaction. This allowed for the fast and easy generation of a diverse library, limited only by our access to suitable boronic acids. Microwave-assisted Suzuki-Miyaura reactions on this scaffold have since proved successful, resulting in significantly reduced synthesis times.

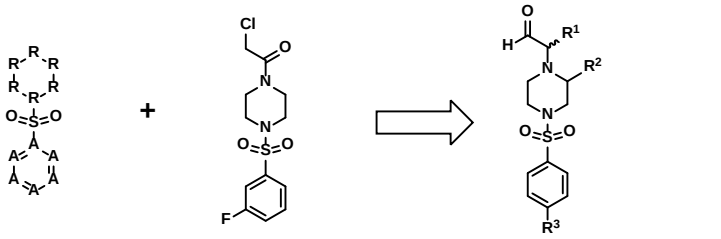

Figure 1: Figure to show the design and modification of the drug, bound in crystal structure 5REK.

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PO8 Discovery and Optimization of Potent and CNS Penetrant M_5-Selective PAMs Derived from the ML326 Isatin Scaffold

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The pharmacology of the M_5 muscarinic acetylcholine receptor (mAChR) is the least studied of the five mAChR subtypes due to both low expression levels in CNS tissue and a historic lack of selective tool compounds.[1,2] Studies on M_5 knockout animals have indicated that the receptor is implicated in the etiology of Alzheimer's disease, schizophrenia, and Substance Use Disorder.[3,4] There is still an unmet need to develop potent, selective, and drug-like molecules to further elucidate the biological function of M_5 mAChR. Currently, the M_5 positive allosteric modulator (PAM) ML326 is one of the most potent and selective in its class, however, its use in *in-vivo* studies is limited due to its low potency and suboptimal pharmacokinetic properties.[2] The present work aims to explore new chemical space in order to improve potency, explore replacements to the ML326 isatin chemotype, and optimize pharmacokinetic properties.

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PO9 Assay validation for inhibitors of *M. tuberculosis* coenzyme A biosynthesis: investigation and screening of known and new inhibitors of MtCoaBC

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In recent years an increasing number of inhibitors have been tested against the second bifunctional enzyme in the coenzyme A (CoA) biosynthetic pathway, CoaBC, due to a study indicating it as a bactericidal target in *Mycobacterium tuberculosis*.[1] Despite this promising discovery, several factors have complicated the identification of potent inhibitors that translate to whole cell activity that can subsequently move through clinical trials. A critical factor in the CoaBC-targeting drug discovery efforts has been the lack of a validated assay that is amenable to high throughput screening, or that can at least be used to confirm initial hits resulting from an HTS. We therefore set out to identify appropriate assay parameters and conditions that would be able to optimally screen for and identify inhibitors of MtCoaBC. An initial sample set of reaction intermediate mimics that employ a triazole moiety as a phosphodiester bioisostere were synthesized and tested using a systems-based assay of the truncated MtCoaBC biosynthetic pathway. This was done to investigate whether the compounds would undergo metabolic activation and be transformed into inhibitors. Only two compounds showed positive results in these tests. We then proceeded to synthesize the phosphorylated analogs of these compounds to allow for the evaluation of their in vitro binding of the target. Specifically, we planned to use a biophysical assay to circumvent the complex kinetic analysis involved with the standard activity assay. This study is an important contribution to the antituberculosis drug discovery efforts that aims to target enzymes involved in CoA biosynthesis and utilization.

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PO10 Nucleophilic annulative amination: Access to novel 3-aminoindole derivatives and their biological evaluations

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Tuberculosis (TB), a bacterial infection caused by *Mycobacterium tuberculosis (Mtb)* is one of the deadly diseases in the world. World Health Organization (WHO) reported that in 2018, that 1.5 million people died from TB while an estimated 10 million worldwide were infected with this disease.[1] Several drugs have been developed to address this including the first line (Rifampicin, Ethambutol), the second line (Levofloxacin, Streptomycin) and those developed later especially for MDR-TB such as Linezolid and Amoxicillin.[2] However, the use of these drugs is under threat due to the emergence of multi-drug, prolonged treatment time and extensively-drug resistant TB strains, thus hampering efforts to combat this disease.[3] The indole motif is present in a large number of therapeutic substances such as oxypertine, acemetacin and panobinostat.[4] Owing to its diverse biological properties, of particular interest is 3-aminoindole derivatives as potential anti-TB agents. Aminoindoles were found to possess various biological activities, for example, 7-aminoindoles were found to be active against diabetes and cancer.[5] 5-Aminoindole derivatives were found to be HIV protease inhibitors, while melatonin was used for the treatment of strokes.[6] Additionally, Schiff bases of indoline-2,3-dione (isatin) were found to exhibit anti-TB activity.[7] Therefore, this poster will explore on the synthesis of 3-aminoindole derivatives (**Figure 1**) starting from iodoanilines (one pot synthesis) and their biological activity against *Mycobacterium tuberculosis* (H37Rv) including their cytotoxicity. The most active 3-aminoindole derivative possessed an MIC_{90} of 7.813 µM while all 3-aminoindole derivatives were not active against Mouse Raw 264.7 macrophages at the highest concentration of 78 µg/mL.

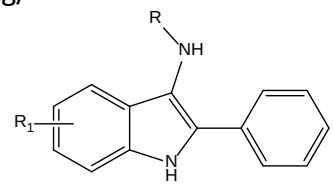

Figure 1: General representation of 3-Aminoindole derivatives

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PO11 Design and synthesis of novel benzimidazole derivatives with anti-tb activity

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Tuberculosis (TB) is the world's most life-threatening disease caused by the bacteria *Mycobacterium tuberculosis* (*M.tb*). It is the most common infectious disease in developing countries and infects one-third of the world's population.[1] Despite the availability of potent anti-TB drugs, TB mortality rate has remained relatively high globally, mainly due to the long treatment duration of these drugs and increased rate of resistance towards these TB regimens.[2] Therefore, the above mentioned drawbacks necessitate for the development of new anti-TB agents that are active against TB, extensively drug-resistant (XRD)TB, and multi-drug-resistant (MDR) TB.[3] *N*-Heterocyclic compounds consisting of the benzimidazole scaffolds are amongst several bioactive pharmacophores reported to exhibit anti-TB activity.[4] This poster will unveil different synthetic approaches undertaken to design and synthesize novel benzimidazole derivatives based on the structure of compound **1** with promising anti-TB activities.

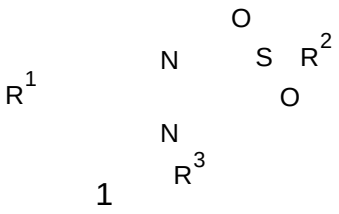

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Figure 1

Reference

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PO12 Profiling of Senna didymobotrya extracts for activity against breast and cervical cancer and characterisation of active compounds

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Cancer is the uncontrolled growth of abnormal cells in the body. Cancer develops when the body's normal control mechanism stops working[1]. According to the World Health Organization (WHO), cancer is a leading cause of death worldwide, accounting for 10 million deaths in 2020 and the numbers are projected to rise to an estimated 13.1 million deaths in 2030 (about a 70% increase)[2]. Senna didymobotrya is widely used for the treatment of human and livestock diseases. It is traditionally used for the treatment of sexually transmitted diseases, purgatives, appetizer, skin diseases, insecticidal, antibiotics, external parasites infections, diarrhea, dysentery, skeletal muscle abscesses and venereal diseases[3]. The study was aimed at investigating the anticancer properties of Senna didymobotrya and the isolation of bioactive compounds. Extraction of the plant was done using five solvents of different polarities (Acetone, hexane, dichloromethane, methanol, and hot water). Isolation of active fractions was done using thin layer chromatography and column chromatography. The plant extracts were subjected to phytochemical analysis to determine the presence or absence of various chemical constituents such as terpenes/terpenoids, alkaloids, phenols, flavonoids, steroids, saponin, phlobatannins, and tannins. The isolated fractions were evaluated for anticancer activity against raw 264.7 macrophage cells (Normal cells), cervical cancer HeLa cells and breast cancer MCF-7 cells. All fractions were selective for killing HeLa cervical cancer cells and MCF-7 breast cancer cells over 264.7 crude macrophage cells. Two compounds were elucidated from the study using NMR and HPLC-MS. The compounds whose structures were elucidated are Stigmasterol and 4b,5,6,7,8,8a-hexahydro-2-isopropyl-8,8,8a-trimethylphenanthrene-3,4-diol (Abietane).

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PO13 Oxidative coupling of naphthols on bismuth promoted Pt, Pd and Ag nanocatalysts

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Aryl-aryl bond formations are of great importance in synthetic organic chemistry for biomimetic of natural products.[1] Clean catalytic methods are often employed for these reactions. Oxidative coupling of naphthols is one of the reaction principle used to achieve this goal. Noble metals nanoparticles have found applications in catalysis, in particular for oxidation reactions, as they are themselves not easily oxidised. This research project aims to replace the stoichiometric reagents with environmentally friendly oxidant such as H_2O_2 on carbon supported noble metal catalysts for the oxidation of 1-naphthols (Figure 2). It also aims to determine the effect of noble metals and promoters on the oxidation of 1-naphthols. Bi promoted Pt, Pd and Ag catalysts supported on activated carbon (AC) were prepared by electroless deposition (ED). The catalysts were characterised by ICP-OES, N_2 physisorption, XRD, SEM, HRTEM and TGA. The catalysts were tested for the oxidative coupling of substituted 1-naphthols in different solvents. 5%Pt-5%Bi/AC contains hexagonal $BiPO_4$ nanorods, 5%Pt-5%Bi/AC contains BiOCl lamellae, and on 5%Ag-5%Bi/AC, $Bi_6(NO_3)_4(OH)_2O_6{\cdot}2H_2O$-containing hexagonal dart-flight features were observed. In the oxidation of 2-methyl-1-naphthol (**1**) (Figure 2), Pt catalyst offers high activity than Pd and Ag catalysts, which reflect their relative intrinsic activities.

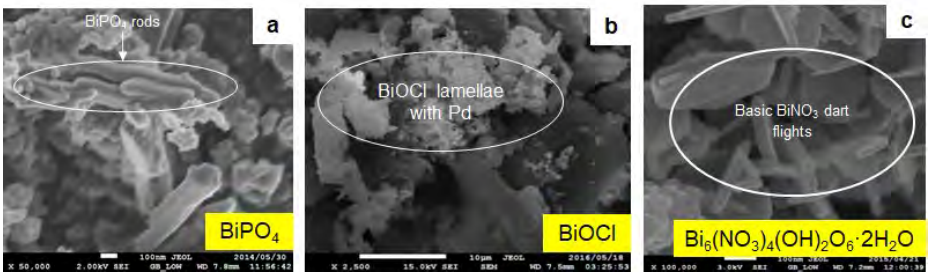

Figure 1: SEM images of 5%Pt-5%Bi/AC (a), 5%Pd-5%Bi/AC (b) and 5%Ag-5%Bi/AC (c)

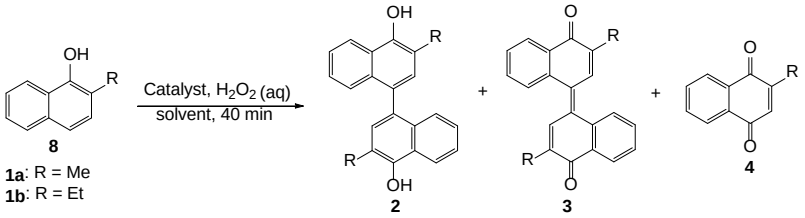

Figure 2: Oxidation of substituted 1-naphthols over noble metal catalysts

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PO14 Stereoselective effects of molecularly imprinted polymers on a photochemical reaction of novel potential antimalarial compounds

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Isomeric by-products formed during organic reactions often produce different and even opposite pharmacological and toxicological properties driven by structural differences, as such, there is always a need to isolate the obtained products prior to clinical use to elucidate the biological activities that result because of structural differences. Molecularly imprinted polymers (MIPs) are artificial receptors obtained using imprinting technology. They are robust molecular recognition elements that mimic natural recognition biological receptors and antibodies. The research undertaken reports on MIPs as a fast, inexpensive, and highly efficient method of separating the isomers as opposed to other analytical methods. Isomers were obtained by photoirradiation of the trans isomer in the presence of trans templated MIPs and vice versa. A further probe into the stereochemical implications resulting from using MIPs as microreactors was carried out.[1] Novel trans-chloroquine derivatives where photo irradiated with UV light of wavelength 254 nm for 24h in the presence of trans-templated MIPs as microreactors to simultaneously separate and enhance the photochemical reaction time.[2]

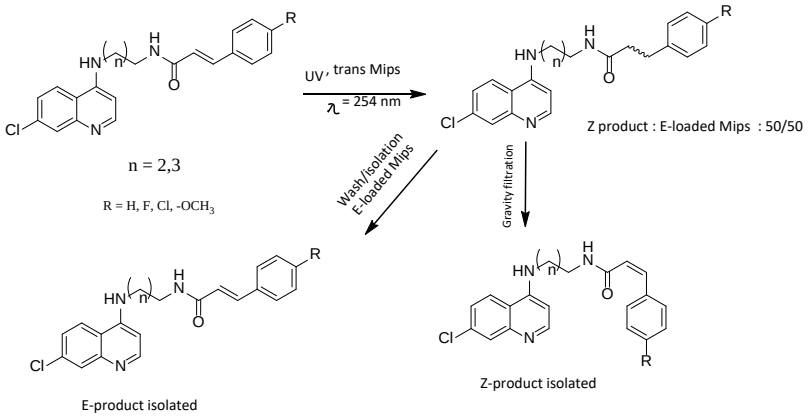

Figure 1: Photoirradiation reaction of 4-amino-7chloroquinoline/cinnamic acid conjugate in the presence of MIPs templated with the trans-cinnamic acid conjugate and vice versa

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PO15 Targeting the tumour extracellular environment through rational modification of the SNX class of HSP90 inhibitors

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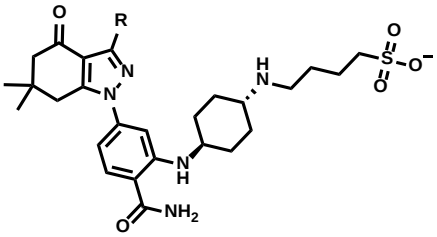
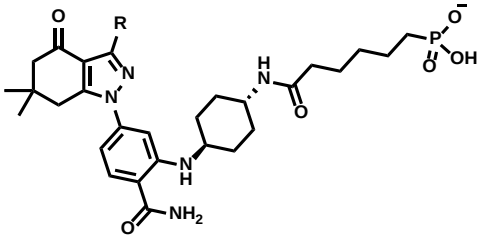
HSP90 remains a valuable target for cancer therapy. Unfortunately, targeting intracellular HSP90 has limitations associated with the compensatory overexpression of HSP70 which is triggered by intracellular HSP90 inhibition. Extracellular HSP90 in involved in numerous pro-oncogenic pathways, including cell signalling and metastasis. Accordingly, targeting HSP90 in the extracellular environment has been postulated as a promising anti-cancer strategy, devoid of the drawbacks associated with intracellular HSP90 inhibition.[1] Most medicinal chemistry studies which focus on intracellular targets tend to focus on measured increases in lipophilicity and structural rigidity to improve cell penetration. Conversely, the development of extracellular inhibitors, typically requires the introduction of disordered polar moieties. To this end, in this study, we synthesized four analogues of the known HSP90 N-terminal inhibitor SNX-2112, all of which were modified include a polar sulfonate (**1,2**) of phosphonate group (**3,4**) at the end of an alkyl chain. Biological assessments carried out to date, confirm that while these compounds retain potent cytotoxicity, they do not inhibit intracellular HSP90, nor do they stimulate the expression of HSP70. While further biological and mechanistic evaluations are ongoing, these preliminary data suggest extracellular HSP90 inhibition.



1. R = CF_3 pIC_{50} = 6.2
2. R = Me pIC_{50} = 6.3



3. R = CF_3 pIC_{50} = 6.6
4. R = Me pIC_{50} = 6.2

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PO16 Biocatalytic Resolution and Stereoconversion of Homoally Alcohols to Tetrahydropyrans and Piperidines

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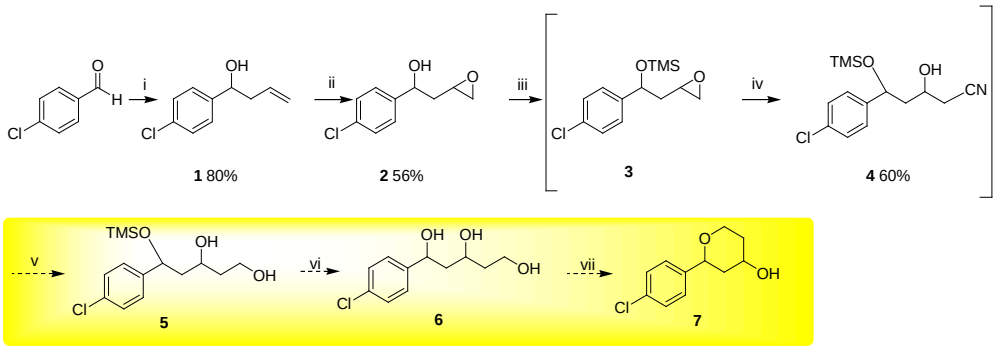
The objective of the study is the biocatalytic resolution and stereoconversion of homoally alcohols to tetrahydropyrans and piperidines. This is important as it is most relevant as it meet several requirements such as excellent selectivities under mild reaction conditions. Enantiomerically pure chiral amines and alcohols are used as key intermediates in a number of pharmaceutical compounds that have a wide range of biological activities. Biological activities of these building blocks have relied on the resolution of racemic substrates using hydrolytic enzymes such as lipases and acylases[1]. The research group at TUT discovered a method for the mild cyclodehydration of 1,2,4-butane triols to 3-hydroxytetrahydrofuran. stereo dependency was observed where the syn-1,2,4-triol isomers gave the anti-THF product exclusively, while the anti-1,2,4-triol isomers gave a mixture of the anti-2,4-diol monotosylate (major) and syn-THF (minor) products[2]. Our interest is to expand the method for the mild cyclodehydration by synthesizing tetrahydropyrans and Piperidines from the synthesis of 1,3,5-pentanetriols and 5-amino-1,3-pentanediols respectively. We tried different method of synthesizing 1,3,5-pentanetriols and we observed early cyclization of compound forming THF. We then protected the OH group on compound **2** to avoid cyclization.



(i)Zn, All·Br, NH_4Cl THF; (ii) *m*-CPBA CH_2Cl_2; (iii) TMSCl, Et_3N, CH_2Cl_2 (iv) ACN,KCN -H_2O, 50^{O}C; (v) H_3O^+, $LiAH_4$-,heat;(vi)deprotection
(vii) Bu_2SnO (5 mol%), p-TsCl (1eq.), Et_3N (1 eq.), DCE, reflux, 4 h

Figure 1: synthesis of 3-hydroxytetrahydropyans

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PO17 Synthesis of substituted 2-(4-(sulfonyl)styryl)quinazolin-4(3h)-one complexes as potential anticancer agents

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As a result of their diverse and different pharmacological effects, nitrogen-containing heterocycles have gotten a lot of interest in recent years. Quinazoline is a type of nitrogen-containing heterocycle with a wide range of biological properties. Among the quinazoline analogues, the substituted 2-(4-(sulfonyl)styryl)quinazolin-4(3H)-one have established themselves as selective and effective inhibitors of the epidermal growth factor receptor tyrosine kinase (EGFR-TK) phosphorylation, which results from competitive binding at the ATP site. The biological activity of the quinazolines and sulphonated derivatives inspired us to merge the two pharmacophores in the same molecular context to develop as a prospective anticancer future biological activity. Computational chemistry will be employed to simulate the biological environment of the drug interaction with the selected proteins responsible for the proliferation of cancer cells. This was achieved by the halogenation of anthranilamide, followed by acetylation of 2-amino-5-iodobenzamide using acetyl chloride and subsequent cyclization of the incipient to afford 2-methylquinazoline, followed by Suzuki cross-coupling in position of the halogen. Condensation of the product with sulphonated salisaldehydes to afford our 2-(4-(sulfonyl)styryl)quinazolin-4(3H)-one.

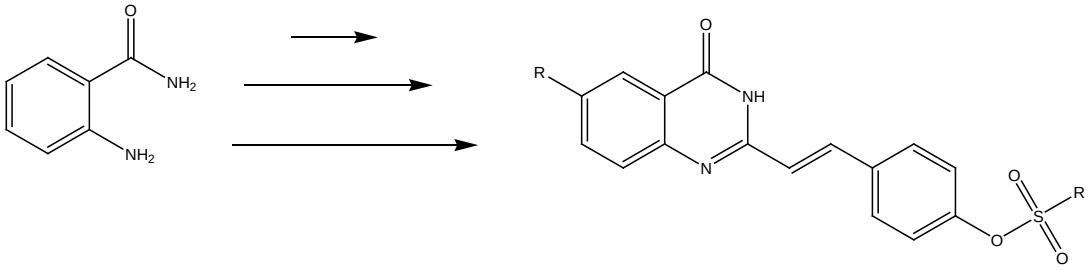

Figure 1: Summary of methodology

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PO18 Synthesis of Quinoline-1,2,3-triazole hybrids for biological evaluation against cancer

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Cancer is one of the leading diseases in the world and is responsible for an increase in the mortality rate in the world [1]. According to the World Health Organisation (WHO), 9.6 million deaths as resulting from cancer have been reported in the year 2018 alone [2]. Both 1,2,3-Triazole and quinoline derivatives have been found to possess biological activities such as anti-bacterial and anti-cancer properties [3-4]. Molecular hybrid compounds of quinoline-1,2,3-triazole were synthesized through Claisen-Schmidt aldol-condensation of 2-amino-3,5-dibromoactophenone with benzaldehyde derivatives to form 2-aminochalones followed by an acid mediated-cyclization reaction to form 2-substituted 2,3-dihydro-quinolin-4(*1H*)-ones, which underwent dehydrogenation and oxidative aromatization to afford 2-substituted quinolin-4(*1H*)ones derivatives. The nucleophilic substitution of the latter with sodium azide yielded the 2-substituted 4-azidoquinolines, which underwent Huisgen cycloaddition reaction to form the 2-substituted 4-triazolo-quinoline derivatives in high yields. Molecular docking and anti-cancer studies were used to estimate the binding free energies and estimate MIC_{50} values of 2-substituted 4-triazolo-quinoline derivatives **6a-6f** against the VEGFR-2 tyrosine kinase reference to Sorafenib as a standard. The 2-substituted 4-triazolo-quinoline derivatives **6a-6f** were biologically tested against the breast-cancer cell line MDA-MB-231 strain where compound **6f** showed a good cytotoxicity compared to other compounds with an IC_{50} of 40.7 µM. The compounds **6a** and **6b** exhibited a good concentration dependent cell adhesion inhibition against the MDA-MB-231 cell line compared to the standard Curcumin. All the synthesised compounds were confirmed using a combination of ^{1}H-NMR, ^{13}C-NMR, FT-IR, and mass spectrometry.

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PO19 Biocatalytic and Stereoselective Synthesis of Chiral Oxygenated Heterocycles

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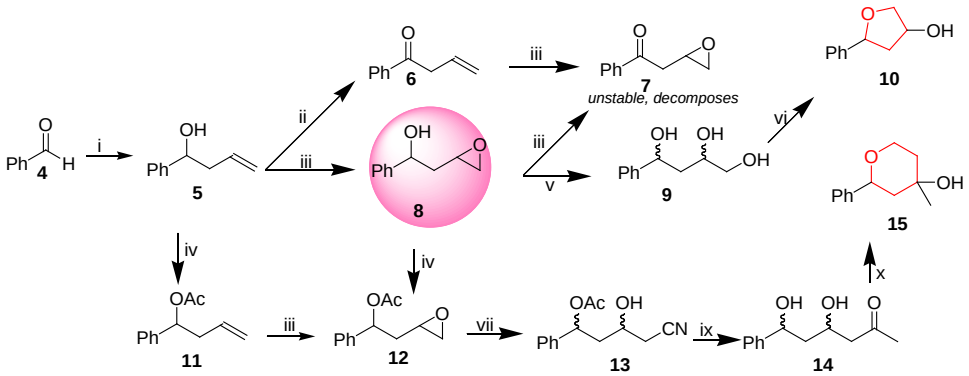
The Flavours and Fragrances industry is a rapidly growing multi-billion dollar global industry, mainly driven by expanding markets in middle-to-low income countries, including South Africa. Heterocyclic compounds are among the key targets in this industry and also the pharmaceutical industry. This includes the commercially available fragrances namely, Clarycet (**1**), Rhubafuran (**2**) and florol (**3**)[1], a key feature of these compounds is that they are heterocycles (tetrahydrofuran or tetrahydropyran) with several chiral centres. We envisioned that chiral tetrahydrofurans and tetrahydropyrans could be synthesised from 1,2,4-triols or 1,3,5-triols via a mild stereoselective cyclodehydration which our research group has demonstrated does not lead to scrambling or loss of stereochemistry[2]. To incorporate biocatalysis early in the synthetic scheme we identified hydroxyepoxide **8** as the key target for enzymatic resolution (Figure 1). Different oxidation ways were tried to form **7** which resulted in poor yields and decomposition. Early results on the lipase acetylation of **8** using porcine pancrease lipase (PPL) are poor (22% after 90 h), but other enzymes are yet to be explored. Cyclisation of **8** to form **10** was obtained in good yield. **15** was obtained via cyclisation after opening oxirane ring **12**.



(i) Zn, All-Br, NH_4Cl THF; (ii) PCC CH_2Cl_2; (iii) *m*-CPBA CH_2Cl_2; (iv) Ac_2O, DMA, pyridine; (v) $HClO_4$ -H_2O, 20^OC; (vi) $HClO_4$ -H_2O, 100^OC;(vii) EtOH, H_2O, KCN; (ix) CH_3MgBr, H_2O; (x) (a). $NaNH_4$; (b) Bu_2SnO, Et_3N, TsCl

Figure 1: Synthesis of a key hydroxyepoxide **8** intermediate, tetrahydrofurans **10** and tetrahydropyrans **15**

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PO20 Synthesis and photoisomerization of conjugated cinnamic acid/chloroquinoline as potential antimalarial agents

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Malaria is a global infectious disease caused by parasites of the Plasmodium genus.[1] Its treatment is difficult due to many factors including the toxicity of the drugs currently in use, and also by the development of resistance by the parasite.[2] Due to the aforementioned difficulties in the treatment of malaria, development of new and better antimalarial agents is needed. Synthesis of the compounds was based on conjugation of cinnamic acid and chloroquinoline pharmacophore as shown in Figure 1. Cinnamolyted-chloroquinoline analogues were photoisomerized by UV irradiation at 245 nm. LC-QTOF-MS/MS analyses of the photoisomerized products revealed the emergence of *cis* isomer which eluted before its synthesized *trans* counterpart, suggesting reduced polarity. This dramatic change in polarity could be further exploited in the future synthesis of other combinatorial drugs with mixed polarities which can aid in synergistic pharmacological properties.

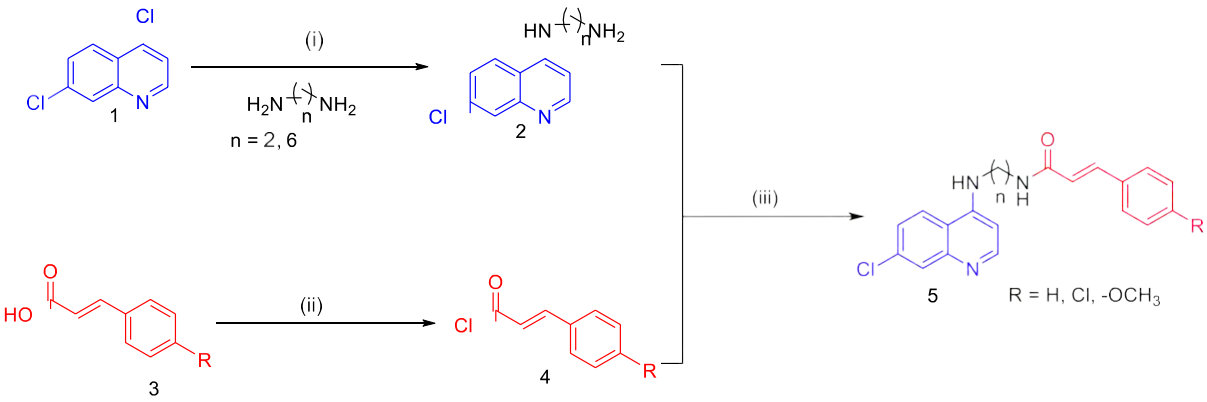

Figure 1: (i) Reflux, 18h, (ii) toluene, 3 drops of DMF, RT, 3 h (iii) Dry DCM, TEA, RT, 18h

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PO21 Identification of active compounds in indigenous plants used for diabetes

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Diabetes is the world's fastest-growing health pandemic. In South Africa, for the period 2016-2018, it was the second most underlying natural cause of death among the general population; among females, it was the leading cause of natural death.[1] There are several drugs, such as metformin and meglitinides, used to treat diabetes. However, many of these drugs have side effects or are excessively expensive.[2] Therefore, effective and affordable new drugs should be developed. Many commercial pharmaceutical drugs are based on natural products. Although plants are a good source of bioactive molecules, there are some limitations in the process of identifying these compounds. In the traditional approach, large amounts of plant material are extracted with organic solvents to yield extracts. This is followed by comprehensive chromatography to produce pure compounds, which are assayed for activity. The overall process is time-consuming and cumbersome. This project aims to identify plants with antidiabetic activity and to develop a strategy to isolate and characterize antidiabetic compounds in extracts of the plants without the need for excessive amounts of plant material and organic solvents. *Sclerocarya birrea* (A.Rich.) Hochst., also known as Marula, is an important tree for different purposes in African countries. A bark concoction is used to treat various diseases like diabetes.[3] The current study is conducted to identify active compounds in the plant extract by enzyme-inhibition studies on α-glucosidase and α-amylase, two enzymes that are targets for the discovery of antidiabetic drugs. Lead-like small-scale (300 mg) extractions were prepared from 19 plants. An α-glucosidase inhibitory assay was conducted on the plant extracts, and three extracts showed activity. LC-MS methods were developed for the extracts. Further investigations focused on *S. birrea*. In ongoing studies, the extract will be fractionated in triplicate into 96-well plates. One plate will be subjected to enzyme-inhibition studies. In the second plate, the wells showing activity will be analyzed by LC-MS-MS to determine the active compounds' retention times and molecular formulas. Preparative HPLC will be used to isolate the active compounds to confirm the structures and activities of these compounds.

Acknowledgements
The authors would like to thank the University of KwaZulu-Natal and NRF for research funds.

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PO22 Synthesis of Coumarin hybrids with potential anti-diabetic activity

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Diabetes mellitus is a group of metabolic diseases illustrated by abnormally high levels of plasma glucose or hyperglycemia. Drugs that are commonly used to treat diabetes produce various complications (most notably high risk of hypoglycaemia, bodyweight gain and gastric symptoms). Amongst these drugs, the α-glucosidase has gained significant attention of medicinal chemists and various potent anti-diabetic agents have been designed and synthesised by inhibition of this enzyme. The α-glucosidase enzyme catalyses the break down of carbohydrates into absorbable monosaccharides leading to increased glucose level in blood.[1] Hence, the inhibition of α-glucosidase reduces blood glucose level by delaying digestion of carbohydrates, and in turn suppresses postprandial hyperglycaemia.[2] Research on coumarins has increased significantly over the years due to their versatile pharmacological and biochemical properties.[3] The major factor being the biological activities that they possess[4] and their low toxicity.[5] Their potential contribution in the prevention and treatment of diseases is an attractive highlight in the pharmaceutical industry.[6] The aim of this project was to synthesize substituted coumarin hybrids and to test their anti-diabetic potential under in vitro conditions. All the synthesized compounds were characterized using NMR, FT-IR and HR-MS. The synthesized compounds will then be tested in vitro for their anti-diabetic activity using the standard drug, acarbose as a control. A structure activity relationship will be studied after the assay and computational studies will be done on the most active compounds.

Acknowledgements
National Research Foundation

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PO23 The design and synthesis of novel lassomycin peptide derivatives to target *Mycobacterium tuberculosis*, the causative agent of tuberculosis

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Tuberculosis (Tb) is one of the world's deadliest infectious diseases caused by a resilient pathogen known as *Mycobacterium tuberculosis* (Mtb) which infects around ten million people each year worldwide and claims over 1.5 million lives anually[1-2]. The emergence of multi-drug resistant (MDR) Tb has become a global challenge in the control, prevention and eradication of the disease[3]. The development of novel anti-Tb agents that use a different mechanism of action to target and kill Mtb is one of the ways that can be employed to overcome this challenge as most currently used anti-Tb drugs target the cell wall of Mtb. Lassomycin (Figure 1a) is a novel anti-microbial lasso peptide (Figure 1b) that was discovered from a soil bacterium, *Lentzea kentuckyensis* sp. and was found to selectively target and kill Mtb with potency that is similar to that of rifampicin, a leading approved anti-Tb drug. Lassomycin was also found to be active against latent Tb and multi-drug resistant (MDR) Tb strains. The peptide targets and binds to the caseinolytic protease and disrupts the regulated protein degradation process essential for cell survival, resulting in accumulation of damaged substrates that causes cell death due to toxicity[4]. Our study involves optimization of lassomycin to improve the effect of binding, peptide penetration to the bacterial cell wall, and to increase the effect of pathogenic cell rupture (potency). Peptides were synthesized using solid phase peptide synthesis strategy (SPPS) and purified using the semi-preparative High Performance Liquid Chromatogram (prep-HPLC). The compounds are analyzed using HPLC coupled to Mass Spectrometry (HPLC-MS).

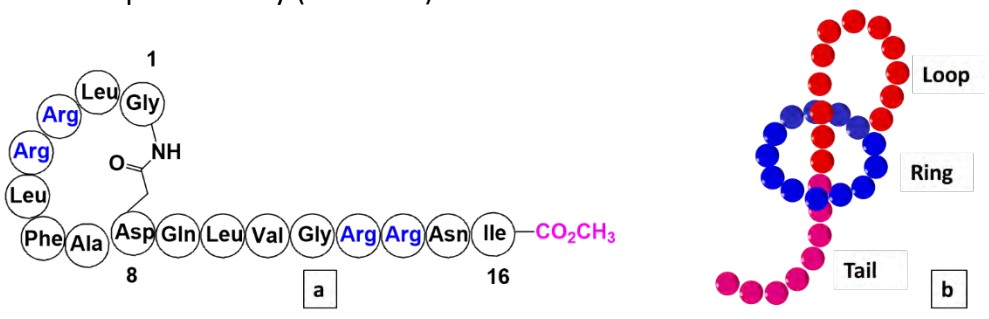

Figure 1: The structure of lassomycin illustrating (a) the sequence and connection of amino acid residues and (b) a depiction of a 3-dimensional lasso structure

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PO24 Towards The Continuous Flow Synthesis of Trimethoprim

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Infectious diseases have been well documented throughout the history of the world. Antimicrobials such as trimethoprim, listed on the World Health Organization's 20th Essential Medicines List (EML) under Key Access antibiotics have been used for both antimicrobial and antimalarial applications. However, China produces the largest quantities of this antimicrobial hence hiking the cost through importation of these medicines. Additionally, much of the production of trimethoprim is heavily reliant on the conventional batch processes. Consequently, we are working on developing local trimethoprim production in Africa exploring the use of continuous flow synthesis, with the goal of improving accessibility. Continuous flow chemistry is well known for its efficiency over batch processes. In this study, we investigated an efficient continuous flow production process for this antimicrobial drug. Herein, we report an optimised continuous flow process for trimethoprim. Batch reactions were done to obtain synthetic standards for all intermediates and to benchmark the continuous flow syntheses. All intermediates in this multistep process were optimised using Little Things Factory reactors. Under optimum flow conditions we obtained a 92% conversion at a residence time of less than 1 h compared to 31% conversion obtained in an overall process of more than 20 h in a batch procedure. In conclusion, we have developed a continuous flow synthesis protocol for trimethoprim and all intermediates in shorter reaction time and higher overall conversion. We also managed to telescope two of steps to achieve a multistep continuous flow process towards the synthesis of trimethoprim.

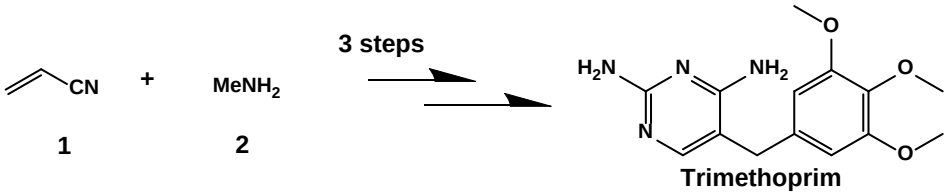

Figure 1: Schematic route for the preparation of Trimethoprim

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PO25 Synthesis, conformational analysis and biological evaluation of benzo[*b*][1,5]thiazepines as α-Glucosidase and/or α-Amylase inhibitors

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The 2.4-diaryl-2,3-dihydrobenzo[b][1,5]thiazepines were made by combining the binucleophilic properties of 2-aminothiophenol and the ambident electrophilic properties of 5-bromo-2-hydroxychalcones[1]. The structures and conformation of the synthesized compounds were determined using spectroscopic methods in combination with a single crystal X-ray diffraction (SC-XRD) approach. Both ^{1}H-NMR & IR spectroscopic techniques confirmed participation of the hydroxyl group in intramolecular hydrogen bonding interaction with a nitrogen atom. SC-XRD confirmed the presence of a six-membered intramolecularly hydrogen bonded pseudo-aromatic ring, which was supported by a DFT method on **2b** as a representative example in the gas phase. In comparison to acarbose (IC50 = 7.56 0.42 M), compounds **2a** (Ar = -C6H5), **2c** (Ar = -C6H4(4-Cl)), and **2f** (Ar = -C6H4(4-CH(CH3)2) showed higher inhibitory action against α-glucosidase. Their respective IC_{50} values were 6.70 ± 0.15 µM, 2.69 ± 0.27 µM and 6.54 ± 0.11 µM. The compound **2f**, which showed enhanced activity against α-glucosidase, also significantly inhibited α-amylase (IC50 = 9.71 0.50 M).

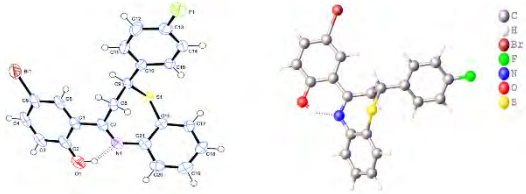

Figure 1: ORTEP diagram of 2b with thermal ellipsoids drawn at 50% probability level (a) and its optimized geometry (b) at the B3LYP/LANL2DZ level. The atom-labelling scheme for this compound is based on the XRD structure and the numbering differs from the systematic one.

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PO26 Synthesis of novel irreversible Janus kinase III Inhibitors

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Tofacitinib is a medically approved Janus kinase 3 (JAK3) inhibitor which is currently being used for the treatment of rheumatoid arthritis; however, the pan-JAK inhibition of this compound causes undesired effects.[1] Due to the severity of the side effects of Tofacitinib, many research groups have focused on the synthesis and development of novel irreversible JAK3 inhibitors. A true JAK3 inhibitor, known as RB1, has recently been reported in the literature and has been shown to reduce the severity of the disease.[2] Since the precise mechanism of JAK3 inhibition precludes rational drug design of novel compounds, it is our desire to generate a structure-activity relationship profile for RB1 as it represents a key lead structure for drug discovery. A library of RB1 derivatives obtained via this approach will be explored for their ability to complex in the lipophilic binding pocket of the JAK3 protein by way of irreversible inhibition. Initially, we will be exploring the addition of acrylamide onto the main scaffold; however, by incorporating different Michael acceptors, we will be able to compare the biological activity of these derivatives with clinically approved drugs. This will be carried out with the potential that these new drug candidates will have improved therapeutic profiles. When these final compounds become available, the inhibition activity of selected analogues will be determined using enzymatic assays.[3] The inhibitors will also be tested for inhibition against the other two members of the JAK family to determine the specificity of the inhibition of JAK3.

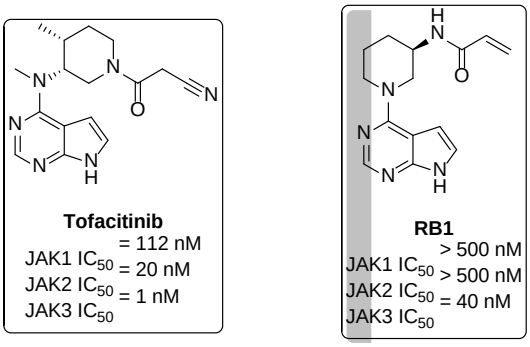

Figure 1: The inhibition concentrations of Tofacitinib and RB1.

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PO27 Reduction of α, β-alkynyl carbonyl compounds using $SnCl_2$ and computational investigation of the reaction mechanism

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The development of an efficient method for the reduction of α, β - alkynyl carbonyl compounds, is mostly important in organic synthesis, playing a crucial role in the synthesis of pharmaceuticals, pesticides, production of polymers and other valuable chemicals[1]. From the literature, no reaction was reported when Tin (II) chloride ($SnCl_2$) was used for the reduction of alkyne to alkane. The aim of this research is to investigate the reduction of conjugated α, β - alkynyl carbonyl compounds into alkanes using commercially available $SnCl_2$ and other metal salts known to reduce the nitro group, such as iron (Fe) and zinc (Zn). Our approach to the synthesis of 1-(6-nitroquinoxaline-2-yl) hex-1-yn-3-one, involves the use of 6-nitroquinoxalin-2-yl-benzenesulfonate compound as a substrate for Sonogashira cross coupling with terminal alkyne to give appreciable yield of 1-(6-nitroquinoxalin-2-yl)hex-1-yn-3-ol compound, followed by oxidizing using PCC or jones reagent to give 1-(6-nitroquinoxalin-2-yl)hex-1-yn-3-one. The oxidised product was used for reduction reaction at different temperatures, time, and equivalences of SnCl2. Our desired product was obtained with yields ranging from 47 - 75%. The optimised conditions were extended to other α, β - alkynyl carbonyl compounds such as 1-(pyrimidine-2-yl) hex-1-yn-3-one and 1-(pyrazine-2-yl) hex-1-yn-3-one and were found to be effective. Computational studies are currently underway to understand the mechanism involved at a molecular level[2].

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PO28 Incorporation of the Dotmatics platform in the WCNDD

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The Warren Center for Drug Discovery is a multi-lab entity that relies on the Dotmatics scientific platform to gather, understand, and share research data and experimental data across the whole center.
The Dotmatics platform consist of different modules:
Studies is subdivided into flexible templates: For our chemists, the Chemistry Electronic Lab Notebook is used to log compound details/synthesis and has a direct link to the Register module for registering new molecules. For our Molecular Pharmacology team, analysis template allows them to generate CRC from raw data. For our DMPK team, templates to uploads their raw data and parse directly into the database.
Register is a compound repository. The registration process assigns them a unique identifier that is then used throughout the database to bring all of the data together.
Gateway stores shared documents. Browser module, is the query side where all our data is linked together from Register, Studies, Inventory and Gateway. This module facilitates exporting data for further analysis with Blueprint, Vortex, excel, pdf, (future Prism) or downloading other documents the team might upload. Blueprint, Vortex and Prism are used by the team to take a deeper dive into the data.

PO29 Synthesis of imidazo [1,2-a]pyridine and pyrazolo [1,5-a]pyridine derivatives as potential kinase inhibitors of *Plasmodium falciparum* parasite

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Malaria is a disease that impacts negatively on the global health status and contributes more to mortality rate in the less developed countries[1]. The diseases arise from the protozoan parasite of genus *Plasmodium*[2]. *Plasmodium* kinases have been found to be important in facilitating several critical stages in the parasite lifecycle[3]. Targeting and inhibiting the activities of the enzymes implicated in the pathogenesis and/or progression of malaria such as P*V*PI4K AND P*f*PKG [4] represent the most effective therapeutic strategy for the treatment of this disease. A series of Imidazopyridines[5], pyrazole[6] exhibit a wide range of pharmacological properties of antimalarial activities. Considering the therapeutic potential of imidazo [1,2-a]pyridine and pyrazolo [1,5-a]pyridine against malaria, a series of novel imidazo [1,2-a]pyridine and pyrazolo [1,5-a]pyridine derivatives have been synthesised and evaluated for their activity as potential kinase inhibitors (P*v*PI4K and P*f*PKG) of plasmodium falciparum parasite.

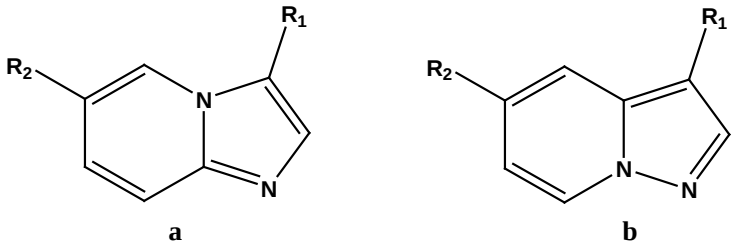

Figure 1a and 1b: Imidazo [1,2-a]pyridine and Pyrazolo [1,5-a]pyridine scaffolds respectively.

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PO30 Studies towards resolving racemic C_4-symmetric inherently chiral calix[4]arenes

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The synthesis of high yielding, enantiopure inherently chiral calixarenes (ICCs) has proven to be one of the greatest challenges regarding calixarene research. Many of the problems that plagued the early days of calixarenes, such as low yields, poor selectivity and painstaking resolution procedures, are still prevalent today. The focus within our group has been on finding approaches to access meta-functionalised ICCs. Most recently, it was demonstrated that a carbamate can act as an effective directing group for meta-functionalisation. The most interesting work was performed on tetracarbamate systems in which it was shown that the carbamate can direct a bromination reaction to produce ICCs with C_4 symmetry. Since the procedures produce a racemic mixture of ICCs, the focus of my research has been on their separation. This has been achieved by using Boc-L-proline as a chiral auxiliary. The brominated tetraproline derivative was produced in good yield and separation of the diastereomers was achieved using preparative TLC. The proline moiety was subsequently removed to produce a pair of pure ICCs (**5a** and **5b**).

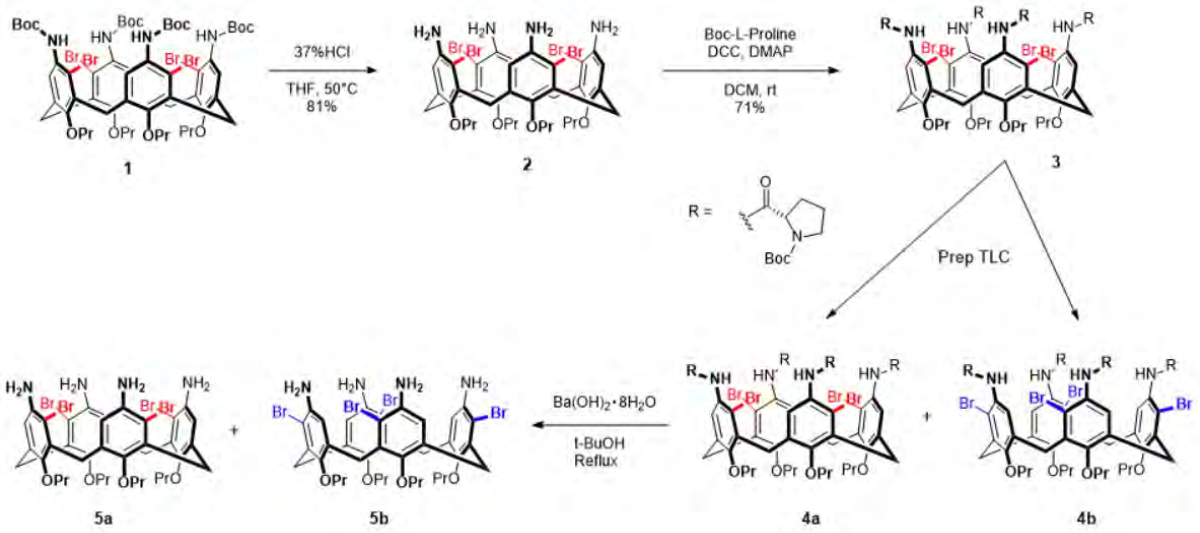

Figure 1: Synthetic route to produce C_4 tetraamino ICCs.

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PO31 Deuterium oxide as a deuterating agent for selective deuteration of chalcones

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Deuterium oxide (D_2O) and deuterium labeled compounds are essential tools for recognizing and studying biological and chemical processes.[1] Deuterium oxide (D_2O) is often used as the primary source for deuterium due to its low cost and toxicity.[1,2] Deuterated compounds are compounds labeled with deuterium and in medicinal chemistry they play important roles since are used to alter the absorption, distribution, metabolism and excretion properties of the investigational drugs.[3] In this presentation, we report a facile method for selective transfer deuteration of activated conjugated alkenes to deuterated alkanes using D_2O as deuterating agent in the presence of palladium catalyst. The deuterium isotope is incorporated in high yields and with good selectivity.

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PO32 Chiral acyl-radicals generated by visible-light enables stereoselective access to 3,3-disubstituted oxindoles

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Explorations in the repurposing of N-acyl chiral auxiliaries for use as novel chiral C1 radical synthons is reported. The acyl radicals are generated under visible-light mediated single electron transfer of N-hydroxyphthalimido ester and its use toward the stereoselective synthesis of 3,3'disubstituted oxindoles via a radical addition-cyclization sequence is demonstrated. Downstream synthetic utility of this method is showcased in the formal synthesis of the natural product (–)-physovenine. TEMPO trapping experiments support the proposed reaction mechanism presented.

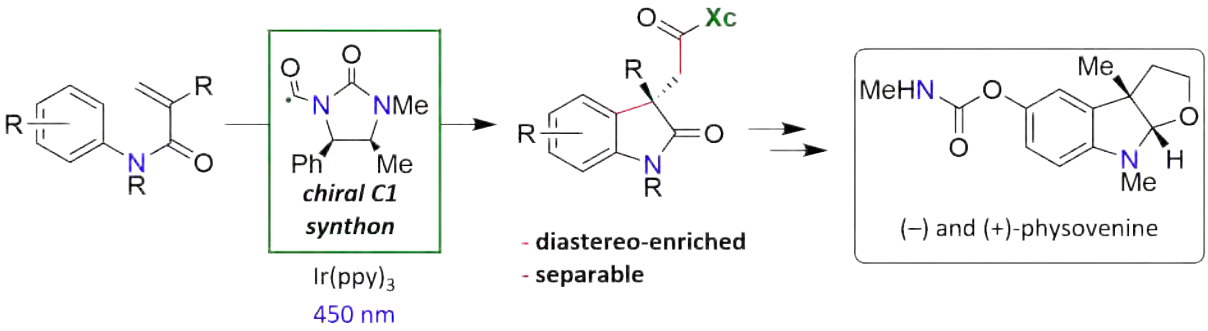

Figure 1

PO33 The effect of chemical properties on the overall *in vivo* biodistribution of radiodiagnostic compounds as visualized by microPET/CT imaging

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The design of pharmaceutically relevant compounds during the drug development process, from a chemist's point of view, focusses on chemical features such as stereochemistry, steric hindrance, molecular modeling and structure-activity relationship. However, when it comes to application of these compounds *in vivo*, there are additional factors that affect the compound's biological distribution, excretion and targeting efficacies which need to be considered[1]. These chemical properties include: molecular weight, lipophilicity and overall charge (if applicable) of a compound. Radiodiagnostic compounds (radiotracers) are compounds that have a radionuclide incorporated into their structure either by organic synthesis methods eg: fluorine-18 or by metal complexation eg: copper-64, gallium-68. Radiotracers are commonly used in nuclear medicine for disease targeting and diagnosis using positron emission tomography (PET) imaging[2]. The advantage of radiotracers is that they can track molecules below toxicity levels in real-time in a living system and therefore allow for establishing disease targeting and efficacy of a new drug by noninvasively investigating the drug's absorption, biodistribution and excretion[3]. This presentation evaluated and compared the *in vivo* biodistribution and excretion of 7 radiotracers using microPET/CT imaging and correlated the results to the chemical properties such as their molecular weight, lipophilicity and overall charge. This investigation highlights how the expected and required targeting of compounds can be influenced by factors that do not form part of the normal descriptive scope used in chemistry drug design.

Acknowledgements
Prof Thomas Ebenhan, Prof Jan Rijn Zeevaart, Ms Jillene Visser, Dr Janie Duvenhage, Ms Johncy Mahluleke

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PO34 Synthesis of 2-thiohydantoin derivatives as antidiabetic drugs

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Diabetes is a chronic condition that arises when the pancreas does not create enough insulin or when the body does not use the insulin that is produced adequately.[1] The rising prevalence of diabetes is expected to continue, and It is of utmost importance that the research on diabetes oral drugs continues to the discovery of better and more affordable diabetes medications.[2] Using the synthetic approach described below, the 2-thiohydantoin derivatives were effectively synthesized in high quantities (*Figure 1*). NMR spectroscopy supported the results, with compounds 5 characterized by the appearance of a singlet peak about 8ppm in their ^{1}H NMR spectra and compounds 6 characterized by 13-17 peaks in their ^{13}C NMR spectra. The final compounds (6) will be sent for biological assays where they will be evaluated for their alpha-glucosidase and alpha-amylase inhibition activities and their toxicity levels.

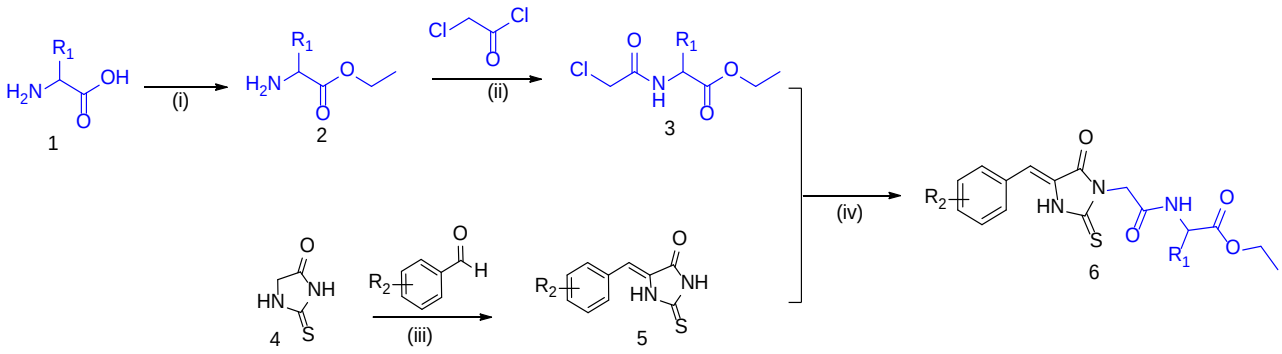

Figure 1: (i) $SOCl_2$, EtOH, reflux, (ii) DCM/H_2O, 0 ^{o}C-rt, (iii) AcOH, NaOAc, reflux, (iv) EtOH, Et_3N, reflux

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PO35 Synthesis and Investigation into the hormone receptor modulatory activity of natural isoflavans & flavonols and their synthetic derivatives in cancer

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Cancer is a burden globally with incidence and mortality rates on the rise. Breast cancer is reportedly the most invasive and prevalent cancer in women, while prostate cancer and lung cancer is the most prevalent in men. Due to the rise in incidence, mortality, and resistance to currently available chemotherapeutics, there is a need to develop new preventative strategies and treatments. Hormone receptor antagonists and inhibitors are widely used therapeutic agents in the treatment of hormone-related cancers. Phytoestrogens are natural products found in many dietary plants, can act as natural anti-cancer agents[1]. In this study we investigate the antagonist activity of natural isoflavans and their synthetic derivatives. We synthesized a small library of non-natural isoflavans and flavonols with different substituents at the 4'-position and tested them for any modulatory activity on CV1 cells transfected with either the estrogen receptor (ER) or the androgen receptor (AR). The synthesis made use of a [4+2] cycloaddition reaction between an *o*-quinone methide and an aryl-substituted enol ether based on the method by Gharpure *et al*[2]. The substituted flavonols were sythesized using the Algar-Flynn-Olyamade reaction[3]. The results of the study may provide structure-activity relationships and aid in the future design of hormone receptor antagonists for cancer prevention and therapy.

Acknowledgements
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PO36 Synthesis of substituted 5,7-dihydrodibenzo[*c*,*e*]oxepines as allocolchicine analogues

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Colchicine is naturally toxic and a secondary metabolite which is present in the *Colchicum autumnale* flower alternatively known as meadow saffron. In cancer research, because of its cytotoxicity, significant interest was gained in the anticancer properties of colchicine.[1] An isomer of colchicine which occurs naturally known as allocolchicine, has since then been applied in cancer research.[2] These compounds are known for targeting and inhibiting tubulin assembly however, the mechanism for this action is not yet fully understood. In this project the focus is on synthesizing 5,7-dihydrodibenzo[c,e]oxepines as allocolchicine analogues by means of palladium catalysed Suzuki-miyaura couplings and ring closures. The project also includes the synthesis of an analogue introducing an azide group to form an amide and in future study the effect that the electron donation of multiple methoxy groups has on the regioselectivity of the azide. The steps of the synthesis involve a bromination, then reduction followed by protection, subsequently the suzuki-miyaura coupling and finally an acidic deprotection and ring closure. The different compounds contain multiple methoxy groups – ranging from zero methoxy groups to three methoxy groups. It is seen that the synthetic yields pertaining to the three methoxy compound, starting material being 3,4,5-trimethoxybenzaldehyde, is the lowest and the trend of yield increases with decreasing methoxy group. The synthesis of compound with no methoxy groups, starting material being 2-bromobenzaldehyde, results in the highest yield. The trend is predicted to be influenced by the electron donation of the methoxy groups as well as possible sterics pertaining to the tert-butyldimethylsilyl group used for the protection. Future work would include biological testing of these compounds as well as introducing the azide group onto the molecules containing methoxy groups.

Acknowledgements
Stellenbosch University and supervisor Prof van Otterlo for support and guidance.

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PO37 Phenylcyclobutenone annulation reactions as new entry towards total syntheses of aglycones gilvocarcins

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Cyclobutenones, with their ring strain and enone moiety are useful intermediates[1,2] which have been shown to undergo annulation reactions *via* ketene intermediates that can cyclize to a naphthol rings[3]. In our work, we hope to employ this chemistry for the synthesis of gilvocarcin natural products. Cyclobutenones could be conveniently accessed through a [2 + 2] cycloaddition of ketenes with alkynes to form cyclobutenones[3]. To assess the generality of this method, we reacted model alkynes **3a-c** with the transient dichloroketene **2**, which was generated *in situ* from trichloroacetyl chloride **1** to yield cyclobutenones **4a-c** (**Figure 1**). A yield of 80% was obtained for terminal alkyne **3a**. A diminished, but fair yield of 68% was obtained when the substrate containing electron donating TMS group **3b** was used. Electron withdrawing substituents directly bonded to the alkyne group (X = Br) proved deleterious to the reaction, as the desired cyclobutenone **4c** was not detected from the reaction between **3c** and ketene **2**. Armed with this information, our current efforts are directed towards utilizing cyclobutenones, synthetized from terminal alkynes (akin to **3a**), in the novel total synthesis of aglycones gilvocarcins.

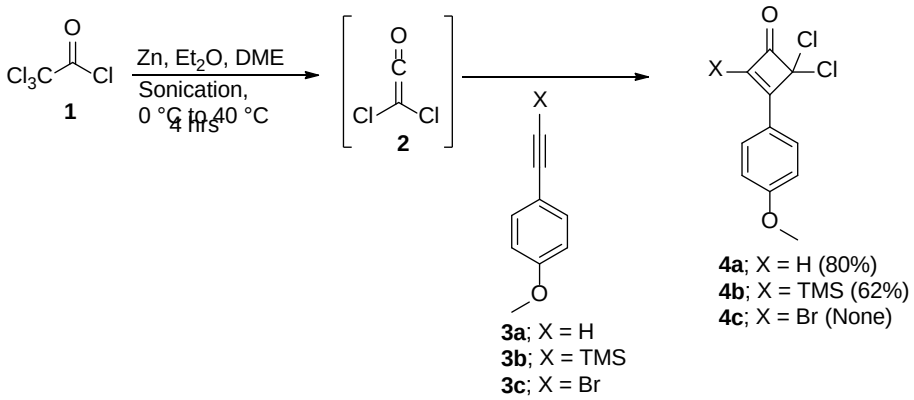

Figure 1. The general scheme of cyclobutenone **4** formation from the transient ketene **2** and alkyne **3**.

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PP1 Computational investigation of Zinc Oxide nanoparticles

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Numerous industries use the photocatalyst ZnO to produce photovoltaic solar cells, optical sensors, and optoelectronic devices.[1] ZnO's use as a photocatalytic degradation catalyst for organic pollutants,[2] has shown potential to reduce the toxicity of many industrial chemicals and dyes. ZnO is a useful photocatalyst[2] due to its strong oxidising power, hydrophobicity, antimicrobial activity,[3] stability, and non-toxicity. However, a disadvantage to ZnO is that its electronic properties indicate a relatively large bandgap of 3.37eV,[3] making it only photo-catalytically active when exposed to UV light.[1] However, research has been conducted to reduce the bandgap by adding modifier metals.[4] Using a Density Functional Theory (DFT) computational model of ZnO nanoparticles will aid the investigation of the electronic properties and reduction of the bandgap. Cubic and hexagonal crystal lattices identified experimentally were obtained and used to create bulk and surface structures of ZnO. The optimised surfaces were used to construct the ZnO nanoparticles. Their structural and electronic properties were studied. The calculated properties were compared to the experimental results described by Oyewo et al.[5] All computational calculations were done on the Lengau cluster at the Centre for High Performance Computing (CHPC)[6] using Materials Studio software. The models were calculated and optimised using Perdew, Burke, and Ernzerhof (PBE) functional within the generalised gradient approximation (GGA). This model will be used to find potential methods to reduce the bandgap and enhance the photocatalytic activity of ZnO nanoparticles.

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PP2 Synthesis, structures, and CO_2 sorption of Cu(II) and Zn(II) two-fold interpenetrated pyridyl diimide metal-organic frameworks

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Metal-organic frameworks (MOFs) are three-dimensional (3D) porous organic-inorganic hybrid materials.[1] MOFs possess high surface areas and large pore volumes.[2] They are also thermally stable, and their pore sizes can be tuned to the desired size.[2] MOFs are potential candidates for several applications in many disciplines, including pharmaceutics and materials science. Here we report the synthesis, structures and CO_2 sorption studies of two 2-fold interpenetrated three dimensional (3D) metal-organic frameworks (MOFs) namely; $\{[Cu(2,6\text{-}NDC)(L1)_{0.5}]\cdot 3DMF\}_n$ (**1**) and $\{[Zn_{0.5}(2,6\text{-}NDC)_{0.5}(L2)_{0.5}]\cdot 2DMF\}_n$ (**2**) where L1 is 5,5'carbonylbis (2-(pyridin-3-ylmethyl) isoindoline-1,3'-dione, L2 is 2,2'-bis(pyridin-4-ylmethyl)-[5,5-biisoindoline]-1,1-3,3'-tetraone, DMF is *N*,*N*'-dimethylformamide, and 2,6-NDC is 2,6-naphthalenedicarboxylic acid. The MOFs were synthesized solvothermally and characterized using single-crystal X-ray diffraction (SCXRD), thermogravimetric analysis (TGA), and powder X-ray diffraction (PXRD). SCXRD revealed that **1** and **2** are 3D and possess 33% and 22% of solvent-accessible volumes. Carbon dioxide sorption experiments were conducted at 195 K and 273 K on the activated phases of **1** (**1-d**) and **2** (**2-d**). **1-d** adsorbs 11 $cm^3\ g^{-1}$ (STP) at 273 K and 30 $cm^3\ g^{-1}$ (STP) at 195 K, while **2-d** adsorbs 35 $cm^3\ g^{-1}$ (STP) at 273 K and 80 $cm^3\ g^{-1}$ (STP) at 195 K.

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PP3 Investigating the self-organization of oxygen atoms on top of nanoporous gold surfaces with and without the effect of additional adsorbates

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The adsorption of carbon monoxide (CO) is a common prototypical reaction in gold-based heterogeneous catalysis, yet many facets of its reactivity are left unexplored. Recently, it was shown that oxygen (O) atoms tend to self-organize on stepped gold (Au) surfaces, forming quasi-ordered Au-O-chains with directional Au-O bonds, which get further stabilized in the presence of admetal silver (Ag) impurities.[1] The previously unexplored dynamic mechanistic picture of nanoporous gold (npAu) surface restructuring and reactivity during catalysis has been explored in-depth in this project with the help of ab initio molecular dynamics simulations, particularly focusing on the adsorption of O atoms on the gold surfaces. Furthermore, these simulations have unearthed how the presence of additional adsorbates such as CO and water alongside Ag surface and subsurface impurities affects the self-organization of O atoms on npAu surfaces, and its effect on the dynamic mechanistic picture of these surfaces. See Figure 1 for the self-organization of randomly placed oxygen atoms adsorbed on top of Au(221).[2]

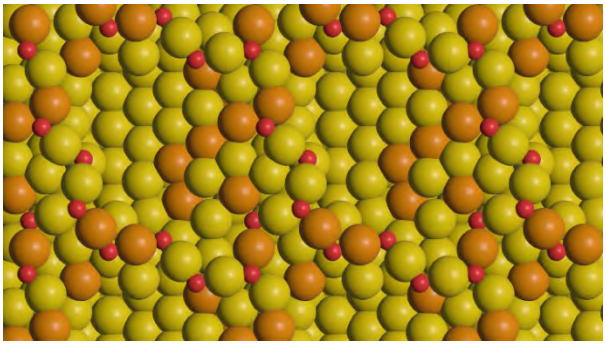

Figure 1: Self-organization of oxygen atoms atop Au(221). Red spheres are oxygen atoms, gold spheres are gold atoms and orange spheres are gold atoms that at the start of the simulation were stepped Au atoms

Acknowledgements
I would like to thank the DFG for providing the funding for this project, as well as the HLRN, RES and CHPC for providing the computational resources.

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PP4 Production of Mg-containing compounds via thermochemical treatment of diamond mine residues

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South Africa and other countries face a variety of environmental problems associated with the management of large volumes of solid mine waste residues[1]. Mine tailings and slimes are a form of environmental pollution through fine dust dispersal, slope instability, mud slides and possible contamination to local surface and ground waters, and also take up vast tracks of land that could possibly be used for other purposes. Mine residues can, however, represent untapped secondary mineral resources, which could be processed to promote sustainability through their conversion to valuable materials or products[2,3]. The aim of our study is to develop a process for the valorisation of diamond mine residues. The extraction of three components from the mine residues and their conversion to produce commercial-grade products are of particular interest. These include magnesium (for the production of magnesium carbonate or magnesium oxide nanoparticles, or layered double hydroxides); iron (for the production of iron nanoparticles) and talc (which can be used in numerous applications). This study reports on the experimental conditions applied to achieve maximum extraction of Mg from the mine residues, using a multistep process which entails the combination of a thermochemical solid-solid treatment step with ammonium sulphate[3,4], which is followed by aqueous dissolution. The reactivity of talc, present in the untreated tailings, with respect to the thermochemical and leaching steps was also investigated[5]. Experimental conditions required to precipitate Mg-containing compounds will be reported. The extent of conversion, from the soluble extracted minerals to the required products, was monitored using a combination of XRD, ICP-OES, SEM and TGA analyses.

Acknowledgements
The project was financially supported by the University of Pretoria and the National Research Foundation of South Africa (NRF Thuthuka Grant No. 117944). Any opinion, finding, conclusion or recommendation expressed in this material is that of the authors and the NRF does not accept any liability in this regard.

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PP5 Development of group contribution methods to predict the enthalpy of formation of energetic salts

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Ionic liquids (ILs) are low-melting salts with liquidity over a wide temperature range that are normally composed of an asymmetric organic cation and an inorganic or organic anion. Although ILs are typically associated with green chemistry due to their low vapour pressure, many are highly toxic and some, explosive. Whereas these properties can be detrimental to the potential of ILs as green solvents, they can be utilized to develop so-called energetic ionic liquids (EILs). Energetic materials include explosives, pyrotechnics, and propellants, which are not only useful for military purposes, but also have civilian, engineering, and mining applications. The assessment of the combustion and detonation properties of energetic liquids or salts require knowledge of the condensed phase standard enthalpy of formation, $\Delta_f H°$. *Ab initio* quantum chemistry can be used to compute gas phase ion pair enthalpies to high accuracy, but are computationally too expensive for large scale screening, and thus rational design. A cost-effective alternative to first-principles calculation is a group contribution method (GCM), which predicts thermodynamic properties of pure components and mixtures using atomic or functional group properties. GCM approximations can be classified into zeroth-, first-, and second-order, which sum the contributions from constituent atoms, bonds, or groups, respectively. In this work, the W1RO *ab initio* composite method was used to calculate $\Delta_f H°$ values for a systematically constructed set of five- and six-membered, N-heterocyclic neutral and charged molecules and ions with selected sidechains, forming the basis of EILs. A first-order GCM was then developed using this computational data. Greater transferability of the underlying group contributions is assured by accounting for ring strain, aromatic stabilization and charged contributions as separate corrections.

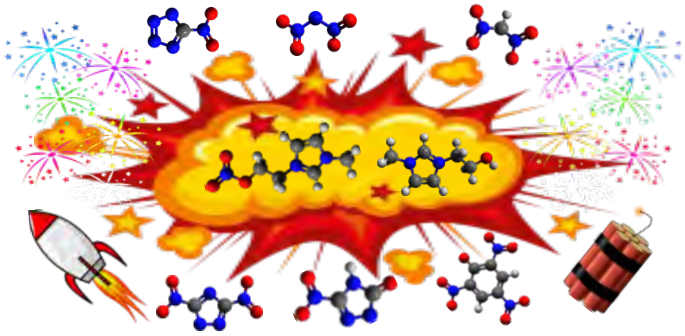

Figure 1

Acknowledgements
The authors acknowledge the Centre for High Performance Computing (CHPC), South Africa, for providing computational resources to this project.

PP6 Gold(III) Complexes of Isoquinolyl-Amide Ligands: Structural, Spectroscopic and DNA Binding Studies

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The structures, spectroscopy, and cytotoxicity of three novel square-planar gold(III) chelates (1–3) with the general formula cis-$AuCl_2(X)$, where X is a bidentate isoquinolylamide ligand (Figure 1), were elucidated using single crystal X-ray diffraction. The Au–N_{amido} and Au–$N_{isoquinolyl}$ distances are 2.00(4), and 2.04(3) Å, respectively. Density functional theory simulations afforded accurate coordination geometries for 1–3 (bond distances and angles within 5% of the X-ray values), while accurate transition energies were limited to those in the UV spectral region. These gold(III) chelates are anticipated to exert their cytotoxicity via DNA intercalation. Fluorescence competitive DNA binding studies were used to measure the binding affinity of the gold(III) mono(isoquinolyl-amide) chelates towards ctDNA. The binding affinities ranged from 1.52×10^5 M^{-1} to 3.14×10^5 M^{-1}. A structure/DNA affinity relationship is proposed. The gold(III) chelate (1) has a higher binding affinity than (2) and (3) which have EWG and EDG on the ortho position of the phenyl ring. One of gold(III) chelates structures exhibited Au···π interactions between the electron deficient gold(III) metal ion and the electron rich isoquinoline ring with an average interaction distance of 3.88 Å in the solid state. There is also some evidence of Au···Au interactions. The ligand structures exhibited extensive hydrogen bonding, which stabilize various supramolecular structures in the solid state.

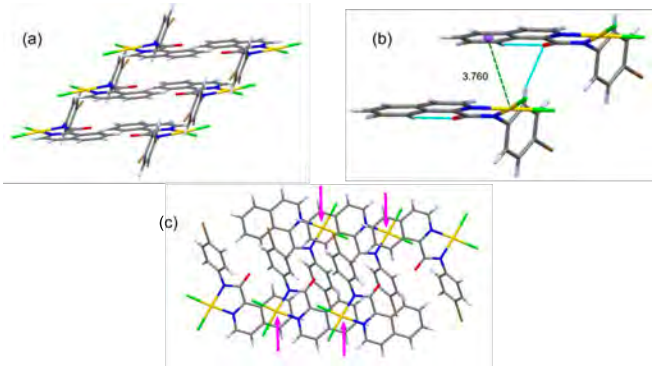

Figure 1. X-ray crystal structure of 2 showing (a) dimers stacked in a stepped pattern, (b) Au···π interactions and (c) shows the Au···π interaction viewed along the b axis.

PP7 (Not so) anomalous lattice expansion of Y(III) and Sc(III) co-doped δ-Bi_2O_3 solid electrolytes

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Significant research has been undertaken to develop electrolytes for solid oxide fuel cells that are fast ion conductors at lower operating temperatures than the most commonly used electrolyte, yttria stabilized zirconia. Of interest in this work are δ-Bi_2O_3-based electrolytes as they have the highest ionic conductivity amongst the solid oxides. The δ-phase of Bi_2O_3 is only stable in the narrow temperature range between 730 °C and 825 °C. However, it has been shown that by co-doping Bi_2O_3 with a range of trivalent cations the δ-phase can be stabilized to room temperature. When co-doping, if the proportion of the larger dopant cation increases at the expense of the smaller dopant cation, there is a slight expansion of the lattice, resulting in an improved oxide ion conductivity. [1] In this work we studied the Y(III) and Sc(III) co-doped system and found that as the proportion of Sc(III) - the smaller dopant cation - increases at the expense of Y(III) - the larger dopant cation – an anomalous lattice expansion is triggered. This confirmed results found by Wang *et al.* [2] They proposed that the lattice expansion was due to the reduction of Sc(III) to Sc(II), but this is highly unlikely since Sc(II) has not been identified before. As such, this work provides a comprehensive characterization of the phase composition of the Bi_2O_3-Y_2O_3-Sc_2O_3 system at various compositions using Rietveld refinement analysis of synchrotron powder X-ray data and proposes a mechanism for the reported lattice expansion.

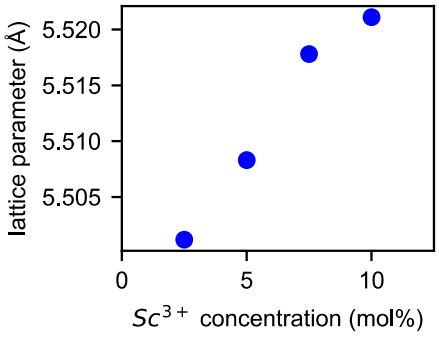

Figure 1: Variation of the cubic lattice parameter with Sc(III) dopant concentration.

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PP8 New insights into the squalene monooxygenase inhibitors for lowering cholesterol in cardiovascular biology using molecular docking and molecular dynamics simulations

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Over the past decades, the drugs called statins have been used in lowering high cholesterol, unfortunately several studies shows that people who are taking statins experience severe side effects especially in elderly patients, women of child birthing possibility, and children. For this reason, we conducted an *in silico* investigation into the squalene monooxygenase inhibitors that have the potential of lowering cholesterol in cardiovascular biology. In this framework, we have performed high throughput calculations, and molecular dynamics simulations. Our discoveries suggest that antimycotic squalene monooxygenase inhibitors, Terbinafine and its derivatives, and anticholesterolemic squalene monooxygenase inhibitors could be the alternative and safer remedies for lowering cholesterol in the future for mammals. From the calculations performed, the compounds show promising results with respect to the binding affinity to the target protein, Molecular dynamics calculations shows that the inhibitors stayed in the binding pocket over 100 ns simulations.

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PP9 A *Python* script for evaluating 3D 'Tolman cone angle'-based steric descriptors of N-substituents and their modulation of the dimer Au..Au distance

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A *Python* script was developed to calculate the Tolman-based cone angles,[1] for one apex coordinate and two 'hard sphere' contact points that are coplanar to a particular ϕ-plane, *i.e.* the sum of the angles defined by the $\overrightarrow{(\text{apex} - \text{contact})}$ vectors and the N-C axis vector of the N-substituent, i.e. θ_{sum} ($\theta_1 + \theta_2$). This plane may be the reference plane (ϕ=0°) or a plane rotated about the N-C axis ($0 < \varphi < 180$), as shown in Fig. 1. Polynomial regressions were performed for several variants in order to evaluate the capacity of Tolman-based cone angle descriptors to model Au..Au distances of the rTPSSh-D3(BJ)/def2-TZVP optimized-geometries (supplied as an XMOL .xyz file) and to explore the response of modifying several underlying parameters and options, used during the cone angle calculation, which included: branching levels (BL), 'hard sphere' radii (R) and whether projections of 'hard spheres' to ϕ-planes were applied or not.[2,3]

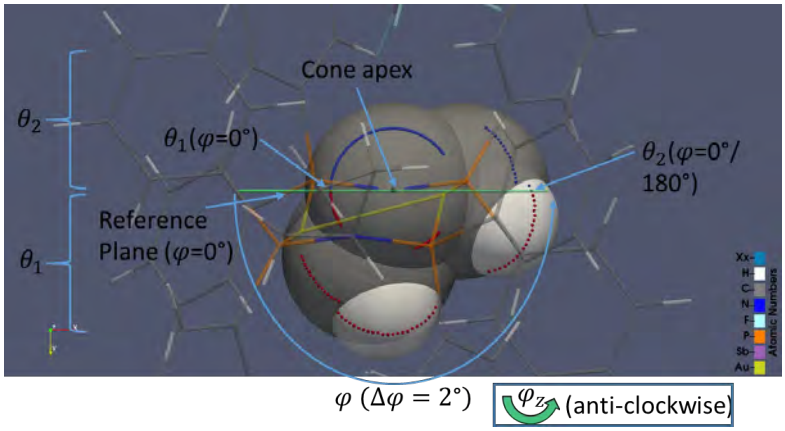

Figure 1: Orthographic view of a stick-representation of bis(μ_2-*bis*(diphenylphosphino)-cyclobutylamine)-di-gold(I)·2SbF_6^- system showing an approximate least-squares P-N-P reference ϕ-plane (ϕ =0°, shown in green) of a PNP-ligand, where the van der Waals sphere intercepts/contacts are shown as red and blue spheres for the range $0 \leq \varphi < 180$ ($\Delta\varphi = 2°$) [R=Bondi vdW radii,[2] BL = 3].

Acknowledgements
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PP10 Synthesis and Substitution Kinetics of Pyridyl *N,N'*-Bidentate Palladium(II) Complexes

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Amongst other metal-based drugs, significant similarities in coordination chemistry of platinum(II) and palladium(II) complexes had advocated studies of palladium(II) complexes as potential antitumor drugs to overcome side effects associated with Pt(II) complexes[1-3]. Considering the mechanism of action of platinum(II) complexes when interacting with DNA and other thiol containing biomolecules in target cells[4-5], we study the unexplored kinetics and mechanistic behavior of *N,N'*-pyridyl Pd(II) complexes, *viz*. dichloro-(2-pyridinemethanamine-*N,N'*)palladium(II) (**PdL1**), dichloro-(*N*-((pyridin-2-yl)methyl)aniline)palladium(II) (**PdL2**), dichloro-(4-fluoro-*N*-((pyridin-2-yl)methyl)aniline)-palladium(II) (**PdL3**), dichloro-(4-bromo-*N*-((pyridin-2-yl)methyl)aniline)-palladium(II) (**PdL4**) under *pseudo* first-order conditions. The Pd(II) complexes were synthesized and structurally characterized using NMR, FT-IR spectroscopy and mass spectrometry. The rate of the substitution of the chloride ligands from the complexes by the nucleophiles was studied as a function of nucleophile concentration and temperature using the stopped-flow and UV-visible spectrophotometric techniques. The observed *pseudo*-first-order rate constants, k_{obs}, appreciably followed the rate law $k_{obs} = k_2[Nu]$. DFT calculations were performed to elucidate the experimental data.

Acknowledgements
The authors gratefully acknowledge financial support from the University of KwaZulu-Natal and the National Research Foundation.

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PP11 The structural investigation of low-temperature rhombohedral bismuth oxide-based electrolytes

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South Africa is struggling to meet the energy demands of a rapidly growing society while being majorly coal-driven in energy supply. Alternative energy sources to consider in dealing with this shortfall are more efficient energy conversion devices such as solid oxide fuel cells (SOFCs). While SOFCs have attractive characteristics such as high specific energy and power density, their performance is limited by high temperature operation and long-term functioning[1,2]. Bismuth oxide electrolytes are studied through structural investigations to explore lowering the operating temperature of SOFCs while still maintaining efficiency[3]. The high-temperature face-centered cubic (fcc) phase of bismuth oxide has been extensively studied, but investigation of the low-temperature rhombohedral phase has largely been neglected. While the rhombohedral phase has lower ionic conductivity than the fcc phase, several characteristics of the rhombohedral phase contribute to its efficiency as an electrolyte material. The rhombohedral phase has a layered structure that provides several pathways for oxide ion conductivity[2,3]. Apart from its desirable low-temperature operation as an electrolyte material, the rhombohedral phase is also structurally stable. Most importantly, the lower ionic conductivity of the rhombohedral phase has the potential to improve upon doping with suitable metal cations[1]. In this work, the structure of the rhombohedral phase was investigated by examining the effects of varying compositions as well as thermal treatments. Stabilized Bi_2O_3 materials were synthesized using the citrate sol-gel method. The materials were characterized with powder X-ray diffraction and phase analysis of the materials showed the results of different dopant ratios and annealing temperatures. Further characterization was completed using thermal analysis to study the thermodynamic behaviour of the stabilized bismuth oxide electrolytes.

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PP12 Understanding the phase evolution of Y(III) and Pb(II) co-doped bismuth oxide electrolyte materials using the sol-gel synthesis

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Fuel cells provide a way to convert chemical energy directly into electrical energy. The primary components are the anode, cathode, and electrolyte[1]. In solid oxide fuels cells, the most commonly used electrolyte is yttrium-doped zirconia but these cells need to operate above 800°C to be sufficiently conducting[2]. This work focuses on using bismuth oxide as an electrolyte due to its extremely high conductivity in its face centered cubic (fcc) structure (Fig.1) which can then be utilized at lower temperatures. Pure bismuth oxide is only stable in the fcc structure between 730-824°C which is not optimal for the cell operation and longevity[3]. Doping bismuth oxide can result in fcc phase stability by also reduces the oxide conductivity. A combination of dopants are often used to optimize the sought-after properties. In this work a combination of yttrium (to stabilize the fcc structure at lower temperatures) and lead (to enhance its conductivity) was use to achieve these properties. Synthesis of the electrolytes were done using the sol-gel method. The gels were calcined for 8 hours at 500°C and annealed at between 700-750°C depending on the concentration of lead. Powder X-ray diffraction (PXRD) and simultaneous thermal analysis (STA) was used to determine the phase and thermal behavior of the materials of the final electrolyte as well as the optimal annealing temperatures and ideal amounts of dopants to stabilize the fcc phase. Additionally, the products from intermediate steps, including pre and post calcination steps, were investigated to build an understanding of the phase evolution of the material during the synthesis process.

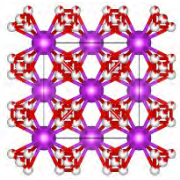

Figure 1: Cubic structure of bismuth oxide

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PP13 A Detailed Kinetic and Mechanistic Study of the Substitution Behaviour of Dinuclear Platinum(II) Phenanthroline Complexes with a Flexible Alkyl Bridging Ligand

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Several metal complexes have been reported to stabilize G-quadruplex DNA, thus leading to potent antitumor activity. However much of the current research has focused mainly on non-covalent binders to stabilize the quadruplex structure with covalent binders being largely excluded.[1-2] Recently, Shao and co-workers, presented a series of dinuclear platinum complexes of the type, [{Pt(dip)Cl}$_2$-(μ-diamine)](NO$_3$)$_2$, where dip = 4,7-diphenyl-1,10-phenanthroline, which contain two dual-functional platinum centers connected by an alkyl linkage. At least one of the complexes demonstrated an ability to stabilize G-quadruplex DNA and was able to cross-link to the quadruplex structure. These complexes offered several advantages: (i) each platinum center coordinated to a dip ligand to offer π-π stacking on G-tetrads, (ii) to enable the cross-linking reaction to the purine based in GQ sequence, one chloride moiety coordinated to each platinum center act as a leaving group and, (iii) an alkyl diamine occupying the last coordination site to link the two [Pt(dip)Cl] headgroups[3] In an effort to understand the mechanism by which Pt-phen derived complexes interact with biological moieties, we propose a detailed kinetic and mechanistic study of the substitution behavior of these, and some analogous complexes comprising linear alkyl linkages of increasing length. Currently, there are no such studies focusing on dinuclear platinum complexes comprising the 1,10-phenanthroline (phen) backbone or analogues thereof. We report here our progress thus far in terms of the synthesis of the mononuclear platinum(II) precursors, bridging with the alkyl diamine linker to form the dinuclear platinum(II) complexes, as well as preliminary computational and kinetic studies of these complexes.

Acknowledgements
We gratefully acknowledge financial support from the National Research Foundation (NRF)

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PP14 First-principles based evaluation of rate constants for R + O2 reactions with R = ethyl, isopropyl, isobutyl, t-butyl and neopentyl

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The kinetics and mechanistic pathways for the reactions of R = ethyl, isopropyl, isobutyl, tert-butyl and neopentyl with molecular oxygen have been studied. The B3LYP/cc-pvtz+d method was used to obtain the initial potential energy surface for each of the five elementary steps. For each transition state, intrinsic reaction coordinate (IRC) procedures were performed to confirm the connection between reactants and product species. The single-point electronic energies of stationary points were further refined using the very accurate composite W1U method. The enthalpies of formation, entropies and heat capacities of all reactants, products, and intermediates were determined and used in the calculation of rate constants. Variational transition state theory and Rice–Ramsperger–Kassel–Marcus theory were used to predict temperature and pressure dependent reaction rate constants at 300-1200 K and 760-1225 torr. Analysis of the results indicates that the entrance channel (O_2 addition to R) leading to the formation RO_2 of all the selected systems is barrieless and that the concerted OOH elimination channel is the most preferred for all systems except neopentyl system. These results are in agreement with published literature[1].

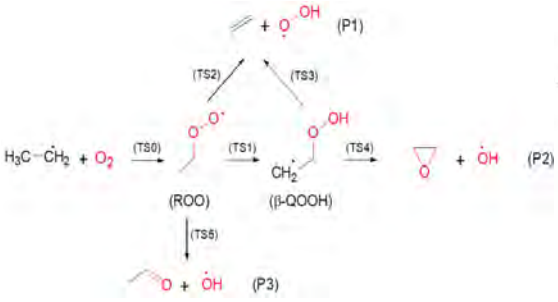

Figure 1: Ethyl + O_2 reaction network

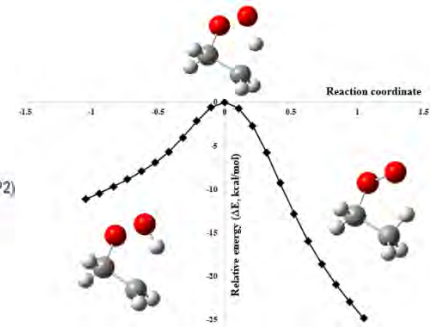

Figure 2: IRC path for isomerization of RO_2 to QOOH

Acknowledgements

We acknowledges the National Research Foundationund and the, Centre for High Performance Computing (CHPC), South Africa, for providing computational resources to this research project.

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PP15 Kinetic and mechanistic investigation into the influence of substituents on the substitution reactions of *cis*-Platinum(II) complexes

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The alteration of the structure of the non-leaving ligand of the *cis*-PtL_2 motif has a direct influence on the binding reactivity of the complexes with DNA as well as subsequent induction of cellular damage and downstream apoptotic processes.[1] The introducing of aromatic planar non-leaving ligands with substituents of variable σ-donor/π-acceptor capacity can result in favourable non-covalent interactions of the complexes with the bases of DNA.[2, 3] Foremost is the fact that the rate at which that occurs can be tuned by attaching substituents of variable σ-donor/π-acceptability. Bidentate Pt(II) complexes containing substituted pyridine-carboxamide chelating spectator ligands with varying substituents of different electronic properties were synthesized and characterized using NMR, FT-IR spectroscopy and mass spectrometry. Substitution reactions of the complexes with biological nucleophiles were studied under *pseudo* first-order conditions. The rate of substitution was investigated as a function of nucleophile concentration and temperature using the Stopped-flow and UV-Visible absorption spectrophotometers. The observed *pseudo* first-order rate constants regressed linearly with concentration on the incoming nucleophiles according to the equation: $k_{obs} = k_2[Nu]$. The reactivity of the complexes depends on the electronic effects and conformational disposition of the ligands. The substitution is associatively activated as supported by the negative entropy of activation values for the reactions.

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PP16 Synthesis and characterization of a series of multicomponent crystals with sulfanilamide derivatives

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Often promising active pharmaceutical ingredients (API) have poor physiochemical properties that inhibit them from being a practical treatment option. This includes poor solubility, dissolution rates or the properties are poor for processability. Crystal engineering is one method for solving this. In this work we combined sulfamethazine (**sz**) with benzoic acid and eight of its various derivatives, forming nine multi-component crystals all together. This includes 2-chloro-4-nitrobenzoic acid (**2c4n**), 2-chloro-5-nitrobenzoic acid (**2c5n**), salicylic acid (**2hba**), 3-hydroxybenzoic acid (**3hba**), 4-hydroxybenzoic acid (**4hba**), 4-bromobenzoic acid (**4Brba**), benzoic acid (**ba**), cinnamic acid (ca) and toluic acid (**ta**). These multi-component crystals were characterized by single crystal X-ray diffraction (SC-XRD), Powder X-ray diffraction (PXRD) and Differential scanning calorimetry (DSC). It was determined that the combination of **sz** and the respective benzoic acid formed a predictable hydrogen bonding pattern in each of the crystal structures: a ring based hydrogen bond motif formed between the carboxylic acid of the benzoic acid and the sulfonamide and pyrimidine ring of **sz** (**Figure 1**). PXRD confirmed that the single crystal represented the bulk material. DSC showed that each of the multi-component crystals, with the exception of **sz + 4brba** and **sz + ca** only had a melting peak. In the case of **sz + 4brba** and **sz+ca** an endothermic peak before melting was observed, which corresponds to a transition to an amorphous form before melting.[1]

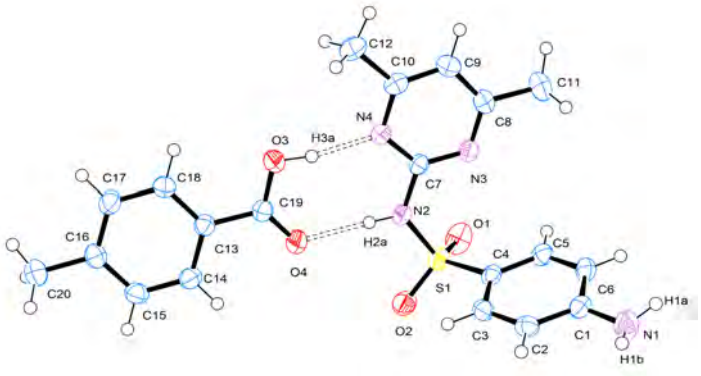

Figure 1: An ORTEP diagram showing the typical hydrogen bonding between a benzoic acid derivative (toluic acid (**ta**) in this case) and sulfamethazine (**sz**).

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PP17 Targeting the *Plasmodium falciparum* cGMP-dependent protein kinase: Machine learning and medicinal chemistry approaches.

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The ever-increasing parasite resistance to currently used antimalarials is why continued research of this disease and the development of structurally and mechanistically novel treatments is crucial. Recently, *P. falciparum* cGMP-dependent protein kinase (PfPKG) has been identified as a prioritised target for antimalarial drug discovery.[1] This enzyme plays a central role in parasite survival and is distinguished from its mammalian counterpart due to a small gatekeeper residue offering small molecule selectivity. Recent work in our research group has led to the development of the Antiplasmodium Chemical Space (APCS) map.[2,3] Generated using a simple principal component analysis algorithm, the map allows one to simply visualise a subset of antiplasmodium chemical space, and based on target class clustering, observe areas of enrichment for activity prediction. Myburgh *et al*. have demonstrated the successful use of the APCS map with respect to identifying new inhibitors of three diverse antimalarial drug targets, including PfPKG.[3] We intend to explore this further with the purpose of increasing the hit rate for discovery of PfPKG inhibitors. To this end, the APCS map was used as a preliminary filtration step to identify a subset of compounds from large online databases that fall in regions of PfPKG inhibitor enrichment. The ability of these compounds to inhibit this target as predicted by the APCS map was refined using a Random Forest machine learning algorithm trained on various descriptor sets. Subsequently, model validation was examined through biological testing of a subset of predicted PfPKG inhibitors. As of now, two hit compounds have been identified. These will undergo a lead optimization phase in an attempt to improve characteristics such as potency, solubility and selectivity. The computational model will also be refined and optimized as more data is collected and used in the training process.

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3. D. Myburgh *et al. Principal Component Analysis of Antiplasmodium Chemical Space Predicts Regions of Enrichment for Discovery of New Inhibitors of β-Hematin Formation, PfPKG and PfDHODH (Manuscript in Preparation)*, **2022**

PP18 Computational study of selected anti-cancer acylphloroglucinols in vacuo and in solution

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Cancer is the second leading cause of mortality worldwide. Drug resistance toward drugs currently in clinical use is increasing, posing the risk of fatalities' increase. Acylphloroglucinols (ACPLs) are a large class of compounds, mostly of plant origin, having a wide range of biological activities. Some of them have shown anticancer properties[1], and this makes them interesting because they have not yet been used for cancer treatment and therefore cancers have not developed resistance to them; they can be explored as lead structures for the development of new drugs[2]. Their molecules are phloroglucinol (1,3,5-trihydroxybenzene) derivatives characterized by the presence of at least one acyl (R-C=O) group; this enables the presence of an intramolecular hydrogen bond (IHB) between the sp^2 O of the acyl group and an *ortho* OH. The current presentation reports the results of a conformational study of 75 ACPLs with anticancer activity. Besides the conformational preferences, the study aimed at computing and comparing molecular descriptors such as the HOMO-LUMO energy gap and dipole moment, which are important for further analyses of the molecules' biological activities. Calculations with fully relaxed geometry were carried out at different levels of theory: Hartree-Fock (HF), Møller-Plesset Perturbation Theory (MP2) and Density Functional Theory (DFT) in vacuo, and HF and DFT in three solvents (chloroform, acetonitrile and water). The results show that the conformational preferences are dominantly influenced by the previously mentioned IHB common to all ACPLs, and other IHBs when present. Because of their role, the characteristics of the IHBs are analysed and compared in detail, both in terms of their parameters and in terms of the changes they cause in the computed IR vibrational frequencies (harmonic approximation) of the donor OH groups. The solvent effects influence the conformational preferences and the other molecular properties, in relation to the conformer types and the solvent polarity; e.g., the HOMO-LUMO energy gap gets smaller as the polarity of the medium increases and the dipole moment gets bigger.

Acknowledgements
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PP19 *In silico* study of the inhibition of PCSK9 for the reduction of atherosclerotic cardiovascular disease

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Over the years, cholesterol has earned a reputation as a high-risk factor for cardiovascular diseases. This is because the high concentrations of cholesterol in the blood may result in a buildup of plaque in the arteries that supply oxygen to the heart. Cholesterol build-up in the arteries interferes with blood flow resulting in atherosclerotic cardiovascular diseases or a heart attack. Cholesterol is an essential molecule in the body, for it is an integral part of the cell membrane and therefore provides the membrane's fluidity. Cholesterol is also essential for a number of cellular processes such as the production of bile, steroid hormones and Vitamin D. Cholesterol is obtained by the body from dietary constituents, and many cells can synthesize their own endogenous cholesterol. There are drugs currently in clinical use that target cholesterol biosynthesis in the body called statins, however they have been associated with severe side effects.[1] Recently US Food and Drug Administration and European Medicines Agency approved proprotein convertase subtilisin/kexin type 9 (PCSK9) inhibitors (alirocumab and evolocumab) as a new class of cholesterol-lowering drugs. Alirocumab and evolocumab reduce cholesterol levels but at a large cost relative to statins.[2-3] This study uses computational methods to elucidate the inhibitory pathways of alirocumab and evolocumab and search for other drugs with better activity and lower cost than evolocumab and alirocumab that target PCSK9.

Acknowledgements
The presenters acknowledge the NRF for funding and CHPC for computational recourses

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PP20 Crystallization of hydrates by sublimation

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Hydrates are common crystalline forms of many pharmaceutical materials and account for a third of pharmaceutical active drug forms[1,2]. A detailed understanding of hydrates is essential to improve the properties of drug forms such as stability, biopharmaceutical properties, and processability[2]. Hydrate formation has been well-explored via common crystallization methods such as mechanochemistry and solution crystallization[3]. Sublimation is based on the crystallization of a solid material from the gas phase and has previously been utilized in several studies as a crystal growth technique[3]. Although recent studies have explored the use of sublimation to selectively form salts and co-crystals, no attempt has been made to investigate whether hydrates of molecular crystals can be formed from sublimation, which formed the basis of this study. A series of organic molecules (Figure 1) with known hydrates were sublimed both in the presence and absence of water and we have shown that molecular crystals with stable hydrates at room temperature sublime as the hydrate in the presence of water, which can be attributed to the strong and dominant hydrogen-bonding interactions present within the hydrate crystal structure. An increase in the quantity of water resulted in an increase in crystalized hydrate for all systems, which correlates well with the stronger hydrogen bonds within these hydrate crystal structures. To further probe this, competition experiments between different hydrates were carried out.

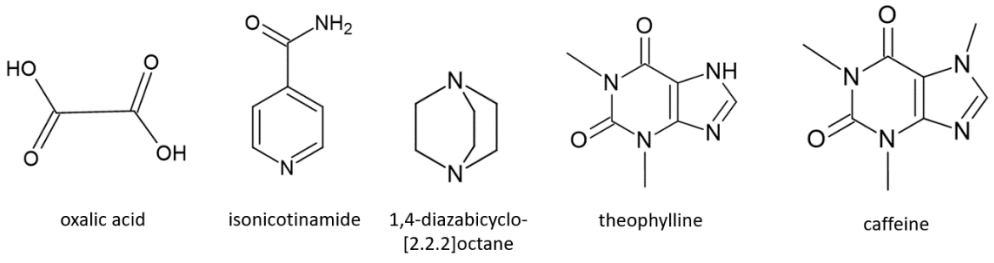

Figure 2: Structures of organic compounds used in this study.

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PP21 Application of the CL&Pol polarizable force field: a study of anion effects on ionic liquid transport properties

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Ionic liquids (ILs) have emerged as potential electrolytes in next-generation batteries with physical properties that align well with the requirements for beyond-lithium technologies, e.g., high thermal stability, low volatility, high ionic conductivity, a large electrochemical window, and the ability to solvate metal salts. IL-based electrolytes typically consist of pyrrolidinium-based cations with varying alkyl chain lengths; however, as the fundamental role of an electrolyte is to transport the metal ion through the solvent, the performance is largely dependent of the nature of the anion; therefore, a more significant focus is placed on the choice and refinement of the anion structure. Transport properties such as low viscosity, high diffusivity and high ionic conductivity are important for peak electrochemical performance, and an in-depth understanding of molecular features that control these properties is therefore key to the development of improved electrolytes. Molecular dynamics (MD) simulation is an important tool that can compliment experimental research for understanding how the thermodynamic and transport properties of ionic liquids are controlled by their underlying structure. In this work, the properties of ILs consisting of symmetric and asymmetric imide-type anions (see Figure 1) are determined with MD using the recently developed CL&Pol Drude-polarisable force field. These properties are analysed and compared to measured values to assess the accuracy of the force field. In addition, the fluidity is explained using the flexibility of the anions, as well as their interaction with the cation.

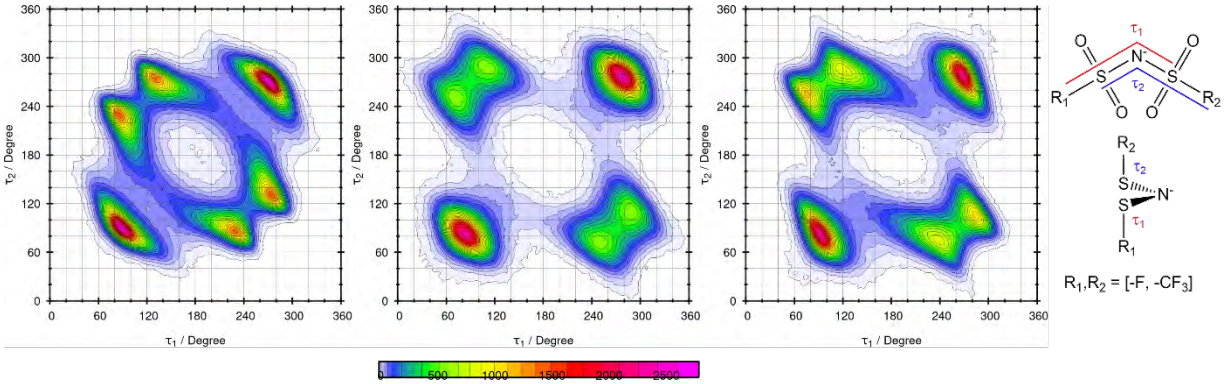

Figure 1: Distribution of anion dihedral angles in N-butyl-N-methylpyrrolidinium bis(trifluoromethanesulfonyl)-imide (left), (fluorosulfonyl)(trifluoromethanesulfonyl)imide (centre) and bis(fluorosulfonyl)imide (right) ILs.

Acknowledgements
The authors acknowledge the Centre for High Performance Computing (CHPC), South Africa, for providing computational resources to this project. Computations were also performed using facilities provided by the University of Cape Town's ICTS High Performance Computing team.

PM2 The Development of Biocompatible Polymeric Scaffolds for Drug Delivery

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The potential of polymeric scaffolds as drug delivery vehicles have been realized since the early 1900's[1], and since the pioneering work by Ringsdorf[2] on the rational design of polymeric drug scaffolds has continued to garner the interest of scientists. It is well known that polymer encapsulated drugs have extended half-lives, enhanced stability, increased aqueous solubility, decreased immunogenicity and antigenicity as well as the ability to specifically target tissues or cells.[3] The advancement of controlled free radical polymerization has enabled the synthesis of well-defined polymeric architectures with predictable molecular weight and low dispersity. The ability of amphiphilic block copolymers (BCPs) to undergo spontaneous self-assembly by solvophobic forces allows for the encapsulation of drug molecules in the core whilst stabilizing the aggregates periphery block polymer.[4] The aim of the project is to develop a method for synthesizing amphiphilic poly(*N*-vinylpyrrolidone)-*block*-poly(D,L-lactide) (PVP-*b*-PLA) in an one-step, one-pot polymerization procedure. The idea behind the orthogonal approach is to combined light mediated reversible addition-fragmentation chain-transfer (RAFT) polymerization and organocatalyzed ring-opening polymerization (ROP). The study exploits the inherent properties of the chain transfer agent (CTA) and find the synergy between the CTA and the ROP co-initiator to achieve orthogonal BCP synthesis, circumventing additional time-consuming purification steps.

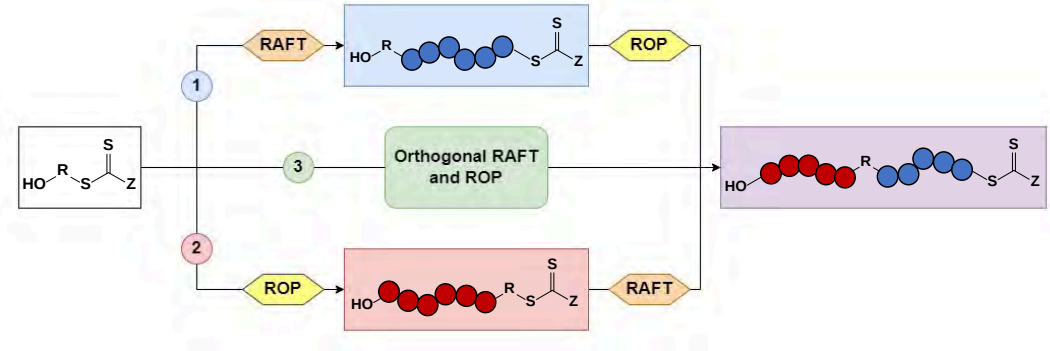

Figure 1: Synthetic strategy towards orthogonal BCP synthesis

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PM3 Surface modification of commercially available thermoplastics for biological applications

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The immobilization of bioactive compounds onto functionalized surfaces has been utilized extensively in biosensors, microarrays, and enzyme reactors.[1] Synthetic polymers, especially commercial thermoplastic films, are ideal for bio-functionalization due to their excellent mechanical properties, durability, and low cost.[1,2] However, the inert nature of these non-polar commercial polymers necessitates surface modification prior to the immobilization of bioactive compounds.[1,2] In this study, a UV-induced surface modification technique was investigated to functionalize commercial thermoplastic films for subsequent biological applications.[2] This UV-induced surface modification method exploits the photo-sensitive nature of dimethylformamide (DMF) and it can be applied in two ways: (i) using DMF in conjunction with vinylic monomers to introduce specific functionalities to the surface or (ii) using DMF to produce an amine-terminated surface.[1,2] Commercial polyethylene (PE), polypropylene (PP), and poly(ethylene terephthalate)(PET) films were considered for functionalization. Attenuated total reflectance Fourier transform (ATR-FTIR) spectra and Orange II staining results determined that PET films were the most susceptible to surface modification via the UV-induced modification method, compared to PE and PP films. Thus, commercial PET films were selected as the base polymer to be functionalized with different bioactive compounds, for two separate biological applications. The first application exploited the ability of the UV-induced method to introduce specific functionalities on the surface to produce a pH indicator. The second application exploited the ability of the UV-induced method to produce an amine-terminated surface to develop a bio-scaffold film for potential microalgae cultivation. Scanning electron microscopy (SEM) and ATR-FTIR data confirmed the surface modification and subsequent immobilization. The performance of each developed application was also evaluated used metrics such as colour response, red cabbage extract stability, and retention of biological activity. In conclusion, our study illustrated the utility of the UV-induced surface modification method for functionalizing inert thermoplastic films, which could then be immobilized with bioactive compounds for various applications.

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PM4 Well-defined styrene-maleic acid (SMA) copolymers for lipid membrane solubilization

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The advent of styrene-maleic acid lipid particle (SMALP) technology has facilitated the direct solubilization of membrane proteins from their native membranes into lipid-containing nanodiscs. Historically, membrane proteins (MPs) have proven difficult to isolate in their native and functional states due to the use of detergents that yield proteins void of lipid molecules in detergent-lipid complexes. The absence of lipids in these complexes can be destabilizing as the interplay between MPs and lipids is important for cellular function. Styrene-maleic acid (SMA) copolymers are thus a viable alternative for MP solubilization. To fully understand the role of SMA in the lipid solubilization process, a uniform copolymer sample, with respect to chain length and CCD is needed. To this end, we synthesized via an iterative RAFT technique, sequence- and length-controlled SMA (2:1) copolymers. The lipid solubilization efficiency and stability of the resultant nanodiscs were investigated. Well-defined SMA copolymers, such as those used in the present study, offer many intriguing possibilities to gain further insights into the mechanism of lipid solubilization via SMA copolymers and the subsequent influence on nanodisc properties.

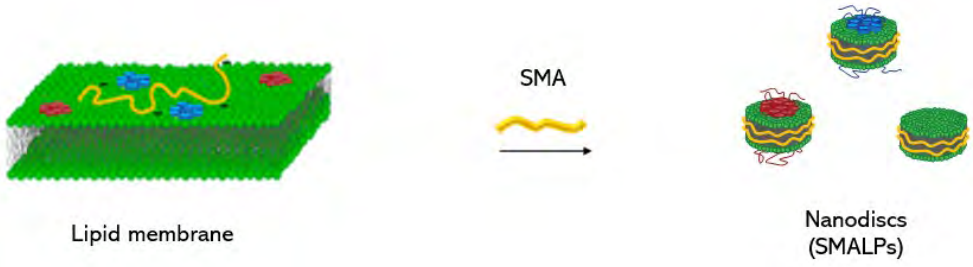

Figure 3: Lipid solubilization via SMA copolymer

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PM5 Designing an antibacterial polymer material for 3d printed consumer and medical devices

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Additive manufacturing is an ideal method for preparing materials with complex geometries,[1] as shown by literature examples with applications in the medical industry in prosthetics, tissue engineering and surgical tools.[2] Common engineering polymers provide good mechanical properties but lack the antibacterial properties needed for the medical field. There is a need, therefore, for polymer materials suitable for additive manufacturing, with antibacterial properties. To achieve this, we developed a method of blending two polymers, i.e. an engineering polymer (polyamide-11) and a quaternary amine functional polymer, antimicrobial polymer), giving give rise to a new polymer blend with properties from both individual polymers. Varying blend ratios were investigated, and blend compatibility was evaluated by determining the Flory-Huggins parameters via differential scanning. A proof-of-concept device, i.e., a surgical forceps, was then printed and post printing parameters evaluated.

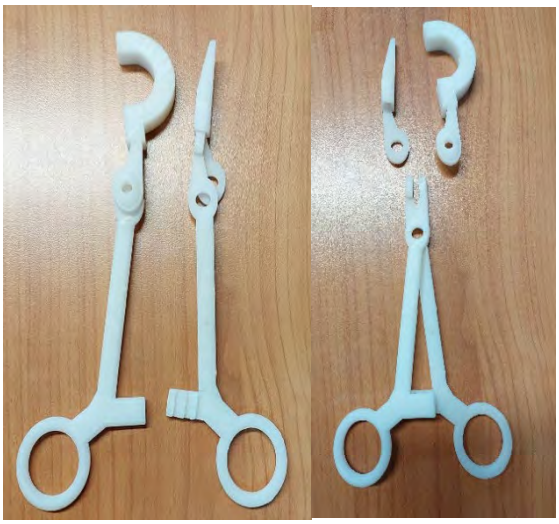

Figure 1: Proof of 3D printed concept - Forceps

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PM6 Comprehensive microstructural analysis of amorphous chain walking polyethylene random copolymers with polar functionalities

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Functionalized polyolefins possess properties that are of interest for various novel nanomaterial applications[1]. The late-transition metal catalysts (based on Ni and Pd) have been successfully employed to synthesize polyethylene with incorporation of polar functionalities in a one pot procedure following the chain-walking mechanism[2]. More interestingly, the chain walking mechanism of the catalysts results in macromolecule with a novel architecture but extraordinary complex molecular topology. Furthermore, palladium catalyst particularly produces polyolefin that is characterized by its highly amorphous nature due to high branch incorporation (up to 100 branches/1000 carbon) with branch-on-branch structures[3, 4]. Additionally, it is known that the branching topology and the overall molecular architecture of chain walking polyethylene are significantly influenced by the reaction conditions, notably ethylene pressure and temperature[5,6]. Herein we report the analytical protocol for a comprehensive study of the influence of synthesis conditions on the molecular structure of ethene-methyl acrylate random copolymers that is synthesized using Pd-catalyst. Preparative fractionation in combination with advanced analytical techniques including quadruple detector high temperature size exclusion chromatography (HT-SEC-4d), high temperature solvent interaction chromatography (HT-SGC), atomic force microscopy (AFM), nuclear magnetic resonance spectroscopy (NMR) unable in-depth understanding of the composition and structural distribution of these macromolecules.

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PM7 Understanding the molecular behaviour of alkali lignin

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The drive towards renewable feedstocks such as lignin for bio-based chemical applications has been of considerable interest. Lignin is desirable as it is produced in millions of tonnes as waste material, and is not in competition with societal needs. The complex heterogenous structure of lignin introduces challenges with understanding its chemical and physical properties, and ultimately its valorization. Molar mass is a molecular parameter providing insight on the properties of lignin. To determine the molar mass of lignin, size exclusion chromatography (SEC) is often implemented. However (1) poor solubility, (2) self-fluorescence and (3) aggregation, present challenges in accurate molar mass determination.[1] In this study SEC coupled to refractive index (RI) and multi-angle laser light scattering (MALLS) detection, in combination with various spectroscopic techniques was used to investigate the mechanisms involved in the size-based separation of alkali lignin (AL) (a technical lignin), see Figure 1 for schematic summary. Preparative SEC enabled the collection of size-based AL fractions, whose molar mass and mode of separation was determined by SEC-RI-MALLS. The self-fluorescence of lignin led to an over estimation of the molar masses, so to understand the fluorescence behavior and its dependence on lignin structural properties, selected fractions were analysed by fluorescence spectroscopy and nuclear magnetic resonance (NMR) spectroscopy.

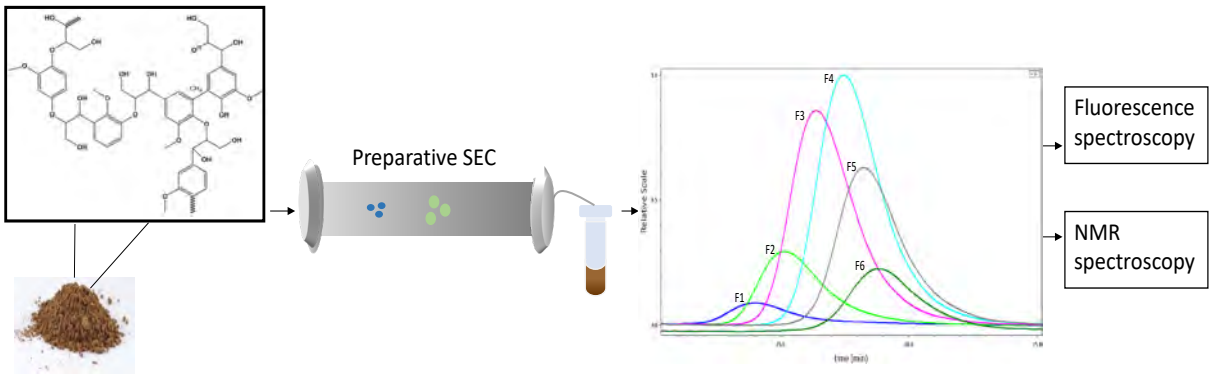

Figure 4: Preparative SEC fractionation of alkali lignin, followed by molar mass analysis by SEC-RI-MALLS, fluorescence emission analysis by fluorescence spectroscopy and chemical structure analysis by NMR spectroscopy.

Reference

1. G. Zinovyev, I. Sulaeva, S. Podzimek, D. Rössner, I. Kilpeläinen, I. Sumerskii, T. Rosenau, A. Potthast, *ChemSusChem*, **2018**, *11*, 3259 – 3268.

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Surname	Name	Theme	Abstract	Day	Venue	Time
Coetzee	Megan	Physical	PP5	Thursday	De Beers	
Cummings	Richard D.	ACS Symposium	KN13	Tuesday	1st Year Argon	11h35-12h20
Cunningham	Randy	Polymer	PM4	Thursday	Endler	
Currie	Dailin	Environmental	PE2	Monday	De Beers	
Danca	Busisiwe	Organic	PO4	Tuesday	De Beers	
Daniels	Miché	Polymer	PM5	Thursday	Endler	
Daramola	Olamide-	Green	C30	Tuesday	1st Year Neon	11h50-12h10
Davoren	Brandon	Industrial	C75	Friday	De Beers 2003	14h30-14h50
de Beer	Shane	Physical	C42	Tuesday	De Beers 2003	15h40-16h00
de Doncker	Stephen	Inorganic	PI3	Monday	De Beers	
de Koning	Charles	Gold Medal	G1	Sunday	Endler	18h00-18h45
de Villiers	Katherine	Inorganic	KN7	Monday	1st Year Neon	16h00-16h40
Dicks	James	Green	C37	Tuesday	1st Year Neon	14h30-14h50
Dikobe	Paki Israel	Environmental	PE3	Monday	De Beers	
Dikotla	Pertunia	Analytical	PA2	Monday	Endler	
Du Preez	Andrea	Analytical	PA3	Monday	Endler	Flash Monday Endler
Duma	Nontokozo	Physical	PP6	Thursday	De Beers	
Dwyer	Cathy	Industrial	KN32	Friday	De Beers 2003	16h00-16h40
Eaby	Alan	Physical	C57	Thursday	De Beers 2003	11h10-11h30
Falch	Anzel	Analytical	C26	Tuesday	Endler	11h30-11h50
Faure	Jessica	Organic	PO5	Tuesday	De Beers	
Feldmann	Wesley	Green	C39	Tuesday	1st Year Neon	15h40-16h00
Forbes	Patricia	Analytical	I1	Monday	Endler	12h10-12h40
Friedrich	Klaus	Inorganic	PI4	Monday	De Beers	
Friščić	Tomislav	Plenary	P2	Tuesday	Endler	9h00-10h00
Fynn	Darren	Physical	PP7	Thursday	De Beers	
Garnie	Larnelle	Inorganic	C21	Monday	1st Year Neon	15h40-16h00
Gebreyohannes	Belete Eshetu	Analytical	PA4	Monday	Endler	
Girdhari	Letisha	Organic	PO6	Tuesday	De Beers	
Golding	Taryn	Inorganic	PI5	Monday	De Beers	
Gondo	Thamani F.	Analytical	C13	Monday	Endler	14h30-14h50
Gould	Khaya	Organic	PO7	Tuesday	De Beers	
Gouws	Shawn	Education	C72	Friday	1st Year Neon	11h10-11h30
Gouws	Shawn	Industrial	PIND1	Monday	De Beers	
Govender	Kimberleigh	Organic	C71	Friday	Endler	11h50-12h10
Hlapisi	Nthabeleng	Inorganic	PI6	Monday	De Beers	
Hlengwa	Sbonelo	Organic	C78	Friday	Endler	14h30-14h50
Hloma	Phathisanani	Analytical	C34	Tuesday	Endler	14h30-14h50
Holme	Thomas A.	Education	KN28	Friday	1st Year Neon	10h30-11h10
Hulme	Alison	Organic	KN27	Friday	Endler	10h30-11h10

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Inger	Joseph	Organic	PO8	Tuesday	De Beers	
Invernizzi	Luke	Young Chemists	C46	Wednesday	1st Year Neon	11h30-11h50
Joseph	Cassiem	Inorganic	PI7	Monday	De Beers	
Kalebaila	Nonhlanhla	Environmental	KN8	Monday	De Beers 2003	16h00-16h40
Kandjo Ngoubeyou	Prisca Stephanie	Environmental	Pe4	Monday	De Beers	
Kaschula	Catherine	Organic	C54	Thursday	1st Year Neon	11h10-11h30
Kelani	Monsuru Temitope	Inorganic	C7	Monday	1st Year Neon	11h10-11h30
Kempkes	Geyan	Analytical	PA5	Monday	Endler	
Kenfack Tsobnang	Patrice	Physical	I20	Thursday	De Beers 2003	12h10-12h40
Kerssebaum	Rainer	NMR	KN26	Thursday	De Beers 2003	16h00-16h40
Khanye	Setshaba	Organic	C70	Friday	Endler	11h30-11h50
Kiwanuka	Mxolisi Junior	Analytical	PA6	Monday	Endler	
Klein	Rosalyn	Green	C29	Tuesday	1st Year Neon	11h30-11h50
Koiki	Babatunde	Environmental	C12	Monday	De Beers 2003	11h50-12h10
Kotze	Timothy	Organic	PO9	Tuesday	De Beers	
Kotzé	Izak A.	NMR	C68	Thursday	De Beers 2003	15h40-16h00
Kunene	Philisiwe	Analytical	PA7	Monday	Endler	
Kuyler	Gestél	Polymer	I6	Monday	1st Year Argon	14h00-14h30
Lau	Tracy	Physical	C58	Thursday	De Beers 2003	11h30-11h50
Lawrence-Moodley	Estee	Industrial	I31	Friday	De Beers 2003	14h00-14h30
Lebeko	Tsepo	Environmental	C84	Wednesday	1st Year Argon	10h30-11h10
Leboho	Tlabo	Organic	PO10	Tuesday	De Beers	
Lekgetho	Tumisang	Green	Pg1	Monday	De Beers	
Leoma	Mofeli Benedict	Physical	PP8	Thursday	De Beers	Flash Tuesday Endler
Lombard	Jean	Physical	C33	Tuesday	De Beers 2003	11h50-12h10
Luckay	Robert	Inorganic	I3	Monday	1st Year Neon	12h10-12h40
Mabaso	Mandla	Environmental	C48	Wednesday	De Beers 2003	11h10-11h30
Mabe	Chepape	Analytical	PA8	Monday	Endler	
Maboya	Winny	Analytical	PA9	Monday	Endler	
Mabunda	Karabo	Analytical	PA10	Monday	Endler	
Machakaire	Tatenda	Analytical	PA11	Monday	Endler	
Madikizela	Lawrence	Analytical	I18	Thursday	Endler	12h10-12h40
Maggott	Emile	Inorganic	Pi8	Monday	De Beers	Flash Monday de Beers
Maharaj	Vinesh	Organic	I19	Thursday	1st Year Neon	12h10-12h40
Mahhumane	Nondumiso	Analytical	PA12	Monday	Endler	
Mahlambi	Precious	Analytical	PA13	Monday	Endler	
Mahlangu	Walter	Analytical	C15	Monday	Endler	15h40-16h00
Maikoo	Sanam	Inorganic	C44	Wednesday	Endler	11h30-11h50
Maiphetlho	Kgomotso	Analytical	PA14	Monday	Endler	

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Makatini	Maya	Organic	I28	Friday	Endler	14h00-14h30
Makgaba	Dinah	Inorganic	PI9	Monday	De Beers	
Makgoathana	Herman	Organic	PO11	Tuesday	De Beers	
Makhura	Winie	Analytical	PA15	Monday	Endler	
Makobe	Samuel	Analytical	C51	Thursday	Endler	11h10-11h30
Makwakwa	Tlou	Green	PG2	Monday	De Beers	
Malaza	Siphelele	Industrial	PIND2	Monday	De Beers	
Malete	Sabina	Analytical	PA16	Monday	Endler	
Maluleke	Blesant Kerryn Tsakane	Organic	PO12	Tuesday	De Beers	
Maluleke	Patience	Analytical	PA17	Monday	Endler	
Manamela	Lebogang	Analytical	C35	Tuesday	Endler	14h50-15h10
Manye	Remofilwe	Inorganic	PI10	Monday	De Beers	
Mapetla	Sabetha	Analytical	PA18	Monday	Endler	
Maphakela	Khuliso	Analytical	C53	Thursday	Endler	11h50-12h10
Maphoru	Mabuatsela	Organic	Po13	Tuesday	De Beers	
Martincigh	Bice	Environmental	KN4	Monday	De Beers 2003	10h30-11h10
Maseko	Nontlantla	Organic	Po14	Tuesday	De Beers	
Maseme	Mametsi	Inorganic	C19	Monday	1st Year Neon	14h30-14h50
Mashale	Kedibone	Analytical	C62	Thursday	Endler	15h40-16h00
Mashazi	Philani	Inorganic	C45	Wednesday	Endler	11h50-12h10
Mashigo	Maria	Analytical	C87	Wednesday	1st Year Argon	11h50-12h10
Mashiloane	Karabo	Environmental	C23	Monday	De Beers 2003	14h50-15h10
Masilela	Vusi Witbooi	Analytical	PA19	Monday	Endler	
Matabane	Lovia	Environmental	PE6	Tuesday	Endler	
Mathabathe	Kgadi	Education	I26	Friday	1st Year Neon	12h10-12h40
Mathenjwa	Gciniwe	Organic	PO15	Tuesday	De Beers	Flash Tuesday de Beers
Mathura	Sadhna	Inorganic	PI11	Monday	De Beers	
Matlhabadie	Dineo	Organic	PO16	Tuesday	De Beers	
Matthews	Cameron	Physical	PP9	Thursday	De Beers	
Maziya	Khona	Environmental	PE7	Tuesday	Endler	
Mbonzhe	Luccile	Inorganic	PI12	Thursday	De Beers	Flash Tuesday de Beers
Mbuyazi	Thandi	Inorganic	PI13	Monday	De Beers	
Mcphail	Kerry	Organic	KN30	Friday	Endler	16h00-16h40
Mdanda	Sipho	Analytical	PA20	Tuesday	Endler	
Mdluli	Njabulo Simanga	Analytical	C2	Monday	Endler	11h30-11h50
Mdluli	Njabulo Simanga	Analytical	PA21	Monday	Endler	
Mehlo	Thembelihle	Industrial	C76	Friday	De Beers 2003	11h30-11h50
Mgiba	Samuel	Analytical	C14	Monday	Endler	14h50-15h10
Mjwara	Pinky Ncomela	Physical	PP10	Thursday	De Beers	Flash Tuesday Endler

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Mkhize	Sinethemba	Inorganic	PI14	Monday	De Beers	
Mngadi	Sihle	Environmental	C24	Monday	De Beers 2003	15h40-16h00
Mngadi	Sihle	Environmental	PE8	Tuesday	Endler	
Mntambo	Thandiwe	Green	PG3	Monday	De Beers	
Moagi	Violet Mamaele	Analytical	PA22	Monday	Endler	
Mofokeng	Nondumiso	Environmental	C11	Monday	De Beers 2003	11h30-11h50
Mokgalaka-Fleischmann	Ntebogeng	Environmental	I17	Wednesday	De Beers 2003	12h10-12h40
Mokganya	Khomotso Jamie	Organic	PO17	Tuesday	De Beers	
Mokoena	Terrinne	Organic	PO18	Tuesday	De Beers	
Molefe	Dan	Polymer	C16	Monday	1st Year Argon	14h30-14h50
Molepo	Kwena	Analytical	PA23	Tuesday	Endler	
Mollo	Vuyo	Analytical	PA24	Tuesday	Endler	
Moloto	Nosipho	Inorganic	KN20	Wednesday	Endler	10h30-11h10
Mona	Lijo	Inorganic	PI15	Monday	De Beers	
Moodley	Brenda	Environmental	I33	Wednesday	1st Year Argon	12h10-12h40
Moodley	Danica	Analytical	C27	Tuesday	Endler	11h50-12h10
Moodley	Thrineshen	Analytical	C3	Monday	Endler	11h50-12h10
Morethe	Moloko	Analytical	C61	Thursday	Endler	14h50-15h10
Morrison	Caitlin	Physical	PP11	Tuesday	De Beers	
Moyo	Babra	Analytical	PA25	Tuesday	Endler	
Moyo	Dennis	Physical	C31	Tuesday	De Beers 2003	11h10-11h30
Msagati	Titus	Analytical	KN5	Monday	Endler	16h00-16h40
Mthiyane	Wakhiwe Mthandi	Inorganic	PI16	Monday	De Beers	
Mubiayi	Pierre	Green	C38	Tuesday	1st Year Neon	14h50-15h10
Mundy	Christine	Education	I30	Friday	1st Year Neon	14h30-14h50
Munnik	Brandon	Inorganic	PI17	Monday	De Beers	
Muzenda	Charles	Analytical	PA26	Monday	Endler	
Naicker	Emileo	Physical	PP12	Tuesday	De Beers	
Naicker	Tricia	Young Chemists	I16	Wednesday	1st Year Neon	12h10-12h40
Ndlangamandla	Nqobile	Inorganic	Pi18	Monday	De Beers	
Ndlela	Lungelo	Physical	PP13	Tuesday	De Beers	
Ndlovu	Malcolm	Inorganic	C20	Monday	1st Year Neon	14h50-15h10
Ndlovu	Matumelo	Organic	PO19	Tuesday	De Beers	
Ndou	Dakalo	Analytical	PA27	Tuesday	Endler	
Ndwabu	Sinayo	Analytical	PA28	Tuesday	Endler	
Nemudzivhadi	Anza	Organic	PO20	Tuesday	De Beers	
Nety	Sol	Analytical	PA29	Tuesday	Endler	Flash Tuesday Endler
Ngcobo	Nkosinathi	Organic	Po21	Thursday	Endler	
Ngcoya	Nomandla	Organic	PO22	Thursday	Endler	

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Ngqinayo	Ntombizanele	Organic	PO23	Thursday	Endler	
Ngubeni	Grace	Analytical	C36	Tuesday	Endler	15h40-16h00
Ngwenya	Sandiso	Organic	PO24	Thursday	Endler	Flash Monday Endler
Nhlapho	Samukelisiwe	Analytical	PA30	Tuesday	Endler	
Nkoana	Jackson	Organic	PO25	Thursday	Endler	
Nkosi	Duduzile	Analytical	PA31	Monday	Endler	
Nkwachukwu	Oluchi	Analytical	PA32	Monday	Endler	
Nokeri	Boitumelo	Analytical	PA33	Tuesday	Endler	
Ntola	Pinkie	Inorganic	PI19	Thursday	De Beers	
Ntombela	Silindile	Analytical	C85	Wednesday	1st Year Argon	11h10-11h30
Nxumalo	Nonhlazeko	Analytical	PA34	Tuesday	Endler	Flash Tuesday Endler
Nxumalo	Winston	Organic	I24	Thursday	1st Year Neon	16h00-16h40
Nyamori	Vincent	Physical	C32	Tuesday	De Beers 2003	11h30-11h50
Obiechefu	Zodidi	Green	C28	Tuesday	1st Year Neon	11h10-11h30
Oddy	Meghan	Organic	C79	Friday	Endler	14h50-15h10
Odularu	Ayodele	Education	C81	Friday	1st Year Neon	15h40-16h00
Odularu	Ayodele	Inorganic	PI20	Thursday	De Beers	
Ojo	Babatope	Analytical	C25	Tuesday	Endler	11h10-11h30
Olaitan Amusat	Sefiu	Analytical	Pa35	Tuesday	Endler	
Olaniyan	Okikiola	Physical	C40	Tuesday	De Beers 2003	14h30-14h50
Olorundare	Foluke Omobola Grace	Analytical	PA36	Monday	Endler	
Oloyede	Solomon O.	Analytical	PA37	Tuesday	Endler	
Onkani	Shirley Priscilla	Environmental	PE10	Tuesday	Endler	
Opeolu	Beatrice	Analytical	I4	Monday	De Beers 2003	12h10-12h40
Otukile	Kgalaletso	Physical	PP14	Tuesday	De Beers	
Ozoemena	Kenneth	ACS Symposium	KN16	Tuesday	1st Year Argon	14h30-14h50
Paca	Athandwe	Inorganic	PI21	Thursday	De Beers	
Papo	Tshephiso	Physical	PP15	Tuesday	De Beers	
Pester	Christian	Polymer	KN2	Monday	1st Year Argon	10h30-11h10
Petrik	Leslie	Environmental	KN21	Wednesday	De Beers 2003	10h30-11h10
Pfukwa	Helen	Analytical	PA38	Monday	Endler	
Pfukwa	Reuben	Polymer	I2	Monday	1st Year Argon	12h10-12h40
Pholosi	Agnes	Environmental	C50	Wednesday	De Beers 2003	11h50-12h10
Ponnusamy	Samy	Green	I13	Tuesday	1st Year Neon	14h00-14h30
Potgieter	Jean-Phillip	Organic	PO26	Thursday	Endler	
Rademeyer	Melanie	Physical	KN24	Thursday	De Beers 2003	10h30-11h10
Rakodi	GH	Inorganic	PI22	Thursday	De Beers	Flash Monday de Beers
Ralepelle	Ursula	Organic	PO27	Thursday	Endler	Flash Monday Endler
Ramoba	Lesetja V.	Inorganic	PI23	Thursday	De Beers	

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Spath	Josef	Organic	PO32	Thursday	Endler	Flash Monday de Beers
Stanvliet	Zahn	Polymer	C18	Monday	1st Year Argon	15h40-16h00
Stechmann	Bahne	Organic	C80	Friday	Endler	15h40-16h00
Stevens	Jeanri	Environmental	C22	Monday	De Beers 2003	14h30-14h50
Stingelin	Natalie	Plenary	P1	Monday	Endler	9h00-10h00
Strydom	Christien	Physical	KN11	Tuesday	De Beers 2003	10h30-11h10
Swanepoel	Cecile	Organic	PO33	Thursday	Endler	
Swarts	Andrew	Inorganic	C9	Monday	1st Year Neon	11h50-12h10
Szweda	Róża	Polymer	KN6	Monday	1st Year Argon	16h00-16h40
Tapala	Kgaugelo	Inorganic	PI29	Thursday	De Beers	Flash Tuesday de Beers
Tenza	Perceverence	Analytical	PA45	Tuesday	Endler	Flash Tuesday Endler
Thiart	Taella	Industrial	C83	Friday	De Beers 2003	14h50-15h10
Thibaud	Jessica	Physical	PP17	Tuesday	De Beers	
Toerien	Rene	Education	KN31	Friday	1st Year Neon	16h00-16h40
Tshilande	Neani	Physical	PP18	Tuesday	De Beers	
Tshishonga	Unarine	Organic	PO34	Thursday	Endler	
Tshiwawa	Tendamudzimu	Physical	PP19	Tuesday	De Beers	
Tshoko	Siphokazi	Green	PG4	Monday	De Beers	
Tsipa	Nikiwe	Organic	PO35	Thursday	Endler	
Tumeli	Tsepo	Inorganic	PI30	Thursday	De Beers	
Turner	Charlotta	Green	KN1	Monday	Endler	10h30-11h10
Tutu	Hlanganani	Analytical	I5	Monday	Endler	14h00-14h30
Tyhali	Akhona	Analytical	PA46	Tuesday	Endler	
van Biljon	Angeline	Analytical	C52	Thursday	Endler	11h30-11h50
van der Klashorst	Gerrit	ACS Symposium	KN14	Tuesday	1st Year Argon	12h20-12h55
van der Merwe	Leandre	Inorganic	PI31	Thursday	De Beers	
van der Merwe	Petra	Analytical	C1	Monday	Endler	11h10-11h30
van Lill	Amy	Organic	PO36	Thursday	Endler	
van Niekerk	Annick	Inorganic	PI32	Thursday	De Beers	
van Steen	Eric W. J.	Physical	KN19	Tuesday	De Beers 2003	16h00-16h40
van Zyl	Werner	Green	I10	Tuesday	1st Year Neon	12h10-12h40
Venter	Gerhard	Physical	C41	Tuesday	De Beers 2003	14h50-15h10
Volkwyn	Alexandra	Physical	PP20	Tuesday	De Beers	
Wang	Shaomeng	ACS Symposium	KN12	Tuesday	1st Year Argon	10h50-11h35
Watts	Paul	Organic	I25	Friday	Endler	12h10-12h40
Wei	Xueting	Young Chemists	C47	Wednesday	1st Year Neon	11h50-12h10
Weigand	Jan	Plenary	P3	Wednesday	Endler	9h00-10h00
Welsh	Athi	Inorganic	C8	Monday	1st Year Neon	11h30-11h50
Williams	Chelsea	Polymer	PM7	Thursday	Endler	

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Wilson	Angela	ACS Symposium	KN17	Tuesday	1st Year Argon	15h50-16h35
Wilson	Tayla	Physical	PP21	Tuesday	De Beers	
Wooding	Madelien	Analytical	C60	Thursday	Endler	14h30-14h50
Wright	Sarah	Organic	PO37	Thursday	Endler	Flash Monday de Beers
Yusuf	Tunde	Environmental	PE13	Tuesday	Endler	
Zeevaart	Jan Rijn	Industrial	I32	Friday	De Beers 2003	15h40-16h00
Zimmermann	Ralf	Analytical	KN22	Thursday	Endler	10h30-11h10
Zinman	Paige	Inorganic	PI33	Thursday	De Beers	
Zitha	Marvin	Inorganic	Pi34	Thursday	De Beers	
Zondo	Sandisiwe	Analytical	C86	Wednesday	1st Year Argon	11h30-11h50
Zungu	Vuyokazi Busisiwe	Environmental	PE14	Tuesday	Endler	
Zwane	Nokalika	Analytical	PA47	Monday	Endler	
Zwane	Xolani Rodger	Analytical	PA48	Tuesday	Endler	