Agenda for 2021 Chemistry PGR symposium, **June 18** and **June 25**, **2021**

Meeting location: Microsoft Teams

Attendees: PGR students, Chemistry staffs and ECRs

Agenda on June 18 (Friday), 2021

Time (UK)	Topic	Presenter
Session 1		
0900-0920	PGR students and staff arrive	
0920 – 0930	Welcome by HoD School Research Director	
Session 2		**Chaired by Professor Donald Macphee**
0930 – 0950 O1	The magnetic phases of $Sr_2Cr_2MnAs_2O_2$	Bor Arah
0950 – 1010 O2	Characterization of trace metals in metal coil	Ahmed Alanazi
1010 – 1030 O3	Application of Acyl-S-acetylcysteamine (Acyl-SNAC) thiosters as synthetic mimic in biosynthetic intermediates acyl- CoAs	Saad Alrashdi
1030 – 1050 O4	The effects of feeding seaweed on bovine methane production, milk yield, basic composition, and iodine content	Ali Alzahrani
1050 – 1110	Coffee Break	
Session 3		**Chaired by Dr Kassim Adebambo**
1110 – 1130 O5	Flavobacterium CIP-J1- A Treasure Box of RiPPs	Subha Arjunan
1130 – 1150 O6	Towards simplified Vancomycin Analogues	Senyu Zheng
1150 – 1210 O7	The effect of a shorter spacer on mesophase behaviour: A comparison of the CB4O.m, CB4O.Om, CB6O.m and CB6O.Om series	Amerigo Zattarin
1210 – 1230 O8	Chemistry in low-dimensional quantum materials	Struan Simpson
1230 – 1250 O9	Anti-sickling activities of some compounds isolated from the leaves of Vernonia amygdalina (Asteraceae) and Ocimum gratissimum (Lamiaceae)	Oluwatofunmilay Diyaolu

Time (UK)	Topic	Presenter
1250 – 1400	Lunch break	
Session 4		**Chaired by Dr Peter Henderson**
1400 – 1420 O10	Study of the Sustainable Transformation of Solid Feedstock into Valuable Chemical Products	Nadege You
1420 – 1440 O11	Electrochemical conversion of glycerol, methanol and formic acid using Au and Pt: Self-poisoning problems to solve	Laura Perez Martinez
1440 – 1500 O12	Alternative synthetic method to prepare liquid crystal dimers using sodium activated aromatic coupling reactions	Calum Gibb
1500 – 1520 O13	High Temperature Fischer Tropsch Sythesis- High Alcohol (C2+) and & lower olefins (C2-C4) production	Belcher Fulele
1520 – 1540 O14	Analysis of formaldehyde in pharmaceuticals	Vittoria Delbono
1540 – 1600 O15	Trace elements in toenails in environmental epidemiology	Camilla Faidutti

Agenda on June 25 (Friday), 2021

Session 4		Chaired by Dr Rebecca Walker
1000 – 1135	5-min Flash presentation	
F1/Poster A1	Non-Symmetric Liquid Crystal Dimers and the search for new twist-bend phases (Poster room A No A1)	Ahlam Alshamari
F2/Poster A2	Observation of high concentrations of unidentified organofluorines in pilot whales stranded in Scotland (Poster room A No A2)	Amnah Alzbedy
F3/Poster A3	Effect of different conditions of growth on the secondary metabolites produced by Streptomyces isolated from the Atacama Desert (Poster room A No A3)	Rishi Vachaspathy Astakala
F4/Poster A4	Photocatalytic Production of Hydrogen by TiO2 and CuO Assembled at the Interface between Two Immiscible Electrolyte Solutions (ITIES) (Poster room A No A4)	Edwin Avella
F5/Poster B1	The Search for the Ferroelectric Nematic Phase (Poster room B No B1)	Stevie Brown
F6/Poster B2	Characterisation of wax synthases to investigate their high promiscuity towards different diacylglycerol and acyl-CoA species (Poster room B No B2)	Federica Casolari
F8/Poster B3	Isolation of natural products from Deep-Water horizon bacterial strains (Poster room B No B3)	Ahmad Ghazal
F9/Poster B4	Determination of Ionic Pathways in the Hexagonal Perovskite Derivative Ba3VMoO8.5 (Poster room B No B4)	Dylan Tawse
F10/Poster C1	Development of a biofilm growth inhibition assay to aid the discovery of natural product antifouling compounds (Poster room C No C1)	Jessica Gomez-Banderas
F11/Poster C2	Identification of Novel Secondary Metabolites by LC-MS Dereplication from the Atacama Desert Fungi (Poster room C No C2)	Gagan Preet
F12/Poster C3	Isolation and structural elucidation of three terpenoids from brine pool fungus (Poster room C No C3)	Joy Ebenezer Rajakulendran
F13/Poster C4	Susceptor-Assisted Microwave Processing of Inorganic Solids (Poster room C No C4)	Brent Sherwood
1130 – 1200	Q & A discussion on flashpresentations	

1200– 1300	Poster presentation	Committee:
1300	Closing Remarks	

Oral and flash presentation committee:
Organic: Rebecca Walker,
Inorganic: Eve Wildman
Physical: Angel Ciscar Cuesta
Analytical: Kassim Adebambo

Poster committee:
Organic: Rebecca Walker,
Inorganic: Eve Wildman
Physical: Alan Mccue
Analytical: Kassim Adebambo

Abstracts for Oral Presentations

Characterization of trace metals in metal coil

Ahmed Alanazi*[1], Professor Donald Macphee 1[1], Professor Joerg Feldmann[2]
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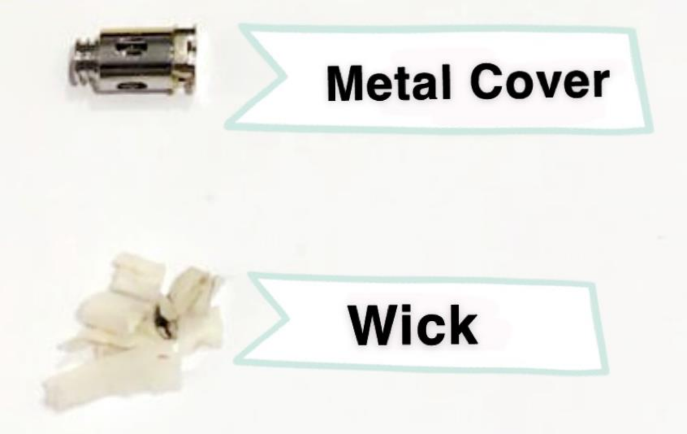

Figure 1: Photo of metal cover and wick samples

The popularity of e-cigarettes has grown in recent times around the world. According to (Hess et al, 2017) the popularity of vaping devices grew tremendously in 2015, raising sales to $3.5 billion. This proliferation is attributable to increased interest among adolescents, as indicated by (Perikleous et al. 2018), who affirm that a third of adolescents in the US consider e-cigarettes less harmful than conventional cigarettes. But some concerns have been expressed regarding the potential risks (Cooper et al. 2016). Amongst these is the ingestion of metals. Some trace metals even though essential could be toxic at certain concentrations, especially when they are inhaled. E-cigarettes have three major components: a battery, an atomizer and an e-liquid- containing cartridge. The atomizer components are metal cover, a wick and brass clamp. The liquid comes in contact with the metal cover via the wick and we have shown that high concentrations of trace metals can be generated in the e-liquids. This part of the study focused on the components of the atomizer as sources of metal contamination. Inductively-coupled plasma- optical emission spectrometry (ICP-OES) was utilized to determine levels of a range of elements in new and used metal covers and wick samples. The results of these analyses are discussed as part of the transport pathway of metals between the e-cigarette and the e-cigarette user.

References

[1] Hess, Catherine Ann, et al. *Environmental Research.* **152**, 221-225 (2016)
[2] Perikleous, Evanthia P., et al. *Frontiers in Public Health.* **6**, 1-9**.** (2018)
[3] Cooper M, Harrell MB, Perry CL. *Health Education Research.* **31**, 429-438. (2016)

Application of Acyl-S-acetylcysteamine (Acyl-SNAC) thiosters as synthetic mimic in biosynthetic intermediates acyl- CoAs

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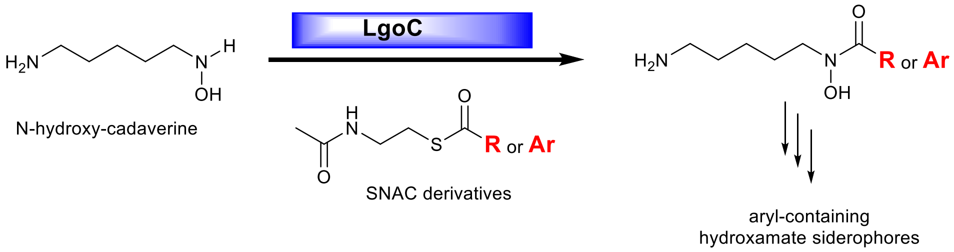
Acyl-CoAs are a family of metabolic intermediates comprised of an acyl group linked by a thioester bond to coenzyme A. Acyl-*S*-(N-acetyl) cysteamines (Acyl-SNACs) are synthetic mimics of Acyl-CoAs and have many applications including their using in the biosynthetic studies of natural products and their derivatives.[1] Acyl-SNAC compounds are synthesized as crucial thioester intermediates to probe the biosynthetic enzymes identified for the pathways of natural products, for example, carbazoles and siderophores.[2]

Siderophores are produced by microorganisms to scavenge iron from the environment, thereby making this essential metal nutrient available to the microbe. More than 500 siderophores are known to date, but only two were identified to be aryl-containing hydroxamate siderophores, legonoxamines A and B from *Streptomyces sp.* MA37. [2,]

In this study, several synthesized SNACs thioester compounds were used to demonstrate that LgoC in the biosynthetic pathway of legonoxamines from *Streptomyces sp.* MA37 is responsible for the key aryl-hydroxamate forming step. Biochemical characterization found that LgoC displays considerable promiscuity for the acylation between N-hydroxy-cadaverine and SNAC (N-acetylcysteamines) thioester derivatives.[2]



Reference

1-Maglangit F, Tong MH, Jaspars M, Kyeremeh K, Deng H. Legonoxamines A-B, two new hydroxamate siderophores from the soil bacterium, Streptomyces sp. MA37. *Tetrahedron Lett*. 2019;60(1):75-79. doi:10.1016/j.tetlet.2018.11.063

2-Maglangit F, Alrashdi S, Renault J, et al. Characterization of the promiscuous: N-Acyl CoA transferase, LgoC, in legonoxamine biosynthesis. *Org Biomol Chem*. 2020;18(12):2219-2222. doi:10.1039/d0ob00320d

The effects of feeding seaweed on bovine methane production, milk yield, basic composition, and iodine content

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The aim of this study was to reduce methane emission from bovines by feeding them seaweed product. A reduction in methane from cattle could contribute to the major goal of the EIT Food consortium to reduce greenhouse gas (GHG) emission from European food production by 40% in 2030. Ruminant enteric fermentation is the single biggest anthropogenic source (~25%) of methane, which has a 28 times higher global warming potential than CO_2 (Chang J, et al., 2019). Seaweed has the potential to inhibit methanogenesis at low inclusion (Li et al., 2016).In addition, seaweed supplementation could have other beneficial side effects such as improving iodine concentration in bovine milk and meat and this would be an excellent way of increasing iodine intake in the general public without food supplements.

A mixed ratio of three kind of seaweed, *Fucus vesiculosus* (FV), *Asparagopsis taxiformis* (AT) and *Ascophyllum nodosum* (AN) in different proportions 0.15%, (AN-FV-AT), 1.75%, (FV-AN) and 0.65%, (AN-FV) of dry matter intake (DMI) were used. The study ran continuously for 49 days (7 weeks) with cows remaining on the same diet treatment throughout the study. Seaweed supplementation did not have a significant effect, 9% reduction of exhaled methane from cattle's compared to control group. However, iodine concentration in bovine meat, milk and milk product have shown a significant increase in all of the three treatment ranging between 168-216% comparing to the control group.

There was no significant effect of feeding AN, FV and AT on methane production or yield, and no effects on milk yield. The seaweed treatments (all three) did have an effect on the iodine concentration in the milk which was double compared to the control treatment.

References

[1] Jinfeng Chang, Shushi Peng, Philippe Ciais, Marielle Saunois, Shree R. S. Dangal, Mario Herrero, Petr Havlík, Hanqin Tian & Philippe Bousquet., *Nature Communications* **Volume 10**, (2019)

[2] Li, X., H. C. Norman, R. D. Kinley, M. Laurence, M. Wilmot, H. Bender, R. de Nys, and N. Tomkins. Asparagopsis taxiformis decreases enteric methane production from sheep. *Animal Production Science* **Volume 58** page 681-688, (2016)

The magnetic phases of $Sr_2Cr_2MnAs_2O_2$

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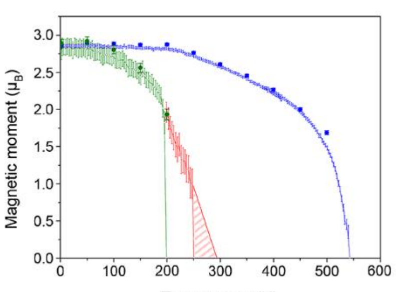

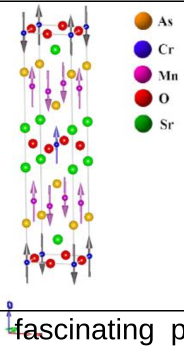

Transition metal oxypnictides can exhibit fascinating properties such as giant or colossal magnetoresistance or superconductivity. I have synthesized and analysed $Sr_2Cr_2MnAs_2O_2$, a member of the $Sr_2Cr_{3-x}Mn_xAs_2O_2$ series. The compounds in this series crystallize in the *I4/mmm* space group, in the tetragonal crystal system. They were targeted because they contain both $M(1)O_2$ and $M(2)_2As_2$ layers, which are the superconducting layers in cuprate and iron based superconductors, respectively. The sample was synthesized via a standard solid state synthesis method, initially analysed with X-ray diffraction (XRD) and later with variable temperature neutron diffraction (ND). Room temperature XRD data was analysed to optimize the synthesis method, while Rietveld refinement with the ND data was used to determine the variation of the crystal and magnetic structures with temperature.

The site occupancies of transition metal sites (Wyckoff positions *2a* and *4d*) and the ordering of their magnetic moments were determined. Our results were compared to $Sr_2Cr_3As_2O_2$[1], $Sr_2Mn_3As_2O_2$[2], and $Sr_2Cr_{0.77}Mn_{2.23}As_2O_2$[3]. In agreement with the observations of Lawrence *et al.*[3], we have determined that Cr^{2+} ions exhibit site selectivity, preferentially occupying the *2a* sites with distorted octahedral/square planar coordination in the $M(1)O_2$ layers, while the Mn^{2+} ions display no selectivity. This was attributed to the crystal field splitting energies of the different coordination environments in conjunction with the electron configurations of Cr^{2+} (d^4) and Mn^{2+} (d^5). Below 540 K, the *4d* site moments order with a C-type antiferromagnetic (AFM) arrangement. Below 200 K, the *2a* site moments couple AFM within the *ab* plane, with even amounts ordering parallel and antiparallel along the *c* axis - this is the first time such an arrangement has been observed in these compounds. Between 200 K and 290 K, the *2a* site moment parallel arrangement along *c* remains, gradually shifting from long- to short-range order. At 1.5 K the magnitude of the magnetic moment's magnitudes are lower than those of analogous magnetic structures in other compounds of the series.

References

[1] Xu, X., Jones, M. A., Cassidy, S. J., Manuel, P., Orlandi, F., Batuk, M., Hadermann, J., Clarke, S. J., *Inorganic Chemistry*, **59 (21)**, 15898–15912 (2020)

[2] Nath, R., Garlea, V. O., Goldman, A. I. and Johnston, D. C., *Physical Review B - Condensed Matter and Materials Physics*, **81 (22)**, p. 224513 (2010)

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Flavobacterium CIP-J1- A Treasure Box of RiPPs

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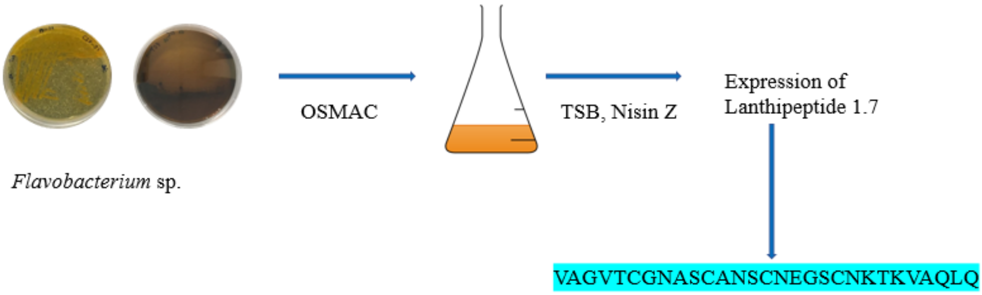

Lanthipeptides are a class of ribosomally synthesized post-translationally modified peptides (RiPPs) that are a promising addition to antibiotics. This class of compounds thought to be majorly produced by gram positive bacteria. With the increasing number of whole genome sequences, it is evident that gram negative bacteria and fungi contain RiPP genes. Flavobacterium CIP-J1 sp. which is a gram-negative bacterium encodes a significant number of RiPP genes that includes multi-precursor peptide. These genes are cryptic under normal laboratory growth conditions. One of the lanthipeptides has been expressed using OSMAC approach, and the presence of this peptide is supported by its mass fragments.

References (bold, 11 pt)

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[2]Zhong, Z., He, B., Li, J. and Li, Y.X., 2020. Challenges and advances in genome mining of ribosomally synthesized and post-translationally modified peptides (RiPPs). *Synthetic and Systems Biotechnology*, *5*(3), pp.155-172.

Analysis of formaldehyde in pharmaceuticals

Vittoria Delbono*[1], Christopher Paul Larch[1], Katrina Carol Newlands[1], Thomas Craven Baddeley[1], John Mervyn David Storey[1]
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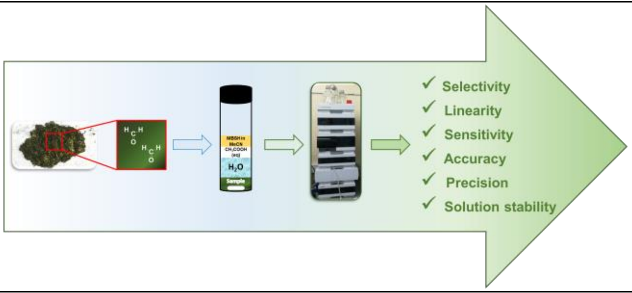

Formaldehyde is commonly used as an alkylating agent in the pharmaceutical industry. According to the Environmental Protection Agency (EPA), formaldehyde can cause both acute and chronic effects to humans through inhalation [1]. Additionally, the ingestion of concentrated formaldehyde can induce the corrosion of the gastrointestinal tract, the inflammation, and the ulceration of the mouth, esophagus and stomach [1]. Consequently, its residual level in drug substances, products and/or their intermediates needs to be accurately quantified.

Formaldehyde is a small, volatile molecule with a weak chromophore (the carbonyl group) and its direct analysis by gas chromatography with flame ionisation detection (GC-FID) and high-performance liquid chromatography with UV detection (HPLC-UV) is difficult. For this reason, the majority of papers found in literature are based upon a derivatisation process prior to the analysis of formaldehyde and these present drawbacks.

A novel HPLC method with UV detection for its quantification in two intermediate and an active pharmaceutical ingredient (API) is presented. The method proposed is based upon a derivatisation reaction between formaldehyde and 4-methylbenzenesulfonohydrazide (MBSH) before analysis by HPLC-UV. Selectivity, linearity, limit of quantification, accuracy, repeatability, intermediate precision and solution stability were successfully assessed as per ICH guideline Q2(R1) [2] and the method has also been validated for different compounds in Good Manufacturing Practice (GMP) laboratories in the United Kingdom (UK) and Taiwan.

Furthermore, the method was adapted for tablets of two different sizes and validation characteristics were successfully proven for these.

Moreover, as it is thought that formaldehyde could potentially be formed by demethylation of the API substance when high pressure is applied during the tableting process or during tablet storage by potential oxidation of the methyl group, its analysis has also been carried out on tablets on stability.

References

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[2] ICH Expert Working Group, Validation of analytica; procedures: text and methodology Q2(R1), 1-13 (2005)

Anti-sickling activities of some compounds isolated from the leaves of *Vernonia amygdalina* (Asteraceae) and *Ocimum gratissimum* (Lamiaceae)

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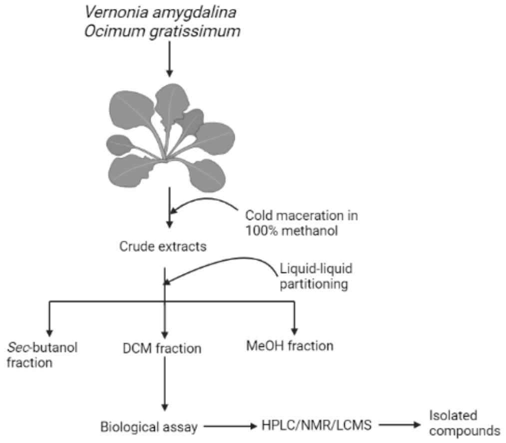

Evaluation of plants such as *Vernonia amygdalina* and *Ocimum gratissimum* with claimed traditional use in the management of sickle cell anaemia in Nigeria and other parts of West Africa could serve as a helpful research strategy in the search for potential anti-sickling drugs and templates. This study aimed at evaluating the anti-sickling potential of *Vernonia amygdalina* and *Ocimum gratissimum* by activity-guided purification and isolation of its active constituents. The crude methanol extracts and the fractions obtained by partitioning were investigated for anti-sickling activity against sodium metabisulphite induced sickling of sickle cell haemoglobin (HbSS). Repeated chromatographic separations were conducted on the most active dichloromethane (DCM) fractions to purify and isolate bioactive compounds for further tests for anti-sickling activity. The characterisation of the isolated compounds was done by mass spectrometry and nuclear magnetic resonance spectroscopy.

The DCM fractions (% sickled erythrocyte ranged from 3.0 to 34.1) exhibited better anti-sickling activity than *sec*-butanol fractions (% sickled erythrocyte ranged from 38.9 to 51.5) as well as the methanol fraction (% sickled erythrocyte ranged from 19.1 to 30.4). Hence, the phytochemical investigation was focused on the DCM fractions, which led to the isolation of vernodalol, lasiopulide, vernonoside A, and loliolide. Vernodalol and vernonioside A showed suitable, comparable anti-sickling activities, with vernodalol exhibiting a slightly better *in vitro* activity. This research reports for the first time anti-sickling principles of vernodalol, lasiopulide, and vernonoside, therefore, provided some justification for the ethnomedicinal use of the plant in the management of sickle cell disease.

High Temperature Fischer Tropsch Sythesis- High Alcohol (C_2+) and & lower olefins (C_2-C_4) production

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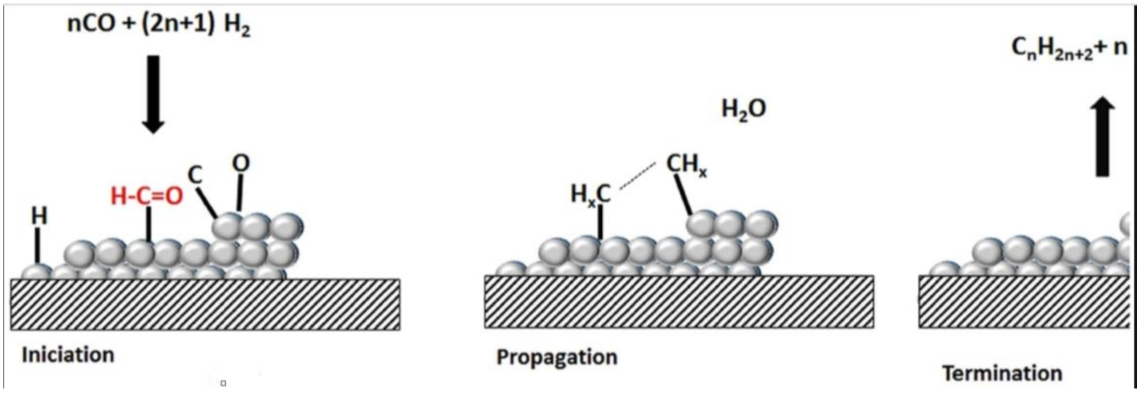
Abstract

Fischer-Tropsch (FT) synthesis is a heterogeneous catalytic reaction that converts synthesis gas (mixture of CO and H_2), obtained from coal, biomass, shale gas and natural gas into clean transportation fuels and hydrocarbons (1). In particular, iron-based catalyst at elevated temperature favour the selective production of C_2-C_4 olefins which are building blocks for the chemical industry. Bimetallic catalyst of copper and iron favour the production of C_{2+} alcohols which are used as fuels or fuel additives. Method of catalyst preparation plays an important role on the catalyst performance and product selectivity. Fe/CNF catalyst were prepared by thermal decomposition of $Fe(CO)_5$ to form nanoparticle which were subsequently dispersed on carbon nanofiber support. Bimetallic catalyst were prepared by simple impregnation of metal precursors onto γ-Al_2O_3 support with different sequential order of impregnation of metal to the support.

Catalyst samples were characterised by XRD, H_2-TPR, N_2 physisorption and IR spectroscopy. The mechanism of catalysed reaction were studied by *operando* DRIFT-MS technique during syngas (CO+H_2) and CO adsorption at different temperatures and pressures. Data obtained from aforementioned techniques was used to interpret; the effect of the support, reaction conditions, sequential impregnation of active metals and give insights into mechanism during syngas adsorption at catalyst surface.



Reference

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Alternative synthetic method to prepare liquid crystal dimers using sodium activated aromatic coupling reactions.

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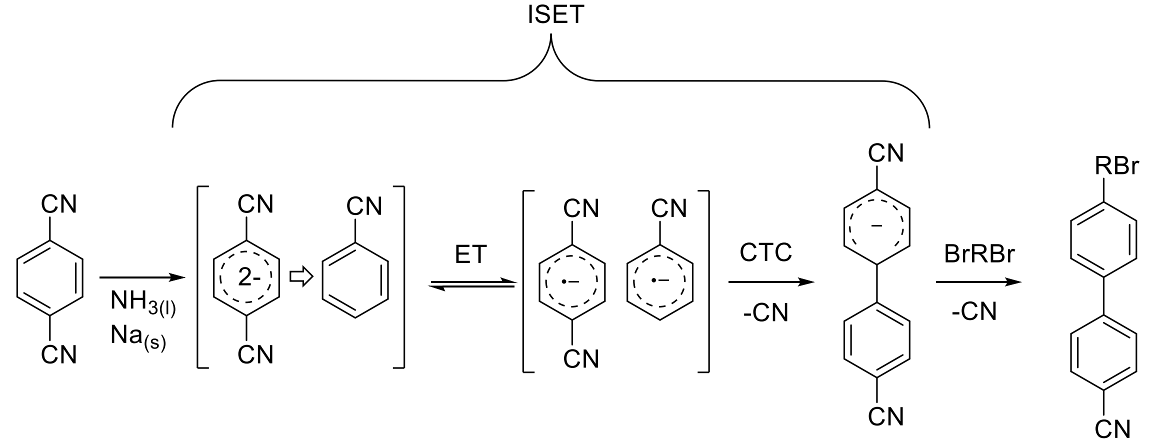

Recent research into the twist-bend nematic (N_{TB})[1] and heliconical twist-bend smectic (SmC_{TB}) [2] phases has been focused on molecules containing aryl - alkyl and aryl - alkoxy spaced mesogens. The synthesis of these materials has remained largely unchanged, with traditional synthetic pathways being plagued by difficult synthetic steps often resulting in low overall yields and using expensive reagents.

Sodium activated aromatic coupling reactions help provide a cheaper, quicker and greener solution in the synthesis of more versatile intermediate compounds, ultimately allowing for more complex final materials.[3][4] By utilising this one pot synthesis for 4-alkyl,4'-cyanobiphenyls and related units, it is possible to quickly create a library of liquid crystal dimers including the widely studied CBnCB series as well as opening new avenues to previously challenging functional group chemistry. This reduction in synthetic steps has put new liquid crystal dimers and higher oligomers within reach.

[1] D. A. Paterson, et al, *Liquid crystals*, 44, 1 (2017).
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[4] E. V. Panteleeva, et al, *European journal of organic chemistry*, 12 (2005).

Electrochemical conversion of glycerol, methanol and formic acid using Au and Pt: Self-poisoning problems to solve.

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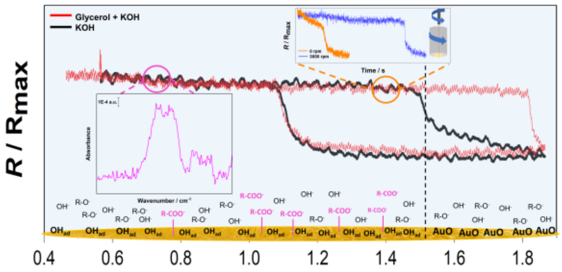

Figure 1. Schematic of the overall glycerol oxidation in presence of Au

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The growing popularity of liquid alcohols or acids versus hydrogen, due to their larger volume energy density and their easy storage and transport without high-pressure necessity, have propelled us to study their electrooxidation. Methanol's oxidation to CO_2 does not require the rupture of any carbon-carbon making the reaction simpler and more efficient than that of higher alcohols, although adsorbed carbon monoxide (CO_{ad}) formed as an intermediate in one of the two possible reaction pathways acts as a poison of Pt-based catalysts. The same problem happens with formic acid. Our research focuses on understanding this adsorption process to design catalysts on which this reaction is inhibited. On the other side, glycerol is a higher alcohol whose partial oxidation on Au without breaking its C–C bonds allows its transformation to value-added products without external energy input or, in particularly favourable cases, coupled to the generation of energy, thereby obtaining a double benefit.

These problems have been studied by combining cyclic voltammetry and potentiostatic current transients with surface-enhanced infrared absorption spectroscopy in the attenuated total reflection mode (ATR-SEIRAS) and, in the case of glycerol, in-situ visible-reflectance.
Our experiments with methanol show that the formation of CO_{ad} occurs, although at a very slow rate, at potentials as negative as -0.4 V *vs.* RHE. We have been able to determine which sites are poisoned first and to identify the active sites, as well as the role played by specifically adsorbing spectator species from the electrolyte by comparing experiments in H_2SO_4 and $HClO_4$. Studying the oxidation of formic acid on Pt, we have seen that the rate of the reaction depends on the potentials, going through a maximum.
In the case of glycerol, we have proved that the oxidation of gold is retarded in presence of glycerol because both reactions compete for the same intermediate, OH_{ad}. Carboxylates resulting from the oxidation of glycerol adsorb on the surface and have an inhibiting effect on the reaction rate acting as a poison of the surface.

In all these cases, our results are relevant for the design of fuel cells capable of generating electricity.

Chemistry in low-dimensional quantum materials

Struan Simpson* and A.C. Mclaughlin
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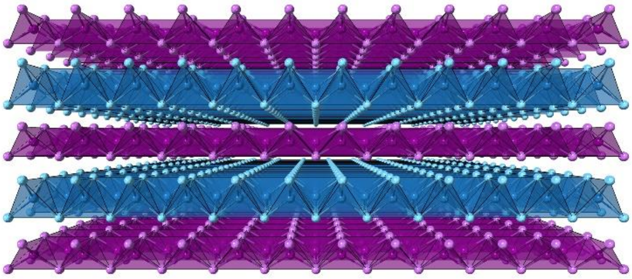

Quantum materials pervade our everyday lives. From computer memory devices, to optical disk drives, to magnetic resonance imaging scanners – multiple contemporary technologies rely on quantum mechanics. However, new materials displaying exotic quantum phenomena are sought to develop next-generation technologies[1]. Such technologies include quantum computers and sensors, which offer considerable advantages over their classical counterparts. The discovery of untapped quantum materials hence remains an essential goal in modern materials research.

We have recently identified two new quantum materials of interest – $CeMnAsO_{0.95}F_{0.05}$ and $Ba_3SrMo_2O_9$. $CeMnAsO_{0.95}F_{0.05}$ is a quasi-2D oxypnictide which presents several signatures of an elusive "many-body localised" state. This phenomenon is unprecedented in solid-state materials with great potential as a novel form of quantum memory[2]. In contrast, $Ba_3SrMo_2O_9$ is a new hexagonal perovskite that segregates into two electronically distinct phases below 230 K. Each phase forms nonmagnetic spin dimers, but segregation appears to be mediated by a unique competition between Mo–Mo bonding and Mo–O–Mo magnetic superexchange. Chemical modifications hence offer a promising route to discover new and fascinating quantum ground states.

Here, we will discuss how our understanding of chemistry may be used to study quantum materials such as $CeMnAsO_{0.95}F_{0.05}$ and $Ba_3SrMo_2O_9$. We have probed the origins of their exotic physical properties by identifying key structure-property relationships. Additionally, further chemical substitutions have allowed us to identify how their physical properties may be tuned. This work serves to illustrate the fundamental role of chemistry in the pursuit of novel quantum materials and technologies.

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Study of the Sustainable Transformation of Solid Feedstock into Valuable Chemical Products

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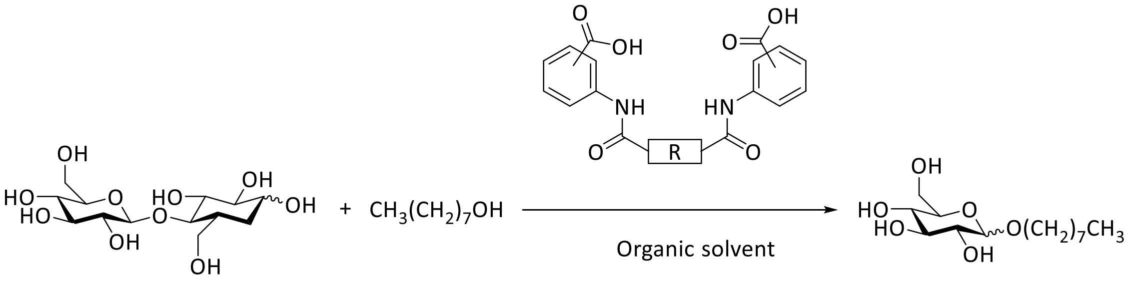
Alkyl polyglucosides (APGs) are a recent green class of non-ionic and amphiphilic surfactants. Made from renewable materials and readily biodegradable, they have become a popular choice for various applications [1]. APGs are manufactured from a carbohydrate and an alcohol via the acid-catalysed Fischer's method. Although the formation of APGs is a straightforward reaction, it typically produces unwanted by-products through caramelization. Currently, a promising option involves performing the conversion of cellulose, main biopolymer in Nature, via catalytic alcoholysis. However, it is a very difficult reaction to achieve due to the highly robust polysaccharide system [2].

This project aims to develop a sustainable production method of APGs from cellulose using organocatalysts that partially mimic lysozyme, a glycoside hydrolase which possesses a glutamic and aspartic acid residue in its active site. We hope that the reaction could be performed under milder conditions and will produce fewer caramelization products. To do so, we have designed a range of new diacid organocatalysts that bear carboxylic acid groups oriented in ways that may assist the alcoholysis of cellulose via a mechanism similar to that observed for the enzymatic hydrolysis of polysaccharides.

The study presented here focused on the alcoholysis of cellobiose (a disaccharide) by 1-octanol. Cellobiose is a simplified system of cellulose chosen for its solubility in common organic solvents. Upon catalytic process with diacid organocatalysts, the one-pot and direct production of octyl glucosides from cellobiose has been achieved by direct alcoholysis. The effect of each catalyst on the conversion rate has been observed and represents a preliminary step in the conversion of cellulose.



α/β–Cellobiose

α/β–Octyl Glucosides

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The effect of a shorter spacer on mesophase behaviour: A comparison of the CB4O.m, CB4O.Om, CB6O.m and CB6O.Om series

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One of the most fascinating liquid crystal phases is the NTB phase, which was first predicted over 35 years ago by Meyer and independently in 2001 by Dozov. At the heart of Dozov's seminal work is the assertion that bent molecules have a natural tendency to pack into bent structures. but nature does not allow pure uniform bend. Thus, spontaneous bend must be accompanied by other deformations of the local director, specifically either twist or splay, forming the heliconical structure of twist-bend or splay-bend nematic phases, respectively. [1,2]

Previous work investigated the first ten homologues of the 1-(4-cyanobiphenyl-4′-yl)-6-(4-alkylanilinebenzylidene-4′-oxy)hexanes (CB6O.m) and their alkoxy-terminated analogues, CB6O.Om. All ten members of the CB6O.m series exhibited an enantiotropic nematic, N, phase, and a monotropic twist-bend nematic, NTB, phase. Only CB6O.10 showed a smectic phase, classified as SmCTB. This change in the local structure on increasing m had no apparent effect on the stability of either nematic phase, and TNTBN and TNI showed a regular dependence on m. On the other hand, the CB6O.Om series just shows an intercalated, anticlinic smectic C, SmCA, phase for m = 3–5. A second smectic phase is seen for m = 4,5 but its monotropic nature precluded detailed investigation. All 10 homologues of the CB6O.Om series exhibit nematic, N, and twist-bend nematic, NTB, phases. [3,4]

In this work, we compare the behaviour of the new CB4O.m series with the CB6O.m series and investigate the possibility of smectic phase behaviour. We also compare the CB6O.Om and CB4O.Om series. Additionally, the effect of the shorter spacer length on the transition temperatures of the other liquid crystal phases was investigated to understand both the effect of central spacer variation and that of varying the terminal chain.

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Towards simplified Vancomycin Analogues

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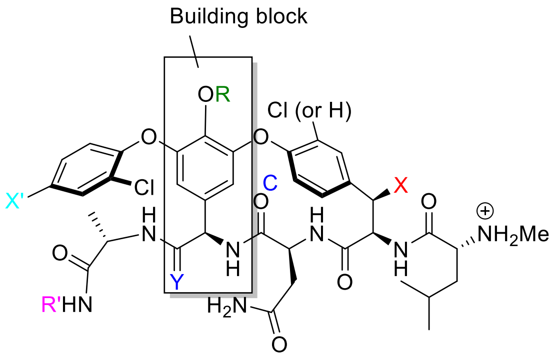

Analogues

X = H, OH, NHMe
R = H, CH_3, CH_2CH_2OH, other
Y = O, H_2, NH
R' = amino acid(s)
X' = H, Cl, CH_2OH, other

Vancomycin is an antibiotic which has been in clinical use for over 60 years to treat bacterial infections. For a long time, Vancomycin has been considered as “last resort” antibiotic. It is classified as a “third-grade antibiotic” for treating serious infections that are resistant to any other antibiotics, including the infection of methicillin-resistant S. aureus [1, 2]. Due to excessive use of antibiotics, vancomycin-resistant bacteria have greatly increased. In resistant bacteria, the last D-ala residue has been replaced by a D-lactate, which prevents vancomycin from binding efficiently to lipid II. The aims of the research are to synthesis a simplified version of vancomycin or modify vancomycin. By using retrosynthesis, we can clearly see where the key point of the whole synthesis is. All the amino acids required for the peptide synthesis are commercially available excepted the phenylglycine derivative. A Key building block is needed for the whole synthesis and methods for macrocyclization also need be studying for further experiments.

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Trace elements in toenails in environmental epidemiology

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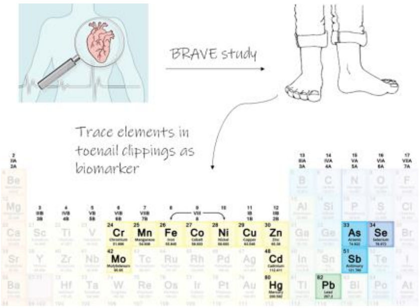

Coronary heart disease is a major cause of death in Bangladesh. However, limited evidence about its determinants in this population is currently available. Beyond conventional risk factors (e.g., smoking and poor diet), environmental risk factors, such as exposure to trace elements from contaminated drinking water or from anthropogenic emissions, are often overlooked [1]. My PhD project aims to determine how exposure to trace elements might contribute to high rates of heart disease in Bangladesh. The project is part of the Bangladesh Risk of Acute Vascular Events (BRAVE) study, a hospital-based case-control study led by the University of Cambridge, which is investigating the effects of environmental, genetic, lifestyle and biochemical factors on coronary heart disease in Bangladesh [2].

We explored the occurrence of trace elements in nail samples of 4,000 participants of the BRAVE study. Preliminary analyses have shown that the distributions of 7 trace elements in cases and controls are significantly different ($p < 0.05$, Mann Whitney Test). Cases have higher median values than controls for Cd, Co, Fe, Mn, Ni, and Sb, while controls have higher median values than cases for Se. However, the significance of some of these trace elements as biomarkers is reduced because their concentrations reflect both endogenous accumulation and high levels of exogenous deposition. Ideally, terrestrial and anthropogenic materials, soil or dust that is adherent to the nail should be removed in order not to be confounding the true concentrations found in toenails. Often, this is not fully possible, and it ultimately affects the suitability of an element for use in epidemiological studies.

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Abstracts for Flash Presentations
(also in poster breakout rooms)

Non-Symmetric Liquid Crystal Dimers and the search for new twist-bend phases

ROOM A Poster A1

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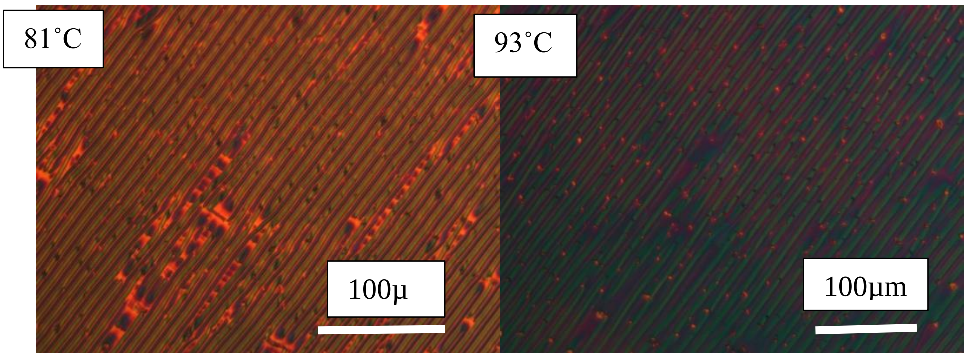

CB10O.1

Liquid crystal dimers are composed of molecules containing two mesogenic groups linked by a flexible spacer. Symmetrical liquid crystalline dimers contain two identical mesogenic units, whereas their non-symmetrical analogues have two different mesogenic groups [1]. This class of materials has attracted very considerable interest in recent years following the discovery of the twist-bend nematic phase [2,3] and, more recently, twist-bend smectic phases [4,5]. The phases are composed of achiral, bent molecules and the director forms a spontaneous helix in which it is tilted with respect to the helical axis. In order to better understand these novel phases and the relationships between molecular structure and the tendency to form these phases, this research aims to identify new examples of them and aims to synthesis a non-symmetric liquid crystal dimer series (CB10O.m) (Figure 1). This structure was chosen as the decyloxy spacer, will endow the necessary molecular curvature for the system to exhibit the twist-bend phases and a range of homologues may be prepared by varying the length of the terminal chain. This will constitute the first extended study of the effects associated with a long spacer on the twist-bend phases.

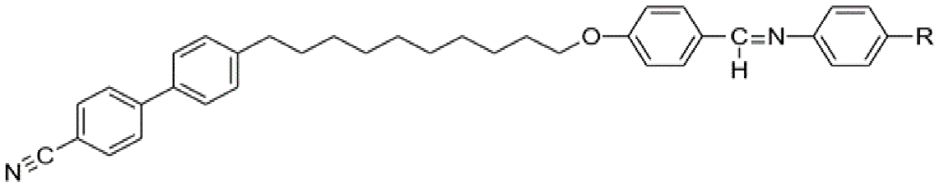

Figure 1: General structure of (CB10O.m), R= CmH2m+1

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Observation of high concentrations of unidentified organofluorines in pilot whales stranded in Scotland

ROOM A Poster A2

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Per- and polyfluoroalkyl substances (PFASs) are a group of anthropogenic chemicals, produced since the 1950s. These chemical when applied on the surfaces of various products make them resistant to moisture, stain, or stickiness. For instance, they could be used to coat cookware so that food does not stick on them. Global detection of these compounds in the environment[1], and human wildlife matrices[2] has increased. The increasing use of such compounds has sparked a lot of environmental concerns since they degrade quite slowly. Exposure to PFAS has been linked to a variety of adverse health effects in humans and wildlife, including immunotoxicity, developmental problems, and cancer. Although new methods are being developed, analyses of PFASs in biota at low concentration levels pose a significant analytical challenge. In this work combustion ion chromatography for total fluorine was applied to measure extractable organic fluorine (EOF) in liver tissue of pilot whales stranded in Scotland and high-performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS) was used for known PFASs. Comparisons between the amounts of known PFASs and EOF in the livers showed that a large proportion of the organic fluorine in liver is of unknown origin. Similar PFAS profiles were observed in liver tissue over the different ages and the proportion of unknown compounds increase with age.

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Effect of different conditions of growth on the secondary metabolites produced by *Streptomyces* isolated from the Atacama Desert

ROOM A Poster A3

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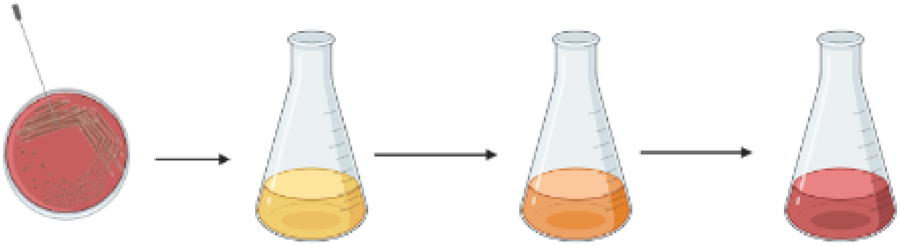

Some organisms produce secondary metabolites, organic compounds which are not directly necessary for the growth, development or the reproduction. Various plant and microbial secondary metabolites have been found to have several uses in human health such as anti-tumour, antibiotic and antiparasitic agents. *Streptomyces* are a genus of bacteria with a high GC content typically found in the soil, and are known for their especially complex secondary metabolism. Another attractive feature of *Streptomyces* is their ability to produce antibiotics which amount to about 80% of currently used antibiotics [1]. Several strains of *Streptomyces* were isolated from the rhizosphere of lupine plants growing in the Atacama Desert, one of the driest places on earth. This project looks at the effect of different growth conditions and nutrient media on the secondary metabolites produced by the S26 strain.

References (bold, 11 pt)

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[2] Image made using biorender.com

Photocatalytic Production of Hydrogen by TiO_2 and CuO Assembled at the Interface between Two Immiscible Electrolyte Solutions (ITIES)

ROOM A Poster A4

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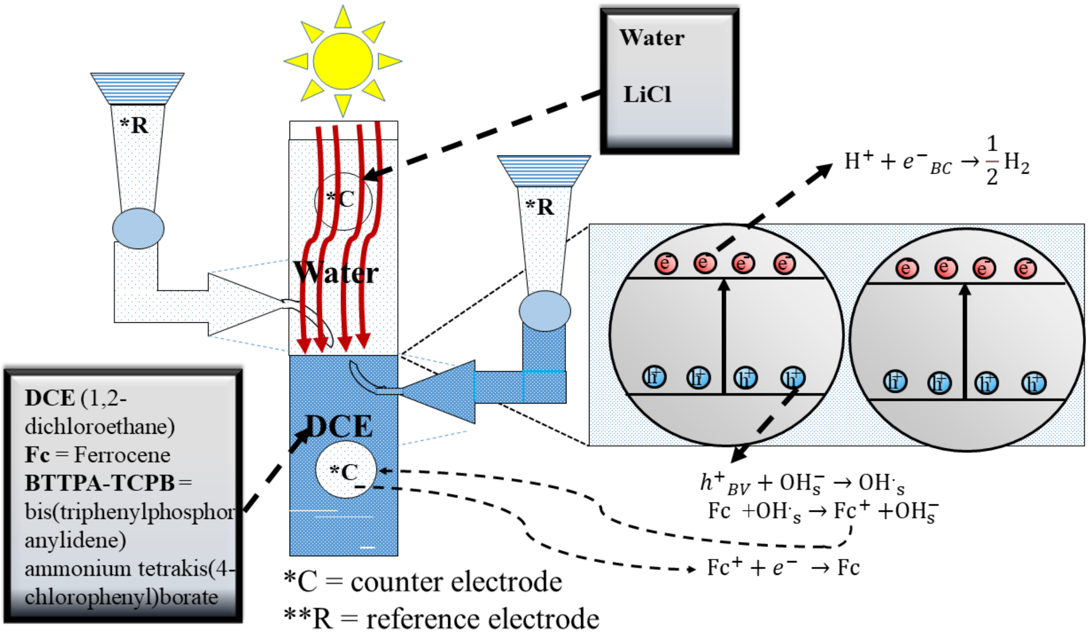

The effect of the assembly of TiO_2 (anatase, 5 nm) and CuO (< 50 nm) nanoparticles at the interface between water and 1,2 dichloro-ethane on their photocatalytic activity was investigated. Photocurrent measurements in the absence of photocatalyst show a slow charge transfer, which can be related to the photo-oxidation of Ferrocene (used as a hole scavenger in the organic phase)[1]. A fast photo-response was observed when TiO_2 was assembled, and a further enhancement in the photocurrents generated was achieved by assembly of a lower bandgap photocatalyst (CuO). All experiments showed a positive photocurrent, suggesting hydrogen production by capturing photogenerated electrons at the aqueous side of the ITIES. Conditions for oxygen evolution with reversed interface polarity and using the electron scavenger Tetracyanoquinodimethane (TCNQ) in the organic phase still need to be optimized.

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The Search for the Ferroelectric Nematic Phase

ROOM B Poster B1

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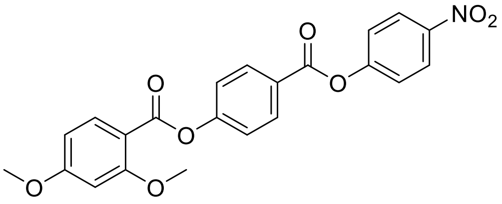
RM734



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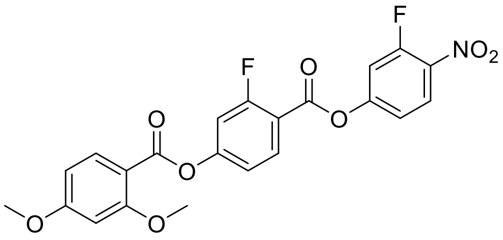

Liquid Crystals are a state of matter that have properties of both solids and liquids. Depending on the arrangement of molecules, liquid crystals can be grouped into different mesophases such as nematics or smectics etc. Since their discovery in the late 1800s, liquid crystals have been studied extensively and have found many uses in society, especially in display devices. [1]

In 2017, both DIO and RM734 were discovered to have an interesting new nematic phase. [2] [3] The identity of this new phase is uncertain. It was initially identified as the splay nematic phase. [4] [5] However recent results have suggested that the ferroelectric nematic phase has been discovered. [6]

My recent work has focused on making alterations to the RM734 molecule shown and making combinations of the RM734 molecule plus the DIO molecule. This work has led to the discovery of three interesting molecules.

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Characterisation of wax synthases to investigate their high promiscuity towards different diacylglycerol and acyl-CoA species

ROOM B Poster B2

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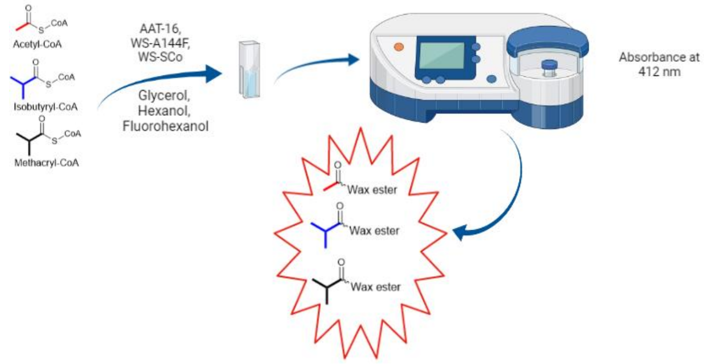

Methyl methacrylate (MMA) is an organic compound produced industrially as a precursor for acrylic plastics (Polymethyl methacrylate, PMMA), or for the production of medical devices, coatings and consumer electronics[1]. The demand for this monomer is exponentially increasing due to its special properties, such as weather and chemical resistance, and numerous novel applications[2]. MMA has currently no equivalent replacement, which will cause a continuous rise in its demand. Methyl methacrylate production has reached 4.8 million metric tonne in 2020, where PMMA production has already surpassed 2.8 million tonne annually[3]. Due to its increasing demand and costly production, alternative biosynthetic routes have been developed in recent years to allow methacrylic acid and its ester.

Wax esters, widely used in cosmetic and food industries, have been exploited and extracted from plants and synthesises from costly precursors[4]. Therefore, low-cost production of these compounds has been receiving particular attention in recent years. To achieve this, great focus has been put on developing methods that exploit enzymatic biosynthesis for the production of wax esters via reactions catalysed by wax esters synthases/diacylglycerol acyltransferases (WS/DGAT). These enzymes are able of catalysing the transesterification of acyl-CoA species with diacylglycerol through their bifunctional activity to yield wax esters. Nevertheless, information regarding the sequences in eukaryotic genomes and promiscuity activities of these enzymes is lacking[5,6]. Thus, this project wishes to characterise three different bacterial wax synthases (AAT-16, WS-A144F and WS-SCo) and investigate their promiscuity towards different diacylglycerol species (glycerol, hexanol and fluorohexanol) and acyl-CoA species (acetyl, isobutyryl and methacryl-CoA). After optimising their overexpression in *E. coli* BL21/pGro7, the wax synthases' kinetics were monitored via DTNB spectrophotometer assay (Ellman's reagent) and product formation was confirmed with LC-MS.

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Isolation of natural products from Deep-Water horizon bacterial strains

ROOM B Poster B3

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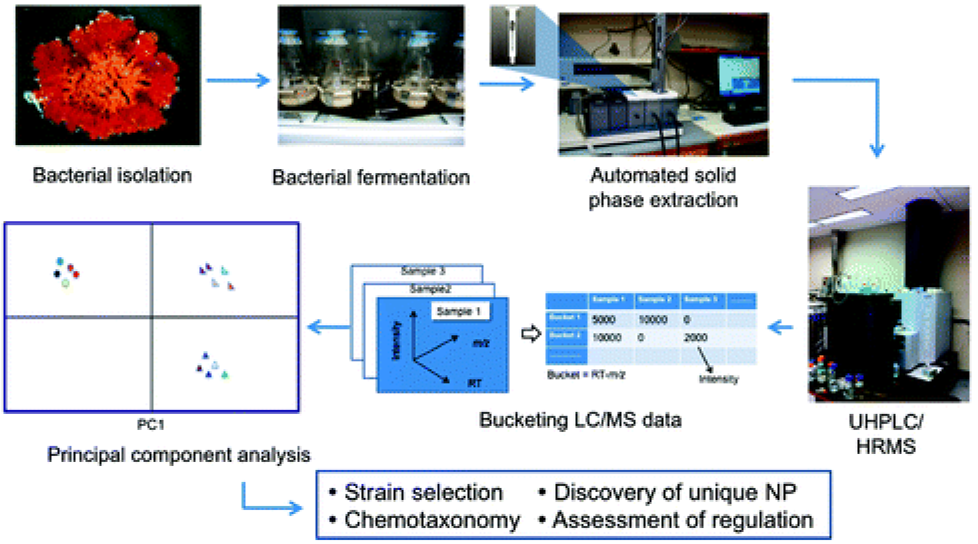

LC-MS based Principal Component Analysis (PCA) has been proven to be an effective tool to distinguish unique and common metabolites. Hence, PCA was chosen as a method to formulate an order of priority for the strains, this was done in tandem with molecular networking (GNPS). The strains that were analyzed using LC-MS based PCA were collected from the Deep-Water Horizon (DWH) oil spill that occurred in 2010. The strain *Halomonas GOS-1* was chosen for large scale culturing (5-6 L culture) to isolate potentially novel natural products.

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Determination of Ionic Pathways in the Hexagonal Perovskite Derivative $Ba_3VMoO_{8.5}$

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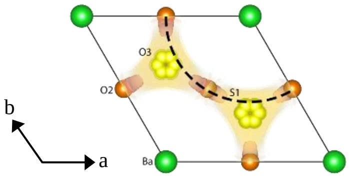

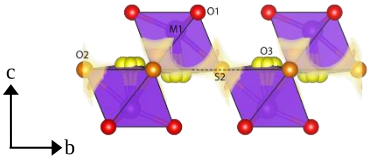

The $Ba_3M'M''O_{8.5}$ structural class of hexagonal perovskite derivatives have been investigated as potential electrolyte materials to be utilised in solid oxide fuel cells. $Ba_3NbMoO_{8.5}$ displays a hybrid structure between that of palmierite and 9R hexagonal perovskite with a disordered array of $M1O_x$ polyhedra [1]. This structure is also presented by other members of the $Ba_3M'M''O_{8.5}$ structural family including $Ba_3NbWO_{8.5}$ and more recently $Ba_3Nb_{1-x}V_xMoO_{8.5}$ [2,3]. Unlike these compounds where the cationic vacancies are distributed across two distinct crystallographic sites, the vacancies are ordered onto one position in $Ba_3VMoO_{8.5}$ resulting in the same structure displayed by $Ba_3VWO_{8.5.}$ This structure is composed of palmierite-like layers of $M1O_x$ units separated by ordered octahedral vacancies [4].

The ratio of tetrahedral to octahedral units varies greatly for the $Ba_3M'M''O_{8.5}$ phases with $Ba_3VMoO_{8.5}$ presenting the highest percentage of tetrahedra in the average structure. This ratio is dependent on the geometrical preference of the cations present, with V^{5+} and Mo^{6+} favouring tetrahedral geometry while Nb^{5+} and W^{6+} typically adopt octahedral geometry [5]. Consequently, in $Ba_3VMoO_{8.5}$ the geometry of the palmierite-like layer is predominantly tetrahedral resulting in a much-reduced distortion of the tetrahedral units while the octahedral units are highly distorted.

Bond-valence site energy (BVSE) calculations were performed to investigate the migration pathways of oxide ions and determine the energy landscape in the average crystal structure of $Ba_3VMoO_{8.5.}$ Two-dimensional conduction pathways along the palmierite layers corresponding to two relative energy barriers are observed and are expected to have the greatest contribution to the overall conductivity of $Ba_3M'M''O_{8.5}$ [3,4].

Investigation into the stability of $Ba_3VMoO_{8.5}$ has determined that it is unstable in both air and O_2 above 300 °C which is likely attributed to the barium non-stoichiometry of the phase. Further optimisation of the synthesis is warranted to allow for the elucidation of the electrical properties.

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Development of a biofilm growth inhibition assay to aid the discovery of natural product antifouling compounds

ROOM C Poster C1

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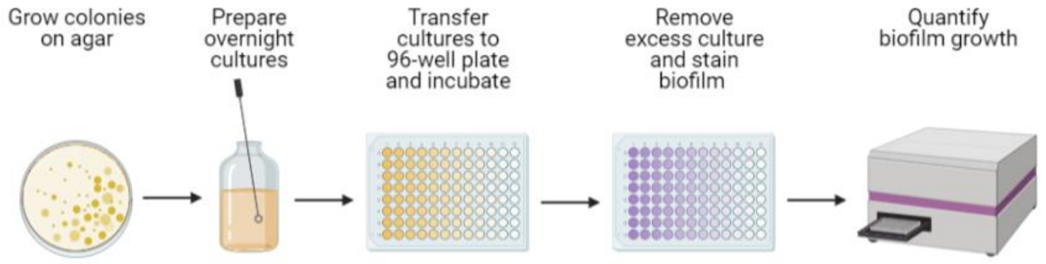

Biofouling is a big issue in both the maritime and oil and gas industries due to the increased drag on vessels, resulting in increased fuel consumption, and the costly task of removing marine growth from oil and gas structures. Fouling is made up of microfouling - an accumulation of microbial cells forming a biofilm layer - and macrofouling which is typically a thick encrustment of hard organisms such as mussels, barnacles and hard corals. Many antifouling solutions are currently being used, however, many of them are showing toxic and accumulative effects within the marine environment [1]. Interestingly, marine invertebrates produce chemical defence compounds to prevent organisms from settling on their surfaces and these natural products could have potential use as non-toxic and environmentally friendly antifouling compounds for use in marine industries. This particular study involves the discovery of antifouling active compounds from marine invertebrates using chromatographic and spectroscopic techniques. The development of an in-house bioassay guided fractionation method is underway to help prioritise samples during the fractionation and isolation process. This method was altered from an existing method [2] and involves the use of five bacterial strains which are key biofilm forming microbes in marine and estuarine environments [3]. The assay involves growing the bacterial strains in liquid culture before allowing them to form biofilms in a 96-well plate. The effect on biofilm growth under the presence of marine invertebrate extracts and pure, isolated compounds can then be quantified using the crystal violet staining method.

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Identification of Novel Secondary Metabolites by LC-MS Dereplication from the Atacama Desert Fungi

ROOM C Poster C2

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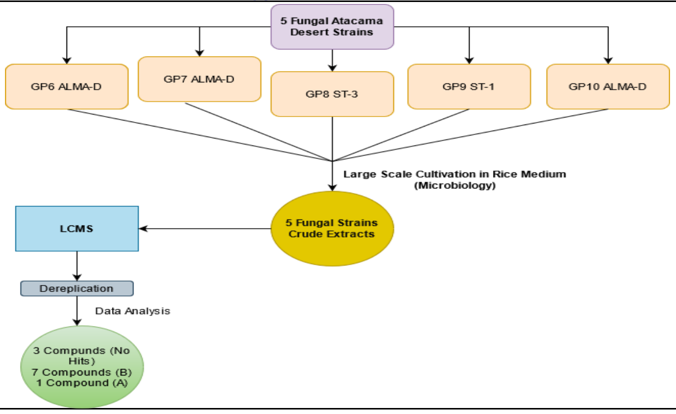

The Atacama Desert in Northern Chile is one of the least explored habitats comprising the driest and one of the most extreme environments on the planet. The microorganisms in this desert experience extreme aridity, high levels of ultraviolet radiation as well as high salinity with an exceptionally low amount of organic carbon[2]. Organic carbon is essential for the microorganisms to grow and support other nutritional requirements[1]. Therefore, in this research project, 5 unknown fungal strains were cultivated on long grain rice media leading to the potential discovery of 3 new compounds through targeted dereplication process of the large scale crude extract which showed no hits in the Antibase and Reaxys databases. Other compounds have not been reported from fungi previously. The dereplication process was applied by using the data generated from HPLC-HRMS analysis which provided an accurate and sensitive analysis. The databases used for the dereplication were NPs Atlas database, ChemFinder database, Reaxys database (NPs and general). Based on LCMS crude extract analysis, several chromatographic techniques will be used to separate and purify the promising compounds and their structures will be characterized using Nuclear Magnetic Resonance (NMR) spectroscopy and Mass Spectrometry (MS).

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Isolation and structural elucidation of three terpenoids from brine pool fungus

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ROOM C Poster C3

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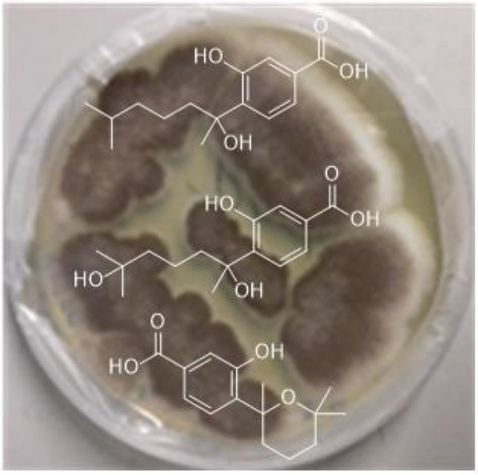

Marine brine pools are classic examples of extreme environments and are characterized by their hypersalinity, anoxic environment and heavy metal accumulation. Due to their high density, brine pools do not mix with the overlying sea water and are considered as mini lakes lying on the bottom of the ocean floor[1]. Microbes that inhabit these pools are highly salt tolerant and are termed halophilic or halotolerant. Natural product chemists have been fascinated by halophilic microbes, since they are capable of producing intriguing compounds which allow them to survive in their extreme environment[2]. Research carried out on the marine obligate halophilic actinomycete *Salinispora* spp. led to the discovery of arenimycin which is a potent antibiotic against rifampin and methicillin-resistant *Staphylococcus aureus* and the potent anticancer protease inhibitor salinosporamide A, therefore making halophilic microbes a promising source for potential new drug leads. In the current study an unknown fungal strain was isolated from a deep-sea brine pool sediment collected at a depth of 1200 m in the North Atlantic Ocean, was fermented on a small scale using six different media, followed by extraction with HP20 resin and organic solvents. Based on dereplication long-grain rice was chosen to culture the fungus on a large scale. The crude extract was subjected to several preparative chromatographic techniques. Subsequently three bisabolane type sesquiterpinoids were isolated and their structures were characterised using Nuclear Magnetic Resonance (NMR) spectroscopy and Mass Spectrometry (MS).

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Susceptor-Assisted Microwave Processing of Inorganic Solids

ROOM C Poster C4

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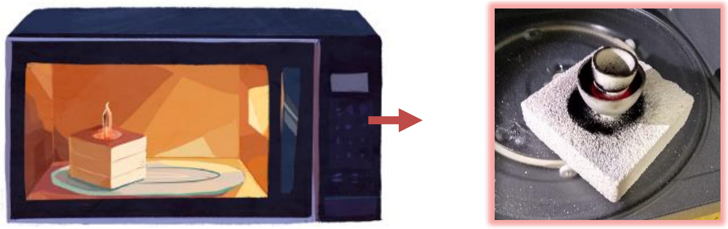

Conventional solid-state synthesis involves homogenisation of reagent powders by grinding followed by calcination at high temperatures; it is a relatively low-cost and straight-forward synthesis technique. Its main drawbacks are the exceptionally high temperatures and heating durations required for the interdiffusion of cations, to form the desired product. This limitation is addressed by susceptor-assisted microwave heating,[1,2, 3] a technique wherein a susceptor (a material that couples strongly to microwaves at room temperature) is used to provide heat to microwave-inactive reagents; once sufficiently hot, these reagents begin to absorb microwaves and subsequently experience a rapid increase in temperature. This process allows significantly reduced reaction times and energy expenditure when compared to a conventional furnace.

This study outlines the principles that govern microwave heating, as well as the experimental setup required for effective heating to take place. The system contains many more variables and so there are more factors to investigate such as the type and amount of susceptor, the microwave power and heating duration, the temperature-dependent dielectric properties of the sample and sample housing, etc. A crucible containing activated charcoal and a pellet composed of $BaCO_3$, Nb_2O_5 and MoO_3 was heated using a domestic 1000 W microwave oven for two 5-minute intervals with intermittent grinding. The result was a predominantly phase-pure product of the hexagonal perovskite oxide-ion conductor $Ba_3NbMoO_{8.5}$. This is a dramatic improvement over the conventional synthesis method, which requires three 48-hour intervals at 1100 °C with intermittent grinding. Optimisation of this technique promises a significant decrease in synthesis times with the possibility of enhanced conductivity properties due to decreased grain growth.

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Abstracts for Poster Presentations
(not presented as flash talks)

Genome mining of novel antimicrobial natural products from new bacterial strains

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ROOM A Poster A5

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Resistance to antibiotics is rising to dangerously high levels in all countries over all the world. 33000 deaths each year from drug-resistant bacteria is estimated in Europe alone and the cost is more than €1.5 billion [1]. As the natural products have been the main source for treatment of diseases and illnesses [2]. The most interesting property of *Streptomyces* is the ability to produce bioactive secondary metabolites, especially antibiotics [3]. Many have suggested that the solution lies in genomics and focusing research efforts on strains that encode genes for the biosynthesis of uncharacterized natural products can dereplicate, streamline, and accelerate the discovery process.

This project is designed to maximise the chance of harnessing a group of previously underexploited antimicrobial natural products using available genomic data and new cultivation technology. We have recently isolated several novel actinomycete strains from geologically unique regions in the world. The genomes of these strains have been sequenced and the bioinformatics analysis indicated that these strains have a huge reservoir for new antimicrobial natural product discovery. We discovered several new bioactive compounds and their related biosynthetic pathways in these bacteria through data mining, genetic manipulation, protein overexpression and enzymology studies.

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Design and synthesis of novel Peptidomimetic inhibitors for SARS-CoV-2

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ROOM B Poster B5

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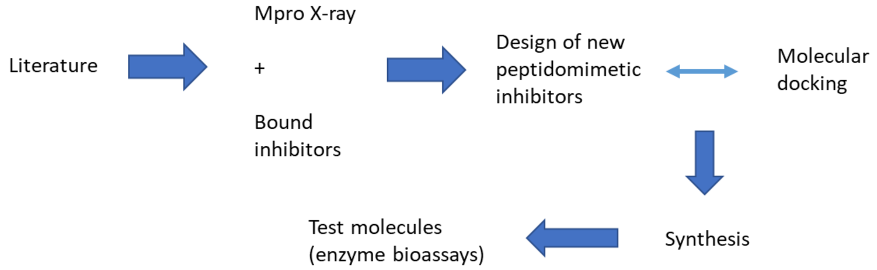

Literature

Mpro X-ray
+
Bound inhibitors

Design of new peptidomimetic inhibitors

Molecular docking

Synthesis

Test molecules (enzyme bioassays)

Abstract: AIM: Design effective peptidomimetic drugs against human coronavirus.
SUMMARISE: Due to the similarity of human coronavirus proteases, inhibitors of Mpro and PLpro are more likely to provide effective treatments against SARS-CoV-2. In this case, the inhibitor was designed and docked through Auto dock vina, and some potential compounds were screened out.
DOCKING OUTCOME: It was found that the tyrosine and benzothiazole structures have a significant inhibitory effect on MPro.
Future research will focus on the synthesis of compounds and the evaluation of their inhibitory effects in vitro.

Key Words: PEPTIDOMIMETICS, DOCKING, DESIGN, SYNTHESIS, BIOLOGICAL EVALUATION

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Isolation of pure compounds from Genus *Acremonium*

ROOM C Poster C5

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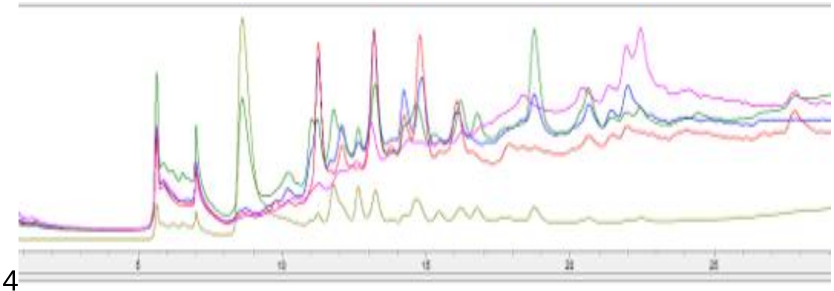

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Figure 1. HPLC chromatogram of *Acremonium* MA146167 sec-butanol fraction.

Microbial sources are important in the field of antimicrobial starting with the discovery of penicillin from a fungus in the 20th century. [1] Most of the antibiotics used clinically today are derived from microorganisms. [2] *Acremonium* MA146167 was previously isolated from sediment obtained from Salar de Chaxa in the Atacama Desert and cultivated in GYM medium. The crude methanol extract obtained from HP-20 solid phase extraction showed good antimicrobial activity against G-ve bacteria, while it showed insignificant antimicrobial activity against G+ve bacteria. The methanol crude extract was subjected to solvent partitioning and five fractions were produced with the sec-butanol fraction produced in the largest quantity. Further fractionation was carried out on this fraction by using MPLC and HPLC techniques. Finally, five compounds were isolated which may need further purification followed by structure elucidation of pure compounds using LC-MS and NMR (H-1, C-13, HSQC, COSY, and HMBC) techniques. Finally, the isolated compounds will be tested for their antimicrobial activity. In subsequent work, isolation of microorganisms from sediment samples recovered from different oceans will be carried out. Species identification will be achieved using DNA sequencing and bioinformatics. These microorganisms will be used to isolate pure compounds, then elucidate and characterize their structures and test their bioactivity.

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Synthetic and biosynthetic studies of antimicrobial peptides

ROOM C Poster C6

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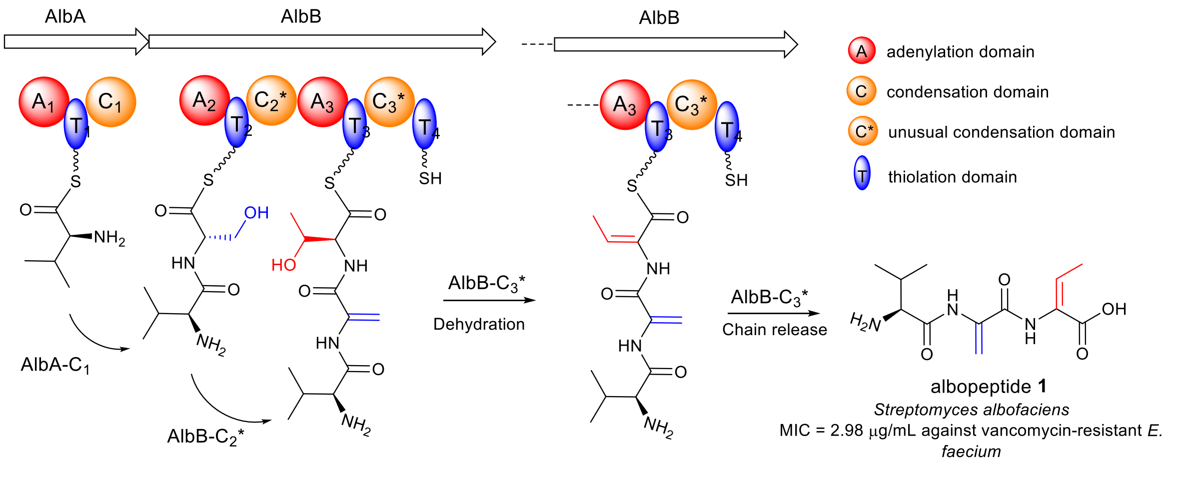

albopeptide **1**
Streptomyces albofaciens
MIC = 2.98 μg/mL against vancomycin-resistant *E. faecium*

Antimicrobial resistance (AMR) constitutes one of the greatest threats to global public health. There is a clear, unmet need for new agents to combat multidrug-resistant (MDR) microbial pathogens[1]. Natural products are an unprecedented starting point for drug discovery. They represent the only validated source of chemical diversity capable of delivering a sustainable pipeline for novel drug candidates[2].

We have recently reported the identification of the new peptidyl NP named albopeptide **1**, which was isolated from the culture broth of the soil bacterium *Streptomyces albofaciens.*[3] Albopeptide contains an unprecedented combination of two contiguous unsaturated residues, Dha-(*E*)-Dhb. It displays narrow-spectrum activity against vancomycin-resistant *Enterococcus faecium. In vitro* pathway reconstitution and detailed biochemical assays together with bioinformatics analysis show that albopeptide originates from a noncanonical NPRS biosynthetic pathway, featured with dehydration processes to form Dha and (*E*)-Dhb residues, catalysed by two unusual condensation domains, respectively.

The aim of this project is to develop a new and efficient synthetic route of albopeptide and its derivatives for structural activity relationship (SAR) studies. In the meantime, the synthetic protocol of putative biosynthetic intermediates during the biosynthesis of albopeptide will be also developed with the aim of characterizing the key enzyme, AlbB-C3*.

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