O1

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

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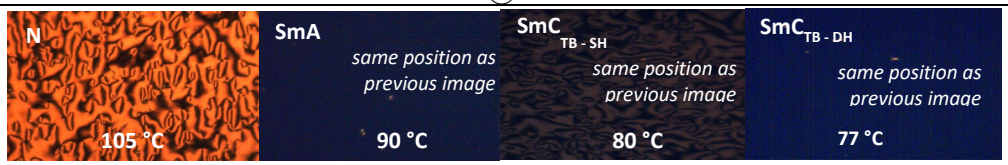

CB10O.16

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 them, this research aims to synthesise a non-symmetric liquid crystal dimer series CB10O.*m* (Figure 1) expected to show new examples of twist-bend phases. This structure was chosen as the decyloxy spacer, will endow the necessary molecular curvature for the system to exhibit the twist-bend behaviour and a range of homologues may be prepared by varying the length of the terminal chain. This is the first study of the effects a long spacer has on the twist-bend phases.

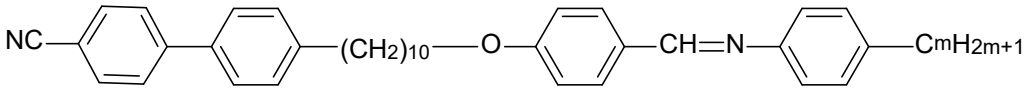

Figure 1: General structure of CB10O.*m*

Acknowledgements
I would like to thank Dr. R. Walker (UoA), Prof. E. Gorecka and Dr. D. Pociecha for their assistance with the phase characterization, as well as Calum Gibb for his support with the synthesis. The Saudi Arabian Cultural Bureau is gratefully acknowledged for the financial support of this research.

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O2

Ionic Conductivity in Hexagonal Perovskite Derivatives

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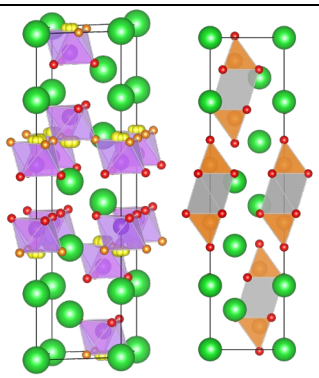

Oxide ion and proton conductors have application as electrolyte materials in solid oxide (SOFC) and proton ceramic fuel cells (PCFC). The greatest limitation with current materials is high operating temperatures resulting in slow start-up times, few compatible materials and poor durability of components. Increasing interest in the use of hydrogen technologies, including ceramic fuel cells, means it is vital the next generation of fuel cell electrolytes are developed with lower operating temperatures.

We have investigated several hexagonal perovskite derivatives which display oxide ion and/or proton conductivity including the BaM'M''$O_{8.5}$ (M' = Nb, V; M'' = Mo, W) crystal family and $Ba_7Nb_4MoO_{20}$. $Ba_7Nb_4MoO_{20}$ exhibits excellent dual ionic conductivity over a wide range of atmospheres [1]. Doping of $Ba_7Nb_4MoO_{20}$ with V^{5+} was performed to determine if it was possible to enhance ionic conductivity further by altering the tetrahedra: octahedra ratio, however this resulted in lower ionic conductivities.

$Ba_3VMoO_{8.5}$ was investigated and found to display a structure similar to $Ba_3NbMoO_{8.5}$ however cation ordering is present resulting in octahedral vacancies which would be expected to hinder oxide ion conductivity. $Ba_3VMoO_{8.5}$ is actually non-stoichiometric with vacancies on Ba and O sites. This results in poor stability preventing measurement of electrical properties. However, BVSE calculations strongly suggest oxide ion conductivity would be present if the phase can be stabilised [2].

Ionic conduction pathways were primarily detected within the palmierite-like (P-L) layer of these materials which consists of a disordered array of tetrahedral and octahedral units. We have now investigated the crystal structure and electrical properties of the palmierites $A_3V_2O_8$ (A = Ba, Sr). Both materials display dual oxide ion and proton conduction with $Sr_3V_2O_8$ exhibiting significant dual ionic conductivity of 1.0 x 10^{-4} S cm^{-1} at 600 °C under humidified air [3]. This is comparable to leading doped proton conductors with structures containing isolated tetrahedra. These materials are currently undoped so this gives promise that doping of $A_3V_2O_8$ may enhance bulk proton and oxide ion conductivity.

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O 3

Developing an enzymatic system for methacrylate intermediates and esters

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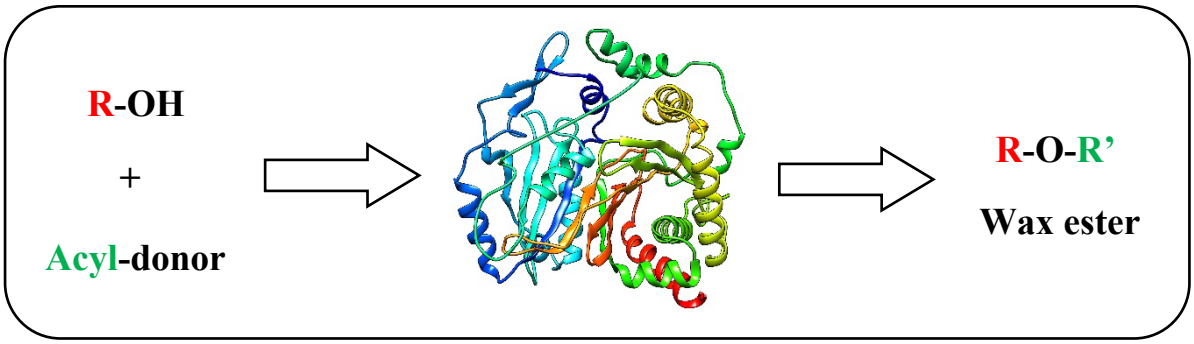

Methyl methacrylate (MMA) is an organic compound used as a precursor in the manufacturing of plastics. MMA production has reached 4.8 million metric tonnes yearly in 2020, with no current equivalent on the market[1]. Furthermore, it is currently produced chemically via half-dozen processes that use carbon fuel feedstocks[2]. As a result, new sustainable manufacturing strategies are needed. The current biosynthetic pathway to MMA occurs not without limitations. Low conversion rates, namely too many side products, and difficulties in separating them, are just a few of the concerns that business is facing. Consequently, several enzymes have been exploited to try and solve these problems. Alcohol acyl transferases (AAT) are a group of enzymes with the ability of producing esters from acyl-donors (such as acyl-CoA) and fatty alcohols as substrates. They have been previously reported as source for biodiesels fuels from *Saccharomyces cerevisiae*[3]. In the biotransformation to MMA, AATs can be used to produce key intermediates, such as acetate, isobutyrate and methacrylate esters. In this project, multiple acyl-donors and alcohols will be investigated as substrates among several transferases from various hosts to design the most optimal enzymatic system to yield methacrylate intermediates and esters.

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O4

A General Route to the Synthesis of Highly Functionalised Pyrazole-containing Heterocycles

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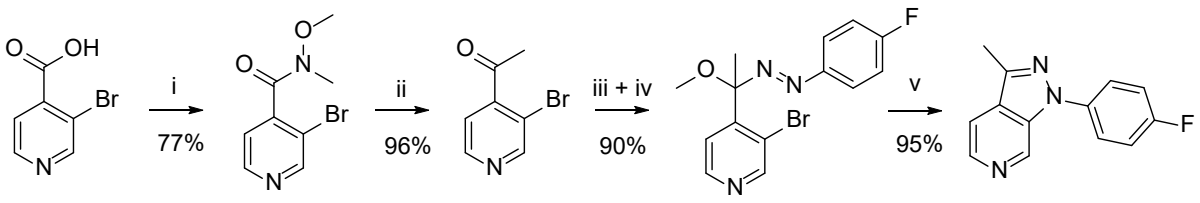

i; EDC HCl, *N,O*-dimethylhydroxylamine HCl, *N*-methylmorpholine, DCM, 24 h, rt.
ii; MeMgBr, THF, 24 h, 0 °C.
iii; 4-fluorophenylhydrazine HCl, TEA, MeOH, 48 h, 70 °C.
iv; DAIB, MeOH, 24 h, rt.
v; TTMSS, ACHN, toluene, 2 h, MW, 160 °C.

Scheme 1: Example synthesis using developed synthetic route.

The pyrazole ring is an important moiety in biological environments and by extension, drug discovery. It has been shown to exhibit high potency across a range of applications including anti-microbial, anti-fungal, anti-cancer, and neuroprotective activity [1]. As such, the incorporation of pyrazoles into fused heterocycles is an interesting avenue for exploration in the development of drug molecules to treat a range of diseases.

Existing methods for forming pyrazole-containing bicyclic systems demonstrate limited variation in the types, isomers, and substitution patterns of scaffolds producible. The majority of documented strategies rely on ionic ring-forming steps, which are sensitive to electronic effects and not tolerant of certain functionality. In contrast, radical cyclisation strategies are generally highly selective and have wide functional group tolerance - making them an attractive choice for a versatile synthetic strategy.

Kunka *et al.* [2], published a synthetic route to produce 1*H*-indazoles by radical cyclisation onto an azo functional group. The route provided a promising starting point for the development of a general route, see Scheme 1, to produce a range of pyrazole-containing heterocycles. The published route was improved by replacing undesirable reagents and laborious techniques and verified on a test indazole. Subsequently, a range of 1*H*-pyrazolopyridine and 1*H*-thienopyrazole scaffolds with varied functionality was prepared.

Future work will target alternative fused heterocycles as well as further varying functionality. The reaction sequence will also be examined, since the ability to introduce specific 'modules' at different stages of the synthetic route increases its overall versatility.

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O5

Hydrogen and Oxygen Production Driven by Photocatalyst Assembled at the Interface between Two Immiscible Electrolyte Solutions (ITIES)

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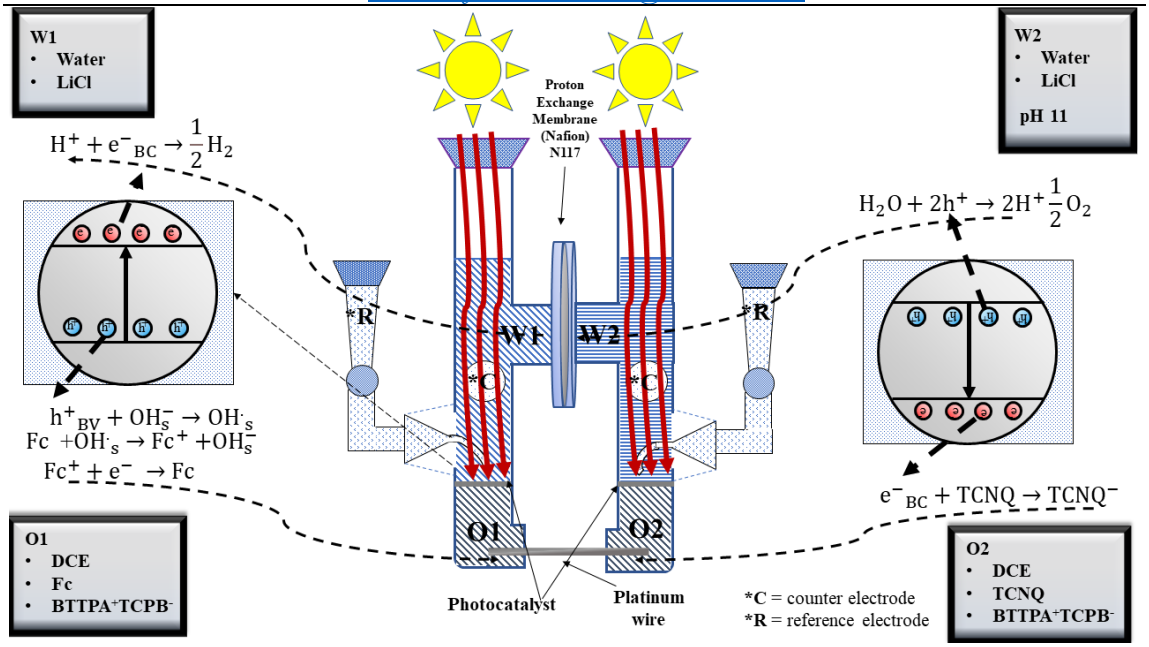

Figure 1. Novel double-interface H-Cell system for photocatalytic water splitting. DCE: 1,2-dichloroethane; Fc: Ferrocene; TCNQ: Tetracyanoquinodimethane; $BTTPA^+$: bis(triphenylphosphoranylidene) ammonium; $TCPB^-$: tetrakis(4-chlorophenyl)borate

Water splitting feasibility using a novel double-ITIES cell connected in series through a Pt wire and a proton exchange membrane (H-cell) was analyzed. Results with a single-interface cell for hydrogen evolution show a small photocurrent of 0.2 µA cm^{-2} in the absence of a photocatalysts assembled at the interface, which can be related to the photo-oxidation of Ferrocene in the organic phase[1]. A larger and faster photo-response was observed when TiO_2 was assembled, with a maximum photocurrent of 2.2 µA cm^{-2}. A *ca.* fivefold enhancement in the photocurrent (11.8 µA cm^{-2}) was achieved by the assembly of CuO, a lower bandgap photocatalyst. However, an opposite effect was seen for oxygen evolution in a single-interface cell, as larger photoactivity (-2 µA cm^{-2}) was found in the absence of a solid photocatalyst assembled at the interface, with TCNQ in the organic phase acting both as photocatalyst and electron scavenger, compared with the photocurrents obtained in the presence of TiO_2 (-0.2 µA cm^{-2}), Fe_2O_3 (-0.1 µA cm^{-2}) or WO_3 (-0.4 µA cm^{-2}). This is most likely due to a low transference of photogenerated electrons from the conduction band of the photocatalyst to the LUMO of TCQN[2]. When two interfaces were coupled, a -0.017 µA cm^{-2} photocurrent was observed, signaling the respective formation of H_2 and O_2 at each interface. Connecting the two aqueous phases through a Nafion membrane suppressed the photocurrent, suggesting that the circuit is now closed by H^+ migrating between the aqueous phases instead of through oxidation and reduction, respectively, of H_2 and O_2.

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O6

A new member of the Mutactimycin family isolated from a *Saccharotrix* found in the Atacama Desert

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The Atacama Desert is one of the driest places on earth. Studies have revealed tremendous potential for biodiversity[1] with new and important secondary metabolites such as Chaxamycins[2] and Abenquines[3] being discovered from organisms found in the desert. One strain isolated from the rhizosphere of lupine plants growing in the Atacama Desert, *Saccharotrix sp* S26, when grown in TSB has produced a new compound (compound 1) which belongs to a family of anti-bacterial compounds known as Mutactimycins. The compound was isolated and characterised using HR-LCMS, ^{1}H, ^{13}C, HSQC, COSY and HMBC NMR techniques. The strain was subsequently co-cultured with a fungal strain belonging to the *Penicillium* genus which was also isolated from the Atacama Desert on a solid rice medium which yielded different secondary metabolites compared to either axenic culture, as seen in figure 2, which shows that the presence of a second organism triggers the production of new secondary metabolites. The compound showed moderate activity against MRSA, a nosocomial pathogen which often causes fatal skin infections.

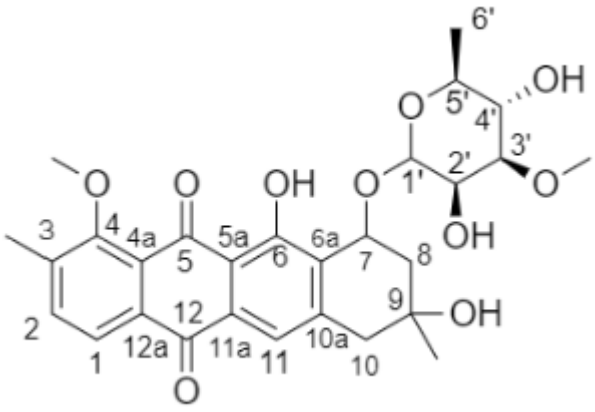

Figure 1: structure of Compound 1

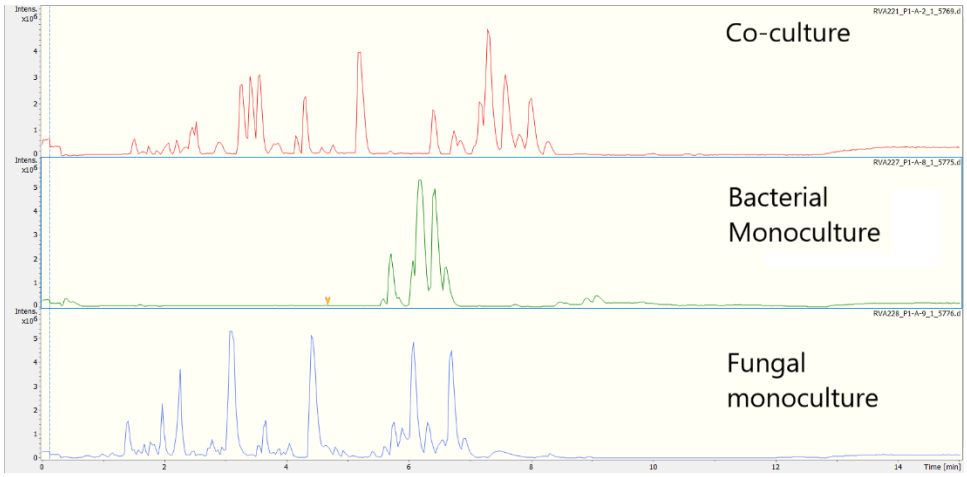

Figure 2: A comparison of the QTOF-HR-ESI-MS chromatograms of the fungal monoculture, bacterial monoculture, and their co-culture in short grain rice.

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O7

The Effect of Fluorination on the Ferroelectric Nematic Phase

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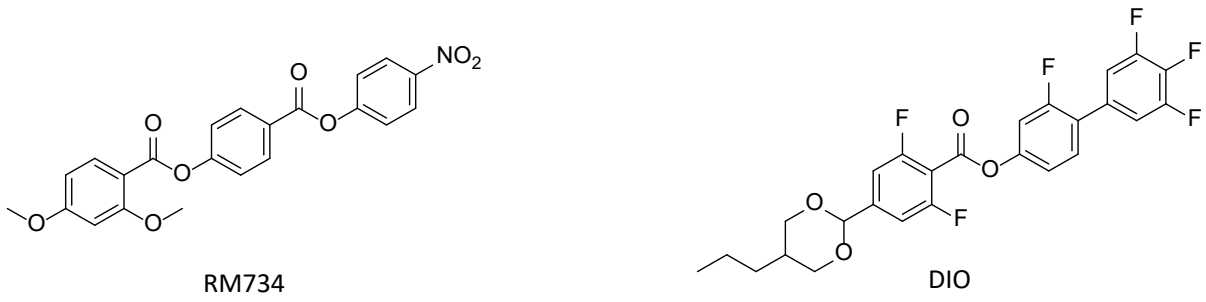

Figure 1 *– Chemical structure of RM734 and DIO*

In the conventional nematic phase, the molecules are dispersed randomly along the director, **n**, and show no long-range positional order. The molecules tend to possess chemically distinct ends which are evenly distributed with respect to the director so that the phase shows apolar character i.e., **n** = **-n**. In 2017, RM734 and DIO, shown in **Figure 1**, were reported separately by two different groups and were shown to exhibit a new nematic phase, [1][2] which was later identified to be the ferroelectric nematic phase. [3]

The ferroelectric nematic phase lacks the inversion symmetry shown in the conventional nematic phase and is polar in nature, it is sensitive to external electric fields giving it suitable properties to be used in future display devices. Direct isotropic to ferroelectric transitions are rare with a few examples being found in literature. [4][5][6]

My research focuses on the effect of fluorination on the ferroelectric nematic phase. Through combinations of RM734 and DIO, and fluorinated analogues of RM734 I was able to produce a library of molecules that show the ferroelectric nematic phase and was able to produce a molecule with a direct isotropic to ferroelectric transition, [6] this was only the second known example of this in literature at the time.

Acknowledgments:

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F1/P1

Genome mining of novel antimicrobial natural products from new bacterial strains

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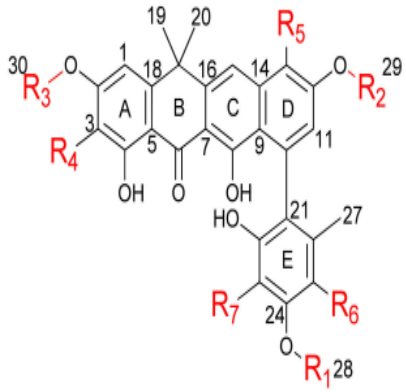
Abstract:

Streptomyces sp MA-37 is a prolific producer of bioactive natural products. The discovery programme in this strain resulted in the isolation and characterization of structurally diverse specialized metabolites, including fluorometabolites, various bacterial alkaloids, and type II polyketides such as accramycin, naphthacemycin or fasamycin derivatives [1-10].



	R_1	R_2	R_3	R_4	R_5	R_6	R_7
Accramycin A **1**	CH_3	CH_3	H	H	H	H	H
Accramycin B **2**	CH_3	CH_3	CH_3	H	H	H	H
Accramycin C **3**	H	CH_3	H	Cl	H	H	H
Accramycin D **4**	CH_3	CH_3	CH_3	Cl	H	H	H
Accramycin E **5**	CH_3	CH_3	H	Cl	Cl	H	H
Accramycin F **6**	CH_3	H	CH_3	Cl	Cl	H	H
Accramycin G **7**	CH_3	CH_3	CH_3	Cl	Cl	H	H
Accramycin H **8**	H	H	CH_3	Cl	H	Cl	Cl
Accramycin I **9**	H	CH_3	CH_3	Cl	Cl	Cl	H
Accramycin J **10**	H	H	CH_3	Cl	Cl	Cl	Cl
Accramycin K **11**	H	CH_3	CH_3	Cl	Cl	Cl	Cl
Naphthacemycin B_1 **12**	H	H	H	H	H	H	H
Fasamycin C **13**	CH_3	H	H	H	H	H	H

Figure (1): some compounds which had been isolated from streptomyces MA-37 strain.

In this project, I will report the isolation and characterization of a new accramycin derivative from a mutated MA37 variant.

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F2/P2

Isolation and identification of pure compounds from fungal strains

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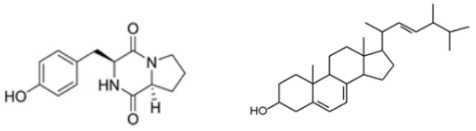

(1) (2)

Antimicrobial resistance is one of the most dangerous problems affecting human health worldwide. This threat has increased over the last years because of the continued overuse of antibiotics and lack of discovery of new drugs.[1] The discovery of new antimicrobials with novel mechanisms of action is now urgent to overcome this problem and the morbidity and mortality associated with it. [2] During my research I isolated two pure compounds from two fungal strains: Maculocin (**1**) ($C_{14}H_{16}N_2O_3$) and ergosterol (**2**) ($C_{28}H_{44}O$). Maculocin was isolated from *Acremonium* PIQ1-14616-BJ-CB-7 which recovered from Atacama Desert soil and cultivated in GYM medium. Maculocin was isolated from the sec-butanol fraction by using MPLC and HPLC techniques. Ergosterol was isolated from fungal strain AWA13 derived from a deep-sea sediment from the North Atlantic Ocean (Cruise ID 64PE391/ 73) then cultivated in rice medium. Ergosterol was isolated from the hexane fraction after it crystalised on the inner wall of the separating funnel during solvent partitioning. The crystals were collected and washed using methanol several times. The structures of **1** and **2** were confirmed by comparing their NMR spectra with the published NMR spectra for these two compounds in the literature. Finally, the isolated compounds will be tested for their antimicrobial activity. In subsequent work, I will continue working on AWA13 crude extract to isolate more pure compounds and I will apply the one-strain-many-compounds approach on other microbial strains which I isolated previously from deep-sea core sediment, then large-scale fermentation and extraction using chemical solvents and subjected to repeated rounds of purification until a pure, active compound is obtained. In addition to that, species identification will be achieved using DNA sequencing and bioinformatics for both fungi: AWA13 and *Acremonium* PIQ1-14616-BJ-CB-7.

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F3/P3

Synthesis of isovalery-dehydrobutyrine-proline thioester for bacterial pyrrolizidine biosynthesis

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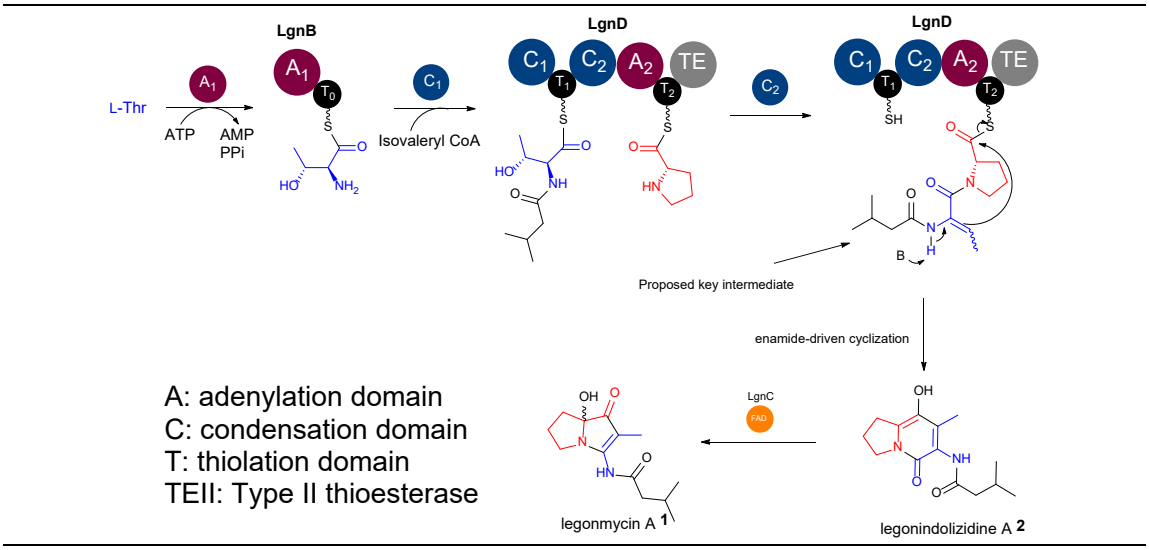

Pyrrolizidine alkaloids (PAs) are a group of naturally occurring alkaloids based on the structure of pyrrolizidine, and they are produced by plants as a defense mechanism against insect herbivores. More than 700 PAs have been identified in over 6,000 plants, and about half of them exhibit hepatotoxicity and they can result in damage to organs in the body, and could be a potential cause of cancer. PAs from bacterial origin are rare. In 2015, we discovered a new bacterial PAs called legonmycin A **1**. Biosynthetic investigation of legonmycins led a conclusion that legonmycin is biosynthesized from three building blocks (precursors/substrates) Pro, Thr and fatty acid CoA to form bicyclic legonindolizidine intermediate **2** (5+6), followed by multistep oxidation/rearrangement to decorate PA ring system (5+5) [1]. Recent studies indicated that two multidomain non-ribosomal peptide synthetases (LgnB and LgnD) together with the newly identified amino-acyl transferase/type II thioesterase (LgnA) are responsible for the assembly of **2**, the last intermediates of the **1** biosynthesis [2]. During the study, protein-tethered isovaleryl(IV)-dehydrobutyrine (Dhb)-Pro-thioester is likely to be the last intermediate for the encarbamide-driven heterocyclization by an unusual Type I thioesterase LgnD-Te to produce **2** [2]. However, the conformation of Dhb in this putative intermediate has remained elusive.

In this presentation, I will report the synthesis of the synthetic mimic IV-(E/Z)Dhb-Pro-SNAC. Once the synthetic molecules are produced, I will compare them with the biosynthetic intermediates with the aim of identifying the correct configuration.

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F4/P4

Design and synthesis of novel Peptidomimetic inhibitors of SARS-CoV2

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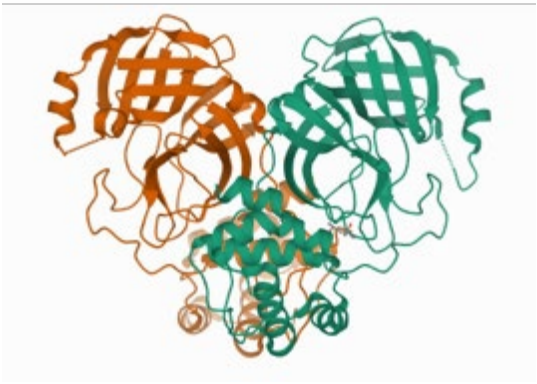

Figure 1. Structure of the main protease of SARS-CoV2[1]

Abstract

The aim of this project was to design new peptidomimetic drugs against human coronaviruses. Due to the similarity of human coronavirus proteases [2], inhibitors of the main protease (Mpro) and papain-like protease (Plpro) enzymes are likely to provide effective treatments against SARS-CoV-2 and other related coronaviruses. In this poster we report the design, docking and synthesis of potential new inhibitors of the Mpro. Docking showed high binding scores for peptidomimetics that contained tyrosine and benzothiazole moieties. We have prepared several such compounds, which will be tested using the Mpro inhibition assay. Future research will focus on the synthesis of more derivatives and the evaluation of the compounds in vitro and in vivo.

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P4

The Effect of Sulfur on Ferroelectric Nematic Liquid Crystals

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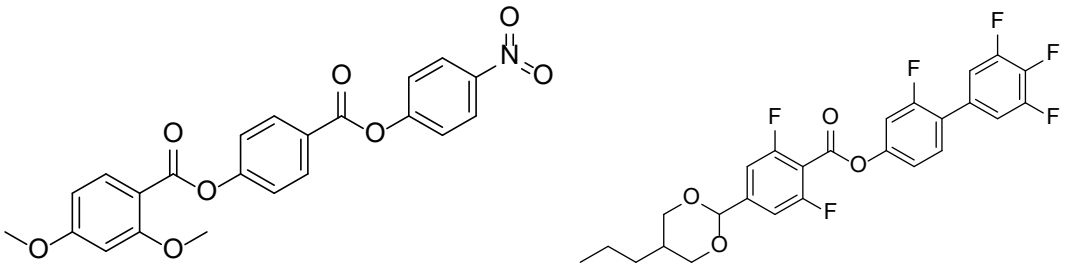

Figure 1 – Structure of RM734 (left) and DIO (right)

The nematic phase (N) is the most fluid and the least ordered liquid crystal phase, in which the molecules are orientated roughly in the same direction along the director, **n**. Due to the molecular orientation around the director, the phase has inversion symmetry, **n** = **-** **n**, therefore the phase is non-polar. In 2017, two new rod-shaped molecules exhibiting a unique phase and a large dipole moment, shown in **Figure 1**, were discovered. The phases exhibited by DIO[1] and RM734[2] were described as polar nematic and splay nematic respectively, but were later determined to be the same: the ferroelectric nematic phase, N_F. [3] In this phase, **n** ≠**-n**, the phase no longer has inversion symmetry and so is polar. The N_F has high response sensitivity to an applied external electric field and this coupled with nematic fluidity [4] gives it exciting potential for applications in the next generation of optical or electrical LC display devices.

Sulfur containing analogues of RM734 have been prepared, replacing the terminal ether and/or one of the ester links with a thioether or thioester respectively. The enhanced polarizability arising from the substitution of a carboxylate ester with a thioester would be expected to increase the clearing temperature, whereas the addition of thioether would decrease it due to the decreased bond angle between C-S-C. [5,6]

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P5

Downstream Processing and Structure Confirmation of Chemoenzymatically Produced Macrocycles

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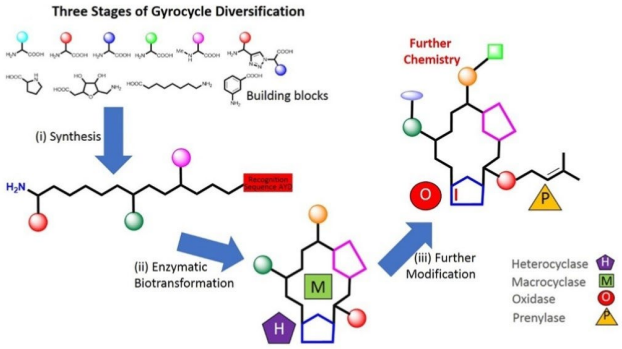

Many cyclic peptides have biological properties ranging from antibacterial to immunosuppressive to anti-tumour and over the last two decades, the dominant trend in peptide drug discovery has been a shift away from naturally derived cyclic peptides and toward cyclic peptide analogues optimised for potency, stability, and pharmacokinetic features [1].
The development of selection procedures also allowed for the discovery of cyclic peptides with unique qualities such as cell membrane penetration, oral bioavailability, chemical stability, metabolic stability, and uniform structure.
There are difficulties associated with cyclic peptide sequence identification by mass spectrometry that hamper the validation of effective peptide synthesis, in addition to the complications in selecting future "applicable" cyclic peptides to develop and study[2].

These project aims to ease those problems by:

- Calculate the physicochemical properties of linear precursors and cyclic peptides with precision and utilise them to improve compound isolation operations.
- To investigate and comprehend the unique mass spectrometry fragmentations in linear precursors and cyclic peptides and to use this information to create a tool that can forecast the most likely fragmentations.
- To provide a tool to compare mass spectrometry fragmentation data from linear precursors and cyclic peptides to expected fragments to ensure successful synthesis.

Mass Spectrometry data has been obtained from different cyclic peptides provided by GyreOx and trends on the fragmentation will be presented.

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P6

Desalination Acid-Base Battery – DABB

Symposium Abstract

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As electricity production in the United Kingdom moves towards renewable sources such as wind and solar, the need to store these theoretically limitless but intermittent sources becomes a necessity [1]. Electrochemical energy conversion offers a highly efficient route, however, typical batteries, such as lithium-ion, are expensive, decrease performance overtime, and most importantly, are restricted by cell construction size [2]. As local commercial and domestic renewable energy grows, a cheap and flexible storage system is required to adapt to growing renewable energy.

Redox-flow batteries (RFBs) offer a solution for this issue as the redox active solutions are stored externally where capacity can be expanded by increased electrolyte tank size [3]. The electrolytes pass through channels separated by ion-selective membranes and go through redox reactions on the opposing electrodes, supplying current through an external circuit. Another energy source in the spotlight is hydrogen fuel cells. As in RFBs, the reactant can be stored externally of the cell to limitless capacity. Hydrogen can be electrochemically synthesised via electrolysis of water which can be powered by renewable sources (green hydrogen), leading to a clean energy loop [4]. However, to obtain hydrogen gas from water, it must be pure and void of parasitic ions, such as chloride which is converted to corrosive chlorine gas if present in water electrolysers. Therefore, to have a clean energy cycle with hydrogen and batteries, a cheap and effective method of achieving deionized water (thereby avoiding having to use valuable fresh-water resources) is also necessary.

Our work offers a 2-for-1 solution, combining a RFB with neutralization dialysis (ND) to store and discharge energy while simultaneously desalinating water. This three-membrane system utilizes the neutralization energy of acid and base in the form of the hydrogen oxidation and evolution reactions (HOR and HER) at the negative and positive electrode respectively. Though the theoretical open cell voltage (OCV) is smaller (0.83 V for neutralisation of pH 0 with pH 14) than a typical hydrogen/oxygen fuel cell (1.23 V), the overall consumption of hydrogen gas is zero as it is being produced and consumed equally on opposite electrodes. Applications of this cell could be seen in sustainable desalination of seawater for consumption or for water splitting in green hydrogen production.

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P7

Assessment of Novel Microbial-derived Pharmaceuticals from *Micromonospora* STR1s-16 and *Rahnella* LBJCSS2801 Strains

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Abstract

Microorganisms from underexplored extreme environments like deep-seas, cold seas, semi-arid, and hyper arid deserts have been shown to produce a range of complex natural products with high biological activity. However, very few natural compounds have been isolated from deep-sea-derived microorganisms and our knowledge of bioprospecting microorganisms from desert habitats is sparse. The aim of this study is to assess the production of novel microbial-derived pharmaceuticals from marine and desert microorganisms. Our collaborators at Newcastle University and University College Cork, Ireland UK, provided the microbial strains *Micromonospora* STR1s-16 and *Rahnella* LBJCSS2801, which were previously isolated from Atacama Desert soils and salmon fish (*Salmon salar*) skin, respectively. The microbial fermentation culture was extracted using organic solvents, the dried crude extract subjected to separation and purification by Kupchan fractionation scheme, and SPE prior to HPLC chromatographic analysis. The preliminary LC-MS analysis of methanolic extract from a small-scale culture of *Micromonospora* STR1s-16 and *Rahnella* LBJCSS2801 strains cultured in ISP2 and LB medium respectively showed interesting peaks with molecular ions that yielded no results when searched in databases (i.e. Reaxys, NPs Atlas). The MS/MS fragmentation data analysis of the hit compound (Corynebactin) was consistent with the MS/MS spectra. The genome of *Rahnella* LBJCSS2801 strain was sequenced, annotated, and genome mining to identify the BGCs using antiSMASH predicted 7 BGCs, and the siderophore gene clusters showed 100% genes similarity to desferrioxamine E. The GNPS dereplication of the *Micromonospora* STR1s-16 and *Rahnella* LBJCSS2801 strains molecular network showed parent ions which were singletons, indicating that their fragmentation patterns did not correlate with that of any other parent ion in the dataset, implying chemical uniqueness. The *Micromonospora* STR1s-16 strain small-scale extract bioactivity screening showed activity against some ESKAPE pathogens, with the zones of inhibition ranging between 4 to 18mm, and the highest zone of inhibition of 18mm against methicillin resistant *S. aureus* DSM2569 (MRSA) as compared to oxolinic acid and ampicillin positive controls. The *Rahnella* LBJCSS2801 strain fermentation extract differed antagonism assays showed activity against fish pathogen *Yersinia ruckeri* DSM18506.

Key Words: *Micromonospora* STR1s-16, *Rahnella* LBJCSS2801, ESKAPE pathogens, Bioactivity assay

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P8

Synthesis and Characterization of Disulphide- and Thioether-linked Liquid Crystal Dimers

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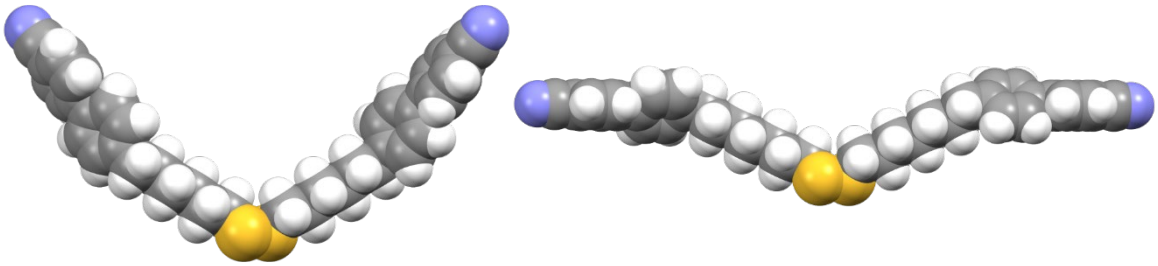

Figure 1 - Molecular models of members of the CBnSSnCB series.

The dependence of the transitional behaviour of liquid crystal dimers on their molecular structure has been the focus of considerable research activity in recent years. Much of this work has centred on the twist bend phases. [1] In order to control the bend of these dimers, various oxygen functionalities have been employed as linkers for the flexible spacers. Sulfur-containing materials, although very similar to oxygen, have not been investigated to the same extent. It has been reported that the introduction of the C-S-C link, having a more acute bond angle than the corresponding C-C-C and C-O-C links, influences the temperature range of the mesophases observed, not to mention the structural modifications induced by a disulphide bond. [2][3] The highly polarizable nature of sulfur atoms enhances the birefringence of these materials which is of great interest in developing liquid crystal display technologies. [4][5][6] Here we present the synthesis and characterization of a series of dimers linked by a disulphide bridge (Figure 1). In addition, we also present examples of thioether-linked dimers and discuss the role that these sulfur links have in the formation of the N_{TB} phase.

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P9

The Synthesis and Stability of $K_2Ba(MoO_4)_2$

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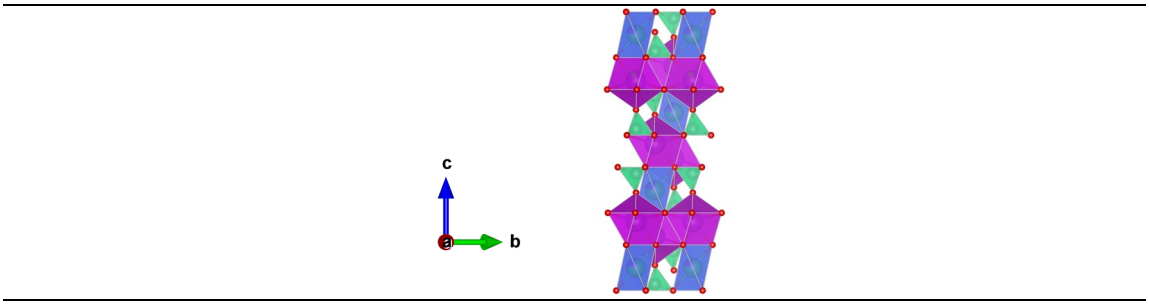

Palmierites are hexagonal perovskite derivative structures which exhibit significant proton and oxide ion conductivity. This is displayed most notably in $Ba_3NbMoO_{8.5}$ and $Ba_7Nb_4MoO_{20}$ which contain palmierite-like layers [1]. These materials have application in SOFCs (solid oxide fuel cells) which desire high conductivity at low temperatures (≤ 600 °C). The palmierite structure contains isolated tetrahedra and recently dual oxide ion and proton conductivity was reported in $A_3V_2O_8$ (A = Ba, Sr) [2].

$K_2Ba(MoO_4)_2$ has been synthesised as it exhibits the desired palmierite oxide structure and has not previously been investigated as an ionic conductor [3]. It was determined that $K_2Ba(MoO_4)_2$ could be synthesised by heating at 850 °C for 10 hr. This step was repeated three times to obtain a phase-pure material. The stability of the phase was then investigated by heating the sample at varying temperatures in a range of 400-1050 °C and analysing by X-ray diffraction. However, $K_2Ba(MoO_4)_2$ was found only to be stable between 700-950 °C which precludes application in a ceramic fuel cell.

Research into another palmierite oxide, $Sr_3V_2O_8$, has begun. This material has previously been reported to have high proton and oxide ion conductivity [2]. In comparison to $Ba_3V_2O_8$, $Sr_3V_2O_8$ has a significantly higher conductivity. This is potentially due to the unit cell size being smaller. It is hoped that chemically doping $Sr_3V_2O_8$ with the smaller Ca^{2+} ion will further increase its oxide ion and/or proton conductivity as the conductivity increases from 1.6×10^{-6} S cm^{-1} to 1.0×10^{-4} S cm^{-1} upon decreasing the size of the A cation from Ba to Sr [2]. $Sr_{3-x}Ca_xV_2O_8$ (x = 0.2, 0.4, 0.6) have successfully been synthesised as phase pure phases.

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P10

The Discovery of Novel Pharmaceuticals from Desert Microorganisms

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Natural products provide a rich source for the discovery of therapeutics. Screening novel microorganisms from underexplored habitats, particularly the extremobiosphere, like desert biomes, is an important strategy to discover new chemical scaffolds and hence chemical diversity[1].

This research project aims to discover novel, potent and selective secondary metabolites from hyper-arid desert microorganisms with potential applications against cancer and inflammatory diseases. All aspects of this programme have been designed to streamline the isolation, identification, and structural characterisation of potentially new bioactive compounds.

Numerous filamentous actinobacteria have been isolated from Atacama Desert soils and assigned to the genus *Streptomyces*[2] in addition to rare and understudied genera, such as *Actinomadura, Saccharothrix*[3] and *Micromonospora*[4]. Thus, for the first part of this project *Micromonospora* strain Y6-2; isolated from the Yungay core region in the Atacama Desert, was selected for bioactive secondary metabolites screening. OSMAC (One Strain Many Compounds) approach[5], LC-MS/MS analysis and molecular networking were used for condition optimization before large scale culture.

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P11

Isolation of Novel Bioactive Molecules against Infectious Diseases from Unexplored Marine Actinomycetes

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Infectious diseases contribute a significant burden globally, particularly with the evolution of multi-drug resistant (MDR) pathogenic strains. MDR is a growing crisis and is estimated to account for about 10 million deaths globally by 2050 [1]. On that basis, the necessity for drug replacement with novel antimicrobial compounds is critical. Deep-sea marine ecosystems host unexplored microbial species which have undergone evolutionary adaptation to the extremophilic conditions, and thus guarantee an untapped diverse source of exceptionally bioactive novel secondary metabolites [2,3]. Meanwhile, only about 10% of rare Actinomycetes have been isolated [4] and they have attracted attention for their novel biochemical diversity [5]. This research aims to screen unexploited marine microorganisms with high potential for the discovery of unique bioactive molecules with novel structural skeletons.

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