THE MONA SYMPOSIUM 2024
(TWENTY NINTH)

NATURAL PRODUCTS & MEDICINAL CHEMISTRY
Kingston, Jamaica
January 3 – 6, 2024

Department of Chemistry
THE UNIVERSITY OF THE WEST INDIES

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Trevor Herbert Yee

(December 29, 1944 – June 20, 2023)

Trevor Herbert Yee completed his High School education at the top of his class in 1962 at **St George's College in Kingston, Jamaica**. He was blessed with an unrelenting curiosity, keen powers of observation, an analytical mind, a retentive memory and a love of the Jamaican landscape. He studied the sciences and, recognised as an outstanding student, he was immediately recruited by his headmaster to tutor the first class preparing to sit the Cambridge 'O-Level' examinations in Biology at the then fledgling companion school, **Campion College**. All the students were successful.

Trevor then proceeded to the UWI in 1964 on a **Jamaica Government Bursary**, and gained in 1967 a BSc degree in Chemistry & Botany with First Class Honours. On an **Alcan Independence Postgraduate Scholarship** he completed, in 1971, a PhD degree in Organic Chemistry under the guidance of the distinguished Professor Wilfred Chan, the "Father of Natural Products Chemistry" in the Caribbean, and the first Organising Secretary of the *Mona Symposium*. A **Canadian (CIDA) Postdoctoral Fellowship** (1971-73) took him to the University of British Columbia to study, with Professor James Kutney, the natural products associated with lower plants. He developed in the process a continuing interest in the botanical and culinary aspects of mushrooms. He has contributed a chapter on *The Fungi* in the Natural History Society of Jamaica's ***Guide to the Blue and John Crow Mountains (2008)***.

While in Canada he pursued a **Certificate in Business Administration**, followed later (1988) by an **MBA**, with Honours, from Nova Southeastern in Florida, forging a route around Academia and into the family business between 1973 and 2001. In 1980 Trevor bought two of the companies involved, serving as Chairman and Managing Director for 20 years. This gave him an opportunity to travel extensively through the region, gaining a broad appreciation of the Caribbean, its business environment, natural environment, flora and its people. Concurrent with

this period, Trevor served the **Jamaica Bureau of Standards** as Chair of the Cosmetics Committee, winning the accolade of **Chairman of the Year** on several occasions. His interest in Academia continued during this "Commercial" phase and he generously supported the activities of the *Mona Symposium* – then named the *Natural Products Symposium*.

Trevor sold the businesses in 2000, and in 2001 returned to the Academic fold, joining the **Natural Products Institute** in the then Faculty of Pure & Applied Sciences at the UWI as Deputy Director, eventually becoming Director. He retired in 2015. During this spell, working with Professor Helen Jacobs, he gained the **first US Patent granted to the UWI**, for a new process to extract the bitter compound (quassin) from bitterwood – once an important export from Jamaica, and an essential ingredient in several internationally prominent beverages. He went on to gain patents in other areas – including processes for weaning butterflies and their destructive caterpillars off from their choice, citrus crop plants on to less valuable, related host plants; and for studies with Professors Paul Reese and Lisa Lindo, on the use of *Eucalyptus* extracts to control diabetes and hypertension, racking up, perhaps the largest number of patents for a local researcher. For the work on *Eucalyptus* extracts, the team involved was awarded by the **Scientific Research Council** in 2012 the **top prize for *Innovation in Science & Technology***. He supervised three PhD and three MPhil students and wrote over 24 research papers and book chapters.

Trevor was an active member of the **Natural History Society of Jamaica** and served as its president for two 2-year stints. People who met him, particularly on Natural History Society field trips, as well as colleagues and students, were inevitably, thoroughly impressed by his encyclopaedic knowledge of the local flora. His enthusiastic observations led to intriguing research questions and ultimately to novel solutions, but also enticed the editor of the magazine ***JamaicaEats*** to invite Trevor to write a column in the Journal from a scientific perspective. Trevor enthusiastically did this for the past four years, combining his scientific and culinary interests in our local flora and fauna. The **Institute of Jamaica** recognised Trevor's contributions to the Nation, with the award of a prestigious **Musgrave Medal** (bronze) for Science (Natural Products) in 2013.

Trevor was truly a National Treasure in his own right and his many contributions are sorely missed. May his soul rest in peace.

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Symposium website:
http://www.monasymposium.com

SPECIAL EVENTS

The 29th Mona Symposium will host a **Reception** and **Concert** on **Wednesday, January 3, 2024** at **7:00** pm at Science Lecture Theatre 3. Come and enjoy the musical stylings of the **UWI Panoridim** steel orchestra.

UWI Panoridim is the oldest steel band in the Jamaica and is a blend of mostly Jamaicans with other Caribbean islanders and a few international students. Their repertoire covers an array of genres, including classical, reggae, latin, pop, folk, dancehall, jazz, and of course soca.

Posters will be displayed in the Chemistry Lecture Theatres 6 and 7 on **Thursday, January 4, 2024** during the poster session at **3:15-5:30 pm**. Please set up your poster by 2:00 pm on Thursday in the assigned area. The posters should be left in place until the end of the meeting. There will be an open bar during this session.

The **Closing Ceremony** will be held on **Friday, January 5, 2024** in the Science Lecture Theatre 3 at **4:20 pm**. Cash prizes will be awarded for the most outstanding posters.

All roads lead to **Lyssons Beach** in St. Thomas for the **Conference Day Trip** on **Saturday, January 6, 2024**. Come and bring your swimwear and sunblock to take a dip in the beautiful Caribbean Sea, or just sit back and relax under a coconut tree. There will be plenty of tantalizing Jamaican cuisine to sample; enjoy some jerk chicken and much more. Please note that the bus will depart from the Department of Chemistry at **8:00 am**, so don't be late!

SCIENTIFIC PROGRAMME

SCIENCE LECTURE THEATRE 3

WEDNESDAY, JANUARY 3, 2024

Morning

8:30 – 9:30	Registration	
9:30 – 10:30	Opening Ceremony and Announcements	
	Opening Remarks:	Dr. Peter L. Ruddock (Chairperson) *University of Technology Jamaica*
	Welcome:	Prof. Sir Hilary Beckles *Vice Chancellor, UWI*
	Greetings:	Prof. Densil Williams *Pro-Vice Chancellor and Principal, UWI, Mona*
	Greetings:	Ms LaTrease Garrison *Chief Operating Officer, American Chemical Society*
	Greetings:	Mrs Joy Spence *Master Blender, Appleton Estate*
	Announcements:	Prof. Paul Reese *The Mona Symposium, Organizing Secretary*
10:30 – 10:45	Coffee Break	
Chairperson	Peter L. Ruddock	
10:45 – 11:25	**Plenary Lecture #1:** **Bill J Baker** Cold-water Chemistry	
11:25 – 11:35	Question and Discussion Period	
11:35 – 11:55	**Short Paper #1:** **Lesley-Ann Giddings** Molecular Indicators of Environmental Change in an Antarctic Polar Desert	
11:55 – 12:00	Question and Discussion Period	
12:00 – 2:00	Lunch Break	

Afternoon

Chairperson:	Andrea Goldson-Barnaby
2:00 – 2:40	**Plenary Lecture #2:** **Hayato Ishikawa** Collective Total Synthesis of Secologanin-Related Natural Products
2:45 – 2:55	Question and Discussion Period
2:55 – 3:15	**Short Paper #2:** **Kareem Abdur-Rashid** Catalytic Synthesis of Cannabinoids
3:15 – 3:20	Question and Discussion Period
3:20 – 3:35	Coffee Break
3:35 – 4:20	**Plenary Lecture #3:** **Patrick Harran** Molecular Amalgamations that Systematically Generate Complex Polycycles
4:20 – 4:30	Question and Discussion Period
4:30 – 4:50	**Short Paper #3:** **James M. Cook** General Strategy to Access Both Natural and Unnatural Enantiomers of C-19 Methyl Containing Sarpagine/Macroline Indole Alkaloids
4:50 – 4:55	Question and Discussion Period
4:55 –5:15	**Short Paper #4:** **M. Jack Mphahlele** Synthesis, Spectroscopic, *In Vitro* and *In Silico* Biological Studies of Sulfonamide Appended Small Drug-Like Molecules Against Chronic Inflammation-Mediated Diseases
5:15 – 5:20	Question and Discussion Period
7:00 – 9:00	**Reception**

THURSDAY, JANUARY 4, 2024

Morning	**Dedicated to the memory of Dr Trevor Yee**
Chairperson:	Rupika Delgoda
9:00 – 9:10	Charah Watson-Francis Reflections on Trevor Yee
9:10 – 9:50	**Plenary Lecture #4:** **Dean J. Tantillo** Walking in the Woods with Quantum Chemistry – Unusual Structures And Reactivity in Terpene Biosynthesis
9:50 – 10:00	Question and Discussion Period
10:00 – 10:20	**Short Paper #5:** **William Irvine** Making Magic Mushrooms More Magical: Molecular Modelling
10:20 – 10:25	Question and Discussion Period
10:25 – 10:40	Coffee Break
10:40 – 11:20	**Plenary Lecture #5:** **Stuart J. Conway** The Development of Chemical Tools to Target and Image Hypoxia
11:20 – 11:30	Question and Discussion Period
11:30 – 11:50	**Short Paper #6:** **Shaunté Cotterell** An Investigation of the Catalytic Activity of Benzothiazol-2-quinoline in Organic Reactions
11:50 – 11:55	Question and Discussion Period
11:55 – 12:05	**Conference Photograph**
12:05 – 2:00	Lunch Break

Afternoon

Chairperson:	Andrew Lamm
2:00 – 2:40	**Plenary Lecture #6:** **Maged Henary** Research Progress on the Synthesis and Biomedical Application of NIR Modified Cyanine Dyes
2:40 – 2:50	Question and Discussion Period
2:50 – 3:10	**Short Paper #7:** **Marcel Denny** The Synthesis and Metal-Sensing Application of 2-Substituted *o*-Naphthoquinone[2,1-*D*] Oxazoles
3:10 – 3:15	Question and Discussion Period
3:15 – 6:00	**Poster Session**

FRIDAY, JANUARY 5, 2024

Morning

Chairperson:	Alexa Redway
9:00 – 9:40	**Plenary Lecture #7:** **Sean Brady** Natural Antibiotics without Natural Processes
9:40 – 9:50	Question and Discussion Period
9:50 – 10:10	**Short Paper #8:** **Andrew Lamm** Complete Genome Sequence of *Nocardia iowensis* DSM 45197^T (= NRRL 5646^T) and its Potential Usefulness
10:10 – 10:15	Question and Discussion Period
10:15 – 10:30	Coffee Break
10:30 – 10:50	**Short Paper #9:** **Ricaldo Pryce** Chemistry and Biology of Novel Rearranged Stemodane Diterpenoids and their Biotransformation by *Exophiala lecanii-corni*
10:50 – 10:55	Question and Discussion Period
10:55 – 11:15	**Short Paper #10:** **Sandra Latchman** Preparation of Stemodane Derivatives and their Biological Activity against the PC-3 Cancer Cell Line
11:15 – 11:20	Question and Discussion Period
11:20 – 11:40	**Short Paper #11:** **Kamaluddin Abdur-Rashid** Asymmetric Catalytic Synthesis of Pharmaceuticals and Cannabinoids
11:40 – 11:45	Question and Discussion Period
11:45 – 2:00	Lunch Break

Afternoon

Chairperson:

2:00 – 2:40	**Plenary Lecture #8:** **Masaki Kita** Modulators of Protein-Protein Interactions from Marine Origin: Target Identification and Mode of Action Studies on Aplyronine A and Stylissatin A
2:40 – 2:50	Question and Discussion Period
2:50 – 3:05	Coffee Break
3:05 – 3:25	**Short Paper #12:** **Sherry-Ann Wint-Turner** Spectroscopic, Redox and Beta-Lactamase Inhibition Properties of Some Hydrazonic Isatin and Hydroxyacetophenone Derivatives: an Experimental, DFT and Molecular Docking Study
3:25 – 3:30	Question and Discussion Period
3:30 – 3:50	**Short Paper #13:** **Joanna Klimek** C2-Symmetrical Terphenyl Derivatives as Small-Molecular Inhibitors of Programmed Cell Death-1/Programmed Death Ligand 1 Protein-Protein Interaction
3:50 – 3:55	Question and Discussion Period
3:55 – 4:15	**Short Paper #14:** **Wiktor Uzar** Synthesis and Biological Activity Evaluation of C2-Symmetric, Small Molecule Inhibitors of PD-L1
4:15 – 4:20	Question and Discussion Period
4:20 – 4:30	Closing Ceremony
7:30	**Conference Dinner**

SATURDAY, JANUARY 6, 2024

8:00	**Day Trip**

ABSTRACTS OF PLENARY LECTURES
AND
SHORT PAPERS

Plenary Lecture #1

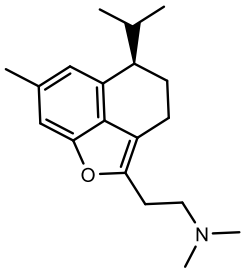
COLD-WATER CHEMISTRY

Bill J. Baker and Many Collaborators

Department of Chemistry, University of South Florida, Tampa, FL 33620

Shallow-water communities of temperate and tropical marine environments harbor significant biodiversity, including metabolite-rich sponges, tunicates and corals. These organisms have been explored for decades as sources of natural product derived or inspired bioactive metabolites to drive drug discovery programs. Less attention has been focused on cold-water habitats that include polar marine environments and the deep-sea. To be sure, the cold-water regions are often difficult to access, but the limited data available suggests biodiversity there is similarly rich in biologically active metabolites. Three examples from our work will be discussed that demonstrate the versatility of cold-water invertebrates as sources of bioactive lead compounds.

Our most recent work has found a deep-sea coral from the Irish continental shelf with activity in a zebrafish model of epilepsy, leading to the isolation of a family of aminated terpenes represented by SHO-05 (**1**).[1] The deep-sea of Antarctica has also been a prolific source of new chemotypes, including the friomaramides (e.g., **2**), with activity against malaria.[2, 3] Finally, our ongoing progress to advance the palmerolides as anticancer agents will be presented.[4]



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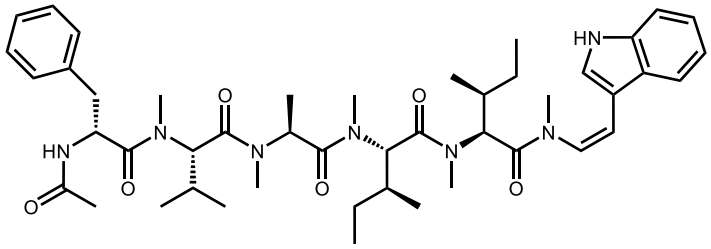

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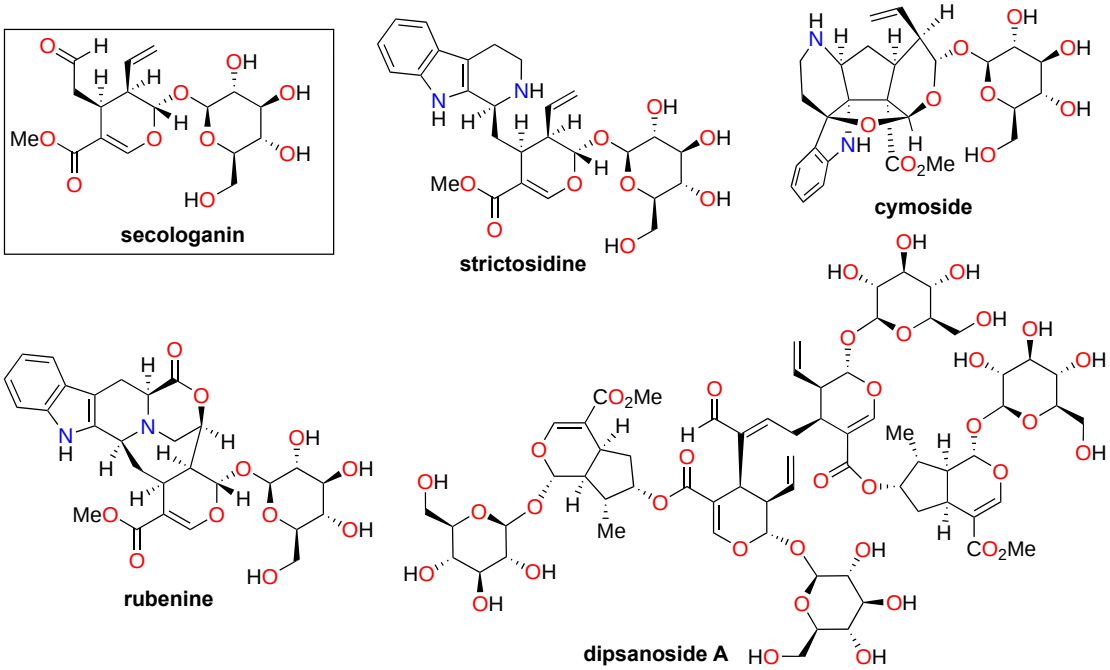
Plenary Lecture #2

COLLECTIVE TOTAL SYNTHESIS OF SECOLOGANIN-RELATED NATURAL PRODUCTS

Hayato Ishikawa

Graduate School of Pharmaceutical Sciences, Chiba University, Chiba 260-8675, Japan

We successfully achieved a collective total synthesis of 39 natural products, including glycosylated monoterpenoid indole alkaloids (MTIAs) and hetero-oligomeric iridoid glycosides (HOIGs) via bioinspired transformations, initiated by the first total synthesis of secologanin.[1] The key strategy of our secologanin synthesis was a rapid and stereoselective construction of the secologanin scaffold through an *anti*-selective organocatalytic Michael reaction/Fukuyama reduction/spontaneous cyclization/Schmidt glycosylation sequence, and we obtained a key intermediate, secologanin tetraacetate, on a decagram scale in seven steps.[2] First, Pictet-Spengler cyclization with L-tryptophan methyl ester or (*R*)-α-cyanotryptamine using secologanin tetraacetate proceeded via different transition states but in the same 3*S* stereoselectivity to give 5-carboxystrictosidine and strictosidine, respectively.[3] These biosynthetic intermediates of MTIAs were converted into complex alkaloids, including rubenine and cymoside, via bioinspired transformation on the highly reactive secologanin reaction sites.[2,3] On the other hand, loganin, the biosynthetic precursor of secologanin, was synthesized from secologanin tetraacetate via a reverse-biogenetically inspired reductive cyclization. These iridoid monomers were condensed via hetero-oligomerization to HOIGs including dipsanoside A.[4]



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Plenary Lecture #3

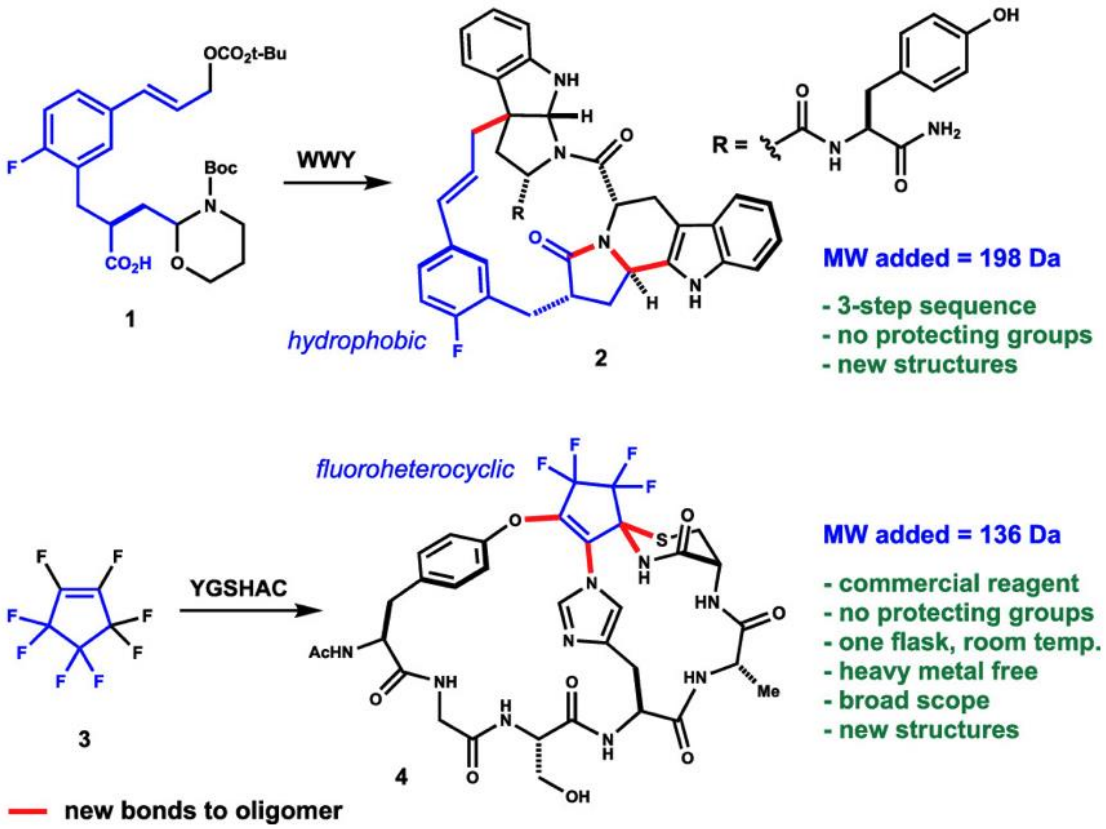
MOLECULAR AMALGAMATIONS THAT SYSTEMATICALLY GENERATE COMPLEX POLYCYCLES

Patrick Harran

Department of Chemistry, University of California, Los Angeles
Los Angeles, CA 90095, USA

Email: harran@chem.ucla.edu

We are developing scaffolding reagents that can be integrated into peptide structure to afford diverse ring systems having embedded heterocyclic motifs. Our experiments run processively, wherein template molecules are reacted incrementally with unprotected oligomers to form composite products. These compounds retain molecular recognition elements in the oligomer, yet display that functionality as part of stable polycyclic structures having improved pharmacological properties. The methodology allows systematic alteration of product topology by engaging a range of native peptide functional groups in carbon–heteroatom and carbon–carbon bond-forming reactions. Our latest discoveries will be discussed in this lecture.



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2) *Proc. Natl. Acad. Sci. USA* (**2020**) 117, 24679-24690

Plenary Lecture #4

WALKING IN THE WOODS WITH QUANTUM CHEMISTRY – UNUSUAL STRUCTURES AND REACTIVITY IN TERPENE BIOSYNTHESIS

Dean J. Tantillo

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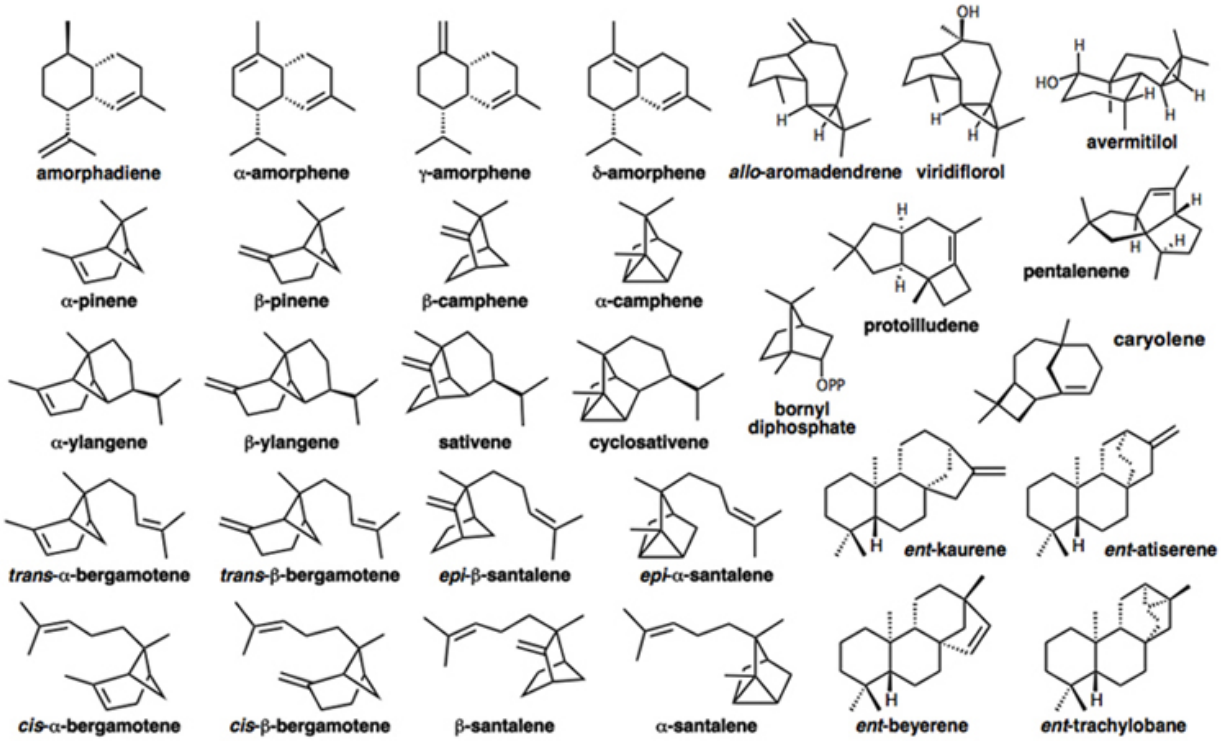
1 Shields Ave, Davis, CA 95616, USA

Applications of quantum chemistry to deciphering structures of terpene natural products and the mechanisms for their formation will be discussed,[1-4] with a focus on reactions that do not conform to the tenets of classic transition state theory.[5,6]



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5. Tantillo, D. J. *Adv. Phys. Org. Chem.* **2021**, *55*, 1-16: "Beyond Transition State Theory – Non-statistical Dynamic Effects for Organic Reactions"
6. Tantillo, D. J. *J. Phys. Org. Chem.* **2021**, *34*, e4202: "Dynamic Effects on Organic Reactivity – Pathways to (and from) Discomfort"

Plenary Lecture #5

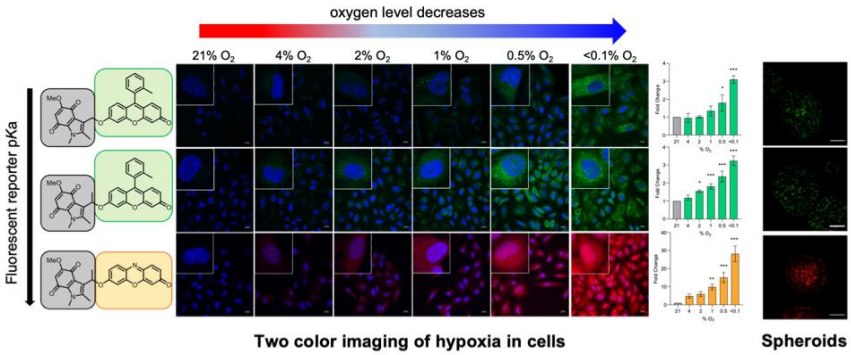
THE DEVELOPMENT OF CHEMICAL TOOLS TO TARGET AND IMAGE HYPOXIA

Stuart J. Conway

Department of Chemistry & Biochemistry, University of California, Los Angeles
Los Angeles, CA 90095, USA

Tumor hypoxia (low oxygen levels) is associated with resistance to all therapeutic approaches to treat cancers, and consequently poor patient prognosis. Hypoxia-activated prodrugs (HAPs), designed to selectively release a bioactive compound in oxygen-deficient cells, while sparing healthy tissue, represent a promising therapeutic strategy for treatment of cancers.[1,2] I will discuss our recent work to develop HAPs applied to a lysine deacetylase (KDAC) inhibitor and PROTACs. We have developed NI-Pano (CH-03), a novel hypoxia-activated version of the clinically approved KDAC inhibitor, panobinostat. We demonstrated the pre-clinical efficacy of NI-Pano, showing that it is stable in normoxic (21% oxygen) conditions but undergoes NADPH-CYP-mediated enzymatic bioreduction to release panobinostat selectively in hypoxia (<0.1% oxygen). Treatment of cells grown in both 2D and 3D culture with NI-Pano induced apoptosis, and decreased clonogenic survival. Importantly, NI-Pano exhibited growth delay effects as a single agent in mouse tumor xenografts. Pharmacokinetic analysis confirmed the presence of effective concentrations of panobinostat in hypoxic mouse xenografts, but not in circulating plasma, or kidneys.[3] Having demonstrated the potential of HAPs against KDACs, we sought to apply this technology to proteolysis targeting chimeras (PROTACs). PROTACs are bifunctional molecules that recruit and E3 ligase, leading to ubiquitination of a protein of interest (POI) and subsequent proteasomal degradation. By adding a bioreductive group to the E3 ligase ligand of VHL- or cereblon-recruiting PROTACs we have developed hypoxia-activated PROTACs (HAP-TACs), which selectively degrade the POI in hypoxia, but not normoxia.

To enable studies of the cellular redox environment, and to support work using HAPs, it is essential to have accurate and effective imaging agents for the complex tumour microenvironment. To this end, we have recently developed a suite of hypoxia-activated fluorophores, based on the indole quinone redox trigger, that image a range of oxygen concentrations in different colours, visualising gradients of hypoxia for the first time.[4] The development of these tools, which enable imaging of the tumour microenvironment with unprecedented detail, will be described.



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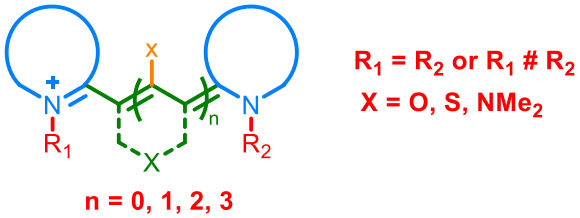
Plenary Lecture #6

RESEARCH PROGRESS IN THE SYNTHESIS AND BIOMEDICAL APPLICATION OF NIR MODIFIED CYANINE DYES

Henary, M.,[1] Buabeng, E. R.,[1] Owens, E.,[1] Narayana, L.,[1] Hyun, H.,[2] Kang, H.,[2] Choi, H.[2]

[1]Department of Chemistry, Center for Diagnostics and Therapeutics, Petit Science Center, Georgia State University, 100 Piedmont Avenue SE, Atlanta, GA 30303, USA.
[2]Gordon Center for Medical Imaging, Department of Radiology, Massachusetts General Hospital and Harvard Medical School, Boston, MA 02114, USA.

The development of near-infrared (NIR-I and II) fluorescence imaging[1-9] has implemented real-time detection of biological cells, tissues[1,3,7] and monitoring the disease processes[2] and even enabling the direct conduct of surgical procedures.[5] NIR-I and II fluorescence imaging provide better imaging contrast and penetration depth, benefiting from the reducing photon scattering, light absorption and autofluorescence.[3-4] Among small molecule NIR fluorescent probes, cyanine dyes[1-9] have been widely used in imaging and biosensing fields due to their good optical properties.[9] Functionalization of the polymethine chain, which can significantly improve the stability of dyes and alter their photophysical properties and biological selectivity, has become a hotspot for structural modification of cyanine dyes in recent years.[1-9] The synthetic methods of NIR modified cyanine dyes are summarized and the progress of the modified cyanine dyes[1-9] and their application in medicine[1-9] is discussed.



General Structure of Cyanine Dyes

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Plenary Lecture #7

NATURAL ANTIBIOTICS WITHOUT NATURAL PROCESSES

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The characterization of small molecules produced by bacteria in laboratory culture has been a key step to developing diverse small molecule therapeutics. As successful as this approach has been for identifying novel bioactive small molecules, extensive sequencing of bacterial genomes and metagenomes has revealed that the bacterial biosynthetic diversity currently accessed in the laboratory represents only a small fraction of what is predicted to exist in nature. This shortcoming arises from both our inability to culture most bacteria in the laboratory and from the fact that most biosynthetic gene clusters remain silent under laboratory fermentation conditions.

We have developed a new bioactive small molecule discovery pipeline that avoids the requirement for either bacterial culture or gene cluster expression. In this purely in vitro approach, which we have termed synthetic-Bioinformatic Natural Products (synBNPs), the structures of natural products encoded by biosynthetic gene clusters are predicted bioinformatically, and the resulting predictions are then chemically synthesized to generate libraries of bioactive small molecules that are inspired by nature. Contrary to other synthetic approaches, all of the structures we produce are inspired by natural selection and, consequently, are expected to exhibit bioactivities at a high rate. In this presentation I will discuss a number of antibiotics we have identified using a synBNP approach.

Plenary Lecture #8

MODULATORS OF PROTEIN–PROTEIN INTERACTIONS FROM MARINE ORIGIN: TARGET IDENTIFICATION AND MODE OF ACTION STUDIES ON APLYRONINE A AND STYLISSATIN A

Masaki Kita,[1] Didik Huswo Utomo,[1] Yiting Sun,[1] Menghua Zhang,[1] and Hideo Kigoshi[2]
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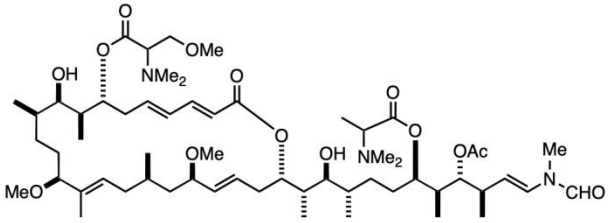
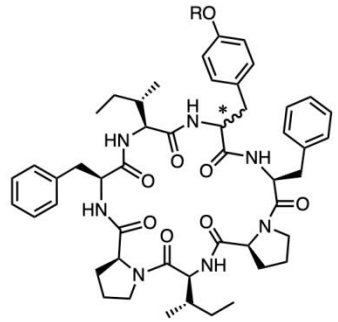
[2] Institute of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan

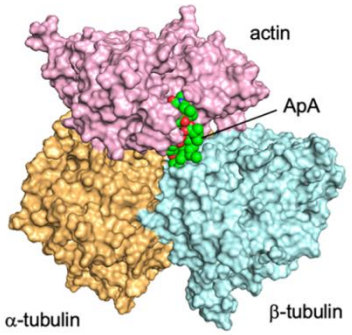
Various marine natural products that target specific biomacromolecules have been discovered, and a few of them have been shown to modulate protein–protein interactions (PPIs).[1] An antitumor macrolide aplyronine A (**1**) from the sea hare *Aplysia kurodai* synergistically binds to tubulin in association with actin, and prevents spindle formation and mitosis in tumour cells.[2] To investigate how **1** stabilizes the PPIs between tubulin a/b-heterodimer and actin to disturb microtubule (MT) dynamics, blind protein–protein docking and molecular dynamics simulations were performed. Two plausible actin–**1**–tubulin HTC models were obtained, and their internal and capping models to potently destabilize MT structure were newly proposed.[3] Stylissatin A (SA, **2**) is a proline-rich cyclic heptapeptide from the marine sponge *Stylissa massa*. A synthetic analog D-Tyr[1]-*t*BuSA (**3**) potently inhibits the nitric oxide production in LPS-stimulated murine RAW264.7 macrophages, the differentiation of murine 3T3-L1 preadipocytes, and their fat accumulation with little cytotoxicity.[4] Using a biotin probe of **2**, acyl-CoA dehydrogenase long chain (ACADL) was initially identified as a target protein. However, SA derivatives localized in another organelle rather than the mitochondria containing ACADL, and they possessed a hitherto unknown PPI inhibitory effect. Our research might contribute to the development of leads for new anti-inflammatory and anti-obesity agents with new mechanism of actions.



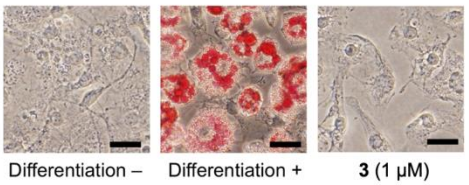
Aplyronine A (ApA, 1)



Stylissatin A (SA, 2) : L-Tyr[1], R = H
3 : D-Tyr[1], R = *t*-Bu



Proposed HTC model



Inhibition of adipocyte differentiation

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Short Paper #1

MOLECULAR INDICATORS OF ENVIRONMENTAL CHANGE IN AN ANTARCTIC POLAR DESERT

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Antarctic soils support active, low diversity microbial communities that produce secondary metabolites, which influence community structure and microbial adaptation to changing climates (e.g., solar radiation and salinity)[1]. Warming events in the McMurdo Dry Valleys, East Antarctica can result in pulses of meltwater from permafrost or snow, generating patches of meltwater seeps in these dry desert soils with distinct biogeochemical conditions compared to the surrounding soil[1]. Here, we characterize the secondary metabolites and their biosynthetic genes associated within and outside a soil seep in the Fryxell Basin (Figure 1). To determine the microbial secondary metabolite response to varying salinity, pH, and limited moisture, soil profiles were collected, and DNA was extracted for 16S rRNA gene amplicon and shotgun metagenome sequencing. Both moist and dry soils contained similar bacterial community compositions. High-quality metagenome assembled genomes (MAGs; 56) were recovered from wet and dry soils, including Actinobacteria (>60% of MAGS). Terpenes, polyketides, and ribosomally synthesized and post-translationally modified peptide biosynthetic gene clusters were predominantly found in MAGs. However, no significant difference was observed in the secondary metabolite biosynthetic gene clusters (BGCs) associated with microbes from either wet or dry soils. Liquid chromatography/mass spectrometry and probe-based techniques detected secondary metabolites, such as tetracyclines, ectoines, and desferrioxamines, in soils and their representative bacteria. Notably, a differential abundance of metabolite features was observed in bacteria cultivated at environmentally-relevant pH extremes (8–11). Thus, while the bacterial composition and BGCs are similar in wet and dry soils, the differential production of secondary metabolites suggests that these molecules are associated with the bacterial community response to changing environmental conditions. We suggest that the differential expression of secondary metabolites may influence microbial adaptation to the McMurdo Dry Valleys soils.

Figure 1. Lake Fryxell in the McMurdo Dry Valleys, Antarctica (orange circle on inset map).

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Short Paper #2

CATALYTIC SYNTHESIS OF CANNABINOIDS

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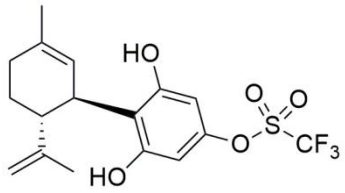
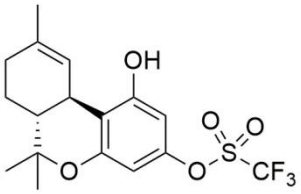
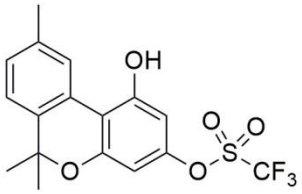
Cannabinoid precursor compounds were prepared and used for the catalytic synthesis of several classes of cannabinoids under mild conditions. The precursors include 3,5-dihydroxy-4-((1*R*,6*R*)-3-methyl-6-(prop-1-en-2-yl)cyclohex-2-enyl)phenyl trifluoromethanesulfonate ((*R*,*R*)-CBD-OTf), (6a*R*,10a*R*)-1-hydroxy-6,6,9-trimethyl-6a,7,8,10a-tetrahydro-6*H*-benzo-[c]chromen-3-yl trifluoromethanesulfonate ((*R*,*R*)-THC-OTf) and 1-hydroxy-6,6,9-trimethyl-6*H*-benzo[c]chromen-3-yl trifluoromethanesulfonate (CBN-OTf). These were used to prepare CBD (and CBD analogues), THC (and THC analogues), and CBN (and CBN analogues). The preparation, characterization and purification of the precursors and cannabinoid products will be presented. The preparation of related cannabinoid precursors, such as (*S*,*S*)-CBD-OTf, (*R*,*S*)-CBD-OTf, (*S*,*R*)-CBD-OTf, (*S*,*S*)-THC-OTf, (*R*,*S*)-THC-OTf and (*S*,*R*)-THC-OTf will also be presented, along with their use for the preparation of (*S*,*S*)-CBD, (*R*,*S*)-CBD, (*S*,*R*)-CBD, (*S*,*S*)-THC, (*R*,*S*)-THC and (*S*,*R*)-THC and related cannabinoid analogues.



(R,R)-CBD-OTf



(R,R)-THC-OTf



CBN-OTf

Short Paper #3

GENERAL STRATEGY TO ACCESS BOTH NATURAL AND UNNATURAL ENANTIOMERS OF C-19 METHYL CONTAINING SARPAGINE/MACROLINE INDOLE ALKALOIDS

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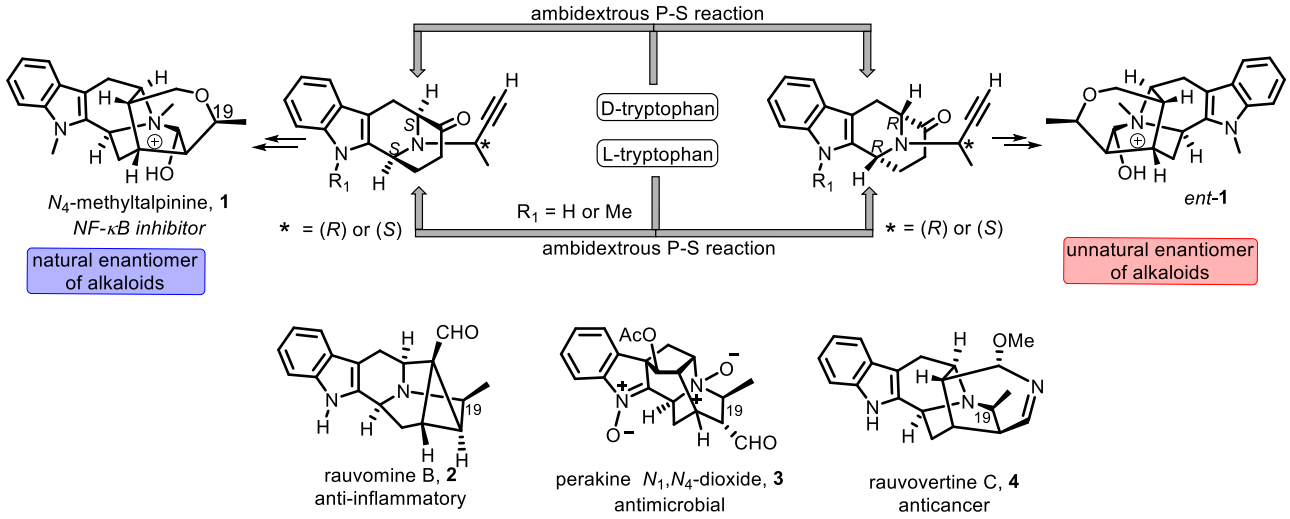
The C-19 methyl substituted indole alkaloids belong to a small sub-class of sarpagine/macroline/ajmaline alkaloids containing >70 alkaloids. A few alkaloids from this group (e.g., **1**-**4**) have been reported to possess important bioactivity ranging from anti-inflammatory to anticancer activity, while the activity of the majority of the alkaloids remain unexplored. We envisioned that a systematic and comprehensive screening of these alkaloids, including their unnatural enantiomers (e.g., *ent*-**1**), would uncover much useful biological data, as well as provide insights for the rational design for a diversified SAR study. An effective method for accessing the alkaloids is a prerequisite for that purpose. Our endeavour in this vein has resulted in an ambidextrous and practical approach, which allows access to the natural and unnatural enantiomers of these alkaloids from either D- or L-tryptophan, at will. The general approach and completion of the total synthesis of a few alkaloids from this group including the potent NFκB inhibitor N4-methyltalpinine will be presented.



Short Paper #4

SYNTHESIS, SPECTROSCOPIC, *IN VITRO* AND *IN SILICO* BIOLOGICAL STUDIES OF SULFONAMIDE APPENDED SMALL DRUG-LIKE MOLECULES AGAINST CHRONIC INFLAMMATION-MEDIATED DISEASES

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The prevalence of the secondary sulfonamido group (-$NHSO_2R$) in drugs of pharmacological importance, including anti-inflammatory agents, makes it an important template in the context of drug design and development. This moiety is capable of establishing strong electrostatic (π-cation, attractive charge interaction) and hydrogen bonding interactions with a wide range of functional groups of biological receptors more so than the carboxylic acid, amide and ester surrogates. These drug-like features afford the sulfonamide-appended compounds their ability to inhibit a wide range of enzymes, including carbonic anhydrases, HIV protease, cyclooxygenase, acetylcholinesterase and butyrylcholinesterase. Our group's interest in sulfonamide derivatives is not limited to drug development [1]. Their conformations and crystalline structures also continue to attract attention to explore intramolecular and intermolecular non-covalent interactions, control molecular conformations and improve the physicochemical properties (durability, solubility and bioavailability) of the drug molecules. We study these properties using a combination of spectroscopic and single crystal X-ray diffraction techniques complemented with density functional theory (DFT) methods [2,3].

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Short Paper #5

MAKING MAGIC MUSHROOMS MORE MAGICAL: MOLECULAR MODELLING

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Nearly all mushrooms of the *Psilocybe* genus contain the natural product psilocybin, which is a psychoactive alkaloid derived from L-tryptophan. Considering their use in ancient times, as well as their psychedelic properties, these 'magic mushrooms' have re-emerged with psychotherapeutic potential for treating an array of neurological disorders, which has triggered increased pharmaceutical interest.[1,2] However, the psilocybin biosynthesis pathway was only recently defined and, as such, little exists in the way of structural data. Accordingly, this pathway was structurally characterised by generating homology models for the four *Psilocybe cubensis* enzymes involved in psilocybin biosynthesis (PsiD, a decarboxylase; PsiH, a monooxygenase; PsiK, a phosphotransferase; PsiM, a methyltransferase).[3] Following initial model generation and alignment with the identified structural templates, repeated refinement of the models was carried out using secondary structure prediction, geometry evaluation, energy minimization, and molecular dynamics simulations in water. The final models were then evaluated using molecular docking interactions with their substrates, i.e., psilocybin precursors (L-tryptophan, tryptamine, 4-hydroxytryptamine, and norbaeocystin/baeocystin), all of which generated feasible binding modes for the expected biotransformation. Further plausibility of the psilocybin → aeruginascin, 4-hydroxytryptamine → norpsilocin, and tryptamine → *N*,*N*-dimethyltryptamine conversions, all mediated by the generated model for PsiM, suggests valid routes of formation for these key secondary metabolites. The structural characterization of these enzymes and their binding modes can lead to a better understanding of psylocibin synthesis, thereby paving the way for the development of novel substrates and selective inhibitors, as well as improved biotechnological manipulation and production of psilocybin in vitro.

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Short Paper #6

AN INVESTIGATION OF THE CATALYTIC ACTIVITY OF BENZOTHIAZOL-2-QUINOLINE IN ORGANIC REACTIONS

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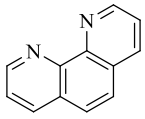
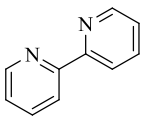
Copper is an economic and environmentally abundant transition metal that can exist in a range of oxidation states and chemical morphologies. The ready accessibility, benign nature and diverse applications of copper ion based catalytic systems make further developments of these systems of continued importance to the synthetic community.[1] The ligands that promote copper-catalysed reactions are predominantly electron rich, *N*,*N*-donor ligands, with 1,10-phenanthroline (**L1**) and 2,2'-bipyridine (**L2**) being the most common.[2,3] Benzothiazol-2-quinoline (**L3**) has also been reported to bind favourably to copper ions via its nitrogen atoms.[4] However, the literature on these complexes has primarily focused on their photophysical properties rather than their use in catalysis. In comparison to other nitrogen heterocycles, the use of benzothiazoles as ligands in transition metal catalysts is far less explored. In these reports the catalytic complexes contained group 13 and platinum group metal centres and were applied to polymerization and C-C coupling reactions.[5-7]

We hereby present a preliminary survey that explores the use of benzothiazol-2-quinoline (**L3**) as a ligand in the copper-catalysed formation of C-N, C-O and C-S bonds, and compares the reaction efficiency to that of 1,10-phenanthroline (**L1**) and 2,2'-bipyridine (**L2**). Yields for C-O and C-S bond formation reactions via oxidative cyclization, were superior for **L3**, but ligand **L3** was less efficient in *N*-arylation reactions, underperforming both ligands.



L1



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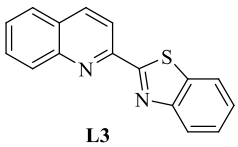

L3

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Short Paper #7

THE SYNTHESIS AND METAL SENSING APPLICATION OF 2-SUBSTITUTED *O*-NAPHTHOQUINONE[2,1-*D*] OXAZOLES

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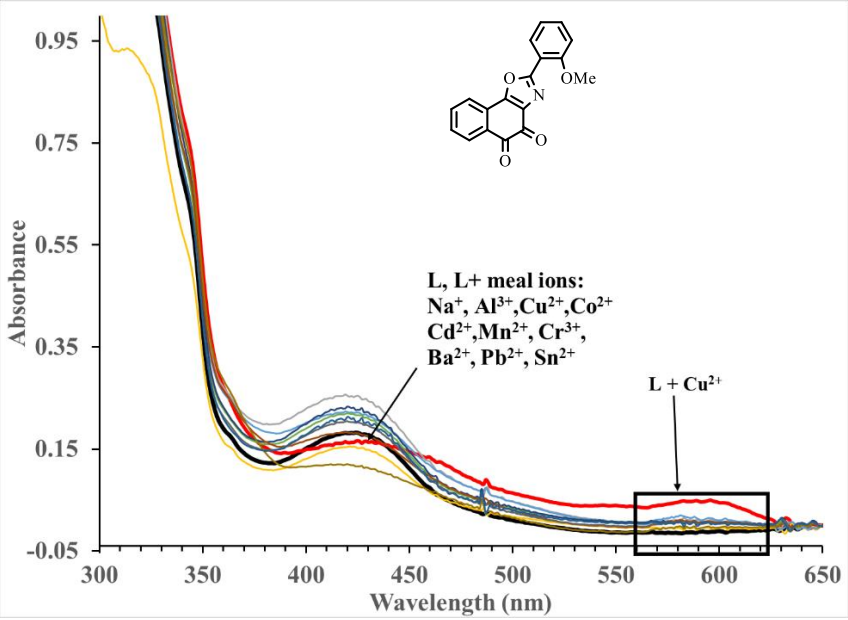
Metals play a pivotal role in our environment and biological processes.[1] However, their presence in high amounts can lead to deleterious effects on both the environment and humans.[1] Naphthoquinones, for example lawsone, have been known to function as chemosensors because they can detect metals ions, such as copper(II), cobalt(II), and mercury(II) among others.[2-4] Consequently, developing chemosensors as a quick and simple way to detect metals ions using these substrates would provide an innovative application of these systems. Hence, we aimed to develop a new, operationally simple protocol for synthesizing some novel naphthoquinone oxazoles with structural similarities to known chemosensing compounds.[3] The 2-substituted *o*-naphthoquinone oxazoles (**1**) were prepared in poor to moderate yield from a modified two step protocol seen within the literature.[5] and then investigated for their chemosensing abilities towards various metals ions. Our substrates showed a colourimetric response for Na^+ and Cu^{2+} ions, preferentially to Co^{2+}, Al^{3+}, Cd^{2+}, Sn^{2+}, Mn^{2+}, Cr^{3+}, Ba^{2+} and Pb^{2+}.



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Short Paper #8

COMPLETE GENOME SEQUENCE OF *NOCARDIA IOWENSIS* DSM 45197^{T} (= NRRL 5646^{T}) AND ITS POTENTIAL USEFULNESS.

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[1]Leibniz Institute DSMZ-German Collection of Microorganisms and Cell Cultures, Braunschweig, Germany.

[3]German Centre of Infection Research, Partner Site Hannover-Braunschweig, Braunschweig, Germany.

We report the complete genome sequence and predicted functional profile of *Nocardia iowensis DSM 45197^{T}*. This spore-forming, mesophilic, Gram-positive, actinomycete bacterium was isolated from garden soil in Osceola, Iowa, USA. *N. iowensis* has been exploited for its production of glycocinnamolyspermidine antibiotics and biotransformation of xenobiotic substances. Other significant features of *N. iowensis* include the first fully characterized carboxylic acid reductase (CAR) and the first bacterial nitric oxide synthase (NOS) system. The genome sequence of *N. iowensis* can facilitate further understanding of its function, as well as the pathogenesis of *Nocardia* spp. *N. iowensis* has a genome size of 8.95 Mbp; about 46% of the coding sequences have no known homologues and were labelled hypothetical proteins. The organism also possesses several antibiotic resistance and virulence genes; is phylogenetically close to significant pathogens; and has a 62% probability of being a human pathogen. This and other findings implies further potential for biomedical and biotechnological research applications.

Short Paper #9

CHEMISTRY AND BIOLOGY OF NOVEL REARRANGED STEMODANE DITERPENOIDS AND THEIR BIOTRANSFORMATION BY *EXOPHIALA LECANII-CORNI*

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[3]Department of Horticulture, Michigan State University, East Lansing, MI 48824, USA

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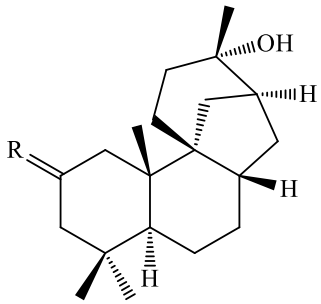
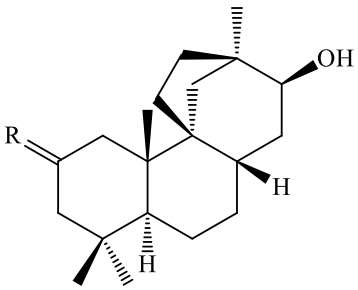
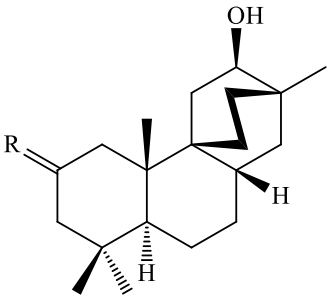
Stemodin (**1**) is a biologically active natural product from *Stemodia maritima*. The compound possesses cytotoxic and antiviral properties and can be obtained in relatively large quantities from the plant.[1] Stemodinone (**2**), also isolated from *S. maritima* (albeit in lower quantities), can be generated by simple oxidation of **1**. In the presence of aqueous acid **2** undergoes solvolytic rearrangement to form 15(13→12)*abeo*-13β-hydroxystemaran-2-one (**3**) and 15(8→9)*abeo*-8β(H)-12β-hydroxystachan-2-one (**4**).[2] The skeleton of **3** is similar to that of the scopadulanes, which inhibit the porcine H^+, K^+-ATPase enzyme, and possess antitumour and antiviral activities against the *Herpes simplex* virus type 1. These natural products also interfere with the nutrient transport of the malarial parasite *Plasmodium falciparum*.[3] The biological activity of compounds bearing the skeleton of **4** have not been explored. Diterpene **2** is readily chemically converted to analogues **5** and **6**. The solvolyses of **1**, **5** and **6** were carried out in order to generate similar products of rearrangement. The biological properties of these novel analogues were assessed and found to possess antioxidant, analgesic as well as cytotoxic properties when assessed against prostate cancer cells *in-vitro.* The analogues also served as substrates for transformation by the fungus *Exophiala lecanii-corni*. The aim is the production of a series of novel compounds for bioassay. *E. lecanii-corni* has previously been exploited as a catalyst for steroid biotransformation. However, its potential for microbial functionalization of terpenes is yet to be investigated. Preliminary studies have shown that the enzymes within the fungus are able to carry out redox as well as hydroxylation reactions at remote carbon centres within these novel terpenes.



1 R= αOH, βH
2 R= O
5 R= βOH, αH
6 R= H_2



7 R= αOH, βH
3 R= O
9 R= βOH, αH
11 R= H_2



8 R= αOH, βH
4 R= O
10 R= βOH, αH
12 R= H_2

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Short Paper #10

PREPARATION OF STEMODIN DERIVATIVES AND THEIR BIOLOGICAL ACTIVITY AGAINST THE PC-3 CANCER CELL LINE

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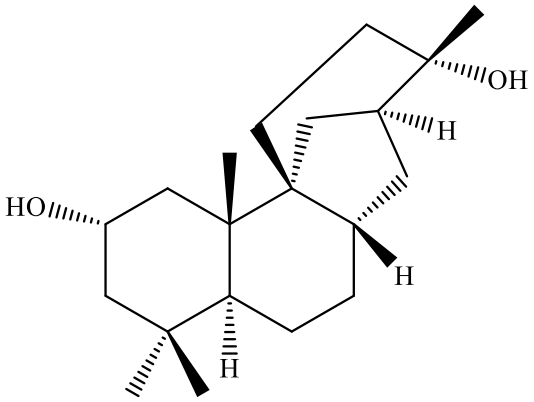
Stemodia maritima is a perennial herb which grows 1 to 2 metres in height. It is found in saline and brackish areas in Jamaica, Bahamas, South America, the Greater Antilles, Curaçao and Grand Cayman.[1] In the Caribbean it is used to treat dropsy, stomach ache, body pain, swellings and venereal diseases.[2] Stemodin (1), the most abundant natural product isolated from this plant, has a unique tetracyclic stemodane core.[3] The diterpene has attracted significant interest because of its structural similarity to aphidicolin, which possesses antiviral and antitumour activity.[4] Both compounds possess a *trans*-fused A/B ring system. However, the B/C rings of stemodin are *cis*-fused, whereas, in aphidicolin are *trans*. Stemodin also exhibits antiviral and antitumour activity which makes it a suitable starting material for chemical manipulation.[2,5] Derivatives of stemodin were prepared by redox reactions and these were tested against the PC-3 cancer cell line. Results will be reported.



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Short Paper #11

ASYMMETRIC CATALYTIC SYNTHESIS OF PHARMACEUTICALS AND CANNABINOIDS

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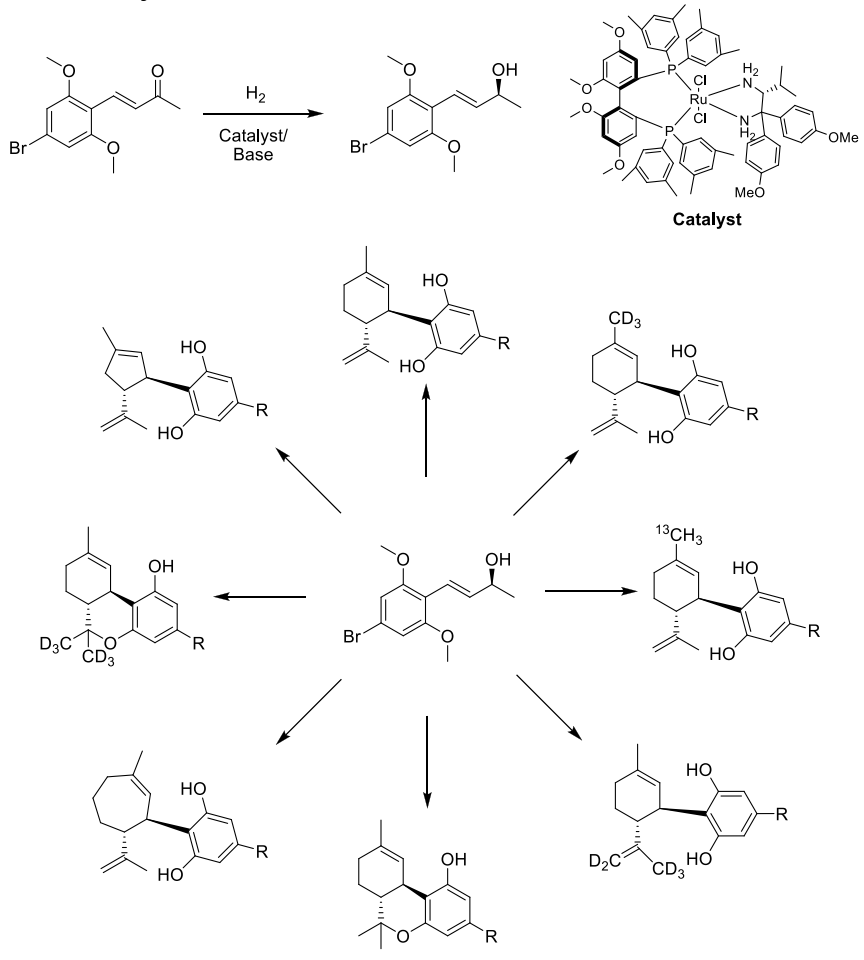
Homogeneous catalytic hydrogenation is a versatile method that can be exploited for the asymmetric synthesis of chiral alcohols and amines, which can be used for the preparation of pharmaceuticals, agrochemicals, flavours, fragrances and materials. In general, the incorporation of catalysis in manufacturing processes reduces wastes, increases profitability, and offsets and deters generic competition. Our laboratory specializes in homogeneous catalysis, and over the past two decades we have worked on behalf of and in partnership with several companies for the development of products using catalysis. Examples of pharmaceutical products that were developed for both branded and generic pharmaceutical companies will be presented.

The global interest in cannabinoids for pharmaceutical research and applications, provided us the opportunity to extend our use of catalysis for the manufacture of single component, pure cannabinoids. Our work using homogeneous catalytic hydrogenation for the preparation of new chiral scaffolds for the synthesis of cannabinoids and their derivatives will also be discussed.



Short Paper #12

SPECTROSCOPIC, REDOX AND BETA-LACTAMASE INHIBITION PROPERTIES OF SOME HYDRAZONIC ISATIN AND HYDROXYACETOPHENONE DERIVATIVES: AN EXPERIMENTAL, DFT AND MOLECULAR DOCKING STUDY

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Isatin, a heterocyclic indole derivative, also called 2,3 dioxindole or 1H-indole-2,3-dione, is a pervasive compound whose derivatives are found in both plants, such as Isatis tinctoria, and humans as a metabolic derivative of adrenaline.[1] However, this compound was first synthesized in 1841 by Erdmann and Laurent via oxidation of indigo blue by nitric and chromic acids[2]. This compound and its derivatives represent a very fascinating class of compounds with pertinent biological properties[1]. Like isatin, hydrazones also represent a class of compounds that has been extensively explored by researchers due to their interesting biological and pharmacological activities. Additionally, they possess some interesting metal chelating properties, hence, they tend to form interesting coordination complexes[3].

Hence, this exploratory study examines the spectroscopic and redox characteristics of hydrazonic compounds, derived from isatin and acetophenone. The vibrational attributes and solvent dependent optical features were explored via Fourier Transform Infrared (FT-IR) and UV-Vis absorption spectroscopies. Additionally, cyclic and square wave voltammetries were applied in investigating the redox properties of these compounds, indicating that their oxidation occurs via an electron transfers coupled with rapid chemical processes: EC mechanism, results which are corroborated by density functional theoretical (DFT) calculations. The Beta-lactamase inhibition potential of all compounds was probed via molecular docking calculations revealing exergonic binding potentials similar to known beta-lactamase inhibitors.

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Short Paper #13

C2-SYMMETRICAL TERPHENYL DERIVATIVES AS SMALL-MOLECULAR INHIBITORS OF PROGRAMMED CELL DEATH-1/PROGRAMMED DEATH LIGAND 1 PROTEIN-PROTEIN INTERACTION

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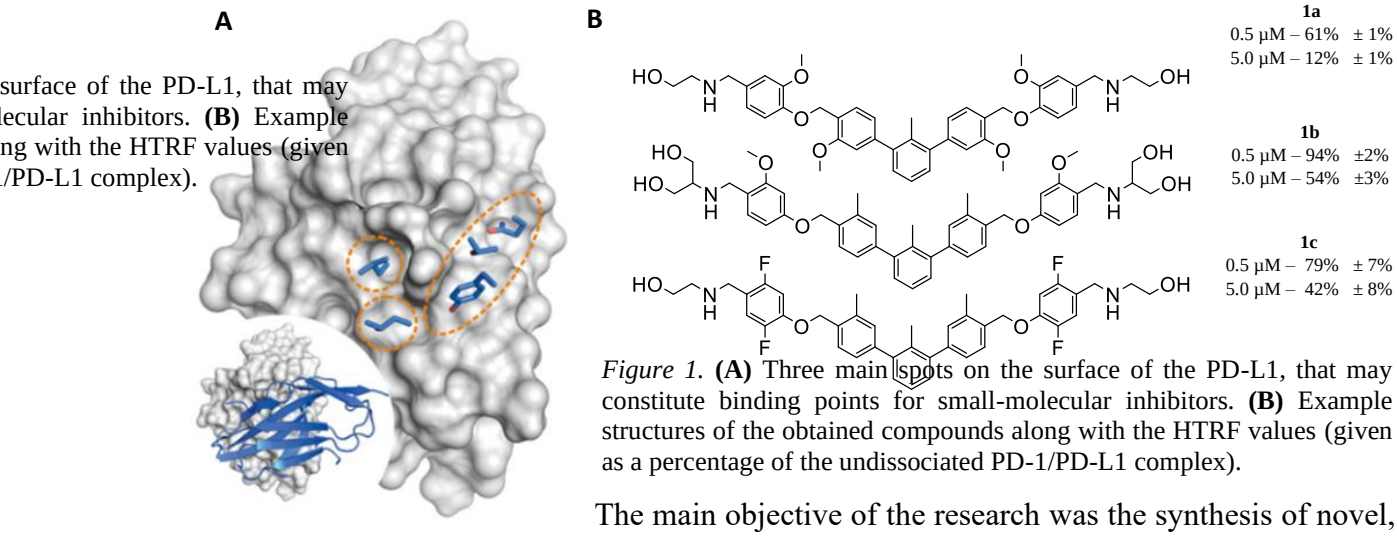
The PD-1/PD-L1 pathway represents an immune checkpoint mechanism responsible for regulating host's immune response against pathogenic agents. PD-1 is a cell surface receptor that plays a pivotal role in down-regulating the immune system by suppressing activation and proliferation of T-cell. Activation of PD-1 occurs through its complex formation with PD-L1. The expression of these proteins, among others, has been confirmed on cells of numerous malignant tumors, contributing significantly to cancer therapy. Activation of the PD-1/PD-L1 pathway facilitates immune evasion of tumor cells by suppressing T-cells functions, which precludes effective anti-cancer therapy. Targeting the PD-1/PD-L1 immunologic pathway with small-molecules gives high expectancy of advancing cancer therapy. Disrupting the activation of the PD-1/PD-L1 pathway with appropriately designed inhibitors allows for the sustained activity and performance of T-cells.



surface of the PD-L1, that may
lecular inhibitors. **(B)** Example
ng with the HTRF values (given
/PD-L1 complex).

Figure 1. **(A)** Three main spots on the surface of the PD-L1, that may constitute binding points for small-molecular inhibitors. **(B)** Example structures of the obtained compounds along with the HTRF values (given as a percentage of the undissociated PD-1/PD-L1 complex).

The main objective of the research was the synthesis of novel, small-molecular inhibitors of PD-1/PD-L1 pathway. Compounds were designed to be symmetrical, centered around the terphenyl core, causing the PD-L1 dimerization that hinders its interactions with PD-1. The potency of PD-1/PD-L1 complex formation inhibition was assessed using homogenous time-resolved fluorescence (HTRF) assay.

ACKNOWLEDGEMENTS
The research has been supported by a grant from the Priority Research Area SciMat under the Strategic Programme Excellence Initiative at Jagiellonian University.

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Short Paper #14

SYNTHESIS AND BIOLOGICAL ACTIVITY EVALUATION OF C2-SYMMETRIC, SMALL-MOLECULE INHIBITORS OF PD-L1

Wiktor Uzar,[1,2] Joanna Klimek,[1] Radosław Kitel,[1] Tad A. Holak,[1] Damian Muszak,[1] Łukasz Skalniak[1] Ewa Surmiak[1*]

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PD-1 (programmed cell death protein 1) belongs to the group of immune-checkpoint proteins. It is expressed on the surface of immune system cells, including T lymphocytes. The PD-1/PD-L1 signaling pathway is responsible for regulating the degree of immune response. The interaction of PD-1 with its ligand, PD-L1, leads to attenuation of the effector functions of T lymphocytes, which ultimately results in their exhaustion.

Cancer cells are capable of evading immune control by presenting PD-L1 on their surface, which has been observed to be overexpressed in various types of tumors. It has been demonstrated that blocking of PD-1 or PD-L1 can restore immune surveillance against cancer cells by engaging T lymphocytes in the fight against tumor cells.

In recent years monoclonal antibodies (mAbs) targeting immune-checkpoints have been introduced as a standard care for a number of cancers. However, mAbs exhibit several limitations. Therefore, there is a strong need for the development of new modalities overcoming the drawbacks of mAbs.

Here, we designed and synthesised a set of small-molecule compounds based on a biphenyl core (**Figure 1**). Their activity was assessed in HRTF (Homogeneous Time Resolved Fluorescence) assay and ICB (immune checkpoint blockade) assay. Additionally, we evaluated the electrostatic complemantarity of tested compounds.

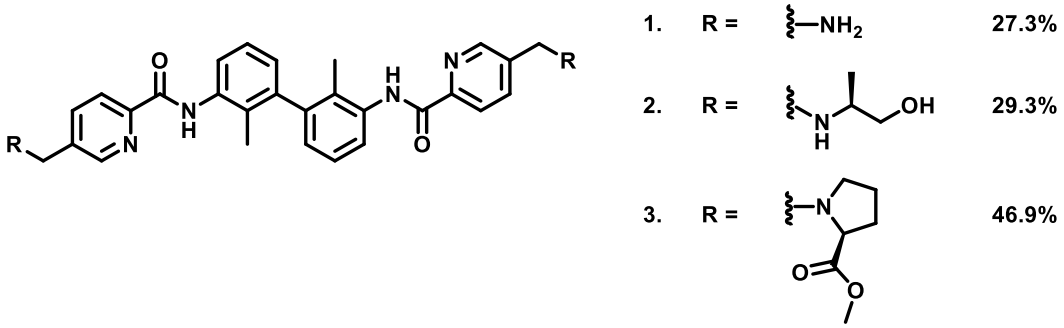

Figure. 1 The structures of investigated compounds, along with the corresponding HTRF values at a 5 nM inhibitors, expressed as the percentage of the undissociated PD-1/PD-L1 complex.

ACKNOWLEDGEMENTS

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ABSTRACTS OF POSTER PRESENTATIONS

Poster #1

UNLOCKING SUSTAINABLE ENERGY: A STUDY ON THE BIOMETHANE POTENTIAL OF CASSAVA STARCH

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Addressing wastewater challenges and promoting sustainable energy, the Scientific Research Council (SRC) employs the patented Biodigester Septic Tank (BST) to enhance wastewater treatment. This technology efficiently digests organic waste, yielding biogas as a renewable energy resource. The biogas composition, approximately 60% methane and 40% carbon dioxide, positions it as a versatile combustible gas with a higher ignition temperature than traditional sources such as diesel oil and propane (Brown, J, 2003). Optimizing biogas production involves understanding Biomethane Potential (BMP), the maximum methane yield through anaerobic digestion (Jingura & Kamusoko, 2017).

To assess diverse trade effluent streams, the SRC conducted a study on the BMP of cassava starch as a substrate in the Biodigester Septic Tank. Using a manometric method to measure changes in headspace pressure as an indicator of gas production, a bench-scale study evaluated the activity of cassava starch/digested slurry mixtures at varied ratios. Mixtures were placed in sterile glass bottles, and the headspace was evacuated to achieve a gas pressure of 0 mbar. Reaction mixtures were incubated at room temperature for 12 days, with gas pressure readings taken twice daily. The results concluded that a test ratio of 10% cassava starch:90% digested slurry generated the highest quantity of biogas (2.28 mbar), while a test ratio of 20% digested slurry:80% cassava starch also experienced notable gas production (1.47 mbar).

These findings suggest the potential use of agricultural effluent streams for biogas generation, providing cleaner energy for various industrial processes. Establishing a Biomethane Potential (BMP) database enables industries to assess effluent stream viability for alternative energy through BST systems. This study offers early insights into the promising application of varied substrates in biogas generation within the BST framework, laying the foundation for industries to consider sustainable and decentralized energy solutions—a critical stride towards a greener future.

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Poster #2

DESIGN AND ANALYSIS OF BIODIESEL PRODUCTION FROM HIGH FREE FATTY ACID WASTE COOKING OIL

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Trinidad and Tobago imports over 17 million litres of cooking oil annually and thus produces a large amount of waste cooking oil.[1] While it is known that waste cooking oil can be used to produce biodiesel, high amounts of free fatty acids and water can negatively affect yields. Trinidad's local vendors tend to reuse their cooking oil at high temperatures many times, thus producing waste cooking oil that is very high in free fatty acids, water content, and particulates, making it difficult to utilise for biodiesel production. Waste cooking oil sourced from different types of local food vendors (KFC, Doubles producers, and Chinese restaurants) were assessed in terms of environmental impact and energy intensity of processing. Novel and conventional alkali and acidic catalysts were also compared. Potential waste streams and environmental management plans were then evaluated. Using the most sustainable options, a biodiesel production plant that uses locally produced high free fatty acid cooking oil as the raw material with an annual capacity of 11 million litres was designed, simulated, and assessed in terms of overall sustainability.

Reference

1. Trinidad and Tobago Central Statistical Office, 2017

Poster #3

THERMAL STABILITY OF ACKEE (*BLIGHIA SAPIDA*) ARIL OIL AND CHANGES IN ITS α-TOCOPHEROL AND β-CAROTENE CONTENT UPON HEATING

Zoie Aimey[1], Andrea Goldson-Barnaby[1], Coniel Roye[2]

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Jamaican ackee, *Blighia sapida,* is a widely known fruit of which the main current processing method is canning. This process generates significant amounts of waste ackee aril which have immense potential for the creation of value-added products and may serve as a source of edible oil. The thermal stability of ackee aril oil and changes in its nutritive value upon heating were explored. Thermal stability was determined based on the oil's smoke point and changes in its acid value, free fatty acid content, free radical scavenging activity, carotenoid and tocopherol content upon heating. Thin Layer Chromatography and Nuclear Magnetic Resonance Spectroscopy were also utilized to analyse the samples. There was an increase in the percentage free fatty acid (16.7 %) and acid value (16.4 %). Ackee aril oil exhibited high free radical scavenging activity (98.51 ± 0.71 %), which is partially attributed to its carotenoid content (44.32 ± 0.58 ppm). The concentration of α-tocopherol (1.699 µg/g) in the oil was low and decreased by 60 % upon heating, while the β-carotene content (4.79 ± 0.12 ppm) increased by 125 %. The ^{1}H and ^{13}C NMR spectra of the heated and unheated oils appeared similar except for an unidentified peak observed at 4.684 ppm in the ^{1}H NMR of the heated ackee aril oil. The smoke point (232 °C) of the extracted oil was comparable to that found in literature for "refined extra light" olive oil (240 °C). Ackee aril oil is also high in oleic acid, which contributed significantly to the nutritive value of the oil. The structure for the major triglyceride present within ackee aril oil, 1-oleoyl-2-stearoyl-3-oleoyl-sn-glycerol, was also proposed.

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Poster #4

BETA CAROTENE CONTENT OF *BLIGHIA SAPIDA* (ACKEE) ARILLI UTILIZING DIFFERENT PROCESSING METHODS AND DETECTION OF THE FLAVOUR COMPONENT 9-OCTADECENAL

Debbie Ann Phillips[1], Nashana Murray[1], Maryam Kolahi[2], Raymond Reid[1], Andrea Goldson-Barnaby[1]

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Blighia sapida, also known as ackee, is a fruit originating from West Africa which is widely consumed in Jamaica. After harvesting, the edible arilli is separated from the seed and pod. The arilli is then blanched and sautéed with codfish. The impact of various processing methods (uncooked, cooked, uncooked frozen, cooked frozen, and canned) on the beta-carotene content of the arilli was measured utilizing a spectroscopic assay. The findings revealed a strong relationship between the processing method utilized and the beta-carotene concentration of the ackees. Canned ackee exhibited the highest beta-carotene content (1.33 ± 0.11 ppm). This is possibly due to high temperature processing breaking down cellular structures and releasing beta-carotene. Uncooked arilli had the lowest beta-carotene content (0.71 ± 0.06 ppm). Temperature was a significant factor impacting beta-carotene concentration suggesting that the processing method plays a crucial role in shaping the nutritional composition of *Blighia sapida* arilli. Gas Chromatography Mass Spectrometry analysis of arilli oil extracts detected the presence of 9-octadecenal which may contribute to the flavour of the arilli.

References

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2. Wray, D.: Goldson-Barnaby, A., Bailey, D. *Int. J. Fruit Sci*. **2020**. 20(2), S910-S924.

Poster #5

POLYMER CHARACTERIZATION AND TRACE ELEMENTS IN PAPER-BASED FOOD PACKAGING: A JAMAICAN CASE STUDY

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Plastics have served as a major food packaging material over the years, based on their economic costs, durability, and barrier properties. However, their detrimental impact on the environment and human health remains a significant drawback. The food packaging industry worldwide, crucial for ensuring food safety and security, is currently undergoing a transformative shift towards biodegradable alternatives, as demonstrated by Jamaica's 2019 ban on non-biodegradable plastics. Paper-based alternatives are now being used to make food contact containers. However, synthetic polymers are incorporated to improve their functionality. This study investigates the growing use of paper-based food containers as plastic substitutes. It addresses regulatory gaps regarding overall organic and inorganic composition.

The polymers in 24 samples of paper-based food containers and straws sold in Jamaica were examined using Fourier Transform Infrared (FTIR) Spectrometry. Cellulose (100%), polyethylene (42%), and polystyrene (21%) emerged as the major components; plastics were identified in at least 15 of the samples. However, making distinctions between the derivatives of these polymers is challenging using this technique. The straw samples analysed did not contain plastics and met their requirements based on regulatory prohibitions. Though marketed as environmentally friendly packaging, the compositions of the packaging materials varied, as 7 of the 15 samples labelled as paper were found to contain an undeclared plastic polymer. The moisture content, ash content, total organic carbon content, and microscopic imagery were utilized to categorise their organic and inorganic properties.

Instrumental Neutron Activation Analysis (INAA) showed the presence of aluminium as a major non-polymeric layer in some samples. The study's future phase will focus on further elemental characterisation and the health risks of potentially harmful metal migration.

This comprehensive examination of paper-based food packaging materials and their potential implications for both consumer health and environmental sustainability, integrates various analytical techniques. This research is relevant to academia, food packaging industry members, policymakers, consumers, and other stakeholders, thus playing a crucial role in ensuring consumer health and promoting the sustainable development of the food packaging industry.

Poster #6

A DFT AND EXPERIMENTAL STUDY OF THE SPECTROSCOPIC AND CU(II)-SENSING PERFORMANCE OF SOME BENZYLIDENE-BASED COMPOUNDS

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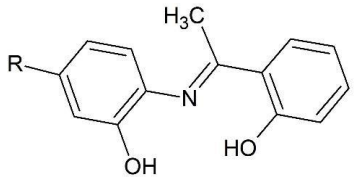

R = NO_2, Cl, H, CH_3, OH

A thorough investigation into the electronic and spectroscopic properties of a series of benzylideneaniline-type compounds was carried out using a combination of experimental and high-quality molecular modelling techniques. Calculations carried out at the DFT/B3LYP/6-31++G(d,p) level revealed highly twisted structures for all compounds and electron density distribution patterns which were heavily substituent-dependent. Such structural and electronic features manifested in the spectroscopic properties and copper-sensing capabilities of the compounds. Indeed, compounds exhibit a selective colorimetric response for Cu(II) producing a distinct colour change from colourless to purple as a result of an metal-ligand charge transfer (MLCT) process. Further investigation of the copper(II)-sensing revealed exergonic binding (~25 kJ mol^{-1}) resulting from an interaction of enthalpic and entropic effects. Furthermore, compounds produce detection limits as low as 0.16 ppm, offering greater sensitivity than methods based on the well-regarded technique Flame Atomic Absorption Spectroscopy (FAAS). Whereas only Zn(II) diminishes the accuracy of Cu(II) determination for the unsubstituted derivative (R = H) , the other derivatives investigated experienced significant interference from several metal ions at equimolar levels- a consequence of hard-soft interactions and the basicity of binding sites. The modulation of such effects can be achieved through modification of the core structure through substitution.

Poster #7

GREEN ALDOL CONDENSATION PRODUCTS WITH NMR SPECTROSCOPY STUDIES: TRANS-CINNAMALDEHYDE & ACETOPHENONE

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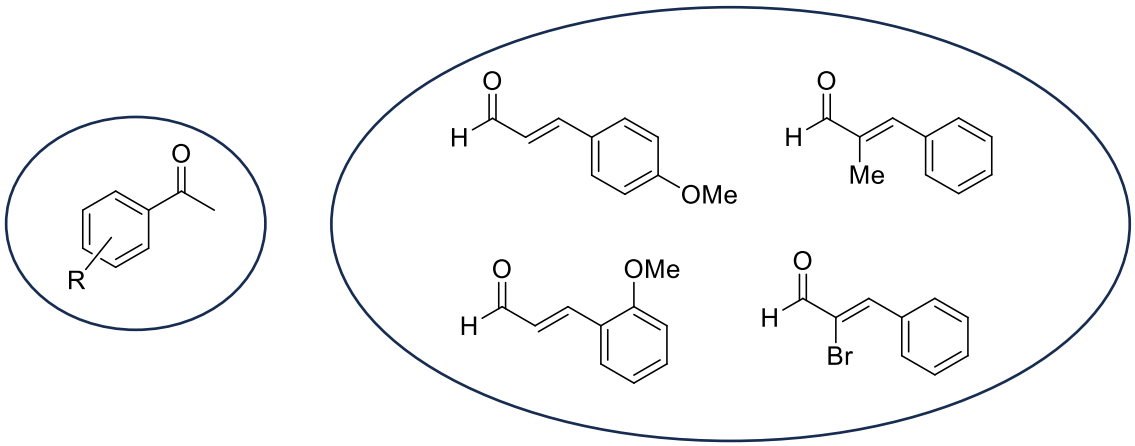
Chalcones are α,β-unsaturated ketones consisting of two aromatic rings separated by an unsaturated carbon chain. Traditionally these chalcones have been synthesized using a one-step Aldol Condensation. In this study, a broader series of Aldol products arising from trans-cinnamaldehyde (and derivatives) and a variety of acetophenone derivatives were investigated by NMR spectroscopy (1-D and 2-D. Using readily available starting materials, these reactions are fast, easy and solventless, making the synthesis of these products a great example of green chemistry.

By varying the acetophenone derivatives, we are aiming to see the variation in the NMR spectra when the ketones are condensed with the available trans-cinnamaldehyde derivatives. By comparing the spectral data of these compounds, students will get an insight to how substituent effects can and does affect the coupling patterns and the ppm appearance of these novel compounds in the NMR spectra. In addition, C-13 NMR (Dept and proton decoupled) is an important analytical and easier tool for analysis as compared to the proton spectra. The variety of NMR experiments available 1-D (proton and carbon), 2-D (COSY, HSQC, HMBC) make the study of these compounds a valuable instructional tool for structural elucidation.



Poster #8

STUDIES TOWARDS THE SYNTHESIS OF HYDROXYUREA ANALOGUES

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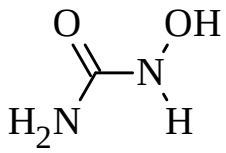
Sickle cell disease (SCD) arises from a defect in the β-globin molecules in haemoglobin (Hb) of red blood cells (RBC). Globally, there are 7.74 million individuals with sickle cell disease, 60% of which are individuals of African descent.[1] In Jamaica, 1 in every 150 individuals has SCD and as a result suffer from, pain crises, jaundice, anaemia and stroke.[2,3] Hydroxyurea (**1**) is a drug approved by the United States' Food and Drug Administration utilized in treating SCD via a series of mechanisms involving the release of nitric oxide which is crucial to increase fetal haemoglobin levels. Despite the effectiveness of hydroxyurea (**1**) in alleviating the symptoms of SCD by increasing the concentration of fetal haemoglobin in the blood, there is a need to synthesize analogues with milder side effects and a greater capacity to release nitric oxide.



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Herein, we present the successful synthesis of various hydroxyurea analogues.

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Poster #9

IDENTIFICATION OF TERPENE CHEMOTYPES OF THE ESSENTIAL OILS OBTAINED THROUGHOUT THE FLOWERING STAGE OF MEDICINAL CANNABIS *SATIVA* L. CULTIVARS AND THEIR BIOLOGICAL ACTIVITY.

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Cannabis *sativa* L. is regarded as one of the oldest cultivated plant species.[1] With a century of global prohibition, scientific information relating to its chemical diversities and taxonomy remains largely obscured.[2] This veil of restriction has given rise to a landscape marked by discrepancies, disarray, and an absence of standardization concerning the diverse array of cannabis varieties and their phytochemical compositions. Among the myriad of constituents present in cannabis cultivars, terpenes emerge as particularly notable secondary metabolites. They contribute to the various organoleptic properties and effect of each cannabis variety while also possessing a wide array of biological activities.[3] They are also highly distinguishing compounds, surpassing cannabinoids in their capacity for distinctiveness.[4] Despite this, there has been an overall neglect in cannabis terpene research in favour of their more widely known cannabinoid counterparts.

This study aims to assess the terpene profiles and biological activities of vegetatively propagated medicinal Cannabis *sativa* L. essential oils (EOS) throughout the flowering stage (from weeks 5 till maturity). EOs are extracted via hydro distillation with the Clevenger apparatus and then subsequently analyzed by Gas Chromatography coupled with a Flame Ionization detector (GC-FID) and Gas Chromatography–Mass spectrometry (GC–MS). The antibacterial activity of EOs will also be analyzed using disk diffusion and tube dilution method to determine the minimum inhibitory concentrations (MIC). Lastly, the larvicidal activity of each oil will be assessed against 3rd instar *Aedes aegypti* (Rockerfeller) mosquito larvae.

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Poster #10

MONOSACCHARIDE COMPOSITION OF SARGASSUM SPECIES (*S. FLUITANS, S. NATANS I & S. NATANS VIII*) FROM PALISADOES, JAMAICA.

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During the Period of 2011 – 2019, many western regions, including the Caribbean, experienced massive inundation events from the pelagic, brown alga *Sargassum*. Various industries including the tourism and fisheries sector were severely impacted, leading many researchers to investigate the source and cause of the inundation events, and potential uses of the Sargassum seaweed.

This research probed into the composition of selected monosaccharides from the invasive species *S. fluitans, S. natans I & S. natans VIII*, collected in February 2019 along the Palisadoes are in Jamaica and serves a primer investigation into the constituents of these *Sargassum* species, with an aim to guide possible uses. Results showed that in general there was a low cellulosic glucose content for all samples investigated and a greater mannuronic acid content than guluronic acid content for these samples. Also, the highest monosaccharides contents observed was for mannuronic acid, galacturonic acid, galactose, guluronic acid and fucose, with *S. natans VIII* having the highest mannitol content (> 5 µg/mg biomass) among the samples tested.

Poster #11

THE INVESTIGATION OF THE ANTIDEPRESSANT EFFECTS OF EXTRACTS OF *ARACHIS HYPOGAEA* (PEANUT) TESTA IN MICE

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Depression is a life threatening condition that affects the population worldwide. Depression can present itself during childhood or adulthood and can cause turmoil and distress [2] . The prevalence of depression in the Jamaican population in 2005, was reportedly 8% [1] . Based on the anatomy of the brain, most of the dopaminergic, serotonergic, and noradrenergic neurons are situated in the brainstem and midbrain. This indicates that the monoaminergic system is applicable in the maintenance of brain functions including Mood, sleep, appetite, cognition, and focus [4]. The Monoamine Hypothesis implies that depression is a result of depleted serotonin, norepinephrine, and dopamine in the brain. The monoaminergic system is the main drug target for antidepressant treatment [5]. *Arachis hypogaea* is a potent bio-resource for resveratrol. However, recent studies have shown that *Arachis hypogaea* have anti-fungal, anti-microbial, antioxidant, anticancer, antiviral, antihypertensive, anti-mutagenic, anti-inflammatory, and neuroprotective properties [3]. In Jamaican folklore, the peanut *(Arachis hypogaea)* testa is purported to "improve mood" when it is brewed as a tea. However, there is a lack of scientific evidence to support this claim. This experiment used two animal models of depression to investigate the antidepressant effects of various extracts of the *Arachis hypogaea* testa.

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Poster #12

BIOPESTICIDE ACTIVITY OF *MYRISTICA FRAGRANS* ESSENTIAL OIL AGAINST *AEDES AEGYPTI* LARVAE

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In Jamaica, the use of synthetic insecticides in vector control strategies continue to be hindered by increasing insecticide resistance in *Aedes aegypti* mosquito populations [1,2]. As a result, transmission of the dengue virus, which is the causative agent of the endemic dengue infection, remains a major challenge. With this in mind, the researchers sought to investigate the biopesticide activity of the popular Jamaican herb *Myristica fragrans* (nutmeg) as a potential natural alternative to the current synthetic agents in use. To evaluate this potential, the essential oil was extracted from the seed kernels of the nutmeg and was screened against the routinely targeted third instar larval stage of the *Aedes aegypti* laboratory strain 'Rockefeller' mosquitoes as well as field *Aedes aegypti* mosquitoes collected from Kitson Town, Jamaica. We discovered that the essential oil possessed significant larvicidal activity, with LC50 values of 7.179 ppm for the laboratory strain and 15.82 ppm for the field strain. Gas-chromatography mass spectrometry analysis of the oil revealed 30 compounds of which α-Thujene, Terpinolene, o-Cymene and trans-Piperitol were found to be the most abundant constituents. Interestingly, previous studies have attributed the larvicidal activity of nutmeg to Myristicin [3] and sabinene [4] with LC50 values of 22.9 ppm and 27.3 ppm respectively. However, these constituents were only found in trace amounts in the oil from the current study suggesting that the observed larvicidal activity may not be due to these constituents. Therefore, future work will focus on identifying the active principle in the oil responsible for the observed potent larvicidal activity and mechanistic studies to determine the mode of action of the oil.

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Poster #13

COBALT(II) AND COPPER(II) PINCER COMPLEXES BEARING FUNCTIONALIZED PYRIDYL BENZOTHIAZOLES AND (THIO)AMIDES FOR ELECTROCATALYTIC HYDROGEN EVOLUTION REACTION (HER)

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A series of pincer ligands, bis-*N*-(2,5-dimethoxyphenyl)pyridine-2,6- dicarbothioamide (**pdcta**), *N*-(2,5- dimethoxyphenyl)-6-[(2,5- dimethoxyphenyl)carbamothioyl]pyridine-2-carboxamide (**pcta**), bis-*N*-(4-chlorophenyl)pyridine-2,6-dicarbothioamide (**Cl-pdcta**), 6-(6-chloro-1,3-benzothiazol-2-yl)-*N*-(4-chlorophenyl)pyridine-2-carbothioamide (**Cl-pbcta**), 6-(4,7-dimethoxy-2-benzothiazoyl)-*N*-(2,5-dimethoxyphenyl)-pyridinecarbothioamide (**pbcta**) and 6-(4,7-dimethoxy-2-benzothiazoyl)-*N*-(2,5-dimethoxyphenyl)-pyridinecarboxamide (**pbca**) were prepared using standard procedures. The corresponding pincer complexes were prepared by reacting an equivalence of $M(CH_3CO_2)_2.xH_2O$ (where M = Co(II) (x = 4) or Cu(II) (x = 1)) with an equivalence of the respective ligand. The Cu(II) complexes had an effective magnetic moment between 1.8 and 2.1 B.M., consistent with a d^9 cconfiguration while the Co(II) complexes had an effective magnetic moment between 4.7 and 5.2 B.M., consistent with a high spin d^7 configuration. Voltammetric measurements indicated that the $[Cu(CH_3CO_2)(H_2O)(L)].xH_2O$ complexes where L = **pdcta** (x = 0) or **pcta** (x = 2) and $[Co(CH_3CO_2)(H_2O)(L)].xH_2O$ complexes where L = **Cl-pdcta** (x = 3), **Cl-pbcta** (x = 2) or **pbcta** (x = 0) were efficient homogeneous hydrogen evolution electrocatalysts when acetic acid (pK_a = 22.3) and trifluoracetic acid (pK_a = 12.7) in acetonitrile and *p*-toluene sulfonic acid in DMF (pK_a = 2.6) were used as the proton sources. $[Co(CH_3CO_2)(H_2O)$**pbca**] decomposed in the presence of both acids. When the chloro-containing Co(II) complexes were used in acetic acid under non-aqueous conditions, rate constants (k_{obs}) in the range of 10^3-10^4 s^{-1} at excellent overpotentials of 0.2 V were achieved, which were well in agreement with similar systems studied for electrocatalytic H_2 production. Faradaic efficiencies exceeding 90% were consistently obtained for all the complexes using acetic acid in DMF or MeCN. The catalytic studies supported a ECEC mechanism for the cobalt-catalytized proton reduction process, where the first electrochemical step was attributed to the reduction of Co^{II} to Co^{I} and the first chemical step involves the protonation of Co^{I} to form the Co^{III}-H.

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Notes