SCIENCE CONFERENCE 2023

National Library of Wales, Aberystwyth, and online.

Thursday 15 June 2023

Coleg Cymraeg Cenedlaethol

CYMRAEG

Ariennir gan Lywodraeth Cymru
Funded by Welsh Government

SCIENCE CONFERENCE 2023

National Library of Wales, Aberystwyth and online.

Timetable

09:30 **Registration**

09:45 **Welcome** – **Elin Rhys, Founder and Chair, Telesgop**

10:00 **Session 1**

Chair: Elin Rhys, Founder and Chair, Telesgop

Bedwyr ab Ion Thomas

Developing therapies to treat prion diseases (or how to conjure mosters to battle zombies!)

Llinos Honeybun

Developing a Drug Screen for CLN3 Disease

Aled Lloyd

Computational studies of drug commitment in human aquaporin 1

11:15 **Break**

11:30 **Session 2**

Chair: Dr Rhys Morris, Bristol University

Cai Stoddard-Jones

Unlocking the internal mechanisms of the outbursts of centaur 29P/Schwassmann-Wachmann

Liam Edwards

Eclipse in COVID time - polarized light observations of the Sun's corona during total eclipse on December 14th 2020

12:20 **Lunch / Poster Competition Adjudication**

13:30 **Session 3**

Chair: Dr Heulyn Jones, Cardiff University

Megan Kendall

Understanding Oxide Formation on Carbon Steel Tubes During High Temperature Processing

Oliver Tomos Wright

Cooperative Redox Enhancement exhibited by Bimetallic Catalysts

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14:20 **Session 4**

Chair: Dr Deri Tomos, Emeritus Professor, Bangor Univeristy

Carwyn Sion Hughes

Developing New Nanomedicines to Target Breast Cancer

Maisie Edwards

The importance of the use of the Welsh language within the provision of basic healthcare services, specifically family medicine

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15:10 **Session 5**

Chair: Dr Cennydd Jones, Aberystwyth University

Dr Eifiona Thomas Lane

Welsh Food Experiences, Sustaining Community and Place: responding to the Future Generations Targets

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15:35 **Poster competition winners announced**

15:45 **Finish**

Contributors

Bedwyr ab Ion Thomas

Medicine Discovery Unit, Cardiff University
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Biography

I graduated from The University of Oxford in 2019 with a master's degree in Chemistry (MChem) before returning to my hometown to further my studies. I am currently in my final year as a PhD Student within The Medicines Discovery Institute at Cardiff University. The goal of my research is to develop therapies for neurodegenerative diseases (prion diseases) through Medicinal Chemistry. To reach this ambitious goal, I have utilised a myriad of scientific disciplines, such as synthetic and computational chemistry, biochemistry, and biology. Throughout my research, new ground is being broken both scientifically, and in Welsh.

Developing therapies to treat prion diseases (or how to conjure mosters to battle zombies!)

Prion diseases are rare, neurodegenerative, transmissible, and are always fatal. Currently, there exists no effective therapy or treatment. This project's aim is to try and offer a path with therapeutic potential with the hope of developing it further as a possible treatment for prion diseases. Within the context of neurodegenerative diseases, an interesting aspect of prion diseases is their transmissibility. Equally as interesting is their mode of transmission, which is achieved when the native prion protein misfolds and induces further misfolding of the protein, leading to the formation of amyloids, plaques, and, ultimately, neurotoxicity and neurodegeneration. Examples of these types of diseases include mad cow disease, and Creutzfeldt-Jakob disease in humans. One route that has therapeutic potential is the use of PROTAC technology (*proteolysis targeting chimeras*) to degrade the native prion protein to stop the spread of the disease. Contrary to "traditional" small molecule drugs, which can work by

binding to a target protein to modulate its functions, PROTACs aim to hijack the ubiquitin-proteasome system to degrade the target protein, which ultimately, in effect, hinders the active protein within the cell. During my research as a PhD student, I designed a series of PROTAC degraders by computational modelling and went on to synthesize them using synthetic organic chemistry. Furthermore, proof-of-principle assays were conducted to determine if it is possible to degrade the native prion protein in the cell, and if these PROTACs have therapeutic potential.

Llinos Honeybun

Biosciences, Cardiff University
@LlinosHoneybun

Biography

Llinos Honeybun is a PhD student at Cardiff University researching new treatments for CLN3 disease, a rare neurodegenerative disease in children. She studied pharmacology as an undergraduate at the University of Bath before undertaking a master's degree in forensic science at the University of Strathclyde in Glasgow. Before starting her PhD, Llinos worked in the NHS genetics laboratories focusing on cancer genetics helping guide to patients' treatment to targeted small molecule therapies. Before that, she worked for Welsh company BBI Solutions as a research and development scientist creating novel lateral flow devices.

In her research in Cardiff, Llinos hopes to repurpose medicines to treat the CLN3 disease; a disease that currently has no effective treatments. To achieve this, she is developing a specialist drug screening assay and hopes to be screening compounds within the next year.

Developing a Drug Screen for CLN3 Disease

CLN3 (ceroid lipofuscinosis neuronal, 3) disease causes progressive neurodegeneration in children; the first symptoms are seen in children aged 4 to 8 years with patients starting to lose their sight. Some children suffer from epileptic seizures which worsen to the point where there is no effective treatment. Gradually cognitive and behavioral problems are seen before they lose the ability to walk, talk, swallow etc. In all cases, death came early. CLN3 is a very rare disease affecting 1:33,000-50,000 people worldwide with no effective treatment available.

CLN3 disease is caused by mutations in the CLN3 gene that prevent the protein from working; the most common mutation is a 1kb deletion in chromosome 16 of the CLN3 gene. The CLN3 protein exists as a channel on the membrane of the lysosome which is an essential structure that exists in every cell and digests and

recycles cellular material. So far, we don't know the exact role of the CLN3 protein so one part of my project is to try to reveal what type of transmembrane channel CLN3 is.

The main aim of my project is to investigate new treatments for CLN3 disease. I am trying to reveal more about what happens in CLN3 cells by studying changes in the levels of different markers e.g. proteins or fats. I am creating a test that compares cells with the most common CLN3 mutation seen in patients with healthy cells to determine any changes and then intend to screen collections of drugs against it. I am refining the test to ensure that the changes are representative of the disease and clear enough to see any differences after treatment with drugs. The hope is to discover treatments that modify the disease and slow down the neurodegeneration rather than treating symptoms.

Aled Lloyd

Faculty of Medicine, Health and Life Sciences,
Swansea University

Biography

Having completed his Master's degree in Chemistry and Drug Discovery at the University of Bath, Aled returned to his hometown to study postgraduate Medicine at Swansea University Medical school. He remained in the city to continue his medical training and since then, has specialised in Nephrology and General Medicine and worked as a registrar in the field throughout South Wales. Aled has since undertaken a sabbatical from his medical training to undertake a PhD at Swansea University. Now in his second year, Aled's work looks at computer chemical modelling of proteins in the kidney and how existing drugs interact with these proteins

Computational studies of drug commitment in human aquaporin 1

Introduction

Both bumetanide and furosemide have been shown in-vitro to bind to the cytoplasmic surface of animal AQP1 resulting in inhibition of water transport[1,2]. This is a finding of some interest as it has been conventionally believed that diuretic effects of these medications is due to the inhibition of the sodium/chloride cotransporter, There is little evidence of other drug interactions with human AQP1. The aim of this study was to characterise the interaction between human AQP1, bumetanide and furosemide using computational methods. Additionally, a drug repurposing screen of existing licensed medication was planned to explore new therapeutic options.

Methods

Threading modelling using the I-TASSER server and suite was undertaken to obtain monomeric structures of human AQP1. Saftware was written to download 3D chemical structures of all medication listed in the British National Formulary from the NCBI PubChem database. PLANTS software was used to establish the compound's

most energetically favourable binding positions. Visual inspection of these structures using UCSF Chimera was then performedto establish which compounds were most likely to exhibit an interaction with the protein.

Results

The most energetically favourable conformation of furosemide binding to the cytoplasmic opening of the intrinsic pore of the AQP1 monomer is different to those previously published. One end of the furosemide molecule binds to a pocket on the cytoplasmic surface of the pore opening, the other protruding into the pore in cork like conformation. The 10 most energetically favourable conformations identified in the docking simulation using PLANTS were all away from the pore.
1002 medicinal compounds were tested against the cytoplasmic opening of human AQP1. 198 were bound in the water pore as 45 of these compounds were bound with a higher calculated binding energy than furosemide.

Discussion

Using PLANTS and a model based entirely on human AQP1, we have identified a different orientation of furosemide binding to previously published models. Analysis of the binding site suggests furosemide could impede water flow through the protein by occluding the pore. We were unable to reproduce the lid like conformation of Migliati and co-workers with respect to the binding of bumetanide[2]
One of the weaknesses of docking studies is low sensitivity for active ligands. Molecular dynamic studies of these results are planned to further assess the most relevant interactions.

Conclusion

We have identified a different binding conformation for the interaction between furosemide and AQP1. Our repurposing screen identified 45 compounds for further investigation using molecular dynamics methodology.

Cai Stoddard-Jones

School of Physics and Astronomy, Cardiff University
@senoj_draddots / @comet_chasers (engagement project)

Biography

I'm originally from Ynys Môn, and I studied my undergraduate degree at Cardiff University. Loving Cardiff so much, I've stayed there to work towards my PhD. My project is a hybrid of comet astronomy, and astronomy education and outreach with schools. In my free time, I enjoy playing guitar, supporting Wrexham and the Scarlets, and cross-stitching.

Unlocking the internal mechanisms of the outbursts of centaur 29P/Schwassmann-Wachmann

29P/Schwassmann-Wachmann is odd. With its circular orbit, no tails, and often outbursting, 29P is an anomaly. The biggest mistery is why is it so active, and what's causing these violent outbursts? The main theory is cryo-volcanoes, but a lot more research needs to be done before we are certain. Maybe you're asking, what is a comet and why are they important? I'll be discussing this, by explaining how comets and asteroids formed during the early Solar System.

Liam Edwards

Physics Department, Aberystwyth University

@LiamTEdwards

Biography

Originally from Anglesey, Liam graduated from Aberystwyth University in 2019 with an Integrated Masters degree in Astrophysics. He received a research scholarship from the Coleg Cymraeg Cenedlaethol to study a PhD in Physics in the Solar System Physics research group at Aberystwyth University and began his studies in September 2019. During his doctorate, Liam contributed to several programs on BBC Radio Cymru, such as Post Prynhawn, Yfory Newydd and the Aled Hughes program discussing topics from asteroids and black holes to solar storms and his research on the outer atmosphere of the Sun - the 'corona'. More information about his research can be found on his website: Liam Edwards - Home (aber.ac.uk)

Eclipse in COVID time - polarized light observations of the Sun's corona during total eclipse on December 14th 2020

Total solar eclipses are unique opportunities to observe the lower part of the corona, the Sun's extended atmosphere, where the solar wind is accelerated to supersonic speeds. Observing this region is essential to being able to explore the processes that power the solar wind and can lead to better forecasts of extreme space weather events. On 14 December 2020, a team from Aberystwyth University managed to observe a total solar eclipse in Argentina. Due to bad weather, this was the only team with scientific equipment that managed to successfully observe this eclipse. A new instrument was designed for the eclipse and built to measure visible light from the corona, the Coronal Imaging Polariser (CIP) – aptly named as we only get a 'snapshot' of the corona during an eclipse. The instrument has a polarizer that automatically rotates to six polarization angles (0, 30, 60, 90, 120, and 150 degrees), taking five images of different exposure times at each angle (0.001s, 0.01s, 0.1s , 1s, and 3s). The process of calibrating the instrument and processing the images will be

discussed together with results from the plasma density of the corona during the eclipse, which is an important parameter to understand the acceleration of the solar wind. I will conclude by talking about new work that will use the density to estimate the strength of the corona's magnetic field - an extremely rare measurement, and of great importance to the field.

Megan Kendall

Materials and Engineering Department, Swansea University

@MEKendall369

Biography

Megan graduated from the University of Sheffield in 2021 with an MEng degree in Mechanical Engineering. During her degree, she worked on industrial projects related to materials integrity, non-destructive testing (NDT) and computational modelling. She has also completed a research placement with the Insigneo Institute for Computational Medicine, looking at mobility sensors to monitor long-term patient health.

Megan is now in the second year of an EngD (Industrial Doctorate) sponsored by TATA Steel, as part of the Materials and Manufacturing Academy (M2A) at Swansea University. Her research focuses on using computational techniques to improve the understanding of how steel responds to high temperature processing.

Understanding Oxide Formation on Carbon Steel Tubes During High Temperature Processing

Low carbon steel conveyance tubes for building and industrial services applications are manufactured via a high-frequency welded, hot-finished process route. Welded tubes exhibit better geometric consistency, machinability, and mechanical properties than their seamless equivalent. However, microstructural inhomogeneity is introduced by the temperature gradient established due to the localised heating effect of welding and its effect on carbon solid solubility. A 900°C heat treatment is applied to the tubes to normalise the microstructure and mechanical properties across the fusion line, heat affected zone (HAZ) and bulk material, and relieve residual stresses evolved by thermal deformation and oxidative microstructural distortion. However, the growth of a multi-species oxide surface scale can negatively

affect product cosmetic quality and performance.

Scale growth is especially problematic for conveyance tubes due to the rapid stretch reduction process, performed to achieve customer-specified wall thickness and tube length dimensions, which introduces intense heat, mechanical stress, and tool-surface interaction, and accelerates inconsistent scale spallation. The negative consequences of spallation include degradation of protective passive properties from the scale, material yield loss, and poor surface quality.

Computationally driven proactive management of scale kinetics, and adhesion on conveyance tube steel grades could contribute to improved manufacturing agility, product quality, and customer satisfaction. This study explores the scope within computational thermodynamic modelling software, namely Thermo-calc DICTRA, to explore external oxidation kinetics and adhesion, specifically under tube manufacturing conditions, using the moving phase boundary methodology. After initial model development, the aim is to explore two parameters; geometry, as the most significant differentiating factor of tube compared to slab manufacturing; and silicon content, as one of the greatest and most variable alloy element contributions across the two steel grades of interest to conveyance tube production.

Oliver Tomos Wright

Cardiff Catalysis Institute, School of Chemistry,
Cardiff University
@olwrighty

Biography

Originally from Mold, Oliver graduated in Chemistry with Industrial Experience in 2022 from Bangor University, having received a scholarship from the Coleg Cymraeg Cenedlaethol. In 2020, he took up an industrial placement, taking the position of research technician at the BioComposites Centre within Bangor University. Here, he primarily investigated the emission of volatile organic compounds (VOCs) from natural building materials. In his final year, he specialized in the synthesis and use of organocatalysts in addition reactions.

Since October 2022, Oliver is in his first year of PhD studies at Cardiff Catalysis Institute under the supervision of Professor Graham Hutchings. His research aims at the design of novel selective heterogeneous catalysts for redox reactions.

Cooperative Redox Enhancement exhibited by Bimetallic Catalysts

Oliver Wright[a], Xiaoyang Huang[a], Mark Douthwaite[a], Kai Wang[a], Liang Zhao[a], Richard J. Lewis[a], Samuel Pattisson[a], Isaac Daniel[a], Sultan Althahban[a,], Steven McIntosh[b], Christopher J. Kiely[b] & Graham Hutchings[a]

[a]Cardiff Catalysis Institute, Cardiff University

[b]Lehigh University, Bethlehem, PA, USA

In oxidation reactions catalysed by metal nanoparticles, the rate of oxygen reduction can be a limiting factor. This is evident in the oxidative dehydrogenation of alcohols. This is an important reaction in industrial synthetic chemistry for the production of aldehydes and ketones, which act as essential commercial chemicals. Gold nanoparticles are very efficient for the dehydrogenation of alcohol to aldehyde but are less effective for oxygen reduction. The inverse is true for palladium nanoparticles. This imbalance can be overcome by creating a gold and palladium alloy, which gives

both reactions a higher activity; however, the electrochemical potential of the alloy is a compromise between the two metals, which means that while the oxygen reduction reaction in the alloy can be improved, the catalytic dehydrogenation activity is severely limited. We are able to show that by separating the gold and palladium components in bimetallic catalysts, almost double the reaction rate can be achieved. This can be demonstrated using physical mixtures of monometallic gold and palladium catalysts and bimetallic catalysts, consisting of spatially separated gold and palladium regions or Janus structures. Furthermore, we can show electrochemically that these improvements are attributable to the coupling of two separate redox processes, which occur at isolated gold and palladium sites. A recent derivation of kinetic models for this system confirms and demonstrates the significant improvements driven by this new effect. The discovery of this catalytic effect (**Co**operative **R**edox **E**nhancement-**CORE**) offers a novel approach to designing multicomponent heterogeneous catalysts.

Carwyn Sion Hughes

School of Pharmacy and Pharmaceutical Sciences, Cardiff University

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Biography

I am originally from Llannerch-y-medd in Anglesey. In 2017 I began studying my undergraduate degree in Medical Pharmacology at Cardiff University's School of Medicine. Upon finishing my degree in 2020 I relocated to the School of Pharmacy and Pharmaceutical Sciences to study a postgraduate degree in Cancer Biology and Therapeutics. In 2021, again at the School of Pharmacy, I was given the opportunity by the Coleg Cymraeg Cenedlaethol to join with the research team of Professor Arwyn T. Jones that has an interest in developing new treatments for cancer and other diseases. At present I am researching an developing polymeric nanoparticles as a treatment for breast cancer.

Developing New Nanomedicines to Target Breast Cancer

Some cancer cells possess unique characteristics that differentiate them from healthy cells. In some types of breast cancer this can lead to the overproduction of a protein known as HER2, that can be found on the surface of the cell. In this project we have developed nanoparticles that contain the anti-cancer drug doxorubicin and are decorated with Herceptin, which is an antibody used in the clinic to target HER2 on breast cancer cells. This allows us to target HER2 overproducing cells exclusively. The aim is this will ensure that doxorubicin is delivered to the cancer cells only thereby preventing any damage to the body's healthy cells.

Maisie Edwards

Medical and Health Care Studies, MSc by Research, Swansea University
@maisieefa

Biography

My name is Maisie. I'm a Masters by Research student at Swansea University, but originally from Newport. I studied Population Health and Medical Sciences as an undergraduate degree, also at Swansea University. I began this research process as part of my undergraduate degree when examining the importance of Welsh language provision within primary health care. This year, I am focusing on the use/lack of use of the Welsh language within general healthcare for people with chronic conditions. Recently, I have presented my research at the Caring in Welsh Conference and the Postgraduate Research Conference at the Faculty of Medicine, Health and Life Science at the university. My supervisor and I have also formed links with a doctor and researchers in the Basque Country, who are carrying out research on improving language barriers within health for speakers of minority languages. We also had the opportunity to share our work at their annual conference, which includes contributors from all over the world.

The importance of the use of the Welsh language within the provision of basic healthcare services, specifically family medicine

Effective communication is an integral part of healthcare and has been reinforced by previous studies. However, in Wales, GPs are not required to provide verbal consultations through the Welsh language. A lack of use of a specific language can compromise patients' health opportunities and lead to misunderstandings. Due to the lack of current regulations and data, the main aim of the study is to collect the public's perceptions in relation to the use of the Welsh language in primary healthcare services. By holding discussions with experts in the field, focus groups and a questionnaire, the intention is to assess the demand for more rights and the benefits of increasing the bilingual provision. A combination of qualitative and quantitative analysis techniques is used in order to collate the main perceptions of

the public and interpret their experiences. A strong relationship was observed between respondents who spoke Welsh in the household, with people stating that they would benefit from an increase in bilingual provision. Despite the fact that 69% believe they would benefit from an increase in bilingual provision, only 18.3% have asked for a Welsh-speaking doctor when arranging an appointment. The qualitative data highlighted possible reasons for this, such as awareness of the challenges facing the healthcare services and concerns about waiting longer for a consultation. Therefore, the importance of strategies such as the 'Active Offer' can be seen in order to remove the burden from patients. Using studies that examine the use of other official minority languages in the provision of healthcare services, the main aspects can be drawn and applied to benefit the Welsh context. Carrying out joint studies with other organisations could increase the current data available and required in order to inform changes to the regulations. Increasing the provision available in primary healthcare is even more important as GPs are often the population's main link to healthcare services.

Dr Eifiona Thomas Lane

School of Natural Sciences, Bangor University.
@DrEifiona

Biography

Eifiona is a lecturer in Geography and Environmental Planning at Bangor University with a research interest in many aspects of sustainable communities, e.g. food security, the rural economy (especially agriculture and heritage conservation), and also the challenges of managing designated areas, e.g. National Parks and AONB.

Welsh Food Experiences, Sustaining Community and Place: responding to the Future Generations Targets

Rebecca Jones, Eifiona Thomas Lane, Ian Harris a Sian Pierce, Geography, School Natural Sciences, Prifysgol Bangor University.

This presentation will share the results of independent primary research which examines a range of examples of food and drink experiences from the upper part of the food chain, a key economic sector in Wales. Their relevance to the Strategy for Creating and Sustaining Place (Welsh Government 2020) is discussed as is the contribution that food and food experiences make to realizing the Future Wellbeing Targets which is the Welsh Government's interpretation of the UN Sustainable Development Goals (Welsh Government 2015). These targets offer a unique research context for exploring developing the resilience of local communities and strengthening the Welsh rural food chains and economy (Thomas Lane et al. 2016). Using a multi methods approach, original primary data is combined for exploration e.g. food celebrations, branding and 'craft' products (Morgan et al. 2022), with experiences of lack of access to food and solutions offered by redistributing food through Food Hubs. The research discusses how food can contribute towards strengthening the circular economy (Welsh Government 2021) and to building the resilience of rural communities.

The case studies investigated represent a variety of food experiences, many of which are based on innovative partnerships established during the lockdown period (Jones et al., 2022). Currently, local authorities in Wales are establishing food partnerships and strategic food plans, however, this research questions whether future resourcing and commitment exists to ensure long-term change that will ensure that sustainable food from Wales is available to everyone in Wales. In the light of devolved governments talks, Scotland and Wales, about the 'right to food', the presentation triggers a timely discussion about sustainable food policies and strategies that can practically contribute to strengthening and protecting the whole chain food 'from the field to the kitchen'.

Poster Competition

A poster competition is held for undergraduate and postgraduate students. We ask that the poster expresses a scientific idea through the medium of Welsh. Adjudication will take place on the day of the conference. Thank you to everyone for applying.

Thank you

Thanks to everyone for their contribution to the Scientific Conference hosted by the Coleg Cymraeg Cenedlaethol.

The Coleg Cymraeg Cenedlaethol will be tweeting about the Conference. Join the conversation and remember to follow @GwyddCCC account and use the hashtag #cynhadleddwyddonol. The contributors' Twitter handle can be found in this program.

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