Dial-a-Molecule

An EPSRC Grand Challenge Network

July 2015

Welcome to the July 2015 Edition of the Dial-a-Molecule Newsletter. In this edition we are covering highlights from our Annual Meeting which was held earlier this month, promoting Network Activities we have planned for the remainder of the year and letting you know of some external events relevant to the Dial-a-Molecule Community.

In this edition…

Dates for your Diaries: Upcoming Meetings:

- Lead-Oriented Synthesis: Exploring Drug-Relevant Chemical Diversity on **25 September**
- Smart Materials: Efficiency, Complexity and Design on **21 October**

Meeting Report: Chemical Synthesis in the 21st Century – The 2015 Dial-a-Molecule Annual Meeting

External Events:

- Understanding and Optimising Chemical Processes through Statistical Methodologies, 9-11 September, Durham University
- International Chemical Identifier (InChI) QR Code Consultation Workshop

Funding Opportunities: ECR Travel Bursaries

Connect

www.dial-a-molecule.org

@DaM_Challenge

Dial-a-Molecule EPSRC Grand Challenge

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The Grand Challenge is owned by the community and we value your input and feedback, so if there is anything you think the Network should support or get involved in, please get in touch

Lead-Oriented Synthesis: Exploring Drug Relevant Chemical Diversity

GSK Stevenage, 25 September 2015

The ready availability of structurally novel lead molecules with appropriately controlled molecular properties (e.g. logP, molecular weight and fraction of sp^3 atoms) is crucial to the ability of the pharmaceutical industry to bring new small molecule drugs to market. However, it is now recognised that access to such lead molecules is poorly served not only by many current commercial libraries but also by the synthetic methods widely adopted within industry and many of those developed in academic laboratories. In this meeting, approaches to rectifying this issue will be presented both from academia and industry, with the hope of stimulating a broader recognition of, and solutions to, the challenges of lead-oriented synthesis

The meeting is free to attend, but to facilitate with catering we ask you to register at www.dial-a-molecule.org.

Registrations close 4 September 2015

Organising Committee: *Prof. Steve Marsden & Prof. Adam Nelson*

Keynote Speaker:
Prof. Jeffrey Bode (ETH Zurich)
"Cross Coupling 2.0"

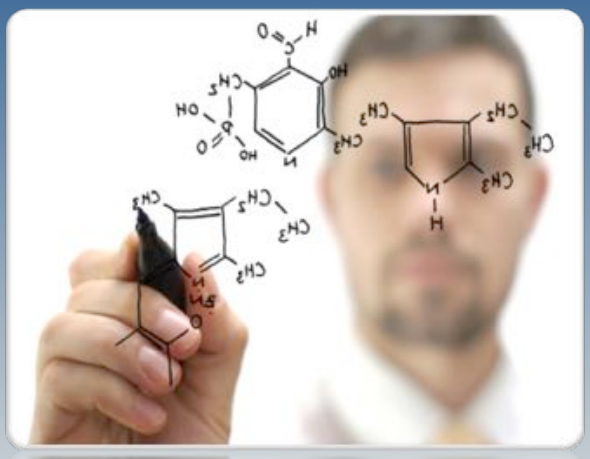
Invited Speakers:
Dr Ian Churcher (GSK)
"How Synthetic Chemistry Can Drive the Discovery of Drugs of the Future"

Dr Jason Kettle (AstraZeneca)
"Design and Exploitation of Novel Medicinal Chemistry Reagent Sets"

Prof. Steve Marsden (University of Leeds)
"Synthetic Strategies for the Efficient Exploration of Lead-Like Space"

Prof. Peter O'Brien (University of York)
"Exploring 3-D Pharmaceutical Space: Lead-oriented and Fragment-oriented Synthesis"

Prof. David Spring (University of Cambridge)
"Enriching Chemical Space to Drug Undruggable Targets"



Early Career Researcher Travel Bursaries

Dial-a-Molecule have bursaries available to help ECR's attend our meetings. These cover travel expenses and accommodation costs and can be applied for on meeting application forms.

Note: ECR's are defined as post-doctoral research fellows and academic staff in the first three years of their first academic appointment.

Smart Materials: Efficiency, Complexity and Design

University of Warwick, 21 October 2015

A one-day meeting designed to bring **synthetic** and **polymer** chemists together.

The UK is a global leader in polymer synthesis, and academic activity in the area continues to deliver palpable economic advantage to society. Building on the advances delivered in the use of polymers in smart, functional materials will require a step-change in the synthetic chemistry which underpins the subject; only by ensuring access to new generations of functionalized high-value monomers and delivering improved methods for polymerisation will advances continue.

Confirmed Speakers: **Prof. Cameron Alexander** (University of Nottingham), **Dr Fransisco Fernandez-Trillo** (University of Birmingham), **Dr Matthew Gibson** (University of Warwick), **Prof. Alan Rowan** (Radboud University of Nijmegen), **Dr Helen Willcock** (Loughborough University)

Understanding and Optimising Chemical Processes through Statistical Methodologies

Durham University, 9-11 September 2015

The Industrial Statistics Research Unit (ISRU) at Newcastle University, together with the Department of Chemistry at Durham University, are running a 3 day course on Understanding and Optimising Chemical Processes through Statistical Methodologies.

The program will involve a series of workshops involving experimental design, analysis and interpretation of data that explore scoping, screening, optimisation and robustness methods. The event is targeted at scientists, working in industry and academia, and at all scales from research through to manufacturing. Registration and contact details can be found by clicking on this link

International Chemical Identifier (InChI) QR Code Consultation Workshops

IUPAC and the InChI Trust are examining the development of a QR code (2D bar code) version of the InChI and wish to consult with Industry, Regulatory and Academic Sector users to identify and prioritise additional information that could/should be included in the QR code at a series of workshops.

More information can be found at this link

Dial-a-Molecule Steering Group

PI: Prof Richard Whitby *(University of Southampton)*

Co-I: Prof Steve Marsden *(University of Leeds)*

Co-I: Prof David Harrowven *(University of Southampton)*

Dr Robin Attrill *(GSK)*

Dr John Clough*(Syngenta)*

Prof Asterios Gavriilidis *(UCL)*

Dr Iain Gladwell *(Pfizer)*

Dr Mimi Hii *(Imperial College London)*

Dr David Hollinshead *(STB Associates)*

Prof John Leonard *(Royal Society of Chemistry)*

Dr Harris Makatsoris *(Brunel University)*

Dr Andrew Russell *(University of Reading)*

Ms Natasha Richardson *(EPSRC)*

Mrs Gillian Smith *(Gillian Smith Associates)*

Prof Joe Sweeney *(University of Huddersfield)*

Dr Matt Tozer

Prof Nick Turner *(University of Manchester)*

Chemical Synthesis in the 21st Century

The 3rd Dial-a-Molecule Annual Meeting

30 June & 1 July, University of Warwick

"**Chemical Synthesis in the 21st Century**" was the third running of the Dial-a-Molecule Annual Meeting series. Returning to the University of Warwick, the meeting was held on the 30 June and 1 July 2015 and was attended by 66 delegates over the two days. The meeting included a number of different elements, including keynote lectures, updates from Dial-a-Molecule supported projects, posters, an exhibition showcasing technology developed within the Network and discussion sessions designed to implement and advance objectives set out in the Roadmap.

Professor David Procter (University of Manchester) delivered the first of the two keynote lectures, describing research his group is undertaking towards identifying new methods for target synthesis by utilizing copper catalysts and metal-free cross-coupling reactions. **Dr Rebecca Goss** (University of St Andrews) followed in the afternoon with a very informative account of how synthetic chemistry can be combined with synthetic biology techniques to 'Dial-a-Molecule'.

After **Gill Smith** (Project Coordinator) gave an overview of the three Dial-a-Molecule inspired Manufacturing the Future projects, **Prof Asterios Gavriilidis** (UCL) and **Prof Kevin Booker-Milburn** (University of Bristol) provided updates on the projects they respectively lead: "Sustainable manufacturing in multiphase continuous reactors: Aerobic Oxidations" and "Factory in a Fume Cupboard: Reagentless flow reactors as enabling techniques for manufacture".

Since the 2014 Edition of the Annual Meeting, Dial-a-Molecule has supported a number of small projects centered on advancing areas within the Roadmap. **Dr Thomas Chamberlain** (University of Leeds) gave an update on the project looking at developing carbon nanoreactor stabilized nanoparticle catalysts, and **Dr Bao Nguyen** (University of Leeds) described the progress his team have made on electrochemically switchable catalysts in flow. **Dr Natalie Fey** (University of Bristol) provided a progress report on the collaborative projects she is involved with, looking at the use of descriptor-led ligand screening in organometallic catalysis. **Dr Richard Bourne** (University of Leeds) rounded off the mini-project updates with his work on optimizing reactions using statistical designs – both in the research and undergraduate laboratories. **Prof Steve Marsden** (University of Leeds) closed the meeting with an introduction to the European Lead Factory, and explained the opportunities available for academics to become involved.

A highlight of the meeting for many was the exhibition which showcased technology developed in research labs across the Network. Each research consortium was given 4 minutes to give a quick introduction to the technology, which was followed by a hands-on exhibition. There was a wide variety of items on show, including electrochemical flow cells and reactors, calorimeters, photochemical reactors, 3D printed flow reactors, mechanical grinding jars, wireless sensors and PCA maps developed for solvent selection.

A unique aspect of Dial-a-Molecule meetings is the breakout discussion sessions that centre on specific objectives of the Roadmap. Seven of these sessions were held over the two days. Outputs from the sessions have been summarized and can be found on the website.