

Dial-a-Molecule

An EPSRC Grand Challenge Network

August 2015

A warm welcome to the August Edition of the Dial-a-Molecule Newsletter. In this issue, we would like to draw your attention to the two upcoming events the Network are organizing, and some external activities relevant to the Network.

In this edition...

Dates for your Diaries: Upcoming Dial-a-Molecule Meetings:

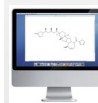
- Lead-Oriented Synthesis: Exploring Drug Relevant Chemical Diversity, 25th September, GSK Stevenage
- Smart Materials: Efficiency, Complexity & Design, 21st October, University of Warwick

External Events:

- Measurement, Information and Innovation: Digital Disruption in the Chemical Sciences, 20 October
- Understanding and Optimising Chemical Processes through Statistical Methodologies: 9-11 September

Funding Opportunities: ECR Travel Bursaries

Connect



www.dial-a-molecule.org



@DaM_Challenge



Dial-a-Molecule EPSRC
Grand Challenge

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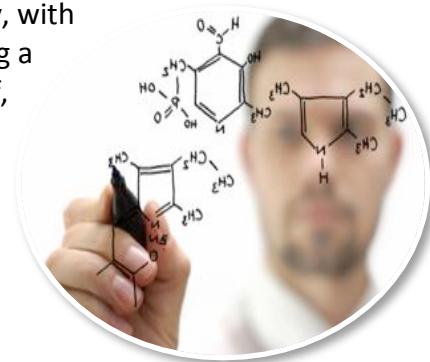
The Grand Challenge is owned by the community and we value your input and feedback, so if there is anything you think the Network should support or get involved in, please get in touch

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 sp³ 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, organised by the **EPSRC Dial-a-Molecule Grand Challenge Network**, 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.



[Register Now!](#)

The meeting is free to attend, but to facilitate with catering we ask you to register via the following link. Travel bursaries for Early Career Researchers are available and should be applied for upon registration.

Registrations close Friday 4th September

Program

09:45 Registration and Coffee

Session One: Chair – Prof Steve Marsden

10:30 Welcome and Housekeeping

10:40 How synthetic chemistry can drive the discovery of drugs of the future
Dr Ian Churcher (GSK)

11:00 Exploring 3-D pharmaceutical space: Lead-oriented synthesis and fragment-oriented synthesis
Prof. Peter O'Brien (University of York)

11:40 LLAMA: An open-access tool to guide lead-oriented synthesis
Prof Adam Nelson (University of Leeds) & Dr Richard Doveston (TU Eindhoven)

12:00 Lunch and Freeware demonstration

Session Two: Chair – Prof Adam Nelson

13:15 Synthetic strategies for the efficient exploration of lead-like space
Prof Steve Marsden (University of Leeds)

13:55 Design and exploitation of novel medicinal chemistry reagent sets
Dr Jason Kettle (AstraZeneca)

14:35 Enriching chemical space to drug undruggable targets
Prof. David Spring (University of Cambridge)

15:15 Afternoon Refreshments

15:45 Cross coupling 2.0
Prof Jeffrey Bode (ETH Zurich)

16:45 Concluding remarks and close of meeting

Smart Materials: Efficiency, Complexity and Design

University of Warwick, 21 October 2015

A meeting 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 polymerization will advances continue.

This meeting will consist of short presentations followed by facilitated round-table discussions which will be focused on identifying technology gaps and creating new collaborative frameworks.

Registration Details: The meeting is free to attend, but to facilitate with catering we ask you to register at the following [link](#). Travel bursaries for Early Career Researchers are available and should be applied for upon registration.

Organising Committee: Prof. Joe Sweeney and Prof. Rachel O'Reilly

Confirmed Speakers:

Prof Cameron Alexander
University of Nottingham

Dr Francisco Fernandez-Trillo
University of Birmingham

Dr Matthew I. Gibson
University of Warwick

Prof Alan Rowan
Radboud University of Nijmegen

Dr Helen Willcock
Loughborough University

Funding Opportunities:

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.

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 Peter Clark - *Knowledge Transfer Network*
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 - *Consultant*
3 Prof Nick Turner - *University of Manchester*



Other events....

A selection of conferences, meetings and workshops of relevance to the Network

Understanding and Optimising Chemical Processes through Statistical Methodologies

9 – 11 September, Durham University

The **Industrial 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 include a series of workshops involving experimental design, analysis and

interpretation of data that explore scoping, screening, optimization and robustness methods. The event is targeted at scientists, working in industry and academia, and at all scales from research through to manufacturing.

More information, including registration and contact details, can be found at the following [link](#).

Measurement, Information and Innovation: Digital Disruption in the Chemical Sciences

20 October, Royal Society of Chemistry (Burlington House), London

A one day meeting organized by two RSC Interest Groups: the **Automation and Analytical Management Group (AAMG)** and the **Chemical Information and Computer Applications Group (CICAG)** to address the challenges, opportunities and issues that arise through the digital transformation of laboratory work.

Please visit the [events website](#) for more information, including speakers and registration details.