

Dial-a-Molecule

An EPSRC Grand Challenge Network

March 2015

A warm welcome to the March 2015 Edition of the Dial-a-Molecule Newsletter. We are pleased that we can now officially announce the dates and location for the Dial-a-Molecule Annual Meeting for 2015, and are in the process of securing some exciting speakers. Keep watching this space for more information!

In this edition...

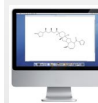
Dates for your Diaries: Upcoming Meetings:

- From Big Data to Chemical Information: 22 April
- Dial-a-Molecule 3rd Annual Meeting: 30 June & 1 July

Funding Opportunities:

- Dial-a-Molecule Mobility Grants
- ECR Travel Bursaries

Connect



www.dial-a-molecule.org



@DaM_Challenge



Dial-a-Molecule EPSRC
Grand Challenge

Contact

Dr Kelly Kilpin

Network Coordinator

K.J.Kilpin@soton.ac.uk

Tel: +44 (0) 2380 597314

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

Event: From Big Data to Chemical Information

Royal Society of Chemistry, 22 April 2015

An event jointly organized by Dial-a-Molecule and the RSC Chemical Information and Computer Applications Group



Large and complex data sets, often referred to as “Big Data”, can be difficult to manage and analyse using conventional processes and software tools. Such data sets exist in many disciplines, and chemistry is no exception. Most chemists are familiar with the huge growth in the number of compounds registered in databases in the public domain, the majority of which have data associated

with them. Many will also have struggled with increasingly large data sets generated through their work, often stored in spreadsheets with limited analytical capabilities.

To download a registration form, please visit www.dial-a-molecule.org

Program

10.00 Registration and tea/coffee

The Rise and Impact of Big Data

10.30 **Welcome and Introduction.** Dr Helen Cooke, CICAG Committee Chair

10.40 **Big data and the Dial-a-Molecule Grand Challenge.** Prof Richard Whitby, PI Dial-a-Molecule Grand Challenge Network, University of Southampton

11.00 **Big, broad and blighted data.** Prof Jeremy G. Frey, Department of Chemistry, University of Southampton

11.20 **Digital disruption in the laboratory: joined-up science?** Mr John Trigg, Automation and Analytical Management Group, RSC

11.40 **Big data chemistry.** Prof Jonathan Goodman, Department of Chemistry, University of Cambridge

12.00 Discussion

12.20 Lunch

Approaches to Managing Big Data and Maximising Opportunities

13.20 **Managing and searching large chemical structure data resources.** Dr Mark J Forster, Chemical Indexing Unit Team Leader, Syngenta R&D

13.40 **Data-Rich Organic Chemistry: Enabling and innovating the study of chemical reactions.** Prof Donna Blackmond, The Scripps Research Institute

14.00 **Use of data standards and metadata in information exchange.** Rachel Uphill, Early IP and Data Strategy Business Consultant, R&D IT, GlaxoSmithKline

14.20 **100 million compounds, 100K protein structures, 2 million reactions, 4 million journal articles, 20 million patents and 15 billion substructures: Is 20TB really big data?** Dr Noel O'Boyle, Senior Software Engineer at NextMove Software, Cambridge

14.40 **Dealing with the wealth of open source data.** Dr John Holliday, Senior Research Manager, Information School, University of Sheffield

15.20 Tea/Coffee

15.40 **Keynote: Activities at the Royal Society of Chemistry to gather, extract and analyze big datasets in chemistry.** Dr Tony Williams, Vice President of Strategic Development, Royal Society of Chemistry

Dial-a-Molecule Annual Meeting III

30 June – 1 July 2015

We are pleased to be able to announce that the Dial-a-Molecule Annual Meeting will be returning for a 3rd year.

This year we will go back to the **University of Warwick** where we officially launched the Dial-a-Molecule Roadmap almost 3 years ago!

Plenty has happened since then so save these dates! Registrations will open in the next few weeks.

Annual Meeting III Highlights

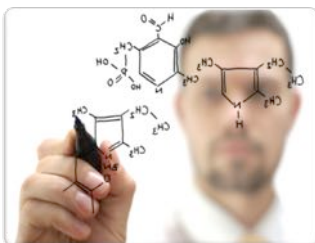
- Plenary Lectures from leading International speakers
- Updates from the Dial-a-Molecule Inspired Manufacturing the Future Projects
- Outputs from Dial-a-Molecule Proof of Concept studies
- Stars of Tomorrow Poster Session
- Technology Exhibition from Network Members
- Breakout sessions around areas central to Dial-a-Molecule

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 Mobility Grants

The activity aims to promote inter-disciplinary and academic-industry collaborations by funding travel and accommodation for short term visits and exchanges. These may involve several people and more than one visit. We expect a typical award to be £1-2000 and we aim to fund up to 40 exchanges over 3 yrs. Applications may be made at any time and we aim to turn-around in < 1 month.

For an application form, please visit the resources tab at www.dial-a-molecule.org

Dial-a-Molecule Steering Group

PI: Prof Richard Whitby (*University of Southampton*), **Co-I:** Prof Steve Marsden (*University of Leeds*), **Co-I:** Prof David Harrowen (*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 (*RSC/AstraZeneca*), Dr Harris Makatsoris (*Brunel University*), Dr Andrew Russell, (*University of Reading*), Ms Natasha Richardson (*EPSRC*), Dr Gillian Smith (*Gillian Smith Associates*), Prof Joe Sweeney, (*University of Huddersfield*), Dr Matt Tozer (*Peakdale Molecular Ltd*), Prof Nick Turner (*University of Manchester*)