Dial-a-Molecule

An EPSRC Grand Challenge Network

February 2015

Welcome to the February 2015 Edition of the Dial-a-Molecule Newsletter. We have a busy calendar for the next few months, so please read on to find out about the meetings that we have planned and some funding opportunities that are available.

In this edition…

Dates for your Diaries: Upcoming Meetings:

- Closed Loop Optimisation of Synthesis: 16 April
- From Big Data to Chemical Information: 22 April
- Making Molecules to Make Materials: An Exclusive ECR Event: 19-20 May
- Dial-a-Molecule 3rd Annual Meeting: 30 June & 1 July

Meeting Report: Catalytic Sustainability in the Future

Funding Opportunities:

- Dial-a-Molecule Mobility Grants
- 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

Event: Closed Loop Optimisation of Synthesis

GSK Stevenage, 16 April 2015

The optimisation of synthetic procedures is a time consuming process which is rarely carried out as efficiently as would be desirable. Automated reaction equipment, and in-line/in-situ analytical tools are becoming more readily available, but these still rely on the chemist to set-up reactions, analyse the outcomes, and decide which experiment(s) to do next.

Join us for a discussion on how to "Close the Loop" and utilise computer algorithms and automated equipment to remove the drudgery from optimising synthetic procedures.

Registrations close 22 March 2015

Organising Committee: *Richard Whitby, Andrew Richards, Robin Attrill & Gill Smith*

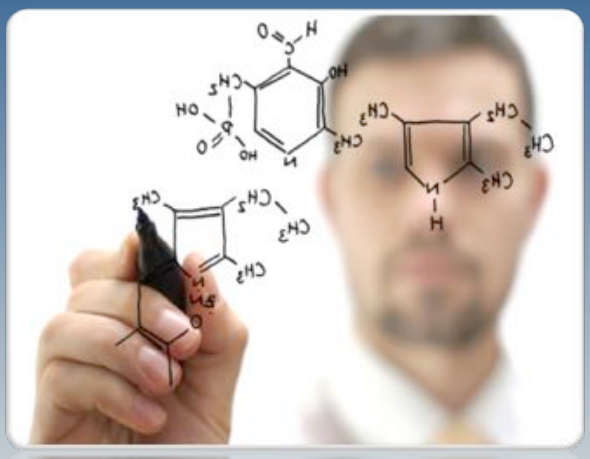
Plenary Speakers:

- **Dr Richard Bourne (University of Leeds)**
  Automated optimisation in continuous flow reactors
- **Prof Martyn Poliakoff (University of Nottingham)**
  Self-optimising and other reactions
- **Prof Lee Cronin (University of Glasgow)**
  Using configurable robotics, algorithms and randomness to discover and synthesise new molecules

Also included on the program

- Update from the Dial-a-Molecule inspired "Manufacturing the Future: Closed Loop Optimisation for Sustainable Chemical Manufacture" team
- Flash Poster Session
- Exhibition from key technology suppliers

*Visit **www.dial-a-molecule.org** for the full program*



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.

Event: From Big Data to Chemical Information

Royal Society of Chemistry, 22 April

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**. Professor Richard Whitby, PI Dial-a-Molecule Grand Challenge Network, University of Southampton

11.00 **Big, broad and blighted data**. Professor 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**. Professor 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 **Classification: square pegs and undetermined holes**. Dr Julie Wilson, Reader, University of York

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

Making Molecules to Make Materials

An Exclusive ECR Event

19-20 May 2015, Weetwood Hall Conference Centre and Hotel, Leeds

Dial-a-Molecule and our sister Grand Challenge Beyond the Molecule: Directed Assembly are joining forces to host an event **exclusively for Early Career Researchers** from across the two Networks.

We hope to encourage participants from a wide spread of disciplines, including - but not limited to - chemists, biochemists, chemical engineers, materials scientists, modelers, theoreticians, experimental or instrumental scientists.

The meeting will be structured around informal activities, with plenty of chances to show off your research through flash presentations, discuss your interests in a relaxed environment and discover what else is going on across the Networks and meet new people in the area. There will also be an Industry meet and great session to learn what Industry want and how to get in touch with them, and opportunities to speak to funding agencies.

There will be no charge to attend the meeting, although participants will need to meet their own travel costs. Meals and accommodation are included. We anticipate that this event will be extremely popular and to maximise networking opportunities numbers are limited!

If you would like to attend, please apply online via the Dial-a-Molecule website.

Applications close March 15 2015

ECR's are defined as 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 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)

Mr Simon Rushworth *(KTN)*

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)

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

Catalytic Sustainability in the Future

Meeting Report

Event Organisers: Dr David Mills & Dr Kelly Kilpin

The University of Manchester, School of Chemistry, hosted the Dial-a-Molecule Event "Catalytic Sustainability in the Future" in the Ellen Wilkinson building, lecture theatre C5.1, on 13th February 2015 from 1100-1900. Eighty people registered for and attended the event.

The Conference consisted of eight talks, across a broad range of subjects that encompassed the theme of catalytic sustainability, split into three sessions: After an introduction by **Prof Steve Marsden** (Leeds), the plenary lecture was delivered by **Prof. Laurent Maron** (Toulouse), who discussed the potential for f-element complexes in the catalytic activation of environmentally relevant small molecules. **Prof. Igor Larrosa** (Manchester) kindly stepped in at the last minute and discussed selective C–H activation chemistry at the meta-position of aromatic rings with late d-transition metal catalysts.

Dr Jonathan Moseley (CatScI Ltd) gave a talk on probing reaction mechanisms to identify by-products and therefore modify reaction conditions to increase yields and **Dr Bao Nguyen** (Leeds) discussed how X-ray absorption techniques can be applied to probe reaction mechanisms. **Dr Mimi Hii** (Imperial) gave a talk on mechanistic investigations coupled with a discussion on the suitability of batch and flow processes and **Dr Katherine Wheelhouse** (GSK) concluded the session by giving an industrial insight on precious metal catalysis and the development of catalytic processes by non-precious metal systems.

Prof. Matthew Davidson (Bath) discussed early transition metalcatalysis, focusing on hafnium and zirconium polymerisation systems mediating bio-polymer formation and **Prof. David Procter** (Manchester) concluded the formal program by speaking about copper-catalysed C–C bond-forming reactions and the potential of using samarium(II) systems in catalytic processes.

These speakers were supported by eleven flash presentations: Dr Matthew Edmundson (Edinburgh), Dr Fabrizio Ortu (Manchester), Dr Rebecca Melen (Cardiff), Dr Thomas Chamberlain (Nottingham), Mr Benjamin Zelenay (Imperial), Dr G. Richard Stevenson (UEA), Dr Sara Evangelisti (UCL), Dr David Mills (Manchester), Dr Jason Camp (Huddersfield), Dr James Walton (Durham) and Dr Daniele Leonori (Manchester).

Following the oral programme a poster session with refreshments was held in the foyer of the Chemistry Building, with 20 posters presented. Feedback for the event was very positive and we thank the speakers for giving a varied and entertaining programme.

DPM & KJK