Dial-a-Molecule Newsletter

Welcome to August's edition of the Dial-a-Molecule newsletter. July has been a month full of Dial-a-Molecule workshops. This edition of our newsletter includes meeting reports from workshops held under the Catalysis theme and Lab of the future theme. Also we are happy to announce our upcoming Rapid Reaction Analysis Workshop to be held at University of Strathclyde, Glasgow, U.K. on 7-8 September 2011. But first the meetings reports …

Meeting Report

Selectivity, Sustainability, Predictability: Multi-Disciplinary Issues for 21st Century Catalysis

7-8 July 2011

AstraZeneca, Alderley Park Conference Centre

The first of this summer's **Dial-a-Molecule** Grand Challenge meetings, a highly successful 2-day event under the Catalysis theme, took place on **7th - 8th July 2011** at **AstraZeneca's Alderley Park Conference Centre**. The meeting brought together 33 scientists from across industry and academia, and spanning a range of disciplines from outside synthetic chemistry including heterogeneous catalysis, surface science, membrane biology, chemical engineering, theoretical chemistry, physical organic chemistry and computing.

The programme was divided into three focused sessions. Each of the sessions started with informative and provocative assessments of the state of the art and key future directions from invited speakers, before the delegates split into small working groups to more tightly define new thematic areas of research. The first session **on New Reactivity: Target Driven Catalysis** featured talks from Nick Turner from CoEBio3 at Manchester (*The role of biocatalysis and synthetic biology*), Gerry Rassias from GlaxoSmithKline (*Industrial perspectives on the areas of need for new catalysis*), Joe Harrity from Sheffield (*Defining parameters to assess what makes an ideal catalytic reaction*) and Ron Grigg from Leeds (*Highlighting the potential of reactions that multiply orthogonal functionality in a single transformation*).

The second session focused on **Intervention-free Synthesis by Phase-Distinct Multi-Dimensional Catalysis**. Paula Booth from the School of Biochemistry at Bristol offered perspectives on compartmentalisation and active membrane transport from biology. Frontiers in phase-tagging of homogeneous catalysts and controllable activation were defined in presentations from Mark Muldoon (Queen's Belfast, liquid-liquid phase systems) and Chris Frost (Bath, magnetic nanoparticles for solid-liquid phase partitioning). Stan Golunski from the Cardiff Catalysis Institute outlined challenges and opportunities for fine chemical synthesis using heterogeneous catalysis.

The final scientific session addressed **Engineering Control Through Fundamental Mechanistic Understanding**. Jeremy Harvey (Bristol) discussed the state of maturity of theoretical approaches towards understanding and, in the future, predicting/designing reactivity, as well as summarising some of the roles that theoretical and chemoinformatic studies can play in **Dial-a-Molecule** as a whole. Paul Murray (CatSci) described the application of screening and statistical analysis approaches not just to reaction optimisation but also to developing predictive models for reaction/process design. John Atherton (Huddersfield) gave a perspective on the necessity of whole-systems approaches to a kinetic understanding of processes. Finally, Sven Schroeder from the School of Chemical Engineering at Manchester presented studies outlining the application of XPS and related techniques to reaction analysis in parallel platforms.

The outputs from the meeting, summarised in a plenary session, were not only tightly developed challenges for inclusion in the **Dial-a-Molecule** roadmap, but also new research groupings and networks stimulated through the discussions. Overall this was a highly interactive, stimulating and enjoyable two days, which will hopefully be replicated in the forthcoming meetings in the other Dial-a-Molecule challenge themes.

The organisers would like to thank AstraZeneca for their generous hospitality in hosting this meeting.

Additional information on the Catalysis theme and on the meeting can be obtained from Prof. Steve Marsden or from our network coordinator.

Meeting Report

Predicting reaction outcomes and developing perfect reactions

25-26 July 2011

Syngenta, Jeallot's Hill Research Centre, UK

The **Predicting Reaction Outcomes and Developing Perfect Reactions** meeting took place on the **25th -26th July 2011** at **Syngenta, Jealott's Hill Research Centre** in Bracknell, UK. Thirty two delegates attended the meeting, from across industry and academia and spanning a range of disciplines from computer science, statistics to chemical engineering and organic synthesis.

The programme was divided between informative, provocative assessments of the state of the art and key future directions from invited speakers and small group discussions on new thematic areas of research.

The meeting was opened by Prof. Whitby who presented the aims of the Dial-a-Molecule Grand Challenge and the objectives of this meeting. Dr. Sophie Schirmer (University of Cambridge) presented the view of a mathematician on modelling, control and optimization of chemical reactions.

The first session of talks focused on the need for optimal reactions. The session was kicked-off by a plenary presentation of Dr. Martin Owen (GSK) on Innovation, intrapreneurship and information. This was followed by a talk underlining the importance of efficient synthesis to the crop protection chemicals industry delivered by Dr. John Clough (Syngenta) and the views of Dr. John Knight (Scientific Update) on what makes a perfect synthetic transformation.

The series of talks continued in the afternoon with presentations on models and control for optimal reactions started by Dr. Harris Makatsoris (Brunel University) on unsupervised exploration of chemical spaces. The discussions were continued by Dr. John Slattery (University of York) on the designing new catalysis *in silico*, Dr. Dave Woods (University of Southampton) on statistically designed experiments for reaction optimisation and understanding and Dr. Vivek Dua (UCL) on decomposition approach for parameter estimation. Dr. Sebastian Mosbach (University of Cambridge) and Dr. Martyn Deal, (Radleys) concluded the session with discussions on automated model building for gas-phase chemical kinetics and reaction control in organic synthesis.

The final part of DAY 1 was dedicated to small group discussions. They were started by Dr. Frank Langbein (Cardiff University) who presented the draft roadmap of the Optimum reaction and route design focus area and focused on identifying opportunities on modelling, optimising and controlling reactions.

DAY 2 was started by Dr. Dave Woods (University of Southampton) who presented feedback from the first session of discussion on DAY 1. This was followed by Prof. Peter Johnson's (University of Leeds) plenary talk on the challenges and opportunities in reaction prediction. Next was Dr. David Blackmore (Pfizer) who asked us to think about the value of mining internal data sets for a better understanding of chemical reactivity. The series of talks was closed by the excellent presentation of Prof. Costas Pantelides (Process Systems Enterprise/Imperial College) on model-based reactor design when moving from laboratory to commercial scale.

The rest of the second day was dedicated to small group discussion on refinement of the roadmap and identifying opportunities on predicting reactivity and building models from data as well as identifying proposals topics to be taken forward. The heated debates identified three essential proposals that will be further developed by the Dial-a-Molecule members.

The first proposal relates to **Synthetic Route Finding and Modelling**. Here the aim is to devise computational methods to determine the most efficient route and optimal reaction conditions to synthesise a molecule. If you would like to get involved in this activity please contact Dr. Frank Langbein at F.C.Langbein@cs.cardiff.ac.uk or Dr. Richard Stephenson at g.r.stephenson@uea.ac.uk .

The second proposal that will be taken forward and developed by the Dial-a-Molecule members is **Modelling and Optimisation of Reactions**. This activity will deliver a validated method to estimate potential for successful reaction optimisation (or risk of failure to optimise to acceptable level). For more information and to get involved please contact Dr. Dave Woods at D.Woods@soton.ac.uk . The activity will extend to the more general problem of reaction outcome prediction when the substrates are a variable.

The final one is the need of a **National Centre for the study of reactions** recognising that the equipment and expertise needed are currently too expensive for individual departments to support. The main mission will be to use high throughput methods to determine the variation in reaction outcomes with respect to the substrates, and in collaboration with a range of research groups to use statistical and computational methods to allow reliable prediction of outcomes in untested cases. It would also promote the use of systematic study (and optimisation) of reactions by providing access to equipment and skills, and act as a central repository of data so generated. If you would like be involved in discussions on this activity please contact Prof. Richard Whitby at rjw1@soton.ac.uk .

The organisers would like to thank Syngenta for their generous hospitality in hosting this meeting.

Meeting Report

The Smart Laboratory: Towards a national ELN

28-29 July 2011

Chilworth Manor, Southampton, UK

The Smart Laboratory: Towards a national ELN thematic meeting organized by the Lab of the Future theme of the **Dial-a-Molecule** Grand Challenge, took place on the 28th–29th July 2011 in the beautiful Edwardian manor house of Chilworth Manor. It was tackling the often repeated observation that we must capture information on all reactions carried out, not just the most successful, if we are to progress to **'Dial-a-Molecule'**. A big step would be the implementation of an ELN system in academia, which formed the main theme of the meeting. The meeting included showcases from ELN developers, current users of ELN sharing their experience and views on existing systems as well as small group discussions on topics such as a 'wish list' of capabilities of an ELN, how could a national roll-out of ELN's be funded and implemented, how to collect more data with less effort, and store it in a more usable form and more.

The meeting was opened by Prof. Whitby who presented the aims of the **Dial-a-Molecule** Grand Challenge and the objectives of this meeting. The introduction was followed up by the excellent plenary lecture by Dr. Richard Bolton (GSK) who introduced the Pistoia Alliance and their working groups to the attendees underlying the importance of data sharing. There then followed the first of the many talks sharing the experience of current users on ELN presented by Dr. Robin Attrill (GSK) who presented the benefits that ELN brought to the activities of a large pharmaceutical company such as GSK.
These talks were followed by presentations from ELN developers who were supporting the meeting: IDBS, Accelrys, Perkin Elmer (CambridgeSoft) and ACD/Labs. Each of them presented their latest developments on this rapidly evolving market as well as insights into their future plans, providing an excellent introduction for the discussion planned in the afternoon.

The afternoon session was opened by a presentation from open-source ELN developers represented at this meeting by Dr. Simon Coles and Prof. Jeremy Frey (University of Southampton) who presented their plans for The Smart Research Framework: LabTrove, blog3 and LabBroker. The session broke out into small group discussions with each of the ELN developer present at the meeting to answer crucial questions such as: Why has uptake of ELNs in academia been poor?, What features would make adoption compelling?, What other features would we like? and Any problems that would limit adoption?.
The session was closed by Dr. Martin Sweet (EPSRC) who introduced the audience to the new research data policy adopted by EPSRC, introduced on 1 May 2011 with full compliance expected by 1 May 2015.

DAY 1 was concluded by a session of informal discussions around demonstrations stations provided by each of ELN developers which provided an ideal opportunity for delegates to find out and try the products on offer.

DAY 2 was kicked-off by Prof. Whitby who gave a brief review of the discussion from DAY 1. The introduction was followed by an excellent plenary talk from Dr. Brian Brooks (University of Cambridge) on the intelligent fume cupboard project from the research group of Dr. Murray-Rust. The project aimed to find improved ways that computers can help chemists in the lab and explores technologies such as speech recognition, video, infra-red and ultrasonic sensors, touch screens, laser keyboards, etc.
The talk was an excellent starting point for the following small group discussions on equipment and techniques that can help us to get more useful information into an ELN with less effort.

Dr. Dovey (JISC) presented means through which JISC can help universities to modernize and improve their digital infrastructure ensuring that UK remains world-class in research, teaching and learning.
The morning session was concluded by two excellent presentations delivered by Dr. Tim Dickens (University of Cambridge) and Mr. John Leonard (AstraZeneca) giving valuable insights from users that have already adopted the use of ELNs. They made a compelling case for the adoption of an ELN and, as Dr. Dickens eloquently said: *The question now is not if we should adopt it but rather when and how*.

The afternoon session was entirely dedicated to small group discussions focussed on four main topics: how can an ELN system be financed, what is the best strategy to deploy an ELN system, what disciplines outside of synthetic chemistry should be involved at this stage, and defining a common format for data exchange.

The major outputs from the meeting were to establish a group to lead the development of an open standard for electronic storage of experimental procedures and data, and to work with developers to pilot the use of electronic lab notebooks at selected universities. If you are interested in either initiative please let us know by email at dialamol@soton.ac.uk or contact Prof. Richard Whitby at rjw1@soton.ac.uk .

Meeting Information

Rapid Reaction Analysis

7-8 September 2011

University of Strathclyde, Glasgow, UK

Synopsis: Real-time analysis is key to advancements in a number of areas, e.g. design and optimisation of reactions, within Dial-A-Molecule. The meeting will look at: the technologies that are currently available and how they have been or could be used for real-time reaction analysis; and, identification of developments required in instrumentation and data analysis methodologies to enable wider use of real-time reaction analysis.

The meeting will bring together scientists and engineers from a wide range of disciplines to define short- to long-term challenges in the area, which will be used to produce a roadmap. Hence, the meeting provides an ideal opportunity for networking and new collaborations with a view to developing potential ideas for research proposals.

Registration Link: http://www.personal.soton.ac.uk/dialamol/conference1/registration_rra.php

Agenda for the meeting:

DAY 1, 7th September 2011

10.00 - 10.30 Registration and coffee
10.30 - 11.00 Introductory talk
11.00 - 13.00 Presentations from academics and industrialists on examples of use of reaction analysis (end-users and technology providers)
13.00 - 14.00 Lunch Break
14.00 - 15.30 Small-group discussions (needs and requirements from reaction analysis, barriers to wider use of current technology, areas where developments required)
15.30 - 16.00 Coffee Break
16.00 - 17.00 Feedback from small-group discussions
18.30 Dinner

DAY 2, 8th September 2011

Challenge 1: Instrumentation
09:00 - 09.30 Summary of development areas identified on DAY 1
09:30 - 10.30 Small-group discussions on how to move areas forward (short-, medium-, and long-term)
10.30 - 11.00 Coffee Break
11.00 - 12.00 Feedback from small-group discussions
12.00 - 13.00 Lunch Break
Challenge 2: Data analysis
13.00 - 13.30 Summary of development areas identified on DAY 1
13:30 - 14.30 Small-group discussions on how to move areas forward (short-, medium-, and long-term)
14.30 - 15.30 Feedback from small-group discussions
15.30 - 16.00 Coffee Break

Overnight accommodation is arranged and provided by **Dial-a-Molecule** at **Premier Inn Hotel (George Square)**. If you require accommodation for additional nights please contact Premier Inn Hotel at http://www.premierinn.com/en/home.action or at 0871 527 8440.

Please note that delegates will be responsible for their own travel expenses.

Please let us know if you cannot attend the event as we will charge you if you fail to attend on the day without notifying us with 2 weeks in advance.