Welcome to the April's edition of the Dial-a-Molecule newsletter. New and exciting things have been happening in the Dial-a-Molecule network. We have expanded our presence on the _connect platform, reports from 3 meetings and announcement of several upcoming meetings.

Dial-a-Molecule on the _connect platform

Recently Dial-a-Molecule has expanded its presence on the web to the _connect platform managed by the Technology Strategy Board which provides a virtual meeting space for all 16 Knowledge Transfer Networks, other supporting groups and FP7. If you are already member of _connect join the Dial-a-Molecule Group in the Chemistry Innovation Network and participate in the discussions, if not registration takes < 5 minutes. The website is accessible without joining, but you will not be able to participate in discussions. Membership helps you to meet people with related research interests and establish new and fruitful collaborations.

MEETING REPORT
DIAL-A-MOLECULE INDUSTRY FOCUS MEETING

The Dial-a-Molecule INDUSTRY FOCUS MEETING took place at the SCI, London on Monday, 11th April and was well attended by representatives of companies from across the chemical-using industries, including pharmaceuticals, agrochemicals, catalysis and fine chemicals. Technology and solution providers, ranging from equipment suppliers to modelling and cheminformatics companies, were also represented together with key people from professional bodies and research councils, including the RSC and MRC.

Since the launch of the Grand Challenge in October 2010 9 focus area have been developed under the themes of Lab of the Future & Synthetic Route Selection (4 focus areas), Catalytic Paradigms for 100% efficient synthesis (3 focus areas) and A Step Change in Molecular Synthesis (2 focus areas). Industry input was invaluable in initially developing these themes, but the INDUSTRY FOCUS MEETING was important to give the themes a broader industrial steer & to make them as industry relevant, academically challenging and fundable as possible.

There was strong support for the proposed themes and focus areas and the meeting has allowed these areas to be more tightly focused and prioritised.

- Detail on the themes and the champions in these areas can be found through the website.
- A summary of the industry input will shortly be available on the website on which we welcome your feedback.

We hope that the theme meetings for the Grand Challenge will interest you and that you'll be able to contribute your expertise, ideas or support. Inclusivity is essential for this activity & the true test for the Grand Challenge will be the quality of the roadmap which is developed and quality and depth of the research proposals, or collaborations it generates.

If you have any questions please contact either Prof Richard Whitby (University of Southampton, PI) or Dr Stephen Hillier (Chemistry Innovation KTN).

MEETING REPORT
DIAL-A-MOLECULE AT EXTERNAL COLLABORATION WORKSHOP

Dial-a-Molecule was represented at a Royal Society of Chemistry "Precompetitive Workshop" entitled "Getting the most out of external collaborations" held in London on 28th March. The meeting was organised by Dr David Fox of Pfizer and Dr Ellen Friel of the Royal Society of Chemistry. David, who is a Visiting Senior Industrial Fellow at the RSC, is a member of the **Dial-a-Molecule** steering group. The aim of the workshop was to discuss how the open innovation agenda impacts on interactions between and amongst the pharmaceutical industry and academia. Around 60 delegates were present, representing over 15 companies, 14 Universities, and funding agencies including EPSRC, BBSRC, MRC and the TSB. The day featured plenary presentations from Will Barton, the Head of Technology at the TSB, and Malcolm Skingle, the Director of Academic Liaison at GSK, as well as supporting talks describing exemplar case studies of different collaboration models, and networking poster sessions, including one on **Dial-a-Molecule** presented by Steve Marsden.

Meet a member

Asterios Gavriilidis is a member of the Steering Group for the Next Generation Reaction Platforms focus area in Dial-a-Molecule network. As professor of Chemical Reaction Engineering at University College London, his expertise is on chemical and catalytic reaction engineering, and over the last ten years he has specialised in the area of flow microreaction technology. His group has worked on the design, development and evaluation of high temperature gas phase and low temperature multiphase microstructured reactors, using in addition to experimental approaches various modelling tools, such as CFD simulations. The reactors have been used to perform various types of reactions including catalytic oxidations, hydrogenations, epoxidations, ozonolysis etc. Some highlights of the group's research are: studies on design and fabrication of zeolite-based microstructured reactors for liquid phase reactions, studies on catalytic falling film microstructured reactors for hydrogenation reactions; demonstration of microfabricated reactors for in situ Raman and EXAFS measurements during gas phase catalysis. Find out more about Prof Asterios Gavriilidis and other members on our website.

The outcomes of the meeting are the five working groups listed at the end of this article. Each of these areas impacts upon **Dial-a-Molecule**, either in terms of driving new demands on molecular synthesis, or in changing the way we think about establishing collaborations to achieve these goals. The groups will be meeting for the first time shortly to discuss how to drive the areas forward, and we will report back on any future developments from the working groups in future newsletters. Anyone interested in getting involved in the networks should contact Dr Ellen Friel at the RSC (friele@rsc.org).

Working groups (**Dial-a-Molecule** steering group members on the groups shown in parentheses):

1) Establishment of a national compound screening bank (Joe Sweeney);
2) Developing a more effective communication bridge across pharma, SMEs and academia (Stephen Hillier);
3) Translational chemical synthesis (Steve Marsden, Joe Sweeney);
4) A shared model for collaborative agreements (David Hollinshead);
5) A model for supporting better interactions with SME companies (David Hollinshead and Stephen Hillier).

MEETING REPORT
DIAL-A-MOLECULE AT DATA TO KNOWLEDGE MEETING

Dial-a-Molecule was represented at the Data to Knowledge meeting held on 29-30 March 2011 at AstraZeneca, Alderley Park. The meeting was organised jointly by the RSC Molecular Spectroscopy

Group and the British Mass Spectrometry Society. It covered topics such as automated data processing, the use of historical data & databases, predictive tools, peak deconvolution & principal component analysis applied to the analysis and interpretation of mass spectrometry, NMR spectroscopy,vibrational spectroscopy & chromatographic data.

Since its launch meeting Dial-a-Molecule has recognised that the capability to rapidly, ideally in real time, analyse the components in a reaction is crucial in achieving its aims. Dr. John Langley has presented a poster on behalf of Dial-a-Molecule which was well received by the attendees and underlined once again the need to set-up a new focus area dedicated to this topic.

Dial-a-Molecule is currently searching for volunteers (champions) to lead the Real-time Analysis focus area and help us organise provocative meetings and generate collaborative proposals that will drive the Dial-a-Molecule agenda forward in this critical area. If you are such a person please contact us at dialamol@soton.ac.uk.

Volunteers wanted

Do you have a bright idea and are searching for collaborations? **Dial-a-Molecule** is looking for volunteers to organise meetings to promote research collaborations in a theme area. Please contact the network coordinator (dialamol@soton.ac.uk).

UPCOMING MEETINGS

The ambitions of Dial-a-Molecule are straightforward:

- To facilitate the formation of effective networks & consortia to address the themes of Dial-a-Molecule
- To establish new collaborations and initiated grant proposals (or alternative funding mechanisms)
- To raise the profile of Synthesis as a Grand Challenge.

These ambitions will be realised through a series of theme meetings.

MEETING ANNOUNCEMENT
SELECTIVITY, SUSTAINABILITY, PREDICTABILITY: MULTI-DISCIPLINARY ISSUES FOR 21ST CENTURY CATALYSIS

The Catalysis theme of **Dial-a-Molecule** will be running a 2-day meeting at **AstraZeneca's Alderley Park** site on **7th/8th July 2011**. The meeting will be built around three overlapping themes: Engineering control (improved understanding of catalyst activity, selectivity and longevity), New reactivity in catalysis (processes that proliferate complexity and functionality simultaneously, by harnessing new reactivity or re-wiring existing pathways such as in biocatalysis) and Intervention free synthesis (cascaded processes, whether by highly selective one-pot, multi-reaction processes, or temporally, spatially and/or phase-separated reactions).

The meeting will involve short, provocative presentations from invited experts from inside and outside the synthetic chemical community (*eg* experts in biocatalysis, engineering, complex kinetics, computational chemistry, spectroscopists/spectrometrists etc) aimed at stimulating discussion. These will be followed by small working groups, the aim of which is to define new areas for study, the resource/teams needed and to put a timeframe on developments. The outputs from the meeting will form an important part of the Dial-a-Molecule roadmap.

Due to space issues, attendance at the meeting is restricted to ca. 40 delegates and will be by application. Further details of the meeting, speakers and application process will be publicized through the **Dial-a-Molecule** network in the upcoming period.

For more information concerning the meeting and on the catalysis theme please contact Prof Steve Marsden or email us at dialamol@soton.ac.uk.

OTHER MEETINGS PROPOSED FOR JUNE – SEPTEMBER 2011

1. ***Making a reaction perfect***. How can we develop reactions so that they always give high yields and clean products? The meeting will cover discussions about rapid optimisation of a particular transformation as well as the experimental and theoretical study of a reaction type so that success in unknown cases can be predicted reliably. Both software and hardware development have crucial parts to play. The purpose of the meeting is to better understand the state of the art in the various fields and thus identify links and initiate collaborations towards the goal of achieving optimum reaction design. It will also discuss how such methods can be deployed for routine use in U.K. academia. The meeting is currently being planned for July.
2. ***Prediction of Reaction Outcomes and Synthetic Routes***. How can we best use available reaction data and /or computer models to predict the outcome and optimum conditions for unknown reactions (and is such data of sufficient quality)? How can we identify the optimum synthetic route to a target under constraints (scale, cost, sustainability, time, available reaction platform etc)? How can the information in existing reaction databases presented to chemists in a way that allows better selection of reaction conditions and synthetic routes. The meeting will bring together mathematicians, computer scientists, chemists and others to tackle the above problems which lay at the heart of achieving Dial-a-Molecule.
3. ***The Smart Laboratory*.** Collection of complete reaction data on all reactions carried out has been identified as a key enabling step towards Dial-a-Molecule and this meetings aim is to develop a route to allow it. The use of Electronic Lab Notebook's (ELNs) to collect and allow re-use of such data seems central. Questions to be tackled include: why are academics not using ELN's; what properties of an ELN would drive universal acceptance; how do we get information into an ELN with minimum work for the chemist; can universal standards for reaction data be developed to enable interchange between different systems as well as allowing efficient automated harvesting of information; IP issues; how might a national ELN be rolled out, and how might it be paid for?
4. ***Reactor Platforms for the Lab of the future***. The meeting aims to define the near-, medium- and long-term prospects and impact of new innovative and integrated technology for carrying out synthesis as well as developing the business case for the adoption of the technology.
5. ***Reagentless Synthesis.*** Reactions driven by direct energy input rather than from an additional component (reagent) are ideally suited to sequencing, particularly using flow techniques, as by-products are not inherent. Examples include thermal, photochemical, microwave, THz radiation, ultrasound and electrochemical techniques. The meeting will define the scope of 'Reagentless Synthesis', identify particular opportunities for development and suitable topics for collaboration.
6. ***1000 Click Reactions/Perfect reactions (provisional title).*** The term 'click chemistry' has come to refer to a specific reaction rather than, as originally intended, any reaction which meets particular criteria for yield and robustness. The meeting aims to promote the development of many more 'click' transformations. It will set-out criteria on how to judge new '*click*' processes, identify key transformations in need of optimisation to 'click' status, and desirable reactions that at present have no adequate method to achieve them in very high yield.
7. ***Holistic approach to molecular synthesis.*** The holistic approach is a novel approach to synthesis where maximisation of complexity build-up and minimisation of steps is central. This meeting will make a case for the development of such reactions and identify strategies to tackle it, realistic goals for short, medium and long-term together with teams to take the ideas forward.

If you are interested in any of the meetings and you would like to get involved in the planning please let us know by email to dialamol@soton.ac.uk.