

Dial-a-Molecule

An EPSRC Grand Challenge network

An EPSRC **Dial-a-Molecule** Grand Challenge theme meeting

Predicting reaction outcomes and developing perfect reactions



25-26 July 2011

Syngenta, Jealott's Hill Research Centre

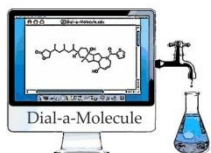
EPSRC

Engineering and Physical Sciences
Research Council

Register online:

www.dial-a-molecule.org/events/

email: dialamol@soton.ac.uk



Predicting reaction outcomes and developing perfect reactions

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Dial-a-Molecule is a Grand Challenge network funded by EPSRC to promote research aimed at promoting a step change in our ability to deliver molecules quickly and efficiently.

How can we make molecules in DAYS not YEARS?

Dial-a-Molecule requires the multi-reaction sequences to make a target, each step of which must be successful. Being able to predict the outcome of novel reactions with high reliability is thus central to achieving the Grand Challenge. Since prediction of ideal reaction conditions in advance is improbable, ways to optimise reactions in real time are also necessary to provide efficient routes.

A multi-disciplinary approach is necessary to tackle this difficult problem including many aspects of chemistry, engineering, mathematics and computer science.

The **Lab of the Future** theme of the EPSRC **Dial-a-Molecule** Grand Challenge will be running a 2-day meeting at **Syngenta, Jealott's Hill Research Centre** on **25-26 July 2011** focused on establishing a roadmap to achieve a step change in the ability to predict the outcome of reactions and to rapidly optimise reactions. It will also establish multi-disciplinary groups to compete for funding to advance the area.

The meeting will tackle questions such as:

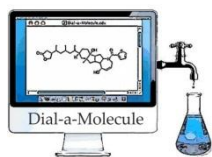
- How can we make more effective use of past experimental data to predict the outcome of novel chemical reactions? Can information from computer models be integrated? How can more and better quality data be made available?
- What are the best approaches to experimentally and theoretically study a reaction type (e.g. Sonogashira) so that optimum conditions and outcomes in all novel cases can be predicted reliably – developing a *perfect reaction*. Should the equipment and software required for high throughput study of reactions become a standard departmental facility (like NMR, MS...)? Is there a case for a national service (central or distributed) for reaction study?
- Can we define a roadmap which leads to the routine auto-optimisation of reactions? What advances in technology, analysis, software are required?
- Is there a case for strongly promoting the use of statistical and/or theoretical methods in routine synthesis?
- What advances in equipment, software and techniques are needed to enable the above? Can technologies currently used in a process environment be reduced in cost, size and ease of use to allow routine use in synthesis? Is there the opportunity to further advance the strong U.K. industry in the provision of equipment and software for reaction chemistry?

There will be presentations on the state of the art in the above areas together with group work to define a roadmap for progress in the area and to develop collaborations to tackle the problems. 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. 30 delegates. Applications for the meeting are now invited by completing the attached form or by on-line registration.

The closing date for applications is **Friday 8th July 2011** but we encourage you to apply early as places are limited.

Please note that although there is no registration fee for the meeting and **Dial-a-Molecule** will arrange and cover the costs of overnight accommodation, delegates will be responsible for their own travel expenses.



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Personal Details

First Name:
Last Name:
Email:
Phone:

Organization:

Department:

Position:

Address:

Please tell us why you are interested in the meeting (<100 words)

Briefly outline any particular areas of expertise/interest relevant to the meeting
(<200 words)

I would be willing, if asked, to present a short (10 minute) summary on a topic of my
choice relevant to the meeting

Topic Title:

☐ Yes

☐ No

I would like to participate at the following days:

☐

Monday, 25th July 2011

☐

Tuesday, 26th July 2011

Please return by **Friday 8th July 2011** to:

Bogdan Ibanescu, Dial-a-Molecule Network Assistant Coordinator.

Email: dialamol@soton.ac.uk

Post: School of Chemistry, University of Southampton, Highfield, Southampton, SO17 1BJ.

Syngenta, Jealott's Hill Research Centre, UK
25-26 July 2011