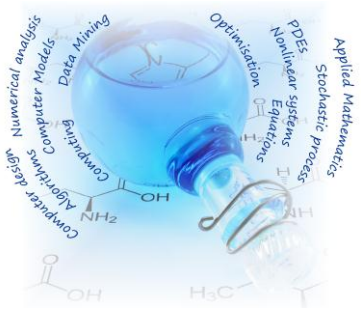
Welcome to July's edition of the Dial-a-Molecule newsletter. This edition is full of information concerning the upcoming events organised by our network. Also we are delighted to welcome two new champions in our network: Dr. Alison Norton (Strathclyde) and Dr. Ian Clegg (Pfizer) who will be joining our core theme in the critical **Rapid Complete Reaction Analysis** focus area. But first let's kick-off with …

Meeting information



Predicting reaction outcomes and developing perfect reactions

25-26 July 2011

Syngenta, Jealott's Hill Research Centre

Synopsis: The meeting will cover topics such as: predicting the outcome of chemical reactions based on experimental data and computer models; prediction of the optimum synthetic route to a target under constraints (scale, cost, sustainability, time, available reaction platform etc); rapid (auto) optimisation of reactions; study of a reaction type to allow reliable prediction of outcomes in unknown cases. The meeting aims to build collaborations between chemists, engineers, mathematicians and computer scientists to bring fresh approaches to the above problems.

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

Program of the Meeting:

DAY 1, Monday 25th July 2011

10:00 – 10:30	Coffee and registration
10:30 – 11:00	Introductory talks
11:00 – 12:20	Talks 1: **The Need for Optimal Reactions**.
13:30 – 15:00	Talks 2: **Models and Control for Optimal Reactions.**
15:30 – 17:30	Group work 1: **Roadmap and Proposals - Control and Models**
19:00 – 20:00	Conference Dinner
20:00	Informal discussions on potential collaborative proposals

DAY 2, Tuesday 26th July 2011

09:00 – 10:10	Talks 3: **Predicting Reactivity from Experimental Data.**
10:30 – 12:30	Group work 2: **Roadmap and Proposals - Models and Data**
13:30 – 15:00	Group work 3: **Funding and Proposals**
15:30 – 16:00	Group discussions to develop proposal outlines
16.00 – 16:30	Round up and ways forwards
16:30	Meeting Close

The Smart Laboratory: Towards a national ELN
28-29 July 2011
Best Western Chilworth Manor, Southampton, UK

Synopsis: The meeting is focussed on the acquisition and sharing of laboratory data, particularly on reactions and compounds. How to collect more data with less effort, and store it in a more usable form? A plan for the adoption of Electronic Laboratory Notebooks (ELNs) in academia and the establishment of a national framework for the sharing of experimental data are intended outputs.

The meeting will involve presentation form current users of ELN, sharing their experience and views on existing systems, showcases from providers of ELN's. These will be followed by small working groups, the aims of which are to develop a plan for implementation of national ELN and a business case for funding it. The outputs from the meeting will form an important part of the Dial-a-Molecule roadmap.

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

Program of the Meeting:

DAY 1: Thursday, 28th July 2011

10:00 – 10:30	Registration & Coffee
10:30 – 10:40	Welcome message
10:40 – 11:30	Plenary presentations from Dr. Richard Bolton (GSK) and Dr. Martin Sweet (EPSRC)
11.25 – 14:30	Electronic Lab Notebooks – the view from developers (IDBS, Accelrys, Cambridgesoft and ACD/Labs).
14:30 – 16:40	Round table discussions with ELN developers.
16:40 – 17:00	UMF project, Prof. Jeremey Frey, Dr. Simon Coles, University of Southampton.
17:00 – 17.30	Open discussions on the priority order for characteristics of an ELN.
18:30 – 20:00	Conference Dinner
20:00	Informal discussions with ELN developers and networking

DAY 2: Friday, 29th July 2011

9.00 – 9:10	Summary from DAY 1 and looking to the future of Smart laboratory
9:10 – 9:30	The intelligent FC project, Dr. Brian Brooks, University of Cambridge.
9:30 – 10:30	Workshop session: Equipment and techniques to get more information into an ELN with less effort.
11:00 – 11:20	JISC – University modernisation: rational and approaches.
11:20 – 12:30	Round table discussions session 1
13:30 – 15:00	Round table discussions session 2
15:30 – 16:30	General discussion on the way forward.
16:30	Meeting close

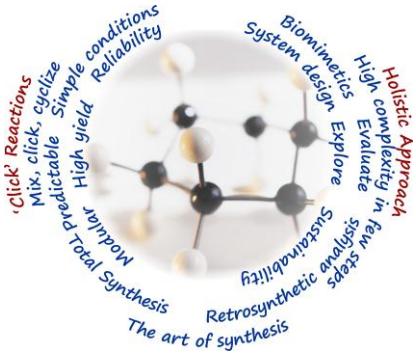
Welcome to Ian

Since the last newsletter, we've recruited a new champion into the core team. Dr Ian Clegg from Pfizer will be joining our existing champions taking forward the critical **Rapid Complete Reaction Analysis** focus area.

Ian is an Associate Research Fellow for PAT working for Pfizer Worldwide R&D. His remit is to apply the full range of PAT technologies during development and scale up of APIs and Solid Oral Pharmaceutical products.

He holds a BSc in Chemistry and also a PhD in Instrumentation and Analytical Science (both from the University of Manchester). Ian is a member of the Royal Society of Chemistry, an associate member of the Institution of Chemical Engineers and is also a member of the EPSRC peer review college.

Ian started his career with ICI and held a variety of roles in Research, Development and Engineering where he designed, developed and commissioned measurement / PAT systems on manufacturing units and within R&D. Prior to joining Pfizer, Ian also had a senior consultancy role working for ABB in the area of measurement science and PAT.



A Step Change in Synthesis

2-3 August 2011

AstraZeneca Macclesfied Research Centre, Cheshire, UK

Synopsis: The meeting will consider two approaches to **Dial-a-Molecule** challenge. One is to develop many *perfect reactions* which always work and can be readily sequenced so that the number of steps in a synthesis is unimportant. The other is to develop a holistic approach in which minimisation of the number of steps is the goal. Topics will include: What are *click reactions*, how can they be developed, and which would have most impact; Reagentless synthesis; How can synthetic planning incorporate reactions which achieve maximum increase in complexity; Can we invent *molecule specific* multi-bond forming reactions *on-the-fly* to achieve rapid synthesis. Meeting outputs are expected to include the formation of groups to develop fundable proposals to promote a step change in synthesis.

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

Program of the Meeting:

DAY 1: Tuesday, 2nd August 2011

10:00 – 10:30	Arrival and registration
10:30 – 10:45	Opening of the meeting and welcome message
10:45 – 11:30	Thematic presentations
11:30 – 12:30	Round table discussion*:* **Focus areas in A step change in molecular synthesis theme**
13:30 – 13:45	Workshop session: **A step change in molecular synthesis** roadmap
13:45 – 15:00	Round table discussions: **Emerging themes in synthesis**
15:30 – 15:45	Feedback from first round table discussions
15:45 – 17:00	Round table discussions: **Refining the key themes in synthesis**
17:00 – 17:15	Workshop session: **A step change in molecular synthesis** roadmap
19:00 – 21:00	Conference Dinner
21:00 – 22:00	Networking session

DAY 2: Wednesday, 2nd August 2011

09:30 – 10:00	Introduction to the day and feedback from discussions on DAY 1
10:00 – 13:00	Sandpit session: **Future collaborations in synthesis ***
14:00 – 14:30	Closing remarks from the Steering Group
14:30	Meeting close

* Additional time is reserved for a second sandpit session after the lunch break, if requested by participants.

CLiDE: Chemical Literature Data Extraction

CLiDE is a chemistry intelligent equivalent of Optical Character Recognition (OCR) software. Just as an OCR can recognize characters from a scanned images of printed text, CLiDE can recognize structures, reactions and text from scanned images of printed chemistry literature.

The software saves users hours of redrawing structures from printed material, as it transforms the *images* into a *real structures* that can then be input into databases.

The latest edition CLiDE v4 comes in three flavors: CLiDE Standard, CLiDE Professional and CLiDE Batch.

The CLiDE software was originally written at the University of Leeds, UK. It is currently developed and maintained by Keymodule Ltd, UK, and marketed by SimBioSys Inc.

Reactor platforms for the 21st century lab: Synthesis-on-Demand at minimum waste

11-12 August 2011

GSK, Stevenage Research Centre, UK

Synopsis:

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. It will create a map of the state of the art and perform gap analysis, identify trends and project them into a development roadmap.

It is an ideal opportunity for networking and partnering environment for grant proposal preparation or technology development and transfer to industrial collaborators and fostering strong links and collaborations at the biology – chemist –engineering interface.

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

Program:

DAY 1: Thursday, 11th August 2011: Roadmap for the future Workshop

09:30 – 10:00	Coffee and registration - Posters
10:00 – 10:15	Welcome and introduction
10:15 – 11:40	Invited talks – **Framing the challenge**
11:40 – 13:00	2 min Flash presentation from meeting participants
13:00 – 14:00	Lunch and networking - Posters
14:00 – 14:45	Breakout session 1: **Defining future research agendas**
15:45 – 16:30	Breakout session 2: **Defining future research agendas**
16:30 – 17:15	Debate and feedback
17:15	Meeting close
19:00 – 20:00	Meeting dinner
20:00	Informal discussions on potential collaborative proposals

DAY 2: Friday, 12th August 2011: Sandpit

09:00 – 09:30	Coffee and registration - Posters
09:30 – 09:45	Welcome and introduction to the day, feedback from Day 1
09:45 – 10:45	Sandpit session 1: **Idea generation**
11:00 – 12:30	Sandpit session 2: **Forming of collaborations and idea refinement**
12:30 – 13:30	Lunch and networking - Posters
13:30 – 14:30	Sandpit Session 3: **Partnering and next steps**
14:30 – 15:00	Debate and feedback
15:00 – 15:15	Closing remarks and next steps
15:15	Meeting close

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