Predicting Reaction Outcomes and Developing Perfect Reactions

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, chaired by Prof. Whitby, 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.

Most 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 one is the need of a National Centre for the study of reactions whose main mission will be to determine the scope of reactions with respect to the substrates, and to use statistical and computational methods to allow reliable prediction of outcomes in untested cases. Also it will promote the use of systematic study (and optimisation) of reactions, and act as a central repository of data so generated. If you would like to get involved in this activity please contact Prof. Richard Whitby at rjw1@soton.ac.uk .

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