

## A Step Change in Synthesis meeting at AstraZeneca, Macclesfield on 2-3 August 2011



On 2<sup>nd</sup> and 3<sup>rd</sup> August 2011 *A step-change in molecular synthesis* theme of the EPSRC **Dial-a-Molecule** Grand Challenge organized a two day '**A step-change in synthesis**' workshop. Hosted at AstraZeneca Macclesfield site the workshop was attended by 31 delegates from academia and the chemical industry. The meeting included presentations from the champions of the theme and small group discussions on the emerging themes in synthesis. It was aimed at identifying which projects are required to increase our ability to generate new molecules faster and more efficiently.

The meeting was opened by Dr Andrew Russell (University of Reading) who presented the aims of the **Dial-a-Molecule** Grand Challenge and the objectives of this meeting. The introduction was followed up by Dr David Hollinshead's (AstraZeneca) presentation underlining the importance of the meeting from industry's point of view. Dr Andrew Russell (University of Reading) - *An interplay of theory and synthesis – the way forward?*, Prof. David Harrowven (University of Southampton) – *Approaches and Issues*, and Prof. Kevin Booker-Milburn (University of Bristol) - *Complex Molecule Synthesis: A Self-Critical Analysis*, framed the meeting and the current challenges facing synthesis as well as setting out two approaches to resolving these issues: 1000 Click Reactions and a Holistic Approach to Synthesis.

The excellent presentations were followed by a session of round table discussions focused on identifying key focus areas and challenges in the *A step-change in molecular synthesis* theme. The debate continued in the afternoon session with round table discussions on the emerging themes in synthesis, aiming to identify the next big opportunities. This session also included considered discussion on the **Dial-a-Molecule** roadmap, identifying the main challenges, achievements and activities necessary to reach a step-change in our ability to generate new molecules.

DAY 1 of the workshop ended with a voting session on the identified challenges such as: smart ways of identifying the key transformations and identifying 'magic reactions' which would dramatically shorten the synthesis (using computational tools); definition of a set of benchmark reactions & reaction validation tools and gaining fundamental understanding of reactions; new perfect reactions: activated Click – Catalytic, Photolytic, Electrolytic, *Harmless 3<sup>rd</sup> component*; late stage functionalization: beyond C-H functionalization; OMIC approach to new reaction discovery: toolbox development: generic protocols for critical transformations and use of computation/Data mining/ spectroscopy to design new reactions. This vote will inform future discussions on areas to take forward for further study.



The second day of the workshop was kicked-off by a plenary presentation from Prof. Joe Sweeney (University of Reading) and a review on the discussions from the first day delivered by Dr Andrew Russell (University of Reading) Was this summary done by Kevin?. Both presentations set the scene for the discussion that followed in the sandpit session.

The sandpit session was dedicated to discussion on the next projects to be carried forward and developed by Dial-a-Molecule members based on the challenges identified in the first day.

No doubt the meeting may be considered a success. The interesting presentations pointing out the main objectives of the **Dial-a-Molecule** project whilst the challenges in today's synthesis opened the door for discussions meant to clarify main aspects for '*A step-change in molecular synthesis*' theme. From the fruitful discussions among participants, a lot of valuable ideas arose that will form the foundation for the future development of the **Dial-a-Molecule** Grand Challenge.

The organising committee would like to thank all the delegates who attended as well the AstraZeneca for hosting the meeting and the support provided.