

Selectivity, Sustainability, Predictability: Multi-Disciplinary Issues for 21st Century Catalysis



The first of this summer's **Dial-a-Molecule** Grand Challenge meetings, a highly successful 2-day event under the catalysis theme, took place on 7th-8th July at AstraZeneca's Alderley Park conference centre. The meeting brought together 33 scientists from across industry and academia, and spanning a range of disciplines from outside synthetic chemistry including heterogeneous catalysis, surface science, membrane biology, chemical engineering, theoretical chemistry, physical organic chemistry and computing.

The programme was divided into three focused sessions. Each of the sessions started with informative and provocative assessments of the state of the art and key future directions from invited speakers, before the delegates split into small working groups to more tightly define new thematic areas of research. The first session on "*New Reactivity: Target Driven Catalysis*" featured talks from Nick Turner from CoEBio3 at Manchester (**The role of biocatalysis and synthetic biology**), Gerry Rassias from GlaxoSmithKline (**Industrial perspectives on the areas of need for new catalysis**), Joe Harrity from Sheffield (**Defining parameters to assess what makes an 'ideal' catalytic reaction**) and Ron Grigg from Leeds (**Highlighting the potential of reactions that multiply orthogonal functionality in a single transformation**).

The second session focused on "*Intervention-free Synthesis by Phase-Distinct Multi-Dimensional Catalysis*". Paula Booth from the School of Biochemistry at Bristol offered perspectives on compartmentalisation and active membrane transport from biology. Frontiers in phase-tagging of homogeneous catalysts and controllable activation were defined in presentations from Mark Muldoon (Queen's Belfast, liquid-liquid phase systems) and Chris Frost (Bath, magnetic nanoparticles for solid-liquid phase partitioning). Stan Golunski from the Cardiff Catalysis Institute outlined challenges and opportunities for fine chemical synthesis using heterogeneous catalysis.

The final scientific session addressed "*Engineering Control Through Fundamental Mechanistic Understanding*". Jeremy Harvey (Bristol) discussed the state of maturity of theoretical approaches towards understanding and, in the future, predicting/designing reactivity, as well as summarising some of the roles that theoretical and chemoinformatic studies can play in **Dial-a-Molecule** as a whole. Paul Murray (CatSci) described the application of screening and statistical analysis approaches not just to reaction optimisation but also to developing predictive models for reaction/process design. John Atherton (Huddersfield) gave a perspective on the necessity of whole-systems approaches to a kinetic understanding of processes. Finally, Sven Schroeder from the School of Chemical Engineering at Manchester presented studies outlining the application of XPS and related techniques to reaction analysis in parallel platforms.



The outputs from the meeting, summarised in a plenary session, were not only tightly developed challenges for inclusion in the **Dial-a-Molecule** roadmap, but also new research groupings and networks stimulated through the discussions. Overall this was a highly interactive, stimulating and enjoyable two days, which will hopefully be replicated in the forthcoming meetings in the other **Dial-a-Molecule** challenge themes.

The organisers would like to thank AstraZeneca for their generous hospitality in hosting this meeting.

A copy of the talks together with completed diagrams for each of the 3 focus area of the Catalysis theme can be downloaded from the Forum section of the Dial-a-molecule website as well as from the Catalysis sub-group on the Connect platform from Technology Strategy Board agency.

Please note that you need to be a member of these groups to access the documents. If you would like access please let us know by email at dialamol@soton.ac.uk