Closed Loop Optimisation of Synthesis

GSK, Stevenage, 16th April 2015

Organisers: Prof Richard Whitby, Dr Robin Attrill, Mr Andrew Richards and Dr Gill Smith

"**Closed Loop Optimisation of Synthesis**" was a very successful one-day symposium organised by the EPSRC Dial-a-Molecule Grand Challenge Network, and held at GSK's Stevenage site. The meeting was designed to bring together researchers from chemistry and beyond, with both academic and industrial backgrounds, to discuss the state of the art and new developments in the field of closed loop optimisation.

The day began with a welcome from *Dr Robin Attrill (GSK)* and was followed by *Andy Richards (GSK)* who described the benefits of closed loop methodologies when developing chemical processes, and identified opportunities for their application within the pharmaceutical industry. The first session concluded with a plenary presentation from *Dr Richard Bourne (University of Leeds)* who outlined the work his group is involved with in automated optimisation in continuous flow reactors, utilising Design of Experiments, Simplex, Snobfit and other algorithms together with appropriate on-line analysis, such as quantitative MS.

The second session featured short talks from the Dial-a-Molecule inspired "Closed Loop Optimisation for Sustainable Chemical Manufacture" project team. *Prof Richard Whitby (University of Southampton)*, *Prof Dave Woods (University of Southampton) Dr Alison Nordon (University of Southampton)* and *Prof Alexei Lapkin (University of Cambridge)* discussed the ongoing collaborative efforts towards enabling the development and operation of new, agile, more cost effective and sustainable chemical manufacturing processes. Flash poster presentations concluded the morning session.

Following the lunch break, *Prof Martyn Poliakoff (University of Nottingham)* delivered a most entertaining plenary lecture describing work carried out at Nottingham around self-optimising reactions using on-line IR. *Chris Selway (Cyclofluidic Ltd)* then spoke about closed loop optimisation using non-linear regression analysis applied to drug discovery, with future application to synthesis and the session drew to a close with *Dr Ewan Mercer (Perceptive Engineering*) presenting the results of collaborative efforts towards the control of novel continuous crystallisation reactors for flexible manufacturing.

Dr Frank Langbein (Cardiff University) opened the final session of the day with his talk on the optimal control of chemical reactions at the quantum level with data-driven models, and was followed by *Prof Lee Cronin (University of Glasgow)* who spoke about research his group is carrying out on using configurable robotics, algorithms and randomness to discover and synthesise new

molecules by breaking the current synthetic methodology paradigm. The formal part of the day concluded with all speakers involved in a panel discussion that debated some of the merits of closed loop optimisation. Some animated discussions continued during the closing reception.

Approximately 100 delegates attended the one day meeting, making it one of the most popular theme meetings that Dial-a-Molecule have run. Alongside the scientific program, the day featured a lively exhibition from leading technology suppliers: Advion, Amigo-Chem, Cambridge Reactor Designs, Gilson, HEL Group, JMP, Mettler-Toledo, Radleys, Syrris, Uniqsis and Vapourtec.