

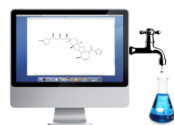
Programme for RSC CICAG – Dial-a-Molecule Meeting



CICAG
Chemical Information and
Computer Applications Group



ROYAL SOCIETY
OF CHEMISTRY



Dial-a-Molecule
An EPSRC Grand Challenge Network

“From Big Data to Chemical Information”

RSC Chemical Information and Computer Applications Group (CICAG) and
Dial-a-Molecule Grand Challenge Network

Wed. 22nd April 2015, Royal Society of Chemistry at Burlington House, Piccadilly, London W1J 0BA

10.00 Registration and tea/coffee

The Rise and Impact of Big Data

Session Chair: Dr Helen Cooke, CICAG Committee Chair

10.30 *Welcome and Introduction.* Dr Helen Cooke, CICAG Committee Chair

10.40 *Big data and the Dial-a-Molecule Grand Challenge.* Professor Richard Whitby, PI Dial-a-Molecule Grand Challenge Network, University of Southampton

11.00 *Big, broad and blighted data.* Professor Jeremy G. Frey, Department of Chemistry, University of Southampton

11.20 *Digital disruption in the laboratory: joined-up science?* Mr John Trigg, Automation and Analytical Management Group, RSC

11.40 *Big data chemistry.* Professor Jonathan Goodman, Department of Chemistry, University of Cambridge

12.00 Discussion

12.20 Lunch

Approaches to Managing Big Data and Maximising Opportunities

Session Chair: Professor Richard Whitby, PI Dial-a-Molecule Grand Challenge Network, University of Southampton

13.20 *Managing and searching large chemical structure data resources.* Dr Mark J Forster, Chemical Indexing Unit Team Leader, Syngenta R&D

13.40 *Classification: square pegs and undetermined holes.* Dr Julie Wilson, Reader, University of York

14.00 *Use of data standards and metadata in information exchange.* Rachel Uphill, Early IP and Data Strategy Business Consultant, R&D IT, GlaxoSmithKline

14.20 *100 million compounds, 100K protein structures, 2 million reactions, 4 million journal articles, 20 million patents and 15 billion substructures: Is 20TB really big data?* Dr Noel O'Boyle, Senior Software Engineer at NextMove Software, Cambridge

14.40 *Dealing with the wealth of open source data.* Dr John Holliday, Senior Research Manager, Information School, University of Sheffield

15.00 Discussion

15.20 Tea/Coffee

15.40 Keynote: *Activities at the Royal Society of Chemistry to gather, extract and analyze big datasets in chemistry.* Dr Tony Williams, Vice President of Strategic Development, Royal Society of Chemistry

16.20 Discussion

16.40 Meeting closes