



## Measurement, Information and Innovation: Digital Disruption in the Chemical Sciences

Tuesday 20<sup>th</sup> October 2015, RSC, Burlington House, Piccadilly, London

### **10.00 Registration and Coffee**

10.30 Welcome and Introduction, Dr Helen Cooke, CICAG

### **Session 1: Data acquisition**

Session Chair: Professor Jonathan Goodman, CICAG and Department of Chemistry, University of Cambridge.

10.40 *The purpose, practicalities, pitfalls and policies of managing and sharing data in the UK.* Dr Danny Kingsley, Head of Scholarly Communication, Cambridge University.

11.00 *Allotrope Foundation, how a data standard and taxonomy for analytical data will support data integration and knowledge generation.* Dr Gerhard Noelken, Technology and Innovation Group, Pfizer Pharmaceutical Sciences.

11.20 *Why we should embrace learnings from other industries.* Peter Boogaard, Industrial Lab Automation.

11.40 Discussion

### **Session 2: Data and Information Management**

Session Chair: Dr Helen Cooke, CICAG

12.00 *Automation in analytical laboratories: A teaching perspective.* Professor Krishna Persaud, School of Chemical Engineering and Analytical Science, University of Manchester.

### **12.20 Lunch**

13.15 *HELM (Hierarchical Editing Language for Macromolecules): A Pistoia Alliance project providing a standard for the storage and exchange of macromolecule structural information in the information ecosystem.* John Wise, Executive Director Business Development - Europe, Pistoia Alliance.

13.35 *Ensuring the machine learner gets the right tuition and AI gets its nose; standardisation and benchmarking in diagnostic marker discovery in exhaled breath.* Professor C.L. Paul Thomas, Centre for Analytical Science, Chemistry Department, Loughborough University.

13.55 Discussion

### **Session 3: Information and Knowledge from Data**

Session Chair: Mr John Trigg, AAMG

14.15 *Building the utopian dream – toward the integrated, paperless drug discovery lab.* Dr Allan Jordan, Head of Chemistry, Drug Discovery Unit, Cancer Research UK Manchester Institute.

14.35 *Using machine learning and cloud technologies for point-of-care in vitro diagnostics.* Dr Omer Casher, Chief Data Officer, SIME Diagnostics, Stevenage Bioscience Catalyst.

### **14.55 Tea/Coffee**

15.15 *Enabling creative scientists to focus on science: automation, workflows, dashboards, insight, aha!!!.* Martin Owen, Data to Insight Activist, GlaxoSmithKline.

15.35 Discussion

### **Session 4: How do we Get There: Meeting Summary and Structured Discussion**

Session Chair: Professor Jeremy Frey, Department of Chemistry, University of Southampton.

15.55 *Building the links.* Mr Richard Kidd, Royal Society of Chemistry.

16.05 Discussion

16.30 Meeting Closes