Chemical Structure Representation: What Would Dalton Do Now?

Thursday 22 June 2017

Central Teaching Hub, University of Liverpool, Liverpool L69 7BX

10.00   Registration & tea/coffee

Session Chair: Dr Helen Cooke, CICAG

10.30   **Welcome and Introduction**

10.40   **IUPAC: the role of international organisations in nomenclature and terminology in the internet age**
Professor Jeremy Frey, *Department of Chemistry, University of Southampton*

11.05   **Indescribable structure: finding words for the future**
Professor Jonathan Goodman, *Department of Chemistry, University of Cambridge*

11.25   **Biology: bigger models, bigger confusion**
Dr David C Briggs, *Department of Life Sciences, Imperial College London*

11.45   **Chemical structure representation challenges encountered when curating the CSD**
Dr Matt Lightfoot, *Editor in Chief, Cambridge Structural Database, CCDC*

12.05   **Panel Discussion**

12.25   **Lunch & tours of the Teaching Hub**

Session Chair: Dr Neil Berry, University of Liverpool

13.25   **Keynote: Describing chemical substances and chemical structures: we have a long way to go**
Dr Evan Bolton, Chemistry Program Head, US National Center for Biotechnology Information (*NCBI)*

14.10   **Using data science techniques to put molecules in context**
Dr Aileen Day, *Data Scientist, Royal Society of Chemistry*

14.30   **Chemical Structure Representation of Inorganic Salts and Mixtures of Gases: A Newer System of Chemical Philosophy**
Dr Roger Sayle, *CEO and Founder, NextMove Software Ltd*

14.50   **Tea/Coffee**

15.10   **Extracting Medicinal Chemistry Knowledge by a secure Matched Molecular Pair Analysis Platform: standardization of SMIRKS enables knowledge exchange**
Dr Al Dossetter, *Managing Director, MedChemica Ltd*

15.30   **InChIs are part of the solution**
Mr Richard Kidd, *Publisher, Royal Society of Chemistry and Treasurer, InChI Trust*

15.50   **HELM: Setting the standard for biomolecular information exchange**
Claire Bellamy, *HELM Project & CSCS Expert Community Manager, Pistoia Alliance*

16.10   **Panel Discussion**

16.30   Meeting close