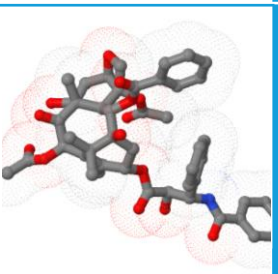
Computational Prediction of Reaction Outcomes and Optimum Synthetic Routes



An event organised by the Dial-a-Molecule EPSRC Grand Challenge Network

***When**: 10th-11th September 2014*

***Where**: Weetwood Hall Conference Centre and Hotel, Leeds, UK*

***Who:** Chemists, Engineers, Mathematicians, Computer Scientists*

We are now living and working in an information age – but is synthetic chemistry taking full advantage of the large amounts of experimental data routinely available and the computing power available to enrich and manipulate it?

Data is the key to 'Dial-a-Molecule'

The Dial-a-Molecule EPSRC Grand Challenge Network invites you to participate in this two day workshop to discuss new ways in which to *represent, manipulate, utilise* and consequently *add value* to the large amounts of data available, and produced in the laboratory each day.

***This workshop will cover*:**

Analysis of complex reaction data, combination with computed data, and use to:

- Predict unknown reaction outcomes
- Design synthetic routes
- Drive the development of new chemistry

The programme will consist of plenary talks to present some of the best current approaches to the problems, short presentations by participants on their potential contributions and interests, alongside brain-storming sessions to suggest ways forward and develop collaborations.

This meeting is free to attend but registration via the website is required. If overnight accommodation is needed this can be booked at the subsidised price of £70. Bursaries for Early Career Researchers to aid with travel and accommodation are available and should be applied for at the time of registration.

Registration will be open until 22nd August 2014

Places are limited and registration will be on a first-in first-served basis.

To register and for further meeting details please visit www.dial-a-molecule.org

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The Challenges and Some Possible Approaches

***Predicting Unknown Reaction Outcomes*:**

- Better ways of using reaction databases
  - Statistical approaches
  - Machine learning
  - How to represent molecules and transformations?
  - Enriching data with theoretical calculations
  - Prediction of possible side reactions
  - How to use richer data
- Systematic experimental and computational investigation of specific reactions to make them 'predictable'
- Theoretical Approaches

Designing Synthetic Routes:

- Ways to visualise the data in reaction databases to allow more effective use (c.f the usual approach which is to extrapolate from the closest few analogues)
- Extracting rules from data (and avoiding errors due to the nature of data)
- Alternatives to the 'lossy' extraction rules (i.e. using full data)
- Expert systems and crowd-sourced knowledge/judgements
- Mechanism based approaches
- Calculation based approaches

Applications to New Chemistry:

- Identify currently unknown transformations which would have the most impact on accessing molecules
- Identify which transformations have most impact on efficiently accessing molecular space to justify further development.
- Identify a sub-set of key 'click' reactions which if realised would allow reasonable access to most molecular space
- Identify a 'holistic approach' (minimum steps) route to molecules
- Predicting (all) possible products from given starting materials, reagents and conditions – knowledge, mechanism and theoretical approaches
- Using the above approaches with calculation of properties (spectral, chromatographic etc) to enable identification of components of complex reaction mixtures.

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