

# UK-QSAR Meeting, Dept. of Chemistry, University of Cambridge: 30<sup>th</sup> September 2014

Hosted by the CCDC

The 2014 Autumn Meeting of the UK-QSAR and Chemoinformatics Group will take place on Tuesday, 30<sup>th</sup> September at the Department of Chemistry, Lensfield Road, Cambridge CB2 1EW -

<http://www.ch.cam.ac.uk/> .

The schedule for the day is shown below.

- 09:00-09:30 REGISTRATION
- 09:30-09:45 UK-QSAR GROUP BUSINESS / WELCOME
- 09:45-10:15 Jason Cole, CCDC; "Generating Small Molecule Conformations from Structural Data"
- 10:15-10:45 Yi Mok, ICR; "Increasing the coverage of medicinal chemistry-relevant space in fragment screening"
- 10:45-11:00 POSTER FLASH TALKS
- 11:00-11:30 TEA / COFFEE / POSTERS
- 11:30-12:00 Yasaman Kalantar Motamedi, University of Cambridge; Title TBA
- 12:00-12:30 Samuel Webb, Lhasa; "Feature combinations networks with statistical (Q)SAR models: interpretation and knowledge mining"
- 12:30-13:00 Noel O'Boyle, NextMove Software, and Jonas Bostrom, AstraZeneca; "Evidence-based Medicinal Chemistry using Matched Molecular Series"
- 13:00-14:00 LUNCH / POSTERS
- 14:00-14:30 Alicia Higuerele, University of Cambridge; "What can we learn from the evolution of protein-ligand interactions to aid design of new therapeutics?"
- 14:30-15:00 Andrea Bortolato, Heptares; "Decoding the role of solvent in ligand-protein binding kinetics"
- 15:00-15:30 Gerard Van Westen, EBI; "Physicochemical Property Trends in Allosteric and Orthosteric Binders and their Predicted Presence in Chemical Databases"
- 15:30-16:00 CLOSING REMARKS / POSTER PRIZE / TEA AND COFFEE

## **Posters;**

Please let us know on the registration form if you would like to present a poster at the event. The maximum number of posters we can accommodate is 12 - if the number of submissions received is greater than this, priority will be given to submissions from PhD students and younger researchers in academia and industry. The recommended poster format is A0 portrait – boards are 2m tall by 1m wide. Presenters should be prepared to give a quick one minute “advertisement”, explaining why people should visit their poster, in the Poster Flash Talks slot, before the mid-morning break. A poster prize will be presented at the end of the day, sponsored by the Cambridge Crystallographic Data Centre (CCDC).

## **Evening Meal;**

As is traditional, an evening meal has been organised for Monday 29<sup>th</sup> September, at the historic Eagle pub, 8 Bene't Street, Cambridge CB2 3QN. Each attendee must cover their own costs for this meal. Please indicate on the registration form if you wish to attend.

## **Travel;**

The Department of Chemistry is located approximately 20 minutes' walk from Cambridge railway station. Please use postcode CB2 1EW on a map server site. Please enter the building at the western end.

Unfortunately, there are very few, if any, visitor car parking places at the department. It is recommended that drivers either;

- use the Cambridge Park and Ride sites (see <http://www.cambridgeshire.gov.uk/transport/around/park-ride/>),
- park in the nearby Queen Anne multi-storey car park, Gonville Place, Cambridge CB1 1ND, about 5 minutes' walk from the venue (see <https://www.cambridge.gov.uk/queen-anne-terrace-car-park>), or
- if you are lucky, find a metered space on Union Road, on the south side of the Chemistry Department (please note that this is a one-way street towards Hills Road; parking is £1 per hour, 8 hrs maximum).

**Accommodation;**

Cambridge has a very wide variety of hotel accommodation. It is recommended that an online booking site (booking.com, Trivago, HRS, Lastminute.com etc.) be consulted, but the following hotels are geographically the closest to the venue;

Lensfield Hotel (1 minute's walk) - <http://www.lensfieldhotel.co.uk/>

Royal Cambridge Hotel (2-3 minutes' walk) - <http://www.sjhotels.co.uk/cambridge>

Gonville Hotel (4-5 minutes' walk) - <http://www.gonvillehotel.co.uk/>