



# MGMS and RSC MMG Young Modellers' Forum 2010

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## Presentations

9.00 – 9.30	<b>Coffee and Registration</b>
9.30 - 9.40	<b>Welcome and Introduction</b> Steve Maginn and Louise Birch
9.40 – 10.00	<b>A method for visualising transient binding sites on protein surfaces</b> Paul Ashford – <i>Birkbeck College, University of London</i>
10.00 – 10.20	<b>Multiscale modelling of an artificial self-replicating system</b> Sabrina Beniken – <i>King's College London</i>
10.20 – 10.40	<b>Translocation of biopolymers through protein nanopores: mechanistic insights from MD simulations.</b> Andrew Guy – <i>University of Southampton</i>
10.40 – 11.00	<b>The use of Voronoi protein-ligand contact statistics in structure-based design</b> Ilenia Giangreco – <i>Università di Bari, Italy</i>
11.00-11.20	<b>Applications of Molecular Modelling (MD) studies and Quartz Crystal Microbalance (QCM) experiments to study the ligand recognition by the major urinary protein (MUP).</b> Julie Roy – <i>University of Nottingham</i>
11.20-11.40	<b>Organic enzyme cofactors: on their properties, intrinsic groupings and conformational variability</b> Julia Fischer – <i>EMBL-EBI, Cambridge</i>
11.40-13.30	<b>Lunch and Poster Session</b>
13.30 – 13.50	<b>Energetics, kinetics and binding pathway reconstruction for enzyme-inhibitor complex from high-throughput molecular dynamics simulations</b> Ignasi Buch – <i>Universitat Pompeu Fabra-IMIM, Spain</i>
13.50 – 14.10	<b>Virtual Screening to Identify Novel Antimalarial Chemotypes</b> Alexandre Lawrenson – <i>University of Liverpool</i>
14.10 – 14.30	<b>Generation of a fragment library that maximally represents a compound collection</b> Michèle Schulz – <i>University of York</i>
14.30 – 15.00	<b>Tea</b>

15.00 - 15.20	<b>QM/MM modelling of the hydroxylation of diclofenac by human cytochrome P450 enzymes</b> Kerensa Houghton – <i>University of Bristol</i>
15.20 – 15.40	<b>Photochemistry and DNA Interactions of Platinum Anticancer Agents: DFT/LFMM Studies</b> Hui-Chung Tai – <i>University of Warwick</i>
15.40 – 16.00	<b>Structure-based virtual screening and validation of UGP inhibitors</b> Waldemar Striker – <i>University of Dundee</i>
16.00	<b>Fun event – “Only Connect”</b>
16.30	<b>Judges Deliberations</b>
16.45	<b>Prize Presentations</b>
17.00	<b>End</b>

## Posters

Poster 1	<b>Theory vs. experiment in probing a prototypical protein-protein interaction</b> Richard Bradshaw – <i>Imperial College London</i>
Poster 2	<b>Large scale conformational changes in aromatic transporters in presence of benzene</b> Pragya Chohan – <i>University of Oxford</i>
Poster 3	<b>A Computational Study into the Role of Defects in BaTiO<sub>3</sub></b> James Dawson – <i>University of Sheffield</i>
Poster 4	<b>Novel half-bonded model for metalloprotein simulation</b> Mahmoud Ibrahim – <i>The University of Manchester</i>
Poster 5	<b>Quantitative mapping of ligand and target binding spaces of chemical probes</b> Felix Krüger – <i>EMBL-EBI, Cambridge</i>
Poster 6	<b>Towards a Multiscale Simulation of Cellular Calcium Signalling in the Cardiac Cell</b> Daniel Mason – <i>University of Southampton</i>
Poster 7	<b>Dynamics based alignment of proteins</b> Marton Munz – <i>University of Oxford</i>
Poster 8	<b>Electrostatic embedding in large scale DFT biomolecular simulations</b> Chris Pittock – <i>University of Southampton</i>
Poster 9	<b>Protein Unfolding Under Force: Crack Propagation in a Network</b> Gareth Shannon – <i>University of Nottingham</i>
Poster 10	<b>Mining of Emerging Structural Patterns for Identification of Toxicophores</b> Richard Sherhod – <i>University of Sheffield</i>
Poster 11	<b>QM/MM study of Oleamide (OLE) hydrolysis and Oleoylmethylester (OME) hydrolysis catalysed by Fatty Acid Amide Hydrolase.</b> Jitnapa Sirirak – <i>University of Bristol</i>
Poster 12	<b>Folding and Dynamics of Lantibiotic Peptide Analogues</b> Eleanor Turpin – <i>University of Nottingham</i>