MGMS and RSC MMG

Young Modellers' Forum 2010

Presentations

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

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

Posters

Poster 1	**Theory vs. experiment in probing a prototypical protein-protein interaction** Richard Bradshaw – *Imperial College London*
Poster 2	**Large scale conformational changes in aromatic transporters in presence of benzene** Pragya Chohan – *University of Oxford*
Poster 3	**A Computational Study into the Role of Defects in $BaTiO_3$** James Dawson – *University of Sheffield*
Poster 4	**Novel half-bonded model for metalloprotein simulation** Mahmoud Ibrahim – *The University of Manchester*
Poster 5	**Quantitative mapping of ligand and target binding spaces of chemical probes** Felix Krüger – *EMBL-EBI, Cambridge*
Poster 6	**Towards a Multiscale Simulation of Cellular Calcium Signalling in the Cardiac Cell** Daniel Mason – *University of Southampton*
Poster 7	**Dynamics based alignment of proteins** Marton Munz – *University of Oxford*
Poster 8	**Electrostatic embedding in large scale DFT biomolecular simulations** Chris Pittock – *University of Southampton*
Poster 9	**Protein Unfolding Under Force: Crack Propagation in a Network** Gareth Shannon – *University of Nottingham*
Poster 10	**Mining of Emerging Structural Patterns for Identification of Toxicophores** Richard Sherhod – *University of Sheffield*
Poster 11	**QM/MM study of Oleamide (OLE) hydrolysis and Oleoylmethylester (OME) hydrolysis catalysed by Fatty Acid Amide Hydrolase.** Jitnapa Sirirak – *University of Bristol*
Poster 12	**Folding and Dynamics of Lantibiotic Peptide Analogues** Eleanor Turpin – *University of Nottingham*