



MGMS and RSC MMG Young Modellers' Forum 2009

Presentations

9.00 – 9.30	Coffee and Registration
9.30 - 9.40	Welcome and Introduction Steve Maginn and Stuart Firth-Clark
9.40 – 10.00	Reactivity and Interaction Studies of Glycolysed Generation 3.5 PAMAM Dendrimers with TLR4-MD2 Complex Teresa Barata – <i>School of Pharmacy, University of London</i>
10.00 – 10.20	Molecular Dynamics Simulations of the β_2-adrenergic Receptor in Complex with a Peptide Derived from the $G\alpha$ Subunit of the Heterotrimeric G_s-protein Angela Götz – <i>Friedrich Alexander University, Erlangen, Germany</i>
10.20 – 10.40	Minor Groove of DNA as Target for Drug Design Gudrun M. Spitzer – <i>University of Innsbruck, Austria</i>
10.40 – 11.00	Fe(H)₂(diphosphine)(diamine) Complexes as Attractive Catalysts for The Hydrogenation of Ketones? Hsin-Yi Tiffany Chen – <i>University College London</i>
11.00-11.20	Defect and Transport Properties of LiFePO₄ Battery Materials Veluz Maria Hart Prieto – <i>University of Bath</i>
11.20-11.40	Assigning Stereochemistry Using GIAO NMR Shift Calculation Steven G. Smith – <i>University of Cambridge</i>
11.40-13.30	Lunch and Poster Session
13.30 – 13.50	Predicting Fragment Positions in Binding Sites Using MCSS (CHARMm) Kamran Haider – <i>University of York</i>

13.50 – 14.10 **Application of Simulation Methods for the Identification of the Allosteric Binding Site in Human Glucokinase**
Nadia Vahdati – *University of Southampton*

14.10 – 14.30 **Screening for Near-Native Protein-Protein Docking Complexes: Use of Residue-Pair Propensity Matrices**
Ja-won Song – *University of Cambridge*

14.30 – 15.00 **Tea**

15.00 - 15.20 **QM/MM Modelling of the Reaction Mechanism of Chorismate Synthase**
Narin Lawan – *University of Bristol*

15.20 – 15.40 **Computational Studies of Water-Mediated Interactions in Ionotropic Glutamate Receptors**
Michelle A. Sahai – *University of Oxford*

15.40 – 16.00 **Evaluation of a Bayesian Inference Network for Ligand-Based Virtual Screening**
Christoph Mueller – *University of Sheffield*

16.00 **Chemical Catchphrase**

16.30 **Judges Deliberations**

16.45 **Prize Presentations**

17.00 **End**

Posters

Poster 1 **Modelling the Hydroxylation of Diclofenac in Human Cytochrome P450 Enzymes**
Kerensa Houghton – *University of Bristol*

Poster 2 ***In Silico* Design of Potential HIF-1 α : p300 Interaction Inhibitors**
Jarmila Husby – *School of Pharmacy, University of London*

Poster 3 **QSARs for a Series of Aminoquinoline Compounds against Chloroquine Sensitive and Resistant Strains of the Malaria Parasite, Along with Hit Expansion Methods to Find Potential Lead-Like Compounds**
Alexandre S. Lawrenson – *University of Liverpool*

- Poster 4 **Catalytic Activity of Fatty Acid Amide Hydrolase: Non-Empirical Analysis of Differential Transition State Stabilization**
Ewa Chudyk – *University of Bristol*
- Poster 5 **RNA- Small Molecules Complexes Database**
Irena Sani – *Birkbeck College, London*
- Poster 6 **Large Scale Molecular Simulations using Brownian Dynamics with Boundary Element Method Electrostatics.**
David Fallaize – *University College London*
- Poster 7 **Molecular Dynamics Using Cooperative Replicas: Folding of Trp-cage Mini-protein**
Neil J. Bruce – *University of Manchester*
- Poster 8 **Molecular Docking and QSAR of Aplyronine A and Analogues: Potent Inhibitors of Actin**
Abrar Hussain – *University of Nottingham*
- Poster 9 **Simulation Studies of the Binding Properties of an Unusual Pleckstrin Homology Domain**
Craig N. Lumb – *University of Oxford*
- Poster 10 **The Sugar Shovel: The Role of Tryptophan in the Glycosyl Transfer Activity of *Trypanosoma cruzi* Trans-Sialidase**
Felicity L. Mitchell – *University of Manchester*
- Poster 11 **How Point Mutations Confer Resistance in BCR-Abl – a Computational Study**
Genevieve Clapton – *University of Southampton*
- Poster 12 **Activation of Integrins by Formation of a Complex with Talin and Membranes: a Coarse-Grained Molecular Dynamic Study**
Antreas Kalli – *University of Oxford*