MGMS and RSC MMG

Young Modellers' Forum 2008

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	**Where Does the Tetrazole Belong? Insight to the Binding Pose of AT1 Antagonists Using Homology Modelling, Molecular Dynamics, and Docking** NJ Maximilian Macaluso – *University of Cambridge*
10.00 – 10.20	**The Determinants of Protein Kinase Inhibitor Selectivity** Duangrudee Tanramluk – *University of Cambridge*
10.20 –10.40	**On the Diversity of Physicochemical Environments Experienced by Identical Ligands in Binding Pockets of Unrelated Proteins** Abdullah Kahraman – *European Bioinformatics Institute*
10.40 – 11.00	**Protein-Protein Interactions as Drug Targets: a View from the Binding Site** Jonathan C. Fuller – *University of Leeds*
11.00-11.20	**Entropic Cost of Molecular Association** Sheeba Jem Irudayam – *University of Manchester*
11.20-11.40	**Haptic Technology in Drug Design: Breaching the Accessibility Barrier** Nicola Zonta – *University of Cardiff*
11.40-13.30	**Lunch and Poster Session**
13.30 – 13.50	**Coarse-Grain Protein Modelling with Hamiltonian Replica Exchange** Mishal Patel – *University of Southampton*

13.50 – 14.10	**Classifiation Models for Aqueous Solubility in the Early Drug Discovery Phase** Christian Kramer - *Universität Erlangen-Nürnberg*
14.10 – 14.30	**Towards High Level QM/MM Calculation of Protein-Ligand Binding Affinities** Katie Shaw – *University of Bristol*
14.30 – 15.00	**Tea**
15.00 - 15.20	**FapR Protein: Functional Study of a Potential Target for Antibiotics Against Gram Positive Bacteria** Olivier Périn – *Institut Pasteur, Paris*
15.20 – 15.40	**Wavelet Compression of GRID Fields for Similarity Searching and Virtual Screening** Richard Martin – *University of Sheffield*
15.40 – 16.00	**Probing Enzyme Catalysis Using High Pressure Molecular Dynamics** Tom McGrory – *University of Manchester*
16.00	**Molecular Mayhem**
16.30	**Judges Deliberations**
16.45	**Presentations**
17.00	**End**

Posters

Poster 1	**Discarding Functional Residues from the Substitution Table Improves Predictions of Active Sites within Three-Dimensional Structures** Sungsam Gong – *University of Cambridge*
Poster 2	**A Computational Method for Examining the Conformational Stability of Family A GPCRs** Lisa M Simpson – *University of Essex*
Poster 3	**Protein Dynamics and Networks of Dynamically-Conserved Residues** Suryani Lukman – *University of Cambridge*

Poster 4	**Use of Reduced Dimensionality Representation and Molecular Dynamics Techniques to Investigate PDZ Domain Similarity and Ligand Specificity** Cristina Sisu – *University of Cambridge*
Poster 5	**Computational Studies of Water-Mediated Interactions in Ionotropic Glutamate Receptors** Michelle A. Sahai – *University of Oxford*
Poster 6	**Dynamics of Phosphate Transport by the Anion-Specific Outer Membrane Protein OprP** Prapasiri Pongprayoon – *University of Oxford*
Poster 7	**Unsatisfied Hydrogen Bond Donors/Acceptors at Buried Protein-Ligand Interfaces** Kamran Haider – *University of York*
Poster 8	**Molecular Dynamics Simulations of Mesophilic and Thermophilic Citrate Synthase** John McGeagh – *University of Bristol*
Poster 9	**QM/MM Study of the Sulfoxidation of Dimethyl Sulphide by Cytochrome P450** Cristina S. Porro – *University of Manchester*
Poster 10	**Specific Ion Effects on Structurally Persistent Micelles – Guiding Experiments with MD Simulations** Christof Jäger - *Universität Erlangen*
Poster 11	**The Role of Complex Formation between Substrates and Efflux Pump Inhibitors (EPIs) in Multidrug-Resistant (MDR) Bacteria** Sheikh Shilbe Rahman – *School of Pharmacy, London*
Poster 12	**Easy and Rapid Method for Dendrimer 3D Structure Generation** Teresa S. Barata - *School of Pharmacy, London*