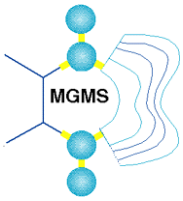

RSC MMG
RSC Molecular Modelling Group

MGMS and RSC MMG

Young Modellers' Forum 2011

Presentations

9.00 – 9.30	**Coffee and Registration**
9.30 – 9.40	**Welcome and Introduction** Steve Maginn and Louise Birch
9.40 – 10.00	**Flexibility Controls Specificity of Snake Venom Metalloproteases** Hannes Wallnoefer, *University of Innsbruck, Austria*
10.00 – 10.20	**Flipping Inositol Phosphates: A Molecular Dynamics Approach to Understanding the Selectivity of Protein Kinase B** Sarah Rosen, *Imperial College London*
10.20 –10.40	**Protein-ligand binding free energies from large-scale DFT calculations with the ONETEP program** Stephen Fox, *University of Southampton*
10.40 – 11.00	**Combination of structure- and ligand-based virtual screening for the discovery of novel non-LBP antiandrogens as chemical tools to treat prostate cancer** Laura Caboni, *Trinity College Dublin, Ireland*
11.00 – 11.20	**Atomic Detail Studies of P-Glycoprotein and Drug Permeation in Model Membranes** Jerome Ma, *University of Oxford*
11.20 – 11.40	**From Development to Application: Molecular Mechanical Study of Halogen Bonding in Drug Discovery** Mahmoud Ibrahim, *University of Manchester*
11.40 – 13.30	**Lunch and Poster Session**
13.30 – 13.50	**Druggability and structural analysis of bromodomain acetylated-lysine binding sites** Lewis Vidler, *Institute of Cancer Research*
13.50 – 14.10	**Advances in Free Energy Calculation: The Enveloping Distribution Sampling Method** Sereina Riniker, *ETH Zurich, Switzerland*
14.10 – 14.30	**Metabolite Space and Metabolite-Likeness** Julio Peironcely, *Leiden University/TNO, The Netherlands*
14.30 – 15.00	**Tea**
15.00 – 15.20	**A Ligand-Assisted Proton Shuttle (LAPS) Mechanism: Using Coordinated Acetate Ligands to Affect Chemical Change** David Johnson, *University of York*
15.20 – 15.40	**Interpreting Experimental Analysis of the Human Ether-a-go-go Related Gene Product (hERG) with Molecular Dynamics**

	and *in-silico* Docking Charlotte Colenso, *University of Bristol*
15.40 – 16.00	**A Novel Computational Approach to Fragment-Based Drug Discovery** Michael Bodnarchuk, *University of Southampton*
16.00	**Fun event – "Name That Molecule"**
16.30	**Judges Deliberations**
16.45	**Prize Presentations**
17.00	**End**

Posters

Poster 1	**Revisiting the General Solubility Equation: *In Silico* Prediction of Aqueous Solubility incorporating the Effect of Topographical Polar Surface Area** Jogoth Ali, *University of Hertfordshire*
Poster 2	**The Development and Application of a simplified QM/MM method for Free Energy Simulations** Michael Carter, *University of Southampton*
Poster 3	**Visualization and Analysis of Helix Flexibility Using Bendix** Caroline Dahl, *University of Oxford*
Poster 4	**Ligand- and Structure-Based Computational Approaches for the Design of Potent and Selective Compounds towards Adenosine Receptors.** David Rodríguez, *Unilever Centre: University of Cambridge*
Poster 5	**Rapid Prediction and Scoring of Water Molecules in Protein Binding Sites** Gregory Ross, *University of Oxford*
Poster 6	**The Assessment of Computationally Derived Protein Ensembles in Protein-Ligand Docking** Barbara Sander, *University of Southampton*
Poster 7	**Actinyl reduction potentials in solution: An assessment of computational methods to achieve experimental accuracy** Krishnamoorthy Arumugam, *University of Manchester*
Poster 8	**The Relationship between Drug-Lipid Interaction Energy and Non-Specific Binding** Callum Dickson, *Imperial College London*
Poster 9	**Understanding the Competing Reactions of Polyurethane Foam Formation: A Computational Study** Jack Gibb, *Unilever Centre: University of Cambridge*
Poster 10	**Exploring the mycolic acid potential energy surface: the ups and downs** Wilma Groenewald, *Bangor University*
Poster 11	**In silico target predictions using machine-learning methods: Naïve Bayes & Parzen-Rosenblatt Window** Alexios Koutsoukas, *Unilever Centre: University of Cambridge*
Poster 12	**An *In Silico* Scaffold Hopping Protocol for Identifying Novel Kinase Inhibitors** Sarah Langdon, *Institute of Cancer Research*