Young Modellers' Forum 2005

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	**Evolution of metal binding sites** James Torrance - *European Bioinformatics Institute*
10.00 – 10.20	**Using multiobjective optimization to study the strengths of different interaction energies in protein-ligand complexes** Sally Mardikian - *University of Sheffield*
10.20 –10.40	**Simulation of conformational transitions and Free Energy Calculations of PcrA DNA Helicase by Targeted Molecular Dynamics and WHAM** Hao Wang - *University of Nottingham*
10.40 – 11.00	**Drug binding to the hERG K^+ channel: a molecular modelling study** Phillip J. Stansfeld - *University of Leicester*
11.00-11.20	**Modelling drug metabolism in cytochrome P450 enzymes** Jolanta Zurek - *University of Bristol*
11.20-11.40	**Online Drug Design** Alasdair Laurie - *University of Leeds*
11.40-13.30	**Lunch and Poster Session**
13.30 – 13.50	**Molecular Surface Property Graphs** Vishwesh Venkatraman - *University of Portsmouth*
13.50 – 14.10	**Where do the protons go: Protonation states in protein-ligand complexes** Paul Czodrowski - *Philipps University Marburg*
14.10 – 14.30	**The Role of Water in Protein-Ligand Interactions: Implications for Rational Drug Design** Caterina Barillari - *University of Southampton*
14.30 – 15.00	**Tea**
15.00 - 15.20	**Investigation of the charge transfer mechanism in 9-mesityl-10-methylacridinium : Rationalizing electron transfer in perpendicular systems.** Ben Allen - *University Of Newcastle Upon Tyne*

15.20 – 15.40	**π-stacking in aromatic structures: a DFT and Atoms in Molecules study** Arturo Robertazzi - *Cardiff University*
15.40 – 16.00	**Modelling Aromatic Interactions via Molecular Mechanics Simulation** Christopher M. Baker – *University of Oxford*
16.00	**Compound Countdown**
16.30	**Judges Deliberations**
16.45	**Presentations**
17.00	**End**

Posters

Poster 1	**Can Clefts Aid the Prediction of Protein-Protein Interfaces** Nick Burgoyne - *University of Leeds*
Poster 2	**A Graph Theoretic Survey of RNA Base Triple Interactions** Mohd Firdaus Raih - *University of Sheffield*
Poster 3	**Scoring Functions and Enrichment: A Case Study on Hsp 90** Chrysi Konstantinou Kirtay - *University of Cambridge*
Poster 4	**QSAR Analysis of NK3 Activity** Natalie Akoma-Mordi – *University College, London*
Poster 5	**The Application of RAPPER to and it's Implications for the Limitations in Comparative Modelling** Nicholas Furnham - *Cambridge University*
Poster 6	**QM/MM Study of the Intramolecular Proton Transfer in Glycine** Phaedra Williams – *University of Bath*
Poster 7	**Regioselectivity of Soluble Epoxide Hydrolase: A QM/MM study** Simon Hoyle – *University of Bristol*
Poster 8	**Molecular Dynamics Simulations of LDAO detergent micelles and of Mistic** Emi Psachoulia - *University of Oxford*
Poster 9	**QSPR investigation into solvation properties of platinum complexes** Steven Oldfield - *Cardiff University*
Poster 10	**Docking and direct design in the binding pocket -libraries for serine protease inhibitors**

Christof Gerlach - *Philipps-Universität Marburg*

Poster 11	**QM/MM modelling of reactions in citrate synthase** Marc van der Kamp - *University of Bristol*
Poster 12	**Molecular Modelling of DNA Compression Caused by Physical Probing Techniques** Verity Hudson - *University of Nottingham*