

Young Modellers Forum – 1st December 2006

9.00-9.30	Coffee and Registration
9.30-9.40	Welcome & Introduction Stuart Firth-Clark and Steve Maginn
9.40-10.00	The Computational Photochemistry of Conjugated Organic Radical Cations Katherine Hall – Imperial College, London
10.00-10.20	A Computational Study of the Fluorescence of 2-aminourine and pyrrolocytosine in Nucleic Acids Samantha Hardman – Birkbeck College, London
10.20-10.40	Understanding Stereoselectivity – Molecular Modelling to Inform Organic Synthesis Robert Paton – University of Cambridge
10.40-11.00	The Mechanism of Induction of the Tetracycline Repressor Protein Ute Seidel – University of Erlangen
11.00-11.20	Ensemble Molecular Dynamics Simulations of Wildtype and Mutant HIV-1 Proteases Reveal Novel Conformations of the Inhibitor Saquinavir S. Kashif Sadiq – UCL, London
11.20-11.40	Modelling MM Polarization in Hybrid QM/MM Calculations Chris Illingworth – University of Essex
11.40-13.30	Lunch and Poster Session
13.30-13.50	Hybrid QM/MM Modelling of the Arg90Cit Mutant of Bacillus Subtilis Chorismate Mutase Reveals Unexpected Complexity of Catalytic Effects Stephen Macrae – University of Bristol
13.50-14.10	Simulations of B-DNA under Torsional Stress Reveal Enhanced Base Breathing Angelo Pugliese – University of Nottingham
14.10-14.30	Graph Theoretic Approaches for Exploring and Analysing RNA 3D Structures Mohd Firdaus Raih – University of Sheffield
14.30-15.00	Tea and Posters
15.00-15.20	Molecular Basis of Substrate Specificity of the Adenylation Domains of Nonribosomal Peptide Synthetases Joanne Hanna – University of Warwick
15.20-15.40	Driving Protein-Ligand Docking by Quantitative Chemical Shifts Perturbations Domingo González-Ruiz – J.W. Goethe University, Frankfurt-am-Main
15.40-16.00	A Fast and Accurate Biomembrane Model Mario Orsi – University of Southampton
16.00	Blockbusters
16.30	Judges Deliberations
16.45	Presentations
17.00	Close

Poster Presentations

Poster 1	Computational Infrared Spectroscopy Studies of Enzyme Interactions Michelle Szeto – University of Bristol
Poster 2	Interaction of DNA with Groove Binding Ligands Mark Broome – University of Warwick
Poster 3	Computational Studies of α-lactone Reactivity Mahmoud Soliman – University of Bath
Poster 4	Study of the Conformational Dynamics of HIV-1 Protease using Reversible Digitally Filtered Molecular Dynamics Sarah Williams – University of Southampton
Poster 5	Conformational Analysis and Molecular Dynamics at the Receptor Level of the Immunodominant Myelin Basic Protein Epitope 87-99 Implicated in Multiple Sclerosis, and its Antagonists Linear Altered Peptide Ligands Efthimia Mantzourani – Universities of Cardiff and Patras
Poster 6	Sequence-Structure-Function Relationships of Viper Venom Serine Proteases Sakthivel Vaiyapuri – University of Reading
Poster 7	VSTx1, a Modifier of Kv Channel Gating, Localizes to the Interfacial Region of Lipid Bilayers Chze Ling Wee – University of Oxford
Poster 8	Contemporary QSAR Classifiers Compared Craig Bruce – University of Nottingham
Poster 9	In Silico Simulation of the Self Association of Amyloidogenic Peptides Oliver Clarke – University of Leeds
Poster 10	The Importance of Water Molecules and Charge Assistance for the Inhibition of TGT Tina Ritschel – Philipps University of Marburg
Poster 11	GARlig: A Fully Automated Tool for Reagent Enumeration and Subset Selection of De Novo Skeletons via Genetic Algorithms Patrick Pfeffer – Philipps University of Marburg
Poster 12	Aromaticity of the Metal Dithiolene Ring During the Nitrate Reduction Pathway Ganga Periyasamy – University of Manchester