



MGMS and RSC MMG Young Modellers' Forum 2007

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	Molecular Dynamics Study of the Structural Stability and Materials Properties of DNA-Intercalated Layered Double Hydroxides Mary-Ann Thyveetil - <i>University College London</i>
10.00 – 10.20	Binding Free Energy Calculation from Molecular Dynamics Simulation Floris P. Buelens - <i>Birkbeck College</i>
10.20 – 10.40	Molecular Spam: Use of a Modified Spam Filter for Classification of Bioactive Molecules and Drug Target Prediction Florian Nigsch - <i>University of Cambridge</i>
10.40 – 11.00	Homology Model Based Virtual Screening for GPCR Ligands using Docking and Target-Biased Scoring Sebastian Radestock - <i>J.W. Goethe-University, Frankfurt</i>
11.00-11.20	Study of the Lysozyme Protein: Use of a Novel Method to Sample Conformational Change J. Fernandez Carmona - <i>University of Southampton</i>
11.20-11.40	A Core Fragment Based Look at Chemical Space Agata Krasowski - <i>University of Dundee</i>
11.40-13.30	Lunch and Poster Session
13.30 – 13.50	<i>In Silico</i> Identification and Characterisation of Ion Binding Sites in Glutamate Receptors Ranjit Vijayan - <i>University of Oxford</i>

13.50 – 14.10	The UV Spectrum of [Zn(pyridine)₄]²⁺ Caroline Norris - <i>University of Sussex</i>
14.10 – 14.30	An Application of Reaction Vectors in <i>De Novo</i> Design Hina Patel - <i>University of Sheffield</i>
14.30 – 15.00	Tea
15.00 - 15.20	Searching New Inhibitors of <i>Trypanosoma cruzi</i> Triosephosphate Isomerase (TcTIM). Docking and Virtual Screening Studies. Jorge Estrada - <i>Universidad de Zaragoza</i>
15.20 – 15.40	Seeing the Trees Through the Forest Craig L. Bruce - <i>University of Nottingham</i>
15.40 – 16.00	Cytochrome P450 Reactivity and Specificity from QM/MM Mechanistic Modelling Richard Lonsdale - <i>University of Bristol</i>
16.00	Compound Countdown
16.30	Judges Deliberations
16.45	Presentations
17.00	End

Posters

Poster 1	Class A β-lactamases: QM/MM Study of their Mechanism of Resistance to Antibiotics. Juliette J. Pradon - <i>University of Bristol</i>
Poster 2	Understanding the Interaction Between Dye Molecules and Cellulose W.H. Hindy Mok - <i>University of Cambridge</i>
Poster 3	Influence of Non-Nucleoside Inhibitors on the Conformation of Wild-Type and Mutant HIV-1 Reverse Transcriptase Studied by Molecular Dynamics Peerapol Nunriam - <i>University of Bristol</i>
Poster 4	Cryptic Chlorination by a Non-Heme Halogenase - a DFT Study Shanthi Pandian - <i>University of Manchester</i>
Poster 5	A QM/MM Investigation into the Biodegradation Mechanism of Chitinase B

Heather Rowlands - *University of Bristol*

Poster 6 **Preferential Solvation Behaviour of Manganese Ions**
Jens Rydén - *University of Sussex*

Poster 7 **Molecular Dynamics Simulations of Transport at Water-Silicate Interface**
Wojtek Gren - *University of Bath*

Poster 8 **Identification of Allosteric Binding Sites in Proteins**
Nadia Vahdati - *University of Southampton*

Poster 9 **ILBP – Flexible Protein Scaffold for Multiple Ligand Transport**
Mari Chikvaidze - *University of Nottingham*

Poster 10 **Capturing Lipid Phases Using a Highly Simplified Lipid Model**
George D. Chellapa - *University of Southampton*

Poster 11 **Self-Assembly and Dynamics of the Influenza A M2 Channel via Coarse Grain MD Simulations**
Timothy Carpenter - *University of Oxford*

Poster 12 **Modelling Interaction of the ITIH4 von Willebrand type A Domain with Fraction C4b of the Classical Complement Pathway**
Alvaro Sebastián - *University of Zaragoza*