

# Young Modellers' Forum 2001 MGMS & RSC MMG

## Programme

November 30th 2001  
Scientific Societies Lecture Theatre, London

9.15 – 9.50	Registration
9.50 – 10.00	<b>Introductions</b> David Manallack (MGMS) and Steve Maginn (RSC MMG)
10.00 – 10.20	<b>MM and QM/MM Dynamics Simulations of the Tetrahedral Intermediate in the Deacylation Step of the Catalytic Mechanism in Serine Proteases</b> Maya Topf
10.20 – 10.40	<b>Simulating the Induced Fit: A Combined QM/MM Docking Approach</b> Frank Beierlein
10.40 – 11.00	<b>QM/MM Studies of the Citrate Synthase Reaction Mechanism</b> Francesca Perruccio
11.00 – 11.20	<b>Asymmetry of LysU Demonstrated Through Molecular Dynamics Simulations and Free Energy Calculations</b> Samantha Hughes
11.20 – 11.40	<b>Bivariate Multicanonical WHAM: An Efficient and Accurate Route to Relative Binding Free Energies and Entropies</b> Christopher Woods
11.40 – 12.00	<b>A Target Selection Informatics Resource for Structural Genomics</b> Ana Rodrigues
12.00 – 1.30	Lunch and <b>POSTERS</b> (details below)
1.30 – 1.50	<b>Computational Modelling of Molecular Motor Proteins</b> Barry Grant
1.50 – 2.10	<b>Evaluation of K<sup>+</sup> Channel Models Using MD Simulations</b> Charlotte Capener
2.10 – 2.30	<b>Homology Modelling of the Novel Cytochrome P450 CYP4X1</b> Lorna Gillett
2.30 – 2.50	<b>Generation and Display of Activity-Weighted Chemical Hyperstructures</b> Nathan Brown
2.50 – 3.20	Coffee and <b>POSTERS</b>
3.20 – 3.40	<b>A QSAR for all Sweet Tasting Compounds</b> Channa Hattotuwigama
3.40 – 4.00	<b>The Application of Neural Networks to Molecular Recognition</b> Thomas Kabir
4.00 – 4.30	<b>University Challenge hosted by Trevor Howe. GSK vs 'The Rest of the World'</b>
4.30 – 4.40	Judges deliberations
4.40 – 5.00	<b>Prizes</b>
5.00 onwards	Networking down the pub [RSC building to be vacated by 5.15 pm please]

## POSTERS

- Poster 1     **The 11  $\beta$ -hydroxysteroid Dehydrogenase Isozymes – Challenges in Drug Design**  
Amber Seigel
- Poster 2     **Residue Pairing Preferences in Beta Sheet Proteins**  
Helen Fooks
- Poster 3     **Modeling and Molecular Dynamics Studies of Human Aquaporin - 1**  
Richard Law
- Poster 4     **A Molecular Surface-Based Method for Optimisation of Protein-Lipid Interfaces in Membrane Protein Simulations**  
José Faraldo-Gómez
- Poster 5     **Molecular Dynamics Simulations of Biomembranes and Small Molecule Permeation**  
Daniele Bemporad
- Poster 6     **Investigating the Mechanism of Dihydrofolate Reductase by Molecular Dynamics Simulations**  
Paul Shrimpton
- Poster 7     **Active and Inactive Conformations of the  $\beta_2$ -Adrenergic Receptor**  
Nathan Kidley
- Poster 8     **Molecular Modelling of Delta-class Glutathione S-Transferases**  
Mike Nagle