

Programme

Monday 7 January

9.30 Registration and Coffee

Session 1

10.55 Opening Remarks

11.00 **Plenary 1: Rebecca Wade** - *Combining Brownian and Molecular Dynamics to simulate protein-protein docking subject to biochemical constraints*

11.35 **T1: Thorsten Kampmann** - *Ligand-unbinding induced refolding of the ABC ATPase RLI*

11.55 **T2: Philip Fowler** - *Do we understand how Potassium channels are able to conduct K⁺ but not Na⁺ ions? Testing the snug-fit, carbonyl repulsion and topological-control hypotheses of ion selectivity.*

12.15 **T3: Hannes Loeffler** - *Molecular Dynamics Simulations of the Periplasmic Glutamine Binding Protein.*

12.35 Lunch

Session 2

14.00 **Plenary 2: Adrian Roitberg** - *Molecular dynamics simulations of subtype C HIV-1 protease*

14.35 **T4: Ingvar Lagerstedt** - *Programming Generalized Born methods for a SIMD Architecture*

14.55 **T5: Christopher Woods** - *QM/MM Free Energy Calculations for Rational Drug Design*

15.15 **T6: Guy Robinson/Charlie Laughton** - *Using CCPB codes on HECToR, some early experiences, first results and opportunities for the future.*

15.35 Tea

Session 3

16.05 **Plenary 3: Marcus Elstner** - *Computer simulation of biophysical processes: application to light driven proton pumps in the bacterial photosynthesis*

16.40 **T7: Pedro Silva** - *Computational studies of heme biosynthesis*

17.00 **T8: Johannes Kaestner** - *Finding Minima and Transition States: the Development of a Geometry Optimiser for Atomistic Simulation Codes*

17.20 End of session

17.30 Poster session with wine reception

19.00 End of day

Tuesday 8 January

Session 4

- 9.00 **Plenary 4: Victor Guallar** - *Heme Electron Transfer: The Propionate Pathway*
9.35 **T9: Ian Williams** - *Computational Modelling of Glycosidase Mechanisms*
10.10 **T10: Marc van der Kamp** - *Modelling the mechanism of citrate synthase: evidence for arginine acting as an acid and failure of B3LYP*
- 10.30 Coffee

Session 5

- 11.00 **Plenary 5: Siewart-Jan Marrink** - *Membrane Proteins in Action*
11.35 **T11: Mario Orsi** - *The development of a coarse-grain biomembrane model and its use in multiscale coarse-grain/atomic-level simulations*
11.55 **T12: Kia Balali-Mood** - *Multi-level simulations of membrane bound Oxidosqualene Cyclase: From Coarse Grained to Atomistic*
12.15 **T13: Sarah Wilsey** - *EPSRC National Service for Computational Chemistry Software (NSCCS)*
- 12.35 Lunch and posters

Session 6

- 14.00 **Plenary 6: Johan Aqvist** - *Computer Simulations of Processes Involved in mRNA Translation on the Ribosome*
14.35 **T14: Alessio Lodola** - *Application of computational models to the design of new inhibitors of fatty acid amide hydrolase*
14.55 **T15: Marcus Kubitzki** - *Simulating Large Conformational Transitions Using Temperature Enhanced Essential Dynamics Replica Exchange (TEE-REX)*
15.15 **T16: Elodie Laine** - *The interplay between the interactions within a protein-protein complex and the conformational sampling of each partner*
- 15.35 Tea

Session 7

- 16.05 **T17: Richard Henchman** - *Liquid-phase partition function from computer simulation*
16.40 **T18: Arumugam Madhumalar** - *Cooperativity in binding of p53 to DNA: a computational study*
- 17.00 CCPB Annual Meeting
17.30 End of Session
- 19.30 Conference Dinner followed by entertainment

Wednesday 9 January

Session 8

- 9.00 **Plenary 7: Mike Sutcliffe** - *Dynamically-coupled enzyme catalysis: insight from simulation of hydrogen tunnelling*
- 9.35 **T19: Chris-Kryton Skylaris** - *A study of the BRCA2-RAD51 complex with classical molecular dynamics and large-scale density functional theory calculations*
- 10.10 **T20: Carla Molteni** - *A metadynamics study of a possible trans-cis proline switch for opening ion channels*
- 10.30 Coffee

Session 9

- 11.00 **Plenary 8: Jan Jensen** - *Prediction and Rationalization of Protein Stability and Activity*
- 11.35 **T21: Syma Khalid** - *OmpG: A Quiet Pore?*
- 11.55 **T22: Josh Berryman** - *Plasticity and Polymorphism of the Glutamine-Rich Amyloid Aggregates*
- 12.15 **T23: Clare-Louise Evans** - *Dynamics and Unfolding of the p62 UBA Domain: Correlations between Simulation and Experimental Data*
- 12.35 Lunch

Session 10

- 14.00 **Plenary 9: Inaki Tunon** - *Computational Design of Biological Catalysts*
- 14.35 **T24: Hans Martin Senn** - *Insights into Enzymatic Halogenation from QM and QM/MM Calculations*
- 14.55 **T25: Robert Deeth** - *Molecular Modelling of Transition-Metal Carboxylate Interactions*
- 15.15 Tea and departure