



MGMS

Young Modellers' Forum 2017

24th November 2017

PROGRAMME

Programme of Oral Presentations

9.15 – 9.50	Coffee and Registration
9.50 – 10.00	Welcome and Introduction
10.00 – 10.20	Carl Mensch, Universities of Antwerp and Ghent Towards a standardized characterization of solution phase protein structure using Raman optical activity
10.20 – 10.40	Luca Iuzzolino, University College London Use of crystal structure informatics for defining the conformational space needed for predicting crystal structures of pharmaceutical molecules
10.40 – 11.00	Can Simon Pervane, University of Southampton Enhancing conformational sampling by modifying the underlying velocity distribution: Digitally filtered hybrid Monte Carlo
11.00 – 11.30	Poster Presenters "Lightning Talks"
11.30 – 11.50	Tea/Coffee break
11.50 – 12.10	Heider A. Hussein, University of Birmingham Structural Investigations and Stabilities of Au-Pd Sub-nanometre Clusters
12.10 – 12.30	Adam Baskerville, University of Sussex Going beyond standard approximations in quantum chemistry
12.30 – 12.50	Hannah Bruce Macdonald, University of Southampton Water networks in protein-ligand complexes using Grand Canonical ensemble methods
12.50 – 14.10	Lunch and Poster Session
14.10 – 14.30	Christian Jorgensen, King's College London Energetics of Ion Permeation in an Open-Activated TRPV1 Channel
14.30 – 14.50	Juan Eiros Zamora, Imperial College Markov State Models of cardiac Troponin dynamics
14.50 – 15.10	Xiuyun Jiang, University College London Simulation of Pump-Probe Experiment in Small Tetraheme Cytochrome
15.10 – 15.30	Pattama Wapeesittipan, University of Edinburgh Allosteric effects in a catalytically impaired variant of Cyclophilin A are unrelated to millisecond time scale motions
15.30 – 15.30	Tea/Coffee break
15.50 – 16.10	Nick Fowler, University of Manchester Prediction of reduction potentials of copper proteins with continuum electrostatics and density functional theory
16.10 – 16.30	Olivia Lynes, University of Lancaster Ab initio Molecular Dynamics Simulations of Hydrated Hydroxide Systems
16.30 – 17.00	Deliberations and Prizes
17.00	End

Programme of Poster Presentations

Poster 1	Leanna Smith, University of Leicester Architectural insights into CHFR structure through homology modelling of the central RING domain
Poster 2	Marc Daemgen, University of Oxford Alternative Binding Mode of Full and Partial Agonists in the Glycine Receptor Stabilises Loop C in an Open Conformation
Poster 3	Angus Voice, University of Bristol Investigating reactivity of covalent drugs by QM/MM modelling
Poster 4	Jacqueline Tan, University of Oxford Understanding regioselectivity in radical cation Diels-Alder reactions using quantum and molecular dynamics
Poster 5	Maeve Kavanagh, Imperial College Excited States of the Photosystem II Reaction Centre
Poster 6	Matthew Dwyer, University of Sheffield The Role of Hydrocarbon Composition on the Thermal Stability of Aviation Fuel
Poster 7	Lee Steinberg, University of Southampton Understanding the Structure of Water Networks through Topological Data Analysis
Poster 8	Sowmya Indrakumar, Technical University of Denmark Characterization of protein-excipient interactions for designing formulation
Poster 9	Ganesh Shahane, Queen Mary University of London Depth-dependent physical properties of model biological lipid bilayers
Poster 10	Joan Clark-Nicholas, University of Edinburgh Exploring the druggability of hPNMT with the JEDI collective variable
Poster 11	Mateusz Bieniek, King's College London and the Francis Crick Institute Fibronectin III 9-10 Adhesion and Material-Driven Fibrillogenesis
Poster 12	Ricardo Parra-Cruz, University of Nottingham Engineering thermostable biocatalysts for CO ₂ capture and utilization purposes

Poster presenters will give their 2 minute "Lightning Talks" in the above order starting at 11:00.

Posters will be on display during the breaks and at lunchtime.