Biochemical Society
Advancing Molecular Bioscience

23–24 October 2014
Charles Darwin House, London, UK

APPLICATION DEADLINE: 25 AUGUST 2014

A Biochemical Society Training Day

Hands-on Introduction to Protein Simulations

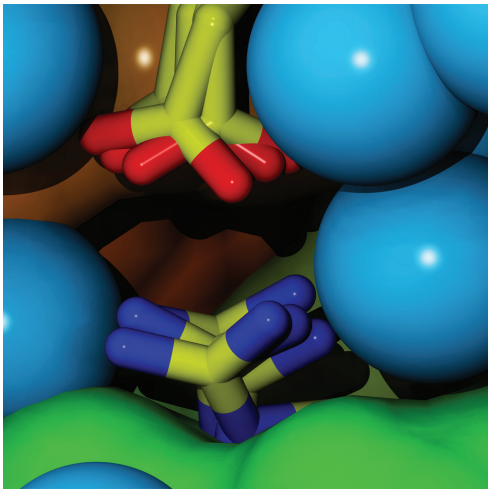

Image kindly supplied by Marcos Sotomayor (Ohio State University, USA)

Organizers:

Amir Khan
Marcos Sotomayor

Overview:

Protein and enzyme function is determined by both structure and dynamic flexibility in solution. Molecular simulations provide insight into conformational transitions that play a critical role in biological activity. This training course will enable biochemists that are non-experts in computational biology to perform protein simulations and evaluate their results, using a free and widely used software package. Participants will leave with the practical knowledge of running and analysing simulations on a protein system.

Topics:

* Visualization and analysis of protein structure
* Theoretical aspects of molecular dynamics simulations
* Preparation of a protein system for molecular dynamics simulations
* Practical aspects of running a simulation
* Output of simulations and analysis of trajectories
* Steered molecular dynamics

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Registration fees starting at £85

This event is CPD approved and attendees can claim 42 credits

Trainers:

Amir Khan	(Trinity College, Dublin, Ireland)
Hannes Loeffler	(Science and Technology Faculties Council, UK)
Marcos Sotomayor	(Ohio State University, USA)
Rachelle Gaudet	(Harvard University, USA)
Valeria Losasso	(Science and Technology Faculties Council, UK)

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