



Queen's University Belfast
10th - 13th of December 2012

Date	Time	Lecture Title	Lecturer	Venue
Monday 10	09:00-10:30 ²	Introduction to Statistical Mechanics and Monte Carlo Methods	Mario Del Popolo	ELTC/SR4 ³
	10:30-11:00	Coffee break		
	11:00-12:30	Introduction to Molecular Dynamics		ELTC/SR4
	12:30-14:00	Lunch break		
	14:00-17:00	Practical session Molecular Dynamics and Monte Carlo		ELTC/IS1 ⁴
Tuesday 11	09:00-10:30	Molecular dynamics of proteins: ion channels	Shozeb Haider	ELTC/SR4
	10:30-11:00	Coffee break		
	11:00-12:30	Molecular dynamics of proteins: G protein coupled receptors	Irina Tikhonova	ELTC/SR4
	12:30-14:00	Lunch break		
	14:00-17:00	Practical session: Molecular dynamics of proteins	S. Haider & I. Tikhonova	ELTC/IS1

¹ Local organizers: Prof. Jorge Kohanoff (j.kohanoff@qub.ac.uk) and Dr. Mario Del Pópolo (m.del-popolo@qub.ac.uk)

² Lectures and tutorials will be split into 40 min sessions and 10 min breaks

³ ELTC/SR4: Elmwood Learning and Teaching Centre – Study Room 4. Queen's University Belfast

⁴ ELTC/IS1: Elmwood Learning and Teaching Centre – Independent Study 1. Queen's University Belfast

Wednesday 12	09:00-10:30	Ab initio Molecular Dynamics	J. Kohanoff	ELTC/SR4
	10:30-11:00	Coffee break		
	11:00-12:30	Tight-binding Molecular Dynamics		ELTC/SR4
	12:30-14:00	Lunch break		
	14:00-17:00	Practical session: Tight-binding Molecular Dynamics	D. Pashov & T. Sheppard	ELTC/IS1
Thursday 13	09:00-10:30	Enhanced sampling methods in Molecular Dynamics I	Gareth Tribello	ELTC/SR4
	10:30-11:00	Coffee break		
	11:00-12:30	Enhanced sampling methods in Molecular Dynamics II		ELTC/SR4
	12:30-14:00	Lunch break		
	14:00-17:00	Enhanced sampling practical session: PLUMED		ELTC/IS1

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