Workshop Program

Monday, 2nd		
9.00-9.50	Alexandre Bonvin	General principles of docking and introduction to HADDOCK
10.00-10.50	Alexandre Bonvin	(parts 1 and 2)
11.20-12.10	Po-chia Chen	Binding of toxins to potassium channels from HADDOCK
14.00-17.00	Alexandre Bonvin	Tutorial on protein-protein docking with HADDOCK
20.00-21.30	Student talks	
Tuesday, 3rd		
9.00-9.50	Alexandre Bonvin	Integrative modeling of macromolecular assemblies
10.00-10.50	Alexandre Bonvin	(parts 1 and 2)
11.20-12.10	Ugur Sezerman	A review of scoring methods for binding
14.00-17.00	Alexandre Bonvin	Tutorial on flexible multi-body docking and SAXS scoring.
20.00-21.30	Student talks	
Wednesday, 4th		
9.00-9.50	Rita Casadio	From protein-protein interaction networks to interaction
10.00-10.50	Rita Casadio	surface patches in proteins (parts 1 and 2)
11.20-12.10	Ugur Sezerman	Scoring the impact of mutations on protein-ligand interactions
14.00-17.00	Pier Luigi Martelli	Tutorial on protein-protein interaction networks
20.00-21.30	Student talks	
Thursday, 5th		
9.00-9.50	Turkan Haliloglu	Protein dynamics in binding
10.00-10.50	Turkan Haliloglu	(parts 1 and 2)
11.20-12.10	Ozlem Keskin	Prediction of protein-protein interactions combining structures and sequence: PRISM
14.00-17.00	Ozlem Keskin	Tutorial on protein-protein interactions
20.00-21.30	Student talks	
Friday, 6th		
9.00-9.50	Turgut Bastug	Free energy methods for calculation of binding free energies
10.00-10.50	Serdar Kuyucak	Free energy calculations for toxin-ion channel complexes and
11.20-12.10	Serdar Kuyucak	glutamate transporters (parts 1 and 2)
14.00-17.00	Turgut Bastug	Tutorial on free energy calculations from MD simulations
20.00-21.30	General discussion	Future of computational methods in description of protein interactions