EJIBCE 2018

Programme

08:30	**Registration**		*Foyer* - FMUP
09:30	**Opening Ceremony**		Room 4 - FMUP
09:35	**K1**: Improving the description of hydrogen bonds in molecular docking using DFT calculations	**Diogo Santos-Martins** The Scripps Research Institute (USA)	
10:05	**OC1**: Molecular Modelling, Analysis of Protein Tunnels and Screening the Binding Trajectories of Inhibitors using the Caver Suite	**Gaspar Pinto** Masaryk University (Czech Republic)	
10:25	**OC2**: An *in silico* predictor of protein dimer interfaces	**António J. Preto** Universidade de Coimbra (Portugal)	
10:45	**Poster Session 1 + Coffee Break**		*Foyer* - FMUP
11:15	**K2**: Computer-Aided Discovery of JAK2-JH2 Inhibitors	**Ana S. Newton** Yale University (USA)	Room 4 - FMUP
11:45	**OC3**: Computational strategies for the engineering of peptide ligases	**Eduardo F. Oliveira** University of Groningen (Netherlands)	
12:05	**OC4**: Computational campaign to discover novel human 20S proteasome inhibitors	**Pedro M. P. Fernandes** Universidade de Lisboa (Portugal)	
12:25	**Lunch** Poster Session 1 Poster Session 2		*Foyer* - FMUP
14:30	**K3**: A Complete Pipeline for Enabling Efficient and Timely NMR Structural Biology on Challenging Pharmaceutical Targets	**Marta G. Carneiro** ZoBio B.V. (Netherlands)	Room 4 - FMUP
15:00	**K4**: The KH type III domain: From an ancestral peptide to three different protein folds	**Joana Pereira** Max-Planck Institute (Germany)	
15:30	**OC5**: PypKa: a python module for flexible Poisson-Boltzmann based pKa calculations with proton tautomerism	**Pedro B. P. S. Reis** Universidade de Lisboa (Portugal)	
15:50	**Poster Session 2 + Coffee Break**		*Foyer* - FMUP
16:30	**K5**: How do buried residues get phosphorylated?	**João Henriques** University of Copenhagen (Denmark)	Room 4 - FMUP
17:00	**OC6**: The impact of using single atomistic long range cutoff schemes with the GROMOS 54A7 force field	**Tomás F. D. Silva** Universidade de Lisboa (Portugal)	
17:20	**OC7**: Accelerating the DszD enzyme for the Biodesulfurization of Crude Oil and Derivatives	**Pedro Ferreira** Universidade do Porto (Portugal)	
17:40	**Closing Ceremony + Awards**		
18:00			

Keynote Oral Communication