ADVANCED WORKSHOPS

June 15th and 16th, 2023 - UC

June 15th   Anfiteatro II

01

Paulo Costa

9:00	Workshop Check In
9:15	**MM/PBSA to estimate ligand-binding affinities**
10:45	Coffee Break
11:00	**MM/PBSA to estimate ligand-binding affinities**
12:00	

02

Francisco Fernandes
Irina Moreira

14:00	Workshop Check In
14:15	**Deep Learning for protein sequence and structure**
15:45	Coffee Break
16:00	**Deep Learning for protein sequence and structure**
17:00	

June 16th   Auditório

03

Miguel Machuqueiro

9:00	Workshop Check In
9:15	**pKa calculations and constant pH MD simulations of proteins**
10:45	Coffee Break
11:00	**pKa calculations and constant pH MD simulations of proteins**
12:00	

04

Manuel Melo

14:00	Workshop Check In
14:15	**Using MDanalysis for structural work, before and after simulation**
15:45	Coffee Break
16:00	**Using MDanalysis for structural work, before and after simulation**
17:00	