



INTERMEDIATE WORKSHOPS

December 19th, 2023 - UC

08:45 Workshop Check In

09:15 **Opening Session**

Auditório

01

Francisco Fernandes

09:30 **Machine learning demystified**

11:00 Coffee Break

02

Sérgio Sousa

11:30 **Protein-ligand docking and library
preparation for virtual screening**

13:00 Lunch Break

Auditório

03

Miguel Machuqueiro

14:30 **pKa calculations of proteins using the
PypKa tool**

16:00 Coffee Break

04

Manuel Melo

16:30 **Coarse-grain simulation using the
Martini 3 model**

18:00 Closing Session

