Program

Wednesday, December 21st 2022

8:30 **Registration**

9:30 **Opening Session**

Pedro Patacho, Councilor for Education and Science, Municipality of Oeiras
Cláudio M. Soares, Dean of the ITQB-NOVA
Manuel N. Melo, 3D-BioInfo-PT-Community

9:45 **Carlos S. H. Shiraishi**

"Virtual screening of a library of natural compounds against COX-2 protein"

10:00 **Gabriel F. Martins**

"Polyphenols as Aggregation Inhibitors: Application to α-Synuclein and Related Peptides"

10:15 **Israa Aljnadi**

"In Silico Studies and Chemical Synthesis of Ligands Targeting c-MYC G-Quadruplex"

10:30 **Marta S. P. Batista**

"Structural characterization of the permeation of water and glycerol derivatives through PfAQP for the development of new antimalarial therapies"

10:45 **Rita I. Teixeira**

"The impact of SARS-CoV-2 Omicron variant on the interaction with human ACE2"

11:00 **Coffee Break and Poster Session I**

11:45 **Wallfuture**

11:55 **Keynote Lecturer – Carla Sousa**

"MD simulations applied to Infection research: improving studies of drug permeation across biomembranes"

12:55 **Tomás F. Silva**

"Tackling the realism of transmembrane peptides simulations with a pH-Gradient/CpHMD approach"

13:05 **Pedro C. Rosado**

"Exploring PBP2a protein to fight β-lactam resistance in MRSA"

13:25 **Rodrigo Barriga**

"Simulating substrate binding sites in the S. aureus Type II NADH Dehydrogenase"

13:40 **Tatiana F. Vieira**

"What can computational methods do to help find new molecules with antimicrobial properties"

13:45 **Lunch**

SPBf Session

15:50 **Armindo Salvador**

Presentation of the Portuguese Biophysical Society (SPBf)

16:00 **Pedro Beltrão**

"Studying protein interactions and domain evolution using AlphaFold"

16:45 **Coffee Break and Poster Session II**

17:30 **Bruno Calçada**

"Development of machine learning models to predict thyroid peroxidase inhibition"

17:45 **João G. N. Sequeira**

"Extending the stochastic titration CpHMD to the CHARMM36m and AMBER14SB force fields"

18:00 **Urszula Orzeł**

"Oligomerization of metabotropic glutamate receptors"

18:15 **Andreia Fortuna**

"Tackling halogen anisotropy in biomolecular simulations: assessment of force field parameters using hydration free energies"

18:30 **Bárbara Bahls Bruni**

"Design and virtual screening of Indoloisoquinoline derivatives as c-MYC G4 binders"

18:45 **Closing Session/Remark**