

VIII EJIBCE

Coimbra, 20 de dezembro 2021

Program

08:30 - REGISTRATION

09:30 - Cláudia Cavadas

Opening Session by the Vice-Rector of the University of Coimbra

09:45 - Irina Moreira

3d-Bioinfo-PT-community inauguration

10:00 - Diana Lousa

"Viral membrane fusion: characterizing and inactivating a crucial step of the infection by devastating pathogens"

10:45 - Joana Pereira

"What is hidden in the darkness? Seeking new families in natural unknown proteins"

11:10 - COFFEE BREAK AND POSTER SESSION I

11:40 – Ona Šivickytė

"A novel US-CpHMD protocol to study the protonation-dependent mechanism of the ATP/ADP carrier"

12:05 - Nuno Oliveira

"A novel US-CpHMD protocol to study the protonation-dependent mechanism of the ATP/ADP carrier"

12:30 - LUNCH AND POSTER SESSION II

14:45 - Bruno Victor

"Identification of membrane Pan-Assay INterference CompoundS (PAINS) using an atomistic Molecular Dynamics protocol"

15:30 – Beatriz Bueschbell

"DRD2 homo-dimers - a world of possibilities"

15:55 - Pedro Suzano

"An US-CpHMD protocol to calculate pH-dependent membrane permeability coefficients of antitumor drugs"

16:20 - COFFEE BREAK AND POSTER SESSION III

16:50 – Luís Borges-Araújo

"SARS-CoV-2 variants impact RBD conformational dynamics and ACE2 accessibility"

17:15 - Tatiana Vieira

"Developed of Inverted Virtual Screening Approaches for the Identification of Protein Targets Associated to the Biological Activity of Specific Molecules"

17:40 – Mariana Valério

"Parainfluenza fusion peptide promotes membrane fusion by assembling into oligomeric pore-like structures"

18:05 - CLOSING SESSION