

# 2ND ANNUAL MEETING

December 18th, 2023 Coimbra

MORNING SESSION

ANFITEATRO I

08:30 Registration

09:30 **Opening Session**

09:40 **Presentation of the Portuguese Biophysical Society (SPBf) | Armindo Salvador**

09:45 **Oral Communication 1 | Inês Pires**

"Are protein pKa predictions affected by the choice of experimental structure?"

10:00 **Oral Communication 2 | Andreia Fortuna**

"Binding free energies using MM-PBSA calculations: an assessment using halogenated ligands"

10:15 **Oral Communication 3 | Fábio Martins**

"Lysinated multiwalled carbon nanotubes with carbohydrate ligands as a doxorubicin nanocarrier: AMD analysis."

10:30 **Keynote I | Rita Melo**

"Data driven and computational tools in radiopharmaceutical research"

11:15 Coffee Break & Poster Session 1

11:45 **Keynote II | Ricardo J. Ferreira**

"Computer-aided drug discovery (CADD) in CROs and open-source software: new approaches to everyday problems."

12:30 **Oral Communication 4 | Beatriz Caniceiro**

"Bridging Quantitative Database Insights with Machine Learning for CPPs"

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**12:45 Oral Communication 5 | João Sequeira**

“Understanding P-gp inhibition by RuCp compounds using a Molecular Docking protocol.”

----- **LUNCH BREAK (13:00 - 15:00)** -----

AFTERNOON SESSION

AUDITÓRIO

**15:00 Oral Communication 6 | Nuno Oliveira**

“Mechanism of the conformational switching in diphtheria toxin translocation (T) domain triggered by protonation”

**15:15 Oral Communication 7 | Sofia Sousa**

“Design of novel KDM4C inhibitors for the treatment of triple negative breast cancer”

**15:30 Oral Communication 8 | Tomás Silva**

“CpH-MetaD: coupling wt-metadynamics and CpHMD in the study of RNA oligomers”

**15:45 Keynote III | Hugo Penedones**

“Scientific Computing meets AI”

**16:30 Coffee Break & Poster Session 2**

**17:00 Round Table**

Hugo Penedones | Luís Valente | Nuno Cerqueira |  
Ricardo J. Ferreira | Irina Moreira

Charting trajectories: Navigating career paths in structural computational biology - a round table discussion on bridging academia and industry

**17:45 Closing Session**