Poster Session 1

10:45 - 11:15 & 12:25 - 13:30

P1. A multi-target approach for hormone-dependent breast cancer: estrogen receptors and aromatase

Almeida, C., Oliveira, A., Amaral C., Ramos, M. J., Correia-da-Silva, G., Teixeira, N. and Fernandes, P. A.

P2. Understanding Structural and Dynamic Differences of GHSRGq and GHSR-Arr Complexes

Barreto, C., Melo, R., Magalhães, P. R., Renault, P., Machuqueiro, M., Moreira, I. S.

P3. The influence of conformational diversity on enzyme catalysis

Calixto, A. R., Ramos, M. J. and Fernandes, P. A.

P4. Coarse grain-molecular dynamics simulations of cyclic peptide nanotubes on biological membranes for different negative charge content

Calvelo, M., Claro, B., Bastos, M., Garcia-Fandiño, R.

P5. From All Atoms to Coarse Grain: Simulating the Molecular Imprinting Process of a Silica Polymer

Concu, R., Cordeiro, M. N.

P6. Estimation of solvation free energies by continuum methods: How to tackle halogenated species?

Nunes, R. and Costa, P. J.

P7. The pH-dependent membrane stability and insertion mechanism of GALA peptide

Dias, J. R., Silva, T., Machuqueiro, M.

P8. Is the 5,10-methylenetetrahydrofolate cofactor through a non-enzymatic or enzymatic mechanism?

Fernandes, H. S., Sousa, S. F., and Cerqueira, N. M. F. S. A.

P9. Text Mining for Recognition of Cancer Biomarkers

Gaspar, A. C., Pires, M. N., Preto, A. J., Moreira, I. S.

P10. The importance of unstructured termini in the aggregation cascade of beta-2-microglobulin: insights from molecular simulations of D76N mutant

Loureiro, R.J.S., Vila-Viçosa, D., Machuqueiro, M., Shakhnovich, E.I, Faísca,P.F.N.

P11. Influence of codon 35 amino acid insertion in HIV-1 protease: insights from molecular dynamics

Luís, J. P, Mata, A. I., Alves, N. G., Simões, C. J. V., Pereira-Vaz, J., Vaz, D.C., Duque, V. and Brito, R. M. M.

P12. pH effects on PG/PC and PS/PC lipid binary mixtures: a CpHMD study

Magalhães, P. R., Vila-Viçosa, D., Silva, T., Machuqueiro, M.

P13. Creation of a Structural Database for Inhibition of BioFilm Formation

Magalhães, R. P., Vieira, T. F., Fernandes, H. S., Cerqueira, N. M. F. S. A., Melo,A., Simões, M., Sousa, S. F.

P14. MENSAdb: A Major Structural Statistical Analysis of Membrane Protein Dimers

Matos-Filipe, P., Preto, A. J., Almeida, A. J., Koukos, P. I., Bonvin, A. M. J. J., Moreira, I. S.

P15. Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization

Melo R., Almeida J. G., Melo A., Cordeiro M. N. D. S., Gumus, Z. H., Cabo-Verde S., Moreira I. S., Correia J. D. G.

P16. Drug-Target Interaction Prediction: End-to-End Deep Learning Approach

Monteiro, N.R.C, Arrais J.P., Ribeiro B.

P17. In silico design of halogenated carbohydrate mimetics as potential halogen-bonding ligands

Nunes, R., Xavier, N. M., and Costa, P. J.

P18. New phosphorylated amino acid parametrization to correctly reproduce their acid/base equilibria, including in protein binding events

Oliveira, N. F. B. M., Pires, I. D. S., Machuqueiro, M.

Poster Session 2

13:30 - 14:30 & 15:50 - 16:30

P19. Exploring the Catalytic Mechanism of the Malonyl-Acetyl Transferase Domain of Human Fatty Acid Synthase

Paiva, P., Sousa, S.F., Ramos, M.J., Fernandes, P.A.

P20. Comparing Molecular Dynamics Force Fields in Bacteria Membrane Models

Peón, A., Claro, B., Bastos, M., Piñeiro, Á., García-Fandiño, R.

P21. Application of QM/MM Methods in the Study of PNPOx

Pina, A., Sousa, S. F., Cerqueira, N. M. F. S. A.

P22. Machine Learning to Predict Binding Affinity of Ligand-Target Interactions

Pinho, X., Preto, A. J., Moreira, I. S.

P23. Unravelling the molecular details of the pH-dependent gating mechanism in the outer membrane protein G

Pires, I. D. S. and Machuqueiro, M.

P24. Estimating pKa shifts of encapsulated drugs through a CpHMD approach

Reis, D., Machuqueiro, M., Vila-Viçosa, D.

P25. Implementation of a biocomputing platform to settle a new drug discovery pipeline towards post-synaptic receptors

Ribeiro R., Giorgetti A.

P26. A Survey of Enzyme Chemistry using the Mechanism and Catalytic Site Atlas

Ribeiro, A. J. M., Tyzack, J. D., Borkakoti, N., Thornton, J. M.

P27. Combined experimental and computational studies devoted to the synthesis of 1,4-lactones

Rocha, J. F., Freitas, D. S. , Noro, J., Teixeira, C. S. S., Sousa, C. E., Sousa, S. F., Alves, M. J., Cerqueira, N. M. F. S. A.

P28. Metabolic Engineering of Cyanobacteria for Bisabolene Production

Rodrigues, J., Dienst, D., Lindberg, P.

P29. A Molecular Dynamics Insight to Non-Structural Protein 1 (NS1) – A Hub Protein Essential for Influenza Infection

Rosário-Ferreira, N., Melo, R., Moreira, I. S., Brito, R. M. M.

P30. The HIV-2 envelope glycoprotein as a differentiated target in structure-function relationships to structural elucidation and characterization

Serra, P., Martins A., Taveira, N., Guedes, R.C.

P31. Carbohydrate-aromatic interactions mimetics: the role of C-Br...pi bonds

Šivickytė, O., Nunes, R., and Costa, P. J.

P32. Experimental and Computational Studies Addressed to 1,3Dipolar Cycloadditions of D-Erythrose 1,3-Dioxane 1,5-Lactone with Regio- and Stereo-selectivity

Sousa, C. E. A., Ribeiro, A. M. P., Fortes, A. G., Cerqueira, N. M. F. S. A., and Alves, M. J.

P33. Single vs Multi Conformational QM/MM approach for enzymatic catalysis: The case of study of the HBPS desulfinase from the 4S pathway

Sousa J. P. M., Sousa S. F., Ramos M. J., Fernandes P. A.

P34. Unraveling the Catalytic Mechanism of Tryptophan Synthase, a Drug Target Against Mycobacterium Tuberculosis

Teixeira, C. S. S., Sousa, S. F., Cerqueira, N. M. F. S. A.

P35. Initial studies on the sensibility of Aquaporin-4 to membrane PAINS

Luz, A.F.S., Victor, B.L.

P36. Evaluation of Different Scoring Functions for Docking and Virtual Screening against GPCR Drug Targets

Vieira, T. F., Magalhães, R. P., Cerqueira, N. M. F. S. A., Sousa, S. F.

P37. Folding of cyclic peptides stabilized by halogen bonds

Vila-Viçosa, D., Nunes, R., Costa, P. J.