Mini Symposium

"Computational methods in drug and materials design"

BRFAA Amphitheater

Wednesday July 3, 2019
9 am – 3 pm

9:00 – 9:30 Keynote Speaker, Prof. Kennie Merz, Department of Chemistry, Department of Biochemistry & Molecular Biology, Michigan State University
"Simulating Coordination Chemistry"

9:30 – 10:00 Dr. Stefan Doerr, Pompeu Fabra University
"Applications of machine learning in molecular simulations"

10.00 – 10.30 Sofia Kyriakidi, Department of Chemistry, University of Athens
"A combined equilibrium and steered Molecular Dynamics simulations study of the drug-binding pathway of candesartan on Angiotensin 1 Receptor"

10.30 – 10.45 Coffee Break

10.45 – 11.15 Dr. Ana Newton, Department of Chemistry, Yale University
"Computer-Aided Discovery of JAK2-JH2 Inhibitors"

11.15 – 11.45 Dr. Sophie Hirakis, Department of Chemistry, University of California San Diego
"Towards universal virtual cell screening: Multiscale spatiokinetic models of cardiac signaling"

11.45 – 12.00 Anastasia Theodoropoulou, Biomedical Research Foundation, Academy of Athens
"Targeting IL-33 as an anti-inflammatrory agent with computer-aided design"

12.00 – 12.15 Alexios Chatzigoulas, Biomedical Research Foundation, Academy of Athens
"Prediction of protein membrane binding interfaces using machine learning"

12.15 – 13.00 Lunch

13.00– 13.15 Dimitris Ntekoumes, Biomedical Research Foundation, Academy of Athens
"Evaluation of the predictive accuracy of free energy calculations in drug design"

13.15 – 13.45 Ioannis Skarmoutsos, National Hellenic Research Foundation
"Computational Modeling of nanoporous materials for sustainable energy and environmental applications"

13.45 – 14.15 Manolis Klontzas, National Hellenic Research Foundation
"Tuning the properties of nanoporous materials with the aid of computational chemistry tools"

14.15 – 14.45 Keynote Speaker – Prof. Manos Mikros, Department of Pharmacy, University of Athens
"Using advanced and analytical tools for efficient discovery of new bioactive compounds"

14.45 – 15.15 Discussion and Closing