



2nd BRF AA Mini Symposium

“Computational methods in drug and materials design”

BRFAA Amphitheater

**Monday June 20, 2022
15.00 – 19.00 (CET)**

15.00 – 15.15 Registration

15.15 – 15.30 Q&A with Prof. Erik Lindahl

“Bioexcel and GROMACS”

15:30 – 16:00 Keynote Speaker, Prof. Erik Lindahl, Professor of Biophysics at the Department of Biochemistry & Biophysics, Science for Life Laboratory, Stockholm University

“Resolving gating and allosteric modulation in ion channels from molecular dynamics simulations & experiments”

16:00 – 16:30 Dr. George Boulougouris, Lecturer, Department of Molecular Biology and Genetics

“Free energy: from Statistical Mechanics to Molecular Simulation”

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956314.

16.30 – 17.00 Keynote Speaker – Prof. Thomas Cheatham, III, School of Pharmacy, University of Utah

“Recent successes in simulations of nucleic acids”

17.00 – 17.15 Coffee Break

17.15 – 17.45 Prof. Thomas Mavromoustakos, Professor of Organic Chemistry, National and Kapodistrian University of Athens

“Rational Drug Design for the treatment of the Hypertension Risk Factor”

17.45 – 18.15 Dr. Alexios Chatzigoulas, Postdoctoral Associate, Biomedical Research Foundation, Academy of Athens

“Predicting protein-membrane interfaces of peripheral membrane proteins using ensemble machine learning”

18.15 – 18.45 Dr. Demeter Tzeli, Associate Professor of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens

“DFT and Semiempirical Calculations: Powerful tools for drug and materials design”

18.45 – 19.00 Discussion and Closing

Zoom Connection Details

Topic: 2nd BRFAA Mini Symposium

Join Zoom Meeting

<https://zoom.us/j/98001118799?pwd=aGdyY01CVXpab3d5RStiZVcwY1pLZz09>

Meeting ID: 980 0111 8799

Passcode: QJBxr9

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