ISQBP
THE INTERNATIONAL SOCIETY OF QUANTUM BIOLOGY & PHARMACOLOGY

ACADEMY OF ATHENS

BRFAA
BIOMEDICAL RESEARCH FOUNDATION ACADEMY OF ATHENS

ISQBP President's Meeting 2024

19 | 23 May 2024

Athens GREECE

www.isqbp2024.org

PROGRAM

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INVITED SPEAKERS



Johan Åqvist
Uppsala University
SWEDEN



Charlie Brooks
University of Michigan
USA



Matthias Buck
Case Western Reserve University
USA



Andrea Cavalli
CECAM
SWITZERLAND



Vlad Cojocaru
Universitatea Babeș-Bolyai
ROMANIA



Marco de Vivo
Italian Institute of Technology
ITALY



José Duca
Novartis Institutes of Biomedical Research
USA



Serdar Durdağı
Bahçeşehir University
TURKEY



Evi Gkeka
Sanofi
FRANCE



Frauke Gräter
Heidelberg Institute for Theoretical Studies
GERMANY



Ellinor Haglund
University of Hawaii Manoa
USA



Sarah Harris
University of Leeds
UK



Fahmi Himo
Stockholm University
SWEDEN



Wonpil Im
Lehigh University
USA



William Jorgensen
Yale University
USA



Themis Lazaridis
City College of New York
USA



Klaus Liedl
University of Innsbruck
AUSTRIA



Alexander MacKerell
University of Maryland
USA



Alessandra Magistrato
Trieste SISSA
ITALY



Nancy Makri
University of Illinois Urbana - Champaign
USA



Thomas Mavromoustakos
University of Athens
GREECE



Kenneth Merz Jr.
Michigan State University
USA



Emmanuel Mikros
University of Athens
GREECE



Sophie Saquin-Mora
CNRS
FRANCE



Modesto Orozco
University of Barcelona
SPAIN



Jean-Philip Piquemal
University of Sorbonne
FRANCE



Carol Post
Purdue University
USA



Nigel Richards
Cardiff University
UK



Adrian E. Roitberg
University of Florida
USA

WELCOME

Dear Colleagues and Friends,

It is a pleasure to welcome you to the ISQBP President's Meeting, 19-23 May 2024 taking place at the historical building of the Academy of Athens, Greece, as well as at the Biomedical Research Foundation of the Academy of Athens (BRFAA), which is the most recent addition to the Life Sciences research organizations in Greece.

The International Society of Quantum Biology and Pharmacology is a Society founded in 1970 to provide a forum for chemists, pharmacologists, and biologists to discuss and extend the impact of computational methodologies in the fields of biology, chemistry, medicinal chemistry, chemical biology, drug discovery, pharmacology, bioinformatics, genomics, and proteomics.

The ISQBP President's Meeting is the flagship event of ISQBP being organized biennially for the past 50 years, providing a forum to promote interdisciplinary collaboration and to honor significant scientific contributions in these fields. In this spirit, the ISQBP awards biennially the Computational Biology award, which is awarded this year to Professor Johan Åqvist, Uppsala University, Sweden, as well as an endowed Lectureship honoring Gilda Loew, which is presented by Professor Kenneth Merz, Jr., Michigan State University, USA. Moreover, three awards for the best contributed talk and poster presentations will be given.

Finally, I would like to extend my heartfelt thanks to the ISQBP Board and Founding Members, who have helped in all aspects to organize the Meeting, to the President of BRFAA for his support, to my lab members for their time, to our sponsors for the financial assistance, and to all of you for making this conference a success!

I wish you an exciting ISQBP President's Meeting 2024 and an enjoyable time in the historical and beautiful city of Athens.



Dr. Zoe Cournia
ISQBP President 2022-2024
Senior Investigator, Biomedical Research Foundation Academy of Athens

PROGRAM

SUNDAY 19 May 2024

ACADEMY OF ATHENS, CENTRAL BUILDING, EAST CONFERENCE ROOM

16:00-18:00	**REGISTRATION**
18:00	**WELCOME REMARKS** • **Zoe Cournia** (ISQBP President) • **Lucas Papademos** (President of the Board, Biomedical Research Foundation, Academy of Athens, Greece)
18:15-18:20	**INTRODUCTION TO THE COMPUTATIONAL BIOLOGY AWARD LAUREATE**
18:20-19:20	**COMPUTATIONAL BIOLOGY AWARD LECTURE** **Johan Åqvist,** Uppsala University, Sweden Computer Simulations of the Temperature Dependence of Enzyme Reactions
19:30-22:00	**WELCOME RECEPTION**

MONDAY 20 MAY 2024

ACADEMY OF ATHENS, CENTRAL BUILDING, EAST CONFERENCE ROOM

09:00-12:40	**FREE ENERGY** Chair: **Marco de Vivo**
09:00-09:30	**William Jorgensen,** Yale University, USA Evolution of Computer-Aided Drug Discovery
09:30-10:00	**Charlie Brooks,** University of Michigan, USA High-throughput approaches to free energy calculations in ligand discovery and protein design
10:00-10:30	**Alex Mackerell,** University of Maryland, USA Site Identification by Ligand Competitive Saturation (SILCS) as a Platform Technology for Computational Investigations of Free Energies of Intermolecular Interactions
10:30-11:15	**COFFEE BREAK**
11:15-11:35	**Jonas Kaidl,** Schrodinger, Germany Is The Functional Response of a Receptor Determined by the Thermodynamics of Ligand Binding?
11:35-12:05	**Klaus Liedl,** University of Innsbruck, Austria Quantifying Thermodynamic Properties in Biological Systems by Grid Inhomogeneous Solvation Theory
12:05-12:25	**Nour Aldin Kahlous,** Uppsala University, Sweden Design of drug efficacy guided by free energy simulations of G protein-coupled receptors
12:25-12:40	**Nishita Mandal,** Adam Mickiewicz University, Poland Beyond the Threshold: Delving into Rare Gate Opening Events in Enzyme Tunnels through Enhanced Molecular Dynamics Simulations
12:40-14:00	**FREE TIME | LUNCH ON YOUR OWN**
14:00-18:20	**BIOMOLECULAR DYNAMICS I** Chair: **Roland Stote**
14:00-14:30	**Carol Post,** Purdue University, USA Syk tyrosine kinase association with immunoreceptors: MD simulation unravels the physical basis for a new phospho-sensor regulating this protein-protein interaction
14:30-15:00	**Ellinor Haglund,** University of Hawaii Manoa, USA Exploring Pierced Lasso Topologies: Novel Insights into Protein Folding, Function, and Therapeutic Potential
15:00-15:20	**Jan Brezovsky,** Adam Mickiewicz University, Poland Exposing unseen passages for ligand transport through proteins and their functional consequences
15:20-15:50	**Frauke Gräter,** Heidelberg Institute for Theoretical Studies, Germany Learning force fields and reactivity to enhance classical biomolecular simulations
15:50-16:30	**COFFEE BREAK**
16:30-17:00	**Wonpil Im,** Lehigh University, USA What can CHARMM-GUI do for you?
17:00-17:20	**Jennifer Sapia,** University of Fribourg, Switzerland Computational insights into the mechanism of triglycerides formation: a study of DGAT1 using molecular dynamics
17:20-17:40	**Paulo Siani,** Università degli Studi di Milano Bicocca, Italy Mechanistic Insights from Molecular Dynamics Simulations in Nanomedicine Research
17:40-18:00	**Thibault Tubiana,** CNRS, France Molecular modelling, homo-oligomerisation and membrane interactions of hepatitis E virus pORF1 replication polyprotein
18:00-18:20	**Fabrizio Pucci,** Université Libre de Bruxelles, Belgium Leveraging structural and (co)evolutionary data for protein fitness prediction

TUESDAY 21 May 2024

ACADEMY OF ATHENS, CENTRAL BUILDING, EAST CONFERENCE ROOM

09:00-12:30	**QUANTUM MECHANICS AND QUANTUM COMPUTING** Chair: **Julian Tirado-Rives**
09:00-09:30	**Jean-Philip Piquemal,** University of Sorbonne, France Hybrid Quantum-classical algorithms for Accurate Quantum Chemistry
09:30-10:00	**Nancy Makri,** University of Illinois, Urbana-Champaign, USA Real-Time Path Integral Simulation of Energy Transfer in Light Harvesting Complexes
10:00-10:20	**Océane Mangel,** Université Grenoble Alpes Study of the Streptomyces tyrosinase reaction mechanism: a dynamic QM/MM approach
10:20-11:00	**COFFEE BREAK**
11:00-11:30	**Fahmi Himo,** Stockholm University, Sweden Mechanism of Vanadium Chloroperoxidase from Quantum Chemical Calculations
11:30-11:50	**Sergio Sousa,** University of Porto, Portugal Probing the Role Played by Different Amino Acid Residues in the Catalytic Mechanism of Plastic PET degrading by QM/MM Methods
11:50-12:10	**Jon Uranga,** University of the Basque Country, Spain A Lysine-Cysteine Redox Switch: The NOS Bridge
12:10-12:30	**Elise White**, University of Bristol, UK Multi-scale simulations provide insights for engineering product outcome of polyketide synthases
12:30-14:00	**RELOCATION FROM THE ACADEMY OF ATHENS TO BRFAA WITH BUSES | LUNCH AT BRFAA**
14:00-16:00	**BIOMOLECULAR DYNAMICS II** Chair: **Annick Dejaegere**
14:00-14:30	**Nigel Richards,** Cardiff University, UK Hidden Conformational Dynamics Controlling Ammonia Transport in Human Asparagine Synthetase
14:30-15:00	**Themis Lazaridis**, City College of New York, USA Classical simulations with proton transfer: insights into proton channels
15:00-15:30	**Sophie Sacquin-Mora,** CNRS, France Investigating the dynamics of protein-protein interfaces in well structured and fuzzy complexes
15:30-16:00	**Matthias Buck,** Case Western Reserve University, USA Learning to use AlphaFoldMultimer and variants - amazing to not so good for transmembrane proteins
16:00-16:30	**COFFEE BREAK**
16:30-17:15	**LOEW LECTURESHIP** Chair: **Zoe Cournia**
	Kennie Merz, Michigan State University, USA Transition Metal Modeling in Aqueous Solution
17:15-17:30	**Nigel Richards,** Cardiff University, UK Remembering Peter Politzer
17:30-20:00	**POSTER SESSION**

WEDNESDAY 22 May 2024

BIOMEDICAL RESEARCH FOUNDATION, ACADEMY OF ATHENS

09:00-12:40	**COMPUTER-AIDED DRUG DESIGN** Chair: **Evi Gkeka**
09:00-09:30	**José Duca,** Novartis Institutes of Biomedical Research, USA Modeling the undruggable; from the computer to the clinic
09:30-10:00	**Marco De Vivo,** Italian Institute of Technology, Italy Targeting the conserved active site of splicing machines
10:00-10:30	**Thomas Mavromoustakos,** University of Athens, Greece Computational Analysis and Drug Discovery
10:30-11:00	**COFFEE BREAK**
11:00-11:20	**Minos Matsoukas,** University of West Attica, Greece Computational approaches in targeting GPCRs and cancer related proteins with small molecules
11:20-11:50	**Serdar Durdağı,** Bahçeşehir University, Turkey Development of New Virtual Screening Methods Incorporating Artificial Intelligence Approaches to Accelerate the Transition from Preclinical to Clinical Stages in Drug Development
11:50-12:20	**Manos Mikros,** University of Athens, Greece In silico tools for the discovery and optimization of new bioactive compounds
12:20-12:40	**Özge Kürkcüoglu,** Instabul Technical University, Turkey In Silico Identification of Allosteric Sites and Modulators on GPCRs Using Residue Network Model and Site Identification by Ligand Competitive Saturation
12:40-14:00	**LUNCH BREAK | POSTER SESSION**
14:00-17:30	**NUCLEIC ACIDS MODELING** Chair: **Thomas Cheatham**
14:00-14:30	**Modesto Orozco,** University of Barcelona, Spain Frontiers in molecular dynamics of nucleic acids
14:30-15:00	**Evi Gkeka,** Sanofi, France Identifying small-molecules binding sites in RNA conformational ensembles with SHAMAN
15:00-15:20	**Nathalie Basdevant,** Université d'Evry Paris Saclay, France DNA translocation through alpha-hemolysin nanopore using the MARTINI coarse-grained force field
15:20-15:40	**Maxime Kermarrec,** Ecole Normale Supérieure de Lyon, France Mapping the Radical Cation Guanine in the nucleosomal DNA using QM/MM approaches
15:40-16:00	**COFFEE BREAK**
16:00-16:30	**Alessandra Magistrato,** Trieste SISSA, Italy Molecular Mechanisms of RNA Metabolism
16:30-17:00	**Vlad Cojocaru,** Universitatea Babeș-Bolyai, Romania Transcription factors meet chromatin under the computational nanoscope
17:00-17:30	**Sarah Harris,** University of Leeds, UK Multi-Scale Simulations of DNA Supercoiling

WEDNESDAY 22 May 2024

BIOMEDICAL RESEARCH FOUNDATION, ACADEMY OF ATHENS

17:30-18:05	**FLASH TALKS** Chair: **Klaus Liedl**
	Isidora Diakogiannaki, University of Naples Federico II, Italy Modeling A40s Aptamer for Advancing Glioblastoma Therapy
	Petr Jurečka, Palacky University Olomouc, Czech Republic Developing Force Field for Nucleic Acids Simulations - Both Canonical and Non-canonical
	Gianfranco Martino, University of Bologna, Italy MD simulatons identify precise and dynamic protein cooperation for the spliceosomal splicing
	Fethiye Aylin Sungur, Istanbul Technical University, Turkey A Multiscale Modelling Study to Elucidate the Citrullination Reaction of the Protein Arginine Deiminase 2 and Identifying New Hit Compounds
	Roxana Geanina Vasarhelyi, Babes-Bolyai University, Romania Exploring RNA-protein interactions: from binding modes to sequence specificity through molecular docking and simulations
	Alessia Visigalli, Italian Institute of Technology, Italy Molecular Dynamics Simulations to study translocation in Human DNA Polymerase
	Merve Yuce, Istanbul Technical University, Turkey Identification of Potent E. coli Ribosome Inhibitors Using a Computationally Efficient Workflow
18:05-19:30	**ISQBP Business Meeting**
20:30	**CONFERENCE DINNER**

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THURSDAY 23 May 2024

BIOMEDICAL RESEARCH FOUNDATION, ACADEMY OF ATHENS

09:00-11:00	**BIOMOLECULAR DYNAMICS AND DRUG DISCOVERY** Chair: **Minos Matsoukas**
09:00-09:30	**Andrea Cavalli,** CECAM, Switzerland Physics-based approaches to computational drug discovery
09:30-10:00	**Vangelis Daskalakis,** University of Patras, Greece CRISPR-Cas proteins: Engineering of "silver-bullets" in the arsenal of gene editing
10:00-10:20	**Nishita Mandal,** Adam Mickiewicz University, Poland Probing Ligand Transport Pathways in Proteins with Buried Active Sites: Insights from Coarse-Grained Molecular Dynamics Simulations
10:20-10:40	**Giulia Paiardi,** Heidelberg University, Germany The role of heparin in spike SARS-COV-2 infection: From a model for heparan sulfates to a starting structure for antivirals
10:40-11:00	**Alexios Chatzigoulas,** Biomedical Research Foundation, Academy of Athens, Greece Predicting protein-membrane interfaces of peripheral membrane proteins using AI
11:00-11:30	**COFFEE BREAK**
11:30-12:40	**FORCE FIELD DEVELOPMENT** Chair: **Zoe Cournia**
11:30-12:00	**Adrian Roitberg,** University of Florida, USA Machine Learning Potentials for Molecular Modeling. ANAKIN, The Next Generation
12:00-12:20	**Franz Waibl,** ETH Zürich, Switzerland Validating small-molecule force fields for simulation of macrocycles
12:20-12:40	**Panagiotis Koukos,** Biomedical Research Foundation, Academy of Athens, Greece Martini 3 force field parameters for protein lipidation post-translational modifications
12:40-12:50	**BEST TALK AND POSTER AWARDS**
12:50	**CLOSING REMARKS AND FAREWELL - END OF CONFERENCE**

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