



2nd Meeting Towards Data FAIRness in Molecular Biophysics



October 7, 2026

Academy of Sciences of Lithuania, Gedimino ave. 3 Vilnius, Lithuania

Time	Presenter	Institution	Title of the Lecture
8:30-9:00	Registration of the participants		
9:00-9:15	Opening Ceremony		
9:05-9:10	Daumantas Matulis <i>Head of the Scientific Committee</i>	Life Sciences Center, Vilnius University, Lithuania	Welcome address
9:10-9:15	Vytautas Nekrošius <i>President of the Lithuanian Academy of Sciences</i>	Lithuanian Academy of Sciences	Welcome address
9:15-11:00	Session 1		
9:15-10:00	Michael Gilson <i>Plenary</i>	Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, USA	BindingDB: A Growing, FAIR, Foundation for Medicinal Chemistry, Molecular Modeling, and AI
10:00-10:20	Jan Dohnálek <i>Invited</i>	The Institute of Biotechnology of the Czech Academy of Sciences, Prague, Czech Republic	Molecular Biophysics Database for Annotated Raw Molecular Biophysics Data
10:20-10:40	Sergey N. Krylov <i>Invited</i>	Department of Chemistry, York University, Toronto, Canada	Disregarded Causes and Costly Consequences of Gross Inaccuracies in Binding Studies: Time to Act
10:40-11:00	Mark Williams <i>Invited</i>	School of Natural Sciences, Birkbeck University of London, UK	TBD
11:00-11:30	Coffee Break		
11:30-13:10	Session 2		
11:30-11:50	Juan Sabín <i>Invited</i>	AFFINImeter, Santiago de Compostela, Spain	From Data to Meaningful Insights: Getting the Most out of Isothermal Titration Calorimetry Measurements
11:50-12:10	Ran Friedman <i>Invited</i>	Faculty of Health and Life Sciences, Linnæus University, Kalmar, Sweden	Accurate calculations of interaction free energies
12:10-12:30	Nathalie Reuter <i>Invited</i>	Faculty of Science and Technology, University of Bergen, Norway	Molecular simulations to understand mechanisms of lipid shuttling by lipid transfer proteins
12:30-12:50	Elena Papaleo <i>Invited</i>	Department of Health Technology, Technical University of Denmark, Lyngby, Denmark	Towards Mechanistic Interpretation of Disease Variants and Drug Resistance with MAVISp
12:50-13:10	Saulius Gražulis	Sector of Crystallography and Chemical Informatics, Vilnius University, Lithuania	Data Management and Reuse in the Machine Learning Age
13:10-14:00	Lunch Break		

14:00-15:50	Session 3		
14:00-14:20	Jan Stránský <i>Invited</i>	The Institute of Biotechnology of the Czech Academy of Sciences, Prague, Czech Republic	Validation of Complex Metadata in MBDB User Entries Utilizing Large Language Models
14:20-14:35	Mattia Utichi	Danish Cancer Institute; Technical University of Denmark, Denmark	Probing LIR-mediated molecular recognition through complementary biophysical approaches
14:35-14:55	Justas Dapkūnas	Life Sciences Center, Vilnius University, Vilnius, Lithuania	Data-driven research in structural bioinformatics: from proteins to biomolecular interactions
14:55-15:10	Pablo Sánchez-Izquierdo Besora	Danish Cancer Institute; Technical University of Denmark, Denmark	Automated non-equilibrium free-energy calculations for predicting the impact of BCL-2 mutations on venetoclax binding
15:10-15:30	Daumantas Matulis	Department of Biothermodynamics and Drug Design, Vilnius University, Lithuania	Protein-Ligand Binding Database (PLBD.org) for Drug Design AI-ML
15:30-15:50	Vytautas Petrauskas	Department of Biothermodynamics and Drug Design, Vilnius University, Lithuania	Accuracy and Precision in Binding Affinity and Inhibition Measurements: Lessons from Carbonic Anhydrase Case Studies
15:50-16:30	Coffee Break		
16:30-17:50	Panel Discussion on FAIR data principles		
18:00-20:00	Evening Mixer		