

TRAINING SCHOOL

Computational Chemistry: Applications in Scientific Research



Organized within the **COST Action CA21101**

"Confined Molecular Systems: from the new generation of materials to the stars" (COSY)

Supported by **CEI KEP Project EUROSCICOMP-BRIDGE**

BANJA LUKA | JUNE 11 – 12, 2026

Day 1 – June 11, 2026 (Lecture hall)

09:00 – 10:00	Registration and Welcome Remarks
10:00 – 11:00	Ab Initio Modelling of Subnanometric Metal Clusters: Jahn-Teller Distortions and Benchmarking of DFT Lecturer: María Pilar de Lara-Castells (CSIC, Spain)
11:00 – 11:30	 Coffee Break
11:30 – 12:30	First-Principles Investigation of Interfacial Interactions Lecturer: Majdi Hochlaf (Université Gustave Eiffel, France)
12:30 – 13:30	Quantum Chemistry Developments in the AI Era Lecturer: Stefan Vučković (University of Fribourg, Switzerland)
13:30 – 15:00	 Lunch Break
15:00 – 16:00	In Silico Methods in Drug Discovery Lecturer: Žarko Gagić (University of Banja Luka, BIH)
16:00 – 17:00	Improving Your Presentation Skills Lecturer: Marina Šekutor (Ruđer Bošković Institute, Croatia)
17:00 – 17:30	Questions and Answers Session

Day 2 – June 12, 2026 (Workshop room)

09:00 – 10:30	Hands-on Session: Navigating Chemical Space: A Hands-on Journey Through Modern Chemoinformatics Lecturer: Črtomir Podlipnik (University of Ljubljana, Slovenia)
10:30 – 11:00	 Coffee Break
11:00 – 13:00	Lecture+Hands-on Session: AI in Drug Design: From Generative Models to Structure-Based Approaches Lecturer: Jurica Novak (Ruđer Bošković Institute, Croatia)
13:00 – 14:30	 Lunch Break
14:30 – 15:15	Mechanistic Insight into Thermal Relaxation of Photoswitches Lecturer: Johannes Dietschreit (University of Vienna, Austria)
15:15 – 16:00	Hands-on Session: Exploring Cholinesterase–Ligand Interactions Lecturer: Relja Suručić (University of Banja Luka, BIH)
16:00 – 17:00	Questions and Closing Remarks

LOCATION: Rectorate of the University of Banja Luka, University Campus
Bulevar vojvode Petra Bojovića 1A, 78000 Banja Luka



COMMITTEES

Organizing & Scientific Boards

Scientific Committee

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