1st International Computational Chemistry Meeting - **ICCM 2026**

Faculty of Science, University of Kragujevac (main building)

Programme

Tuesday, September 8, 2026

09:00 Registration

09:45 (A-I-25) Opening Ceremony

10:00 (A-I-25) **We will dock you – accelerating Drug design with computational chemistry**
Dr. Robert Vianello
Ruđer Bošković Institute, Zagreb, Croatia

10:50 (A-I-25) **Steiner distance and related topological indices in chemical graph theory**
Dr. Yaping Mao
Quinghai Normal University, China

11:25 Coffee Break

12:05 (A-I-25) **Geometric influence on designing topological indices**
Dr. Boris Furtula
University of Kragujevac, Kragujevac, Serbia

12:40 (A-I-25) **Quantifying network similarity through structural features distributions**
Dr. Izudin Redžepović
State University of Novi Pazar, Novi Pazar, Serbia

13:15 Lunch Break
Restaurant Klub 3

15:15 (A-I-21) **Introduction and overview of the WorkShop**
Dr. Rino Ragno
Sapienza University, Rome, Italy

15:30 (A-I-21) **3-D QSAR: Ligand-Based 3-D QSARs**
Dr. Rino Ragno
Sapienza University, Rome, Italy

16:00 (A-I-21) **3-D QSAR: Structure-Based 3-D QSARs**
Dr. Milan Mladenović

University of Kragujevac, Kragujevac, Serbia

16:30 Coffee Break

17:00 (A-I-21) **Build 3-D QSAR model: The www.3d-qsar.com portal**
Dr. Rino Ragno
Sapienza University, Rome, Italy

17:30 (A-I-21) **Registration of users to www.3d-qsar.com portal**

17:45 (A-I-21) www.3d-qsar.com: **Generation of bioactive molecules with Py_MolEdit**
Dr. Rino Ragno
Sapienza University, Rome, Italy

at 20:00 Social Dinner
Restaurant Stara Srbija

Wednesday, September 9, 2026

09:00 (A-I-25) **Oriented electric fields - Universal catalysts**
Dr. Sason Shaik
The Hebrew University, Jerusalem, Israel

09:50 (A-I-25) **Understanding and modelling catalytic reactions with valence bond diagrams**
Dr. Benoit Braida
University of Sorbonne, Paris, France

10:25 Coffee Break

10:55 (A-I-25) **Rethinking electron counting rules for σ-aromaticity**
Dr. Slavko Radenković
University of Kragujevac, Kragujevac, Serbia

11:30 (A-I-25) **Application of comparative binding energy (COMBINE) analysis in the design of BioActive molecules**
Prof. Rino Ragno
Sapienza University, Rome, Italy

12:05 Lunch Break
Restaurant Klub 3

14:30 www.3d-qsar.com: **Conformational search with Py_ConfSearch**

(A-I-21) Dr. Rino Ragno
Sapienza University, Rome, Italy

15:00 www.3d-qsar.com: **LB alignment with Py_Align**
(A-I-21) Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

15:30 www.3d-qsar.com: **Build LB 3-D QSAR model: (Rino Ragno)**
(A-I-21) Dr. Rino Ragno
Sapienza University, Rome, Italy

16:00 Coffee Break

16:30 www.3d-qsar.com: **Py-PDB**
(A-I-21) Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

17:00 www.3d-qsar.com: **Build SB 3-D QSAR model**
(A-I-21) Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

18:00 Guide City Tour

at 20:00 Social Dinner
Restaurant Panorama

Thursday, September 10, 2025

09:00 **Why are the excited states of heterocycles still challenging for theory?**
(A-I-25) Dr. Antonio Prlj
Ruđer Bošković Institute, Zagreb, Croatia

09:50 **How excited-state antiaromaticity drives ring-puckering and isomerization in benzene**
(A-I-25) Dr. Slađana Đorđević
Ruđer Bošković Institute, Zagreb, Croatia
University of Kragujevac, Kragujevac, Serbia

10:25 Coffee Break

10:55 **Optoelectronic properties of new porous metal halide semiconductors**
(A-I-25) Dr. Nourdine Zibouche

Lancaster University, Lancaster, UK

11:30 (A-I-25) **Cryptands & computer chemistry – learning about selective ion complexation**
Dr. Ralph Puchta
University of Erlangen-Nürnberg, Erlangen, Germany

12:05 Lunch Break
Restaurant Klub 3

14:30 Visit to Šumarice Memorial Park

16:00 (A-I-21) www.3d-qsar.com: **Molecular Docking with Py-Docking**
Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

16:30 (A-I-21) Evolution of 3-D QSAR: **Comparative Binding Energy Analysis**
Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

17:00 (A-I-21) www.3d-qsar.com: **Build SB ComBinE model with Py_ComBine**
Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

17:00 Coffee Break

18:00 (A-I-21) www.3d-qsar.com: **Practical sessions on Py-MolEdit, Py-ConfSearch, and Py-Align**
Participants

18:30 (A-I-21) www.3d-qsar.com: **Practical sessions on Py-PDB, and Py-Docking**
Partcipants

at 20:00 Social Dinner
Pizzeria Mali Napulj

Friday, September 11, 2025

09:00 (A-I-25) **Do pnictogen onium cations and aromatic rings form only cation-π interactions? Answers from quantum chemical perspective**
Dr. Dušan Malenov
University of Belgrade, Belgrade, Serbia

09:50 (A-I-25) **Melissa Officinalis l. as a potential source of natural agents for the prevention of gingivitis**
Dr. Svetlana Jeremić
State University of Novi Pazar, Novi Pazar, Serbia

10:25 Coffee Break

10:55 (A-I-25) **Computational design of PROTACs and their ternary complexes**
Dr. Milan Mladenović
University of Kragujevac, Kragujevac, Serbia

11:30 (A-I-21) www.3d-qsar.com: **Practical sessions on Py-CoMFA**
Participants

12:00 Lunch Break
Restaurant Klub 3

14:00 (A-I-21) www.3d-qsar.com: **Practical sessions on Py-ComBinE**
Participants

14:30 (A-I-21) www.3d-qsar.com: **Discussions of the results**
Participants

15:30 (A-I-25) Closing words