



KATEDRA FYZIKÁLNÍ CHEMIE
UNIVERZITY PALACKÉHO V OLMOUCI



INSTITUTE OF MOLECULAR AND
TRANSLATIONAL MEDICINE



9th Advanced *in silico* Drug Design (KFC/ADD) Welcome

Karel Berka, Pavel Polishchuk,

Johannes Kirchmair, Aleix Gimeno Vives, Corin Wagen

Alexandre Varnek, Martin Lepšík, Peter Ertl, Thierry Langer, Jonathon Vandezande,

Marian Novotný, Anna Špačková, Federica Moraca, Hanoach Senderowitz,

Semen Yesylevskyy, Petr Stadlbauer, Aleksandra Ivanova, Niklas Piet Doering,

Valerij Talagayev, Wim Dehaen, Martin Šícho, Marko Jukić, Crtomir Poplipnik, Igor Tetko,

Guzel Minibaeva, Dominik Martinát, Kateřina Storchmannová, Jan Salomon,

Lukáš Gibala, Elizabeth Kolářová, Jindřich Lněnička, Jaromír Kepřt, Václav Bazgier

UP Olomouc, 26.1.-30.1. 2026

Sponsors



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**INSTITUTE OF MOLECULAR AND
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DEPT. of PHYSICAL CHEMISTRY
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Challenge is sponsored by:



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Est. 1573



Johan Gregor Mendel
(1840-1843)



450 years of Palacký University
— genius up —

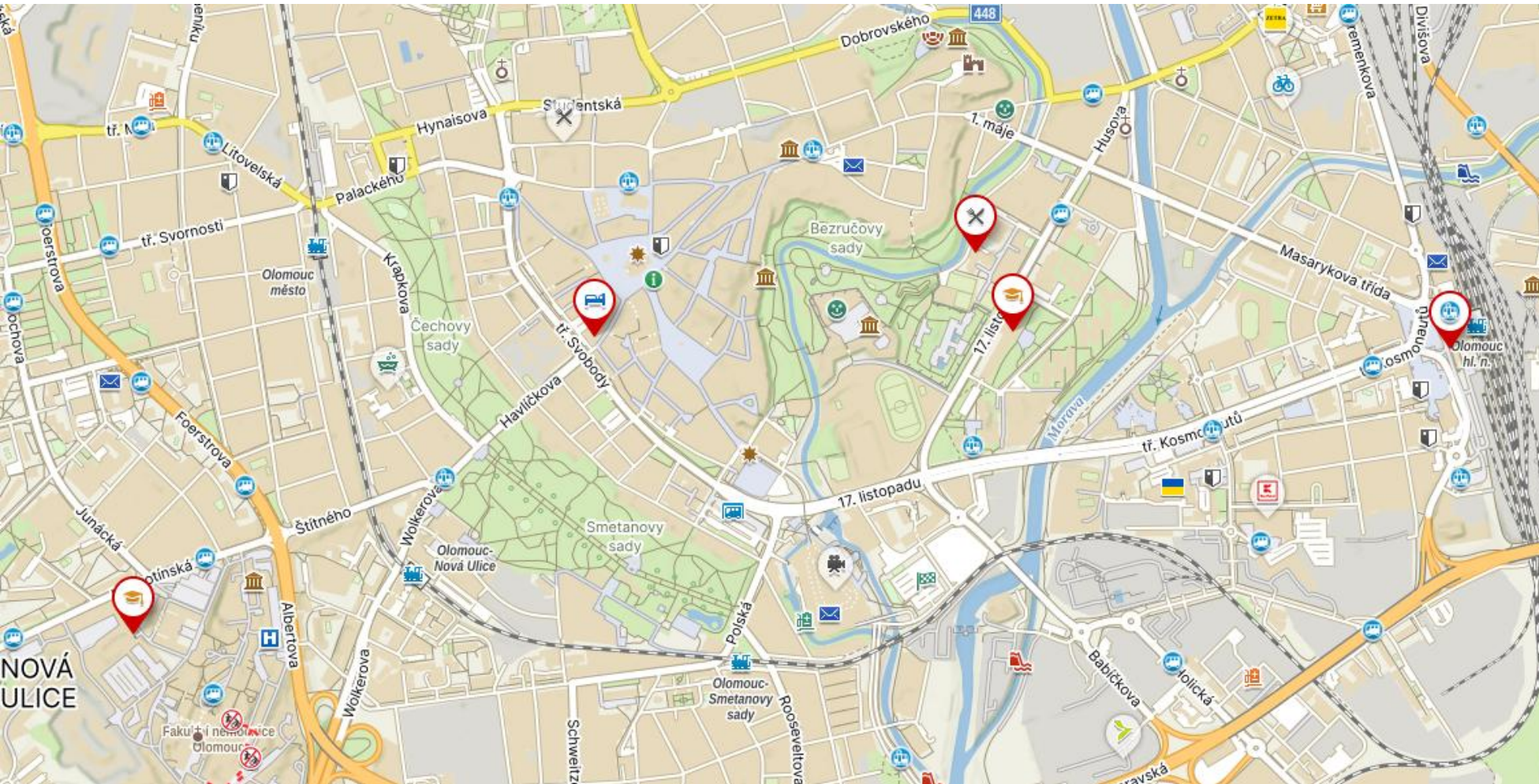
www.upol.cz

Olomouc and the Olomouc Region in Europe



Secret jewel of Central Europe
Lonely Planet guide

Olomouc Map with important points



CONFERENCE DINNER - ...
Restaurace a pohostinství



Faculty of Science UPOL ...
Vysoká škola, univerzita



ACCOMODATION SPEAK...
Ubytování - hotel



Olomouc Main Train Stati...
Zastávka tramvaje, autobusu



IMTM UPOL
Vysoká škola, univerzita

Course Program

Monday, January 26

10:00 - 12:00 Registration (2nd floor)
12:00 - 12:15 Opening of the workshop
12:15 - 13:00 Introduction to drug design (Prof. Karel Berka)
13:00 - 14:00 Introduction to chemoinformatics (Prof. Johannes Kirchmair)
14:00 - 14:30 coffee break
14:30 - 15:00 PDB-Cat (Aleix Gimeno Vives)
15:00 – 16:00 Easy online access to molecular modelling tools with RowanSci (Corin Wagen)
16:00 - 17:00 Poster flash talks
17:00 - 19:00 Poster session (3rd floor)

Tuesday, January 27

8:45 - 9:45 Reaction informatics (Prof. Alexandre Varnek)	
9:45 - 10:45 Alphafoldology (Prof. Karel Berka)	
10:45 - 11:00 coffee break	
11:00 - 12:00 Quantum mechanics in Drug design (Dr. Martin Lepsik)	
12:00 - 13:00 lunch	
13:00 - 14:00 Substructure analysis in drug discovery (Dr. Peter Ertl)	
14:00 - 15:00 Pharmacophore (Prof. Thierry Langer)	
15:00 - 15:20 coffee break	
Session 1	Session 2
15:20 - 17:45 Pharmacophore tutorial (Prof. Thierry Langer)	15:20 - 16:30 RowanSci online platform and tools (Jonathon Vandezande)
	16:30 - 17:45 Online structural analysis – PrankWeb, MOLE, Autodock Vina (Dr. Marian Novotný, Anna Špačková)
18:30 Conference dinner (Kozlovna)	

Wednesday, January 28

8:45 - 9:45 From Classical Docking to AI-Enhanced Scoring (Dr. Federica Moraca)	
9:45 - 10:45 Application of drug design on plant protector (Prof. Hanoach Senderowitz)	
10:45 - 11:00 coffee break	
11:00 - 12:00 Why ML in Drug discovery is not (yet) a silver bullet (Dr. Semen Yesylevskyy)	
12:00 - 13:00 lunch	
Session 1	Session 2
13:00 - 15:00 Docking with EasyDock (Dr. Pavel Polishchuk)	13:00 - 15:00 Docking tutorial (Dr. Federica Moraca)
coffee break	
15:30 – 16:10 Introduction to molecular dynamics (Dr. Petr Stadlbauer)	
16:10 - 17:30 MD with StreaMD (Aleksandra Ivanova)	16:10 - 17:30 MD with OpenMMDL (Niklas Piet Doering, Dr. Valerij Talagayev)
18:20 - Excursion to the Institute of Molecular and Translational Medicine (IMTM)	

Thursday, January 29

8:45 - 9:45 Introduction QSAR modeling (Dr. Win Dehaen)	
9:45 - 10:45 Introduction to de novo design (Dr. Martin Sicho)	
10:45 - 11:00 coffee break	
Session 1	Session 2
11:00 - 12:00 Chemical space visualization (Dr. Martin Sicho)	11:00 - 12:00 The Orange toolbox for pipeline automation (Dr. Marko Jukic, Dr. Crtomir Podlipnik)
12:00 - 13:00 lunch	
13:00 - 15:00 QSAR tutorial in Python (Dr. Wim Dehaen)	13:00 - 15:00 QSAR tutorial with OCHEM online platform (Dr. Igor Tetko)
coffee break	
15:30 - 17:30 De novo design with CReM (Dr. Pavel Polishchuk, Guzel Minibaeva)	15:30 - 17:30 De novo design with DrugEx (Dr. Martin Sicho)

Friday, January 30

8:45 - 14:30 Ligand selection challenge (Dr. Pavel Polishchuk)
14:30 - 15:00 Presentations of winners

Materials, YouTube channel

Materials will be uploaded to **webpage during workshop:**

<https://www.kfc.upol.cz/9add>

YouTube channel - broadcast and store individual videos:

https://www.youtube.com/playlist?list=PLRGiGr8c-LIJ3cS_KX5xSmZncNT2-i_ME

QUESTIONS?

Enjoy Workshop