



KATEDRA FYZIKÁLNÍ CHEMIE
UNIVERZITY PALACKÉHO V OLOMOUCI



INSTITUTE OF MOLECULAR AND
TRANSLATIONAL MEDICINE



8th Advanced *in silico* Drug Design (KFC/ADD) Welcome



Karel Berka, Pavel Polishchuk,

Marián Hajdúch, Johannes Kirchmair, Alexander Varnek, Martin Lepšík,
Semen Yesylevskyy, Thierry Langer, Federica Moraca, Hanoch Senderowitz,
Aleksandra Ivanova, Wim Dehaen, Martin Šícho, Alexander Dömling,
Oleksander Isaev, Thomas Evangelidis, Miroslav Lžičař
Dominik Martinát, Kateřina Storchmannová, Anna Špačková, Jan Salomon,
Jaromír Kepřt, Václav Bazgier, Elizabeth Kolářová, Guzel Minibaeva

UP Olomouc, 27.1.-31.1. 2025



ÚOCHB AV ČR
IOCB PRAGUE



Deep MedChem



Carnegie
Mellon
University



Palacký University Olomouc

Est. 1573



Johan Gregor Mendel
(1840-1843)



450 years of Palacký University
genius up

www.upol.cz

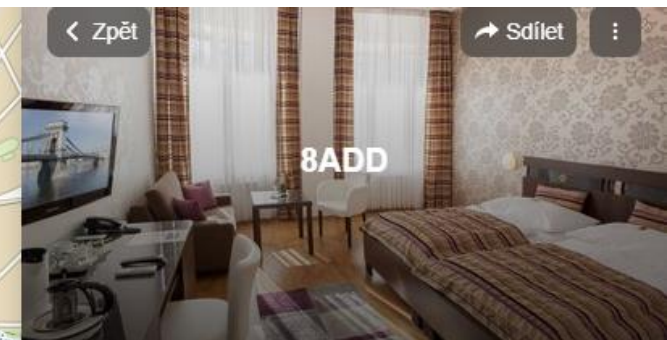


Olomouc and the Olomouc Region in Europe








Secret jewel of Central Europe
Lonely Planet guide 2012-2013

Olomouc Map w important points



Řadit podle: vlastní ✓

-  **Faculty of Science UPOL - ...**
Vysoká škola, univerzita
-  **ACCOMODATION SPEAKE...**
Ubytování - hotel
-  **CONFERENCE DINNER - R...**
Restaurace a pohostinství
-  **Olomouc Main Train Station**
Zastávka tramvaje, autobusu
-  **IMTM UPOL**
Vysoká škola, univerzita

Course Program

Monday - Basics

- 12:15 Welcome (Berka)
- 12:30 Drug design – intro (Berka)
- 13:00 Drug Res. Dev. in Academia (Hajdúch)
- 14:00 Intro Cheminform (Kirchmair)
- 15:15 Chemography (Varnek)
- 16:30 Poster session

Tuesday – Structures

- 9:00 Structure sources (Berka)
- 10:00 QM in drug design (Lepsik)
- 11:15 AI in DD (Yesylevskyy)
- 13:00 Pharmacophores (Langer)
- 14:00 Tutorial – Pharmph (Langer)
- 18:00 Tour Olomouc (Berka)
- 19:00 Workshop dinner (Drápal)

Wednesday – Structure-based methods

- 9:00 Molecular docking (Moraca)
- 10:00 Mol. dynamics (Yesylevskyy)
- 11:15 CFTR Modelling (Senderowitz)
- 13:00 Tutorial – Mol. dock (Moraca)
- 15:15 Tutorial – EasyDock (Minibaeva)
- 16:00 Tutorial - MD (Ivanova)
- 18:30 Excursion to IMTM (Polishchuk)

Thursday – Ligand-based methods

- 9:00 QSAR (Dehaen)
- 10:00 MI Learning (Polishchuk)
- 11:00 De novo design (Šícho)
- 13:00 Tutorial - QSAR (Polishchuk)
- 15:15 Tutorial – ChemSpace (Šícho)
- 16:00 Tutorial – De Novo (Šícho, Polischchuk)

Friday – Applications

- 9:00 Innovative DD tools (Dömling)
- 10:00 Alphafoldology (Berka)
- 11:15 CACHE (Polishchuk)
- 13:00 AIMNet2 (Isaev)
- 14:00 DD w NMR (Evangelidis)
- 14:30 CHEESE (Lžičař)

Materials, YouTube channel

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

<https://www.kfc.upol.cz/8add>

YouTube channel - broadcast and store individual videos:

<https://youtube.com/playlist?list=PLRGiGr8c-LIKHyFNS-fGka-uHGAFAlxqE&si=o-dMPIfP9A-SLEHO>

QUESTIONS?

Enjoy Workshop