



AURORA

7th Advanced *in silico* Drug Design

KFC/ADD

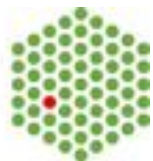
Welcome

Karel Berka, Pavel Polishchuk,

Thierry Langer, Johannes Kirchmair, Semen Yesylevskyy, Genevieve Evans,
Paulyna Magaña, Alžběta Tuerková, Wim Dehaen, Martin Lepšík, Federica Moraca,
Václav Bazgier, Dominik Martinát, Kateřina Storchmannová, Anna Špačková,
Nina Kadášová, Guzel Minibaeva, Aleksandra Ivanova

UP Olomouc, 29.1.-1.2. 2024

EMBL-EBI



INSTITUTE OF PHYSICS
National academy of Sciences of Ukraine



ÚOCHB AV
ČR
IOCB PRAGUE



Palacký University Olomouc

Est. 1573



Johan Gregor Mendel
(1840-1843)



450 years of Palacký University
genius up

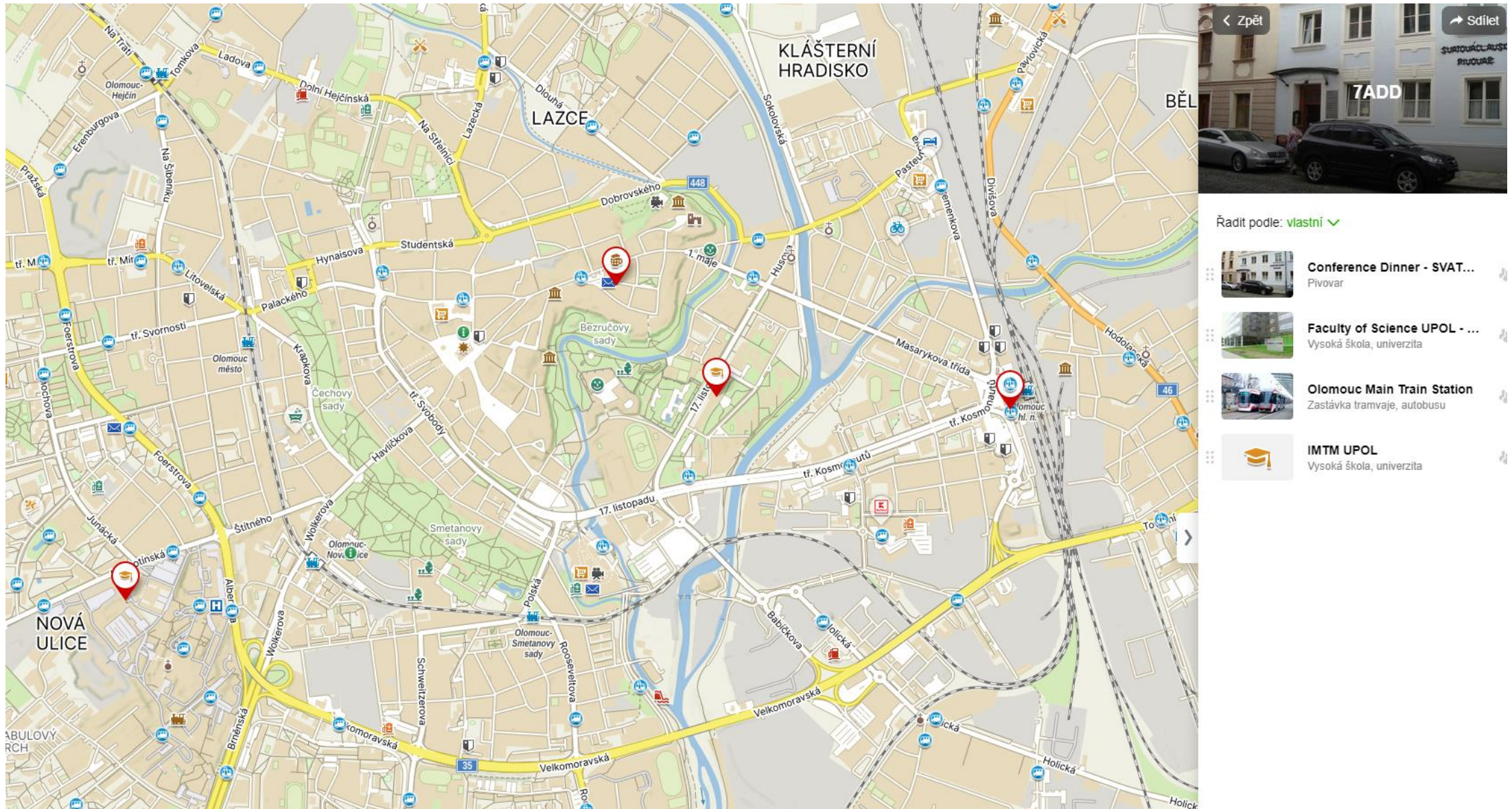
www.upol.cz

Olomouc and the Olomouc Region in Europe



Secret jewel of Central Europe
Lonely Planet guide 2012-2013

Olomouc Map w important points



<https://mapy.cz/s/cozozuluge>

Course Program

Monday - Basics

- 12:20 Welcome
- 12:30 Drug design – intro (Berka)
- 13:15 PDBe/PDBe-KB (Evans, Magaña)
- 15:30 Binding Site identification (Novotny)
- 16:00 Insights from biotech on PROTACs (Tuerkova)
- 17:00 Poster session

Tuesday – Small molecules

- 9:15 Virtual screening (Polishchuk)
- 10:00 QM in drug design (Lepsik)
- 11:15 AI in drug design (Yesylevskyy)
- 13:00 Frequent hitters (Kirchmair)
- 14:00 QSAR (Dehaen)
- 15:15 Tutorial – QSAR (Dehaen)
- 18:00 Tour Olomouc (Berka)
- 19:00 Workshop dinner (S. Vaclav brewery)

Wednesday – Structure-based methods

- 9:15 Alphafoldology (Berka)
- 10:00 Molecular Drug design (Moraca)
- 11:00 Molecular docking (Moraca)
- 13:00 Tutorial – Molecular docking (Moraca)
- 15:30 Tutorial – Molecular dynamics (Ivanova)
- 18:30 Excursion to IMTM (Polishchuk)

Thursday – De novo methods

- 9:15 De novo (Polishchuk)
- 10:30 Tutorial - De novo (Polishchuk)
- 13:00 CACHE (Polishchuk)
- 14:00 Pharmacophore (Langer)
- 15:15 Tutorial – Pharmacophore (Langer)

Friday – Challenge/hackathon

- cancelled

Materials, YouTube channel

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

<https://www.kfc.upol.cz/7add>

YouTube channel - broadcast and store individual videos:

<https://www.youtube.com/playlist?list=PLRGiGr8c-LIJhMBKt0LqcUSjaMIJnET5W>

QUESTIONS?

Enjoy Workshop