



KATEDRA FYZIKÁLNÍ CHEMIE  
UNIVERZITY PALACKÉHO V OLMOUCI



INSTITUTE OF MOLECULAR AND  
TRANSLATIONAL MEDICINE



# 6<sup>th</sup> Advanced *in silico* Drug Design

KFC/ADD

## Welcome

Karel Berka, Pavel Polishchuk,

Thierry Langer, Johannes Kirchmair, Melissa F. Adasme, James Blackshaw,

Wim Dehaen, Mariia Matveieva, Olena Mokshyna, Semen Yesylevskyy,

Václav Bazgier, Dominik Martinát, Kateřina Storchmannová, Anna Špačková,

Alina Kutlushina, Aleksandra Ivanova

UP Olomouc, 30.1.-3.2. 2023



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

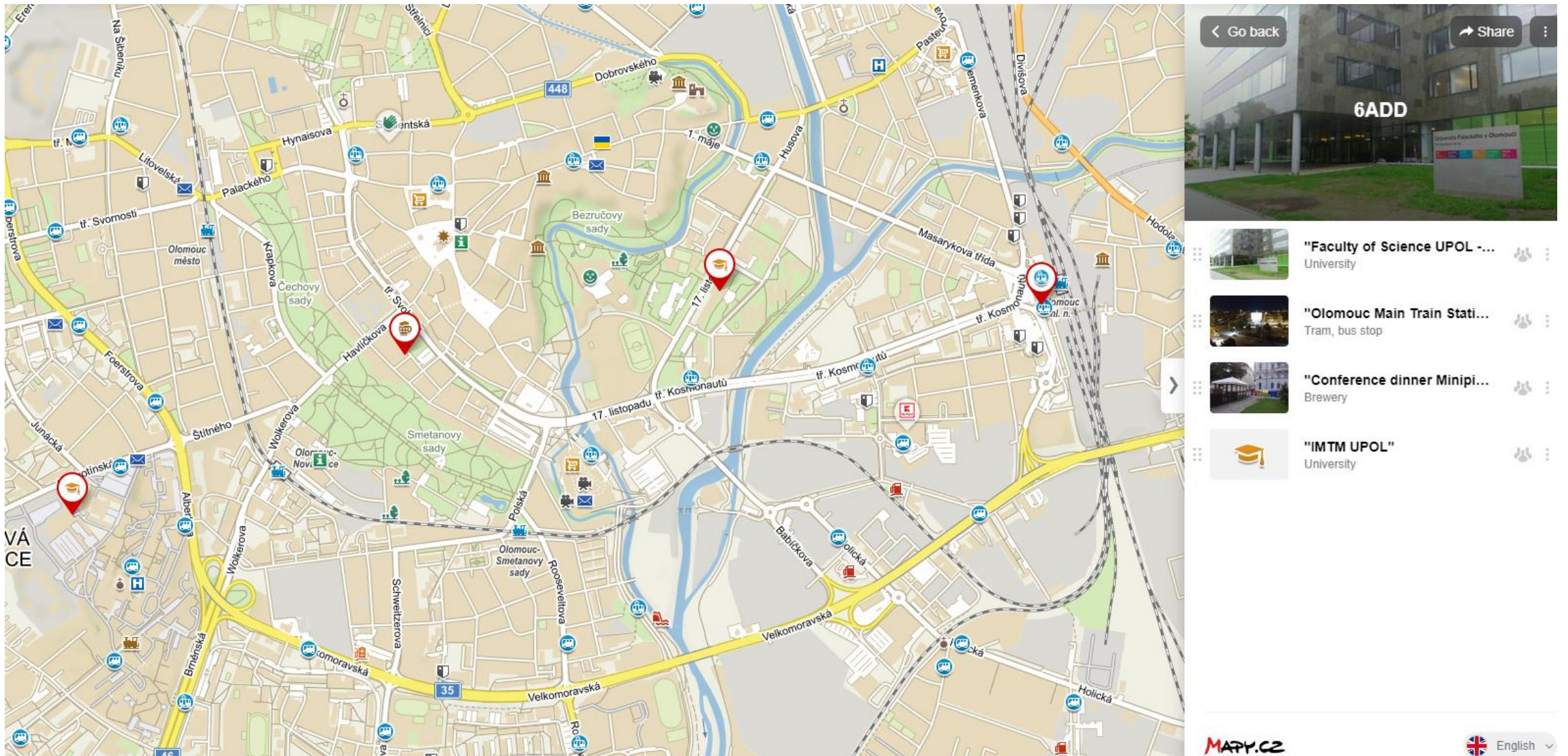
[www.upol.cz](http://www.upol.cz)

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

- 12:30 Welcome
- 12:40 Drug design – intro (Berka)
- 13:30 ChEMBL (Adasme, Blackshaw)
- 15:15 Structural bioinfo tools (Berka)
- 16:00 Alphafoldology (Berka)
- 17:00 Poster session

## Tuesday – Small molecules

- 9:00 Molecular similarity, optimization (Dehaen)
- 9:45 Fantastic natural products (Mokshyna)
- 11:00 Metabolism prediction (Kirchmair)
- 13:00 Pharmacophores (Langer)
- 14:30 Tutorial – Pharmacophores (Langer)
- 17:30 Tour Olomouc (Berka)
- 18:30 Workshop dinner (Moritz brewery)

## Wednesday – Ligand-based methods

- 9:00 QSAR modeling (Matveieva)
- 9:45 Multiple instance learning (Polishchuk)
- 11:00 De novo design (Polishchuk)
- 13:00 Tutorial – QSAR (Kutlushina)
- 15:30 Tutorial – de novo design (Polishchuk)
- 17:00 Poster session

## Thursday – Structure-based methods

- 9:00 Molecular docking basics (Berka)
- 9:45 Molecular dynamics basics (Berka)
- 11:00 Membrane druggability – MD (Yesylevskyy)
- 13:00 Tutorial – Docking (Berka)
- 15:00 Tutorial – High throughput MD (Ivanova)

## Friday – Challenge/hackathon

- 9:00 Challenge (Polishchuk)
- 15:00 Final word (Berka)

# Ligand challenge



- Challenge (Friday)
  - Drug design for selected problem – Pavel Polishchuk
  - Selection of active compounds from the blind set
  - Participation to hackathon is **exam requirement** for [Advanced Rational Drug Design](#) (4 ECTS credits)

# Materials, Zoom, YouTube channel

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

<https://www.kfc.upol.cz/6add>

**Zoom calls**, where you will be able to ask questions:

6ADD Day 1, 12:30-17:00 CET -

<https://cesnet.zoom.us/j/95232474898?pwd=a0ZkYW1WbG9peWdaZEJsK3pnTmxRUT09>

6ADD Day 2, 9:00-14:00 CET -

<https://cesnet.zoom.us/j/96039346433?pwd=MnYzRGJSYIJ4QzIwb3RML0toRnU5Zz09>

6ADD Day 3, 9:00-12:00 CET -

<https://cesnet.zoom.us/j/99946533039?pwd=NmVGcWFjOVBQd0NvODhRT3lwRXFIdz09>

6ADD Day 4, 9:00-12:00 CET -

<https://cesnet.zoom.us/j/92424913495?pwd=c3ovcnBTTkt1QTc3b29rVitqc2dLZz09>

**YouTube channel** - broadcast and store individual videos:

[https://www.youtube.com/playlist?list=PLRGiGr8c-LIKYTDnuWcqSwvGZ\\_rOVkZuB](https://www.youtube.com/playlist?list=PLRGiGr8c-LIKYTDnuWcqSwvGZ_rOVkZuB)

**QUESTIONS?**

**Enjoy Workshop**