



BIOEXCEL WORKSHOP BALKAN EDITION:

ENHANCING BIOMOLECULAR SIMULATIONS

WITH GROMACS, HADDOCK AND PMX

May 21-22, 2025, Sofia, Bulgaria

Organised by



AMBASSADOR PROGRAM

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DISCOVERER



EPICURE
Unlocking European-level HPC Support

Programme

Day 1, May 21: HADDOCK

All indicated times are in the Eastern European Summer Time (EEST) zone (GMT +2)

8:30 – 9:30 Registration

9:30 – 9:45 Opening

9:45 – 10:00 EPICURE presentation

10:00 – 11:00 Lecture:

- Integrative modelling with HADDOCK, Alexandre Bonvin

11:00 – 11:30 Break

11:30 – 13:30 Practical session:

- HADDOCK tutorial on antibody-antigen modelling, Alexandre Bonvin & Vlad Cojocaru

13:30 – 14:30 Lunch break

Day 1, May 21: GROMACS

14:30 – 15:30 Lecture:

- Molecular dynamics using GROMACS, Alessandra Villa

15:30 – 16:00 Break

16:00 – 17:30 Practical session:

- Tutorial: Introduction to Molecular Dynamics simulations, Cathrine Bergh

17:30 – 18:00 Break

18:00 – 19:00 Practical session:

- Tutorial: Enhanced sampling with AWH, Alessandra Villa

20:00 – 22:30 Social dinner

Day 2, May 22: PMX

All indicated times are in the Eastern European Summer Time (EEST) zone (GMT +2)

10:00 – 11:00 Lecture:

- Alchemical free energy calculations with PMX/GROMACS, Bert de Groot

11:00 – 11:30 Break

11:30 – 13:00 Practical session:

- Tutorial on amino acid mutations with PMX, Bert de Groot

13:00 – 14:00 Lunch break

Day 2, May 22: GROMACS performance

14:00 – 15:00 Lecture:

- Efficient use of CPU resources in GROMACS simulations, Andrey Alekseenko

15:00 – 15:30 Break

15:30 – 17:00 Practical session:

- Efficient use of CPU resources in GROMACS simulations, Andrey Alekseenko

17:00 – 17:30 Closing remarks