



# BIOEXCEL WORKSHOP BALKAN EDITION:

*ENHANCING BIOMOLECULAR SIMULATIONS*

*WITH GROMACS, HADDOCK AND PMX*

***May 21-22, 2025, Sofia, Bulgaria***

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# Programme

## Day 1, May 21: HADDOCK

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

9:00 – 9:45 Registration

9:45 – 10:00 Opening

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 – 17:00 Practical session:

- Tutorial: Introduction to Molecular Dynamics simulations, Cathrine Bergh

17:00 – 17:30 Break

17:30 – 19:00 Lecture:

- 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