

Workshop on BioExcel Software Tools

Report of Contributions

Contribution ID: 6

Type: **not specified**

Lecture: BioExcel Building Blocks (BioBB), a software library for interoperable biomolecular simulation workflows

Wednesday 11 February 2026 09:30 (1 hour)

Contribution ID: 7

Type: **not specified**

Practicals: Protein MD setup & Automatic Ligand Parameterization

Wednesday 11 February 2026 11:00 (2 hours)

Contribution ID: 8

Type: **not specified**

Lecture: Integrative modelling with HADDOCK

Wednesday 11 February 2026 14:30 (1 hour)

Contribution ID: 9

Type: **not specified**

Practical: HADDOCK tutorial on antibody-antigen modelling

Wednesday 11 February 2026 16:00 (1h 30m)

Contribution ID: **10**

Type: **not specified**

Lecture: Introduction to alchemical free energy calculations

Thursday 12 February 2026 10:00 (1 hour)

Contribution ID: 11

Type: **not specified**

Practical: Tutorial on ligand modifications with PMX

Thursday 12 February 2026 11:30 (1h 30m)