

Docking for Cheminformatics — Hands-on

Learn docking the right way for discovery-scale cheminformatics. This module covers end-to-end **protein/ligand preparation**, **search/exhaustiveness**, **scoring and consensus rescoring**, and **benchmark-driven validation** (redocking, cross-docking, decoy sets). You will generate audit-ready reports with **enrichment metrics**, **pose QC**, and **reproducible configs**.

Docking for Cheminformatics: Benchmarking & Scoring

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Session 1

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Protein & Ligand Preparation

Target structure curation

[chain/altloc selection](#) [protonation/tautomers \(pH\)](#)
[cofactors/metal handling](#)

Binding site definition

[reference ligand/box](#) [cavity detection](#) [conserved waters](#)

Ligand prep & QC

enumeration (stereo/proto) 3D conformers (ETKDG)
strain/flags & PAINS

Session 2

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Docking Protocols & Parameters

Search/exhaustiveness & sampling

genetic/local search pose clustering constraints &
pharmacophores

Protein flexibility & waters

soft/induced-fit options key waters retained metal
constraints

Workflow hygiene

determinism/seeds runtime/caching
checkpoint/resume

Session 3

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Scoring, Consensus & Benchmarking

Scoring families & rescore

empirical/knowledge-based consensus/rank fusion
MM/GBSA-lite checks

Benchmark design & metrics

redocking/cross-docking decoys (DUD-E-style)
ROC/PR, EF@1%, BEDROC

Pose QC & filters

strain/contacts clashes interaction fingerprints
synthetic feasibility flags

Session 4

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Mini Capstone: Docking Benchmark Report

Design a benchmark (target + decoys) & execute docking

Theory + Practical

Analyze enrichment & pose quality

ROC/PR & EF curves **IFP/contacts summary**
consensus ranking

Deliverables

ranked hit list + poses **benchmark report (PDF/HTML)**
reproducible configs/notebooks