

Molecular Modelling Facility

Instruments in this facility

- HPC Cluster
- AutoDock
- GROMACS
- PyMOL

MOLECULAR MODELLING FACILITY

HPC Cluster

An HPC cluster links many servers so they behave like one very large computer. Jobs are split into pieces that run side by side, so calculations that would tie up a workstation for weeks can finish in hours. It gives research groups a shared, expandable platform for simulation, docking, sequence analysis, and machine learning.

Key Specifications

Parameter	Specifications
Node Count	4 to 100+, depending on configuration
CPUs	Server-grade Intel Xeon or AMD EPYC
Cores per Node	32 to 128
RAM per Node	128 GB to 2 TB
Accelerators	Optional NVIDIA A100, H100, or L40S GPUs
Network Fabric	InfiniBand or 10/25/100 Gb Ethernet
Storage	Lustre or BeeGFS parallel storage, 50 TB to petabyte scale
Operating System	Rocky Linux, Ubuntu, or RHEL
Scheduler	SLURM or PBS
Software Stack	Environment modules, MPI, OpenMP, CUDA, Singularity/Docker
Facilities	Rack-mounted, air or liquid cooled, dual power feeds

Signature Features

- **Parallel Execution:** Spreads work over many cores and nodes at once.
- **Grows With You:** Add compute, GPUs, or disk without rebuilding the system.
- **Fast Interconnect:** Keeps communication delays low for multi-node jobs.
- **GPU Power:** Shortens simulation, docking, and training runs.
- **Fair Queuing:** The scheduler allocates resources across users and projects.
- **Quick Data Access:** Parallel storage copes with very large trajectory and sequence files.
- **Controlled Sharing:** Individual accounts, quotas, and project directories.
- **Stay Online:** Redundant hardware and live monitoring reduce downtime.

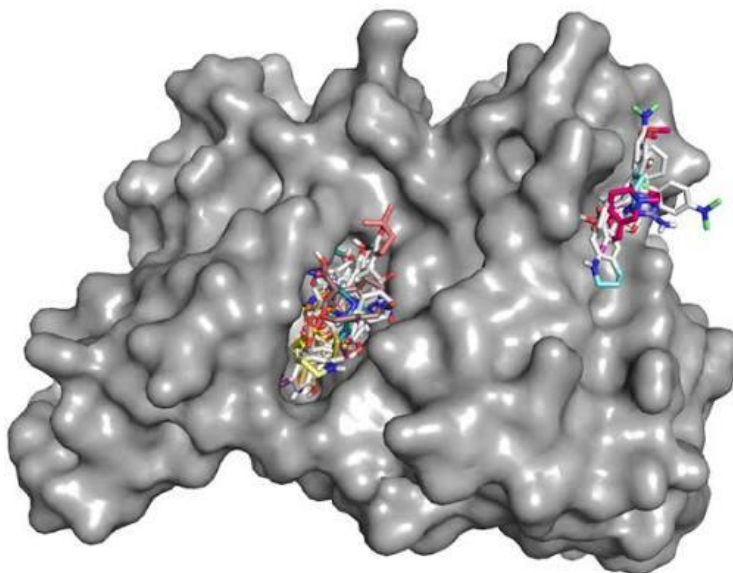
Research Applications

- **Molecular Dynamics:** Long simulations with GROMACS and related engines.
- **Docking Campaigns:** Large-scale ligand screening with AutoDock.
- **Genomics:** Read alignment, assembly, and variant calling.
- **Structural Biology:** Cryo-EM reconstruction and structure prediction.
- **Drug Discovery:** Hit-to-lead work and property prediction.
- **AI Workloads:** Training models on chemical and biological data.

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AutoDock

AutoDock is a free docking program family that predicts how a small molecule, such as a drug candidate or substrate, sits in the binding site of a protein. It generates likely binding poses and ranks them with an estimated binding energy. It comes in three main forms: AutoDock 4, AutoDock Vina, and the GPU-based AutoDock-GPU.



Key Specifications

Parameter	Specifications
Category	Open-source docking software
Origin	Scripps Research
Releases	AutoDock 4, Vina, AutoDock-GPU
Search Methods	Lamarckian genetic algorithm; iterated local search in Vina
Scoring	Empirical, free-energy-based
File Format	PDBQT, prepared from PDB, MOL2, or SDF
Ligand Handling	Flexible across rotatable bonds
Receptor Handling	Optional flexible side chains
Operating Systems	Linux, Windows, macOS
Hardware	Multi-core CPUs; CUDA/OpenCL GPUs
Helper Tools	AutoDockTools, MGLTools, Meeko

Signature Features

- **Pose and Energy Prediction:** Suggests binding orientations with estimated affinities.
- **Flexibility:** Ligand torsions and chosen receptor residues can move.
- **High Throughput:** Vina and the GPU version process large ligand sets quickly.
- **Precomputed Grids:** Affinity maps reduce runtime per dock.

- **No Licence Cost:** Open for academic and commercial use.
- **Easy Automation:** Simple to script for batch runs on a cluster.
- **Common Formats:** Works with standard chemistry and structure files.
- **Strong Support:** Extensive tutorials and an active user base.

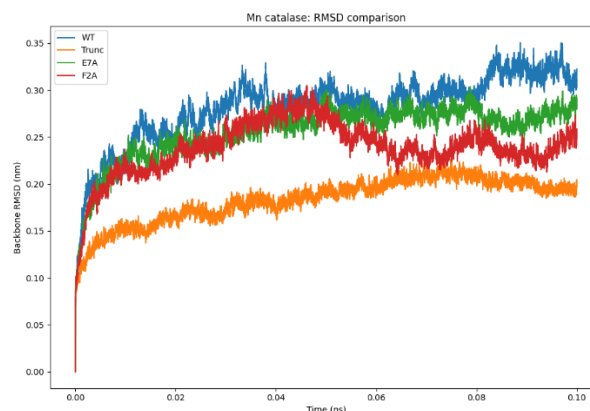
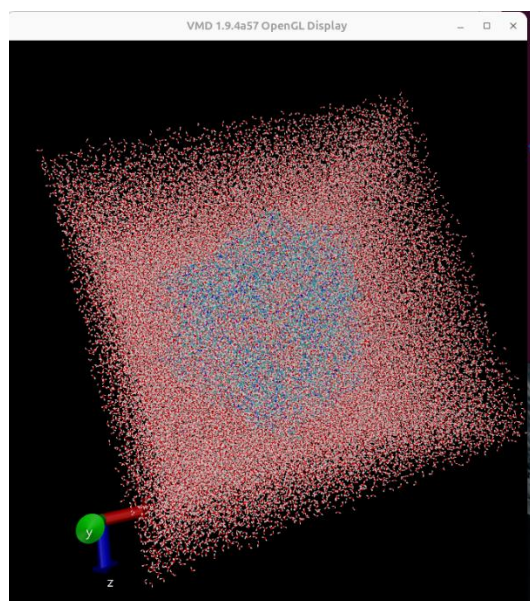
Research Applications

- **Lead Identification:** Ranks candidate compounds against a target.
- **Library Screening:** Filters large compound collections for hits.
- **Interaction Mapping:** Highlights residues and contact types at the binding site.
- **Inhibitor Design:** Guides rational modification of ligands.
- **Repurposing Studies:** Checks existing drugs against new targets.
- **Teaching:** Introduces docking concepts in computational chemistry courses.

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GROMACS

GROMACS is an open-source molecular dynamics engine that calculates how atoms in proteins, lipids, nucleic acids, and other systems move over time. It is known for speed and for scaling well from a single desktop to a large cluster, and it is widely used for protein motion, membranes, and molecular interactions.



Key Specifications

Parameter	Specifications
Category	Open-source MDengine
Licence	GNU LGPL
Force Fields	AMBER, CHARMM, GROMOS, OPLS-AA
Integrators	Leap-frog, velocity Verlet, stochastic dynamics
Long-Range Electrostatics	Particle Mesh Ewald, reaction-field
Ensembles	NVE, NVT, NPT
Parallel Modes	MPI, OpenMP, domain decomposition
GPU Backends	CUDA, SYCL, OpenCL
Input	.gro, .pdb, .top, .mdp, .tpr
Output	.xtc, .trr, .edr, .log
Operating Systems	Linux, macOS, Windows

Signature Features

- **Speed:** Heavily optimised kernels give very high simulation rates.
- **GPU Offload:** Non-bonded forces, PME, and updates can run on the GPU.
- **Scaling:** Efficient from one machine to many nodes.
- **Force Field Choice:** Supports the major biomolecular parameter sets.

- **Enhanced Sampling:** Free energy methods, replica exchange, and umbrella sampling.
- **Built-in Analysis:** Tools for RMSD, RMSF, hydrogen bonds, and energies.
- **Dependable Results:** Mature code validated by a large community.
- **Documentation:** Detailed manuals, tutorials, and user forums.

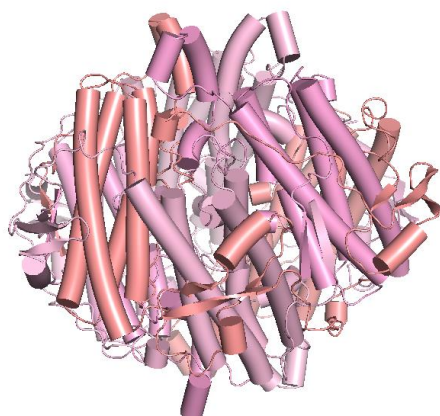
Research Applications

- **Protein Behaviour:** Conformational change, stability, and folding.
- **Docking Validation:** Tests whether a docked pose stays bound over time.
- **Membrane Studies:** Lipid bilayers, channels, and transporters.
- **Free Energy Estimation:** Binding and solvation energies.
- **DNA/RNA Work:** Structure and interaction dynamics.
- **Soft Matter:** Polymers, nanomaterials, and related systems.

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PyMOL

PyMOL is a 3D molecular graphics program for viewing, analysing, and rendering proteins, nucleic acids, and small molecules. It creates high-quality figures and animations and can be automated with Python. Researchers and students use it to interpret docking and simulation output.



Key Specifications

Parameter	Specifications
Category	Molecular visualisation software
Maintainer	Schrödinger (created by Warren DeLano)
Editions	Open-source and commercial/incentive builds
Readable Files	PDB, mmCIF, MOL2, SDF, CCP4 maps, DCD/XTC trajectories
Display Styles	Cartoon, surface, sticks, spheres, ribbon, mesh, lines
Image Rendering	Ray tracing for print-ready output
Automation	PyMOL command language and Python API
Exports	PNG, MP4/MPEG, .pse sessions
Operating Systems	Windows, macOS, Linux
Graphics Needs	OpenGL support; optional stereo 3D

Signature Features

- **Figure-Ready Images:** Ray-traced output with adjustable lighting and colours.
- **Many Representations:** Switch views to reveal different structural detail.
- **Contact Analysis:** Show hydrogen bonds, polar contacts, and pocket residues.
- **Superposition:** Align structures and report RMSD.
- **Scriptable:** Automate routines and write custom plugins.

- **Animation:** Build rotations and trajectory movies.
- **Maps and Surfaces:** Display density, electrostatics, and cavities.
- **Saved Sessions:** Store a full scene to share or reproduce later.

Research Applications

- **Structure Inspection:** Explore domains, folds, and active sites.
- **Docking Review:** Inspect AutoDock poses and interactions.
- **Trajectory Viewing:** Follow motions from GROMACS runs.
- **Mutation Mapping:** Place variants on the structure to judge impact.
- **Publication Graphics:** Prepare images for papers, posters, and theses.
- **Teaching:** Demonstrate molecular concepts in class.