

Resource Summary Report

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PLUMED 2

RRID:SCR_021952

Type: Tool

Proper Citation

PLUMED 2 (RRID:SCR_021952)

Resource Information

URL: <https://www.plumed.org/>

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Description: Open source, community developed library that provides range of different methods, which include enhanced sampling algorithms, free energy methods, tools to analyze vast amounts of data produced by molecular dynamics simulations. PLUMED 2 is complete rewrite of the code in object oriented programming language C plus plus. This new version introduces greater flexibility and greater modularity, which both extends its core capabilities and makes it far easier to add new methods and CVs. It also has simpler interface with the MD engines and provides single software library containing both tools and core facilities.

Synonyms: PLUgin for MolEcular Dynamics 2

Resource Type: software library, software resource, software toolkit

Defining Citation: [DOI:10.1016/j.cpc.2013.09.018](https://doi.org/10.1016/j.cpc.2013.09.018)

Keywords: Molecular dynamics analysis, enhanced sampling algorithms, free energy methods, PLUMED

Funding: CeCAM ;
European Research Council ;
Marie Curie Intra European Fellowship ;
MIUR grant FIRB ;
SISSA

Availability: Free, Available for download, Freely available

Resource Name: PLUMED 2

Resource ID: SCR_021952

Alternate URLs: www.plumed-code.org

License: Lesser GNU General Public License

Record Creation Time: 20220421T050137+0000

Record Last Update: 20260919T195500+0000

Ratings and Alerts

No rating or validation information has been found for PLUMED 2.

No alerts have been found for PLUMED 2.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 34 mentions in open access literature.

Listed below are recent publications. The full list is available at [dkNET](#) .

Rapetti D, et al. (2026) Making PLUMED Fly: A Tutorial on Optimizing Performance. The journal of physical chemistry. B, 130(9), 2504.

Boucher RC, et al. (2026) Photoreceptor outer segment disk rim curvature relies on a tetraspanin interaction web. The Journal of biological chemistry, 302(6), 113136.

Schnapka V, et al. (2026) Atomic resolution ensembles of intrinsically disordered proteins with AlphaFold. Nature communications, 17(1).

Cao H, et al. (2026) Inhibiting Mrt4-rRNA interaction with fumaramidmycin-based derivatives as an antifungal strategy. Nature communications, 17(1).

Falconieri A, et al. (2025) The evolution of eukaryotic linear motifs governing the function of androgen receptor from fish to Homo sapiens. Nucleic acids research, 53(14).

Tian X, et al. (2025) Electrochemical potential-driven water dynamics control CO₂ electroreduction at the Ag/H₂O interface. Nature communications, 16(1), 10636.

Liao L, et al. (2025) Structural basis of calcium-dependent C1ql1/BAI3 assemblies in synaptic connectivity. Nature communications, 16(1), 11444.

Tosello Gardini A, et al. (2025) Machine learning-driven molecular dynamics unveils a bulk phase transformation driving ammonia synthesis on barium hydride. Nature communications, 16(1), 2475.

Acharya A, et al. (2025) Dynamic Coupling between Tom22 Motions and Tom40 Pore Dynamics Modulates Ion Transport in the Mitochondrial TOM Complex. Journal of

chemical information and modeling, 65(22), 12475.

Paissoni C, et al. (2025) A conformational fingerprint for amyloidogenic light chains. *eLife*, 13.

Creazzo F, et al. (2025) DFT-metadynamics insights on the origin of the oxygen evolution kinetics at the (100)-WSe₂ surface. *iScience*, 28(3), 112045.

Posani E, et al. (2025) Ensemble refinement of mismodeled cryo-EM RNA structures using all-atom simulations. *Nature communications*, 16(1), 4549.

Tao E, et al. (2025) Drugs exhibit diverse binding modes and access routes in the Nav1.5 cardiac sodium channel pore. *The Journal of general physiology*, 157(2).

Guo SC, et al. (2024) Dynamics of activation in the voltage-sensing domain of *Ciona intestinalis* phosphatase Ci-VSP. *Nature communications*, 15(1), 1408.

Moura ACM, et al. (2024) Studying Conformational Properties of Transmembrane Domain of KCNE3 in a Lipid Bilayer Membrane Using Molecular Dynamics Simulations. *Membranes*, 14(2).

Erlebach A, et al. (2024) A reactive neural network framework for water-loaded acidic zeolites. *Nature communications*, 15(1), 4215.

Hoff SE, et al. (2024) Accurate model and ensemble refinement using cryo-electron microscopy maps and Bayesian inference. *PLoS computational biology*, 20(7), e1012180.

Nieto-Fabregat F, et al. (2024) Computational toolbox for the analysis of protein-glycan interactions. *Beilstein journal of organic chemistry*, 20, 2084.

Schneider A, et al. (2024) Biocatalytic stereocontrolled head-to-tail cyclizations of unbiased terpenes as a tool in chemoenzymatic synthesis. *Nature communications*, 15(1), 4925.

Wrabel TM, et al. (2024) Secondary Binding Site of CYP17A1 in Enhanced Sampling Simulations. *Journal of chemical information and modeling*, 64(19), 7679.