

Resource Summary Report

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MDAnalysis

RRID:SCR_025610

Type: Tool

Proper Citation

MDAnalysis (RRID:SCR_025610)

Resource Information

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

Proper Citation: MDAnalysis (RRID:SCR_025610)

Description: Software object oriented Python library to analyze trajectories from molecular dynamics simulations in many popular formats.

Resource Type: software toolkit, software resource, software library, source code

Keywords: analyze molecular dynamics simulations, molecular dynamics simulations, molecular dynamics,

Availability: Free, Available for download, Freely available,

Resource Name: MDAnalysis

Resource ID: SCR_025610

Alternate URLs: <https://github.com/MDAnalysis/mdanalysis>,
<https://pypi.org/project/MDAnalysis/>,

License: GNU GPL v2

Record Creation Time: 20240814T053254+0000

Record Last Update: 20260805T044549+0000

Ratings and Alerts

No rating or validation information has been found for MDAnalysis.

No alerts have been found for MDAnalysis.

Data and Source Information

Usage and Citation Metrics

We found 18 mentions in open access literature.

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

Berselli A, et al. (2026) The effect of ionic strength on PETase enzymes: An experimental and computational study. *Protein science : a publication of the Protein Society*, 35(1), e70386.

Avstrikova M, et al. (2025) Hidden complexity of $\alpha 7$ nicotinic acetylcholine receptor desensitization revealed by MD simulations and Markov state modeling. *Proceedings of the National Academy of Sciences of the United States of America*, 122(7), e2420993122.

He Y, et al. (2025) Screening and analysis of malt pentapeptide DPP-IV inhibitory activity. *NPJ science of food*, 9(1), 224.

Lesovoy D, et al. (2025) Insight into Malt1 activation mechanism through synergetic approach of AlphaFold, MD Simulation and NMR dynamic analyses. *bioRxiv : the preprint server for biology*.

Bozdaganyan M, et al. (2025) Exploring tubulin-paclitaxel binding modes through extensive molecular dynamics simulations. *Scientific reports*, 15(1), 8378.

Kakoulidis P, et al. (2025) Comparative structural insights and functional analysis for the distinct unbound states of Human AGO proteins. *Scientific reports*, 15(1), 9432.

Phan TM, et al. (2025) Optimized protein-water interactions and torsional refinements yield balanced atomistic protein force fields. *Nature communications*, 16(1), 10562.

Rizuan A, et al. (2025) Structural details of helix-mediated multimerization of the conserved region of TDP-43 C-terminal domain. *Nature communications*, 16(1), 10528.

Van Wyk RJ, et al. (2025) Carboxy-Amidated AamAP1-Lys has Superior Conformational Flexibility and Accelerated Killing of Gram-Negative Bacteria. *Biochemistry*, 64(4), 841.

Toay S, et al. (2025) Genetic mutations disrupt the coordinated mode of tyrosinase's intramelanosomal domain. *Protein science : a publication of the Protein Society*, 34(8), e70209.

Motso A, et al. (2025) GRK-biased adrenergic agonists for the treatment of type 2 diabetes and obesity. *Cell*.

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).

Abramsson ML, et al. (2025) Engineering cardiolipin binding to an artificial membrane protein reveals determinants for lipid-mediated stabilization. *eLife*, 14.

Swarnkar A, et al. (2024) Determinants of chemoselectivity in ubiquitination by the J2 family of ubiquitin-conjugating enzymes. *The EMBO journal*, 43(24), 6705.

Kameda T, et al. (2024) Protocol for calculating binding free energy of RNA:RNA interactions through molecular dynamics simulations using adaptive biasing force technique. *STAR protocols*, 5(3), 103223.

López-Ríos de Castro R, et al. (2024) Lessons learned during the journey of data: from experiment to model for predicting kinase affinity, selectivity, polypharmacology, and resistance. *bioRxiv : the preprint server for biology*.

Zhang X, et al. (2024) Molecular basis for chemokine recognition and activation of XCR1. *Proceedings of the National Academy of Sciences of the United States of America*, 121(48), e2405732121.

Reddy T, et al. (2016) The Role of the Membrane in the Structure and Biophysical Robustness of the Dengue Virion Envelope. *Structure (London, England : 1993)*, 24(3), 375.