

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 library, software resource, software toolkit, 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: 20260829T183414+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 28 mentions in open access literature.

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

de Assis JN, et al. (2026) Insect-resistant soybean genotypes accumulate rutin and its O-methylated derivative narcissin, a more potent flavonol targeting *Anticarsia gemmatalis* digestive and detoxification enzymes and reducing larval survival. *Journal of the science of food and agriculture*, 106(10), 5921.

Vidal-Gironès Ò, et al. (2026) Enzyme Reset: Water-Mediated Tautomerization Restores the Catalytic Asparagine in Protein O-Fucosyltransferase 1. *Journal of chemical information and modeling*, 66(10), 6086.

Frezzini M, et al. (2026) Rationalizing Enhanced Affinity of Engineered T-Cell Receptors in Cancer Immunotherapy Through Interaction Energy Calculations and Residue Correlation Analysis. *Proteins*, 94(2), 529.

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.

Li Y, et al. (2026) The intrinsic disorder challenge for AlphaFold: A case study of G3BP1 and pathogenic peptide. *iScience*, 29(5), 115737.

Yan L, et al. (2026) The Erlin1/2 complex is a dynamic scaffold for membrane microdomain assembly on the endoplasmic reticulum. *Molecular cell*, 86(7), 1362.

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.

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

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 intra-melanosomal domain. *bioRxiv : the preprint server for biology*.

Alshahrani M, et al. (2025) Neutral Frustration Landscape Architecture of SARS-CoV-2 Spike-Antibody Interfaces Shapes Immune Evasion Mechanisms for Ultrapotent Neutralizing Antibodies and Determines Pathways of Viral Adaptation: Insights from Integrative Computational Approach. *bioRxiv : the preprint server for biology*.

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.

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

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

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).