

Resource Summary Report

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OpenMM

RRID:SCR_000436

Type: Tool

Proper Citation

OpenMM (RRID:SCR_000436)

Resource Information

URL: <https://openmm.org/>

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Description: Software toolkit to run modern molecular simulations. It can be used either as a standalone application for running simulations, or as a library that enables accelerated calculations for molecular dynamics on high-performance computer architectures.

Synonyms: OpenMM 8, OpenMM, OpenMM 7, OpenMM 4

Resource Type: standalone software, software resource, simulation software, software application

Defining Citation: [PMID:28746339](#), [PMID:23316124](#), [PMID:38154096](#),
[DOI:10.1021/acs.jpcb.3c06662](https://doi.org/10.1021/acs.jpcb.3c06662)

Keywords: modeling, molecular dynamics, molecular simulation

Funding: NIGMS U54 GM072970;
NIGMS R01 GM062868;
NCI P30 CA008748

Availability: Free, Available for download, Freely available

Resource Name: OpenMM

Resource ID: SCR_000436

Alternate IDs: nif-0000-23334

Alternate URLs: <https://github.com/openmm/openmm>, <https://openmm.org/>,
<https://openmm.org/documentation>, <https://github.com/openmm>

Old URLs: <https://simtk.org/home/openmm>

License: MIT, LGPL

Record Creation Time: 20220129T080201+0000

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Ratings and Alerts

No rating or validation information has been found for OpenMM.

No alerts have been found for OpenMM.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 12 mentions in open access literature.

Listed below are recent publications. The full list is available at [kravitz2](#) .

Yan X, et al. (2025) Intra-condensate demixing of TDP-43 inside stress granules generates pathological aggregates. *Cell*, 188(15), 4123.

Luo S, et al. (2023) Examining asymmetric pairwise pre-reaction and transition states in enzymatic catalysis by molecular dynamics simulation and quantum mechanics/molecular mechanics calculation. *STAR protocols*, 4(2), 102263.

Xie T, et al. (2022) Rational exploration of fold atlas for human solute carrier proteins. *Structure (London, England : 1993)*, 30(9), 1321.

Liao VWY, et al. (2020) Heterologous expression of concatenated nicotinic ACh receptors: Pros and cons of subunit concatenation and recommendations for construct designs. *British journal of pharmacology*, 177(18), 4275.

Malone SA, et al. (2019) Defective AMH signaling disrupts GnRH neuron development and function and contributes to hypogonadotropic hypogonadism. *eLife*, 8.

Fudenberg G, et al. (2017) FISH-ing for captured contacts: towards reconciling FISH and 3C. *Nature methods*, 14(7), 673.

Harrigan MP, et al. (2017) Markov modeling reveals novel intracellular modulation of the human TREK-2 selectivity filter. *Scientific reports*, 7(1), 632.

Lee J, et al. (2016) CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. *Journal of chemical theory and computation*, 12(1), 405.

G??tz AW, et al. (2014) Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. *Journal of chemical theory and computation*, 10(4), 1631.

Doyle B, et al. (2014) Chromatin loops as allosteric modulators of enhancer-promoter interactions. *PLoS computational biology*, 10(10), e1003867.

Lindert S, et al. (2013) Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. *Journal of chemical theory and computation*, 9(11), 4684.

Ensign DL, et al. (2009) The Fip35 WW domain folds with structural and mechanistic heterogeneity in molecular dynamics simulations. *Biophysical journal*, 96(8), L53.