Resource Summary Report

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OpenMM

RRID:SCR_000436
Type: Tool

Proper Citation

OpenMM (RRID:SCR_000436)

Resource Information

URL: https://simtk.org/home/openmm

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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 7, OpenMM 4

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

Defining Citation: PMID:28746339, PMID:23316124

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

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 11 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

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.

Götz 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.