Resource Summary Report

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Molecular Dynamics Workflow (BioKepler)

RRID:SCR_014389
Type: Tool

Proper Citation

Molecular Dynamics Workflow (BioKepler) (RRID:SCR_014389)

Resource Information

URL: https://github.com/nbcrrolls/workflows/tree/master/Production/AmberGPUMDSimulation

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Description: A workflow for running molecular dynamics simulations. It can be used for all-atom molecular dynamic simulations, which involve five steps of minimization, one step of heating, three steps of equilibration, and one or more instances of production. The input is a set of directories that include the MD simulation input scripts, system topology and coordinate files. Output files are list of plots, simulation trajectories, intermediate files, restart files, and the like.

Synonyms: Molecular Dynamics Workflow, AmberGPUMDSimulation, Molecular Dynamics Workflow Software, Amber GPUMD Simulation

Resource Type: data processing software, workflow software, software resource, software application

Keywords: workflow, MD, molecular dynamics, simulation, software, bio.tools

Funding: NIGMS P41GM103426

Availability: Requires Linux

Resource Name: Molecular Dynamics Workflow (BioKepler)

Resource ID: SCR_014389

Alternate IDs: biotools:ambergpumdsimulation

Alternate URLs: http://nbcr.ucsd.edu/data/downloads/workflows/,

https://bio.tools/ambergpumdsimulation

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Record Last Update: 20250430T055927+0000

Ratings and Alerts

No rating or validation information has been found for Molecular Dynamics Workflow (BioKepler) .

No alerts have been found for Molecular Dynamics Workflow (BioKepler) .

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 1 mentions in open access literature.

Listed below are recent publications. The full list is available at dkNET.

Purawat S, et al. (2017) A Kepler Workflow Tool for Reproducible AMBER GPU Molecular Dynamics. Biophysical journal, 112(12), 2469.