**GROMACS**

RRID:SCR_014565  
Type: Tool

**Proper Citation**

GROMACS (RRID:SCR_014565)

**Resource Information**

**URL:** [http://www.gromacs.org](http://www.gromacs.org)

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**Description:** Software package created to perform molecular dynamics. Molecular dynamics package mainly designed for simulations of proteins, lipids, and nucleic acids. Can also be used for research on non-biological systems, such as polymers.

**Synonyms:** Gromacs

**Resource Type:** software toolkit, simulation software, software application, software resource

**Defining Citation:** PMID:26620784, DOI:10.1016/0010-4655(95)00042-E

**Keywords:** simulation, molecular dynamics, software package, software toolkit, biochemical, molecule, protein, lipid, nucleic acid, bond interaction, bio.tools

**Funding Agency:** European Research Council, Swedish eScience Research Center, Stream Computing Performance Engineers, Nvidia, Swedish Research Council, Swedish Foundation for Strategic Research, Swedish National Infrastructure for Computing, Swedish Foundation for International Cooperation in Research and Higher Education

**Availability:** Free, Available for download

**Resource Name:** GROMACS

**Resource ID:** SCR_014565
Alternate IDs: biotools:gromacs, OMICS_05081


Record Creation Time: 20220129T080321+0000

Record Last Update: 20240616T053831+0000

Ratings and Alerts

No rating or validation information has been found for GROMACS.

No alerts have been found for GROMACS.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 5794 mentions in open access literature.

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


Rao S, et al. (2024) Three-step docking by WIPI2, ATG16L1, and ATG3 delivers LC3 to the phagophore. Science advances, 10(6), eadj8027.


Ceccacci S, et al. (2024) A label free chemoproteomic-based platform to disclose cannabidiol molecular mechanism of action on chronic myelogenous leukemia cancer cells. Heliyon, 10(1), e24196.


Chavan RS, et al. (2024) Synergistic effects of Momordica charantia, Nigella sativa, and Anethum graveolens on metabolic syndrome targets: In vitro enzyme inhibition and in silico analyses. Heliyon, 10(2), e24907.


Valdivia A, et al. (2024) Binding of Cholesterol to the N-Terminal Domain of the NPC1L1 Transporter: Analysis of the Epimerization-Related Binding Selectivity and Loop Mutations. Journal of chemical information and modeling, 64(1), 189.


Chirasani VR, et al. (2024) Structural and functional interactions between the EF hand domain and S2-S3 loop in the type-1 ryanodine receptor ion channel. The Journal of biological chemistry, 300(2), 105606.


Ren K, et al. (2024) Thioacetamide Additive Homogenizing Zn Deposition Revealed by In Situ Digital Holography for Advanced Zn Ion Batteries. Nano-micro letters, 16(1), 117.