

Resource Summary Report

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Desmond

RRID:SCR_014575

Type: Tool

Proper Citation

Desmond (RRID:SCR_014575)

Resource Information

URL: https://www.deshawresearch.com/resources_desmond.html

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Description: Software designed to perform high-speed molecular dynamic simulations of biological systems on conventional commodity clusters, supercomputers and GPUs. This code uses novel parallel algorithms and numerical techniques to achieve high performance and accuracy on platforms with a large number of processors. It can be used with a single computer.

Resource Type: simulation software, software application, software resource

Keywords: simulation, supercomputer, commodity cluster, gpu, parallel algorithm, biological system, parallel algorithms, computer, processor

Availability: Open source, Free for non-commercial use, Commercial entities must contact Schrodinger LLC

Resource Name: Desmond

Resource ID: SCR_014575

License: Commercial License available through Schrödinger, LLC

Record Creation Time: 20220129T080321+0000

Record Last Update: 20260912T195818+0000

Ratings and Alerts

No rating or validation information has been found for Desmond.

No alerts have been found for Desmond.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 946 mentions in open access literature.

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

Yang Q, et al. (2026) Molecular mechanism of resistance to lonafarnib conferred by mutations in the cysteine-rich region of respiratory syncytial virus fusion glycoprotein and discovery of a lonafarnib-derived antiviral PROTAC. *Journal of virology*, 100(1), e0148725.

Feher A, et al. (2026) A kinetic trap mechanism underlies hHv1 inhibition by NZ-58. *The Journal of general physiology*, 158(4).

Tian JL, et al. (2026) Design of a sustained-release nanosystem for ultra-efficient absorption of anthocyanins and regulating lung damage through the "lung-gut" axis. *Journal of advanced research*, 81, 27.

Beigh S, et al. (2026) Ginkgolide as a Promising Multi-Target Therapeutic for Alzheimer's Disease: Targeting ApoE4 and Beyond. *Current pharmaceutical design*, 32(15), 1200.

Aeimlapa R, et al. (2026) Vildagliptin and Omarigliptin Differentially Bind to DPP-4 Homodimers and Modulate Osteoclast-Mediated Bone Resorption. *Comprehensive Physiology*, 16(1), e70103.

Qiang Y, et al. (2026) USP1 driven mitotic dysregulation and PLK1 stabilization confer Lenvatinib resistance in hepatocellular carcinoma. *Journal of experimental & clinical cancer research : CR*, 45(1).

Chernitsky-Hamd D, et al. (2026) Plasmodium falciparum Chloroquine Resistance Transporter (PfCRT) Is a Redox-Dependent Drug Transporter. *Biochemistry*, 65(7), 1033.

Al Mashud MA, et al. (2026) Computational identification of Terminalia arjuna phytochemicals as potential 3?-HSD3 inhibitors. *Scientific reports*, 16(1).

Saber MA, et al. (2026) Pan-genome and reverse vaccinology for a multi-epitope vaccine against circulating post-2022 Monkeypox virus strains. *PloS one*, 21(6), e0351881.

Geng M, et al. (2026) Cytoplasmic retention of IRF3 binding Vimentin competitively with ERK1/2 mitigates acute myeloid leukemia through TFEB nuclear translocation. *Cell communication and signaling : CCS*, 24(1).

Pandey P, et al. (2026) Cannabidiophorol (CBDP) acts as a negative allosteric modulator at two distinct sites of cannabinoid receptor 1. *Communications chemistry*, 9(1).

Huang Y, et al. (2026) SHP-1 agonist SC-43 limits methicillin-resistant Staphylococcus aureus infection through inhibition of heme biosynthesis. *EMBO molecular medicine*, 18(5), 1990.

Alam MJ, et al. (2026) Molecular Docking and MD Modeling Techniques for the Development of Novel ROS1 Kinase Inhibitors. *Pharmaceuticals* (Basel, Switzerland), 19(2).

Yu Z, et al. (2026) Multi-target modulation of the homologous recombination pathway by resveratrol promotes DNA damage repair in POI: integrated network pharmacology, molecular dynamics simulation, and experimental validation. *International journal of surgery* (London, England), 112(4), 9404.

Bauer M, et al. (2026) Receptor Binding, Functional Activity, and Cell Viability Assessment of Novel Marine-Based Hybrid Peptides from *Raja porosa*. *Marine drugs*, 24(5).

Roshdy E, et al. (2026) Design and Synthesis of Bis-Triazole-Linked Benzenesulfonamides as Selective Carbonic Anhydrase IX/XII Inhibitors with Chemosensitizing Activity. *Journal of medicinal chemistry*, 69(9), 11365.

El-Bayaa MN, et al. (2026) Design, click-based synthesis, molecular docking, molecular dynamics and anticancer activity of new isoindoline-1,3-dione- triazole-glycopyranosyl hybrids. *Scientific reports*, 16(1).

Alanzi AR, et al. (2026) In silico identification and validation of vaccine and drug targets in *Coccidioides posadasii* through integrated genomic, proteomic, and molecular modeling approaches. *Medicine*, 105(23), e49169.

Yadav M, et al. (2026) Bio-Assisted Synthesis of Reduced Graphene Oxide Nanosheets From Graphene Oxide: Promising and Efficient Cytotoxic and Antidiabetic Potency in In Vitro, Kinetic, and In Silico Models. *International journal of biomaterials*, 2026, 5521416.

Aguti R, et al. (2026) Critical Assessment of a Structure-Based Pipeline for Targeting the Long Noncoding RNA MALAT1. *Journal of chemical information and modeling*, 66(7), 4187.