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: software application, simulation software, software resource

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

Funding:

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: 20250508T065533+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 723 mentions in open access literature.

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

Marczak M, et al. (2025) The HECT ubiquitin-protein ligases UPL1 and UPL2 are involved in degradation of Arabidopsis thaliana ACC synthase 7. Physiologia plantarum, 177(1), e70030.

Elsaman T, et al. (2025) Examining Prenylated Xanthones as Potential Inhibitors Against Ketohexokinase C Isoform for the Treatment of Fructose-Driven Metabolic Disorders: An Integrated Computational Approach. Pharmaceuticals (Basel, Switzerland), 18(1).

Ghasemi M, et al. (2025) Substituted piperazine conjugated to quinoline-thiosemicarbazide as potent ?-glucosidase inhibitors to target hyperglycemia. Scientific reports, 15(1), 1871.

Arshad F, et al. (2025) Core-genome guided novel therapeutic targets identification and chimeric vaccine designing against Rickettsia rickettsii. Scientific reports, 15(1), 921.

Wang D, et al. (2025) Identification of Downregulated MECR Gene in Parkinson's Disease Through Integrated Transcriptomic Analysis and Validation. International journal of molecular sciences, 26(2).

Naveed M, et al. (2025) Fragment optimized chalcone derivatives targeting OmpA protein as a therapeutic approach against multidrug resistant Acinetobacter baumannii. Scientific reports, 15(1), 3917.

Ishaq S, et al. (2025) Evaluation of fluorinated phospholipid analogs: A study on ADMET profiles, molecular docking and dynamics simulation in anticancer therapy. Heliyon, 11(2), e41739.

Halder D, et al. (2025) Exploring target selectivity in designing and identifying PI3K? inhibitors for triple negative breast cancer with fragment-based and bioisosteric replacement approach. Scientific reports, 15(1), 1890.

Er-Rajy M, et al. (2025) An in-depth study of indolone derivatives as potential lung cancer

treatment. Scientific reports, 15(1), 2199.

Loyau J, et al. (2025) Biparatopic binding of ISB 1442 to CD38 in trans enables increased cell antibody density and increased avidity. mAbs, 17(1), 2457471.

Németh BZ, et al. (2025) The High-Affinity Chymotrypsin Inhibitor Eglin C Poorly Inhibits Human Chymotrypsin-Like Protease: Gln192 and Lys218 Are Key Determinants. Proteins, 93(2), 543.

Moghadam Farid S, et al. (2025) Synthesis, biological evaluations, and in silico assessments of phenylamino quinazolinones as tyrosinase inhibitors. Scientific reports, 15(1), 846.

Patel JIA, et al. (2025) Mechanistic insights into gut microbe derived siderophores and PHD2 interactions with implications for HIF-1? stabilization. Scientific reports, 15(1), 1113.

Naimuzzaman M, et al. (2025) Computational and In silico study of novel fungicides against combating root rot, gray mold, fusarium wilt, and cereal rust. PloS one, 20(1), e0316606.

Guerguer FZ, et al. (2025) Moroccan natural products for multitarget-based treatment of Alzheimer's disease: A computational study. PloS one, 20(1), e0313411.

Guerguer FZ, et al. (2025) Potential Azo-8-hydroxyquinoline derivatives as multi-target lead candidates for Alzheimer's disease: An in-depth in silico study of monoamine oxidase and cholinesterase inhibitors. PloS one, 20(1), e0317261.

Bheemireddy S, et al. (2025) Computational analysis of the effect of a binding protein (RbpA) on the dynamics of Mycobacterium tuberculosis RNA polymerase assembly. PloS one, 20(1), e0317187.

Schneider C, et al. (2024) A Novel AMPK Inhibitor Sensitizes Pancreatic Cancer Cells to Ferroptosis Induction. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 11(31), e2307695.

Abchir O, et al. (2024) Exploration of alpha-glucosidase inhibitors: A comprehensive in silico approach targeting a large set of triazole derivatives. PloS one, 19(9), e0308308.

Malasala S, et al. (2024) Enabling systemic identification and functionality profiling for Cdc42 homeostatic modulators. Communications chemistry, 7(1), 271.