

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: 20260805T044328+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 875 mentions in open access literature.

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

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.

Bayouth A, et al. (2025) Integrated Network Pharmacology and Molecular Dynamics Reveal Multi-Target Anticancer Mechanisms of Myrtus communis Essential Oils. *Pharmaceuticals (Basel, Switzerland)*, 18(10).

Deng Z, et al. (2025) PNPO-Mediated Oxidation of DVL3 Promotes Multiple Myeloma Malignancy and Osteoclastogenesis by Activating the Wnt/ β -Catenin Pathway. *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*, 12(5), e2407681.

Gadewal N, et al. (2025) In silico screening of phytochemicals against chromatin modifier, SETD7 for remodeling of the immunosuppressive tumor microenvironment in renal cancer. *Molecular diversity*, 29(5), 4359.

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

Ahmed MZ, et al. (2025) Immunoinformatic-driven design and evaluation of multi-epitope mRNA vaccine targeting HIV-1 gp120. *Frontiers in immunology*, 16, 1480025.

Güner Y, İmzaz ÖZ, et al. (2025) A Computationally Efficient Method to Generate Plausible Conformers for Ensemble Docking and Binding Free Energy Calculations. *Journal of chemical information and modeling*, 65(15), 8137.

Alshehri B, et al. (2025) Exploring the interplay between LDHA and ABCC1 in breast cancer using computational approach. *Discover oncology*, 16(1), 1471.

Tran MH, et al. (2025) Revealing inhibitory activity of luteolin from Vietnamese *Jatropha Podagrica* Hook against *Staphylococcus aureus* by integrating in vitro and in silico approaches. *Scientific reports*, 15(1), 28537.

Oak S, et al. (2025) The deubiquitinase inhibitor WP1130 drives nuclear aggregation and reactivation of mutant p53 for selective cancer cell targeting. *The FEBS journal*, 292(11), 2823.

Shao J, et al. (2025) Designing polymersomes with surface-integrated nanoparticles through hierarchical phase separation. *Nature communications*, 16(1), 2445.

Mohamed AAK, et al. (2025) In silico molecular studies of Phosphinogold(I) thiocarbohydrate complexes: insights into multi-target anticancer mechanisms. *Frontiers in chemistry*, 13, 1533026.

Zang HJ, et al. (2025) Neuroprotective effects of chemical constituents from *Nicotiana tabacum* L. in Parkinson's disease. *Natural products and bioprospecting*, 15(1), 67.

Carvalho M, et al. (2025) Understanding behaviour change maintenance after attending a self-management education and support programme for type 2 diabetes: A longitudinal qualitative study. *Diabetic medicine : a journal of the British Diabetic Association*, 42(6), e70032.

Khan SA, et al. (2025) Network pharmacology and in silico analysis reveal *Kochia fructus* as a potential therapeutic against atopic dermatitis through immunomodulatory pathway interactions. *PloS one*, 20(4), e0320818.

Tareq MMI, et al. (2025) Development of a potential vaccine against Capripox virus implementing reverse vaccinology and pan-genomic immunoinformatics. *PloS one*, 20(7), e0326310.

Mohamed AI, et al. (2025) Exploring the Chemical Profile, Antioxidants, and Anti-Diabetic Properties of Coffee Beans From Selected East African Countries: A Comparative In Vitro and Computational Study. *Food science & nutrition*, 13(7), e70527.

Siddiquee NH, et al. (2025) Molecular activity of bioactive phytochemicals for inhibiting host cell attachment and membrane fusion interacting with West Nile Virus envelope glycoprotein. *PloS one*, 20(4), e0321902.

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

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.