Resource Summary Report

Generated by RRID on Aug 12, 2026

Molinspiration

RRID:SCR_018525
Type: Tool

Proper Citation

Molinspiration (RRID:SCR_018525)

Resource Information

URL: https://www.molinspiration.com/

Proper Citation: Molinspiration (RRID:SCR_018525)

Description: Broad range of cheminformatics software tools supporting molecule manipulation and processing, including SMILES and SDfile conversion, normalization of molecules, generation of tautomers, molecule fragmentation, calculation of various molecular properties needed in QSAR, molecular modelling and drug design, high quality molecule depiction, molecular database tools supporting substructure and similarity searches. Molinspiration tools are platform independent and may be run on any PC, Mac, UNIX or LINUX machine. Software is distributed in form of engines, which may be used as stand-alone computational engines, used to power web-based tools, or incorporated into larger in-house Java applications.

Resource Type: software toolkit, software resource

Keywords: Cheminformatics, molecule manipulation, molecule processing, molecule normalization, tautomer generation, molecule fragmentation, molecular property calculation, molecular modeling, drug design, FASEB list

Availability: Free, Freely available

Resource Name: Molinspiration

Resource ID: SCR_018525

Record Creation Time: 20220129T080340+0000

Record Last Update: 20260810T040742+0000

Ratings and Alerts

No rating or validation information has been found for Molinspiration.

No alerts have been found for Molinspiration.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 389 mentions in open access literature.

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

Chen Q, et al. (2026) Antifungal potential of naphthoquinone derivatives: screening of shikonin-based compounds and mechanistic insights into 5,8-dihydroxy-1,4-naphthoquinone against Candida albicans in vitro and in vivo. Microbiology spectrum, 14(4), e0243825.

Siame C, et al. (2026) In silico evaluation of garlic-derived organosulfur compounds as multi-target inhibitors of breast cancer biomarkers. PloS one, 21(5), e0348369.

Mondal J, et al. (2026) Integrated In Silico and In Vitro Study of Copper Nanocatalyzed Carbonyl-Functionalized Triazoles-Inducing S Phase Cell Cycle Arrest and Apoptosis in MCF-7. ChemistryOpen, 15(1), e202500543.

Altharawi A, et al. (2026) Synthesis, molecular modelling, and evaluation of new mono- and bis-isoxazolines as antibacterial agents: in vitro and in silico analysis. RSC advances, 16(29), 26399.

Du S, et al. (2026) Skin-penetrating peptides derived from computational simulation improve transdermal absorption and facilitate topical treatment of melanoma. Acta pharmaceutica Sinica. B, 16(2), 1140.

Meier L, et al. (2026) In Silico Studies and Biological Evaluation of Thiosemicarbazones as Cruzain-Targeting Trypanocidal Agents for Chagas Disease. Pharmaceutics, 18(1).

Bahia IAF, et al. (2026) Comparative pharmacoinformatic and quantum descriptor insights from BFM/GBTLI guidelines to phase I/II compounds for acute lymphoblastic leukemia (ALL). Scientific reports, 16(1).

Cabrera-Pérez LC, et al. (2026) Ex vivo and in silico evaluations of (E)-5-((benzo[d]thiazol-2-ylimino)(methylthio)methylamino)-2-hydroxybenzoic acid as a ?3-adrenoreceptor agonist exerting anti-obesity, anti-inflammatory and hepatoprotective effects on Zucker rats. PloS one, 21(3), e0344359.

Wakid MH, et al. (2026) Kaempferol activity on Cryptosporidium parvum infection in an experimentally infected immunocompromised mouse model: In silico and in vivo investigations. Pharmaceutical biology, 64(1), 27.

Shakour N, et al. (2026) Rational Design of Novel Inhibitors: Integrating 3D-QSAR and Molecular Dynamics. BioMed research international, 2026, 4138899.

Fotopoulos I, et al. (2026) Coumarin-Amino Acid Hybrids Used as Possible Multifactorial Anti-Inflammatory Agents. International journal of molecular sciences, 27(10).

Kadda S, et al. (2026) Applications of Opuntia ficus-indica (L.) mill seed oil from eastern morocco including chemical profiling, antibacterial activity, and docking. Scientific reports, 16(1).

Jia Y, et al. (2026) Computational and preliminary screening of anti-caries active compounds of Caesalpinia sappan. Scientific reports, 16(1).

Ashfaq A, et al. (2026) Chemoinformatic Approaches to Identify Bioactive Inhibitors Against Type I Dehydroquinase (DHQ1) Enzyme of Typhoidal Salmonella. Bioinformatics and biology insights, 20, 11779322261418889.

Ka?mierczak T, et al. (2026) Interaction of diosmetin, diosmin and diosmetin-7-O-glucoside with human erythrocytes, their model membrane, hemoglobin and redox-active metal ions. Frontiers in molecular biosciences, 13, 1814932.

Singh N, et al. (2025) Computational drug discovery of phytochemical alkaloids targeting the NACHT/PYD domain in the NLRP3 inflammasome. Scientific reports, 15(1), 16677.

Wang R, et al. (2025) Novel Isatin-Chalcone Hybrid Molecules: Design, Synthesis and Anti-Neuroinflammatory Activity Evaluation. Molecules (Basel, Switzerland), 30(7).

Islam MD, et al. (2025) Synthesis, antibacterial activity, in silico ADMET prediction, docking, and molecular dynamics studies of substituted phenyl and furan ring containing thiazole Schiff base derivatives. PloS one, 20(3), e0318999.

Hidalgo M, et al. (2025) The antioxidant property of CAPE depends on TRPV1 channel activation in microvascular endothelial cells. Redox biology, 80, 103507.

Boyer R, et al. (2025) LPS2336, a New TREK-1 Channel Activator Identified by High Throughput Screening. Biomolecules, 15(5).