Resource Summary Report

Generated by T1D on Aug 1, 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 resource, software toolkit

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: 20260801T042833+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 263 mentions in open access literature.

Listed below are recent publications. The full list is available at T1D .

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.

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

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.

Vats P, et al. (2025) Comparative analysis of phytocompounds and repurposed drugs against dengue virus serotypes employing an in silico study. Scientific reports, 15(1), 27878.

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.

Pesquet E, et al. (2025) Physiological roles of lignins - tuning cell wall hygroscopy and biomechanics. The New phytologist, 248(6), 2674.

?astawiecka E, et al. (2025) Design, synthesis and bioactivity evaluation of phosphinanes as potential anticancer agents. Scientific reports, 15(1), 28229.

Khan K, et al. (2025) Zapotin mitigates breast cancer progression by targeting PKC? mediated glycolytic pathway regulation. BMC cancer, 25(1), 798.

Vats P, et al. (2025) Correction: Comparative analysis of phytocompounds and repurposed drugs against dengue virus serotypes employing an in silico study. Scientific reports, 15(1), 44405.

Pastuch-Gawo?ek G, et al. (2025) Effect of Glycoconjugation on Cytotoxicity and Selectivity of 8-Aminoquinoline Derivatives Compared to 8-Hydroxyquinoline. Molecules (Basel, Switzerland), 30(2).

Wang Z, et al. (2025) Exploration of small molecules as inhibitors of potential BACE1 protein to treat amyloid cerebrovascular disease by employing molecular modeling and simulation approaches. PloS one, 20(3), e0317716.

Cook AL, et al. (2025) Identification of nonsense-mediated decay inhibitors that alter the tumor immune landscape. eLife, 13.

Haitian-Li , et al. (2025) Exploring the Mechanism of Action of Berberine on Arrhythmia After Myocardial Infarction: A Network Pharmacology, Molecular Docking, and Cellular Experimental Study. Cardiovascular therapeutics, 2025, 5632985.

Gill JH, et al. (2025) Development of novel benzamide class I selective lysine deacetylase inhibitors as potent anticancer agents. Journal of enzyme inhibition and medicinal chemistry, 40(1), 2520612.

Krug SA, et al. (2025) Application of preclinical absorption, distribution, metabolism, elimination in vitro techniques for the characterization and compound library optimization of novel antibiotic gallium salophen. Drug metabolism and disposition: the biological fate of chemicals, 53(6), 100080.

Andola P, et al. (2025) Application of chemical similarity and bioisosteres to find allosteric inhibitors of type 2 lipid kinase ?. Scientific reports, 15(1), 33890.

Kourat O, et al. (2025) Structural, nonlinear optical, and molecular docking studies of schiff base compounds as multi-target inhibitors of AChE, BChE, and carbonic anhydrases. Scientific reports, 15(1), 34818.

Naglah AM, et al. (2025) In Vitro Enzymatic and Computational Assessments of Pyrazole-Isatin and Pyrazole-Indole Conjugates as Anti-Diabetic, Anti-Arthritic, and Anti-Inflammatory Agents. Pharmaceutics, 17(3).

Zhu TW, et al. (2025) Screening potential anti-osteoarthritis compounds using molecular docking based on MAPK and NF?B pathways and validating their anti-osteoarthritis effect. PloS one, 20(3), e0319686.

do Nascimento Martinez L, et al. (2025) In vitro and in silico evaluation of synthetic compounds derived from bi-triazoles against asexual and sexual forms of Plasmodium falciparum. Malaria journal, 24(1), 74.