Resource Summary Report

Generated by T1D on Aug 3, 2026

MacroModel

RRID:SCR_016747
Type: Tool

Proper Citation

MacroModel (RRID:SCR_016747)

Resource Information

URL: https://www.schrodinger.com/macromodel

Proper Citation: MacroModel (RRID:SCR_016747)

Description: Software package for molecular modeling. Computes free energy changes using free energy perturbation method. Used to examine molecular conformations, molecular motion, and intermolecular interactions, such as those in a ligand-receptor complex.

Resource Type: simulation software, software resource, software application

Keywords: molecular, modeling, free, energy, changes, perturbation, method, conformation, motion, interaction, ligand, receptor, complex

Availability: Commercially available, Free version available

Resource Name: MacroModel

Resource ID: SCR_016747

Alternate URLs: https://en.freedownloadmanager.org/Windows-PC/MacroModel.html

Record Creation Time: 20220129T080332+0000

Record Last Update: 20260803T040729+0000

Ratings and Alerts

No rating or validation information has been found for MacroModel.

No alerts have been found for MacroModel.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 137 mentions in open access literature.

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

Kang S, et al. (2025) Discovery of a selective dual-specificity tyrosine phosphorylation-regulated kinase 1B inhibitor with anti-adipogenic and anti-diabetic activities. Frontiers in pharmacology, 16, 1645033.

Varró N, et al. (2025) Betaine-Conjugated ß-Peptide Foldamers: Influence of Quaternary Charge on Self-Organization and MorphologyFormation. ChemistryOpen, 14(12), e202500340.

Farag A, et al. (2025) Repurposing rupatadine as topical treatment against methicillin-resistant Staphylococcus aureus. AMB Express, 15(1), 132.

Al-Sanea MM, et al. (2023) Design, synthesis, and biological investigation of oxadiazolyl, thiadiazolyl, and pyrimidinyl linked antipyrine derivatives as potential non-acidic anti-inflammatory agents. Journal of enzyme inhibition and medicinal chemistry, 38(1), 2162511.

Balouch M, et al. (2023) Computational Prodrug Design Methodology for Liposome Formulability Enhancement of Small-Molecule APIs. Molecular pharmaceutics, 20(4), 2119.

Federico S, et al. (2022) Azetidin-2-one-based small molecules as dual hHDAC6/HDAC8 inhibitors: Investigation of their mechanism of action and impact of dual inhibition profile on cell viability. European journal of medicinal chemistry, 238, 114409.

Lachowicz JI, et al. (2022) Thymosin ?4 Is an Endogenous Iron Chelator and Molecular Switcher of Ferroptosis. International journal of molecular sciences, 23(1).

Fois B, et al. (2021) Flavonoids and Acid-Hydrolysis derivatives of Neo-Clerodane diterpenes from Teucrium flavum subsp. glaucum as inhibitors of the HIV-1 reverse transcriptase-associated RNase H function. Journal of enzyme inhibition and medicinal chemistry, 36(1), 749.

Rösch AT, et al. (2021) Rotational Isomerism of an Amide Substituted Squaraine Dye: A Combined Spectroscopic and Computational Study. The Journal of organic chemistry, 86(18), 13100.

Matiadis D, et al. (2021) Curcumin Derivatives as Potential Mosquito Larvicidal Agents against Two Mosquito Vectors, Culex pipiens and Aedes albopictus. International journal of molecular sciences, 22(16).

Meleddu R, et al. (2021) Exploring New Scaffolds for the Dual Inhibition of HIV-1 RT Polymerase and Ribonuclease Associated Functions. Molecules (Basel, Switzerland), 26(13).

Oliveira D, et al. (2021) 2-(2-Methyl-2-nitrovinyl)furan but Not Furvina Interfere with Staphylococcus aureus Agr Quorum-Sensing System and Potentiate the Action of Fusidic Acid against Biofilms. International journal of molecular sciences, 22(2).

Rodríguez-Salarichs J, et al. (2021) Versatile Lipases from the Candida rugosa-like Family: A Mechanistic Insight Using Computational Approaches. Journal of chemical information and modeling, 61(2), 913.

Kiper AK, et al. (2021) Identification of a critical binding site for local anaesthetics in the side pockets of Kv 1 channels. British journal of pharmacology, 178(15), 3034.

Saldanha LL, et al. (2021) Hypoglycemic active principles from the leaves of Bauhinia holophylla: Comprehensive phytochemical characterization and in vivo activity profile. PloS one, 16(9), e0258016.

Bellone ML, et al. (2021) Limonoids from Guarea guidonia and Cedrela odorata: Heat Shock Protein 90 (Hsp90) Modulator Properties of Chisomicine D. Journal of natural products, 84(3), 724.

Marchetti G, et al. (2020) Syk Inhibitors: New Computational Insights into Their Intraerythrocytic Action in Plasmodium falciparum Malaria. International journal of molecular sciences, 21(19).

Pruijssers AJ, et al. (2020) Remdesivir Inhibits SARS-CoV-2 in Human Lung Cells and Chimeric SARS-CoV Expressing the SARS-CoV-2 RNA Polymerase in Mice. Cell reports, 32(3), 107940.

Tsuchiya Y, et al. (2020) Molecular Design Based on Donor-Weak Donor Scaffold for Blue Thermally-Activated Delayed Fluorescence Designed by Combinatorial DFT Calculations. Frontiers in chemistry, 8, 403.

Purgatorio R, et al. (2020) Pharmacophore Modeling and 3D-QSAR Study of Indole and Isatin Derivatives as Antiamyloidogenic Agents Targeting Alzheimer's Disease. Molecules (Basel, Switzerland), 25(23).