

# Resource Summary Report

Generated by [RRID](#) on Aug 2, 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:** software resource, software application, simulation software

**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:** 20260801T190552+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

## Usage and Citation Metrics

We found 137 mentions in open access literature.

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

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  $\beta$ -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  $\gamma$ 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).