Resource Summary Report

Generated by FDI Lab - SciCrunch.org on May 28, 2025

Ligprep

RRID:SCR_016746
Type: Tool

Proper Citation

Ligprep (RRID:SCR_016746)

Resource Information

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

Proper Citation: Ligprep (RRID:SCR_016746)

Description: Software tool to correct and optimize the ligands by generating different protonation states, stereochemistry, tautomers, and ring conformations. Used to generate accurate, energy minimized 3D molecular structures.

Abbreviations: Ligprep

Synonyms: LigPrep, LigandPreparation, Ligand preparation

Resource Type: software resource, simulation software, software application

Keywords: correct, optimize, ligand, protonation, stereochemistry, tautomer, conformation, energy, minimized, 3D, moleular, structure

Funding:

Availability: Commercially available

Resource Name: Ligprep

Resource ID: SCR_016746

Record Creation Time: 20220129T080332+0000

Record Last Update: 20250528T061340+0000

Ratings and Alerts

No rating or validation information has been found for Ligprep.

No alerts have been found for Ligprep.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 43 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

Che T, et al. (2024) Structural mechanism of human HCN1 hyperpolarization-activated channel inhibition by ivabradine. The Journal of biological chemistry, 300(11), 107798.

Peixoto C, et al. (2024) Discovery of Clinical Candidate GLPG3970: A Potent and Selective Dual SIK2/SIK3 Inhibitor for the Treatment of Autoimmune and Inflammatory Diseases. Journal of medicinal chemistry, 67(7), 5233.

Schneider C, et al. (2024) A Novel AMPK Inhibitor Sensitizes Pancreatic Cancer Cells to Ferroptosis Induction. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 11(31), e2307695.

Pedersen CN, et al. (2024) Cryo-EM structure of the dopamine transporter with a novel atypical non-competitive inhibitor bound to the orthosteric site. Journal of neurochemistry, 168(9), 2043.

Pietru? W, et al. (2023) Tuning the Biological Activity of PI3K? Inhibitor by the Introduction of a Fluorine Atom Using the Computational Workflow. Molecules (Basel, Switzerland), 28(8).

Grychowska K, et al. (2023) Impact of the Substitution Pattern at the Basic Center and Geometry of the Amine Fragment on 5-HT6 and D3R Affinity in the 1H-Pyrrolo[3,2-c]quinoline Series. Molecules (Basel, Switzerland), 28(3).

Szczepa?ska K, et al. (2023) Dual Piperidine-Based Histamine H3 and Sigma-1 Receptor Ligands in the Treatment of Nociceptive and Neuropathic Pain. Journal of medicinal chemistry, 66(14), 9658.

Pietru? W, et al. (2023) Isomeric Activity Cliffs-A Case Study for Fluorine Substitution of Aminergic G Protein-Coupled Receptor Ligands. Molecules (Basel, Switzerland), 28(2).

Grychowska K, et al. (2023) Superiority of the Triple-Acting 5-HT6R/5-HT3R Antagonist and MAO-B Reversible Inhibitor PZ-1922 over 5-HT6R Antagonist Intepirdine in Alleviation of Cognitive Deficits in Rats. Journal of medicinal chemistry, 66(21), 14928.

Lettl C, et al. (2023) Selective killing of the human gastric pathogen Helicobacter pylori by mitochondrial respiratory complex I inhibitors. Cell chemical biology, 30(5), 499.

Jahid S, et al. (2022) Structure-based design of CDC42 effector interaction inhibitors for the treatment of cancer. Cell reports, 39(1), 110641.

Anju A, et al. (2022) Virtual screening of quinoline derived library for SARS-COV-2 targeting viral entry and replication. Journal of biomolecular structure & dynamics, 40(18), 8464.

Wang Y, et al. (2022) Scutellarein attenuates atopic dermatitis by selectively inhibiting transient receptor potential vanilloid 3 channels. British journal of pharmacology, 179(20), 4792.

Staro? J, et al. (2021) Tuning the activity of known drugs via the introduction of halogen atoms, a case study of SERT ligands - Fluoxetine and fluvoxamine. European journal of medicinal chemistry, 220, 113533.

Montanari S, et al. (2021) New Coumarin Derivatives as Cholinergic and Cannabinoid System Modulators. Molecules (Basel, Switzerland), 26(11).

Sun K, et al. (2021) Saikosaponin D exhibits anti-leukemic activity by targeting FTO/m6A signaling. Theranostics, 11(12), 5831.

Muralidharan A, et al. (2021) Identification and characterization of novel candidate compounds targeting 6- and 7-transmembrane ?-opioid receptor isoforms. British journal of pharmacology, 178(13), 2709.

Huang T, et al. (2021) Andrographolide prevents bone loss via targeting estrogen-related receptor-?-regulated metabolic adaption of osteoclastogenesis. British journal of pharmacology, 178(21), 4352.

Yang Y, et al. (2020) Sitravatinib, a Tyrosine Kinase Inhibitor, Inhibits the Transport Function of ABCG2 and Restores Sensitivity to Chemotherapy-Resistant Cancer Cells in vitro. Frontiers in oncology, 10, 700.

Fujimori I, et al. (2020) Discovery of Novel and Highly Selective Cyclopropane ALK Inhibitors through a Fragment-Assisted, Structure-Based Drug Design. ACS omega, 5(49), 31984.