Resource Summary Report

Generated by NIF on Aug 4, 2026

Mcule

RRID:SCR_018921
Type: Tool

Proper Citation

Mcule (RRID:SCR_018921)

Resource Information

URL: https://mcule.com/

Proper Citation: Mcule (RRID:SCR_018921)

Description: Software drug discovery platform to integrate purchasable chemical space with molecular modeling tools. Chemical marketplace for drug discovery with services based around small molecule compound sourcing. Integrated molecular modeling tools, compound database, IT infrastructure and compound procurement service with web interface. Virtual screens can be run to identify new hits and modeling applications can be used to improve their affinity and other properties.

Resource Type: portal, web service, data access protocol, data or information resource, software resource

Keywords: Drug discovery platform, molecular modeling, molecular modeling tools, compound database, IT infrastructure, compound procurement service, web interface, virtual screening, modeling application

Availability: Restricted

Resource Name: Mcule

Resource ID: SCR_018921

Record Creation Time: 20220129T080342+0000

Record Last Update: 20260804T043721+0000

Ratings and Alerts

No rating or validation information has been found for Mcule.

No alerts have been found for Mcule.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 26 mentions in open access literature.

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

Zhang Y, et al. (2025) Network pharmacology study on the mechanism of berberine in Alzheimer's disease model. NPJ science of food, 9(1), 16.

Lima RJV, et al. (2025) Modeling, virtual screening, and enzymatic docking of trehalose 6-phosphate phosphatase and evaluation of the insecticidal effect of phthalimide, N-(p-tolylsulfonyl) on Aedes aegypti (Diptera: Culicidae). Pest management science, 81(8), 4777.

Shin DH, et al. (2025) Targeting TGF-?-Smad2/3-JNK1-mediated SIRT1 activity overcomes the chemoresistance of KRAS mutation lung cancer. Experimental & molecular medicine, 57(9), 2022.

Eyster C, et al. (2025) Mechanistic studies of PFKFB2 reveal a novel inhibitor of its kinase activity. PloS one, 20(5), e0317167.

Eyster C, et al. (2024) Mechanistic studies of PFKFB2 reveals a novel inhibitor of its kinase activity. bioRxiv : the preprint server for biology.

Sobhani N, et al. (2024) Artificial intelligence-powered discovery of small molecules inhibiting CTLA-4 in cancer. BJC reports, 2.

Ilyas S, et al. (2024) Exploring the therapeutic potential of Emblica officinalis natural compounds against hepatocellular carcinoma (HCC): a computational approach. EXCLI journal, 23, 1440.

Kant R, et al. (2024) Antimicrobial activity of compounds identified by artificial intelligence discovery engine targeting enzymes involved in Neisseria gonorrhoeae peptidoglycan metabolism. Biological research, 57(1), 62.

Joshi RP, et al. (2023) AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. Journal of chemical information and modeling, 63(5), 1438.

Molyneaux K, et al. (2023) A novel binding pocket in the D2 domain of protein tyrosine phosphatase mu (PTPmu) guides AI screen to identify small molecules that modulate tumour cell adhesion, growth and migration. Journal of cellular and molecular medicine, 27(22), 3553.

Ogun OJ, et al. (2023) Molecular Structural Analysis of Porcine CMAH-Native Ligand Complex and High Throughput Virtual Screening to Identify Novel Inhibitors. Pathogens (Basel, Switzerland), 12(5).

Ghorayshian A, et al. (2023) Discovery of novel RAR? agonists using pharmacophore-based virtual screening, molecular docking, and molecular dynamics simulation studies. PloS one, 18(8), e0289046.

Lucia A, et al. (2023) Metabolic perturbation studies using a Nash Equilibrium model of liver machine perfusion: modeling oxidative stress and effect of glutathione supplementation. Frontiers in systems biology, 3, 1260315.

Ahmad S, et al. (2022) Carvacrol protects against carbonyl osmolyte-induced structural modifications and aggregation to serum albumin: Insights from physicochemical and molecular interaction studies. International journal of biological macromolecules, 213, 663.

Al-Rashedi NAM, et al. (2022) Prediction of potential inhibitors against SARS-CoV-2 endoribonuclease: RNA immunity sensing. Journal of biomolecular structure & dynamics, 40(11), 4879.

Ali F, et al. (2022) In silico analysis of AhyI protein and AI-1 inhibition using N-cis-octadec-9z-enoyl-l-homoserine lactone inhibitor in Aeromonas hydrophila. Microbial pathogenesis, 162, 105356.

Lucia A, et al. (2022) Modeling energy depletion in rat livers using Nash equilibrium metabolic pathway analysis. Scientific reports, 12(1), 3496.

Hamdy R, et al. (2021) Iterated Virtual Screening-Assisted Antiviral and Enzyme Inhibition Assays Reveal the Discovery of Novel Promising Anti-SARS-CoV-2 with Dual Activity. International journal of molecular sciences, 22(16).

Marzano S, et al. (2021) Targeting of Telomeric Repeat-Containing RNA G-Quadruplexes: From Screening to Biophysical and Biological Characterization of a New Hit Compound. International journal of molecular sciences, 22(19).

Ntie-Kang F, et al. (2021) Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. Journal of cheminformatics, 13(1), 64.