Resource Summary Report

Generated by RRID on Aug 15, 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 or information resource, data access protocol, 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: 20260815T042800+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 46 mentions in open access literature.

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

Jossart J, et al. (2026) Screening for novel chemical scaffolds targeting PCNA identifies the Hsp90alpha inhibitor SNX-2112. Current research in structural biology, 11, 100183.

Koh YC, et al. (2026) Oleic Acid-Esterified Octacosanol as a Functional Ingredient to Counter Obesity-Associated Lipid Dysregulation through PPAR-Targeted Regulation. Journal of agricultural and food chemistry, 74(3), 2761.

López-Cánovas DJ, et al. (2026) Buckwheat Flavonoids Modulate Inflammation in RAW 264.7 Macrophages at Physiologically Relevant Concentrations via the LPS/COX-2 Pathway. Journal of agricultural and food chemistry, 74(11), 9441.

Albahri G, et al. (2026) Anti-Inflammatory Activity of Mandragora autumnalis Ethanolic Extract: In Vitro and Cellular Mechanistic Insights. Pharmaceuticals (Basel, Switzerland), 19(3).

Chang N, et al. (2026) Identification of compounds that repress DUX4 expression in facioscapulohumeral muscular dystrophy. bioRxiv : the preprint server for biology.

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.

Li L, et al. (2025) Based on Network Pharmacology and Gut Microbiota to Explore the Underlying Mechanism of Huangqi Gegen Decoction for Treating Metabolic-Associated Fatty Liver Disease. Food science & nutrition, 13(11), e71133.

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.

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

Ferrara BT, et al. (2025) C-Terminal Analogues of Camostat Retain TMPRSS2 Protease Inhibition: New Synthetic Directions for Antiviral Repurposing of Guanidinium-Based Drugs in Respiratory Infections. International journal of molecular sciences, 26(14).

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.

Ortiz-González C, et al. (2025) Identification and Characterization of ERK2 Dimerization Inhibitors by Integrated In Silico and In Vitro Screening. International journal of molecular sciences, 26(23).

Aruge S, et al. (2024) Impact of MTHFD2 Expression in Bladder/Breast Cancer and Screening of Its Potential Inhibitor. ACS omega, 9(44), 44193.

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.

Schneider NO, et al. (2024) Synthesis and Evaluation of 5-(Heteroarylmethylene)hydantoins as Glycogen Synthase Kinase-3? Inhibitors. Pharmaceuticals (Basel, Switzerland), 17(5).

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.

Ilyas S, et al. (2024) Mechanistic Exploration of Smilax glabra Roxb. in Osteoarthritis: Insights from Network Pharmacology, Molecular Docking, and In Vitro Validation. Pharmaceuticals (Basel, Switzerland), 17(10).

Li LZ, et al. (2023) Molecular mechanism of the effect of Gegen Qinlian decoction on COVID-19 comorbid with diabetes mellitus based on network pharmacology and molecular docking: A review. Medicine, 102(44), e34683.