

Resource Summary Report

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Molecular Operating Environment

RRID:SCR_023932

Type: Tool

Proper Citation

Molecular Operating Environment (RRID:SCR_023932)

Resource Information

URL: <https://www.chemcomp.com/Products.htm>

Proper Citation: Molecular Operating Environment (RRID:SCR_023932)

Description: Drug discovery platform to integrate visualization, modeling and simulation in single package. Integrated computer aided molecular design platform.

Abbreviations: MOE

Synonyms: Chemical Computing Group ULC Molecular Operating Environment, Molecular Operating Environment (MOE)

Resource Type: software application, software resource

Keywords: Chemical Computing Group ULC., drug discovery, visualization, modeling, simulation, molecular design,

Availability: Restricted

Resource Name: Molecular Operating Environment

Resource ID: SCR_023932

Record Creation Time: 20230812T050218+0000

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Ratings and Alerts

No rating or validation information has been found for Molecular Operating Environment.

No alerts have been found for Molecular Operating Environment.

Data and Source Information

Usage and Citation Metrics

We found 27 mentions in open access literature.

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

Botelho FD, et al. (2026) PROTAC-Mediated Ternary Complex Stability with Ricin Toxin A: A Computational Perspective. ACS omega, 11(7), 11685.

Mishra SK, et al. (2026) Identification of enzymatically modified isoquercitrin as a therapeutic lead for myotonic dystrophy type 1. NAR molecular medicine, 3(1), ugag007.

Mellouk A, et al. (2026) Mechanism of trans-envelope bacterial polysaccharide secretion in Class-3 outer-membrane polysaccharide export (OPX) protein systems. Nature communications, 17(1), 732.

Osman ST, et al. (2026) Repurposing SGLT2 and DPP-4 inhibitors for mild cognitive impairment in type 2 diabetes mellitus: Insights from proteomics, target prediction and molecular docking. British journal of pharmacology, 183(10), 2533.

Shivkumar A, et al. (2025) Nootropic benzothiazoles promote dendritic spine formation by targeting fascin-1. The Journal of biological chemistry, 301(9), 110572.

Abdelazim AA, et al. (2025) In-silico screening and analysis of missense SNPs in human CYP3A4/5 affecting drug-enzyme interactions of FDA-approved COVID-19 antiviral drugs. Scientific reports, 15(1), 2153.

Elanany MM, et al. (2025) CCR4-NOT Transcription Complex Subunit 7 (CNOT7) Protein and Leukocyte-Associated Immunoglobulin-like Receptor-1 in Breast Cancer Progression: Clinical Mechanistic Insights and In Silico Therapeutic Potential. International journal of molecular sciences, 26(15).

Zhou K, et al. (2025) Nobiletin protected against hypertrophic cardiomyopathy via targeting PPAR γ . Frontiers in pharmacology, 16, 1628625.

Tangpeerachaikul A, et al. (2025) Zidesamtinib Selective Targeting of Diverse ROS1 Drug-Resistant Mutations. Molecular cancer therapeutics, 24(7), 1005.

Metwaly A, et al. (2024) In silico and in vitro evaluation of the anti-virulence potential of patuletin, a natural methoxy flavone, against Pseudomonas aeruginosa. PeerJ, 12, e16826.

Carr SC, et al. (2024) Two ubiquitous aldo-keto reductases in the genus Papaver support a patchwork model for morphine pathway evolution. Communications biology, 7(1), 1410.

Gao B, et al. (2024) The evolutionary novelty of insect defensins: from bacterial killing to toxin neutralization. Cellular and molecular life sciences : CMLS, 81(1), 230.

Samy A, et al. (2024) Network pharmacology, molecular docking, and dynamics analyses to predict the antiviral activity of ginger constituents against coronavirus infection. *Scientific reports*, 14(1), 12059.

Zheng YY, et al. (2024) Inosine-Induced Base Pairing Diversity during Reverse Transcription. *ACS chemical biology*, 19(2), 348.

Ahmad I, et al. (2024) Antioxidant activity, metabolic profiling, in-silico molecular docking and ADMET analysis of nano selenium treated sesame seed bioactive compounds as potential novel drug targets against cardiovascular disease related receptors. *Heliyon*, 10(7), e27909.

Abd El Maksoud EA, et al. (2024) Potential therapeutic biomolecules of hymenopteran venom against SARS-CoV-2 from Egyptian patients. *Scientific reports*, 14(1), 15363.

Wang C, et al. (2024) Isatin improves oligoasthenospermia caused by busulfan by regulating GSH/GPX4 axis to inhibit ferroptosis. *Frontiers in pharmacology*, 15, 1489956.

Saito H, et al. (2024) DMDA-PatA mediates RNA sequence-selective translation repression by anchoring eIF4A and DDX3 to GNG motifs. *Nature communications*, 15(1), 7418.

Shan J, et al. (2024) Comprehensive analysis of the potential biological significance of CCL5 in pan-cancer prognosis and immunotherapy. *Scientific reports*, 14(1), 22138.

Afsar T, et al. (2023) Truncated DNM1 variant underlines developmental delay and epileptic encephalopathy. *Frontiers in pediatrics*, 11, 1266376.