Resource Summary Report

Generated by NIF on Aug 13, 2026

MOE

RRID:SCR_014882
Type: Tool

Proper Citation

MOE (RRID:SCR_014882)

Resource Information

URL: http://www.chemcomp.com/MOE-Molecular_Operating_Environment.htm

Proper Citation: MOE (RRID:SCR_014882)

Description: Drug discovery software package which can be used in structure-based design, fragment-based design, pharmacophore discovery, medicinal chemistry, protein and antibody modelling, and molecular modeling and simulations. Each aspect of the software package has its own unique features: for example, features for structure-based design include active site detection, scaffold replacement, multi fragment search, and solvent analysis.

Resource Type: software resource

Keywords: drug discovery, software package, structure based design, fragment based design, pharmacophore, medicinal chemistry, protein modeling, antibody modeling, molecular modeling, molecular simulations

Resource Name: MOE

Resource ID: SCR_014882

License URLs: http://www.chemcomp.com/legal.htm

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260808T190036+0000

Ratings and Alerts

No rating or validation information has been found for MOE.

No alerts have been found for MOE.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 27 mentions in open access literature.

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

Yang Q, et al. (2026) Molecular mechanism of resistance to lonafarnib conferred by mutations in the cysteine-rich region of respiratory syncytial virus fusion glycoprotein and discovery of a lonafarnib-derived antiviral PROTAC. Journal of virology, 100(1), e0148725.

Huang Y, et al. (2026) SR-B1-Mediated Transplacental Transfer of Hydrophobic Toxicants Disrupts Fetal Development During Barriergenesis. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 13(23), e15742.

Unmuth L, et al. (2026) Antigen-directed single domain antibody-based TNFR1 agonists elicit preferential killing of HER2-overexpressing cancer cells. iScience, 29(4), 115327.

Powell T, et al. (2025) Determining T-cell receptor binding orientation and Peptide-HLA interactions using cross-linking mass spectrometry. The Journal of biological chemistry, 301(5), 108445.

Yan X, et al. (2025) Intra-condensate demixing of TDP-43 inside stress granules generates pathological aggregates. Cell, 188(15), 4123.

Sampathkumar P, et al. (2024) Targeted protein degradation systems to enhance Wnt signaling. eLife, 13.

Jiang H, et al. (2024) Targeting C21orf58 is a Novel Treatment Strategy of Hepatocellular Carcinoma by Disrupting the Formation of JAK2/C21orf58/STAT3 Complex. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 11(15), e2306623.

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.

Ray R, et al. (2024) Eliciting a single amino acid change by vaccination generates antibody protection against group 1 and group 2 influenza A viruses. Immunity, 57(5), 1141.

Dimitrov S, et al. (2023) Evaluation of Acute and Sub-Acute Toxicity, Oxidative Stress and Molecular Docking of Two Nitrofuranyl Amides as Promising Anti-Tuberculosis Agents. Biomolecules, 13(8).

Pelizzari-Raymundo D, et al. (2023) A novel IRE1 kinase inhibitor for adjuvant glioblastoma treatment. iScience, 26(5), 106687.

Fern??ndez-Quintero ML, et al. (2022) Paratope states in solution improve structure prediction and docking. Structure (London, England : 1993), 30(3), 430.

Angelova VT, et al. (2022) Development of New Antimycobacterial Sulfonyl Hydrazones and 4-Methyl-1,2,3-thiadiazole-Based Hydrazone Derivatives. Antibiotics (Basel, Switzerland), 11(5).

Helsen C, et al. (2022) Exploiting Ligand-binding Domain Dimerization for Development of Novel Androgen Receptor Inhibitors. Molecular cancer therapeutics, 21(12), 1823.

Dayal A, et al. (2021) Pore mutation N617D in the skeletal muscle DHPR blocks Ca2+ influx due to atypical high-affinity Ca2+ binding. eLife, 10.

Geeraerts SL, et al. (2021) Repurposing the Antidepressant Sertraline as SHMT Inhibitor to Suppress Serine/Glycine Synthesis-Addicted Breast Tumor Growth. Molecular cancer therapeutics, 20(1), 50.

Shaw J, et al. (2020) Rationally derived inhibitors of hepatitis C virus (HCV) p7 channel activity reveal prospect for bimodal antiviral therapy. eLife, 9.

Guthmiller JJ, et al. (2020) Polyreactive Broadly Neutralizing B cells Are Selected to Provide Defense against Pandemic Threat Influenza Viruses. Immunity, 53(6), 1230.

Zhao Y, et al. (2020) Identification of a G-Protein-Independent Activator of GIRK Channels. Cell reports, 31(11), 107770.

Tariq H, et al. (2019) Antioxidant, Antimicrobial, Cytotoxic, and Protein Kinase Inhibition Potential in Aloe vera L. BioMed research international, 2019, 6478187.