Resource Summary Report

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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: 20260725T190803+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 23 mentions in open access literature.

Listed below are recent publications. The full list is available at kravitz2 .

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.

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.

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.

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

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.

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

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

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.

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

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

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.

Dönerta? HM, et al. (2019) Identifying Potential Ageing-Modulating Drugs In Silico. Trends in endocrinology and metabolism: TEM, 30(2), 118.

Ding Y, et al. (2017) A haplotype in CFH family genes confers high risk of rare glomerular nephropathies. Scientific reports, 7(1), 6004.

Di Matteo A, et al. (2017) Structural investigation of nucleophosmin interaction with the tumor suppressor Fbw7?. Oncogenesis, 6(9), e379.

Temml V, et al. (2013) Interaction of Carthamus tinctorius lignan arctigenin with the binding site of tryptophan-degrading enzyme indoleamine 2,3-dioxygenase. FEBS open bio, 3, 450.