Resource Summary Report

Generated by NIF on Jul 30, 2026

ChEMBL

RRID:SCR_014042
Type: Tool

Proper Citation

ChEMBL (RRID:SCR_014042)

Resource Information

URL: https://www.ebi.ac.uk/chembl/

Proper Citation: ChEMBL (RRID:SCR_014042)

Description: Collection of bioactive drug-like small molecules that contains 2D structures, calculated properties and abstracted bioactivities. Used for drug discovery and chemical biology research. Clinical progress of new compounds is continuously integrated into the database.

Synonyms: ChEMBLdb, Chembl, ChEMBL Database

Resource Type: data or information resource, database

Defining Citation: PMID:21948594

Keywords: database, compound, data, bioassay, bioactive, molecule, drug, discovery

Funding: Wellcome Trust ;
EMBL Member States ;
Medicines for Malaria Ventures ;
EU Innovative Medicines Initiative ;
GSK ;
Syngenta ;
Pfizer

Availability: Public, Free, Freely available, Acknowledgement requested

Resource Name: ChEMBL

Resource ID: SCR_014042

Alternate IDs: r3d100010539

Alternate URLs: https://doi.org/10.17616/R3C320, https://doi.org/10.17616/R3C320

Record Creation Time: 20220129T080318+0000

Record Last Update: 20260729T044341+0000

Ratings and Alerts

No rating or validation information has been found for ChEMBL.

No alerts have been found for ChEMBL.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 2433 mentions in open access literature.

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

Zhang Q, et al. (2026) Synergistic effects of Akebia saponin D and Semaglutide on diabetic nephropathy and osteoporosis via the Klotho?p53 signaling axis. International journal of molecular medicine, 57(1).

Wang X, et al. (2025) Integrative machine learning and transcriptomic analysis identifies key molecular targets in MNPN-associated oral squamous cell carcinoma pathogenesis. Frontiers in bioinformatics, 5, 1664576.

Malarvizhi GL, et al. (2025) Rationally Designed Functionalized Phytochemical-Conjugated Fullerene Quantum Dots Inhibiting Viral Chaperone Activity and RNA-Dependent RNA Polymerase in Nipah Virus. FASEB journal : official publication of the Federation of American Societies for Experimental Biology, 39(15), e70890.

Puleo N, et al. (2025) Identification of a TNIK-CDK9 Axis as a Targetable Strategy for Platinum-Resistant Ovarian Cancer. Molecular cancer therapeutics, 24(4), 639.

Lyu TT, et al. (2025) The sodium-glucose co-transporter 2 inhibitor, empagliflozin, attenuates pulmonary vascular remodelling by inhibiting the phosphorylation of PDGF

receptor-?. British journal of pharmacology.

Fontenot R, et al. (2025) Clinical outcomes of DNA-damaging agents and DNA damage response inhibitors combinations in cancer: a data-driven review. Frontiers in oncology, 15, 1577468.

Hoque A, et al. (2025) Molecular Machine Learning Approach to Enantioselective C-H Bond Activation Reactions: From Generative AI to Experimental Validation. Chemical science, 16(29), 13276.

Hasib FMY, et al. (2025) Structural, Functional and Inhibitory Annotations of Lumpy Skin Disease Virus Hypothetical Protein LSDV004: An In-Silico Study. Veterinary medicine and science, 11(4), e70437.

Kaushik AC, et al. (2025) Integrative machine learning approach for identification of new molecular scaffold and prediction of inhibition responses in cancer cells using multi-omics data. Briefings in functional genomics, 24.

Pérez-Ribera M, et al. (2025) SingleFrag: a deep learning tool for MS/MS fragment and spectral prediction and metabolite annotation. Briefings in bioinformatics, 26(4).

Sankar J, et al. (2025) ML enhanced bioactivity prediction for angiotensin II receptor: A potential anti-hypertensive drug target. Scientific reports, 15(1), 25367.

Krasnov L, et al. (2025) BigSolDB 2.0, dataset of solubility values for organic compounds in different solvents at various temperatures. Scientific data, 12(1), 1236.

Wang J, et al. (2025) Integrated 4D label-free proteome and SUMOylated proteome in glioma uncover novel pathological mechanisms and pave the way for precision therapy. Cell insight, 4(4), 100253.

Campanelli L, et al. (2025) New insights into the molecular biology of Alzheimer's-like cerebral amyloidosis achieved through multi-omics approaches. PloS one, 20(9), e0330859.

Stephens DR, et al. (2025) A genome-scale drug discovery pipeline uncovers therapeutic targets and a unique p97 allosteric binding site in Schistosoma mansoni. Proceedings of the National Academy of Sciences of the United States of America, 122(35), e2505710122.

Guo DQ, et al. (2025) Analyzing the potential targets and mechanisms of liver damage induced by acetyl tributyl citrate plasticizer using network toxicology, molecular docking and in vitro experiments. Frontiers in pharmacology, 16, 1636576.

Qin Z, et al. (2025) Molecular mechanism of resveratrol in suppressing lung adenocarcinoma based on network pharmacology and molecular docking. Medicine, 104(36), e44489.

Gong H, et al. (2025) Exploring the causal relationship and molecular mechanisms between Methyl-4-hydroxybenzoic acid (MEP) and Alzheimer's disease: a mendelian randomization, multi-omics, and network toxicology approach. Toxicology research, 14(4), tfaf113.

Liu X, et al. (2025) DFusMol: predicting molecular properties based on dual-channel attention. Frontiers in molecular biosciences, 12, 1623620.

Duong Nguyen TT, et al. (2025) PGxDB: an interactive web-platform for pharmacogenomics research. Nucleic acids research, 53(D1), D1486.