Resource Summary Report

Generated by NIF on Aug 20, 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: database, data or information resource

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: 20260821T042916+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 3035 mentions in open access literature.

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

Wei S, et al. (2026) Risk assessment for hydrophobic disinfectants and antiseptics as contaminants in freshwater using risk quotient and network pharmacology approaches. iScience, 29(7), 116339.

Jiang M, et al. (2026) Analysis of the molecular mechanism underlying di(2-ethylhexyl) phthalate-induced bladder carcinogenesis via network toxicology and molecular docking approaches: An observational study. Medicine, 105(6), e47378.

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.

Ravegnini G, et al. (2026) Identification of MBT3T as a new effective therapeutic option in imatinib-resistant gastrointestinal stromal tumors (GISTs). Journal of experimental & clinical cancer research : CR, 45(1).

Baskaran SP, et al. (2026) sCentInDB: a database of essential oil chemical profiles of Indian medicinal plants. Molecular diversity, 30(1), 789.

Yang X, et al. (2026) Polyethylene terephthalate microplastics exposure enhances the risk of ulcerative colitis: insights from multiomics integration, machine learning, and molecular docking reveal intestinal toxicity mechanisms. International journal of surgery (London, England), 112(1), 735.

Jaladanki CK, et al. (2026) Integrating multi-structure covalent docking with machine-learning consensus scoring enhances potency ranking of human acetylcholinesterase inhibitors. Briefings in bioinformatics, 27(1).

Zuo Y, et al. (2026) FKSUDDAPre: A drug-disease association prediction framework based on F-TEST feature selection and AMDKSU resampling with interpretability analysis. PLoS computational biology, 22(2), e1013947.

Grewal S, et al. (2026) Computational strategies for unraveling insights from known inhibitors for further lead optimization: A case study on Celecoxib analogues. Scientific reports, 16(1), 6720.

Koyama T, et al. (2026) Chemical genomics language model toward reliable and explainable compound-protein interaction exploration. Journal of cheminformatics, 18(1), 29.

McKean EL, et al. (2026) Drug repurposing to combat multidrug-resistant hookworm. Biology open, 15(2).

Hu J, et al. (2026) Environmental toxicant ochratoxin A induces psoriasis based on network toxicology machine learning and molecular docking analyses. Scientific reports, 16(1), 6419.

Garai U, et al. (2026) Benchmarking deep learning models for predicting anticancer drug potency (IC50) with insights for medicinal chemists. Communications chemistry, 9(1).

Cui F, et al. (2026) Revealing the Action Mechanism of Exogenous Hydrogen Sulfide Intervention in Colorectal Cancer Pathogenesis Based on Multiomics Analysis and Experimental Validation. Human mutation, 2026, 5595505.

Ghamsary MS, et al. (2026) Interpretable machine learning rationalizes carbonic anhydrase inhibition via conformal and counterfactual prediction. Scientific reports, 16(1).

Zhang J, et al. (2026) The shared genetic architecture underlying the autoimmune and cardiovascular disease: a multivariate genome-wide analysis. Cardiovascular diabetology, 25(1), 44.

Kubincov?? A, et al. (2026) A simple compound prioritization method for drug discovery considering multi-target binding. Digital discovery, 5(3), 1204.

de Oliveira Borges JA, et al. (2026) Modifying Antibiotic Activity of Synthetic Thiadiazine Analogs Against MDR Bacteria and ADMET Analysis. ChemistryOpen, 15(4), e202500260.

Tsoukas E, et al. (2026) G.AI.A: An Integrated Machine-Learning Platform for Predicting Bioaccumulation and Ecotoxicity of Pharmaceuticals. Journal of chemical information and modeling, 66(3), 1414.

Melzi A, et al. (2026) Copper biosorption by Serratia plymuthica: crucial role of tightly bound extracellular polymeric substances in planktonic and biofilm systems. Biodegradation, 37(1), 25.