Resource Summary Report

Generated by SPARC SAWG on Sep 5, 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: EMBL Member States ;
EU Innovative Medicines Initiative ;
GSK ;
Medicines for Malaria Ventures ;
Pfizer ;
Syngenta ;
Wellcome Trust

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

Record Creation Time: 20220129T080318+0000

Record Last Update: 20260903T235232+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 SPARC SAWG .

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).

Zheng J, et al. (2026) PMADS: an integrated database of curated and proteomics-inferred associations between protein post-translational modifications and drug sensitivity. Nucleic

acids research, 54(D1), D1569.

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).

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.

Qiang H, et al. (2026) Language model-guided anticipation and discovery of mammalian metabolites. Nature, 651(8104), 211.

Yang X, et al. (2026) Novel metabolic adaptation driven by glycoside hydrolase family 25 protein contributes to increasing trimethoprim-sulfamethoxazole resistance in clinical human Brucella melitensis isolates in China. Antimicrobial agents and chemotherapy, 70(3), e0128425.

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

Liang Y, et al. (2026) Deciphering the mechanism of aristolochic acid I-driven hepatocellular carcinoma through integrated network toxicology and bioinformatics. Naunyn-Schmiedeberg's archives of pharmacology, 399(6), 7973.

Santura A, et al. (2026) Natural Product-like Fragments Unlock Novel Chemotypes for a Kinase Target?Exploring Options beyond the Flatland. Journal of chemical information and modeling, 66(4), 2249.

Ferolito BR, et al. (2026) Leveraging large-scale biobanks for therapeutic target discovery. HGG advances, 7(1), 100556.

Vazquez-Mendoza LH, et al. (2026) Multicomplex Pharmacophore Modeling of Estrogen Receptors Suggests the Probable Repurposing of Procaterol as an Antiproliferative Agent Against Breast Cancer Cells. International journal of molecular sciences, 27(1).

de Sousa DS, et al. (2026) Ligand and structure-based toxicological assessment of (thio)semicarbazones on cholinesterases. Journal of computer-aided molecular design, 40(1), 40.

Xie Z, et al. (2026) Integrative multi-omics and radiogenomic profiling decodes NNK-related tumor remodeling and prognostic stratification in pancreatic cancer. International journal of surgery (London, England), 112(4), 10062.

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

Fu X, et al. (2026) Rosuvastatin Upregulates RCOR1 to Repress C10ORF10 Transcription and Alleviate Oxidative Stress and Plaque Formation in Atherosclerosis. The Kaohsiung journal of medical sciences, 42(3), e70106.

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.