Resource Summary Report

Generated by NIF on May 14, 2025

ChEMBL

RRID:SCR_014042
Type: Tool

Proper Citation

ChEMBL (RRID:SCR_014042)

Resource Information

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

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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: service resource, data repository, data or information resource, database, storage service 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

Record Creation Time: 20220129T080318+0000

Record Last Update: 20250514T061642+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 2017 mentions in open access literature.

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

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

Geng J, et al. (2025) Network Mendelian randomisation analysis deciphers protein pathways linking type 2 diabetes and gastrointestinal disease. Diabetes, obesity & metabolism, 27(2), 866.

Murray JD, et al. (2025) Establishing a Pharmacoinformatics Repository of Approved Medicines: A Database to Support Drug Product Development. Molecular pharmaceutics, 22(1), 408.

Du H, et al. (2025) CovalentInDB 2.0: an updated comprehensive database for structure-based and ligand-based covalent inhibitor design and screening. Nucleic acids research, 53(D1), D1322.

Qian L, et al. (2025) Physiologically Based Pharmacokinetic Modeling of Cannabidiol, Delta-9-Tetrahydrocannabinol, and Their Metabolites in Healthy Adults After Administration by Multiple Routes. Clinical and translational science, 18(1), e70119.

Zheng H, et al. (2025) Dissecting Causal Relationships Between Antihypertensive Drug, Gut Microbiota, and Type 2 Diabetes Mellitus and Its Complications: A Mendelian Randomization Study. Journal of clinical hypertension (Greenwich, Conn.), 27(1), e14968.

Xu Y, et al. (2025) Exploring potential drug targets for SLE through Mendelian randomization

and network pharmacology. PloS one, 20(1), e0316481.

Lin TE, et al. (2025) Identification of a Potent CDK8 Inhibitor Using Structure-Based Virtual Screening. Journal of chemical information and modeling, 65(1), 378.

Viesi E, et al. (2025) APBIO: bioactive profiling of air pollutants through inferred bioactivity signatures and prediction of novel target interactions. Journal of cheminformatics, 17(1), 13.

Yamane F, et al. (2025) Identification of dequalinium as a potent inhibitor of human organic cation transporter 2 by machine learning based QSAR model. Scientific reports, 15(1), 2581.

Kore M, et al. (2025) Development and experimental validation of a machine learning model for the prediction of new antimalarials. BMC chemistry, 19(1), 28.

Liu S, et al. (2025) Multi-Omics Analysis for Identifying Cell-Type-Specific Druggable Targets in Alzheimer's Disease. medRxiv : the preprint server for health sciences.

Orlov AA, et al. (2025) From High Dimensions to Human Insight: Exploring Dimensionality Reduction for Chemical Space Visualization. Molecular informatics, 44(1), e202400265.

Li VOK, et al. (2025) DeepDrug as an expert guided and AI driven drug repurposing methodology for selecting the lead combination of drugs for Alzheimer's disease. Scientific reports, 15(1), 2093.

Yoshimori A, et al. (2025) Context-dependent similarity analysis of analogue series for structure-activity relationship transfer based on a concept from natural language processing. Journal of cheminformatics, 17(1), 5.

Li R, et al. (2025) Deep learning-based discovery of compounds for blood pressure lowering effects. Scientific reports, 15(1), 54.

DeCorte J, et al. (2025) Interpretable Deep-Learning pKa Prediction for Small Molecule Drugs via Atomic Sensitivity Analysis. Journal of chemical information and modeling, 65(1), 101.

Tang S, et al. (2025) PepTune: De Novo Generation of Therapeutic Peptides with Multi-Objective-Guided Discrete Diffusion. ArXiv.

Zhang M, et al. (2025) Topical transdermal administration of lenalidomide nanosuspensions-based hydrogels against melanoma: In vitro and in vivo studies. International journal of pharmaceutics: X, 9, 100316.

Yuan Y, et al. (2025) Serine/threonine protein kinase mediates rifampicin resistance in Brucella melitensis through interacting with ribosomal protein RpsD and affecting antioxidant capacity. mSystems, 10(1), e0110924.