Resource Summary Report

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ChemDB: The UC Irvine ChemDB

RRID:SCR_007594
Type: Tool

Proper Citation

ChemDB: The UC Irvine ChemDB (RRID:SCR_007594)

Resource Information

URL: http://cdb.ics.uci.edu

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Description: A database of general chemical information. The datasets are comprised of various available chemical datasets annotated with interesting properties to train and test machine-learning prediction and searching methods. Tools provided include ChemicalSearch, Virtual Chemical Space, Reaction Explorer, Datasets, and supplemental material. ChemicalSearch is a tool that allows users to find a chemical by basic criteria like molecular weight and predicted logP, or by the more abstract notion of structural similarity. Virtual Chemical Space is a tool which lets users interactively deconstruct target compounds into component precursors and reconstruct similar building-blocks into combinatorial libraries representing the virtual chemical space near the target compound. Reaction Explorer is a synthesis explorer and mechanism explorer. It provides an interactive system for learning and practicing reactions, syntheses and mechanisms in organic chemistry, with advanced support for the automatic generation of random problems, curved-arrow mechanism diagrams, and inquiry-based learning.

Synonyms: ChemDB

Resource Type: data or information resource, database

Keywords: chemical, chemical property, chemical reaction, chemistry, compound, organic chemistry, synthesis, software

Resource Name: ChemDB: The UC Irvine ChemDB

Resource ID: SCR_007594

Alternate IDs: nif-0000-02657

Record Creation Time: 20220129T080242+0000

Record Last Update: 20260806T054444+0000

Ratings and Alerts

No rating or validation information has been found for ChemDB: The UC Irvine ChemDB.

No alerts have been found for ChemDB: The UC Irvine ChemDB.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 14 mentions in open access literature.

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

Wan Z, et al. (2025) Applications of Artificial Intelligence in Drug Repurposing. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 12(14), e2411325.

Ittycheria SS, et al. (2025) Discovery of potential small molecule inhibitors against ??-hCG: an in silico study with in vitro validation. RSC advances, 15(25), 19561.

Chakraborty C, et al. (2024) The changing scenario of drug discovery using AI to deep learning: Recent advancement, success stories, collaborations, and challenges. Molecular therapy. Nucleic acids, 35(3), 102295.

Neal M, et al. (2023) Genome-scale metabolic modeling of the human gut bacterium Bacteroides fragilis strain 638R. PLoS computational biology, 19(10), e1011594.

Hashemi ZS, et al. (2021) In silico Approaches for the Design and Optimization of Interfering Peptides Against Protein-Protein Interactions. Frontiers in molecular biosciences, 8, 669431.

Tanoli Z, et al. (2021) Exploration of databases and methods supporting drug repurposing: a comprehensive survey. Briefings in bioinformatics, 22(2), 1656.

Carpio LE, et al. (2021) Computational strategies for the discovery of biological functions of health foods, nutraceuticals and cosmeceuticals: a review. Molecular diversity, 25(3), 1425.

McCoubrey LE, et al. (2021) Harnessing machine learning for development of microbiome therapeutics. Gut microbes, 13(1), 1.

Azam MW, et al. (2020) ACD: Antimicrobial chemotherapeutics database. PloS one, 15(6), e0235193.

Jackson SS, et al. (2020) A 35-Year Review of Pre-Clinical HIV Therapeutics Research Reported by NIH ChemDB: Influences of Target Discoveries, Drug Approvals and Research Funding. Journal of AIDS & clinical research, 11(11).

Awale M, et al. (2014) A multi-fingerprint browser for the ZINC database. Nucleic acids research, 42(Web Server issue), W234.

Zaman A, et al. (2012) Docking studies and network analyses reveal capacity of compounds from Kandelia rheedii to strengthen cellular immunity by interacting with host proteins during tuberculosis infection. Bioinformation, 8(21), 1012.

Nasr RJ, et al. (2009) Large scale study of multiple-molecule queries. Journal of cheminformatics, 1(1), 7.

Plested AJ, et al. (2009) Engineering a high-affinity allosteric binding site for divalent cations in kainate receptors. Neuropharmacology, 56(1), 114.