Resource Summary Report

Generated by dkNET on Apr 27, 2025

RDKit: Open-Source Cheminformatics Software

RRID:SCR_014274
Type: Tool

Proper Citation

RDKit: Open-Source Cheminformatics Software (RRID:SCR_014274)

Resource Information

URL: http://www.rdkit.org/

Proper Citation: RDKit: Open-Source Cheminformatics Software (RRID:SCR_014274)

Description: An open-source cheminformatics and machine-learning toolkit that is useable from Java or Python. It includes a collection of standard cheminformatics functionality for molecule I/O, substructure searching, chemical reactions, coordinate generation (2D or 3D), fingerprinting, etc., as well as a high-performance database cartridge for working with molecules using the PostgreSQL database. Documentation is available on the main website.

Synonyms: RDKit, RDKit Open-Source Cheminformatics and Machine Learning

Resource Type: software toolkit, software resource

Keywords: cheminformatics, machine learning, software toolkit, open source, python, c++, FASEB list

Funding:

Availability: Open source, Acknowledgement requested

Resource Name: RDKit: Open-Source Cheminformatics Software

Resource ID: SCR_014274

Alternate IDs: OMICS_14853

Alternate URLs: https://github.com/rdkit https://sourceforge.net/projects/rdkit/

Old URLs: https://sources.debian.org/src/python3-rdkit/

License: BSD, Creative Commons Attribution-ShareAlike 3.0 License

Record Creation Time: 20220129T080319+0000

Record Last Update: 20250426T060354+0000

Ratings and Alerts

No rating or validation information has been found for RDKit: Open-Source Cheminformatics Software.

No alerts have been found for RDKit: Open-Source Cheminformatics Software.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 390 mentions in open access literature.

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

Xiao M, et al. (2025) Drug molecular representations for drug response predictions: a comprehensive investigation via machine learning methods. Scientific reports, 15(1), 20.

Kretschmer F, et al. (2025) Coverage bias in small molecule machine learning. Nature communications, 16(1), 554.

Baei B, et al. (2025) Pharmacophore modeling and QSAR analysis of anti-HBV flavonols. PloS one, 20(1), e0316765.

Škuta C, et al. (2025) ECBD: European chemical biology database. Nucleic acids research, 53(D1), D1383.

Herrera LPT, et al. (2025) GPCRdb in 2025: adding odorant receptors, data mapper, structure similarity search and models of physiological ligand complexes. Nucleic acids research, 53(D1), D425.

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.

Ge J, et al. (2025) PROTAC-DB 3.0: an updated database of PROTACs with extended pharmacokinetic parameters. Nucleic acids research, 53(D1), D1510.

Yang QF, et al. (2025) G4LDB 3.0: a database for discovering and studying G-quadruplex and i-motif ligands. Nucleic acids research, 53(D1), D91.

Ziaikin E, et al. (2025) BitterDB: 2024 update on bitter ligands and taste receptors. Nucleic acids research, 53(D1), D1645.

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

Liu T, et al. (2025) BindingDB in 2024: a FAIR knowledgebase of protein-small molecule binding data. Nucleic acids research, 53(D1), D1633.

Gallo K, et al. (2024) Withdrawn 2.0-update on withdrawn drugs with pharmacovigilance data. Nucleic acids research, 52(D1), D1503.

Köck Z, et al. (2024) Cryo-EM structure of cell-free synthesized human histamine 2 receptor/Gs complex in nanodisc environment. Nature communications, 15(1), 1831.

Tang B, et al. (2024) Automated molecular structure segmentation from documents using ChemSAM. Journal of cheminformatics, 16(1), 29.

Zhou L, et al. (2024) Activating SRC/MAPK signaling via 5-HT1A receptor contributes to the effect of vilazodone on improving thrombocytopenia. eLife, 13.

Banerjee P, et al. (2024) ProTox 3.0: a webserver for the prediction of toxicity of chemicals. Nucleic acids research, 52(W1), W513.

Pahl A, et al. (2024) Illuminating Dark Chemical Matter Using the Cell Painting Assay. Journal of medicinal chemistry, 67(11), 8862.

Liu Y, et al. (2024) TransGEM: a molecule generation model based on Transformer with gene expression data. Bioinformatics (Oxford, England), 40(5).

Ugrani S, et al. (2024) Inhibitor design for TMPRSS2: insights from computational analysis of its backbone hydrogen bonds using a simple descriptor. European biophysics journal : EBJ, 53(1-2), 27.

Karwounopoulos J, et al. (2024) Insights and Challenges in Correcting Force Field Based Solvation Free Energies Using a Neural Network Potential. The journal of physical chemistry. B, 128(28), 6693.