Resource Summary Report

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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 resource, software toolkit

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

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/

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 312 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

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 (2024) Withdrawn 2.0-update on withdrawn drugs with pharmacovigilance data.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

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.

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.

Gu Y, et al. (2024) DBPP-Predictor: a novel strategy for prediction of chemical drug-likeness based on property profiles. Journal of cheminformatics, 16(1), 4.

Steshin IS, et al. (2024) Free Energy Barriers for Passive Drug Transport through the Mycobacterium tuberculosis Outer Membrane: A Molecular Dynamics Study. International journal of molecular sciences, 25(2).

Zhidkov ME, et al. (2024) Comparative Evaluation of the Antibacterial and Antitumor Activities of 9-Phenylfascaplysin and Its Analogs. Marine drugs, 22(2).

Tian Z, et al. (2024) PMhub 1.0: a comprehensive plant metabolome database. Nucleic acids research, 52(D1), D1579.

Wu J, et al. (2024) Large-scale comparison of machine learning methods for profiling prediction of kinase inhibitors. Journal of cheminformatics, 16(1), 13.

Soffer A, et al. (2024) MolOptimizer: A Molecular Optimization Toolkit for Fragment-Based Drug Design. Molecules (Basel, Switzerland), 29(1).

Manelfi C, et al. (2024) "DompeKeys": a set of novel substructure-based descriptors for efficient chemical space mapping, development and structural interpretation of machine learning models, and indexing of large databases. Journal of cheminformatics, 16(1), 21.

Sahu A, et al. (2023) Identification of core therapeutic targets for Monkeypox virus and repurposing potential of drugs against them: An in silico approach. Computers in biology and medicine, 161, 106971.

Fan C, et al. (2023) Characterizing RNA-binding ligands on structures, chemical information, binding affinity and drug-likeness. RNA biology, 20(1), 431.

Soares JX, et al. (2023) The Chemical Space of Marine Antibacterials: Diphenyl Ethers, Benzophenones, Xanthones, and Anthraquinones. Molecules (Basel, Switzerland), 28(10).

Park JE, et al. (2023) Specific inhibition of an anticancer target, polo-like kinase 1, by allosterically dismantling its mechanism of substrate recognition. Proceedings of the National Academy of Sciences of the United States of America, 120(35), e2305037120.

Abe K, et al. (2023) Deep learning driven de novo drug design based on gastric proton pump structures. Communications biology, 6(1), 956.

Shen C, et al. (2023) Molecular geometric deep learning. Cell reports methods, 3(11), 100621.

Devillers J, et al. (2023) Nonlinear SAR Modelling of Mosquito Repellents for Skin Application. Toxics, 11(10).

Abdel-Rehim A, et al. (2023) Protein-ligand binding affinity prediction exploiting sequence constituent homology. Bioinformatics (Oxford, England), 39(8).

Huang M, et al. (2023) In Silico Prediction of Metabolic Reaction Catalyzed by Human Aldehyde Oxidase. Metabolites, 13(3).

Avram S, et al. (2023) DrugCentral 2023 extends human clinical data and integrates veterinary drugs. Nucleic acids research, 51(D1), D1276.