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 toolkit, software resource

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/

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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 465 mentions in open access literature.

Listed below are recent publications. The full list is available at kravitz2 .

Zhang L, et al. (2026) Gut microbiome-mediated transformation of dietary phytonutrients is associated with health outcomes. Nature microbiology, 11(1), 94.

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

Hoba SN, et al. (2025) Parallel synthesis of 5'-amino-5'-deoxy-adenosine derivatives for focused chemical space exploration and their application as methyltransferase inhibitors. RSC medicinal chemistry.

Li X, et al. (2025) Irinotecan alleviates chemoresistance to anthracyclines through the inhibition of AARS1-mediated BLM lactylation and homologous recombination repair. Signal transduction and targeted therapy, 10(1), 214.

Wei Z, et al. (2025) Integrating network pharmacology, IPA, and molecular docking to reveal the anti-osteoporosis effects of EA and EB via the FAK pathway. Frontiers in pharmacology, 16, 1532665.

Zhang S, et al. (2025) Sequence-based virtual screening using transformers. Nature communications, 16(1), 6925.

Ladika G, et al. (2025) Exploring Postharvest Metabolic Shifts and NOX2 Inhibitory Potential in Strawberry Fruits and Leaves via Untargeted LC-MS/MS and Chemometric Analysis. Metabolites, 15(5).

Steigemann P, et al. (2025) Identification of NUV-244 as a PNPLA3 I148M degrading small molecule. iScience, 28(5), 112384.

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

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

Rocha S, et al. (2025) Flavonoids as Potential Modulators of Pancreatic Lipase Catalytic Activity. Pharmaceutics, 17(2).

Gadiya Y, et al. (2025) Predicting Antimicrobial Class Specificity of Small Molecules Using Machine Learning. Journal of chemical information and modeling, 65(5), 2416.

Scott T, et al. (2025) Drugit: crowd-sourcing molecular design of non-peptidic VHL binders. Nature communications, 16(1), 3548.

Guo Q, et al. (2025) UMAP-based clustering split for rigorous evaluation of AI models for virtual screening on cancer cell lines. Journal of cheminformatics, 17(1), 94.

Tivon B, et al. (2025) Computational Design of Lysine Targeting Covalent Binders Using Rosetta. Journal of chemical information and modeling, 65(11), 5612.

Amorim J, et al. (2025) In silico-driven identification of potent CDK9 inhibitors through bioisosteric replacement and multi-stage virtual screening. Scientific reports, 16(1), 4.

Dong R, et al. (2025) Exploring the repository of de novo-designed bifunctional antimicrobial peptides through deep learning. eLife, 13.

Cabrera M, et al. (2025) CADD-based discovery of novel oligomeric modulators of PKM2 with antitumor activity in aggressive human glioblastoma models. Heliyon, 11(3), e42238.

Jia X, et al. (2025) Application of Machine Learning and Mechanistic Modeling to Predict Intravenous Pharmacokinetic Profiles in Humans. Journal of medicinal chemistry, 68(7), 7737.

Nguyen ATN, et al. (2025) Structure-based discovery of positive allosteric modulators of the A1 adenosine receptor. Proceedings of the National Academy of Sciences of the United States of America, 122(28), e2421687122.