

Resource Summary Report

Generated by [PRECISE-TBI](#) on Jul 31, 2026

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/>

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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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Record Creation Time: 20220129T080319+0000

Record Last Update: 20260729T044326+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 465 mentions in open access literature.

Listed below are recent publications. The full list is available at [PRECISE-TBI](#) .

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

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.

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

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

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

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

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

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).

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

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.

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.

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.

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*.

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

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.

Nogueira VHR, et al. (2025) Fuzz Testing Molecular Representation Using Deep Variational Anomaly Generation. *Journal of chemical information and modeling*, 65(4), 1911.

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.

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

Huang C, et al. (2025) Modeling glycans with AlphaFold 3: capabilities, caveats, and limitations. *Glycobiology*, 35(10).