

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/>

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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 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/>

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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 618 mentions in open access literature.

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

van Tienen LM, et al. (2026) Systematic cysteine scanning identifies a druggable pocket in oncogenic KRAS. Cell chemical biology, 33(2), 241.

Sordyl D, et al. (2026) MODOMICS: a database of RNA modifications and related information. 2025 update and 20th anniversary. Nucleic acids research, 54(D1), D219.

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

Moretti S, et al. (2026) MetaNetX: a bridge between metabolic resources for enhanced curation and multi-omics data harmonization. Nucleic acids research, 54(D1), D617.

Zhan M, et al. (2026) UGTformer: a pretrained graph transformer model for predicting UDP-glucuronosyltransferase-mediated drug metabolism. Journal of cheminformatics, 18(1).

Liu D, et al. (2026) Efficient global accuracy estimation for protein complex structural models using multi-view representation learning. Cell reports methods, 6(2), 101312.

Natter Perdiguero A, et al. (2026) Genetic Incorporation of Diverse Noncanonical Amino Acids for Histidine Substitution. Journal of the American Chemical Society, 148(13), 13619.

Vichentijevikj I, et al. (2026) Prompt-to-Pill: Multi-Agent Drug Discovery and Clinical Simulation Pipeline. Bioinformatics advances, 6(1), vbaf323.

Beidja C, et al. (2026) Improving hERG Cardiotoxicity Prediction via SMILES Transformer, Molecular Fingerprints, and Layer-Wise Self-Adaptive Graph Attention Network. ACS omega, 11(11), 17484.

Lu Z, et al. (2026) AI-driven de novo design of BRAF inhibitors with enhanced binding affinity and optimized drug-likeness. PeerJ, 14, e20541.

Durai P, et al. (2026) ToxiVerse: A Public Platform for Chemical Toxicity Data Sharing and Customizable Predictive Modeling. *bioRxiv : the preprint server for biology*.

Wang K, et al. (2026) Hypergraph learning with multi-dimensional metabolite feature extractions and static-dynamic attention mechanisms to fill missing reactions in metabolic networks. *Briefings in bioinformatics*, 27(3).

K?rbo?a KK, et al. (2026) Structure-Based Virtual Screening of Plant-Derived Flavonoids as Putative GLUT9 Binders with Antioxidant Properties. *Molecules (Basel, Switzerland)*, 31(4).

Fischer S, et al. (2026) Hydrophobic tuning with non-canonical amino acids in a copper metalloenzyme. *Nature chemistry*, 18(7), 1269.

Ali A, et al. (2026) Elucidating the binding mechanism of *Caralluma tuberculata* metabolites with type 2 diabetes targets through molecular docking and dynamics simulations. *PloS one*, 21(4), e0343905.

Saurith-Coronell O, et al. (2026) Computational Identification of Potential Novel Allosteric IHF Inhibitors Using QSAR Modeling to Inhibit Plasmid-Mediated Antibiotic Resistance. *International journal of molecular sciences*, 27(6).

Antony P, et al. (2026) QSAR and scaffold-based optimization of HMGR inhibitors using cheminformatics and machine learning. *Frontiers in bioinformatics*, 6, 1764859.

Gutierrez-Rus LI, et al. (2026) Substrate scope of ancestral versus modern family-1 glycosidases. *Protein science : a publication of the Protein Society*, 35(7), e70676.

Lissner R, et al. (2026) A new role for lipoproteins LpqZ and FecB in orchestrating mycobacterial cell envelope biogenesis. *mBio*, 17(1), e0211925.

Zhu S, et al. (2026) MetabFlow: a comprehensive metabolic map for exogenous natural products. *Nucleic acids research*, 54(D1), D607.