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/

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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 Kravitz .

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.

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.

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

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

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).

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.

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

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

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

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.

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.

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

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).

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).

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.

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.

Amin SA, et al. (2026) KidneyTox_v1.0 enables explainable artificial intelligence prediction of nephrotoxicity in small molecules. Scientific reports, 16(1), 5099.

Zhu J, et al. (2026) MGTbind: a comprehensive database of molecular glue ternary interactome. Nucleic acids research, 54(D1), D1500.