**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/](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.

**Resource Type:** Resource, software resource, software toolkit

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

**Availability:** Open source, Acknowledgement requested

**Website Status:** Last checked up

**Resource Name:** RDKit: Open-Source Cheminformatics Software

**Resource ID:** SCR_014274

**Alternate URLs:** [https://github.com/rdkit](https://github.com/rdkit) [https://sourceforge.net/projects/rdkit/](https://sourceforge.net/projects/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 129 mentions in open access literature.

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


Armstrong DR, et al. (2020) PDBe: improved findability of macromolecular structure data in the PDB. Nucleic acids research, 48(D1), D335-D343.


Douguet D, et al. (2020) sensaas: Shape-based Alignment by Registration of Colored Point-


