

Resource Summary Report

Generated by [NIF](#) on Jul 31, 2026

CDK

RRID:SCR_023985

Type: Tool

Proper Citation

CDK (RRID:SCR_023985)

Resource Information

URL: <https://cdk.github.io/>

Proper Citation: CDK (RRID:SCR_023985)

Description: Open Source software modular Java libraries for cheminformatics.

Synonyms: cdk, Chemistry Development Kit

Resource Type: software toolkit, software resource, software library

Keywords: Java libraries, cheminformatics,

Availability: Free, Available for download, Freely available

Resource Name: CDK

Resource ID: SCR_023985

Alternate URLs: <https://sources.debian.org/src/cdk/>

License: LGPL-2.1

Record Creation Time: 20230824T050211+0000

Record Last Update: 20260731T043142+0000

Ratings and Alerts

No rating or validation information has been found for CDK.

No alerts have been found for CDK.

Data and Source Information

Usage and Citation Metrics

We found 7 mentions in open access literature.

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

Gadaleta D, et al. (2024) Comprehensive benchmarking of computational tools for predicting toxicokinetic and physicochemical properties of chemicals. Journal of cheminformatics, 16(1), 145.

Cerrato G, et al. (2024) AI-based classification of anticancer drugs reveals nucleolar condensation as a predictor of immunogenicity. Molecular cancer, 23(1), 275.

Harding SD, et al. (2024) The IUPHAR/BPS Guide to PHARMACOLOGY in 2024. Nucleic acids research, 52(D1), D1438.

Gadaleta D, et al. (2024) Quantitative structure-activity relationships of chemical bioactivity toward proteins associated with molecular initiating events of organ-specific toxicity. Journal of cheminformatics, 16(1), 122.

Priyadarsinee L, et al. (2024) Molecular Property Diagnostic Suite for COVID-19 (MPDSCoVID-19): an open-source disease-specific drug discovery portal. GigaByte (Hong Kong, China), 2024, gigabyte114.

McGibbon M, et al. (2023) From intuition to AI: evolution of small molecule representations in drug discovery. Briefings in bioinformatics, 25(1).

Emonts J, et al. (2023) An overview of descriptors to capture protein properties - Tools and perspectives in the context of QSAR modeling. Computational and structural biotechnology journal, 21, 3234.