Resource Summary Report

Generated by dkNET on Aug 17, 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 library, software resource

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: 20260817T040703+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

Source: SciCrunch Registry

Usage and Citation Metrics

We found 10 mentions in open access literature.

Listed below are recent publications. The full list is available at dkNET .

Galarion LH, et al. (2026) AntibioticDB: An Updated and Improved Open-Access Database for the Antibacterial Research and Development Community. ACS infectious diseases, 12(3), 1135.

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

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.

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

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.

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

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.

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

Delre P, et al. (2022) Ligand-based prediction of hERG-mediated cardiotoxicity based on the integration of different machine learning techniques. Frontiers in pharmacology, 13, 951083.

Venkatraman V, et al. (2022) Drugsniffer: An Open Source Workflow for Virtually Screening Billions of Molecules for Binding Affinity to Protein Targets. Frontiers in pharmacology, 13, 874746.