Resource Summary Report

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OrChem

RRID:SCR_008865

Type: Tool

Proper Citation

OrChem (RRID:SCR_008865)

Resource Information

URL: http://orchem.sourceforge.net

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Description: OrChem is an extension for the Oracle 11G database that adds registration and indexing of chemical structures to support fast substructure and similarity searching. The cheminformatics functionality is provided by the Chemistry Development Kit. OrChem provides similarity searching with response times in the order of seconds for databases with millions of compounds, depending on a given similarity cut-off. For substructure searching, it can make use of multiple processor cores on today"s powerful database servers to provide fast response times in equally large data sets. OrChem is an Oracle chemistry plug-in using the Chemistry Development Kit (CDK). The CDK is an open source Java library for Chemoinformatics and Bioinformatics. Or Chem is maintained by the chemoinformatics and metabolism team of the European Bioinformatics Institute. Oracle Data cartridges extend the capabilities of the Oracle server. For chemistry various commercial cartridges exist that facilitate searching and analyzing chemical data. OrChem also provides functionality like this, but is not a cartridge. It doesn't need Oracle's extensibility architecture because its Java components run as Java stored procedures inside the Oracle standard JVM (Aurora). OrChem is suitable for Oracle 11G and onwards. Starting with Oracle 11g release 1 (11.1) there is a just-in-time(JIT) compiler for Oracle JVM environment. A JIT compiler for Oracle JVM enables much faster execution because it manages the invalidation, recompilation, and storage of code without an external mechanism. This new Oracle feature makes Java classes perform better than before.

Abbreviations: OrChem

Resource Type: software resource, source code

Defining Citation: PMID:20298521

Keywords: oracle, chemistry, cdk, similarity search, chemical structure, cheminformatics,

bioinformatics, plugin

Funding:

Availability: GNU Lesser General Public License

Resource Name: OrChem

Resource ID: SCR_008865

Alternate IDs: nlx_149252

Record Creation Time: 20220129T080249+0000

Record Last Update: 20250419T055150+0000

Ratings and Alerts

No rating or validation information has been found for OrChem.

No alerts have been found for OrChem.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 1 mentions in open access literature.

Listed below are recent publications. The full list is available at <u>dkNET</u>.

Rijnbeek M, et al. (2009) OrChem - An open source chemistry search engine for Oracle(R). Journal of cheminformatics, 1(1), 17.