

FREE SOFTWARE SESSION PRESENTATION

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OrChem

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Background

Registration, indexing and searching of chemical structures in relational databases is one of the core areas of cheminformatics.

However, little detail has been published on the inner workings of search engines and their development has been mostly closed-source. We decided to develop an open source chemistry extension for Oracle, the de facto database platform in the commercial world.

Results

Here we present OrChem, 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.

Availability

OrChem is free software and can be redistributed and/or modified under the terms of the GNU Lesser General Public License as published by the Free Software Foundation. All software is available via <http://orchem.sourceforge.net>.

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