JChem PostgreSQL Cartridge History of Changes

October 29th, 2019: JChem PostgreSQL Cartridge 5.0

Improvements

- PostgreSQL 12 is the only supported PostgeSQL version from now on.
- Monitoring of index creation progress is enabled. Documentation
- Cache size decreased by 20% for target-type datasets.
- 15% indexing speed improvement.
- 20-50% search speedup for frequent queries
- Vacuum speed up for large tables.
- Cost estimation has been improved, joined queries run faster.

Bugfixes

- Nitrogen in marked stereo configuration matched unmarked chiral center.
- Small ring cis double bond stereo configurations were recognized as trans in case of trans perspective drawing in 3D.

September 23rd, 2019: JChem PostgreSQL Cartridge 4.4

Improvements

- JChem Service can be installed on other instance than the PostgreSQL database.
- Pseudo formula handling has been added to chemical terms .
- Allow NULL values in queries and molecular columns of tables.
- Standardize method added.

August 13th, 2019: JChem PostgreSQL Cartridge 4.3

No changes.

March 11th, 2019: JChem PostgreSQL Cartridge 4.2

Bugfixes

- Chemical term evaluation could cause OperationAbortedException because of concurrency problems.
- Initializing jchem-psql service sometimes failed because of missing log folder.

October 2nd, 2018: JChem PostgreSQL Cartridge 4.1

Improvements

- Enabled logical replication of indexed chemical data.

Bugfixes

- A memory leak during indexing is fixed.

May 10th, 2018: JChem PostgreSQL Cartridge 4.0

Improvements

- Default fingerprint size is reduced from 1024 to 512.
- Upgrade of Thrift to 0.11.0.

Bugfixes

- Copy of binary data was erroneous.
- Chemical terms returning a list of values (e.g. logD) did not return the values.
- Polymers with ambiguous aromatic rings in end groups could not be indexed.

December 7th, 2017: JChem PostgreSQL Cartridge 3.0

Improvements

- PostgreSQL 10 is supported from now on.
- Parallel sequential scan mode is supported.
- Indexing speed has been increased.
- Log4j logging is implemented. Documentation
- New cache parameters are provided for performance tuning of searches. Documentation

Bugfixes

- Peptide sequence file format was not handled correctly in the searches. From now on the 3-letter peptide format works in searches.
- Duplicate search could be slow when the target structure contained charged hydrogen atom.

September 20th, 2017: JChem PostgreSQL Cartridge 2.10

Improvements

- Speedup when query contains 5-membered ring with ambiguous aromaticity.

Bugfixes

- Wrong fingerprints were used after copying columns from one molecule subtype to another.

June 9th, 2017: JChem PostgreSQL Cartridge 2.9

Bugfixes

- Similarity search did not always return hits in the order of similarity.
- Molfiles with sgroups embedded in SRU groups were not handled.
- Missing hits could have been experienced in tautomer duplicate search in case of InChi files.
- jchem-psql service could crash if erroneous query structure was applied in a query.
- *Service jchem-psql stop* did not work on some new Ubuntu versions.
- Known issue present in version 2.8 has been solved.

May 17th, 2017: JChem PostgreSQL Cartridge 2.8 (version withdrawn)

Improvements

- Changing MapDB backend to MVStore approximately doubles the speed of the CREATE INDEX processes.

Bugfixes

- Similarity search did not always return hits in the order of similarity.
- Molfiles with sgroups embedded in SRU groups were not handled.
- Missing hits could have been experienced in tautomer duplicate search in case of InChi files.
- jchem-psql service could crash if erroneous query structure was applied in a query.
- *Service jchem-psql stop* did not work on some new Ubuntu versions.

Known issue

- The size of the index files under `/var/lib/jchem-psql/store/` have been hugely increased.

March 10th, 2017: JChem PostgreSQL Cartridge 2.7

Improvements

- Performance of select statements containing conditions for several rows or tables and including substructure search is improved by up to 20 times. Documentation

Bugfixes

- Missing hits could have been experienced in tautomer duplicate search in the case of molecules with aromatic rings.

February 1st, 2017: JChem PostgreSQL Cartridge 2.6

Improvements

- Quick relevance sorting of substructure search hits is provided by using a new chemical indextype SORTEDCHEMINDEX. Documentation

Bugfixes

- Querying with R-group structures did not work without Markush Enumeration license.

November 7th, 2016: JChem PostgreSQL Cartridge 2.5

Improvements

- New method providing fast similarity search has been implemented. Documentation

Bugfixes

- Molecules with small rings containing double bonds could miss duplicates when duplicate search was performed.
- Tautomer duplicate search could result false negative hits.

August 30th, 2016: JChem PostgreSQL Cartridge 2.4

Improvements

- Speed of insert into indexed table has been increased.

Bugfixes

- Index creation threw exception in case of molecules having deuterium atom.
- Tautomer duplicate search could result false positive hits.

August 2nd, 2016: JChem PostgreSQL Cartridge 2.3

Improvements

- Reaction search is supported from now on. Documentation
- Searching structures containing rings is sped-up.

June 28th, 2016: JChem PostgreSQL Cartridge 2.2

Improvements

- JChem PostgreSQL Cartridge is supported on a distributed PostgreSQL Citus database. Documentation

Bugfixes

- Duplicate search could result failing hits in tables indexed with `chemindex`.
- Misleading warning: `WARNING: molecule_ops.cpp:205 Cost estimation values were not calculated` has been fixed.

June 20th, 2016: JChem PostgreSQL Cartridge 2.1

Improvements

- PostgreSQL 9.5 is the only supported PostgeSQL version from now on. PostgreSQL 9.4 is only supported in JChem PostgreSQL Cartridge versions up to 2.0. Documentation

Bugfixes

- Tetrahedral stereo properties were incorrectly evaluated in case of structures where a substituent on the chiral center - e.g., on phosphorus - was connected by double bond.

May 26th, 2016: JChem PostgreSQL Cartridge 2.0

Improvements

- Searches with joined queries and with limit <n> conditions has been improved due to cost estimation and function mode search enhancements.
- Limitation of the number of jchem-psql service sessions is configurable by the administrator. Documentation

Bugfixes

- Searches combining more than three SELECT statements with logical operators could run into dead lock state.
- Relevance calculation threw exception in case of polymer and query structures.
- Relevance calculation could throw license exception even if the postgresql license was present.
- Custom standardizer.xml applied in type definition generated exception when more than one molecules were inserted in one statement.

February 10th, 2016: JChem PostgreSQL Cartridge 1.8

Improvements

- Relevance sorting possibility of the search hits is provided. Documentation
- Collecting invalid molecules during sdf import and (cx)smiles/(cx)smarts import is available.
- New function, `is_valid_molecule` , is introduced.
- Memory size requirement of searches in big tables has been decreased, and further performance tuning possibilities are provided. Documentation

October 20th, 2015: JChem PostgreSQL Cartridge 1.7

Improvements

- Speed of searches - compared to version 1.6 - has been increased.

Bugfixes

- Specified requirement regarding glibc version for running JChem PostgreSQL Cartridge is canceled.

October 7th, 2015: JChem PostgreSQL Cartridge 1.6

Improvements

- From now on, search engine in JChem PostgreSQL Cartridge works on vague bond level half. Previously, it worked on vague bond level 0.

Known issue

- glibc version 2.14 is needed to run JChem PostgreSQL Cartridge.

Bugfixes

- Tautomer substructure search could result false negative hits in case of aromatic structures.

- Index entries were overridden by each other in some cases resulting loss of hits.

August 14th, 2015: JChem PostgreSQL Cartridge 1.5 (version withdrawn)

July 27th, 2015: JChem PostgreSQL Cartridge 1.4

Improvements

- The use of chemical terms is implemented. Documentation
- The performance of searching with combined queries can be tuned by calibration. Documentation