

JChem Microservices History of Changes

August 3rd, 2019: JChem Microservices 19.18.0

No changes.

July 16th, 2019: JChem Microservices 19.17.0

No changes.

July 4th, 2019: JChem Microservices 19.16.0

No changes.

June 27th, 2019: JChem Microservices 19.15.0

Improvements

- Default timeout is lowered to 30 seconds.

June 24th, 2019: JChem Microservices 19.14.0

No changes.

June 17th, 2019: JChem Microservices 19.13.0

No changes.

June 3rd, 2019: JChem Microservices 19.12.0

Improvements

- DB module
 - New endpoint added: substructureHitCountEstimate

May 21st, 2019: JChem Microservices 19.11.0

Bugfixes

- Config server was not visible in Eureka.
- Calculations modul
 - API provided superfluous fields for structure input.

May 7th, 2019: JChem Microservices 19.10.0

Improvements

- Calculations modul has been extended by
 - Batch calculations

March 18th, 2019: JChem Microservices 19.8.0 (removed from the downloadables)

No changes.

Long Term Supported Release - July 30th, 2019: JChem Microservices 19.7.3 (Deuterium. 3)

Long Term Supported Release - June 3rd, 2019: JChem Microservices 19.7.2 (Deuterium. 2)

Long Term Supported Release - April 11th, 2019: JChem Microservices 19.7.1 (Deuterium. 1)

March 8th, 2019: JChem Microservices 19.7.0

No changes.

February 28th, 2019: JChem Microservices 19.6.0

Improvements

- New modul - Markush (Markush Enumeration) - has been implemented.
- Structure manipulation modul has been extended by
 - Extractor
 - Fragmenter
 - Molecule cleaner

Bugfixes

- Substructure search returned NaN if similarity value was requested but could not be calculated. From now on, fingerprint bit distance is returned instead of similarity value.

February 13th, 2019: JChem Microservices 19.4.0

Improvements

- Calculations modul has been extended by
 - Topology analyser
 - Polar surface area
 - Major microspecies

February 4th, 2019: JChem Microservices 19.3.0

Improvements

- Calculations modul has been extended by
 - HBDA
 - logD
 - pKa distribution
 - Canonical tautomerization
 - Dominant tautomerization

January 23rd, 2019: JChem Microservices 19.2.0

No changes.

January 11th, 2019: JChem Microservices 19.1.0

Improvements

- Calculations modul has been extended by
 - Elemental analysis
 - HLB
 - Isoelecztic point
 - logP
 - pKa
 - Solubility
 - Stereoisomer

December 14th, 2018: JChem Microservices 18.30.0

Improvements.

- New modul - Calculations - has been implemented