

# JChem Microservices History of Changes

## November 29th 2019: JChem Microservices 19.25.0

### Improvements

- DB modul
  - Duplicate search takes also higher order stereo information (like axial stereo information) into account.

## November 15th 2019: JChem Microservices 19.24.0

No changes.

## November 8th 2019: JChem Microservices 19.23.0

### Improvements

- New module - Structure Checker - has been implemented providing structure checker and fixer functionalities.

## October 21th 2019: JChem Microservices 19.22.0

### Improvements

- DB modul
  - Cache size decreased by 20%.
  - 15% import speed improvement.
  - 20-50% search speedup for frequent queries

### Bugfixes

- DB modul
  - 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.

**Long Term Supported Release - December 9th, 2019: JChem Microservices 19.21.2 (Europium.2)**

## **Long Term Supported Release - October 18th, 2019: JChem Microservices 19.21.1 (Europium.1)**

### **October 7th 2019: JChem Microservices 19.21.0**

#### **Improvements**

- DB module
  - Memory need decreases in case of datasets with explicit Hydrogens.

#### **Bugfixes**

- DB module
  - Sometimes searches did not stop if search wall time limit was reached.

### **September 18th 2019: JChem Microservices 19.20.0**

No changes.

### **September 2nd 2019: JChem Microservices 19.19.0**

#### **Improvements**

- DB module
  - Double bond stereo information can be ignored during substructure search.

### **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