

chem-bla-ics

Pimp my JavaDoc

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Keywords

Cdk, Javadoc, Literature

Copyright

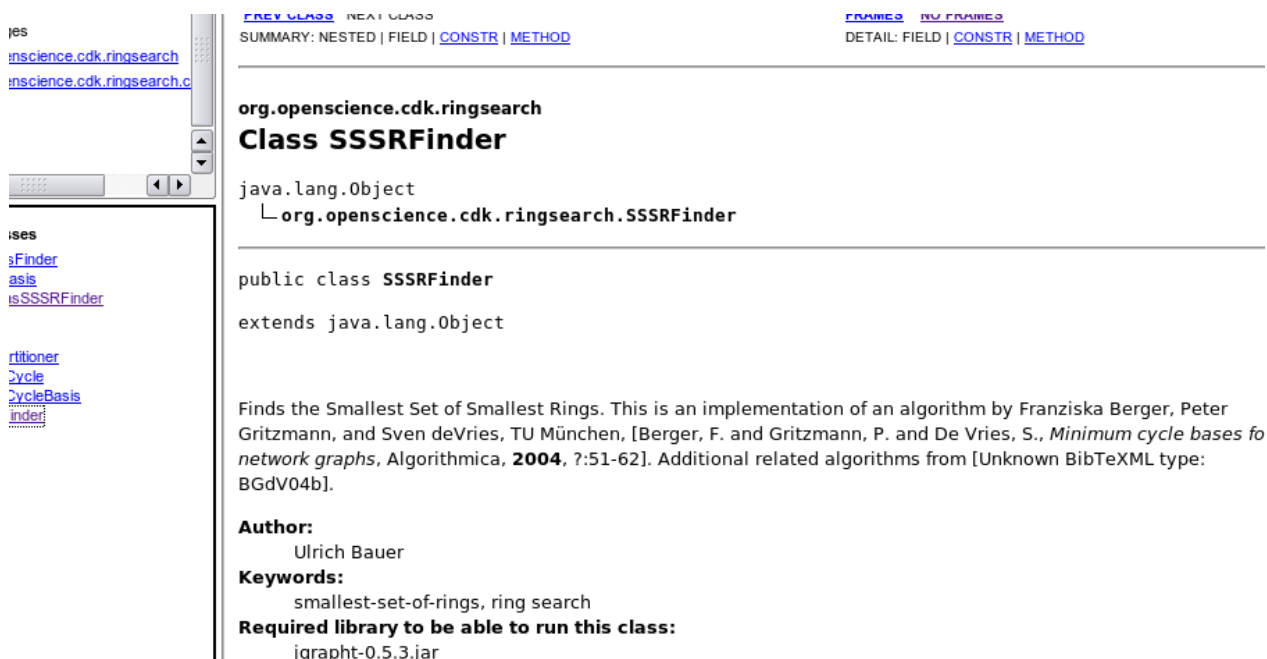
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Jörg's PhD book *Data Mining und Graph Mining auf molekularen Graphen - Chemoinformatik und molekulare Kodierungen für ADME/Tox-QSAR-Analysen* has a dump of the JavaDoc of the `GroupContributionPredictor` in `JOELib` (Figure 3.2, page 43). There are two nice things to the shown JavaDoc: 1. it has links to [Wikipedia](#); 2. it has a Further Reading section.

Now, the `CDK` already links to a bibliography for some time now. However, it would just give a BibTex key, and link to a webpage created from a `BibTeXML` file in which we store all references (`cdk/doc/refs/cheminf.bibx`). Putting the full citation inline makes the JavaDoc more informative, but I wanted to preserve the `@cdk.cite` mechanism we were using.

This weekend I hacked up a nice `CDKciteDoclet` that would read the `BibTeXML` file with `XOM`, and convert items to HTML to put into the pimped JavaDoc:



PREV CLASS NEXT CLASS
SUMMARY: NESTED | FIELD | CONSTR | METHOD
FRAMES NO FRAMES
DETAIL: FIELD | CONSTR | METHOD

org.openscience.cdk.ringsearch
Class SSSRFinder

java.lang.Object
└─org.openscience.cdk.ringsearch.SSSRFinder

```
public class SSSRFinder
extends java.lang.Object
```

Finds the Smallest Set of Smallest Rings. This is an implementation of an algorithm by Franziska Berger, Peter Gritzmann, and Sven deVries, TU München, [Berger, F. and Gritzmann, P. and De Vries, S., *Minimum cycle bases for network graphs*, *Algorithmica*, **2004**, 7:51-62]. Additional related algorithms from [Unknown BibTeXML type: BGdV04b].

Author:
Ulrich Bauer

Keywords:
smallest-set-of-rings, ring search

Required library to be able to run this class:
iqrapt-0.5.3.jar