Pimp my JavaDoc

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Keywords

Cdk, Javadoc, Literature

Abstract

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.
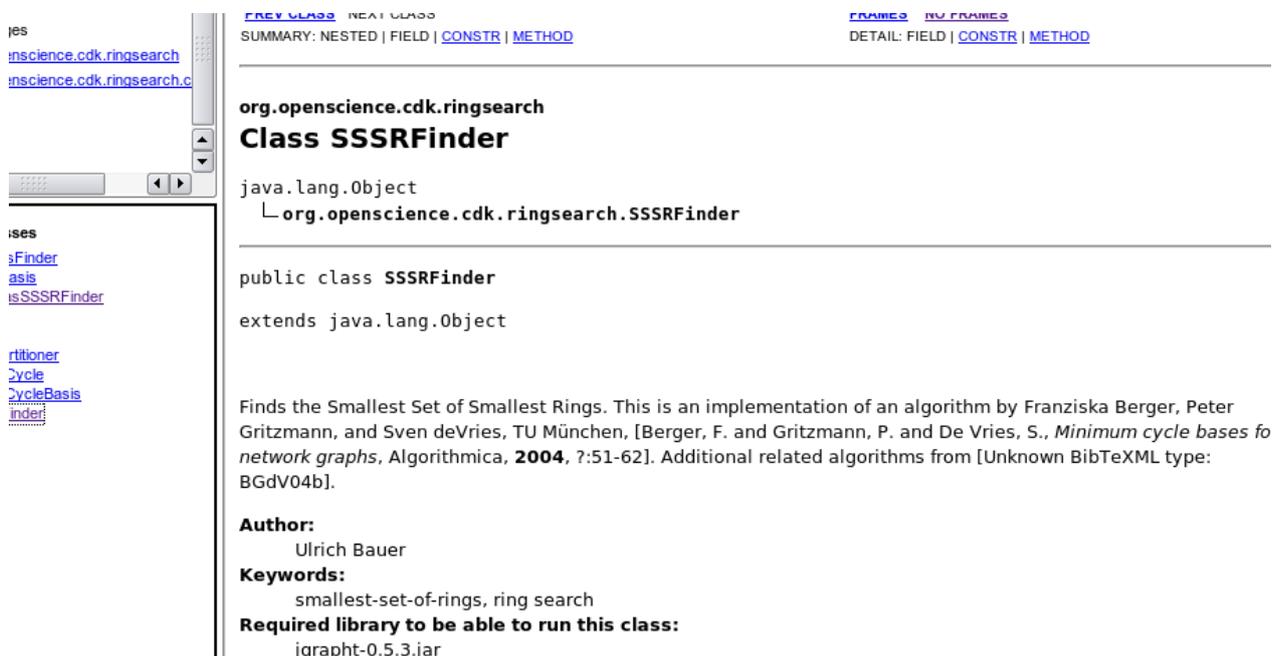
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Jörg's PhD book *Data Mining und Graph Mining auf molekularen Graphen - Chemoinformatik und molekulare Kodierungen für ADME/Tox-QSAR-Analysen* has a dump of the JavaDoc of the `GroupContributionPredictor` in JOELib (Figure 3.2, page 43). There are 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: