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Recent Developments of the Chemistry Development Kit

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Keywords

Cdk, Cheminf, Qsar

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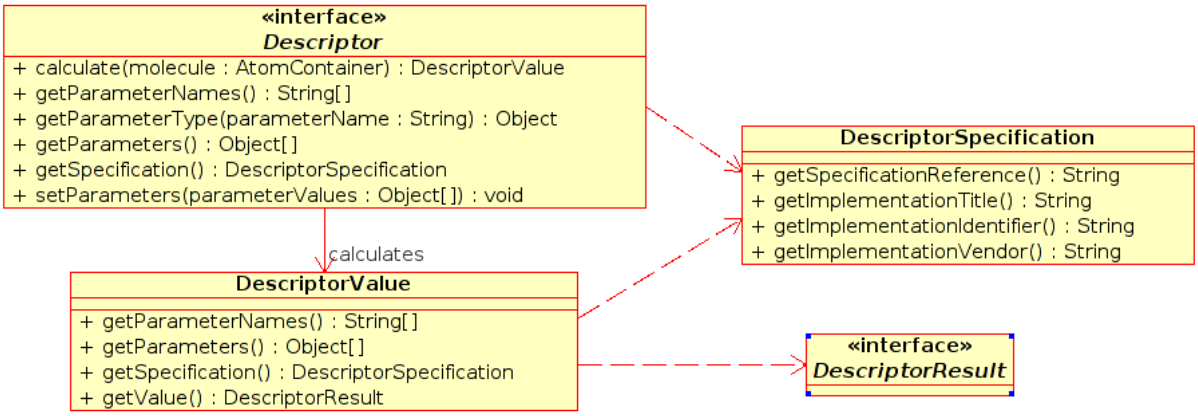
Recent Developments of the Chemistry Development Kit (CDK) - *An Open-Source Java Library for Chemo- and Bioinformatics* (green OA) discusses (reasonably) recent additions to the CDK. It appeared in issue 17 of this years Current Pharmaceutical Design volume, after being too long in the queue after being accepted; but I am happy that it is out now.

The article discusses CDK's QSAR capabilities (the class designs and an overview of provided descriptors), the 3D model builder (see also C. Hoppe, CDK News, 1(2):4-5) and and the interface to the statistical software R (see also CDK News, vol.2, issue 1). The article is part of a small special issue on Computational Applications in Medicinal Chemistry.

CDK's QSAR package comes with one main requirement: **the outcome of QSAR descriptor calculations must be reproducable**. *"Science must be reproducable"*; I'm sure someone once said this :) Therefore, each QSAR descriptor has a specification pointing the a unique algorithm found in an ontology (see diagram below). This QSAR descriptor ontology is maintained by the qsar.sf.net project, which is project independent, and even welcomes proprietary programs to discuss interoperability.



And calculated descriptors are explicitely linked to this specification again, though it is up to the user to do with this what he wants:

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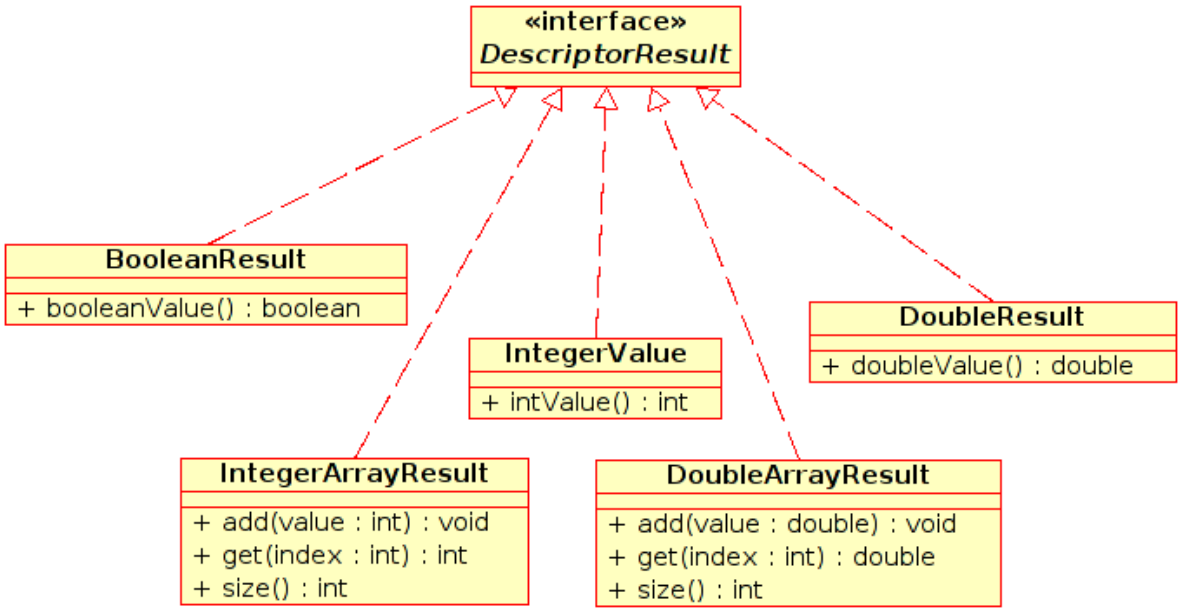

Note that code has evolved since this publication, so class, interface and method names may have changed a bit.