chem-bla-ics

Molecular QSAR descriptors in the CDK

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Abstract
Rajarshi has patched trunk last night with his work to address a few practical issues in the molecular descriptor module of the CDK (and I peer reviewed this work yesterday). One major change is that the IMolecularDescriptor calculate() method no longer throws an Exception, but returns Double.NaN instead. The Exception is stored in the DescriptorValue for convenience.

Rajarshi has patched trunk last night with his work to address a few practical issues in the molecular descriptor module of the CDK (and I peer reviewed this work yesterday). One major change is that the IMolecularDescriptor `calculate()` method no longer throws an `Exception`, but returns `Double.NaN` instead. The Exception is stored in the `DescriptorValue` for convenience. This simplifies the QSAR descriptor calculation considerably, and, importantly, makes it more robust to the input. Though only by propagating errors into descriptor matrix. *Just make sure your molecular structures have explicit hydrogens and 3D coordinates, and you're fine.*

Anyway, Rajarshi also added a new page to CDK Nightly to list the available descriptors:

CDK Descriptor Summary (2008-07-23)

A summary of the currently available descriptors listing the descriptor name and the names of the individual values. Follow the links to get a more detailed description of the descriptor and any parameters that it may take.

Quick links: Molecular Bond Atom

Molecular Descriptors

Descriptor	*Definition*	*Values*
ALOGP	Calculates atom additive logP and molar refractivity values as described by Ghose and Crippen and	ALogP ALogp2 AMR
APol	Descriptor that calculates the sum of the atomic polarizabilities (including implicit hydrogens).	apol
AminoAcidCount	Returns the number of amino acids found in the system	nA nR nN nD nC nF nQ nE nG nH