Subject: Re: translation of the idcodes
Posted by thomas on Fri, 23 Oct 2020 13:05:22 GMT
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The idcode is a canonical very compact text representation of a molecule.
Its creation requires ring and aromaticity perception and much more complicated, complete enhanced stereo perception. It also includes sub-structure query features and this way is somewhat comparable to an isomeric SMARTS. The best way for another software package to create or read it, is to use the original source code, which is available for anybody and any purpose in the OpenChemLib project on Github.

LigandScout is an example of a commercial software package that can read idcodes and DataWarrior conformer files.

Whether OpenBabel will support OpenChemLib idcodes once, is not in our hands.

Thomas