Subject: Incomplete SMILES related to double bonds
Posted by Christoph on Tue, 30 May 2017 12:26:07 GMT
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Hello,

the SMILES which DataWarrior creates do not seem to be specific enough. E.g. for double bonds it does not encode the direction of the adjacent bonds.

See also point 3.3.2 in www.daylight.com/dayhtml/doc/theory/theory.smiles.html

This is a very important problem, and for me also urgent because on the SMILES all my work on the molecules is based and nearly every compound has double bonds.

Best wishes,
Christoph

Subject: Re: Incomplete SMILES related to double bonds
Posted by thomas on Fri, 02 Jun 2017 20:24:09 GMT
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Hello Christoph,

this is not really a bug. The problem is that DataWarrior generates a normal SMILES, not an 'isomeric SMILES'. Only the latter contains the stereo configuration of double bonds and tetrahedral center. The SMILES generation is a really historic functionality and was never enhanced to the isomeric level, because at Actelion we never had the need for it, because even isomeric SMILES don't support the enhanced stereo representation that we use as internal standard. However, since the external world uses SMILES rather often and in triggered by the need to correctly interpret Wikipedia compounds I have enhanced the SMILES interpreter to fully support isomeric SMILES. Enhancing also the SMILES export accordingly is an obvious thing to do. I cannot promise anything, but I will look into the matter...

Thomas

Subject: Re: Incomplete SMILES related to double bonds
Posted by Christoph on Sun, 04 Jun 2017 11:39:28 GMT
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Hi Thomas,

Thank you very much for your answer and looking into this issue.

Saving the structures in DataWarrior in the SDF-format (2D) does preserve the stereocenters, is this correct? Then a workaround in the meantime until DataWarrior is updated would be to save

the compounds as SDF-File and then convert it with obabel to obtain isomeric SMILES.

Best wishes,
Christoph

Subject: Re: Incomplete SMILES related to double bonds
Posted by Christoph on Fri, 09 Jun 2017 12:25:00 GMT
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Short Update: I have tested this idea with a few compounds, it seems to work.