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