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