

Wikidata script for SMILES, SMARTS, and CXSMILES depiction

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Keywords

Wikidata, Cdk, Cxsmiles, Dagstuhl, Smiles

Abstract

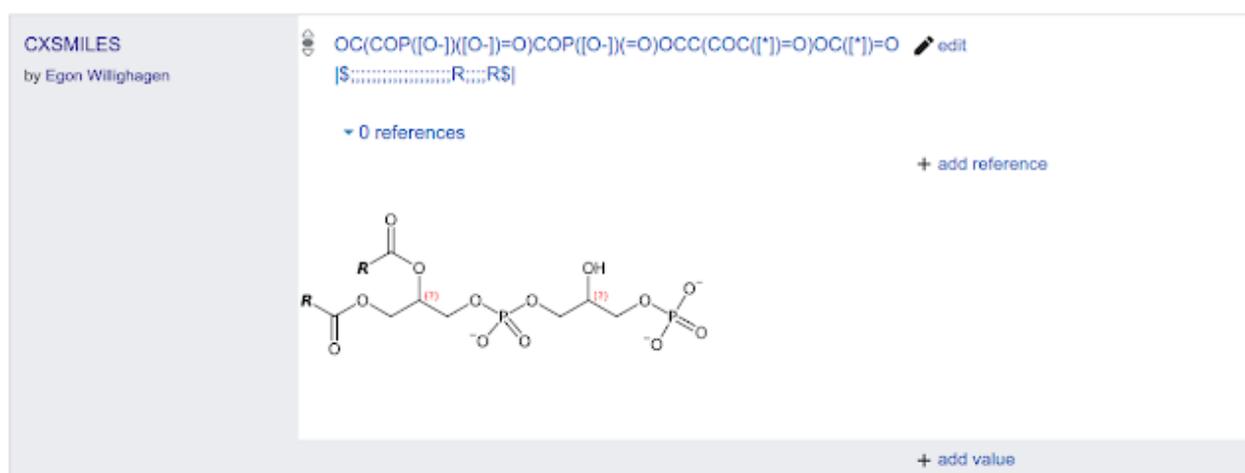
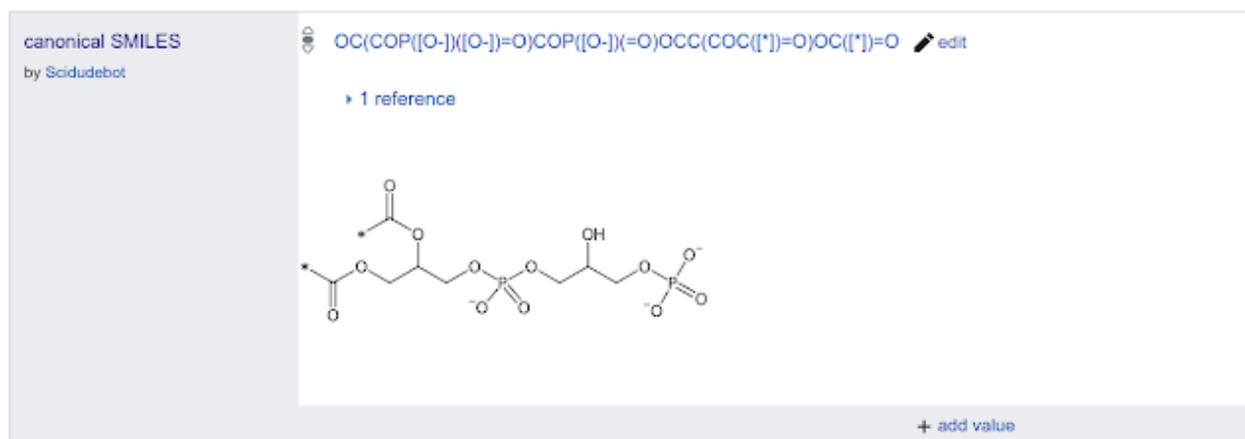
In August I reported about 2D depiction of (CX)SMILES in Wikidata via linkouts (going back to 2017). Based on a script by Magnus Manske, I wrote a Wikidata gadget that uses the same CDK Depict (VHP4Safety mirror) to depict the 2D structure in Wikidata itself:

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chem-bla-ics

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Note the depiction of the undefined (CIP) stereochemistry on two atoms. Thanks to [Adriano](#) and [John](#) for working that out.

More about CXSMILES in Wikidata in [this Dagstuhl meeting results write up](#).