

# Wikidata script for SMILES, SMARTS, and CXSMILES depiction

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## Keywords

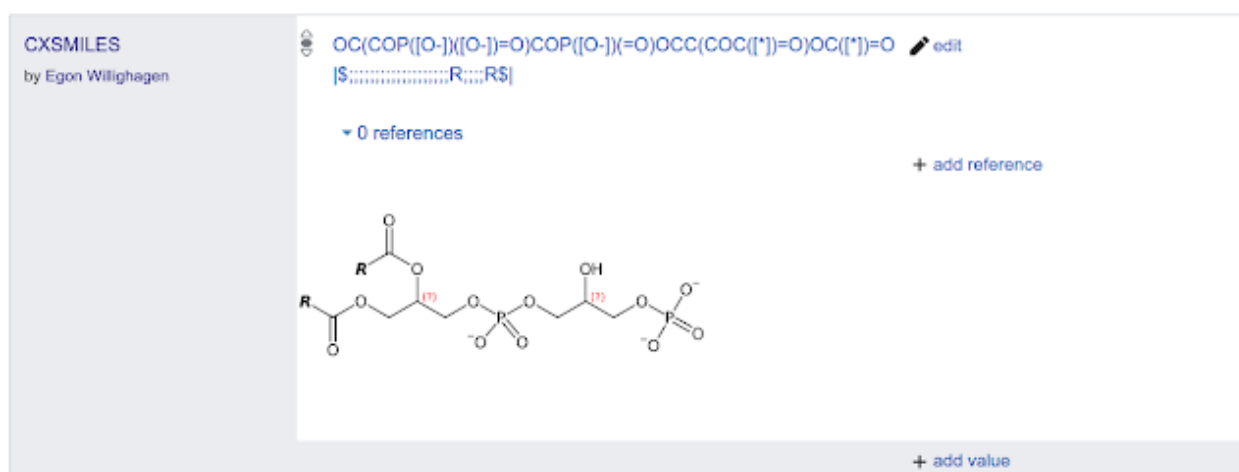
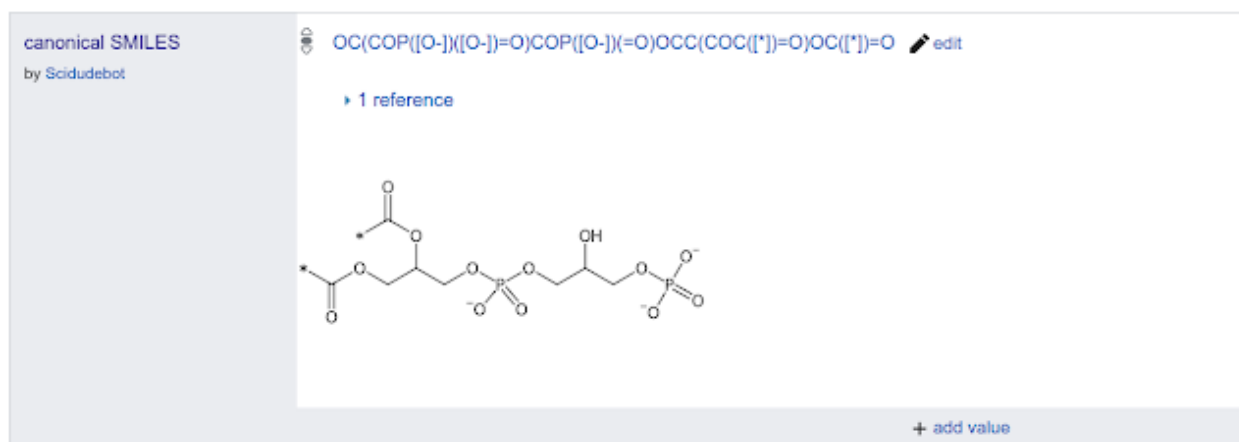
Wikidata, Cdk, Cxsmiles, Dagstuhl, Smiles

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## chem-bla-ics

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:



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](#).