chem-bla-ics

Wikidata script for SMILES, SMARTS, and CXSMILES depiction

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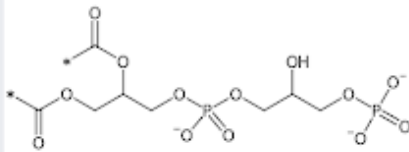## Keywords

Wikidata, Cdk, Cxsmiles, Dagstuhl, Smiles

Copyright

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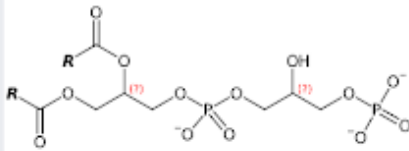
Note the depiction of the undefined (CIP) stereochemistry on two atoms. Thanks to Adriano and John for working that out.

More about CXSMILES in Wikidata in this Dagstuhl meeting results write up.