
Subject: Re: Stereoisomers conformer generation and Inchikeys

Posted by [nbehrnd](#) on Tue, 14 Sep 2021 07:01:37 GMT

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An improvement is on the way. Based on a separate exchange, Thomas mentioned the assignments of InChI/InChiKey provided by DataWarrior are revised and, where necessary, are going to be corrected.

For the moment, alternatives may be the online conversion of individual of structures,[1] or one of the reference implementations distributed by the InChI Trust[2] which, by a command like

```
./inchi-1 test.sdf -AuxNone -Tabbed -Key
```

write InChI and InChiKeys of structures in test.sdf into a tabulator separated .txt file.

Norwid

[1], examples

http://www.cheminfo.org/Chemistry/Cheminformatics/Generate_InChI/index.html

<https://chemdrawdirect.perkinelmer.cloud/js/sample/index.htm> l# (Structure -> Get InChI)

[2] <https://www.inchi-trust.org/downloads/>
