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Subject: Re: Stereoisomers conformer generation and Inchikeys

Posted by [thomas](#) on Mon, 20 Sep 2021 22:39:41 GMT

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Many thanks to Norwid and Mattia for pointing out the discrepancies of created Inchis and Inchi-Keys with the ones produced by OpenBabel and also for providing a test data set. The issues were mainly caused by a bug in the conversion of the tetrahedral stereo configuration for the jni-inchi (1.0.3) library from 2010 that DataWarrior used to create inchis. During the recent days DataWarrior was updated to using a new open-source project jna-inchi from Daniel Lowe, which is based on the inchi-trust code 1.0.6 from 2020. The stereo issues have also been fixed. The current development update contains all fixes and a new jniinchi.jar (which actually is the jnainchi.jar). The dev update link appears on the download page after checking the 'Read and Understood' checkbox.

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