
Subject: Re: Stereoisomers conformer generation and Inchikeys

Posted by [nbehrnd](#) on Sun, 31 Oct 2021 19:03:32 GMT

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It should be noted that tautomers share standard an InChI and standard InChIKey in common.

One FAQ by the InChI trust (though by 2012-05-12) explains this by

«different tautomers have the same connectivity/hydrogen layer»[1]

With the current version of InChI executables (1.06, December 2020), it is possible e.g., to add what InChI defines as «Fixed H layer», which offers to discern the tautomers. However, currently this may yield a non-standard InChI (i.e., the string does not start with InChI=1S/, but InChI=1/). Thus, their use in a search in databases[2] may refer to more than one chemical entity.

Norwid

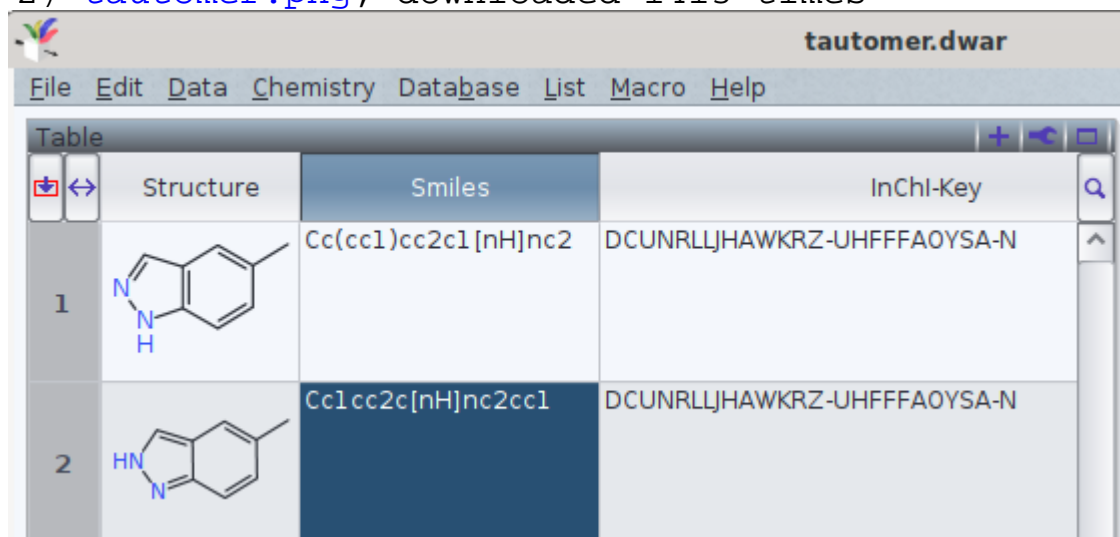
[1] <https://www.inchi-trust.org/technical-faq-2/>

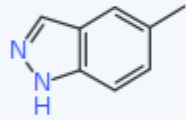
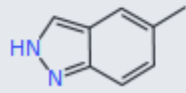
[2] «Many InChIs and quite some feat» by Warr, W.A., J. Comput. Aided Mol. Des., 2015, 29: 681. <https://doi.org/10.1007/s10822-015-9854-3>

File Attachments

1) [tautomer.dwar](#), downloaded 606 times

2) [tautomer.png](#), downloaded 1413 times



	Structure	Smiles	InChI-Key
1		<chem>Cc(cc1)cc2c1[nH]nc2</chem>	DCUNRLLJHAWKRZ-UHFFFAOYSA-N
2		<chem>Cc1cc2c[nH]nc2cc1</chem>	DCUNRLLJHAWKRZ-UHFFFAOYSA-N