

InChIKey collision: the DIY copy/pastables

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Keywords

Inchi

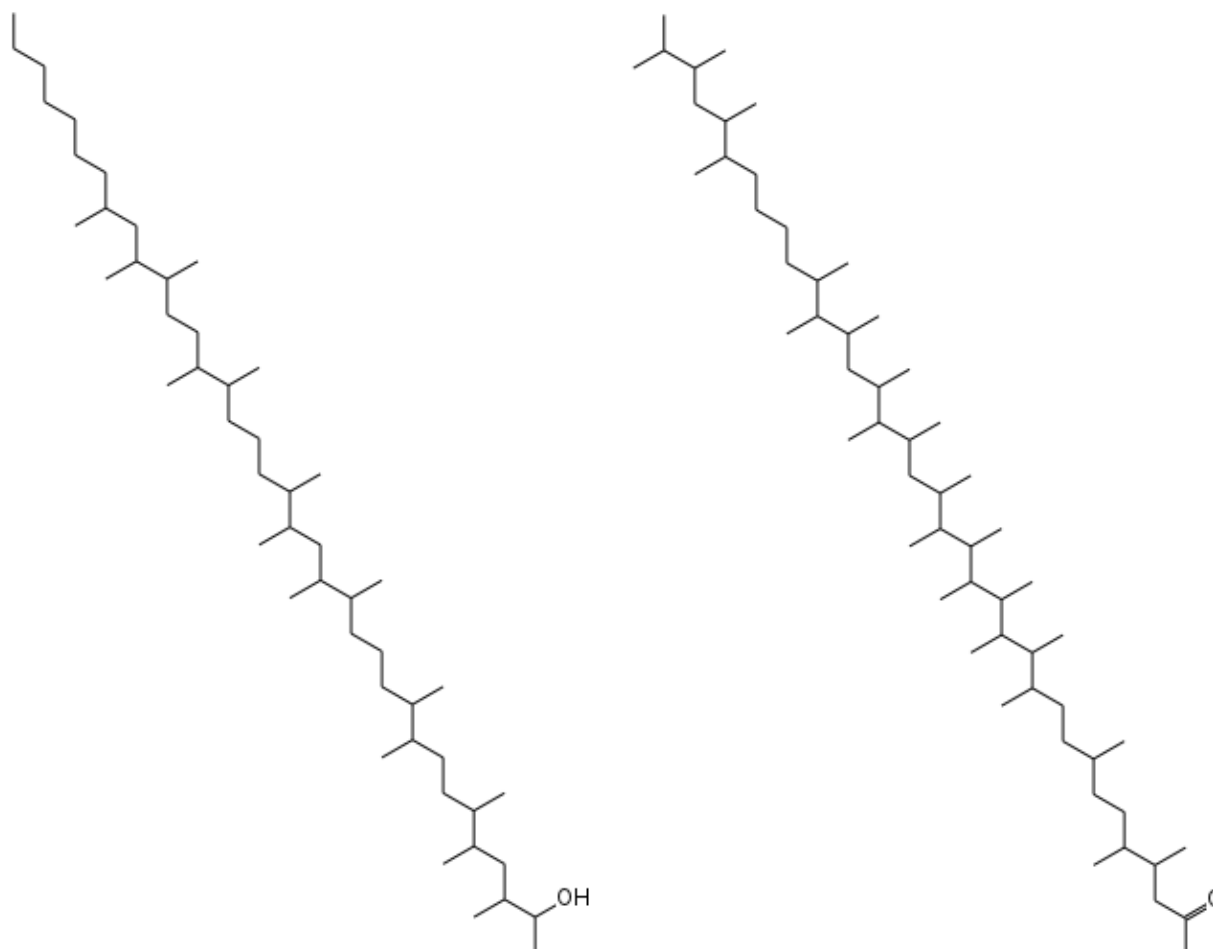
Abstract

About two weeks ago, the ChemConnector blog reported an InChIKey collision detected by Prof. Goodman . Unlike the previous collision, this one was based solely on the graph and not on stereochemistry.

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About two weeks ago, the ChemConnector blog [reported an InChIKey collosion](#) detected by [Prof. Goodman](#). Unlike the previous collision, this one was based solely on the graph and not on stereochemistry. The two molecules both have the InChIKey OCPAUTFLLNMYSX-UHFFFAOYSA-N:



The compounds are really different, the molecular formulas are $C_{50}H_{102}O$ and $C_{57}H_{114}O$ respectively. The SMILESes are

[OC(C)C(C)CC(C)C(C)CCC(C)C(C)CCCC(C)C(C)CC(C)C(C)CCCC(C)C(C)CCC(C)C(C)CC(C)CCCCCCC]

{.chem:smiles} and

[O=C(C)CC(C)C(C)CCC(C)CCC(C)C(C)C(C)C(C)C(C)C(C)C(C)CC(C)C(C)C(C)CC(C)C(C)C(C)CCCC(C)C(C)CC(C)C(C)C]

{.chem:smiles}. The IUPAC names are useful to have as copy/pastables too (e.g. with the [OPSIN](#)-based ‘[Molecule from IUPAC name](#)’-wizard in [Bioclipse](#) 2.5, which has been updated to the latest OPSIN version this week): 3,5,6,9,10,14,15,17,18,22,23,26,27,29-tetradecamethylhexatriacontan-2-ol and 4,5,8,11,12,13,14,15,16,17,18,20,21,22,24,25,26,31,32,34,35-henicosamethylhexatriacontan-2-one.

I am adding these structures to the [pharmbio.org course book](#) and the matching Bioclipse plugin this weekend.