

InChIKey collision: the DIY copy/pastables

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Keywords

Inchi

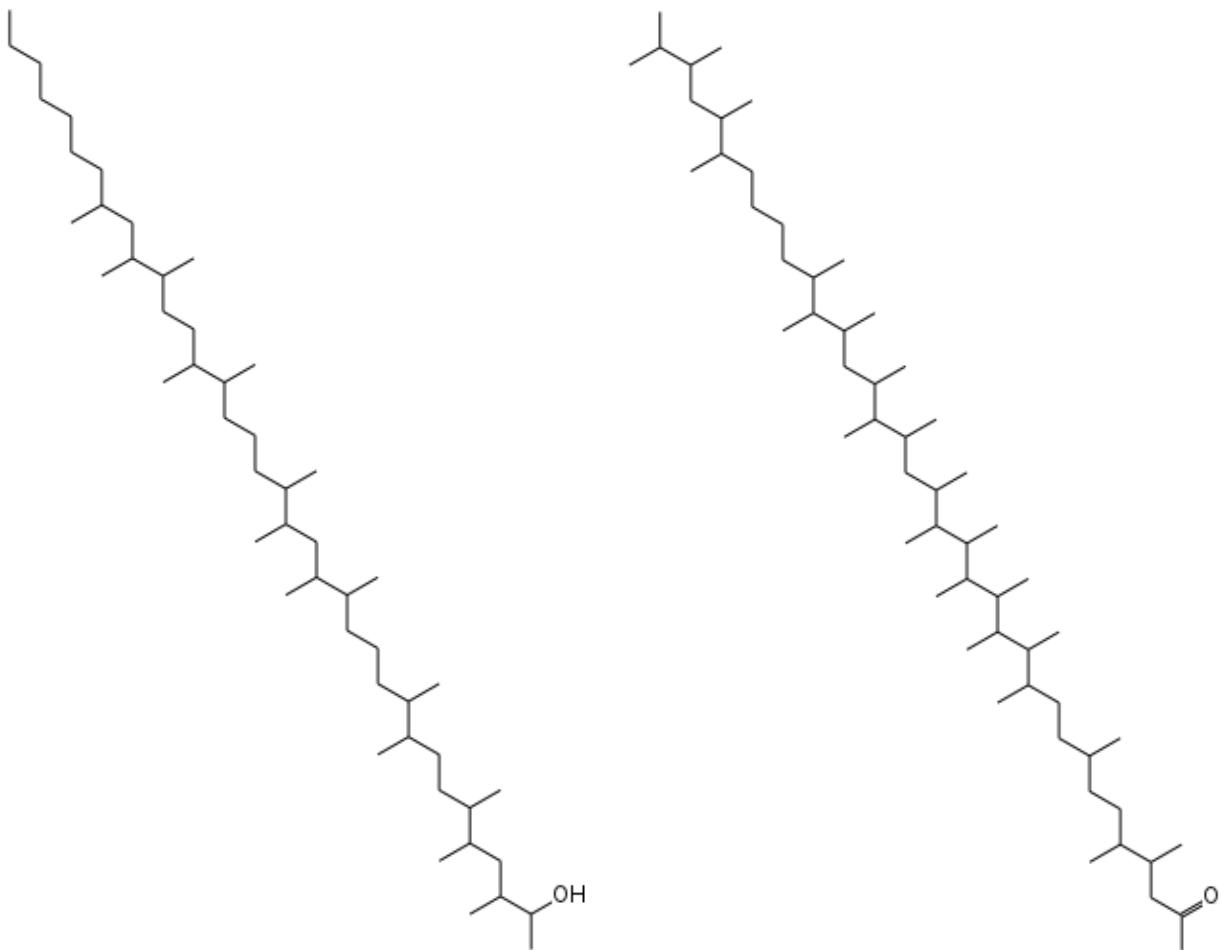
Abstract

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 collision](#) 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 OCPAUTFLNMYSX-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

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