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InChIKey collision: the DIY copy/pastables

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Inchi

Abstract
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.

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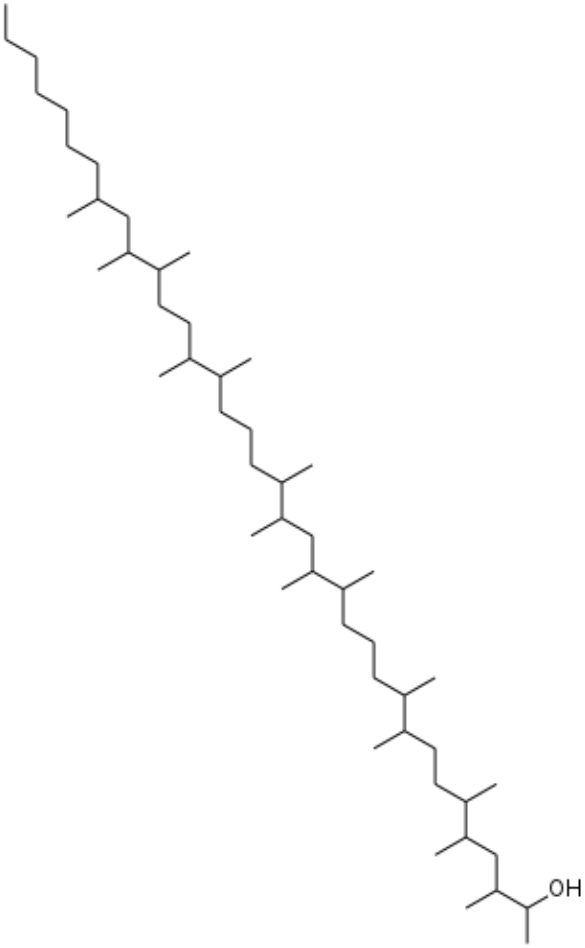
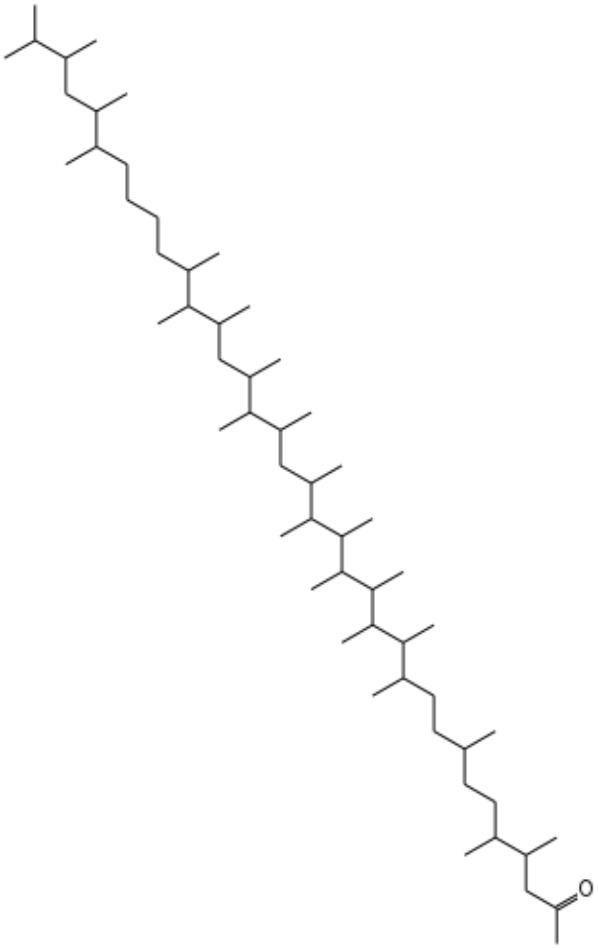
About two weeks ago, the ChemConnector blog reported an InChIKey collosion detected by Prof. Goodman . Unlike the previous collision, this one was based solely on the graph and not on stereochemistry. The two molecules both have the InChIKey OCPAUTFLLNMYSX-UHFFFAOYSA-N:





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)C(C)C(C)CC(C)C(C)C(C)C(C)CC(C)C(C)C(C)C(C)CCCCC(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.