chem-bla-ics

InChIKey collision: the DIY copy/pastables

Published September 17, 2011

Citation
Willighagen, E. (2011, September 17). InChIKey collision: the DIY copy/pastables. *Chem-bla-ics*. https://doi.org/10.59350/pxxek-shz13

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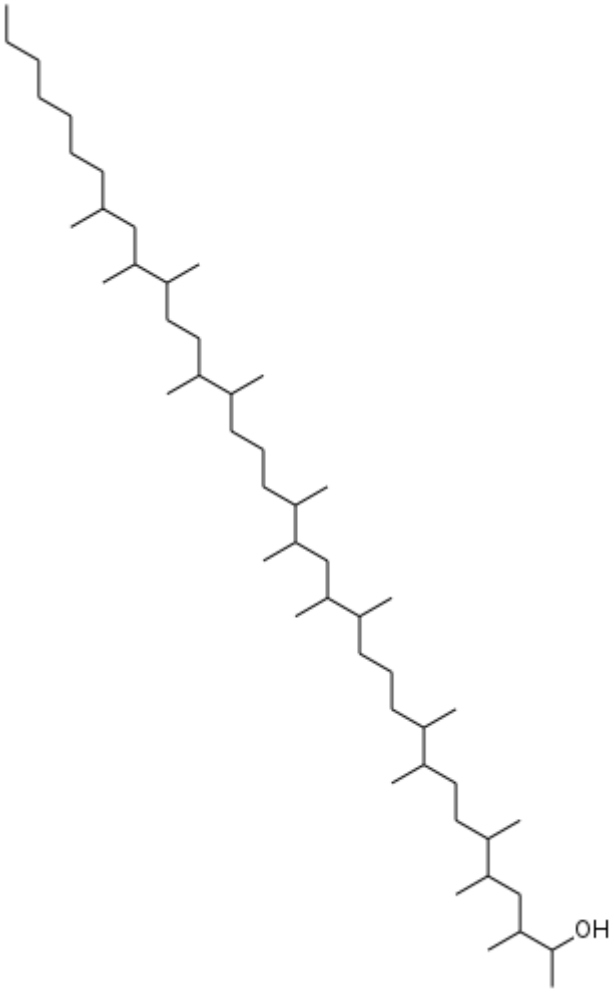
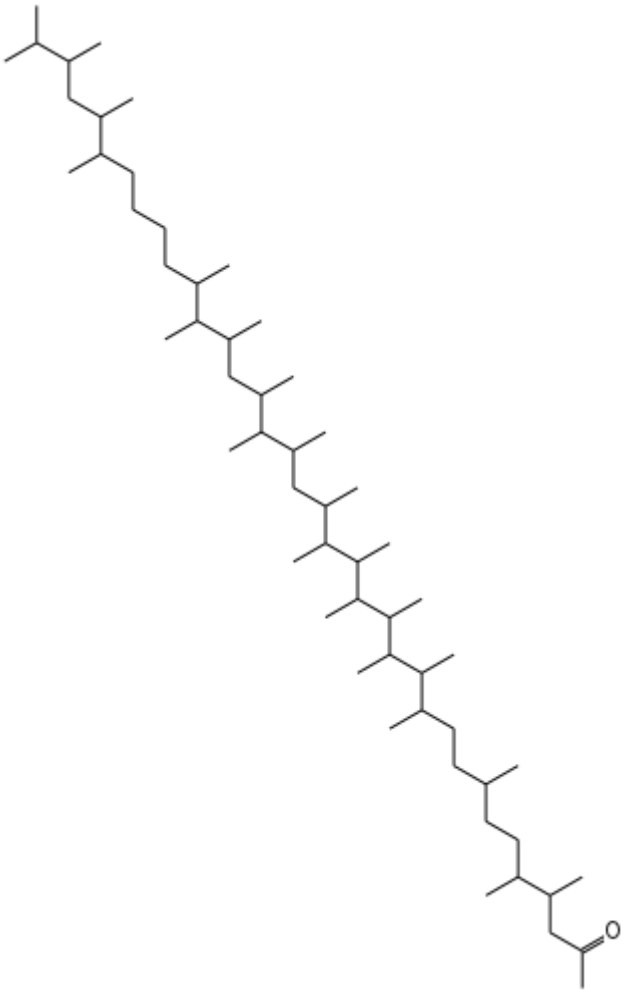
About two weeks ago, the ChemConnector blog reported an InChIKey collosion detected by Prof. Goodman . Unlike the previous collision, this one was based solely on the graph and not on stereochemistry. The two molecules both have the InChIKey OCPAUTFLLNMYSX-UHFFFAOYSA-N:





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.