

InChIKey collision: the DIY copy/pastables

Egon Willighagen 

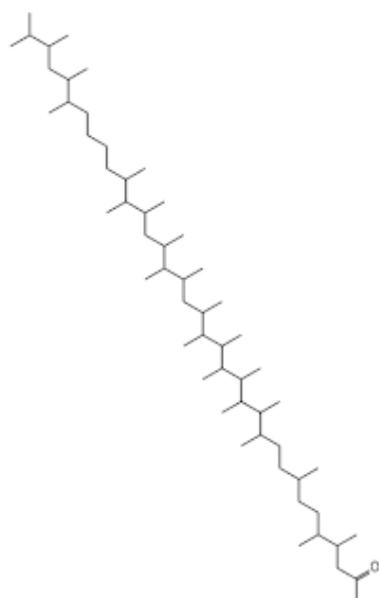
Published September 17, 2011

Citation

Willighagen, E. (2011). InChIKey collision: the DIY copy/pastables. *Chem-bla-ics*. <https://doi.org/10.59350/eg94z-9dg88>

Keywords

Inchi, Inchikey:OCPAUTFLLNMYSX-UHFFFAOYSA-N, Opsin, Smiles, Bioclipse



Copyright

Copyright © Egon Willighagen 2011. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

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 **OCPAUTFLLMYSX-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)CCCCC
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)CC(C)C(C)C(C)CC(C)C(C)C(C)CCCC(C)

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.

References