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Subject: Generate tautomers

Posted by [Christophe](#) on Thu, 27 Oct 2022 09:25:16 GMT

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Hello everyone,

Is there a way to generate tautomers from either 2- or 3D structures with DW and to pool them (as for conformers) into the same target row ?

Thanks

Christophe

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Subject: Re: Generate tautomers

Posted by [nbehrnd](#) on Thu, 27 Oct 2022 10:00:03 GMT

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Christophe,

maybe the answer is «not yet», yet there are multiple programs/services available to generate them. Though his focus was the description of tautomers, one presentation by Marc Niclaus of NIH mentioned their tautomerizer to consider 80+ rules

<https://cactus.nci.nih.gov/tautomerizer/>

requesting SMILES strings as input as an example.

Regards,

Norwid

File Attachments

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1)

[2022-04-12\\_Nicklaus\\_OpenInChIDays\\_2022-04-05\\_Tautomerism\\_\\_inchi days2022 -- inchi presentations.pdf](#), downloaded 95 times

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Subject: Re: Generate tautomers

Posted by [Christophe](#) on Thu, 27 Oct 2022 13:54:59 GMT

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Hi Norwid,

Thanks for your answer and the link.

I also found that the MarvinSketch suite was able to generate tautomers from structures in a friendly way.

Regards

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