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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

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### File Attachments

1)

[2022-04-12\\_Nicklaus\\_OpenInChIDays\\_2022-04-05\\_Tautomerism\\_\\_inchi days2022 -- inchi presentations.pdf](#), downloaded 180 times

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