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

1)

2022-04-12\_Nicklaus\_OpenInChIDays\_2022-04-05\_Tautomerism\_\_inch idays2022 -- inchi presentations.pdf, downloaded 590 times