Subject: Re: Generate tautomers
Posted by nbehrnd on Thu, 27 Oct 2022 10:00:03 GMT

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__inchidays2022 -- inchi presentations.pdf, downloaded 640 times