Subject: Suggestion: tautomer-check
Posted by nbehrnd on Wed, 06 May 2020 13:40:09 GMT
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DataWarrior's model to assign Druglikeness depends on the encoded structure a tautomer is represented. With Ambit-Tautomer, Kochev et al. published an open source tool (Java based), to predict tautormers and to rank their likelyhood. If wanted, their executable may be run without the larger Ambit framework, just by

java -jar ambit-tautomers-2.0.0-SNAPSHOT.jar

Thus, I would like to suggest DataWarrior could implement a function to check if the structures to consider could reasonably yield a tautomer worth to probe equally. This equally could be complementary to your recently published reference tautomer.dwar.

Out of curiosity, I drew a pyridone, a pyrazole, and a thalomide with ACD ChemSketch in two tautomeric forms, exported the SMILES strings (as defined by ACD ChemSketch) into a .smi file:

With openbabel, it was converted into a .sdf accessible for DataWarrior by

obabel -ismi tautomers.smi -osd -O tautomers.sdf

successfully read and used to compute the Druglikeness. At least as the examples about «hydroxypyridine» and the enol form of the thalomide differ in the results examined.

To ease replication of the findings, the relevant files are provided below.

Publication about Ambit-Tautomer: https://doi.org/10.1002/minf.201200133
github-entry about Ambit-Tautomer:
https://github.com/ideaconsult/apps-ambit/tree/master/tautom ers-example

File Attachments

1) tautomers.gif, downloaded 626 times
2) tautomers.smi, downloaded 413 times
3) tautomers.sdf, downloaded 413 times
4) tautomers.dwar, downloaded 441 times
5) tautomer_DW.png, downloaded 706 times