
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 tautomers and to rank their likelihood.

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 thalomid 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 thalomid differ in the results examined.

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

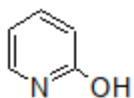
Publication about *Ambit-Tautomer*: <https://doi.org/10.1002/minf.201200133>

github-entry about *Ambit-Tautomer*:

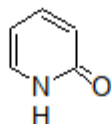
<https://github.com/ideaconsult/apps-ambit/tree/master/tautomers-example>

File Attachments

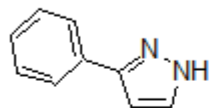
1) [tautomers.gif](#), downloaded 1025 times



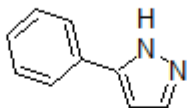
pyridin-2-ol
Oc1ccccn1



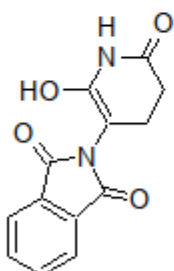
pyridin-2(1H)-one
O=C1C=CC=CN1



3-phenyl-1H-pyrazole
c1ccc(cc1)c2ccnn2

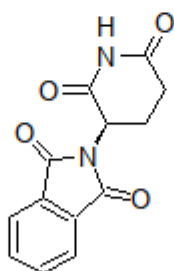


5-phenyl-1H-pyrazole
c1ccc(cc1)c2ccnn2



thalomidone

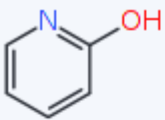
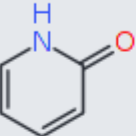
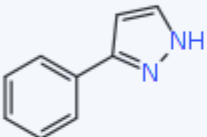
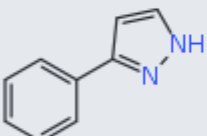
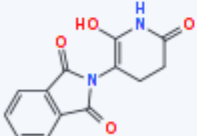
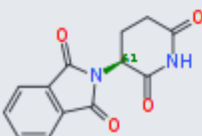
OC=1NC(=O)CCC=1N3C(=O)c2ccccc2C3=O



thalomidone

O=C1NC(=O)CC[C@H]1N3C(=O)c2ccccc2C3=O

- 2) [tautomers.smi](#), downloaded 691 times
- 3) [tautomers.sdf](#), downloaded 674 times
- 4) [tautomers.dwar](#), downloaded 700 times
- 5) [tautomer_DW.png](#), downloaded 1163 times

	Structure	Molecule Name	H-Acceptors	H-Donors	Druglikeness
1		pyridin-2-ol	2	1	-1.88
2		pyridin-2(1H)-one	2	1	-0.23382
3		3-phenyl-1H-pyrazole	2	1	1.3013
4		5-phenyl-1H-pyrazole	2	1	1.3013
5		thalomid_enone	6	2	1.7671
6		thalomid_ketone	6	1	4.3067