
Subject: Re: Aromaticity perception

Posted by [richards99](#) on Sat, 27 Jun 2020 22:14:27 GMT

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Okay, worked out now how to attach the file.

Attached is the SDF file which is problematic for DW, and a snapshot showing the difference between importing as smiles or SDF.

Simon.

File Attachments

1) [Screenshot 2020-06-27 at 23.06.40.png](#), downloaded 1417 times

Table

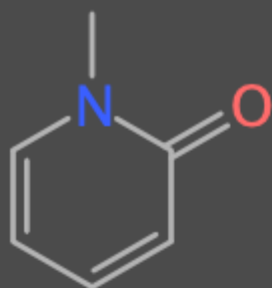


Structure of ...

Molecule

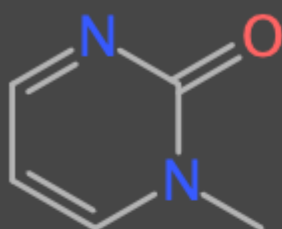


1

Cn1cccc1=O

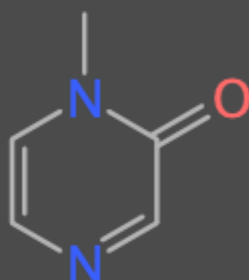
1

2

Cn1cccnc1=O

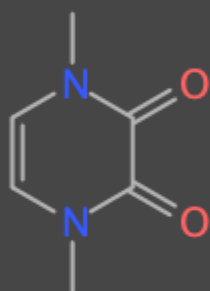
2

3

Cn1ccncc1=O

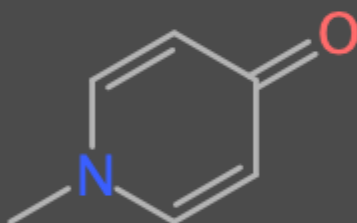
3

4

Cn1ccn(C)c(=O)c1=O

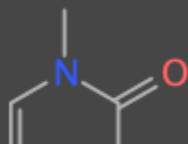
4

5

Cn1ccc(=O)cc1

5

6

Cn1ccc2ncccc2c1=O

6

2) [Aromatised.sdf](#), downloaded 770 times
