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 1320 times

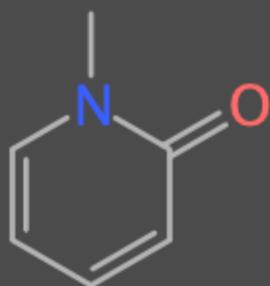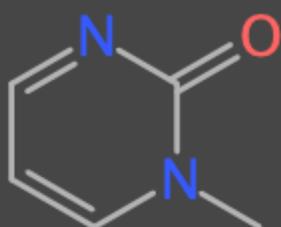| Table		
Structure of ...	**Molecule**	
1	Cn1ccccc1=O	
2	Cn1cccnc1=O	
3	Cn1ccncc1=O	
4	Cn1ccn(C)c(=O)c1=O	
5	Cn1ccc(=O)cc1	
6	Cn1ccc2ncccc2c1=O	
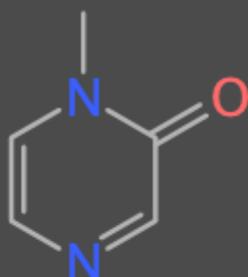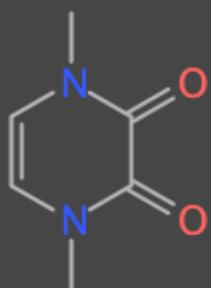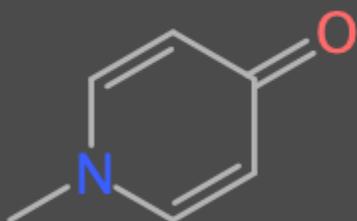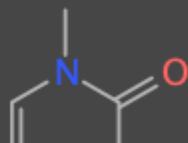
Table

| 1 |
| 2 |
| 3 |
| 4 |
| 5 |

2) Aromatised.sdf, downloaded 735 times