Posted by richards99 on Thu, 25 Jun 2020 20:38:01 GMT

Hi,
There appears to be consistent issues with the import of certain aromatised structures.
Ones I especially notice are N-methylated pyridinones, pyrimidinones, and bicyclic structures.
Data Warrior puts double bonds into the wrong positions, quaternising nitrogens.

It would be useful if the aromaticity perception can be improved otherwise it creates lots of invalid smiles which require manually altering.

Thanks,

Simon.