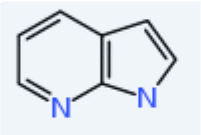
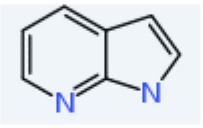
Subject: Substructure issue - bicyclic heterocycles
Posted by amorrison on Fri, 25 Nov 2022 12:21:18 GMT
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Hi Thomas,
I'm having some issues with, in particular, azaindoles being identified in different resonance forms. As a consequence of this, when substructure searching or Core based SAR analysis the two resonance forms are being seen differently. I've tried bringing these in from different mol blocks (ACD, Dotmatics) and also converting the SMILES string in DataWarrior with 'Add structures from name' but all give the same result. I am unable to share the structures but the image attached shows the issue I'm having with some in one resonance form and some in the other. These are closely related structures so not sure why this occuring. I'm currently using DW dev version 30-Jun-2022. Any help would be much appreciated.
Many thanks,
Angus

File Attachments

1) Azaindole.png, downloaded 847 times


N
N

N
N