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 238 times

Subject: Re: Substructure issue - bicyclic heterocycles
Posted by thomas on Sat, 26 Nov 2022 14:43:00 GMT
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Hi Angus,

in principle both ways to kekulize delocalized rings should be compatible and both version should behave the same for all purposes, e.g. substructure search, in DataWarrior. From your description I cannot really build a test scenario, but I assume that the problem disappeared in the current dev version. At some time in summer I added some new substructure features, which caused a problem when generating FragFP fingerprints and with the substructure search itself. To my knowledge the bug is fixed. I suggest to download the newest dev version and to recreate the FragFp of files that are problematic (Data->Delete Column...->FragFp and then Chemistry->From Chemical Structure->Calculate Descriptor->FragFp). If you then still have any issue, please construct a small DataWarrior file with at least one structure in the table and a not working substructure in a filter. But probably that is not necessary anymore...
Thomas

Subject: Re: Substructure issue - bicyclic heterocycles
Posted by amorrison on Thu, 01 Dec 2022 07:15:53 GMT
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Hi Thomas,
Many thanks, that worked and now behaving as expected.
Thanks,