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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

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