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Subject: Compound properties

Posted by [sansun](#) on Fri, 10 Jul 2020 11:41:12 GMT

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I think it would be great to get 'counts' of more structural features.

For instance currently 'Aromatic rings' can be counted but it would be nice to have a separate count for 'carboaromatic and heteroaromatic rings'

Also, I think other properties like aliphatic rings (carbo and hetero), number of carbons, FSp3, etc. are not computable directly by one click.

Probably it would be best to implement RD-Kit descriptors that seem to be quite exhaustive.

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Subject: Re: Compound properties

Posted by [thomas](#) on Sat, 11 Jul 2020 22:26:02 GMT

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thanks for the suggestion. I have added a couple of ring counts to start with...

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