Subject: Compound properties
Posted by sansun on Fri, 10 Jul 2020 11:41:12 GMT
View Forum Message <> Reply to Message

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.

Subject: Re: Compound properties
Posted by thomas on Sat, 11 Jul 2020 22:26:02 GMT
View Forum Message <> Reply to Message

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