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Subject: Medchem rules

Posted by [sansun](#) on Sat, 16 Jul 2022 12:17:30 GMT

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Hi Thomas

I was wondering if you are planning to add a direct way of implementing various MedChem rules such as rule of 5, Veber's criteria, PAINS, etc.?

Currently, we can do it using 'Calculated Column' but not very efficiently. I understand 'creating macro' is another option. However, I found that as the version change, sometimes column name changes and hence, macros created with the previous versions are sometimes incompatible with the new ones.

Thanks

SS

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