Subject: Re: Lilly Medchem Rules
Posted by nbehrnd on Thu, 23 Apr 2020 17:29:06 GMT
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The publication you cite (ACS' Author Choice, thus open access) was published in 2012, J. Med. Chem. currently is aware of 141 publications citing this work; some you might know. The history of commits in the repository notes for Dec 14, 2017 «First working version for version 2», too.

Are there additions / modifications to the set of 275 MedChem rules of the 2012 publication which you would like to suggest to consider today? The approach suggested indeed is complementary to the approach of druglikeness in DW,[1] in turn borrowed from the earlierr OSIRIS Property Explorer.

[1] http://www.openmolecules.org/properties/properties.html#drug score