Subject: Re: Lilly Medchem Rules
Posted by evehom on Tue, 15 Sep 2020 14:29:59 GMT
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Hi Thomas

I think the REOS rules by Pat Walters & colleagues from Vertex (https://www.sciencedirect.com/science/article/abs/pii/S13596 4469701163X?via%3Dihub are substantially easier to implement (but also well-established) since they were written as SMARTS and there are 'only' 117. I can provide you with the list if you are interested.

Cheers/Evert