Subject: Re: Lilly Medchem Rules
Posted by thomas on Fri, 08 May 2020 16:02:07 GMT
View Forum Message <> Reply to Message

I checked the 2012 paper and believe that adding these rules to DataWarrior would be a valuable extension. There have been quite some requests for unwanted feature flagging and it seems Ian Watson and colleagues made an excellent job. However, the effort to add the rules list to DataWarrior would be significant. Like the conversion from SLN to SMARTS, one would have to convert the 2012 rules into idcodes (the openchemlib structure encodings used by DataWarrior) and to write additional code for the more general rules and their combinations with SMARTS. openchemlib query features are not 1:1 compatible with SMARTS, thus in some cases one would have to guess what the intention was and replace with the appropriate query feature.

If the large majority of rules can be expressed with a substructure alone and somebody could translate these rules into idcode using an openchemlib structure editor, that would help a lot...

Thomas