Subject: Enumerating a virtual library
Posted by amorrison on Sun, 13 Sep 2020 06:13:55 GMT
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Hi,
After doing a core based SAR analysis I get cores and R-groups for the compounds that are present. What I would like to do would be to then take these R-groups and enumerate them all to build a virtual library of the full R-group matrix, so that I could calculate for example properties of the virtual compounds. Is there any to do this that would avoid having to draw each r-grp and core in a virtual reaction?
Many thanks,
Angus

Subject: Re: Enumerating a virtual library
Posted by thomas on Sun, 13 Sep 2020 09:47:12 GMT
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No, currently this is a little cumbersome. It seems to me that the most efficient way would be to have an additional checkbox in the SAR dialog 'Enumerate complete matrixes per found scaffold', and an option to either append not existing combinations to the SAR result window or to save all full matrixes into a new file.

Thomas