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