Subject: Decompose R-Groups
Posted by amorrison on Wed, 06 Nov 2024 12:02:57 GMT
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Hi,

I use the decompose R-groups for SAR analysis frequently. Usually DataWarrior does a great job across multiple scaffolds of placing the R-groups in the correct place but in some cases I would like to specify what a particular substitution off the scaffold should be e.g. R1. I don't think this currently possible in the current version of DataWarrior, but would it be easy to implement?

Many thanks,
Angus