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

Subject: Re: Decompose R-Groups
Posted by thomas on Tue, 12 Nov 2024 18:07:24 GMT
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I presume it would need a non-trivial UI to do that, while I am not sure, whether I understand correctly. Do you refer to 'multiple scaffolds' matching the same query? Or actually an undesired scaffold match on a real compound if there are multiple matches because of symmetry?

How would like to indicate critical cases before running the deconvolution or 'correct' assignments for individual rows after it? From an UI perspective both seems rather difficult to do...

Subject: Re: Decompose R-Groups
Posted by amorrison on Sun, 17 Nov 2024 07:34:33 GMT
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Hi Thomas,

Thanks for getting back to me. I guess I was thinking along the lines of providing R group numbers to the scaffold as in the attached image.

No problem at all if this is too difficult from a coding perspective and thanks for getting back to me.

Angus

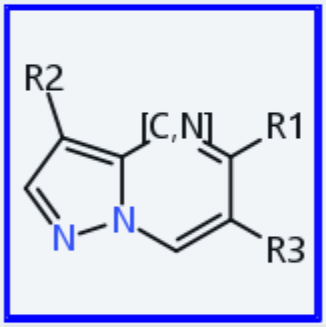
File Attachments
1) R_Grp_Decompose.png, downloaded 813 times

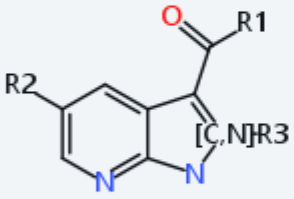
Decompose R-Groups

Structure column: Structure

Determine scaffold as: Custom sub-structure(s)

Define custom scaffold sub-structures:





Use existing columns for scaffold and R-groups

Help

Canc