
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 298 times

 Decompose R-Groups

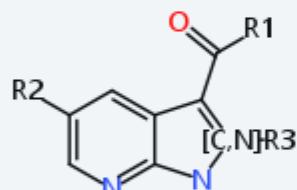
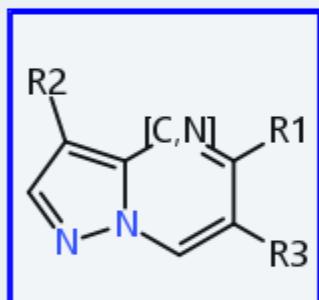
Structure column:

Structure

Determine scaffold as:

Custom sub-structure(s)

Define custom scaffold sub-structures:



Use existing columns for scaffold and R-groups

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