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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...

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