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Subject: R group count

Posted by [amorrison](#) on Sat, 11 Mar 2017 08:00:01 GMT

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Hi Thomas,

First of all let me say what a great bit of software to release for everyone to use.

My question relates to calculating the count of R-groups. I've found the frequency expression in the add calculate value drop down, but this only works by supplying an R-group to calculate for. Is it possible to calculate the frequency of all R-groups in a particular column which I can then use for filtering, e.g. remove all R-groups that only appear once.

Thanks,

Angus

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Subject: Re: R group count

Posted by [thomas](#) on Tue, 21 Mar 2017 20:17:50 GMT

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Hi Angus, if I understand correctly you could actually use the frequency function: frequency(value, column-name)

If you have a column called 'R-Group', then the two parameters passed to the function are: frequency(rGroup, "R-Group")

The first parameter is the variable name that refers to the actual R-group in the respective row, while the second is the column in which this R-Group's occurrence is counted. If you for instance have a column that contains 'methyl' five times and 'ethyl' two times, then a new column is created that has a '5' in every 'methyl' row and a '2' in every row of which the R-group is 'ethyl'.

The trick is to pass a variable as the first parameter and not a static value.

Does this answer your question?

Thomas

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