
Subject: Re: question about 'analyse similarity/activity cliffs' function

Posted by [pmallard](#) on Mon, 30 Sep 2019 12:18:06 GMT

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Dear Thomas,

I have some issue with the structure similarity filter.

I have a large set of structures (>10M) which I imported from csv and FragFp has been automatically calculated.

Most of the structures display well. I am able to a "contain" search and look for molecules containing the structure I just drew.

However the "is similar to [FragFp]" function doesn't work.

No error message is returned however the search is not working and the filter is automatically switched to the "disable filter" mode when I run it

Any clue ?

Many thanks for this excellent software !

PM
