Subject: Re: similarity_search_protocol
Posted by thomas on Thu, 23 Sep 2021 10:10:29 GMT
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The fastest way would be to open the large file, then add a Structure-List (similarity) filter and within the filter with a right mouse click read the query structures into the filter. The play with the similarity slider. SkeletonSpheres would represent chemical similarity best. You can use Flexophores for potential similarity of target activity.

You could calculate conformers for both, the big and the query files. Then, open the big file and do a conformer superpositioning with the query compounds. This would give you shape and pharmacophore point similarity as well as a visual feedback of the best matches.

You could append the big with the query file and create a SOM with maybe 150 nodes per dimension. This gives you an chemical space visualization with where your query molecules are in regard to the 50000.

And as suggested, the 'Find similar compounds in file' calculates all similarities and gives you all the pairs of similar compounds.