Subject: Re: Flexophores
Posted by thomas on Thu, 07 Mar 2019 16:35:50 GMT

most of this should be answered by this:
http://openmolecules.org/forum/index.php?t=msg&goto=484& amp;#msg_484

To your last question: If you want to find out, to which of your few thousand compounds you can find any similar known compounds that has some activity on a Kinase, then I would do these steps:
- within DataWarrior run a ChEMBL query to retrieve all compounds from ChEMBL with a known activity on any Kinase. You may delete less significant result rows, e.g. keep only dose response value and delete any single point measurements, or remove low activity values...
- calculate the SkeletonSpheres and Flexophore descriptors for these actives
- Use the 'Find Similar Compounds In File...' functionality to find for all your compounds the most similar ones from the actives file including target information (using flexophore or SkelSpheres)

Hope this answers the question...

Thomas