Subject: Flexophores
Posted by pc419714@ohio.edu on Sat, 16 Feb 2019 23:57:06 GMT
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I am wondering about clustering using flexophores. This measure is supposed to give you a measure of biological activity..... Does this mean that it predicts binding to specific proteins? Will it tell you what a given molecule will bind if I generated the flexophores and then clustered? It supposedly takes a lot of time and memory so I wanted to make sure before I did it. I just wanted to know which kinases my molecules bind, so I selected find similar compounds in file for a large data set of known kinase inhibitors and found which ones were similar. I did not use the flexophores though. Would the flexophores give me more information on the function of my molecules than skelspheres would? If flexophores do not do this then is there a database I could use to find similar known compounds? I have several thousand molecules in my library.

Thanks again!

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