
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!
