Also, 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? Thanks again!