Subject: Re: Chemistry in 3D
Posted by Christophe on Fri, 18 Mar 2022 09:22:42 GMT
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Dear Norwid,

Thank you. Yes I was talking about these (and others) youtube videos and I was wondering if there were any others about the utilization of DW with 3D chemistry. I didn't find any nor other kind of formats (.pdf ...).

I am a chemist (synthesis and evaluation of compounds with their targets or onto diverse cell lines). I am novice in computation stuff. My interest about the 3D chemistry module is general:
-for example how to choose the algorithm and the minimize energy force field that's best suit with your compounds? Is it really important in my case?
- How many max count conformers do I have to select according a starting structure and how to be sure I get the lower energy ones.

For now, and to start, I'd like to compare (superpose) a known ligand with conformers I would generate from my designed compounds and get a score. I did this kind of experiment with DW and get a PheSA (Pharmacophore enhanced shape alignment) scores. Is it realistic to eliminate some compounds based on this score ?
Basically, I just want to learn more in general so that I can understand the limits and not do or say things that don't make sense. Every little things that could help in the selection process are good to take!!
Best regards
Christophe