Subject: Chemistry in 3D
Posted by Christophe on Thu, 17 Mar 2022 09:56:05 GMT
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Hello everyone,

I read the user manual concerning conformers and 3D chemistry in general and I would like to go a bit deeper.
Does anyone know any good tutorials and/or videos ?
For example I watched the videos of I. Giraud about DW (RSC CICAG Open Source Tools for Chemistry Workshops) and it was really great.
Is there anything comparable for 3D chemistry?

Many thanks

Also: two silly questions:
- When I add a new empty row in DW, it remains invisible and I can't edit it. How to visualize such a row?
- When you click on any rows, it becomes reference cell (red frame around it). How to undo this reference cell selection (to make this red frame disappear)?

Subject: Re: Chemistry in 3D
Posted by nbehrnd on Thu, 17 Mar 2022 21:34:52 GMT
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Dear Christophe,

do you refer to one of the two videos mirrored on youtube?[1,2]

May you specify if your interest concerning «conformers and 3D chemistry» is about the theory behind the scenes, or the choice of one of the algorithms available? For the later, it would help to know what you want to do once the conformers are in obtained. The force-fields offered by DW strive for affordable results in obtained short delay, they may serve as a starting point for computations at higher level of theory with other programs.

(Inferring from the context set above:) The addition of an empty row will fail if the .dwar in question is about conformers already generated and is a container of these (newly generated) 3D coordinates. At stage where the molecules are «only 2D sketches» like on paper, the addition of rows will work.

The red frame is visual aid. To define e.g., the deletion of rows, the range is defined by the cells with the toggled background color (e.g. from default light to dark); this selection moves independently from the red frame.

Norwid

[1] https://www.youtube.com/watch?v=mQCf9GakQW0

[2] https://www.youtube.com/watch?v=Is2hLqqSFvM

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

Subject: Re: Chemistry in 3D
Posted by sansun on Tue, 22 Mar 2022 10:05:57 GMT
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I can answer one of your questions.

The new rows are invisible after addition if you have applied filters. The solution is to disable all filters.

Go to --> Edit
click on
--> disable all filters

Subject: Re: Chemistry in 3D

Posted by nbehrnd on Tue, 22 Mar 2022 12:57:17 GMT
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Dear Christophe,

the conformer generator's aim is the provision e.g., of starting geometries for (in silico) docking experiments and considers only the isolated, single molecule in question. Once the molecule experiences interactions with neighbouring molecules e.g., intermolecular hydrogen bonds may render these predicted energetic minima more shallow/more deep. Then, some conformations might be not longer favourable, and others are locked-in; both render a reliable prediction more demanding. (One reason for prediction contests like the ones by CCDC,[1] or CASP.[2])

The number of conformers per molecule one want to query equally depends on the number of bonds which are conformational flexible. In this perspective, the default of up to 16 is (an empiric) suggestion. DataWarrior neither is the only program to offer this functionality,[3] nor do the force fields provided aim to compete in accuracy and precision with higher level(s) of theory/specialized programs.

Because I have no working experience with the shape alignment and docking you refer to, my suggest were to screen the 500+ citations on ACS's landing page for the the primary publication about DataWarrior,[4] or/and collect advice by others.

Norwid

[1] Reilly et al. Acta Cryst. 2016, B72, 439-459; doi 10.1107/S2052520616007447
[2] https://en.wikipedia.org/wiki/AlphaFold
[3] Ebejer, J. P. et al. J. Chem. Inf. Model. 2012, 52, 1146-1158; doi 10.1021/ci2004658
[4] Sander T. et al. J. Chem. Inf. Model. 2015, 55, 460-473; doi 10.1021/ci500588j

Subject: Re: Chemistry in 3D
Posted by Christophe on Wed, 23 Mar 2022 11:45:37 GMT
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Thanks a lot for all these explanations.
Regards