Subject: Add pharmacophores into the 3D-view ?
Posted by Christophe on Tue, 25 Oct 2022 11:22:54 GMT
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Hello everyone,

I have a file with generated conformers and when I right click into a bound of any structures from the 3D view, I can see "Add pharmacophores" from the list.

When trying to use this great feature from a new file with another set of 3D structures also containing conformers, I cannot see "Add pharmacophores" anymore. Why ?

I must add that I calculated the flexophore descriptor and made a similarity analysis with it for all my structures. Any clue ? I did not find anything about this in the online manual.

Thanks
Christophe

Subject: Re: Add pharmacophores into the 3D-view ?
Posted by thomas on Wed, 09 Nov 2022 17:10:06 GMT
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Dear Christophe,

adding pharmacophores was a feature, which was meant to be available in the 3D-viewer if it was in edit mode only . However, there was a bug in the viewer, which enabled this features also for non-edit mode once another viewer has been opened in edit mode before. Thus, after opening the PheSA or docking dialog you would find this feature also in the molecule context menus of any 3D-viewer. The bug is fixed now and in addition the menu option to show pharmacophores is now available in non-editable 3D views as well.

Thomas