Subject: Set 3D View Alignment

Posted by sbembenek18 on Fri, 11 Oct 2019 17:03:37 GMT

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After orientating a given 3D molecule in the 3D viewer, is it then possible to fix this orientation and have the rest of the molecules use it as well?

My scenario is that I often look at compounds that have been docked, and so they have the protein as the common reference frame and these are the 3D coordinates that are imported into DW. In essence, they have the alignment I want, I simply want to reorientate the 3D view and have it unchanged as I scroll through the molecules.

Scott

Subject: Re: Set 3D View Alignment

Posted by thomas on Fri, 11 Oct 2019 17:34:48 GMT

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Currently, this is not possible. However, I hope to add an option soon that would allow to display and superpose the conformer of the 'current row' (the one with the red frame) to all other rows. In this context, it would make sense to also provide an option to synchronize rotation & translation of all rows with the 'current row'. One way of solving it would be to remember the rotation/translation state of the 'current row' whenever it is updated and apply that to any other row as soon as it is displayed. I will give it a try...

Thomas

Subject: Re: Set 3D View Alignment

Posted by sbembenek18 on Fri, 11 Oct 2019 18:25:21 GMT

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That would be very cool --thanks!