Subject: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by Jo W on Mon, 30 Jan 2023 12:59:02 GMT
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When creating docking scores in DW, you can select whether to protonate the ligand or not.
At the moment I am using this feature with nitrogen heterocyclic ligands.

However, when you use this feature with an EL based on docking scores, the program seems to automatically protonate the nitrogen in nitrogen-containing resulting ligands.

Is there any way to underdo this feature or at least have it as an option?
Many thanks in advance
Jon

Subject: Re: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by thomas on Wed, 01 Feb 2023 00:04:04 GMT
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An option to skip (de-)protonation for docking fitness in evolutionary libraries will be in the next dev version...

Subject: Re: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by Jo W on Wed, 01 Feb 2023 15:23:59 GMT
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Thanks. Do you know approximately when the next development version will be?

Subject: Re: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by thomas on Thu, 02 Feb 2023 11:03:11 GMT
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I assume it is a matter of days, but I need to finish a few changes regarding conformation generation

Subject: Re: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by thomas on Tue, 07 Feb 2023 15:09:40 GMT
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I just deployed an update with this thing solved, but realized that the conformation generation has a fundamental dewsign flaw, which I need to tackle. Thus, another update will follow later...

Subject: Re: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by Jo W on Wed, 08 Feb 2023 23:14:49 GMT
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OK Many Thanks, Thomas. Approximately - are we talking days or weeks for the further update?

Subject: Re: Optional automatic protonation feature of Nitrogen in DW using EL
Posted by thomas on Thu, 09 Feb 2023 21:00:13 GMT
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hopefully before the end of next week...