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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

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