Subject: Optional automatic protonation feature of Nitrogen in DW using EL Posted by Jo W on Mon, 30 Jan 2023 12:59:02 GMT View Forum Message <> Reply to Message

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