Subject: Veiwing PDB Binding Sites in DataWarrior Posted by MedChemProf on Sun, 12 Jan 2025 19:56:00 GMT

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Dear All,

There are downloadable files on the Open Molecules website under the section "All Non-Covalent Binding Sites From the PDB-Database (Dec 2024)" where you can view the binding of a ligand to a protein. There is some description of how the file was created, but I have been unable to reproduce it.

Are there any detailed instructions on how to view or add the information from a PDB into DataWarrior to allow similar viewing? Any help would be appreciated.