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Subject: Re: Viewing PDB Binding Sites in DataWarrior

Posted by [thomas](#) on Thu, 16 Jan 2025 10:15:20 GMT

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Currently, you can download and browse through these binding site files, but DataWarrior cannot create such files itself from e.g. a set of PDB entries. These files were created with a separately developed Java program using OpenChemLib functionality. The mid-term goal is to analyze ligand-protein interaction geometry of different ligand and protein substructure combinations to better visualize and quantify individual interactions, similar to the Rf-interaction concept published by Roche, where they 'forgot' to add the geometry statistics to the papers making it a challenge to reproduce.

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