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.