

## **[P12] Mining chemical databases to obtain knowledge based information of non-covalent interactions.**

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Unconventional non-covalent interactions are gaining popularity in protein-ligand complexes, structural biology, supramolecular chemistry, and crystal growth design. Conventional non-covalent interactions such as hydrogen bonding, ionic bonds, van der Waals' interactions, and hydrophobic effects are well studied. Recently there has been significant interest directed at novel bonds, such as halogen bonds, carbon bonds, and sulfur bonds. With the exponential growth of data in the chemical databases in the recent times, there is significant information that could be obtained by mining these databases. In the study, we made an effort to mine two major structural databases that include Cambridge Structural Database (CSD) and Protein Data Bank (PDB). The databases were sorted through looking for the various nonconventional non-covalent interactions. An understanding of these interactions is crucial in the drug design and crystal growth design. The findings from this research was compiled and will be presented on.