S29-2 NMR screening for FBDD

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NMR is a versatile technique for pharmaceutical industry. From the organic chemistry to MRI, there are really a number of applications of NMR. Among them, biomolecular NMR has been used for structure determination of biomolecule and analyzing the interaction between the target protein and inhibitors.

In the context of FBDD, NMR has been know for fragment screening technique, because NMR is good at detecting the weak binding compound in a accurate manner. Generallly NMR technique for fragment screening is classified into two family Ligand-based technique and Protein-based technique. Protein based technique requires stable Isotope labeled protein and also can be applied for relatively small MW protein target. In ligand based technique such as saturation transfer difference(STD) and waterlogsy, only the NMR signals of the ligands are observed. The disadvantage of STD and waterlogsy is that the non-specific binding is also observed and that Competition experiment is required in order to select the specific binding compound. Due to the diference in the consumption of the protein sample, ligand based technique is generally used recently as a primary screening.