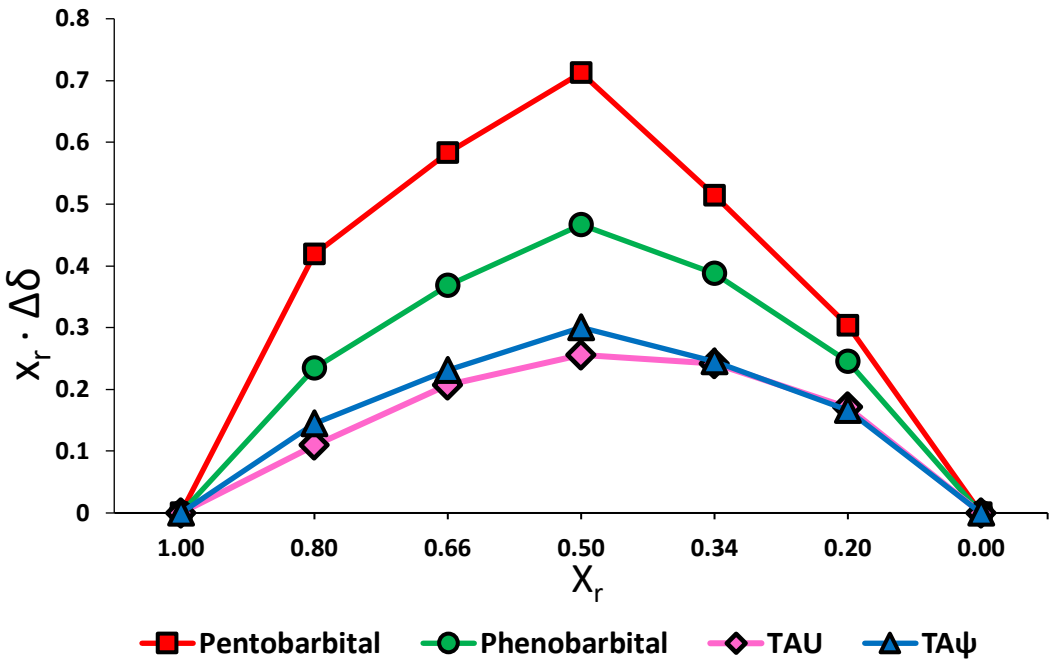
**Supplementary Information**

**Figure S1.** Job Plot for monomer **1** with pentobarbital, phenobarbital, TAU and TAψ. The monomer interacts with the analytes in a 1:1 stoichiometric complex. The experiments were made in $CDCl_3$ using 5mM monomer and template concentration solution. $X_r$ = molar fraction Δδ = chemical shift change.

**Figure S2.** $^1H$ NMR spectra for methanolic extracts from (i) **MIP1** and (ii) **NIP1**. Dried extracts were dissolved in DMSO-$d_6$.

**Figure S3.** Structures of all the monomer **1** conformers considered in the computational study.

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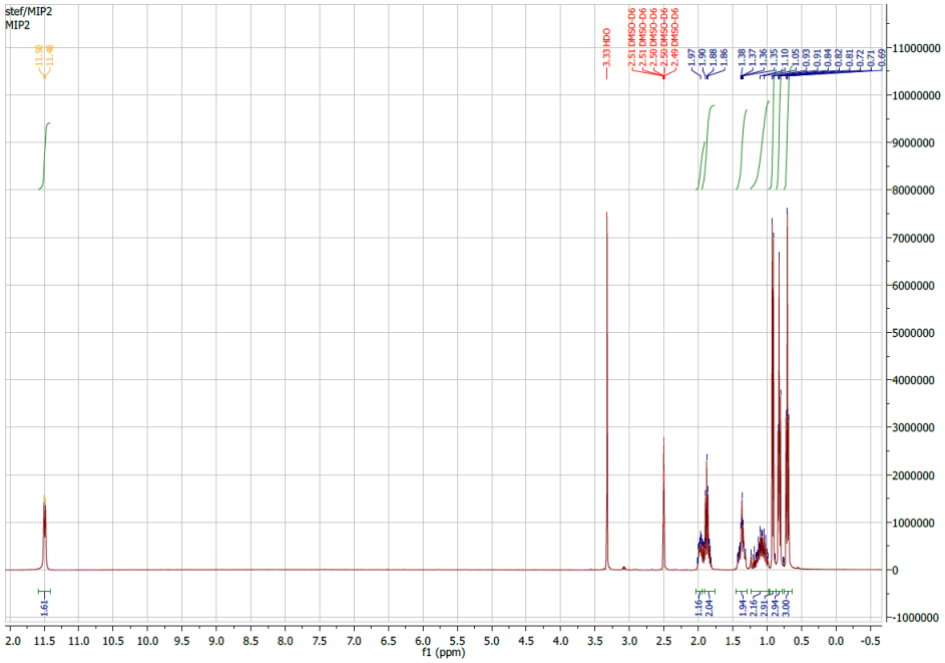
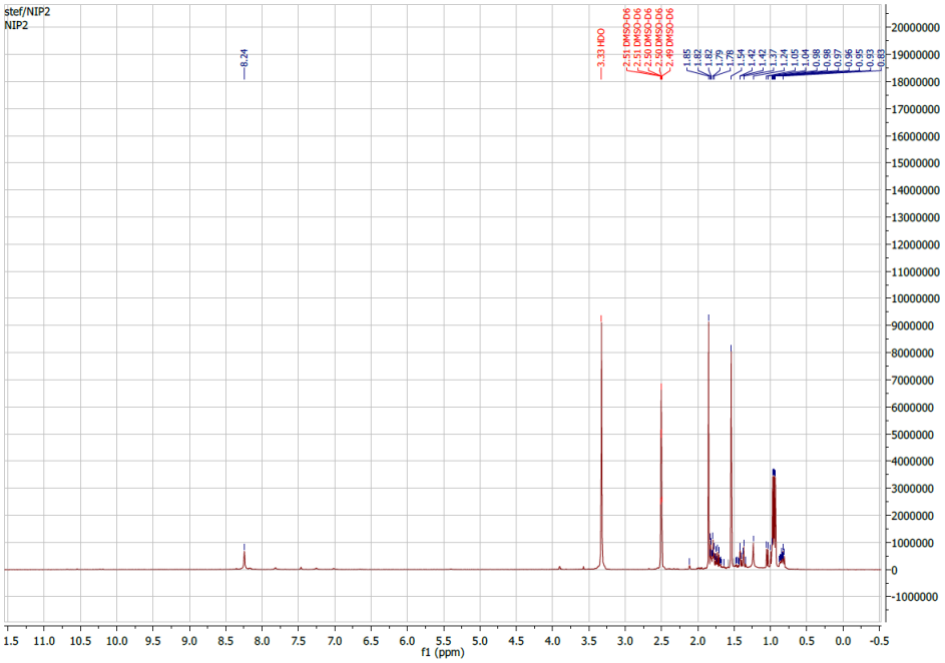
(i) MIP extract (total mass = 288 mg)




(ii) NIP extract (total mass = 2 mg)

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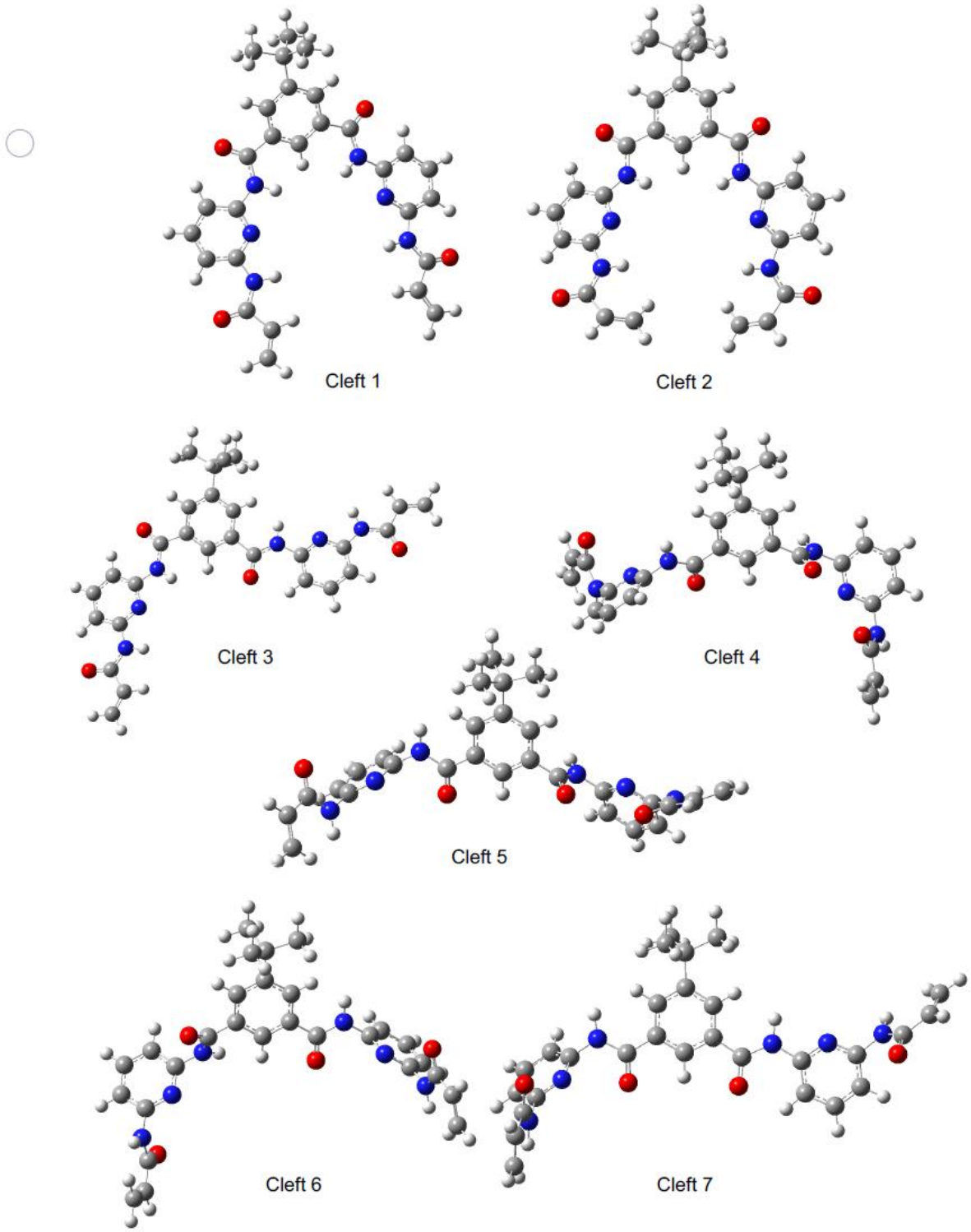


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