

**A**



**B**

**Supplementary Figure S14**. Represent ligand (bergapten) information. **(A)** Represents root mean square deviation (RMSD) values, radius of gyrus (RG) value, intra molecular hydrogen bonds, molecular surface area (MSA), solvent accessible surface area (SASA), and polar surface area (PSA), respectively **(B)** represents structure of bergapten, number of atoms, atomic mass, charge, molecular formula, number of fragments and number of rotatable bonds.