

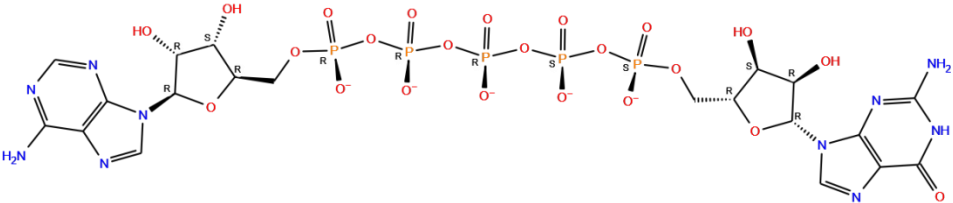
	Docking scores (Kcal/mol)			
	BS-A	BS-B	BS-C	BS-E
 ZINC000261495500	-9.67	-8.02	-7.02	-7.69

Table S4. 2D structure and docking score (expressed in kcal/mol) of the identified ligand within binding sites BS-A, BS-B, BS-C and BS-E.