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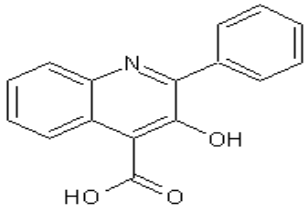
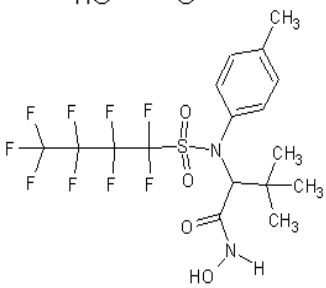
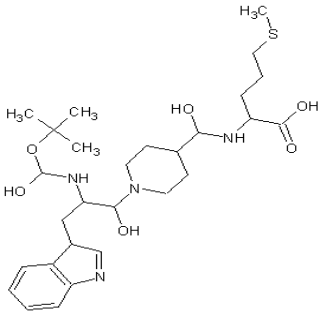
www.bioinformation.net Issue 8 **Hypothesis**

Supplementary material:

Table 1: Three Ligand chosen for Molecular Dynamics Study along with their docking scores (Autodock and Flexidock), key H bond residues and RMSD between Autodock and flexidock conformations.

Ligand Zinc Binding Group	Structure	Docking Energy (Autodock) (Kj/mol)	Docking Energy (Flexidock)	RMSD (Autodock & Flexidock)	H bond residues and distances
Carboxylic Group		-6.09	-297.64	0.093 Å	Ala 189 (1.824 Å) Leu 188 (1.810 Å)
Sulfonamide Hydroxamate		-9.04	-498.68	0.533 Å	Leu 188 (2.325 Å) Ala 189 (1.856 Å) Gln 402 (2.265 Å) His 276 (2.924 Å) His 411 (1.903 Å)
Thio ester based ZBG		-10.02	-642.45	0.078 Å	Leu 188 (2.292 Å) Ala 189 (2.217 Å) Tyr 420 (2.409 Å) Pro 421 (3.459 Å) Tyr 423 (1.747 Å)