BIOINFORMATION

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Supplementary material:

Table 1: The inhibitors with their characteristics of binding screened by Docking server

S. no	Name of the Inhibitor	Estimated free energy (Kcal/Mol)	Estimated Ki (μM)	VdW + HBond+ Dsolv. Energy (Kcal/ Mol)	Electrostatic Energy (Kcal/Mol)	Total Intermolecular Energy (Kcal/ Mol)	Interaction surface
1	Bestatin	-5.46	98.81	-6.6	0.41	-6.2	726.026
2	Sitagliptin	-9.30	0.152	-8.10	-2.28	-10.39	678.630
3	Chloridoxipoxide	-7.25	4.84	-6.16	-1.72	-7.88	706.802
4	Alprazolam	-6.96	7.94	-7.25	0	-7.26	765.015
5	Ergotamine	-6.65	13.33	-8	0.2	-7.8	1139.616
6	Dihydro ergotamine	-6.33	22.78	-8.28	1.21	-7.08	1209.638
7	4,7 Dimethyl 1,10 phenanthroline	-6.23	27.24	-6.06	-0.16	-6.23	577.074
8	9,4hydroxy phenanthroline	-5.61	77.01	-6.19	0.28	-5.91	617.481
9	Camptothecin	-5.53	88.64	-6.55	1.12	-5.43	788.058