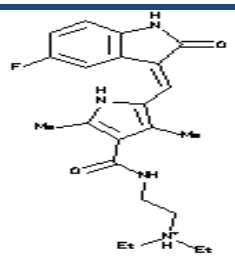
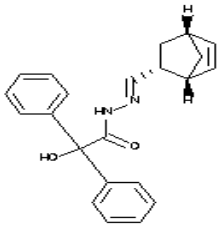
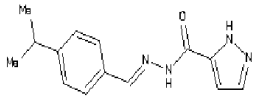
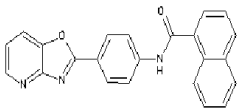
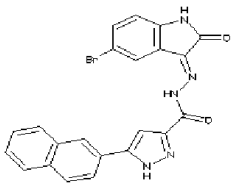
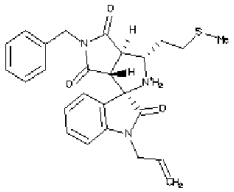
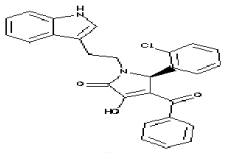
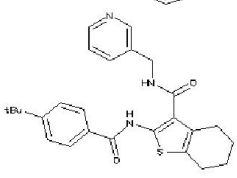
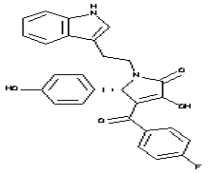
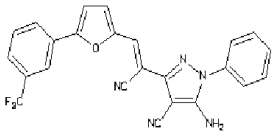
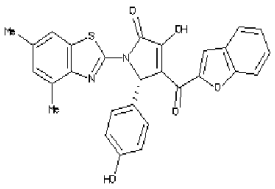
BIOINFORMATION open access

Supplementary material:

Table 1: Virtual screening and Docking results of top 10 molecules with their ZINC ID, IUPAC names, 2D- structures and chemgauss4 scores, Binding energy, Ligand Efficiency, Electrostatic Energy and Hydrogen bonds compared against Sunitinib (Reference Molecule).

S. No.	ZINC ID/ IUPAC Name	2D- STRUCTURE	CHEM GAUSS 4 SCORE	Binding Energy	Ligand Efficiency	Electrostatic Energy	No. of hydrogen bonds
1.	Sunitinib (Z)-N-(2-(Diethylamino)ethyl)-5-((5-fluoro-2-oxoindolin-3-ylidene)methyl)-2,4-dimethyl-1H-pyrrole-3-carboxamide		---	-3.18	-0.11	-0.98	1
2.	ZINC04652104 N'-[(E)-bicyclo[2.2.1]hept-5-en-2-ylmethylidene]-2-hydroxy-2,2-diphenylacetohydrazide		-11.532516	-3.41	-0.13	-0.4	1
3.	ZINC00484682 N'-(4-isopropylbenzylidene)-1H-pyrazole-5-carbohydrazide		-11.364313	-4.15	-0.22	-0.21	2
4.	ZINC00677022 N-(4-[1,3]oxazolo[4,5-b]pyridin-2-ylphenyl)-1-naphthamide		-11.015993	-3.62	-0.13	-0.23	1
5.	ZINC09065134 N'-[(3E)-5-bromo-2-oxo-1,2-dihydro-3H-indol-3-ylidene]-3-(naphthalen-2-yl)-1H-pyrazole-5-carbohydrazide		-10.864721	-4.76	-0.16	-0.48	2
6.	ZINC08439539 1'-allyl-2-benzyl-4-[2-(methylsulfanyl)ethyl]-1',3a,3',4,6,6a-hexahydrospiro(pyrrolo[3,4-c]pyrrole-6,3'-[2'H]-indole)-1,2',3(2H,3aH)-trione		-10.814221	-2.61	-0.08	-0.5	2
7.	ZINC00626508 4-benzoyl-5-(2-chlorophenyl)-3-hydroxy-1-[2-(1H-indol-3-yl)ethyl]-1,5-dihydro-2H-pyrrol-2-one		-10.766582	-3.33	-0.1	-0.38	2
8.	ZINC05944355 2-{[(4-tert-butylphenyl)carbonyl]amino}-N-(pyridin-3-ylmethyl)-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxamide		-10.676544	-4.88	-0.15	-0.15	1
9.	ZINC01414763 4-[(4-fluorophenyl)carbonyl]-3-hydroxy-5-(4-hydroxyphenyl)-1-[2-(1H-indol-3-yl)ethyl]-1,5-dihydro-2H-pyrrol-2-one		-10.668797	-3.06	-0.09	-0.12	3

10.	ZINC08424401 5-amino-3-[(Z)-1-cyano-2-{5-[3-(trifluoromethyl)phenyl]furan-2-yl}ethenyl]-1-phenyl-1H-pyrazole-4-carbonitrile		-10.663716	-3.55	-0.11	-0.27	0
11.	ZINC00703128 4-(1-benzofuran-2-ylcarbonyl)-1-(4,6-dimethyl-1,3-benzothiazol-2-yl)-3-hydroxy-5-(4-hydroxyphenyl)-1,5-dihydro-2H-pyrrol-2-one		-10.663416	-3.71	-0.1	-0.33	3