#Ligand	TotalEnergy	VDW	
cav7b3o_NAG-Roccustyrna_fr1-0.pdb	-66.829	-66.829	
cav7b3o_NAG-Roccustyrna_fr2-0.pdb	-916.588	-916.588	
cav7b3o_NAG-Roccustyrna_fr3-0.pdb	254.912	254.912	
cav7b3o_NAG-Roccustyrna_fr4-0.pdb	-699.511	-699.511	
cav7b3o_NAG-Roccustyrna_fr5-0.pdb	433.157	433.157	
cav7b3o_NAG-Roccustyrna_fr6-0.pdb	-836.801	-836.801	
cav7b3o_NAG-Roccustyrna_fr7-0.pdb	-921.261	-921.261	
cav7b3o_NAG-Zanamivir_CID_60855-0.pdb	-760.641	-760.641	
cav7b3o_NAG-Vidarabine_CID_21704-0.pdb	-748.082	-748.082	
cav7b3o_NAG-Valganciclovir_CID_135413535-0.pdb	440.317	440.317	
cav7b3o_NAG-Tenofovir_CID_464205-0.pdb	-651.681	-651.681	
cav7b3o_NAG-Taribavirin_CID_451448-0.pdb	-683.847	-683.847	
cav7b3o_NAG-Sorivudine_CID_5282192-0.pdb	827.878	827.878	
cav7b3o_NAG-Sofosbuvir_CID_45375808-0.pdb	365.728	365.728	
cav7b3o_NAG-Ritonavir_CID_392622-0.pdb	187.185	187.185	
cav7b3o_NAG-Penciclovir_CID_135398748-0.pdb	-701.763	-701.763	
cav7b3o_NAG-Nelfinavir_CID_64143-0.pdb	416.592	416.592	
cav7b3o_NAG-Merimepodib_CID_153241-0.pdb	-906.535	-906.535	
cav7b3o_NAG-Maribavir_CID_471161-0.pdb	-773.868	-773.868	
cav7b3o_NAG-Lopinavir_CID_92727-0.pdb	405.558	405.558	
cav7b3o_NAG-Indinavir_CID_5362440-0.pdb	-877.687	-877.687	
cav7b3o_NAG-Inarigivir_CID_6912016-0.pdb	-899.455	-899.455	
cav7b3o_NAG-Galidesivir_CID_10445549-0.pdb	-71.061	-71.061	
cav7b3o_NAG-Famciclovir_CID_3324-0.pdb	931.425	931.425	
cav7b3o_NAG-Faldaprevir_CID_42601552-0.pdb	249.487	249.487	
cav7b3o_NAG-Darunavir_CID_213039-0.pdb	-782.833	-782.833	
cav7b3o_NAG-Cytarabine_CID_6253-0.pdb	-672.819	-672.819	
cav7b3o_NAG-Boceprevir_CID_10324367-0.pdb	743.783	743.783	
cav7b3o_NAG-Atazanavir_CID_148192-0.pdb	109.706	109.706	
cav7b3o_NAG-Asunaprevir_CID_16076883-0.pdb	-84.684	-84.684	
cav7b3o_NAG-Amprenavir_CID_65016-0.pdb	-968.745	-968.745	
cav7b3o_NAG-GissitorviffirnaTM1-0.pdb	-750.669	-750.669	
cav7b3o_NAG-GissitorviffirnaTM4-0.pdb	-722.111	-722.111	
cav7b3o_NAG-GissitorviffirnaTM6-0.pdb	405.563	405.563	
cav7b3o_NAG-GissitorviffirnaTM7-0.pdb	-836.518	-836.518	
cav7b3o_NAG-GissitorviffirnaTM8-0.pdb	-956.717	-956.717	
cav7b3o_NAG-GissitorviffirnaTM9-0.pdb	-926.811	-926.811	
cav7b3o_NAG-Roccustyrna_gs1-0.pdb	142.473	142.473	
cav7b3o_NAG-Roccustyrna_gs2-0.pdb	-722.258	-722.258	
cav7b3o_NAG-Roccustyrna_gs3-0.pdb	235.026	235.026	
cav7b3o_NAG-Roccustyrna_gs4-0.pdb	-158.093	-158.093	
cav7b3o_NAG-Roccustyrna_gs5-0.pdb	375.218	375.218	
cav7b3o_NAG-Roccustyrna_gs6-0.pdb	-67.403	-67.403	
cav7b3o_NAG-Roccustyrna_gs8-0.pdb	747.658	747.658	

AverConPair

121.304
184.848
982.051
145.278
226.667
141.316
190.571
21
231.053
20.52
218.421
242.941
18.2
24.25
14.12
23.5
21.475
224.242
195.417
14.087
132.889
173.333
224.211
207.391
151.053
142.632
234.706
174.324
101.569
12.902
210.571
213.182
22.05
101.795
140.526
169.474
206.471
183.043
25
116.809
132.745
151.875
22.35
18.34