#Ligand	TotalEnergy	VDW	
cav6w63_X77-Roccustyrna_fr1-0.pdb	-107.309	-107.309	
cav6w63_X77-Roccustyrna_fr2-0.pdb	-928.431	-928.431	
cav6w63_X77-Roccustyrna_fr3-0.pdb	298.096	298.096	
cav6w63_X77-Roccustyrna_fr4-0.pdb	-928.899	-928.899	
cav6w63_X77-Roccustyrna_fr5-0.pdb	279.472	279.472	
cav6w63_X77-Roccustyrna_fr6-0.pdb	-97.628	-97.628	
cav6w63_X77-Roccustyrna_fr7-0.pdb	-101.803	-101.803	
cav6w63_X77-Zanamivir_CID_60855-0.pdb	-671.306	-671.306	
cav6w63_X77-Vidarabine_CID_21704-0.pdb	-867.989	-867.989	
cav6w63_X77-Valganciclovir_CID_135413535-0.pdb	117.198	117.198	
cav6w63_X77-Tenofovir_CID_464205-0.pdb	-746.343	-746.343	
cav6w63_X77-Taribavirin_CID_451448-0.pdb	-752.318	-752.318	
cav6w63_X77-Sorivudine_CID_5282192-0.pdb	-19.902	-19.902	
cav6w63_X77-Sofosbuvir_CID_45375808-0.pdb	920.626	920.626	
cav6w63_X77-Ritonavir_CID_392622-0.pdb	100.496	100.496	
cav6w63_X77-Penciclovir_CID_135398748-0.pdb	-774.458	-774.458	
cav6w63_X77-Nelfinavir_CID_64143-0.pdb	750.347	750.347	
cav6w63_X77-Merimepodib_CID_153241-0.pdb	-934.382	-934.382	
cav6w63_X77-Maribavir_CID_471161-0.pdb	-78.437	-78.437	
cav6w63_X77-Lopinavir_CID_92727-0.pdb	384.976	384.976	
cav6w63_X77-Indinavir_CID_5362440-0.pdb	-998.427	-998.427	
cav6w63_X77-Inarigivir_CID_6912016-0.pdb	-112.232	-112.232	
cav6w63_X77-Galidesivir_CID_10445549-0.pdb	-700.998	-700.998	
cav6w63_X77-Famciclovir_CID_3324-0.pdb	894.867	894.867	
cav6w63_X77-Faldaprevir_CID_42601552-0.pdb	295.914	295.914	
cav6w63_X77-Darunavir_CID_213039-0.pdb	-993.399	-993.399	
cav6w63_X77-Cytarabine_CID_6253-0.pdb	-763.034	-763.034	
cav6w63_X77-Boceprevir_CID_10324367-0.pdb	917.605	917.605	
cav6w63_X77-Atazanavir_CID_148192-0.pdb	230.683	230.683	
cav6w63_X77-Asunaprevir_CID_16076883-0.pdb	-774.514	-774.514	
cav6w63_X77-Amprenavir_CID_65016-0.pdb	-914.979	-914.979	
cav6w63_X77-GissitorviffirnaTM1-0.pdb	-750.278	-750.278	
cav6w63_X77-GissitorviffirnaTM4-0.pdb	-800.626	-800.626	
cav6w63_X77-GissitorviffirnaTM6-0.pdb	159.089	159.089	
cav6w63_X77-GissitorviffirnaTM7-0.pdb	-95.747	-95.747	

AverConPair
117.536
212.727
172.564
178.889
171.176
175.526
201.429
178.261
287.368
17.36
236.316
280.588
18.1
183.611
5.74
257.778
26.5
185.455
207.917
876.087
159.111
195.128
242.105
146.087
167.544
185.263
288.235
218.919
100.196
129.216
202.571
204.091
26.7
146.154
164.211