




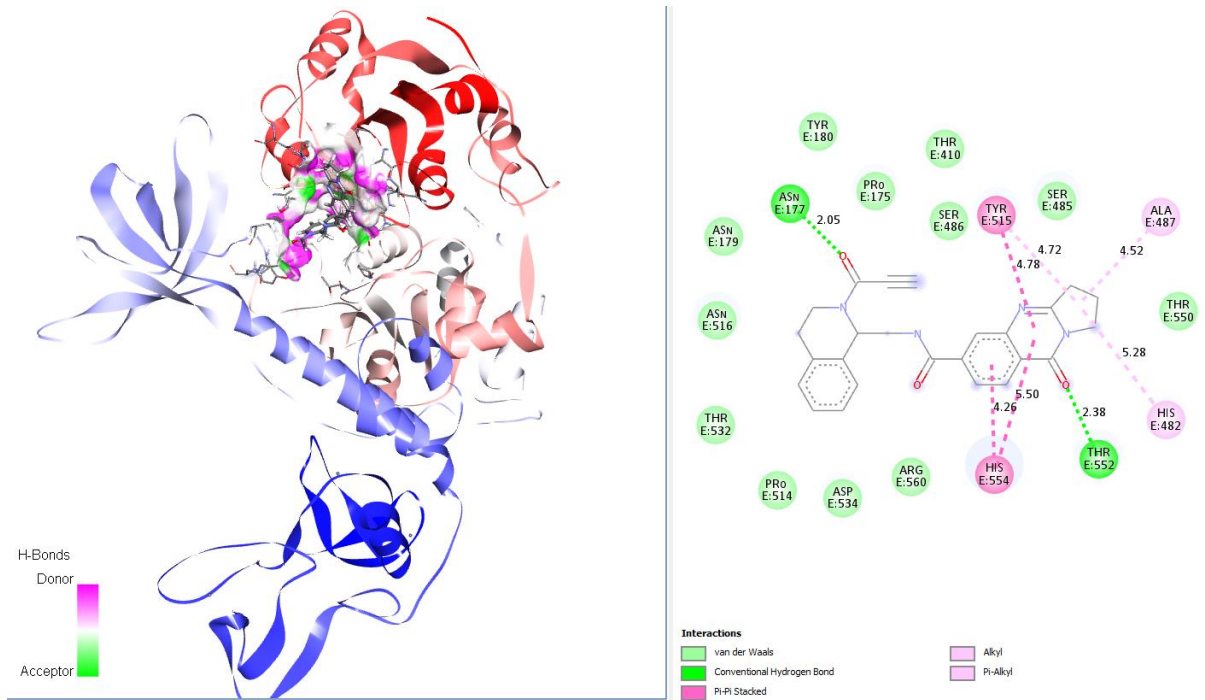








EN300-06233

Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
	Compound 583	CFCC(N1CCc2c3c4c1ccccc4n2)C#CC	Core 6 EN300-06233 + EN300-21202	-8.788888889
	Compound 536	CC(N1CCc2c3c4c1ccccc4n2)C#CC	Core 6 EN300-06233 + EN300-18074	-8.733333333
	Compound 535	CC(NCC1c2c3c4c1ccccc4n2)C#CC	Core 6 EN300-18074 + EN300-06233	-8.466666667
	Compound 656	CC#CC(N1CCc2c3c4c1ccccc4n2)C#CC	Core 6 EN300-06233 + EN300-91328	-8.177777778
	Compound 582	CFCC(NCC1c2c3c4c1ccccc4n2)C#CC	Core 6 EN300-21202 + EN300-06233	-8.144444444

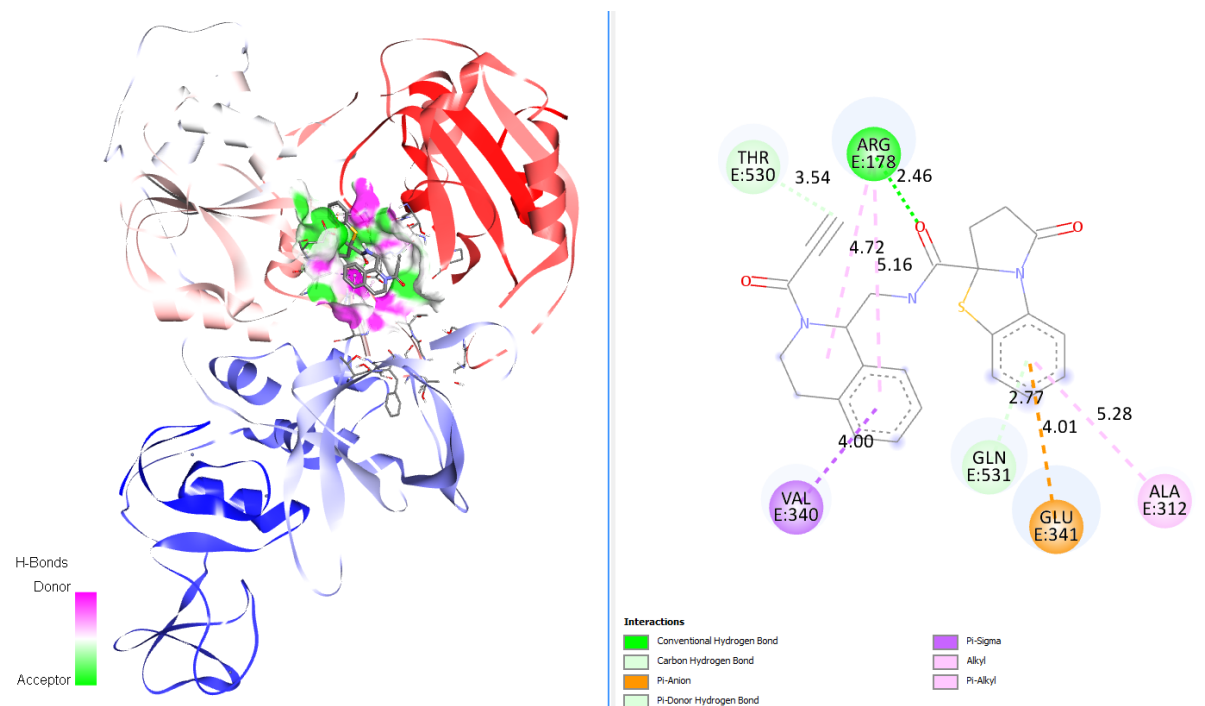
Example compound 583, -9.1 kcal/mol



EN300-10273

Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
	Compound 435	C#CC(N1CCc2ccccc12)C(=O)c3ccccc3	Core 6 EN300-10273 + EN300-21202	-8.62222222
	Compound 434	C#CC(NCC1c2ccccc12)C(=O)c3ccccc3	Core 6 EN300-21202 + EN300-10273	-8.11111111
	Compound 378	CC(NCC1c2ccccc12)C(=O)c3ccccc3	Core 6 EN300-18074 + EN300-10273	-8.1
	Compound 517	CC#CC(N1CCc2ccccc12)C(=O)c3ccccc3	Core 6 EN300-10273 + EN300-91328	-8.03333333
	Compound 516	CC#CC(NCC1c2ccccc12)C(=O)c3ccccc3	Core 6 EN300-91328 + EN300-10273	-8.02222222
	Compound 379	CC(N1CCc2ccccc12)C(=O)c3ccccc3	Core 6 EN300-10273 + EN300-18074	-8.02222222

Example compound 435, -8.9 kcal/mol

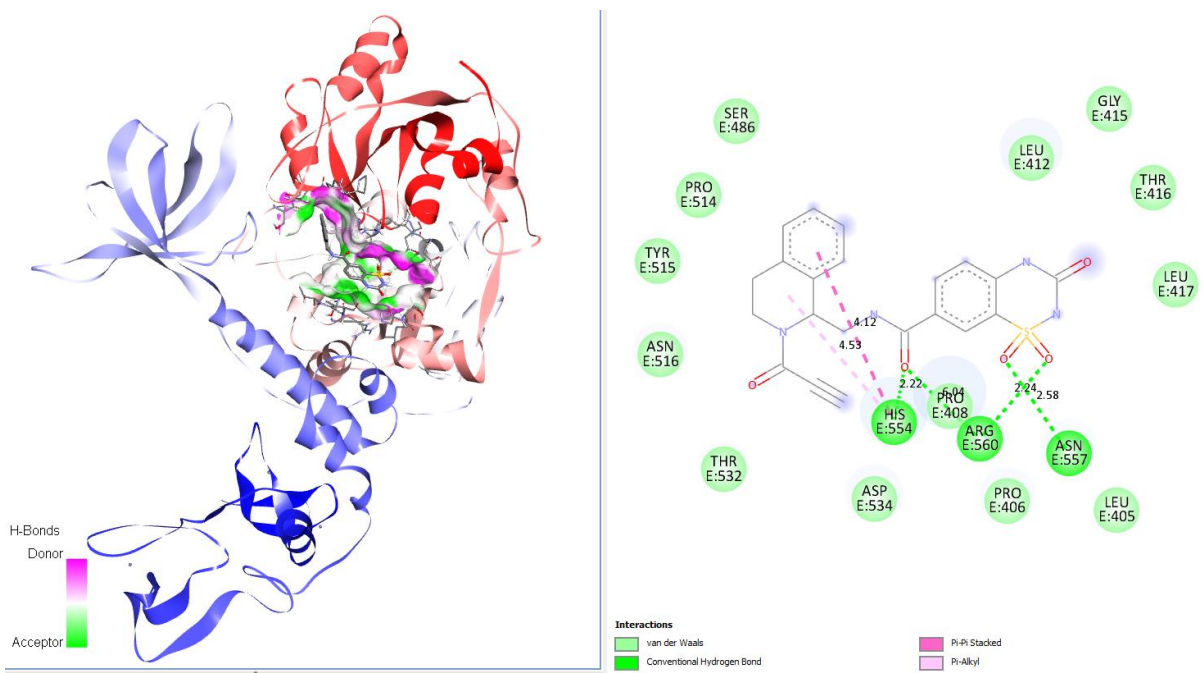


EN300-1703690



Table	Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
1		Compound 16	C#CC(N1CCc2c	Core 6 EN300-1703690 + EN300-21202	-8.896666667
2		Compound 6	CC(N1CCc2c	Core 6 EN300-1703690 + EN300-18074	-8.533333333
3		Compound 5	CC(NCC1c2c	Core 6 EN300-18074 + EN300-1703690	-8.355555556
4		Compound 15	C#CC(NCC1c	Core 6 EN300-21202 + EN300-1703690	-8.111111111
5		Compound 42	CC#CC(N1CC	Core 6 EN300-1703690 + EN300-91328	-8.044444444

Structures	Core 6 EN300-1703690 + EN300-21202	Core 6 EN300-1703690 + EN300-18074	Core 6 EN300-18074 + EN300-1703690	Core 6 EN300-21202 + EN300-1703690	Core 6 EN300-1703690 + EN300-91328
Molecule Name: Compound 16 RuVINA, kcal/mol): -8.89666667	Molecule Name: Compound 6 RuVINA, kcal/mol): -8.53333333	Molecule Name: Compound 5 RuVINA, kcal/mol): -8.35555556	Molecule Name: Compound 15 RuVINA, kcal/mol): -8.11111111	Molecule Name: Compound 42 RuVINA, kcal/mol): -8.04444444	

Example compound 16, -9.3 kcal/mol

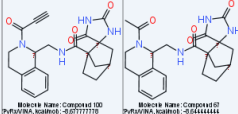


EN300-11687666

Table	Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
1		Compound 100	C#CC1N1CCCc2c1	Core 6 EN300-11687666 + EN300-21202	-8.677777778
2		Compound 67	CC1N1CCCc2c1	Core 6 EN300-11687666 + EN300-18074	-8.644444444

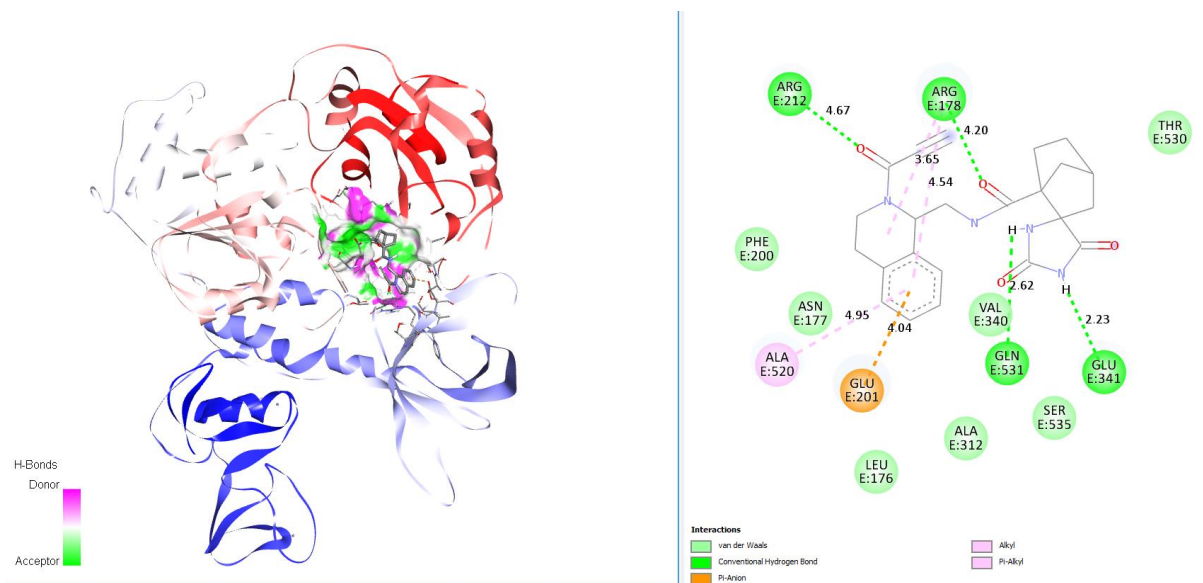
Structures

Core 6 EN300-11687666 + EN300-21202 Core 6 EN300-11687666 + EN300-18074






Molecule Name: Compound 100 Molecule Name: Compound 67
 Pyruvina Acetate Pyruvina Acetate
 -8.677777778 -8.644444444

Example compound 100, -9.3 kcal/mol.

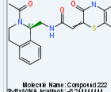


EN300-6750792

Table	Structure	Molecule Name	smiles	ID	Average bindi ng energy (kcal/mol)
1		Compound 222	CC(N1CCc2c1	Core 6 EN300-6750792 + EN300-18074	-8.244444444
2		Compound 223	CC(NCC1c2c1	Core 6 EN300-18074 + EN300-6750792	-8.066666667
3		Compound 287	C#CC(N1OCc1	Core 6 EN300-6750792 + EN300-21202	-8


Structures

Core 6 EN300-6750792 + EN300-18074



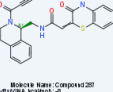
Block6 Rank: Compound 222
PylarVWA kcal/mol: -8.244444444

Core 6 EN300-18074 + EN300-6750792



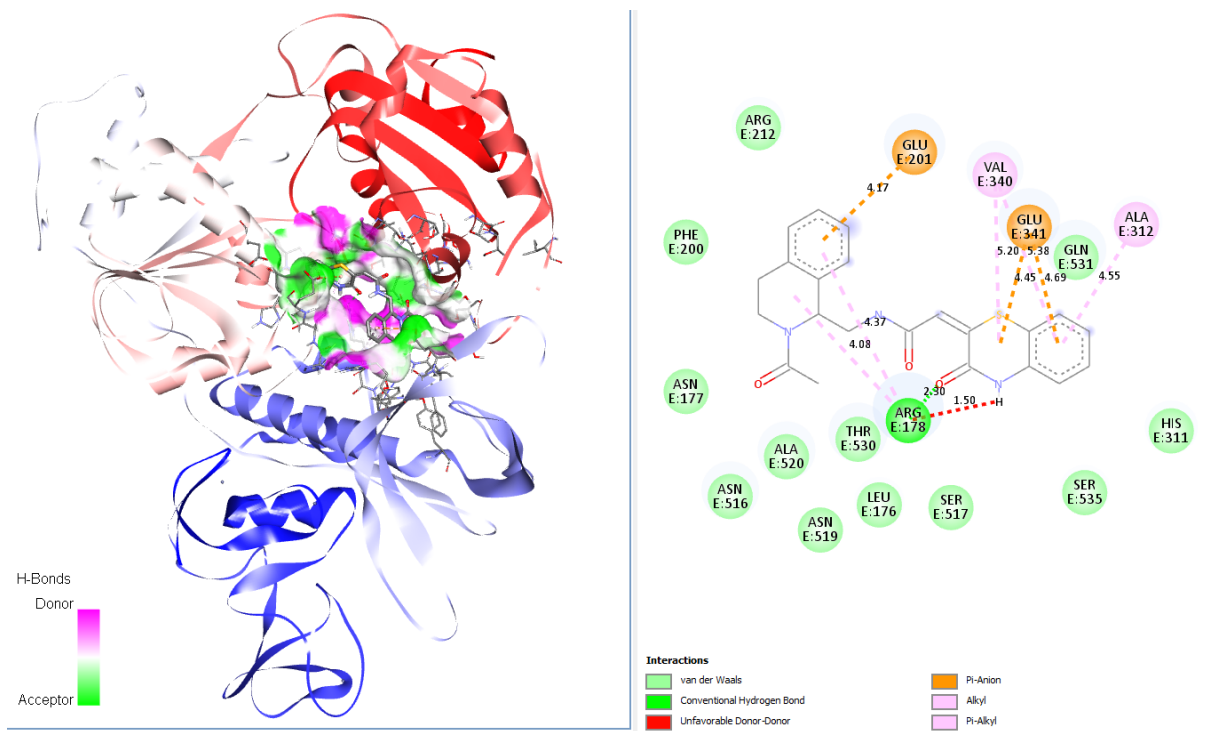
Block6 Rank: Compound 223
PylarVWA kcal/mol: -8.066666667

Core 6 EN300-6750792 + EN300-21202








Block6 Rank: Compound 287
PylarVWA kcal/mol: -8

Example compound 222, -8.7 kcal/mol.



EN300-113123

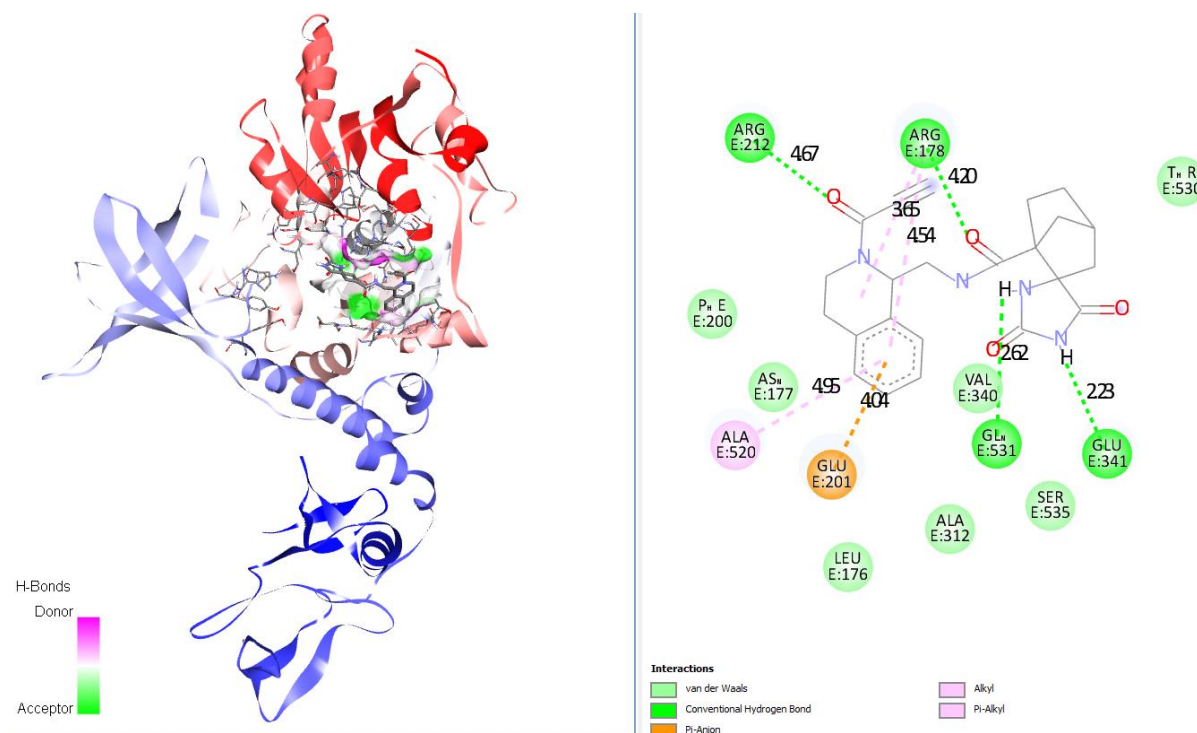
Table	Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
1		Compound 40	C#CC(N1CCC	Core 6 EN300-113123 + EN300-21202	-8.155555566
2		Compound 39	C#CC(NCC1c	Core 6 EN300-21202 + EN300-113123	-8.033333333

Structures	Core 6 EN300-113123 + EN300-21202	Core 6 EN300-21202 + EN300-113123
		

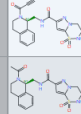
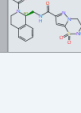
Molecule Name: Compound 40
PyFuVWA, kcal/mol: -8.155555566

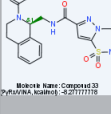
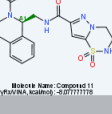
Molecule Name: Compound 39
PyFuVWA, kcal/mol: -8.033333333

Example compound 40, -8.7 kcal/mol.

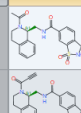
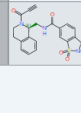


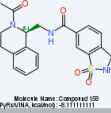
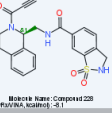
EN300-754603

Table	Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
1		Compound 33	C#CC(N1CCc2c1	Core 6 EN300-754603 + EN300-21202	-8.277777778
2		Compound 11	CC(N1CCc2c1	Core 6 EN300-754603 + EN300-18074	-8.077777778





Structures
<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p>Core 6 EN300-754603 + EN300-21202</p>  <p>Molecule Name: Compound 33 PyPLUVINA_Ischem03_2711111118</p> </div> <div style="text-align: center;"> <p>Core 6 EN300-754603 + EN300-18074</p>  <p>Molecule Name: Compound 11 PyPLUVINA_Ischem03_2711111118</p> </div> </div>

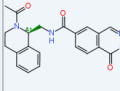
EN300-26871972

Table	Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
1		Compound 158	CC(N1CCc2c1	Core 6 EN300-26871972 + EN300-18074	-8.111111111
2		Compound 228	C#CC(N1CCc2c1	Core 6 EN300-26871972 + EN300-21202	-8.1

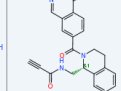
Structures
<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p>Core 6 EN300-26871972 + EN300-18074</p>  <p>Molecule Name: Compound 158 PyPLUVINA_Ischem03_2711111111</p> </div> <div style="text-align: center;"> <p>Core 6 EN300-26871972 + EN300-21202</p>  <p>Molecule Name: Compound 228 PyPLUVINA_Ischem03_2711111111</p> </div> </div>

EN300-6758811

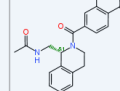
Structure	Molecule Name	smiles	ID	Average binding energy (kcal/mol)
	Compound 248	<chem>CC(N)CCc2c</chem>	Core 6 EN300-6758811 + EN300-18074	-8.165666667
	Compound 311	<chem>C#CC(N)CCc2c</chem>	Core 6 EN300-21202 + EN300-6758811	-8.1
	Compound 249	<chem>CC(N)CCc2c</chem>	Core 6 EN300-18074 + EN300-6758811	-8.077777778
	Compound 310	<chem>C#CC(N)CCc2c</chem>	Core 6 EN300-6758811 + EN300-21202	-8.066666667



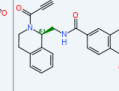
Molecule Name: Compound 248
k_uVINA, kcal/mol: -8.166666667



Molecule Name: Compound 311
k_uVINA, kcal/mol: -8.1



Molecule Name: Compound 249
k_uVINA, kcal/mol: -8.077777778



Molecule Name: Compound 310
k_uVINA, kcal/mol: -8.066666667