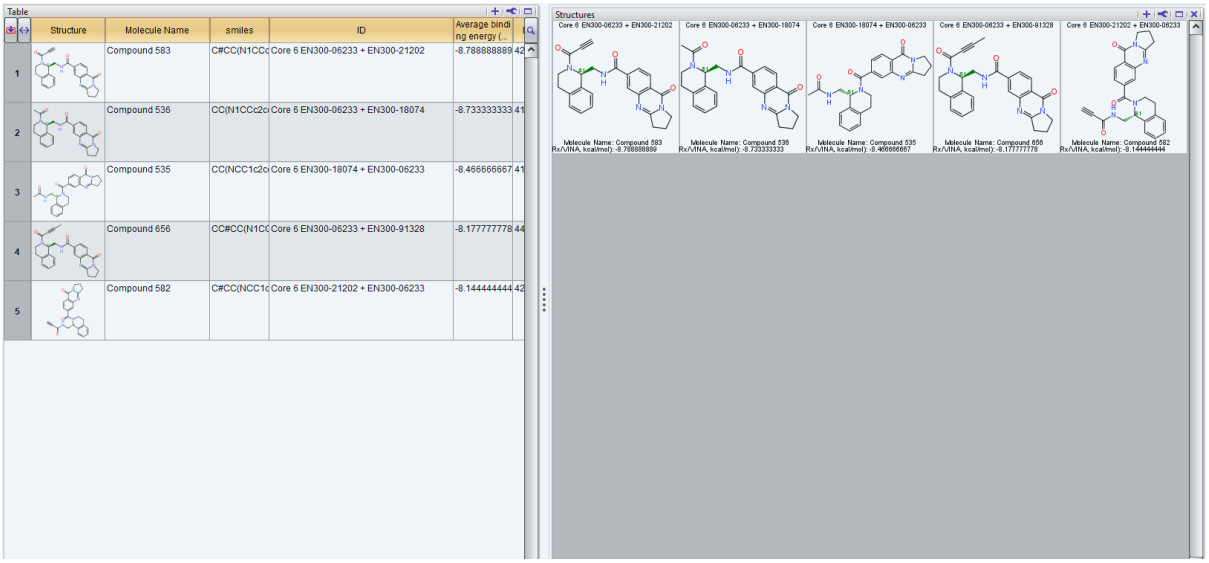
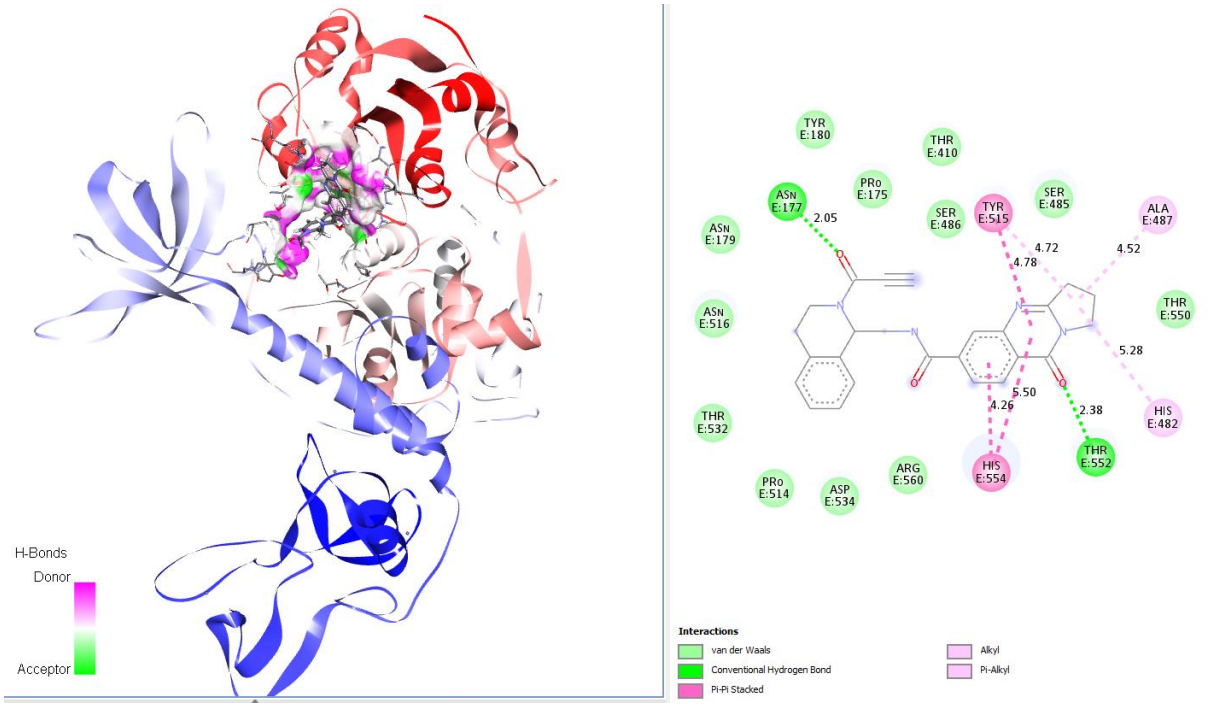
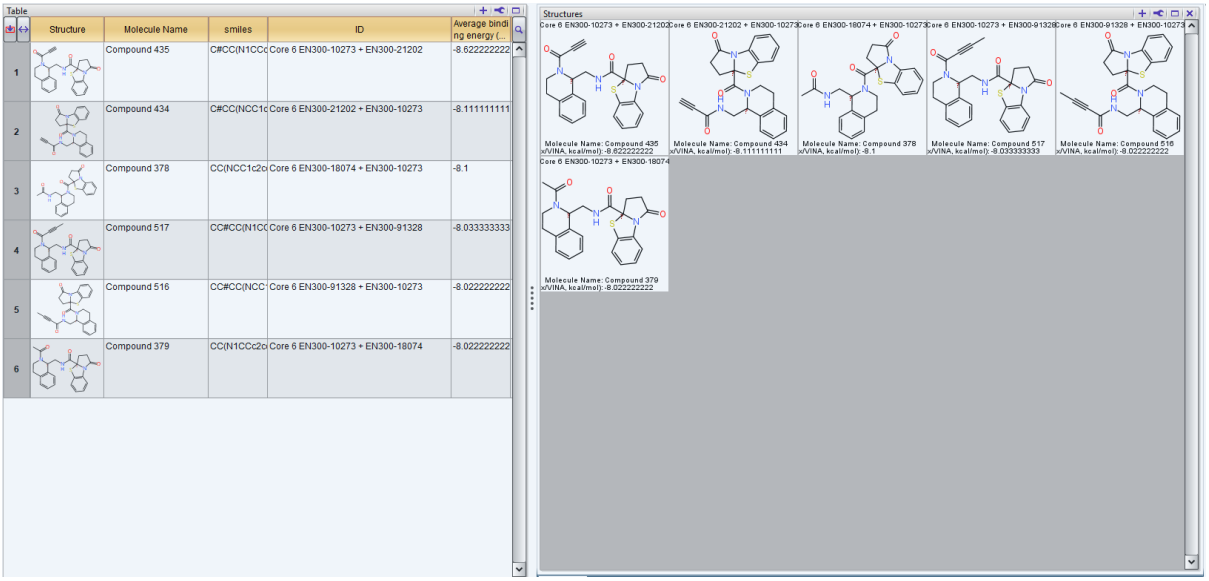
EN300-06233



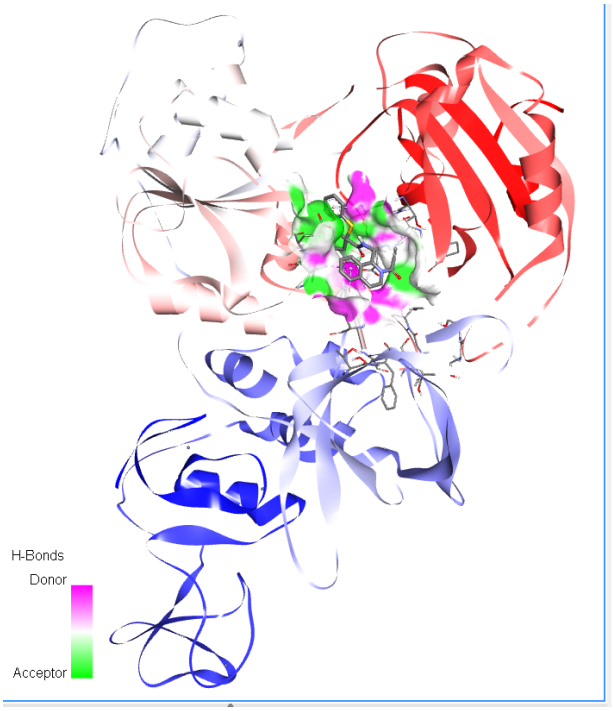
Example compound 583, -9.1 kcal/mol

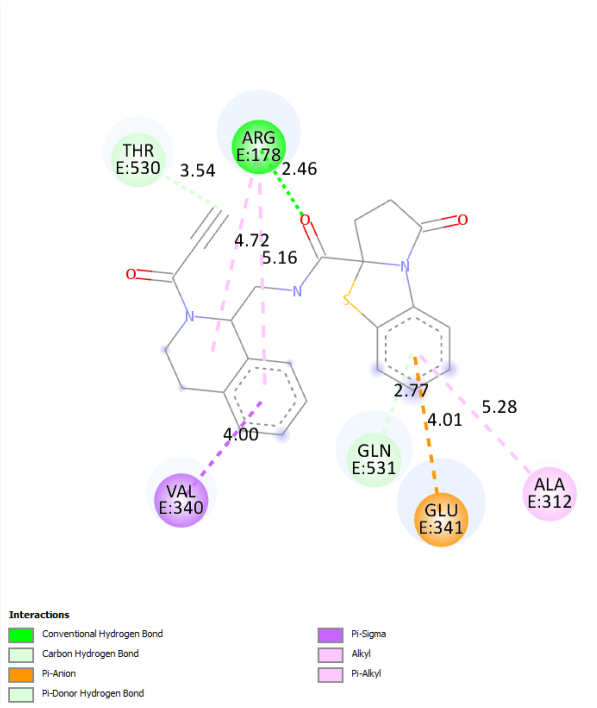


EN300-10273

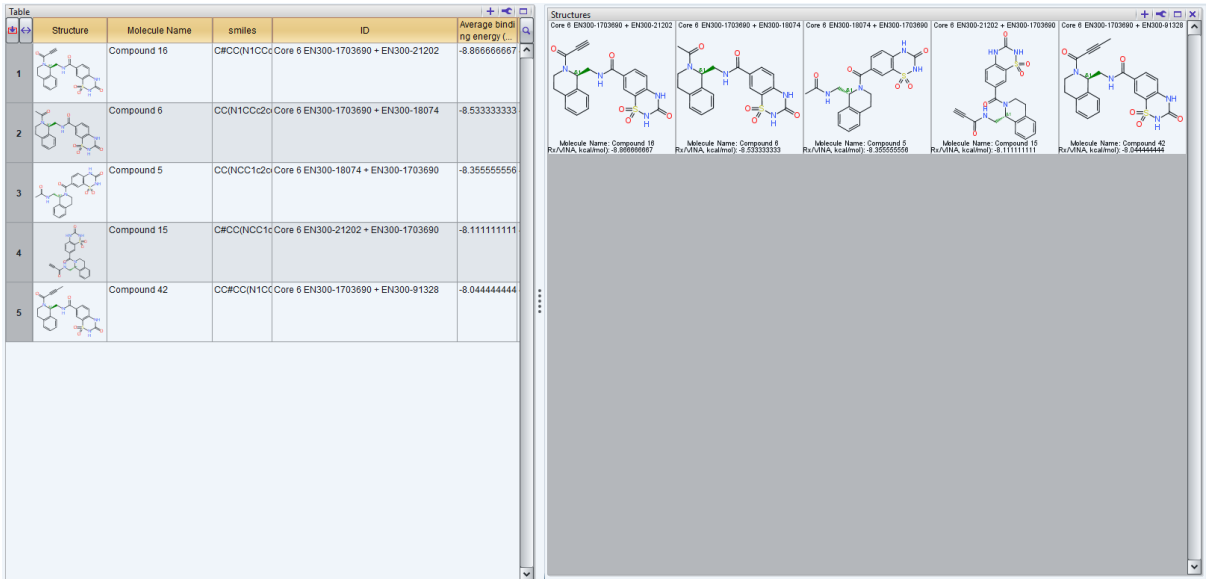


Example compound 435, -8.9 kcal/mol

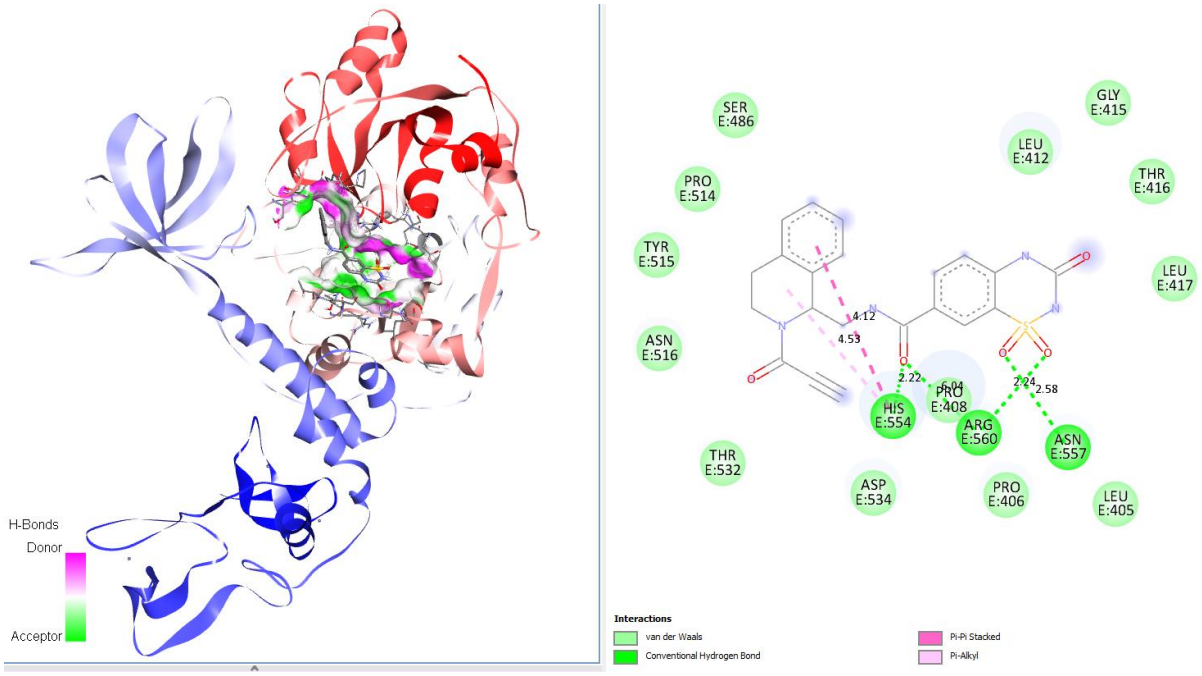




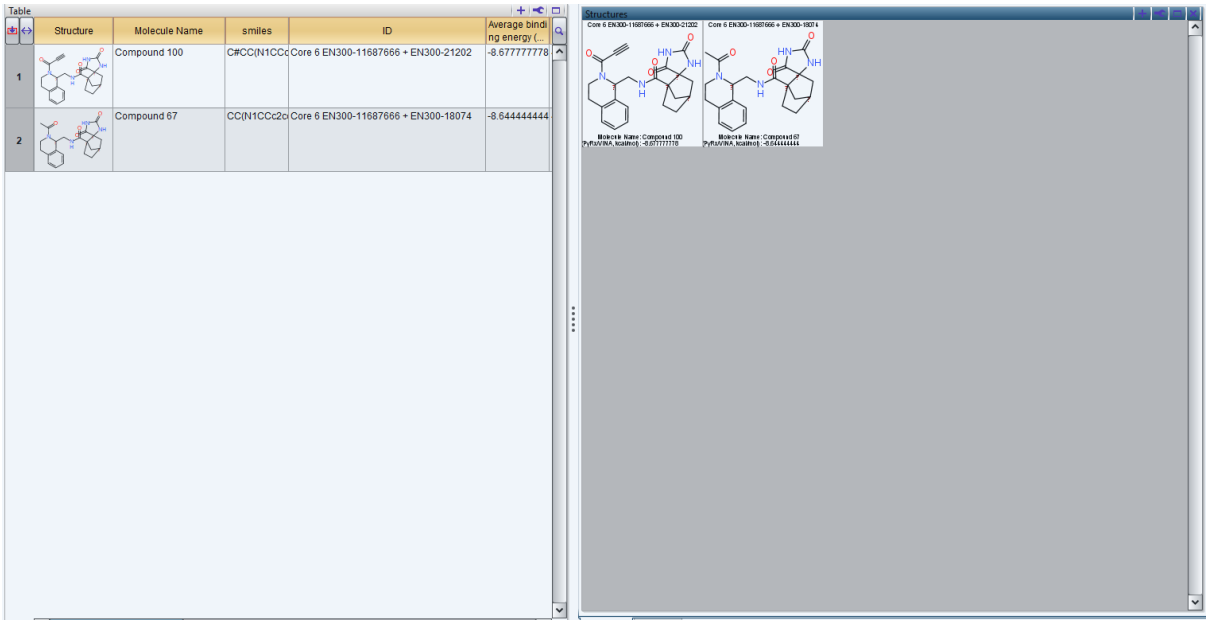
EN300-1703690



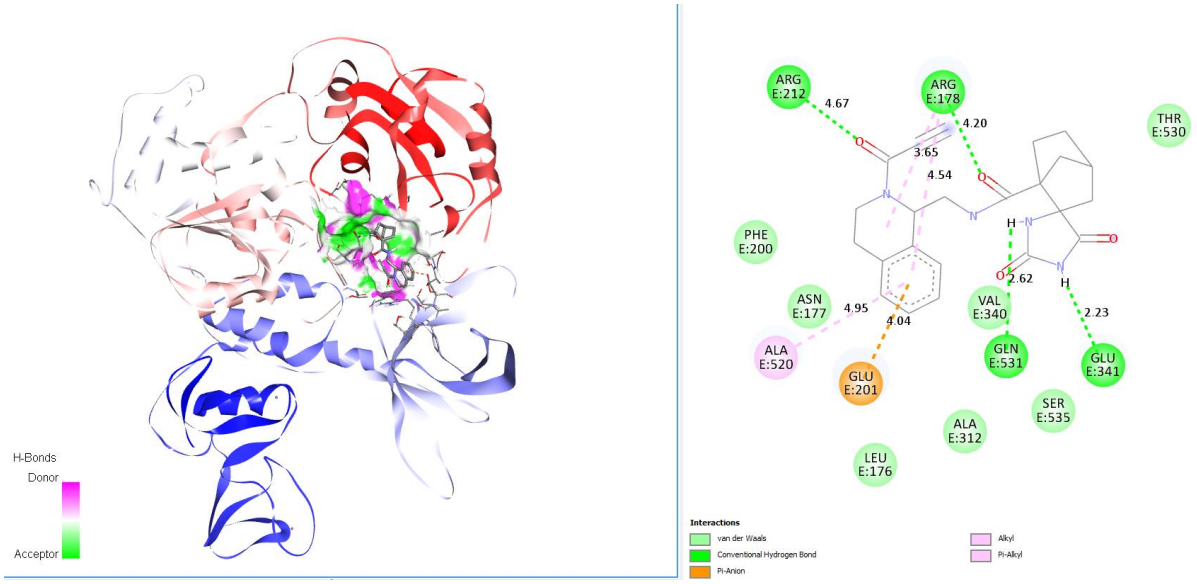
Example compound 16, -9.3 kcal/mol



EN300-11687666



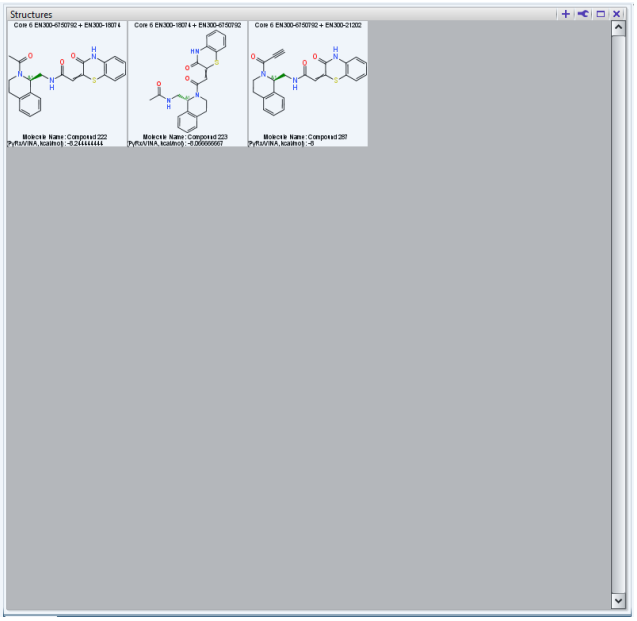
Example compound 100, -9.3 kcal/mol.



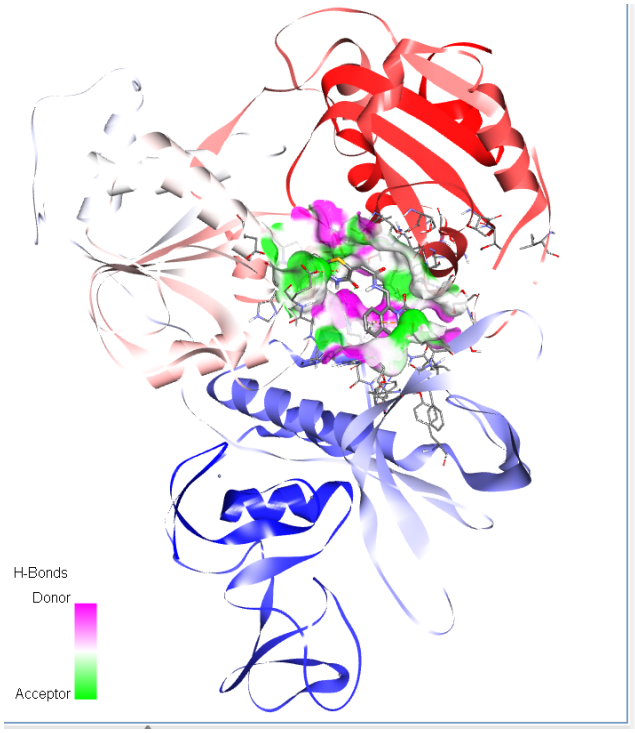
EN300-6750792

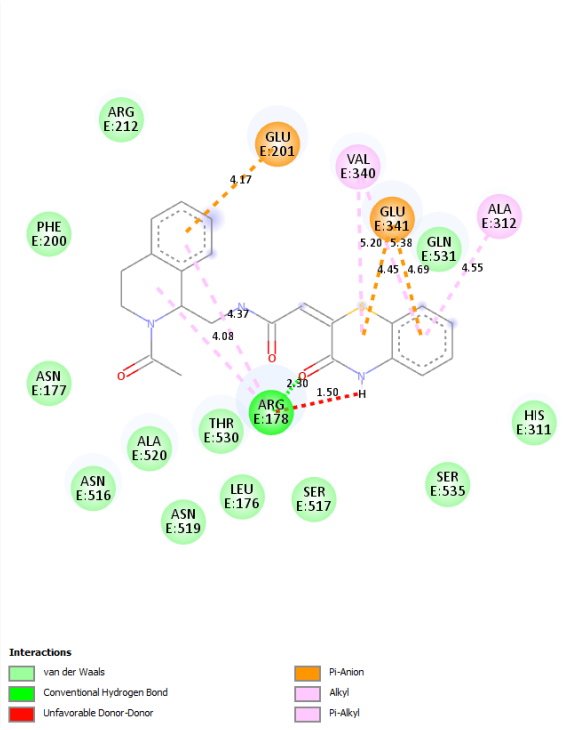
Table

	Structure	Molecule Name	smiles	ID	Average binding energy (...
1		Compound 222	CC(N1CCc2c	Core 6 EN300-6750792 + EN300-18074	-8.244444444
2		Compound 223	CC(NCC1c2c	Core 6 EN300-18074 + EN300-6750792	-8.066666667
3		Compound 287	C#CC(N1CCc	Core 6 EN300-6750792 + EN300-21202	-8

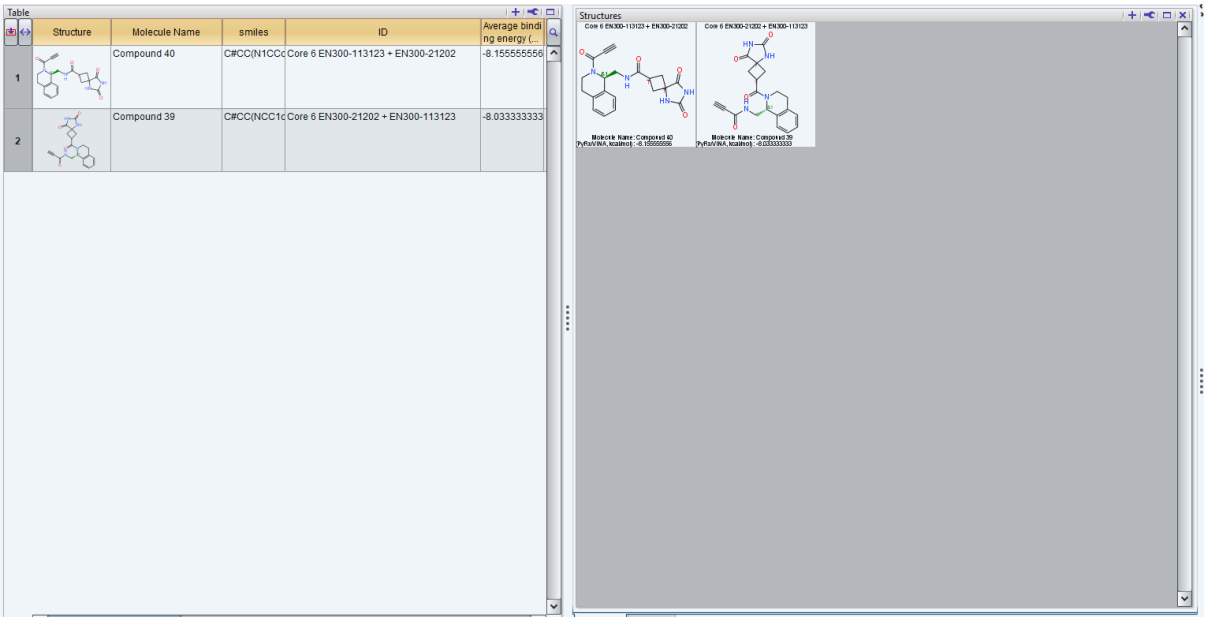


Example compound 222, -8.7 kcal/mol.

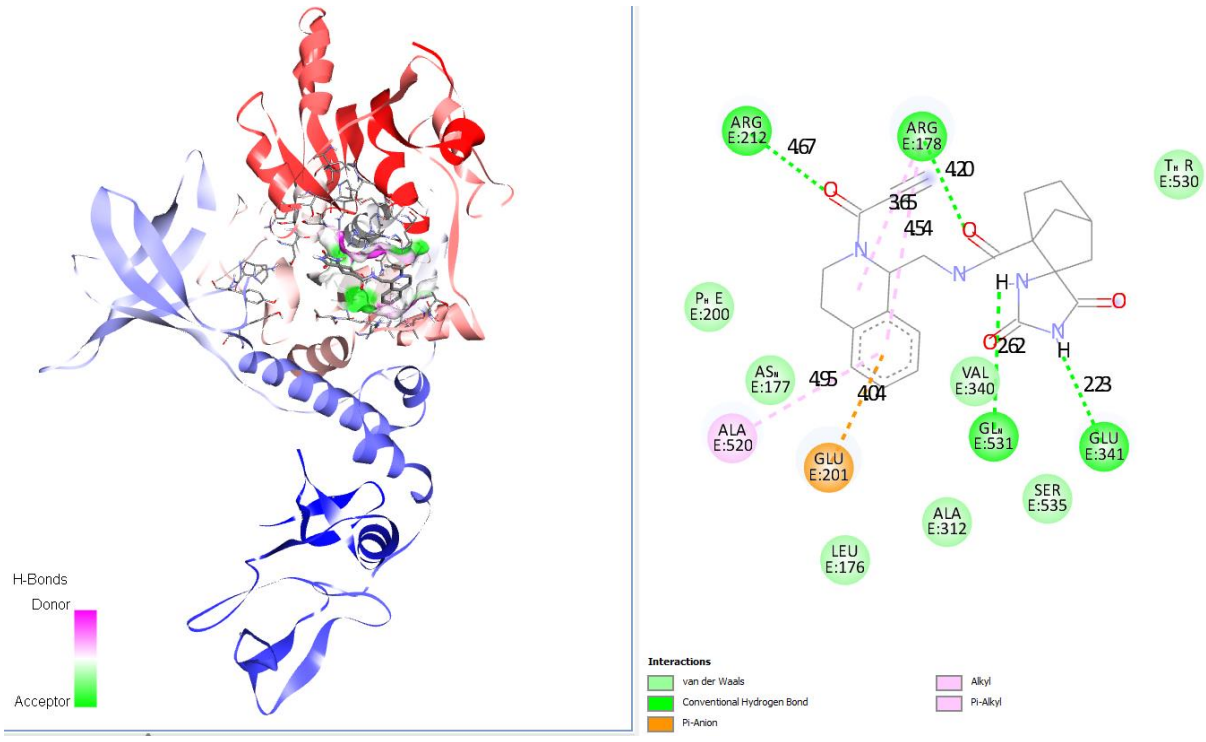




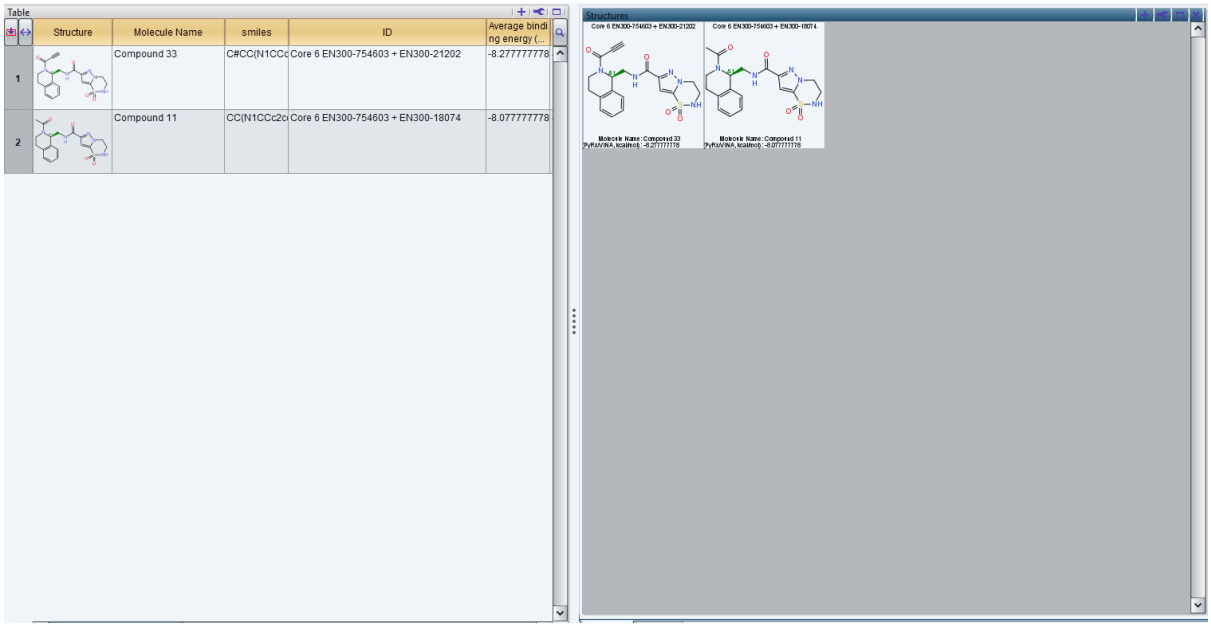
EN300-113123



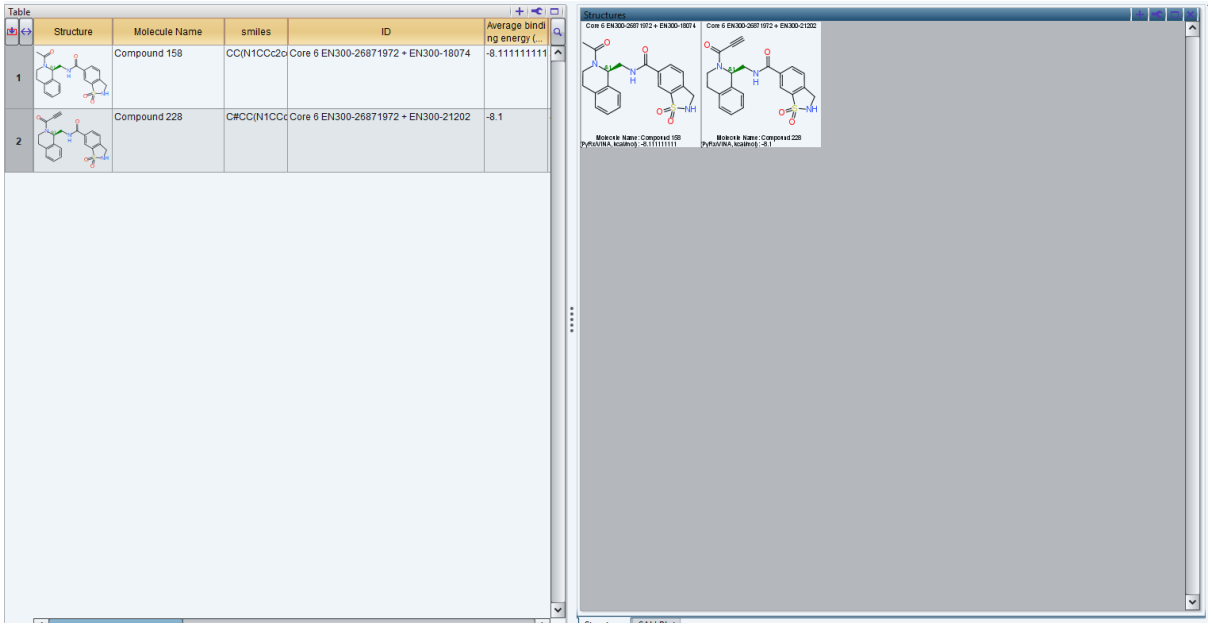
Example compound 40, -8.7 kcal/mol.



EN300-754603



EN300-26871972



EN300-6758811