Absolute Binding Free Energies (kcal/mol)

Model	igb=1	igb=2	igb=5	pb
LIG	-30.0639	-10.3997	-2.5644	21.0105
ZINC19169954	21.2655	24.4560	21.9282	50.7823
ZINC19369903	5.7792	9.7970	10.3785	41.2878
ZINC19369905	0.8506	4.3569	3.4888	30.6430

Relative Binding Free Energies (kcal/mol)

Model	igb=1	igb=2	igb=5	pb	docking
LIG	0.0000	0.0000	0.0000	0.0000	-9.7
ZINC19369905	30.9145	14.7566	6.0532	9.6325	-10.9
ZINC19369903	35.8431	20.1967	12.9429	20.2773	-11.0
ZINC19169954	51.3294	34.8557	24.4926	29.7718	-5.7

Conclusion: autodock-vina docking scoring function cannot discriminate LIG, ZINC19369905 and ZINC19369903, while all the four GB/PB models can explain why the native ligand "LIG" is much better than the compounds identified by docking scoring.