

Compound Stability Classification Summary

Compound ID	DrugBank Ref	ΔG (kJ/mol)	RMSD lig (Å)	H-bonds	RMSF pocket (Å)	Stability
57582435	DB07874	-33.21	4.38	0.05	1.101	Marginal
15167710	DB07738	-29.21	3.92	0.01	1.185	Marginal
24768527	DB07019	-28.21	3.20	1.92	1.339	Stable
67537520	DB07874	-27.61	5.96	0.50	1.393	Marginal
67538061	DB07874	-26.92	6.59	1.06	1.224	Marginal
52944109	DB07874	-25.60	5.61	0.89	1.554	Marginal
52948174	DB07874	-25.21	5.06	1.23	1.449	Marginal
52946915	DB07874	-24.89	4.06	1.17	1.345	Marginal
52940810	DB07874	-24.84	4.81	0.10	1.181	Marginal
16113857	DB07519;DB07874	-24.17	5.79	0.07	1.871	Marginal
59305370	DB07874	-24.05	4.86	0.37	1.801	Marginal
67538655	DB07874	-24.05	3.24	1.48	1.671	Marginal
71713952	DB12285	-22.84	6.37	0.70	1.107	Marginal
67538244	DB07874	-22.51	4.69	0.48	1.960	Marginal
16114585	DB07874	-22.45	5.33	0.75	1.294	Marginal
59790311	DB07519;DB07874	-22.28	6.55	1.15	1.347	Marginal
67537716	DB07874	-21.81	4.87	0.25	1.632	Marginal
67538838	DB07874	-21.68	3.02	1.17	1.329	Marginal
44177328	DB07993	-20.91	8.39	0.76	1.831	Marginal
52945793	DB07874	-20.51	4.76	0.08	1.548	Marginal
16114587	DB07874	-20.46	4.65	0.60	1.648	Marginal
52940974	DB07519;DB07874	-19.09	5.13	0.02	1.360	Marginal
52942848	DB07874	-18.96	4.85	1.15	1.333	Marginal
42628075	DB07415	-16.61	2.41	1.05	1.280	Marginal
3663276	DB07303	-15.62	3.71	0.74	1.316	Marginal
972703	DB07737	-14.53	3.56	0.28	1.912	Marginal
3083714	DB02378	-14.46	10.83	0.59	1.176	Marginal