

Associated content. Table 1. Coordinates of restricted areas (grid boxes) in Dockthor and Autodock Vina software

Protein	Axis		
	X	Y	Z
Protein Spike Open	200	225	250
Protein Spike Closed	210	213	255
RBD	-27	22	26
Mpro	-20	23	66
NSP 10	75	3	4
NSP 16	87	16	17
Polymerase	-7	30	-30

Associated content. Table 2. Drug and viral interaction proteins.

Drugs	Viral protein
abacavir	Polymerase
adefovir	Polymerase
amprenavir	Main protease
atazanavir	Main protease
daclastavir	Non structural protein 10 and 16
darunavir	Main protease
didanosine	Polymerase
dolutegravir	Spike protein
efavirenz	Polymerase
emtricitabine	Polymerase
enfuvirtide	Spike protein
entecavir	Polymerase
Primaquine phosphate	Spike protein
galidesivir	Polymerase
indinavir	Main protease
lamivudine	Polymerase
lopinavir	Main protease
nelfinavir	Main protease
nevirapine	Polymerase
raltegravir	Spike protein
ribavirin	Polymerase
saquinavir	Main protease
simeprevir	Main protease
sofosbuvir	Polymerase

stavudine	Polymerase
Quinine sulfate	Spike protein
Tenofovir	polymerase
tipranavir	Main protease
veruprevir	Main protease
zanamivir	Spike protein
zidovudin	polymerase
Arbidol	Spike protein
Camostat	Main protease
Crysin	Main protease
Emodin	Spike protein
Favipiravir	Polymerase
nFCCI3	Spike protein
Niclosamine	Spike protein
Oseltamivir	Spike protein
Ganciclovir	Spike protein
Penciclovir	polymerase
Phaitanthrin D	All
Remdesivir	Spike protein
Sovalvi	Spike protein
SSAA09E2	Spike protein
Umefenovir	Spike protein

Associated content. Table 3. Results of Molecular Docking.

Drug	Viral Protein	Platform	Affinity (Kcal/mol)	glob	TVdW	ACE	inside	H-bonds	S L/L	S H/H	S buried	Stotal	Match 1
Dolutegravir	RBD	DockThor		17630	-20978			1.44	55.19	50.19	193.67	319.22	0.3301
Dolutegravir	RBD	PatchDock		-43,96	-18,19	-9,49	0,45	1.25	21.90	67.85	245.63	325.96	0.2753
Dolutegravir	RBD	Autodock Vina	-8.1					0.19	27.78	60.82	204.43	330.12	0.2684
Dolutegravir	Protein Spike Open	DockThor		18470	-16882			0,52	14,62	51,77	154,62	325,76	0,2038
Dolutegravir	Protein Spike Open	PatchDock		-51,76	-14,11	-16,66	0,19	0.01	37.02	68.29	286.83	325.62	0.3234
Dolutegravir	Protein Spike Open	Autodock Vina	-7.5					0.35	21.14	42.40	189.55	330.31	0.1924
Dolutegravir	Protein Spike Closed	DockThor		18110	-19795			1.70	37.28	45.00	174.05	321.83	0.2557
Dolutegravir	Protein Spike Closed	PatchDock		-41,29	-19,35	-5,98	0,5	0.71	14.37	88.42	261.01	325.13	0.3162
Dolutegravir	Protein Spike Closed	Autodock Vina	-9.5					2.11	13.23	73.67	266.39	332.02	0.2617
Enfuvirtide	RBD	DockThor											
Enfuvirtide	RBD	PatchDock		-5,61	-5,07	-3,1	11,94	0.00	0.00	4.24	49.68	3121.46	0.0014
Enfuvirtide	RBD	Autodock Vina	-17.1					1.24	2.91	284.05	482.65	3171.46	0.0905
Enfuvirtide	Protein Spike Open	DockThor											
Enfuvirtide	Protein Spike Open	PatchDock		-10,78	-3,54	-3,44	1,28	0.92	0.00	45.00	90.19	3111.78	0.0145
Enfuvirtide	Protein Spike Open	Autodock Vina	-17.2					1.40	21.46	279.93	442.78	3181.47	0.0947
Enfuvirtide	Protein Spike Closed	DockThor											
Enfuvirtide	Protein Spike Closed	PatchDock		-3,94	-1,54	-1,35	0,81	5.15	112.28	900.81	1432.00	3127.23	0.324
Enfuvirtide	Protein Spike Closed	Autodock Vina	-16.9					3.97	105.19	277.97	475.62	3166.90	0.121
Raltegravir	RBD	DockThor		75454	-19225			0.14	14.11	117.59	182.02	375.11	0.3511
Raltegravir	RBD	PatchDock		-45,02	-20,9	-7,54	1,88	0.40	46.58	84.05	245.57	362.28	0.3606
Raltegravir	RBD	Autodock Vina	-6.8					2.15	34.87	61.58	203.54	369.93	0.2607
Raltegravir	Protein Spike Open	DockThor		76698	-20352			0.31	19.24	117.53	201.39	380.74	0.3592
Raltegravir	Protein Spike Open	PatchDock		-51,64	-12,7	-18,02	0,49	1.81	30.95	95.76	276.45	361.21	0.3508
Raltegravir	Protein Spike Open	Autodock Vina	-8.7					2.39	36.77	92.72	246.96	358.16	0.3615
Raltegravir	Protein Spike Closed	DockThor		75032	-13074			2.88	10.82	98.92	184.68	377.65	0.2906

Raltegravir	Protein Spike Closed	PatchDock		-52,98	-17,57	-14,25	0,34	0.59	50.70	103.04	312.21	362.47	0.4241
Raltegravir	Protein Spike Closed	Autodock Vina	-6.9					0.83	61.26	69.43	191.83	376.32	0.3473
Zanamivir	RBD	DockThor		-19546	0.149			2.77	0.00	108.42	108.42	294.43	0.3682
Zanamivir	RBD	PatchDock		-33,32	-11,77	-8,06	1,53	1.83	0.00	186.71	242.27	294.62	0.6337
Zanamivir	RBD	Autodock Vina	-6.7					4.67	0.00	186.20	245.63	308.16	0.6042
Zanamivir	Protein Spike Open	DockThor		-23254	-10800			0.94	0.00	158.41	171.20	298.15	0.5313
Zanamivir	Protein Spike Open	PatchDock		-41,55	-12,16	-13,63	0,24	0.96	0.00	196.96	254.24	296.64	0.664
Zanamivir	Protein Spike Open	Autodock Vina	-6.7					4.89	0.00	196.71	228.29	293.29	0.6707
Zanamivir	Protein Spike Closed	DockThor		-22346	-1143			2.75	0.00	115.38	151.83	297.15	0.3883
Zanamivir	Protein Spike Closed	PatchDock		-38,59	-14,35	-9,88	0,3	1.50	0.00	180.44	264.11	296.07	0.6095
Zanamivir	Protein Spike Closed	Autodock Vina	-6.4					2.36	0.00	160.57	203.48	307.40	0.5223
Daclastavir	NSP 10	DockThor		2666	-38447			0.98	11.33	106.39	317.59	676.82	0.1739
Daclastavir	NSP 10	PatchDock		-63	-21,57	-16,91	2,88	0.00	6.01	89.24	313.60	623.72	0.1527
Daclastavir	NSP 10	Autodock Vina	-8.4					0.98	24.94	86.26	339.30	642.71	0.173
Daclastavir	NSP 16	DockThor		4273	-27863			1.57	7.47	105.44	293.29	667.45	0.1692
Daclastavir	NSP 16	PatchDock		-57,2	-20,64	-14,58	3,52	0.00	48.48	76.20	372.46	621.57	0.2006
Daclastavir	NSP 16	Autodock Vina	-9.0					0.00	49.24	43.73	243.35	672.58	0.1382
Amprenavir	Main Protease	DockThor		-7246	-16268			3.29	2.28	76.58	182.78	460.05	0.1714
Amprenavir	Main Protease	PatchDock		-46,59	-7,28	-16,6	3,55	0.00	16.14	72.47	315.44	446.26	0.1986
Amprenavir	Main Protease	Autodock Vina	-6.0					2.83	11.96	116.58	225.76	414.11	0.3104
Atazanavir	Main Protease	DockThor		49045	-20881			3.17	4.49	79.24	191.07	621.63	0.1347
Atazanavir	Main Protease	PatchDock		-48,81	-14,27	-13,23	3,61	0.67	34.49	69.30	211.89	610.44	0.17
Atazanavir	Main Protease	Autodock Vina	-6.5					0.00	38.04	82.02	232.59	433.79	0.2768
Darunavir	Main Protease	DockThor		-5143	-17889			1.96	1.39	71.14	189.05	482.45	0.1503
Darunavir	Main Protease	PatchDock		-51,33	-16,88	-16,47	3,5	0.34	37.97	111.33	356.51	501.19	0.2979
Darunavir	Main Protease	Autodock Vina	-6,5					1.73	31.08	142.40	263.35	464.62	0.3734
Etravirine	Main Protease	DockThor	16	12504	-14232			1.96	1.39	71.14	189.05	482.45	0.1503
Etravirine	Main Protease	PatchDock		-43,27	-16	-12,31	3,24	1.88	16.58	132.72	268.60	355.63	0.4198
Etravirine	Main Protease	Autodock Vina	-6.0					0.02	1.77	122.21	186.01	382.58	0.3241

Indinavir	Main Protease	DockThor		98155	-20266			2.23	3.73	88.23	189.36	555.49	0.1655
Indinavir	Main Protease	PatchDock		-48,04	-18,14	-14,63	5,15	0.94	16.71	108.04	307.21	570.94	0.2185
Indinavir	Main Protease	Autodock Vina	-7.1					0.65	75.06	103.23	314.23	536.70	0.3322
Lopinavir	Main Protease	DockThor		31261	-16998			1.95	11.71	50.13	188.79	532.14	0.1162
Lopinavir	Main Protease	PatchDock		-53.13	-10,86	-17,88	3,94	0.14	21.27	77.09	341.32	531.89	0.1849
Lopinavir	Main Protease	Autodock Vina	-7.2					0.00	92.97	51.90	311.77	554.87	0.2611
Nelfinavir	Main Protease	DockThor		59199	-18636			0.98	22.15	33.73	178.92	510.17	0.1095
Nelfinavir	Main Protease	PatchDock		-50,62	-13,31	-16,82	4	0.00	21.39	48.92	322.78	508.40	0.1383
Nelfinavir	Main Protease	Autodock Vina	-6.6					1.02	48.54	55.19	257.34	467.84	0.2217
Ritonavir	Main Protease	DockThor		5379	-25079			2.42	4.75	51.26	226.83	569.23	0.0984
Ritonavir	Main Protease	PatchDock		-54,65	-15,68	-18,86	7,01	1.00	56.20	46.90	304.74	583.98	0.1765
Ritonavir	Main Protease	Autodock Vina	-5.9					1.92	53.42	64.94	332.53	568.41	0.2082
Saquinavir	Main Protease	DockThor		56193	-17876			1.70	42.21	67.28	201.58	568.15	0.1927
Saquinavir	Main Protease	PatchDock		-46,84	-13,89	-12,26	2,83	0.74	2.85	95.69	345.69	535.56	0.184
Saquinavir	Main Protease	Autodock Vina	-7.0					0.90	71.01	61.77	295.31	535.63	0.2479
Simeprevir	Main Protease	DockThor		15364	-23813			1.64	6.96	58.73	216.14	614.68	0.1069
Simeprevir	Main Protease	PatchDock		-46,22	-13,98	-14,27	3,8	0.00	42.85	92.28	360.18	586.64	0.2303
Simeprevir	Main Protease	Autodock Vina	-8.6					1.97	21.77	85.44	306.13	581.69	0.1843
Tipranavir	Main Protease	DockThor		36977	-6915			1.17	9.30	18.10	127.53	425.93	0.0643
Tipranavir	Main Protease	PatchDock		-45,96	-17,36	-12,06	4,07	0.00	0.13	9.24	106.14	468.67	0.02
Tipranavir	Main Protease	Autodock Vina	-6.9					0.10	83.04	4.18	252.65	443.04	0.1969
Veruprevir	Main Protease	DockThor		51976	-21735			0.43	25.00	51.77	179.49	580.12	0.1323
Veruprevir	Main Protease	PatchDock		-47,04	-15,48	-12,7	6,58	0.00	16.27	81.14	296.20	578.48	0.1684
Veruprevir	Main Protease	Autodock Vina	-8.0					0.45	13.99	89.94	268.73	564.75	0.184
Abacavir	Polymerase	DockThor		-25545	-14361			1.38	0.06	101.45	143.67	283.53	0.358
Abacavir	Polymerase	PatchDock		-46,93	-10,22	-15,93	1,44	1.39	0.00	141.39	221.96	275.05	0.5141
Abacavir	Polymerase	Autodock Vina	-5.8					0.97	3.99	133.67	175.82	268.80	0.5121
Adefovir	Polymerase	DockThor		-30543	0.416			3.77	0.00	128.16	128.35	218.04	0.5878
Adefovir	Polymerase	PatchDock		-31,66	-9,15	-10,23	1,22	0.83	3.04	127.09	195.31	231.58	0.5619
Adefovir	Polymerase	Autodock Vina	-5.3					1.92	0.00	165.63	172.34	233.73	0.7086
Didanosine	Polymerase	DockThor		-12248	-4609			1.56	0.00	91.33	99.87	205.19	0.4451
Didanosine	Polymerase	PatchDock		-33	-12,94	-8	0,7	1.84	40.44	64.11	178.10	195.95	0.5336

Didanosine	Polymerase	Autodock Vina	-6.2					1.03	28.61	67.02	150.50	200.19	0.4777
Efavirenz	Polymerase	DockThor		-7939	-12629			1.28	0.00	0.00	103.42	235.63	0
Efavirenz	Polymerase	PatchDock		-32,71	-9,62	-9,52	1,35	0.00	5.19	0.00	182.91	227.40	0.0228
Efavirenz	Polymerase	Autodock Vina	-7.6					0.96	128.04	0.00	157.34	226.51	0.5653
Emtricitabine	Polymerase	DockThor		-21244	-10348			1.91	0.00	62.91	109.37	197.08	0.3192
Emtricitabine	Polymerase	PatchDock		-34,96	-10,54	-10,04	0,65	0.90	68.16	26.52	178.22	190.75	0.4964
Emtricitabine	Polymerase	Autodock Vina	-5.9					1.12	0.19	67.66	130.25	196.46	0.3454
Entecavir	Polymerase	DockThor		-26527	-7639			1.49	0.00	138.86	141.07	234.94	0.591
Entecavir	Polymerase	PatchDock		-37,89	-13,86	-10	1,56	2.52	50.19	85.57	214.36	232.46	0.584
Entecavir	Polymerase	Autodock Vina	-6.4					0.88	9.37	96.77	163.22	243.22	0.4364
Primaquine Phosphate	RBD	DockThor		5,996	-2,13			1.62	0.00	53.16	103.29	274.87	0.1934
Primaquine Phosphate	RBD	PatchDock		-40,8	-11,63	-12,19	1,79	0.42	0.00	79.87	212.02	275.19	0.2902
Primaquine Phosphate	RBD	Autodock Vina	-4,9					1.55	18.73	60.88	130.31	254.17	0.3132
Primaquine Phosphate	Proteina Spike Open	DockThor		10076	-11274			0.98	12.21	101.83	172.40	273.35	0.4172
Primaquine Phosphate	Proteina Spike Open	PatchDock		-40,2	-7,38	-14,29	0,31	0.34	65.19	88.35	248.86	279.75	0.5488
Primaquine Phosphate	Proteina Spike Open	Autodock Vina	-5,6					0.74	22.72	105.38	236.83	270.13	0.4742
Primaquine Phosphate	Proteina Spike Closed	DockThor		6456	-6755			1.96	20.89	79.05	135.12	277.02	0.3608
Primaquine Phosphate	Proteina Spike Closed	PatchDock		-39,75	-13,54	-10,76	0,06	2.15	48.23	97.28	239.55	278.99	0.5216
Primaquine Phosphate	Proteina Spike Closed	Autodock Vina	-5,1					0.94	12.53	82.21	184.62	271.31	0.3492
Galidesivir	Polymerase	DockThor		-24508	-9942			3.28	0.00	119.68	123.48	240.95	0.4967
Galidesivir	Polymerase	PatchDock		-36,69	-11,65	-10,64	0,32	2.44	1.14	159.81	199.36	233.67	0.6888
Galidesivir	Polymerase	Autodock Vina	-6.1					3.24	0.00	141.39	142.21	239.93	0.5893
Lamivudine	Polymerase	DockThor		-30225	-10335			1.88	0.00	68.73	114.74	195.00	0.3525
Lamivudine	Polymerase	PatchDock		-32,64	-12,91	-8,2	1,04	1.31	58.42	52.91	179.05	194.68	0.5719
Lamivudine	Polymerase	Autodock Vina	-5.6					2.07	0.00	88.42	142.91	196.77	0.4494
Nevirapine	Polymerase	DockThor		26809	-11614			0.97	0.00	0.13	130.12	226.96	0.0006
Nevirapine	Polymerase	PatchDock		-41,42	-11,78	-11,37	0,51	0.53	73.48	0.13	192.97	218.61	0.3367
Nevirapine	Polymerase	Autodock Vina	-7.5					0.91	11.90	0.06	179.49	222.02	0.0539
Ribavirin	Polymerase	DockThor		0.834	-2839			2.84	0.00	137.21	137.21	216.26	0.6345

Ribavirin	Polymerase	PatchDock		-37,9	-11,8	-11,89	0,31	3,79	0,00	171.64	188.41	211.89	0.81
Ribavirin	Polymerase	Autodock Vina	-6.7					2.30	0.00	170.57	174.55	213.74	0.798
Sofosbuvir	Polymerase	DockThor		-34751	-19244			2.23	17.28	91.77	211.52	440.68	0.2475
Sofosbuvir	Polymerase	PatchDock		-43,79	-12,08	-14,56	1,92	0,49	123.92	41.83	295.75	406.26	0.408
Sofosbuvir	Polymerase	Autodock Vina	-7.8					1.14	105.57	37.72	309.80	416.50	0.344
Stavudine	Polymerase	DockThor		-30817	-3685			1.78	0.00	26.65	93.80	196.64	0.1355
Stavudine	Polymerase	PatchDock		-31,42	-12,11	-7,48	0,65	0,08	70.00	3.48	166.33	184.05	0.3992
Stavudine	Polymerase	Autodock Vina	-5,8					0.06	12.72	21.96	126.01	191.26	0.1813
Quinine Sulphate	RBD	DockThor		42303	-2260			1.67	4.49	55.00	82.91	290.44	0.2048
Quinine Sulphate	RBD	PatchDock		-41,86	-16,03	-10,89	0,73	1,09	47.59	54.24	230.31	300.94	0.3384
Quinine Sulphate	RBD	Autodock Vina	-6,5					0.53	37.09	40.76	180.88	311.02	0.2503
Quinine Sulphate	Proteina Spike Open	DockThor		46,281	-10,311			0.97	7.40	35.89	131.14	295.57	0.1465
Quinine Sulphate	Proteina Spike Open	PatchDock		-49,12	-11,58	-16,83	0,07	0,00	10.57	57.40	247.46	301.89	0.2251
Quinine Sulphate	Proteina Spike Open	Autodock Vina	-6,9					0.92	26.77	53.48	207.59	299.42	0.268
Quinine Sulphate	Proteina Spike Closed	DockThor		46,029	-12,789			1.13	9.49	69.30	169.43	295.93	0.2662
Quinine Sulphate	Proteina Spike Closed	PatchDock		-47,53	-18,61	-11,53	0,39	1,26	0.76	71.90	245.44	301.71	0.2408
Quinine Sulphate	Proteina Spike Closed	Autodock Vina	-7,1					0.98	43.42	56.96	222.78	299.74	0.3349
Tenofovir	Polymerase	DockThor		-23159	1468			0.93	0.00	100.50	112.53	241.77	0.4157
Tenofovir	Polymerase	PatchDock		-31,29	-12,32	-8,26	0,98	2,18	23.61	136.77	231.39	242.35	0.6618
Tenofovir	Polymerase	Autodock Vina	-6.7					4.12	2.22	172.53	215.95	250.39	0.6979
Zidovudin	Polymerase	DockThor		-29704	-8487			2.40	0.00	96.77	153.48	248.54	0.3894
Zidovudin	Polymerase	PatchDock		-35,72	-10,98	-12,14	1,67	1,61	10.95	77.66	208.03	238.11	0.3721
Zidovudin	Polymerase	Autodock Vina	-6.4					0.79	57.34	85.57	211.83	247.21	0.5781
Arbidol	RBD	DockThor		18930	-14403			0,02	10,51	41,45	167,85	362,34	0,1434
Arbidol	RBD	PatchDock		-49,02	-9,11	-15,63	1,79	0,00	45.25	56.83	266.58	363.91	0.2805
Arbidol	RBD	Autodock Vina	-5					0,02	35,76	20,63	143,92	338,41	0,1666
Arbidol	Proteina Spike Open	DockThor		14143	-17751			1,49	10,51	69,37	205,82	354,75	0,2252
Arbidol	Proteina Spike Open	PatchDock		-51,06	-10,85	-19,18	0,82	0,00	90.31	62.21	323.22	370.12	0.4121

Arbidol	Proteina Spike Open	Autodock Vina	-6.2					0.00	24.56	68.80	223.10	350.32	0.2665
Arbidol	Proteina Spike Closed	DockThor		21629	-14546			0,18	35,7	39,56	175,82	360,51	0,2088
Arbidol	Proteina Spike Closed	PatchDock		-47,32	-16,09	-11,59	0,21	1.25	21.58	70.88	292.46	367.33	0.2517
Arbidol	Proteina Spike Closed	Autodock Vina	-6.2					0,91	66,45	38,67	247,78	358,92	0,2929
Camostat	Main Protease	DockThor		-11353	-9902			2,17	0	86,9	142,85	366,84	0,2369
Camostat	Main Protease	PatchDock		-35,87	-15,37	-9,62	4,33	0.00	47.53	89.05	240.19	364.73	0.3745
Camostat	Main Protease	Autodock Vina	-5.4					0,09	50,95	121,14	211,77	376,7	0,4568
Crysin	Main Protease	DockThor		9523	-13738			1,79	0,38	0	113,23	212,08	0,0018
Crysin	Main Protease	PatchDock		-40,36	-15,13	-10,96	0,68	0.30	42.47	0.00	172.28	208.67	0.2035
Crysin	Main Protease	Autodock Vina	-6.8					0,57	29,37	0	169,05	220	0,1335
Darunavir	Main Protease	DockThor		-5143	-17889			1.39	71.14	189.05	482.45	0.1503	0.0095
Darunavir	Main Protease	PatchDock		-51,33	-16,88	-16,47	3,5	0.34	37.97	111.33	356.51	501.19	0.2979
Darunavir	Main Protease	Autodock Vina	-6.8					1,92	16,9	151,64	274,68	453,09	0,372
Emodin	RBD	DockThor		10500	-10751			0,54	22,21	0	87,66	207,27	0,1072
Emodin	RBD	PatchDock		-42,09	-15,09	-11,43	0,4	1.01	22.21	0.00	186.77	210.30	0.1056
Emodin	RBD	Autodock Vina	-6,2					1,38	0,19	0	128,67	219,81	0,0009
Emodin	Proteina Spike Open	DockThor		2823	-12643			0,33	11,58	0	145,57	206,32	0,0561
Emodin	Proteina Spike Open	PatchDock		-38,05	-11,8	-12,26	0,6	0.44	50.89	0.00	184.49	213.86	0.238
Emodin	Proteina Spike Open	Autodock Vina	-7.0					1.15	20.82	0.00	132.21	213.10	0.0977
Emodin	Proteina Spike Closed	DockThor		8500	-1507			0,1	22,66	0	96,07	209,49	0,1082
Emodin	Proteina Spike Closed	PatchDock		-37,97	-13,73	-10,11	0,33	0.10	39.68	0.00	175.00	214.05	0.1854
Emodin	Proteina Spike Closed	Autodock Vina	-7.2					0,86	12,53	0	144,24	218,04	0,0575
Favipiravir	Polymerase	DockThor		22.029	-9401			1,34	5,44	35,63	90,38	129,68	0,3167
Favipiravir	Polymerase	PatchDock		-27,96	-13,17	-5,03	0,03	1.06	0.00	58.35	109.30	120.06	0.486
Favipiravir	Polymerase	Autodock Vina	-5.6					0,92	32,02	39,05	119,18	128,8	0,5518
nFCCL3	RBD	DockThor		31648	-27093			0	85,63	0	209,68	396,13	0,2162
nFCCL3	RBD	PatchDock		-51,5	-17,26	-13,34	0,25	0.01	64.24	0.00	284.11	386.64	0.1661
nFCCL3	RBD	Autodock Vina	-7,1					0	142,34	0	270,5	405,25	0,3512

nFCCL3	Proteina Spike Open	DockThor		32090	-25925			0	45,63	0	194,81	397,02	0,1149
nFCCL3	Proteina Spike Open	PatchDock		-58,05	-13,48	-20,15	0,35	0,00	102,66	0,00	299,61	387,34	0,265
nFCCL3	Proteina Spike Open	Autodock Vina	-7.3					0,00	75,06	0,00	276,89	392,96	0,191
nFCCL3	Proteina Spike Closed	DockThor		31288	-20466			0,85	22,72	0	190,95	393,6	0,0577
nFCCL3	Proteina Spike Closed	PatchDock		-49,11	-19,82	-9,79	0,48	0,06	120,12	0,00	299,05	386,25	0,311
nFCCL3	Proteina Spike Closed	Autodock Vina	-7.2					0,46	32,59	0	258,6	399,48	0,0816
Nicosamide	RBD	DockThor		12601	-10555			1,13	20,19		116,07	228,73	0,0883
Nicosamide	RBD	PatchDock		-39,21	-15,62	-10,21	3,57	0,98	94,49	0,63	185,00	216,77	0,4388
Nicosamide	RBD	Autodock Vina	-5,5					0	1,65	38,86	136,45	235,13	0,1723
Nicosamide	Proteina Spike Open	DockThor		10895	-13121			1,09	0,89	0	131,83	230,76	0,0039
Nicosamide	Proteina Spike Open	PatchDock		-47,37	-13,79	-15,33	0,22	0,01	0,00	0,00	135,88	192,08	0
Nicosamide	Proteina Spike Open	Autodock Vina	-7.2					0,00	147,72	21,39	222,21	254,36	0,6648
Nicosamide	Proteina Spike Closed	DockThor		13859	-5812			0,75	19,18	0	128,99	230,25	0,0833
Nicosamide	Proteina Spike Closed	PatchDock		-41,44	-16,79	-9,48	0,63	1,31	53,29	0,19	195,76	218,15	0,2452
Nicosamide	Proteina Spike Closed	Autodock Vina	-6.8					3,24	8,73	49,56	164,49	241,51	0,2414
Oseltamivir	RBD	DockThor		-9030	-4939			1,69	0	82,97	123,92	328,97	0,2522
Oseltamivir	RBD	PatchDock		-41,59	-14,57	-10,74	2,16	2,62	98,29	69,75	290,18	343,23	0,4896
Oseltamivir	RBD	Autodock Vina	-5,9					0,94	57,34	78,1	208,22	332,59	0,4072
Oseltamivir	Proteina Spike Open	DockThor		-11111	-12487			2	16,52	79,49	167,91	328,02	0,2927
Oseltamivir	Proteina Spike Open	PatchDock		-43,63	-12,36	-14,33	0,71	0,79	25,06	91,07	286,96	342,76	0,3388
Oseltamivir	Proteina Spike Open	Autodock Vina	-6.1					0,73	63,86	82,97	263,16	329,69	0,4454
Oseltamivir	Proteina Spike Closed	DockThor		-1884	-11166			1,94	17,4	67,59	166,52	324,35	0,262
Oseltamivir	Proteina Spike Closed	PatchDock		-36,49	-13,64	-9,58	0,82	0,50	78,29	87,53	303,41	340,31	0,4873
Oseltamivir	Proteina Spike Closed	Autodock Vina	-5.9					1,01	59,49	83,54	236,20	316,58	0,4518
Ganciclovir	RBD	DockThor		-54089	16220			1,28	0	133,86	134,3	326,64	0,4098
Ganciclovir	RBD	PatchDock		-32,39	-16,33	-4,09	2,4	3,56	0,00	226,58	297,59	321,20	0,7054

Ganciclovir	RBD	Autodock Vina	-6,3					3,33	0,00	164,74	183,22	320,18	0,5145
Ganciclovir	Proteina Spike Open	DockThor		-59019	22239			3,98	0	121,33	121,64	342,34	0,3544
Ganciclovir	Proteina Spike Open	PatchDock		-42,08	-13,54	-13,44	0,55	3,44	14,62	199,62	285,63	321,52	0,6663
Ganciclovir	Proteina Spike Open	Autodock Vina	-6,8					1,95	1,84	198,60	238,48	317,01	0,6323
Ganciclovir	Proteina Spike Closed	DockThor		-49996	0,613			2,9	0	130,5	147,15	33,8	0,391
Ganciclovir	Proteina Spike Closed	PatchDock		-40,05	-15,89	-9,04	0,19	1,91	0,00	160,95	253,79	319,30	0,5041
Ganciclovir	Proteina Spike Closed	Autodock Vina	-7,9					3,56	0,00	172,91	282,59	311,89	0,5544
Penciclovir	Polymerase			-33,11	-8,7	-11,23	0,41	11,93	0,125	0,35	0,51	147,53	192,78
Penciclovir	Polymerase			-42,863	-8,598			4,77	0,444	2,71	0,00	157,28	162,15
Penciclovir	Polymerase		-5,6					4,64	0,5	2,40	0,00	134,68	135,88
Phaitanthrin_D	RBD	DockThor		7869	-13352			0,98	4,05	44,43	119,68	228,16	0,2125
Phaitanthrin_D	RBD	PatchDock		-48,72	-18,36	-12,97	0,23	0,00	26,01	73,54	186,90	231,76	0,4295
Phaitanthrin_D	RBD	Autodock Vina	-8,2					0,56	20,13	86,64	140,63	231,83	0,4606
Phaitanthrin_D	Proteina Spike Open	DockThor		5442	-16277			0,91	1,39	47,21	121,45	228,60	0,2126
Phaitanthrin_D	Proteina Spike Open	PatchDock		-44,79	-13,89	-14,7	0,12	0,92	23,73	40,89	206,71	232,90	0,2775
Phaitanthrin_D	Proteina Spike Open	Autodock Vina	-7,9					0,79	11,90	75,63	175,06	233,93	0,3742
Phaitanthrin_D	Proteina Spike Closed	DockThor		6372	-18721			1,59	16,96	78,61	180,57	228,41	0,4184
Phaitanthrin_D	Proteina Spike Closed	PatchDock		-41,63	-14,99	-10,77	1,01	1,83	12,21	39,24	212,40	233,35	0,2205
Phaitanthrin_D	Proteina Spike Closed	Autodock Vina	-8,2					0,85	8,48	77,15	178,92	230,44	0,3716
Phaitanthrin_D	Main Protease	DockThor		6269	-20518			0,82	7,59	57,72	168,86	228,66	0,2856
Phaitanthrin_D	Main Protease	PatchDock		-43,19	-11,88	-13,57	0,53	0,02	33,61	80,76	181,33	233,42	0,49
Phaitanthrin_D	Main Protease	Autodock Vina	-7,0					1,75	18,04	58,35	148,42	233,29	0,3274
Phaitanthrin_D	Polymerase	DockThor		6057	-20704			0,01	3,54	87,47	152,15	227,27	0,4004
Phaitanthrin_D	Polymerase	PatchDock		-47,73	-18,57	-11,57	0,48	0,94	12,59	48,10	218,92	231,33	0,2624
Phaitanthrin_D	Polymerase	Autodock Vina	-8,2					1,38	40,95	69,87	181,9	231,52	0,4787
Phaitanthrin_D	NSP 10	DockThor		7,021	-16,473			0,98	13,42	59,94	121,71	227,15	0,323
Phaitanthrin_D	NSP 10	PatchDock		-42,37	-9,29	-13,47	1,6	1,28	0,76	108,86	189,11	233,22	0,47
Phaitanthrin_D	NSP 10	Autodock Vina	-9,4					0	4,3	12,34	92,53	232,08	0,0717

Phaitanthrin_D	NSP 16	DockThor		8,164	-20,514			0,04	6,77	82,21	159,11	229,62	0,3875
Phaitanthrin_D	NSP 16	PatchDock			-15,79	-9,16	1,62	0,84	6,65	74,87	171,01	231,14	0,3527
Phaitanthrin_D	NSP 16	Autodock Vina	-8,4					0	0,51	59,75	124,05	232,27	0,2594
Rendesvir	Polymerase	DockThor		-26981	-20979			1,62	46,45	98,92	225,95	541,58	0,2684
Rendesvir	Polymerase	PatchDock			-13,31	-18,06	1,84	1,32	7,34	157,66	351,32	473,10	0,3488
Rendesvir	Polymerase	Autodock Vina	-8,1					1,51	77,59	79,56	370,69	516,63	0,3042
Ribavirin	Polymerase	DockThor		0,982	-3282			2,32	0	137,4	137,4	216,32	0,6352
Ribavirin	Polymerase	PatchDock			-11,8	-11,89	0,31	3,79	0,00	171,64	188,41	211,89	0,81
Ribavirin	Polymerase	Autodock Vina	-6,7					4,29	0	166,39	169,62	218,67	0,7609
Sovalvi	RBD	DockThor		-32695	-17130			1,05	33,61	78,99	182,21	406,7	0,2769
Sovalvi	RBD	PatchDock			-12,58	-6,51	1,22	1,56	37,09	66,64	348,28	406,82	0,255
Sovalvi	RBD	Autodock Vina											
Sovalvi	Proteina Spike Open	DockThor		-34248	-18440			2,12	0	81,58	163,16	430	0,1894
Sovalvi	Proteina Spike Open	PatchDock			-17,56	-13,07	0,07	0,26	57,34	95,63	358,73	405,51	0,3772
Sovalvi	Proteina Spike Open	Autodock Vina											
Sovalvi	Proteina Spike Closed	DockThor		-32445	-19246			2,08	1,52	49,24	228,22	407,59	0,1245
Sovalvi	Proteina Spike Closed	PatchDock			#VALOR!	-11,19	0,16	1,64	53,80	60,51	369,36	408,42	0,2799
Sovalvi	Proteina Spike Closed	Autodock Vina											
SSAA09E2	RBD	DockThor		12089	-6154			1,95	0	69,43	126,26	288,79	0,2404
SSAA09E2	RBD	PatchDock			-15,61	-11,14	1,12	0,67	15,51	104,37	236,26	280,83	0,4269
SSAA09E2	RBD	Autodock Vina	-6,8					1,37	2,34	89,37	192,15	296,83	0,309
SSAA09E2	Proteina Spike Open	DockThor		12512	-16127			1,75	36,01	98,54	190,5	291,83	0,4611
SSAA09E2	Proteina Spike Open	PatchDock			-14,37	-15,69	0,28	0,98	19,05	109,93	242,08	278,91	0,4624
SSAA09E2	Proteina Spike Open	Autodock Vina	-6,6					0,93	3,29	115,00	218,67	301,38	0,3925
SSAA09E2	Proteina Spike Closed	DockThor		11813	-20100			0,96	9,62	144,05	222,4	290,88	0,5283
SSAA09E2	Proteina Spike Closed	PatchDock			-17,03	-9,75	0,18	0,32	22,21	129,43	236,26	280,68	0,5403
SSAA09E2	Proteina Spike Closed	Autodock Vina	-5,4					0,99	8,80	96,96	158,92	290,82	0,3637
Umefenovir	RBD	DockThor		18532	-15090			1,77	27,47	37,34	158,86	350,38	0,185

Umefenovir	RBD	PatchDock			-9,11	-15,63	1,79	0,00	45,25	56,83	266,58	363,91	0,2805
Umefenovir	RBD	Autodock Vina	-6,5					0,85	110,88	28,92	204,43	351,69	0,3975
Umefenovir	Proteina Spike Open	DockThor		12884	-16859			1,26	25,06	69,62	172,4	361,58	0,2619
Umefenovir	Proteina Spike Open	PatchDock			-10,85	-19,18	0,82	0,00	90,31	62,21	323,22	370,12	0,4121
Umefenovir	Proteina Spike Open	Autodock Vina	-5.1					1,44	13,61	48,61	170,82	347,91	0,1788
Umefenovir	Proteina Spike Closed	DockThor		20361	-16066			0,12	44,43	27,53	171,71	358,91	0,2005
Umefenovir	Proteina Spike Closed	PatchDock			-16,09	-11,59	0,21	1,25	21,58	70,88	292,46	367,33	0,2517
Umefenovir	Proteina Spike Closed	Autodock Vina	-5.6					0,40	68,16	0,44	243,86	358,48	0,1914