

## Supporting Information

# Accelerating the repurposing of FDA-approved drugs against Coronavirus Disease-19 (COVID-19)

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**Table S1.** Ligand structure (SMILES) and CAS ID of the selected compounds (See also Table 1 in the main text).

Ligand	SMILES	CAS
Olaparib	<chem>c1cccc2c1c(n[nH]c2=O)Cc1cc(c(cc1)F)C(=O)N1CCN(CC1)C(=O)C1CC1</chem>	763113-22-0
Dutasteride	<chem>C1=C[C@]2([C@H](NC1=O)CC[C@@H]1[C@@H]2CC[C@]2([C@H]1CC[C@@H]2C(=O)Nc1cc(ccc1C(F)(F)F)C(F)(F)F)C)C</chem>	164656-23-9
Dolutegravir	<chem>c1(cc(c(cc1)CNC(=O)c1cn2c(c(c1=O)[O-])C(=O)N1[C@H](C2)OCC[C@H]1C)F)F</chem>	1051375-16-6
Conivaptan	<chem>C(=O)(Nc1ccc(cc1)C(=O)N1c2c(c3c(CC1)[nH+]c([nH]3)C)cccc2)c1c(cccc1)c1cccc1</chem>	168626-94-6
Velpatasvir	<chem>c1cccc(c1)[C@H](C(=O)N1C[C@H](C[C@H]1c1[nH]c(c1)C)C(=O)N1C[C@H](C[C@H]1c1[nH]c(c1)COc1c2cc2c(c1)c1c(cc2)nc([nH]1)[C@H]1N([C@H](CC1)C)C(=O)[C@@H](NC(=O)OC)C(C)C)COC)NC(=O)OC</chem>	1377049-84-7
Lomitapide	<chem>[N@H+]1(CC[C@H](CC1)NC(=O)c1c(cccc1)c1ccc(cc1)C(F)(F)F)CCCC[C@]1(c2c(c3c1cccc3)cccc2)C(=O)NC(C(F)(F)F)</chem>	182431-12-5
Entrectinib	<chem>c1cc2c(cc1Cc1cc(cc(c1)F)F)c(n[nH]2)NC(=O)c1ccc(cc1NC1CCOCC1)N1CCN(CC1)C</chem>	1108743-60-7
Bromocriptine	<chem>N12[C@]([C@H]3N(C(=O)[C@@H]2CC(C)C)CCC3)(O[C@](C1=O)(NC(=O)[C@@H]1C=C2c3c4c(C[C@@H]2N(C1)C)c([nH]c4ccc3)Br)C(C)C)O</chem>	22260-51-1
Peficitinib	<chem>C1[C@@H]2CC3(C[C@@H](C2NC4=C5C=CNC5=NC=C4C(=O)N)CC1C3)O</chem>	944118-01-8
Dihydroergotamine	<chem>C1[C@@H]2c3cccc4[nH]cc(c34)C[C@@H]2[N@@H+](C)C[C@@H]1C(=O)N[C@@]1(C)C(=O)N2[C@@H](Cc3cccc3)C(=O)N3CCC[C@H]3[C@@]2(O)O</chem>	6190-39-2
Rutin	<chem>c1(c(c(=O)c2c(o1)cc(cc2O)O)O)[C@H]1O[C@@H](CO[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](O2)C)O)O)O)[C@@H]([C@@H]([C@H]1O)O)O)c1cc(c(cc1)O)O</chem>	207671-50-9

**Table S2.** Predicted docking score of Olaparib against the viral protein panel.

<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>
4wm7	-11.80	4k7f	-10.80	4uo7	-10.50
3t3c	-11.80	4g43	-10.80	4uo7	-10.50
3t3c	-11.80	4g42	-10.80	4uo7	-10.50
4lsv	-11.60	4cey	-10.80	4uo7	-10.50
4j4x	-11.60	3rwi	-10.80	4uo0	-10.50
2wrc	-11.60	3rwd	-10.80	4uo0	-10.50
2wr3	-11.60	3kna	-10.80	4uo0	-10.50
3nxu	-11.50	3b0w	-10.80	4uo0	-10.50
2wrh	-11.50	2wre	-10.80	4uo0	-10.50
2wrf	-11.50	2hjk	-10.80	4uo0	-10.50
4i2p	-11.40	2bvo	-10.80	4uo0	-10.50
2i4v	-11.40	2axg	-10.80	4uo0	-10.50
4o4g	-11.30	1ida	-10.80	4uo0	-10.50
3kql	-11.30	4qrs	-10.70	4uo0	-10.50
3kql	-11.30	3klv	-10.70	4uo0	-10.50
3kql	-11.30	3bwa	-10.70	4uo0	-10.50
2bvp	-11.30	1syv	-10.70	4uo0	-10.50
3fku	-11.20	1hhh	-10.70	4uo0	-10.50
4mmr	-11.10	4uo3	-10.60	4rw7	-10.50
4e78	-11.10	4uo3	-10.60	4qru	-10.50
4e78	-11.10	4uo3	-10.60	4i7f	-10.50
4e7a	-11.00	4uo3	-10.60	4fnk	-10.50
4e7a	-11.00	4uo3	-10.60	4cdw	-10.50
4cdu	-11.00	4uo0	-10.60	3kqn	-10.50
3s11	-11.00	4uo0	-10.60	3hky	-10.50
3rwe	-11.00	4uo0	-10.60	3hkw	-10.50
2wrg	-11.00	4uo0	-10.60	3gsr	-10.50
2wrg	-11.00	4qru	-10.60	3gso	-10.50
2wrg	-11.00	4e5e	-10.60	2wre	-10.50
2wrg	-11.00	4cew	-10.60	4uo7	-10.40
2wrg	-11.00	4cdq	-10.60	4rw6	-10.40
1oop	-11.00	3u7s	-10.60	4mkb	-10.40
4u6h	-10.90	3u7s	-10.60	4gua	-10.40
4qrs	-10.90	3rwh	-10.60	4g9z	-10.40
4q6r	-10.90	3rwh	-10.60	4g9f	-10.40
4q6r	-10.90	3rwc	-10.60	4cqy	-10.40
4k7f	-10.90	3rwc	-10.60	4cdx	-10.40
4j4w	-10.90	3kqn	-10.60	3vcl	-10.40
4i2q	-10.90	3kqn	-10.60	3vcl	-10.40
4f3z	-10.90	3gsq	-10.60	3rwg	-10.40
3rwe	-10.90	3gso	-10.60	3rwg	-10.40
3koa	-10.90	3ggg	-10.60	3r4b	-10.40
3i6l	-10.90	3bwa	-10.60	3bw9	-10.40
2i4x	-10.90	1r6a	-10.60	3bw9	-10.40
1klm	-10.90	1p9u	-10.60	3bew	-10.40
4wm8	-10.80	4uo7	-10.50	2ygc	-10.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
2i4d	-10.40	3gsw	-10.20	4mkb	-9.90
1hhk	-10.40	3gsq	-10.20	4m8y	-9.90
1hhj	-10.40	2wr2	-10.20	4lst	-9.90
1hhi	-10.40	1izh	-10.20	4j4v	-9.90
4uo5	-10.30	4pv9	-10.10	4j4v	-9.90
4uo5	-10.30	4mgu	-10.10	4j4v	-9.90
4uo5	-10.30	4lsr	-10.10	4j4v	-9.90
4unx	-10.30	4j4u	-10.10	4j4s	-9.90
4rw9	-10.30	3cj0	-10.10	4j4s	-9.90
4o44	-10.30	2wre	-10.10	4fnk	-9.90
4j4r	-10.30	2wr1	-10.10	3n0i	-9.90
4g9z	-10.30	2wr1	-10.10	3lkh	-9.90
3r4b	-10.30	2wa1	-10.10	3iyw	-9.90
3d0h	-10.30	2hcs	-10.10	3iyw	-9.90
3bev	-10.30	1izi	-10.10	3h98	-9.90
3alw	-10.30	1a41	-10.10	3ggg	-9.90
2ygc	-10.30	4uny	-10.00	3cj5	-9.90
2wr2	-10.30	4qhk	-10.00	3ciz	-9.90
2wr0	-10.30	4opa	-10.00	3ciz	-9.90
2wr0	-10.30	4mka	-10.00	2ygb	-9.90
2wr0	-10.30	4mk7	-10.00	2ygb	-9.90
2wr0	-10.30	4mk7	-10.00	4unw	-9.80
2wr0	-10.30	4lkj	-10.00	4unw	-9.80
2i4w	-10.30	4j6r	-10.00	4rw8	-9.80
2i4u	-10.30	4hkj	-10.00	4m30	-9.80
2gec	-10.30	4fqv	-10.00	4kps	-9.80
2gec	-10.30	4fqv	-10.00	4j4v	-9.80
1quv	-10.30	4fqj	-10.00	4ej8	-9.80
4uo2	-10.20	3ztj	-10.00	4e5l	-9.80
4uo2	-10.20	3vbo	-10.00	3vbr	-9.80
4uo2	-10.20	3lkh	-10.00	3ok9	-9.80
4uo2	-10.20	3kqh	-10.00	3oah	-9.80
4uo2	-10.20	3kms	-10.00	3mj5	-9.80
4uo2	-10.20	3iyw	-10.00	3mj5	-9.80
4unx	-10.20	3iyw	-10.00	3cj5	-9.80
4unx	-10.20	3iyw	-10.00	3cj2	-9.80
4unx	-10.20	3iyw	-10.00	3cj2	-9.80
4rw4	-10.20	3gsx	-10.00	3cj0	-9.80
4rw4	-10.20	3gsx	-10.00	2hu0	-9.80
4mka	-10.20	2wr1	-10.00	1v3d	-9.80
4mk9	-10.20	2uv0	-10.00	1v3d	-9.80
4mk9	-10.20	2uv0	-10.00	1pk0	-9.80
4j4y	-10.20	2htw	-10.00	4unw	-9.70
4fqr	-10.20	4uo3	-9.90	4jo8	-9.70
4fqr	-10.20	4uo3	-9.90	4fvu	-9.70
4a92	-10.20	4uo3	-9.90	4ejl	-9.70
4a92	-10.20	4uo3	-9.90	4ej8	-9.70
3gsw	-10.20	4uo3	-9.90	4e5f	-9.70

PDB	Docking score	PDB	Docking score	PDB	Docking score
4cqw	-9.70	3hky	-9.50	4jb9	-9.30
4bh0	-9.70	3cj4	-9.50	4eee	-9.30
4bac	-9.70	3alx	-9.50	3tid	-9.30
3sdy	-9.70	2wr2	-9.50	3nf8	-9.30
3sdy	-9.70	2vvw	-9.50	3gsr	-9.30
3pqy	-9.70	2vvw	-9.50	3d23	-9.30
3n0i	-9.70	2uv0	-9.50	3cj4	-9.30
3hkw	-9.70	2uv0	-9.50	2xi5	-9.30
3h98	-9.70	2uv0	-9.50	2xi5	-9.30
3h2l	-9.70	2uv0	-9.50	2mgu	-9.30
3gsv	-9.70	2uv0	-9.50	1v3e	-9.30
3gsv	-9.70	2uv0	-9.50	4i2q	-9.20
3gsu	-9.70	2uv0	-9.50	4e5g	-9.20
3gsu	-9.70	2hty	-9.50	4dag	-9.20
3d0g	-9.70	1v2i	-9.50	4bgy	-9.20
3cj3	-9.70	1n5a	-9.50	3kmq	-9.20
3cj3	-9.70	4pg2	-9.40	2xra	-9.20
2wre	-9.70	4mj1	-9.40	2wr7	-9.20
2wre	-9.70	4mds	-9.40	2wr4	-9.20
2uv0	-9.70	4i2p	-9.40	1n59	-9.20
1idb	-9.70	4fqi	-9.40	4uo6	-9.10
1b53	-9.70	4fqi	-9.40	4uo6	-9.10
4uo8	-9.60	4f3i	-9.40	4mg3	-9.10
4mk8	-9.60	4cr0	-9.40	4gaj	-9.10
4m8x	-9.60	4adf	-9.40	4e5j	-9.10
4lsu	-9.60	4adf	-9.40	4dgd	-9.10
4iv3	-9.60	4adf	-9.40	3u82	-9.10
4ejl	-9.60	4adf	-9.40	3u82	-9.10
3hkw	-9.60	4adf	-9.40	3tie	-9.10
3h2l	-9.60	4adf	-9.40	3tie	-9.10
2wre	-9.60	3se9	-9.40	3se8	-9.10
2uv0	-9.60	3sdy	-9.40	3se8	-9.10
Spike RBD	-9.50	3nf8	-9.40	3rki	-9.10
4mze	-9.50	3mlh	-9.40	3ku3	-9.10
4mze	-9.50	3i6g	-9.40	3ku3	-9.10
4mk8	-9.50	3cpl	-9.40	2z35	-9.10
4mj0	-9.50	3cpl	-9.40	1v3e	-9.10
4m8y	-9.50	2vvx	-9.40	4gaj	-9.00
4m8x	-9.50	2vvx	-9.40	4g9f	-9.00
4lsu	-9.50	2hu4	-9.40	4e5i	-9.00
4jpk	-9.50	2hu4	-9.40	4bh4	-9.00
4gag	-9.50	2hu4	-9.40	4bh4	-9.00
4gag	-9.50	2hu4	-9.40	4bh4	-9.00
4f3i	-9.50	1v2i	-9.40	4bh4	-9.00
4e92	-9.50	4pv9	-9.30	3ro5	-9.00
4e91	-9.50	4pv9	-9.30	3nwf	-9.00
4e76	-9.50	4mms	-9.30	3nf7	-9.00
3tid	-9.50	4mds	-9.30	3bwa	-9.00

PDB	Docking score	PDB	Docking score	PDB	Docking score
3avf	-9.00	4gv3	-8.70	4gu3	-8.60
2xwy	-9.00	4gu4	-8.70	4gu3	-8.60
2x83	-9.00	4gu4	-8.70	4gu3	-8.60
2uv0	-9.00	4gu4	-8.70	4g8g	-8.60
2oy0	-9.00	4gu4	-8.70	4dgc	-8.60
2iph	-9.00	4gu4	-8.70	4dgc	-8.60
2ghw	-9.00	4gu4	-8.70	4dgc	-8.60
1v3c	-9.00	4g8g	-8.70	4dgc	-8.60
1v3b	-9.00	4fqy	-8.70	4cqy	-8.60
4qhn	-8.90	4fqy	-8.70	3zp6	-8.60
4pv8	-8.90	4cqx	-8.70	3zp1	-8.60
4mg3	-8.90	4cqr	-8.70	3zp0	-8.60
4gzf	-8.90	4cqy	-8.70	3s13	-8.60
4gzf	-8.90	4bh3	-8.70	3nf6	-8.60
4egt	-8.90	4bh3	-8.70	3nf6	-8.60
3v3m	-8.90	4bh3	-8.70	2x5i	-8.60
3v3m	-8.90	4bh3	-8.70	2ht5	-8.60
3sv8	-8.90	4bgw	-8.70	1v3b	-8.60
3ebj	-8.90	4bgw	-8.70	4jkg	-8.50
2x83	-8.90	3zp2	-8.70	4iv1	-8.50
2oy0	-8.90	3o4l	-8.70	4fp8	-8.50
2iph	-8.90	3d0i	-8.70	4fp8	-8.50
2iph	-8.90	3ava	-8.70	4ejd	-8.50
2ge7	-8.90	3ava	-8.70	4ejd	-8.50
1v3c	-8.90	3alz	-8.70	4ejd	-8.50
4fqi	-8.80	2c36	-8.70	4dgc	-8.50
4ffz	-8.80	2c36	-8.70	4dgc	-8.50
4cqy	-8.80	1b50	-8.70	4cqu	-8.50
4cqp	-8.80	Main	-8.60	4bh2	-8.50
4cqp	-8.80	protease	-8.60	4bh2	-8.50
4cqp	-8.80	5ajm	-8.60	3lqa	-8.50
4bgz	-8.80	5ajm	-8.60	3ku5	-8.50
3zpb	-8.80	5ajm	-8.60	3ku5	-8.50
3zpb	-8.80	5ajm	-8.60	3iyp	-8.50
3zp3	-8.80	5ajm	-8.60	3avn	-8.50
3vbh	-8.80	5ajm	-8.60	2htu	-8.50
3ku6	-8.80	4qrt	-8.60	1rzk	-8.50
3ku6	-8.80	4mmu	-8.60	4qhl	-8.40
3d23	-8.80	4kpq	-8.60	4jkg	-8.40
3avl	-8.80	4gu3	-8.60	4fb3	-8.40
2iph	-8.80	4gu3	-8.60	4eq0	-8.40
1v3c	-8.80	4gu3	-8.60	4cqu	-8.40
1sys	-8.80	4gu3	-8.60	4cqu	-8.40
1sk7	-8.80	4gu3	-8.60	4cqu	-8.40
1r6a	-8.80	4gu3	-8.60	4cqu	-8.40
4i31	-8.70	4gu3	-8.60	3nw8	-8.40
4i31	-8.70	4gu3	-8.60	3nfa	-8.40
4gv3	-8.70	4gu3	-8.60	3nfa	-8.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
3nf9	-8.40	4gve	-8.10	2xpx	-7.90
3nf9	-8.40	4dkp	-8.10	2me4	-7.90
3nf6	-8.40	4bgx	-8.10	2ge8	-7.90
3avj	-8.40	4bgx	-8.10	4oph	-7.80
3avc	-8.40	3ztn	-8.10	4mj1	-7.80
4qru	-8.30	3zpa	-8.10	4lkk	-7.80
4pv8	-8.30	3su1	-8.10	4eqj	-7.80
4mza	-8.30	3rwj	-8.10	4dko	-7.80
4jpi	-8.30	3rwj	-8.10	4bh1	-7.80
4eq0	-8.30	3rwi	-8.10	4bh1	-7.80
4cqu	-8.30	3nfa	-8.10	4bh1	-7.80
3uf5	-8.30	3nf7	-8.10	3su2	-7.80
3p8o	-8.30	3nf7	-8.10	3rwf	-7.80
3nwa	-8.30	3avl	-8.10	3rwf	-7.80
3nwa	-8.30	3avg	-8.10	3a07	-7.80
3nf9	-8.30	3avb	-8.10	2wh6	-7.80
3nf9	-8.30	2zu4	-8.10	2q7c	-7.80
3nf8	-8.30	2yol	-8.10	2q7c	-7.80
3nf8	-8.30	2yol	-8.10	2q7c	-7.80
3nf6	-8.30	2axf	-8.10	2lsp	-7.80
2zu5	-8.30	4qrt	-8.00	1rpi	-7.80
2wh6	-8.30	4lss	-8.00	1rpi	-7.80
2hcn	-8.30	4g9d	-8.00	4mj0	-7.70
2c7u	-8.30	4cqz	-8.00	4gye	-7.70
1yh3	-8.30	4cqz	-8.00	4gye	-7.70
1rzj	-8.30	4cqq	-8.00	4g1o	-7.70
4mza	-8.20	4co6	-8.00	4ejd	-7.70
4ep3	-8.20	3sv7	-8.00	4ejd	-7.70
4ep3	-8.20	3suf	-8.00	4ejd	-7.70
4dgd	-8.20	3oah	-8.00	3su3	-7.70
4cqs	-8.20	3avh	-8.00	3su3	-7.70
4cqs	-8.20	3ava	-8.00	3su2	-7.70
4cqr	-8.20	3ava	-8.00	3su2	-7.70
4cqp	-8.20	2xze	-8.00	3su1	-7.70
4cqp	-8.20	2vvy	-8.00	3su0	-7.70
4cqp	-8.20	2bvq	-8.00	3sud	-7.60
3nfa	-8.20	4uo4	-7.90	3sit	-7.60
3nf7	-8.20	4qrt	-7.90	3sit	-7.60
3avh	-8.20	4mmv	-7.90	3sit	-7.60
3avg	-8.20	4mmt	-7.90	3sit	-7.60
3avb	-8.20	4i32	-7.90	3sit	-7.60
3avb	-8.20	4dkq	-7.90	3sit	-7.60
3avb	-8.20	3vbf	-7.90	3gsw	-7.60
2ghv	-8.20	3vbf	-7.90	2ztz	-7.60
2axf	-8.20	3uqi	-7.90	4gv9	-7.50
1v3c	-8.20	3uqi	-7.90	4ffy	-7.50
1rv7	-8.20	3su6	-7.90	4ejd	-7.50
1p9s	-8.20	2xpx	-7.90	4ejd	-7.50

PDB	Docking score	PDB	Docking score	PDB	Docking score
4ejd	-7.50	2xya	-7.10	2zol	-6.70
4e92	-7.50	2wfo	-7.10	4oyd	-6.60
4dga	-7.50	2ca1	-7.10	4nwk	-6.60
4dga	-7.50	1qz8	-7.10	3u83	-6.60
4c1w	-7.50	4lcx	-7.00	3avn	-6.60
3su0	-7.50	3sv9	-7.00	2yhh	-6.60
2yka	-7.50	3sv6	-7.00	2y1s	-6.60
2me2	-7.50	3sv6	-7.00	4nwl	-6.50
1rq9	-7.50	3sud	-7.00	4b4n	-6.50
4oyd	-7.40	3su5	-7.00	4b4n	-6.50
4b8e	-7.40	3su4	-7.00	3u83	-6.50
4b8e	-7.40	3su4	-7.00	2v6q	-6.50
4b8e	-7.40	3gzf	-7.00	2l2f	-6.50
3w39	-7.40	2zty	-7.00	4g1l	-6.40
3rkc	-7.40	1qr8	-7.00	3avk	-6.40
3p8n	-7.40	4i33	-6.90	4ipz	-6.30
4lkh	-7.30	4g8i	-6.90	4ipz	-6.30
4ejk	-7.30	3sug	-6.90	4ipz	-6.30
4ejk	-7.30	3m5i	-6.90	4ipz	-6.30
4dmn	-7.30	2wfo	-6.90	4ipz	-6.30
4dmn	-7.30	2vxw	-6.90	4ipz	-6.30
4dgb	-7.30	2q5u	-6.90	4ipz	-6.30
4dgb	-7.30	2q5u	-6.90	4ipz	-6.30
3sv7	-7.30	2q5u	-6.90	4ipz	-6.30
3sue	-7.30	2q5u	-6.90	4ipz	-6.30
3su5	-7.30	2q5u	-6.90	4ipz	-6.30
3sis	-7.30	2q5u	-6.90	4c1w	-6.30
3m5h	-7.30	2m3m	-6.90	4mod	-6.20
3ifu	-7.30	2hfz	-6.90	4mod	-6.20
3gsn	-7.30	2g69	-6.90	4ipz	-6.20
3avk	-7.30	2g69	-6.90	4epj	-6.20
2zu1	-7.30	1zsd	-6.90	4epj	-6.10
2yhf	-7.30	1qr9	-6.90	2c86	-6.10
Papain	-7.20	3sug	-6.80	2c3a	-6.10
protease	-7.20	3su6	-6.80	4ejr	-6.00
4lsp	-7.20	3s12	-6.80	3vie	-6.00
4g9d	-7.20	3avj	-6.80	4adq	-5.90
4g8i	-7.20	2q7c	-6.80	2mkr	-5.90
4ekx	-7.20	2q7c	-6.80	3kqk	-5.80
3vie	-7.20	2q7c	-6.80	3giv	-5.80
2xze	-7.20	2m3l	-6.80	4adq	-5.70
1z8r	-7.20	2gvf	-6.80	2vxj	-5.70
1f08	-7.20	4nwk	-6.70	3vtt	-5.50
4g1g	-7.10	3zd0	-6.70	4kol	-5.40
4ejk	-7.10	3b71	-6.70	3i6k	-5.40
3sv9	-7.10	3b71	-6.70	4kom	-5.30
3su5	-7.10	3avc	-6.70	4g2k	-5.20
3sis	-7.10	2zu3	-6.70	3vtt	-5.20



PDB	Docking score	PDB	Docking score	PDB	Docking score
4ep2	-5.10	4uoa	-4.60	3m5g	-2.50
2x9m	-5.10	4g2k	-4.50	4dge	-1.50
4ep2	-5.00	1hhg	-4.30	3vu5	-1.30
4kon	-4.90	2jw8	-3.90	2zsv	-1.10
2me3	-4.90	4lki	-3.70	2zsv	-1.00
2l3h	-4.90	1knz	-3.20	4e0r	-0.50
3j22	-4.80	4qhm	-2.90	3m5j	-0.40
3j23	-4.70	2wrb	-2.70	4fqm	-0.10

**Table S3.** Predicted docking score of Dutarestide against the viral protein panel.

PDB	Docking score	PDB	Docking score	PDB	Docking score
4wm7	-12.80	4uo5	-11.60	3rwe	-11.30
3t3c	-12.60	4j4w	-11.60	3rwc	-11.30
3t3c	-12.50	3vcl	-11.60	3rwc	-11.30
3nxu	-12.50	3vcl	-11.60	3lkh	-11.30
2i4x	-12.40	3bw9	-11.60	3kqn	-11.30
4j4x	-12.30	2wrg	-11.60	3kqn	-11.30
2i4v	-12.30	2wrg	-11.60	3kqn	-11.30
4rw6	-12.20	1p9u	-11.60	3kql	-11.30
3r4b	-12.20	1ida	-11.60	3kql	-11.30
2i4d	-12.10	4uo5	-11.50	3koa	-11.30
4wm8	-12.00	4uo5	-11.50	3i6l	-11.30
3bwa	-12.00	4rw7	-11.50	3gso	-11.30
3b0w	-12.00	4qru	-11.50	2hcs	-11.30
2axg	-12.00	4qru	-11.50	2bvp	-11.30
4q6r	-11.90	4qrs	-11.50	1hhk	-11.30
4q6r	-11.90	4m30	-11.50	4uo0	-11.20
4k7f	-11.90	4g9f	-11.50	4uo0	-11.20
4k7f	-11.90	4cew	-11.50	4m8y	-11.20
3r4b	-11.90	4lsv	-11.40	4j4v	-11.20
1oop	-11.90	3rwg	-11.40	4e78	-11.20
1hhh	-11.90	3rwg	-11.40	3rwe	-11.20
4rw4	-11.80	3kql	-11.40	3ok9	-11.20
4rw4	-11.80	3bew	-11.40	3lkh	-11.20
4o44	-11.80	1idb	-11.40	3gso	-11.20
4g42	-11.80	1hhj	-11.40	4uo2	-11.10
3u7s	-11.80	4m8y	-11.30	4uo2	-11.10
3u7s	-11.80	4j4v	-11.30	4uo2	-11.10
2i4w	-11.80	4j4v	-11.30	4uo2	-11.10
3rwd	-11.70	4j4v	-11.30	4uo0	-11.10
3ggg	-11.70	4j4v	-11.30	4uo0	-11.10
3bw9	-11.70	3ztj	-11.30	4uo0	-11.10
2wrg	-11.70	3vbr	-11.30	4uo0	-11.10
2wrg	-11.70	3rwi	-11.30	4uo0	-11.10
2wrg	-11.70	3rwh	-11.30	4uo0	-11.10
2i4u	-11.70	3rwh	-11.30	4j4y	-11.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
4gua	-11.10	4unx	-10.90	4ejl	-10.70
4fqj	-11.10	4unw	-10.90	4e5e	-10.70
3h98	-11.10	4unw	-10.90	3hkw	-10.70
3h98	-11.10	4opa	-10.90	3hkw	-10.70
2hjk	-11.10	4mkb	-10.90	3gsw	-10.70
2bvo	-11.10	4fnk	-10.90	3fku	-10.70
1hhi	-11.10	3vbo	-10.90	3cj3	-10.70
4uo7	-11.00	3tie	-10.90	3cj3	-10.70
4uo7	-11.00	3tie	-10.90	3cj0	-10.70
4uo7	-11.00	3s11	-10.90	3cj0	-10.70
4uo7	-11.00	3ciz	-10.90	2ygc	-10.70
4uo7	-11.00	3ciz	-10.90	2ygc	-10.70
4uo7	-11.00	2wrh	-10.90	1syv	-10.70
4uo3	-11.00	2wre	-10.90	4rw9	-10.60
4uo3	-11.00	2wr1	-10.90	4pg2	-10.60
4uo3	-11.00	2uv0	-10.90	4o4g	-10.60
4uo3	-11.00	2uv0	-10.90	4mka	-10.60
4uo3	-11.00	2uv0	-10.90	4mka	-10.60
4uo2	-11.00	2uv0	-10.90	4mk8	-10.60
4uo2	-11.00	2uv0	-10.90	4mk8	-10.60
4uo0	-11.00	2gec	-10.90	4ejl	-10.60
4uo0	-11.00	1r6a	-10.90	4bac	-10.60
4uo0	-11.00	1n59	-10.90	3cj4	-10.60
4uo0	-11.00	1izh	-10.90	3cj2	-10.60
4uo0	-11.00	4uo0	-10.80	3bwa	-10.60
4uo0	-11.00	4mkb	-10.80	2uv0	-10.60
4qrs	-11.00	4i2q	-10.80	4pv9	-10.50
4m8x	-11.00	3kqh	-10.80	4mmr	-10.50
4m8x	-11.00	2wre	-10.80	4mk9	-10.50
4cey	-11.00	2wre	-10.80	4j4u	-10.50
3kna	-11.00	2wre	-10.80	4e7a	-10.50
3gsr	-11.00	2wre	-10.80	4e7a	-10.50
3gsq	-11.00	2wre	-10.80	4a92	-10.50
3gsq	-11.00	2wr3	-10.80	3cj5	-10.50
3ggu	-11.00	2wr0	-10.80	3cj4	-10.50
3bev	-11.00	2wa1	-10.80	3cj2	-10.50
2wr1	-11.00	2vvw	-10.80	2ygb	-10.50
2wr1	-11.00	2uv0	-10.80	2ygb	-10.50
2wr0	-11.00	2uv0	-10.80	4fnk	-10.40
2wr0	-11.00	2uv0	-10.80	4e5l	-10.40
2wr0	-11.00	2uv0	-10.80	4e5f	-10.40
2wr0	-11.00	2uv0	-10.80	3nf7	-10.40
2vvw	-11.00	4unx	-10.70	3n0i	-10.40
1izi	-11.00	4unx	-10.70	3h2l	-10.40
4uo0	-10.90	4unw	-10.70	3h2l	-10.40
4uo0	-10.90	4rw8	-10.70	3cpl	-10.40
4uo0	-10.90	4mk9	-10.70	3cj5	-10.40
4unx	-10.90	4j4r	-10.70	2wrf	-10.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
2wr4	-10.40	3tid	-10.00	2oy0	-9.70
2wr2	-10.40	3nf9	-10.00	1sk7	-9.70
2wr2	-10.40	3nf8	-10.00	4uny	-9.60
2wr2	-10.40	3nf8	-10.00	4lsu	-9.60
1quv	-10.40	3klv	-10.00	4j4s	-9.60
4g43	-10.30	3ebj	-10.00	4j4s	-9.60
4e5g	-10.30	3d0g	-10.00	4cdx	-9.60
4cqy	-10.30	3avh	-10.00	3se9	-9.60
4bh0	-10.30	2vxx	-10.00	3nf6	-9.60
4a92	-10.30	2vxx	-10.00	2x83	-9.60
3nf7	-10.30	2hty	-10.00	2x83	-9.60
3hky	-10.30	1a41	-10.00	1r6a	-9.60
3hky	-10.30	4uo3	-9.90	4uo6	-9.50
3gsw	-10.30	4mj1	-9.90	4mmu	-9.50
3cpl	-10.30	4i2p	-9.90	4fqr	-9.50
1pk0	-10.30	4gag	-9.90	4ffz	-9.50
4mgu	-10.20	4ej8	-9.90	4egt	-9.50
4lst	-10.20	4cdu	-9.90	4e91	-9.50
4f3z	-10.20	3nf9	-9.90	3uf5	-9.50
4e78	-10.20	3avg	-9.90	3ava	-9.50
3tid	-10.20	4pv9	-9.80	4g8g	-9.40
3nf7	-10.20	4pv9	-9.80	4fqy	-9.40
3nf7	-10.20	4mds	-9.80	4fqy	-9.40
3n0i	-10.20	4mds	-9.80	4fqr	-9.40
2wr7	-10.20	4lsu	-9.80	4cqy	-9.40
2hu0	-10.20	4kpp	-9.80	4bh2	-9.40
2gec	-10.20	4i2p	-9.80	4bh2	-9.40
1n5a	-10.20	4gaj	-9.80	3se8	-9.40
4u6h	-10.10	4ej8	-9.80	3se8	-9.40
4qhk	-10.10	4adf	-9.80	3nfa	-9.40
4mk7	-10.10	4adf	-9.80	3d23	-9.40
4lsr	-10.10	4adf	-9.80	3ava	-9.40
4cdq	-10.10	3iyw	-9.80	1v3e	-9.40
3nf8	-10.10	3iyw	-9.80	1v2i	-9.40
3hkw	-10.10	3iyw	-9.80	1v2i	-9.40
2uv0	-10.10	3iyw	-9.80	4pv8	-9.30
1klm	-10.10	3iyw	-9.80	4kps	-9.30
4uo3	-10.00	3d0h	-9.80	4g8g	-9.30
4uo3	-10.00	2xi5	-9.80	4dag	-9.30
4uo3	-10.00	4jo8	-9.70	4co6	-9.30
4uo3	-10.00	4gag	-9.70	3zp1	-9.30
4qhn	-10.00	4cqy	-9.70	3oah	-9.30
4mk7	-10.00	4bgz	-9.70	3nfa	-9.30
4mj0	-10.00	4adf	-9.70	3nfa	-9.30
4g9f	-10.00	3nf6	-9.70	3nfa	-9.30
4cdw	-10.00	3lqa	-9.70	3nf6	-9.30
4adf	-10.00	3iyw	-9.70	3mlh	-9.30
4adf	-10.00	2xwy	-9.70	3i6g	-9.30

PDB	Docking score	PDB	Docking score	PDB	Docking score
3d23	-9.30	3avb	-9.00	3avb	-8.80
2z35	-9.30	3ava	-9.00	2mgu	-8.80
2ghw	-9.30	2xi5	-9.00	1v3b	-8.80
1v3c	-9.30	5ajm	-8.90	5ajm	-8.70
1v3c	-9.30	5ajm	-8.90	4uo8	-8.70
1v3c	-9.30	4uo6	-8.90	4mg3	-8.70
1v3b	-9.30	4qhl	-8.90	4iv1	-8.70
4jb9	-9.20	4pv8	-8.90	4fqi	-8.70
4bgy	-9.20	4mj1	-8.90	4fqi	-8.70
4bgw	-9.20	4g9z	-8.90	4cqp	-8.70
4bgw	-9.20	4fqi	-8.90	4cqp	-8.70
3v3m	-9.20	4cqu	-8.90	4cqp	-8.70
3nf9	-9.20	4cqu	-8.90	4cqp	-8.70
3ku3	-9.20	4cqu	-8.90	3zpa	-8.70
3ku3	-9.20	4cqr	-8.90	3zp6	-8.70
1b53	-9.20	4cqr	-8.90	3zp0	-8.70
4gaj	-9.10	4cqq	-8.90	3rwj	-8.70
4fp8	-9.10	4cqq	-8.90	3oah	-8.70
4fp8	-9.10	4cqq	-8.90	3nf6	-8.70
4cqz	-9.10	3zp2	-8.90	3mj5	-8.70
4cqz	-9.10	3ro5	-8.90	3mj5	-8.70
4bh1	-9.10	3nw8	-8.90	3avg	-8.70
4bh1	-9.10	3gsv	-8.90	2oy0	-8.70
3zpb	-9.10	3bwa	-8.90	2c36	-8.70
3zpb	-9.10	3avb	-8.90	2c36	-8.70
3zp3	-9.10	2ht5	-8.90	4ejd	-8.60
3v3m	-9.10	1v3d	-8.90	4cqp	-8.60
3rki	-9.10	1v3d	-8.90	4bgx	-8.60
3o4l	-9.10	1rzj	-8.90	3ku5	-8.60
3nf9	-9.10	5ajm	-8.80	3ku5	-8.60
3ava	-9.10	5ajm	-8.80	3gsx	-8.60
3alz	-9.10	5ajm	-8.80	3gsr	-8.60
2wrc	-9.10	4mg3	-8.80	2xra	-8.60
1v3e	-9.10	4g9z	-8.80	2vvy	-8.60
1v3c	-9.10	4cr0	-8.80	2hu4	-8.60
1rzk	-9.10	4cqu	-8.80	2hu4	-8.60
4i7f	-9.00	4cqu	-8.80	2htw	-8.60
4e76	-9.00	4cqu	-8.80	2htu	-8.60
4cqs	-9.00	4cqp	-8.80	2ge8	-8.60
4cqs	-9.00	4bh1	-8.80	1yh3	-8.60
4bgx	-9.00	3vbh	-8.80	4mza	-8.50
3nwf	-9.00	3sdy	-8.80	4mza	-8.50
3nf8	-9.00	3sdy	-8.80	4f3i	-8.50
3ku6	-9.00	3s13	-8.80	4f3i	-8.50
3ku6	-9.00	3rwj	-8.80	4eq0	-8.50
3gsv	-9.00	3gsx	-8.80	4ejd	-8.50
3avl	-9.00	3gsu	-8.80	4ejd	-8.50
3avb	-9.00	3avl	-8.80	4dkq	-8.50

PDB	Docking score	PDB	Docking score	PDB	Docking score
4cqy	-8.50	4i2q	-8.10	2q7c	-7.80
4bh4	-8.50	4fb3	-8.10	2bvq	-7.80
3u82	-8.50	4e5j	-8.10	2axf	-7.80
3pqy	-8.50	4bh3	-8.10	1sys	-7.80
3gsu	-8.50	4bh3	-8.10	4nwk	-7.70
3avn	-8.50	4bh3	-8.10	4i31	-7.70
3avj	-8.50	4bh3	-8.10	4i31	-7.70
3avc	-8.50	3alw	-8.10	4fvu	-7.70
2zu5	-8.50	2iph	-8.10	3sv9	-7.70
2zu4	-8.50	2iph	-8.10	3sit	-7.70
2wh6	-8.50	2iph	-8.10	3sit	-7.70
2hu4	-8.50	2iph	-8.10	2zu1	-7.70
2hu4	-8.50	2hfz	-8.10	4qrt	-7.60
Main protease	-8.40	1rpi	-8.10	4mmt	-7.60
4qrt	-8.40	4qru	-8.00	4ejd	-7.60
4lkj	-8.40	4mze	-8.00	4ejd	-7.60
4hkj	-8.40	4gzf	-8.00	4ejd	-7.60
4bh4	-8.40	4gve	-8.00	4dgd	-7.60
4bh4	-8.40	4fqv	-8.00	4dgc	-7.60
3u82	-8.40	4ep3	-8.00	4bh4	-7.60
3alx	-8.40	4e92	-8.00	3sv9	-7.60
2ge7	-8.40	3rwf	-8.00	3sit	-7.60
1rv7	-8.40	2xze	-8.00	3sit	-7.60
1rpi	-8.40	1rq9	-8.00	3m5h	-7.60
4gv3	-8.30	4qrt	-7.90	3gsn	-7.60
3ztn	-8.30	4oph	-7.90	3avf	-7.60
3sdy	-8.30	4mmv	-7.90	2zty	-7.60
3rwi	-8.30	4jkg	-7.90	2q7c	-7.60
3nwa	-8.30	4i32	-7.90	2lsp	-7.60
3nwa	-8.30	4gzf	-7.90	2g69	-7.60
2xze	-8.30	4fqv	-7.90	2g69	-7.60
2ghv	-8.30	4ejk	-7.90	2axf	-7.60
4lsp	-8.20	4ejk	-7.90	4ipz	-7.50
4gv3	-8.20	2xya	-7.90	4eq0	-7.50
4dgd	-8.20	2hcn	-7.90	4dco	-7.50
4dga	-8.20	4mj0	-7.80	4dgc	-7.50
4dga	-8.20	4jkg	-7.80	4dgc	-7.50
3avh	-8.20	4ep3	-7.80	4dgc	-7.50
2c7u	-8.20	4ejd	-7.80	4dgc	-7.50
1p9s	-8.20	4eee	-7.80	4dgc	-7.50
Spike RBD	-8.10	4e5i	-7.80	3sv6	-7.50
Papain protease	-8.10	3vbf	-7.80	3sud	-7.50
4mms	-8.10	3vbf	-7.80	3gsw	-7.50
4lss	-8.10	3sis	-7.80	3avk	-7.50
4j6r	-8.10	3sis	-7.80	2ca1	-7.50
4iv3	-8.10	3rwf	-7.80	4jpi	-7.40
		2wh6	-7.80	4ipz	-7.40
		2q7c	-7.80	4ipz	-7.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
4ipz	-7.40	4nwk	-7.00	3kmq	-6.40
4ffv	-7.40	3uqi	-7.00	2v6q	-6.40
4ejd	-7.40	3uqi	-7.00	2q7c	-6.40
3u83	-7.40	3su3	-7.00	4mod	-6.30
3su3	-7.40	3su2	-7.00	4mod	-6.30
3kms	-7.40	3su0	-7.00	4epj	-6.30
4oyd	-7.30	3su0	-7.00	4ekx	-6.30
4ipz	-7.30	3s12	-7.00	3sv7	-6.30
4ipz	-7.30	3d0i	-7.00	3sug	-6.30
4ipz	-7.30	2yka	-7.00	3sug	-6.30
4ipz	-7.30	1b50	-7.00	2q5u	-6.30
4ipz	-7.30	4gye	-6.90	2q5u	-6.30
4g9d	-7.30	4gye	-6.90	2q5u	-6.30
4dkp	-7.30	4eqj	-6.90	2q5u	-6.30
4dgb	-7.30	4ejd	-6.90	1zsd	-6.30
3w39	-7.30	3sv6	-6.90	4nwl	-6.20
3u83	-7.30	3su6	-6.90	4i33	-6.20
3su6	-7.30	3sit	-6.90	3suf	-6.20
3su2	-7.30	4oyd	-6.80	3rkc	-6.20
3su1	-7.30	4b8e	-6.80	3avc	-6.20
3sit	-7.30	3vie	-6.80	2q5u	-6.20
3m5i	-7.30	3su4	-6.80	2q5u	-6.20
3ifu	-7.30	3su4	-6.80	2me2	-6.20
3gzf	-7.30	2me4	-6.80	2m3l	-6.20
2xpx	-7.30	4gv9	-6.70	3zd0	-6.10
4ipz	-7.20	4dgb	-6.70	2zu3	-6.10
4e92	-7.20	4b8e	-6.70	1z8r	-6.10
4dmn	-7.20	2yol	-6.70	1qr9	-6.10
3p8n	-7.20	2yol	-6.70	4g8i	-6.00
2xpx	-7.20	2yhf	-6.70	3avj	-6.00
2vxw	-7.20	4g9d	-6.60	4b4n	-5.90
2gvf	-7.20	3sud	-6.60	2l2f	-5.90
4mze	-7.10	3su5	-6.60	2c86	-5.90
4jpk	-7.10	3su5	-6.60	2c3a	-5.90
4ipz	-7.10	3b71	-6.60	4adq	-5.80
4dmn	-7.10	3b71	-6.60	3avk	-5.80
4dkr	-7.10	3a07	-6.60	4b4n	-5.70
4c1w	-7.10	2wfo	-6.60	4g8i	-5.60
4b8e	-7.10	2q7c	-6.60	4adq	-5.60
3sv8	-7.10	2q7c	-6.60	3avn	-5.60
3sv7	-7.10	4ipz	-6.50	3sue	-5.40
3su2	-7.10	4ejk	-6.50	3giv	-5.40
3su1	-7.10	4c1w	-6.50	3kqk	-5.30
3p8o	-7.10	3su5	-6.50	2vxj	-5.30
2ztz	-7.10	2yhh	-6.50	3iyp	-5.20
2zol	-7.10	2y1s	-6.50	2x9m	-5.20
1qz8	-7.10	2wfo	-6.50	2x5i	-5.20
1f08	-7.10	4ejr	-6.40	3i6k	-5.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
4uo4	-5.00	2m3m	-4.30	2zsv	-1.30
3vtt	-5.00	2me3	-4.20	2zsv	-1.10
3vtt	-5.00	4ep2	-3.70	4uoa	-0.60
2mkr	-5.00	4ep2	-3.70	4e0r	-0.50
1qr8	-4.90	4qhm	-3.00	3m5g	-0.40
3j23	-4.70	4epj	-3.00	4fqm	-0.30
3vie	-4.60	2l3h	-2.60		
3j22	-4.40	4dge	-1.80		

**Table S 4.** Predicted docking score of Dolutegravir against the viral protein panel.

PDB	Docking score	PDB	Docking score	PDB	Docking score
4cey	-11.30	2uv0	-10.60	2i4w	-10.30
3koa	-11.30	2uv0	-10.60	2i4u	-10.30
4g42	-11.10	2uv0	-10.60	2hty	-10.30
4cdu	-11.10	2uv0	-10.60	1syv	-10.30
3t3c	-11.10	2uv0	-10.60	4uo3	-10.20
3t3c	-11.10	2htw	-10.60	4mkb	-10.20
4j4x	-11.00	4wm7	-10.50	4mk7	-10.20
4fvu	-11.00	4pv9	-10.50	4lkj	-10.20
3kql	-11.00	4fnk	-10.50	4k7f	-10.20
3kql	-11.00	4f3z	-10.50	4k7f	-10.20
4wm8	-10.90	3vcl	-10.50	4fqr	-10.20
4lsv	-10.90	3kna	-10.50	4fqr	-10.20
4cdq	-10.90	3fku	-10.50	4e76	-10.20
3kql	-10.90	3b0w	-10.50	3r4b	-10.20
4cew	-10.80	2i4v	-10.50	3pqy	-10.20
1klm	-10.80	4g43	-10.40	3lkh	-10.20
4g9z	-10.70	3u7s	-10.40	3lkh	-10.20
4g9z	-10.70	3u7s	-10.40	3i6l	-10.20
4cdx	-10.70	3rwd	-10.40	3cj5	-10.20
3nxu	-10.70	3kqn	-10.40	3bwa	-10.20
2uv0	-10.70	3kqn	-10.40	3bwa	-10.20
2uv0	-10.70	3kqn	-10.40	3bw9	-10.20
2uv0	-10.70	3hkw	-10.40	2wrf	-10.20
2uv0	-10.70	3cj3	-10.40	2hu0	-10.20
2uv0	-10.70	2wrh	-10.40	2hjk	-10.20
4cdw	-10.60	2bvp	-10.40	2gec	-10.20
3vcl	-10.60	1hhk	-10.40	2gec	-10.20
2wrg	-10.60	4e78	-10.30	2axg	-10.20
2wrg	-10.60	4e78	-10.30	4uo3	-10.10
2wrg	-10.60	3ztj	-10.30	4mka	-10.10
2wrg	-10.60	3s11	-10.30	4gua	-10.10
2wrg	-10.60	3rwc	-10.30	4fnk	-10.10
2uv0	-10.60	3rwc	-10.30	3r4b	-10.10
2uv0	-10.60	3cj3	-10.30	3o4l	-10.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
3cj5	-10.10	4uo2	-9.90	2wr0	-9.90
3bew	-10.10	4uo0	-9.90	2hu4	-9.90
3bev	-10.10	4uo0	-9.90	2hu4	-9.90
2wre	-10.10	4uo0	-9.90	2hu4	-9.90
2i4x	-10.10	4uo0	-9.90	1oop	-9.90
2hcs	-10.10	4uo0	-9.90	1ida	-9.90
2bvo	-10.10	4uo0	-9.90	4uo7	-9.80
1r6a	-10.10	4uo0	-9.90	4uo7	-9.80
1p9u	-10.10	4uo0	-9.90	4uo7	-9.80
1hhj	-10.10	4uo0	-9.90	4uo7	-9.80
1hhi	-10.10	4uo0	-9.90	4uo7	-9.80
1hhh	-10.10	4uo0	-9.90	4uo7	-9.80
4unw	-10.00	4uo0	-9.90	4uo2	-9.80
4unw	-10.00	4uo0	-9.90	4uo0	-9.80
4u6h	-10.00	4uo0	-9.90	4unw	-9.80
4rw4	-10.00	4uo0	-9.90	4rw6	-9.80
4qru	-10.00	4uo0	-9.90	4qrs	-9.80
4qru	-10.00	4uo0	-9.90	4qrs	-9.80
4q6r	-10.00	4rw4	-9.90	4j4y	-9.80
4o44	-10.00	4q6r	-9.90	4i2p	-9.80
4o4g	-10.00	4mmr	-9.90	4ejl	-9.80
4j4u	-10.00	4mk9	-9.90	4e5i	-9.80
4ej8	-10.00	4mk8	-9.90	3vbr	-9.80
3rwi	-10.00	4g9f	-9.90	3iyw	-9.80
3rwh	-10.00	4ej8	-9.90	3iyw	-9.80
3rwh	-10.00	3se9	-9.90	3hky	-9.80
3rwg	-10.00	3rwg	-9.90	3h98	-9.80
3ok9	-10.00	3rwe	-9.90	3gsw	-9.80
3klv	-10.00	3rwe	-9.90	3cj2	-9.80
3hky	-10.00	3iyw	-9.90	3ciz	-9.80
3hkw	-10.00	3iyw	-9.90	2wr2	-9.80
3ciz	-10.00	3iyw	-9.90	2wr1	-9.80
3bw9	-10.00	3hkw	-9.90	2wr1	-9.80
2ygc	-10.00	3h2l	-9.90	1v3d	-9.80
2ygc	-10.00	3h2l	-9.90	1v3d	-9.80
2wrc	-10.00	3ggg	-9.90	1izi	-9.80
2i4d	-10.00	3ggg	-9.90	4uo8	-9.70
1idb	-10.00	2wre	-9.90	4pg2	-9.70
4uo5	-9.90	2wre	-9.90	4j4w	-9.70
4uo5	-9.90	2wre	-9.90	4j4s	-9.70
4uo5	-9.90	2wre	-9.90	4g9f	-9.70
4uo3	-9.90	2wre	-9.90	4ejl	-9.70
4uo3	-9.90	2wr3	-9.90	4e7a	-9.70
4uo3	-9.90	2wr1	-9.90	4e7a	-9.70
4uo2	-9.90	2wr0	-9.90	4e5e	-9.70
4uo2	-9.90	2wr0	-9.90	4cqW	-9.70
4uo2	-9.90	2wr0	-9.90	4cqV	-9.70
4uo2	-9.90	2wr0	-9.90	4cqu	-9.70



PDB	Docking score	PDB	Docking score	PDB	Docking score
4cqr	-9.70	3nf8	-9.50	4e5l	-9.30
4bh2	-9.70	3nf8	-9.50	4dag	-9.30
3h98	-9.70	3nf6	-9.50	4cqu	-9.30
3gsw	-9.70	3nf6	-9.50	4bh0	-9.30
3gsr	-9.70	3mlh	-9.50	3vbo	-9.30
3gso	-9.70	3iyw	-9.50	3tie	-9.30
3ebj	-9.70	2ygb	-9.50	3tie	-9.30
3cj4	-9.70	2ygb	-9.50	3tid	-9.30
3cj4	-9.70	2wr2	-9.50	3sdy	-9.30
2hu4	-9.70	1quv	-9.50	3nfa	-9.30
1n5a	-9.70	Main		3nfa	-9.30
1izh	-9.70	protease	-9.40	3ku5	-9.30
4uo3	-9.60	4mmu	-9.40	3iyp	-9.30
4uo3	-9.60	4mms	-9.40	3cj2	-9.30
4uo3	-9.60	4mgu	-9.40	3avc	-9.30
4uo3	-9.60	4m30	-9.40	2x5i	-9.30
4uo3	-9.60	4j4v	-9.40	2vvw	-9.30
4rw8	-9.60	4j4v	-9.40	1v3c	-9.30
4mka	-9.60	4j4v	-9.40	1v3b	-9.30
4mk8	-9.60	4j4r	-9.40	1v3b	-9.30
4m8x	-9.60	4cqz	-9.40	1v2i	-9.30
4j6r	-9.60	4bgw	-9.40	5ajm	-9.20
4j4v	-9.60	4adf	-9.40	5ajm	-9.20
4i2p	-9.60	4adf	-9.40	4unx	-9.20
4fqj	-9.60	4adf	-9.40	4unx	-9.20
4eee	-9.60	4adf	-9.40	4unx	-9.20
4cqz	-9.60	4adf	-9.40	4unx	-9.20
4cqu	-9.60	4adf	-9.40	4unx	-9.20
4bgw	-9.60	4a92	-9.40	4mg3	-9.20
3kqh	-9.60	3nf9	-9.40	4lkk	-9.20
3gso	-9.60	3nf9	-9.40	4kpp	-9.20
2wr4	-9.60	3nf7	-9.40	4hkj	-9.20
2wa1	-9.60	3nf7	-9.40	4cqp	-9.20
4uny	-9.50	3gsr	-9.40	4bac	-9.20
4rw7	-9.50	3gsq	-9.40	4a92	-9.20
4qhk	-9.50	3gsq	-9.40	3zp0	-9.20
4mze	-9.50	2wr7	-9.40	3tid	-9.20
4mze	-9.50	2wr2	-9.40	3sdy	-9.20
4m8y	-9.50	1v3e	-9.40	3sdy	-9.20
4m8y	-9.50	1v3e	-9.40	3ku5	-9.20
4m8x	-9.50	1v3c	-9.40	3ku3	-9.20
4j4v	-9.50	1v2i	-9.40	3d0g	-9.20
4j4v	-9.50	1a41	-9.40	3cpl	-9.20
4i7f	-9.50	4rw9	-9.30	3cj0	-9.20
4i2q	-9.50	4mkb	-9.30	3cj0	-9.20
4cqu	-9.50	4lsr	-9.30	3avg	-9.20
3se8	-9.50	4j4v	-9.30	3avb	-9.20
3se8	-9.50	4eq0	-9.30	2vvw	-9.20
				5ajm	-9.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
4qru	-9.10	4fqv	-8.90	3rki	-8.70
4opa	-9.10	4fp8	-8.90	3lqa	-8.70
4mk9	-9.10	4ffz	-8.90	3gsn	-8.70
4mg3	-9.10	4eq0	-8.90	3d23	-8.70
4lst	-9.10	4e91	-8.90	3ava	-8.70
4kps	-9.10	4e5f	-8.90	3ava	-8.70
4j4s	-9.10	4bgx	-8.90	2z35	-8.70
4gag	-9.10	3zp6	-8.90	2xi5	-8.70
4gag	-9.10	3zp1	-8.90	2xi5	-8.70
4egt	-9.10	3su6	-8.90	2wh6	-8.70
4e5g	-9.10	3nf8	-8.90	2oy0	-8.70
3zp3	-9.10	3nf8	-8.90	2c36	-8.70
3oah	-9.10	3mj5	-8.90	2c36	-8.70
3ku6	-9.10	3mj5	-8.90	1sk7	-8.70
3ku6	-9.10	3gsv	-8.90	1pk0	-8.70
3gsx	-9.10	3d23	-8.90	4fqi	-8.60
3gsx	-9.10	3bwa	-8.90	4fqi	-8.60
3d0i	-9.10	2zu4	-8.90	4dgd	-8.60
3cpl	-9.10	2xra	-8.90	4dga	-8.60
3avb	-9.10	2mgu	-8.90	4dga	-8.60
3alz	-9.10	1n59	-8.90	4cqx	-8.60
2xwy	-9.10	5ajm	-8.80	4cqr	-8.60
2vvx	-9.10	4qhn	-8.80	4cqp	-8.60
2ht5	-9.10	4mj1	-8.80	4cqp	-8.60
1v3c	-9.10	4mj0	-8.80	4cqp	-8.60
1v3c	-9.10	4mds	-8.80	4cqp	-8.60
1b50	-9.10	4jo8	-8.80	4bgz	-8.60
5ajm	-9.00	4i2q	-8.80	3zp2	-8.60
4pv9	-9.00	4gv3	-8.80	3nwa	-8.60
4mk7	-9.00	4g9d	-8.80	3nf7	-8.60
4gaj	-9.00	4f3i	-8.80	3nf7	-8.60
4gaj	-9.00	4e5j	-8.80	3ifu	-8.60
4fp8	-9.00	4dgd	-8.80	3i6g	-8.60
3n0i	-9.00	4cqu	-8.80	3avj	-8.60
3n0i	-9.00	4bgy	-8.80	2hfz	-8.60
3gsu	-9.00	3v3m	-8.80	Spike RBD	-8.50
3gsu	-9.00	3oah	-8.80	4uo6	-8.50
3d0h	-9.00	3ku3	-8.80	4uo6	-8.50
3avh	-9.00	3gsv	-8.80	4oyd	-8.50
2vvx	-9.00	3avh	-8.80	4fqy	-8.50
1yh3	-9.00	2oy0	-8.80	4fqy	-8.50
4qrt	-8.90	1rzj	-8.80	4fqi	-8.50
4pv9	-8.90	4mds	-8.70	4fb3	-8.50
4mza	-8.90	4jpk	-8.70	4f3i	-8.50
4mza	-8.90	4gv3	-8.70	4ejk	-8.50
4g8g	-8.90	4cqp	-8.70	4ejk	-8.50
4g8g	-8.90	3zpa	-8.70	4ejk	-8.50
4fqv	-8.90	3v3m	-8.70	4cqp	-8.50

PDB	Docking score	PDB	Docking score	PDB	Docking score
4cqq	-8.50	4dgc	-8.20	3kms	-8.00
4cqq	-8.50	4dgc	-8.20	2iph	-8.00
3zpb	-8.50	4dgc	-8.20	2iph	-8.00
3zpb	-8.50	4cqu	-8.20	2hcn	-8.00
3s13	-8.50	4cqs	-8.20	1f08	-8.00
3nwa	-8.50	4cqs	-8.20	4uo4	-7.90
3avl	-8.50	4bh4	-8.20	4qrt	-7.90
2x83	-8.50	4bh4	-8.20	4oph	-7.90
1rzk	-8.50	4bh4	-8.20	4mmt	-7.90
4qhl	-8.40	4bh4	-8.20	4jpi	-7.90
4jb9	-8.40	4bh1	-8.20	4gye	-7.90
4gve	-8.40	4bh1	-8.20	4gye	-7.90
4cr0	-8.40	4bh1	-8.20	3uf5	-7.90
4cqq	-8.40	3nf9	-8.20	3su0	-7.90
4bgx	-8.40	3avg	-8.20	3rwj	-7.90
3ztn	-8.40	2zu5	-8.20	3rwj	-7.90
3u82	-8.40	2iph	-8.20	3nwf	-7.90
3u82	-8.40	2ghw	-8.20	2vvy	-7.90
3su1	-8.40	2ge7	-8.20	1p9s	-7.90
3avn	-8.40	4pv8	-8.10	1b53	-7.90
3avb	-8.40	4pv8	-8.10	4gv9	-7.80
3avb	-8.40	4eqj	-8.10	4ejd	-7.80
3ava	-8.40	4ep3	-8.10	4ejd	-7.80
3ava	-8.40	4ep3	-8.10	4ejd	-7.80
3alx	-8.40	4dkr	-8.10	4ejd	-7.80
2yol	-8.40	4dgc	-8.10	4ejd	-7.80
2yol	-8.40	4dgc	-8.10	4dkq	-7.80
2x83	-8.40	4dgc	-8.10	4dko	-7.80
2htu	-8.40	4co6	-8.10	3sis	-7.80
5ajm	-8.30	4bh3	-8.10	3nw8	-7.80
4gzf	-8.30	4bh3	-8.10	3nf6	-7.80
4gzf	-8.30	4bh3	-8.10	3nf6	-7.80
4e92	-8.30	4bh3	-8.10	3avn	-7.80
4bh2	-8.30	3vbh	-8.10	2iph	-7.80
3suf	-8.30	3vbf	-8.10	2c7u	-7.80
3su0	-8.30	3vbf	-8.10	1rv7	-7.80
3nfa	-8.30	3ro5	-8.10	4mj1	-7.70
3nfa	-8.30	3kmq	-8.10	4ejd	-7.70
3nf9	-8.30	3avf	-8.10	4dgb	-7.70
2axf	-8.30	1sys	-8.10	3su2	-7.70
2axf	-8.30	4lsu	-8.00	3su2	-7.70
1r6a	-8.30	4lsu	-8.00	3sis	-7.70
4qrt	-8.20	4i32	-8.00	3s12	-7.70
4mmv	-8.20	4g8i	-8.00	3rwi	-7.70
4i31	-8.20	4dkp	-8.00	3p8o	-7.70
4i31	-8.20	3sv8	-8.00	3p8n	-7.70
4g9d	-8.20	3sud	-8.00	3avl	-7.70
4e92	-8.20	3su2	-8.00	4dgb	-7.60

PDB	Docking score	PDB	Docking score	PDB	Docking score
3uqi	-7.60	3sug	-7.30	2zol	-6.70
3avk	-7.60	3sue	-7.30	2yhh	-6.70
2bvq	-7.60	2zu1	-7.30	2y1s	-6.70
1rq9	-7.60	2yka	-7.30	2q7c	-6.70
4iv3	-7.50	2xpx	-7.30	2q7c	-6.70
4g8i	-7.50	2xpx	-7.30	4b4n	-6.60
3sud	-7.50	2q7c	-7.30	4b4n	-6.60
3m5i	-7.50	2q7c	-7.30	3avj	-6.60
3m5h	-7.50	2q7c	-7.30	2q7c	-6.60
3gzf	-7.50	2ghv	-7.30	2q5u	-6.60
3alw	-7.50	1rpi	-7.30	2q5u	-6.60
2xya	-7.50	3sv7	-7.20	2q5u	-6.60
2wh6	-7.50	3sv7	-7.20	2q5u	-6.60
2wfo	-7.50	3su1	-7.20	2q5u	-6.60
2ge8	-7.50	3avc	-7.20	2q5u	-6.60
2ca1	-7.50	2xze	-7.20	1zsd	-6.60
4uoa	-7.40	2wfo	-7.20	4mod	-6.50
4c1w	-7.40	2v6q	-7.20	4mod	-6.50
3uqi	-7.40	4oyd	-7.10	4lkh	-6.50
3su3	-7.40	4nwk	-7.10	3vie	-6.50
3su3	-7.40	4lss	-7.10	3su5	-6.50
3sit	-7.40	4c1w	-7.10	3rkc	-6.50
3sit	-7.40	4b8e	-7.10	3avk	-6.50
3sit	-7.40	4b8e	-7.10	2g69	-6.50
3sit	-7.40	4b8e	-7.10	2g69	-6.50
3sit	-7.40	3sv9	-7.10	4nwk	-6.40
3sit	-7.40	3sv9	-7.10	4i33	-6.40
3rwf	-7.40	3su6	-7.10	3b71	-6.40
3rwf	-7.40	2zty	-7.10	3b71	-6.40
3gsw	-7.40	3w39	-7.00	2l2f	-6.40
2xze	-7.40	3a07	-7.00	4epj	-6.30
2lsp	-7.40	2zu3	-7.00	3u83	-6.30
1z8r	-7.40	2vxw	-7.00	3su4	-6.30
1rpi	-7.40	1qr9	-7.00	4ipz	-6.20
1qz8	-7.40	1qr8	-7.00	4ipz	-6.20
Papain	-7.30	4lsp	-6.90	4ipz	-6.20
protease	-7.30	4g2k	-6.90	4ipz	-6.20
4mj0	-7.30	3sv6	-6.90	4ipz	-6.20
4iv1	-7.30	2yhf	-6.90	4ipz	-6.20
4ffy	-7.30	2me2	-6.90	4ipz	-6.20
4ekx	-7.30	2gvf	-6.90	4ipz	-6.20
4ejd	-7.30	4g2k	-6.80	4ipz	-6.20
4ejd	-7.30	3sv6	-6.80	4ipz	-6.20
4ejd	-7.30	3su5	-6.80	3u83	-6.20
4dmn	-7.30	3m5g	-6.80	3su4	-6.20
4dmn	-7.30	4nwl	-6.70	4ipz	-6.10
3vie	-7.30	3su5	-6.70	4ipz	-6.10
3sug	-7.30	2ztz	-6.70	4epj	-6.00

PDB	Docking score	PDB	Docking score	PDB	Docking score
2c3a	-6.00	4ep2	-4.70	4dge	-1.60
2m3l	-5.90	1hhg	-4.70	4gu3	-1.40
2vxj	-5.80	3j23	-4.50	4gu3	-1.40
2c86	-5.80	3j22	-4.50	4gu3	-1.40
4ejr	-5.60	4lcx	-4.40	4gu3	-1.40
2me4	-5.60	4lki	-3.90	4gu3	-1.40
2me3	-5.60	2l3h	-3.90	4gu3	-1.40
3giv	-5.50	4qhm	-3.30	4gu3	-1.40
2m3m	-5.50	2jw8	-3.00	4gu3	-1.40
4adq	-5.40	4g1g	-2.80	4gu3	-1.40
3kqk	-5.40	3vu5	-2.70	4gu3	-1.40
2x9m	-5.40	4gu4	-2.00	4gu3	-1.40
4adq	-5.30	4gu4	-2.00	4gu3	-1.40
3zd0	-5.30	4gu4	-2.00	4g1o	-1.30
3vtt	-5.30	4gu4	-2.00	2zsv	-1.30
3vtt	-5.30	4gu4	-2.00	2zsv	-1.10
2mkr	-5.30	4gu4	-2.00	4kol	-1.00
3m5j	-5.10	3vu5	-2.00	4e0r	-0.70
4ep2	-5.00	1knz	-2.00	4fqm	-0.10
3i6k	-4.90	4kom	-1.70		

**Table S5.** Predicted docking score of Conivaptan against the viral protein panel.

PDB	Docking score	PDB	Docking score	PDB	Docking score
4wm7	-13.90	3rwd	-11.60	4fnk	-11.20
3b0w	-13.10	3kqh	-11.60	3t3c	-11.20
3nxu	-12.70	2wrc	-11.60	3rwi	-11.20
4f3z	-12.30	1hhj	-11.60	3kqn	-11.20
4mmr	-11.90	4g42	-11.50	3kqn	-11.20
3bw9	-11.90	2wrg	-11.50	3kqn	-11.20
1idb	-11.90	2wrg	-11.50	3gsr	-11.20
3bwa	-11.80	2wrg	-11.50	3fku	-11.20
4m8y	-11.70	2wrg	-11.50	2wr3	-11.20
4m8y	-11.70	1hhk	-11.50	2gec	-11.20
4m8x	-11.70	4j4v	-11.40	2axg	-11.20
4m8x	-11.70	4j4v	-11.40	1hhh	-11.20
3r4b	-11.70	4j4v	-11.40	4unx	-11.10
3bwa	-11.70	4j4v	-11.40	4unx	-11.10
3bw9	-11.70	4j4v	-11.40	4unx	-11.10
2wr1	-11.70	3gso	-11.40	4unx	-11.10
2wr1	-11.70	3gso	-11.40	4qru	-11.10
2i4x	-11.70	2wrg	-11.40	4j4u	-11.10
2hjk	-11.70	4k7f	-11.30	4i2p	-11.10
2hcs	-11.70	2i4u	-11.30	4i2p	-11.10
2bvp	-11.70	2gec	-11.30	4fqr	-11.10
2bvo	-11.70	4qru	-11.20	4fqr	-11.10
1syv	-11.70	4qrs	-11.20	3vcl	-11.10
1klm	-11.70	4k7f	-11.20	3u7s	-11.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
3t3c	-11.10	4bac	-10.80	4uo0	-10.50
3rwe	-11.10	3s11	-10.80	4uo0	-10.50
3rwe	-11.10	3pqy	-10.80	4uo0	-10.50
3rwc	-11.10	3gsq	-10.80	4lsr	-10.50
3rwc	-11.10	2wrh	-10.80	4cey	-10.50
3gsw	-11.10	2wr1	-10.80	4cew	-10.50
3ggu	-11.10	4rw4	-10.70	4cdx	-10.50
1r6a	-11.10	4pg2	-10.70	4cdw	-10.50
1hhi	-11.10	4mka	-10.70	3tid	-10.50
4uo3	-11.00	4mk8	-10.70	3koa	-10.50
4uo3	-11.00	4j4y	-10.70	3hkw	-10.50
4uo3	-11.00	4ejl	-10.70	3h98	-10.50
4uo3	-11.00	4ejl	-10.70	3h2l	-10.50
4uo3	-11.00	4ej8	-10.70	3h2l	-10.50
4rw8	-11.00	4e7a	-10.70	3cj2	-10.50
4rw7	-11.00	4e7a	-10.70	2wr0	-10.50
4j4x	-11.00	4adf	-10.70	2wr0	-10.50
4j4w	-11.00	4adf	-10.70	2wr0	-10.50
4g9f	-11.00	4adf	-10.70	2wr0	-10.50
4cdu	-11.00	4adf	-10.70	2wr0	-10.50
4bh0	-11.00	4adf	-10.70	4uo5	-10.40
3u7s	-11.00	4adf	-10.70	4uo5	-10.40
3lkh	-11.00	4a92	-10.70	4uo0	-10.40
3lkh	-11.00	3ztj	-10.70	4mk9	-10.40
3i6l	-11.00	3rki	-10.70	4fnk	-10.40
3gsw	-11.00	1p9u	-10.70	4e5e	-10.40
2i4d	-11.00	1izi	-10.70	3se8	-10.40
4unw	-10.90	4uny	-10.60	3rwg	-10.40
4unw	-10.90	4mk8	-10.60	2wa1	-10.40
4qrs	-10.90	4cdq	-10.60	1v3d	-10.40
3vcl	-10.90	4a92	-10.60	1v3d	-10.40
3rwh	-10.90	3vbr	-10.60	1a41	-10.40
3rwh	-10.90	3vbo	-10.60	4uo0	-10.30
3iyw	-10.90	3tid	-10.60	4uo0	-10.30
3iyw	-10.90	3r4b	-10.60	4uo0	-10.30
3iyw	-10.90	3n0i	-10.60	4mkb	-10.30
3iyw	-10.90	3n0i	-10.60	4j4s	-10.30
3iyw	-10.90	3hkw	-10.60	4j4s	-10.30
3iyw	-10.90	3hkw	-10.60	4gua	-10.30
3iyw	-10.90	3h98	-10.60	3se8	-10.30
3gsq	-10.90	3bev	-10.60	3rwg	-10.30
2xi5	-10.90	2i4w	-10.60	3ku3	-10.30
2xi5	-10.90	2i4v	-10.60	3cj5	-10.30
4uo5	-10.80	4uo0	-10.50	3cj2	-10.30
4unw	-10.80	4uo0	-10.50	1quv	-10.30
4q6r	-10.80	4uo0	-10.50	1ida	-10.30
4q6r	-10.80	4uo0	-10.50	4wm8	-10.20
4o44	-10.80	4uo0	-10.50	4uo0	-10.20
4ej8	-10.80	4uo0	-10.50	4uo0	-10.20

PDB	Docking score	PDB	Docking score	PDB	Docking score
4uo0	-10.20	3cj4	-10.00	4fqi	-9.60
4rw4	-10.20	3cj4	-10.00	4dag	-9.60
4mka	-10.20	2ygc	-10.00	4cqW	-9.60
4mk7	-10.20	2ygc	-10.00	3zp2	-9.60
4lsv	-10.20	2wre	-10.00	3u82	-9.60
4g43	-10.20	2wre	-10.00	4qhl	-9.50
4e78	-10.20	1b53	-10.00	4gag	-9.50
4e78	-10.20	4uo2	-9.90	4gag	-9.50
3tie	-10.20	4uo2	-9.90	4fp8	-9.50
3tie	-10.20	4qhk	-9.90	4cqz	-9.50
3kql	-10.20	4pv9	-9.90	3u82	-9.50
3kql	-10.20	4j4r	-9.90	3kql	-9.50
3hky	-10.20	4fqy	-9.90	3cpl	-9.50
3cj5	-10.20	4fqy	-9.90	5ajm	-9.40
3cj3	-10.20	3cj3	-9.90	5ajm	-9.40
3bew	-10.20	3cj0	-9.90	5ajm	-9.40
2vVx	-10.20	4rw6	-9.80	4mza	-9.40
2vVx	-10.20	4pv9	-9.80	4mza	-9.40
1izh	-10.20	4mk9	-9.80	4mj0	-9.40
4uo7	-10.10	4jb9	-9.80	4j6r	-9.40
4uo2	-10.10	4e5f	-9.80	4egt	-9.40
4uo2	-10.10	4cqQ	-9.80	4cqz	-9.40
4uo0	-10.10	3se9	-9.80	4cqX	-9.40
4uo0	-10.10	3hky	-9.80	4cqQ	-9.40
4uo0	-10.10	3ggU	-9.80	3zpb	-9.40
4rw9	-10.10	3d0g	-9.80	3zpb	-9.40
4mkb	-10.10	3ciz	-9.80	3zp1	-9.40
4mk7	-10.10	3alz	-9.80	3vbh	-9.40
4mgu	-10.10	2wr7	-9.80	3klv	-9.40
4fqj	-10.10	2wr2	-9.80	3d0h	-9.40
4e5g	-10.10	2wr2	-9.80	3cpl	-9.40
3ok9	-10.10	2wr2	-9.80	3alx	-9.40
3cj0	-10.10	2hu4	-9.80	2vVw	-9.40
2ygb	-10.10	2hu4	-9.80	2c36	-9.40
2ygb	-10.10	2hu4	-9.80	2c36	-9.40
4uo7	-10.00	2hu4	-9.80	5ajm	-9.30
4uo7	-10.00	1n5a	-9.80	4uo6	-9.30
4uo7	-10.00	4uo6	-9.70	4uo3	-9.30
4uo7	-10.00	4lst	-9.70	4uo3	-9.30
4uo7	-10.00	4cqQ	-9.70	4o4g	-9.30
4uo2	-10.00	3ciz	-9.70	4mds	-9.30
4uo2	-10.00	2wre	-9.70	4mds	-9.30
4e76	-10.00	1v3c	-9.70	4jo8	-9.30
4cqV	-10.00	1v3c	-9.70	3mlh	-9.30
3kna	-10.00	1rzj	-9.70	3avf	-9.30
3ebj	-10.00	4qhn	-9.60	2wrf	-9.30
3d23	-10.00	4gaj	-9.60	2wre	-9.30
3d23	-10.00	4gaj	-9.60	2wr4	-9.30

PDB	Docking score	PDB	Docking score	PDB	Docking score
2oy0	-9.30	4cr0	-9.00	4cqp	-8.80
2hty	-9.30	4cqs	-9.00	4bgz	-8.80
4mmu	-9.20	4bh1	-9.00	3zpa	-8.80
4g9f	-9.20	4bgy	-9.00	3sdy	-8.80
4g8g	-9.20	4bgx	-9.00	3sdy	-8.80
4fqi	-9.20	3nfa	-9.00	3lqa	-8.80
4fqi	-9.20	3nf6	-9.00	2htw	-8.80
4e5j	-9.20	3nf6	-9.00	1sk7	-8.80
4cqr	-9.20	3gsv	-9.00	5ajm	-8.70
4co6	-9.20	2wre	-9.00	4u6h	-8.70
4bgx	-9.20	2wre	-9.00	4m30	-8.70
3ku6	-9.20	2uv0	-9.00	4i7f	-8.70
3ku6	-9.20	2uv0	-9.00	4fqv	-8.70
3ifu	-9.20	2uv0	-9.00	4f3i	-8.70
2x83	-9.20	2uv0	-9.00	4cqy	-8.70
2vww	-9.20	2uv0	-9.00	4cqu	-8.70
2hu0	-9.20	2uv0	-9.00	4cqu	-8.70
1r6a	-9.20	2uv0	-9.00	4cqu	-8.70
4uo3	-9.10	2uv0	-9.00	4cqu	-8.70
4opa	-9.10	2uv0	-9.00	4bh2	-8.70
4mj1	-9.10	2uv0	-9.00	4bh2	-8.70
4mg3	-9.10	2uv0	-9.00	3nwf	-8.70
4mg3	-9.10	2uv0	-9.00	3nw8	-8.70
4g8g	-9.10	2ghw	-9.00	2x83	-8.70
4fp8	-9.10	4pv8	-8.90	1v2i	-8.70
4e91	-9.10	4mj1	-8.90	1v2i	-8.70
4dgd	-9.10	4kps	-8.90	4lsu	-8.60
4cqr	-9.10	4g9z	-8.90	4f3i	-8.60
4bh1	-9.10	4ffz	-8.90	4b8e	-8.60
4bh1	-9.10	4dkq	-8.90	4b8e	-8.60
4bgw	-9.10	4cqs	-8.90	3zp0	-8.60
3zp3	-9.10	4bgw	-8.90	3sv6	-8.60
3oah	-9.10	3s13	-8.90	3oah	-8.60
3nfa	-9.10	3ku5	-8.90	3avh	-8.60
3ku3	-9.10	3ku5	-8.90	1v3e	-8.60
3i6g	-9.10	1v3e	-8.90	1p9s	-8.60
3gsv	-9.10	1sys	-8.90	4qru	-8.50
2xwy	-9.10	5ajm	-8.80	4lsu	-8.50
2xra	-9.10	4mj0	-8.80	4ep3	-8.50
2oy0	-9.10	4iv3	-8.80	4ep3	-8.50
2ht5	-9.10	4fqv	-8.80	4b8e	-8.50
1v3b	-9.10	4cqu	-8.80	3nf9	-8.50
4uo3	-9.00	4cqu	-8.80	3nf9	-8.50
4uo3	-9.00	4cqp	-8.80	3avg	-8.50
4pv8	-9.00	4cqp	-8.80	3ava	-8.50
4kpq	-9.00	4cqp	-8.80	3ava	-8.50
4i2q	-9.00	4cqp	-8.80	2zu5	-8.50
4e5l	-9.00	4cqp	-8.80	2z35	-8.50



PDB	Docking score	PDB	Docking score	PDB	Docking score
2htu	-8.50	3nf8	-8.20	3su5	-7.90
1pk0	-8.50	3nf6	-8.20	3gsx	-7.90
Main protease	-8.40	3nf6	-8.20	3gsx	-7.90
4g9z	-8.40	3gsu	-8.20	2zu4	-7.90
3ztn	-8.40	3gsu	-8.20	2zu1	-7.90
3sdy	-8.40	3bwa	-8.20	2q7c	-7.90
3ro5	-8.40	3avl	-8.20	2q7c	-7.90
3nf9	-8.40	3avb	-8.20	2q7c	-7.90
3nf9	-8.40	2ge8	-8.20	2mgu	-7.90
3nf7	-8.40	1yh3	-8.20	2ca1	-7.90
3nf7	-8.40	1n59	-8.20	2axf	-7.90
3avh	-8.40	4qrt	-8.10	4gzf	-7.80
3avc	-8.40	4oph	-8.10	4gzf	-7.80
1rv7	-8.40	4i31	-8.10	4gv9	-7.80
Papain protease	-8.30	4i31	-8.10	4ejk	-7.80
4uo8	-8.30	3sv9	-8.10	3sv7	-7.80
4qrt	-8.30	3sv7	-8.10	2lsp	-7.80
4pv9	-8.30	3rwi	-8.10	2c7u	-7.80
4mmv	-8.30	3mj5	-8.10	1rq9	-7.80
4gve	-8.30	3mj5	-8.10	1rpi	-7.80
4e5i	-8.30	3avl	-8.10	1oop	-7.80
3zp6	-8.30	3avj	-8.10	4lss	-7.70
3nf8	-8.30	2yka	-8.10	4ejk	-7.70
3nf8	-8.30	1v3c	-8.10	4ejd	-7.70
3nf7	-8.30	1v3c	-8.10	4dkp	-7.70
3nf7	-8.30	1v3b	-8.10	3sit	-7.70
3avb	-8.30	4mms	-8.00	3sit	-7.70
3avb	-8.30	4lkj	-8.00	3sit	-7.70
3avb	-8.30	4ffv	-8.00	3sit	-7.70
3ava	-8.30	4dkr	-8.00	3sit	-7.70
3ava	-8.30	3v3m	-8.00	3sit	-7.70
3ava	-8.30	3v3m	-8.00	3gsr	-7.70
2xze	-8.30	3uf5	-8.00	2ztz	-7.70
2v6q	-8.30	3avg	-8.00	2ge7	-7.70
4i32	-8.20	2hcn	-8.00	1rpi	-7.70
4dko	-8.20	2ghv	-8.00	Spike RBD	-7.60
4dgd	-8.20	4jpk	-7.90	4lsp	-7.60
3sv9	-8.20	4i2q	-7.90	4ipz	-7.60
3su1	-8.20	4hkj	-7.90	4gv3	-7.60
3rwj	-8.20	4fvu	-7.90	4gv3	-7.60
3rwj	-8.20	4fb3	-7.90	4ejk	-7.60
3o4l	-8.20	3vbf	-7.90	4ejd	-7.60
3nwa	-8.20	3vbf	-7.90	4ejd	-7.60
3nwa	-8.20	3sug	-7.90	4bh3	-7.60
3nfa	-8.20	3sug	-7.90	4bh3	-7.60
3nfa	-8.20	3su6	-7.90	4bh3	-7.60
3nfa	-8.20	3su5	-7.90	4bh3	-7.60
3nf8	-8.20	3su5	-7.90	3su1	-7.60

PDB	Docking score	PDB	Docking score	PDB	Docking score
3rwf	-7.60	4ejd	-7.20	2q5u	-6.80
3rwf	-7.60	3sis	-7.20	2q5u	-6.80
3d0i	-7.60	3avk	-7.20	2q5u	-6.80
2xze	-7.60	2iph	-7.20	2q5u	-6.80
2axf	-7.60	4eq0	-7.10	2q5u	-6.80
4mmt	-7.50	4ejd	-7.10	2q5u	-6.80
4ipz	-7.50	4ejd	-7.10	1z8r	-6.80
4ipz	-7.50	4dmn	-7.10	1qr9	-6.80
4ipz	-7.50	3kmq	-7.10	4ekx	-6.70
4ipz	-7.50	2zol	-7.10	4dga	-6.70
4dgc	-7.50	4jpi	-7.00	4dga	-6.70
3uqi	-7.50	4gye	-7.00	3vie	-6.70
3uqi	-7.50	4gye	-7.00	3m5i	-6.70
3sv8	-7.50	4eee	-7.00	2yhf	-6.70
3su3	-7.50	4e92	-7.00	2y1s	-6.70
3su3	-7.50	4e92	-7.00	2m3l	-6.70
3su0	-7.50	4dmn	-7.00	4i33	-6.60
3m5h	-7.50	4bh4	-7.00	3s12	-6.60
2zty	-7.50	4bh4	-7.00	3kms	-6.60
2wh6	-7.50	4bh4	-7.00	4oyd	-6.50
2gvf	-7.50	4bh4	-7.00	3p8n	-6.50
4uo4	-7.40	3su2	-7.00	3avc	-6.50
4iv1	-7.40	3su2	-7.00	2iph	-6.50
4dgc	-7.40	3su0	-7.00	2iph	-6.50
4dgc	-7.40	3rkc	-7.00	4nwk	-6.40
4dgc	-7.40	3gsw	-7.00	3u83	-6.40
4dgc	-7.40	2yol	-7.00	3u83	-6.40
4dgc	-7.40	2yol	-7.00	3su4	-6.40
3sud	-7.40	2wfo	-7.00	3su4	-6.40
3su6	-7.40	2q7c	-7.00	2wfo	-6.40
3su2	-7.40	2q7c	-7.00	2l2f	-6.40
3avn	-7.40	2q7c	-7.00	4qrt	-6.30
3alw	-7.40	2c86	-7.00	4nwk	-6.30
2xya	-7.40	4dgb	-6.90	3sv6	-6.30
2iph	-7.40	4b4n	-6.90	2me4	-6.30
2bvq	-7.40	4b4n	-6.90	1f08	-6.30
4oyd	-7.30	3w39	-6.90	4c1w	-6.20
4jki	-7.30	2vxw	-6.90	3p8o	-6.20
4jki	-7.30	2g69	-6.90	2xpx	-6.20
4ipz	-7.30	2g69	-6.90	2xpx	-6.20
4epj	-7.30	1rzk	-6.90	2m3m	-6.20
3sis	-7.30	4nwl	-6.80	4mze	-6.10
3gzf	-7.30	4eq0	-6.80	4mze	-6.10
3a07	-7.30	4dgb	-6.80	4mod	-6.10
2vvy	-7.30	3b71	-6.80	4ejd	-6.10
2me2	-7.30	3b71	-6.80	4ejd	-6.10
1qz8	-7.30	2yhh	-6.80	4ejd	-6.10
1b50	-7.30	2wh6	-6.80	3sud	-6.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
3gsn	-6.10	4adq	-5.70	3j22	-5.00
2zu3	-6.10	4adq	-5.70	1qr8	-5.00
2c3a	-6.10	2vxj	-5.70	4epj	-4.40
4mod	-6.00	4g8i	-5.60	4qhm	-3.50
4ipz	-6.00	4c1w	-5.60	2l3h	-3.30
4g9d	-6.00	3suf	-5.60	4lcx	-2.70
3giv	-6.00	3sue	-5.60	4dge	-1.60
3avj	-6.00	3vtt	-5.40	4lkk	-1.20
2hfz	-6.00	3vtt	-5.40	4g2k	-1.00
4ipz	-5.90	3vie	-5.40	4g2k	-0.90
4ipz	-5.90	3i6k	-5.40	2zsv	-0.90
4ipz	-5.90	3avn	-5.40	2zsv	-0.90
4ipz	-5.90	4eqj	-5.30	4e0r	-0.50
4g9d	-5.90	3zd0	-5.30	4fqm	-0.30
4g8i	-5.90	3kqk	-5.30		
3avk	-5.90	4ep2	-5.20		
1zsd	-5.90	2mkr	-5.20		
4ipz	-5.80	2me3	-5.20		
4ejr	-5.80	4ep2	-5.10		
2x9m	-5.80	3j23	-5.00		

**Table S6.** Predicted docking score of Velpatasvir against the viral protein panel.

PDB	Docking score	PDB	Docking score	PDB	Docking score
4j4x	-13.00	4uo0	-11.80	4uo0	-11.50
4g42	-12.90	4uo0	-11.80	4bh0	-11.50
3alz	-12.80	4unw	-11.80	3t3c	-11.50
2bvo	-12.60	4unw	-11.80	3ok9	-11.50
3ztj	-12.40	4rw8	-11.80	3h2l	-11.50
3fku	-12.40	4j4v	-11.80	3gsw	-11.50
1hhj	-12.40	4j4v	-11.80	3ciz	-11.50
4qru	-12.30	4j4v	-11.80	2wrg	-11.50
3koa	-12.30	4e78	-11.80	2wre	-11.50
3bwa	-12.30	3r4b	-11.80	2i4u	-11.50
2hjk	-12.30	3gsw	-11.80	1izi	-11.50
2axg	-12.30	3gso	-11.80	4mkb	-11.40
1hhk	-12.30	3bw9	-11.80	4mkb	-11.40
4uo5	-12.20	2wr0	-11.80	4mka	-11.40
4unw	-12.20	1hhi	-11.80	4mk8	-11.40
4qru	-12.20	1hhh	-11.80	4k7f	-11.40
4qrs	-12.20	4uo7	-11.70	3t3c	-11.40
2bvp	-12.20	4uo3	-11.70	3rwc	-11.40
1syv	-12.20	4uo2	-11.70	3gsq	-11.40
4uo7	-12.10	4uo0	-11.70	3ggg	-11.40
4uo5	-12.10	4uo0	-11.70	3cj2	-11.40
3rwi	-12.10	4uo0	-11.70	3bev	-11.40
3bwa	-12.10	4rw9	-11.70	2wre	-11.40
4uo7	-12.00	4j4v	-11.70	1izh	-11.40
4qrs	-12.00	4j4v	-11.70	4mka	-11.30
4o44	-12.00	4e78	-11.70	4mk8	-11.30
4mk9	-12.00	4e7a	-11.70	4j4y	-11.30
4mk9	-12.00	4e7a	-11.70	4a92	-11.30
3i6l	-12.00	3rwe	-11.70	4a92	-11.30
2wrh	-12.00	3rwe	-11.70	3vcl	-11.30
2i4v	-12.00	3r4b	-11.70	3s11	-11.30
4g9f	-11.90	3gsr	-11.70	3rwh	-11.30
3lkh	-11.90	4uo7	-11.60	3rwh	-11.30
3lkh	-11.90	4uo3	-11.60	3rwg	-11.30
3gso	-11.90	4uo2	-11.60	3rwd	-11.30
3bw9	-11.90	3vcl	-11.60	3h2l	-11.30
2wr1	-11.90	3rwg	-11.60	2wre	-11.30
2wr1	-11.90	3kqh	-11.60	2wr4	-11.30
2wr1	-11.90	2wrg	-11.60	2wr2	-11.30
4uo7	-11.80	2wrg	-11.60	2wr2	-11.30
4uo7	-11.80	2wrg	-11.60	2wa1	-11.30
4uo0	-11.80	2wrg	-11.60	4uo5	-11.20
4uo0	-11.80	4uo3	-11.50	4uo2	-11.20
4uo0	-11.80	4uo3	-11.50	4cqy	-11.20
4uo0	-11.80	4uo3	-11.50	3u82	-11.20

PDB	Docking score	PDB	Docking score	PDB	Docking score
3u82	-11.20	2ygc	-10.80	2wre	-10.50
3rwc	-11.20	1quv	-10.80	2vww	-10.50
3ku6	-11.20	1klm	-10.80	2vww	-10.50
3ggu	-11.20	4uo6	-10.70	4uo3	-10.40
3cj5	-11.20	4uo2	-10.70	4uo2	-10.40
3ciz	-11.20	4pv9	-10.70	4uo0	-10.40
2wre	-11.20	4mk7	-10.70	4uo0	-10.40
2wr0	-11.20	4i2p	-10.70	4uo0	-10.40
2wr0	-11.20	2wre	-10.70	4jo8	-10.40
2i4x	-11.20	5ajm	-10.60	4j4r	-10.40
1ida	-11.20	5ajm	-10.60	4i7f	-10.40
4m8y	-11.10	5ajm	-10.60	4gag	-10.40
4k7f	-11.10	5ajm	-10.60	4gag	-10.40
4j4u	-11.10	4uo0	-10.60	4fqi	-10.40
3ku6	-11.10	4m8y	-10.60	4cqq	-10.40
3h98	-11.10	4jkp	-10.60	4cey	-10.40
3cj5	-11.10	4j4w	-10.60	3zpb	-10.40
3cj4	-11.10	4g43	-10.60	3zp6	-10.40
3cj2	-11.10	4cqz	-10.60	3zp3	-10.40
2wr0	-11.10	4cqr	-10.60	3zp2	-10.40
2i4w	-11.10	4cqp	-10.60	3tie	-10.40
2i4d	-11.10	4cqp	-10.60	3tie	-10.40
1idb	-11.10	3zp1	-10.60	3tid	-10.40
4mk7	-11.00	3tid	-10.60	3ku3	-10.40
4m8x	-11.00	3kqn	-10.60	3iyw	-10.40
4gua	-11.00	3cpl	-10.60	3iyw	-10.40
3u7s	-11.00	2wr7	-10.60	3iyw	-10.40
3u7s	-11.00	5ajm	-10.50	3iyw	-10.40
3hkw	-11.00	5ajm	-10.50	3d23	-10.40
3h98	-11.00	4wm7	-10.50	3d23	-10.40
3cj4	-11.00	4uo0	-10.50	2ygb	-10.40
3cj3	-11.00	4pg2	-10.50	2wrf	-10.40
3cj0	-11.00	4opa	-10.50	4uo0	-10.30
2wr0	-11.00	4jkp	-10.50	4uo0	-10.30
4wm8	-10.90	4cqz	-10.50	4qhk	-10.30
4uo6	-10.90	4cqp	-10.50	4lsr	-10.30
3hky	-10.90	4cqp	-10.50	4j4s	-10.30
3hkw	-10.90	4cqp	-10.50	4gaj	-10.30
3gsq	-10.90	4cqp	-10.50	4gaj	-10.30
3cj3	-10.90	4bgx	-10.50	4fnk	-10.30
3bew	-10.90	4bgx	-10.50	4f3z	-10.30
2ygc	-10.90	4bgw	-10.50	4ejl	-10.30
2wr2	-10.90	4bgw	-10.50	4cqs	-10.30
4m8x	-10.80	3kqn	-10.50	4cqs	-10.30
4ejl	-10.80	3kqn	-10.50	4cqr	-10.30
3hky	-10.80	3iyw	-10.50	4cqq	-10.30
3hkw	-10.80	3iyw	-10.50	4cqq	-10.30
3cj0	-10.80	3cpl	-10.50	4co6	-10.30

PDB	Docking score	PDB	Docking score	PDB	Docking score
4bgy	-10.30	3sdy	-9.90	2uv0	-9.50
3zpa	-10.30	3rki	-9.90	2uv0	-9.50
3s13	-10.30	3nf8	-9.90	2uv0	-9.50
3mlh	-10.30	3kql	-9.90	2uv0	-9.50
3ebj	-10.30	3d0g	-9.90	2uv0	-9.50
2ygb	-10.30	1v3b	-9.90	2uv0	-9.50
1p9u	-10.30	1v2i	-9.90	2uv0	-9.50
1n5a	-10.30	1pk0	-9.90	1v3b	-9.50
4uo3	-10.20	4hkj	-9.80	4mg3	-9.40
4uo3	-10.20	4dag	-9.80	4kps	-9.40
4uo3	-10.20	4cew	-9.80	4e76	-9.40
4uo0	-10.20	3nf8	-9.80	4cdq	-9.40
4unx	-10.20	3nf8	-9.80	3nf7	-9.40
4unx	-10.20	3nf8	-9.80	3nf6	-9.40
4unx	-10.20	1r6a	-9.80	3ku5	-9.40
4j4s	-10.20	4rw4	-9.70	3ku5	-9.40
4fqy	-10.20	4mmu	-9.70	2xra	-9.40
4fqy	-10.20	4lsv	-9.70	2uv0	-9.40
4cqu	-10.20	4ej8	-9.70	4i2q	-9.30
4cqu	-10.20	4cdw	-9.70	4e5l	-9.30
3zp0	-10.20	3se8	-9.70	4e5g	-9.30
2xwy	-10.20	3kql	-9.70	3uf5	-9.30
1v2i	-10.20	3d0h	-9.70	3i6g	-9.30
4uo3	-10.10	2x83	-9.70	4q6r	-9.20
4unx	-10.10	1a41	-9.70	4q6r	-9.20
4ej8	-10.10	4o4g	-9.60	3nfa	-9.20
4cqu	-10.10	4mj1	-9.60	3nfa	-9.20
3zpb	-10.10	4jb9	-9.60	3mj5	-9.20
3n0i	-10.10	4g9f	-9.60	2wrc	-9.20
2xi5	-10.10	4ffz	-9.60	2mgu	-9.20
4uo2	-10.00	4cr0	-9.60	4fnk	-9.10
4pv9	-10.00	4bgz	-9.60	4bh1	-9.10
4i2p	-10.00	3se8	-9.60	4bh1	-9.10
4fqj	-10.00	3nf6	-9.60	2xi5	-9.10
4cqu	-10.00	2uv0	-9.60	2htw	-9.10
4cqu	-10.00	4mgu	-9.50	1v3e	-9.10
4bac	-10.00	4fp8	-9.50	1v3e	-9.10
3se9	-10.00	4fp8	-9.50	1rzj	-9.10
3sdy	-10.00	4cdx	-9.50	4rw7	-9.00
3sdy	-10.00	4adf	-9.50	4qhl	-9.00
3kql	-10.00	3nf7	-9.50	4g8g	-9.00
3b0w	-10.00	3nf7	-9.50	4g8g	-9.00
2hcs	-10.00	3nf7	-9.50	4bh1	-9.00
4qhn	-9.90	3nf6	-9.50	3nf9	-9.00
4mj0	-9.90	3nf6	-9.50	3mj5	-9.00
4cqW	-9.90	3ku3	-9.50	3ava	-9.00
4cqu	-9.90	3avl	-9.50	2x83	-9.00
4cdu	-9.90	2uv0	-9.50	2wr3	-9.00

PDB	Docking score	PDB	Docking score	PDB	Docking score
2hu4	-9.00	2z35	-8.50	1r6a	-7.90
2hu0	-9.00	2oy0	-8.50	4i2q	-7.80
4mza	-8.90	2hu4	-8.50	4e92	-7.80
3nf9	-8.90	1rq9	-8.50	4dkr	-7.80
3nf9	-8.90	4mds	-8.40	4dko	-7.80
3lqa	-8.90	4fqv	-8.40	4adf	-7.80
3alx	-8.90	3avn	-8.40	4adf	-7.80
2ghw	-8.90	3avj	-8.40	2oy0	-7.80
2gec	-8.90	3avc	-8.40	4e92	-7.70
1n59	-8.90	2hu4	-8.40	4bh4	-7.70
4rw4	-8.80	2gec	-8.40	4bh4	-7.70
4qru	-8.80	1b53	-8.40	2ge8	-7.70
4oyd	-8.80	4mds	-8.30	2bvq	-7.70
4mza	-8.80	4f3i	-8.30	2axf	-7.70
4mg3	-8.80	4e5j	-8.30	4mmt	-7.60
4fvu	-8.80	1v3d	-8.30	4mj1	-7.60
3nf9	-8.80	1v3c	-8.30	4kpq	-7.60
2vvx	-8.80	4lsp	-8.20	3o4l	-7.60
2vvx	-8.80	4fqv	-8.20	3nxu	-7.60
2hty	-8.80	3kna	-8.20	3klv	-7.60
2ghv	-8.80	2htu	-8.20	3gsw	-7.60
1b50	-8.80	2hcn	-8.20	3avh	-7.60
4pv9	-8.70	4mms	-8.10	3avb	-7.60
4mj0	-8.70	4m30	-8.10	3ava	-7.60
4gzf	-8.70	4lss	-8.10	3ava	-7.60
4e5f	-8.70	4g9z	-8.10	2yka	-7.60
4e5e	-8.70	4f3i	-8.10	2axf	-7.60
3rwi	-8.70	3ztn	-8.10	Papain	-7.50
3n0i	-8.70	3vbr	-8.10	protease	-7.50
3ava	-8.70	3ro5	-8.10	4qrt	-7.50
2zu1	-8.70	2gvf	-8.10	4g9z	-7.50
2uv0	-8.70	4lkj	-8.00	4bh2	-7.50
2uv0	-8.70	4j6r	-8.00	3rwf	-7.50
2iph	-8.70	4adf	-8.00	3gsv	-7.50
2iph	-8.70	3avl	-8.00	2zu5	-7.50
4rw6	-8.60	1v3d	-8.00	1sys	-7.50
4pv8	-8.60	Spike RBD	-7.90	1qz8	-7.50
4gzf	-8.60	Main	-7.90	4gv3	-7.40
2iph	-8.60	protease	-7.90	3avk	-7.40
2iph	-8.60	4e91	-7.90	3avb	-7.40
2hu4	-8.60	4dkq	-7.90	3avb	-7.40
1v3c	-8.60	4dkp	-7.90	2c7u	-7.40
1v3c	-8.60	4dgb	-7.90	4qrt	-7.30
1v3c	-8.60	4adf	-7.90	4mze	-7.30
4pv8	-8.50	3rwj	-7.90	4dgd	-7.30
4adf	-8.50	3rwj	-7.90	3rwf	-7.30
3nfa	-8.50	3avg	-7.90	4e5i	-7.20
3nfa	-8.50	3avb	-7.90	3su1	-7.20

PDB	Docking score	PDB	Docking score	PDB	Docking score
3kmq	-7.20	3su2	-6.60	3sud	-5.70
3gsx	-7.20	3su0	-6.60	3su1	-5.70
3avh	-7.20	3alw	-6.60	3avf	-5.70
2zty	-7.20	2yol	-6.60	4u6h	-5.60
2lsp	-7.20	2ht5	-6.60	4lst	-5.60
4i33	-7.10	2g69	-6.60	4fqi	-5.60
4fb3	-7.10	4dmn	-6.50	4ekx	-5.60
4dgd	-7.10	3sv8	-6.50	3su5	-5.60
4bh3	-7.10	3gsu	-6.50	2x9m	-5.60
4bh2	-7.10	2yol	-6.50	2q5u	-5.60
3vbh	-7.10	2wh6	-6.50	2q5u	-5.60
3su4	-7.10	1p9s	-6.50	2q5u	-5.60
3su4	-7.10	4ejr	-6.40	2q5u	-5.60
2ztz	-7.10	4dmn	-6.40	2q5u	-5.60
2vxw	-7.10	4b4n	-6.40	4nwl	-5.50
4qrt	-7.00	3su6	-6.40	3sv9	-5.50
4bh3	-7.00	3su2	-6.40	2v6q	-5.50
3vbo	-7.00	3pqy	-6.40	2q7c	-5.50
3s12	-7.00	4dgc	-6.30	4mmv	-5.40
3oah	-7.00	4dgc	-6.30	4eq0	-5.40
3gsv	-7.00	4b4n	-6.20	3p8o	-5.40
1rpi	-7.00	3su3	-6.20	2q7c	-5.40
4gv3	-6.90	3gsr	-6.20	3vie	-5.30
4dgb	-6.90	1rpi	-6.20	3sv7	-5.30
4bh3	-6.90	4bh4	-6.10	3sue	-5.30
4bh3	-6.90	2q7c	-6.10	3giv	-5.30
3w39	-6.90	4i32	-6.00	2xpx	-5.30
3nwf	-6.90	4gye	-6.00	4i31	-5.20
3m5h	-6.90	4gv9	-6.00	3sv6	-5.20
3gsx	-6.90	4dgc	-6.00	3sv6	-5.20
3gsu	-6.90	4dgc	-6.00	3b71	-5.20
2zol	-6.90	4dgc	-6.00	2xpx	-5.20
2wh6	-6.90	3vbf	-6.00	4b8e	-5.10
2ca1	-6.90	3b71	-6.00	3sud	-5.10
2c3a	-6.90	3avj	-6.00	3su3	-5.10
1sk7	-6.90	2zu4	-6.00	3d0i	-5.10
1f08	-6.90	4mmr	-5.90	4nwk	-5.00
4jpi	-6.80	4bh4	-5.90	4cqx	-5.00
3v3m	-6.80	3su5	-5.90	4b8e	-5.00
3v3m	-6.80	3su5	-5.90	3sv9	-5.00
3su2	-6.80	2q7c	-5.90	3sug	-5.00
3nwa	-6.80	4oyd	-5.80	3sug	-5.00
3nwa	-6.80	4fqi	-5.80	3p8n	-5.00
2ge7	-6.80	4ejd	-5.80	3ifu	-5.00
4mze	-6.70	3vbf	-5.80	3i6k	-5.00
4jpk	-6.70	3gzf	-5.80	1rv7	-5.00
2xya	-6.70	2q7c	-5.80	4nwk	-4.90
2g69	-6.70	4dgc	-5.70	4ipz	-4.90



PDB	Docking score	PDB	Docking score	PDB	Docking score
4i31	-4.90	4ep3	-4.20	4ejd	-2.90
4adq	-4.90	3su6	-4.20	4uo8	-2.50
3suf	-4.90	4ep3	-4.10	4qhm	-2.40
3nw8	-4.90	3kms	-4.10	2vvy	-2.40
3kqk	-4.90	3gsn	-4.10	3su0	-2.30
2q7c	-4.90	4b8e	-4.00	2wfo	-2.30
2q5u	-4.90	2yhf	-4.00	4egt	-2.00
4lsu	-4.80	2c36	-4.00	3vtt	-1.80
4ipz	-4.80	1zsd	-4.00	4oph	-1.60
4gve	-4.80	2xze	-3.80	3sis	-1.50
4adq	-4.80	2vxj	-3.80	4ipz	-1.20
3sv7	-4.80	2c36	-3.80	4ipz	-1.20
2mkr	-4.80	4g8i	-3.70	4dge	-1.10
4ejd	-4.70	4dga	-3.60	4ipz	-0.90
4ejd	-4.70	3j23	-3.60	3m5i	-0.90
4ffy	-4.60	3j22	-3.60	2zsv	-0.80
2wfo	-4.60	3avk	-3.60	2zsv	-0.80
2m3l	-4.60	4dga	-3.50	4ipz	-0.50
4eq0	-4.50	4eee	-3.40	4fqr	-0.50
3u83	-4.50	3bwa	-3.40	4e0r	-0.40
3u83	-4.50	4iv3	-3.20	4cqy	-0.30
1z8r	-4.50	3uqi	-3.20	4fqr	-0.20
4g8i	-4.40	2zu3	-3.20		
2c86	-4.30	4lsu	-3.00		

**Table S7.** Predicted docking score of Lomitapide against the viral protein panel.

<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>
3fku	-12.70	2axg	-11.30	3se9	-11.00
3nxu	-12.40	4q6r	-11.20	3kqn	-11.00
3s11	-12.10	4mk9	-11.20	3kqn	-11.00
3b0w	-12.10	4j4w	-11.20	3kqh	-11.00
2wrg	-12.10	4i2p	-11.20	3h98	-11.00
3ztj	-12.00	4gua	-11.20	3h98	-11.00
2wrg	-12.00	4fqr	-11.20	3d23	-11.00
4wm8	-11.90	4fqr	-11.20	3cj2	-11.00
3t3c	-11.90	4fnk	-11.20	1ida	-11.00
2wrg	-11.90	3t3c	-11.20	4uo7	-10.90
2wrg	-11.90	3iyw	-11.20	4uo2	-10.90
4wm7	-11.80	3iyw	-11.20	4uo2	-10.90
2wrg	-11.80	3iyw	-11.20	4lsv	-10.90
2hcs	-11.80	3cj0	-11.20	4k7f	-10.90
4i2p	-11.70	4uo3	-11.10	3n0i	-10.90
4o4g	-11.60	4unx	-11.10	3kqn	-10.90
4g42	-11.60	4qrs	-11.10	3ggg	-10.90
3rwg	-11.60	4mkb	-11.10	3ciz	-10.90
4uo3	-11.50	4mka	-11.10	3bwa	-10.90
4e5l	-11.50	4mka	-11.10	3bw9	-10.90
4bac	-11.50	4i2q	-11.10	2i4x	-10.90
3rwg	-11.50	4dag	-11.10	2i4v	-10.90
3cj3	-11.50	4cqy	-11.10	4uo3	-10.80
2bvp	-11.50	3vcl	-11.10	4o44	-10.80
2bvo	-11.50	3u7s	-11.10	3vcl	-10.80
4rw4	-11.40	3u7s	-11.10	3lkh	-10.80
4mk8	-11.40	3kql	-11.10	3gso	-10.80
4j4u	-11.40	3kql	-11.10	3ciz	-10.80
4f3z	-11.40	3kql	-11.10	3bwa	-10.80
4e91	-11.40	3iyw	-11.10	3bw9	-10.80
3cj5	-11.40	3iyw	-11.10	2wre	-10.80
2hu4	-11.40	3gsq	-11.10	2i4w	-10.80
2hu4	-11.40	3d23	-11.10	1syv	-10.80
2hu4	-11.40	3cj5	-11.10	1r6a	-10.80
4uo3	-11.30	3cj2	-11.10	1hhj	-10.80
4rw4	-11.30	4unx	-11.00	4uo3	-10.70
4j4s	-11.30	4unx	-11.00	4pv9	-10.70
4e5e	-11.30	4unx	-11.00	4m30	-10.70
3iyw	-11.30	4unw	-11.00	4lkj	-10.70
3i6l	-11.30	4unw	-11.00	4j4x	-10.70
3hkw	-11.30	4rw8	-11.00	3koa	-10.70
3h2l	-11.30	4qrs	-11.00	3gsr	-10.70
3h2l	-11.30	4q6r	-11.00	3gsq	-10.70
3cj3	-11.30	4j4s	-11.00	3cj4	-10.70
2hu4	-11.30	4g9f	-11.00	3cj4	-10.70
2hjk	-11.30	4bh0	-11.00	3bew	-10.70

PDB	Docking score	PDB	Docking score	PDB	Docking score
2wre	-10.70	3hkw	-10.40	3tid	-10.10
1p9u	-10.70	3gso	-10.40	3tid	-10.10
1klm	-10.70	3ggu	-10.40	3rwe	-10.10
1izh	-10.70	2wr3	-10.40	3bev	-10.10
4uo3	-10.60	2vww	-10.40	2wrc	-10.10
4uo3	-10.60	4uo0	-10.30	1pk0	-10.10
4uo3	-10.60	4uo0	-10.30	1idb	-10.10
4mk7	-10.60	4uo0	-10.30	4mze	-10.00
4k7f	-10.60	4uo0	-10.30	4mmr	-10.00
4j4v	-10.60	4rw9	-10.30	4mk9	-10.00
4fnk	-10.60	4mg3	-10.30	4mk8	-10.00
4e7a	-10.60	4m8x	-10.30	4mgu	-10.00
4cew	-10.60	4lsu	-10.30	4jkp	-10.00
4adf	-10.60	4lsu	-10.30	4i7f	-10.00
3rwh	-10.60	4g9z	-10.30	4fqj	-10.00
3rwc	-10.60	4ejl	-10.30	4cdu	-10.00
3kna	-10.60	4e5j	-10.30	4cdq	-10.00
3hky	-10.60	4adf	-10.30	4bh2	-10.00
3hky	-10.60	4adf	-10.30	4a92	-10.00
3cj0	-10.60	4adf	-10.30	1izi	-10.00
3alx	-10.60	2wrf	-10.30	4uo7	-9.90
4rw7	-10.50	2wre	-10.30	4uo2	-9.90
4mk7	-10.50	2wre	-10.30	4uo0	-9.90
4j4v	-10.50	2i4u	-10.30	4uo0	-9.90
4j4v	-10.50	4uo2	-10.20	4uo0	-9.90
4j4v	-10.50	4uo0	-10.20	4uo0	-9.90
4ej8	-10.50	4uo0	-10.20	4rw6	-9.90
4e7a	-10.50	4uo0	-10.20	4m8y	-9.90
4cey	-10.50	4uo0	-10.20	4jkp	-9.90
3rwh	-10.50	4uo0	-10.20	4g9z	-9.90
3rwd	-10.50	4mkb	-10.20	4fqj	-9.90
3rwc	-10.50	4jo8	-10.20	4cr0	-9.90
3r4b	-10.50	4j4v	-10.20	4bh2	-9.90
2i4d	-10.50	4hkj	-10.20	3zp2	-9.90
2hty	-10.50	4g43	-10.20	3cpl	-9.90
4uo8	-10.40	3vbo	-10.20	2ygc	-9.90
4uo0	-10.40	3rki	-10.20	2ht5	-9.90
4j6r	-10.40	2wre	-10.20	1v3d	-9.90
4j4y	-10.40	2wre	-10.20	1rzj	-9.90
4i2q	-10.40	2vww	-10.20	1n5a	-9.90
4ej8	-10.40	4uo3	-10.10	4uo7	-9.80
4adf	-10.40	4uo3	-10.10	4uo7	-9.80
4adf	-10.40	4uo2	-10.10	4unw	-9.80
3vbr	-10.40	4uo2	-10.10	4qhn	-9.80
3rwe	-10.40	4uny	-10.10	4pv9	-9.80
3r4b	-10.40	4pv9	-10.10	4pg2	-9.80
3ok9	-10.40	4mze	-10.10	4mza	-9.80
3n0i	-10.40	4ejl	-10.10	4m8x	-9.80

PDB	Docking score	PDB	Docking score	PDB	Docking score
4lsr	-9.80	4cqy	-9.50	2vvx	-9.30
4e5f	-9.80	4cdw	-9.50	2vvx	-9.30
3tie	-9.80	3zp6	-9.50	2htw	-9.30
3ebj	-9.80	3zp0	-9.50	4qru	-9.20
3cpl	-9.80	3u82	-9.50	4gag	-9.20
3avg	-9.80	3lqa	-9.50	4bh4	-9.20
2wrh	-9.80	3i6g	-9.50	3nf9	-9.20
2wr0	-9.80	3gsw	-9.50	3nf8	-9.20
1v3d	-9.80	3d0h	-9.50	3nf8	-9.20
1hhi	-9.80	3avn	-9.50	3nf6	-9.20
4uo0	-9.70	3ava	-9.50	3nf6	-9.20
4mza	-9.70	3ava	-9.50	3alz	-9.20
4mds	-9.70	2xi5	-9.50	2z35	-9.20
4mds	-9.70	2wr2	-9.50	2xwy	-9.20
4fvu	-9.70	2wr0	-9.50	2wr2	-9.20
4e5g	-9.70	2wr0	-9.50	2wr0	-9.20
4a92	-9.70	2iph	-9.50	2wa1	-9.20
3u82	-9.70	2iph	-9.50	2htu	-9.20
3tie	-9.70	2iph	-9.50	1v2i	-9.20
3lkh	-9.70	2gec	-9.50	1v2i	-9.20
3avh	-9.70	1b53	-9.50	1sk7	-9.20
2ygc	-9.70	4qrt	-9.40	1hbk	-9.20
2ygb	-9.70	4cdx	-9.40	4uo5	-9.10
2ygb	-9.70	4bh3	-9.40	4uo5	-9.10
2xra	-9.70	4bh3	-9.40	4lst	-9.10
2wr0	-9.70	3rwi	-9.40	4iv3	-9.10
4uo0	-9.60	3oah	-9.40	4gaj	-9.10
4uo0	-9.60	3nf9	-9.40	4g8g	-9.10
4mms	-9.60	3nf7	-9.40	4e5i	-9.10
4g8g	-9.60	3gsv	-9.40	4bh4	-9.10
4fqv	-9.60	3avl	-9.40	3zpb	-9.10
4fqv	-9.60	3avj	-9.40	3se8	-9.10
4cqx	-9.60	3avh	-9.40	3klv	-9.10
4bh4	-9.60	3ava	-9.40	2bvq	-9.10
3hkw	-9.60	2gec	-9.40	1quv	-9.10
3gsw	-9.60	1hhh	-9.40	5ajm	-9.00
2wr7	-9.60	Spike RBD	-9.30	4qru	-9.00
2wr4	-9.60	4uo6	-9.30	4qhl	-9.00
2iph	-9.60	4uo5	-9.30	4gaj	-9.00
2hu0	-9.60	4g9f	-9.30	4cqq	-9.00
4uo7	-9.50	4cqw	-9.30	4bh4	-9.00
4uo7	-9.50	4bh3	-9.30	3v3m	-9.00
4uo6	-9.50	4bh3	-9.30	3nf9	-9.00
4opa	-9.50	3se8	-9.30	3mlh	-9.00
4m8y	-9.50	3sdy	-9.30	3avl	-9.00
4e78	-9.50	3nf7	-9.30	3ava	-9.00
4e78	-9.50	3avb	-9.30	1sys	-9.00
4dgd	-9.50	2x83	-9.30	1a41	-9.00

PDB	Docking score	PDB	Docking score	PDB	Docking score
4qru	-8.90	2uv0	-8.70	4gye	-8.30
4mj0	-8.90	2uv0	-8.70	4gve	-8.30
4gv3	-8.90	2axf	-8.70	4bgy	-8.30
4f3i	-8.90	4mmv	-8.60	4bgw	-8.30
3zp3	-8.90	4gv3	-8.60	4bgw	-8.30
3vbh	-8.90	4fqy	-8.60	3su6	-8.30
3sv8	-8.90	4f3i	-8.60	3su2	-8.30
3su1	-8.90	4cqs	-8.60	3sdy	-8.30
3s13	-8.90	4cqr	-8.60	3rwf	-8.30
3avf	-8.90	3nf9	-8.60	3rwf	-8.30
3avb	-8.90	3nf7	-8.60	3nw8	-8.30
2wr2	-8.90	2xi5	-8.60	3avc	-8.30
2ghw	-8.90	2wr1	-8.60	2yol	-8.30
2ge8	-8.90	2c7u	-8.60	2oy0	-8.30
1v3b	-8.90	2axf	-8.60	1v3c	-8.30
Main protease	-8.80	1n59	-8.60	1v3c	-8.30
4oph	-8.80	4mj1	-8.50	4mg3	-8.20
4jb9	-8.80	4mj1	-8.50	4kps	-8.20
4ffz	-8.80	4kpq	-8.50	4fqy	-8.20
4bh1	-8.80	4gag	-8.50	4fp8	-8.20
3ro5	-8.80	4fqi	-8.50	4cqu	-8.20
3nfa	-8.80	4cqs	-8.50	4cqu	-8.20
3d0g	-8.80	4co6	-8.50	3zp1	-8.20
2wr1	-8.80	3nf7	-8.50	3uf5	-8.20
2uv0	-8.80	3ku6	-8.50	3suf	-8.20
2uv0	-8.80	3avk	-8.50	3su2	-8.20
2uv0	-8.80	1v3b	-8.50	3su0	-8.20
2uv0	-8.80	1rq9	-8.50	3ku3	-8.20
2uv0	-8.80	1p9s	-8.50	3ku3	-8.20
2uv0	-8.80	5ajm	-8.40	2zu4	-8.20
2uv0	-8.80	4uo0	-8.40	2ztz	-8.20
2uv0	-8.80	4qhk	-8.40	2ge7	-8.20
2uv0	-8.80	4pv8	-8.40	4qrt	-8.10
2uv0	-8.80	4oyd	-8.40	4pv8	-8.10
2uv0	-8.80	4mj0	-8.40	4dko	-8.10
1b50	-8.80	4fb3	-8.40	4bgx	-8.10
4j4r	-8.70	4cqu	-8.40	3zpb	-8.10
4fqi	-8.70	4cqq	-8.40	3v3m	-8.10
4cqu	-8.70	3ztn	-8.40	3sud	-8.10
4cqr	-8.70	3sdy	-8.40	3o4l	-8.10
3nwa	-8.70	3rwi	-8.40	3nf8	-8.10
3nwa	-8.70	3ku6	-8.40	3nf6	-8.10
3nfa	-8.70	2yol	-8.40	3nf6	-8.10
3mj5	-8.70	2mgu	-8.40	3gsv	-8.10
3alw	-8.70	1r6a	-8.40	2xze	-8.10
2zu5	-8.70	4uo4	-8.30	2x83	-8.10
2wr1	-8.70	4i32	-8.30	2hcn	-8.10
2wh6	-8.70	4i31	-8.30	5ajm	-8.00

PDB	Docking score	PDB	Docking score	PDB	Docking score
5ajm	-8.00	4eq0	-7.80	3kms	-7.50
5ajm	-8.00	4e92	-7.80	3ifu	-7.50
5ajm	-8.00	4dgd	-7.80	3gsu	-7.50
4jpk	-8.00	4dgc	-7.80	2q7c	-7.50
4iv1	-8.00	4dgc	-7.80	2q7c	-7.50
4gzf	-8.00	4dgc	-7.80	2q5u	-7.50
4gzf	-8.00	4dgb	-7.80	4dgc	-7.40
4fp8	-8.00	4cqu	-7.80	3sv9	-7.40
4dkp	-8.00	4bh1	-7.80	3sit	-7.40
4cqz	-8.00	4bgz	-7.80	3gsr	-7.40
4cqz	-8.00	4bgx	-7.80	3avg	-7.40
4cqq	-8.00	4b8e	-7.80	1v3c	-7.40
4cqp	-8.00	3uqi	-7.80	1qr9	-7.40
4cqp	-8.00	3sv7	-7.80	1oop	-7.40
4cqp	-8.00	3sue	-7.80	4ekx	-7.30
4cqp	-8.00	3rwj	-7.80	3sv6	-7.30
3vbf	-8.00	3rwj	-7.80	3sv6	-7.30
3nwf	-8.00	3nf8	-7.80	3su3	-7.30
3nfa	-8.00	2q5u	-7.80	3sit	-7.30
3nfa	-8.00	4cqu	-7.70	3sit	-7.30
3ku5	-8.00	3mj5	-7.70	2vvy	-7.30
2xze	-8.00	3gsx	-7.70	2q7c	-7.30
2oy0	-8.00	3avb	-7.70	2c86	-7.30
2ghv	-8.00	2q5u	-7.70	4lss	-7.20
2c36	-8.00	1v3e	-7.70	4dgb	-7.20
1rv7	-8.00	1v3e	-7.70	3sis	-7.20
4qrt	-7.90	4u6h	-7.60	3m5h	-7.20
4mmu	-7.90	4eq0	-7.60	2q5u	-7.20
4mmt	-7.90	4ep3	-7.60	2ca1	-7.20
4lsp	-7.90	4egt	-7.60	4ejd	-7.10
4ep3	-7.90	4b8e	-7.60	3su2	-7.10
4e76	-7.90	4b8e	-7.60	3gzf	-7.10
4dkq	-7.90	3sud	-7.60	3bwa	-7.10
4dgc	-7.90	3p8o	-7.60	2vxw	-7.10
4cqp	-7.90	3kmq	-7.60	2q7c	-7.10
4cqp	-7.90	3d0i	-7.60	2gvf	-7.10
4bh1	-7.90	3avb	-7.60	4gv9	-7.00
3zpa	-7.90	2zu1	-7.60	4ejd	-7.00
3uqi	-7.90	2q7c	-7.60	4e92	-7.00
3su6	-7.90	1rpi	-7.60	3w39	-7.00
3ku5	-7.90	1f08	-7.60	3sit	-7.00
3gsx	-7.90	4i31	-7.50	3pqy	-7.00
3gsu	-7.90	4gye	-7.50	3avk	-7.00
2zol	-7.90	4dgc	-7.50	3a07	-7.00
2q5u	-7.90	3vbf	-7.50	2zty	-7.00
2q5u	-7.90	3sv9	-7.50	2yhh	-7.00
2c36	-7.90	3su3	-7.50	2c3a	-7.00
1v3c	-7.90	3su0	-7.50		

PDB	Docking score	PDB	Docking score	PDB	Docking score
Papain	-6.90	4ejk	-6.40	1qr8	-5.40
protease	-6.90	4ejd	-6.40	4ejr	-5.30
4c1w	-6.90	4ejd	-6.40	3i6k	-5.20
3su5	-6.90	3u83	-6.40	3vtt	-5.10
3sis	-6.90	3u83	-6.40	3giv	-5.10
2yka	-6.90	3su5	-6.40	2x9m	-5.00
2xpx	-6.90	3p8n	-6.40	2vxj	-5.00
1rpi	-6.90	2y1s	-6.40	2l3h	-5.00
4oyd	-6.80	2wh6	-6.40	4ipz	-4.90
4nwk	-6.80	2mkr	-6.40	4ipz	-4.80
4jpi	-6.80	2m3l	-6.40	4ipz	-4.80
4ipz	-6.80	2lsp	-6.40	4adq	-4.80
4ejd	-6.80	4g8i	-6.30	4adq	-4.80
4ejd	-6.80	4dga	-6.30	2hfz	-4.80
4eee	-6.80	4dga	-6.30	4ipz	-4.70
4dkr	-6.80	3avc	-6.30	3vtt	-4.70
3sv7	-6.80	2wfo	-6.30	2me3	-4.70
3rkc	-6.80	2me2	-6.30	3kqk	-4.60
3b71	-6.80	4ipz	-6.20	4ipz	-4.50
3b71	-6.80	3su4	-6.20	4ipz	-4.40
3vie	-6.70	3su4	-6.20	4ep2	-4.30
3sit	-6.70	3sit	-6.20	4lki	-4.10
1z8r	-6.70	2wfo	-6.20	4lkh	-4.10
4nwl	-6.60	2g69	-6.20	3j23	-4.10
4ffy	-6.60	4ejk	-6.10	3j22	-4.10
4dmn	-6.60	4ejk	-6.10	3vie	-3.90
4dmn	-6.60	2zu3	-6.10	4ep2	-3.70
4b4n	-6.60	2v6q	-6.10	4gu4	-3.20
3su1	-6.60	2q7c	-6.10	4gu4	-3.20
3gsn	-6.60	4ipz	-6.00	4gu4	-3.10
3avn	-6.60	3sug	-6.00	4gu4	-3.10
3avj	-6.60	2g69	-6.00	4gu4	-3.10
2xya	-6.60	4mod	-5.90	4gu4	-3.10
4i33	-6.50	3sug	-5.90	4qhm	-2.90
4ejd	-6.50	2m3m	-5.90	3iyp	-2.80
4ejd	-6.50	1zsd	-5.80	2x5i	-2.80
4ejd	-6.50	1yh3	-5.80	4ipz	-2.50
4b4n	-6.50	4nwk	-5.70	4gu3	-2.30
3su5	-6.50	4ipz	-5.70	4gu3	-2.30
3s12	-6.50	4c1w	-5.70	4gu3	-2.30
3gsw	-6.50	4lkk	-5.60	4gu3	-2.30
2yhf	-6.50	4ipz	-5.60	4uoa	-2.20
2me4	-6.50	4g8i	-5.60	4gu3	-2.20
1rzk	-6.50	3zd0	-5.60	4gu3	-2.20
1qz8	-6.50	2xpx	-5.60	4gu3	-2.20
4g9d	-6.40	2l2f	-5.60	4gu3	-2.20
4g9d	-6.40	4mod	-5.40	4gu3	-2.20
4epj	-6.40	4eqj	-5.40	4gu3	-2.20

<b>PDB</b>	<b>Docking score</b>
4gu3	-2.20
4gu3	-2.20
3m5i	-1.70
4epj	-1.30
3m5g	-1.20
4kom	-1.10

<b>PDB</b>	<b>Docking score</b>
4dge	-1.00
2jw8	-1.00
3m5j	-0.90
2zsv	-0.50
2zsv	-0.40
4g2k	-0.30

<b>PDB</b>	<b>Docking score</b>
4e0r	-0.20
4g2k	-0.10



**Table S8.** Predicted docking score of Entrectinib against the viral protein panel.

<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>
4j4x	-13.00	4cdx	-11.30	4uo0	-10.90
3s11	-12.20	3t3c	-11.30	4rw4	-10.90
2wrh	-12.20	3kql	-11.30	4rw4	-10.90
4wm8	-12.10	3kql	-11.30	3u7s	-10.90
4o4g	-12.00	3bw9	-11.30	3rwe	-10.90
4g42	-12.00	1r6a	-11.30	3rwe	-10.90
4j4y	-11.90	4uo7	-11.20	3r4b	-10.90
1izh	-11.90	4uo7	-11.20	3ok9	-10.90
4wm7	-11.80	4qru	-11.20	3lkh	-10.90
4e78	-11.80	4j4u	-11.20	3lkh	-10.90
2i4x	-11.80	4hkj	-11.20	3h98	-10.90
4e78	-11.70	4fnk	-11.20	3h98	-10.90
3kqh	-11.70	3rwd	-11.20	3gso	-10.90
3fku	-11.60	2i4w	-11.20	3bw9	-10.90
2wrg	-11.60	4qru	-11.10	3bev	-10.90
2wrg	-11.60	4qrs	-11.10	2wre	-10.90
2wrg	-11.60	3wrg	-11.10	2wre	-10.90
2wrg	-11.60	3wrg	-11.10	2wre	-10.90
2wrg	-11.60	3kql	-11.10	2wre	-10.90
1klm	-11.60	2wrc	-11.10	2wre	-10.90
4lsv	-11.50	2bvo	-11.10	1n5a	-10.90
4j4w	-11.50	1hhh	-11.10	1hhi	-10.90
4i2p	-11.50	4uo2	-11.00	4uo5	-10.80
4gua	-11.50	4pv9	-11.00	4uo0	-10.80
4cew	-11.50	4mka	-11.00	4q6r	-10.80
4cdu	-11.50	4k7f	-11.00	4q6r	-10.80
3nxu	-11.50	4k7f	-11.00	4j4s	-10.80
2i4d	-11.50	4g9f	-11.00	4j4s	-10.80
2hjk	-11.50	4a92	-11.00	3u7s	-10.80
4rw7	-11.40	4a92	-11.00	3se9	-10.80
4g43	-11.40	3ztj	-11.00	3bwa	-10.80
4f3z	-11.40	3i6l	-11.00	2ygb	-10.80
4cey	-11.40	3gsw	-11.00	2ygb	-10.80
3t3c	-11.40	3bew	-11.00	2wr2	-10.80
3kqn	-11.40	2wrf	-11.00	2i4v	-10.80
3kqn	-11.40	2wre	-11.00	1izi	-10.80
3kqn	-11.40	1v2i	-11.00	4uo5	-10.70
3koa	-11.40	1v2i	-11.00	4uo5	-10.70
3b0w	-11.40	1p9u	-11.00	4qrs	-10.70
2wr3	-11.40	1hhk	-11.00	4qhk	-10.70
2bvp	-11.40	4uo2	-10.90	4o44	-10.70
4uo7	-11.30	4uo2	-10.90	4mka	-10.70
4uo7	-11.30	4uo2	-10.90	4mg3	-10.70
4uo7	-11.30	4uo0	-10.90	4mg3	-10.70
4uo7	-11.30	4uo0	-10.90	4m8y	-10.70
4i2p	-11.30	4uo0	-10.90	4m8y	-10.70

PDB	Docking score	PDB	Docking score	PDB	Docking score
4j4v	-10.70	4mmr	-10.50	1v3d	-10.40
4i2q	-10.70	4mk9	-10.50	4uo2	-10.30
4fvu	-10.70	4m8x	-10.50	4uo2	-10.30
4e7a	-10.70	4m8x	-10.50	4unw	-10.30
3r4b	-10.70	4fqj	-10.50	4unw	-10.30
3ggg	-10.70	3rwi	-10.50	4unw	-10.30
3cpl	-10.70	3rwh	-10.50	4mkb	-10.30
2wr2	-10.70	3rwh	-10.50	4mk9	-10.30
2vww	-10.70	3n0i	-10.50	4jkg	-10.30
2vww	-10.70	3klv	-10.50	4j6r	-10.30
2axg	-10.70	3cpl	-10.50	4e5j	-10.30
1ida	-10.70	3alx	-10.50	4e5e	-10.30
4uo3	-10.60	2wr4	-10.50	4cdw	-10.30
4uo3	-10.60	2wr1	-10.50	3pqy	-10.30
4uo3	-10.60	2uv0	-10.50	3ku6	-10.30
4uo3	-10.60	2uv0	-10.50	3ku6	-10.30
4rw6	-10.60	2uv0	-10.50	3iyw	-10.30
4mkb	-10.60	2uv0	-10.50	3iyw	-10.30
4mk8	-10.60	2uv0	-10.50	3iyw	-10.30
4m30	-10.60	2uv0	-10.50	3iyw	-10.30
4e7a	-10.60	2uv0	-10.50	3gsr	-10.30
4e5l	-10.60	2uv0	-10.50	3ggg	-10.30
3vcl	-10.60	2i4u	-10.50	2wr2	-10.30
3vcl	-10.60	1syv	-10.50	2wa1	-10.30
3vbr	-10.60	4uo3	-10.40	2gec	-10.30
3rwc	-10.60	4uo0	-10.40	4pg2	-10.20
3n0i	-10.60	4uo0	-10.40	4opa	-10.20
3h2l	-10.60	4uo0	-10.40	4j4v	-10.20
3gso	-10.60	4uo0	-10.40	4j4v	-10.20
3bwa	-10.60	4uo0	-10.40	4fqj	-10.20
2wr1	-10.60	4uo0	-10.40	4ej8	-10.20
2wr1	-10.60	4uo0	-10.40	4ej8	-10.20
2wr0	-10.60	4uo0	-10.40	4e5i	-10.20
2wr0	-10.60	4qhn	-10.40	4bac	-10.20
2wr0	-10.60	4mk8	-10.40	3rwc	-10.20
2wr0	-10.60	4i7f	-10.40	3iyw	-10.20
2wr0	-10.60	4fqj	-10.40	3gsw	-10.20
2uv0	-10.60	4fnk	-10.40	3d23	-10.20
2uv0	-10.60	4cdq	-10.40	3d23	-10.20
2uv0	-10.60	3vbo	-10.40	2hcs	-10.20
2uv0	-10.60	3iyw	-10.40	1pk0	-10.20
1idb	-10.60	3gsq	-10.40	4uo3	-10.10
1hhj	-10.60	3gsq	-10.40	4rw9	-10.10
4uo0	-10.50	3cj5	-10.40	4pv9	-10.10
4uo0	-10.50	3cj2	-10.40	4mk7	-10.10
4uo0	-10.50	2hu0	-10.40	4j4v	-10.10
4uo0	-10.50	2gec	-10.40	4j4v	-10.10
4uo0	-10.50	1v3d	-10.40	4cqy	-10.10

PDB	Docking score	PDB	Docking score	PDB	Docking score
3u82	-10.10	4rw8	-9.80	4adf	-9.60
3u82	-10.10	4qru	-9.80	4adf	-9.60
3rki	-10.10	4mms	-9.80	4adf	-9.60
3lqa	-10.10	4mds	-9.80	3v3m	-9.60
3hkw	-10.10	4mds	-9.80	3uf5	-9.60
2htw	-10.10	4lst	-9.80	3sdy	-9.60
4uo3	-10.00	4lsr	-9.80	3ku5	-9.60
4uo3	-10.00	4jo8	-9.80	3kna	-9.60
4uo3	-10.00	4j4r	-9.80	3hky	-9.60
4uo3	-10.00	4ejl	-9.80	3d0g	-9.60
4unx	-10.00	3tie	-9.80	3cj3	-9.60
4unx	-10.00	3tie	-9.80	1v3c	-9.60
4unx	-10.00	3nf9	-9.80	1v3c	-9.60
4pv9	-10.00	3nf9	-9.80	1v3c	-9.60
4mgu	-10.00	3mj5	-9.80	1v3b	-9.60
4fqv	-10.00	3mj5	-9.80	4uo8	-9.50
4cqr	-10.00	3hkw	-9.80	4fqy	-9.50
4bh0	-10.00	3ciz	-9.80	4eq0	-9.50
3se8	-10.00	2ygc	-9.80	4cqw	-9.50
3ciz	-10.00	2ygc	-9.80	3zp0	-9.50
3alz	-10.00	2ht5	-9.80	3vbh	-9.50
2xi5	-10.00	1v3e	-9.80	3v3m	-9.50
2xi5	-10.00	1b53	-9.80	3sdy	-9.50
1quv	-10.00	5ajm	-9.70	3hky	-9.50
1a41	-10.00	4uo6	-9.70	3avj	-9.50
4mk7	-9.90	4lsu	-9.70	2zu5	-9.50
4gaj	-9.90	4lsu	-9.70	2x83	-9.50
4gaj	-9.90	4jkg	-9.70	4u6h	-9.40
4g8g	-9.90	4g9f	-9.70	4qrt	-9.40
4g8g	-9.90	4ejl	-9.70	4mmu	-9.40
4fqv	-9.90	4e76	-9.70	4mj1	-9.40
4dag	-9.90	4e5f	-9.70	4mj0	-9.40
4cqr	-9.90	3mlh	-9.70	4jb9	-9.40
4bgz	-9.90	3ku3	-9.70	4gag	-9.40
3tid	-9.90	3hkw	-9.70	4cqs	-9.40
3tid	-9.90	3cj4	-9.70	3ku5	-9.40
3se8	-9.90	3cj4	-9.70	3d0h	-9.40
3h2l	-9.90	2wr7	-9.70	2vvx	-9.40
3ebj	-9.90	1v3e	-9.70	2hu4	-9.40
3cj5	-9.90	1v3c	-9.70	4iv3	-9.30
3cj3	-9.90	5ajm	-9.60	4i2q	-9.30
3cj2	-9.90	4g9z	-9.60	4fp8	-9.30
3cj0	-9.90	4g9z	-9.60	4fp8	-9.30
3cj0	-9.90	4fqy	-9.60	4eq0	-9.30
2hty	-9.90	4e5g	-9.60	4dkp	-9.30
Main protease	-9.80	4adf	-9.60	4cqx	-9.30
4uo6	-9.80	4adf	-9.60	4bgw	-9.30
		4adf	-9.60	3zp2	-9.30

PDB	Docking score	PDB	Docking score	PDB	Docking score
3sdy	-9.30	4qhl	-9.00	3ava	-8.80
3nf9	-9.30	4oph	-9.00	2c36	-8.80
3nf9	-9.30	4fqr	-9.00	1rzj	-8.80
3nf6	-9.30	4fqr	-9.00	1r6a	-8.80
2xra	-9.30	4cqq	-9.00	4uny	-8.70
2x83	-9.30	4cqq	-9.00	4mza	-8.70
2mgu	-9.30	4cqq	-9.00	4mza	-8.70
2hu4	-9.30	4cqp	-9.00	4mj1	-8.70
2hu4	-9.30	4cqp	-9.00	4ffz	-8.70
2hu4	-9.30	4cqp	-9.00	4cqz	-8.70
1v3b	-9.30	4bgx	-9.00	4bh3	-8.70
1b50	-9.30	3nfa	-9.00	4bh2	-8.70
4unx	-9.20	3nf6	-9.00	4bgx	-8.70
4mze	-9.20	3avg	-9.00	3uqi	-8.70
4gag	-9.20	2iph	-9.00	3sv8	-8.70
4e91	-9.20	2iph	-9.00	3nfa	-8.70
4cqy	-9.20	1oop	-9.00	3nfa	-8.70
4cqs	-9.20	1n59	-9.00	3nf7	-8.70
4bgy	-9.20	4pv8	-8.90	3nf7	-8.70
4bgw	-9.20	4lkj	-8.90	3nf7	-8.70
3ztn	-9.20	4egt	-8.90	3i6g	-8.70
3s13	-9.20	4dko	-8.90	3gsx	-8.70
3o4l	-9.20	4cqu	-8.90	3gsx	-8.70
3ku3	-9.20	4bh1	-8.90	2xwy	-8.70
3kmq	-9.20	4bh1	-8.90	1p9s	-8.70
2vvx	-9.20	4bh1	-8.90	4mze	-8.60
2oy0	-9.20	3rwj	-8.90	4gv3	-8.60
2c7u	-9.20	3rwj	-8.90	4gv3	-8.60
4mmv	-9.10	3nf8	-8.90	4cr0	-8.60
4kpq	-9.10	3nf8	-8.90	4cqu	-8.60
4fqi	-9.10	3nf8	-8.90	4cqu	-8.60
4f3i	-9.10	3nf6	-8.90	4cqu	-8.60
4f3i	-9.10	3avh	-8.90	4co6	-8.60
4cqp	-9.10	3avb	-8.90	4bh3	-8.60
4cqp	-9.10	2iph	-8.90	4bh3	-8.60
4cqp	-9.10	2iph	-8.90	4bh3	-8.60
3oah	-9.10	2c36	-8.90	3zpb	-8.60
3nwf	-9.10	1sk7	-8.90	3zp3	-8.60
3nwa	-9.10	4jpk	-8.80	3zp1	-8.60
3nwa	-9.10	4cqz	-8.80	3nf7	-8.60
3nfa	-9.10	3uqi	-8.80	3gsv	-8.60
3nf6	-9.10	3nf8	-8.80	3avl	-8.60
3kms	-9.10	3gsv	-8.80	2zu4	-8.60
3gsn	-9.10	3gsr	-8.80	2yka	-8.60
3avf	-9.10	3d0i	-8.80	5ajm	-8.50
3ava	-9.10	3avc	-8.80	5ajm	-8.50
3ava	-9.10	3avb	-8.80	5ajm	-8.50
2htu	-9.10	3ava	-8.80	5ajm	-8.50

PDB	Docking score	PDB	Docking score	PDB	Docking score
4qrt	-8.50	4dgc	-8.20	3su5	-7.80
4lsp	-8.50	4dgc	-8.20	3su5	-7.80
4kps	-8.50	4dgc	-8.20	3su5	-7.80
4gye	-8.50	4dgc	-8.20	3su1	-7.80
4gye	-8.50	4dgb	-8.20	3avk	-7.80
4fb3	-8.50	4bh4	-8.20	2hfz	-7.80
4ejd	-8.50	4b8e	-8.20	4qrt	-7.70
4ejd	-8.50	4b8e	-8.20	4mj0	-7.70
4ejd	-8.50	4b8e	-8.20	4lss	-7.70
4eee	-8.50	3su2	-8.20	4iv1	-7.70
4dga	-8.50	3gsu	-8.20	4ejd	-7.70
4cqu	-8.50	2q7c	-8.20	4dkq	-7.70
4cqu	-8.50	2q7c	-8.20	3su6	-7.70
3zpb	-8.50	1qz8	-8.20	3su6	-7.70
3zpb	-8.50	4mmt	-8.10	3su3	-7.70
3nw8	-8.50	4dgc	-8.10	2zty	-7.70
3gzf	-8.50	3p8n	-8.10	2gvf	-7.70
3avn	-8.50	3gsw	-8.10	1rzk	-7.70
3avl	-8.50	3avg	-8.10	1rv7	-7.70
3avb	-8.50	2z35	-8.10	1f08	-7.70
2q7c	-8.50	2wfo	-8.10	4nwl	-7.60
2oy0	-8.50	2bvq	-8.10	4g9d	-7.60
2ge7	-8.50	1rq9	-8.10	4g8i	-7.60
4pv8	-8.40	4nwk	-8.00	4e92	-7.60
4i32	-8.40	4gv9	-8.00	3vbf	-7.60
4i31	-8.40	4ep3	-8.00	3vbf	-7.60
4i31	-8.40	3p8o	-8.00	3sv9	-7.60
4dgd	-8.40	1sys	-8.00	3sv9	-7.60
3zpa	-8.40	Spike RBD	-7.90	3sv6	-7.60
3rwi	-8.40	4i33	-7.90	3sv6	-7.60
3rwf	-8.40	4dgc	-7.90	3sue	-7.60
3rwf	-8.40	4bh2	-7.90	3su3	-7.60
3oah	-8.40	3sud	-7.90	3avh	-7.60
2hcn	-8.40	3su1	-7.90	2zu1	-7.60
2ghw	-8.40	3su0	-7.90	2yhh	-7.60
4gzf	-8.30	3ro5	-7.90	2lsp	-7.60
4gzf	-8.30	2xpx	-7.90	2axf	-7.60
4dgb	-8.30	2wfo	-7.90	2axf	-7.60
4dga	-8.30	2vvy	-7.90	1rpi	-7.60
4bh4	-8.30	2ge8	-7.90	3sis	-7.50
4bh4	-8.30	Papain	-7.80	3sis	-7.50
4bh4	-8.30	protease	-7.80	3avn	-7.50
3gsu	-8.30	4oyd	-7.80	3avc	-7.50
3avk	-8.30	4gve	-7.80	2xpx	-7.50
3avb	-8.30	4ep3	-7.80	2wh6	-7.50
4g9d	-8.20	4ejd	-7.80	2ca1	-7.50
4e92	-8.20	3suf	-7.80	3w39	-7.40
4dgd	-8.20	3sud	-7.80	3sv7	-7.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
3rkc	-7.40	3sit	-6.90	4ipz	-5.80
2yol	-7.40	3sit	-6.90	4ipz	-5.80
2y1s	-7.40	3b71	-6.90	2me3	-5.80
2xze	-7.40	3b71	-6.90	2l2f	-5.80
2wh6	-7.40	2q7c	-6.90	4ipz	-5.70
2ghv	-7.40	2q7c	-6.90	4ipz	-5.70
4g8i	-7.30	2q7c	-6.90	4ipz	-5.70
4ekx	-7.30	4ejk	-6.80	4ipz	-5.70
3su0	-7.30	3vie	-6.80	4mod	-5.60
3bwa	-7.30	3u83	-6.80	4ipz	-5.60
2yol	-7.30	3su4	-6.80	4ipz	-5.60
2xze	-7.30	3su4	-6.80	2x9m	-5.60
2xya	-7.30	3sit	-6.80	2vxj	-5.60
1rpi	-7.30	2ztz	-6.80	2me4	-5.60
4jpi	-7.20	3alw	-6.70	4uo4	-5.50
4ejk	-7.20	2v6q	-6.70	4ipz	-5.50
4dkr	-7.20	4ffy	-6.60	4adq	-5.50
3sv7	-7.20	2yhf	-6.60	4adq	-5.50
3su2	-7.20	2c86	-6.60	3giv	-5.50
3su2	-7.20	4nwk	-6.50	2m3m	-5.50
2g69	-7.20	2m3l	-6.50	3vie	-5.30
3sug	-7.10	2me2	-6.40	2mkr	-5.30
3m5h	-7.10	2g69	-6.40	3j22	-5.00
3ifu	-7.10	2c3a	-6.40	3vtt	-4.90
3a07	-7.10	4c1w	-6.30	3j23	-4.90
2vxw	-7.10	3s12	-6.30	2l3h	-4.70
1z8r	-7.10	2zu3	-6.30	4epj	-4.60
1yh3	-7.10	2q5u	-6.30	3vtt	-4.60
4oyd	-7.00	2q5u	-6.30	4ep2	-4.10
4ejk	-7.00	2q5u	-6.30	3m5g	-4.10
4ejd	-7.00	2q5u	-6.30	1hhg	-4.10
4ejd	-7.00	2q5u	-6.30	4ep2	-3.90
4dmn	-7.00	2q5u	-6.30	4g2k	-3.80
4dmn	-7.00	1qr8	-6.30	4g2k	-3.50
4b4n	-7.00	4epj	-6.20	4qhm	-3.10
4b4n	-7.00	4c1w	-6.20	4lki	-3.10
3sug	-7.00	3kqk	-6.10	4lkh	-3.10
3sit	-7.00	3i6k	-6.10	4lkk	-1.90
3sit	-7.00	1zsd	-6.10	4dge	-1.30
3avj	-7.00	4ipz	-6.00	2zsv	-1.00
2zol	-7.00	4eqj	-6.00	2zsv	-1.00
1qr9	-7.00	3zd0	-6.00	4e0r	-0.50
4ejd	-6.90	4ejr	-5.90	4g1g	-0.30
4ejd	-6.90	4mod	-5.80	4fqm	-0.20
3u83	-6.90	4ipz	-5.80	2x5i	-0.10
3sit	-6.90	4ipz	-5.80		

**Table S 9.** Predicted docking score of Bromocriptine against the viral protein panel.

<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>
3u7s	-12.80	3koa	-10.50	4rw8	-10.10
3u7s	-12.70	3cj5	-10.50	4qru	-10.10
3nxu	-11.80	2wr0	-10.50	4mk7	-10.10
3kqn	-11.60	4uo3	-10.40	4mk7	-10.10
4j4x	-11.50	4qrs	-10.40	4j4w	-10.10
3kqn	-11.50	4qrs	-10.40	4j4u	-10.10
3kqn	-11.50	4mk9	-10.40	4fnk	-10.10
1ida	-11.30	3hky	-10.40	4ej8	-10.10
4j4s	-11.20	3hky	-10.40	4ej8	-10.10
4j4s	-11.20	3ggu	-10.40	3t3c	-10.10
4a92	-11.10	3cj5	-10.40	3cj4	-10.10
3lkh	-11.10	3cj2	-10.40	2wrg	-10.10
2i4v	-11.10	2i4w	-10.40	2wrg	-10.10
4uo3	-11.00	2i4u	-10.40	2wrg	-10.10
4g42	-11.00	1p9u	-10.40	2wrg	-10.10
4uo7	-10.90	4uo3	-10.30	4rw9	-10.00
4uo7	-10.90	4uo3	-10.30	4mkb	-10.00
4uo7	-10.90	4uo3	-10.30	4e5e	-10.00
4uo7	-10.90	4rw4	-10.30	4bac	-10.00
4uo7	-10.90	4rw4	-10.30	3vbo	-10.00
4a92	-10.90	4qru	-10.30	3tid	-10.00
3hkw	-10.90	4pg2	-10.30	3ok9	-10.00
3hkw	-10.90	4mkb	-10.30	3h2l	-10.00
3hkw	-10.90	4j4v	-10.30	3h2l	-10.00
4uo7	-10.80	4j4v	-10.30	3d23	-10.00
3cj0	-10.80	3cj2	-10.30	3d23	-10.00
1quv	-10.80	2wr1	-10.30	3cpl	-10.00
4o44	-10.70	2wr0	-10.30	3cj4	-10.00
3cj0	-10.70	1syv	-10.30	3bew	-10.00
2wr0	-10.70	1r6a	-10.30	2ygb	-10.00
2i4x	-10.70	4uo5	-10.20	2ygb	-10.00
4q6r	-10.60	4uo5	-10.20	2wr4	-10.00
4q6r	-10.60	4mk8	-10.20	4qhk	-9.90
4mka	-10.60	4mk8	-10.20	4j4v	-9.90
4e7a	-10.60	4j4y	-10.20	4gua	-9.90
4e7a	-10.60	4j4v	-10.20	4e78	-9.90
3kqh	-10.60	4j4v	-10.20	4e78	-9.90
3cj3	-10.60	3ztj	-10.20	3tie	-9.90
3cj3	-10.60	3h98	-10.20	3tie	-9.90
3ciz	-10.60	3h98	-10.20	2wre	-9.90
3ciz	-10.60	2wrg	-10.20	2wre	-9.90
2wr0	-10.60	2wr1	-10.20	1n5a	-9.90
2i4d	-10.60	2wr1	-10.20	4uo0	-9.80
4mka	-10.50	2axg	-10.20	4uo0	-9.80
4bh0	-10.50	4wm8	-10.10	4uo0	-9.80
3t3c	-10.50	4uo5	-10.10	4uo0	-9.80

PDB	Docking score	PDB	Docking score	PDB	Docking score
4uo0	-9.80	4unw	-9.60	4cqu	-9.40
4uo0	-9.80	4rw7	-9.60	4cqu	-9.40
4uo0	-9.80	4pv9	-9.60	4cqu	-9.40
4uo0	-9.80	4pv9	-9.60	4cqu	-9.40
4uo0	-9.80	4o4g	-9.60	4cqr	-9.40
4uo0	-9.80	4i2q	-9.60	4cqr	-9.40
4uo0	-9.80	4fqy	-9.60	4adf	-9.40
4uo0	-9.80	4fp8	-9.60	4adf	-9.40
4uo0	-9.80	4cqw	-9.60	4adf	-9.40
4uo0	-9.80	3s11	-9.60	4adf	-9.40
4uo0	-9.80	3rwe	-9.60	4adf	-9.40
4uo0	-9.80	3kql	-9.60	4adf	-9.40
4uo0	-9.80	3kql	-9.60	3rki	-9.40
4uo0	-9.80	3kql	-9.60	3gsq	-9.40
4unw	-9.80	3ebj	-9.60	3bw9	-9.40
4unw	-9.80	5ajm	-9.50	2wr2	-9.40
4pv9	-9.80	5ajm	-9.50	2wr2	-9.40
4jo8	-9.80	5ajm	-9.50	2hcs	-9.40
3mlh	-9.80	5ajm	-9.50	1hhi	-9.40
3cpl	-9.80	5ajm	-9.50	4uo2	-9.30
2ygc	-9.80	5ajm	-9.50	4uo2	-9.30
2ygc	-9.80	4opa	-9.50	4uo2	-9.30
2wre	-9.80	4j4r	-9.50	4uo2	-9.30
2gec	-9.80	4fqr	-9.50	4uo2	-9.30
2gec	-9.80	4fqj	-9.50	4uo2	-9.30
2bvo	-9.80	3tid	-9.50	4uny	-9.30
1idb	-9.80	3rwe	-9.50	4mj1	-9.30
1hhk	-9.80	3nf6	-9.50	4m8y	-9.30
Main protease	-9.70	3n0i	-9.50	4k7f	-9.30
4mk9	-9.70	3lkh	-9.50	4fnk	-9.30
4mds	-9.70	3ku3	-9.50	4cqv	-9.30
4mds	-9.70	3kna	-9.50	4bgx	-9.30
4fqy	-9.70	2wr2	-9.50	4bgx	-9.30
4cqq	-9.70	2wr0	-9.50	3vbh	-9.30
4cqq	-9.70	2hjk	-9.50	3s13	-9.30
4cqq	-9.70	4uo3	-9.40	3r4b	-9.30
4cqq	-9.70	4uo3	-9.40	3nf8	-9.30
3vbr	-9.70	4uo3	-9.40	3nf7	-9.30
3se8	-9.70	4gaj	-9.40	3n0i	-9.30
3se8	-9.70	4gaj	-9.40	3gsu	-9.30
3rwd	-9.70	4gag	-9.40	3bev	-9.30
3fku	-9.70	4gag	-9.40	2xwy	-9.30
3bwa	-9.70	4g9f	-9.40	2vux	-9.30
2wrh	-9.70	4fqr	-9.40	1a41	-9.30
2wre	-9.70	4e5f	-9.40	4unx	-9.20
2wre	-9.70	4cr0	-9.40	4unx	-9.20
2wre	-9.70	4cqu	-9.40	4unx	-9.20
2wa1	-9.70	4cqu	-9.40	4rw6	-9.20



PDB	Docking score	PDB	Docking score	PDB	Docking score
4qhn	-9.20	4uo3	-9.00	4bgw	-8.70
3zp3	-9.20	4mj0	-9.00	3zpb	-8.70
3zp1	-9.20	4m30	-9.00	3zp0	-8.70
3sdy	-9.20	4m8y	-9.00	3u82	-8.70
3sdy	-9.20	4kpq	-9.00	3u82	-8.70
3sdy	-9.20	4jb9	-9.00	3rwg	-8.70
3rwh	-9.20	4g43	-9.00	3rwg	-8.70
3rwh	-9.20	4e5g	-9.00	2xra	-8.70
3rwc	-9.20	4dag	-9.00	2vvx	-8.70
3rwc	-9.20	4cqp	-9.00	2oy0	-8.70
3r4b	-9.20	4bh1	-9.00	1v3e	-8.70
3nf7	-9.20	4bh1	-9.00	1v3b	-8.70
3iyw	-9.20	4bh1	-9.00	4uo6	-8.60
3iyw	-9.20	3v3m	-9.00	4mza	-8.60
3iyw	-9.20	3se9	-9.00	4m8x	-8.60
3iyw	-9.20	3gso	-9.00	4ejl	-8.60
3iyw	-9.20	2vvw	-9.00	4e76	-8.60
3iyw	-9.20	1hhj	-9.00	4cqz	-8.60
3i6l	-9.20	1hhh	-9.00	4bgw	-8.60
3gsw	-9.20	4uo3	-8.90	3zpa	-8.60
3gso	-9.20	4m8x	-8.90	3zp2	-8.60
3bwa	-9.20	4kps	-8.90	3nfa	-8.60
3avl	-9.20	4hkj	-8.90	3ku6	-8.60
3ava	-9.20	4ffz	-8.90	3ku6	-8.60
3ava	-9.20	4ejl	-8.90	3ku3	-8.60
1v3d	-9.20	3zp6	-8.90	3klv	-8.60
1v3d	-9.20	3vcl	-8.90	3d0h	-8.60
1klm	-9.20	3rwi	-8.90	3alz	-8.60
4unx	-9.10	3nf7	-8.90	2hty	-8.60
4lst	-9.10	3nf7	-8.90	1v3b	-8.60
4k7f	-9.10	3ku5	-8.90	1rzj	-8.60
4cqp	-9.10	3gsq	-8.90	1oop	-8.60
4cqp	-9.10	3ggg	-8.90	1b53	-8.60
4cqp	-9.10	3b0w	-8.90	4lsv	-8.50
4cqp	-9.10	3avj	-8.90	4i2q	-8.50
4cqp	-9.10	2vvw	-8.90	4cqz	-8.50
4cew	-9.10	1izi	-8.90	4bgz	-8.50
3v3m	-9.10	4i2p	-8.80	3nwa	-8.50
3nf8	-9.10	4fp8	-8.80	3nwa	-8.50
3gsr	-9.10	4cqs	-8.80	3nfa	-8.50
3d0g	-9.10	4cqs	-8.80	3nfa	-8.50
3bw9	-9.10	4co6	-8.80	3nfa	-8.50
2wr7	-9.10	3zpb	-8.80	3nf8	-8.50
2hu4	-9.10	3vcl	-8.80	3avh	-8.50
2hu4	-9.10	3ku5	-8.80	2uv0	-8.50
2hu4	-9.10	2hu0	-8.80	2uv0	-8.50
2hu4	-9.10	1v3e	-8.80	2uv0	-8.50
2bvp	-9.10	4lsr	-8.70	2uv0	-8.50

PDB	Docking score	PDB	Docking score	PDB	Docking score
2htw	-8.50	2iph	-8.20	4pv8	-7.70
4wm7	-8.40	1v3c	-8.20	4dkq	-7.70
4mj1	-8.40	1v3c	-8.20	4dgd	-7.70
4fqi	-8.40	1v3c	-8.20	4cey	-7.70
4bgy	-8.40	4uo6	-8.10	3ztn	-7.70
3nf9	-8.40	4qhl	-8.10	3uf5	-7.70
3nf6	-8.40	4mza	-8.10	3oah	-7.70
3avf	-8.40	4iv3	-8.10	3gsu	-7.70
2z35	-8.40	3nwf	-8.10	3alx	-7.70
2uv0	-8.40	3nf9	-8.10	2wh6	-7.70
2uv0	-8.40	3avg	-8.10	2vvy	-7.70
2uv0	-8.40	2x83	-8.10	2hcn	-7.70
2uv0	-8.40	2iph	-8.10	1n59	-7.70
2uv0	-8.40	2ht5	-8.10	4lsp	-7.60
2uv0	-8.40	1v3c	-8.10	4fvu	-7.60
2uv0	-8.40	4mmr	-8.00	4f3i	-7.60
2uv0	-8.40	4eq0	-8.00	4f3i	-7.60
2oy0	-8.40	4cqx	-8.00	4e5l	-7.60
2mgu	-8.40	4bh4	-8.00	4dkp	-7.60
1v2i	-8.40	4bh4	-8.00	4cdq	-7.60
1v2i	-8.40	4bh4	-8.00	3vbf	-7.60
1sk7	-8.40	4bh2	-8.00	3su1	-7.60
1rv7	-8.40	4bh2	-8.00	3nw8	-7.60
1izh	-8.40	3ro5	-8.00	3avb	-7.60
4mmu	-8.30	3o4l	-8.00	3avb	-7.60
4mgu	-8.30	3avn	-8.00	2ge8	-7.60
4g8g	-8.30	2wr3	-8.00	4qru	-7.50
4g8g	-8.30	2gvf	-8.00	4f3z	-7.50
4eq0	-8.30	1rzk	-8.00	4cqy	-7.50
3nf8	-8.30	1b50	-8.00	3vbf	-7.50
2wrf	-8.30	4mms	-7.90	3rwi	-7.50
2ge7	-8.30	4i2p	-7.90	3oah	-7.50
1r6a	-8.30	4gve	-7.90	3nf6	-7.50
1pk0	-8.30	4egt	-7.90	3nf6	-7.50
4mj0	-8.20	2xi5	-7.90	3mj5	-7.50
4mg3	-8.20	2xi5	-7.90	3mj5	-7.50
4mg3	-8.20	2x83	-7.90	3i6g	-7.50
4lsu	-8.20	2wrc	-7.90	3gsw	-7.50
4lsu	-8.20	2ghw	-7.90	3avc	-7.50
4j6r	-8.20	2c7u	-7.90	4i31	-7.40
4i7f	-8.20	1p9s	-7.90	4i31	-7.40
4fb3	-8.20	4pv8	-7.80	4cdx	-7.40
4e5j	-8.20	4g9f	-7.80	4cdw	-7.40
3lqa	-8.20	3nf9	-7.80	3avl	-7.40
2zu5	-8.20	3nf9	-7.80	3ava	-7.40
2zu4	-8.20	3gsv	-7.80	3ava	-7.40
2iph	-8.20	Spike RBD	-7.70	2htu	-7.40
2iph	-8.20	4qrt	-7.70	2c36	-7.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
2c36	-7.40	4iv1	-6.90	4i33	-6.50
4qrt	-7.30	4ejd	-6.90	4e91	-6.50
4oyd	-7.30	4ejd	-6.90	4bh3	-6.50
4i32	-7.30	4e5i	-6.90	4bh3	-6.50
4dko	-7.30	4dgc	-6.90	4bh3	-6.50
3avk	-7.30	4b8e	-6.90	4bh3	-6.50
3avb	-7.30	3su0	-6.90	3vie	-6.50
3avb	-7.30	3sis	-6.90	3su3	-6.50
3a07	-7.30	3gsx	-6.90	3su3	-6.50
2zty	-7.30	3gsx	-6.90	3sit	-6.50
2yka	-7.30	1yh3	-6.90	2ztz	-6.50
2q7c	-7.30	4lss	-6.80	2g69	-6.50
2ghv	-7.30	4gv3	-6.80	2bvq	-6.50
4fqi	-7.20	4gv3	-6.80	1f08	-6.50
4fqi	-7.20	4dkr	-6.80	4oph	-6.40
4cdu	-7.20	4b8e	-6.80	4lkj	-6.40
3w39	-7.20	2wh6	-6.80	4gv9	-6.40
3sud	-7.20	2q7c	-6.80	4g9z	-6.40
3gsr	-7.20	2g69	-6.80	4fqv	-6.40
3avh	-7.20	1rpi	-6.80	4ejk	-6.40
3avg	-7.20	4qrt	-6.70	4dmn	-6.40
2q7c	-7.20	4jpp	-6.70	4dmn	-6.40
4dgc	-7.10	4jpk	-6.70	3ifu	-6.40
4dgc	-7.10	4g9z	-6.70	3gsn	-6.40
4dgc	-7.10	4ffy	-6.70	3bwa	-6.40
4dgc	-7.10	4e92	-6.70	3avc	-6.40
4dgc	-7.10	4e92	-6.70	2yhf	-6.40
4bh4	-7.10	3su6	-6.70	2xpx	-6.40
3su2	-7.10	3sis	-6.70	2me2	-6.40
3su2	-7.10	3m5h	-6.70	4nwl	-6.30
3rwj	-7.10	2zu1	-6.70	4gye	-6.30
3rwj	-7.10	2v6q	-6.70	4fqv	-6.30
3rwf	-7.10	1rpi	-6.70	4ejd	-6.30
3rwf	-7.10	4oyd	-6.60	3u83	-6.30
3gsv	-7.10	4gzf	-6.60	3u83	-6.30
3gsu	-7.10	4gzf	-6.60	3sv6	-6.30
2xya	-7.10	4dgb	-6.60	3sv6	-6.30
2xpx	-7.10	4dgb	-6.60	3su5	-6.30
Papain	-7.00	3uqi	-6.60	2nze	-6.30
protease	-7.00	3sv8	-6.60	2vxw	-6.30
4ejd	-7.00	3sit	-6.60	1sys	-6.30
4dgd	-7.00	3sit	-6.60	4jpk	-6.20
4b8e	-7.00	3sit	-6.60	4epj	-6.20
3pqy	-7.00	3sit	-6.60	4ep3	-6.20
2lsp	-7.00	3sit	-6.60	4ep3	-6.20
2ca1	-7.00	2zol	-6.60	4eee	-6.20
1rq9	-7.00	2yol	-6.60	4b4n	-6.20
1qz8	-7.00	1qr8	-6.60	3sv9	-6.20

PDB	Docking score	PDB	Docking score	PDB	Docking score
3sud	-6.20	4mod	-5.80	4dga	-4.70
3su6	-6.20	4mod	-5.80	3vtt	-4.70
3su5	-6.20	4mmv	-5.80	2hfz	-4.70
3su5	-6.20	4gye	-5.80	4dga	-4.60
3su4	-6.20	4ekx	-5.80	3zd0	-4.60
3su4	-6.20	4ejd	-5.80	4g8i	-4.50
3su2	-6.20	3sug	-5.80	4ep2	-4.50
3su1	-6.20	3gzf	-5.80	1z8r	-4.50
3kmq	-6.20	2yol	-5.80	4g9d	-4.40
3b71	-6.20	4mmt	-5.70	4ep2	-4.40
2yhh	-6.20	4c1w	-5.70	3j23	-4.40
2y1s	-6.20	3uqi	-5.70	3j22	-4.40
2q5u	-6.20	3i6k	-5.70	4uo8	-4.10
2q5u	-6.20	3avk	-5.70	4epj	-3.90
2q5u	-6.20	3alw	-5.70	2l3h	-3.80
2q5u	-6.20	2m3l	-5.70	4ejk	-3.60
2q5u	-6.20	4mze	-5.60	2m3m	-3.60
2q5u	-6.20	2xze	-5.60	4ipz	-3.50
4u6h	-6.10	2q7c	-5.60	4ipz	-3.40
4nwk	-6.10	2q7c	-5.60	2me3	-3.40
4jkg	-6.10	2q7c	-5.60	4qhm	-3.30
4ejr	-6.10	2c3a	-5.60	4ipz	-2.90
4ejd	-6.10	4mze	-5.50	4ipz	-2.90
4ejd	-6.10	3sue	-5.50	4ipz	-2.80
4ejd	-6.10	2x9m	-5.50	4ipz	-1.90
4b4n	-6.10	4adq	-5.40	4dge	-1.60
3sug	-6.10	4adq	-5.40	4eqj	-1.50
3suf	-6.10	2me4	-5.40	2zsv	-1.10
3su0	-6.10	2l2f	-5.40	2zsv	-1.00
3s12	-6.10	4ipz	-5.30	4e0r	-0.70
3p8o	-6.10	4c1w	-5.20	4gu4	-0.60
3p8n	-6.10	3avn	-5.20	4gu4	-0.60
3kms	-6.10	2mkr	-5.20	4gu4	-0.60
2wfo	-6.10	1qr9	-5.20	4gu4	-0.60
2axf	-6.10	4g8i	-5.10	4gu4	-0.60
4nwk	-6.00	3vtt	-5.10	4gu4	-0.50
4g9d	-6.00	1zsd	-5.10	3m5i	-0.40
3sv7	-6.00	3kqk	-5.00	4gu3	-0.10
3d0i	-6.00	3giv	-5.00	4gu3	-0.10
3b71	-6.00	4ejk	-4.90	4gu3	-0.10
2wfo	-6.00	3vie	-4.90	4gu3	-0.10
4ejd	-5.90	2zu3	-4.90	4gu3	-0.10
3sv9	-5.90	2vxj	-4.90	4gu3	-0.10
3sv7	-5.90	4ipz	-4.80	4gu3	-0.10
3rc	-5.90	4ipz	-4.80	4gu3	-0.10
3avj	-5.90	4ipz	-4.70	4gu3	-0.10
2c86	-5.90	4ipz	-4.70	4gu3	-0.10
2axf	-5.90	4ipz	-4.70	4gu3	-0.10

<b>PDB</b>	<b>Docking score</b>
4gu3	-0.10

<b>PDB</b>	<b>Docking score</b>
4fqm	-0.10

**Table S 10.** Predicted docking score of Peficitinib against the viral protein panel.

PDB	Docking score	PDB	Docking score	PDB	Docking score
3u7s	-12.70	2wr0	-10.50	2wrg	-10.00
3u7s	-12.60	4rw4	-10.40	2wrg	-10.00
3nxu	-11.50	4rw4	-10.40	2wrg	-10.00
3kqn	-11.30	4mk9	-10.40	2wr1	-10.00
3kqn	-11.30	3t3c	-10.40	2wr0	-10.00
3kqn	-11.30	3kqh	-10.40	2bvo	-10.00
4uo7	-11.20	4qru	-10.30	4mkb	-9.90
4uo7	-11.20	4qru	-10.30	4mkb	-9.90
4j4x	-11.20	4qrs	-10.30	4mka	-9.90
4uo7	-11.10	3hky	-10.30	4mk8	-9.90
4uo7	-11.10	3hky	-10.30	4mk7	-9.90
4uo7	-11.10	2i4d	-10.30	4j4v	-9.90
4uo7	-11.10	4wm8	-10.20	4j4v	-9.90
4o44	-11.10	4uo5	-10.20	4j4v	-9.90
4a92	-11.10	4pg2	-10.20	4j4v	-9.90
3lkh	-11.10	4j4w	-10.20	4j4v	-9.90
4j4s	-11.00	3tie	-10.20	4gua	-9.90
4j4s	-11.00	3tie	-10.20	3mlh	-9.90
4a92	-11.00	2i4w	-10.20	3cj4	-9.90
4uo3	-10.90	2i4u	-10.20	3cj2	-9.90
4uo3	-10.90	2axg	-10.20	3bev	-9.90
4uo3	-10.90	1syv	-10.20	2wrg	-9.90
3hkw	-10.90	4rw8	-10.10	2gec	-9.90
3hkw	-10.80	4mka	-10.10	2gec	-9.90
3hkw	-10.80	4mk8	-10.10	Main protease	-9.80
3cj0	-10.80	4j4y	-10.10	4uo0	-9.80
2i4v	-10.80	4j4u	-10.10	4uo0	-9.80
4uo3	-10.70	3h98	-10.10	4uo0	-9.80
4uo3	-10.70	3h98	-10.10	4uo0	-9.80
3koa	-10.70	3bew	-10.10	4uo0	-9.80
3cj0	-10.70	2wr0	-10.10	4uo0	-9.80
2i4x	-10.70	1p9u	-10.10	4uo0	-9.80
4uo5	-10.60	1n5a	-10.10	4uo0	-9.80
4g42	-10.60	1idb	-10.10	4uo0	-9.80
4e7a	-10.60	1ida	-10.10	4uo0	-9.80
4e7a	-10.60	4rw9	-10.00	4uo0	-9.80
4bh0	-10.60	4bac	-10.00	4unw	-9.80
3t3c	-10.60	3vbo	-10.00	4unw	-9.80
3cj5	-10.60	3d23	-10.00	4qhk	-9.80
1quv	-10.60	3d23	-10.00	4mk7	-9.80
4uo5	-10.50	3cj4	-10.00	3tid	-9.80
4qrs	-10.50	3cj2	-10.00	3rwe	-9.80
3cj3	-10.50	3ciz	-10.00	3lkh	-9.80
3cj3	-10.50	2ygc	-10.00	4uo0	-9.70
3ciz	-10.50	2ygc	-10.00	4uo0	-9.70
2wr0	-10.50	2wrg	-10.00	4uo0	-9.70
				4uo0	-9.70

PDB	Docking score	PDB	Docking score	PDB	Docking score
4uo0	-9.70	3kql	-9.50	4e78	-9.30
4uo0	-9.70	3kql	-9.50	4cr0	-9.30
4uo0	-9.70	3kna	-9.50	4cqy	-9.30
4unw	-9.70	3fku	-9.50	4adf	-9.30
4rw6	-9.70	3cpl	-9.50	4adf	-9.30
4g9f	-9.70	3bwa	-9.50	4adf	-9.30
4fqy	-9.70	2ygb	-9.50	4adf	-9.30
3vbr	-9.70	2ygb	-9.50	4adf	-9.30
3tid	-9.70	2xwy	-9.50	4adf	-9.30
3s11	-9.70	2wre	-9.50	3s13	-9.30
3rwe	-9.70	2wre	-9.50	3r4b	-9.30
3h2l	-9.70	2wre	-9.50	3r4b	-9.30
3h2l	-9.70	2wre	-9.50	3ok9	-9.30
3cpl	-9.70	2wre	-9.50	3gsr	-9.30
3bwa	-9.70	2wre	-9.50	2wr0	-9.30
3bw9	-9.70	1klm	-9.50	1hhk	-9.30
2wrh	-9.70	1hhi	-9.50	1hhh	-9.30
2wr4	-9.70	4uny	-9.40	5ajm	-9.20
2wr1	-9.70	4q6r	-9.40	4uo2	-9.20
2wr1	-9.70	4q6r	-9.40	4uo2	-9.20
2hjk	-9.70	4opa	-9.40	4uo2	-9.20
1r6a	-9.70	4gag	-9.40	4unx	-9.20
4uo0	-9.60	4gag	-9.40	4unx	-9.20
4rw7	-9.60	4g43	-9.40	4mds	-9.20
4mk9	-9.60	4fqj	-9.40	4mds	-9.20
4jo8	-9.60	3ztj	-9.40	4m8x	-9.20
4j4r	-9.60	3rwc	-9.40	4kpp	-9.20
4i2q	-9.60	3rwc	-9.40	4gaj	-9.20
4fqy	-9.60	3ku3	-9.40	4gaj	-9.20
4e78	-9.60	3ebj	-9.40	4fqr	-9.20
4cqy	-9.60	2wr2	-9.40	4e5f	-9.20
3nf6	-9.60	2wr2	-9.40	4e5e	-9.20
3n0i	-9.60	2wr2	-9.40	4cqu	-9.20
3cj5	-9.60	1a41	-9.40	4cqu	-9.20
2wa1	-9.60	5ajm	-9.30	4cqu	-9.20
4pv9	-9.50	5ajm	-9.30	4cqu	-9.20
4pv9	-9.50	5ajm	-9.30	4cqu	-9.20
4o4g	-9.50	5ajm	-9.30	4cqu	-9.20
4mmu	-9.50	5ajm	-9.30	4bgx	-9.20
4k7f	-9.50	4uo2	-9.30	3vbh	-9.20
4cqq	-9.50	4uo2	-9.30	3v3m	-9.20
4cqq	-9.50	4uo2	-9.30	3gsw	-9.20
4cqq	-9.50	4unx	-9.30	3gsw	-9.20
3rwd	-9.50	4pv9	-9.30	3gso	-9.20
3rki	-9.50	4fqr	-9.30	3d0g	-9.20
3nf6	-9.50	4fnk	-9.30	3avl	-9.20
3n0i	-9.50	4ej8	-9.30	3ava	-9.20
3kql	-9.50	4ej8	-9.30	3ava	-9.20

PDB	Docking score	PDB	Docking score	PDB	Docking score
2zu5	-9.20	4uo3	-8.90	4co6	-8.70
2hcs	-9.20	4m8y	-8.90	3zp2	-8.70
4m8y	-9.10	3zp6	-8.90	3zp0	-8.70
4k7f	-9.10	3vcl	-8.90	3nf8	-8.70
4fnk	-9.10	3se9	-8.90	3alz	-8.70
4e5g	-9.10	3se8	-8.90	2xra	-8.70
4bgx	-9.10	3se8	-8.90	2wr7	-8.70
3zp3	-9.10	3rwg	-8.90	2vvx	-8.70
3v3m	-9.10	3ku5	-8.90	2vvx	-8.70
3sdy	-9.10	3klv	-8.90	2vvw	-8.70
3sdy	-9.10	3iyw	-8.90	2oy0	-8.70
3sdy	-9.10	3iyw	-8.90	2htw	-8.70
3rwi	-9.10	3iyw	-8.90	1v3b	-8.70
3rwh	-9.10	3i6l	-8.90	4lst	-8.60
3rwh	-9.10	3ggu	-8.90	4lsr	-8.60
3gsq	-9.10	1izi	-8.90	4iv3	-8.60
3gso	-9.10	4mj1	-8.80	4hkj	-8.60
3bw9	-9.10	4m30	-8.80	4dag	-8.60
2hu4	-9.10	4m8x	-8.80	4cqz	-8.60
2hu4	-9.10	4jb9	-8.80	3zpa	-8.60
2hu4	-9.10	4i2p	-8.80	3ku6	-8.60
1v3d	-9.10	4fp8	-8.80	3ku6	-8.60
1v3d	-9.10	4fp8	-8.80	3gsq	-8.60
4uo3	-9.00	4ffz	-8.80	2vvw	-8.60
4uo3	-9.00	4cqs	-8.80	2hty	-8.60
4uo3	-9.00	4cqs	-8.80	1v3b	-8.60
4unx	-9.00	4cqp	-8.80	1b53	-8.60
4qhn	-9.00	4cqp	-8.80	4fqi	-8.50
4mj0	-9.00	4cqp	-8.80	4ejl	-8.50
4lsu	-9.00	4cqp	-8.80	4e5j	-8.50
4ejl	-9.00	4cqp	-8.80	4cqz	-8.50
4cqr	-9.00	4cqp	-8.80	4bh1	-8.50
4cqr	-9.00	4bgw	-8.80	4bh1	-8.50
4cew	-9.00	4bgw	-8.80	4bh1	-8.50
3nf8	-9.00	3zpb	-8.80	4bgz	-8.50
3nf8	-9.00	3zpb	-8.80	3zp1	-8.50
3nf7	-9.00	3vcl	-8.80	3u82	-8.50
3nf7	-9.00	3rwg	-8.80	3u82	-8.50
3nf7	-9.00	3ku5	-8.80	3nwa	-8.50
3nf7	-9.00	3ku3	-8.80	3nwa	-8.50
3iyw	-9.00	3iyw	-8.80	3nfa	-8.50
3iyw	-9.00	3b0w	-8.80	3d0h	-8.50
3ggu	-9.00	1v3e	-8.80	2uv0	-8.50
3avj	-9.00	1v3e	-8.80	2uv0	-8.50
2hu4	-9.00	4uo6	-8.70	2uv0	-8.50
2bvp	-9.00	4kps	-8.70	2uv0	-8.50
1hhj	-9.00	4i7f	-8.70	2uv0	-8.50
4uo3	-8.90	4i2p	-8.70	2uv0	-8.50



PDB	Docking score	PDB	Docking score	PDB	Docking score
2uv0	-8.50	4mg3	-8.10	4dkq	-7.60
2uv0	-8.50	4i2q	-8.10	4dkp	-7.60
2uv0	-8.50	4bgy	-8.10	3ztn	-7.60
2uv0	-8.50	3lqa	-8.10	3vbf	-7.60
2uv0	-8.50	3avf	-8.10	3vbf	-7.60
2uv0	-8.50	2x83	-8.10	3su6	-7.60
2hu0	-8.50	2x83	-8.10	3rwi	-7.60
2ht5	-8.50	2htu	-8.10	3mj5	-7.60
1sk7	-8.50	2gvf	-8.10	3mj5	-7.60
1rzj	-8.50	4wm7	-8.00	3gsw	-7.60
4g8g	-8.40	4lsv	-8.00	2q7c	-7.60
4g8g	-8.40	4eq0	-8.00	2c36	-7.60
4eq0	-8.40	4bh4	-8.00	4qru	-7.50
4e76	-8.40	4bh2	-8.00	4pv8	-7.50
3nfa	-8.40	4bh2	-8.00	4lsp	-7.50
2zu4	-8.40	3oah	-8.00	4f3z	-7.50
2mgu	-8.40	3nwf	-8.00	4dgd	-7.50
1izh	-8.40	3nfa	-8.00	4cdu	-7.50
4uo6	-8.30	3nfa	-8.00	4cdq	-7.50
4j6r	-8.30	3nf9	-8.00	3uf5	-7.50
4e5l	-8.30	3avn	-8.00	3avc	-7.50
3nf9	-8.30	3avg	-8.00	3avb	-7.50
3nf8	-8.30	3alx	-8.00	3avb	-7.50
3avh	-8.30	2wh6	-8.00	3ava	-7.50
2z35	-8.30	2oy0	-8.00	2iph	-7.50
2xi5	-8.30	2ghw	-8.00	2iph	-7.50
2ge7	-8.30	4gve	-7.90	1rq9	-7.50
1v2i	-8.30	4egt	-7.90	4oyd	-7.40
1v2i	-8.30	4cqx	-7.90	4mms	-7.40
1rv7	-8.30	3o4l	-7.90	4i32	-7.40
1r6a	-8.30	3i6g	-7.90	4i31	-7.40
1pk0	-8.30	2wrc	-7.90	4i31	-7.40
1b50	-8.30	2iph	-7.90	4f3i	-7.40
4mj1	-8.20	2hcn	-7.90	4e92	-7.40
4lsu	-8.20	1rzk	-7.90	4e92	-7.40
2xi5	-8.20	4qrt	-7.80	4cqy	-7.40
2wrf	-8.20	4fb3	-7.80	4cey	-7.40
1v3c	-8.20	3nf9	-7.80	3oah	-7.40
1v3c	-8.20	3nf9	-7.80	3nf6	-7.40
1v3c	-8.20	3gsv	-7.80	3nf6	-7.40
1v3c	-8.20	1oop	-7.80	3avl	-7.40
1p9s	-8.20	4mmr	-7.70	3ava	-7.40
4qhl	-8.10	4g9f	-7.70	2q7c	-7.40
4mza	-8.10	4fvu	-7.70	2q7c	-7.40
4mza	-8.10	3gsv	-7.70	2lsp	-7.40
4mj0	-8.10	3avk	-7.70	2iph	-7.40
4mgu	-8.10	2vvy	-7.70	2ge8	-7.40
4mg3	-8.10	4oph	-7.60	2c36	-7.40

PDB	Docking score	PDB	Docking score	PDB	Docking score
4qrt	-7.30	2wr3	-7.00	3sit	-6.60
4fqi	-7.30	4gye	-6.90	3sit	-6.60
4f3i	-7.30	4ejd	-6.90	3gzf	-6.60
4cdw	-7.30	4dgd	-6.90	2zol	-6.60
3su1	-7.30	4dgc	-6.90	2me2	-6.60
3avb	-7.30	4dgc	-6.90	4lkj	-6.50
3avb	-7.30	4dgc	-6.90	4g9z	-6.50
2zty	-7.30	4dgc	-6.90	4g9z	-6.50
2ghv	-7.30	4dgc	-6.90	4fqv	-6.50
2c7u	-7.30	4dgc	-6.90	4ep3	-6.50
4pv8	-7.20	3sis	-6.90	4ep3	-6.50
4fqi	-7.20	2xpx	-6.90	4ejd	-6.50
4dko	-7.20	2g69	-6.90	4e91	-6.50
3w39	-7.20	2ca1	-6.90	4dmn	-6.50
3sud	-7.20	4lss	-6.80	4dkr	-6.50
3ro5	-7.20	4ejd	-6.80	4bh3	-6.50
3pqy	-7.20	4e5i	-6.80	4bh3	-6.50
2yka	-7.20	2wh6	-6.80	4bh3	-6.50
1yh3	-7.20	2g69	-6.80	4bh3	-6.50
1n59	-7.20	Spike RBD	-6.70	3vie	-6.50
Papain	-7.10	4oyd	-6.70	3sv6	-6.50
protease	-7.10	4jpk	-6.70	3su5	-6.50
4qrt	-7.10	4gv9	-6.70	3su5	-6.50
4iv1	-7.10	4ffy	-6.70	3su5	-6.50
4cdx	-7.10	4dgb	-6.70	3su0	-6.50
4b8e	-7.10	4dgb	-6.70	2ztz	-6.50
3gsu	-7.10	4b8e	-6.70	2xze	-6.50
3gsu	-7.10	4b4n	-6.70	1sys	-6.50
3avh	-7.10	4b4n	-6.70	1qr8	-6.50
3a07	-7.10	3rkc	-6.70	4nwl	-6.40
1qz8	-7.10	3nw8	-6.70	4fqv	-6.40
4bh4	-7.00	3m5h	-6.70	4eee	-6.40
4bh4	-7.00	3kmq	-6.70	3su6	-6.40
4bh4	-7.00	2yol	-6.70	3su4	-6.40
3su2	-7.00	2bvq	-6.70	3su4	-6.40
3su2	-7.00	1rpi	-6.70	3su1	-6.40
3su2	-7.00	1rpi	-6.70	3ifu	-6.40
3su0	-7.00	4jpk	-6.60	2yhf	-6.40
3sis	-7.00	4i33	-6.60	2v6q	-6.40
3rwj	-7.00	4dmn	-6.60	1f08	-6.40
3rwj	-7.00	4b8e	-6.60	4gzf	-6.30
3rwf	-7.00	3sv8	-6.60	4gzf	-6.30
3gsx	-7.00	3su3	-6.60	4gv3	-6.30
3gsx	-7.00	3su3	-6.60	4gv3	-6.30
3gsr	-7.00	3sit	-6.60	4ejd	-6.30
3avg	-7.00	3sit	-6.60	4ejd	-6.30
2zu1	-7.00	3sit	-6.60	4ejd	-6.30
2xya	-7.00	3sit	-6.60	3sv9	-6.30

PDB	Docking score	PDB	Docking score	PDB	Docking score
3sv9	-6.30	2q5u	-5.80	4g8i	-4.80
3rwf	-6.30	2q5u	-5.80	3zd0	-4.80
3p8n	-6.30	2q5u	-5.80	3avn	-4.80
3b71	-6.30	4mze	-5.70	2vxj	-4.80
3b71	-6.30	4mze	-5.70	4ipz	-4.70
2xpx	-6.30	4mmv	-5.70	4ipz	-4.70
2vxw	-6.30	4ejr	-5.70	4g9d	-4.70
4nwk	-6.20	2x9m	-5.70	4dga	-4.70
4jpi	-6.20	2q7c	-5.70	4ep2	-4.60
4jki	-6.20	2c3a	-5.70	4ep2	-4.60
3sv6	-6.20	4mod	-5.60	3j23	-4.50
3suf	-6.20	4mod	-5.60	3j22	-4.50
3sud	-6.20	4ejd	-5.60	4ipz	-4.00
3kms	-6.20	3vtt	-5.60	3vie	-4.00
3gsn	-6.20	3uqi	-5.60	4uo4	-3.50
3bwa	-6.20	3sue	-5.60	4uo8	-3.30
4mmt	-6.10	3avc	-5.60	4ipz	-3.30
4epj	-6.10	4ejk	-5.50	4eqj	-3.00
3u83	-6.10	4adq	-5.50	4ipz	-2.90
3u83	-6.10	3sug	-5.50	4qhm	-2.80
3sv7	-6.10	3avk	-5.50	4ipz	-2.80
3s12	-6.10	4ekx	-5.40	4ipz	-2.70
3d0i	-6.10	4c1w	-5.40	4ipz	-2.60
2wfo	-6.10	3i6k	-5.40	4ipz	-2.40
2wfo	-6.10	3giv	-5.40	4epj	-1.80
2axf	-6.10	3alw	-5.40	2l3h	-1.70
2axf	-6.10	2me4	-5.40	4dge	-1.60
4u6h	-6.00	2m3l	-5.40	2zsv	-1.10
4nwk	-6.00	2l2f	-5.40	2zsv	-1.10
4ejd	-6.00	4g9d	-5.30	3m5i	-1.00
4ejd	-6.00	4dga	-5.30	4gu4	-0.90
3sv7	-6.00	1qr9	-5.30	4gu4	-0.90
3sug	-6.00	4c1w	-5.20	4gu4	-0.90
2yhh	-6.00	4adq	-5.20	4gu4	-0.90
2xze	-6.00	3vtt	-5.20	4gu4	-0.90
3uqi	-5.90	1z8r	-5.20	4gu4	-0.90
3p8o	-5.90	3kqk	-5.10	4e0r	-0.70
3avj	-5.90	2mkr	-5.10	4gu3	-0.40
2y1s	-5.90	1zsd	-5.10	4gu3	-0.40
2q5u	-5.90	2zu3	-5.00	4gu3	-0.40
2c86	-5.90	2me3	-5.00	4gu3	-0.40
4gye	-5.80	4ipz	-4.90	4gu3	-0.40
4ejk	-5.80	4ejk	-4.90	4gu3	-0.30
2yol	-5.80	2m3m	-4.90	4gu3	-0.30
2q7c	-5.80	2hfz	-4.90	4gu3	-0.30
2q7c	-5.80	4ipz	-4.80	4gu3	-0.30
2q5u	-5.80	4ipz	-4.80	4gu3	-0.30
2q5u	-5.80	4g8i	-4.80	4gu3	-0.30

<b>PDB</b>	<b>Docking score</b>
4gu3	-0.30

<b>PDB</b>	<b>Docking score</b>
4fqm	-0.30

**Table S 11.** Predicted docking score of Dihydroergotamine against the viral protein panel.

<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>	<b>PDB</b>	<b>Docking score</b>
3nxu	-13.00	2wrg	-10.90	3lkh	-10.50
3kqn	-11.90	2wrg	-10.90	3hky	-10.50
3kqn	-11.90	2wrg	-10.90	3hky	-10.50
3kqn	-11.90	2wrg	-10.90	3hkw	-10.50
3kqh	-11.80	4rw9	-10.80	3hkw	-10.50
3iyw	-11.80	4qru	-10.80	3cj4	-10.50
3iyw	-11.80	4mk8	-10.80	2wr1	-10.50
3iyw	-11.80	4mk8	-10.80	2i4u	-10.50
3iyw	-11.80	4fnk	-10.80	1hhk	-10.50
3iyw	-11.80	3tid	-10.80	4mkb	-10.40
3iyw	-11.80	3h2l	-10.80	4mkb	-10.40
2wr0	-11.40	3bwa	-10.80	4mka	-10.40
2wr0	-11.40	2hjk	-10.80	4mka	-10.40
2wr0	-11.40	2bvp	-10.80	4mk7	-10.40
2wr0	-11.40	2axg	-10.80	4mk7	-10.40
4uo3	-11.30	1syv	-10.80	4k7f	-10.40
4uo3	-11.30	4rw8	-10.70	4g9f	-10.40
4uo3	-11.30	4qrs	-10.70	4fnk	-10.40
3vbr	-11.30	4o44	-10.70	4e78	-10.40
2wr0	-11.30	4j4x	-10.70	4e78	-10.40
4g42	-11.10	3gso	-10.70	4a92	-10.40
3vbo	-11.10	3cpl	-10.70	4a92	-10.40
3u7s	-11.10	3cj3	-10.70	3ztj	-10.40
3u7s	-11.10	2ygb	-10.70	3i6l	-10.40
3cj2	-11.10	1n5a	-10.70	3d23	-10.40
4mk9	-11.00	4uo5	-10.60	3d23	-10.40
4mk9	-11.00	4pg2	-10.60	3cj4	-10.40
4fqr	-11.00	4j4y	-10.60	3cj0	-10.40
4e7a	-11.00	4bh0	-10.60	3b0w	-10.40
4e7a	-11.00	3lkh	-10.60	2wr4	-10.40
3vcl	-11.00	3cpl	-10.60	2wr1	-10.40
3vcl	-11.00	3cj5	-10.60	2wr1	-10.40
3tie	-11.00	3cj5	-10.60	1hhi	-10.40
3tie	-11.00	3cj3	-10.60	4uo3	-10.30
3h98	-11.00	3cj0	-10.60	4uo2	-10.30
3cj2	-11.00	3ciz	-10.60	4uo2	-10.30
3bwa	-11.00	3bw9	-10.60	4uo2	-10.30
2hcs	-11.00	2ygc	-10.60	4uo2	-10.30
2bvo	-11.00	2ygc	-10.60	4uo2	-10.30
1r6a	-11.00	2ygb	-10.60	4uo2	-10.30
4qru	-10.90	2htu	-10.60	3rwe	-10.30
4qrs	-10.90	1quv	-10.60	3koa	-10.30
4fqr	-10.90	4uo5	-10.50	3kna	-10.30
3h98	-10.90	4uo5	-10.50	3gsw	-10.30
3h2l	-10.90	4j4w	-10.50	3ciz	-10.30
2wrg	-10.90	3tid	-10.50	3bw9	-10.30

PDB	Docking score	PDB	Docking score	PDB	Docking score
2wrh	-10.30	4lsu	-10.00	3sdy	-9.80
2i4v	-10.30	4g43	-10.00	3sdy	-9.80
2gec	-10.30	4cdw	-10.00	3rwc	-9.80
2gec	-10.30	3se8	-10.00	3ggg	-9.80
1v2i	-10.30	3se8	-10.00	2wa1	-9.80
1v2i	-10.30	3rwi	-10.00	2ht5	-9.80
1ida	-10.30	3rwh	-10.00	1v3b	-9.80
4wm8	-10.20	3rwg	-10.00	1p9u	-9.80
4uo7	-10.20	3rwg	-10.00	4rw7	-9.70
4uo7	-10.20	3rwd	-10.00	4lsr	-9.70
4uo7	-10.20	3gsq	-10.00	4j4v	-9.70
4uo7	-10.20	3gsq	-10.00	4j4v	-9.70
4uo7	-10.20	3gso	-10.00	4j4v	-9.70
4uo7	-10.20	3fku	-10.00	4j4v	-9.70
4uo3	-10.20	2vww	-10.00	4j4v	-9.70
4uny	-10.20	2i4d	-10.00	4j4u	-9.70
4pv9	-10.20	1v3d	-10.00	4j4s	-9.70
4pv9	-10.20	1v3d	-10.00	4j4s	-9.70
4k7f	-10.20	1hhj	-10.00	4i2p	-9.70
4gua	-10.20	4uo0	-9.90	4gaj	-9.70
4cew	-10.20	4uo0	-9.90	4gag	-9.70
3rwe	-10.20	4uo0	-9.90	4gag	-9.70
3hkw	-10.20	4uo0	-9.90	4cey	-9.70
2i4w	-10.20	4uo0	-9.90	2vww	-9.70
4uo0	-10.10	4uo0	-9.90	2hty	-9.70
4uo0	-10.10	4uo0	-9.90	4unw	-9.60
4uo0	-10.10	4uo0	-9.90	4unw	-9.60
4m8x	-10.10	4uo0	-9.90	4unw	-9.60
4e5e	-10.10	4uo0	-9.90	4mza	-9.60
4cdu	-10.10	4uo0	-9.90	3s11	-9.60
3rwh	-10.10	4rw4	-9.90	3ava	-9.60
3r4b	-10.10	4opa	-9.90	3ava	-9.60
3ok9	-10.10	4cdx	-9.90	1pk0	-9.60
3kql	-10.10	4bac	-9.90	1izh	-9.60
3kql	-10.10	3sdy	-9.90	4uo3	-9.50
3kql	-10.10	3rwc	-9.90	4uo3	-9.50
3gsw	-10.10	3r4b	-9.90	4uo3	-9.50
3bev	-10.10	3n0i	-9.90	4uo3	-9.50
2wr2	-10.10	3n0i	-9.90	4uo3	-9.50
2wr2	-10.10	3gsr	-9.90	4rw6	-9.50
2wr2	-10.10	3bew	-9.90	4mza	-9.50
1idb	-10.10	4unx	-9.80	4mms	-9.50
1a41	-10.10	4unx	-9.80	4m8y	-9.50
4uo0	-10.00	4unx	-9.80	4m8y	-9.50
4uo0	-10.00	4unx	-9.80	4fqy	-9.50
4uo0	-10.00	4qhn	-9.80	3zp1	-9.50
4uo0	-10.00	4lst	-9.80	3t3c	-9.50
4lsu	-10.00	4cdq	-9.80	3rki	-9.50

PDB	Docking score	PDB	Docking score	PDB	Docking score
3ebj	-9.50	4fqi	-9.20	3zp2	-9.00
2i4x	-9.50	4ffz	-9.20	3zp0	-9.00
2hu4	-9.50	4dgd	-9.20	3nwa	-9.00
2hu4	-9.50	4cqy	-9.20	3nwa	-9.00
2hu4	-9.50	4cqs	-9.20	3mlh	-9.00
2hu4	-9.50	4bgz	-9.20	3ku3	-9.00
1v3c	-9.50	3zp6	-9.20	3ku3	-9.00
Spike RBD	-9.40	3o4l	-9.20	3klv	-9.00
4j4r	-9.40	2oy0	-9.20	3ggg	-9.00
4fqy	-9.40	2oy0	-9.20	3alx	-9.00
4fqv	-9.40	5ajm	-9.10	2xra	-9.00
4ej8	-9.40	5ajm	-9.10	2wrf	-9.00
4ej8	-9.40	5ajm	-9.10	4mj1	-8.90
4e5g	-9.40	5ajm	-9.10	4jo8	-8.90
4e5f	-9.40	5ajm	-9.10	4ejl	-8.90
4dag	-9.40	5ajm	-9.10	4egt	-8.90
4cqu	-9.40	4q6r	-9.10	4cqu	-8.90
4adf	-9.40	4q6r	-9.10	4cqu	-8.90
4adf	-9.40	4mmu	-9.10	4cqr	-8.90
4adf	-9.40	4mj0	-9.10	4cqr	-8.90
4adf	-9.40	4kps	-9.10	4cqq	-8.90
4adf	-9.40	4i2p	-9.10	4cqq	-8.90
4adf	-9.40	4g8g	-9.10	4cqq	-8.90
3t3c	-9.40	4g8g	-9.10	4cqp	-8.90
2xwy	-9.40	4e76	-9.10	4cqp	-8.90
1v3c	-9.40	4cr0	-9.10	4cqp	-8.90
1sk7	-9.40	4cqy	-9.10	4cqp	-8.90
1klm	-9.40	4cqs	-9.10	3ztn	-8.90
1hhh	-9.40	4bgx	-9.10	3nf9	-8.90
4o4g	-9.30	4bgx	-9.10	3nf9	-8.90
4mj1	-9.30	3zpb	-9.10	3nf7	-8.90
4m8x	-9.30	3zpb	-9.10	3nf7	-8.90
4jb9	-9.30	2zu5	-9.10	3nf6	-8.90
4gaj	-9.30	2wr7	-9.10	3nf6	-8.90
4cqu	-9.30	Main	-9.00	3d0h	-8.90
3alz	-9.30	protease	-9.00	3avg	-8.90
2wre	-9.30	4qhk	-9.00	2htw	-8.90
2wre	-9.30	4mmr	-9.00	2c36	-8.90
2wre	-9.30	4i7f	-9.00	2c36	-8.90
2wre	-9.30	4i2q	-9.00	4pv9	-8.80
2wre	-9.30	4fvu	-9.00	4gve	-8.80
2wre	-9.30	4fp8	-9.00	4cqz	-8.80
1izi	-9.30	4fp8	-9.00	4cqz	-8.80
4rw4	-9.20	4ejl	-9.00	4cqu	-8.80
4lsv	-9.20	4cqy	-9.00	4cqu	-8.80
4kpq	-9.20	4cqp	-9.00	4cqp	-8.80
4fqv	-9.20	4co6	-9.00	4bgw	-8.80
4fqj	-9.20	3zpa	-9.00	3v3m	-8.80

PDB	Docking score	PDB	Docking score	PDB	Docking score
3v3m	-8.80	3nf7	-8.50	4bh3	-8.20
3avh	-8.80	3nf7	-8.50	4bh3	-8.20
2vvx	-8.80	3avl	-8.50	4bh3	-8.20
2vvx	-8.80	3avb	-8.50	4bh3	-8.20
2hu0	-8.80	3avb	-8.50	3vbh	-8.20
1v3e	-8.80	2z35	-8.50	3sit	-8.20
1p9s	-8.80	2x83	-8.50	3rwj	-8.20
4uo6	-8.70	2wr3	-8.50	3rwj	-8.20
4uo6	-8.70	1v3e	-8.50	3lqa	-8.20
4m30	-8.70	1rzj	-8.50	3i6g	-8.20
4bh1	-8.70	4pv8	-8.40	3gsr	-8.20
4bgw	-8.70	4mgu	-8.40	3d0g	-8.20
3nfa	-8.70	4i32	-8.40	3avj	-8.20
3nfa	-8.70	4dgd	-8.40	3ava	-8.20
3nf8	-8.70	3nwf	-8.40	3ava	-8.20
3nf8	-8.70	3nf9	-8.40	2xi5	-8.20
3ku6	-8.70	3mj5	-8.40	2xi5	-8.20
3ku6	-8.70	3mj5	-8.40	4pv8	-8.10
3avn	-8.70	3ku5	-8.40	4f3z	-8.10
3avl	-8.70	3gsx	-8.40	3vbf	-8.10
2x83	-8.70	3gsx	-8.40	3vbf	-8.10
2wrc	-8.70	3gsv	-8.40	3sit	-8.10
2iph	-8.70	3gsv	-8.40	3sit	-8.10
2ghv	-8.70	2mgu	-8.40	3sit	-8.10
1r6a	-8.70	1rv7	-8.40	3sit	-8.10
4wm7	-8.60	1oop	-8.40	3ro5	-8.10
4qhl	-8.60	4mg3	-8.30	3oah	-8.10
4mj0	-8.60	4mds	-8.30	3nf6	-8.10
4g9f	-8.60	4i31	-8.30	3nf6	-8.10
4fqi	-8.60	4fb3	-8.30	2ghw	-8.10
4fqi	-8.60	4e5l	-8.30	4i2q	-8.00
4bh1	-8.60	3su0	-8.30	4gv3	-8.00
4bh1	-8.60	3nf9	-8.30	3uqi	-8.00
3zp3	-8.60	3ku5	-8.30	3uqi	-8.00
3s13	-8.60	3gsu	-8.30	3su6	-8.00
3nfa	-8.60	3gsu	-8.30	3avb	-8.00
3nf8	-8.60	3avf	-8.30	2zty	-8.00
3nf8	-8.60	1v3c	-8.30	2me2	-8.00
2iph	-8.60	1v3c	-8.30	2lsp	-8.00
2iph	-8.60	4mg3	-8.20	2ge8	-8.00
1b53	-8.60	4mds	-8.20	1v3b	-8.00
4qru	-8.50	4i31	-8.20	1n59	-8.00
4bgy	-8.50	4dgc	-8.20	4uo8	-7.90
3u82	-8.50	4dgc	-8.20	4gv3	-7.90
3u82	-8.50	4dgc	-8.20	4f3i	-7.90
3su0	-8.50	4dgc	-8.20	4eq0	-7.90
3se9	-8.50	4dgc	-8.20	4bh2	-7.90
3nfa	-8.50	4dgc	-8.20	4bh2	-7.90



PDB	Docking score	PDB	Docking score	PDB	Docking score
3su2	-7.90	2q7c	-7.50	4gv9	-7.00
3su2	-7.90	2q7c	-7.50	4g9z	-7.00
3avh	-7.90	2q7c	-7.50	4ejk	-7.00
2zol	-7.90	2iph	-7.50	3su2	-7.00
2hcn	-7.90	2c7u	-7.50	3kmq	-7.00
4oph	-7.80	1qz8	-7.50	2xze	-7.00
4f3i	-7.80	4iv1	-7.40	2q7c	-7.00
3sit	-7.80	4hkj	-7.40	2q7c	-7.00
3avc	-7.80	4gzf	-7.40	2q7c	-7.00
3avb	-7.80	4gzf	-7.40	1rq9	-7.00
2xya	-7.80	4eee	-7.40	4oyd	-6.90
2uv0	-7.80	4dkq	-7.40	4lkj	-6.90
2uv0	-7.80	3sv8	-7.40	4jpk	-6.90
2uv0	-7.80	3sis	-7.40	4dkr	-6.90
2uv0	-7.80	3rwf	-7.40	4dgb	-6.90
2uv0	-7.80	3alw	-7.40	4dgb	-6.90
2uv0	-7.80	2zu1	-7.40	3u83	-6.90
2uv0	-7.80	2yka	-7.40	3u83	-6.90
2uv0	-7.80	2ca1	-7.40	3su4	-6.90
2uv0	-7.80	4lss	-7.30	3su4	-6.90
2uv0	-7.80	4lsp	-7.30	3s12	-6.90
2uv0	-7.80	4dkp	-7.30	3pqy	-6.90
2uv0	-7.80	3uf5	-7.30	3gsw	-6.90
2ge7	-7.80	3m5h	-7.30	2xpx	-6.90
4eq0	-7.70	3d0i	-7.30	2g69	-6.90
4e5j	-7.70	3bwa	-7.30	2g69	-6.90
4bh4	-7.70	2q5u	-7.30	1rpi	-6.90
3sud	-7.70	2q5u	-7.30	4nwk	-6.80
3su1	-7.70	2q5u	-7.30	4jpk	-6.80
3sis	-7.70	2q5u	-7.30	4jpk	-6.80
3avk	-7.70	2q5u	-7.30	4jpk	-6.80
2zu4	-7.70	4e92	-7.20	4ejd	-6.80
2vvy	-7.70	4e92	-7.20	4ejd	-6.80
4qrt	-7.60	4dko	-7.20	4ejd	-6.80
4iv3	-7.60	3rwi	-7.20	4e91	-6.80
4g9z	-7.60	2q5u	-7.20	4e5i	-6.80
4cqy	-7.60	2axf	-7.20	3su6	-6.80
4bh4	-7.60	2axf	-7.20	3b71	-6.80
4bh4	-7.60	1rzk	-7.20	2xze	-6.80
4bh4	-7.60	4u6h	-7.10	2xpx	-6.80
3nw8	-7.60	4qrt	-7.10	2bvq	-6.80
1sys	-7.60	4ejk	-7.10	4nwk	-6.70
Papain protease	-7.50	3w39	-7.10	4ep3	-6.70
4qrt	-7.50	2ztz	-7.10	3gsn	-6.70
4j6r	-7.50	2gvf	-7.10	3b71	-6.70
3rwf	-7.50	1f08	-7.10	2wh6	-6.70
3avg	-7.50	1b50	-7.10	1zsd	-6.70
		4oyd	-7.00	1rpi	-6.70

PDB	Docking score	PDB	Docking score	PDB	Docking score
4ffv	-6.60	2vxw	-6.20	2mkr	-5.30
4epj	-6.60	4mmt	-6.10	2hfv	-5.30
4ep3	-6.60	4i33	-6.10	4ipz	-5.10
4ejr	-6.60	4gye	-6.10	4ipz	-5.10
4dmn	-6.60	4ekx	-6.10	4g8i	-5.10
4dmn	-6.60	4b4n	-6.10	4g8i	-5.10
4dga	-6.60	4b4n	-6.10	1qr8	-5.10
3su1	-6.60	2c3a	-6.10	2vxj	-5.00
3gzf	-6.60	4b8e	-6.00	4g9d	-4.90
2yol	-6.60	4b8e	-6.00	4ep2	-4.80
2yol	-6.60	4b8e	-6.00	4ipz	-4.70
2wh6	-6.60	3zd0	-6.00	4ipz	-4.70
4dga	-6.50	3vie	-6.00	4g9d	-4.70
3avj	-6.50	3p8o	-6.00	3j23	-4.70
2wfo	-6.50	3avk	-6.00	3j22	-4.70
2v6q	-6.50	2c86	-6.00	2me3	-4.70
2me4	-6.50	4c1w	-5.90	4eqj	-4.50
2m3l	-6.50	3sv9	-5.90	4ep2	-4.50
4gye	-6.40	3sv6	-5.90	4ipz	-4.40
4ejd	-6.40	3su5	-5.90	4ipz	-4.20
4ejd	-6.40	3su5	-5.90	2l3h	-4.00
4ejd	-6.40	3su5	-5.90	4ipz	-3.80
4c1w	-6.40	3kqk	-5.90	4ipz	-3.80
3suf	-6.40	2y1s	-5.90	4qhm	-3.60
3su3	-6.40	4mod	-5.80	4epj	-3.60
3su3	-6.40	4mod	-5.80	4ipz	-3.40
3kms	-6.40	2yhh	-5.80	4ipz	-3.40
3ifu	-6.40	2l2f	-5.80	4gu4	-2.70
2wfo	-6.40	4nwl	-5.70	4gu4	-2.70
1qr9	-6.40	4ipz	-5.70	4gu4	-2.70
3rkc	-6.30	4ipz	-5.70	4gu4	-2.70
3p8n	-6.30	3sv7	-5.70	4gu4	-2.60
3oah	-6.30	3sug	-5.70	4gu4	-2.60
3a07	-6.30	3sug	-5.70	3m5i	-2.40
1yh3	-6.30	3sud	-5.70	4gu3	-1.80
4mze	-6.20	2x9m	-5.70	4gu3	-1.80
4mze	-6.20	4mmv	-5.60	4gu3	-1.80
4ejd	-6.20	4ejk	-5.60	4gu3	-1.80
4ejd	-6.20	3sv6	-5.60	4gu3	-1.80
4ejd	-6.20	3i6k	-5.60	4gu3	-1.80
3vie	-6.20	3avc	-5.60	4gu3	-1.80
3sv9	-6.20	1z8r	-5.60	4gu3	-1.80
3sv7	-6.20	4adq	-5.50	4gu3	-1.80
3sue	-6.20	4uo4	-5.40	4gu3	-1.80
3giv	-6.20	4adq	-5.40	4gu3	-1.80
3avn	-6.20	3vtt	-5.40	4gu3	-1.70
2zu3	-6.20	3vtt	-5.40	4dge	-1.70
2yhf	-6.20	2m3m	-5.40	2zsv	-1.40

<b>PDB</b>	<b>Docking score</b>
2zsv	-1.30
4e0r	-0.70

<b>PDB</b>	<b>Docking score</b>
4fqm	-0.10

**Table S12.** Predicted docking score of Rutin against the viral protein panel

PDB	Docking score	PDB	Docking score	PDB	Docking score
3kql	-12.10	3bev	-10.50	4mk8	-10.00
3kql	-12.10	4lsr	-10.40	4jkp	-10.00
3kql	-12.10	4j4v	-10.40	4jkp	-10.00
4uny	-11.20	4fqr	-10.40	4g42	-10.00
3koa	-11.00	4fqr	-10.40	4ejl	-10.00
4e7a	-10.90	4e78	-10.40	3u7s	-10.00
4e7a	-10.90	4e78	-10.40	3u7s	-10.00
3t3c	-10.90	3kqn	-10.40	3cj4	-10.00
3fku	-10.90	3ggg	-10.40	3cj2	-10.00
4lsv	-10.80	4uo7	-10.30	2wr1	-10.00
3se8	-10.80	4uo7	-10.30	2wr1	-10.00
3se8	-10.80	4uo7	-10.30	2wr1	-10.00
4uo2	-10.70	4uo7	-10.30	1syv	-10.00
4uo2	-10.70	4uo7	-10.30	1pk0	-10.00
4uo2	-10.70	4uo3	-10.30	1idb	-10.00
4uo2	-10.70	4uo3	-10.30	4mk7	-9.90
4uo2	-10.70	4uo3	-10.30	4jb9	-9.90
4uo2	-10.70	4uo3	-10.30	4j4x	-9.90
4uo0	-10.70	4uo3	-10.30	3rwc	-9.90
4uo0	-10.70	4rw6	-10.30	3rwc	-9.90
4uo0	-10.70	4j4s	-10.30	3cj0	-9.90
4uo0	-10.70	4j4s	-10.30	4uo0	-9.80
4j4u	-10.70	3s11	-10.30	4rw4	-9.80
4fnk	-10.70	3b0w	-10.30	4rw4	-9.80
3t3c	-10.70	2hty	-10.30	4pv9	-9.80
4uo0	-10.60	4uo3	-10.20	4mk7	-9.80
4uo0	-10.60	4uo3	-10.20	4lst	-9.80
4uo0	-10.60	4fvu	-10.20	4ejl	-9.80
4uo0	-10.60	4e5g	-10.20	2ygc	-9.80
4uo0	-10.60	3ggg	-10.20	2bvo	-9.80
4uo0	-10.60	2wrg	-10.20	2axg	-9.80
4uo0	-10.60	1p9u	-10.20	1hhh	-9.80
4uo0	-10.60	4uo7	-10.10	4rw9	-9.70
4uo0	-10.60	4mkb	-10.10	4rw7	-9.70
4uo0	-10.60	4j6r	-10.10	4mka	-9.70
4uo0	-10.60	4j4y	-10.10	4mk8	-9.70
4uo0	-10.60	4j4v	-10.10	4j4r	-9.70
4j4w	-10.60	4j4v	-10.10	4e76	-9.70
3nxu	-10.60	4j4v	-10.10	4e5e	-9.70
4unw	-10.50	4j4v	-10.10	4adf	-9.70
4unw	-10.50	3kqh	-10.10	4adf	-9.70
4unw	-10.50	3bew	-10.10	4adf	-9.70
4fnk	-10.50	2hu0	-10.10	4adf	-9.70
3kqn	-10.50	4uo5	-10.00	4adf	-9.70
3kqn	-10.50	4uo5	-10.00	4adf	-9.70
3kna	-10.50	4uo5	-10.00	3lkh	-9.70

PDB	Docking score	PDB	Docking score	PDB	Docking score
3lkh	-9.70	2hcs	-9.50	3hkw	-9.30
3gsw	-9.70	2bvp	-9.50	3h98	-9.30
3ebj	-9.70	1quv	-9.50	3gsw	-9.30
3cj2	-9.70	1izi	-9.50	3gsv	-9.30
3bwa	-9.70	4uo3	-9.40	3gsq	-9.30
2ygc	-9.70	4uo3	-9.40	3gsq	-9.30
2wr2	-9.70	4uo3	-9.40	2xra	-9.30
2wr2	-9.70	4qrs	-9.40	2wre	-9.30
2wr2	-9.70	4qrs	-9.40	2wre	-9.30
4pg2	-9.60	4opa	-9.40	2wre	-9.30
4o44	-9.60	4mk9	-9.40	2wre	-9.30
4lsu	-9.60	4m8x	-9.40	2i4w	-9.30
4fqj	-9.60	4gua	-9.40	2hjk	-9.30
3rwg	-9.60	4g9f	-9.40	2ghw	-9.30
3rwg	-9.60	4g8g	-9.40	2gec	-9.30
3r4b	-9.60	4g8g	-9.40	1v2i	-9.30
3r4b	-9.60	4cey	-9.40	1v2i	-9.30
3iyw	-9.60	4cew	-9.40	5ajm	-9.20
3iyw	-9.60	4a92	-9.40	4wm7	-9.20
3iyw	-9.60	3vbr	-9.40	4unx	-9.20
3iyw	-9.60	3vbo	-9.40	4unx	-9.20
3iyw	-9.60	3rwi	-9.40	4unx	-9.20
3iyw	-9.60	3klv	-9.40	4unx	-9.20
3hkw	-9.60	3h98	-9.40	4qru	-9.20
3cj4	-9.60	3gsv	-9.40	4qru	-9.20
2ygb	-9.60	3cj5	-9.40	4o4g	-9.20
2ygb	-9.60	3ciz	-9.40	4mgu	-9.20
2ht5	-9.60	3ciz	-9.40	4m8y	-9.20
1r6a	-9.60	2wre	-9.40	4m8y	-9.20
Main protease	-9.50	2i4x	-9.40	4lkj	-9.20
4rw8	-9.50	2i4v	-9.40	4i2p	-9.20
4q6r	-9.50	2i4u	-9.40	4gaj	-9.20
4q6r	-9.50	1v3d	-9.40	4gaj	-9.20
4mms	-9.50	1v3d	-9.40	4g9z	-9.20
4mkb	-9.50	1hhi	-9.40	4fqv	-9.20
4mka	-9.50	4wm8	-9.30	4bh2	-9.20
4mk9	-9.50	4i2q	-9.30	4bh2	-9.20
4m30	-9.50	4gag	-9.30	3v3m	-9.20
4m8x	-9.50	4gag	-9.30	3tid	-9.20
4lsu	-9.50	4fp8	-9.30	3rwh	-9.20
4g43	-9.50	4fp8	-9.30	3rwh	-9.20
4fqj	-9.50	4f3z	-9.30	3gsu	-9.20
3ztj	-9.50	4e5f	-9.30	3gsr	-9.20
3vcl	-9.50	3v3m	-9.30	3bwa	-9.20
3gso	-9.50	3u82	-9.30	3bw9	-9.20
3cj3	-9.50	3u82	-9.30	3alz	-9.20
3cj0	-9.50	3rwd	-9.30	2wrh	-9.20
2i4d	-9.50	3i6l	-9.30	2wrg	-9.20

PDB	Docking score	PDB	Docking score	PDB	Docking score
2wrg	-9.20	4fqy	-9.00	4mj1	-8.80
2wrg	-9.20	4fb3	-9.00	4i7f	-8.80
2wrg	-9.20	4cdw	-9.00	4gu3	-8.80
2wre	-9.20	4bgx	-9.00	4gu3	-8.80
2wr0	-9.20	4bac	-9.00	4gu3	-8.80
2hu4	-9.20	3vcl	-9.00	4gu3	-8.80
2hu4	-9.20	3sdy	-9.00	4dgb	-8.80
2hu4	-9.20	3sdy	-9.00	4cqW	-8.80
2hu4	-9.20	3sdy	-9.00	4cdx	-8.80
2htw	-9.20	3bw9	-9.00	3ku6	-8.80
2gec	-9.20	3avf	-9.00	3ku6	-8.80
1klm	-9.20	2xi5	-9.00	3ku3	-8.80
5ajm	-9.10	2xi5	-9.00	2wr7	-8.80
4kps	-9.10	2wrf	-9.00	1v3e	-8.80
4k7f	-9.10	1ida	-9.00	1v3c	-8.80
4k7f	-9.10	1hhk	-9.00	1v3c	-8.80
4g9f	-9.10	5ajm	-8.90	1v3c	-8.80
4fqy	-9.10	4qhk	-8.90	1v3c	-8.80
4fqv	-9.10	4mmu	-8.90	1sk7	-8.80
4bh4	-9.10	4gu4	-8.90	1n5a	-8.80
4bh4	-9.10	4gu4	-8.90	1a41	-8.80
4bh4	-9.10	4gu4	-8.90	4qru	-8.70
3rwe	-9.10	4gu4	-8.90	4mds	-8.70
3rwe	-9.10	4gu4	-8.90	4kpp	-8.70
3n0i	-9.10	4gu4	-8.90	4ej8	-8.70
3n0i	-9.10	4gu3	-8.90	4ej8	-8.70
3ku3	-9.10	4gu3	-8.90	4egt	-8.70
3h2l	-9.10	4gu3	-8.90	4cqz	-8.70
3h2l	-9.10	4gu3	-8.90	4cqr	-8.70
3gsu	-9.10	4gu3	-8.90	4bh0	-8.70
3gso	-9.10	4gu3	-8.90	4a92	-8.70
3d23	-9.10	4gu3	-8.90	3vbf	-8.70
3d23	-9.10	4gu3	-8.90	3tid	-8.70
3cj5	-9.10	4cqs	-8.90	3gsx	-8.70
3cj3	-9.10	4cqs	-8.90	3gsx	-8.70
2wr4	-9.10	4cdU	-8.90	3gsr	-8.70
2wr0	-9.10	4cdq	-8.90	3alx	-8.70
2wr0	-9.10	4bgx	-8.90	2oy0	-8.70
2wr0	-9.10	3ok9	-8.90	4uo8	-8.60
2wa1	-9.10	3oah	-8.90	4mj0	-8.60
1rzj	-9.10	3nf8	-8.90	4mds	-8.60
1hhj	-9.10	3nf8	-8.90	4dgb	-8.60
4uo0	-9.00	3mlh	-8.90	4dag	-8.60
4jo8	-9.00	3hkw	-8.90	4cqV	-8.60
4hkj	-9.00	2wr0	-8.90	4cqp	-8.60
4gv3	-9.00	2hcn	-8.90	4cqp	-8.60
4gv3	-9.00	1v3e	-8.90	4cqp	-8.60
4g9z	-9.00	1izh	-8.90	4bgw	-8.60

PDB	Docking score	PDB	Docking score	PDB	Docking score
4bgw	-8.60	3rwf	-8.40	2c36	-8.20
3zp6	-8.60	3rwf	-8.40	2c36	-8.20
3zp2	-8.60	3lqa	-8.40	1oop	-8.20
3zp1	-8.60	3i6g	-8.40	1f08	-8.20
3vbh	-8.60	2wr3	-8.40	4qhl	-8.10
3vbf	-8.60	2htu	-8.40	4mza	-8.10
3oah	-8.60	1p9s	-8.40	4mza	-8.10
3hky	-8.60	4qhn	-8.30	4mmr	-8.10
3hky	-8.60	4gve	-8.30	4mg3	-8.10
2x83	-8.60	4e5l	-8.30	4eee	-8.10
2oy0	-8.60	4bh3	-8.30	4dgc	-8.10
4pv9	-8.50	3ztn	-8.30	4dgc	-8.10
4pv9	-8.50	3rki	-8.30	4dgc	-8.10
4pv8	-8.50	3o4l	-8.30	4dgc	-8.10
4i2p	-8.50	3nwf	-8.30	4dgc	-8.10
4ffz	-8.50	3nwa	-8.30	4dgc	-8.10
4cr0	-8.50	3nwa	-8.30	4cqz	-8.10
4cqx	-8.50	3nf9	-8.30	3sis	-8.10
4cqy	-8.50	3nf9	-8.30	3s13	-8.10
4cqy	-8.50	3nf6	-8.30	3rwj	-8.10
4cqy	-8.50	3nf6	-8.30	3rwj	-8.10
4cqp	-8.50	3mj5	-8.30	3nf6	-8.10
4bh4	-8.50	3ku5	-8.30	3nf6	-8.10
3zpb	-8.50	3ku5	-8.30	3d0h	-8.10
3zpb	-8.50	3cpl	-8.30	3cpl	-8.10
3zp0	-8.50	3bwa	-8.30	3avb	-8.10
3tie	-8.50	3ava	-8.30	2zty	-8.10
3tie	-8.50	3ava	-8.30	2z35	-8.10
3nw8	-8.50	2wrc	-8.30	2uv0	-8.10
2vww	-8.50	4cqu	-8.20	2uv0	-8.10
1v3b	-8.50	4cqu	-8.20	2uv0	-8.10
1r6a	-8.50	4cqu	-8.20	2uv0	-8.10
5ajm	-8.40	4cqu	-8.20	2uv0	-8.10
5ajm	-8.40	4cqu	-8.20	2uv0	-8.10
5ajm	-8.40	4cqu	-8.20	2uv0	-8.10
4f3i	-8.40	4bh1	-8.20	2uv0	-8.10
4f3i	-8.40	4bh1	-8.20	2uv0	-8.10
4e5j	-8.40	4bh1	-8.20	2uv0	-8.10
4dgd	-8.40	3nf9	-8.20	2uv0	-8.10
4cqp	-8.40	3nf9	-8.20	1v3b	-8.10
4cqp	-8.40	3d0g	-8.20	1rv7	-8.10
4bh3	-8.40	3avg	-8.20	4u6h	-8.00
4bh3	-8.40	3avb	-8.20	4pv8	-8.00
4bh3	-8.40	3avb	-8.20	4mj1	-8.00
4bgy	-8.40	3alw	-8.20	4co6	-8.00
3zpa	-8.40	2zu5	-8.20	3nfa	-8.00
3zp3	-8.40	2zu1	-8.20	3nf7	-8.00
3se9	-8.40	2xwy	-8.20	3avl	-8.00

PDB	Docking score	PDB	Docking score	PDB	Docking score
3avh	-8.00	3kms	-7.70	3sv6	-7.30
3avb	-8.00	2iph	-7.70	3su2	-7.30
3ava	-8.00	2axf	-7.70	3rkc	-7.30
2zu4	-8.00	1n59	-7.70	3kmq	-7.30
2uv0	-8.00	4gye	-7.60	3avj	-7.30
1sys	-8.00	4gv9	-7.60	2xze	-7.30
1rzk	-8.00	3su6	-7.60	2vvx	-7.30
4fqi	-7.90	3rwi	-7.60	2mgu	-7.30
4fqi	-7.90	3nfa	-7.60	2ghv	-7.30
4dgd	-7.90	3nfa	-7.60	1qz8	-7.30
4cqr	-7.90	3nf8	-7.60	Spike RBD	-7.20
3nf7	-7.90	3avg	-7.60	Papain protease	-7.20
3ava	-7.90	2lsp	-7.60	4qrt	-7.20
2yka	-7.90	4mj0	-7.50	4i33	-7.20
2vvx	-7.90	4iv1	-7.50	4i32	-7.20
2vww	-7.90	4dkq	-7.50	4i31	-7.20
2axf	-7.90	3suf	-7.50	4gzf	-7.20
1b50	-7.90	3sud	-7.50	4g9d	-7.20
4mg3	-7.80	3su2	-7.50	4eq0	-7.20
4ffy	-7.80	3su2	-7.50	4dco	-7.20
4ekx	-7.80	3su0	-7.50	3sv8	-7.20
4e92	-7.80	3nf8	-7.50	3sud	-7.20
4cqy	-7.80	3ifu	-7.50	3avk	-7.20
4bgz	-7.80	3gsw	-7.50	3avc	-7.20
3su0	-7.80	2wh6	-7.50	2yhf	-7.20
3sit	-7.80	2vvy	-7.50	1yh3	-7.20
3sit	-7.80	2iph	-7.50	4i31	-7.10
3sit	-7.80	2iph	-7.50	3sv9	-7.10
3sit	-7.80	1b53	-7.50	3sv7	-7.10
3sit	-7.80	4oyd	-7.40	3gsn	-7.10
3pqy	-7.80	4oph	-7.40	3a07	-7.10
3nfa	-7.80	4eq0	-7.40	2xya	-7.10
3nf7	-7.80	4e5i	-7.40	2wh6	-7.10
3nf7	-7.80	4dkr	-7.40	2ge7	-7.10
3avl	-7.80	3w39	-7.40	2ca1	-7.10
3avh	-7.80	3sv7	-7.40	3sis	-7.00
3avc	-7.80	3su1	-7.40	3p8o	-7.00
2x83	-7.80	3avn	-7.40	2xze	-7.00
2iph	-7.80	2ge8	-7.40	2wfo	-7.00
4uo6	-7.70	2c7u	-7.40	4qrt	-6.90
4uo6	-7.70	2bvq	-7.40	4nwk	-6.90
4qrt	-7.70	4iv3	-7.30	4mmt	-6.90
4mze	-7.70	4e91	-7.30	4lsp	-6.90
4mze	-7.70	4dkp	-7.30	4ejk	-6.90
4jpk	-7.70	4b8e	-7.30	3sv9	-6.90
4gye	-7.70	4b8e	-7.30	3sug	-6.90
4e92	-7.70	4b8e	-7.30	3sug	-6.90
3ro5	-7.70	3uf5	-7.30	3su3	-6.90



PDB	Docking score	PDB	Docking score	PDB	Docking score
3su3	-6.90	4ejd	-6.30	4b4n	-5.70
4eqj	-6.80	4ejd	-6.30	3kqk	-5.70
4ep3	-6.80	3sv6	-6.30	2yhh	-5.70
4ep3	-6.80	3su6	-6.30	4ipz	-5.60
4dga	-6.80	3su1	-6.30	4g9d	-5.60
4c1w	-6.80	2m3l	-6.30	2zol	-5.60
4c1w	-6.80	2gvf	-6.30	2y1s	-5.60
3sue	-6.80	2c3a	-6.30	2vxj	-5.60
3mj5	-6.80	4oyd	-6.20	1qr9	-5.60
3gzf	-6.80	4ejd	-6.20	4ipz	-5.50
2yol	-6.80	4dmn	-6.20	4ipz	-5.40
2yol	-6.80	3su5	-6.20	2m3m	-5.40
4gzf	-6.70	3su5	-6.20	1qr8	-5.40
4dga	-6.70	3su5	-6.20	4ejr	-5.30
3uqi	-6.70	3sit	-6.20	4ipz	-5.20
3p8n	-6.70	3avn	-6.20	4ipz	-5.20
2v6q	-6.70	2zu3	-6.20	4ipz	-5.20
2q5u	-6.70	4g8i	-6.10	3avk	-5.20
2q5u	-6.70	4ejk	-6.10	4ipz	-5.10
2hfz	-6.70	4ejk	-6.10	4ipz	-5.10
4mmv	-6.60	4ejd	-6.10	4ipz	-5.10
4jpi	-6.60	4ejd	-6.10	4ipz	-5.10
3u83	-6.60	3vie	-6.10	1zsd	-5.10
3u83	-6.60	3avj	-6.10	4mod	-4.80
2vxw	-6.60	2ztz	-6.10	4mod	-4.80
2q5u	-6.60	2xpx	-6.10	4adq	-4.80
2q5u	-6.60	2xpx	-6.10	3zd0	-4.80
2q5u	-6.60	2g69	-6.10	3vtt	-4.80
2q5u	-6.60	4nwk	-6.00	4adq	-4.70
4uo4	-6.50	4ejd	-6.00	3vtt	-4.60
4lss	-6.50	3vie	-6.00	3i6k	-4.60
4epj	-6.50	2q7c	-6.00	2me3	-4.60
3uqi	-6.50	2q7c	-6.00	2mkr	-4.50
3su4	-6.50	2q7c	-6.00	4ep2	-4.40
3su4	-6.50	2me2	-6.00	2x9m	-4.40
3m5h	-6.50	2l2f	-6.00	4g8i	-4.30
2q7c	-6.50	2g69	-6.00	4epj	-4.30
2q7c	-6.50	4ejd	-5.90	2me4	-4.30
2q7c	-6.50	2c86	-5.90	1hhg	-4.20
1rpi	-6.50	1z8r	-5.90	2l3h	-4.10
4nwl	-6.40	1rpi	-5.90	4ep2	-3.80
4dmn	-6.40	3s12	-5.80	4lkk	-3.70
3d0i	-6.40	3giv	-5.80	3j23	-3.70
2wfo	-6.40	3b71	-5.80	3j22	-3.70
1rq9	-6.40	3b71	-5.80	4qhm	-3.20
4i2q	-6.30	4ipz	-5.70	4g2k	-3.20
4ejd	-6.30	4ipz	-5.70	4lki	-3.00
4ejd	-6.30	4b4n	-5.70	4g1l	-2.80

<b>PDB</b>	<b>Docking score</b>
4lkh	-2.70
4g1g	-2.70
4lcx	-2.40
4kol	-1.90
4dge	-1.10
4g2k	-0.90
2zsv	-0.80
4kon	-0.70
2zsv	-0.70
4e0r	-0.30
4kom	-0.20
4g1o	-0.10
4fqm	-0.10