表五　Serine protease 家族系列之抑制劑與登革熱NS3 protease其分子接合排名的結果

Rank	Title	Lig#	Conf#	Pose#	Score	GScore	E(Cvdw)	Eintern	Emodel	Ehbond	Emetal	Eclash	E(Coul)	E(vdW)	RMSD
1	dengue_NS2A/2B	2	174	193	-5.97	-5.97	-53.2	25.9	-104.1	-4	0	0.1	-24.6	-28.5	--
2	1a5g_BIC	9	130	346	-7.12	-7.12	-43.6	10.4	-71.5	-3.6	0	0	-11.2	-32.4	--
3	1ba8_4res	20	328	372	-8.2	-8.2	-44.8	8.9	-70.3	-5.4	0	0	-13.6	-31.1	--
4	1dy9_BOC	54	225	58	-7.38	-7.38	-50.8	19.1	-69.7	-4.7	0	0.2	-20.1	-30.7	--
5	1abj_PHE	10	301	121	-5.02	-5.02	-38.1	5.8	-64.7	-3.2	0	0.1	-12	-26.1	--
6	1hpg_5res	49	489	383	-6.87	-6.87	-46.3	10.8	-62.6	-3.4	0	0	-14.1	-32.2	--
7	MbBBI	55	867	135	-5.48	-5.48	-51.2	10.7	-61.7	-2.3	0	0.3	-13.7	-37.5	--
8	1a4w_4res	7	595	383	-7.16	-7.16	-46.1	13.7	-61.5	-2.8	0	0	-10.4	-35.6	--
9	1bmm_BM2	34	658	111	-6.92	-6.92	-45.4	9.3	-59.8	-4.7	0	0	-16.2	-29.2	--
10	1dy8	53	303	374	-6.85	-6.85	-48.5	13.3	-59.1	-3.1	0	0	-10.7	-37.8	--
11	1bmm_BM9	35	224	355	-8.08	-8.08	-42.1	5.4	-55.3	-4.5	0	0	-16.4	-25.7	--
12	1a46_4res	6	403	305	-7.54	-7.54	-43.4	15.8	-54.8	-3.2	0	0	-14.1	-29.3	--
13	1awg_GR3	16	250	171	-8.82	-8.82	-40.4	8.8	-54.6	-5.2	0	0	-14.8	-25.6	--
14	1aq7_AEB	13	924	137	-5.96	-5.96	-43.3	56.9	-49.5	-3.7	0	0	-15.7	-27.6	--
15	1bhx_5res	26	293	377	-6.38	-6.38	-34.9	6	-49.2	-4.7	0	0.2	-12.4	-22.5	--
16	1bjv_GB8	33	35	182	-6.11	-6.11	-35.9	2.3	-48	-1.2	0	0	-7.6	-28.3	--
17	1awf_GR4	15	348	350	-5.53	-5.53	-39.6	16.6	-47.1	-1.5	0	0	-15.9	-23.7	--
18	1b5g_3res	19	261	361	-5.79	-5.79	-31.5	8.5	-47	-1.3	0	0	-3.9	-27.6	--
19	1eb1_3res	44	415	277	-7.9	-7.9	-36	12.6	-46.4	-6.4	0	0	-12.5	-23.5	--
20	1c1w_BAH	41	6	237	-7.04	-7.04	-32.8	2.7	-43.8	-4	0	0	-11.2	-21.6	--
21	1c2d_BAK	43	2	207	-6.26	-6.26	-29.6	1.8	-40.8	-3.8	0	0	-7.3	-22.3	--
22	1ae8_AZL	11	304	202	-6.09	-6.09	-35.7	14.7	-39.8	-4	0	0.1	-15.8	-19.9	--
23	1az8_IN4	18	111	78	-6.21	-6.21	-32.1	5.9	-39.4	-2.5	0	0	-8.5	-23.6	--
24	1o2g_696	50	1	70	-5.75	-5.75	-28.2	0.1	-39	-1.2	0	0	-4	-24.2	--
25	1c1s_BAB	40	1	199	-7.05	-7.05	-27.7	0	-38	-2	0	0	-7.9	-19.8	--
26	1c1p_BAI	39	7	369	-5.86	-5.86	-29	0.9	-37.8	-1	0	0	-2.4	-26.5	--
27	1gi5_123	29	2	275	-5.46	-5.46	-29.8	0.9	-37.7	-1	0	0	-7.1	-22.7	--
28	1gi7_120	31	2	195	-6.46	-6.46	-29.4	1.6	-37.7	-1.9	0	0	-6.1	-23.3	--
29	1gi6_124	30	1	235	-5.8	-5.8	-28.9	0.2	-37.2	-1.2	0	0	-6.4	-22.4	--
30	1gi0_BMZ	27	1	398	-6.29	-6.29	-28.5	1.2	-37	-1.9	0	0	-5.8	-22.8	--
31	1c1w_TYS	42	45	138	-5.83	-5.83	-32.4	7	-36.5	-2.8	0	0.3	-13.2	-19.2	--
32	1gi2_122	28	1	357	-6.08	-6.08	-26.4	0.1	-36	-1.7	0	0.3	-5.8	-20.7	--
33	1bju_GB6	32	10	163	-4.96	-4.96	-28.5	1.6	-35.9	-1.1	0	0	-6.2	-22.2	--
34	1eb2_BPO	45	103	262	-5.3	-5.3	-28.1	3.3	-35.8	-1.3	0	0	-6.6	-21.5	--
35	1aht_APA	12	8	86	-5.62	-5.62	-29.3	2	-35.2	-2.7	0	0	-13.6	-15.7	--
36	1ay6_4res	17	570	173	-2.91	-2.91	-26.4	17.5	-34.4	-2.5	0	0.1	-8.5	-17.9	--
37	1rt1_MKC	1	20	395	-5.64	-5.64	-29	4.6	-33.7	-1.7	0	0	-5.4	-23.6	--
38	1gj4_132	47	3	346	-5.3	-5.3	-25.3	0.3	-33.3	-0.8	0	0	-1.8	-23.5	--
39	1bcr_AIP	23	52	293	-6.71	-6.71	-28.7	15.4	-31.8	-6.6	0	0.1	-16.1	-12.6	--
40	1bcu_PRL	25	1	287	-5.16	-5.16	-25.1	0	-31.6	-0.9	0	0	-3	-22.1	--
41	1c2k_ABI	52	1	125	-5.5	-5.5	-22.7	0	-29.3	-1.2	0	0.1	-4.5	-18.2	--
42	1tng_AMA	51	1	91	-3.76	-3.76	-18.8	0.7	-28.4	-1.9	0	0	-5.1	-13.7	--
43	1gbt_GBS	46	5	317	-5.46	-5.46	-18.7	3	-22.6	-2.3	0	0	-5.4	-13.4	--
44	1c1n_BAM	38	1	2	-5.8	-5.8	-17.9	0.9	-22.4	-2.1	0	0	-4.6	-13.3	--