

Potential Compounds Interacting in a Specific Potential Site in SARS-CoV-2 Variants, Selected by Molecular Docking

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Supplementary Information

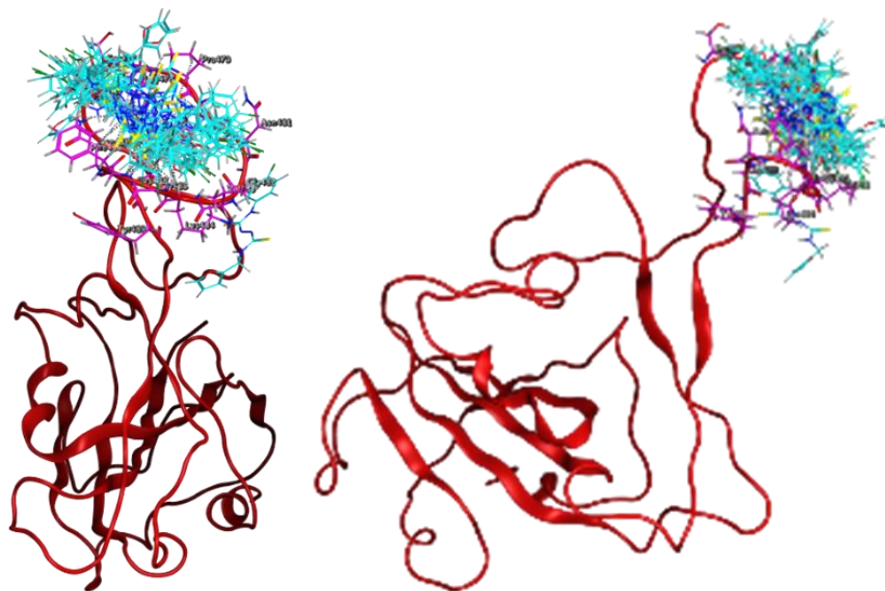


Fig. S1. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V1 (cyan).

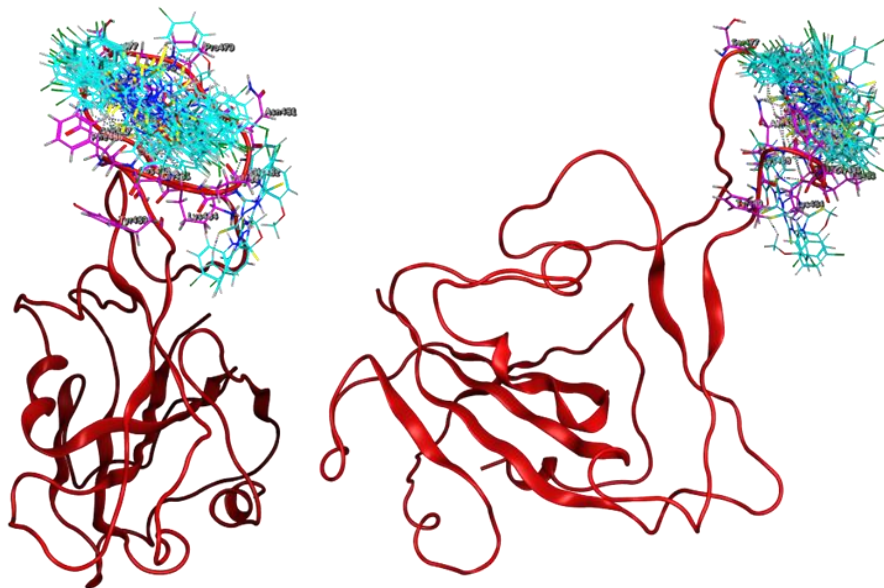


Fig. S2. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V2 (cyan).

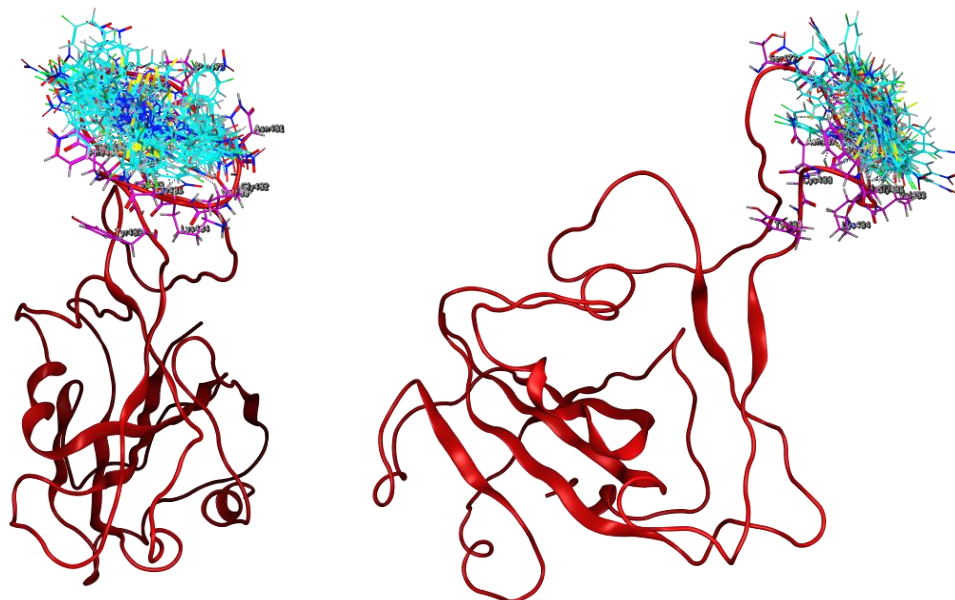


Fig. S3. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V3 (cyan).

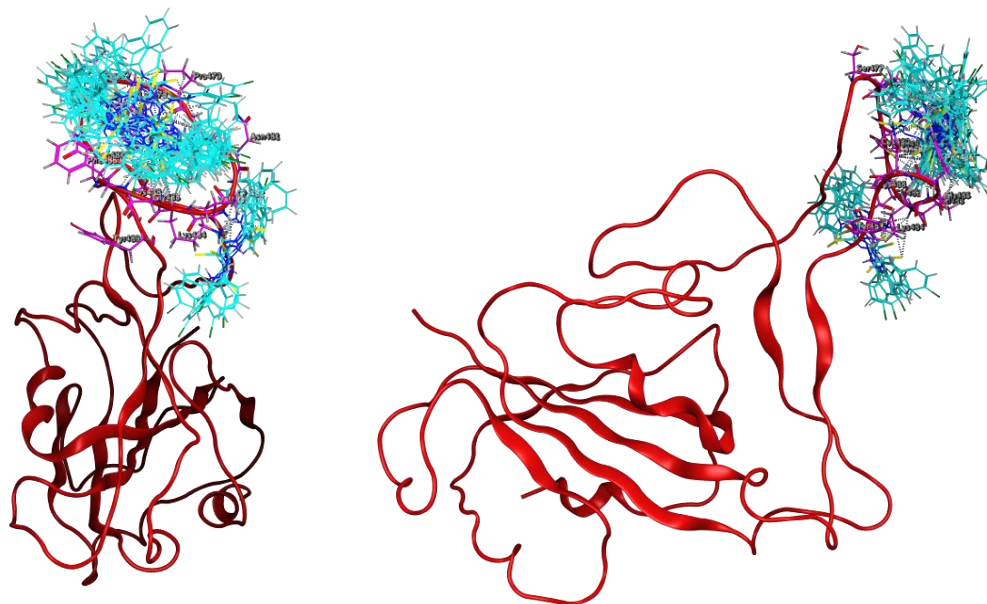


Fig. S4. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V4 (cyan).

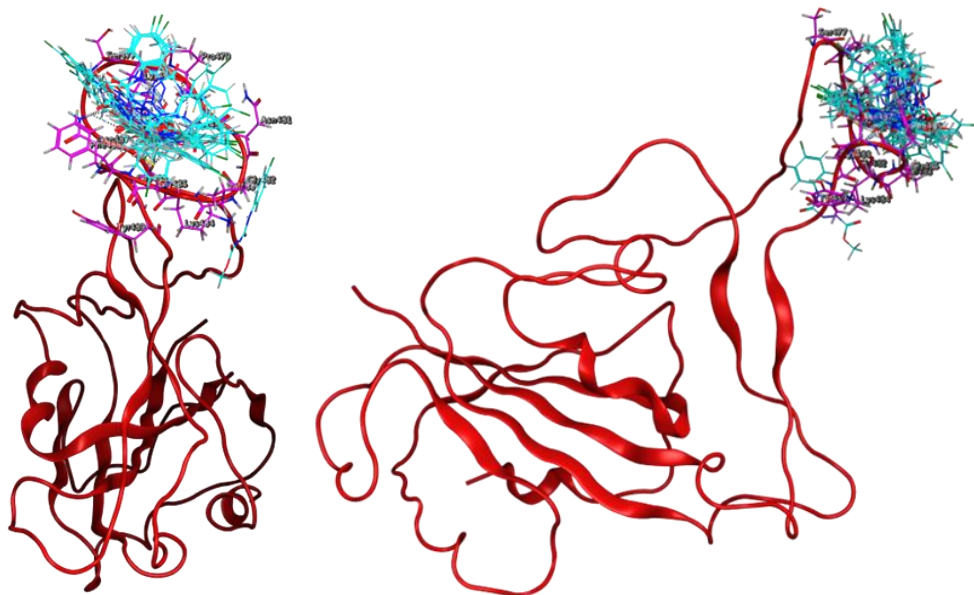


Fig. S5. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V5 (cyan).

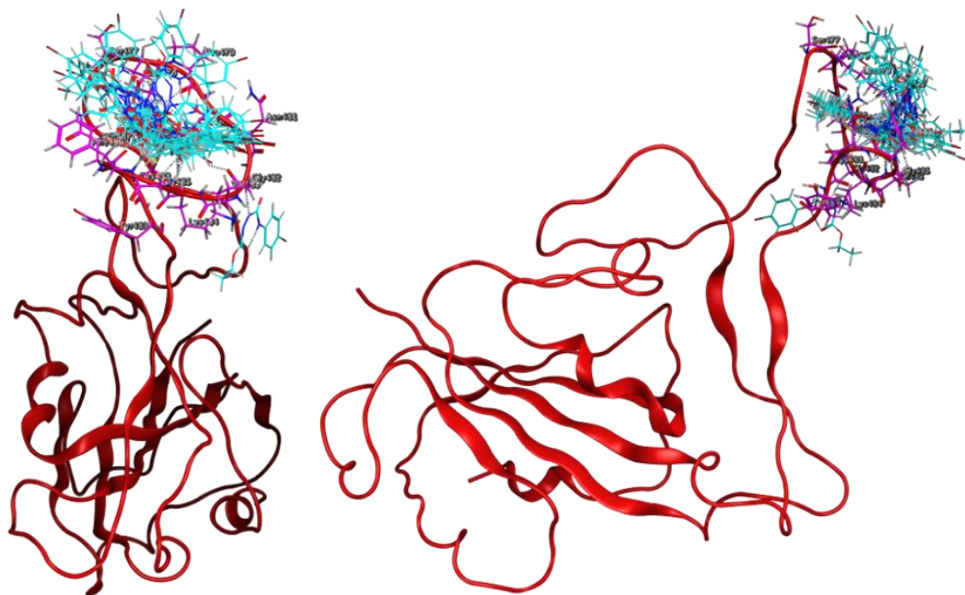


Fig. S6. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V6 (cyan).

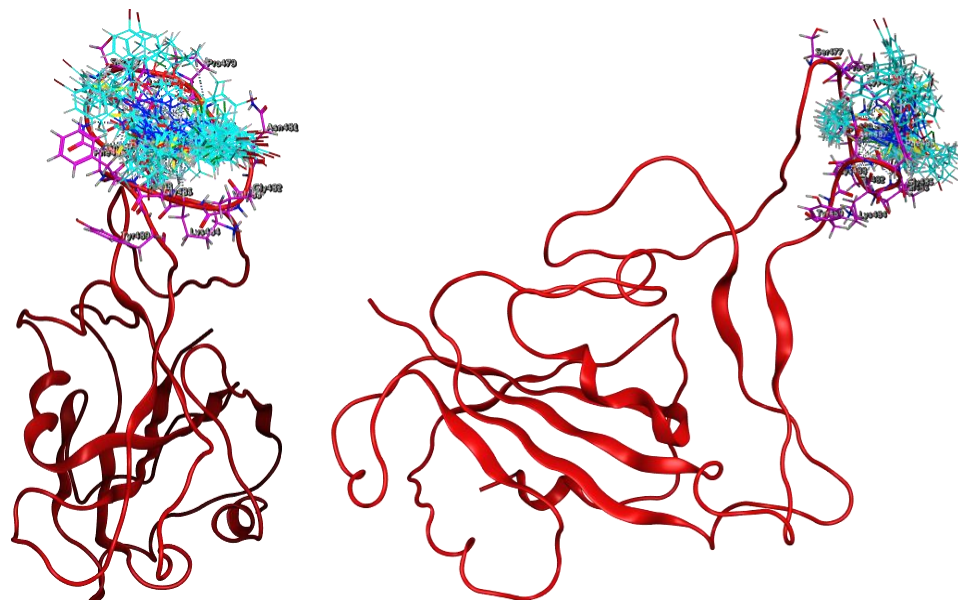


Fig. S7. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V7 (cyan).

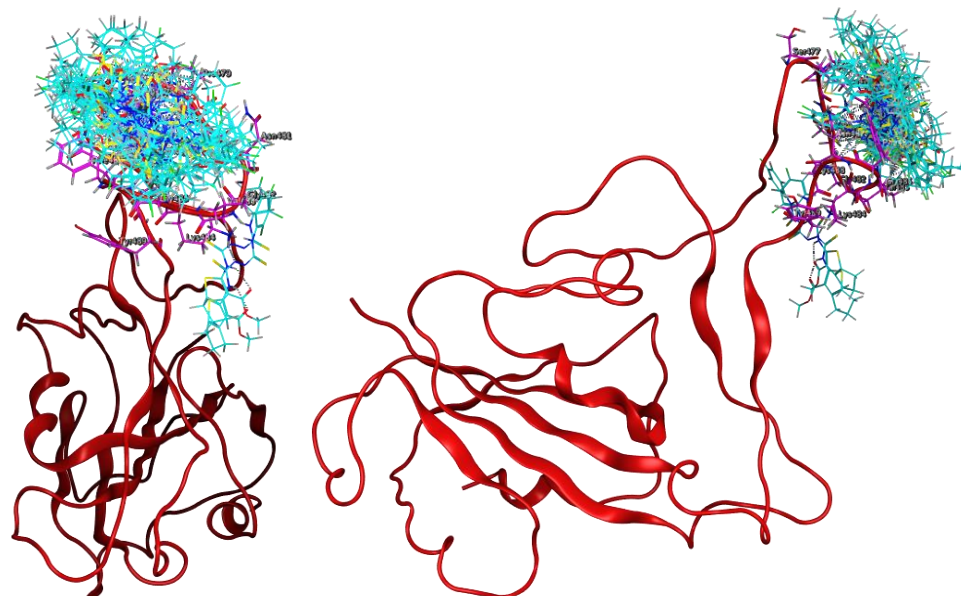


Fig. S8. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V8 (cyan).

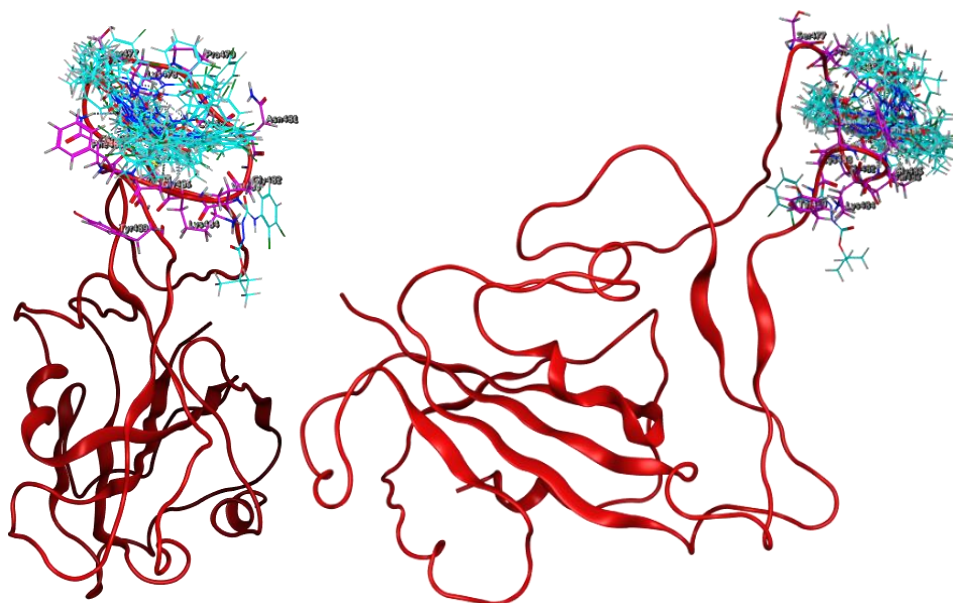


Fig. S9. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V9 (cyan).

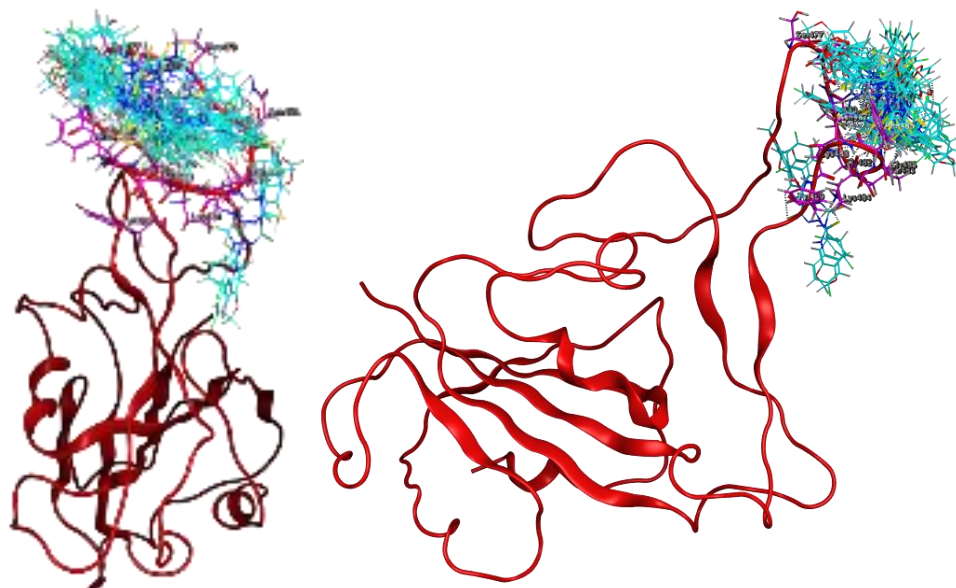


Fig. S10. RBD (red) shows amino acids Ser477, Lys478, Pro479, Cys480, Asn481, Gly482, Val483, Lys484, Gly485, Phe486, Asn487, Cys488, and Tyr489 (Pink) as the specific region chosen for molecular docking with 30 conformers of compound V10 (cyan).

Table S1. $\Delta G_{\text{binding}}$ of 30 conformers of each compound. Determining the average and SD.

Compound	Conformer	$\Delta G_{\text{binding}}$
V1	1	-18.686377
V1	2	-17.658157
V1	3	-17.13052
V1	4	-16.921801
V1	5	-15.976783
V1	6	-15.718482
V1	7	-15.501602
V1	8	-15.293103
V1	9	-15.262588
V1	10	-14.811193
V1	11	-14.61214
V1	12	-13.555136
V1	13	-13.494007
V1	14	-12.93611
V1	15	-12.84235
V1	16	-12.589936
V1	17	-12.493842
V1	18	-12.307854
V1	19	-11.720221
V1	20	-11.596713
V1	21	-11.37906
V1	22	-10.802212
V1	23	-10.653204
V1	24	-10.447802
V1	25	-10.401533
V1	26	-10.400471
V1	27	-10.25163
V1	28	-10.246284
V1	29	-10.088652
	30	-10.036956
	Average $\Delta G_{\text{binding}}$	-13.19389063
	SD	2.59033886
V2	1	-19.9643
V2	2	-18.2029
V2	3	-17.8069
V2	4	-17.1437
V2	5	-16.561

V2	6	-16.5154
V2	7	-15.6107
V2	8	-14.0753
V2	9	-13.0868
V2	10	-12.9705
V2	11	-12.7524
V2	12	-12.6726
V2	13	-12.5635
V2	14	-12.368
V2	15	-12.3005
V2	16	-12.2604
V2	17	-12.0565
V2	18	-11.9918
V2	19	-11.582
V2	20	-11.0982
V2	21	-10.8888
V2	22	-10.5471
V2	23	-10.5295
V2	24	-10.4914
V2	25	-10.4373
V2	26	-10.1899
V2	27	-9.53721
V2	28	-9.50362
V2	29	-9.47532
V2	30	-9.46523
	Average $\Delta G_{\text{binding}}$	-12.8216
	SD	2.898923
V3	1	-21.796642
V3	2	-17.265633
V3	3	-16.58713
V3	4	-16.314447
V3	5	-15.389739
V3	6	-14.457866
V3	7	-13.961026
V3	8	-13.943815
V3	9	-13.211155
V3	10	-12.742643
V3	11	-12.692279
V3	12	-12.313154

V3	13	-12.18643
V3	14	-12.061255
V3	15	-12.042846
V3	16	-11.865976
V3	17	-11.674777
V3	18	-11.343977
V3	19	-11.299106
V3	20	-11.27394
V3	21	-11.211271
V3	22	-10.810858
V3	23	-10.756661
V3	24	-10.737947
V3	25	-10.731977
V3	26	-10.485266
V3	27	-10.431793
V3	28	-10.336724
V3	29	-10.282219
V3	30	-10.249594
	Average $\Delta G_{\text{binding}}$	-12.6819382
	SD	2.620132592
V4	1	-22.4904
V4	2	-20.8875
V4	3	-20.1693
V4	4	-18.8663
V4	5	-18.0306
V4	6	-17.517
V4	7	-16.2575
V4	8	-14.5402
V4	9	-13.9276
V4	10	-13.4629
V4	11	-13.185
V4	12	-12.1585
V4	13	-11.9927
V4	14	-11.6477
V4	15	-11.6194
V4	16	-11.2061
V4	17	-10.3772
V4	18	-10.2186
V4	19	-10.1111

V4	20	-9.6707
V4	21	-9.43412
V4	22	-9.43222
V4	23	-9.12834
V4	24	-9.10504
V4	25	-9.09465
V4	26	-8.99905
V4	27	-8.97505
V4	28	-8.93571
V4	29	-8.93288
V4	30	-8.84972
	Average $\Delta G_{\text{binding}}$	-12.6407756
	SD	4.11093937
V5	1	-15.8968
V5	2	-15.2694
V5	3	-14.111
V5	4	-13.7013
V5	5	-13.6061
V5	6	-13.29
V5	7	-13.2769
V5	8	-13.1059
V5	9	-13.0548
V5	10	-12.8968
V5	11	-12.7982
V5	12	-12.5754
V5	13	-12.4411
V5	14	-12.2883
V5	15	-12.2495
V5	16	-12.2487
V5	17	-12.0011
V5	18	-11.9949
V5	19	-11.9849
V5	20	-11.8974
V5	21	-11.5305
V5	22	-11.3164
V5	23	-11.2972
V5	24	-11.2383
V5	25	-11.2061
V5	26	-11.0891

V5	27	-10.9581
V5	28	-10.8865
V5	29	-10.74
V5	30	-10.7326
	Average $\Delta G_{\text{binding}}$	-12.3895
	SD	1.283996
V6	1	-17.002621
V6	2	-15.295253
V6	3	-15.169549
V6	4	-13.446736
V6	5	-13.311315
V6	6	-13.304582
V6	7	-13.144269
V6	8	-13.132564
V6	9	-12.840862
V6	10	-12.746133
V6	11	-12.457322
V6	12	-12.446866
V6	13	-12.262386
V6	14	-12.155668
V6	15	-12.117506
V6	16	-11.969082
V6	17	-11.858397
V6	18	-11.779815
V6	19	-11.709128
V6	20	-11.488421
V6	21	-11.425038
V6	22	-11.393922
V6	23	-11.367608
V6	24	-11.349224
V6	25	-11.193339
V6	26	-11.085744
V6	27	-11.037675
V6	28	-10.860701
V6	29	-10.624154
V6	30	-10.392555
	Average $\Delta G_{\text{binding}}$	-12.3456145
	SD	1.46638364

V7	1	-21.457426
V7	2	-16.007965
V7	3	-15.236149
V7	4	-14.839081
V7	5	-13.778248
V7	6	-13.695765
V7	7	-13.295493
V7	8	-13.230945
V7	9	-13.063475
V7	10	-12.95778
V7	11	-12.654613
V7	12	-12.288958
V7	13	-12.278214
V7	14	-12.039289
V7	15	-12.02095
V7	16	-11.456208
V7	17	-11.310762
V7	18	-11.309491
V7	19	-11.276503
V7	20	-10.751863
V7	21	-10.707392
V7	22	-10.703274
V7	23	-10.653432
V7	24	-10.434417
V7	25	-10.411265
V7	26	-10.347705
V7	27	-10.27549
V7	28	-10.086998
V7	29	-10.041161
V7	30	-10.007354
	Average $\Delta G_{\text{binding}}$	-12.2872555
	SD	2.37861257
V8	1	-17.369316
V8	2	-15.779747
V8	3	-15.366351
V8	4	-14.262696
V8	5	-13.820786
V8	6	-13.311613
V8	7	-13.250729

V8	8	-13.056003
V8	9	-12.666632
V8	10	-12.433752
V8	11	-12.368236
V8	12	-12.08449
V8	13	-12.060993
V8	14	-11.809308
V8	15	-11.58612
V8	16	-11.524674
V8	17	-11.513528
V8	18	-11.281415
V8	19	-11.140031
V8	20	-11.118045
V8	21	-11.004594
V8	22	-10.881783
V8	23	-10.770062
V8	24	-10.604631
V8	25	-10.48492
V8	26	-10.260252
V8	27	-10.050845
V8	28	-10.016213
V8	29	-9.9025431
V8	30	-9.5279827
	Average $\Delta G_{\text{binding}}$	-12.0436097
	SD	1.8567417
V9	1	-19.997381
V9	2	-18.184566
V9	3	-15.336789
V9	4	-15.336338
V9	5	-15.061238
V9	6	-13.939891
V9	7	-13.271586
V9	8	-13.146473
V9	9	-11.918232
V9	10	-11.539254
V9	11	-11.478748
V9	12	-11.388349
V9	13	-11.252321
V9	14	-11.209301

V9	15	-11.196795
V9	16	-11.177901
V9	17	-11.03306
V9	18	-10.896284
V9	19	-10.80202
V9	20	-10.660067
V9	21	-10.659122
V9	22	-10.633187
V9	23	-10.265592
V9	24	-10.167326
V9	25	-10.16215
V9	26	-10.092634
V9	27	-10.061651
V9	28	-10.060814
V9	29	-9.8499031
V9	30	-9.7733116
	Average $\Delta G_{\text{binding}}$	-12.0184095
	SD	2.51498247
V10	1	-18.22258
V10	2	-16.535313
V10	3	-16.164967
V10	4	-14.076038
V10	5	-13.908955
V10	6	-13.510151
V10	7	-12.893141
V10	8	-12.740181
V10	9	-12.120993
V10	10	-12.013804
V10	11	-11.997242
V10	12	-11.960196
V10	13	-11.918236
V10	14	-11.81843
V10	15	-11.600704
V10	16	-11.335879
V10	17	-11.25161
V10	18	-11.172141
V10	19	-11.002528
V10	20	-10.90007
V10	21	-10.885937

V10	22	-10.515842
V10	23	-10.398866
V10	24	-10.265138
V10	25	-9.9886818
V10	26	-9.9246674
V10	27	-9.8883467
V10	28	-9.7532597
V10	29	-9.6994123
V10	30	-9.6534767
	Average $\Delta G_{\text{binding}}$	-11.9372262
	SD	2.11628099

Table S2. Interaction report of each conformer of compound V1. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD	Interaction	Distance
1	S	CYS 480	H-donor	3.5
	S	CYS 488	H-donor	3.39
	S	GLY 485	H-acceptor	3.58
	S	PHE 486	H-acceptor	3.86
	N	LYS 478	ionic	1.32
	N	LYS 478	ionic	0.76
	S	LYS 478	ionic	3.81
	S	LYS 478	ionic	3.07
2	S	CYS 480	H-donor	3.18
	N	LYS 478	ionic	1.48
	S	LYS 478	ionic	2.51
	6-ring	PHE 486	pi-H	4.36
3	S	CYS 488	H-donor	4.31
	S	PHE 486	H-acceptor	2.5
	N	LYS 478	ionic	1.55
	N	LYS 478	ionic	0.97
	S	LYS 478	ionic	2.68
	5-ring	LYS 478	pi-H	4.21
4	S	CYS 480	H-donor	3.26
	S	CYS 488	H-donor	2.38
	S	PHE 486	H-acceptor	3.98
	S	CYS 488	H-acceptor	4.37
	N	LYS 478	ionic	1.83
	N	LYS 478	ionic	1.14
	S	LYS 478	ionic	3.07

5	S	CYS	480	H-donor	4.22
	N	LYS	478	ionic	1.17
	N	LYS	478	ionic	1.53
	S	LYS	478	ionic	3.14
	S	LYS	478	ionic	3.93
6	S	CYS	488	H-donor	3.58
	S	PHE	486	H-acceptor	2.75
	N	LYS	478	ionic	0.84
	N	LYS	478	ionic	1.66
	S	LYS	478	ionic	2.82
7	S	ASN	487	H-acceptor	3.67
	N	LYS	478	ionic	1.34
	N	LYS	478	ionic	1.09
	S	LYS	478	ionic	3.85
	S	LYS	478	ionic	3.12
8	S	CYS	480	H-donor	2.48
	S	CYS	488	H-donor	1.79
	S	LYS	484	H-acceptor	4.08
	S	CYS	488	H-acceptor	4.38
	N	PHE	486	H-acceptor	3.31
	N	LYS	478	ionic	1.05
	N	LYS	478	ionic	1.64
	S	LYS	478	ionic	3.04
9	S	CYS	480	H-donor	3.85
	N	LYS	478	ionic	1.45
	N	LYS	478	ionic	1.08
	S	LYS	478	ionic	3.66
	S	LYS	478	ionic	3.38
	6-ring	PHE	486	pi-H	4.59
10	S	CYS	480	H-donor	3.63
	S	GLN	474	H-acceptor	4.23
	N	LYS	478	ionic	1.34
	N	LYS	478	ionic	1.85
	S	LYS	478	ionic	2.95
11	S	PHE	486	H-acceptor	2.93
	N	LYS	478	ionic	1.94
	N	LYS	478	ionic	1.22
	S	LYS	478	ionic	2.72
12	N	LYS	478	H-acceptor	2.08
	S	LYS	478	H-acceptor	3.17

	S	CYS	480	H-acceptor	3.58
	N	LYS	478	ionic	2.08
	N	LYS	478	ionic	2.47
	S	LYS	478	ionic	3.84
	5-ring	LYS	478	pi-cation	3.51
13	S	GLY	485	H-acceptor	4.01
	S	PHE	486	H-acceptor	3.26
	S	PHE	486	H-acceptor	3.64
	N	LYS	478	ionic	1.58
	N	LYS	478	ionic	1.84
	S	LYS	478	ionic	3.12
14	N	LYS	478	H-acceptor	1.77
	N	LYS	478	ionic	1.77
	N	LYS	478	ionic	2.32
	S	LYS	478	ionic	3.36
	5-ring	LYS	478	pi-cation	4.35
15	S	GLY	485	H-acceptor	4.43
	S	PHE	486	H-acceptor	4.15
	N	LYS	478	ionic	1.74
	N	LYS	478	ionic	1.8
	S	LYS	478	ionic	3.79
	S	LYS	478	ionic	3.67
16	S	CYS	480	H-donor	3.56
	S	CYS	488	H-donor	2.81
	N	LYS	478	H-acceptor	2.21
	S	LYS	478	H-acceptor	3.7
	S	PHE	486	H-acceptor	3.34
	N	LYS	478	ionic	2.73
	N	LYS	478	ionic	2.21
	S	LYS	478	ionic	3.7
17	S	CYS	480	H-donor	3.77
	S	CYS	488	H-donor	3.33
	S	GLY	485	H-acceptor	3.29
	S	PHE	486	H-acceptor	3.48
	N	LYS	478	ionic	1.5
	N	LYS	478	ionic	2.16
	S	LYS	478	ionic	3.19
	6-ring	ASN	481	pi-H	3.77
18	S	CYS	480	H-donor	3.87
	S	CYS	488	H-donor	1.66

	S	CYS	488	H-acceptor	3.21
	N	LYS	478	ionic	1.73
	N	LYS	478	ionic	2.01
	S	LYS	478	ionic	3.61
	S	LYS	478	ionic	3.95
	5-ring	GLY	485	pi-H	3.84
19	N	LYS	478	ionic	2.34
	N	LYS	478	ionic	2.11
	S	LYS	478	ionic	3.66
20	S	PRO	479	H-acceptor	4.27
	S	GLY	485	H-acceptor	4.15
	S	PHE	486	H-acceptor	3.99
	N	LYS	478	ionic	1.69
	N	LYS	478	ionic	1.8
	S	LYS	478	ionic	3.44
	S	LYS	478	ionic	3.98
21	N	LYS	478	H-acceptor	2.39
	S	GLY	485	H-acceptor	3.36
	S	LYS	478	H-acceptor	3.8
	N	LYS	478	ionic	3.04
	N	LYS	478	ionic	2.39
	S	LYS	478	ionic	3.49
22	S	CYS	480	H-donor	3.91
	N	LYS	478	ionic	1.86
	N	LYS	478	ionic	1.32
	S	LYS	478	ionic	3.97
	S	LYS	478	ionic	3.32
23	S	LYS	478	H-acceptor	3
	N	LYS	478	ionic	2.6
	N	LYS	478	ionic	3.51
	S	LYS	478	ionic	3
24	CL	GLY	482	H-donor	3.25
	N	LYS	478	H-acceptor	2.72
	S	LYS	478	H-acceptor	3.26
	N	LYS	478	ionic	3.28
	N	LYS	478	ionic	2.72
	S	LYS	478	ionic	3.94
25	N	LYS	478	ionic	2.54
	N	LYS	478	ionic	2.08
	S	LYS	478	ionic	3.38

26	N	LYS	478	H-acceptor	1.79
	N	LYS	478	ionic	1.79
	N	LYS	478	ionic	2.4
	S	LYS	478	ionic	3.34
27	S	CYS	480	H-donor	4.12
	N	LYS	478	H-acceptor	2.17
	N	ASN	487	H-acceptor	3.22
	S	CYS	488	H-acceptor	2.89
	N	LYS	478	ionic	2.17
	N	LYS	478	ionic	2.42
28	S	LYS	478	ionic	4
	S	CYS	480	H-donor	4.11
	S	LYS	478	H-acceptor	3.93
	S	GLN	474	H-acceptor	3.49
	S	CYS	480	H-acceptor	4.03
	N	LYS	478	ionic	2.79
	N	LYS	478	ionic	3.36
29	S	LYS	478	ionic	3.93
	N	ASN	487	H-acceptor	3.42
	S	CYS	488	H-acceptor	2.55
	N	LYS	478	ionic	2.36
	N	LYS	478	ionic	1.85
	S	LYS	478	ionic	3.57
	6-ring	PHE	486	pi-H	4.32

Table S3. Interaction report of each conformer of compound V2. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD	Interaction	Distance	
1	S	CYS	480	H-donor	2.62
	N	LYS	478	ionic	0.65
	N	LYS	478	ionic	0.87
	S	LYS	478	ionic	3.19
	S	LYS	478	ionic	3.54
2	S	PHE	486	H-acceptor	2.97
	N	LYS	478	ionic	1.53
	N	LYS	478	ionic	0.83
	S	LYS	478	ionic	2.87
3	S	CYS	480	H-donor	2.77
	S	CYS	488	H-donor	3.69
	N	LYS	478	ionic	1.2
	S	LYS	478	ionic	2.76
	S	LYS	478	ionic	3.93
	6-ring	PHE	486	pi-H	4.41

4	S	LYS	478	H-acceptor	2.08
	S	CYS	480	H-acceptor	4.37
	N	LYS	478	ionic	1.94
	N	LYS	478	ionic	1.04
	S	LYS	478	ionic	2.8
	6-ring	PHE	486	pi-pi	3.89
5	S	ASN	487	H-acceptor	3.96
	N	LYS	478	ionic	1.65
	N	LYS	478	ionic	0.8
	S	LYS	478	ionic	2.88
6	S	CYS	480	H-acceptor	3.71
	N	LYS	478	ionic	0.87
	N	LYS	478	ionic	0.54
	S	LYS	478	ionic	3.49
	S	LYS	478	ionic	3.22
	6-ring	GLY	485	pi-H	4.22
7	S	CYS	480	H-donor	3.47
	S	CYS	488	H-donor	3.17
	S	GLY	485	H-acceptor	3.43
	S	PHE	486	H-acceptor	3.71
	N	LYS	478	ionic	0.82
	N	LYS	478	ionic	1.24
	S	LYS	478	ionic	3.18
	S	LYS	478	ionic	3.66
8	S	PRO	479	H-acceptor	3.19
	S	PHE	486	H-acceptor	4.14
	S	PHE	486	H-acceptor	3.65
	N	LYS	478	ionic	1.99
	N	LYS	478	ionic	1.33
	S	LYS	478	ionic	2.7
9	S	CYS	480	H-donor	3.58
	N	LYS	478	ionic	1.68
	N	LYS	478	ionic	1.21
	S	LYS	478	ionic	2.87
	6-ring	PHE	486	pi-H	4.6
10	S	PRO	479	H-acceptor	3.85
	N	LYS	478	ionic	1.39
	N	LYS	478	ionic	1.34
	S	LYS	478	ionic	3.68
	S	LYS	478	ionic	3.37
11	S	CYS	480	H-donor	2.43
	N	LYS	478	ionic	1.61
	N	LYS	478	ionic	0.82
	S	LYS	478	ionic	2.84
12	S	GLY	485	H-acceptor	4.07
	S	PHE	486	H-acceptor	3.3
	S	PHE	486	H-acceptor	3.65
	N	LYS	478	ionic	1.95
	N	LYS	478	ionic	1.57
S	LYS	478	ionic	3.06	

13	S	GLY	485	H-acceptor	3.71
	N	LYS	478	ionic	2.39
	N	LYS	478	ionic	1.46
	S	LYS	478	ionic	2.42
14	N	LYS	478	H-acceptor	2.02
	S	LYS	478	H-acceptor	2.5
	N	LYS	478	ionic	3.07
	N	LYS	478	ionic	2.02
	S	LYS	478	ionic	2.52
15	S	GLY	485	H-acceptor	2.63
	S	PHE	486	H-acceptor	3.43
	N	LYS	478	ionic	2.13
	N	LYS	478	ionic	1.39
	S	LYS	478	ionic	2.61
	6-ring	PHE	486	pi-pi	3.84
16	N	LYS	478	ionic	2.14
	N	LYS	478	ionic	1.18
	S	LYS	478	ionic	2.52
17	N	LYS	478	ionic	2.42
	N	LYS	478	ionic	1.44
	S	LYS	478	ionic	2.42
18	N	LYS	478	H-acceptor	2.24
	S	PRO	479	H-acceptor	3.89
	S	GLY	485	H-acceptor	4.19
	S	GLY	485	H-acceptor	4.27
	N	LYS	478	ionic	2.76
	N	LYS	478	ionic	2.24
	S	LYS	478	ionic	3.64
19	S	ASN	487	H-acceptor	4.04
	S	CYS	488	H-acceptor	4.28
	N	LYS	478	ionic	1.93
	N	LYS	478	ionic	1.53
	S	LYS	478	ionic	4
	S	LYS	478	ionic	3.43
20	S	CYS	480	H-donor	2.83
	N	LYS	478	ionic	2.24
	N	LYS	478	ionic	1.66
	S	LYS	478	ionic	3.37
21	S	PRO	479	H-acceptor	3.96
	S	GLY	485	H-acceptor	4.17
	S	PHE	486	H-acceptor	4.14
	N	LYS	478	ionic	1.62
	N	LYS	478	ionic	1.61
	S	LYS	478	ionic	3.56
	S	LYS	478	ionic	3.77
22	S	CYS	480	H-donor	2.57
	S	LYS	484	H-acceptor	4.47
	N	LYS	478	ionic	2.2
	N	LYS	478	ionic	1.25
	S	LYS	478	ionic	2.7

	6-ring	PHE	486	pi-H	4.48
23	S	ASN	487	H-acceptor	3.68
	N	LYS	478	ionic	1.34
	N	LYS	478	ionic	1.74
	S	LYS	478	ionic	2.92
24	N	LYS	478	H-acceptor	1.76
	S	GLY	485	H-acceptor	2.97
	S	PHE	486	H-acceptor	2.99
	N	LYS	478	ionic	1.76
	N	LYS	478	ionic	1.95
	S	LYS	478	ionic	3.66
25	S	LYS	478	ionic	3.82
	S	CYS	488	H-donor	3.85
	S	PHE	486	H-acceptor	3.68
	N	LYS	478	ionic	2.79
	N	LYS	478	ionic	1.6
26	S	LYS	478	ionic	1.77
	S	GLN	474	H-acceptor	4.49
	S	PHE	486	H-acceptor	3.3
	S	PHE	486	H-acceptor	3.22
	N	LYS	478	ionic	2.28
	N	LYS	478	ionic	1.49
27	S	LYS	478	ionic	2.6
	N	LYS	478	ionic	2.01
	N	LYS	478	ionic	2.8
	S	LYS	478	ionic	2.88

Table S4. Interaction report of each conformer of compound V3. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD	Interaction	Distance	
1	S	CYS	488	H-donor	2.76
	S	PHE	486	H-acceptor	2.97
	N	LYS	478	ionic	0.89
	N	LYS	478	ionic	0.89
	S	LYS	478	ionic	3.37
	S	LYS	478	ionic	3.41
2	C	GLY	482	H-donor	2.89
	S	PHE	486	H-acceptor	2.9
	N	LYS	478	ionic	1.21
	N	LYS	478	ionic	1.41
	S	LYS	478	ionic	3.44
	S	LYS	478	ionic	3.63
3	S	ASN	487	H-acceptor	3.8
	N	LYS	478	ionic	1.04
	N	LYS	478	ionic	2.04

	S	LYS	478	ionic	2.65
4	S	GLY	485	H-acceptor	3.21
	S	PHE	486	H-acceptor	2.93
	N	LYS	478	ionic	1.25
	N	LYS	478	ionic	1.52
	S	LYS	478	ionic	3.33
	S	LYS	478	ionic	3.77
5	N	LYS	478	ionic	1.08
	N	LYS	478	ionic	2.12
	S	LYS	478	ionic	2.27
6	S	LYS	478	H-acceptor	2.77
	N	LYS	478	ionic	1.55
	N	LYS	478	ionic	2.25
	S	LYS	478	ionic	3.17
7	N	LYS	478	ionic	1.09
	N	LYS	478	ionic	1.72
	S	LYS	478	ionic	2.93
8	N	LYS	478	ionic	1.6
	N	LYS	478	ionic	1.42
	S	LYS	478	ionic	3.92
	S	LYS	478	ionic	3.3
9	S	GLY	485	H-acceptor	3.64
	N	LYS	478	ionic	1.01
	N	LYS	478	ionic	2.27
	S	LYS	478	ionic	1.96
	6-ring	PHE	486	pi-pi	3.37
10	N	LYS	478	ionic	2.06
	N	LYS	478	ionic	1.9
	S	LYS	478	ionic	3.97
	S	LYS	478	ionic	3.66
11	S	GLY	485	H-acceptor	4.26
	N	LYS	478	ionic	1.96
	N	LYS	478	ionic	2.39
	S	LYS	478	ionic	3.59
12	N	LYS	478	ionic	2.19
	N	LYS	478	ionic	2.66
	S	LYS	478	ionic	3.43
13	S	CYS	488	H-donor	3.59
	N	LYS	478	H-acceptor	1.99
	S	LYS	478	H-acceptor	3.05

	S	GLY	485	H-acceptor	3.58
	S	PHE	486	H-acceptor	3.83
	N	LYS	478	ionic	2.71
	N	LYS	478	ionic	1.99
	S	LYS	478	ionic	3.05
14	C	GLY	482	H-donor	2.48
	S	CYS	488	H-donor	4.26
	S	PHE	486	H-acceptor	2.97
	N	LYS	478	ionic	1.87
	N	LYS	478	ionic	2.27
	S	LYS	478	ionic	3.45
15	N	LYS	478	ionic	1.57
	N	LYS	478	ionic	2.3
	S	LYS	478	ionic	2.43
16	S	GLY	485	H-acceptor	3.91
	S	PHE	486	H-acceptor	3.46
	N	LYS	478	ionic	1.66
	N	LYS	478	ionic	1.79
	S	LYS	478	ionic	3.61
	S	LYS	478	ionic	3.8
17	N	LYS	478	ionic	2.65
	N	LYS	478	ionic	2.61
18	N	LYS	478	ionic	2.36
	N	LYS	478	ionic	2.66
	S	LYS	478	ionic	3.37
19	S	ASN	487	H-acceptor	3.34
	N	LYS	478	ionic	1.67
	N	LYS	478	ionic	2.21
	S	LYS	478	ionic	2.98
20	S	PHE	486	H-acceptor	4.12
	N	LYS	478	ionic	2.57
	N	LYS	478	ionic	1.5
	S	LYS	478	ionic	1.98
21	N	LYS	478	H-acceptor	2.28
	N	LYS	478	ionic	2.28
	N	LYS	478	ionic	3.16
	S	LYS	478	ionic	2.83
22	S	GLY	485	H-acceptor	4.03
	S	PHE	486	H-acceptor	3.64
	N	LYS	478	ionic	2.64

	N	LYS	478	ionic	2.39
	S	LYS	478	ionic	3.69
23	N	LYS	478	H-acceptor	2.49
	S	LYS	478	H-acceptor	3.54
	N	LYS	478	ionic	3.15
	N	LYS	478	ionic	3.97
	S	LYS	478	ionic	3.54
	24	N	CYS	480	H-donor
N		CYS	480	H-donor	3.34
N		CYS	488	H-donor	3.31
S		CYS	480	H-donor	3.39
N		LYS	478	ionic	2.11
N		LYS	478	ionic	3.26
S		LYS	478	ionic	1.73
25	C	GLY	482	H-donor	2.87
	S	CYS	488	H-donor	3.56
	S	LYS	478	H-acceptor	2.7
	S	PHE	486	H-acceptor	3.47
	N	LYS	478	ionic	2.18
	N	LYS	478	ionic	3.1
	S	LYS	478	ionic	2.7
26	S	CYS	480	H-acceptor	3.32
	S	ASN	481	H-acceptor	3.57
	N	LYS	478	ionic	2.75
	N	LYS	478	ionic	3.08
	S	LYS	478	ionic	3.69
27	N	LYS	478	ionic	2.05
	N	LYS	478	ionic	2.77
	S	LYS	478	ionic	2.75
28	S	PHE	486	H-acceptor	4.29
	N	LYS	478	ionic	3.02
	N	LYS	478	ionic	1.73
	S	LYS	478	ionic	1.33
29	S	GLY	485	H-acceptor	3.39
	S	PHE	486	H-acceptor	3.22
	N	LYS	478	ionic	3.14
	N	LYS	478	ionic	2.66
	S	LYS	478	ionic	3.64
	6-ring	LYS	478	pi-H	3.9
30	N	LYS	478	H-acceptor	2.46

	S	CYS	480	H-acceptor	4.21
	N	LYS	478	ionic	2.46
	N	LYS	478	ionic	2.62

Table S5. Interaction report of each conformer of compound V4. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD		Interaction	Distance
1	S	CYS	488	H-donor	3.36
	S	PHE	486	H-acceptor	2.3
	N	LYS	478	ionic	1.02
	N	LYS	478	ionic	0.96
	S	LYS	478	ionic	3.42
	S	LYS	478	ionic	3.42
2	S	CYS	480	H-donor	2.44
	S	CYS	488	H-donor	2.67
	S	GLY	485	H-acceptor	4.13
	N	LYS	478	ionic	0.87
	N	LYS	478	ionic	0.72
	S	LYS	478	ionic	3.39
	S	LYS	478	ionic	3.37
6-ring	GLY	485	pi-H	4.1	
3	S	CYS	480	H-acceptor	3.51
	N	LYS	478	ionic	1.08
	N	LYS	478	ionic	1.17
	S	LYS	478	ionic	3.41
	S	LYS	478	ionic	3.51
	6-ring	CYS	480	pi-H	4.3
4	S	CYS	480	H-acceptor	3.92
	S	PHE	486	H-acceptor	3.35
	N	LYS	478	ionic	0.87
	N	LYS	478	ionic	1.16
	S	LYS	478	ionic	3.25
	S	LYS	478	ionic	3.6
	6-ring	ASN	481	pi-H	3.71
5	S	ASN	487	H-acceptor	3.64
	N	LYS	478	ionic	1.3
	N	LYS	478	ionic	0.82
	S	LYS	478	ionic	3.66
	S	LYS	478	ionic	3.26
	6-ring	ASN	481	pi-H	4.85

6	S	CYS	480	H-donor	3.8
	S	CYS	488	H-donor	3.43
	S	GLY	485	H-acceptor	3.43
	S	PHE	486	H-acceptor	3.54
	N	LYS	478	ionic	1.67
	N	LYS	478	ionic	0.99
	S	LYS	478	ionic	3.05
7	S	ASN	487	H-acceptor	4.12
	N	LYS	478	ionic	1.3
	N	LYS	478	ionic	0.91
	S	LYS	478	ionic	3.64
	S	LYS	478	ionic	3.31
8	N	LYS	478	ionic	0.84
	N	LYS	478	ionic	1.65
	S	LYS	478	ionic	2.77
	6-ring	ASN	481	pi-H	4.63
9	N	PHE	486	H-acceptor	2.74
	N	LYS	478	ionic	1.05
	N	LYS	478	ionic	2.02
	S	LYS	478	ionic	2.29
10	S	CYS	480	H-donor	3.56
	S	CYS	488	H-donor	2.68
	S	PHE	486	H-acceptor	3.98
	S	CYS	488	H-acceptor	4.45
	N	LYS	478	ionic	1.63
	N	LYS	478	ionic	2.23
	S	LYS	478	ionic	2.75
11	S	GLY	485	H-acceptor	4.36
	S	PHE	486	H-acceptor	3.23
	N	LYS	478	ionic	1.83
	N	LYS	478	ionic	2.15
	S	LYS	478	ionic	3.57
	6-ring	PHE	486	pi-pi	3.95
12	S	GLY	485	H-acceptor	4.32
	S	PHE	486	H-acceptor	4.25
	N	LYS	478	ionic	2.02
	N	LYS	478	ionic	1.78
	S	LYS	478	ionic	3.51
13	S	ASN	487	H-acceptor	2.86
	N	LYS	478	ionic	1.82

	N	LYS	478	ionic	2.13
	S	LYS	478	ionic	3.16
14	S	PHE	490	H-acceptor	3.04
	N	LYS	484	ionic	2.79
	N	LYS	484	ionic	2.13
	S	LYS	484	ionic	3.01
	N	LYS	478	ionic	1.73
15	N	LYS	478	ionic	1.54
	S	LYS	478	ionic	3.87
	S	LYS	478	ionic	3.42
	S	GLY	485	H-acceptor	3.55
16	N	LYS	478	ionic	1.37
	N	LYS	478	ionic	2.63
	S	LYS	478	ionic	1.62
	6-ring	PHE	486	pi-pi	3.28
	S	CYS	480	H-donor	3.99
17	S	CYS	488	H-donor	3.7
	S	PHE	486	H-acceptor	3.86
	N	LYS	478	ionic	2.5
	N	LYS	478	ionic	1.49
	S	LYS	478	ionic	2.16
	S	CYS	480	H-donor	3.36
18	S	CYS	488	H-donor	2.44
	S	PHE	486	H-acceptor	3.5
	N	LYS	478	ionic	1.51
	N	LYS	478	ionic	1.99
	S	LYS	478	ionic	2.88
	6-ring	ASN	481	pi-H	3.81
	6-ring	PHE	486	pi-pi	3.44
	S	PHE	486	H-acceptor	3.55
19	S	PHE	486	H-acceptor	3.57
	S	GLN	474	H-acceptor	3.95
	N	LYS	478	ionic	1.65
	N	LYS	478	ionic	2.7
	S	LYS	478	ionic	2
	S	CYS	480	H-donor	3.88
20	S	CYS	488	H-donor	4.09
	S	PRO	479	H-acceptor	4.01
	S	GLY	485	H-acceptor	3.57
	S	PHE	486	H-acceptor	4.1

	N	LYS	478	ionic	2.43
	N	LYS	478	ionic	1.81
	S	LYS	478	ionic	3.37
21	S	PRO	479	H-acceptor	2.7
	N	LYS	478	ionic	2.91
	N	LYS	478	ionic	2.06
	S	LYS	478	ionic	2.32
	6-ring	GLY	485	pi-H	4.56
22	N	LYS	478	ionic	2.76
	N	LYS	478	ionic	2.73
	S	LYS	478	ionic	3.99
23	S	PRO	479	H-acceptor	3.06
	N	LYS	478	ionic	2.91
	N	LYS	478	ionic	1.91
	S	LYS	478	ionic	2.35
24	S	CYS	480	H-acceptor	3.82
	N	LYS	478	ionic	2.53
	N	LYS	478	ionic	2.18
	S	LYS	478	ionic	3.7
	6-ring	PHE	486	pi-pi	3.75
25	N	LYS	478	H-acceptor	2.83
	N	LYS	478	ionic	2.83
	N	LYS	478	ionic	3.58
	S	LYS	478	ionic	3.31

Table S6. Interaction report of each conformer of compound V5. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD		Interaction	Distance
1	O	ASN	487	H-acceptor	3.44
	N	LYS	478	ionic	1.56
	N	LYS	478	ionic	0.9
	O	LYS	478	ionic	3.49
	O	LYS	478	ionic	2.62
2	O	CYS	480	H-donor	3.41
	O	CYS	488	H-donor	1.65
	N	LYS	478	ionic	1.91
	N	LYS	478	ionic	1.12
	O	LYS	478	ionic	3.8
	O	LYS	478	ionic	3.17
3	O	CYS	480	H-donor	2.68

	N	LYS	478	ionic	1.87
	N	LYS	478	ionic	1.96
	O	LYS	478	ionic	3.25
	O	LYS	478	ionic	3.03
4	N	LYS	478	ionic	1.94
	N	LYS	478	ionic	1.16
	O	LYS	478	ionic	3.96
	O	LYS	478	ionic	2.13
5	O	PHE	486	H-acceptor	2.46
	N	LYS	478	ionic	2.09
	N	LYS	478	ionic	1.84
	O	LYS	478	ionic	3.54
	O	LYS	478	ionic	3.31
6	O	CYS	480	H-donor	1.56
	O	CYS	488	H-donor	2.33
	N	LYS	478	ionic	2.55
	N	LYS	478	ionic	1.82
	O	LYS	478	ionic	2.71
7	O	CYS	480	H-donor	2.06
	O	CYS	488	H-donor	2.64
	CL	GLN	474	H-donor	2.51
	N	LYS	478	ionic	2.75
	N	LYS	478	ionic	2.28
	O	LYS	478	ionic	3.41
8	N	CYS	480	H-donor	3.75
	N	CYS	480	H-donor	3.06
	O	PHE	486	H-acceptor	3.32
	N	LYS	478	ionic	2.14
	N	LYS	478	ionic	2.66
	O	LYS	478	ionic	2.9
	O	LYS	478	ionic	3.82
9	N	LYS	478	H-acceptor	1.83
	N	LYS	478	ionic	2.57
	N	LYS	478	ionic	1.83
	O	LYS	478	ionic	3.94
	6-ring	PHE	486	pi-H	3.75
10	O	CYS	480	H-donor	3.51
	O	CYS	488	H-donor	3.37
	O	LYS	478	H-acceptor	2.29
	N	LYS	478	ionic	1.39

	N	LYS	478	ionic	2.24
	O	LYS	478	ionic	2.29
	O	LYS	478	ionic	3.98
11	O	CYS	480	H-donor	2.64
	O	CYS	488	H-donor	2.59
	N	LYS	478	ionic	1.72
	N	LYS	478	ionic	1.5
	O	LYS	478	ionic	3.59
	O	LYS	478	ionic	3.17
	12	N	LYS	478	H-acceptor
O		ASN	487	H-acceptor	3.15
N		LYS	478	ionic	1.63
N		LYS	478	ionic	1.62
O		LYS	478	ionic	3.53
O		LYS	478	ionic	3.9
13	N	CYS	480	H-donor	3.68
	N	CYS	488	H-donor	3.36
	N	LYS	478	H-acceptor	1.98
	N	LYS	478	ionic	2.55
	N	LYS	478	ionic	1.98
	O	LYS	478	ionic	3.08
14	O	PHE	486	H-acceptor	3.13
	N	LYS	478	ionic	2.67
	N	LYS	478	ionic	1.81
	O	LYS	478	ionic	2.12
15	N	LYS	484	H-acceptor	2.11
	N	LYS	484	ionic	3.11
	N	LYS	484	ionic	2.11
	O	LYS	484	ionic	2.25
16	O	PHE	486	H-acceptor	3.29
	N	LYS	478	ionic	1.94
	N	LYS	478	ionic	1.84
	O	LYS	478	ionic	3.21
	O	LYS	478	ionic	3.92
17	O	CYS	480	H-donor	2.94
	O	CYS	488	H-donor	3.06
	CL	GLN	474	H-donor	2.88
	N	LYS	478	ionic	2.5
	N	LYS	478	ionic	2.39
	O	LYS	478	ionic	3.46

	O	LYS	478	ionic	3.95
18	N	LYS	478	ionic	1.74
	N	LYS	478	ionic	1.48
	O	LYS	478	ionic	3.4
	O	LYS	478	ionic	2.13
	O	LYS	478	ionic	2.13
19	O	CYS	480	H-donor	1.92
	O	CYS	488	H-donor	2.26
	N	LYS	478	ionic	2.43
	N	LYS	478	ionic	1.96
	O	LYS	478	ionic	3.94
	O	LYS	478	ionic	3.16
20	O	CYS	480	H-donor	1.87
	CL	GLN	474	H-donor	2.42
	N	LYS	478	ionic	2.77
	N	LYS	478	ionic	2.38
	O	LYS	478	ionic	3.55
21	N	CYS	480	H-donor	3.6
	O	PHE	486	H-acceptor	2.61
	O	ASN	487	H-acceptor	2.32
	O	ASN	487	H-acceptor	3.07
	N	LYS	478	ionic	2.92
	N	LYS	478	ionic	3.56
	O	LYS	478	ionic	2.96
22	N	LYS	478	ionic	2.05
	N	LYS	478	ionic	2.01
	O	LYS	478	ionic	3.38
	O	LYS	478	ionic	3.55
23	N	PRO	479	H-donor	2.46
	O	CYS	488	H-donor	4.04
	O	GLN	474	H-acceptor	3.05
	N	LYS	478	ionic	3.3
	O	LYS	478	ionic	3
24	N	PHE	486	H-donor	2.87
	O	CYS	480	H-donor	2.21
	CL	GLN	474	H-donor	2.49
	N	PHE	486	H-acceptor	2.91
	O	PHE	486	H-acceptor	2.62
	N	LYS	478	ionic	2.86
	N	LYS	478	ionic	2.82
	O	LYS	478	ionic	3.75

25	N	LYS	478	ionic	2.57
	N	LYS	478	ionic	2.08
	O	LYS	478	ionic	3.9
26	N	CYS	480	H-donor	2.24
	N	PHE	486	H-donor	3
	O	CYS	480	H-donor	2.55
	O	CYS	480	H-donor	3.53
	N	LYS	478	H-acceptor	3.29
	N	LYS	478	ionic	3.51
	N	LYS	478	ionic	3.29
27	N	CYS	480	H-donor	4.18
	N	CYS	480	H-donor	3.62
	C	ALA	475	H-donor	2.87
	N	LYS	478	ionic	1.88
	N	LYS	478	ionic	2.83
	O	LYS	478	ionic	1.95
28	N	LYS	478	ionic	1.64
	N	LYS	478	ionic	2.49
	O	LYS	478	ionic	2.58
	O	LYS	478	ionic	3.07
29	N	CYS	480	H-donor	2.9
	N	CYS	480	H-donor	2.59
	O	LYS	478	H-acceptor	2.75
	O	PHE	486	H-acceptor	3.04
	N	LYS	478	ionic	3.3
	O	LYS	478	ionic	2.75
30	N	LYS	478	ionic	2.6
	N	LYS	478	ionic	1.57
	O	LYS	478	ionic	1.86

Table S7. Interaction report of each conformer of compound V6. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD	Interaction	Distance	
1	O	CYS	488	H-donor	3.83
	O	PHE	486	H-acceptor	2.61
	N	LYS	478	ionic	2.1
	N	LYS	478	ionic	1.57
	O	LYS	478	ionic	3.98
	O	LYS	478	ionic	2.63
2	N	CYS	480	H-donor	4.21

	O	CYS	480	H-donor	2.5
	O	CYS	488	H-donor	3.11
	N	LYS	478	ionic	2.05
	N	LYS	478	ionic	1.7
	O	LYS	478	ionic	3.84
	O	LYS	478	ionic	3.01
3	N	LYS	478	H-acceptor	1.8
	N	LYS	478	ionic	2.59
	N	LYS	478	ionic	1.8
	O	LYS	478	ionic	3.87
4	N	CYS	480	H-donor	2.67
	N	CYS	480	H-donor	2.88
	N	LYS	478	H-acceptor	2.86
	O	PHE	486	H-acceptor	3.3
	N	LYS	478	ionic	2.86
	N	LYS	478	ionic	3.16
	O	LYS	478	ionic	3.85
	O	LYS	478	ionic	3.61
5	O	CYS	480	H-donor	3.55
	O	CYS	488	H-donor	3.44
	N	LYS	478	ionic	1.66
	N	LYS	478	ionic	1.41
	O	LYS	478	ionic	3.19
	O	LYS	478	ionic	3.21
6	N	CYS	480	H-donor	3.61
	O	PHE	486	H-acceptor	2.7
	N	LYS	478	ionic	2.73
	N	LYS	478	ionic	3.16
	O	LYS	478	ionic	3.33
7	O	CYS	488	H-donor	2.31
	N	LYS	478	ionic	2.16
	N	LYS	478	ionic	1.42
	O	LYS	478	ionic	3.92
	O	LYS	478	ionic	3.47
8	N	CYS	480	H-donor	3.08
	N	CYS	480	H-donor	2.63
	N	LYS	478	H-acceptor	2.84
	N	PHE	486	H-acceptor	3.58
	N	LYS	478	ionic	2.84
	N	LYS	478	ionic	2.96

	O	LYS	478	ionic	3.45
9	N	LYS	478	ionic	1.26
	N	LYS	478	ionic	2.07
	O	LYS	478	ionic	2.44
	O	LYS	478	ionic	3.96
10	N	CYS	480	H-donor	2.45
	N	CYS	480	H-donor	3.55
	O	LYS	478	H-acceptor	2.63
	N	LYS	478	ionic	2.81
	N	LYS	478	ionic	3.12
	O	LYS	478	ionic	2.63
	6-ring	VAL	483	pi-H	3.78
11	N	CYS	480	H-donor	2.77
	N	CYS	480	H-donor	3.29
	O	LYS	478	H-acceptor	2.3
	N	LYS	478	ionic	2.69
	N	LYS	478	ionic	2.82
	O	LYS	478	ionic	2.3
12	N	CYS	480	H-donor	2.45
	N	CYS	480	H-donor	2.79
	N	LYS	478	H-acceptor	3.02
	O	PHE	486	H-acceptor	3.53
	O	CYS	488	H-acceptor	2.88
	N	LYS	478	ionic	3.02
	N	LYS	478	ionic	3.34
	O	LYS	478	ionic	3.88
	O	LYS	478	ionic	3.9
13	BR	GLY	482	H-donor	1.55
	N	LYS	478	H-acceptor	2.14
	N	LYS	478	ionic	2.71
	N	LYS	478	ionic	2.14
14	N	LYS	478	ionic	1.98
	N	LYS	478	ionic	1.71
	O	LYS	478	ionic	3.8
	O	LYS	478	ionic	2.56
15	N	PHE	486	H-acceptor	3.61
	N	LYS	478	H-acceptor	1.74
	O	GLY	485	H-acceptor	2.71
	O	GLY	485	H-acceptor	2.78
	O	PHE	486	H-acceptor	3.04

	N	LYS	478	ionic	2.77
	N	LYS	478	ionic	1.74
	O	LYS	478	ionic	2.6
16	N	CYS	480	H-donor	3.06
	N	CYS	488	H-donor	2.81
	O	CYS	480	H-donor	3.75
	N	LYS	478	H-acceptor	2.5
	O	GLY	485	H-acceptor	3.11
	O	LYS	478	H-acceptor	2.58
	N	LYS	478	ionic	2.81
	N	LYS	478	ionic	2.5
	O	LYS	478	ionic	3.91
	O	LYS	478	ionic	3.81
17	O	PHE	486	H-acceptor	3.3
	N	LYS	478	ionic	2.02
	N	LYS	478	ionic	2.05
	O	LYS	478	ionic	3.06
	O	LYS	478	ionic	3.82
18	O	CYS	480	H-donor	1.89
	BR	GLN	474	H-donor	2.3
	N	LYS	478	ionic	2.77
	N	LYS	478	ionic	2.39
	O	LYS	478	ionic	3.57
19	N	CYS	480	H-donor	2.77
	N	CYS	480	H-donor	2.97
	O	CYS	480	H-donor	3.32
	N	LYS	478	H-acceptor	2.17
	O	CYS	480	H-acceptor	3.15
	N	LYS	478	ionic	2.17
	N	LYS	478	ionic	3.26
	O	LYS	478	ionic	1.92
20	O	PHE	486	H-acceptor	3.1
	O	ASN	487	H-acceptor	2.07
	N	LYS	478	ionic	2.45
	N	LYS	478	ionic	2.21
	O	LYS	478	ionic	3.9
	O	LYS	478	ionic	3.57
21	N	CYS	480	H-donor	2.27
	O	CYS	480	H-donor	3.09
	N	LYS	478	H-acceptor	2.86

	N	LYS	478	ionic	3.24
	N	LYS	478	ionic	2.86
	O	LYS	478	ionic	3.83
22	N	CYS	480	H-donor	3.7
	O	CYS	480	H-donor	3.91
	N	PHE	486	H-acceptor	3.37
	O	ASN	487	H-acceptor	2.59
	N	LYS	478	ionic	2.43
	N	LYS	478	ionic	2.16
	O	LYS	478	ionic	3.18
23	N	LYS	478	ionic	2.47
	N	LYS	478	ionic	1.48
	O	LYS	478	ionic	2.07
24	N	CYS	480	H-donor	2.62
	N	CYS	488	H-donor	2.66
	O	CYS	480	H-donor	3.26
	N	LYS	478	H-acceptor	2.57
	O	GLY	485	H-acceptor	3.03
	N	LYS	478	ionic	3.28
	N	LYS	478	ionic	2.57
O	LYS	478	ionic	3.22	
25	N	LYS	478	ionic	2.28
	N	LYS	478	ionic	2.03
	O	LYS	478	ionic	3.88
	O	LYS	478	ionic	3.18
26	O	CYS	480	H-donor	3.04
	O	CYS	488	H-donor	2.46
	N	PHE	486	H-acceptor	2.67
	N	PHE	486	H-acceptor	3.11
	N	LYS	478	ionic	2.67
	N	LYS	478	ionic	3.05
	O	LYS	478	ionic	3.41
	6-ring	VAL	483	pi-H	4.01
	6-ring	GLY	485	pi-H	4.79
27	N	CYS	480	H-donor	1.88
	N	CYS	480	H-donor	2.8
	O	CYS	480	H-donor	2.65
	N	LYS	478	H-acceptor	3.13
	O	LYS	478	H-acceptor	3.22
	O	PHE	486	H-acceptor	3.02

	N	LYS	478	ionic	3.13
	N	LYS	478	ionic	3.84
	O	LYS	478	ionic	3.22
28	N	LYS	478	H-acceptor	2.14
	N	LYS	478	ionic	2.14
	N	LYS	478	ionic	2.62
	O	LYS	478	ionic	3.4
	O	LYS	478	ionic	2.66
29	N	LYS	478	H-acceptor	2.41
	N	LYS	478	ionic	2.61
	N	LYS	478	ionic	2.41
	O	LYS	478	ionic	3.68
	6-ring	PHE	486	pi-pi	3.92

Table S8. Interaction report of each conformer of compound V7. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD		Interaction	Distance
1	S	CYS	488	H-donor	2.98
	BR	ASN	481	H-donor	2.24
	S	PHE	486	H-acceptor	2.5
	N	LYS	478	ionic	0.93
	N	LYS	478	ionic	0.89
	S	LYS	478	ionic	3.37
	O	LYS	478	ionic	2.95
	6-ring	ASN	481	pi-H	4.36
2	BR	ASN	481	H-donor	2.74
	S	GLY	485	H-acceptor	3.25
	S	PHE	486	H-acceptor	2.98
	S	PHE	486	H-acceptor	3.87
	N	LYS	478	ionic	1.62
	N	LYS	478	ionic	1.31
	S	LYS	478	ionic	3.78
	O	LYS	478	ionic	2.99
3	S	CYS	480	H-donor	4.13
	S	GLY	485	H-acceptor	3.1
	O	PHE	486	H-acceptor	3
	N	LYS	478	ionic	2.17
	N	LYS	478	ionic	1.16
	O	LYS	478	ionic	2.51
4	S	CYS	488	H-donor	4.25

	N	PHE	486	H-acceptor	3.61
	S	PHE	486	H-acceptor	3.26
	N	LYS	478	ionic	2.25
	N	LYS	478	ionic	1.21
	O	LYS	478	ionic	2.54
5	N	CYS	480	H-donor	3.51
	N	CYS	480	H-donor	3.16
	N	LYS	478	H-acceptor	2
	S	GLY	485	H-acceptor	4.13
	S	PHE	486	H-acceptor	3.91
	CL	ASN	481	H-acceptor	2.65
	N	LYS	478	ionic	2
	N	LYS	478	ionic	2.54
	S	LYS	478	ionic	3.26
	O	LYS	478	ionic	3.14
6	S	ASN	487	H-acceptor	3.34
	S	ASN	487	H-acceptor	3.71
	O	LYS	478	H-acceptor	2.21
	CL	LYS	478	H-acceptor	3.58
	N	LYS	478	ionic	2.08
	N	LYS	478	ionic	1.07
	O	LYS	478	ionic	2.21
7	S	GLY	485	H-acceptor	3.86
	S	PHE	486	H-acceptor	3.47
	S	PHE	486	H-acceptor	4.32
	N	LYS	478	ionic	1.35
	N	LYS	478	ionic	2.03
	S	LYS	478	ionic	2.88
8	N	LYS	478	H-acceptor	2.73
	N	LYS	478	H-acceptor	2.26
	S	CYS	480	H-acceptor	2.92
	N	LYS	478	ionic	2.77
	N	LYS	478	ionic	2.26
9	S	CYS	480	H-donor	3.8
	S	CYS	488	H-donor	2.03
	N	PHE	486	H-acceptor	3.06
	S	CYS	488	H-acceptor	4.26
	CL	LYS	478	H-acceptor	3.35
	N	LYS	478	ionic	2.28
	N	LYS	478	ionic	1.34

	O	LYS	478	ionic	3.23
10	N	LYS	478	H-acceptor	2.26
	S	LYS	478	H-acceptor	3.47
	S	CYS	480	H-acceptor	3.43
	N	LYS	478	ionic	2.35
	N	LYS	478	ionic	2.26
11	S	LYS	478	H-acceptor	2.37
	S	CYS	480	H-acceptor	4.02
	O	PHE	486	H-acceptor	2.69
	N	LYS	478	ionic	2.19
	N	LYS	478	ionic	3.06
	S	LYS	478	ionic	2.84
	O	LYS	478	ionic	3.26
12	N	CYS	488	H-donor	3.65
	S	CYS	480	H-donor	2.28
	S	CYS	488	H-donor	2.47
	S	LYS	484	H-acceptor	3.31
	S	GLY	485	H-acceptor	3.15
	N	LYS	478	ionic	2.38
	N	LYS	478	ionic	1.55
	O	LYS	478	ionic	2.04
13	O	CYS	480	H-donor	2.22
	N	PHE	486	H-acceptor	2.82
	S	GLY	485	H-acceptor	3.32
	N	LYS	478	ionic	2.5
	N	LYS	478	ionic	2.32
	O	LYS	478	ionic	3.35
14	N	LYS	478	ionic	2.61
	N	LYS	478	ionic	1.7
	O	LYS	478	ionic	3.68
15	N	CYS	480	H-donor	3.46
	N	CYS	480	H-donor	3.13
	N	LYS	478	H-acceptor	2.4
	N	PHE	486	H-acceptor	3.69
	S	GLY	485	H-acceptor	3.57
	S	PHE	486	H-acceptor	3.75
	N	LYS	478	ionic	2.4
	N	LYS	478	ionic	2.64
	S	LYS	478	ionic	3.84
	O	LYS	478	ionic	3.23

16	N	PHE	486	H-acceptor	3.09
	S	LYS	478	H-acceptor	3.19
	N	LYS	478	ionic	2.31
	N	LYS	478	ionic	2.81
	S	LYS	478	ionic	3.39
17	N	CYS	480	H-donor	3.44
	O	CYS	480	H-donor	2.01
	S	GLY	485	H-acceptor	4.23
	S	PHE	486	H-acceptor	3.61
	S	PHE	486	H-acceptor	4.04
	N	LYS	478	ionic	1.7
	N	LYS	478	ionic	2.34
	S	LYS	478	ionic	2.89
	O	LYS	478	ionic	3.76
18	S	GLY	485	H-acceptor	3.69
	S	PHE	486	H-acceptor	3.54
	N	LYS	478	ionic	1.92
	N	LYS	478	ionic	1.8
	S	LYS	478	ionic	3.9
	O	LYS	478	ionic	3.15
19	N	CYS	480	H-donor	3.26
	N	CYS	480	H-donor	3.05
	N	LYS	478	H-acceptor	2.78
	N	PHE	486	H-acceptor	3.35
	S	GLY	485	H-acceptor	2.65
	S	PHE	486	H-acceptor	2.52
	N	LYS	478	ionic	2.78
	N	LYS	478	ionic	3.05
	S	LYS	478	ionic	3.95
	O	LYS	478	ionic	3.81
20	N	LYS	478	H-acceptor	2.22
	O	LYS	478	H-acceptor	2.61
	N	LYS	478	ionic	3.15
	N	LYS	478	ionic	2.22
	O	LYS	478	ionic	2.61
21	O	CYS	480	H-donor	2.32
	N	LYS	478	H-acceptor	2.12
	N	PHE	486	H-acceptor	3.38
	S	GLY	485	H-acceptor	3.5
	S	PHE	486	H-acceptor	3.18

	S	PHE	486	H-acceptor	4.07
	N	LYS	478	ionic	2.12
	N	LYS	478	ionic	2.51
	S	LYS	478	ionic	3.36
	O	LYS	478	ionic	3.61
22	N	LYS	478	ionic	1.83
	N	LYS	478	ionic	1.92
	S	LYS	478	ionic	3.53
	O	LYS	478	ionic	3.62
23	N	CYS	488	H-donor	3.46
	S	CYS	480	H-donor	3.16
	S	CYS	488	H-donor	3.53
	S	GLY	485	H-acceptor	3.19
	N	LYS	478	ionic	2.04
	N	LYS	478	ionic	1.69
	O	LYS	478	ionic	3.07
24	N	LYS	478	H-acceptor	2.03
	S	GLY	485	H-acceptor	3.92
	S	PHE	486	H-acceptor	4.12
	N	LYS	478	ionic	2.03
	N	LYS	478	ionic	2.45
	S	LYS	478	ionic	3.52
	O	LYS	478	ionic	3.87
25	S	PRO	479	H-acceptor	3.85
	S	CYS	480	H-acceptor	3.13
	N	LYS	478	ionic	3
	N	LYS	478	ionic	2.44
	O	LYS	478	ionic	2.72
26	N	LYS	478	ionic	2.12
	N	LYS	478	ionic	2.54
	S	LYS	478	ionic	3.35
	O	LYS	478	ionic	3.9
27	N	LYS	478	ionic	2.48
	N	LYS	478	ionic	1.72
	O	LYS	478	ionic	2.49
28	N	CYS	480	H-donor	3.26
	O	CYS	480	H-donor	1.89
	N	PHE	486	H-acceptor	3.65
	N	LYS	478	H-acceptor	2.3
	S	GLY	485	H-acceptor	4.17

	N	LYS	478	ionic	2.73
	N	LYS	478	ionic	2.3
	O	LYS	478	ionic	3.57
29	O	CYS	480	H-donor	2.91
	CL	PRO	479	H-donor	2.93
	N	PHE	486	H-acceptor	2.82
	N	LYS	478	H-acceptor	2.42
	S	GLY	485	H-acceptor	3.39
	N	LYS	478	ionic	2.36
	N	LYS	478	ionic	2.42
	S	LYS	478	ionic	3.89
	O	LYS	478	ionic	3.01
	30	N	CYS	480	H-donor
N		LYS	478	H-acceptor	3
S		GLY	485	H-acceptor	2.91
S		PHE	486	H-acceptor	3.58
O		CYS	488	H-acceptor	3.03
N		LYS	478	ionic	3
N		LYS	478	ionic	3.19
O		LYS	478	ionic	3.67

Table S9. Interaction report of each conformer of compound V8. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD	Interaction	Distance	
1	S	CYS	480	H-donor	3.63
	S	CYS	488	H-donor	3.44
	S	PHE	486	H-acceptor	3.96
	N	LYS	478	ionic	1.03
	N	LYS	478	ionic	2.03
	S	LYS	478	ionic	2.45
2	C	GLY	482	H-donor	2.34
	S	CYS	480	H-donor	2.88
	S	CYS	488	H-donor	3.4
	N	LYS	478	H-acceptor	1.5
	S	LYS	478	H-acceptor	2.7
	O	LYS	478	H-acceptor	2.41
	N	LYS	478	ionic	2.47
	N	LYS	478	ionic	1.5
	S	LYS	478	ionic	2.7
3	C	GLY	482	H-donor	2.59

	S	CYS	480	H-donor	3.18
	S	CYS	488	H-donor	3.61
	O	LYS	478	H-acceptor	2.8
	N	LYS	478	ionic	2.39
	N	LYS	478	ionic	1.24
	S	LYS	478	ionic	2.3
4	S	PHE	486	H-acceptor	4.15
	S	PHE	486	H-acceptor	3.83
	S	PRO	479	H-acceptor	3.69
	N	LYS	478	ionic	1.67
	N	LYS	478	ionic	1.72
	S	LYS	478	ionic	3.47
5	S	LYS	478	ionic	3.93
	S	GLY	485	H-acceptor	3.91
	S	PHE	486	H-acceptor	3.48
	S	PHE	486	H-acceptor	3.95
	N	LYS	478	ionic	1.79
	N	LYS	478	ionic	1.7
6	S	LYS	478	ionic	3.68
	S	LYS	478	ionic	3.77
	S	GLY	485	H-acceptor	3.64
	S	PHE	486	H-acceptor	3.03
	S	PHE	486	H-acceptor	3.65
	N	LYS	478	ionic	1.82
7	N	LYS	478	ionic	1.53
	S	LYS	478	ionic	3.97
	S	LYS	478	ionic	3.36
	S	GLY	485	H-acceptor	4.07
	S	PHE	486	H-acceptor	4.07
	N	LYS	478	ionic	1.62
8	N	LYS	478	ionic	1.87
	S	LYS	478	ionic	3.45
	S	LYS	478	ionic	3.95
	S	LYS	478	ionic	1.83
9	N	LYS	478	ionic	1.7
	S	LYS	478	ionic	3.74
	S	LYS	478	ionic	3.73
	S	PHE	486	H-acceptor	3.84
	S	PRO	479	H-acceptor	3.37
	N	LYS	478	ionic	1.55

	N	LYS	478	ionic	2.21
	S	LYS	478	ionic	2.83
10	S	LYS	478	H-acceptor	2.51
	S	GLY	485	H-acceptor	3.71
	N	LYS	478	ionic	1.61
	N	LYS	478	ionic	2.18
	S	LYS	478	ionic	3.03
		N	LYS	478	H-acceptor
11	S	GLY	485	H-acceptor	4.31
	S	PHE	486	H-acceptor	3.24
	S	LYS	478	H-acceptor	2.99
	S	CYS	480	H-acceptor	4.34
	N	LYS	478	ionic	2.25
	N	LYS	478	ionic	1.88
	S	LYS	478	ionic	3.68
		N	LYS	478	ionic
12	N	LYS	478	ionic	1.82
	S	LYS	478	ionic	3.23
		S	CYS	480	H-donor
13	N	LYS	478	H-acceptor	1.75
	N	LYS	478	ionic	1.48
	N	LYS	478	ionic	1.75
	S	LYS	478	ionic	3.11
		S	PHE	486	H-acceptor
14	S	PHE	486	H-acceptor	3.75
	N	LYS	478	ionic	1.77
	N	LYS	478	ionic	2.26
	S	LYS	478	ionic	2.94
		O	LYS	478	H-acceptor
15	N	LYS	478	ionic	2.61
	N	LYS	478	ionic	2.1
	S	LYS	478	ionic	3.43
		S	ALA	475	H-donor
16	S	GLN	474	H-acceptor	4.4
	S	ASN	487	H-acceptor	2.73
	S	ASN	487	H-acceptor	3.23
	N	LYS	478	ionic	2.55
	N	LYS	478	ionic	1.33
	S	LYS	478	ionic	1.78
		N	LYS	478	H-acceptor

	S	LYS	478	H-acceptor	3.25
	S	CYS	480	H-acceptor	4.01
	N	LYS	478	ionic	2.73
	N	LYS	478	ionic	2.23
	S	LYS	478	ionic	3.7
18	S	GLY	485	H-acceptor	3.12
	S	GLY	485	H-acceptor	3.09
	S	PHE	486	H-acceptor	4.24
	S	LYS	478	H-acceptor	2.8
	N	LYS	478	ionic	2.76
	N	LYS	478	ionic	2.18
	S	LYS	478	ionic	2.95
19	N	LYS	478	H-acceptor	2.48
	S	GLY	485	H-acceptor	3.85
	N	LYS	478	ionic	3.04
	N	LYS	478	ionic	2.48
	S	LYS	478	ionic	3.65
	5-ring	PHE	486	pi-pi	3.94
20	S	PHE	486	H-acceptor	4.12
	S	PHE	486	H-acceptor	4.28
	S	PRO	479	H-acceptor	4.47
	N	LYS	478	ionic	1.96
	N	LYS	478	ionic	2.18
	S	LYS	478	ionic	3.46
	5-ring	PHE	486	pi-pi	3.44
21	S	CYS	480	H-donor	2.1
	C	PHE	486	H-donor	2.85
	S	CYS	480	H-acceptor	3.78
	S	ASN	481	H-acceptor	4.35
	N	LYS	478	ionic	2.65
	N	LYS	478	ionic	2.77
22	N	LYS	478	ionic	1.76
	N	LYS	478	ionic	2.05
	S	LYS	478	ionic	3.27
23	N	LYS	478	H-acceptor	3
	S	GLY	485	H-acceptor	3.77
	O	LYS	478	H-acceptor	2.65
	N	LYS	478	ionic	3.93
	N	LYS	478	ionic	3
	S	LYS	478	ionic	3.09

24	S	LYS	478	H-acceptor	3.27
	O	LYS	478	H-acceptor	2.44
	N	LYS	478	ionic	2.99
	N	LYS	478	ionic	2.34
	S	LYS	478	ionic	3.27
25	S	PRO	479	H-acceptor	4.12
	S	PHE	486	H-acceptor	4.5
	N	LYS	478	ionic	2.53
	N	LYS	478	ionic	1.7
	S	LYS	478	ionic	2.51
26	S	PRO	479	H-acceptor	4.12
	S	PHE	486	H-acceptor	3.13
	N	LYS	478	ionic	2.23
	N	LYS	478	ionic	1.51
	S	LYS	478	ionic	2.65
27	S	CYS	488	H-donor	4.39
	S	LYS	478	H-acceptor	3.55
	S	PHE	486	H-acceptor	2.1
	N	LYS	478	ionic	3.03
	N	LYS	478	ionic	2.46
	S	LYS	478	ionic	3.55
28	N	PHE	486	H-acceptor	3.07
	S	PHE	486	H-acceptor	2.87
	N	LYS	478	ionic	2.56
	N	LYS	478	ionic	2.5
	S	LYS	478	ionic	3.86
29	N	LYS	484	ionic	2.16
	N	LYS	484	ionic	3.2
	S	LYS	484	ionic	1.99

Table S10. Interaction report of each conformer of compound V9. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD		Interaction	Distance
1	O	CYS	480	H-donor	3.87
	O	CYS	488	H-donor	3.14
	O	PHE	486	H-acceptor	3.2
	N	LYS	478	ionic	1.37
	N	LYS	478	ionic	0.77
	O	LYS	478	ionic	3.33
	O	LYS	478	ionic	2.87

2	O	GLY	482	H-acceptor	2.16
	N	LYS	484	ionic	1.03
	N	LYS	484	ionic	1.67
	O	LYS	484	ionic	2.69
	O	LYS	484	ionic	2.45
	6-ring	GLU	471	pi-H	4.07
3	O	GLY	485	H-acceptor	3.1
	N	LYS	478	ionic	2.21
	N	LYS	478	ionic	1.2
	O	LYS	478	ionic	2.26
4	O	CYS	488	H-donor	3.3
	O	ASN	487	H-acceptor	2.87
	O	PHE	486	H-acceptor	2.92
	CL	LYS	478	H-acceptor	3.68
	N	LYS	478	ionic	2.04
	N	LYS	478	ionic	1.18
	O	LYS	478	ionic	3.94
	O	LYS	478	ionic	3.05
5	N	LYS	478	ionic	1.4
	N	LYS	478	ionic	1.95
	O	LYS	478	ionic	2.55
	O	LYS	478	ionic	3.48
6	O	CYS	488	H-donor	4.23
	O	LYS	478	H-acceptor	2.76
	O	PHE	486	H-acceptor	2.56
	N	LYS	478	ionic	2.39
	N	LYS	478	ionic	1.75
	O	LYS	478	ionic	2.76
7	CL	PHE	486	H-donor	2.69
	N	LYS	478	H-acceptor	1.79
	CL	LYS	478	H-acceptor	2.77
	N	LYS	478	ionic	2.16
	N	LYS	478	ionic	1.79
	O	LYS	478	ionic	3.56
	O	LYS	478	ionic	3.32
8	N	LYS	478	H-acceptor	1.7
	O	GLY	485	H-acceptor	3.26
	O	PHE	486	H-acceptor	3.45
	N	LYS	478	ionic	1.8
	N	LYS	478	ionic	1.7

	O	LYS	478	ionic	3.19
	O	LYS	478	ionic	3.74
9	O	CYS	488	H-donor	4.24
	O	LYS	478	H-acceptor	2.15
	O	PHE	486	H-acceptor	3.01
	N	LYS	478	ionic	1.75
	N	LYS	478	ionic	2.61
	O	LYS	478	ionic	2.15
10	N	LYS	478	H-acceptor	2.27
	O	LYS	478	H-acceptor	2.96
	N	LYS	478	ionic	3.07
	N	LYS	478	ionic	2.27
	O	LYS	478	ionic	2.96
11	N	CYS	480	H-donor	3.03
	N	CYS	480	H-donor	2.64
	N	LYS	478	H-acceptor	2.9
	O	PHE	486	H-acceptor	3.16
	N	LYS	478	ionic	2.9
	N	LYS	478	ionic	3.21
	O	LYS	478	ionic	3.79
	O	LYS	478	ionic	3.69
12	N	LYS	478	H-acceptor	2.67
	O	LYS	478	H-acceptor	3.07
	O	PHE	486	H-acceptor	2.9
	N	LYS	478	ionic	2.67
	N	LYS	478	ionic	3.45
	O	LYS	478	ionic	3.17
	O	LYS	478	ionic	3.31
13	N	CYS	480	H-donor	2.68
	O	CYS	480	H-donor	3.37
	N	LYS	478	H-acceptor	2.37
	O	LYS	478	H-acceptor	2.57
	N	LYS	478	ionic	3.26
	N	LYS	478	ionic	2.37
	O	LYS	478	ionic	2.57
14	O	CYS	480	H-donor	3.05
	O	CYS	488	H-donor	3.44
	CL	GLY	476	H-donor	3.01
	O	GLY	485	H-acceptor	3.17
	N	LYS	478	ionic	2.73

	N	LYS	478	ionic	2.18
	O	LYS	478	ionic	3.24
15	N	CYS	480	H-donor	3.24
	N	CYS	480	H-donor	2.81
	N	LYS	478	H-acceptor	2.62
	O	LYS	478	H-acceptor	3.01
	N	LYS	478	ionic	2.62
	N	LYS	478	ionic	2.81
	O	LYS	478	ionic	3.82
	O	LYS	478	ionic	3.01
	16	O	CYS	480	H-donor
N		PHE	486	H-acceptor	2.62
N		PHE	486	H-acceptor	3.15
N		LYS	478	ionic	2.6
N		LYS	478	ionic	2.25
O		LYS	478	ionic	2.75
17	N	LYS	478	H-acceptor	1.59
	N	LYS	478	ionic	1.59
	N	LYS	478	ionic	2.74
	O	LYS	478	ionic	1.84
18	N	CYS	480	H-donor	3.35
	N	CYS	480	H-donor	1.99
	O	CYS	480	H-donor	2.12
	N	LYS	478	H-acceptor	2.66
	O	LYS	478	H-acceptor	2.99
	CL	ASN	481	H-acceptor	2.51
	N	LYS	478	ionic	2.66
	N	LYS	478	ionic	3.46
	O	LYS	478	ionic	2.99
19	N	LYS	478	ionic	2.63
	N	LYS	478	ionic	2.51
	O	LYS	478	ionic	3.71
20	N	CYS	480	H-donor	3.37
	N	CYS	488	H-donor	3.24
	O	CYS	480	H-donor	2.95
	O	CYS	480	H-donor	4.13
	N	LYS	478	H-acceptor	2.46
	N	PHE	486	H-acceptor	3.61
	O	GLY	485	H-acceptor	3.29
	O	ASN	487	H-acceptor	2.97

	N	LYS	478	ionic	3.14
	N	LYS	478	ionic	2.46
	O	LYS	478	ionic	2.93
21	N	LYS	478	ionic	2.97
	N	LYS	478	ionic	1.99
	O	LYS	478	ionic	2.39
22	N	CYS	480	H-donor	2.88
	N	CYS	488	H-donor	2.66
	O	CYS	480	H-donor	2.79
	O	CYS	488	H-donor	3.25
	N	LYS	478	H-acceptor	2.56
	O	GLY	485	H-acceptor	3.26
	O	ASN	487	H-acceptor	3.5
	N	LYS	478	ionic	2.98
	N	LYS	478	ionic	2.56
O	LYS	478	ionic	3.7	
23	O	CYS	488	H-donor	2.01
	N	LYS	478	ionic	3.28
	N	LYS	478	ionic	3.18
	O	LYS	478	ionic	3.56
24	N	CYS	480	H-donor	1.97
	O	CYS	480	H-donor	2.71
	O	CYS	480	H-donor	3.08
	N	LYS	478	H-acceptor	3.49
	O	GLY	485	H-acceptor	3.28
	N	LYS	478	ionic	3.9
25	N	LYS	478	ionic	3.49
	N	LYS	478	ionic	1.9
	N	LYS	478	ionic	1.78
	O	LYS	478	ionic	3.38
26	O	LYS	478	ionic	3.43
	N	LYS	478	ionic	2.08
	N	LYS	478	ionic	2.47
27	O	LYS	478	ionic	2.88
	O	CYS	480	H-donor	3.22
	N	LYS	478	H-acceptor	3.24
	O	GLY	485	H-acceptor	3.07
	N	LYS	478	ionic	3.24
	N	LYS	478	ionic	3.4
O	LYS	478	ionic	3.89	

	O	LYS	478	ionic	3.28
28	O	CYS	480	H-donor	2.63
	N	PHE	486	H-acceptor	3.24
	N	LYS	478	ionic	2.68
	N	LYS	478	ionic	3.13
	O	LYS	478	ionic	3.48
29	O	CYS	480	H-donor	1.85
	O	CYS	488	H-donor	2.86
	N	LYS	478	ionic	3.44
	N	LYS	478	ionic	2.87
30	O	CYS	480	H-donor	3.21
	CL	LYS	478	H-acceptor	2.46
	N	LYS	478	ionic	3.12
	N	LYS	478	ionic	2.24
	O	LYS	478	ionic	2.78

Table S11. Interaction report of each conformer of compound V10. Number of conformer, Atom of compound, Residue in RBD, Type of interaction and Distance in angstroms.

Conformer	Ligand	Residues in RBD		Interaction	Distance
1	S	CYS	488	H-donor	3.22
	S	PHE	486	H-acceptor	1.96
	N	LYS	478	ionic	1.01
	N	LYS	478	ionic	1.46
	S	LYS	478	ionic	3.05
	S	LYS	478	ionic	3.92
2	S	GLY	485	H-acceptor	3.69
	S	PHE	486	H-acceptor	3.08
	S	PHE	486	H-acceptor	3.63
	N	LYS	478	ionic	1.49
	N	LYS	478	ionic	1.4
	S	LYS	478	ionic	3.69
	S	LYS	478	ionic	3.44
3	S	CYS	480	H-donor	3.55
	S	CYS	488	H-donor	3.27
	S	PHE	486	H-acceptor	3.8
	N	LYS	478	ionic	1.3
	N	LYS	478	ionic	2.05
	S	LYS	478	ionic	2.77
	6-ring	GLY	485	pi-H	4.13
4	S	CYS	488	H-donor	4.27

	S	PHE	486	H-acceptor	3.22
	N	LYS	478	ionic	1.36
	N	LYS	478	ionic	2.34
	S	LYS	478	ionic	2.34
5	S	CYS	488	H-donor	4.21
	S	LYS	478	H-acceptor	2.32
	S	PHE	486	H-acceptor	3.28
	N	LYS	478	ionic	1.46
	N	LYS	478	ionic	2.49
	S	LYS	478	ionic	2.32
6	S	CYS	488	H-donor	3.93
	S	PHE	486	H-acceptor	2.8
	N	LYS	478	ionic	1.5
	N	LYS	478	ionic	2.05
	S	LYS	478	ionic	3.08
7	N	LYS	478	H-acceptor	1.64
	S	LYS	478	H-acceptor	2.05
	N	LYS	478	ionic	2.66
	N	LYS	478	ionic	1.64
	S	LYS	478	ionic	2.51
8	S	ASN	487	H-acceptor	3.05
	N	LYS	478	ionic	1.68
	N	LYS	478	ionic	1.72
	S	LYS	478	ionic	3.41
9	C	ASN	481	H-donor	2.92
	S	PRO	479	H-acceptor	4.23
	S	GLY	485	H-acceptor	4.21
	S	PHE	486	H-acceptor	3.91
	S	PHE	486	H-acceptor	4.42
	N	LYS	478	ionic	2.12
	N	LYS	478	ionic	1.8
	S	LYS	478	ionic	3.5
10	N	LYS	478	H-acceptor	1.72
	N	LYS	478	ionic	1.72
	N	LYS	478	ionic	2.64
	S	LYS	478	ionic	2.54
11	C	ASN	481	H-donor	2.52
	S	GLY	485	H-acceptor	3.59
	N	LYS	478	ionic	1.54
	N	LYS	478	ionic	2.48

	S	LYS	478	ionic	2.25
12	S	CYS	480	H-donor	3.14
	S	LYS	478	H-acceptor	3.29
	S	GLN	474	H-acceptor	4.44
	N	LYS	478	ionic	2.03
	N	LYS	478	ionic	2.64
	S	LYS	478	ionic	3.29
13	N	PHE	486	H-donor	2.98
	C	GLY	476	H-donor	2.39
	N	PHE	486	H-acceptor	2.84
	S	CYS	480	H-acceptor	3.78
	S	ASN	481	H-acceptor	4.44
	N	LYS	478	ionic	2.77
14	N	LYS	478	ionic	2.76
	C	GLY	482	H-donor	2.81
	S	CYS	480	H-donor	4.32
	S	CYS	488	H-donor	3.44
	S	LYS	478	H-acceptor	2.58
	S	PHE	486	H-acceptor	3.13
	N	LYS	478	ionic	1.9
	N	LYS	478	ionic	2.77
15	S	LYS	478	ionic	2.58
	N	PHE	486	H-acceptor	2.76
	N	LYS	478	ionic	2.1
	N	LYS	478	ionic	2.14
16	S	LYS	478	ionic	3.71
	S	PHE	486	H-acceptor	4.15
	S	PRO	479	H-acceptor	3.21
	N	LYS	478	ionic	1.69
	N	LYS	478	ionic	2.76
	S	LYS	478	ionic	2.08
17	6-ring	CYS	480	pi-H	4.15
	S	CYS	480	H-donor	4.16
	S	CYS	488	H-donor	3.41
	S	PHE	486	H-acceptor	4.18
	S	ASN	487	H-acceptor	4.34
	N	LYS	478	ionic	1.73
	N	LYS	478	ionic	2.66
18	S	LYS	478	ionic	2.08
	N	LYS	478	H-acceptor	2.35

	N	LYS	478	H-acceptor	2.54
	S	LYS	478	H-acceptor	3.31
	S	CYS	480	H-acceptor	3.8
	N	LYS	478	ionic	2.35
	N	LYS	478	ionic	2.54
19	S	GLU	471	H-acceptor	4.46
	N	LYS	484	ionic	3.25
	N	LYS	484	ionic	1.95
	S	LYS	484	ionic	1.18
20	N	CYS	480	H-donor	2.57
	S	CYS	488	H-donor	3.49
	S	ASN	481	H-acceptor	3.09
	S	LYS	478	H-acceptor	2.42
	S	PHE	486	H-acceptor	3.28
	N	LYS	478	ionic	3.87
	S	LYS	478	ionic	2.42
21	S	CYS	480	H-donor	3.83
	S	CYS	488	H-donor	4.32
	N	LYS	478	H-acceptor	1.85
	S	GLY	485	H-acceptor	4.42
	N	LYS	478	ionic	2.82
	N	LYS	478	ionic	1.85
	S	LYS	478	ionic	2.59
22	N	LYS	484	H-acceptor	2.84
	S	LYS	484	H-acceptor	2.51
	N	LYS	484	ionic	2.84
	N	LYS	484	ionic	3.9
	S	LYS	484	ionic	2.51
23	N	LYS	484	ionic	2.54
	N	LYS	484	ionic	3.17
	S	LYS	484	ionic	3.02
24	S	CYS	480	H-donor	2.96
	S	CYS	488	H-donor	3.19
	S	LYS	478	H-acceptor	3.94
	S	LYS	484	H-acceptor	4.11
	S	GLY	485	H-acceptor	3.22
	S	PHE	486	H-acceptor	4.25
	N	LYS	478	ionic	2.14
	N	LYS	478	ionic	2.3
	S	LYS	478	ionic	3.94

	S	LYS	478	ionic	3.9
25	S	LYS	478	H-acceptor	3.33
	S	PRO	479	H-acceptor	3.66
	N	LYS	478	ionic	2.42
	N	LYS	478	ionic	3.08
	S	LYS	478	ionic	3.33
	6-ring	CYS	480	pi-H	4.4
26	N	LYS	478	ionic	2.5
	N	LYS	478	ionic	3.41
	S	LYS	478	ionic	2.59
27	N	CYS	480	H-donor	3.29
	N	CYS	480	H-donor	3.79
	N	CYS	488	H-donor	3.48
	S	CYS	480	H-donor	4.43
	N	PHE	486	H-acceptor	3.29
	S	ASN	487	H-acceptor	2.93
	S	VAL	483	H-acceptor	3.8
	S	GLY	485	H-acceptor	3.33
	N	LYS	478	ionic	2.27
	N	LYS	478	ionic	3.06
	S	LYS	478	ionic	2.73
28	C	SER	477	H-donor	3.1
	S	LYS	478	H-acceptor	4.01
	S	PHE	486	H-acceptor	2.4
	N	LYS	478	ionic	2.78
	N	LYS	478	ionic	3.15
29	N	LYS	478	H-acceptor	2.94
	S	ASN	487	H-acceptor	2.7
	N	LYS	478	ionic	3.39
	N	LYS	478	ionic	2.94
30	N	LYS	478	H-acceptor	2.91
	S	GLY	485	H-acceptor	4.14
	S	PHE	486	H-acceptor	3.25
	N	LYS	478	ionic	2.91
	N	LYS	478	ionic	3.07

Table S12. Toxicity – PreADMET | Prediction of ADME/Tox of compounds V1–V10.

V1		V2	
algae_at	0.00644171	algae_at	0.00132146
Ames_test	mutagen	Ames_test	mutagen
Carcino_Mouse	negative	Carcino_Mouse	positive
Carcino_Rat	positive	Carcino_Rat	negative
daphnia_at	0.00702006	daphnia_at	0.00116108
hERG_inhibition	medium_risk	hERG_inhibition	medium_risk
medaka_at	0.000159833	medaka_at	5.68E-06
minnow_at	0.000197558	minnow_at	8.56E-06
TA100_10RLI	negative	TA100_10RLI	negative
TA100_NA	positive	TA100_NA	negative
TA1535_10RLI	positive	TA1535_10RLI	negative
TA1535_NA	negative	TA1535_NA	negative
V3		V4	
algae_at	0.00320439	algae_at	0.00121747
Ames_test	mutagen	Ames_test	non-mutagen
Carcino_Mouse	negative	Carcino_Mouse	positive
Carcino_Rat	negative	Carcino_Rat	negative
daphnia_at	0.00181617	daphnia_at	0.000723365
hERG_inhibition	medium_risk	hERG_inhibition	medium_risk
medaka_at	1.23E-05	medaka_at	2.43E-06
minnow_at	1.77E-05	minnow_at	7.73E-06
TA100_10RLI	positive	TA100_10RLI	negative
TA100_NA	negative	TA100_NA	negative
TA1535_10RLI	negative	TA1535_10RLI	negative
TA1535_NA	negative	TA1535_NA	negative
V5		V6	
algae_at	0.0693099	algae_at	0.0436064
Ames_test	mutagen	Ames_test	mutagen
Carcino_Mouse	positive	Carcino_Mouse	positive
Carcino_Rat	negative	Carcino_Rat	positive
daphnia_at	0.371863	daphnia_at	0.237821

hERG_inhibition	low_risk	hERG_inhibition	low_risk
medaka_at	0.197798	medaka_at	0.0890793
minnow_at	0.173668	minnow_at	0.080496
TA100_10RLI	negative	TA100_10RLI	positive
TA100_NA	negative	TA100_NA	negative
TA1535_10RLI	negative	TA1535_10RLI	negative
TA1535_NA	negative	TA1535_NA	negative
V7		V8	
algae_at	0.00412247	algae_at	0.000939495
Ames_test	mutagen	Ames_test	mutagen
Carcino_Mouse	positive	Carcino_Mouse	negative
Carcino_Rat	negative	Carcino_Rat	positive
daphnia_at	0.00684831	daphnia_at	0.00135228
hERG_inhibition	medium_risk	hERG_inhibition	medium_risk
medaka_at	0.000130801	medaka_at	7.60E-06
minnow_at	0.000249373	minnow_at	5.21E-06
TA100_10RLI	positive	TA100_10RLI	negative
TA100_NA	positive	TA100_NA	positive
TA1535_10RLI	negative	TA1535_10RLI	negative
TA1535_NA	negative	TA1535_NA	negative
V9		V10	
algae_at	0.011453	algae_at	0.00339983
Ames_test	mutagen	Ames_test	mutagen
Carcino_Mouse	positive	Carcino_Mouse	negative
Carcino_Rat	negative	Carcino_Rat	positive
daphnia_at	0.049338	daphnia_at	0.00350968
hERG_inhibition	low_risk	hERG_inhibition	medium_risk
medaka_at	0.00456803	medaka_at	4.19E-05
minnow_at	0.0106336	minnow_at	2.79E-05
TA100_10RLI	positive	TA100_10RLI	negative
TA100_NA	positive	TA100_NA	negative
TA1535_10RLI	positive	TA1535_10RLI	negative

TA1535_NA	negative	TA1535_NA	negative
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Table S13. ADME - PreADMET | Prediction of ADME/Tox of compounds V1–V10.

V1		V2	
AlogP98_value	4.3952	AlogP98_value	6.1324
AMolRef	93.6769	AMolRef	109.65
BBB	1.25008	BBB	3.75911
Buffer_solubility_mg_L	7.87547	Buffer_solubility_mg_L	0.0492061
Caco2	24.615	Caco2	31.6479
CYP_2C19_inhibition	Non	CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non	CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non	CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non	CYP_2D6_substrate	Non
CYP_3A4_inhibition	Non	CYP_3A4_inhibition	Non
CYP_3A4_substrate	Weakly	CYP_3A4_substrate	Weakly
HIA	93.00804	HIA	94.628173
MDCK	63.3816	MDCK	62.7075
Pgp_inhibition	Non	Pgp_inhibition	Inhibitor
Plasma_Protein_Binding	92.511148	Plasma_Protein_Binding	97.273276
Pure_water_solubility_mg_L	0.314331	Pure_water_solubility_mg_L	0.00371765
Skin_Permeability	-3.9701	Skin_Permeability	-3.5609
Solvation_Free_Energy	-5.460000**	Solvation_Free_Energy	-10.140000**
V3		V4	
AlogP98_value	5.109	AlogP98_value	6.3928
AMolRef	107.7979	AMolRef	114.8322
BBB	0.26507	BBB	3.84716
Buffer_solubility_mg_L	0.0579492	Buffer_solubility_mg_L	0.0138886
Caco2	16.3434	Caco2	27.0769

CYP_2C19_inhibition	Non	CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Inhibitor	CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non	CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non	CYP_2D6_substrate	Non
CYP_3A4_inhibition	Non	CYP_3A4_inhibition	Non
CYP_3A4_substrate	Weakly	CYP_3A4_substrate	Weakly
HIA	90.504603	HIA	94.773325
MDCK	0.0578833	MDCK	69.4596*
Pgp_inhibition	Inhibitor	Pgp_inhibition	Inhibitor
Plasma_Protein_Binding	99.690331	Plasma_Protein_Binding	92.014303
Pure_water_solubility_mg_L	0.0101463	Pure_water_solubility_mg_L	0.000562234
Skin_Permeability	-4.05249	Skin_Permeability	-3.18211
Solvation_Free_Energy	- 17.910000**	Solvation_Free_Energy	-10.520000**
V5		V6	
AlogP98_value	1.4231	AlogP98_value	1.8559
AMolRef	57.1112	AMolRef	64.6772
BBB	0.652511	BBB	0.848326
Buffer_solubility_mg_L	631.401**	Buffer_solubility_mg_L	155.146**
Caco2	17.6648	Caco2	17.8502
CYP_2C19_inhibition	Non	CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non	CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non	CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non	CYP_2D6_substrate	Non
CYP_3A4_inhibition	Non	CYP_3A4_inhibition	Non
CYP_3A4_substrate	Non	CYP_3A4_substrate	Non
HIA	84.958071	HIA	87.970389

MDCK	175.282	MDCK	46.1615
Pgp_inhibition	Non	Pgp_inhibition	Non
Plasma_Protein_Binding	64.393396	Plasma_Protein_Binding	75.706107
Pure_water_solubility_mg_L	121.654	Pure_water_solubility_mg_L	51.5406
Skin_Permeability	-4.01568	Skin_Permeability	-4.02124
Solvation_Free_Energy	- 12.710000**	Solvation_Free_Energy	-12.880000**
V7		V8	
AlogP98_value	4.6688	AlogP98_value	5.7999
AMolRef	88.3095	AMolRef	116.4544
BBB	3.6804	BBB	0.64903
Buffer_solubility_mg_L	0.553627	Buffer_solubility_mg_L	0.053158
Caco2	24.5874	Caco2	15.2765
CYP_2C19_inhibition	Non	CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non	CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non	CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non	CYP_2D6_substrate	Non
CYP_3A4_inhibition	Non	CYP_3A4_inhibition	Inhibitor
CYP_3A4_substrate	Substrate	CYP_3A4_substrate	Substrate
HIA	93.875491	HIA	91.870397
MDCK	0.387438*	MDCK	0.0884738
Pgp_inhibition	Inhibitor	Pgp_inhibition	Inhibitor
Plasma_Protein_Binding	95.788061	Plasma_Protein_Binding	88.685027
Pure_water_solubility_mg_L	0.261377	Pure_water_solubility_mg_L	0.00480063
Skin_Permeability	-2.69569	Skin_Permeability	-4.50742
Solvation_Free_Energy	-7.270000**	Solvation_Free_Energy	-12.550000**
V9		V10	

AlogP98_value	3.0188	AlogP98_value	4.9991
AMolRef	75.7198	AMolRef	99.7769
BBB	1.92678	BBB	0.966992
Buffer_solubility_mg_L	417.587**	Buffer_solubility_mg_L	0.119754
Caco2	19.5549	Caco2	22.4951
CYP_2C19_inhibition	Non	CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non	CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non	CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non	CYP_2D6_substrate	Non
CYP_3A4_inhibition	Non	CYP_3A4_inhibition	Inhibitor
CYP_3A4_substrate	Substrate	CYP_3A4_substrate	Weakly
HIA	89.7329	HIA	92.425185
MDCK	9.73139	MDCK	1.39403
Pgp_inhibition	Non	Pgp_inhibition	Inhibitor
Plasma_Protein_Binding	84.755967	Plasma_Protein_Binding	95.56514
Pure_water_solubility_mg_L	4.96097	Pure_water_solubility_mg_L	0.00996553
Skin_Permeability	-3.18134	Skin_Permeability	-4.60257
Solvation_Free_Energy	- 11.660000**	Solvation_Free_Energy	-15.690000**

Table S14. Properties predicted by PhysChem - ACD/Labs of compounds V1–V10.

V1		V2	
Density:	1.5±0.1 g/cm ³	Density:	1.5±0.1 g/cm ³
Boiling Point:	460.6±55.0 °C at 760 mmHg	Boiling Point:	505.1±60.0 °C at 760 mmHg
Vapour Pressure:	0.0±1.1 mmHg at 25°C	Vapour Pressure:	0.0±1.3 mmHg at 25°C
Enthalpy of Vaporization:	72.1±3.0 kJ/mol	Enthalpy of Vaporization:	77.5±3.0 kJ/mol
Flash Point:	232.3±31.5 °C	Flash Point:	259.3±32.9 °C

Index of Refraction:	1.718	Index of Refraction:	1.75
Molar Refractivity:	92.2±0.3 cm ³	Molar Refractivity:	107.9±0.3 cm ³
#H bond acceptors:	5	#H bond acceptors:	5
#H bond donors:	4	#H bond donors:	4
#Freely Rotating Bonds:	8	#Freely Rotating Bonds:	8
#Rule of 5 Violations:	0	#Rule of 5 Violations:	1
ACD/LogP:	3.24	ACD/LogP:	5.07
ACD/LogD (pH 5.5):	2.7	ACD/LogD (pH 5.5):	4.31
ACD/BCF (pH 5.5):	66.28	ACD/BCF (pH 5.5):	1115.93
ACD/KOC (pH 5.5):	699.28	ACD/KOC (pH 5.5):	5277.83
ACD/LogD (pH 7.4):	2.54	ACD/LogD (pH 7.4):	4.17
ACD/BCF (pH 7.4):	46.2	ACD/BCF (pH 7.4):	793.9
ACD/KOC (pH 7.4):	487.45	ACD/KOC (pH 7.4):	3754.79
Polar Surface Area:	125 Å ²	Polar Surface Area:	122 Å ²
Polarizability:	36.5±0.5 10 ⁻²⁴ cm ³	Polarizability:	42.8±0.5 10 ⁻²⁴ cm ³
Surface Tension:	73.6±3.0 dyne/cm	Surface Tension:	74.4±3.0 dyne/cm
Molar Volume:	233.8±3.0 cm ³	Molar Volume:	264.8±3.0 cm ³
V3		V4	
Density:	1.6±0.1 g/cm ³	Density:	1.5±0.1 g/cm ³
Boiling Point:	522.2±60.0 °C at 760 mmHg	Boiling Point:	535.8±52.0 °C at 760 mmHg
Vapour Pressure:	0.0±1.4 mmHg at 25°C	Vapour Pressure:	0.0±1.4 mmHg at 25°C
Enthalpy of Vaporization:	79.6±3.0 kJ/mol	Enthalpy of Vaporization:	81.2±3.0 kJ/mol
Flash Point:	269.6±32.9 °C	Flash Point:	277.8±30.7 °C
Index of Refraction:	1.734	Index of Refraction:	1.817

Molar Refractivity:	104.7±0.3 cm ³	Molar Refractivity:	114.2±0.3 cm ³
#H bond acceptors:	8	#H bond acceptors:	4
#H bond donors:	4	#H bond donors:	4
#Freely Rotating Bonds:	9	#Freely Rotating Bonds:	7
#Rule of 5 Violations:	0	#Rule of 5 Violations:	1
ACD/LogP:	4.17	ACD/LogP:	5.28
ACD/LogD (pH 5.5):	3.07	ACD/LogD (pH 5.5):	4.43
ACD/BCF (pH 5.5):	126.04	ACD/BCF (pH 5.5):	1366.15
ACD/KOC (pH 5.5):	1107.24	ACD/KOC (pH 5.5):	6089.09
ACD/LogD (pH 7.4):	2.87	ACD/LogD (pH 7.4):	4.15
ACD/BCF (pH 7.4):	80.45	ACD/BCF (pH 7.4):	719.49
ACD/KOC (pH 7.4):	706.77	ACD/KOC (pH 7.4):	3206.84
Polar Surface Area:	167 Å ²	Polar Surface Area:	112 Å ²
Polarizability:	41.5±0.5 10 ⁻²⁴ cm ³	Polarizability:	45.3±0.5 10 ⁻²⁴ cm ³
Surface Tension:	77.8±3.0 dyne/cm	Surface Tension:	81.1±3.0 dyne/cm
Molar Volume:	261.1±3.0 cm ³	Molar Volume:	262.9±3.0 cm ³
V5		V6	
Density:	1.4±0.1 g/cm ³	Density:	1.6±0.1 g/cm ³
Boiling Point:		Boiling Point:	
Vapour Pressure:		Vapour Pressure:	
Enthalpy of Vaporization:		Enthalpy of Vaporization:	
Flash Point:		Flash Point:	
Index of Refraction:	1.602	Index of Refraction:	1.605
Molar Refractivity:	59.0±0.3 cm ³	Molar Refractivity:	66.4±0.3 cm ³
#H bond acceptors:	6	#H bond acceptors:	6

#H bond donors:	3	#H bond donors:	3
#Freely Rotating Bonds:	3	#Freely Rotating Bonds:	4
#Rule of 5 Violations:	0	#Rule of 5 Violations:	0
ACD/LogP:	1.72	ACD/LogP:	2.43
ACD/LogD (pH 5.5):	1.28	ACD/LogD (pH 5.5):	1.77
ACD/BCF (pH 5.5):	5.57	ACD/BCF (pH 5.5):	13.03
ACD/KOC (pH 5.5):	118.85	ACD/KOC (pH 5.5):	218.46
ACD/LogD (pH 7.4):	1.22	ACD/LogD (pH 7.4):	1.71
ACD/BCF (pH 7.4):	4.81	ACD/BCF (pH 7.4):	11.41
ACD/KOC (pH 7.4):	102.68	ACD/KOC (pH 7.4):	191.42
Polar Surface Area:	79 Å ²	Polar Surface Area:	79 Å ²
Polarizability:	23.4±0.5 10 ⁻²⁴ cm ³	Polarizability:	26.3±0.5 10 ⁻²⁴ cm ³
Surface Tension:	54.4±3.0 dyne/cm	Surface Tension:	53.6±3.0 dyne/cm
Molar Volume:	172.1±3.0 cm ³	Molar Volume:	192.8±3.0 cm ³
V7		V8	
Density:	1.5±0.1 g/cm ³	Density:	1.6±0.1 g/cm ³
Boiling Point:		Boiling Point:	551.1±60.0 °C at 760 mmHg
Vapour Pressure:		Vapour Pressure:	0.0±1.5 mmHg at 25°C
Enthalpy of Vaporization:		Enthalpy of Vaporization:	83.1±3.0 kJ/mol
Flash Point:		Flash Point:	287.1±32.9 °C
Index of Refraction:	1.634	Index of Refraction:	1.741
Molar Refractivity:	87.8±0.3 cm ³	Molar Refractivity:	113.8±0.3 cm ³
#H bond acceptors:	5	#H bond acceptors:	6
#H bond donors:	3	#H bond donors:	4

#Freely Rotating Bonds:	6	#Freely Rotating Bonds:	9
#Rule of 5 Violations:	0	#Rule of 5 Violations:	1
ACD/LogP:	4.19	ACD/LogP:	6.04
ACD/LogD (pH 5.5):	3.79	ACD/LogD (pH 5.5):	4.76
ACD/BCF (pH 5.5):	446.85	ACD/BCF (pH 5.5):	2417.74
ACD/KOC (pH 5.5):	2744.46	ACD/KOC (pH 5.5):	9177.74
ACD/LogD (pH 7.4):	3.76	ACD/LogD (pH 7.4):	4.59
ACD/BCF (pH 7.4):	413.22	ACD/BCF (pH 7.4):	1673.53
ACD/KOC (pH 7.4):	2537.96	ACD/KOC (pH 7.4):	6352.73
Polar Surface Area:	94 Å ²	Polar Surface Area:	167 Å ²
Polarizability:	34.8±0.5 10 ⁻²⁴ cm ³	Polarizability:	45.1±0.5 10 ⁻²⁴ cm ³
Surface Tension:	56.5±3.0 dyne/cm	Surface Tension:	78.1±3.0 dyne/cm
Molar Volume:	245.7±3.0 cm ³	Molar Volume:	281.7±3.0 cm ³
V9		V10	
Density:	1.4±0.1 g/cm ³	Density:	1.6±0.1 g/cm ³
Boiling Point:		Boiling Point:	462.8±55.0 °C at 760 mmHg
Vapour Pressure:		Vapour Pressure:	0.0±1.1 mmHg at 25°C
Enthalpy of Vaporization:		Enthalpy of Vaporization:	72.4±3.0 kJ/mol
Flash Point:		Flash Point:	233.7±31.5 °C
Index of Refraction:	1.58	Index of Refraction:	1.763
Molar Refractivity:	77.8±0.3 cm ³	Molar Refractivity:	97.6±0.3 cm ³
#H bond acceptors:	6	#H bond acceptors:	6
#H bond donors:	3	#H bond donors:	4
#Freely Rotating Bonds:	4	#Freely Rotating Bonds:	7

#Rule of 5 Violations:	0	#Rule of 5 Violations:	0
ACD/LogP:	3.37	ACD/LogP:	3.71
ACD/LogD (pH 5.5):	3.05	ACD/LogD (pH 5.5):	2.81
ACD/BCF (pH 5.5):	122.87	ACD/BCF (pH 5.5):	80.48
ACD/KOC (pH 5.5):	1088.86	ACD/KOC (pH 5.5):	802.96
ACD/LogD (pH 7.4):	2.98	ACD/LogD (pH 7.4):	2.6
ACD/BCF (pH 7.4):	104.79	ACD/BCF (pH 7.4):	48.96
ACD/KOC (pH 7.4):	928.64	ACD/KOC (pH 7.4):	488.45
Polar Surface Area:	79 Å ²	Polar Surface Area:	131 Å ²
Polarizability:	30.8±0.5 10 ⁻²⁴ cm ³	Polarizability:	38.7±0.5 10 ⁻²⁴ cm ³
Surface Tension:	48.9±3.0 dyne/cm	Surface Tension:	85.4±3.0 dyne/cm
Molar Volume:	233.6±3.0 cm ³	Molar Volume:	236.4±3.0 cm ³