Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental Material

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Residue	Atomic group	Binding pocket radius (Å)	Distance (Å)	Energy (Kcal/mol)			
				ε=1	ε=2	ε=10	ε=40
GLY151	iv(C30)H; v(N4)H	2.0	2.35; 1.89	-14.19	-9.88	-6.63	-6.15
GLY153	iii(C35)O	2.0	1.87	-13.70	-10.68	-5.42	-4.53
THR83	iii(C21)CH2; iv(C32)NH2+	2.5	2.44; 3.89	2.55	2.47	0.59	-0.29
MET84	iii(C22)NH3+	2.5	2.30	-30.46	-29.61	-24.86	-23.44
ARG85	iii(C22)NH3+	2.5	2.04	79.82	54.12	14.11	4.98
ASP129	v(C45)NH2+	2.5	2.25	-66.89	-43.52	-14.26	-7.68
PHE130	v(N5)H	2.5	2.09	-10.55	-5.99	-3.66	-2.92
TYR150	v(C42)H	2.5	2.47	-3.30	-1.42	-1.60	-1.66
ASN152	iv(C32)NH2+	2.5	2.15	-27.09	-26.75	-18.63	-16.47
TYR161	iii(C35)O; v(C45)NH2+	2.5	1.97; 4.78	-12.92	-10.88	-8.79	-8.18
GLY82	iv(C32)NH2+	3.0	2.77	-1.71	-0.82	-0.61	-0.43
HIS51	iv(C32)NH2+	3.0	2.86	-3.97	-0.81	2.10	2.49
PRO132	i(C14)H; v(C42)H	3.0	2.64; 260	-6.43	-3.77	-2.02	-1.89
GLY133	v(C39)H	3.0	3.13	3.65	0.83	0.70	0.36
THR134	v(C39)H	3.0	3.06	4.09	1.02	0.80	0.76
VAL154	iii(C21)H	3.0	2.50	5.21	3.57	1.27	0.57
VAL155	ii(C2)H	3.0	2.47	-17.98	-12.94	-5.16	-3.17
ASP81	iv(C32)NH2+	3.5	3.39	-111.19	-67.13	-16.04	-4.40
VAL52	v(C39)H	3.5	4.27	-0.71	-0.39	0.05	0.14
LYS131	v(C45)NH2+	3.5	5.53	48.46	21.83	4.52	1.06
ILE86	iii(C22)NH3+	4.0	3.90	-5.72	-4.79	-0.98	-0.21
TRP50	iv(C32)NH2+	4.0	3.46	7.14	5.07	2.07	1.57
ARG54	iv(C32)NH2+	4.0	3.73	64.18	41.05	10.20	2.52
ASP75	iv(C32)NH2+	4.0	3.59	-66.90	-49.48	-13.27	-3.08
VAL36	v(C39)OH	4.5	4.49	-4.16	-3.61	-2.96	-2.81
VAL72	iv(C32)NH2+	4.5	4.05	-1.77	-2.99	-1.22	-0.36
GLY37	v(C39)H	5.0	5.22	1.63	0.60	0.23	0.08
MET49	iv(C29)H; v(N4)H	5.5	5.38; 5.76	-14.67	-14.23	-14.61	-14.84
LEU128	v(C41)H	5.5	5.28	0.38	0.13	-0.04	-0.07
GLY136	v(C38)H	5.5	5.27	4.67	1.27	0.14	-0.01
VAL162	iii(C18)H	5.5	5.37	-0.81	-0.77	-0.30	-0.79
VAL162	v(C38)H	5.5	5.02	-0.47	-0.16	-0.13	-0.47
VAL78	iv(C32)NH2+	5.5	6.36	-4.16	-0.79	0.42	-0.05
VAL38	v(C39)OH	6.0	6.51	-1.69	-0.99	-0.30	-0.20
SER137	v(C38)H	6.0	6.10	0.39	0.20	-0.25	-0.17
GLY164	iii(C35)O	6.0	6.21	-3.95	0.28	0.03	-0.30
ILE76	iii(C22)NH3+	6.5	6.61	1.71	1.36	0.78	0.09
THR77	iii(C22)NH3+	6.5	6.62	-3.92	-4.59	-0.79	-0.33
ASP79	iii(C22)NH3+; iv(C32)NH2+	6.5	6.64; 6.92	-110.09	-64.97	-14.45	-3.64
LYS74	iv(C32)NH2+	6.5	6.44	50.34	28.53	5.83	1.34
GLU101	v(C38)H; v(C45)NH2+	6.5	6.84; 6.91	-43.20	-23.06	-5.01	-1.22
PRO102	v(C39)H	6.5	6.93	-0.82	-0.24	-0.04	-0.18
GLY159	v(C45)NH2+	6.5	6.65	-1.67	-0.39	-0.10	-0.23
ASP80	iv(C32)NH2+	7.5	7.39	-84.31	-44.89	-8.39	-2.00
GLY0	iv(C32)NH2+	7.5	6.98	-3.33	-2.80	-0.80	-0.21
GLN35	v(C39)H	7.5	7.12	2.47	0.93	0.18	0.05
MET75	iii(C22)NH3+	9.5	9.15	-17.08	-15.94	-15.57	-15.47
ALA127	v(C41)H	9.5	9.12	-0.18	-1.15	0.02	0.03
LYS157	iii(C22)NH3+	9.5	9.72	36.33	20.89	4.74	1.66
THR34	v(C39)OH	10.0	10.30	1.72	0.54	0.11	0.07
GLY39	v(C39)H	10.0	10.29	-0.83	-0.13	-0.03	-0.05
PRO138	v(C41)H	10.0	9.90	-0.71	-0.25	-0.14	-0.13
ASN158	ii(C2)H	10.0	9.96	5.79	1.68	0.42	0.16
ARG24	v(C39)H	10.5	10.57	29.58	17.06	3.96	0.92
GLY55	iv(C32)NH2+	10.5	10.08	1.69	0.68	0.12	0.03
ALA70	iv(C32)NH2+	10.5	10.32	0.10	1.99	0.59	0.10
ILE77	iv(C32)NH2+	10.5	9.89	-3.00	-1.41	-0.38	-0.15
ILE98	v(C41)H	10.5	10.36	-3.09	-1.16	-0.05	-0.02
ILE123	iv(C42)H	10.5	10.39	-1.12	-0.47	0.01	0.05
ALA125	iii(C35)O	10.5	10.46	0.82	0.25	0.24	0.07
ILE165	v(C38)H	10.5	10.20	-0.81	0.29	0.07	0.03
LEU51	v(C39)H	11.0	11.72	-4.94	-3.04	-0.04	0.01
LYS26	v(C39)H	11.0	11.83	29.97	16.10	3.64	0.87
GLN27	v(C39)H	11.0	11.59	1.12	0.39	0.08	0.00
LYS104	v(C45)NH2+	11.0	11.12	41.68	23.03	4.55	0.99
PHE109	v(C42)H	11.0	10.88	-0.79	-0.19	-0.09	-0.08
TYR23	v(C39)H	11.5	11.33	-0.07	-0.08	-0.16	-0.10
THR118	iii(C22)NH3+	11.5	11.08	0.98	0.56	0.15	0.03
GLY124	iii(C35)O	11.5	11.51	-2.11	-1.00	-0.30	-0.12
GLY148	v(C41)H	11.5	11.35	3.64	1.86	0.49	0.15
GLN167	iv(C32)NH2+	11.5	11.44	-2.15	-1.85	-0.53	-0.16
HIS72	iii(C18)H	12.0	11.87	-0.80	-0.12	-0.08	-0.12
VAL3	iv(C32)NH2+	12.0	11.82	0.05	-1.36	-0.12	0.10
PHE46	v(C39)OH	12.0	12.65	-0.07	-1.13	-0.11	-0.02
HIS47	v(C39)H	12.0	12.52	-0.01	1.42	0.35	0.20
ALA56	iv(C32)NH2+	12.0	11.76	-0.02	-0.13	0.01	0.00
THR111	v(C42)H	12.0	11.77	1.17	0.07	-0.04	-0.04
THR68	v(C42)H	12.5	12.25	1.45	0.39	-0.05	0.01
GLY69	v(C42)H	12.5	12.34	0.52	0.16	0.09	0.05
VAL22	v(C39)H	12.5	12.24; 12.28	0.03	-0.08	0.08	0.10
LEU58	v(C39)H	12.5	13.20	0.01	0.21	0.03	0.00
TRP69	iv(C32)NH2+	12.5	12.42	-0.07	-0.46	-0.04	0.00
GLY103	v(C39)H	12.5	12.28	-0.01	-0.08	-0.03	0.00
GLN117	iii(C22)NH3+	12.5	12.33	-1.14	-1.21	-0.37	-0.19
LEU4	iv(C32)NH2+	13.0	13.14	-0.01	0.54	-0.12	0.00
VAL40	v(C39)H	13.0	12.53	-0.05	-0.67	-0.17	-0.10
TYR79	iv(C32)NH2+	13.0	12.81	-0.12	-0.52	-0.20	-0.10
TRP83	iv(C32)NH2+	13.0	12.79	1.15	0.69	0.13	-3.02
PRO106	v(C41)H	13.0	12.65	0.00	0.36	0.10	0.10
LYS107	v(C45)NH2+	13.0	12.59	27.93	15.54	3.52	0.85
THR168	iv(C32)NH2+	13.0	13.29	-2.47	-0.66	-0.18	-0.05
THR52	v(C39)OH	13.5	14.38	-0.20	-0.15	-0.09	-0.10

TABLE I: Interaction layer, minimal distance and MFCC binding energies between each one of the 131 amino acid residues of the serine protease of the dengue virus NS2B-NS3 surrounding by the inhibitor Bz-nKRR-H. The energy values were calculated within the GGA-D/PBE/DNP theory with ε =1, ε=2, ε=10 and ε=40. We have adopted a bold red (blue) color for negatively (positively) charged residues. Besides, the residues with normal (italic) font represent those located in NS3 (NS2B) protein, and the shadows means the residues within the same pocket radius r.