

Genome-wide mining for Hevein-like lectins from *Selaginella moellendorffii* and their potential molecular mimicry with SARS-CoV2 spike glycoprotein

Supplementary File S1

Tables

Table S1: trRosetta templates used for lectin homology modeling

ID	Template	Confidence	Coverage	Identity	E-value	Z-score
Smo446851	2DKV_A	100.0	89.9	62.9	2.9E-34	63.357
	6LNR_A	100.0	88.3	54.1	8.5E-36	65.895
	3W3E_A	99.9	75.6	64.0	1.3E-21	42.420
	4TX7_A	99.8	77.2	62.9	2.6E-20	40.244
	1DXJ_A	99.9	75.9	62.0	1.7E-22	43.870
Smo443112	2DKV_A	100.0	88.8	63.6	9.2E-35	63.931
	6LNR_A	100.0	88.4	54.5	2.2E-35	63.921
	3W3E_A	99.9	74.7	64.5	7.2E-22	42.712
	4TX7_A	99.8	76.2	62.9	1.5E-20	40.581
	1DXJ_A	99.9	75.0	62.4	1.6E-22	43.822
Smo437354	3D30_A	99.8	62.5	25.0	2.3E-19	33.403
	1N10_A	99.7	71.0	23.0	9.3E-19	32.541
	2HCZ_X	99.7	71.5	28.5	9.5E-19	32.514
	4JS7_A	99.7	60.5	18.0	1.4E-18	32.253
	4JJO_A	99.7	60.5	21.0	2.7E-18	31.887

Z-score: Normalized score of the raw alignment. Z-score > 11 indicates a reliable hit, E-value: values closer to 0 indicate a more significant hit.

Table S2: Predicted TM-score for each lectin model.

ID	TM-score	ID	TM-score
Smo446851	0.879	Smo443112	0.858
Smo35272	0.467	Smo7_99416	0.590
Smo125663	0.520	Smo437354	0.740
Smo425957	0.443	Smo99732	0.722
Smo403798	0.513	Smo139127	0.689

Table S3: The binding site residues of the lectins

Lectin	Hevein domain	Active residues in the binding site
Smo446851	22-58	S38, W40, G41, W42, G44, D48, H49
Smo35272	1-38, 39-76, 77-113, 120-154	S93, F95, G96, Y97, G99, F104, S136, F138, G139, Y140, G142, Y147
Smo125663	19-49, 57-91	S73, F75, G76, Y77, G79, Y84
Smo425957	38-68	S54, F56, G57, Y58, G60, Y65
Smo403798	38-72	S54, F56, G57, Y58, G60, A64, F65
Smo443112	22-58	S38, W40, G41, W42, G44, D48, H49
Smo99416	23-59, 44-99	S39, Y41, G42, Y43, G45, Y50
Smo437354	26-57	S37, W39, G40, Y41, G43, Y48
Smo99732	30-62	S41, F43, G44, Y45, G47, Y52
Smo139127	19-53	S35, F37, G38, Y39, G41, Y46

Table S4: The hydrogen bonds formed in protein-protein interactions of mutant S protein RBD and lectins.

Mutant	Lectin	# of H-bonds	Interacting residues		Docking score●	Confidence score*	MM/GBSA ●
			S protein	Lectins			
K417N	Smo446851	5	Leu335, Lys444, Asn450, Arg466	Gln316, Ser108, Glu112, Gln166	-182.71	0.66	-11.11
	Smo125663	8	Thr345, Ser349, Tyr351, Arg355, Tyr449, Leu452, Arg466	Arg74, Glu,83, Thr81, Gln36, Ser82, Glu83, Ser44	-179.18	0.64	-11.70
	Smo99732	5	Ser349, Asn354, Asp467, Ser469	Tyr45, Asp25, Tyr52, Thr48	-193.45	0.70	-32.78
L452R	Smo446851	4	Thr333, Thr345	Gly244, Glu112, Lys239	-177.70	0.64	-14.48
	Smo125663	2	Thr345, Phe347	Gln22, Arg59	-177.76	0.64	-06.97
	Smo99732	2	Arg453, Glu516	Gln61, Thr5	-186.23	0.67	-31.41
T478K	Smo446851	1	Leu582	Pro33	-197.06	0.72	-9.54
	Smo125663	7	Thr345, Trp353, Arg355, Arg454, Arg466, Thr470	Arg27, Asn67, Ser42, Gly50, Tyr84	-206.57	0.76	-19.55
	Smo99732	5	Ser349, Asp467, Ile468, Ser469	Tyr45, Tyr52, Thr48	-195.79	0.71	-34.52
E484K	Smo446851	6	Asn540, Asn542, Asp745, Glu748, Asp843	Arg4, Gln165	-201.87	0.74	-29.16
	Smo125663	5	Thr354, Arg454, Arg466, Thr470	Arg27, Ser42, Gly50, Tyr84	-201.53	0.74	-16.47
	Smo99732	1	Tyr449	Lys2	-164.55	0.57	-8.93
E501Y	Smo446851	0	—	—	-166.31	0.58	9.94
	Smo125663	2	Ser359, Asn450	Glu9, Arg74	-207.24	0.76	-10.63
	Smo99732	3	Asn354, Arg357, Asn360, Lys444	Lys20, Ser6	-205.90	0.75	-28.79

●Docking score and the free binding energy MM/GBSA are in Kcal/mol

*Confidence score > 0.7, the two molecules would be very likely to bind; between 0.5 and 0.7, the two molecules would be possible to bind; < 0.5, the two molecules would be unlikely to bind.

Figures

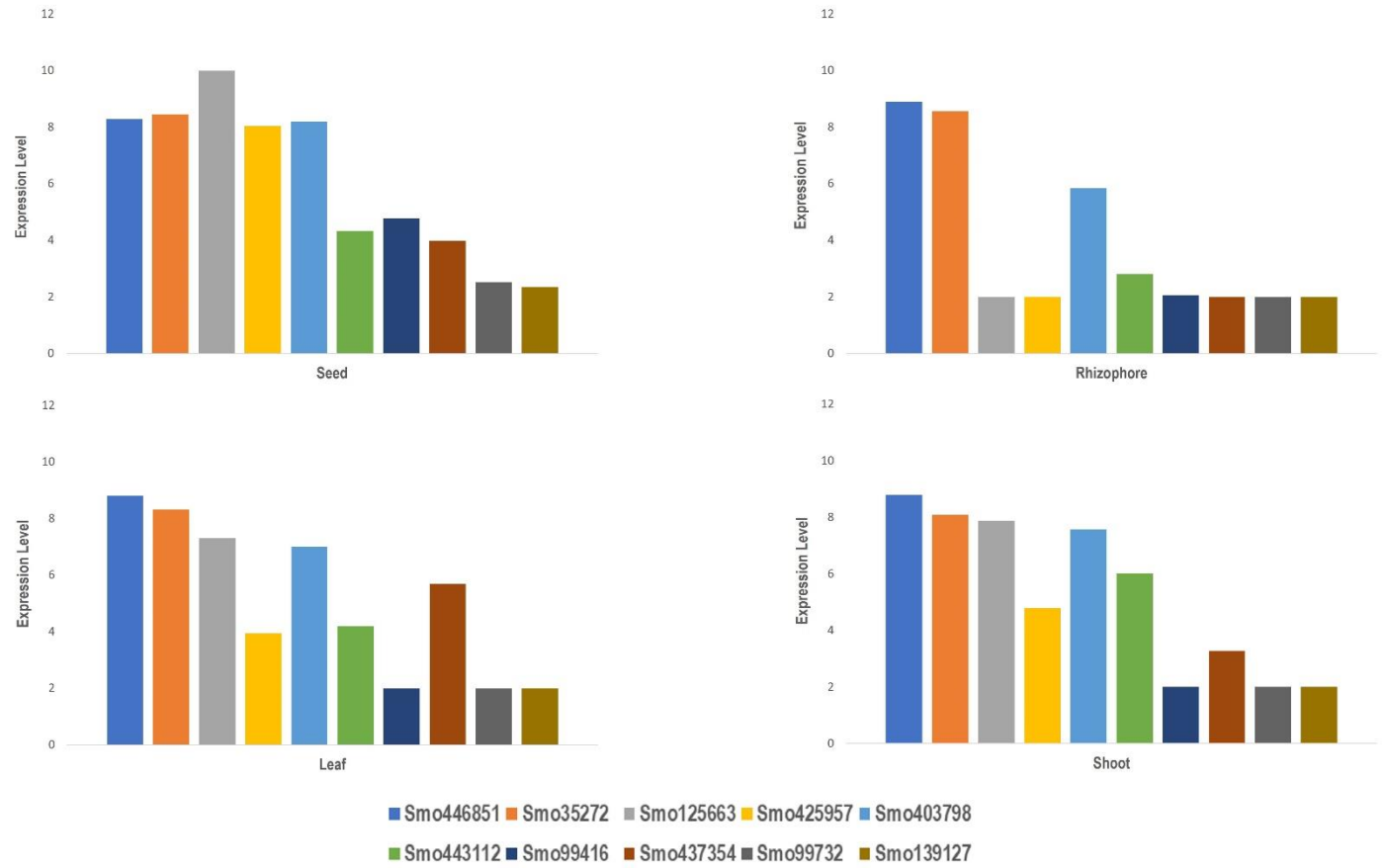


Figure S1: Expression profile of Hevein-like genes from *Selaginella moellendorffii* in different tissues/organs.

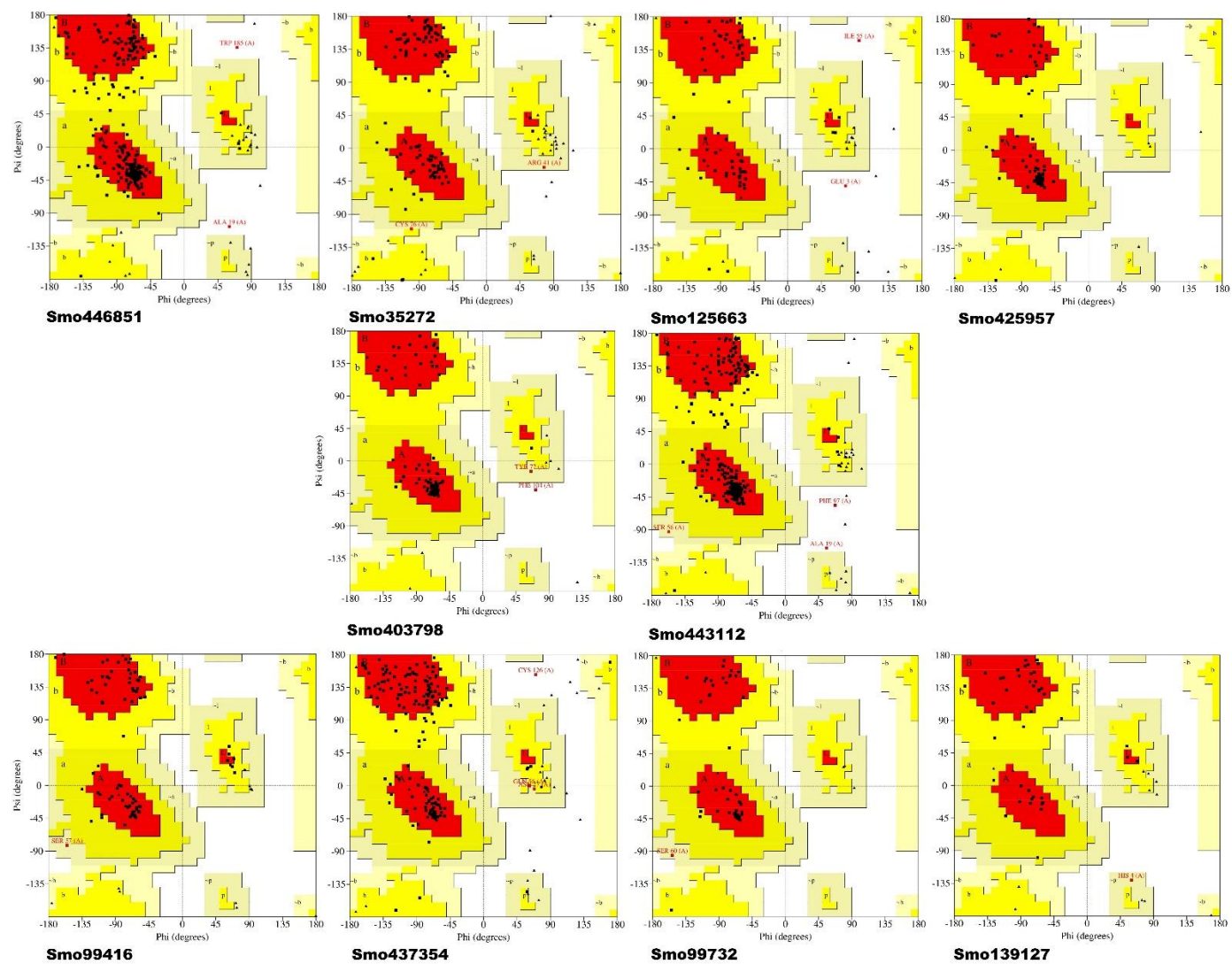


Figure S2: The Ramachandran plots for the Hevein-like lectin model structures.

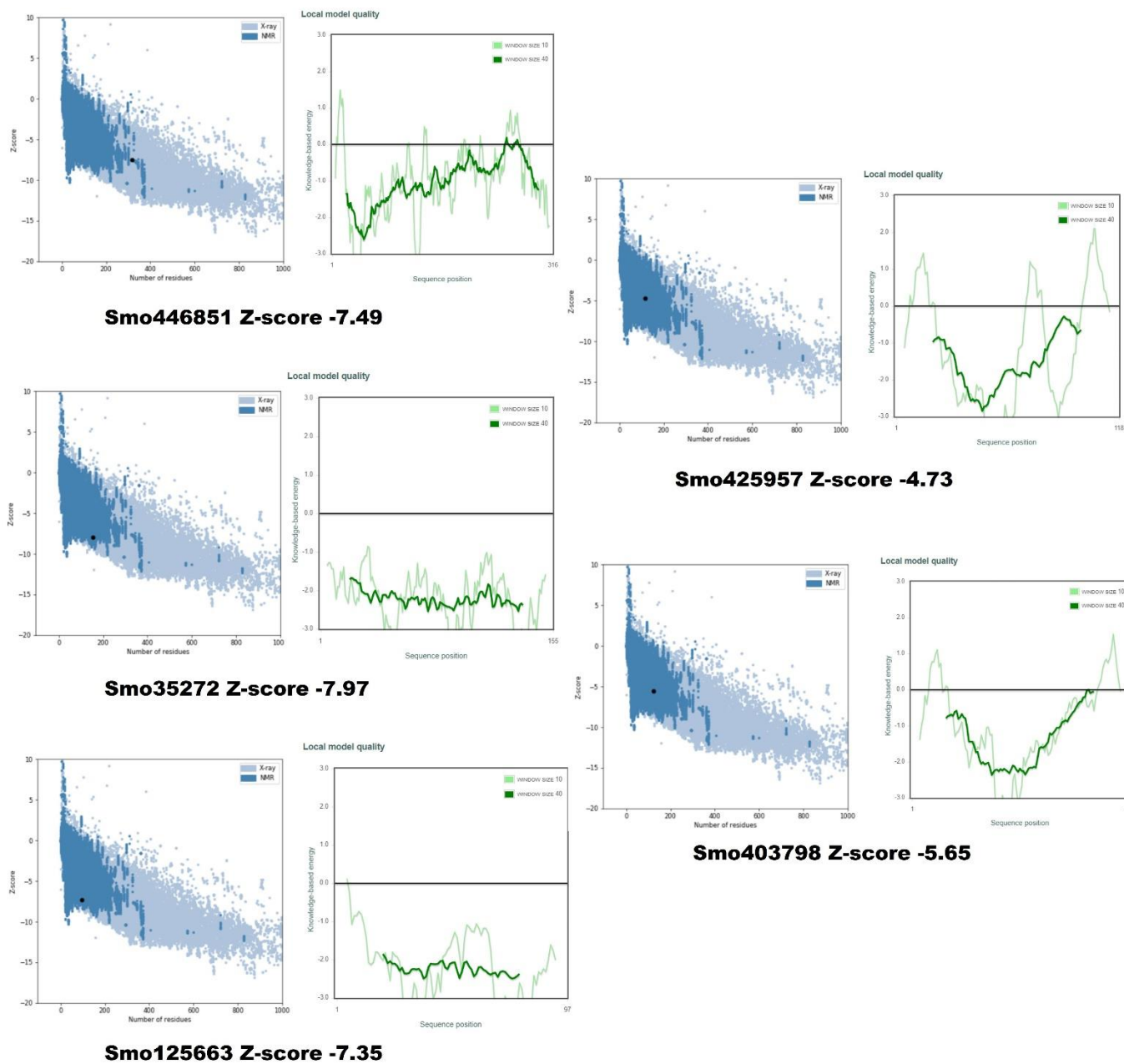


Figure S3-A: The quality and Z-score of the Hevein-like lectin structural models (five models).

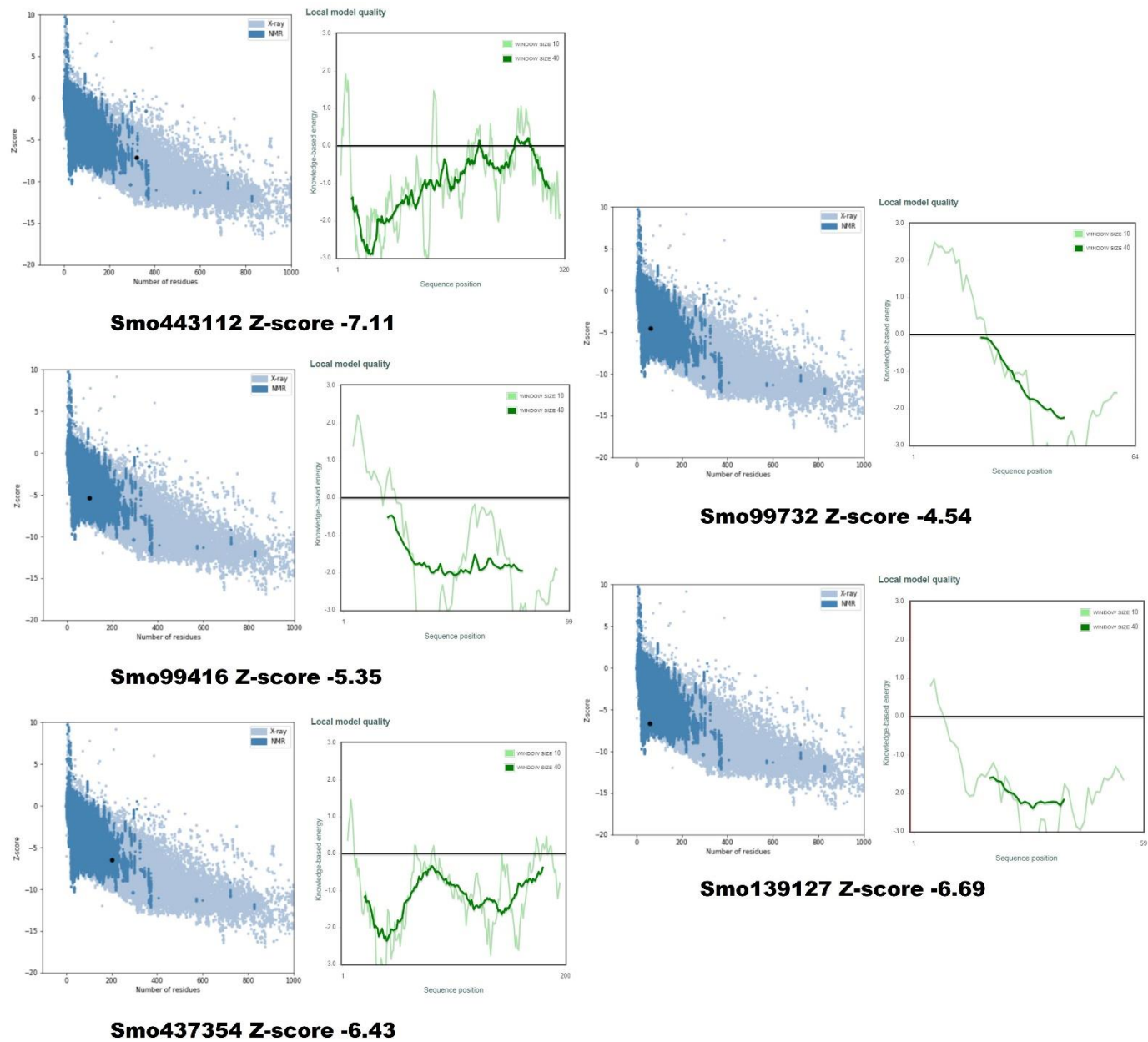


Figure S3-B: The quality and Z-score of the Hevein-like lectin structural models (five models).

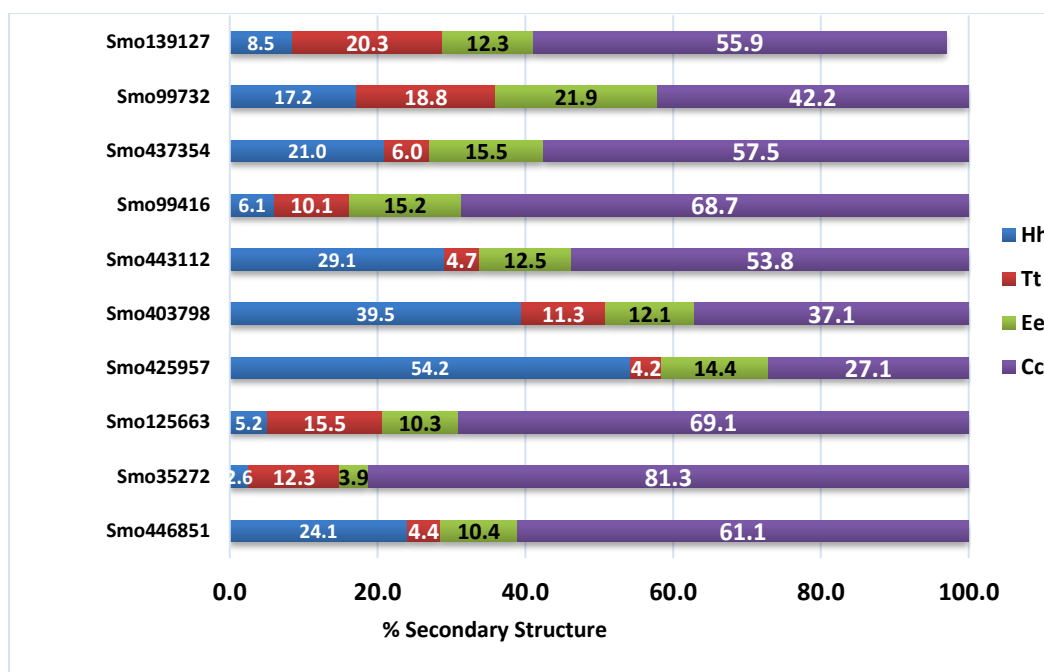


Figure S4: Prediction of the secondary structure of Hevein-like lectins from *Selaginella moellendorffii*. Hh: α -helices, Tt: β -turns, Cc: Random Coil, Ec: Extended strand.

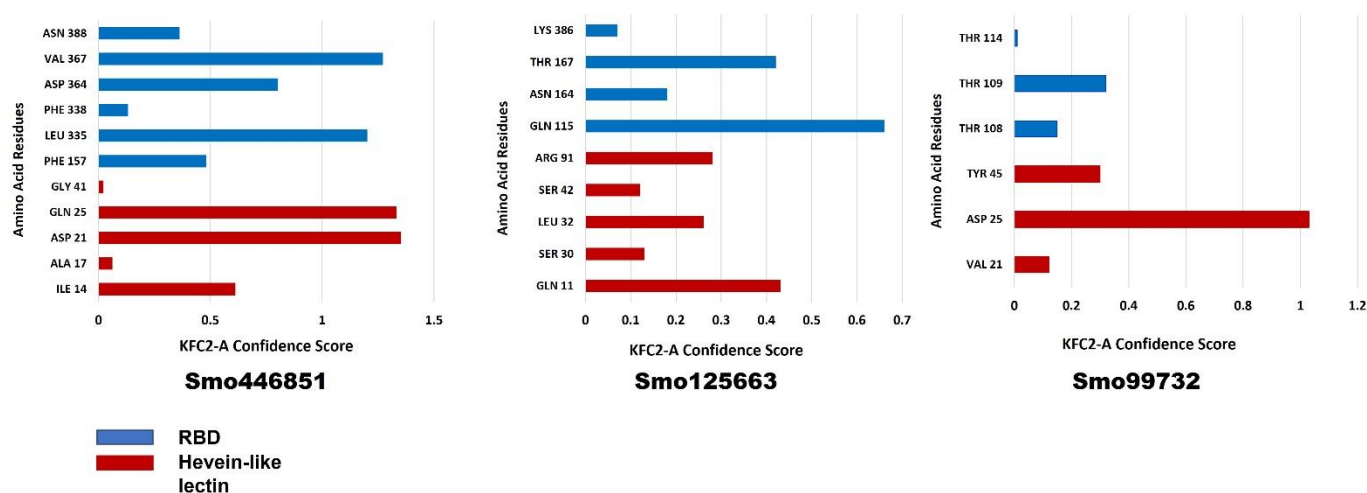


Figure S5: Hot-spot residue scores predicted by KFC-2 for the PPI involving SARS-CoV-2 S glycoprotein.

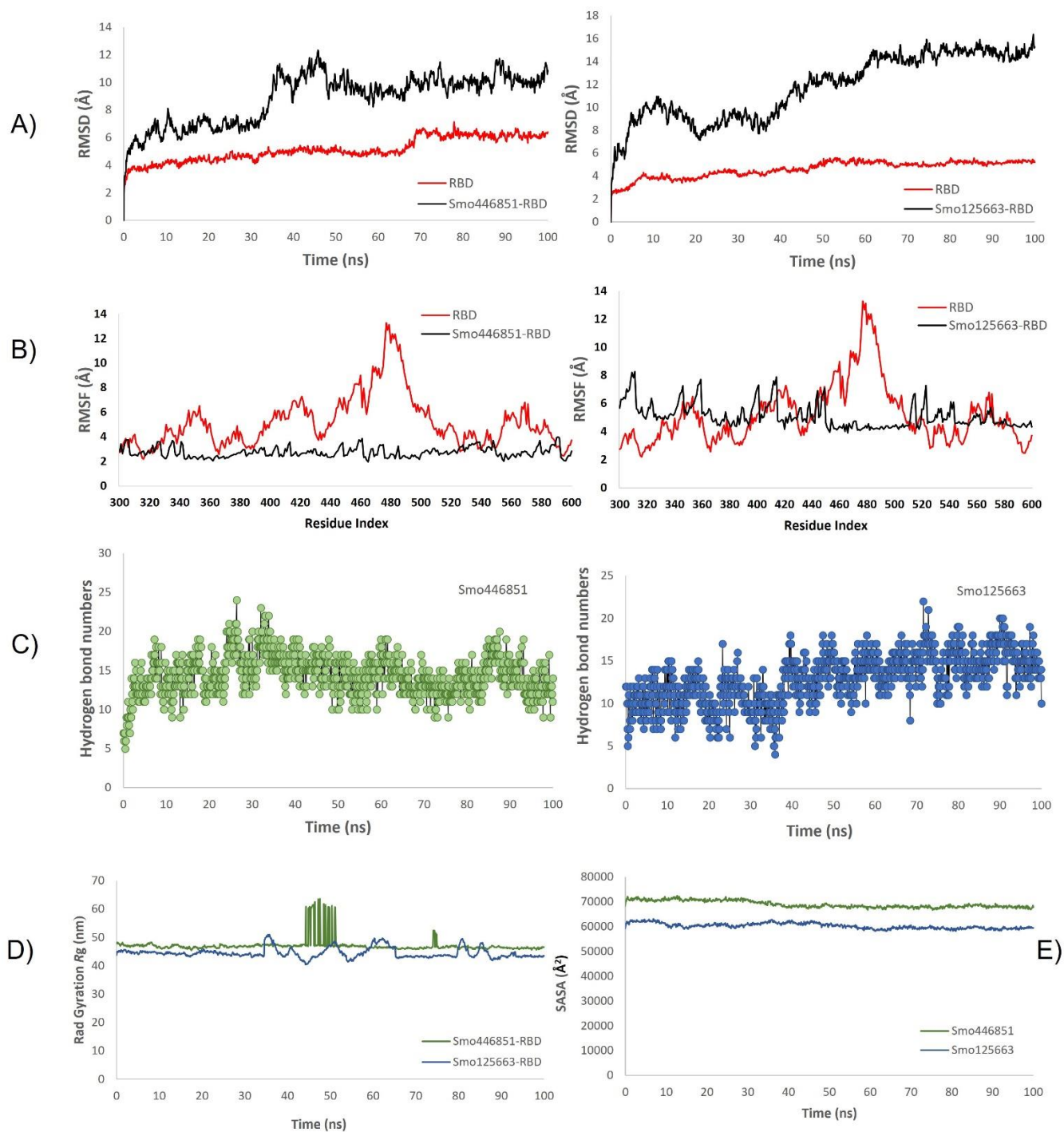


Figure S6: Molecular dynamic simulation (MDS) for the spike protein's RBD complexed with Smo446851 and Smo125663. A) RMSD, B) RMSF, C) Number of hydrogen bonds, D) Radius gyration, E) SASA.

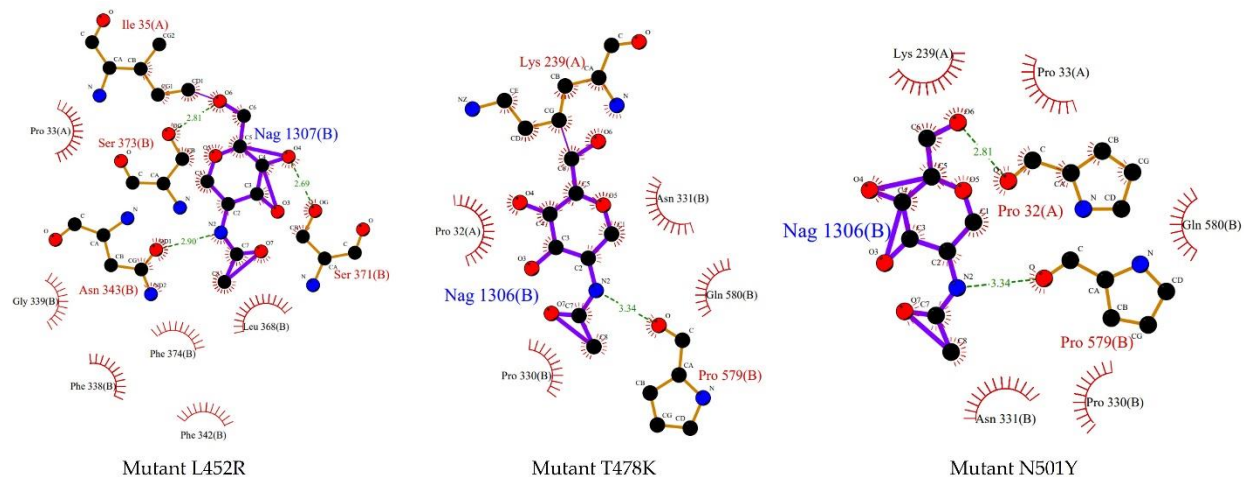


Figure S7: NAG1306 and NAG1307 of mutant spike proteins interactions with Smo446851 Hevein domain active residues