

Supplementary Materials

Supplementary Table 1. A summary of the glutelin type-B 5-like protein details used for the homology modeling

Protein type/label	Length	Amino acid sequence	Ascension number
Glutelin type-B 5-like	256	MESSAANPRGRPPSGRGPAKSDEPRQHIAEHHVRARERERSENA LLRETESQRRRQGNDRDYQQADGRGHSPDDQDQMCRMKVTMNLQ ARPWHQRRPALPAEDEGHEPDRPQLPILNSLQVSVERGTLSQDV AVPPLYTTAGAQSVVYAVRGSARLQLVDNIGAAVFDGELRRGQL LVVPEFFVVLTEAGKDGVEYIAFRNDASPVTSRIAGPGSVLRGL PVGVIAASYNVPAKDAMKLKDSGGGGGGGGTSESEL	RLM98351

Supplementary Table 2. A summary of the glutelin type-B 5-like homology templates used for the homology modeling

Protein sequence alignment	Identities	E-value	Positives	Gaps	Score
Pro-11S globulin of pumpkin (2E9Q_A)	58/128(45%)	2e-32	90/128 (70%)	1/128 (0%)	124 bits (311)
11s globulin protein from Amaranthus (3QAC_A)	48/128(38%)	4e-26	83/128 (64%)	1/128 (0%)	106 bits (265)
Pro-11s seed globulin from pea (3KSC_A)	50/131(38%)	2e-25	82/131 (62%)	1/131 (0%)	104 bits (260)
Proglycinin mutant of soybean (1UD1_A)	47/130(36%)	2e-24	83/130 (63%)	1/130 (0%)	102 bits (254)
Proglycinin mutant of soybean (1FXZ_A)	47/130(36%)	2e-24	83/130 (63%)	1/130 (0%)	102 bits (253)

*Five letters in parenthesis in column 1 are the identity number of the proteins in the protein database (PDB)

Supplementary Table 3. Summary of glutelin type-B 5-like protein models quality assessment score

Model template	Swiss-Model Server				Robetta Server			
	Mol probity score	Clash	Ramachandra favored score (%)	QMEAN Z score	Mol probity score	Clash	Ramachandra favored score (%)	QMEAN Z score
2E9Q	2.27	9.61	94.01	-2.67	1.23	1.04	93.4	-0.81
3QAC	1.66	1.93	89.22	-4.06	1.27	0.78	90.87	-1.59
3KSC	1.82	1.69	92.42	-3.27	1.35	1.30	91.73	-1.10
1UD1	1.38	0.65	93.21	-3.53	1.32	1.30	92.44	1.25
1FXZ	1.82	4.66	88.89	-3.37	1.49	2.85	93.7	-2.00

Supplementary Table 4. Percentage of secondary structure element per the three-dimensional structure of glutelin type-B 5-like protein molecule after 1 ns simulation under different simulation conditions.

Treatments	Coil (%)	Beta-sheet (%)	Beta-bridge (%)	Bend (%)	Turns (%)	Alpha helix (%)	3-helix (%)
300K, 0 V/nm	37.30	23.10	0.85	17.6	11.66	6.53	2.92
300K, 0.1 V/nm	36.3	23.9	0.97	18.6	12.2	5.35	2.58
300K, 1 V/nm	37.27	22.59	1.06	17.65	12.84	4.80	3.78
300K, 3 V/nm	37.59	22.16	1.01	18.98	12.38	5.41	2.46
350K, 0 V/nm	36.88	23.07	0.85	19.04	11.43	5.67	3.01
350K, 0.1 V/nm	37.56	23.04	1.11	18.30	12.07	5.71	2.10
350K, 1 V/nm	36.71	23.65	0.80	19.28	11.03	5.75	2.72
350K, 3 V/nm	36.36	23.05	0.87	18.73	10.86	7.64	2.23
400K, 0 V/nm	36.44	22.03	1.30	20.96	10.41	5.91	2.82
400K, 0.1 V/nm	38.74	21.77	0.88	19.24	9.37	7.00	2.89
400K, 1 V/nm	38.15	22.13	1.17	20.32	10.96	4.40	2.84
400K, 3 V/nm	38.21	22.16	0.84	21.39	10.93	3.60	2.80