BIOINFORMATION

Supplementary material:

Table 1: Ramachandran Plot scores and other protein validations score for 3D model of serine proteinase of *Heterodera glycines* and all Plant serine proteinase inhibitors

Ramachandran Plot Scores	SP_HG	SPI_PG	SPI_PGn	SPI_PO	SPI_VM	SPI_VMn
% Amino acid in most favored regions	73.6%	82.5%	80.6%	88.8%	90.1%	73.7%
% Amino acid in additional allowed regions	21.3%	14.4%	16.1%	9.0%	9.9%	22.4%
% Amino acids in generously allowed regions	3.6%	2.1%	3.2%	1.1%	0.0%	3.9%
% Amino acids in disallowed regions	1.5%	1.0%	0.0%	1.1%	0.0%	0.0%
ProSA Z-Score	-5.82	-3.49	-3.44	-3.49	-3.13	-3.76
Errat Score	86.97	78.00	95.08	75.82	81.96	77.41
Overall G-factor	-0.37	-0.28	-0.36	-0.14	-0.19	-0.38
Verfy_3D score	0.73	0.35	0.51	0.38	0.33	0.51

Table 2: Most favorable protein interacting residues for SP_HG and SPIs predicted by the PPI-pried server.

Proteins	Favorable protein binding site Amino acid
SP_HG	40A, 41V, 46S, 62H, 66S, 68I,101S,103V,104N, 105N, 107N, 109G, 110Y, 113D, 153R, 158S, 202S, 205S, 221, 222G, 224A, & 225Q
SPI_PG	44P, 45C, 46C, 47D, 49C, 51C, 53D, 54S, 55I, 56P, 57P, 92T, 94F, 93D 95C, 96Y, &97K
SPI_PGn	44P, 46C, 47D, 48K, 49C, 50M, 51C, 52A, 53D, 54S, 57P, 58I, 59C, 60Q, 61C, 62T, 94C, 95Y & 107D
SPI_PO	44P, 46C, 47D, 48H, 49C, 50M, 51C, 53D, 54S, 57P, 58I, 59C, 60Q, 61C, 62T, 94C, 95Y & 96K
SPI_VM	47K, 49C, 51D, 52Q, 53C, 55C, 56T, 57K, 58S, 59I, 61P, 62K, 63C, 64R, 69R, 73C, &102P
SP_VMn	42S, 45S, 46T, 47P, 48C, 50D, 51L, 52C, 54C, 56P, 57S, 58I, 59P, 60P, 61Q & 62C

Table 3: Various energy values for each best complex of SPIs with SP_HG generated by Fiber Dock Server. Attractive and Repulsive Van-der wall (VDW) forces for each complex are positive and negative respectively. ACE stand for Atomic Contact Energy whereas HB shows minimum Hydrogen bond energy.

Sr. No	Proteinase Inhibitors	Global Energy (Kj/mole)	Attractive VDW (Kj/mole)	Repulsive VDW (Kj/mole)	ACE (Kj/mole)	HB (Kj/mole)
1	SPI_PG	-24.34	-21.27	11.38	-8.91	-2.19
2	SPI_PGn	-24.08	-17.85	15.49	-12.92	-1.33
3	SPI_PO	-25.81	-17.82	8.79	-7.39	-2.16
4	SPI_VM	-23.43	-16.24	14.97	-10.96	-1.09
5	SPI_VMn	-24.14	-14.79	13.62	-11.79	-2.91