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Supplementary

In silico analysis and transcript levels of non-specific lipid transfer proteins (SiLTPI.5 and SiLTPII.1) under abiotic stresses in sesame (*Sesamum indicum*)

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Supplementary Tables

Table S1 Hydrogen bond analysis of SiLTPI.5-(ergo)sterol binding over final 40 ns of simulations. In total, 18 hydrogen bond calculations were analyzed with a distance cutoff of 3.5 Å and an angle cutoff of 30°

Donor	Acceptor	Occupancy (%)
ERG1-Main-O	ASP64-Side-OD1	2.68%
ERG1-Main-O	ASP64-Side-OD2	4.72%
GLN68-Side-NE2	ERG1-Main-O	0.87%
ERG1-Main-O	GLN68-Side-OE1	0.80%
ERG1-Main-O	ASP79-Main-O	0.26%
ERG1-Main-O	LYS90-Main-O	0.55%
ERG1-Main-O	GLN68-Side-NE2	0.01%
ERG1-Main-O	MET78-Main-O	0.03%
ERG1-Main-O	ASP79-Side-OD1	0.01%
ASP87-Main-N	ERG1-Main-O	6.20%
ERG1-Main-O	ASP87-Main-O	0.22%
ERG1-Main-O	SER85-Side-OG	0.20%
ERG1-Main-O	SER83-Side-OG	1.04%
SER83-Side-OG	ERG1-Main-O	0.40%
ERG1-Main-O	ASP87-Side-OD2	0.15%
ERG1-Main-O	ASP87-Side-OD1	0.27%
LYS90-Side-NZ	ERG1-Main-O	0.02%
SER85-Side-OG	ERG1-Main-O	0.20%

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Table S2 Hydrogen bond analysis of SiLTPII.1-(ergo)sterol binding over final 40 ns of simulations. In total, 13 hydrogen bond calculations were analyzed with a distance cutoff of 3.5 Å and an angle cutoff of 30°

Donor	Acceptor	Occupancy (%)
LYS41-Side-NZ	ERG1-Main-O	0.05%
ERG1-Main-O	CYS68-Side-OT2	0.01%
ERG1-Main-O	CYS68-Side-OT1	0.01%
ARG67-Side-NH1	ERG1-Main-O	0.89%
ARG67-Main-N	ERG1-Main-O	1.43%
ERG1-Main-O	ARG67-Side-NH1	0.01%
ARG67-Side-NH2	ERG1-Main-O	1.34%
ARG67-Side-NE	ERG1-Main-O	2.38%
ERG1-Main-O	MET40-Side-SD	0.02%
ERG1-Main-O	TYR65-Main-O	0.01%
ERG1-Main-O	ARG67-Side-NH2	0.01%
ERG1-Main-O	ARG67-Side-NE	0.01%
CYS37-Side-SG	ERG1-Main-O	0.01%

Supplementary Figures

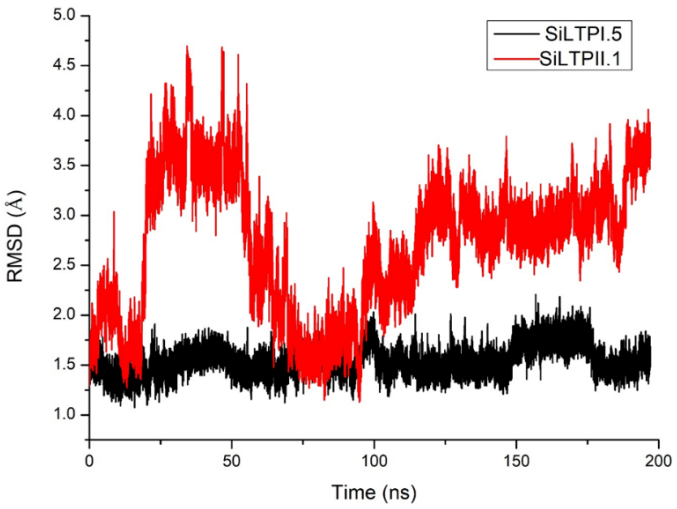

Fig. S1 Root-mean-square deviation (RMSD) of protein backbone compared with initial structure over 200 ns

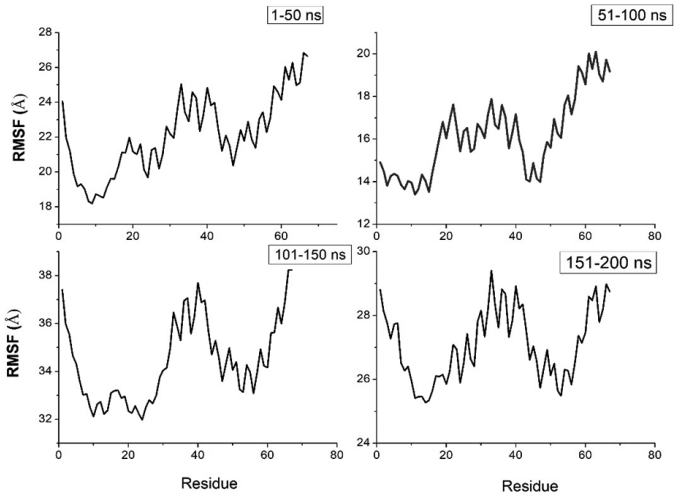

Fig. S3 Root-mean-square fluctuation (RMSF) per residue upon SiLTPII.1-(ergo)sterol binding

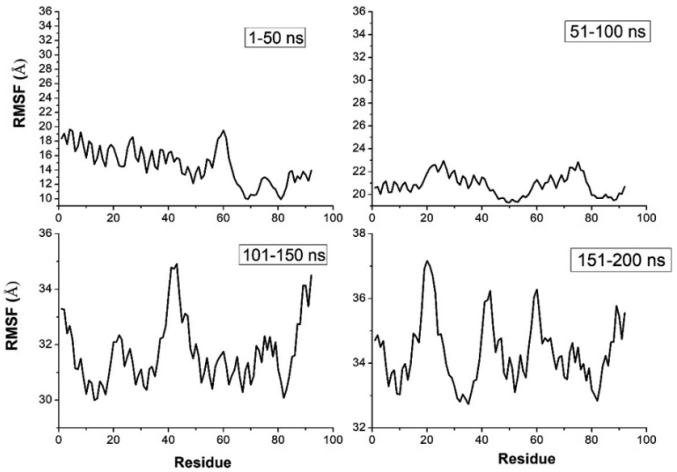

Fig. S2 Root-mean-square fluctuation (RMSF) per residue upon SiLTPI.5-(ergo)sterol binding