

Supplementary material:

Table 1: Parameters considered for protein structure quality analysis of sigma 1 and sigma 2 GSTs of *A. gossypii*

Parameter	Standard Range	Sigma 1 GST	Sigma 2 GST
Sequence Identity	50	48%	43.8%
E value	Less	3.9E-44	3.7E-41
QMEANscore4	0-1	0.722	0.714
QMEAN Z score	Not too much negative	-0.962	-1.076
ERRAT	91-95	84.375	92.746
Verify 3D	Pass	Pass	Pass
Ramachandran plot (Residues in most favoured regions)	Above 90%	91.6%	89.6%

Table 2: Active site residue predicted for model sigma 1 and sigma 2 GSTs

GST class	Residues involved in active site
Sigma 1 GST	LEU 87, ILE 88, ILE 90, ASN 91, ASN 94, ILE 95, PHE 128, TYR 129, LYS 132, PHE 133, ILE 136, VAL 137, ASN 140, PHE 144, VAL 145, ASN 146, GLY 147.
Sigma 2 GST	LEU 87, ILE 88, ILE 90, ALA 91, ASN 94, ILE 95, PHE 128, TYR 129, ARG 132, PHE 133, ILE 136, ASN 140, PHE 144, VAL 145, ASN 146.

Table 3: XP docking of insecticides and plant natural compounds with model sigma 1 GST (accession No: JN989964.1) of *A. gossypii*

S.No.	Compound Name	PubChem ID	Sigma 1 GST from <i>A. gossypii</i>			Bond distance (Å)
			Glide score	H- bonding score	H-bond Interaction	
1	Tannin	250395	-8.9	-4.6	GLU 139(O) : L(H)	2.35
					GLU 139(O) : L(H)	1.653
					ASN 140(H) : L(O)	2.092
					GLU 139(O) : L(H)	1.758
2	Piperonyl butoxide	5794	-6.8	-4.6	ASN 140(H) : L(O)	2.003
					ASN 146(H) : L(O)	2.192
					ASN 140(H) : L(O)	1.741
3	α-mangostin	5281650	-6.6	-2.1	ASN 146(O) : L(H)	2.203
					ASN 146(O) : L(H)	2.054
4	Capsaicin	1548943	-6.4	-1.2	ASN 140(O) : L(H)	2.381
					PHE 144(H) : L(O)	2.046
5	Ellagic acid	5281855	-6.2	-2.4		

Table 4: XP docking of insecticides and plant natural compounds with sigma 2 GST (accession No: JN989965.1) of *A. gossypii*

S.No.	Compound Name	PubChem ID	Sigma 2 GST from <i>A. gossypii</i>			Bond Distance (Å)
			Glide Score	H-bonding score	H-bond Interaction	
1	Tannins	250395	-8.4	-5.2	ASN 94(H) : L(O)	2.009
					LEU 87(O) : L(H)	2.245
					ASN 140(H) : L(O)	2.099
					ARG 132(H) : L(O)	1.922
2	Gossypol	3503	-6.2	-3.2	GLU 139(O) : L(H)	2.018, 1.719
					PHE 144(O) : L(H)	2.120
3	Ellagic acid	5281855	-6.1	-2.0	ASN 140(H) : L(O)	2.136
					PHE 144 (O) : L(H)	2.050
4	Quercetin	5280343	-5.9	-2.4	ASN 146(H) : L(O)	2.115
					ASN 140(O) : L(H)	1.929
5	α-mangostin	5281650	-5.8	-1.9	ASN 94(H) : L(O)	2.485
					ASN 146(H) : L(O)	2.303
					ASN 140(O) : L(H)	2.029