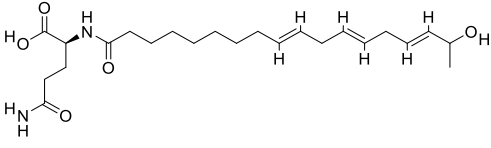
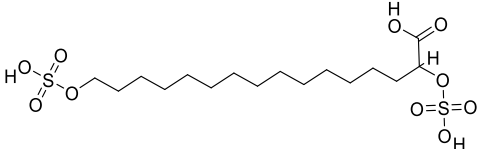
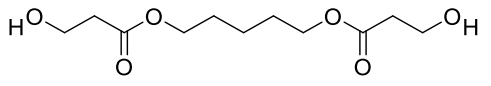
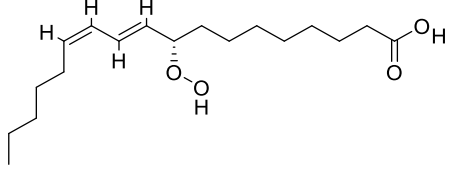
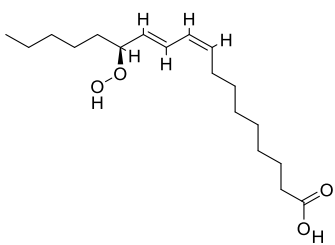
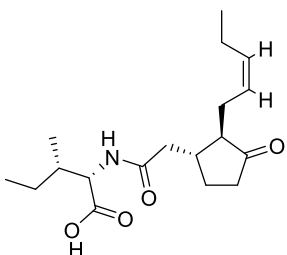


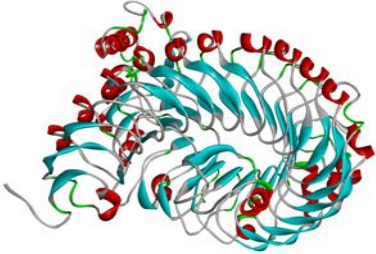
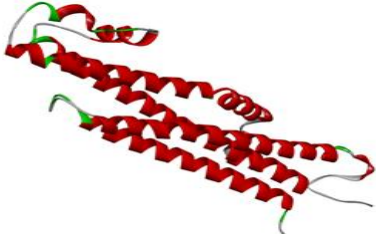
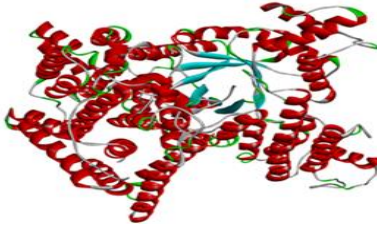
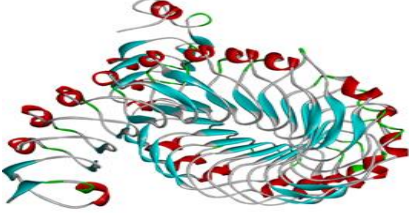
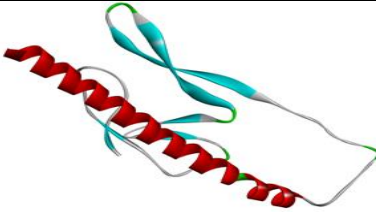
Table 1: Two-dimensional structural information of selected ligands involved in herbivory induced plant defense pathway

Name	Chemical name	IUPAC name	Physiochemical properties	Structure
Volicitin	N-[17-hydroxylinolenoyl]-L-glutamine	(2S)-5-amino-2-[[[(9E,12E,15E)-17-hydroxyoctadeca-9,12,15-trienoyl]amino]-5-oxopentanoic acid	MW = 422.6 g/mol XlogP3 = 3.2 HBD = 4 HBA = 5 RB = 18 TPSA = 130Å ²	
Caeliferin	2,16-Bis (Sulfooxy)Hexadecanoic Acid	2,16-Bis (Sulfooxy)Hexadecanoic Acid	MW = 448.6 g/mol XlogP3 = 4 HBD = 3 HBA = 10 RB = 19 TPSA = 181Å ²	
Bruchins	1,5-Pentanediol Bis(3-Hydroxypropanoate)	5-(3-Hydroxypropanoyloxy) pentyl 3-hydroxypropanoate	MW = 248.27 g/mol XlogP3 = -0.4 HBD = 2 HBA = 6 RB = 12 TPSA = 93.1 Å ²	
9(S) hydroperoxy	(9S,10E,12Z)-9-Hydroperoxy-10,12-Octadecadienoic Acid	(9S,10E,12Z)-9-hydroperoxyoctadeca-10,12-dienoic acid	MW = 312.4 g/mol XlogP3 = 5.4 HBD = 2	

			HBA = 4 RB = 15 TPSA = 66.8 Å ²	
13(S) hydroperoxy	(9Z,11E,13S)-13-hydroperoxyoctadeca-9,11-dienoic acid	(9Z,11E,13S)-13-hydroperoxyoctadeca-9,11-dienoic acid	MW = 312.4 g/mol XlogP3 = 5.4 HBD = 2 HBA = 4 RB = 15 TPSA = 66.8 Å ²	
JA-IIe	(2S,3S)-3-methyl-2-[[2-[(1R,2R)-3-oxo-2-[(Z)-pent-2-enyl]cyclopentyl]acetyl]amino]pentanoic acid	(2S,3S)-3-methyl-2-[[2-[(1R,2R)-3-oxo-2-[(Z)-pent-2-enyl]cyclopentyl]acetyl]amino]pentanoic acid	MW = 323.4 g/mol XlogP3 = 2.7 HBD = 2 HBA = 4 RB = 9 TPSA = 83.5 Å ²	

*MW = Molecular weight, XlogP3 = Partition coefficient, HBD = Hydrogen bond donor, HBA = Hydrogen bond acceptor, RB = Rotatable bond, and TPSA = Total polar surface area.

Table 2: Plant receptors for insect elicitors and receptors involved in herbivory induced plant defense pathway

Organism	Protein	UniProt ID	Predicted 3D structure
<i>Solanum lycopersicum</i>	Systemin	Q8GUQ5	
<i>Arabidopsis thaliana</i>	Systemin receptor 1(SYR1)	A0A178VIM4	
<i>Zea mays</i>	Plant elicitor peptide 1 (Pep1)	P04711	
<i>Arabidopsis thaliana</i>	PEP receptors (PEPR)	Q9FZ59	
<i>Vigna unguiculata</i>	Inceptin	Q2LGZ2	

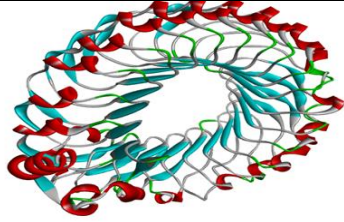
<i>Vigna radiata</i>	Leucine-rich repeat receptor kinase (LRR-RK)	A0A1S3VQX5	
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Table 3: Docking result of interactions between insect and plant elicitor molecules involved in herbivory induced plant defense pathway

Ligand	Receptor	Binding energy (Kcal/mol)	No of Hydrogen bond	Interacting residues	Bond distance(Å)
Volicitin	Systemin	-6.9	1	ND2-asn744:O4	2.89
Volicitin	PEP1	-6.8	2	N-arg567:O4 N-Glu566:O4	3.05 2.91
Caeliferin	Systemin	-5.7	5	N-phe253:O13 O-ser276:O13 N-lys254:O12 OD2-asp232:O28 OG-ser207:O23	2.98 3.17 2.87 2.98 3.06
Caeliferin	PEP1	-5.2	3	O-phe917:O13 NH2-arg911:O11 O-thr88:O23	2.89 3.16 3.11
Bruchins	Systemin	-4.3	2	OD1-asn117:O4 N-asn119:O4	2.83 3.09
Bruchins	PEP1	-4.5	5	O-ala736:O6 O-glu735:O6 N-val739:O6 O-lys606:O4 OH-tyr728:OH	2.70 2.82 2.90 2.78 3.14

Table 4: Docking result of interactions between plant elicitor and receptor molecules involved in herbivory induced plant defense pathway

Protein complex	No of hydrogen bonds	Interaction residues	Bond distance(Å)	Binding affinity (Kcal/mol)
Inceptin-LRR	1	O-ala103:OH-tyr436	2.59	-9.3
Systemin-SYR1	8	arg232:asp173	2.95	-8.2
		arg187:phe659	2.25	
		gly177:arg652	2.33	
		lys200:gly653	2.23	
		tyr172:gly653	3.14	
		ala201:tyr337	2.76	
		asp226:ser198	2.76	
		his221:lys223	2.46	
PEP-PEP1	5	OD1-asn595:OG-ser92	2.02	-8.3
		O-pro608:N-thr66	2.39	
		C-asp436:NH2-arg109	2.99	
		Oh-tyr436:O-met113	2.97	
		OH-tyr578:N-phe44	2.04	

Table 5: Docking result of hydroxyperoxide lyase (HPL) and allene oxide synthase (AOS) interactions with their ligands during jasmonic acid synthesis pathway in plants

Ligand	Receptor	Binding affinity (kcal/mol)	No. of Hydrogen bond	Interacting residues	Bond distance(Å)
9(S) Hydroperoxy	Allene Oxide Synthase (AOS)	-6.3	2	O-lys463:O4 OG1-thr132:O1	3.10 3.19
9(S) Hydroperoxy	Hydroxyperoxide lyase (HPL)	-5.8	3	O-phe286:O2 ND2-asn424:O3 O-lys463:O4	2.79 3.20 3.21
13(S) Hydroperoxy	Allene Oxide Synthase (AOS)	-6.0	4	O-ser384:O4 O-phe131:O4 O-asn315:O2 O-phe314:O2	3.20 3.00 2.97 2.55
13(S) Hydroperoxy	Hydroxyperoxide lyase (HPL)	-6.7	3	ND2-asn424:O2 N-tyr359:O2 NZ-lys97:O1	3.16 3.17 3.06