Supplementary material:

Table 1: Target protein and template protein considered for the study

Target protein	Uniprot ID	Length	Template protein	PDB ID	e-value
Polyphenol oxidase	A8D6D7	139 AA.	Catechol oxidase from Ipomoea batatas (Sweet Potatoes)	1BT1	4e-42
Lipoxygenase	A8D7D8	156 AA.	Crystal structure of delta 413-417:gs I805w Lox	3FG3	0.004
Eugenol o-methyltransferase	B2ZA12	200 AA.	Crystal structure of isoflavone o-methyltransferase homolog	2QYO	1e-35
Eugenol o-methyltransferase	B2ZA16	200 AA.	Crystal structure of Bchu involved in bacteriochlorophyll C biosynthesis	1X19	0.23
Eugenol o-methyltransferase	B2ZA17	154 AA.	Crystal structure analysis of isoflavone o-methyltransferase	1FP2	3e-23
Phenylalanine ammonia-lyase	B6VQV5	145 AA.	Phenylalanine ammonia-lyase (Pal) from *Petroselinum crispum*	1W27	2e-62
Chavicol o-methyltransferase	B6VQV6	257 AA	Crystal structure of isoflavanone 4'-o-methyltransferase complexed with (+)-6a-hydroxymaackiain	1ZGA	1e-56
Chavicol o-methyltransferase	D3KYA1	356 AA.	Crystal structure of a putative o-methyltransferase	2R3S	0.005

Table 2: Amino acid composition (%) of *Ocimum* proteins

Proteins Amino acids	A8D6D7	A8D7D8	B2ZA12	B2ZA16	B2ZA17	B6VQV5	B6VQV6	D3KYA1
Alanine(A)	5	7.1	8.5	8.5	9.7	11.7	7.8	7.6
Cysteine(C)	0	1.3	2.0	2.0	1.3	0.7	2.3	2.0
Aspartic acid(D)	6.5	5.8	3.5	3.5	3.9	2.1	7.8	6.5
Glutamic acid(E)	2.2	6.4	5.0	5.0	6.5	6.9	5.4	5.3
Phenylalanine(F)	6.5	1.3	4.0	4.0	5.2	4.1	4.3	4.5
Glycine(G)	7.2	6.4	5.5	5.5	5.8	9.7	7.4	5.6
Histidine(H)	2.9	5.8	7.0	7.0	7.1	2.8	3.5	3.9
Isoleucine(I)	3.6	7.7	5.0	5.0	3.2	7.6	5.8	6.2
Lysine(K)	2.9	7.1	5.5	5.5	4.5	4.1	6.2	5.9
Leucine(L)	5.8	11.5	10.5	10	9.1	15.2	8.6	10.1
Methionine(M)	3.6	1.9	5.5	5.5	5.2	1.4	4.3	4.5
Asparagine(N)	7.2	5.1	4.5	4.5	4.5	4.8	3.9	4.8
Proline(P)	10.8	5.1	5.0	5.0	4.5	6.2	3.9	3.9
Glutamine(Q)	4.3	3.8	3.0	3.0	1.9	2.8	1.9	3.9
Arginine(R)	5.8	4.5	4.0	4.0	3.9	1.4	2.7	2.5
Serine(S)	7.2	5.1	7.0	7.0	5.8	5.5	4.7	6.2
Threonine(T)	7.2	7.1	5.0	5.0	5.8	6.2	5.8	5.1
Valine(V)	4.3	3.2	6.0	6.5	7.1	6.2	8.9	7.3
Tryptophan(W)	2.2	1.3	2.0	2.0	2.6	0	2.3	2.0
Tyrosine(Y)	5.0	2.6	1.5	1.5	1.9	0.7	2.3	2.2

Table 3: Hydrophilic and hydrophobic residues content

Accession Number	Hydrophobic residues (%)	Hydrophilic residues (%)	Net hydrophobic residues content
A8D6D7	48.9	30.9	High
A8D7D8	45.5	25	High
B2ZA12	52	23	High
B2ZA16	52	23	High
B2ZA17	52.6	21.4	Very high
B6VQV5	62.1	20.7	Very high
B6VQV6	53.3	21	Very high
D3KYA1	51.7	24.2	Very High

Table 4: Physiochemical characters as predicted by Expasy's prot-param program

Uniprot ID	Protein	Sequence length	M.wt.	pI	-R	+R	Extinction Coefficient	Instability Index	Aliphatic Index	GRAVY
A8D6D7	Polyphenol oxidase	139	15815.6	7.45	12	12	26930	34.50	54.03	-0.660
A8D7D8	Lipoxygenase	156	17511.9	6.82	19	18	17085-16960	57.08	91.35	-0.494
B2ZA12	Eugenol o-methyltransferase	200	22492.1	8.38	17	19	26720-26470	48.32	86.35	-0.114
B2ZA16	Eugenol o-methyltransferase	200	22478.1	8.38	17	19	26720-26470	46.93	85.85	-0.112
B2ZA17	Eugenol o-methyltransferase	154	17386.9	6.39	16	13	26595-26470	48.62	78.57	-0.161
B6VQV5	Phenylalanine ammonia-lyase	145	15121.5	5.28	13	8	1490-1490	30.71	118.48	0.423
B6VQV6	Chavicol o-methyltransferase	257	28569.8	5.22	34	23	42315-41940	30.88	89.88	-0.003

D3KYA1	Chavicol o-methyltransferase	356	39950	5	42	30	50795-50420	38.34	92.30	-0.038

Table 5: Presence of disulphide (ss) bond as predicted by Cys_Rec

Accession number	CYS_REC	Score
A8D6D7	No cystein found	-
A8D7D8	Cys_114	-6.8
	Cys_124	-18.4
B2ZA12	Cys_5	-7.9
	Cys_12	-17.4
	Cys_129	-31.4
	Cys_151	-31.4
B2ZA16	Cys_5	-7.9
	Cys_12	-17.4
	Cys_129	-28.6
	Cys_151	-34.8
B2ZA17	Cys_83	-25.8
	Cys_105	-33.0
B6VQV5	Cys_17	-24.7
B6VQV6	Cys_6	-29.3
	Cys_62	-24.1
	Cys_84	-26.7
	Cys_130	-36.6
	Cys_186	-36.7
	Cys_225	-27.0
D3KYA1	Cys_37	-25.0
	Cys_97	-16.8
	Cys_153	-26.7
	Cys_175	-25.6
	Cys_221	-42.8
	Cys_277	-29.2
	Cys_316	-35.5

Table 6: Calculated secondary structure elements by Profunc

Secondary Structure	B2ZA12	B2ZA17	B6VQV6	D3KYA1	B2ZA16	A8D7D8	A8D6D7	B6VQV5
Strand	5.0%	2.6%	11.7%	13.8%	6.5	12.2%	0.0%	5.5%
Alpha helix	58.5%	48.1%	46.7%	45.2%	43.5%	18.6%	38.1%	53.8%
3-10 helix	1.5%	1.9%	2.3%	1.4%	1.0%	5.1%	2.2%	2.8%
Other	35.0%	47.4%	39.3%	39.6%	49.0%	64.1%	59.7%	37.9%
Total residues	200	154	257	356	200	156	139	145
Beta sheets	1	1	2	2	1	1	-	1
Beta alpha beta motifs	-	-	4	3	2		-	-
Strands	3	2	7	9	3	4	-	3
Helices	15	11	15	19	11	6	7	7
Helix-helix interactions	25	13	20	23	8	1	6	8
Beta turns	8	14	14	25	16	16	14	8
Gamma turns	3	3	1	3	3	5	3	-
Beta hairpins	1	1	-	2	-	3	-	2
Beta bulges	-	-	-	2	-	1	-	1

Table 7: Protein submitted in PMDB

Uniprot ID	Protein name	PMID
B6VQV6	chavicol o-methyltransferase	PM0077211
D3KYA1	chavicol o-methyltransferase	PM0077212
A8D6D7	Polyphenol oxidase	PM0077059
A8D7D8	Lipoxygenase	PM0077191
B2ZA16	Eugenol o-methyltransferase	PM0077192
B2ZA17	Eugenol o-methyltransferase	PM0077201
B6VQV5	Phenylalanine ammonia-lyase	PM0077206