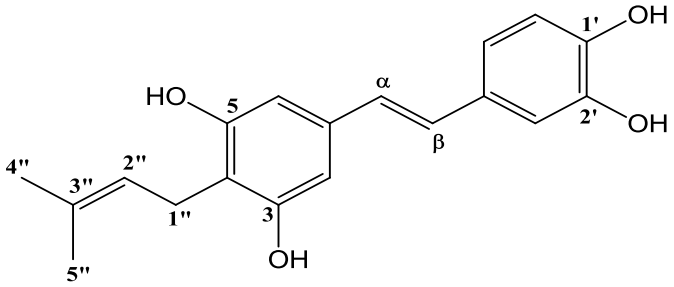
^{1}H-NMR of Arachidin 5

H	δ_H (multiplicity, *J* in Hz)
2 and 6	6.58 (s)
3′	7.05 (d, 2.1)
5′	6.87 (dd, 2.1, 8.3)
6′	6.83 (d, 8.3)
α	6.77 (d, 16.5)
β	6.86 (d, 16.5)
1″	3.36 (d, 7.1)
2″	5.30 (t, 7.1 Hz)
4″	1.77 (s)
5″	1.65 (s)



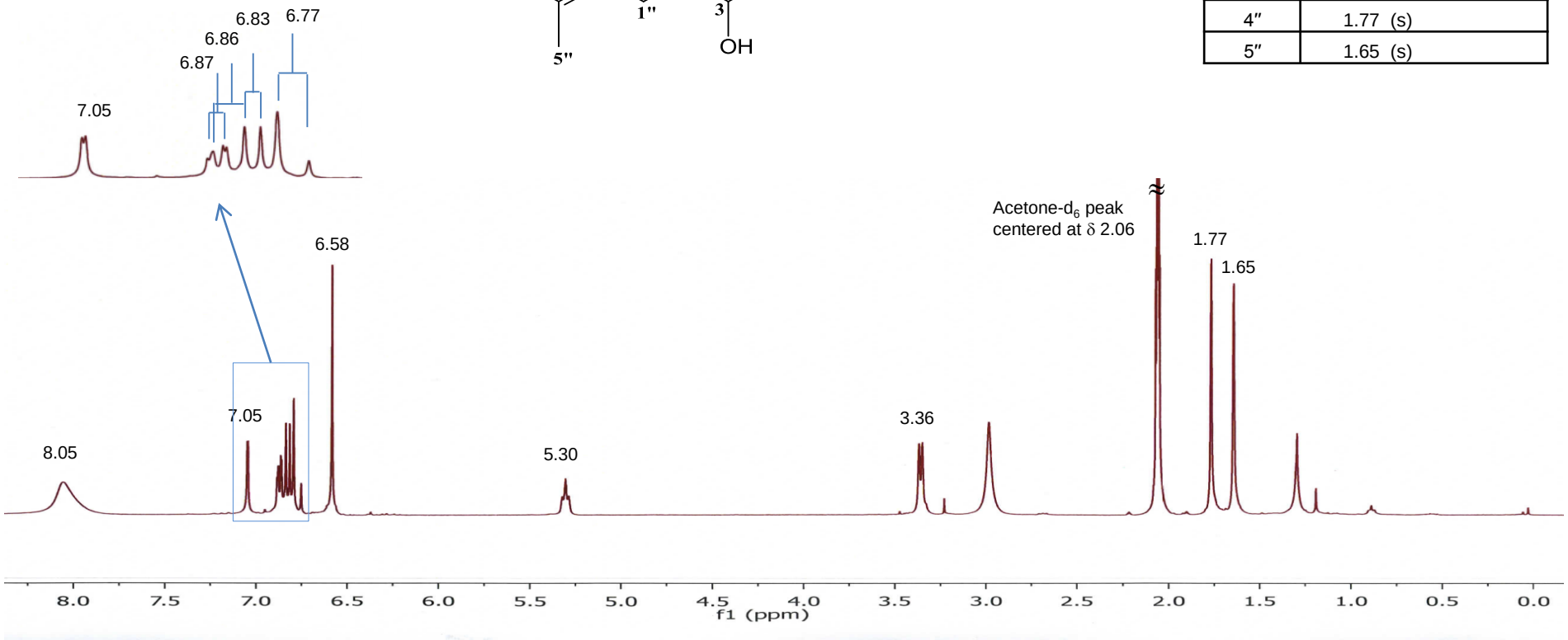
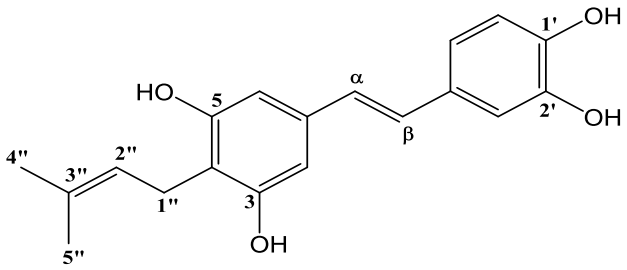


Figure S1. ^{1}H NMR analysis of arachidin-5. ^{1}H NMR was recorded at 400 MHz in acetone-d_6 on a Bruker AV-400 NMR spectrometer.

^{13}C-NMR of Arachidin 5



Carbon	δ_C
1	137.3
2 and 6	105.8
3 and 5	157.0
4	115.2
1′	146.2
2′	146.0
3′	113.7
4′	130.7
5′	119.8
6′	116.3
α	127.0
β	128.4
1″	23.1
2″	124.4
3″	130.9
4″	26.0
5″	17.9

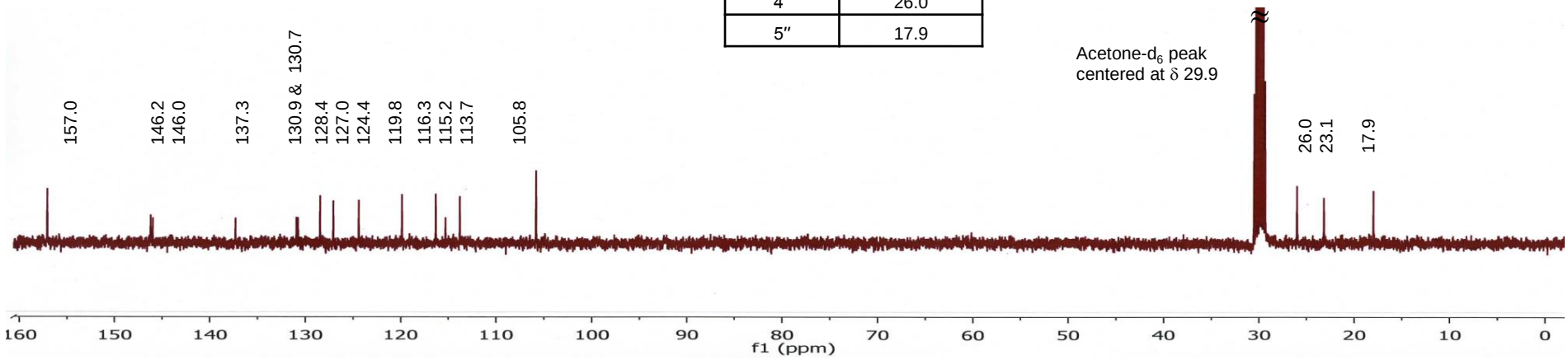


Figure S2. ^{13}C NMR analysis of arachidin-5. ^{13}C NMR was recorded at 100 MHz in acetone-d_6 on a Bruker AV-400 NMR spectrometer.

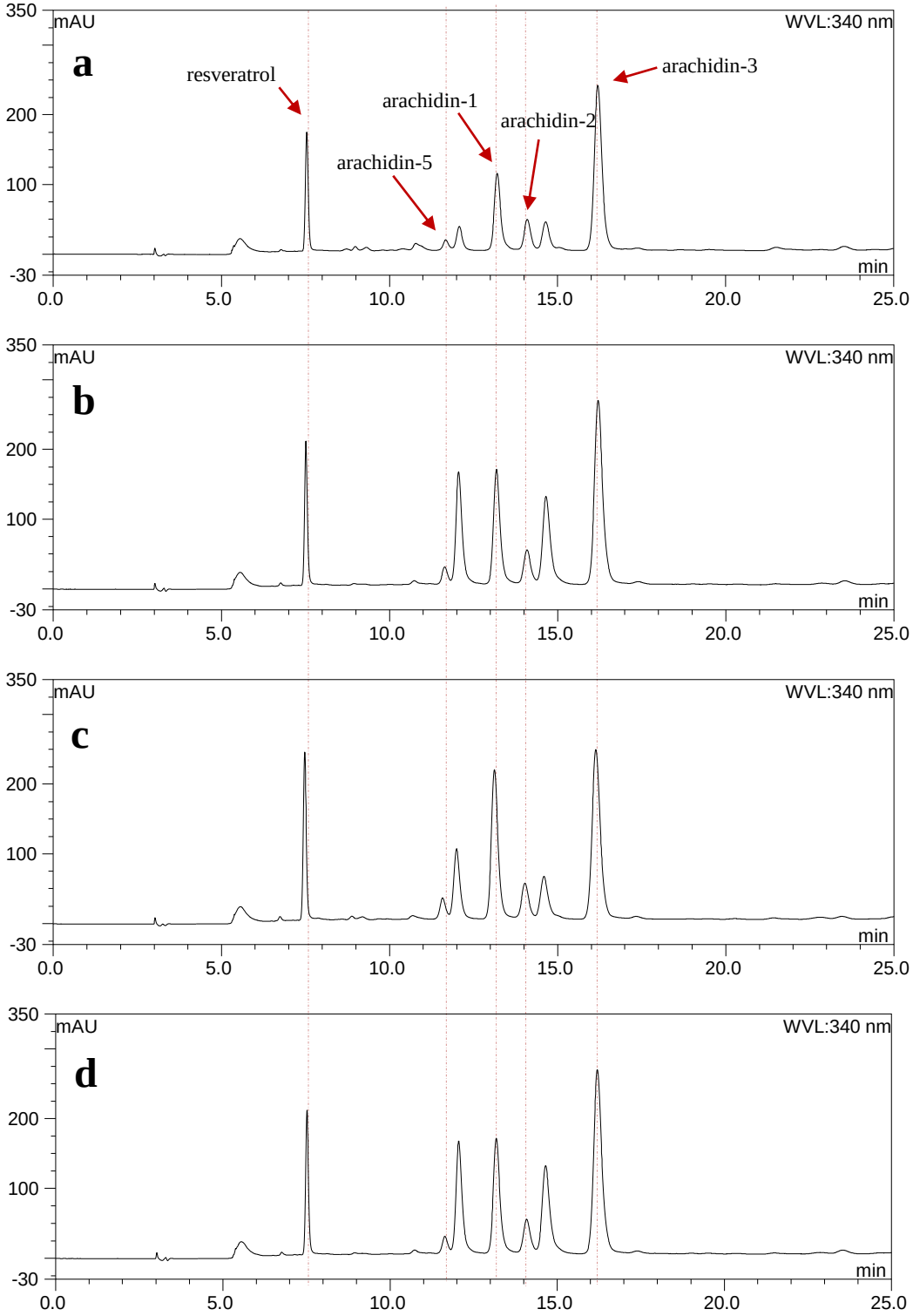


Figure S3. Effect of mevastatin on the production of stilbenoids in elicited peanut hairy root culture. HPLC chromatograms (UV 340 nm) of ethyl acetate extracts from peanut hairy root cultures after 48-hour treatment with **(a)** 100 µM methyl jasmonate (MeJA) and 9 g/L methyl-β-cyclodextrin (CD); **(b)** 100 µM MeJA, 9 g/L CD, and 1 µM mevastatin; **(c)** 100 µM MeJA, 9 g/L CD, and 10 µM mevastatin and **(d)** 100 µM MeJA, 9 g/L CD, and 100 µM mevastatin.

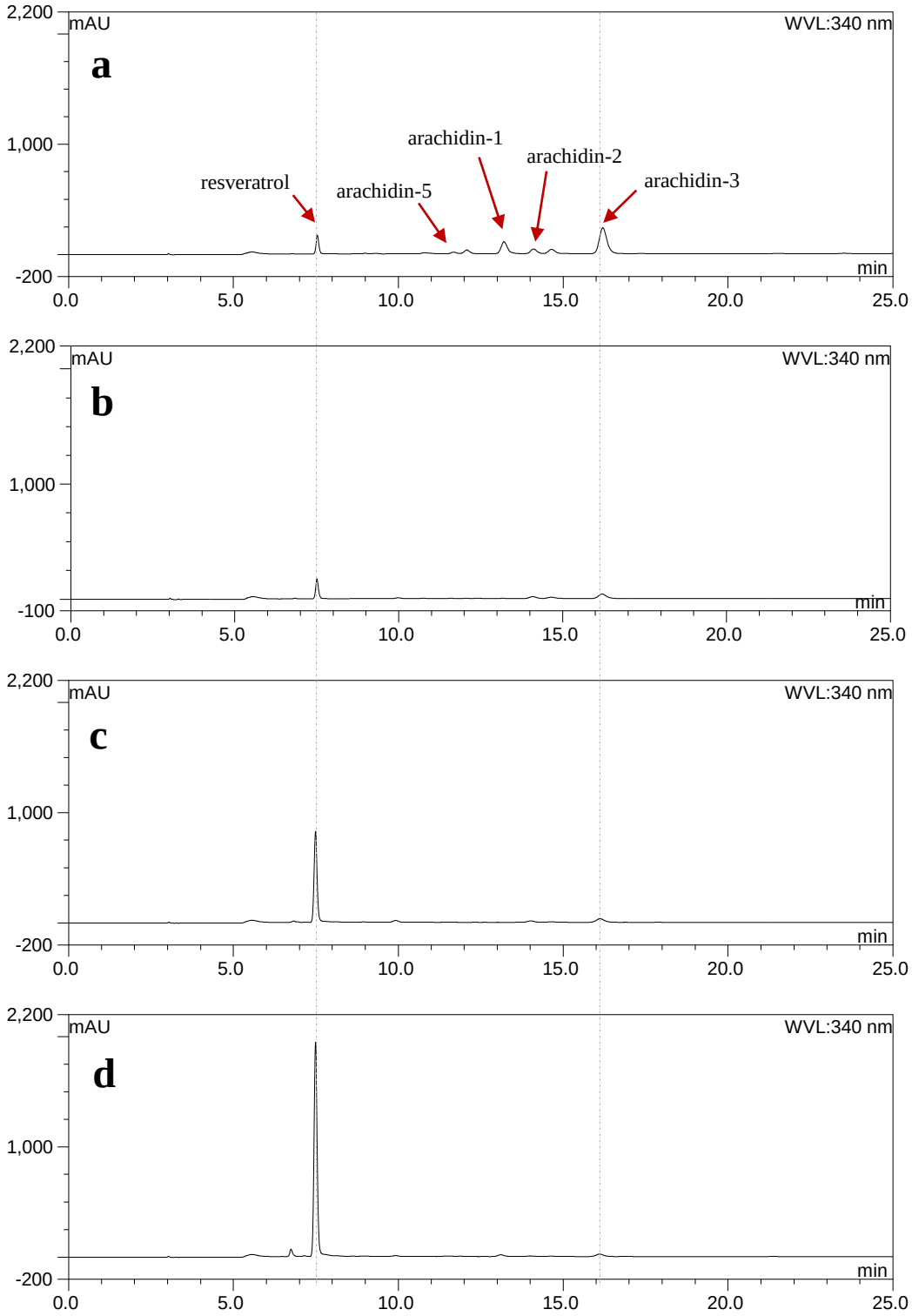


Figure S4. Effect of clomazone on the production of stilbenoids in elicited peanut hairy root culture. HPLC chromatograms (UV 340 nm) of ethyl acetate extracts from peanut hairy root cultures after 48-hour treatment with **(a)** 100 µM methyl jasmonate (MeJA) and 9 g/L methyl-β-cyclodextrin (CD); **(b)** 100 µM MeJA, 9 g/L CD, and 1 µM clomazone; **(c)** 100 µM MeJA, 9 g/L CD, and 10 µM clomazone and **(d)** 100 µM MeJA, 9 g/L CD, and 100 µM clomazone.

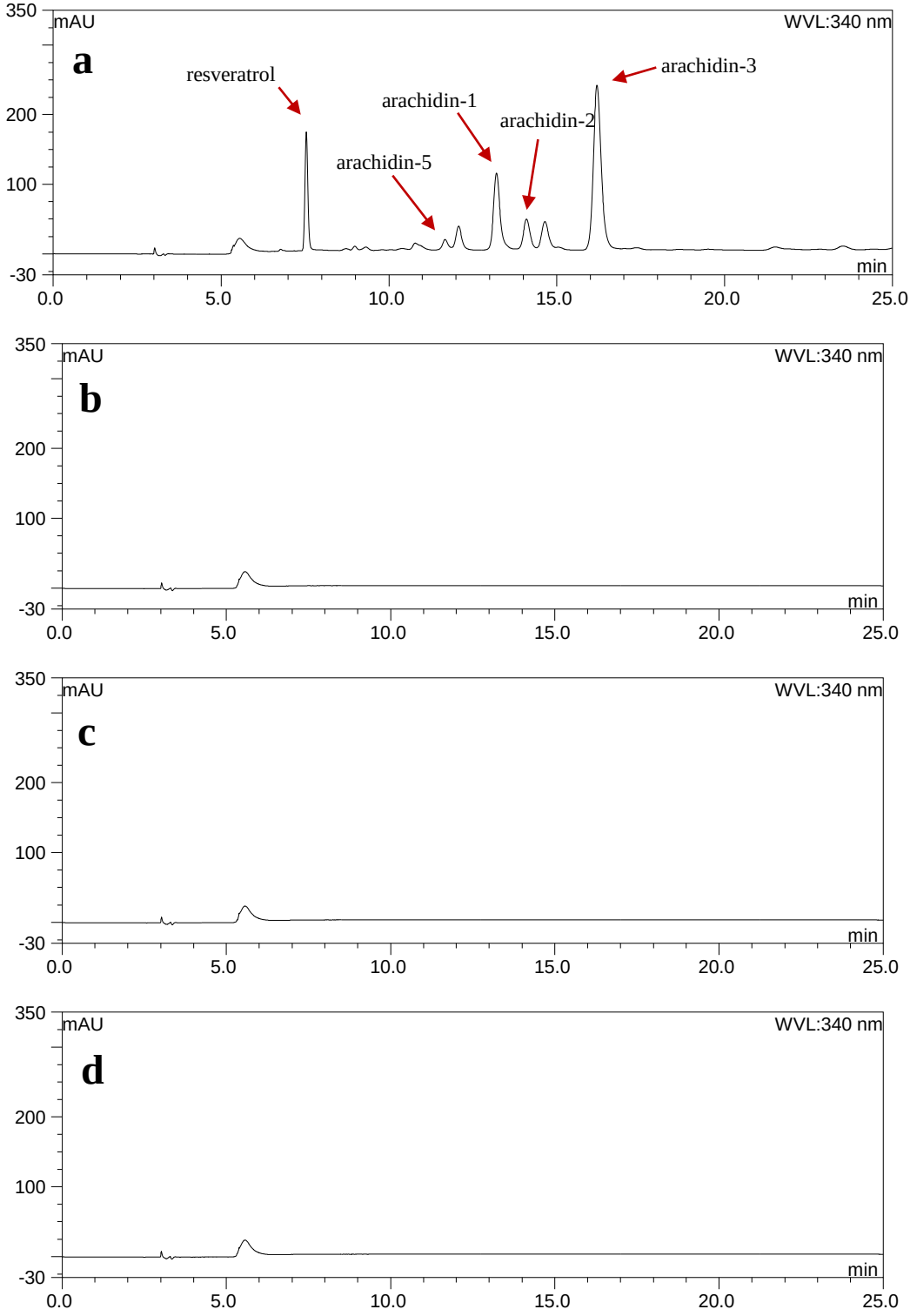


Figure S5. Effect of clomazone on the production of stilbenoids in non-elicited peanut hairy root culture. HPLC chromatograms (UV 340 nm) of ethyl acetate extracts from peanut hairy root cultures after 48-hour treatment with **(a)** 100 µM methyl jasmonate and 9 g/L methyl-β-cyclodextrin; **(b)** 10 µM clomazone; (**c**) 50 µM clomazone and **(d)** 100 µM clomazone.

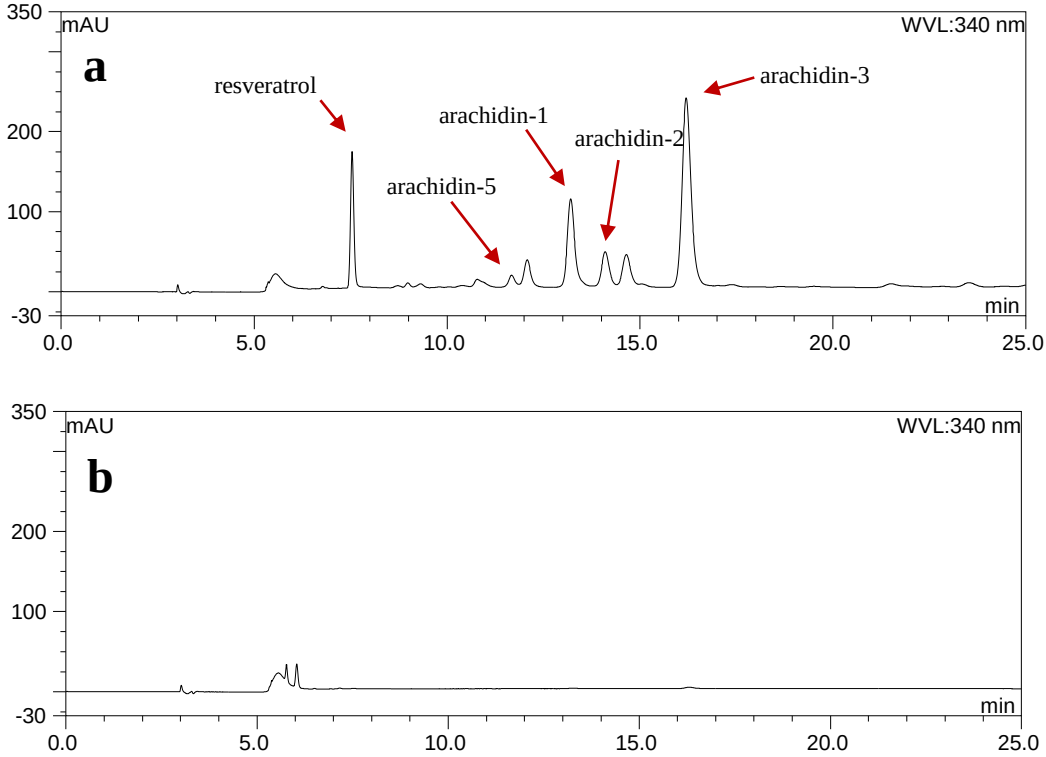


Figure S6. Comparison of stilbenoid yields from the culture medium and root tissue. Ethyl acetate extracts were prepared from elicited peanut hairy root cultures. HPLC chromatograms (UV 340 nm) of ethyl acetate extract from **(a)** culture medium and **(b)** lyophilized root tissue. Cultures were elicited for 48 hours with 100 µM methyl jasmonate and 9 g/L methyl-β-cyclodextrin.

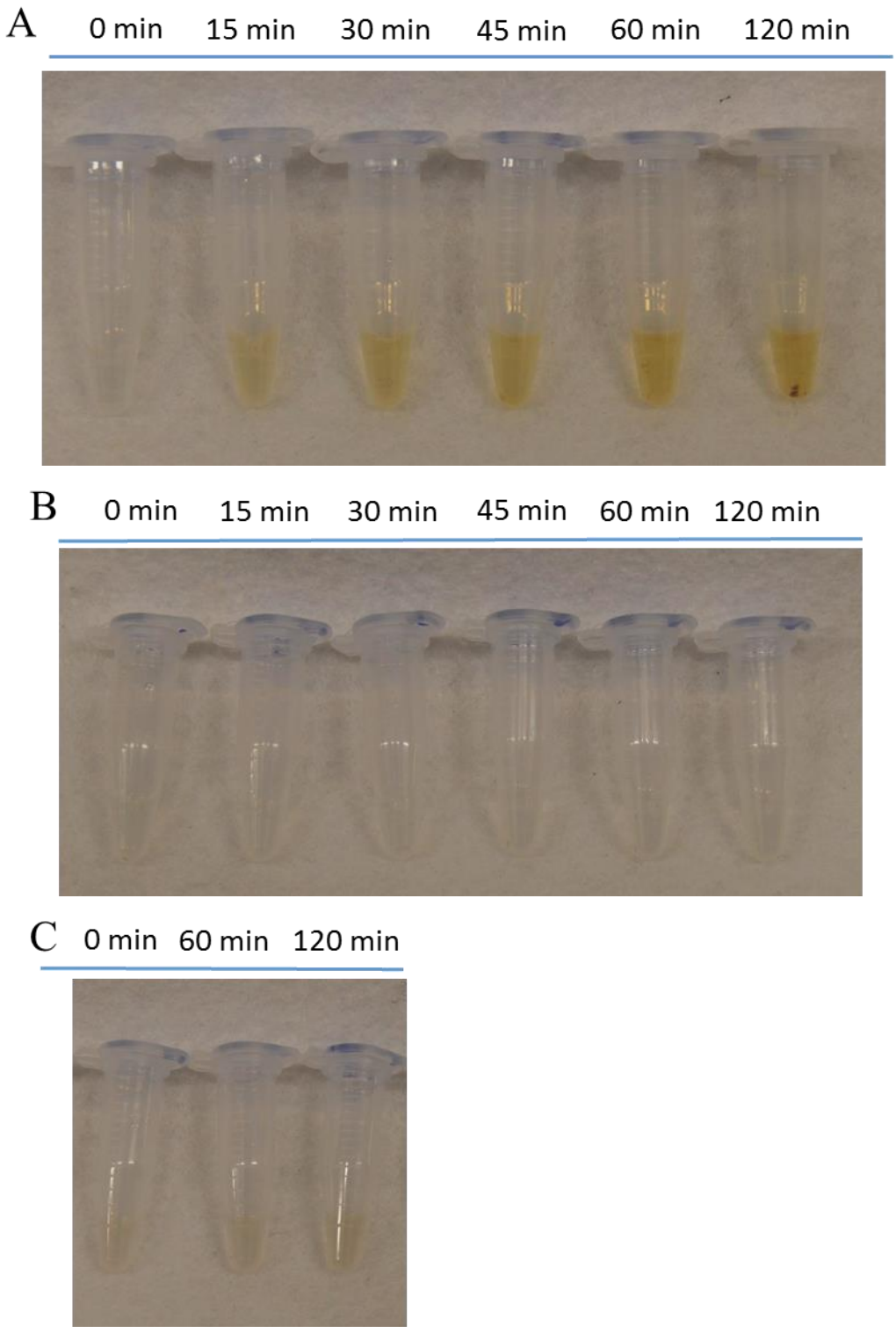


Figure S7. Color of resveratrol degradation reaction mixtures at various incubation time points. One millimolar of resveratrol was co-incubated with (**A**) 25 µg/mL crude cell-free extract from non-elicited peanut hairy roots, (**B**) 25 µg/mL crude cell-free extract with additional 5 mM DTT and (**C**) heat denatured protein as control group.

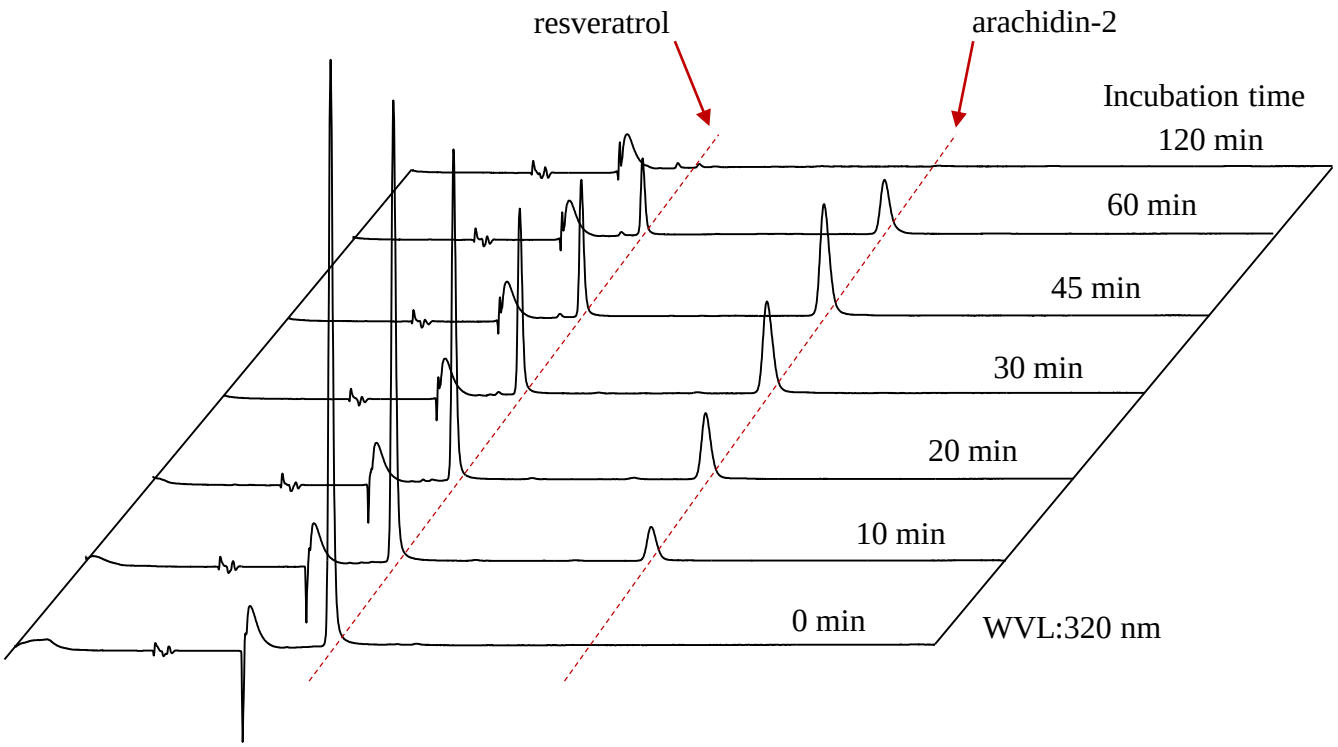


Figure S8. Time course of resveratrol prenyltansferase assay without DTT and subsequent degradation of resveratrol and arachidin-2 in the reaction. Assays were done for 0 to 120 min. HPLC chromatograms (UV 320 nm) of ethyl acetate extracts from the reaction mixture of 30 µg microsomal fraction, 100 µM resveratrol, 300 µM DMAPP, and 10 mM $MgCl_2$. Assays were done for 0, 10, 20, 30 , 45, 60 or 120 min in a pH 9.2 Tris-HCl buffer.

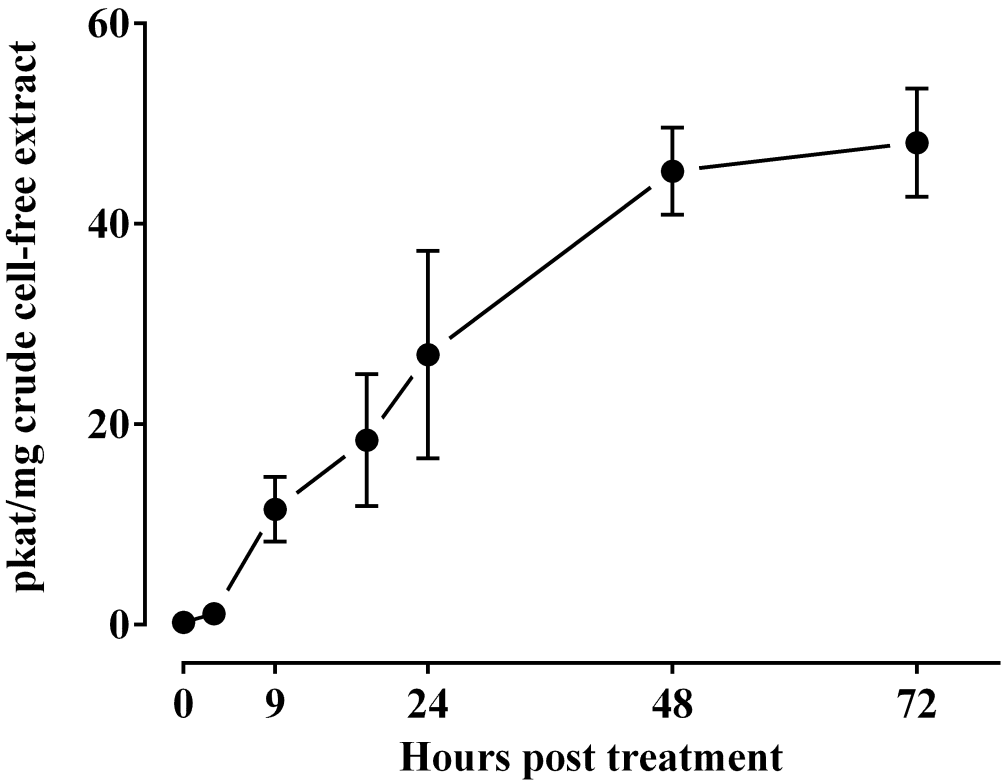


Figure S9. Time course of prenyltransferase activity in crude cell-free extract of peanut hairy roots upon the treatment with 100 µM methyl jasmonate and 9 g/L methyl-β-cyclodextrin.

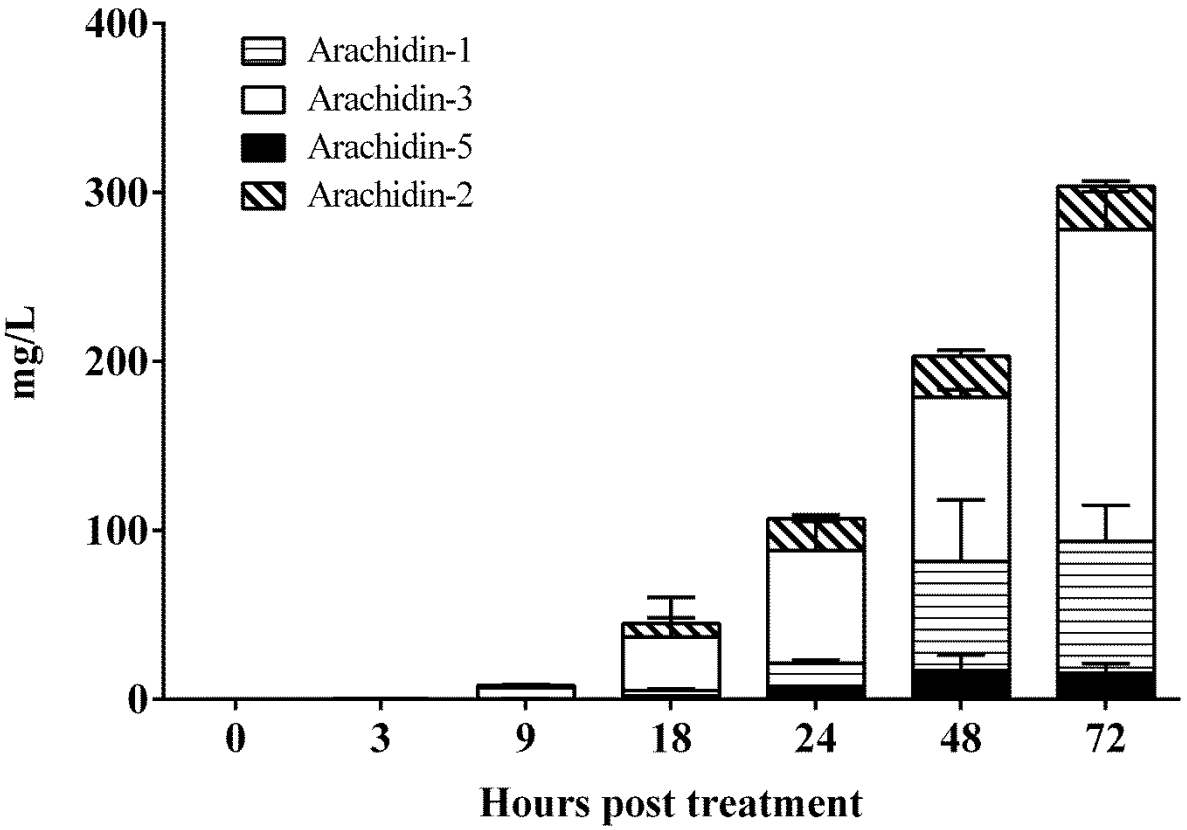


Figure S10. Accumulation of prenylated stilbenoids, arachidin-1, arachidin-3, arachidin-5 and arachidin-2 in the medium of peanut hairy root culture upon the treatment with 100 µM methyl jasmonate and 9 g/L methyl-β-cyclodextrin.

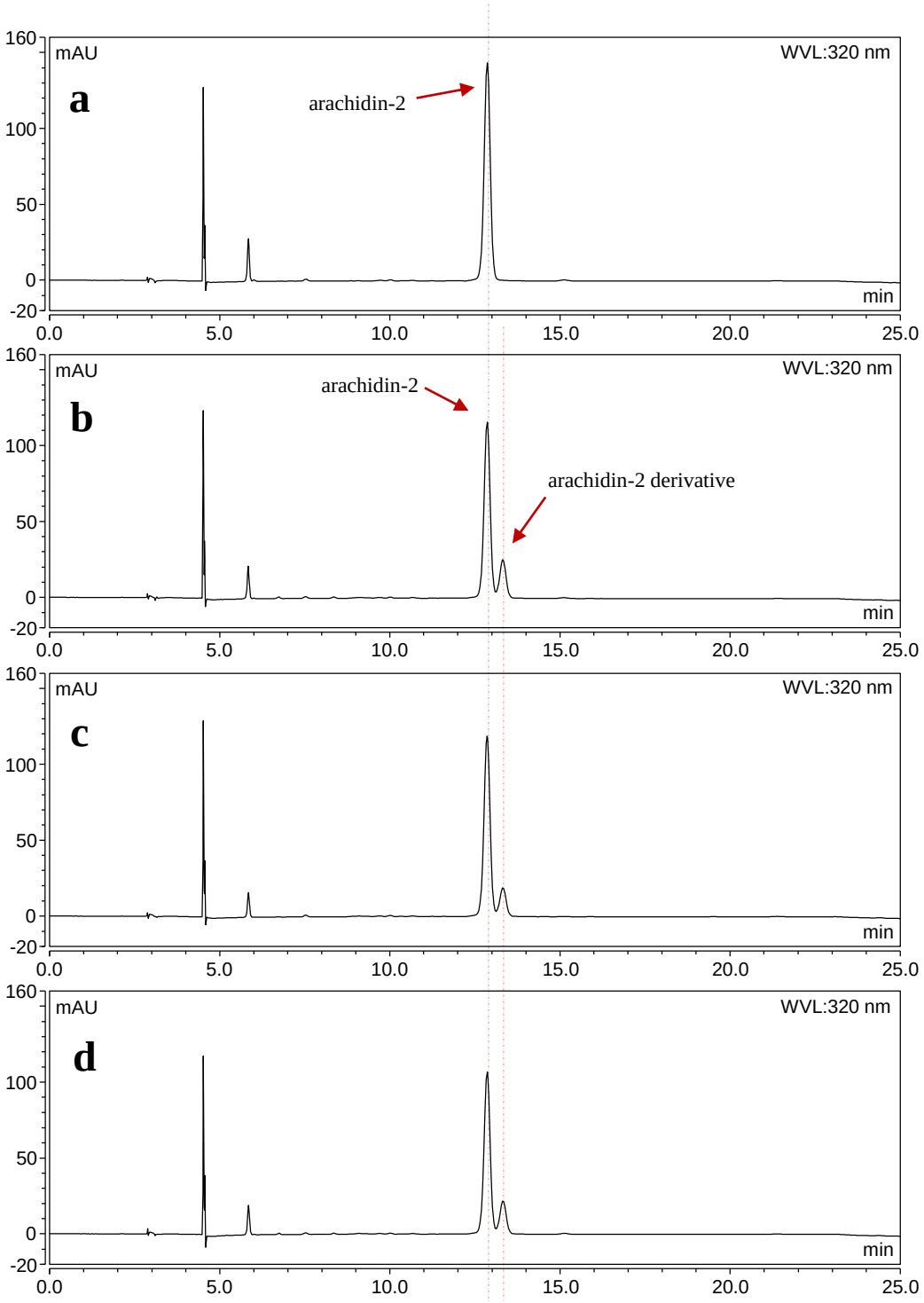


Figure S11. Biotransformation of arachidin-2 by protein extracts from elicited peanut hairy root culture. HPLC chromatograms (UV 320 nm) of ethyl acetate extracts from the 60 min reaction contained **(a)** 100 µM arachdin-2 with 30 µg heat-denatured crude cell-free protein extract as control; **(b)** 30 µg crude cell-free protein extract; **(c)** 30 µg microsomal fraction and **(d)** 30 µg 156,000 g supernatant. All reactions were done in a pH 9.2 Tris-HCl buffer with 5 mM DTT.

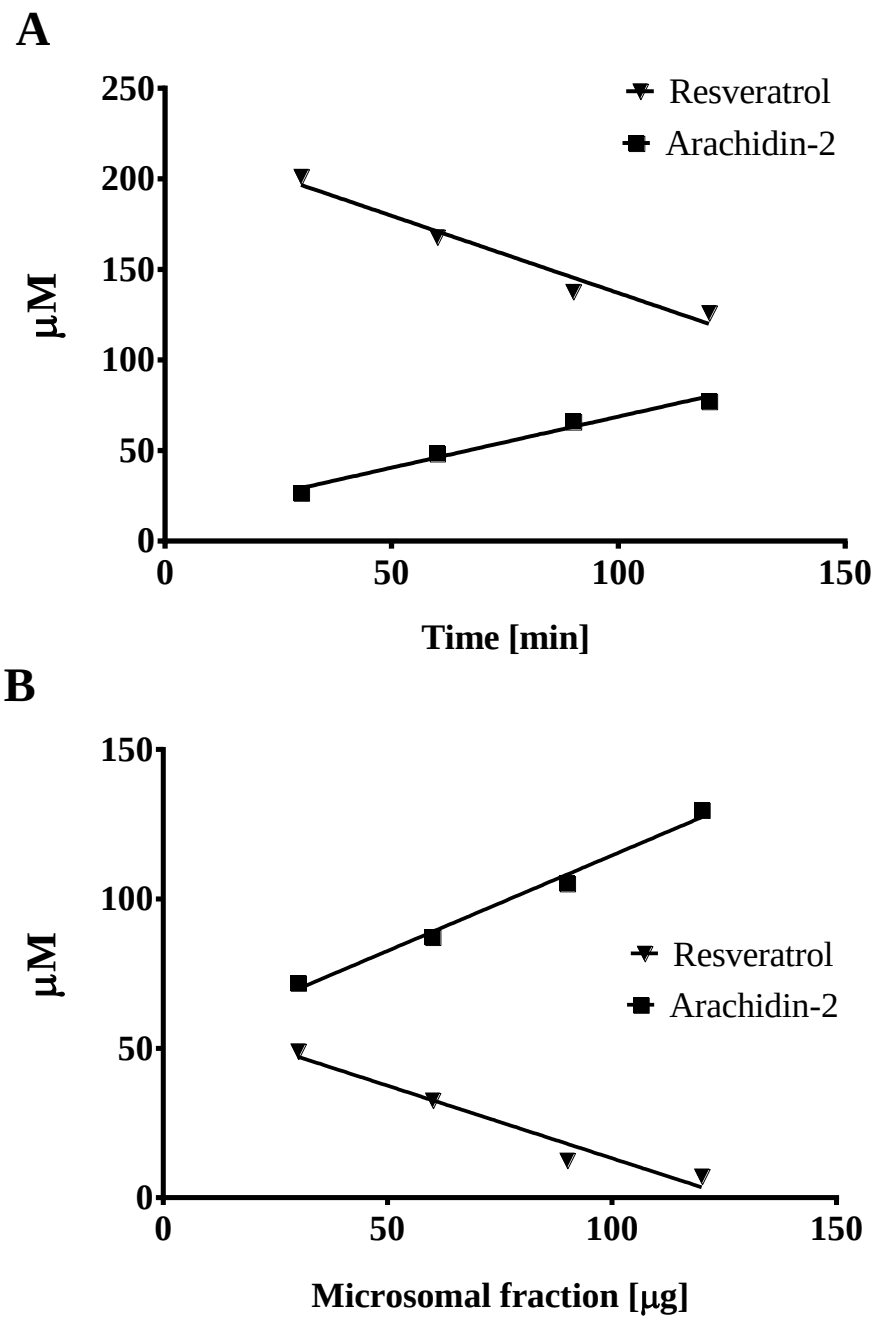


Figure S12. Resveratrol prenyltransferase activity. **A**, Concentrations of remaining resveratrol and generated arachidin-2 from the reaction mixtures with varying incubation times (30, 60 , 90 and 120 min) were measured by HPLC. **B**, Concentrations of remaining resveratrol and generated arachidin-2 from the reaction mixtures with varying amounts of microsomal fraction (30, 60, 90 and 120 µg) were measured by HPLC.

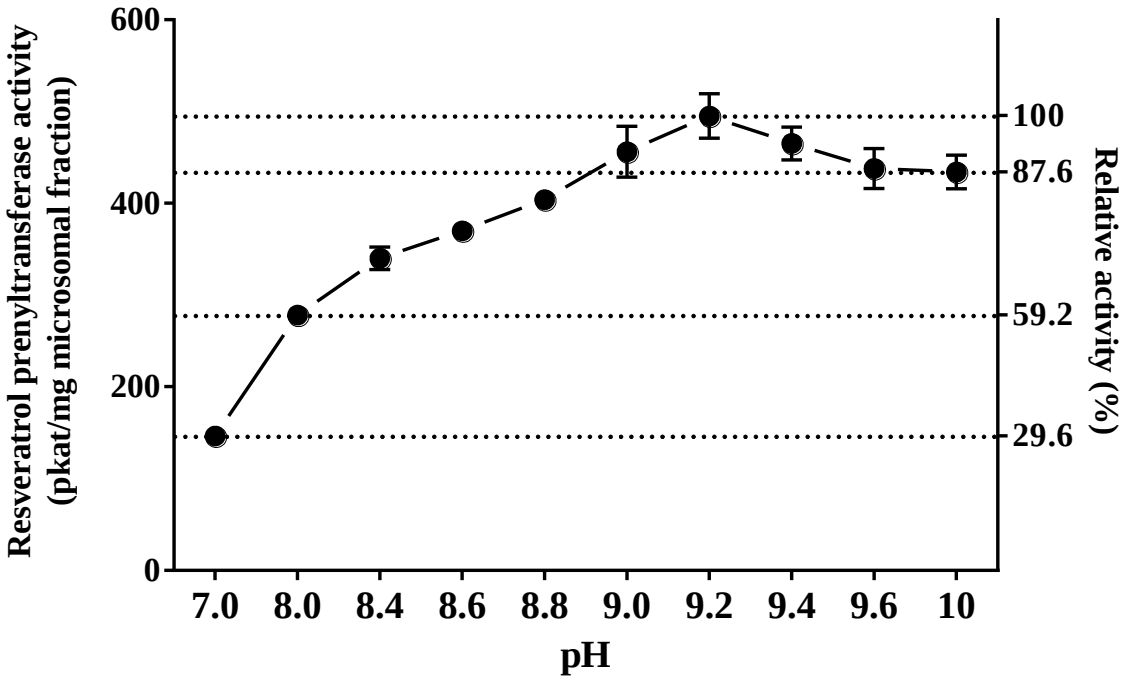


Figure S13. pH dependency of resveratrol prenyltransferase activity. Resveratrol prenyltransferase activity at various pH values was measured using 100 mM Tris-HCl buffer at pH 7.0, 8.0, 8.4, 8.6, 8.8, 9.0, 9.2, 9.4, 9.6 and 10. . Tris-HCl buffer has been reported to have a range between 7.0 and 9.2. Other reports suggest a range between 7.0 and 9.0. We initially tested the stilbenoid prenyltransferase activity with Tris-HCl buffer between 7.0 and 9.2 and the activity increased in this range. In order to ensure that the optimum pH for activity was 9.2, we increased the pH up to 10 and found that the activity decreased after 9.2.

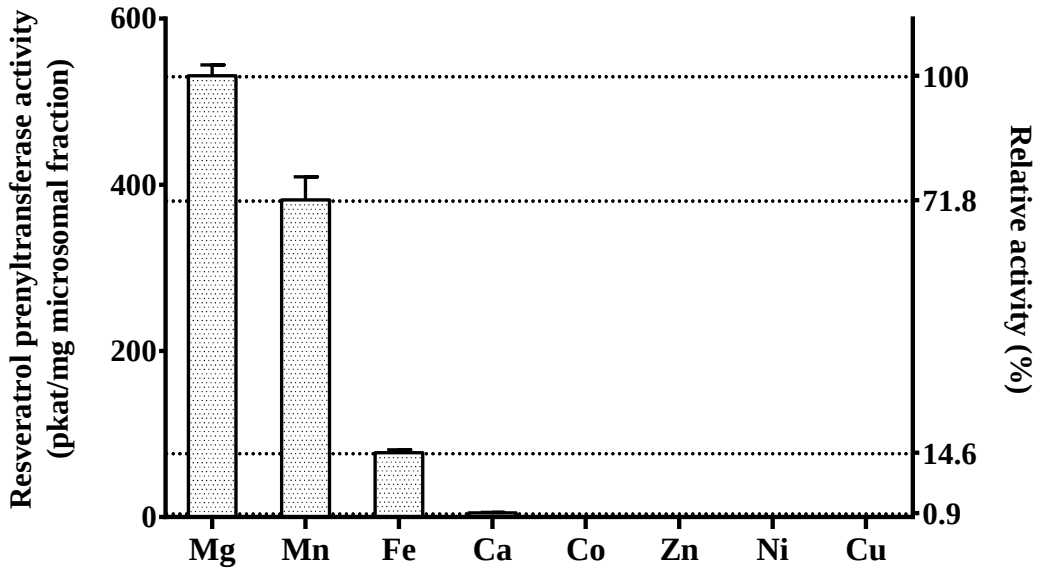


Figure S14. Divalent cation requirement for resveratrol prenyltransferase activity. Resveratrol prenyltransferase activity was compared in the presence of various divalent cations: Mg^{2+}, Mn^{2+}, Fe^{2+}, Ca^{2+}, Co^{2+}, Zn^{2+}, Ni^{2+} and Cu^{2+}. The activity in the presence of Mg^{2+} is shown as 100%.

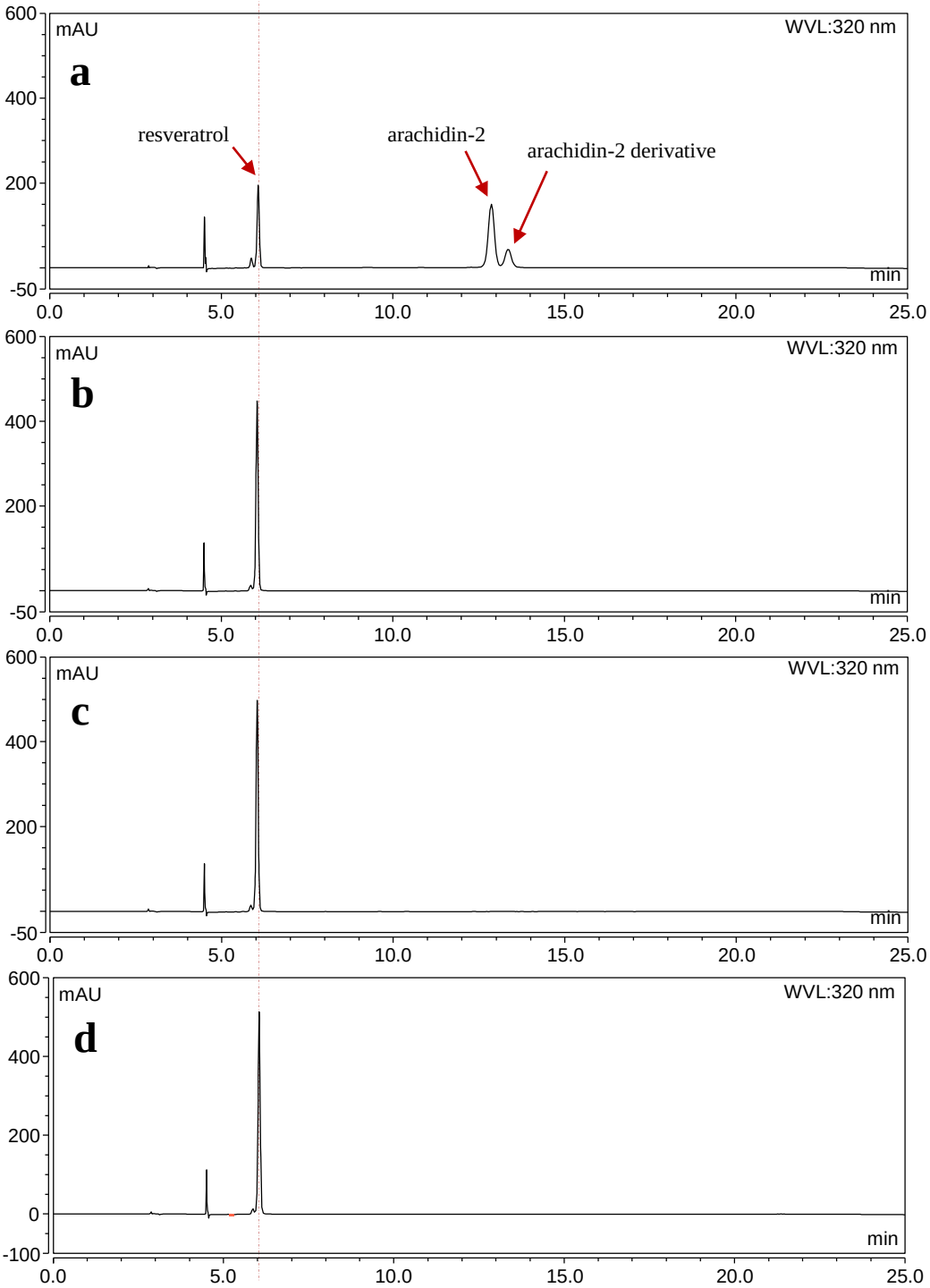


Figure S15. Biochemical characterization of resveratrol prenyltransferase in microsomal fraction of elicited peanut hairy root. HPLC chromatogram (UV 320 nm) of ethyl acetate extract of a 60 min incubation mixture containing **(a)** standard reaction (30 µg microsomal fraction, 100 µM resveratrol, 300 µM DMAPP, 10 mM $MgCl_2$ and 5 mM DTT in a pH 9.2 Tris-HCl buffer); **(b)** standard reaction without divalent cation added; **(c)** standard reaction with 300 µM IPP instead of DMAPP and **(d)** standard reaction with 30 µg microsomal fraction isolated from non-elicited peanut hairy root instead of 30 µg microsomal fraction isolated from elicited peanut hairy root.

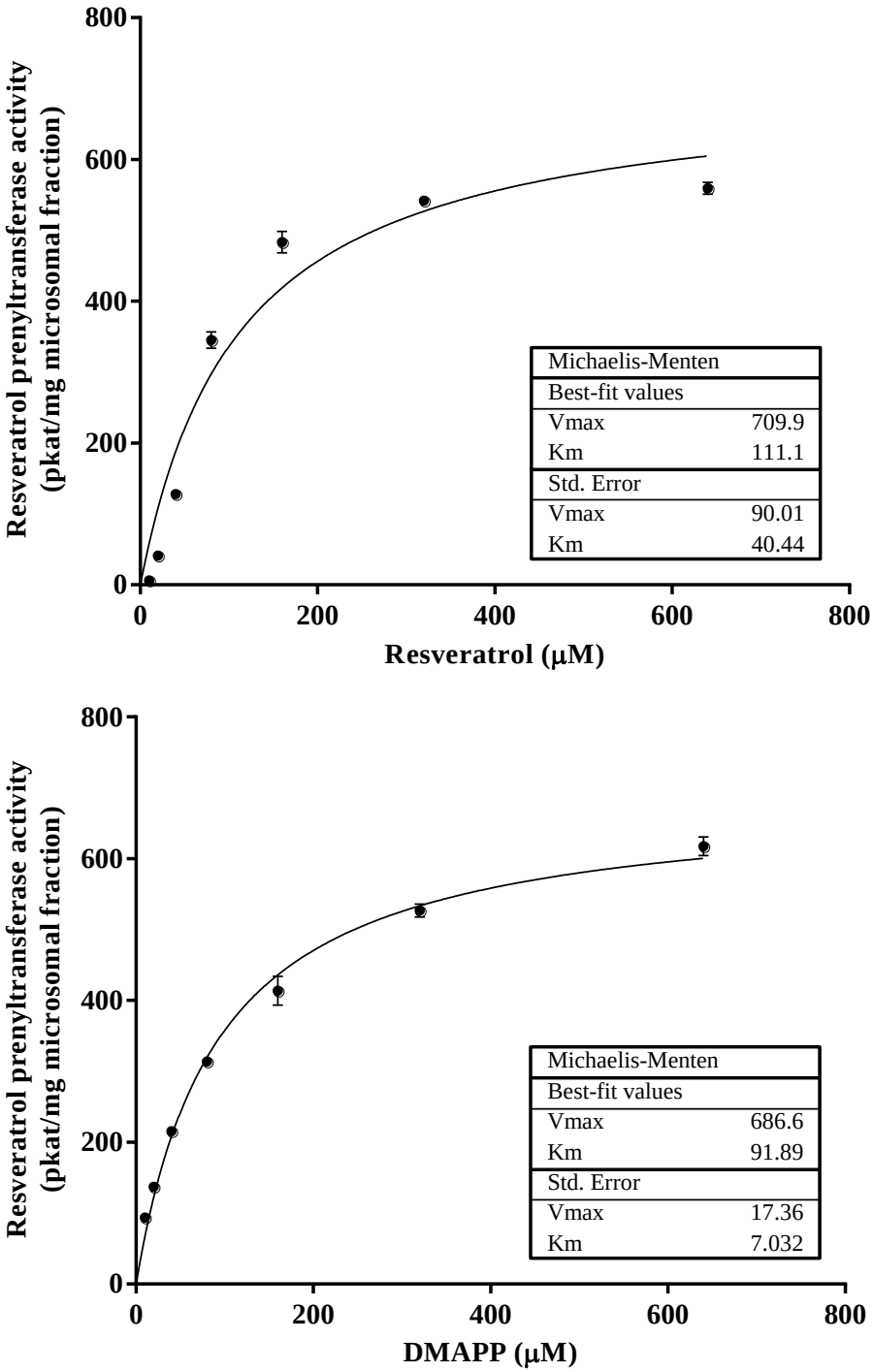


Figure S16. Effects of resveratrol and DMAPP concentrations on resveratrol prenyltransferase activity. Enzymatic activity was measured with a microsomal fraction from peanut hairy roots. The apparent K_m and V_{max} values for resveratrol and DMAPP were determined with varying concentrations of resveratrol (10 - 640 μM) and of DMAPP (10 - 640 μM) respectively and calculated via nonlinear regression analysis with Michaelis-Menten equation by Graphpad Prism 6 software.

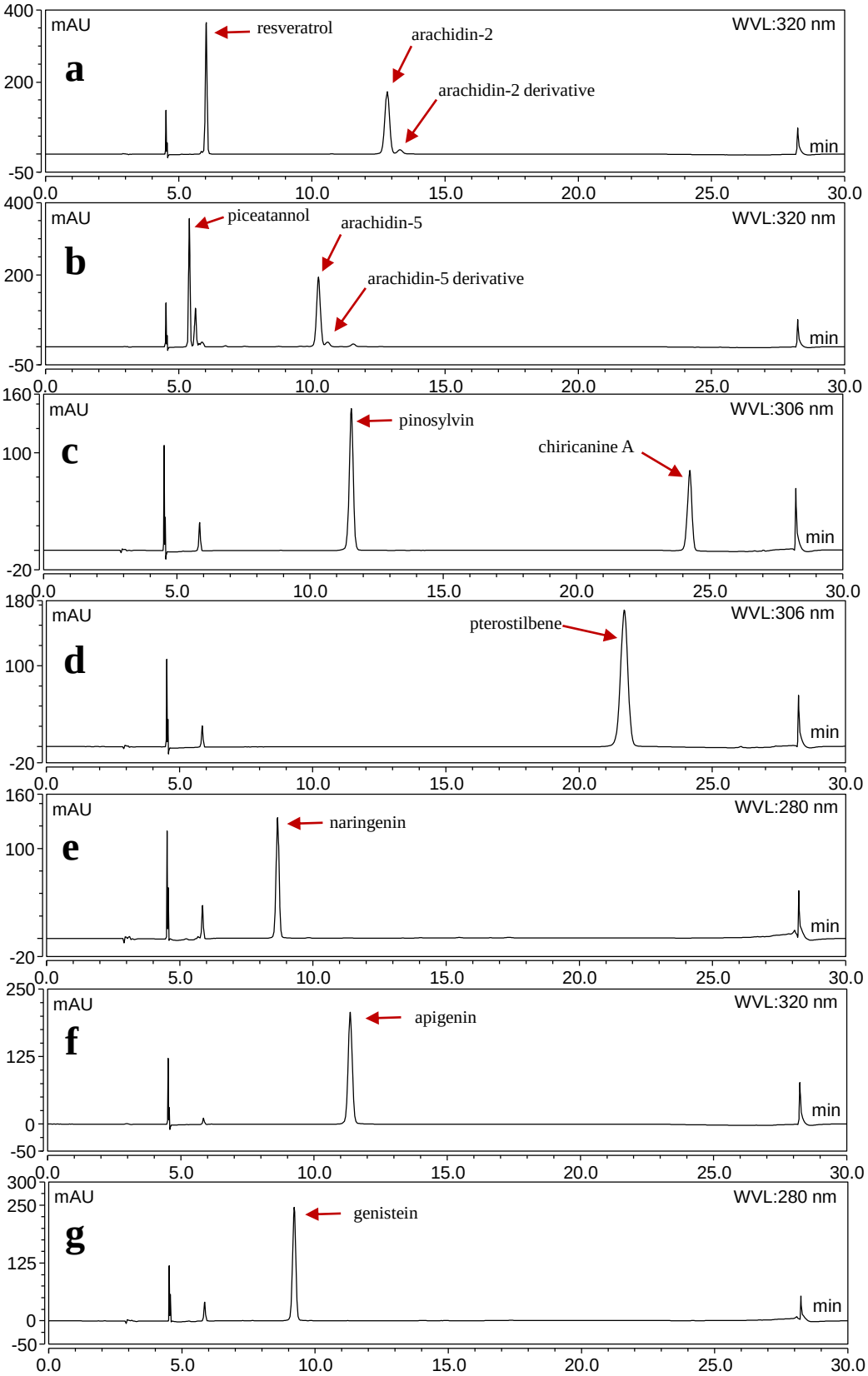


Figure S17. Substrate specificity of resveratrol prenyltransferase in microsomal fraction of elicited peanut hairy root. HPLC chromatograms (UV 320 nm) of ethyl acetate extracts of a 60 min incubation mixture containing 30 µg microsomal fraction with 300 µM DMAPP, 10 mM $MgCl_2$ and 5 mM DTT, and 100 µM prenyl acceptors (**a**, resveratrol; **b**, piceatannol; **c**, pinosylvin; **d**, pterostilbene; **e**, naringenin; **f**, apigenin and **g**, genistein) in a pH 9.2 Tris-HCl buffer.

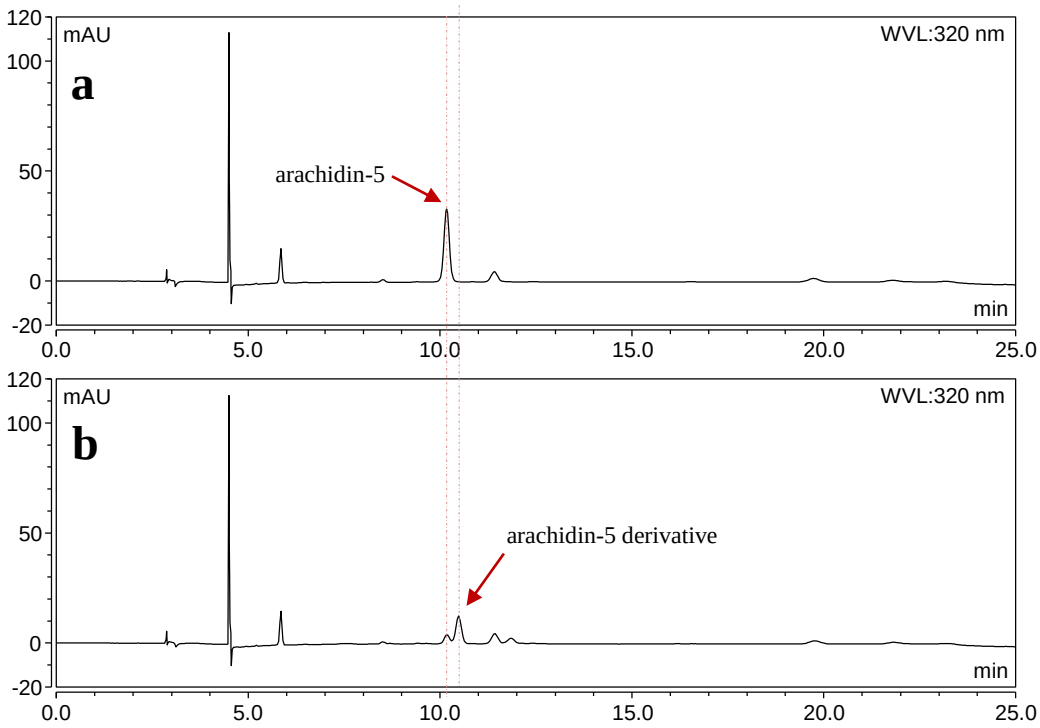
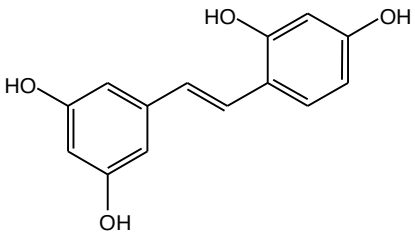
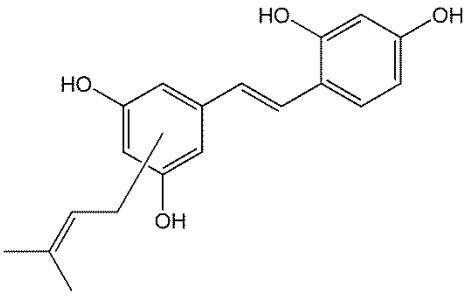


Figure S18. Biotransformation of arachidin-5 by protein fractions from elicited peanut hairy root culture. HPLC chromatograms (UV 320 nm) of ethyl acetate extracts from the 60 min incubation mixtures contained 40 µM arachidin-5 with **(a)** 30 µg heated microsomal fraction as control and **(b)** 30 µg microsomal fraction. All reactions were done in a pH 9.2 Tris-HCl buffer with 5 mM DTT.

A

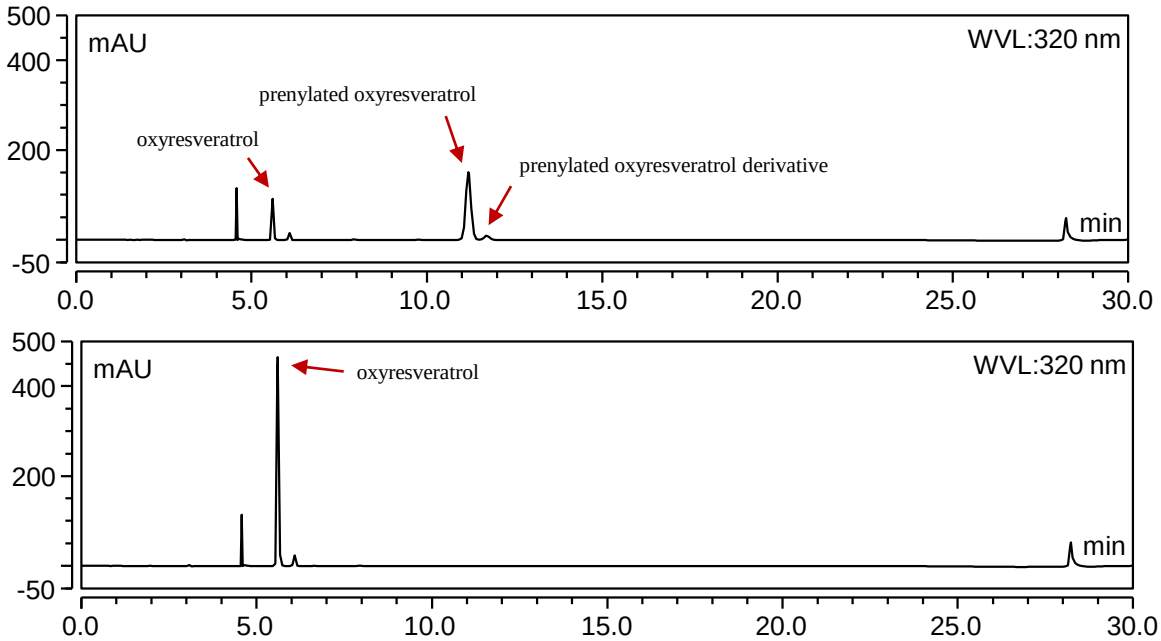


Oxyresveratrol



Prenylated oxyresveratrol

B



C

No	Analyte	t_R (min)	UV (nm)	$[M+H]^+$ (m/z)	MS^2 ions	MS^3 ions
1	Oxyresveratrol	5.61	237, 302, 328	245	**227**	**209,** 199, 157
2	Prenylated oxyresveratrol	11.19	225,304, 328	313	**257**	**239,** 215, 211
3	Prenylated oxyresveratrol derivative	11.72	233, 357	311	**293**, 283, 255	107

a, MS^2 ions in bold were the most abundant ion and subjected to MS^3 fragmentation.

Figure S19. Substrate specificity of resveratrol prenyltransferase in microsomal fraction of elicited peanut hairy root. **A**, Chemical structures of oxyresveratrol and its prenylated product. **B,** HPLC chromatograms (UV 320 nm) of ethyl acetate extraction of reaction mixtures contained 100 µM oxyresveratrol, 300 µM DMAPP, 10 mM $MgCl_2$, 5 mM DTT and 30 µg microsomal fraction **(above)**; heated denatured microsomal fraction **(below)** in a pH 9.2 Tris-HCl buffer for 60 min. **C,** HPLC-PDA-ESI-MS^3 analysis of oxyresveratrol, prenylated oxyresveratrol and its derivative.

Table S1. Protein sequences used for performing blast analysis against *Arachis* genomic and transcriptomic databases and their accession numbers

Flavonid prenyltransferase	Plant species	Protein ID
SfN8DT-1	*Sophora flavescens*	BAG12671
SG6DT	*Sophora flavescens*	BAK52291
GmG4DT	*Glycine max*	BAH22520
LaPT1	*Lupinus albus*	AER35706
GuA6DT	*Glycyrrhiza uralensis*	AIT11912
SfFPT	*Sophora flavescens*	AHA36633

Table S2. Alignment results of various flavonoid prenyltransferases with translated CDS of *Arachis duranensis* and *Arachis ipaensis* gene models.

Queried flavonid prenyltransferase	***A. duranensis***			***A. ipaensis***		
	Sequence ID	Identities[a]	Positives[b]	Sequence ID	Identities	Positives
SfN8DT-1	XP_015934049.1	228/413(55%)	284/413(68%)	XP_016201377.1	226/412(55%)	282/412(68%)
SG6DT	XP_015934049.1	225/397(57%)	276/397(69%)	XP_016201377.1	225/397(57%)	274/397(69%)
GmG4DT	XP_015934049.1	220/406(54%)	280/406(68%)	XP_016201377.1	218/406(54%)	277/406(68%)
LaPT1	XP_015934049.1	205/411(50%)	269/411(65%)	XP_016201377.1	206/411(50%)	271/411(65%)
GuA6DT	XP_015934049.1	258/410(63%)	313/410(76%)	XP_016201377.1	256/410(62%)	309/410(75%)
SfFPT	XP_015934049.1	221/410(54%)	279/410(68%)	XP_016201377.1	220/410(54%)	276/410(67%)

a: Value of identities is defined by the number of identical residues divided by the length of the matched sequence in the alignment.

b: Value of positives is defined by the number of conservative substitutions divided by the length of the matched sequence in the alignment.

Table S3. Available transcriptome databases of *Arachis* (Updated by June 9, 2016)

Database ID	Plant subspecies
WGS_VDB://GBIP01	*Arachis duranensis*
WGS_VDB://GBIQ01	*Arachis ipaensis*
WGS_VDB://GBIU01	*Arachis duranensis*
WGS_VDB://GBIW01	*Arachis ipaensis*
WGS_VDB://GBIX01	*Arachis hypogaea var. vulgaris*
WGS_VDB://GBJE01	*Arachis hypogaea var. vulgaris*
WGS_VDB://GBJF01	*Arachis duranensis*
WGS_VDB://GBJH01	*Arachis hypogaea var. vulgaris*
WGS_VDB://GBJI01	*Arachis hypogaea var. vulgaris*
WGS_VDB://GBJL01	*Arachis ipaensis*
WGS_VDB://GAER01	*Arachis hypogaea*
WGS_VDB://GAIG01	*Arachis hypogaea*
WGS_VDB://GBIR01	*Arachis duranensis*
WGS_VDB://GBIV01	*Arachis duranensis*
WGS_VDB://GBIY01	*Arachis hypogaea var. vulgaris*
WGS_VDB://GBIZ01	*Arachis hypogaea var. vulgaris*
WGS_VDB://GBJK01	*Arachis duranensis*
WGS_VDB://GBJP01	*Arachis ipaensis*
WGS_VDB://GDBK01	*Arachis stenosperma*
WGS_VDB://GDKN01	*Arachis hypogaea*
WGS_VDB://GATE01	*Arachis hypogaea*
WGS_VDB://GBHK01	*Arachis hypogaea*
WGS_VDB://GBIS01	*Arachis ipaensis*
WGS_VDB://GBJG01	*Arachis ipaensis*
WGS_VDB://GDDN01	*Arachis hypogaea*
WGS_VDB://GEFP01	*Arachis hypogaea*
Number of databases	27
Number of sequences	18,285,871
Entrez query	txid3817 [ORGN]

Table S4. Alignment results of various flavonoid prenyltransferases with translated transcripts of *Arachis duranensis*, *Arachis ipaensis* and *Arachis hypogaea*.

Queried flavonoid prenyltransferase	***A. duranensis***			***A. ipaensis***			***A. hypogaea***		
	Sequence ID	Identities[a]	Positives[b]	Sequence ID	Identities	Positives	Sequence ID	Identities	Positives
SfN8DT-1	GBIV01008945.1	228/413(55%)	284/413(68%)	GBJP01042076.1	226/412(55%)	282/412(68%)	GBIY01019957.1	227/412(55%)	283/412(68%)
SG6DT	GBIV01008945.1	229/409(56%)	282/409(68%)	GBJP01042076.1	225/397(57%)	274/397(69%)	GBJE01046074.1	230/409(56%)	281/409(68%)
GmG4DT	GBIV01008945.1	220/406(54%)	280/406(68%)	GBJP01042076.1	218/406(54%)	277/406(68%)	GBJE01046074.1	220/406(54%)	280/406(68%)
LaPT1	GBIV01008945.1	204/411(50%)	269/411(65%)	GBJP01042076.1	206/411(50%)	271/411(65%)	GBIY01019957.1	205/411(50%)	270/411(65%)
GuA6DT	GBIV01008945.1	258/410(63%)	313/410(76%)	GBJP01042076.1	256/410(62%)	309/410(75%)	GBJE01046074.1	258/410(63%)	311/410(75%)
SfFPT	GBIV01008945.1	221/410(54%)	279/410(68%)	GBJP01042076.1	220/410(54%)	276/410(67%)	GBIY01019957.1	221/410(54%)	277/410(67%)

a: Value of identities is defined by the number of identical residues divided by the length of the matched sequence in the alignment.

b: Value of positives is defined by the number of conservative substitutions divided by the length of the matched sequence in the alignment.

Table S5. Chloroplast transit peptide predictions of sequences identified from *Arachis* transcripts.

Sequence ID	ChloroP 1.1 Server - prediction results[a]					TargetP 1.1 Server - prediction results[a]						iPSORT prediction results
	Length	Score	cTP	CS score	cTP length	cTP	mTP	SP	other	Loc	RC	
GBJP01042076.1	409	0.51	Y	0.806	12	0.484	0.166	0.072	0.16	C	4	having a chloroplast transit peptide
GBIV01008945.1	409	0.538	Y	-0.705	34	0.566	0.276	0.03	0.102	C	4	having a chloroplast transit peptide
GBIY01019957.1	409	0.531	Y	-0.025	12	0.608	0.158	0.047	0.191	C	3	having a chloroplast transit peptide
GBJE01046074.1	409	0.544	Y	-0.838	34	0.557	0.298	0.032	0.1	C	4	having a chloroplast transit peptide

a: Outputs interpretation of ChloroP and TargetP results are descrpted on http://www.cbs.dtu.dk/services/ChloroP-1.1/pages/output-expl.php & http://www.cbs.dtu.dk/services/TargetP-1.1/output.php respectively.