

Supplementary Information

Dissertation Chapter 4

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Supplementary Table S1. List of mint transcriptomes analyzed along with species abbreviations and subfamily.

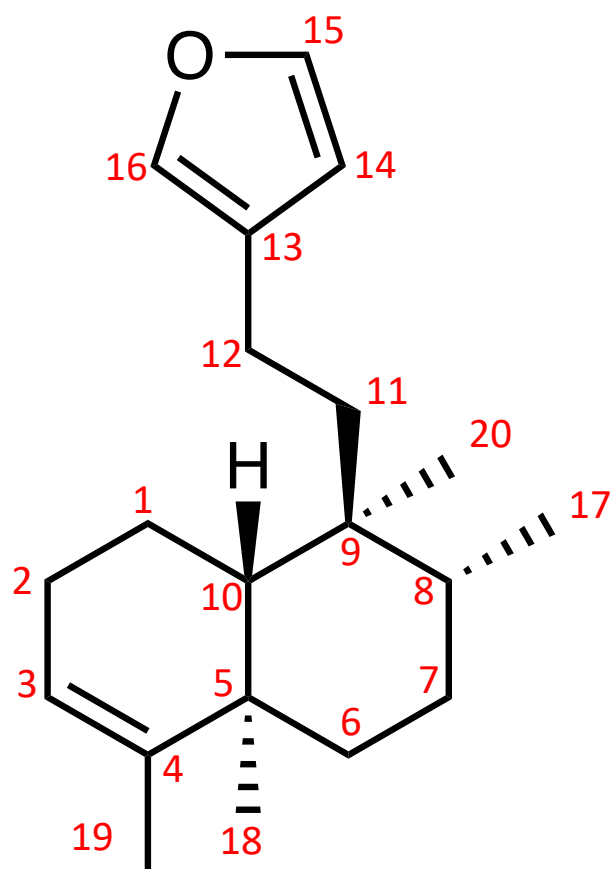
Code	Species	Subfamily	Code	Species	Subfamily
AGFO	<i>Agastache foeniculum</i> (Pursh) Kuntze	Nepetoideae	NECA	<i>Nepeta cataria</i> L.	Nepetoideae
AJRE	<i>Ajuga reptans</i> L.	Ajugoideae	NEMU	<i>Nepeta mussinii</i> Spreng. ex Henckel.	Nepetoideae
BAPS	<i>Ballota pseudodictamnus</i> (L.) Benth.	Lamioideae	OCBA	<i>Ocimum basilicum</i> L.	Nepetoideae
BEOF	<i>Betonica officinalis</i> L. [syn. <i>Stachys officinalis</i> (L.) Trevis.]	Lamioideae	ORMA	<i>Origanum majorana</i> L.	Nepetoideae
CAAM	<i>Callicarpa americana</i> L.	Callicarpoideae	ORVU	<i>Origanum vulgare</i> L.	Nepetoideae
CLBU	<i>Clerodendrum bungei</i> Steud.	Ajugoideae	PEAT	<i>Perilla frutescens</i> (L.) Britton	Nepetoideae
COCA	<i>Collinsonia canadensis</i> L.	Nepetoideae	PEBA	<i>Perovskia atriplicifolia</i> Benth.	Peronematoideae
COPY	<i>Cornutia pyramidata</i> L.	Symphorematoideae	PEFR	<i>Petraeovitex bambusetorum</i> King & Gamble	Nepetoideae
COTO	<i>Congea tomentosa</i> Roxb.	Premnoideae	PHFR	<i>Phlomis fruticosa</i> L.	Lamioideae
GLHE	<i>Glechoma hederacea</i> L.	Nepetoideae	PLBA	<i>Plectranthus barbatus</i> Andrews	Nepetoideae
GMPH	<i>Gmelina philippensis</i> Cham.	Premnoideae	POCA	<i>Pogostemon cablin</i> (Blanco) Benth.	Lamioideae
HOSA	<i>Holmskioldia sanguinea</i> Retz.	Scutellarioideae	PRMI	<i>Premna microphylla</i> Turcz.	Premnoideae
HYOF	<i>Hyssopus officinalis</i> L.	Nepetoideae	PRLA	<i>Prostanthera lasianthos</i> Labill.	Prostantheroideae
HYSU	<i>Hyptis suaveolens</i> (L.) Poit.	Nepetoideae	PRVU	<i>Prunella vulgaris</i> L.	Nepetoideae
LAAL	<i>Lamium album</i> L.	Lamioideae	ROOF	<i>Rosmarinus officinalis</i> L.	Nepetoideae
LAAN	<i>Lavandula angustifolia</i> Mill.	Nepetoideae	ROMY	<i>Rothea myricoides</i> (Hochst.) Steane & Mabb.	Ajugoideae
LECA	<i>Leonurus cardiaca</i> L.	Lamioideae	SAHI	<i>Salvia hispanica</i> L.	Nepetoideae
LELE	<i>Leonotis leonurus</i> (L.) R.Br.	Lamioideae	SAOF	<i>Salvia officinalis</i> L.	Nepetoideae
LYAM	<i>Lycopus americanus</i> Muhl. ex W.P.C.Barton	Nepetoideae	SCBA	<i>Scutellaria baicalensis</i> Georgi	Scutellarioideae
MAVU	<i>Marrubium vulgare</i> L.	Lamioideae	TEGR	<i>Tectona grandis</i> L.f.	Tectonoideae
MEOF	<i>Melissa officinalis</i> L.	Nepetoideae	TECA	<i>Teucrium canadense</i> L.	Ajugoideae
MEPI	<i>Mentha × piperita</i> L.	Nepetoideae	THVU	<i>Thymus vulgaris</i> L.	Nepetoideae
MESP	<i>Mentha spicata</i> L.	Nepetoideae	VIAG	<i>Vitex agnus-castus</i> L.	Viticoideae
MODI	<i>Monarda didyma</i> L.	Nepetoideae	WEFR	<i>Westringia fruticosa</i> (Willd.) Druce	Prostantheroideae

Supplementary Table S2. List primers used in this study.

Name	Primer direction	Primer sequence
CpCYP76BK1	F	ATGGATTTCATCTACGCTAGTC
	R	TCATGCAGTCTCAATGGGA
CbCYP76BK1	F	ATGGATTTCTCAGCAATTGTCATTGCTGC
	R	TCACACCTTTATTGGAACAGCCTTAAGG
HsCYP76BK1	F	ATGGATTTCTCTTCACTTGTCATTGTTG
	R	TCATGTCTTGATTGGAATAGCCTTGAG
PbCYP76BK1	F	ATGAACAAGAAACAGTTGGAAAAAGAATGG
	R	TCATGTCTTTATTGGAATAGCCTTGAGGG
SbaiCYP76BK1	F	ATGGATTTCACTTCACTTGTCATAGT
	R	TCATGTCTTGACTGGAATAGCCTT
TchCYP76BK1	F	ATGGATTTATCCACAGTCGCCATTGC
	R	
CamCYP76BK1	F	CAATACTAAAAATGGATTTCTTTGCACTTGT
	R	CAATAGCTTCATGCCTTTATTGGAAT
ArCYP76BK1	F	ATGGAAGTGTCCACAGTTGTA
	R	TCGATCATCCCTTAATTGGAATAGC
ArCYP76AH20	F	ATGGATAACTATGCAATTTTCATTGCTCTG
	R	TCAACACTTGAATGGAATAGCCCTG
ArCYP76AH60	F	ATGGATCTGAATACAATTTTGATTGCTGTTG
	R	TCATTTCTTGATCGGAAAAGCCTTGAG
ArCYP76B128	F	ATGGATTTCTCACCATTATCCTTGGA
	R	CTAGAGGGCGATGGGCACAG
ArCYP76S78	F	ATGTACACTTTTATCTCGATGGATTTTCTCAC
	R	TTACAATTTCACTGGAAGTGCCTTGAG
ArCYP76A134	F	GAGGAGCTAAAACCTTCCACTCTAAAC
	R	CCGCTCCCTTGGTAACAAATTCCTT
ArCYP76BV1	F	TGCTGTTATCCTCTGTATTCATT
	R	CACACATGTACACCTTCCATTCC
CYP76AH62	F	GGAAGAACTAAATGGATCTCTATG
	R	ATAATCAGGGCCTAATTGGAATAATCC
CYP76AH63	F	GGAAGAACTAAATGGATCTCTATG
	R	CATTTCAATAAATCAGGGCCTAATTGG
CYP76A133	F	ATGGCGTGGCTTCATT
	R	TTATTTTCGTTCTCTTGGAAGT
CYP71D719	F	ATGGAGTTTGAGTTTCCATCAACAC
	R	TCATTTAACCTGCTGCAAAGGT
CYP82D365	F	ATGGAAGTCTAGCTATGTCATT
	R	CTAATAAAGATTAGGAGATAGTCTTGG
CYP76S80	F	ATGAATCCAACTCCGAAAGAAAAAC
	R	GCATCTAAATTCAGGATTCAGTCC
CYP71AT245	F	ATGATTCCTCTGATATTATTAAGCTTG
	R	CTAAATAGCATATTTCTTAGGTACAAG

Supplementary Table S3. GenBank accession numbers for genes cloned in this study.

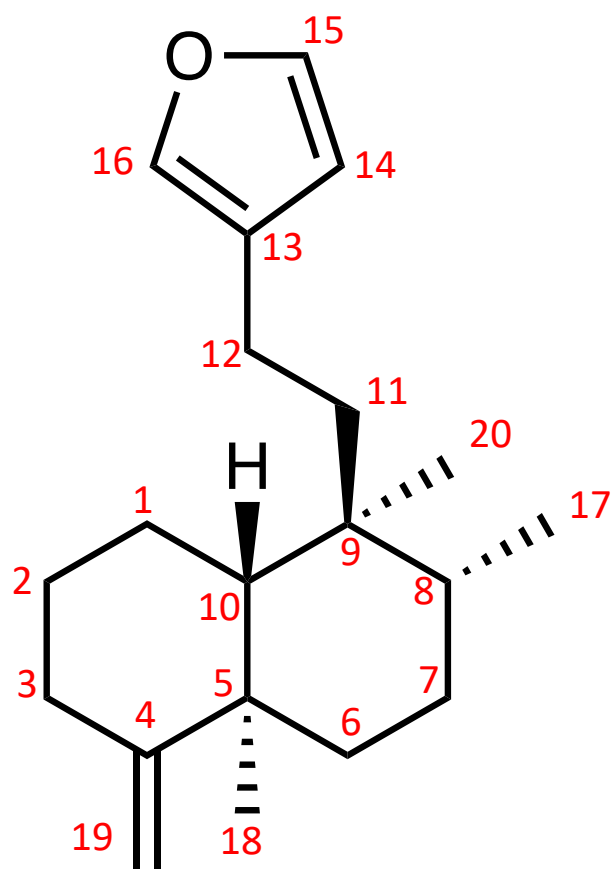
Gene name	Accession #
CamCYP82D365	OQ675287
CamCYP71D719	OQ675289
CamCYP71AT245	OQ675278
CamCYP76AH62	OQ675281
CamCYP76AH63	OQ675282
CamCYP76S79	OQ675279
CamCYP76A133	OQ675294
ArCYP76BK1	OQ675304
CamCYP76BK1	OQ675305
CbCYP76BK1	OQ675306
HsCYP76BK1	OQ675307
PbCYP76BK1	OQ675308
SbaiCYP76BK1	OQ675309
TchCYP76BK1	OQ675310
ArCYP76A134	OQ675311
ArCYP76S78	OQ675312
ArCYP76AH20	OQ675313
ArCYP76AH60	OQ675314
ArCYP76B128	OQ675315
ArCYP76BV1	OQ675316



Carbon #	$^{13}\text{C}$ $\delta$	$^1\text{H}$ $\delta$
1	18.35	1.62/1.43
2	26.97	2.05
3	120.67	5.2
4	144.67	-
5	38.34	-
7	27.53	1.43
8	36.39	1.57
9	38.87	-
10	46.55	1.44
12	18.27	2.32/2.23
13	126.02	-
14	111.16	6.26
15	142.74	7.34
16	138.55	7.2
17	16.09	0.83
18	19.96	1.01
19	18.02	1.59
20	18.35	0.74

Supplementary Figure 1. NMR chemical shift assignments of **1**. Connectivity was deduced from  $^1\text{H}$ ,  $^{13}\text{C}$ , HSQC, HMBC, and COSY correlations (Supplementary Fig. 2).  $\text{CDCl}_3$  was used as the solvent, and  $\text{CDCl}_3$  peaks were referenced to 7.26 and 77.00 ppm for  $^1\text{H}$  and  $^{13}\text{C}$  spectra, respectively. Absolute stereochemistry was assigned based on the configuration the precursor kolavenyl diphosphate.



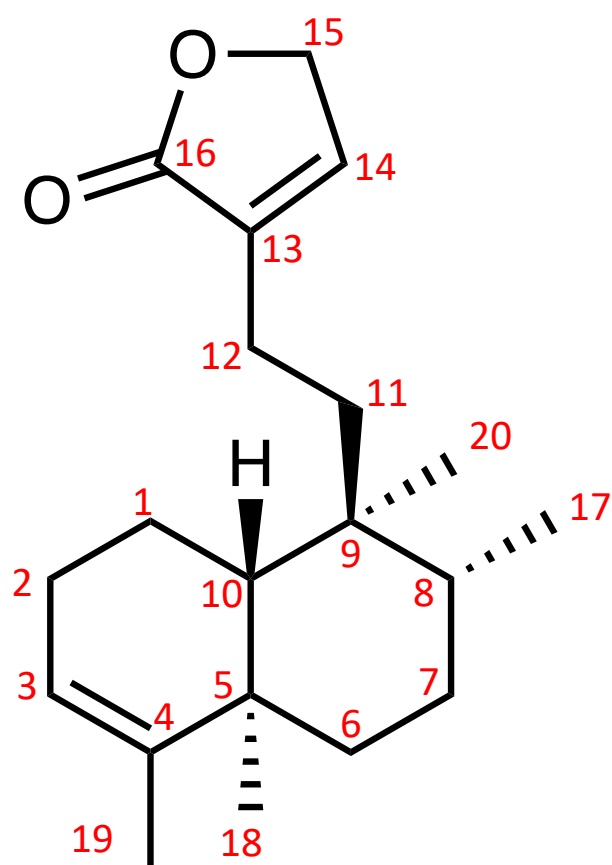


Carbon #	$^{13}\text{C}$ $\delta$	$^1\text{H}$ $\delta$
1	23	1.29
2	28.7	1.88
3	33.3	2.12/2.3
4	160.6	-
5	40.1	-
6	37.4	1.54/1.6
7	27.5	1.46, 1.51
8	36.7	1.51
9	39	-
10	48.7	1.17
11	38.4	1.47/1.57
12	18.1	2.14, 2.27
13	125.8	
14	111.3	6.24
15	142.7	7.33
16	138.5	7.18
17	16.3	0.83
18	21.1	1.05
19	102.7	4.51
20	18.3	0.75

Supplementary Figure 3. NMR chemical shift assignments of **2**. Connectivity was deduced from  $^1\text{H}$ ,  $^{13}\text{C}$ , HSQC, HMBC, and COSY correlations (Supplementary Fig. 4).  $\text{CDCl}_3$  was used as the solvent, and  $\text{CDCl}_3$  peaks were referenced to 7.26 and 77.00 ppm for  $^1\text{H}$  and  $^{13}\text{C}$  spectra, respectively. Absolute stereochemistry was assigned based on the configuration the precursor isokolavenyl diphosphate.

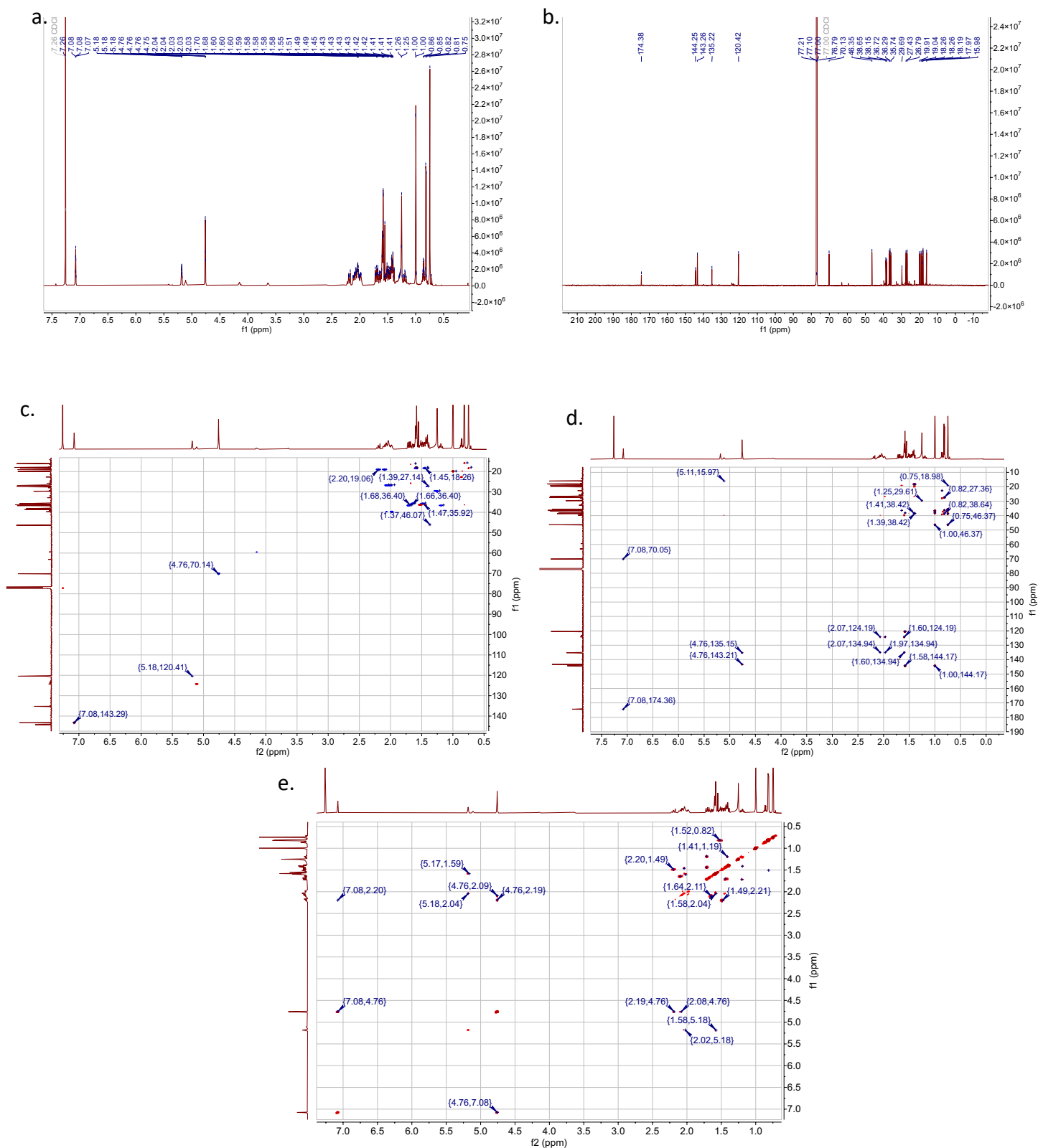




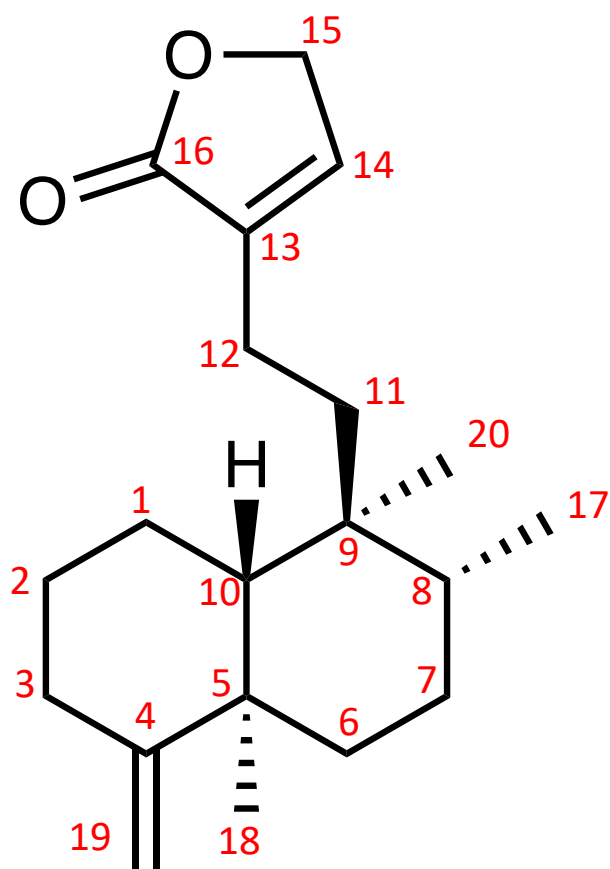


Carbon #	$^{13}\text{C}$ $\delta$	$^1\text{H}$ $\delta$
1	18.26	1.39/1.45, 1.57
2	19.04	2.1, 2.2
3	120.42	5.19
4	144.25	-
5	38.15	-
6	36.72	1.72, 1.2
7	27.43	
8	36.29	1.51
9	38.65	-
10	46.35	1.41
11	35.74	1.65, 1.46/1.49
12	26.79	1.98/2.07
13	135.22	-
14	143.26	7.08
15	70.13	4.76
16	174.38	-
17	17.97	1.59
18	19.91	1
19	18.19	0.75
20	15.98	1.6, 0.82

Supplementary Figure 5. NMR chemical shift assignments of **3**. Connectivity was deduced from  $^1\text{H}$ ,  $^{13}\text{C}$ , HSQC, HMBC, and COSY correlations (Supplementary Fig. 6).  $\text{CDCl}_3$  was used as the solvent, and  $\text{CDCl}_3$  peaks were referenced to 7.26 and 77.00 ppm for  $^1\text{H}$  and  $^{13}\text{C}$  spectra, respectively. Absolute stereochemistry was assigned based on the configuration the precursor kolavenyl diphosphate.

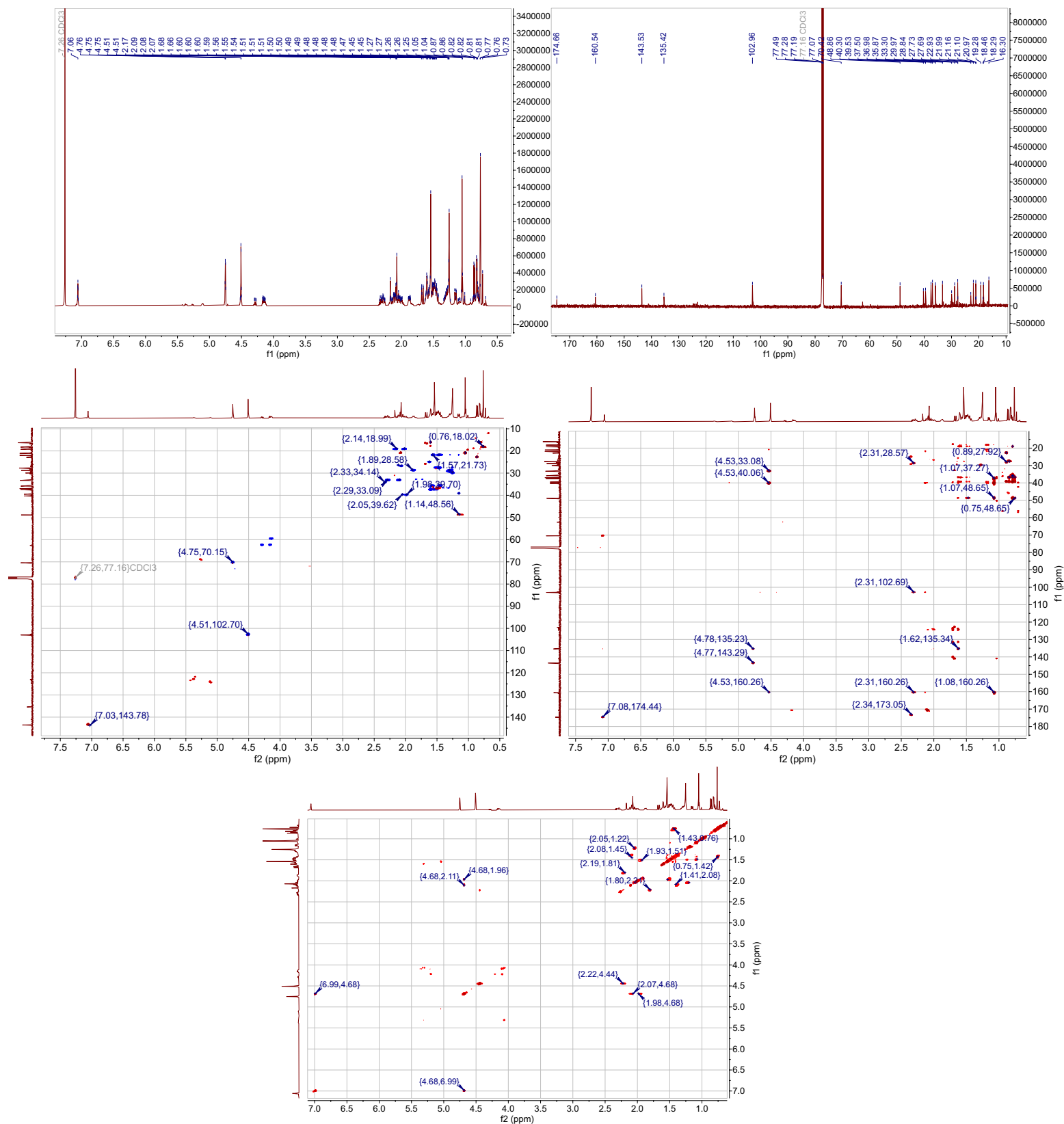


Supplementary Figure 6. NMR spectra of **3**. (a)  $^1\text{H}$  NMR spectrum, (b)  $^{13}\text{C}$  NMR spectrum, (c) HSQC spectrum, (d) HMBC spectrum, (e) COSY spectrum. CDCl<sub>3</sub> was used as the solvent, and CDCl<sub>3</sub> peaks were referenced to 7.26 and 77.00 ppm for  $^1\text{H}$  and  $^{13}\text{C}$  spectra, respectively.

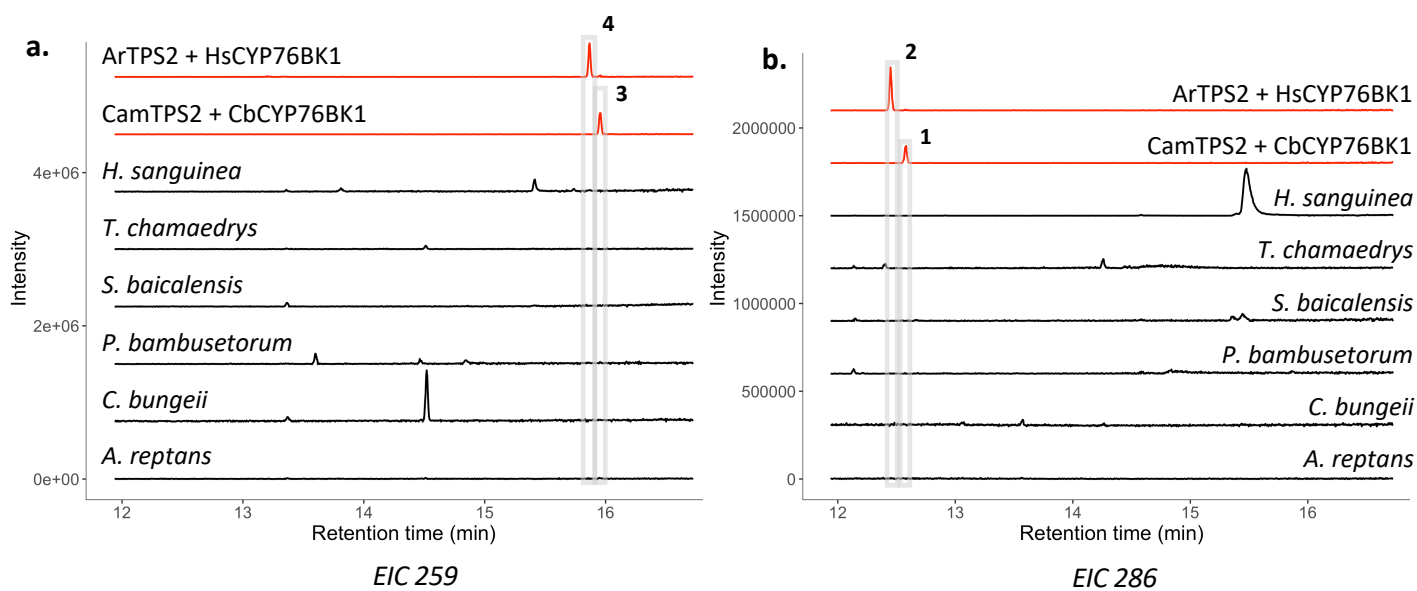


Carbon #	$^{13}\text{C}$ $\delta$	$^1\text{H}$ $\delta$
1	21.77	1.55/1.45
2	28.58	1.32/1.86
3	33.23	2.11/2.27
4	160.4	-
5	40.2	-
6	37.4	1.6
7	27.45	1.48
8	36.7	1.5
9	39.2	-
10	48.6	1.5
11	35.7	1.46/1.56
12	19	2.01/2.15
13	135.3	-
14	143.2	-
15	70.17	4.75
16	174.7	
17	16.2	0.82
18	20.85	1.06
19	102.5	4.5
20	18.2	0.76

Supplementary Figure 7. NMR chemical shift assignments of **4**. Connectivity was deduced from  $^1\text{H}$ ,  $^{13}\text{C}$ , HSQC, HMBC, and COSY correlations (Supplementary Fig. 8).  $\text{CDCl}_3$  was used as the solvent, and  $\text{CDCl}_3$  peaks were referenced to 7.26 and 77.00 ppm for  $^1\text{H}$  and  $^{13}\text{C}$  spectra, respectively. Absolute stereochemistry was assigned based on the configuration the precursor isokolavenyl diphosphate.



Supplementary Figure 8. NMR spectra of **4**. (a) <sup>1</sup>H NMR spectrum, (b) <sup>13</sup>C NMR spectrum, (c) HSQC spectrum, (d) HMBC spectrum, (e) COSY spectrum. CDCl<sub>3</sub> was used as the solvent, and CDCl<sub>3</sub> peaks were referenced to 7.26 and 77.00 ppm for <sup>1</sup>H and <sup>13</sup>C spectra, respectively.



Supplementary Figure 9. GC-MS analysis of plant extracts. None of these extracts have peaks aligning with enzyme products **1**, **2**, **3**, or **4**. However, some of the visible peaks in these EIC chromatograms could be unidentified terpenoid structures.