Table 3. Volatile headspace constituents from *Agave palmeri* and *Datura wrightii* identified by GC-MS

Peak no. Fig. 2	Ret. t. (min)	Compound	*Agave palmeri* (%)	*Datura wrightii* (%)	MW	Molecular formula	notes	Structure class
	2.77	Dimethyl disulfide	<1		94	$C_2H_6S_2$	b, d, e	Disulfide
	3.52	2-hexanone		<1	100	$C_6H_{12}O$	d, e	Ketone
7	5.00	Ethyl isovalerate	3.4		130	$C_7H_{14}O_2$	b, d, e	Ester
8	6.48	Xylene	9.7		106	C_8H_{10}	d, e, i	Aromatic
	7.70	Unk. monoterpene	<1		136	$C_{10}H_{16}$		Terpene
	7.88	A-thujene	<1		136	$C_{10}H_{16}$	d, j	Terpene
9	8.23	A-pinene	16.3		136	$C_{10}H_{16}$	b, d, e	Terpene
	8.45	Ethyl tiglate	<1		128	$C_7H_{12}O_2$	b, d, e	Ester
10	8.82	Camphene	11.0		136	$C_{10}H_{16}$	b, d, e	Terpene
	9.22	Benzaldehyde	<1	<1	106	C_7H_6O	c, d, e, f	Aromatic
	9.38	Ethyl hexanoate	<1		144	$C_8H_{16}O_2$	d	Ester
	9.57	Sabinene	<1	<1	136	$C_{10}H_{16}$	b, c, d, e, j	Terpene
11	9.73	β-pinene	14.8		136	$C_{10}H_{16}$	b, d, e	Terpene
1	10.07	Beta-myrcene	<1	2.5	136	$C_{10}H_{16}$	b, c, d, e	Terpene
12	10.60	Ethyl hexenoate	4.7		142	$C_8H_{14}O_2$	d	Ester
	10.82	Methyl sorbate	<1		126	$C_7H_{10}O_2$	b, d, f	Ester
	11.03	Cymene	<1		134	$C_{10}H_{14}$	b, d, e	Terpene
13	11.18	Limonene	12.7	<1	136	$C_{10}H_{16}$	b, d, e	Terpene
	11.21	Cineol		<1	154	$C_{10}H_{18}O$	c, d	Terpene
2	11.29	Benzyl alcohol		9.5	109	C_7H_8O	c, d, e	Aromatic
	11.57	Ethyl isohexenoate	<1		142	$C_8H_{14}O_2$	d	Ester
3	11.82	Beta-ocimene	<1	32.4	136	$C_{10}H_{16}$	c, e, d, j	Terpene
14	12.02	Ethyl sorbate[k]	2.0		140	$C_8H_{12}O_2$	b, d, f, h	Ester
	12.04	Acetophenone		<1	120	C_8H_8O	d, e	Aromatic
	12.42	Unk. monoterpene	<1		136	$C_{10}H_{16}$		Terpene
		Methyl benzoate		2.6	136	$C_8H_8O_2$	c, d, e, f, g	Ester
15	12.67	Ethyl sorbate	16.9		140	$C_8H_{12}O_2$	b, d, e	Ester
	12.74	Linalool		<1	154	$C_{10}H_{18}O$	c, d, e, f	Terpene
	12.78	Ethyl sorbate[k]	<1		140	$C_8H_{12}O_2$	b, d	Ester
	12.88	Nonanal		<1	142	$C_9H_{18}O$	c, d, e, f	Aldehyde
	13.25	Phenethanol	<1		122	$C_8H_{10}O$	c, b, d, e, f	Aromatic
	14.03	Propyl sorbate[k]	<1		154	$C_9H_{14}O_2$	b, d, f	Ester
	14.20	Ethyl benzoate	<1		150	$C_9H_{10}O_2$	d, e, f	Ester
	14.55	Propyl sorbate[k]	<1		154	$C_9H_{14}O_2$	b, d, f	Ester
4	14.63	Methylsalicyclate		3.9	152	$C_8H_8O_3$	c, d, e,	Aromatic
	14.75	Propyl sorbate	<1		154	$C_9H_{14}O_2$	b, d, e, f, g, h	Ester
	14.92	Decanal	<1		156	$C_{10}H_{20}O$	c, d, e	Aldehyde
	15.38	Propyl sorbate[k]	<1		154	$C_9H_{14}O_2$	b, d, f	Ester
	15.36	Nerol		<1	154	$C_{10}H_{18}O$	c, d, e, f	Terpene

Peak no. Fig. 2	Ret. t. (min)	Compound	*Agave palmeri* (%)	*Datura wrightii* (%)	MW	Molecular formula	notes	Structure class
	15.87	Butyl sorbate	<1		154	$C_{10}H_{16}O_2$	d	Ester
5	15.94	Geraniol		35.5	154	$C_{10}H_{18}O$	c, d, e, f	Terpene
	16.36	Geranial		1.6	152	$C_{10}H_{16}O$	c, d, e, f	Terpene
	16.61	Neral		1.1	152	$C_{10}H_{16}O$	c, d, e	Terpene
	17.85	Cycklosativene	<1		204	$C_{15}H_{32}$	d	Terpene
	17.88	Geranyl acetate		<1	196	$C_{12}H_{20}O_2$	c, d, e	Terpenoid
	18.13	Benzyl pentanoate	<1		192	$C_{12}H_{16}O_2$	c, d	Ester
	18.13	Tetradecane		<1	198	$C_{14}H_{30}$	d, e	Alkane
	18.83	Alloaromadendrene	<1		204	$C_{15}H_{32}$	d	Sesquiterpene
	19.10	Pentadecane	<1	<1	212	$C_{15}H_{32}$	d, e, f	Alkane
6	19.13	A-farnesene		2.3	204	$C_{15}H_{24}$	c, d, e, f	Terpene
	19.88	Hexadecane	<1		226	$C_{16}H_{34}$	d, e	Alkane
	20.55	Heptadecane	<1		240	$C_{17}H_{36}$	d, f	Alkane
	21.14	Benzyl benzoate		<1	212	$C_{14}H_{12}O_2$	c, d, e, f	Ester
	21.24	Octadecane	<1		254	$C_{18}H_{38}$	d, e, f	Alkane
	22.00	Nonadecane	<1		268	$C_{19}H_{40}$	d, e, f	Alkane

[a]Compounds are listed in order of GC retention time. Compound numbers shown in the first column correspond with Fig. 2.

[b]Also observed by R. A. Raguso (1).

[c]Also observed by Raguso *et al*. (2).

[d]Determined by comparison to spectra in the National Institute of Standards and Technology (NIST) 1998 spectral library.

[e]Determined by comparison of spectra and retention times with standard samples.

[f]Confirmed by accurate mass measurement (observed mass within 5 mDa of calculated mass).

[g]Standard samples prepared by transesterification reactions under acidic conditions.
[h]Double bond stereochemistry not determined.

[i]Regiochemistry undetermined.

[j]Determined by comparison to retention indices published by Helmig *et al*. (3).

[k]Isomer.

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