Progress in Essential Oils

Brian M. Lawrence, Consultant

Rose Oil and Extracts

Although rose oil and extracts are produced from more than one species of rose, this review is totally devoted to Rosa damascena Mill., which is grown commercially in Bulgaria, Turkey and to a lesser extent, India and Morocco.

Lindström and Jaquier (1993) analyzed a sample of Bulgarian rose oil to determine the enantiomeric distribution of a number of constituents. The results of this study are summarized as follows:

(1R,5R)-(+)-α-pinene (2 percent): (1S,5S)-(-)-α-pinene (98 percent)
(1R,5R)-(+)-β-pinene (8 percent): (1S,5S)-(-)-β-pinene (92 percent)
(1R,5R)-(+)-sabinene (17 percent): (1S,5S)-(-)-sabinene (83 percent)
(4R)-(+)-limonene (60 percent): (4S)-(-)-limonene (40 percent)
(4R)-(+)-α-terpineol (47 percent): (4S)-(-)-α-terpineol (53 percent)
(4S)-(+)-terpinen-4-ol (27 percent): (4R)-(-)-terpinen-4-ol (73 percent)
(3R)-(+)-citronellol (< 0.1 percent): (3S)-(-)-citronellol (> 99.9 percent)
(3S)-(+)-linalool (42 percent): (3R)-(-)-linalool (58 percent)
(1R)-(+)-camphor (69 percent): (1S)-(-)-camphor (31 percent)
(2R)-(+)-(E)-α-ionone (> 99.9 percent): (2S)-(-)-(E)-α-ionone (< 0.1 percent)
(2R,4S)-(+)-*cis*-rose oxide (< 0.1 percent): (2S,4R)-(-)-*cis*-rose oxide (> 99.9 percent)
(2S,4S)-(+)-*trans*-rose oxide (0.6 percent): (2R,4R)-(-)-*trans*-rose oxide (99.4 percent)
(+)-nerol oxide (50 percent): (-)-nerol oxide (50 percent)
(2S,5S)-(+)-theaspirane A (37 percent): (2R,5R)-(-)-theaspirane A (63 percent)
(2S,5R)-(+)-theaspirane B (77 percent): (2R,5S)-(-)-theaspirane B (23 percent)

The authors noted that camphor, (E)-α-ionone and the two theaspiranes had not previously been identified in rose oil. This finding was important because α-ionone and the two theaspiranes could probably contribute to the complex aroma characteristics of Bulgarian rose oil as they are strong smelling compounds.

Brud and Konpacka-Brud (1994) compared the composition of one sample of Bulgarian and two samples of Turkish rose oils. The results of this comparative study are shown in T-1. The authors also repeated the results of an earlier report of Ohloff (1978) in which the important odor constituents of six components were compared as shown in T-2.

Vuillemier et al. (1995) selected five components of rose oil and rose absolute to study their evaporation rates from the skin using headspace analysis. The comparative differences in these five components between the oil and absolute can be seen in T-3. Unfortunately, the authors compared a Grasse-produced rose absolute (which may have been obtained from *R. canina* and not *R. damascena* as is Bulgarian rose oil).

Wang et al. (1995) used multidimensional GC analysis with one of the columns being a chiral phase to determine the enantiomeric distribution of limonene and linalool in rose oil. They found that these two compounds were present in the following ratios:

(4R)-(+)-limonene (51.1 percent): (4S)-(-)-limonene (48.9 percent)
(3S)-(+)-linalool (4.7 percent): (3R)-(-)-linalool (95.3 percent)

Bayle and Casabianca (1996) examined the enantiomeric distribution of citronellol in a variety of rose oils and extracts. The results of this study are summarized in T-4. Furthermore, for comparative purposes the authors reported that the enantiomeric distribution of synthetic citronellol and citronellol isolated from Chinese and Bourbon geranium oil was as follows:

synth. citronellol: (3R)-(+)- (49.8-50.0 percent): (3S)-(-)- (50.0-50.2 percent)
rhodinol ex Chinese geranium oil: (3R)-(+)- (48.5 percent): (3S)-(-)- (51.5 percent)
rhodinol ex Bourbon geranium oil: (3R)-(+)- (23-30 percent): (3S)-(-)- (40-54 percent)

Comparative percentage composition of Bulgarian and Turkish rose oils **T-1**

Compound	Bulgarian rose oil	Turkish rose oil	Compound	Bulgarian rose oil	Turkish rose oil
ethanol	1.43	0-5.14	citronellol	33.40	28.20-45.04
valeraldehyde	0.07	0-0.05	nerol	5.90	3.60-6.62
3-hexenal*	0.26	0.08-0.16	geraniol + neral	18.47	11.87-26.33
α-pinene	0.73	0.04-0.50	geranial + carvone	0.72	0.57-0.87
camphene + heptanal	0.14	0.01-0.07	citronellyl acetate	0.53	0.51-0.72
β-pinene	0.03	0.02-0.03	neryl acetate	0.06	0.04-0.09
myrcene + hexanol	0.50	0-0.30	(E)-cinnamaldehyde + pentadecane	0.21	0.30-0.50
heptanol	0.02	0-0.01	geranyl acetate	1.60	1.10-1.23
hexyl acetate	0.01	0-0.01	eugenol + (E)-β-damascenone	1.20	1.01-1.19
6-methyl-5-hepten-2-one	0.04	0.02	methyl eugenol + hexadecane	2.37	1.42-3.26
octanal	0.05	0.02	heptadecane + heptadecene*	1.90	1.80-2.44
benzaldehyde	0.10	0.01-0.03	octadecane + octadecene*	0.30	0.25-0.67
octanol	0.07	0.01-0.02	(E,E)-farnesol	0.87	0.36-1.61
linalool	2.18	0.54-0.95	nonadecane + nonadecene*	14.51	13.06-16.17
cis-rose oxide + nonanol	0.43	0.10-0.38	eicosane + eicosene*	1.07	0.85-0.86
trans-rose oxide	0.17	0.07-0.18	heneicosane + heneicosene*	4.28	3.30-3.87
nonanal	0.09	0.03-0.07	docosane + tricosane + tetracosane + pentacosane	1.11	0.74-0.92
2-phenethyl alcohol + decanal + terpinen-4-ol	1.45	1.88-2.58			

*correct isomer not identified

Odor importance of six selected rose oil constituents **T-2**

Compound	Average % composition	Threshold (ppb)	Percentage odor impact
citronellol	38.00	40	4.0
geraniol	14.00	75	0.8
nerol	7.00	300	0.1
cis- & *trans*-rose oxide	0.46	0.5	4.0
(E)-β-damascenone	0.14	0.009	69.9

Comparison of the amounts of five selected components in rose oil and absolute **T-3**

Compound	Rose oil	Rose absolute
linalool	1.33	1.13
2-phenethyl alcohol	1.71	65.54
citronellol	49.21	9.82
geraniol	14.33	4.20
methyl eugenol	2.75	0.75

Finally, they examined the enantiomeric distribution of citronellol in one commercial oil and one concrete and two concretes to which synthetic citronellol had been added as shown in T-5. From these results the authors determined that 7 percent synthetic citronellol had been added to the Bulgarian rose oil and 8 percent had been added to the Bulgarian rose concrete.

Enantiomeric distribution (%) of citronellol in various samples of rose oil and extracts **T-4**

Citronellol origin	(3R)-(+)	(3S)-(-)
Turkish rose oil	0.5-1.0	99.0-99.5
Bulgarian rose oil	0.5-0.7	99.3-99.5
Iranian rose oil	1.0	99.0
Turkish rose concrete	0.8	99.4
Bulgarian rose concrete	0.5-1.0	99.0-99.5
Moroccan rose concrete	0.6	99.4
Turkish rose absolute	0.4-1.0	99.0-99.6
Moroccan rose absolute	0-0.3	99.7-100
Rose-de-Mai concrete	0	100
Rose-de-Mai absolute	0-1.0	99.0-100

Enantiomeric distribution of citronellol in some selected rose isolates **T-5**

Citronellol origin	(3R)-(+)	(3S)-(-)
commercial sample Bulgarian oil	11.0	89.0
commercial sample Bulgarian concrete	35.0	65.0
Bulgarian rose concrete with 1.5 percent synthetic citronellol addition	16.0	84.0
Rose-de-Mai absolute with 1.0 percent synthetic citronellol addition	13.2	86.8

Using supercritical CO_2 extraction to fractionate rose concrete, Reverchon and Della Porta (1996) showed that a superior product to rose oil could be produced. They used a single step extraction at 80 bar and 40°C followed by a two stage seperation at 80 bar and -16°C and 15 bar at 0°C. Three fractions were taken in the second separator; 1. 80 bar at 40°C after 60 min; 2. 80 bar at 40°C between 420-480 min and 3. 120 bar at 40°C after odor exhaustion. The waxes were obtained from the first separator (15 bar at 0°C). Each of the fractions were analyzed by GC/MS, the results of which can be found in T-6.

It was reported by Naqvi and Mandal (1997) that in India rose oil is often adulterated with low volatility compounds such as polyethylene glycol, dioctyl phthalate and diethyl phthalate. Although the two phthalates can be detected at higher temperatures especially when a non-polar GC column is used, if polyethylene gylcol (PEG) is used they will not elute from the GC column. Naqvi and Mandal recommended that IR spectra of rose oil containing absorption peaks at 1651, 1459, 1404, 1087, 1042 and 883 cm^{-1} are indicative of adulteration of the oil with PEG. Also, as phthalates possess a strong C=O absorption at 1728 cm^{-1} and three other additional peaks at 1287, 1125 and 1074 cm^{-1}. Adulteration of rose oil with them is readily detectable.

Boelens and Boelens (1997) compared the composition of hydrodistilled Bulgarian and Turkish rose oils with a supercritical extract of Bulgarian rose as shown in T-7.

The composition of a steam distilled oil, an absolute and a supercritical fluid CO_2 (SFC) extract of *R. damascena* concrete of Bulgarian origin was the subject of analysis by Reverchon et al. (1997). The constituents found in the oil and extracts can be seen in T-8. The authors also collected the rose waxes (stearoptenes) from the SFC and determined that they comprised a series of paraffins of odd carbon numbers C_{23}-C_{47} with C_{29} being most abundant.

Currently, *R. damascena* is cultivated in India in Kashmir, Himachal Pradesh, Pushkar (Rajasthan) and Hasayan, Etah, Ghazipur (Uttar Pradesh). Naqvi and Mandal (1997) analyzed rose oil produced in different regions of India and compared them with an oil of Bulgarian origin (see T-9).

A commercial sample of a rose extract was analyzed by Antonelli and Fabbri (1999). The composition of this extract was reported to be as follows:

(Z)-3-hexenol (0.23 percent)
heptanal (0.11 percent)
α-pinene (0.68 percent)
β-pinene (0.14 percent)
myrcene (0.32 percent)
linalool (2.39 percent)
2-phenethyl alcohol (2.24 percent)
terpinen-4-ol (0.27 percent)
α-terpineol (0.66 percent)
nerol (8.98 percent)
citronellol (32.67 percent)
neral (0.55 percent)
geraniol (18.50 percent)
geranial (0.92 percent)
eugenol (1.24 percent)
geranyl acetate (0.88 percent)
methyl eugenol (1.79 percent)
β-caryophyllene (0.59 percent)
α-humulene (0.28 percent)
pentadecane (0.28 percent)
heptadecene* (0.22 percent)
heptadecane (1.79 percent)
octadecane (0.15 percent)
nonadecene* (3.04 percent)
nonadecane (9.86 percent)
eicosane (0.85 percent)
heneicosane (3.57 percent)
docosane (0.09 percent)
tricosane (0.72 percent)
pentacosane (0.20 percent)
heptacosane (0.17 percent)
nonacosane (0.08 percent)

*correct isomer not identified

Trace amounts (< 0.01 percent) of sabinene and hexadecane were also characterized in this same extract.

The use of a technique known as multilayer coil counter current chromatography to isolate the volatile precursors in rose flowers was described by Winterhalter et al. (1998) and Knapp et al. (1998). To prepare the rose flowers for this analysis 10 kg of flowers were

Percentage composition of rose concrete and its fractions obtained using supercritical CO_2 extraction **T-6**

Compound	Concrete	Fraction 1	Fraction 2	Fraction 3	Waxes
heptanol	0.01	0.12	-	-	-
α-pinene	0.31	1.25	0.02	-	-
benzaldehyde	0.50	0.41	0.41	-	-
β-pinene	0.09	0.55	t	-	-
3-octanol	0.21	0.44	0.56	0.79	-
myrcene	0.52	1.28	0.96	0.53	-
o-cymene	0.05	0.10	0.11	-	-
limonene	0.26	0.46	0.70	0.27	-
o-cresol	0.17	0.67	0.17	-	-
β-ocimene*	0.17	0.15	0.42	0.26	-
γ-terpinene	0.06	0.07	0.05	-	-
octanol	0.03	0.07	0.08	0.13	-
terpinolene	t	0.07	-	-	-
α-terpinyl acetate	0.05	0.08	0.10	-	-
linalool	0.04	0.25	0.07	-	-
2-nonanol	0.11	0.23	0.10	-	-
2-phenethyl alcohol	25.05	57.26	34.04	0.98	-
rose oxide*	t	0.11	0.09	-	-
menthone	0.11	0.29	0.41	0.56	-
pulegol*	0.02	0.07	0.03	-	-
isomenthone	0.02	0.05	0.06	-	-
menthol	0.03	0.11	0.14	-	-
isomenthol	0.26	0.71	0.90	1.40	-
methyl phenylacetate	0.10	0.50	0.13	-	-
verbenone	1.09	2.70	1.53	-	-
citronellol	4.67	9.15	10.79	0.09	-
myrtenyl acetate	0.13	0.57	0.22	0.17	-
2-phenethyl acetate	2.66	6.22	7.67	-	-
neral or geranial*	0.15	0.54	-	-	-
citronellyl formate	0.15	0.15	-	-	-
menthyl acetate	0.16	0.40	0.46	0.68	-
eugenol	0.97	2.08	1.52	-	-
geranyl acetate	0.13	0.50	0.05	-	-
methyl eugenol	0.50	1.09	0.88	-	-
β-caryophyllene	0.18	0.53	0.42	0.11	-
α-guaiene	0.11	0.30	0.13	-	-
β-selinene	0.08	0.22	0.16	-	-
valencene	0.21	0.48	0.27	-	-
pentadecane	0.24	0.47	0.46	-	-
tetradecanol	0.14	0.20	0.46	-	-
heptadecane	1.33	1.23	3.31	3.97	-
hexadecanol	3.22	1.54	6.94	21.30	1.37
nonadecane	12.79	3.96	15.54	52.10	4.36
heneicosane	1.32	0.16	1.12	3.57	0.50
eicosane	9.62	1.10	6.32	11.86	6.86
docosane	0.36	0.03	0.15	0.16	0.53
tricosane	5.33	0.27	1.66	0.63	15.33
tetracosane	0.39	0.07	0.04	0.23	1.61
pentacosane	3.94	0.22	0.26	0.22	19.71
hexacosane	0.40	0.08	t	t	1.60
heptacosane	10.51	0.45	0.03	t	34.57
nonacosane	5.86	-	0.05	t	7.24
henetriacotane	5.35	-	-	t	6.22

*correct isomer not identified; t = trace (< 0.01 percent)

Comparative percentage composition of rose oil and a supercritical fluid CO_2 (SFC) extract of Bulgarian rose **T-7**

Compound	Bulgarian rose oil	Turkish rose oil	SFC Bulgarian rose
α-pinene	0.60-0.80	0.60	0.73
sabinene	0.03-0.05	0.10	0.07
β-pinene	0.10-0.20	0.20	0.14
myrcene	0.25-0.40	0.10	0.22
α-terpinene	0.02-0.03	0.05	0.01
p-cymene	0.01-0.03	0.10	0.01
limonene	0.05-0.10	0.20	1.28
(Z)-β-ocimene	0.05-0.10	0.05	-
(E)-β-ocimene	0.05-0.10	0.05	0.03
γ-terpinene	0.03-0.05	0.05	0.02
terpinolene	0.05	0.05	0.01
ethanol	1.50-3.00	0.50	1.42
isoamyl alcohol	0.05-0.10	0.05	-
2-methylbutanol	0.05-0.10	0.05	0.01
hexanol	0.10-0.20	0.23	0.12
heptanol	0.05	0.01	0.09
nonanol	0.03	-	0.03
acetaldehyde	0.01-0.02	-	-
valeraldehyde	0.05-0.10	-	-
benzaldehyde	-	0.05	-
heptanal	0.10	0.02	0.04
octanal	-	0.01	-
nonanal	0.01-0.05	0.05	0.04
decanal	0.03	-	0.03
rosefuran	0.02	0.02	0.01
cis-rose oxide	0.20-0.30	0.36	0.09
trans-rose oxide	0.10-0.15	0.19	0.04
nerol oxide	0.05-0.10	0.05	0.03
linalool	2.10-2.30	0.81	0.11
2-phenethyl alcohol	1.70-2.00	1.85	67.53
terpinen-4-ol	0.20-0.30	0.46	0.02
α-terpineol	0.60-0.80	0.25	-
γ-terpineol†	0.05-0.10	-	-
myrtenol	-	0.04	-
myrtenal	-	0.01	-
α-citronellal	-	0.01	-
citronellal	-	0.06	-
α-citronellol	0.10	-	-
citronellol	27.50-28.00	45.00	7.77
nerol	7.80-8.60	10.10	2.15
carveol*	0.05-0.10	0.14	0.02
neral	0.50-0.70	0.82	0.19
geraniol	16.00-17.00	20.50	4.15
geranial	0.50-1.00	1.34	0.33
2-phenethyl acetate	0.20-0.25	0.52	0.32
neryl formate	-	0.01	-
geranyl formate	-	0.02	-
methyl geranate	0.05-0.10	0.06	0.02
methyl nerate	0.02	-	-
α-terpinyl acetate	0.05-0.10	-	-
citronellyl acetate	0.40-0.50	0.94	0.22
neryl acetate	0.05-0.10	0.16	0.04
geranyl acetate	0.70-0.80	2.04	0.43
eugenol	1.10-1.20	0.99	1.19
methyl eugenol	1.60-1.70	2.85	0.71
β-damascone‡	< 0.01	< 0.01	-
β-damascenone	0.015	0.015	t
α-copaene	0.01-0.05	0.01	-
β-caryophyllene	0.50-0.60	0.54	0.18
α-guaiene	0.30-0.40	0.51	0.14
α-humulene	0.25-0.30	0.35	0.10
germacrene D	0.50-0.60	0.97	0.26
δ-guaiene	0.50-0.60	0.38	0.10
aromadendrene	0.10-0.20	-	0.05
γ-cadinene	0.05-0.10	0.05	-
δ-cadinene	0.05-0.10	0.05	0.01
elemol	0.10-0.20	-	-
valerianol	0.05-0.10	-	-
α-cadinol	0.05-0.10	-	-
α-muurolol	-	0.01	-
β-eudesmol	0.20-0.40	0.15	-
guaiol	0.01-0.02	-	0.01
(E,Z)-farnesol	1.40-1.50	1.38	0.11
tetradecane	0.05-0.10	-	-
pentadecane	0.50-0.60	-	0.26
hexadecane + hexadecene*	0.02	-	0.22
heptadecane + heptadecene*	1.50-1.70	-	0.84
octadecane + octadecene*	0.35	0.05	0.17
nonadecane + nonadecene*	14.00-15.00	3.05	3.85
eicosane + eicosene*	1.30-1.50	0.11	0.29
heneicosane + heneicosene*	4.00-5.00	0.10	0.78
docosane + docosene*	0.30	0.02	0.09
tricosane + tricosene*	1.00-1.20	-	0.23
tetracosane + tetracosene*	0.05-0.10	-	0.07
pentacosane + pentacosene*	0.50	-	0.11
hexacosane	0.50	-	0.72
ethyl hexadecanoate	0.05	-	0.02
2-phenethyl dodecanoate	0.05	-	-

*correct isomer not identified; †natural occurrence not substantiated; ‡(E)-isomer

Percentage composition of an oil, absolute and a supercritical fluid (SFC) CO_2 extract of rose **T-8**

Compound	Oil	Absolute	SFC	Compound	Oil	Absolute	SFC
heptanol	0.1	-	0.1	2-phenethyl acetate	14.8	2.4	7.5
α-pinene	0.1	0.4	0.2	neral or geranial*	0.7	0.1	0.3
benzaldehyde	0.1	0.5	0.6	citronellyl formate	-	0.1	0.1
β-pinene	t	0.1	0.1	menthyl acetate	-	1.6	0.1
3-octanol	0.7	1.9	0.1	eugenol	3.5	0.4	2.9
myrcene	0.8	0.7	0.5	geranyl acetate	0.6	-	0.3
o-cymene	0.1	0.1	0.1	methyl eugenol	2.0	0.4	1.2
limonene	0.6	1.3	0.2	β-caryophyllene	0.8	0.4	0.3
o-cresol	0.1	0.2	0.6	α-guaiene	0.5	0.1	0.2
β-ocimene*	0.3	0.3	0.2	β-selinene	0.4	0.1	0.2
γ-terpinene	0.1	0.1	0.1	valencene	1.0	0.1	0.3
octanol	0.1	0.2	0.1	pentadecane	1.0	-	0.4
terpinolene	-	t	0.1	methyltetradecane*	-	t	0.2
α-terpinyl acetate†	0.1	0.1	0.2	tetradecanol	0.4	-	0.1
linalool	0.2	0.1	0.1	heptadecane	3.5	1.5	1.6
2-nonanol	0.1	0.1	0.1	hexadecanol	3.3	3.5	2.6
2-phenethyl alcohol	10.4	28.3	50.0	nonadecane	10.0	15.2	7.8
rose oxide*	-	t	0.1	heneicosene*	0.5	1.5	0.6
menthone	0.5	1.2	0.1	heneicosane	1.7	12.0	3.4
pulegol*	0.1	t	0.1	docosane	0.3	0.5	0.1
isomenthone	0.1	0.2	0.1	tricosane	1.1	7.0	0.9
menthol	0.1	0.4	0.2	tetracosane	1.5	0.4	0.1
isomenthol	1.1	3.0	0.1	methyltetracosane*	1.4	-	-
methyl phenylacetate	0.2	0.1	0.2	pentacosane	1.5	4.3	0.1
verbenone	5.6	0.9	2.8	hexacosane	0.5	0.2	-
citronellol	26.1	3.8	11.4	heptacosane	0.8	2.7	-
myrtenyl acetate	0.5	0.5	0.2	nonacosane	-	1.0	-

*correct isomer not identified; t = trace (< 0.1 percent); †incorrect identification based on GC elution order

harvested at their full bloom stage and homogenized in ice-cold 80 percent aqueous methanol. After filtration and vacuum concentration to remove the solvent the aqueous mixture was freeze-dried to yield 260 g of a crude extract. Column chromatographic separation of the extract (in 26 g portions) over XAD-2 yielded 40 g of an aroma precursor concentrate after rinsing the column with water and elution of the retained material with methanol. This aroma precursor concentrate was then subjected to separation into fractions using multilayer coil counter current chromatography (MLCCC).The first four fractions were hydrolyzed with acid using simultaneous distillation and extraction at pH 2.5 for 1 h. The resulting mixtures were subjected to analysis by GC/MS from which the following compounds were characterized:

2,6-dimethyl-7-octene-2,6-diol
2,6-dimethyl-1,7-octadiene-3,6-diol
3,7-dimethyl-5-octene-1,7-diol
2,6-dimethyl-7-octene-1,6-diol
(Z)-2,6-dimethyl-2,7-octadiene-1,6-diol
(2Z,5E)-3,7-dimethyl-2,5-octadiene-1,7-diol
(E)-2,6-dimethyl-2,7-octadiene-1,6-diol
3,7-dimethyloctane-1,7-diol
(2E,5E)-3,7-dimethyl-2,5-octadiene-1,7-diol
3,7-dimethyl-6-octene-1,3-diol
3,7-dimethyl-7-octene-1,6-diol
(2Z)-3,7-dimethyl-2,7-octadiene-1,6-diol
(2Z)-3,7-dimethyl-2,6-octadiene-1,4-diol
(2E)-3,7-dimethyl-2,7-octadiene-1,6-diol
(2E)-3,7-dimethyl-2,6-octadiene-1,4-diol
2,6-dimethyloctane-1,8-diol
(Z)-3,7-dimethyl-2-octene-1,8-diol
(E)-2,6-dimethyl-2-octene-1,8-diol
(2E,6Z)-dimethyl-2,6-octadiene-1,8-diol
(E)-3,7-dimethyl-2-octene-1,8-diol
(2E,6E)-2,6-dimethyl-2,6-octadiene-1,8-diol

Knapp et al. showed that (S)-3,7-dimethyl-5-octene-1,7-diol was the precursor of the rose oxides. Winterhalter et al. also isolated and characterized 3-hydroxy-7,8-didehydro-β-ionol-9-O-β-D-glucopyranoside from one of the MLCCC fractions as the precursor of (E)-β-damascenone.

Baser and Kürkcüoglu (1998) and Kürkcüoglu and Baser (2003) reported that the main constituents of Turkish rose oil produced either in a factory or in the

Percentage composition of rose oil produced in five locations in India and Bulgaria **T-9**

Compound	1	2	3	4	5	6
ethanol	0.09	0.80	0.46	0.75	0.64	1.43
α-pinene	0.43	0.31	0.16	0.03	t	0.73
camphene	0.11	0.64	0.16	t	t	0.14
β-pinene	0.25	0.26	0.10	t	t	0.03
myrcene	t	0.12	0.08	t	t	0.50
cis-rose oxide	0.31	0.26	0.17	0.19	0.04	0.43
(Z)-3-hexenol	0.08	0.06	t	t	t	0.26
trans-rose oxide	0.13	0.17	0.07	0.08	0.02	0.17
3-hexanol	0.28	0.12	0.11	0.29	t	0.26
heptanol	t	0.13	0.05	0.02	t	0.01
decanal	0.21	0.14	0.04	0.06	0.34	t
linalool	3.83	1.42	2.98	1.41	1.74	2.10
benzaldehyde	0.04	0.05	0.06	0.07	2.48	0.10
octanol	0.11	0.41	t	0.02	t	0.05
nonanol	0.03	t	t	0.08	0.02	0.09
citronellyl acetate	0.29	2.08	2.78	0.26	0.42	0.53
neral or geranial*	0.06	3.26	4.82	0.70	1.26	0.72
geranyl acetate	0.17	1.10	1.21	3.04	4.70	1.60
citronellol	31.86	35.81	31.57	30.80	12.88	33.40
nerol	10.95	13.62	13.20	14.54	7.32	5.92
geraniol	24.91	30.12	32.46	35.84	24.69	18.40
2-phenethyl alcohol	1.50	1.82	2.08	2.93	3.94	1.45
nonadecane	6.50	0.53	0.50	1.59	16.31	14.60
eicosane	1.60	0.02	0.13	1.11	1.74	1.70
(E)-cinnamaldehyde	t	t	t	1.30	0.10	0.20
methyl eugenol	t	t	t	t	0.23	2.30
heneicosane	1.74	2.96	1.64	1.32	6.75	4.20
eugenol	2.30	0.22	t	0.37	0.48	1.20
dodecane	0.10	0.08	0.08	0.10	0.35	0.18

t = trace (< 0.01 percent); *correct isomer not identified; 1. Kashmir, 2. Himachal Pradesh, 3. Aligarb (Uttar Pradesh), 4. Lucknow (Uttar Pradesh), 5. Kodaikanal (Tamil Nadu), 6. Bulgaria

Comparative percentage composition of the main constituents of factory and village produced Turkish rose oil **T-10**

Compound	Factory produced oil	Village produced oil
citronellol	31-46	25-39
geraniol	9-17	20-32
nerol	5-9	8-13
2-phenethyl alcohol	1-3	2-4
stearoptenes	14-26	12-20
citronellol/geraniol ratio	2.3-4.8	0.8-1.9

villages varied as can be seen in T-10. They also reported that the main components of Turkish rose absolute made from concretes that were produced by different manufacturers also varied as shown in T-11. Furthermore, the same authors noted that rose absolute of Turkish origin contains the following major components:

2-phenethyl alcohol (67.5 percent)
citronellol (8.3 percent)
geraniol (5.1 percent)
nerol (2.1 percent)
eugenol (1.5 percent)
methyl eugenol (0.7 percent)
nonadecane (2.0 percent)
1-nonadecene (2.8 percent)

It is surprising that the data above is somewhat dissimilar to the data reported in T-11.

For comparison purposes, Baser and Kürkcüoglu reported that the main components of Bulgarian rose absolute were as follows:

2-phenethyl alcohol (59.0 percent)
citronellol (10.0 percent)
geraniol (5.0 percent)
nerol (2.0 percent)
methyl eugenol (1.4 percent)
nonadecane (2.4 percent)
1-nonadecene (7.1 percent)

Using a direct sampling technique, Baser and Kürkcüoglu obtained the headspace volatiles of a living

Comparative percentage composition of the selected components of rose absolute made from rose concrete by different producers **T-11**

Compound	Producer			
	Ercetin	Gülbirlik	Gürkan	Konur
2-phenethyl alcohol	61	50-54	66	50
citronellol	7	10-18	8	10
geraniol	7	6-8	5	11
nerol	3	3	2	4
eugenol	2	2	1	2
methyl eugenol	1	1-2	1	1
nonadecane	5	5-7	7	6
1-nonadecene	5	3-5	< 1	5

Comparative percentage composition of rose water **T-12**

Compound	Hexane extraction	SPME headspace	Immersion SPME	
			diluted	undiluted
2-phenethyl alcohol	50	3	4	10
citronellol	13	34	31	45
geraniol	13	21	22	11
nerol	5	10	11	5
eugenol	5	3	5	5
methyl eugenol	4	13	13	16
nonadecane	0.24	2	1	-
1-nonadecene	0.05	0.5	0.3	-

Turkish rose flower that were trapped on Porpak Q over a 2-h period (between 10 AM-noon) as shown below:

2-phenethyl alcohol (59.2 percent)
citronellol (18.06 percent)
nonadecane (3.28 percent)
α-pinene (2.80 percent)
geraniol* (2.11 percent)
benzyl alcohol (2.01 percent)
heptadecane (1.20 percent)
citronellyl acetate (1.05 percent)
geranyl acetate (0.89 percent)
methyl eugenol (0.88 percent)
2-phenethyl acetate (0.71 percent)
pentadecane (0.68 percent)
nerol (0.47 percent)
(E,E)-α-farnesene (0.34 percent)
heneicosane (0.29 percent)

*impure

The same authors also reported the composition of Turkish rose water by various analytical procedures such as hexane extraction, headspace SPME and immersion headspace SPME on diluted and undiluted rose water. The results of this comparative study on rose water can be found in T-12.

Oka et al. (1999) showed that the majority of volatiles were released from flowers of *R. damascena* on opening between 3:30 AM to 8:30 AM. To obtain this conclusion, the authors measured the quantitative release of 2-phenethyl alcohol, geraniol, citronellol, 2-phenethyl acetate, methyl benzoate, limonene, myrcene, β-pinene and *cis*- and *trans*-rose oxide over a 24-h period.

Gupta et al. (2001) examined the composition of a water distilled oil of fresh flowers of *R. damascena* (cv. Noorjahan) produced in Lucknow (UP). Using both peak enrichment and relative retention indices on two capillary columns of different polarity as the method of component identification the oil was found to contain the following components:

α-pinene (0.1 percent)
sabinene (0.1 percent)
myrcene (1.4 percent)
heptanal (0.1 percent)
limonene (0.2 percent)
1,8-cineole (0.2 percent)
(Z)-β-ocimene (0.2 percent)
(E)-β-ocimene (0.4 percent)
octanal (0.2 percent)
cis-rose oxide (0.1 percent)
trans-rose oxide (0.1 percent)
nonanal (0.1 percent)
decanal (0.1 percent)
linalool (0.7 percent)

Percentage composition of the flower oils of Kannauj and Ranisahiba rose **T-13**

Compound	Kannauj rose oil	Ranisahiba rose oil	Compound	Kannauj rose oil	Ranisahiba rose oil
sabinene	0.2	-	nerol	5.6	7.1
myrcene	0.2	-	2-phenethyl acetate	1.1	1.1
1,8-cineole	0.2	0.1	geraniol	39.3	16.7
octanal	-	t	benzyl alcohol	-	t
cis-rose oxide	0.3	0.1	nonadecane	8.0	4.3
(Z)-3-hexenol	-	0.2	9-nonadecene	5.7	0.8
trans-rose oxide	-	10.1	2-phenethyl alcohol	1.6	-
nonanal	-	0.1	β-ionone*	0.2	0.6
cis-linalool oxide†	-	0.1	eicosane	0.6	1.0
trans-linalool oxide†	-	0.1	eicosene*	0.7	0.3
decanal	0.1	0.1	methyl eugenol	-	0.1
benzaldehyde	-	0.1	(E)-nerolidol	0.3	0.3
linalool	1.0	1.6	heneicosene*	0.4	0.3
β-caryophyllene	0.4	1.1	benzyl tiglate	-	0.3
terpinen-4-ol	-	0.6	eugenol	0.5	0.4
α-guaiene	-	0.2	docosane	1.0	0.4
citronellyl acetate	0.5	0.8	docosene*	-	0.2
α-humulene	-	t	tricosane	1.1	5.6
neral	2.2	0.3	(E,E)-farnesol	1.3	0.2
α-terpineol	-	0.5	tetracosane	0.2	0.5
neryl acetate	-	0.7	pentacosane	1.2	3.6
geranial	1.1	1.0	hexacosane	0.2	0.5
geranyl acetate	1.8	0.4	benzyl benzoate	-	0.1
citronellol	6.7	31.4	heptacosane	0.7	2.6

*correct isomer not identified; t = trace (< 0.1 percent)

β-caryophyllene (0.5 percent)
terpinen-4-ol (0.1 percent)
citronellyl acetate (0.5 percent)
α-humulene (0.3 percent)
neral (0.4 percent)
α-terpineol (0.5 percent)
neryl acetate (0.2 percent)
geranial (0.6 percent)
benzyl acetate (0.1 percent)
geranyl acetate (1.8 percent)
citronellol (20.8 percent)
nerol (11.8 percent)
β-damascenone* (0.1 percent)
2-phenethyl acetate (0.1 percent)
geraniol (25.3 percent)
nonadecane (8.5 percent)
(Z)-9-nonadecene (1.2 percent)
2-phenethyl alcohol (1.7 percent)
β-ionone* (0.1 percent)
eicosane (1.2 percent)
eicosene* (0.1 percent)
methyl eugenol (0.4 percent)
heneicosane (5.0 percent)
heneicosene* (0.1 percent)
benzyl tiglate (0.1 percent)
eugenol (1.0 percent)
docosane (0.1 percent)
tricosane (1.3 percent)
(E,E)-farnesol (2.1 percent)
tetracosane (0.1 percent)
pentacosane (0.9 percent)
benzyl benzoate (0.2 percent)

*correct isomer not identified

Application of traditional plant breeding practices by Patra et al. (2001) led to the selection and development of an oil-rich strain of *R. damascena* in India. A comparative analysis of the flower oils of the standard cultivated rose (Kannauj rose) and the newly developed Ranisahiba rose can be seen in T-13.

Kubeczka and Formacek (2002) used a combination of GC and ^{13}C-NMR to compare the compositions of Turkish and Bulgarian rose oils. Their results are found summarized in T-14.

Using a 300 L stainless steel distillation pot and batch size of 35-40 kg of fresh rose flowers (*R. damascena*) Babu et al. (2002) distilled three batches of flowers under different gauge pressures (atmospheric, 0.21 kg/cm^2, 0.42 kg/cm^2, 0.58 kg/cm^2 and 0.80 kg/cm^2) which corresponded to 96°C, 105°C, 110°C, 114°C and 117°C. The composition of the oils produced at these temperatures can be seen in T-15. The authors also compared the volatile composition of rose water produced from rose distillation that was performed under high pressure with that produced at

Comparative percentage composition of Turkish and Bulgarian rose oils

T-14

Compound	Turkish rose oil	Bulgarian rose oil	Compound	Turkish rose oil	Bulgarian rose oil
ethanol	1.92	1.54	neral	0.40	0.56
valeraldehyde	0.11	0.05	α-terpineol	0.11	0.06
α-pinene	0.53	0.78	heptadecane	2.35	2.34
β-pinene	0.13	0.15	geranial	0.64	0.93
sabinene	0.05	0.04	geranyl acetate	0.74	0.91
myrcene	0.28	0.39	citronellol	42.19	29.35
heptanal	0.15	0.10	nerol	5.91	8.28
limonene	0.08	0.07	2-phenethyl acetate	0.71	0.46
2-methylbutanol	0.15	t	geraniol	12.00	17.10
isoamyl alcohol	0.20	t	nonadecane	10.80	10.10
cis-rose oxide	0.55	0.21	2-phenethyl alcohol	1.95	2.71
trans-rose oxide	0.25	0.13	nonadecene*	2.61	2.47
nonanal	0.09	0.06	eicosane	0.80	0.92
decanal	0.33	0.32	methyl eugenol	2.50	1.70
benzaldehyde + β-bourbonene	0.19	t	heneicosane	3.19	4.19
linalool	1.45	2.47	heneicosene*	0.12	0.16
α-guaiene	0.39	0.42	eugenol	0.38	1.35
β-caryophyllene	0.54	0.61	tricosane	0.56	1.00
terpinen-4-ol	0.41	0.28	(E,E)-farnesol	0.59	1.45
citronellyl acetate	0.57	0.54	pentacosane	0.12	0.27
α-humulene	0.29	0.27			

*correct isomer not identified

Comparative percentage composition of rose oil distilled at different pressures and temperatures

T-15

Compound	Pressure and temperature of distillation				
	atmospheric 96°C	0.21 kg/cm^2 105°C	0.42 kg/cm^2 110°C	0.58 kg/cm^2 114°C	0.80 kg/cm^2 117°C
α-pinene	1.02-1.28	t	-	0.18-1.82	0.23-0.47
sabinene	0.08-0.14	-	-	-	t
myrcene	0-0.50	-	-	0.02-0.26	t
β-pinene	0.48-0.78	0.14-0.22	t	0.25-0.49	0.10-0.34
2-phenethyl alcohol	3.63-5.01	3.10-4.50	4.08-10.18	4.40-13.76	6.51-8.75
linalool	0.61-1.01	-	-	-	0.59-3.75
cis-rose oxide	0.17-0.21	t	t	t	0.09-0.15
trans-rose oxide	0.08-0.12	-	-	-	t
terpinen-4-ol	0.16-0.22	t	0.21-0.39	0.04-0.20	0.12-0.36
α-terpineol	0.50-1.22	0.16-0.94	2.02-3.40	1.04-2.60	1.87-2.57
citronellol + nerol	35.39-36.89	27.62-28.04	30.85-33.31	30.47-36.71	37.15-40.01
geraniol	19.33-23.33	15.16-15.58	16.01-18.85	15.91-25.15	23.76-29.24
eugenol	1.84-2.24	1.12-2.60	0.25-2.87	1.72-2.32	2.86-3.82
damascone*	0-0.29	0.04-0.46	0.02-0.60	0.01-0.77	0.03-0.47
geranyl acetate	2.59-3.85	3.00-4.68	2.12-6.04	3.16-4.06	2.08-3.04
β-ionone	0.11-0.29	t	t	t	t
methyl eugenol	0.64-0.80	0.14-0.68	0.53-0.83	0.72-0.82	0.76-1.50
β-bourbonene	0.83-1.27	0.58-1.84	0.43-0.71	0.39-0.59	0.07-0.83
β-elemene	0.45-0.67	0.62-0.70	0.12-0.24	0-0.41	0.18-0.20
β-caryophyllene	0.45-0.71	0.52-0.70	0.21-0.31	0.11-0.27	0.13-0.25
α-humulene	0.71-1.29	0.40-0.70	0.26-0.52	0.39-0.49	0.11-0.45
α-cadinene	0.31-0.47	0.40-0.78	0.37-0.63	0.31-0.43	0-0.39
docosane†	0.19-0.61	0.24-0.80	t	0-0.35	0.12-0.22
heptadecane	1.48-5.14	5.99-6.05	3.99-6.23	1.67-3.49	0.51-2.33
farnesol*	1.49-3.95	4.96-6.00	2.44-3.68	1.31-3.15	1.21-1.89
9-eicosene*	1.78-2.42	4.73-5.27	2.15-4.97	2.02-4.64	1.14-1.86
nonadecane	14.50-16.34	23.18-26.16	10.77-23.79	10.87-23.89	6.19-8.37

*correct isomer not identified; †incorrect identification based on elution order

atmospheric pressure. The volatiles were either obtained from the rose distillation water either by a redistillation using a Clevenger system or by extraction with methylene chloride as can be seen in T-16.

Jirovetz et al. (2002) analyzed the oil and solid phase microextraction (SPME) headspace volatiles of fresh rose flowers and rose oil of Bulgarian origin. The results of this comparative study are shown summarized in T-17.

Aydinli and Tutas (2003) compared the composition of rose absolute produced using 96 percent ethanol at -25°C and -20°C from the same batch of Turkish rose concrete. The results of this study are shown in T-18.

Baser et al. (2003) reported the production statistics for rose flowers, rose oil and rose concrete in Turkey for the years 1998-2000. These statistics are shown in T-19. The same authors also found that a rose oil produced by a single supplier over a 16-year period possessed the following range in main components:

citronellol (30.9-43.9 percent)
geraniol (9.3-14.1 percent)
nonadecane (8.3-14.7 percent)
nerol (5.2-7.6 percent)
1-nonadecene (2.6-4.9 percent)
methyl eugenol (2.7-4.0 percent)
heneicosane (2.5-4.2 percent)
geranyl acetate (1.0-2.2 percent)
linalool (0.6-2.1 percent)
2-phenethyl alcohol (1.2-1.9 percent)
β-caryophyllene (0.7-1.6 percent)
citronellyl acetate (0.7-1.4 percent)
germacrene D (0.7-1.4 percent)
(E,E)-farnesol (0.6-1.4 percent)

Although these components contribute to the aroma of rose oil, the authors reported that over the years time frame the interesting odor contributors ranged in composition as follows:

Comparative percentage composition of the volatiles isolated from rose distillation water by redistillation or methylene chloride extraction **T-16**

Compound	Rose distillation water produced under high pressure		Rose distillation water produced at atmospheric pressure	
	redistillation	$MeCl_2$ extraction	redistillation	$MeCl_2$ extraction
α-pinene	0.10	0.37	-	t
sabinene	t	-	-	0.10
myrcene	t	-	t	t
β-pinene	t	-	0.17	t
2-phenethyl alcohol	5.41	55.16	2.49	63.12
linalool	10.98	7.93	23.04	6.62
cis-rose oxide	0.18	t	0.28	t
trans-rose oxide	t	t	t	t
terpinen-4-ol	0.71	0.31	0.77	0.24
α-terpineol	6.37	2.79	9.20	2.63
citronellol + nerol	32.40	13.02	34.89	11.05
geraniol	31.09	12.23	21.30	8.56
eugenol	4.20	3.47	2.79	3.52
damascone*	0.05	0.07	0.02	0.04
geranyl acetate	0.54	0.15	-	0.34
β-ionone*	-	-	0.02	0.04
methyl eugenol	1.70	0.71	1.52	0.61
β-bourbonene	t	-	-	-
β-elemene	t	-	-	-
β-caryophyllene	t	-	-	-
α-humulene	t	-	-	-
α-cadinene	t	-	-	-
docosane†	t	-	-	-
heptadecane	0.48	0.51	1.87	t
farnesol*	0.45	-	-	-
9-eicosene*	0.24	-	-	-
nonadecane	1.07	t	-	t

*correct isomer not identified; †incorrect identification based on GC elution order

(E)-β-damascenone (0.03 percent)[a]
cis-rose oxide (0.3-1.0 percent)[b]
trans-rose oxide (0.1-0.5 percent)[b]
rosefuran (< 0.1-0.1 percent)[c]
nerol oxide (< 0.1-0.2 percent)[d]
isonerol oxide (0.01-0.02 percent)[e]
rosefuran epoxide (0.02-0.04 percent)[f]
(E)-3,7-dimethyl-5-octene-1,7-diol (0.1-0.4 percent)[g]
(2Z,5E)-3,7-dimethyl-2,5-octadiene-1,7-diol (0.02-0.1 percent)[c]
(2E,5E)-3,7-dimethyl-2,5-octadiene-1,7-diol (0.02 percent)[a]

[a]one sample year; [b]16 sample years; [c]nine sample years; [d]15 sample years; [e]six sample years; [f]eight sample years; [g]three sample years

In addition to repeating some of their earlier results (cf. Baser and Kürkcüoglu 1998 and Kürkcüoglu and Baser 2003) the authors also extracted fresh rose flowers using a solvent system of 1,1,1,2-tetrafluroethane-dimethyl ether (90:10) over a time period of 45 min-24 h. The main components found in extracts produced after 45 min, 5 h, 8 h and 24 h extraction can be seen in T-20. The authors reported that the best yield (69.6 percent) was obtained after 45 min.

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Percentage composition of Bulgarian rose flower SPME headspace volatiles and Bulgarian rose oil

T-17

Compound	rose headspace volatiles	rose oil	Compound	rose headspace volatiles	rose oil
acetaldehyde	t	-	linalool	4.08	3.14
methyl acetate	t	t	β-bourbonene	0.18	0.16
ethanol	0.14	0.03	linalyl acetate	0.42	0.31
valeraldehyde	0.16	0.05	β-elemene	0.24	0.25
2-butanol	0.05	0.01	citronellyl formate	0.24	0.18
α-pinene	0.32	0.17	terpinen-4-ol	0.14	0.08
isobutanol	0.18	0.11	β-caryophyllene	1.32	1.20
hexanal	0.33	0.19	citronellyl acetate	2.49	2.16
β-pinene	0.29	0.23	α-humulene	t	t
sabinene	0.21	0.14	(E)-β-farnesene	0.05	0.07
myrcene	0.31	0.54	neral	0.55	0.47
δ-3-carene	0.27	0.22	heptadecane	0.43	0.65
heptanal	0.31	0.15	geranial	0.37	0.31
isoamyl alcohol	0.09	0.06	(E)-β-damascenone	0.09	0.05
limonene	1.24	1.02	α-terpineol	0.18	0.14
1,8-cineole	0.52	0.26	neryl acetate	0.34	0.26
(Z)-β-ocimene	0.33	0.29	geranyl acetate	0.32	0.24
p-cymene	0.10	0.08	citronellol	34.77	35.93
(Z)-3-hexenol	1.02	0.84	nerol	3.81	3.69
(E)-β-ocimene	0.82	0.72	2-phenethyl acetate	t	t
terpinolene	0.11	0.05	α-cadinene	t	t
1-hexen-3-ol	0.72	0.66	(Z)-β-damascenone[o]	0.08	0.04
hexanol	0.81	0.52	geraniol	28.13	25.72
cis-rose oxide	0.77	0.54	isogeraniol	t	t
trans-rose oxide	0.62	0.38	damascone*	0.16	0.27
nonanol	0.28	0.24	nonadecane	0.75	5.12
tetrahydrolinalool[‡]	0.14	0.12	β-ionone*	1.99	1.82
acetic acid	0.12	0.05	9-eicosene*	0.14	2.61
butyl tiglate	t	0.04	2-phenethyl alcohol	1.42	1.13
cis-linalool oxide[†]	0.17	0.12	methyl eugenol	3.42	3.25
trans-linalool oxide[†]	0.14	0.10	nerolidol*	0.72	0.66
trans-sabinene hydrate	t	t	eugenol	1.29	1.18
citronellal	0.15	0.08	docosane	-	t
δ-elemene	t	-	farnesol*	0.18	0.14
benzaldehyde	0.08	0.03	eugenyl acetate	t	0.07

*correct isomer not identified; [†]furanoid form; [‡]questionable identity; [o]should be (E)-isomer

Percentage composition of rose absolute produced from Turkish rose concrete using different conditions

T-18

Compound	Absolute 1	Absolute 2	Compound	Absolute 1	Absolute 2
geranyl acetate	0.37	0.48	methyl eugenol	0.65	0.74
citronellol	11.26	10.62	heneicosane	0.14	0.10
nerol	2.42	2.47	eugenol	1.04	0.59
geraniol	5.58	5.65	farnesol*	0.33	0.18
2-phenethyl alcohol	73.80	72.73	unidentified	3.13(10)[a]	5.83(13)[a]
nonadecane	1.79	1.19	Absolute Yield (%)	61.37	63.93

*correct isomer not identified; [a]number of unidentified compounds

Production (metric tonnes) of rose and rose products in Turkey 1998-2000 **T-19**

Year	Rose flowers	Rose oil	Rose concrete
1998	9,200	1.8	2.5
1999	8,600	1.6	2.2
2000	6,200	1.4	2.3

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Comparative main component composition of extracts of fresh rose produced after different extraction times **T-20**

Compound	Extraction time			
	45 min	5 h	8 h	24 h
2-phenethyl alcohol	69.6	41.4	19.8	25.6
nonadecane	6.1	20.5	25.1	5.5
citronellol	3.8	16.5	16.8	1.1
benzyl alcohol	1.9	4.7	5.7	1.5
heptadecane	0.8	3.3	4.0	0.3
geraniol	1.5	1.8	1.8	2.9
germacrene D	< 0.1	1.4	2.2	< 0.1
nonocosane	-	0.7	0.9	3.5
1-nonacosene	-	0.6	1.1	1.1
pentacosane	-	0.3	-	4.2
tricosane	1.3	0.3	0.8	5.0
heneicosane	3.4	0.2	0.6	6.7
heptacosane	-	-	0.8	9.3
unidentified	11.6	8.3	20.4	35.5

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