

# Analytical Determination of Allergenic Fragrances in Indoor Air

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**Table S1.** Compounds detected through SIM-A.

Compound	MW	CAS	Retention time	Quantitative m/z	Confirmation m/z
$\alpha$ -Pinene	136.23	7785-70-8	4.25	91, 93	136
$\beta$ -Pinene	136.23	18172-67-1	4.95	91, 94	136
$\alpha$ -Terpinene	136.23	99-86-5	5.67	79, 121	136
Limonene	136.23	5989-27-5	5.93	93, 68	136
Benzyl alcohol	108.14	100-51-6	6.02	79, 107	108
Linalool	154.25	78-70-6	7.55	93, 71	121
Menthol	156.27	89-78-1	9.63	95, 81	138
Terpineol $\alpha$	154.25	98-55-5	10.17	59, 93	121
Citronellol	156.27	106-22-9	11.19	81, 95	123
Geraniol	154.25	106-24-1	12.01	69, 93	123
Anise alcohol	138.16	105-13-5	12.89	109, 137	138
trans-Anethole	148.2	4180-23-8	13.02	117, 147	148
Cinnamyl alcohol	134.18	104-54-1	13.6	92, 115	134
Eugenol	164.2	97-53-0	15.23	103, 149	164
$\beta,\beta,3$ - Trimethylbenzenepropanol	178.27	103694-68-4	16.92	91, 105	106
$\beta$ -Caryophyllene	204.35	87-44-5	17.25	91, 93	133
Ebanol 1	208.34	67801-20-1	17.88	169, 194	108
Isoeugenol (E)	164.2	5932-68-1	18.06	131, 149	164
Ebanol 2	208.34	67801-20-1	18.15	169, 194	108
$\alpha$ -Santalol	220.35	115-71-9	24.15	93, 94	122
$\alpha$ -Amylcinnamyl alcohol	204.31	101-85-9	24.33	104, 215	133
$\beta$ -Santalol	220.35	77-42-9	25.12	93, 94	122
trans,trans-Farnesol	222.37	106-28-5	25.15	81, 93	107
Musk xylene	297.26	81-15-2	28.33	127, 297	282
Musk ketone	294.3	81-14-1	30.77	280, 294	279
Sclareol	308.5	515-03-7	35.16	95, 109	177

**Table S2.** Compounds detected through SIM-B.

Compound	MW	CAS	Retention time	Quantitative m/z	Confirmation m/z
Benzaldehyde	106.121	100-52-7	4.66	105	106, 51
Salicylaldehyde	122.12	90-02-8	6.28	122	65, 121
Terpinolene	136.23	586-62-9	7.33	121	93, 136
Camphor	152.23	464-49-1	8.88	81	95, 108
Methyl salicylate	152.15	119-16-8	10.29	120	92, 152
Folione	154.21	111-12-6	10.42	123	95, 111
Neral	152.23	5392-40-5	11.63	119	69, 84
Carvone	150.22	2244-16-8	11.74	108	54, 82
Linalyl acetate	196.29	115-95-7	12.04	121	80, 93
Geranial	152.23	141-27-5	12.51	152	84, 83
Cinnamaldehyde	132.16	14371-10-9	12.53	131	103, 132
$\alpha$ -Hexylcinnamaldehyde	216.32	101-86-0	12.98	71	59, 95
DMBCA acetate	192.25	151-05-1	14.06	132	91, 117
$\alpha$ -Damascone	192.3	43052-87-5	15.79	123	69, 192
Geranyl acetate	196.29	105-87-1	16.00	136	68, 93
$\beta$ -Damascenone (Rose Ketone-4)	190.28	23696-85-7	16.10	175	69, 190
$\delta$ -Damascone(Rose Ketone-1)	192.3	57378-68-4	16.38	123	69, 192
Vanillin	152.15	121-335	16.47	151	152, 81
(E)- $\beta$ -Damascone	192.3	23726-91-2	17.02	177	123, 192
Coumarin	229.16	91-64-5	17.66	146	89, 118
$\alpha$ -Isomethylionone	206.32	127-51-5	18.98	150	135, 206
Eugenyl acetate	206.24	93-28-7	20.26	164	131, 149
Butylphenyl methylpropional (Lilyal)	204.31	80-54-6	20.28	189	147, 204
3-Propylidenephthalide	174.2	17369-59-4	21.50	159	104, 174
Amyl salicylate	208.25	2050-08-0	21.54	120	138, 208
Isoeugenyl acetate	206.24	93-29-8	22.59	164	131, 149
$\alpha$ -Amylcinnamaldehyde,	202.29	78605-96-6	23.41	129	201, 202
Hydroxyisohexyl 3-cyclohexene carboxaldehyde (HICC-3)	210.32	31906-04-4	23.60	136	177, 192
ISO E@ $\beta$	234.38	54464-57-2	23.87	191	109, 121
ISO E@ $\gamma$	234.38	68155-67-9	23.65	191	109, 121
Hydroxyisohexyl 4-cyclohexene carboxaldehyde (HICC-4)	210.32	51414-25-6	23.76	136	177, 192
ISO E@ $\alpha$	234.38	68155-66-8	24.01	191	109, 121
$\alpha$ -Hexylcinnamaldehyde (Jasmonal)	216.32	101-86-0	25.75	129	215, 216
Benzyl benzoate	212.24	120-51-4	26.15	105	194, 212
$\alpha$ -Acetyl cedrene	246.39	32388-55-9	26.36	161	119, 231
Galaxolide 1	258.4	1222-05-5	28.09	243	213, 258
Galaxolide 2	258.4	1222-05-5	28.12	243	213, 258
Benzyl salicylate	228.24	118-58-1	28.41	91	65, 228
Hexadecanolactone	254.41	109-29-5	29.75	83	97, 111
Dihydroambrettolide					
Benzyl cinnamate	238.28	103-41-3	32.76	131	192, 193

**Table S3.** Percent recovery of the standards during in the tests for the extraction procedure setting. TMP, *trimethylpentane*. DCM, *dichloromethane*.

Compound	TEST A (%R $\pm$ SD)			TEST B (%R $\pm$ SD)		
	5.5 ml TMP	10 ml DCM	10 ml DCM	5.5 ml n-hexane	10 ml Acetone	10 ml Acetone
Salicylaldehyde	9.7 $\pm$ 4.0	11.2 $\pm$ 3.6	12.2 $\pm$ 0.2	10.0 $\pm$ 3.7	31.4 $\pm$ 3.0	20.8 $\pm$ 2.2
Camphor	8.8 $\pm$ 3.1	21.4 $\pm$ 3.1	11.3 $\pm$ 1.2	9.2 $\pm$ 2.8	28.8 $\pm$ 5.1	21.1 $\pm$ 3.8
Folione	9.8 $\pm$ 4.1	22.4 $\pm$ 2.9	10.5 $\pm$ 0.7	10.1 $\pm$ 3.2	23.4 $\pm$ 4.2	20.5 $\pm$ 3.2
Neral	11.2 $\pm$ 5.2	24.0 $\pm$ 3.6	10.8 $\pm$ 1.1	10.7 $\pm$ 4.7	28.4 $\pm$ 3.4	23.5 $\pm$ 1.7
Carvone	9.8 $\pm$ 3.4	25.7 $\pm$ 3.3	12.3 $\pm$ 0.8	10.3 $\pm$ 3.2	27.4 $\pm$ 2.8	22.7 $\pm$ 2.5
Geranial	9.5 $\pm$ 3.2	20.2 $\pm$ 3.1	9.4 $\pm$ 0.4	9.2 $\pm$ 3.2	25.7 $\pm$ 2.7	19.7 $\pm$ 3.4
DMBCA	9.9 $\pm$ 2.8	22.1 $\pm$ 3.7	11.2 $\pm$ 0.6	9.7 $\pm$ 3.0	25.1 $\pm$ 3.3	15.6 $\pm$ 1.9
Geranyl acetate	11.8 $\pm$ 2.5	27.3 $\pm$ 4.0	10.8 $\pm$ 0.8	12.9 $\pm$ 1.2	22.9 $\pm$ 3.4	19.7 $\pm$ 2.1
$\beta$ -Damascenone	9.5 $\pm$ 3.3	23.3 $\pm$ 3.6	9.5 $\pm$ 1.3	9.1 $\pm$ 3.2	24.6 $\pm$ 2.6	21.2 $\pm$ 3.7
$\delta$ -Damascone	9.3 $\pm$ 2.3	23.6 $\pm$ 4.1	10.0 $\pm$ 2.0	10.1 $\pm$ 2.2	33.8 $\pm$ 1.8	24.3 $\pm$ 2.3
$\beta$ -Damascone	9.1 $\pm$ 1.7	20.7 $\pm$ 4.2	9.2 $\pm$ 0.3	8.7 $\pm$ 2.0	29.2 $\pm$ 2.3	25.1 $\pm$ 1.8
Coumarin	9.1 $\pm$ 2.1	25.5 $\pm$ 4.9	10.7 $\pm$ 2.5	10.5 $\pm$ 1.7	28.3 $\pm$ 2.3	21.1 $\pm$ 2.5
$\alpha$ -Isomethylionone	12.2 $\pm$ 3.4	21.9 $\pm$ 4.2	13.4 $\pm$ 1.8	11.3 $\pm$ 2.8	35.1 $\pm$ 2.0	25.6 $\pm$ 2.0
Eugenyl acetate	10.3 $\pm$ 2.9	17.5 $\pm$ 3.4	10.3 $\pm$ 2.8	11.3 $\pm$ 1.9	21.9 $\pm$ 2.6	23.6 $\pm$ 3.1
3-Propylidenephthalide	10.8 $\pm$ 4.3	22.0 $\pm$ 6.1	17.1 $\pm$ 2.3	11.6 $\pm$ 3.4	25.3 $\pm$ 5.4	20.6 $\pm$ 2.6
$\alpha$ -Amylcinnamaldehyde	9.3 $\pm$ 2.1	13.7 $\pm$ 1.7	7.6 $\pm$ 1.2	9.2 $\pm$ 2.1	28.4 $\pm$ 2.9	22.2 $\pm$ 1.8
ISO E <sup>®</sup> Y	10.0 $\pm$ 2.0	10.1 $\pm$ 2.1	4.9 $\pm$ 0.4	9.2 $\pm$ 1.8	22.8 $\pm$ 2.3	19.8 $\pm$ 2.2
Musk xylene	7.5 $\pm$ 2.1	11.4 $\pm$ 2.3	4.9 $\pm$ 0.4	8.8 $\pm$ 1.6	38.3 $\pm$ 3.1	22.8 $\pm$ 1.4
Musk ketone	9.4 $\pm$ 2.6	10 $\pm$ 1.1	7.7 $\pm$ 0.5	9.6 $\pm$ 2.5	31.5 $\pm$ 1.2	25.3 $\pm$ 2.1
Benzyl cinnamate	8.8 $\pm$ 3.5	22.5 $\pm$ 3.2	10.5 $\pm$ 1.0	10.1 $\pm$ 3.0	31.7 $\pm$ 3.2	25.6 $\pm$ 2.9

**Table S4.** Percentage Recovery (%R) and Standard Deviation (SD) of the method at three levels of native compounds

Compound/Classes <sup>1</sup>	Level 1 (100 ng)		Level 2 (3000 ng)		Level 3 (7500 ng)	
	%R	SD	%R	SD	%R	SD
<b>Terpenes, Terpenoids, Aldehydes</b>						
Terpinolene	81.8	3	63.1	5	78.5	8
Neral	71.4	7	86.9	4	92.2	1
Geranial	66.7	6	85.1	7	91.9	4
Carvone	64.6	9	75.7	3	93.7	3
Cinnamaldehyde	51.8	2	75.8	9	85.9	1
Hydroxycitronellal	60.9	1	83.9	13	95.2	5
Vanillin	70.1	1	110	4	114	10
Lylial	60.7	1	64.1	4	88.2	5
a-Amylcinnamaldehyde	70.9	1	85.1	3	91.4	4
a-Hexylcinnamaldehyde	63.5	2	50.9	8	127	14
<b>Salicylates</b>						
Salicylaldehyde	77.1	8	92.7	7	83.4	14
Methyl salicylate	63.8	4	86.3	3	95.3	4
Amyl salicylate	50.1	3	66.6	4	84.9	2
Benzyl salicylate	58.7	2	72.1	9	140	1
<b>Ketones</b>						
Camphor	82.7	7	77.9	1	86.9	8
Folione	72.8	4	88.7	3	97.7	0
a-Damascone	63.4	1	55.4	4	90.2	4
β-Damasconone	69.3	1	66.2	5	86.2	6
δ-Damascone	70.4	0	68.7	4	86.3	6
β-Damascone	72.4	1	73	5	91.3	6
Coumarin	67.1	5	70.7	5	86.4	4
a-Isomethylionone	79.6	1	70.5	4	89.8	6
3-Propylidenephthalide	69.1	0	77.9	2	83.3	3
ISO E®Y	78.3	3	83.1	1	92.2	3
ISO E®β	58.7	2	62.7	1	90.7	7
ISO E®α	70.4	3	63.5	2	109	2
a-Acetyl cedrene	71.4	5	57.4	8	136	20
Hexadecanolactone	96.2	10	62.3	7	142	29
<b>Acetate</b>						
Linalyl acetate	72	7	88.9	4	112	
DMBCA	74.8	2	82	6	92.5	5
Geranyl acetate	66.9	1	70.4	5	84.3	3
Eugenyl acetate	75.4	1	81.2	4	88.9	5
Isoeugenyl acetate	61.7	1	76.3	2	87.6	3
<b>Musks</b>						
Musk xylene	90	5	90.5	11	92.4	6

Musk ketone	65.4	1	76.9	5	73.6	3
Galaxolide 1	73.3	2	57.9	7	131	27
Galaxolide 2	69.2	6	52	4	134	20
<b>Esters</b>						
Benzyl benzoate	74.1	10	48.2	7	125	14
Benzyl cinnamate	79.3	5	88.1	5	115	8
<b>Light Terpenes</b>						
$\alpha$ -Pinene	18	3	39.1	3	43.9	2
$\beta$ -Pinene	27.6	11	46.1	1	39.5	2
$\alpha$ -Terpinene	40.3	4	41.1	5	55	12
Limonene	25.3	6	83.5	6	49.7	8
<b>Alcoli</b>						
Linalool	56.1	3	63.2	6	69.2	8
Menthol	56.4	10	68.2	7	105	2
Terpineol $\alpha$	54.6	3	65.7	8	72.7	1
Citronellol	50.1	9	85.6	17	120	3
Geraniol	71	12	143	22	131	1
Cinnamyl alcohol	79.4	11	127	27	93.8	7
trans-Anethole	52.1	1	64.1	8	71.6	6
Eugenol	34	6	68.4	13	64.4	3
$\beta$ -Caryophyllene	61.3	1	51.7	3	78.5	8
Isoeugenol (E)	46.1	15	70.7	7	60.5	6
$\beta$ - Santalol	99.8	17	220	24	90.2	7
$\beta,\beta,3$ -Tmbp	82	21	79.4	8	152	13
Sclareol	76.5	4	114	10	115	1
<b>Unreable compounds</b>						
Benzaldehyde	-4145	1306	-3389	171	120	23
HICC-4	77.2	1	127	2	88.7	2
HICC-3	43.7	2	79.5	3	77.8	2
Benzyl alcohol	-118	185	164	12	66.4	8
Anise alcohol	89.5	11	261	55	192	5
Ebanol 1	1092	909	16866	1159	21238	1191
Ebanol 2	89.5	5	103	5	134	2
trans,trans-Farnesol	3465	927	6255	354	10414	217
a-Santalol	154	15	54.4	4	199	8
a-Amylcinnamyl alcohol	196	10	298	7	302	2

<sup>1</sup>The compounds were divided on the basis of common characteristics, by functional group or similar behavior shown during extraction. White was subtracted for each data reported.

**Table S5.** % of ng lost during the sampling for Breakthrough evaluation

Classes/Compounds	First sampling %ng loss	Second Sampling %ng loss
<b>Terpenes, Terpenoids,</b>		
<b>Aldheydes</b>		
Terpinolene	ND	1.55
Neral	ND	0.18
Geranial	ND	0.21
Carvone	0.32	0.17
Cinnamaldehyde	0.07	0.07
Hydroxycitronellal	ND	ND
Vanillin	2.63	2.68
Lylial	0.11	0.12
a-Amylcinnamaldehyde	0.24	0.24
a-Hexylcinnamaldehyde	0.11	0.16
<b>Salicylates</b>		
Salicylaldehyde	12.8	14.2
Methyl salicylate	0.27	0.21
Amyl salicylate	0.21	0.23
Benzyl salicylate	0.58	0.58
<b>Ketones</b>		
Camphor	4.9	6.9
Folione	ND	0.26
a-Damascone	ND	ND
β-Damascenone	0.15	0.16
δ-Damascone	ND	0.99
(E)-β-Damascone	0.16	0.17
Coumarin	0.10	0.12
a-Isomethylionone	0.15	0.16
3-Propylidenephthalide	0.14	0.14
ISO E®Y	ND	0.52
ISO E®β	ND	0.3
ISO E®α	ND	10.4
a-Acetyl cedrene	0.07	0.07
Hexadecanolactone	ND	ND
<b>Acetate</b>		
Linalyl acetate	ND	ND
DMBCA	0.12	0.13
Geranyl acetate	ND	0.18
Eugenyl acetate	0.16	0.16
Isoeugenyl acetate	<LOQ	LOQ
<b>Musks</b>		

Musk xylene	ND	ND
Musk ketone	ND	1.67
Galaxolide 1	0.07	0.07
Galaxolide 2	0.07	0.09
<b>Esters</b>		
Benzyl benzoate	0.13	0.14
Benzyl cinnamate	0.29	ND
<b>Light Terpenes</b>		
$\alpha$ -Pinene	5.41	4.9
$\beta$ -Pinene	4.46	4.54
$\alpha$ -Terpinene	0.81	1.1
Limonene	2.76	1.27
<b>Alcoli</b>		
Linalool	0.24	0.19
Menthol	0.45	0.33
Terpineol $\alpha$	0.44	0.28
Citronellol	<LOQ	<LOQ
Geraniol	0.31	0.29
Cinnamyl alcohol	ND	ND
trans-Anethole	ND	0.12
Eugenol	<LOQ	0.13
$\beta$ -Caryophyllene	0.19	0.18
Isoeugenol (E)	0.3	0.51
$\beta$ - Santalol	ND	0.54
$\beta,\beta,3$ -Tmbp	<LOQ	<LOQ
Sclareol	ND	ND
<b>Unreable compounds</b>		
Benzaldehyde	137	88.8
HICC-4	2	ND
HICC-3	1	<LOQ
Benzyl alcohol	12.1	3.58
Anise alcohol	0.07	0.09
Ebanol 1	20.4	10.4
Ebanol 2	2.18	4.18
trans,trans-Farnesol	ND	6.22
$\alpha$ -Santalol	ND	1.05
$\alpha$ -Amylcinnamyl alcohol	ND	2.54
Benzyl alcohol	12.1	3.58

<sup>1</sup>The compounds were divided on the basis of common characteristics, by functional group or similar behavior shown during extraction. White was subtracted for each data reported. ND: not detected



**Table S6.** Results of the semi-quantitative determination of fragrances in the house and in the coffee bar.

Compound ng/m3	House	Coffee shop
Terpinolene	64.4	138
Vanillin	25.1	182
Lylial	10.9	49.4
a-Hexylcinnamaldehyde	168	92.1
Methyl salicylate	23.3	40.5
Amyl salicylate	72.8	162
Benzyl salicylate	235	182
ISO E®β	< LOQ	< LOQ
ISO E®α	< LOQ	< LOQ
Linalyl acetate	436	242
Galaxolide 1	97.6	46.3
Galaxolide 2	92.7	40.8
Benzyl benzoate	46.8	57.2
Linalool	634	266
Menthol	458	2450
Terpineol α	73.1	70
Citronellol	111	73.5
Geraniol	52.4	19.4
β-Caryophyllene	12.3	17.6
Isoeugenol (E)	3.15	3.85