Method for Predicting Odor Intensity of Perfumery Raw Materials Using Dose−Response Curve Database

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We provide data concerning with relative standard deviation (RSD) of the gas chromatography analysis, the odor properties of PRMs obtained in this study, the result of root mean square error calculations, and the panelists' ability to make evaluations used to verify the prediction accuracy of the model, as follows.

- RSD of each PRM with GC−MS (Table S1)
- odor properties of PRMs (Table S2)
- RMSE in both unshuffled and shuffled parameter in single in single component (Table S3 and Figure S1)
- evaluation ability of each panelist (Table S4)

- possibility of differences related to genes or experience among the panelists (Table S4 and Figure S2)

- predicted odor intensity of mixture sample and average grade of perceived odor intensity (Table S5)

- five conditions shuffled parameter with other PRMs (Table S6)

- RMSE both unshuffled and shuffled odor property in SC model (Table S7)

- the case in which the SC model was unfit (Figure S3)

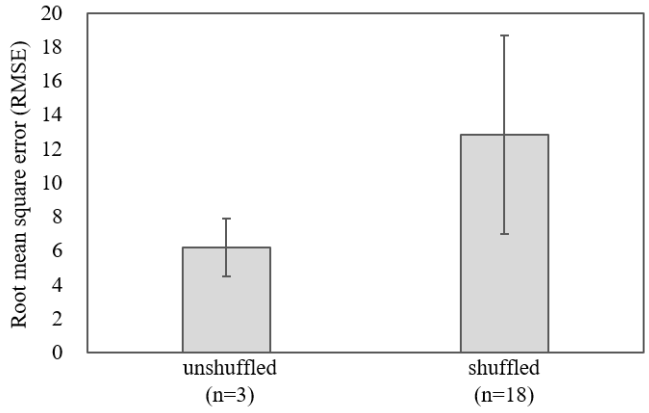


Figure S1. The average of RMSE in unshuffled and shuffled OISC parameter

The bar graph shows the average of RMSE in unshuffled or shuffled odor properties shown in Table 4. The average of the former RMSE is 6.22, while that the latter is 12.85. The error bars represent standard deviation.

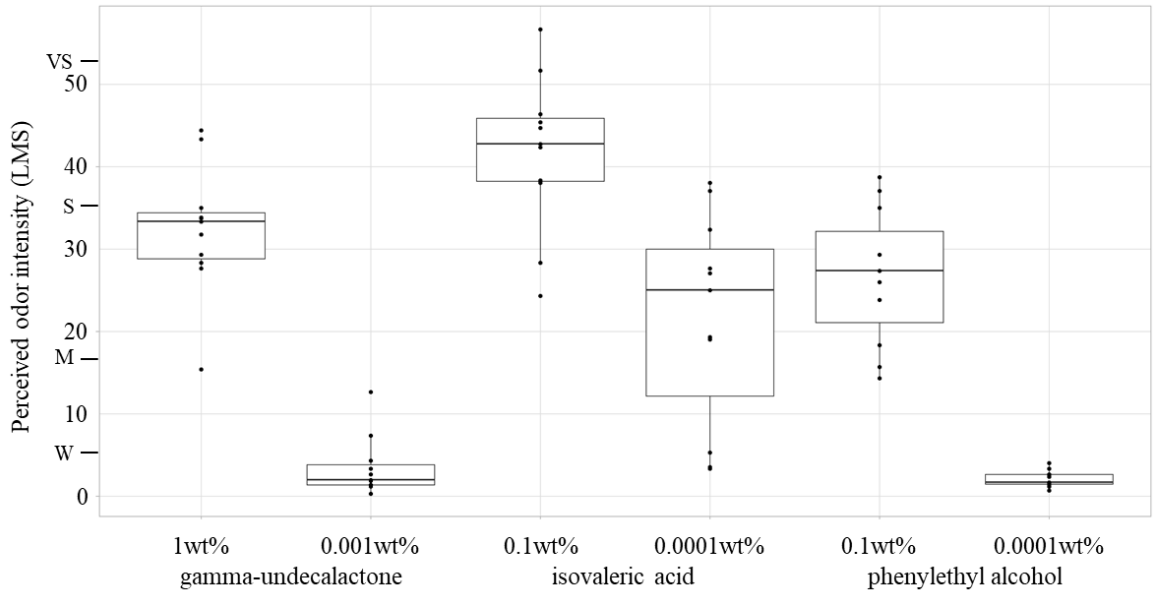
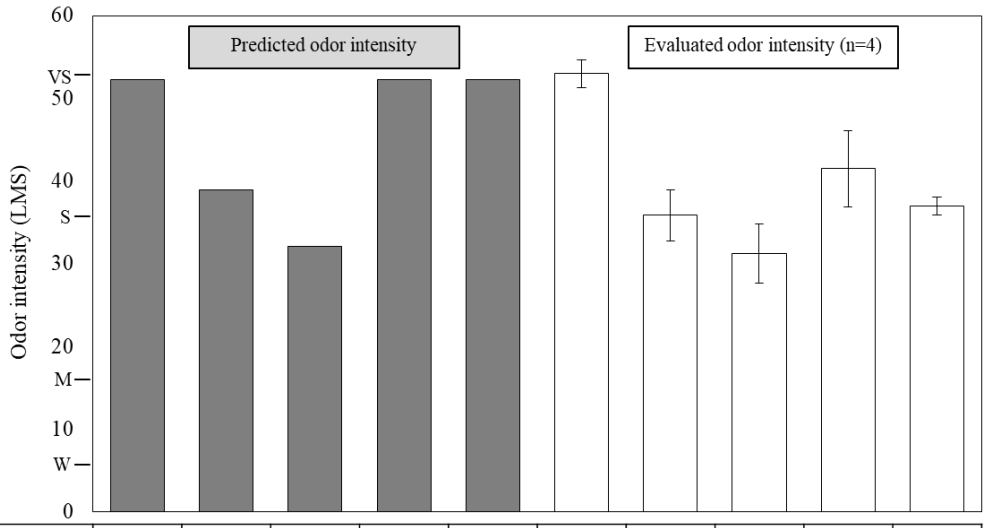


Figure S2. Individual differences in the evaluation of RPMs

The box plots show the median and distribution of perceived odor intensity of RPMs evaluated by each subject (n = 11). Each dot represents an intensity value given by each subject. Boxes represent the upper and lower quartiles around the median value. The dashes represent the extremes of the range and indicate outliers. This result shows a degree of individual variability in odor intensity evaluations.



249.4 µg/L air cis-3-hexenol	+	-	-	+	+	+	-	-	+	+
10.3 µg/L air alpha-damascone	-	+	-	+	+	-	+	-	+	+
2.2 µg/L air ethyl butyrate	-	-	+	-	+	-	-	+	-	+

Figure S3. Examples of PRM mixtures with perceived odor intensity which does not follow the SC model

The left-hand grey bars show odor intensity of each PRM and their mixtures predicted by the SC model and the OISC. The right-hand white bars show the evaluated intensity of the corresponding PRM samples (n = 4, S.E.). In contrast with predicted values, the evaluated odor intensity of the mixtures does not agree with the intensity of their single components, with the highest odor intensity value given for *cis*-3-hexenol. The addition of alpha-damascone and ethyl butyrate to *cis*-3-hexenol decreased the odor intensity of the resulting mixtures, possibly due to masking effect or receptor antagonism.

Table S1. The Relative Standard Deviation (RSD) of each PRM as Determined Using GC−MS

component	peak area			RSD (%)
	sample1	sample2	sample3	
floramat	824973964	808365542	826872458	1.0%
raspberry ketone	220883242	220138881	231170164	2.2%
ethylene brassylate	1041453750	979206866	1000912956	2.6%
damascenone	1076379050	972237009	1020743870	4.2%
terpirosa	672551902	617452140	679224455	4.2%
citral	669277987	593502827	641452871	4.9%
gamma-decalactone	4239795	4074377	4666317	5.8%

Table S2. The Parameter of each PRM Utilized in this Study

Cas no.	compound	odor property		
		I_{max_i}	C_i	D_i
37609-25-9	(5Z)-cyclohexadec-5-en-1-one	14.50	-2.48	0.27
470-82-6	1,8-cineol	58.98	1.41	0.86
112-45-8	10-undecenal	60.03	0.29	0.75
3391-86-4	1-octen-3-ol	41.28	0.93	0.62
2442-10-6	1-octen-3-yl acetate	54.08	1.66	0.87
29895-73-6	2-(phenylmethyl)-1,3-dioxan-5-ol	40.75	-1.85	0.55
140-88-5	2,6-nonadienal	48.08	0.42	0.85
28069-72-9	2,6-nonadienol	47.41	-0.27	0.60
110-41-8	2-methyl undecanal	48.30	0.67	0.53
3452-97-9	3,5,5-trimethyl-1-hexanol	41.11	1.76	0.38
122-97-4	3-phenylpropyl alcohol	41.32	0.02	0.38
534-15-6	acetaldehyde dimethyl acetal	66.44	3.02	0.92
513-86-0	acetoin	49.69	0.90	0.76
98-86-2	acetophenone	67.67	0.97	0.68
80449-58-7	acetyl cedrene	37.09	-0.64	0.61
93-28-7	acetyl eugenol	18.31	-0.82	0.43
93-29-8	acetyl isoeugenol	29.42	-2.35	0.54
77-83-8	aldehyde c-16 strawberry	37.65	0.23	0.48
79-78-7	allyl alpha-ionone	30.67	-0.57	0.26
124899-75-8	allyl amyl glycolate	59.50	0.15	0.60
2705-87-5	allyl cyclohexane propionate	45.18	0.96	0.49

68901-15-5	allyl cyclohexyl glycolate	36.20	-1.08	0.40
142-19-8	allyl heptanoate	40.73	0.69	0.69
123-68-2	allyl hexanoate	61.79	1.60	0.80
7493-74-5	allyl phenoxyacetate	24.82	-0.02	0.25
43052-87-5	alpha-damascone	49.33	0.35	0.54
127-41-3	alpha-ionone	37.15	1.31	0.19
7785-26-4	alpha-pinene	47.36	2.08	0.79
99-86-5	alpha-terpinene	56.48	1.50	0.77
98-55-5	alpha-terpineol	34.59	0.83	0.48
139504-68-0	amber core	6.93	0.05	0.37
3738-00-9	ambrotech	23.86	-0.67	0.11
6790-58-5	ambroxan	29.65	-0.91	0.47
122-40-7	amyl cinnamaldehyde	30.79	-1.86	0.34
2050-08-0	amyl salicylate	15.20	-1.20	0.11
105-13-5	anis alcohol	24.23	-1.15	0.37
123-11-5	anis aldehyde	39.89	0.67	0.40
104-21-2	anisyl acetate	19.56	-0.73	0.45
104-20-1	anisyl acetone	29.82	-1.19	0.45
67845-30-1	bark carbaldehyde	41.75	-0.43	0.61
100-52-7	benzaldehyde	62.02	1.23	0.69
140-11-4	benzyl acetate	35.31	0.74	0.43
100-51-6	benzyl alcohol	30.28	1.49	0.33
120-51-4	benzyl benzoate	13.25	-2.37	0.16
104-57-4	benzyl formate	31.57	1.67	0.55
103-28-6	benzyl isobutyrate	29.67	1.31	0.37
103-37-7	benzyl n-butyrate	39.93	0.53	0.33
122-63-4	benzyl propionate	34.24	0.86	0.28
118-58-1	benzyl salicylate	7.20	-2.78	0.60
87-44-5	beta-caryophyllene	20.21	1.71	0.10
35044-68-9	beta-damascone	47.67	-0.15	0.49
14901-07-6	beta-ionone	53.35	-0.09	0.68
23267-57-4	beta-ionone epoxide	9.25	-0.06	0.11

127-91-3	beta-pinene	44.33	2.08	0.60
58567-11-6	boisambrene forte	8.90	-0.51	0.67
507-70-0	borneol	43.67	-0.07	0.52
123-86-4	butyl acetate	81.23	2.54	0.89
109-21-7	butyl butyrate	60.49	2.29	0.67
28940-11-6	calone	44.56	-0.65	0.46
79-92-5	camphene	41.88	2.38	0.36
464-49-3	camphor	51.04	1.47	0.51
5462-06-6	canthoxal	35.03	-0.57	0.23
33704-61-9	cashmerane	35.04	0.95	0.63
77-53-2	cedrol	6.73	-0.80	0.14
77-54-3	cedryl acetate	29.89	-0.94	0.29
67874-81-1	cedryl methyl ether	18.80	0.25	0.41
13171-00-1	celestolide	14.74	-2.03	0.38
4407-36-7	cinnamic alcohol	34.87	-1.61	0.36
104-55-2	cinnamic aldehyde	40.44	0.62	0.07
103-54-8	cinnamyl acetate	41.42	-1.39	0.62
928-96-1	*cis*-3-hexenol	57.45	0.85	0.59
3681-71-8	*cis*-3-hexenyl acetate	71.83	1.35	0.84
25152-85-6	*cis*-3-hexenyl benzoate	34.77	-1.53	0.52
16491-36-4	*cis*-3-hexenyl butyrate	50.27	0.97	0.71
31501-11-8	*cis*-3-hexenyl hexanoate	49.56	0.71	0.58
41519-23-7	*cis*-3-hexenyl isobutyrate	56.99	1.89	0.43
65405-77-8	*cis*-3-hexenyl salicylate	23.36	-1.17	0.13
67883-79-8	*cis*-3-hexenyl tiglate	44.85	0.01	0.63
21662-09-9	*cis*-4-decenal	60.69	0.42	0.77
6728-31-0	*cis*-4-heptenal	79.63	-0.06	0.70
35854-86-5	*cis*-6-nonen-1-ol	26.97	-0.65	0.47
2277-19-2	*cis*-6-nonenal	59.93	-0.19	0.87
488-10-8	*cis*-jasmone	40.15	-0.35	0.28
5392-40-5	citral	44.11	0.66	0.66
106-23-0	citronellal	52.79	0.58	0.52

26489-01-0	citronellol	32.29	0.72	0.53
150-84-5	citronellyl acetate	39.95	0.08	0.39
105-85-1	citronellyl formate	54.74	0.97	0.65
97-89-2	citronellyl isobutyrate	24.90	0.65	0.44
91-64-5	coumarin	26.79	-0.68	0.77
122-03-2	cumin aldehyde	49.53	1.29	0.47
103-95-7	cyclamen aldehyde	29.71	-0.70	0.44
25485-88-5	cyclohexyl salicylate	10.07	-1.09	0.51
80-71-7	cyclotene	46.43	-0.59	0.32
23726-93-4	damascenone	55.82	-1.50	0.44
112-31-2	decanal	76.62	-0.46	0.74
112-30-1	decanol	14.99	-0.54	0.50
34131-98-1	decatone	22.65	-0.50	0.14
13019-22-2	decenol	19.69	-0.98	0.37
57378-68-4	delta-damascone	50.03	0.60	0.72
705-86-2	delta-decalactone	40.11	-0.91	0.10
713-95-1	delta-dodecalactone	27.46	-1.83	0.35
3301-94-8	delta-nonalactone	35.68	0.01	0.19
710-04-3	delta-undecalactone	32.98	-1.23	0.13
108-59-8	diethyl malonate	35.24	1.30	0.36
17283-81-7	dihydro beta-ionone	29.83	0.64	0.45
2785-87-7	dihydro eugenol	34.34	1.70	0.17
1128-08-1	dihydro jasmone	39.88	-0.06	0.44
18479-58-8	dihydro myrcenol	45.47	0.88	0.83
58985-02-7	dihydro terpineol	44.64	1.54	0.46
151-05-3	dimethy benzyl carbinyl acetate	34.97	1.21	0.45
100-86-7	dimethyl benzyl carbinol	19.81	1.34	0.39
10094-34-5	dimethyl benzyl carbinyl butyrate	32.43	0.47	0.30
2550-11-0	dimethyl octenone	42.75	1.58	0.49
103-05-9	dimethyl phenyl ethyl carbinol	35.47	0.31	0.47
13254-34-7	dimetol	42.89	0.76	0.58
101-84-8	diphenyl oxide	40.00	0.96	0.42

112-54-9	dodecanal	50.27	0.94	0.29
56973-85-4	dynascone	54.96	-0.06	0.97
7452-79-1	ethyl 2-methyl butyrate	77.55	0.63	1.21
141-78-6	ethyl acetate	35.06	2.95	0.35
141-97-9	ethyl acetoacetate	44.94	1.36	0.45
93-89-0	ethyl benzoate	49.90	0.16	0.51
105-54-4	ethyl butyrate	81.16	2.62	1.20
4192-77-2	ethyl cinnamate	26.90	-1.52	0.56
110-38-3	ethyl decanoate	27.80	0.80	0.48
106-30-9	ethyl heptanoate	50.58	1.70	0.70
123-66-0	ethyl hexanoate	71.87	2.67	0.88
97-62-1	ethyl isobutyrate	71.42	1.66	1.03
108-64-5	ethyl isovalerate	65.79	0.66	1.06
10339-55-6	ethyl linalool	45.38	0.61	0.69
4940-11-8	ethyl maltol	49.29	-1.59	0.61
123-29-5	ethyl nonanoate	33.54	1.48	0.18
106-32-1	ethyl octanoate	45.22	1.27	0.56
121-39-1	ethyl phenyl glycidate	30.43	-0.65	0.09
105-37-3	ethyl propionate	73.76	3.26	0.72
35044-59-8	ethyl safranate	51.12	1.22	0.58
118-61-6	ethyl salicylate	45.06	-0.58	0.48
121-32-4	ethyl vanillin	43.45	-1.06	0.45
97-53-0	eugenol	34.29	-0.76	0.59
1632-73-1	fenchyl alcohol	52.15	1.04	0.42
67634-25-7	floralate	40.01	0.56	0.49
68480-15-9	floralol	29.91	1.34	0.43
67634-14-4	floralozone	42.47	0.33	0.36
67801-64-3	floramat	26.92	0.37	0.55
5182-36-5	floropal	41.51	0.22	0.48
63500-71-0	florosa	35.09	0.73	0.53
4621-04-9	folrosia	49.73	0.98	0.46
6413-10-1	fructone	42.03	1.05	0.63

80623-07-0	fruitate	44.72	1.18	0.69
4166-20-5	furaneol	48.78	-0.94	0.56
1222-05-5	galaxolide	16.67	-1.14	0.56
706-14-9	gamma-decalactone	25.69	-0.83	0.24
2305-05-7	gamma-dodecalactone	28.30	-1.18	0.14
695-06-7	gamma-hexalactone	51.21	1.71	0.53
104-61-0	gamma-nonalactone	34.60	-0.09	0.45
104-50-7	gamma-octanoic lactone	40.87	1.09	0.27
99-85-4	gamma-terpinene	43.25	1.18	0.55
104-67-6	gamma-undecalactone	33.76	-0.52	0.77
108-29-2	gamma-valerolactone	30.71	1.63	0.38
106-24-1	geraniol	29.88	0.17	0.35
105-87-3	geranyl acetate	25.52	-0.43	0.35
106-29-6	geranyl butyrate	38.10	-0.61	0.26
68133-79-9	geranyl cyclopentanone	29.58	-1.96	0.45
68901-32-6	glycolierral	19.89	-0.16	0.44
3720-16-9	gravenone	36.42	0.30	0.23
134-28-1	guaiyl acetate	14.76	-0.90	0.35
1205-17-0	helional	23.06	-1.91	0.47
120-57-0	heliotropine	29.56	0.23	0.41
55418-52-5	heliotropyl acetone	8.37	-1.98	0.47
141773-73-1	helvetolide	7.05	-0.75	0.22
111-71-7	heptanal	60.55	1.89	0.82
111-70-6	heptanol	30.50	0.60	0.33
67583-77-1	herbavert	23.26	3.40	0.64
66-25-1	hexanal	80.92	1.16	0.88
111-27-3	hexanol	45.98	1.66	0.73
142-92-7	hexyl acetate	48.92	1.66	0.84
2639-63-6	hexyl butyrate	45.58	1.24	0.56
6259-76-3	hexyl salicylate	7.79	-1.72	0.68
107-75-5	hydroxy citronellal	23.94	-0.42	0.32
107-74-4	hydroxy citronellol	8.53	-1.61	0.14

18096-62-3	indoflor	25.86	-0.19	0.08
120-72-9	indole	43.59	-0.19	0.54
2983-37-1	irotyl	38.22	1.65	0.50
54464-57-2	ISO E super	29.16	-0.18	0.43
123-92-2	isoamyl acetate	84.97	3.07	0.90
123-51-3	isoamyl alcohol	48.56	1.42	0.78
87-20-7	isoamyl salicylate	26.58	-0.20	0.32
124-76-5	isoborneol	44.10	-0.78	0.61
125-12-2	isobornyl acetate	30.17	0.53	0.51
110-19-0	isobutyl acetate	71.78	2.89	0.75
1335-66-6	isocyclocitral	59.65	1.38	0.66
39872-57-6	isodamascone	33.57	1.02	0.44
97-54-1	isoeugenol	39.34	-0.54	0.31
23787-90-8	isolongifolanone	31.42	-0.34	0.51
491-07-6	isomenthone	45.96	1.27	0.68
40379-24-6	isononyl acetate	30.08	2.05	0.38
61699-38-5	jasmacyclat	38.94	0.63	0.33
1322-17-4	Jasmonyl	41.77	-0.60	0.37
117933-89-8	karanal	48.88	-1.32	0.50
36306-87-3	kephalis	26.06	-0.21	0.39
112-53-8	lauryl alcohol	10.53	-1.15	0.70
6485-40-1	*l*-carvone	48.78	1.31	0.69
67633-96-9	liffarome	54.43	0.87	0.57
80-54-6	lilial	35.47	-0.67	0.26
73018-51-6	lime oxide	61.96	1.82	0.65
7392-19-0	limetol	43.19	2.39	0.96
138-86-3	limonene	52.62	1.71	0.50
78-70-6	linalool	50.63	0.08	0.65
60047-17-8	linalool oxide	40.96	1.51	0.60
115-95-7	linalyl acetate	43.52	1.79	0.35
115-99-1	linalyl formate	39.82	0.30	0.62
78-35-3	linalyl isobutyrate	34.29	1.02	0.33

2216-51-5	*l*-menthol	33.06	0.66	0.46
14073-97-3	*l*-menthone	46.69	1.27	0.60
31906-04-4	lyral	25.22	-2.18	0.09
118-71-8	maltol	37.51	-1.32	0.41
20407-84-5	mandarine aldehyde	47.26	-1.39	0.38
39255-32-8	manzanate	70.38	1.26	1.22
106-72-9	melonal	45.92	-0.64	0.95
67707-75-9	melusat	39.70	1.87	0.59
58985-18-5	menthanyl acetate	48.48	1.48	0.75
121-98-2	methyl anisate	17.84	0.64	0.12
134-20-3	methyl anthranilate	30.49	1.36	0.59
93-58-3	methyl benzoate	30.42	1.56	0.48
93-08-3	methyl beta-naphthyl ketone	37.39	-1.23	0.73
623-42-7	methyl butyrate	61.90	1.27	0.89
103-26-4	methyl cinnamate	39.82	0.01	0.44
24851-98-7	methyl dihydrojasmonate	15.83	-0.70	0.37
127-51-5	methyl ionone-gamma	45.02	0.26	0.63
93-16-3	methyl isoeugenol	37.97	-1.75	0.44
112-12-9	methyl nonyl ketone	40.05	0.29	0.38
111-80-8	methyl octine carbonate	51.90	-0.83	0.61
119-36-8	methyl salicylate	54.43	1.71	0.73
82356-51-2	muscenone delta	12.56	-0.72	0.73
541-91-3	muscone	2.90	-1.71	0.37
37677-14-8	myrac aldehyde	34.47	-0.18	0.27
123-35-3	myrcene	49.14	1.05	0.80
1118-39-4	myrcenyl acetate	34.34	1.46	0.49
106-25-2	nerol	29.66	0.68	0.52
7212-44-4	nerolidol	39.68	-0.88	0.49
93-18-5	nerolin bromelia	43.31	-0.10	0.55
93-04-9	nerolin yara yara	34.08	-0.10	0.31
141-12-8	neryl acetate	29.85	-0.08	0.40
124-19-6	nonanal	52.35	1.35	0.82

143-08-8	nonanol	29.81	1.18	0.34
4674-50-4	nootkatone	27.13	-2.24	0.36
128-51-8	nopyl acetate	24.10	1.30	0.38
70788-30-6	norlimbanol	23.30	-0.46	0.75
13877-91-3	ocimene	46.66	2.22	0.57
4430-31-3	octahydrocoumarin	29.65	-0.54	0.49
124-13-0	octanal	78.17	1.33	1.13
111-87-5	octanol	40.11	0.60	0.51
112-14-1	octyl acetate	42.69	1.77	0.52
88-41-5	*o-tert*-butylcyclohexyl acetate	30.91	1.21	0.44
106-44-5	*p*-cresol	51.68	-0.19	0.63
140-39-6	*p*-cresyl acetate	35.62	0.95	0.68
104-93-8	*p*-cresyl methyl ether	55.95	2.30	0.84
99-87-6	*p*-cymene	53.33	1.61	0.51
106-02-5	pentalide	6.29	-1.36	0.18
90397-38-9	peranat	31.66	1.65	0.29
2111-75-3	perillaldehyde	56.27	0.93	0.56
103-60-6	phenoxy ethyl isobutyrate	28.83	-0.47	0.21
3558-60-9	phenyl ethyl methyl ether	50.53	1.26	0.79
55066-48-3	phenyl hexanol	28.72	-0.72	0.70
101-48-4	phenylacetaldehyde dimethyl acetal	41.82	0.26	0.58
103-45-7	phenylethyl acetate	38.38	1.35	0.57
60-12-8	phenylethyl alcohol	20.15	0.05	0.58
103-48-0	phenylethyl isobutyrate	37.51	1.10	0.45
122-70-3	phenylethyl propionate	34.30	0.87	0.32
99-82-1	*p*-menthane	28.99	3.34	0.50
2511-00-4	poirenate	38.02	-0.38	0.40
2109-22-0	pollenal II	60.08	1.17	0.63
1191-16-8	prenyl acetate	72.19	1.94	0.70
105-66-8	propyl butyrate	58.95	2.57	0.82
106-36-5	propyl propionate	53.79	2.74	0.66
98-52-2	*p-tert*-butylcyclohexanol	11.41	0.46	0.70

32210-23-4	*p-tert*-butylcyclohexyl acetate	39.71	1.30	0.63
104-87-0	*p*-tolyl aldehyde	56.18	1.40	0.79
5471-51-2	raspberry ketone	21.91	-0.52	0.35
82461-14-1	rhubafuran	41.03	0.84	0.51
16409-43-1	rose oxide	50.32	1.26	0.69
90-17-5	rosephenone	7.79	-2.29	0.30
60335-71-9	rosyrane	43.92	1.12	0.66
116-26-7	safranal	48.97	0.29	0.71
28219-60-5	sandalmysore core	18.12	-0.19	0.31
83-34-1	skatole	29.64	-2.26	0.35
93-92-5	styrallyl acetate	38.90	1.86	0.45
120-45-6	styrallyl propionate	40.98	1.37	0.41
6658-48-6	suzaral	26.79	-0.96	0.37
20126-76-5	terpinene-4-ol	39.89	1.87	0.44
8000-41-7	terpineol	51.35	0.66	0.58
586-62-9	terpinolene	41.83	1.08	0.68
80-26-2	terpinyl acetate	40.69	0.09	0.50
1247790-47-1	terpirosa	36.61	1.48	0.66
1333-49-9	tetrahydrogeraniol	35.28	-0.21	0.32
78-69-3	tetrahydrolinalool	44.84	0.08	0.54
21145-77-7	tonalide	13.89	-0.66	0.58
3913-81-3	*trans*-2-decenal	20.82	1.39	0.76
928-95-0	*trans*-2-hexen-1-ol	51.49	1.74	0.68
6728-26-3	*trans*-2-hexenal	70.22	1.30	0.70
2497-18-9	*trans*-2-hexenyl acetate	48.31	1.44	0.44
65405-70-1	*trans*-4-decenal	55.22	0.11	0.80
5413-60-5	tricyclodecenyl acetate	41.15	0.71	0.54
113889-23-9	tricyclodecenyl butyrate	24.15	-0.51	0.11
67634-20-2	tricyclodecenyl isobutyrate	30.73	0.21	0.59
17511-60-3	tricyclodecenyl propionate	31.74	0.06	0.61
68039-49-6	triplal	73.42	1.40	0.88
80480-24-6	troenan	25.54	1.71	0.36

112-44-7	undecanal	35.68	0.41	0.19
81782-77-6	undecavertol	61.49	0.41	0.72
4630-07-3	valencene	27.03	0.96	0.28
121-33-5	vanillin	39.02	-1.81	0.00
87731-18-8	violiff	43.25	0.61	0.44

Table S3. Predicted Odor Intensity (Ψ_i) from eq 3 and Odor Intensity of each PRM (limonene, linalool, and methyl ionone-gamma) Evaluated by the Panelists

molecule (i)	$\log C_i^g$	Ψ_i	panelist				average	standard error
limonene	−0.99	0.2	0.0	0.5	0.0		0.2	0.2
	−0.38	0.8	0.1	1.2	5.0		2.1	1.5
	0.01	1.7	0.5	2.0	1.7		1.4	0.5
	0.08	1.9	1.0	1.5	2.8		1.8	0.5
	0.38	3.4	3.0	1.5	12.5		5.7	3.4
	0.62	5.3	6.0	10.3	15.0		10.4	2.6
	0.95	9.4	2.3	3.5	10.7		5.5	2.6
	1.02	10.5	5.0	8.0	15.3		9.4	3.1
	1.08	11.5	17.0	2.0	18.3		12.4	5.2
	1.25	14.9	9.0	3.5	30.5		14.3	8.2
	1.37	17.6	27.0	18.0	31.3		25.4	3.9
	1.67	25.2	39.0	35.0	40.5		38.2	1.6
	1.95	32.5	35.0	27.0	36.7		32.9	3.0
	2.02	34.2	37.0	30.0	43.2		36.7	3.8
	2.37	41.5	44.0	38.0	48.3		43.4	3.0
	2.90	48.2	38.0	51.3	27.0	50.0	41.6	5.7
linalool	−2.55	0.9	3.0	5.5	3.0		3.8	0.8
	−2.21	1.5	5.0	4.8	7.0		5.6	0.7
	−1.87	2.5	4.0	17.0	10.0		10.3	3.8

	−1.61	3.6	13.0	17.0	8.5		12.8	2.5
	−1.55	3.9	5.5	14.7	6.0		8.7	3.0
	−1.45	4.5	2.5	20.0	8.0		10.2	5.2
	−1.21	6.2	7.0	5.0	25.0		12.3	6.4
	−0.87	9.6	17.0	28.5	17.0		20.8	3.8
	−0.61	13.1	15.0	32.0	9.0		18.7	6.9
	−0.45	15.7	7.0	35.0	10.0		17.3	8.9
	−0.22	19.7	9.0	25.0	15.2	5.0	13.6	4.4
	0.12	26.2	15.0	15.0	13.0	17.3	15.1	0.9
	0.38	31.0	18.0	30.0	17.2	6.1	17.8	4.9
	1.09	41.7	35.4	45.0	15.0		31.8	8.8
	1.20	42.9	33.0	30.2	30.5	35.0	32.2	1.1
	1.59	46.0	42.0	52.0	35.0	28.5	39.4	5.0
methyl ionone-gamma	−2.65	0.4	2.0	3.4	2.5		2.6	0.4
	−2.08	1.0	0.5	2.4	0.5		1.1	0.6
	−1.78	1.7	3.3	6.1	0.5		3.3	1.6
	−1.73	1.8	5.3	3.8	1.0		3.4	1.3
	−1.52	2.5	6.0	7.8	0.0		4.6	2.4
	−1.43	2.8	2.0	8.2	4.0		4.7	1.8
	−1.22	3.9	10.0	15.2	4.5		9.9	3.1
	−1.08	4.7	7.4	10.3	3.5		7.1	2.0
	−1.01	5.2	5.0	14.9	4.0		8.0	3.5
	−0.75	7.4	9.0	12.5	3.4		8.3	2.7
	−0.71	7.9	15.3	18.6	6.5		13.5	3.6
	−0.54	9.8	23.0	28.7	6.0		19.2	6.8
	−0.01	17.7	35.4	34.3	9.0		26.2	8.6
	1.00	34.4	47.0	55.0	30.0	70.0	50.5	8.3

Table S4. Within-Subjects Variability and Across-Subjects Variability

panel	gamma-undecalactone				isovaleric acid				phenylethyl alcohol			
	1wt%		0.001wt%		0.1wt%		0.0001wt%		0.1wt%		0.0001wt%	
	ave.	S.D.	ave.	S.D.	ave.	S.D.	ave.	S.D.	ave.	S.D.	ave.	S.D.
1	33.8	3.5	1.4	0.5	42.7	1.5	27.0	8.9	26.0	3.3	1.5	0.5
2	33.3	1.2	2.0	1.7	38.0	2.0	19.0	12.3	38.7	4.0	2.7	2.1
3	43.3	2.9	1.3	1.4	56.7	2.9	27.7	7.5	35.0	5.0	0.7	0.3
4	29.3	5.8	3.3	1.5	42.3	5.5	38.0	4.6	29.3	3.2	2.3	1.5
5	33.7	1.2	12.7	9.2	46.3	4.7	32.3	9.3	27.3	11.0	4.0	3.1
6	35.0	0.0	2.7	1.2	45.3	0.6	25.0	13.2	18.3	2.9	3.3	1.5
7	28.3	5.8	4.3	2.1	28.3	7.6	3.5	2.3	14.3	9.8	1.5	0.5
8	27.7	2.5	1.8	0.3	38.3	2.9	5.3	0.6	23.8	3.2	1.5	0.0
9	44.3	0.6	1.2	0.3	44.7	4.2	37.0	2.6	27.3	1.2	1.7	0.8
10	15.3	9.2	0.3	0.6	24.3	4.0	3.3	0.6	15.7	8.1	1.2	1.3
11	31.7	2.9	7.3	5.1	51.7	2.9	19.3	12.5	37.0	3.6	2.7	0.6
ave. (n=11)	32.4	3.2	3.5	2.2	41.7	3.5	21.6	6.8	26.6	5.0	2.1	1.1
S.D. (n=11)	7.8		3.6		9.3		12.8		8.2		1.0	

Table S5. Predicted Odor Intensity of Mixture Sample and Average Grade of Perceived Odor Intensity

sample	compound	$\log C_i^g$	Ψ_i	Ψ_{mix}	panelist					average	standard error
	limonene	3.14	49.8								
	linalyl acetate	1.96	26.9								
(A)	linalool	1.62	46.2	49.8	32.0	42.0	43.0	34.0	35.0	37.2	2.2
	beta-pinene	2.90	35.3								
	citral	0.35	17.0								
	limonene	2.14	36.9								
	linalyl acetate	0.96	3.8								
(A)	linalool	0.62	35.2	36.9	26.0	27.0	36.0	30.0	28.0	29.4	1.8
	beta-pinene	1.90	18.8								
	citral	-0.65	5.3								
	limonene	1.14	12.6								
	linalyl acetate	-0.04	0.2								
(A)	linalool	-0.38	16.8	16.8	10.0	15.0	7.5	8.0	17.0	11.5	1.9
	beta-pinene	0.90	5.4								

	citral	-1.65	1.3								
	limonene	0.14	2.1								
	linalyl acetate	-1.04	0.0								
(A)	linalool	-1.38	4.9	4.9	2.0	3.0	2.0	5.0	2.5	2.9	0.6
	beta-pinene	-0.10	1.1								
	litral	-2.65	0.3								
	aldehyde c-12 mna	-0.64	3.8								
	triplal	0.99	28.4								
(B)	isobornyl acetate	1.84	28.0	28.4	42.0	40.0	40.0	43.0		41.3	0.8
	nerolin yara yara	-0.22	13.9								
	linalyl acetate	1.63	16.8								
	aldehyde c-12 mna	-1.64	0.6								
	triplal	-0.01	12.4								
(B)	isobornyl acetate	0.84	19.5	19.5	20.0	20.0	25.0	35.0		25.0	3.5
	nerolin yara yara	-1.22	0.9								
	linalyl acetate	0.63	1.5								
	aldehyde c-12 mna	-2.64	0.1								
	triplal	-1.01	4.5								
(B)	isobornyl acetate	-0.16	6.2	6.2	5.0	5.0	8.0	13.0		7.8	1.9
	nerolin yara yara	-2.22	0.0								
	linalyl acetate	-0.37	0.1								
	aldehyde c-12 mna	-3.64	0.0								
	triplal	-2.01	1.5								
(B)	isobornyl acetate	-1.16	1.1	1.5	2.0	2.0	2.0	4.0		2.5	0.5
	nerolin yara yara	-3.22	0.0								
	linalyl acetate	-1.37	0.0								
	aldehyde c-111 len	-1.40	5.7								
	methyl benzoate	0.65	4.0								
(C)				18.3	20.0	34.0	30.0	40.0		31.0	4.2
	methyl ionone-gamma	-0.08	16.5								
	coumarin	-0.94	11.2								

	phenyl ethyl alcohol	1.37	18.3							
	aldehyde c-111 len	-2.40	1.6							
	methyl benzoate	-0.35	0.6							
(C)	methyl ionone-gamma	-1.08	4.7	12.8	15.0	14.0	16.0	26.0	17.8	2.8
	coumarin	-1.94	4.4							
	phenyl ethyl alcohol	0.37	12.8							
	aldehyde c-111 len	-3.40	0.4							
	methyl benzoate	-1.35	0.1							
(C)	methyl ionone-gamma	-2.08	1.0	4.7	5.0	5.0	8.0	17.0	8.8	2.8
	coumarin	-2.94	1.4							
	phenyl ethyl alcohol	-0.63	4.7							
	aldehyde c-111 len	-4.40	0.1							
	methyl benzoate	-2.35	0.0							
(C)	methyl ionone-gamma	-3.08	0.2	1.0	2.0	0.0	3.0	3.0	2.0	0.7
	coumarin	-3.94	0.4							
	phenyl ethyl alcohol	-1.63	1.0							
	cis-3-hexenol	2.01	50.3							
	hexyl acetate	2.02	29.6							
(D)	ethyl butyrate	2.28	34.9	50.3	56.0	55.0	45.0		52.0	3.5
	o-t-b.c.h.acetate	1.83	24.8							
	a-damascone	-0.77	5.5							
	cis-3-hexenol	1.01	32.5							
	hexyl acetate	1.02	15.6							
(D)	ethyl butyrate	1.28	20.1	32.5	30.0	27.0	20.0		25.7	3.0
	o-t-b.c.h.acetate	0.83	9.3							
	a-damascone	-1.77	1.0							
	cis-3-hexenol	0.01	11.2							
	hexyl acetate	0.02	6.1							
(D)				11.2	16.0	14.0	12.0		14.0	1.2
	ethyl butyrate	0.28	10.2							
	o-t-b.c.h.acetate	-0.17	1.3							

	a-damascone	-2.77	0.2							
	cis-3-hexenol	-0.99	2.5							
	hexyl acetate	-0.98	2.1							
(D)	ethyl butyrate	-0.72	4.8	4.8	5.0	6.0	3.0		4.7	0.9
	o-t-b.c.h.acetate	-1.17	0.1							
	a-damascone	-3.77	0.0							
	ionone beta	-0.06	27.2							
	gamma-decalactone	-0.49	20.7							
(E)	linalool	1.73	46.9	46.9	42.0	50.0	37.0		43.0	3.8
	cis-3-hexenyl acetate	1.07	30.0							
	lilial	-0.49	23.6							
	ionone beta	-1.06	10.3							
	gamma-decalactone	-1.49	1.6							
(E)	linalool	0.73	37.0	37.0	24.0	34.0	27.0		28.3	3.0
	cis-3-hexenyl acetate	0.07	12.8							
	lilial	-1.49	1.4							
	ionone beta	-2.06	2.7							
	gamma-decalactone	-2.49	0.0							
(E)	linalool	-0.27	18.7	18.7	8.0	7.0	8.0		7.7	0.3
	cis-3-hexenyl acetate	-0.93	4.4							
	lilial	-2.49	0.0							
	ionone beta	-3.06	0.7							
	gamma-decalactone	-3.49	0.0							
(E)	linalool	-1.27	5.7	5.7	0.5	1.5	1.5		1.2	0.3
	cis-3-hexenyl acetate	-1.93	1.4							
	lilial	-3.49	0.0							

Table S6. Five Conditions for Shuffling PRM Components of Mixtures

unshuffled		shuffled				
sample	component	case1	case2	case3	case4	case5

(A)	beta-pinene	phenyl ethyl alcohol	alpha-damascone	linalyl acetate	ethyl butyrate	phenyl ethyl alcohol
(A)	citral	isobornyl acetate	aldehyde c-12 mna	limonene	beta-ionone	linalyl acetate
(A)	limonene	nerolin yara yara	isobornyl acetate	beta-ionone	phenyl ethyl alcohol	nerolin yara yara
(A), (B)	linalyl acetate	o-t-b.c.h.acetate	nerolin yara yara	phenyl ethyl alcohol	gamma-decalactone	coumarin
(A), (E)	linalool	citral	aldehyde c-111 len	cis-3-hexenyl acetate	o-t-b.c.h.acetate	cis-3-hexenol
(B)	aldehyde c-12 mna	gamma-decalactone	*cis*-3-hexenol	coumarin	*cis*-3-hexenol	citral
(B)	isobornyl acetate	beta-ionone	beta-pinene	beta-pinene	alpha-damascone	isobornyl acetate
(B)	nerolin yara yara	beta-pinene	o-t-b.c.h.acetate	gamma-decalactone	beta-pinene	beta-pinene
(B)	triplal	linalyl acetate	ethyl butyrate	nerolin yara yara	isobornyl acetate	alpha-damascone
(C)	aldehyde c-111 len	ethyl butyrate	phenyl ethyl alcohol	ethyl butyrate	nerolin yara yara	ethyl butyrate
(C)	coumarin	aldehyde c-111 len	limonene	triplal	*cis*-3-hexenyl acetate	linalool
(C)	methyl benzoate	methyl benzoate	coumarin	citral	linalool	*cis*-3-hexenyl acetate
(C)	methyl ionone-gamma	coumarin	beta-ionone	alpha-damascone	citral	gamma-decalactone
(C)	phenyl ethyl alcohol	*cis*-3-hexenyl acetate	linalyl acetate	isobornyl acetate	methyl benzoate	aldehyde c-111 len
(D)	alphalpha-damascone	hexyl acetate	triplal	hexyl acetate	aldehyde c-12 mna	triplal
(D)	*cis*-3-hexenol	lilial	lilial	methyl ionone-gamma	methyl ionone-gamma	methyl ionone-gamma
(D)	ethyl butyrate	triplal	hexyl acetate	aldehyde c-12 mna	hexyl acetate	limonene
(D)	hexyl acetate	methyl ionone-gamma	methyl ionone-gamma	lilial	lilial	lilial
(D)	o-t-b.c.h.acetate	limonene	methyl benzoate	linalool	triplal	aldehyde c-12 mna
(E)	beta-ionone	*cis*-3-hexenol	linalool	aldehyde c-111 len	coumarin	o-t-b.c.h.acetate
(E)	*cis*-3-hexenyl acetate	linalool	gamma-decalactone	*cis*-3-hexenol	aldehyde c-111 len	methyl benzoate
(E)	gamma-decalactone	alpha-damascone	*cis*-3-hexenyl acetate	methyl benzoate	linalyl acetate	beta-ionone
(E)	lilial	aldehyde c-12 mna	citral	o-t-b.c.h.acetate	limonene	hexyl acetate

Table S7. RMSE under of both Unshuffled and Shuffled Odor Properties

sample	unshuffled	shuffled				
	case1	case2	case3	case4	case5	
(A)	**7.86**	14.08	13.29	12.24	19.87	14.31
(B)	**7.05**	1.10	4.52	9.28	7.68	2.47
(C)	**7.12**	13.43	11.50	4.82	9.42	7.30
(D)	**3.80**	14.20	4.60	14.51	7.65	15.17
(E)	**7.61**	2.88	11.07	1.91	10.64	10.80
ave.	**6.69**	9.14	9.00	8.55	11.05	10.01