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Comparison of Volatile Compounds between Wild and Cultivated Roses

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Abstract. **Rose (*Rosa* L.) is an economically important ornamental genus that has been cultivated for its scent for the perfume industry since antiquity. However, most modern roses have lost their fragrance during the later stages of the breeding process. Here, 59 species of *Rosa*, including 24 wild *Rosa* species, 20 Chinese old garden roses, and 15 modern roses, were examined by headspace solid-phase microextraction and gas chromatography–mass spectrometry. Fifty-three volatile organic compounds (VOCs), including terpenoids, benzenoids/phenylpropanoids, and fatty acid derivatives, were detected with qualitative and quantitative analyses. Thirteen common components, including geraniol, citronellol, 2-phenylethanol, 3,5-dimethoxytoluene, 1,3,5-trimethoxybenzene, germacrene D, and cis-3-hexenyl acetate, were found. Furthermore, different wild species or cultivars showed different characteristic compounds. 3,5-Dimethoxytoluene and 1,3,5-trimethoxybenzene were the main compounds in *Rosa odorata* and *Rosa chinensis*, which are the original parents of modern roses. 2-Phenylethanol, citronellol, and geraniol were the main aromatic compounds in *Rosa damascene* and *Rosa centifolia*. Methyl salicylate, eugenol, methyl eugenol, and benzyl acetate were lost during domestication and breeding of wild *Rosa* species to Chinese old garden roses and then to modern cultivars. Geranyl acetate, neryl acetate, and dihydro-β-ionol were gained during this time and showed higher amounts across the rose breeding process. Natural and breeding selection may have caused volatile compound gains and losses. These findings provide a platform for mining scent-related genes and for breeding improved ornamental plants with enhanced flower characteristics to develop new essential oil–producing plants.**

Roses are used as ornamental plants in gardens, as cut flowers, and as potted flowers but also have economic value as sources of essential oils for perfumes and cosmetics (Yan et al., 2014; Zhou et al., 2020a). The genus *Rosa* comprises ≈200 species, and just 10–15 species have contributed to the creation of more than 35,000 complex hybrid rose cultivars (Channelière et al., 2002), resulting in a relatively narrow genetic background for these roses (Qiu et al., 2013). Among the original parents of those rose cultivars, 10 species originated from China, including *Rosa chinensis* var. *chinensis*, *Rosa odorata* var. *odorata*, *Rosa rugosa*, *Rosa multiflora* var. *multiflora*, and *Rosa moyesii* (Chen, 2001). Breeding efforts have focused on the development of rose cultivars with cold and disease resistance, certain flower forms, and long vase life. However, scent traits have largely been lost during the later stages of the breeding process (Channelière et al., 2002).

Floral fragrance is an evolutionary adaptation of plants to attract pollinators and resist herbivores; it also enhances the aesthetic value of ornamental plants (Dudareva et al., 2004; Scalliet et al., 2008). At present, more than 1700 floral volatile components have been identified from plants, and these components are mainly classified into three categories: terpenes, phenylpropanes, and fatty acid derivatives (Feng et al., 2021; Piechulla and Pott, 2003). Previous studies on the floral scents of roses have mainly focused on oil-bearing and modern roses. *R. damascena* Mill. was reported to have more than 127 components, mainly including 2-phenylethanol, citronellol, geraniol, and nerol (Kovats, 1987). Recently, the scent compositions and emissions of numerous rose cultivars were reported (Shalit et al., 2004). Aromatic alcohols, monoterpenes, sesquiterpenes, and various esters were found in Fragrant Cloud rose (Guterman et al., 2002). The scented modern rose 'Jinyindao' and its spontaneous nonscented rose offspring were evaluated by solid-phase microextraction followed by gas chromatography–mass spectrometry (GC/MS), and the results showed that the relative contents of 1-ethenyl-4-methoxy-benzene and benzothiazole were significantly different between the two roses (Yan et al., 2011). *R. odorata* and *R. chinensis* germplasms contained benzodiazepines and sesquiterpenoids as their characteristic substances, whereas 1,3,5-trimethoxybenzene was significantly higher in *R. chinensis* than in *R. odorata*, and 3,5-dimethoxytoluene and phenylethanol were not found in *R. chinensis* (Zhou et al., 2020b).

At present, there are few studies on how wild germplasms and Chinese old garden roses have contributed to the floral scent trait of modern varieties. Here, we present a detailed biochemical analysis of the major volatiles produced from 24 *Rosa* germplasm resources, 20 old garden cultivars, and 15 modern roses with strong scents. The results provide a theoretical basis for the further research and development of new aromatic varieties and the discovery of floral genes. Characterization of the marked differences in volatile components among these species allowed us to examine the mechanisms by which the metabolic diversity of rose flavor components may have been gained and lost.

Materials and Methods

Plant materials. Fifty-nine *Rosa* germplasm resources were used in this study, including 24 wild *Rosa* species belonging to 9 sections of the subgroup of *Rosa* (Table 1), 20 Chinese old garden roses, and 15 modern roses with distinct aromatic odors (Supplemental Table 1). The *Rosa* germplasm resources were collected from their original places and grafted onto *R.* 'Natal Briar' during 2005–13 (Table 1). Then, they were cultivated in the rose germplasm garden of the Flower Research Institute, Yunnan Academy of Agricultural Sciences, Kunming, Yunnan, PR China (Table 1).

Sampling and preparation. Petals from different flowers on the middle branches of adult plants at the blooming stage (petals were spread out flat, but anthers had not released pollen) were collected from 10:00 to 11:00 AM from March to August due to the different flowering periods of the resources (Feng et al., 2021). Samples were collected and placed in collection tubes in an ice box and

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Table 1. List of wild *Rosa* species tested.

Code	Latin name	Section	Collection or cultivated location	Altitude (m)
R1	*R. chinensis* Jacq. var. *spontanea*	*Chinensis*	Bazhong, Sichuan	750
R2	*R. odorata* var. *odorata*	*Chinensis*	Lijiang, Yunnan	2100
R3	*R. odorata* var. *gigantea*	*Chinensis*	Kunming, Yunnan	2099
R4	*R. odorata* var. *pseudoindica*	*Chinensis*	Kunming, Yunnan	2311
R5	*R. odorata* var. *erubescens*	*Chinensis*	Kunming, Yunnan	2078
R6	*R. centifolia* L.	*Rosa*	Kunming, Yunnan	2099
R7	*R. damascena*	*Rosa*	Kunming, Yunnan	2099
R8	*R. beggeriana* Schrenk	*Cinnamomeae*	Beijing	0
R9	*R. rugosa* Thunb.	*Cinnamomeae*	Kunming, Yunnan	1905
R10	*R. willmottiae* Hemsl. var. *glandulifera*	*Cinnamomeae*	Weixi, Yunnan	3164
R11	*R. multiflora* Thunb. var. *multiflora*	*Synstylae*	Jinning, Yunnan	1920
R12	*R. multiflora* var. *carnea* Thory	*Synstylae*	Kunming, Yunnan	1918
R13	*R. wichurana* Crep.	*Synstylae*	Benzilan, Yunnan	1951
R14	*R. longicuspis* Bertol.	*Synstylae*	Mile, C Yunnan	1965
R15	*R. soulieana* Crép. var. *soulieana*	*Synstylae*	Diqing, NW Yunnan	1951
R16	*R. roxburghii* Tratt.	*Microphyllae*	Wenshan, SE Yunnan	1377
R17	*R. praelucens* Byhouwer	*Microphyllae*	Zhongdian, Yunnan	3508
R18	*R. xanthina* Lindl.	*Pimpinellifoliae*	Beijing	0
R19	*R. sericea* Lindl.	*Pimpinellifoliae*	Lijiang, NW Yunnan	3150
R20	*R. banksiae* Ait. *banksiae*	*Banksianae*	Weixi, NW Yunnan	1987
R21	*R. banksiae* f. *lutea*	*Banksianae*	Lijiang, NW Yunnan	2501
R22	*R. cymosa* Tratt. var. *cymosa*	*Banksianae*	Wenshan, SE Yunnan	1428
R23	*R. Bracteata* Wendl.	*Bracteatae*	Longchuan, W Yunnan	926
R24	*R. laevigata* Mickx.	*Laevigatae*	Funing, SE Yunnan	1000

brought to the laboratory for volatile analysis, with three replicates for each variety.

Measurement of petal volatile compounds. The contents of petal volatile compounds were assayed quantitatively using headspace solid-phase microextraction (HS-SPME) and GC/MS (Yan et al., 2018). One gram of petals was placed into a glass vial for volatile extraction with 10 μl internal standard, and a mixture of 2 μL ethyl caprate (CAS Number 110-38-3, 0.865 $\mu g \cdot \mu L^{-1}$) was dissolved in 1998 μL n-hexane AR (CAS Number 110-54-3). The extraction process lasted for 35 min at 35 °C with a 50-μm divinylbenzene/carboxen/polydimethylsiloxane solid-phase microextraction (SPME) fiber (Supelco, Bellefonte, PA), and the product was detected for 30 min in a 7890B GC system with an 5977A MSD (Agilent Technologies, Santa Clara, CA). The NIST2014 library and Kovats' retention indices were used to identify the volatiles. The following formula was used: the emission rate of the volatile compound ($\mu g \cdot g^{-1}$) = (the area of the component/the area of the internal standard) × the concentration of the internal standard ($\mu g \cdot \mu L^{-1}$) × the volume of the internal standard (μL)/sample weight (g).

Results

Identification of volatiles from wild Rosa *species.* According to the total VOC emission analysis of different stages of rose development using qualitative and quantitative analyses, the results showed a higher emission rate at the blooming stage in section (sect.) *Chinensis*, sect. *Cinnamomeae*, sect. *Rosa*, and sect. *Pimpinellifoliae*. Lower amounts of VOCs were found for sect. *Synstylae*, sect. *Banksianae*, sect. *Microphyllae*, sect. *Laevigatae*, and sect. *Bracteatae* (Fig. 1A). A total of 47 floral volatile compounds were detected by HS-SPME–GC/MS, including 27 terpenoids, 15 aromatic hydrocarbons, and five fatty acid derivatives, which accounted for more than 95% of the total compounds detected (Fig. 2A, Table 1). Thirty-five major components were screened from the 47 volatiles and compared with the standard; these components had a content that exceeded 3 $\mu g \cdot g^{-1}$ in more than 3 of the 24 wild species (Fig. 3A).

Each section of the wild species showed obviously different volatiles (Fig. 3A, Supplemental Table 2). For sect. *Chinensis*, including the *R. odorata* and *R. chinensis* complexes, the results showed that the main aromatic components of *R. odorata* var. *odorata* were alcohols, and the content of phenylethanol was the highest (Fig. 3A). The main volatile component of *R. odorata* var. *gigatea* was aromatic hydrocarbons, and the emission rate of 3,5-dimethoxytoluene was the highest in this species (4274 $\mu g \cdot g^{-1}$) (Table 2). The main volatile components of *R. odorata* var. *pseudoindica* were aromatic hydrocarbons and terpenes, and the content of 1,3,5-trimethoxybenzene was the highest in this species. For the *R. chinensis* complex, flowers mainly produced aromatic hydrocarbons, terpenoids, and fatty acid derivatives, of which 1,3,5-trimethoxybenzene was the characteristic aromatic component. There were some common volatile compounds between *R. odorata* and *R. chinensis*, such as linalool, methyl eugenol, and ylangene. Furthermore,

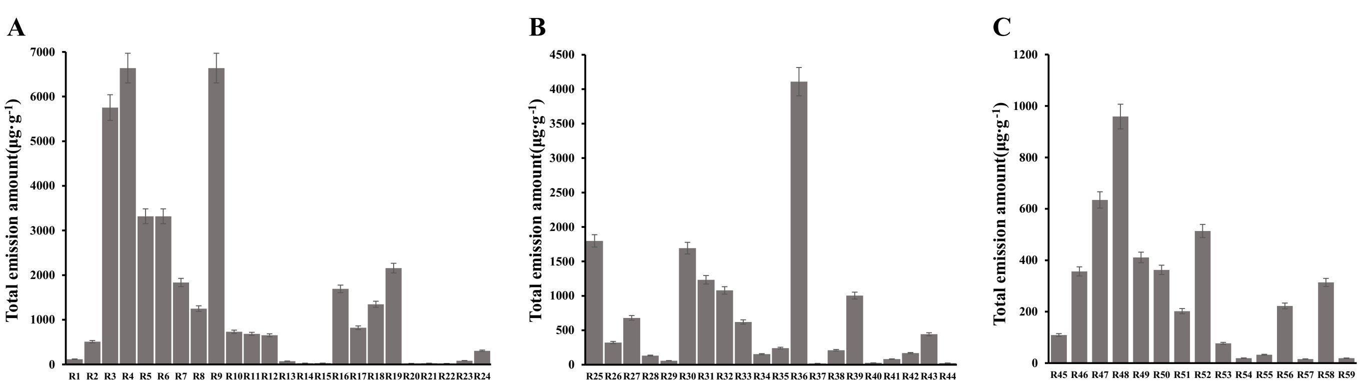

Fig. 1. Quantitative analysis of the total main volatile organic compounds in tested species/cultivars by the internal standard method. (**A**) Wild *Rosa* species. (**B**) Chinese old garden roses. (**C**) Modern roses.

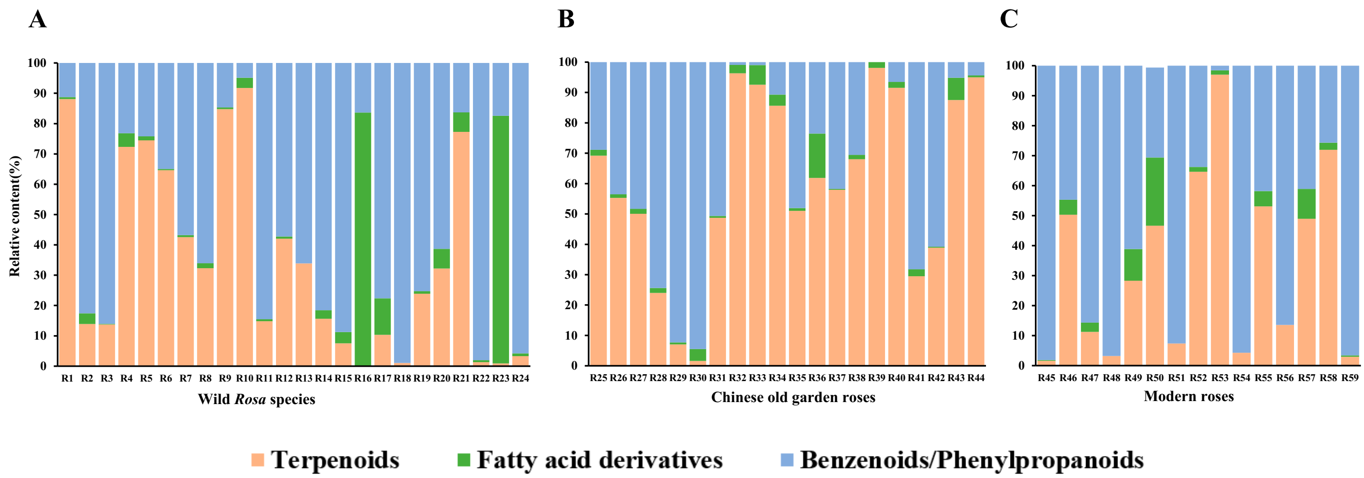

Fig. 2. The relative contents of the three groups of volatile compounds in the tested *Rosa* species/cultivars. (**A**) Wild *Rosa* species. (**B**) Chinese old garden roses. (**C**) Modern roses.

the main characteristic components were strikingly different among these groups. *R. odorata* exhibited the unique compounds 3,5-dimethoxytoluene at 4273 $\mu g \cdot g^{-1}$ and dihydro-β-ionone at 247 $\mu g \cdot g^{-1}$ (Fig. 3A). The emission rates of 1,3,5-trimethoxybenzene and germacrene D were 331 and 1015 $\mu g \cdot g^{-1}$ in *R. chinensis* Jacq. var. *spontanea*, respectively (Table 2).

R. damascene and *R. centifolia* play important roles in sect. *Rosa*. In this study, the results showed that 2-phenylethanol, β-citronellol, and geraniol were the main aromatic components in *R. damascene* and *R. centifolia* (Fig. 3A). However, 2-phenylethanol accounted for 49.95% and 27.44% of the total volatiles in the two species, respectively. In addition, the emission rate was nearly 906 $\mu g \cdot g^{-1}$ in *R. damascene* and 899 $\mu g \cdot g^{-1}$ in *R. centifolia*. However, the rate of β-citronellol emission was strikingly different in *R. damascene* and *R. centifolia*, at 909 and 421 $\mu g \cdot g^{-1}$, respectively (Table 2). Regarding sect. *Cinnamomeae*, three wild species—*R. rugosa*, *R. beggeriana*, and *R. willmottiae* Hemsl var. *glandulifera* Yü et Ku.—were examined by SPME-GC/MS analysis. Twenty-five floral components were identified in these species, including 24 major compounds with greater than 3 μg per gram of petals (Fig. 3A). The main compounds were lower alcohols and terpenes in *R. beggeriana* and *R. willmottiae* Hemsl var. *glandulifera* Yü et Ku., whereas *R. rugosa* showed higher terpenoids, including β-citronellol, geraniol, and 2-phenylethanol, at 4154, 671, and 482 $\mu g \cdot g^{-1}$, respectively (Fig. 3A).

Qualitative and quantitative analyses of volatile components of Chinese old garden roses. Chinese old garden roses have been cultivated by humans since as early as 5000 years ago in China (Wang, 2007) and are used as important rose germplasm resources for breeding cultivars. Old garden roses existed before 1867, the year of the creation of the first modern rose 'La France' (Liorzou et al., 2016). In this study, 20 varieties of Chinese old garden roses were examined for their volatile compound profiles by SPME-GC/MS. A total of 46 VOCs were detected, among which 21 were major compounds, including 14 terpenoids, 4 phenylpropanoids, and 3 fatty acid derivatives (Table 3, Fig. 3B). Terpenoids and benzenoids/phenylpropanoids accounted for more than 90% of the total VOCs, and terpenoids were more abundant than benzenoids/phenylpropanoids, showing different compositions from those of wild *Rosa* species (Fig. 2B). The main floral components identified were geraniol, β-citronellol, germacrene D, dihydro-β-ionol, 3,5-dimethoxytoluene (DMT), 1,3,5-trimethoxybenzene (TMB), phenylethanol, phenethyl acetate, and transrose oxide (Fig. 4B).

'Zixiangrong', 'Huzhongyue', 'Mudanyueji', 'Yipinzhuyi', and 'Huzhongyue' contained high amounts of geraniol at 392 $\mu g \cdot g^{-1}$, DMT at 76 $\mu g \cdot g^{-1}$, citronellol at 63 $\mu g \cdot g^{-1}$, 2-phenylethanol at 76 $\mu g \cdot g^{-1}$, and germacrene D at 173 $\mu g \cdot g^{-1}$ (Supplemental Table 3). The release of total VOCs was in the following order: 'Zixiangrong' > 'Huzhongyue > 'Mudanyueji' > 'Ruanhongxiang' > 'Jinfenlian' > 'Yushizhuang' > 'Old Blush' (Fig. 1B). Furthermore, the results showed that 85% of the Chinese old garden roses examined were strikingly fragrant, suggesting that Chinese old garden roses are a significant germplasm resource for scent breeding of rose.

Qualitative and quantitative analyses of volatile components in modern roses. Modern roses are used as cut flowers, potted plants, and garden plants, at an annual value of more than $10 billion, and high economic value also lies in the use of their petals as a source of natural fragrances and flavorings. However, most modern cut-flower varieties of rose lack distinct fragrances (Yan et al., 2018), and less than 10% of the 35,000 modern rose cultivars are scented (Yan et al., 2021). In this study, 15 cultivars with strong scents were chosen for evaluation by GC/MS.

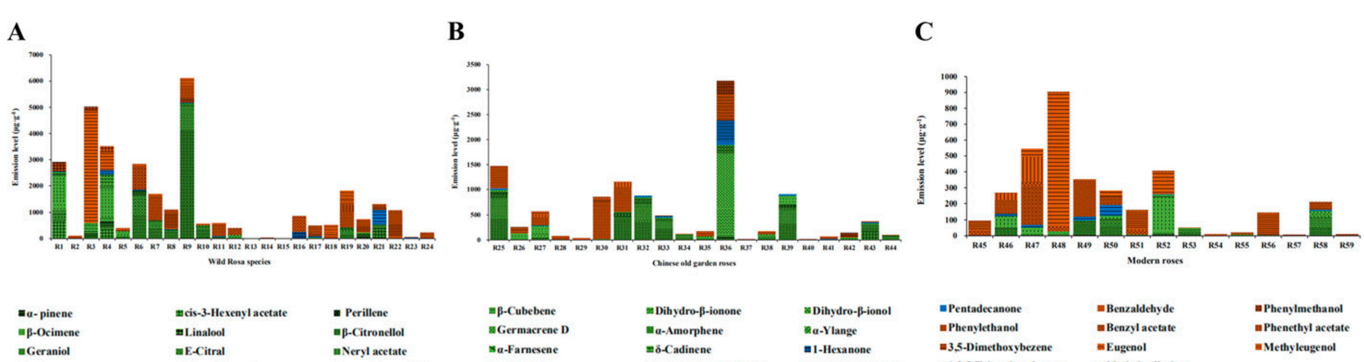

Fig. 3. Diagram showing the emission rates of the main volatile compounds from the tested *Rosa* species/cultivars. (**A**) Wild *Rosa* species. (**B**) Chinese old garden roses. (**C**) Modern roses.

Table 2. Emission rates of the volatile compounds of wild *Rosa* species by quantitative analyses.

	Emission rate (μg·g^{-1})																							
	Chinenses					*Rosa*		*Cinnamomeae*			*Synstylae*					*Microphyllae*		*Pimpinellifoliae*		*Banksianae*		*Laevigatae*		*Bracteatae*
Volatile compounds	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	R20	R21	R22	R23	R24
Terpenoids																								
α-Pinene	-	-	-	-	-	-	5.04	-	-	4.53	-	14.4	-	1.26	0.3	-	-	-	-	-	-	-	-	-
β-Ocimene	-	-	-	-	-	-	-	-		-	3.26	-	-	-	-	-	-	15.1	-	10.	23	-	-	-
Linalool	-	-	-	-	10.4	-	-	-		-	-	-	-	-	-	-	-	-	-	8.72	6.35	4.78	-	-
Perillene	-	-	-	-	-	5.94	3.96	-	14.5	1.90	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Citronellal	-	-	-	-	-		2.52	-	-	2.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-
β-Citronellol	34.9	7.6	-	-	-	909	422	303	4154	365	-	-	-	-	-	-	-	-	184	-	-	-	-	-
Geraniol	233	-	-	33.4	-	668	159	7.92	672	38.3	-	-	-	-	0.6	-	-	-	88	-	-	-	-	-
E-Citral	-	-	-	-	-	31	85.9	15	226	18	25.2	-	-	-	-	-	-	-	-	-	-	-	-	-
Neryl acetate	-	-	-	-	-	25.4	2.34	-	13.9	-	-	-	-	-	-	-	-	-	71.8	-	-	-	-	-
α-Copaene	70.4	-	-	-	7.45	-	-	-	4.6	14.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Geranyl acetate	37.8	-	-	-	-	172	34.9	25.8	44.9	-	55.4	-	-	-	-	-	3.2	-	87.1	8.1	-	-	-	-
Elemene	12.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
trans-Caryophylle-ne	10.3	3.4	301	231	40	14.9	-	-	-	28.8	-	-	3.1	0.8		-	47.7	-	-	138	49.7	-	-	-
β-Cubebene	43.8	-	-	158.8	7.3	-	-	-	-	10.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-
α-Ionone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	19	1.8	-	-	-
Dihydro-β-ionone	23.9	2.1	247	-	8.9	-	-	-	-	-	1.1	70.7	-	0.4	-	-	-	-	-	34.9	1.5	5.4	0.5	-
Dihydro-β-ionol	208	0.5	50.5	-	23.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	19.2	-	4.2	-	-
Germacrene D	1014	-	-	1088	125	-	-	-	42.2	-	-	70.3	-	-	-	-	-	-	-	-	-	-	-	-
α-Amorphene	36.2	-	-	110	8.3	-	-	-	-	-	1.6	-	-	-	-	-	-	-	-	-	-	-	-	-
α-Ylange	-	-	9.3	59.8	5.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
α-Farnesene	-	-	-	-	-	-	-	-	83.2	9.3	-	-	0.3	0.1	-	-	-	-	-	-	3.3	-	-	1.6
δ-Cadinene	143	-	-	365	31.8	-	-	-	-	3	-	16.51	-	-	-	-	-	-	-	-	-	-	-	-
Fatty acid derivatives																								
1-Hexanone	11.6	0.2	-	17.3	-	-	-		5.9	9.9	-	-	-	-	0.12	250	45.5	-	7.8	-	23.5	-		1.10
1-Hexanol	-	0.2	-	41.4	-	-	5.2	7.8	21.8	9.5	0.5	3.1	-	0.1	-	10.5	13.7	-	7.3	10.7	40.7	-	0.1	0.9
cis-3-Hexenyl acetate	675	-	-	397	23	9.6	-	-	-	-	-	-	-	-	-	-	-	-	-	27.9	447	-	-	2.20
Acetic acid, hexyl ester	-	-	-	112.8	5.5	4.95	-	9.9	5.3	-	-	-	-	-	-	-	-	-	-	-	502	-	-	3.52
Pentadecanone	-	-	-	-	-	6.60	5.76	-	-	-	2.45	-	-	0.37	0.39	-	-	-	-	-	-	-	40.07	-
Benzenoids/phenylpropanoids																								
Benzaldehyde	-	-	-	-	-	-	-	40.6	-	-	-	-	-	-	-	-	-	-	-	20.9	9.9	81.3	-	-
Phenylmethanol	-	-	-	-	-	27.1	19.6	555	194	2.6	3.4	-	-	0.2	-	-	96	-	-	200	117	476	8.8	16.6
Methyl benzoate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	9.35	-	-
2-Phenylethanol	7.3	77.2	-	-	-	906	899.1	67.1	482	7.3	391	195	-	12.3	2.23	-	-	79.8	574.8	10	-	101	-	-
4-Methoxystyrene	7.8	-	8.6	-	-	-	-	-	-	-	-	-	-	-	-	603	-	-	-	-	-	-	-	-
Benzyl acetate	-	-	-	-	-	3.9	-	40.6	-	-	-	-	-	-	-	-	281.3	-	-	184	-	292	-	196.3
Methyl salicylate	-	3.12	-	-	-	-	-	-	-	-	0.75	-	-	0.05	-	-	-	-	-	33.57	15.42	3.74	-	-
Benzenepropanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.00	-	-	2.4	-	9.4	-	-
Phenethyl acetate	-	1.2	-	-	-	-	-	10.1	-	-	15.3	38.8	-	0.1	0.3	-	-	-	275	-	58.4	29.7	-	-
3,5-Dimethoxytoluene	-	2.5	4273	688	94.3	44.2	-	-	-	9.4	-	-	-	-	0.5	-	-	118	-	-	-	-	-	-
Eugenol	-	-	-	-	-	-	25.9	2.8	6.6	6.4	81.9	-	-	0.3	8.8	-	-	297	199.7	57.1	14.4	69.4	-	-
Methyl eugenol	-	0.12	11.3	12.7	-	4.6	13.7	1.7	228	2.1	-	-	-	0.4	0.1	-	-	-	307.2	8.1	-	-	-	-
1,3,5-Trimethoxybenzene	331	-	119	185	4.3	6.6	-	1.3	-	-	-	-	-	0.1	0.2	-	-	-	-	-	-	3.3	-	-
trans-Isoeugenol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	24	18		-	-

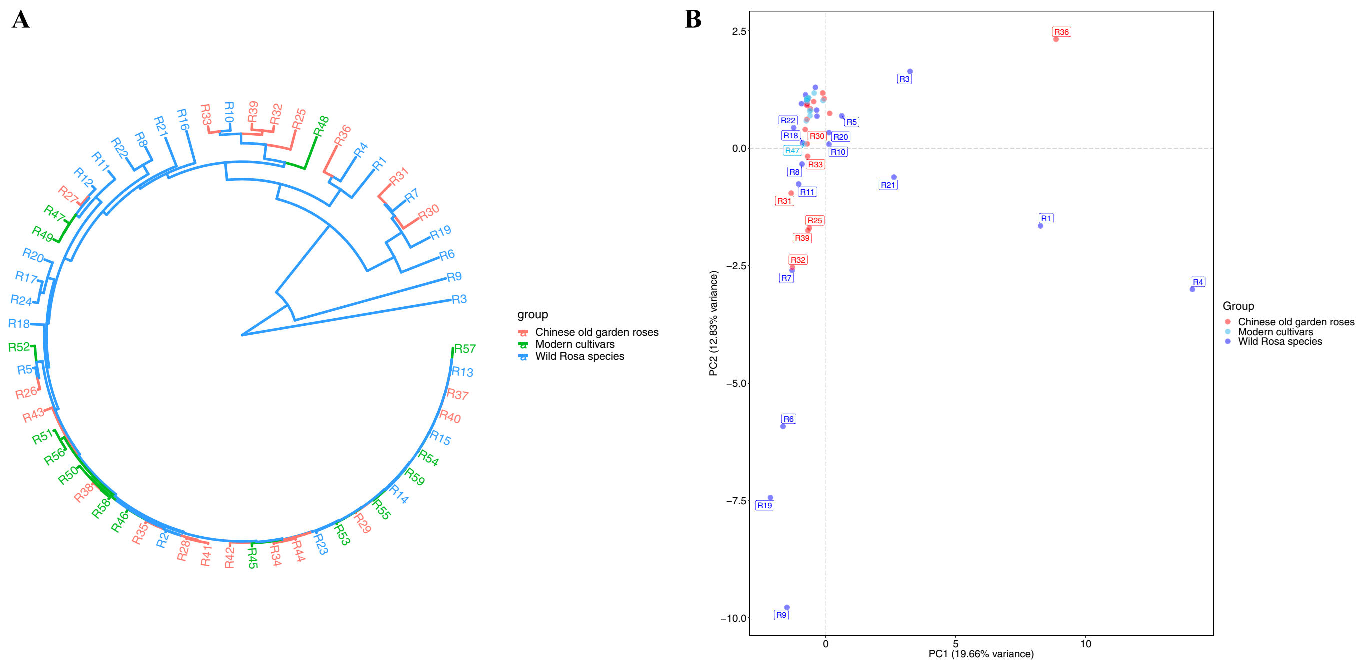

Fig. 4. Dendrogram resulting from hierarchical cluster analysis and principal component analysis (PCA) of wild *Rosa* species, Chinese old garden roses, and modern roses. (**A**) Hierarchical clustering of 59 samples. (**B**) Two-dimensional score plots of the PCA results.

Benzenoids/phenylpropanoids, terpenoids, and fatty acid derivatives were identified in these roses (Supplemental Table 4). Alcohols represented 52.67% of the total volatiles in 'Yunxiang', which contained higher amounts of 2-phenylethanol at 190 $\mu g \cdot g^{-1}$ and β-citronellol at 78 $\mu g \cdot g^{-1}$ (Fig. 1C). A higher release of phenethyl acetate was detected in 'Yunshi No. 1' and 'Yunxiang', at 43 and 30 $\mu g \cdot g^{-1}$, respectively. Terpenes were the main components in 'Hongshuangxi', including citronellol at 54 $\mu g \cdot g^{-1}$, geraniol at 43 $\mu g \cdot g^{-1}$, and germacrene D at 22 $\mu g \cdot g^{-1}$ (Fig. 3C). The three dominant volatile compounds were 3,5-dimethoxybenzene, phenethyl alcohol, and 1,3,5-trimethoxybenzene in 'Jinyindao' and 'Mitang' (Fig. 2C). 3,5-Dimethoxybezene accounted for 87.29% of the total volatiles in 'Mitang', which contained high amounts of this substance at 837 $\mu g \cdot g^{-1}$ (Supplemental Table 5).

Hierarchical cluster analysis and principal component analysis. Hierarchical cluster analysis (HCA) and principal component analysis (PCA) were performed to analyze the correlation between 51 volatile compounds of wild *Rosa* species, Chinese old garden roses, and modern roses. HCA, using the Pearson correlation as the measurement standard, was used to cluster samples into groups by applying the intergroup connection. The Z score method was used to standardize the related variables to obtain the clustering diagram. The results of HCA are shown in Fig. 4A. HCA clustering showed that there were significant differences among wild *Rosa* species in VOC composition and quantity. R3 and R9, two wild *Rosa* species of *R. odorata* var. gigantea and *R. rugosa* Thumb., grouped differently based on their remarkably different VOCs. The modern rose R48, 'Mitang', was separated into another cluster alone because its VOCs may have been inherited from other wild species or old garden roses. The modern roses R47 and R49, wild *Rosa* species R11 and R12, and Chinese old garden rose R27 were grouped together. The modern rose R52, wild rose R5, and Chinese old garden rose R26 were grouped together. The modern roses R46, R50, R51, R56, and R58; wild rose R2; and Chinese old garden roses R28, R35, R38, and R41 were grouped together. The modern roses R45, R53, R54, R55, R57, and R59; wild roses R13, R14, R15, and R23; and Chinese old garden roses R29, R34, R37, R40, and R44 were grouped together. The cultivars that clustered into the same group had the same VOCs both in composition and quantity.

In the PCA, two principal components were constructed and explained 19.66% and 13% of the variability; the cumulative contribution was 32.66%. The wild *Rosa* species were widely dispersed, whereas the Chinese old garden roses and modern roses were relatively concentrated, which was consistent with the HCA results (Fig. 4B).

Comparison of the volatile compositions of wild Rosa *species, Chinese old garden roses, and modern roses.* In the present study, the volatile compounds produced by wild *Rosa* species, Chinese old garden roses, and modern roses were compared by GC/MS. Thirteen common compounds were detected, including geraniol, β-citronellol, 2-phenylethanol, δ-cadinene, 3,5-dimethoxytoluene, 1,3,5-trimethoxybenzene, phenethyl acetate, and germacrene D. However, some common components were present in much lower amounts in modern roses than in wild *Rosa* species and Chinese old garden roses (Table 2), such as 3,5-dimethoxytoluene at 4273 and 688 $\mu g \cdot g^{-1}$ in *R. odorata* var. *gigantea* and *pseudoindica*, respectively. However, the compound 3,5-dimethoxytoluene is quite low in modern roses at 33.5–139.8 $\mu g \cdot g^{-1}$. In addition, phenylpropanoid-related compounds such as 2-phenylethanol contributed greatly to the typical rose scent and were significantly different among the tested roses. These compounds were found at levels above 500 $\mu g \cdot g^{-1}$ in *R. damascene*, *R. centifolia*, and *R. rugosa* Thunb. and at only 7.9–245 $\mu g \cdot g^{-1}$ in most modern roses.

Wild *Rosa* species exhibited 17 main unique compounds, including methyl salicylate, eugenol, methyleugenol, and benzyl acetate, but these compounds were lost in modern roses. On the other hand, geranyl acetate, neryl acetate, and dihydro-β-ionol showed higher levels in old garden roses and modern roses than in wild species, suggesting that they were gained in the process of rose cultivar breeding (Fig. 5).

Discussion

The genus *Rosa* contains ≈200 species, and 95 species of wild *Rosa* are widely distributed in China (Ku and Robertson, 2003; Wissemann and Ritz, 2005). Yunnan is rich in biodiversity and is known for its plants (Jian et al., 2013). Fifty-eight species/varieties of *Rosa* occur in Yunnan (Brichet, 2003; Ku and Robertson, 2003). Wild *Rosa* species from Yunnan played very important roles in the creation of modern roses by providing useful traits, especially tea scents (Scalliet et al., 2008). In the present study, the VOC compositions and quantities of wild *Rosa* species were first detected. Compared with the scent composition of Chinese old garden roses and modern cultivars, the results showed that sect. *Chinensis*, sect. *Rosa*, and sect. *Cinnamomeae* contain higher amounts of fragrant compounds, including DMT, germacrene D, TMB, and phenylethanol,

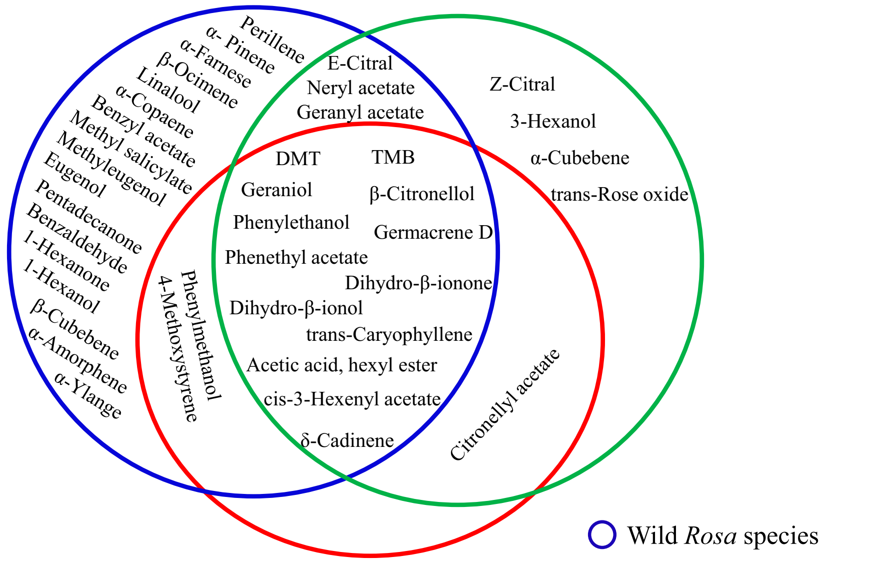

Fig. 5. Comparison of the main components of wild *Rosa* species, Chinese old garden roses, and modern roses.

suggesting that these three sections contributed scent traits to old garden and modern cultivars. Furthermore, the VOC results are in agreement with the genetic relationships found in a previous study (Ku and Robertson, 2003; Qiu et al., 2013).

3,5-Dimethoxytoluene and 1,3,5-trimethoxybenzene are the major scent compounds of *R. odorata* var. *gigantea* and *R. chinensis* Jacq. var. *spontanea*. The two compounds contribute to the characteristic "tea scent." DMT can represent up to 90% of the total flower volatiles in *R. gigantea*, and TMB represents up to 56% of the volatiles in *R. chinensis* Jacq. var. *spontanea*; these roses have fragrances with earthy and spicy notes reminiscent of black tea (Scalliet et al., 2008; Zhou et al., 2020a). The study consistently confirmed that Sect. *Chinensis* played important roles in the history of modern rose breeding, especially regarding fragrance traits (Zhou et al., 2020b). In sect. *Rosa*, *R. damascene*, the damask rose, is the most important species used to produce rose water, essence of rose, and essential oils in the perfume industry (Knudsen et al., 2006). In this study, the content of 2-phenylethanol was the highest in *R. damascena* and represents up to more than half of the total volatiles, suggesting that *R. damascena* contributed the typical scent characteristic to modern rose. In addition, *R. rugosa* has been shown to have much higher amounts of 2-phenylethanol, geraniol, nerol, citronellol, and their derivatives. *R. rugosa* has a long history of cultivation for perfume production since at least the early 1800s in China (Feng et al., 2010). In the breeding process, *R. rugosa* contributed to the typical fragrance of roses due to its unique characteristic terpenoids citronellol and geraniol.

For flowers, scent volatiles attract pollinators and are used as defense compounds against animals and microorganisms (Atkinson, 2018; Prasad et al., 2004). In this study, we compared the volatile compositions among wild *Rosa* species, Chinese old garden roses, and modern cultivars and found strikingly different compounds. Many researchers have reported the large diversity of secondary metabolites that are emitted by plants and their differences between wild species and cultivars (Hanson et al., 1996; Hartmann, 1996; Schwab, 2003). Aharoni et al. (2004) identified markedly different volatile terpenoid flavor components between wild and cultivated strawberry species. Tadmor et al. (2002) found that different volatile compounds negatively affect tomato fruit aroma and that these compounds were selected against during wild species domestication. Hartmann (1996) holds the view that secondary metabolites evolved under the selection pressure of a competitive environment. In this study, the loss of methyl salicylate, eugenol, and methyl eugenol in modern roses might be related to a shift from wild environments and suggested that wild species released specific compounds to survive in adverse environments, to aid in plant reproduction, and to prevent attacks from pests and diseases. Sensitivities to diseases and insects, as well as a lack of fragrance, are some typical shortcomings of modern rose cultivars (Tang et al., 2008, Zhang et al., 2009). The results indicated that the shortcomings of modern cultivars might be due to the loss of these secondary metabolites. Furthermore, the pleasant fragrances geranyl acetate, neryl acetate, and dihydro-β-ionol showed higher levels in these cultivars. The main reason for this result might be that one of the cultivars selected by breeders had VOCs with mild and pleasant aromas that were beneficial to humans. Taken together, our data, along with those in the literature, suggest that the gain and loss of volatile compounds of secondary metabolites are the result of both natural and breeding selection.

Conclusion

In this study, the volatile compounds produced by wild *Rosa* species, Chinese old garden roses, and modern roses were analyzed by GC/MS. The results showed that different wild species/cultivars exhibited characteristic compounds. Methyl salicylate, eugenol, methyl eugenol, and benzyl acetate were lost during domestication and breeding from wild *Rosa* species to Chinese old garden roses and modern cultivars. Geranyl acetate, neryl acetate, citronellyl acetate, and dihydro-β-ionol were gained and produced higher amounts during the rose breeding process. We suggest that natural and breeding selection may have caused volatile compound gains and losses.

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Supplemental Table 1. Chinese old garden roses and modern roses.

Serial code	Latin name	Cultivar	Collection location
R25	Mudan Yueji	Ancient rose	Kunming, Yunnan
R26	Jinou Fanlü	Ancient rose	Kunming, Yunnan
R27	Sichun	Ancient rose	Kunming, Yunnan
R28	Qinglian Xueshi	Ancient rose	Kunming, Yunnan
R29	Yunzhen Xiawei	Ancient rose	Kunming, Yunnan
R30	Jinfenlian	Ancient rose	Kunming, Yunnan
R31	Yipin Zhuyi	Ancient rose	Kunming, Yunnan
R32	Zixiangrong	Ancient rose	Kunming, Yunnan
R33	Zihongxiang	Ancient rose	Kunming, Yunnan
R34	Yingri Hehua	Ancient rose	Kunming, Yunnan
R35	Chunshui Lübo	Ancient rose	Kunming, Yunnan
R36	Huzhongyue	Ancient rose	Kunming, Yunnan
R37	*Rosa chinensis* ‘Slater's crimson China’	Ancient rose	Kunming, Yunnan
R38	Yulinglong	Ancient rose	Kunming, Yunnan
R39	Yushizhuang	Ancient rose	Kunming, Yunnan
R40	*R. chinensis* ‘Old Blush’	Ancient rose	Kunming, Yunnan
R41	Simianjing	Ancient rose	Kunming, Yunnan
R42	Pufuhong	Ancient rose	Kunming, Yunnan
R43	Dafugui	Ancient rose	Kunming, Yunnan
R44	Junang	Ancient rose	Kunming, Yunnan
R45	Jinyindao	Modern roses	Kunming, Yunnan
R46	Yunshi No.1	Modern roses	Kunming, Yunnan
R47	Shuncong	Modern roses	Kunming, Yunnan
R48	Mitang	Modern roses	Kunming, Yunnan
R49	Xiangyun	Modern roses	Kunming, Yunnan
R50	Hongshuangxi	Modern roses	Kunming, Yunnan
R51	Yunxiang	Modern roses	Kunming, Yunnan
R52	Yunfen	Modern roses	Kunming, Yunnan
R53	Fendai	Modern roses	Kunming, Yunnan
R54	Fenzhuangge	Modern roses	Kunming, Yunnan
R55	Yanzhi	Modern roses	Kunming, Yunnan
R56	Fangxiang Furen	Modern roses	Kunming, Yunnan
R57	Xila Zhixiang	Modern roses	Kunming, Yunnan
R58	*R. chinensis* Jacq ‘Grimson Glory’ H .T	Modern roses	Kunming, Yunnan
R59	*R. chinensis* Jacq ‘Jinbian’	Modern roses	Kunming, Yunnan

Supplemental Table 2. Relative content of volatile compounds in wild *Rosa* species.

Retention time	Volatiles	Relative content (%)																							
		Section *Chinensis*					Section *Rosa*		Section *Cinnamomeae*			Section *Synstylae*					Section *Microphyllae*		Section *Pimpinellifoliae*		Section *Banksianae*			Section *Laevigatae*	Section *Bracteatae*
		R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	R20	R21	R22	R23	R24
Terpenoids																									
8.98	α-Pinene	-	-	-	-	-	-	0.28	-	-	0.62	-	2.22	-	4.86	1.12	-	-	-	-	-	-	-	-	-
14.04	β-Ocimene	-	-	-	-	-	-	-	-	-	-	0.48	-	-	-	-	-	-	0.42	-	0.46	0.92	-	-	-
15.98	Linalool	-	-	-	-	2.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.4	0.25	0.23	-	-
16.22	Perillene	-	-	-	-	-	0.18	0.22	-	0.22	0.26	-	-	-	-	-	-	-	-	-	-	-	-	-	-
18.18	Citronellal	-	-	-	-	-	-	0.14	-	-	0.33	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20.71	β-Citronellol	1.05	6.44	-	-	-	27.56	23.44	25.27	62.94	50.03	-	-	-	-	-	-	-	-	8.51	-	-	-	-	-
21.53	Geraniol	7.03	-	-	0.58	-	20.23	8.85	0.66	10.18	5.24	-	-	-	-	2.32	-	-	-	4.08	-	-	-	-	-
22.11	E-Citral	-	-	-	-	-	0.94	4.77	1.25	3.42	2.46	3.7	-	-	-	-	-	-	-	-	-	-	-	-	-
24.49	Megastigma-4,6(E),8(E)-triene	-	0.1	1.46	-	0.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
24.74	Neryl acetate						0.77	0.13	-	0.21	-	-	-	-	-	-	-	-	-	3.33	-	-	-	-	-
24.91	α-Copaene	2.12	-	-	-	1.46	-	-	-	0.07	1.99	-	-	-	-	-	-	-			-	-	-	-	-
25.26	Geranyl acetate	1.14	-	-	-	-	5.2	1.94	2.15	0.68	-	8.15	-	-	-	-	-	0.39	-	4.04	0.37	-	-	-	-
25.51	Elemene	0.38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
26.11	*trans*-Caryophyllene	0.31	2.92	4.54	4.02	7.83	0.45	-	-	-	3.95	-	-	4.28	3.15	0.35	-	5.82	-	-	6.35	1.96	-	-	-
26.25	Bilene	0.94	-	-	0.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
26.35	β-Cubebene	1.32	-	-	2.76	1.42	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
26.43	α-Ionone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.87	0.07	-	-	-
26.57	Dihydro-β-ionone	0.72	1.74	3.72	-	1.75	-	-	-	-	-	0.14	10.87	-	1.56	-	-	-	-	-	1.6	0.06	0.26	0.54	-
26.78	Dihydro-β-ionol	6.27	0.42	0.76	-	4.61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.88	-	0.2	-	-
27.17	α-Humlene	-	-	-	0.32	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
27.25	Bicyclosesquiphellandrene	-	-	-	0.26	0.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
27.76	Germacrene D	30.57	-	-	18.92	24.52	-	-	-	0.64	-	-	10.82	-	-	-	-	-	-	-	-	-	-	-	-
27.61	α-Amorphene	1.09	-	-	1.92	1.62	-	-	-	-	-	0.23	-	-	-	-	-	-	-	-	-	-	-	-	-
28.17	α-Ylange	-	-	0.14	1.04	1.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
28.5	α-Farnesene	-	-	-	-	-	-	-	-	1.26	1.28	-	-	0.36	0.24	-	-	-	-	-	-	0.12	-	-	0.52
28.75	δ-Cadinene	4.29	-	-	6.34	6.22	-	-	-	-	4.23	-	2.54	-	-	-	-	-	-	-	-	-	-	-	-
Fatty acid derivatives																									
4.23	1-Hexanone	0.35	0.1	-	0.3	-	-	-	-	0.09	1.35	-	-	-	-	0.44	14.82	5.55	-	0.36	-	0.93	-	-	0.36
4.46	1-Hexanol	-	0.19	-	0.72	-	-	0.28	0.65	0.33	1.3	0.07	0.47	-	0.1	-	0.62	1.67	-	0.34	0.49	1.61	-	0.13	0.3
11.96	*cis*-3-Hexenyl acetate	20.33	-	-	6.9	4.49	0.29	-	-	-	-	-	-	-	-	-	-	-	-	-	1.28	17.62	-	-	0.72
12.26	Acetic acid, hexyl acetate	-	-	-	1.96	1.07	0.15	-	0.83	0.08	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
17.24	*trans*-Rose oxide	-	-	-	-	-	-	0.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
19.55	Methyl salicylate	-	2.66	-	-	-	-	-	-	-	-	0.11	-	-	0.21	-	-	-	-	-	1.54	0.61	0.18	-	-
32.79	Pentadecanone	-	-	-	-	-	0.2	0.32	-	-	-	0.36	-	-	1.44	1.43	-	-	-	-	-	-	-	48.28	-
Benzenoids/phenylpropanoids																									
10.08	Benzaldehyde	-	-	-	-	-	-	-	3.38	-	-	-	-	-	-	-	-	-	-	-	0.96	0.39	3.91	-	-
13.35	Phenylmethanol	-	-	-	-	-	0.82	1.09	46.27	2.93	0.35	0.5	-	-	0.62	-	-	11.71	-	-	9.16	4.64	22.92	10.58	5.43
15.08	Methyl benzoate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.45	-	-
16.63	Phenylethanol	0.22	65.72	-	-	-	27.44	49.95	5.59	7.3	1	57.57	30.05	-	47.3	8.25	-	-	2.22	26.65	0.46	-	4.86	-	-
18.1	4-Methoxystyrene	0.24	-	0.13	-	-	-	-	-	-	-	-	-	-	-	-	35.69	-	-	-	-	-	-	-	-
18.57	Benzyl acetate	-	-	-	-	-	0.12	-	3.38	-	-	-	-	-	-	-	-	34.31	-	-	8.45	-	14.06	-	64.15
20.37	4-Methylbenzaldehyde	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	10.01	-	-	-	-	-	-	-	-
20.74	Benzenepropanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.61	-	-	0.11	-	0.45	-	-
21.58	Phenethyl acetate	-	1.03	-	-	-			0.84	-	-	2.25	5.97	-	0.39	1.02	-	-	-	12.76	-	2.31	1.43	-	-
21.76	3,5-Dimethoxybenzene	-	2.14	64.38	11.96	18.47	1.34	-	-	-	1.29	-	-	-	-	1.86	-	-	3.29	-	-	-	-	-	-
24.55	Eugenol						-	1.44	0.23	0.1	0.88	12.05	-	-	1.21	32.74	-	-	8.25	9.26	2.62	0.57	3.34	-	-

(Continued on next page)

Supplemental Table 2. (*Continued*)

		Relative content (%)																							
		Section *Chinensis*					Section *Rosa*		Section *Cinnamomeae*			Section *Synstylae*					Section *Microphyllae*		Section *Pimpinellifoliae*		Section *Banksianae*			Section *Laevigatae*	Section *Bracteatae*
Retention time	Volatiles	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	R20	R21	R22	R23	R24
25.83	Methyleugenol	-	0.1	0.17	0.22	-	0.14	0.76	0.14	3.46	0.29	-	-	-	1.56	0.44	-	-	24.95	14.24	0.37	-	-	-	-
25.85	1,3,5-Trimethoxybenzene	9.98	-	1.8	3.22	0.84	0.2	-	0.11	-	-	-	-	-	0.12	0.3	-	-	-	-	-	-	0.16	-	-
25.98	*trans*-Isoeugenol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.1	0.71	-	-	-

Supplemental Table 3. Emission rate of volatile compounds in Chinese old garden roses.

		Emission rate (μg·g^{-1})																			
Retention time	Volatiles	R25	R26	R27	R28	R29	R30	R31	R32	R33	R34	R35	R36	R37	R38	R39	R40	R41	R42	R43	R44
Terpenoids																					
10.108	β-Myrcene	2.52	-	-	-	-	-	-	-	-	0.48	-	-	-	-	3.01	0.70	-	-	-	10.79
11.821	D-Limonene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.17	-	-	-	1.77
14.04	β-Ocimene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.24	-	-	-	5.57
15.98	Linalool	15.28	-	-	-	-	-	-	-	-	1.73	2.15	-	-	-	7.93	0.10	0.20	-	0.93	0.76
20.71	β-Citronellol	412.98	-	-	-	-	2.71	412.27	372.06	219.10	28.66	-	-	-	26.67	300.44	0.23	3.43	-	86.52	7.11
20.86	iso-Geraniol	11.69	-	-	-	-	-	-	-	13.10	-	-	-	-	-	-	-	-	-	-	-
21.11	Z-Citral	12.23	-	-	-	-	-	3.21	28.80	9.75	0.60	-	-	-	1.03	13.85	-	-	-	4.65	0.97
21.53	Geraniol	387.63	-	-	-	-	-	10.60	272.60	138.27	46.12	-	-	-	28.71	265.12	1.77	-	-	14.34	42.23
22.11	E-Citral	23.91	-	-	-	-	-	4.07	46.82	18.56	3.22	-	-	-	2.48	16.26	-	0.20	-	5.84	11.92
23.57	Methyl geranate	8.63	-	-	0.10	-	-	1.48	-	-	0.34	-	-	-	2.29	11.24	-	0.21	-	1.33	1.56
24.32	α-Cubebene	-	7.18	6.39	-	-	-	-	-	-	-	-	32.47	0.07	0.93	-	0.27	-	2.18	-	-
24.39	Citronellyl acetate	27.51	-	-	-	-	-	104.79	30.96	8.57	4.95	-	-	-	-	18.06	-	1.87	-	13.72	1.54
24.74	Neryl acetate	7.73	-	-	-	-	-	2.22	24.60	4.59	1.49	-	-	-	-	19.47	-	0.33	-	12.44	-
24.91	α-Copaene	-	-	-	-	0.07	-	-	-	-	-	-	70.68	0.17	1.52	9.83	0.31	0.27	-	1.46	-
25.26	Geranyl acetate	31.10	-	-	-	-	-	2.10	46.17	9.69	12.85	-	-	-	0.42	45.46	0.56	0.37	-	3.76	29.00
25.51	Elemene	-	-	-	-	-	-	-	-	-	-	-	39.45	-	-	-	-	-	0.29	-	-
25.99	α-Gurjunene	-	0.71	-	-	-	-	-	-	-	-	-	-	-	0.59	1.40	-	-	-	-	-
26.35	β-Cubebene	-	-	2.31	-	-	-	-	-	-	-	0.44	-	-	-	-	-	0.19	-	-	-
26.26	*trans*-Caryophyllene	59.15	12.62	6.05	8.81	-	-	-	11.65	25.70	0.77	25.62	-	-	3.43	9.83	-	-	1.71	1.28	-
26.136	β-Ylangene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.38	-	-	-	-
26.35	β-Cubebene	-	-	-	-	-	-	-	-	-	-	0.85	32.88	-	-	-	-	-	0.98	-	-
26.57	Dihydro-β-ionone	-	4.48	28.47	0.16	1.39	-	1.11	1.08	-	2.24	12.09	54.66	0.07	1.20	-	0.27	-	0.44	-	0.16
26.78	Dihydro-β-ionol	2.52	10.56	83.99	0.82	0.79	-	5.18	7.87	1.30	7.07	10.81	519.85	0.55	10.33	3.81	1.90	0.10	1.51	-	0.46
27.17	α-Humlene	2.88	-	-	-	-	-	-	-	-	-	2.90	20.55	0.05	-	3.51	-	-	-	-	-
27.61	α-Amorphene	-	4.86	-	-	-	-	-	2.27	-	0.55	2.39	-	0.13	1.94	6.22	-	0.51	-	-	-
27.76	Germacrene D	25.17	90.87	107.71	0.31	0.38	12.86	2.10	8.31	10.31	-	21.97	1075.05	2.77	34.25	149.62	0.40	7.68	23.44	20.45	-
28.1	β-Ionone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	8.10
28.26	Biocyclogermacrene	-	2.51	-	-	-	-	-	-	-	-	-	-	-	4.36	15.86	-	0.46	-	-	-
28.5	α-Farnesene	-	-	-	-	-	-	-	-	-	-	12.14	-	-	-	3.91	-	0.43	-	-	-
28.75	δ-Cadinene	3.78	12.72	18.55	-	0.11	2.88	-	1.73	1.99	0.32	3.67	182.46	0.38	5.60	18.97	-	1.54	3.11	2.92	-
Fatty acid derivatives																					
4.23	3-Hexanone	-	-	-	-	0.08	5.25	-	-	-	-	-	-	0.02	-	-	-	-	-	-	-
4.29	2-Hexanone	-	-	-	-	0.12	5.41	-	-	-	-	-	-	-	-	-	-	-	-	-	-
4.46	3-Hexanol	2.52	-	-	0.14	0.06	6.60	-	-	1.92	-	1.69	67.40	-	-	-	0.28	0.12	-	9.69	-
6.54	1-Hexanol	-	3.12	1.36	0.20	-	27.07	-	-	-	-	-	-	-	2.36	-	-	0.43	-	-	-
11.96	*cis*-3-hexenyl acetate	6.83	-	34.52	0.73	-	-	18.99	-	0.99	6.99	-	33.70	0.63	-	21.47	6.27	2.23	21.59	168.97	5.48
12.41	Acetic acid, hexyl ester	21.22	-	8.15	1.11	-	-	1.48	20.17	25.58	5.04	-	419.58	-	-	18.26	-	1.02	0.37	18.63	0.83
16.57	*trans*-Rose oxide	5.21	-	-	-	-	-	-	3.13	3.66	-	-	-	-	0.34	-	-	-	-	-	-
17.19	*cis*-Rose oxide	-	-	-	-	-	-	5.79	1.19	1.18	-	-	-	-	-	-	-	-	-	-	-
Benzenoids/phenylpropanoids																					
13.35	Phenylmethanol	-	-	-	2.95	-	-	1.36	6.36	-	0.55	-	-	-	-	-	-	0.14	-	13.37	1.43
16.63	Phenylethanol	-	-	166.62	36.38	4.53	738.46	481.68	-	-	-	45.91	-	-	55.63	-	-	30.33	-	1.77	-
18.1	4-Methoxystyrene	-	-	-	-	2.15	251.62	-	1.73	2.11	-	-	-	-	-	-	-	-	-	-	3.31
18.57	Benzyl acetate	-	-	-	0.58	-	-	-	-	-	0.25	-	-	-	-	-	-	-	-	2.43	0.32
21.58	Phenethyl acetate	-	-	67.07	14.54	-	-	104.30	-	-	-	-	-	-	-	-	-	15.65	-	-	-
21.76	3,5-Dimethoxybezene	434.38	115.35	41.59	10.65	29.06	67.52	3.08	-	-	-	41.94	518.21	-	0.84	-	-	0.24	-	-	-
24.55	Eugenol	-	-	-	-	-	-	-	-	-	3.28	-	-	-	-	-	-	-	-	-	-
25.83	Methyleugenol	-	-	-	-	-	-	-	-	-	10.19	-	-	-	-	-	-	-	-	-	-
25.85	1,3,5-Trimethoxybezene	-	-	2.72	0.21	0.27	21.32	-	-	2.73	0.51	1.60	266.71	3.46	-	-	0.97	-	86.28	0.80	0.81

Supplemental Table 4. Relative amount of volatile compounds in modern roses.

Retention time	Volatiles	Relative content (%)														
		R45	R46	R47	R48	R49	R50	R51	R52	R53	R54	R55	R56	R57	R58	R59
Terpenoids																
10.108	β-Myrcene	-	0.12	-	-	-	0.23	-	-	-	-	-	-	-	-	-
14.04	β-Ocimene	-	-	-	-	-	-	1.22	-	-	-	-	-	-	-	-
15.98	Linalool	-	-	-	-	0.78	-	-	-	0.33	-	-	-	-	-	-
16.22	Perillene	-	-	-	-	-	-	-	-	-	-	0.3	-	0.22	-	-
20.71	β-citronellol	-	8.55	-	-	16.39	14.94	-	-	29.57	0.82	10.39	-	4.87	17.157	-
20.857	iso-Geraniol	-	-	-	-	-	-	-	-	1.03	-	-	-	-	0.368	-
21.11	Z-Citral	-	1.7	-	-	0.19	-	-	-	2.2	-	-	-	-	2.583	-
21.53	Geraniol	-	-	-	-	0.98	11.77	-	-	22.62	0.25	0.42	-	6.03	19.099	-
22.11	E-Citral	-	-	-	-	-	-	-	-	3.74	-	-	-	0.81	-	-
23.56	Methyl geranate	-	1.47	-	-	1.44	-	-	-	0.57	0.33	2.27	-	0.67	-	-
24.32	α-Cubebene	-	0.46	0.12	-	-	0.29	-	0.74	-	-	0.57	-	-	0.846	-
24.39	Citronellyl acetate	-	2.16	-	-	1.29	1.28	-	-	2.22	-	0.56	-	0.43	0.826	-
24.74	Neryl acetate	-	0.31	-	-	0.22	0.5	-	-	1.08	-		-	1.39	-	-
24.91	α-Copaene	-	1.12	0.19	-	-	0.58	-	2.05	-	-	1.14	-	-	-	-
25.26	Geranyl acetate	-	0.41	-	-	-	0.74	-	-	4.43	-	0.21	-	1.95	0.518	-
25.51	Elemene	-	-	-	-	-	-	-	-	-	-	0.2	-	-	-	-
26.35	β-Cubebene	-	-	-	-	-	-	-	-	-	-	0.25	-	-	-	-
26.11	*trans*-Caryophyllene	1.02	0.94	0.35	0.1	0.4	-	4.25	-	-	-	1.32	0.52	2.04	1.783	0.95
26.43	α-Ionone	-	-	-	-	-	-		-	-	0.33	-	2.19	-	-	-
26.57	Dihydro-β-ionone	-	-	0.36	1.45	-	-	-	1.6	1.15	-	-	0.52	0.37	-	0.11
26.78	Dihydro-β-ionol	-	-	0.83	1.32	-	-	-	2.08	8.12	0.23	-	1.72	0.2	-	0.11
27.76	Germacrene D	0.12	17.13	4.21	0.13	0.22	5.98	0.12	38.1	0.2	-	11.89	-	1.5	10.266	-
27.61	α-Amorphene	-	0.75	0.29	-	-	-	-	1.26	-	-	1.82	-	-	-	0.25
27.96	β-Ionone	-	-	-	-	-	-	-	-	-	-	-	4.76	-	-	-
28.17	α-Ylange	-	-	-	-	-	-	-	-	-	-	-	-	-	0.745	-
28.5	α-Farnesene	-	1.14	0.84	-	0.28	0.36	-	-	-	-	0.48	-	-	0.311	-
28.75	δ-Cadinene	-	2.24	0.54	-	-	-	-	4.8	-	-	2.7	-	-	1.664	-
Fatty acid derivatives																
4.23	3-Hexanone	-	-	0.27	-	-	-	0.45	-	-	-	-	-	-	-	0.3
4.46	2-Hexanol	0.12	0.27	0.31	-	0.35	-	-	-	-	-	0.31	-	-	0.838	0.25
6.17	3-Hexen-1-ol	-	-	-	-	0.57	-	-	-	-	-	0.34	-	-	-	-
6.6	1-Hexanol	-	-	-	-	3.03	1.14	-	-	-	-	2	-	-	-	-
11.96	*cis*-3-Hexenyl acetate	0.23	3.97	2.07	-	4.11	1.46	0.24	3.31	-	0.22	0.76	0.36	-	0.176	-
12.41	Acetic acid, hexyl ester	0.21	4.08	2.72	-	5.77	17.44	-	1.02	1.16	-	1.05	-	4.15	1.847	0.21
16.57	*trans*-Rose oxide	-	-	-	-	0.42	-	-	-	-	-	-	-	-	-	-
17.19	*cis*-Rose oxide	-	0.15	-	-	-	-	-	-	-	-	-	-	-	-	-
Benzenoids/phenylpropanoids																
11.26	Benzyl methyl ether	-	1.28	-	-	0.48	-	-	-	0.17	-	0.21	0.26	0.37	-	-
13.35	Phenylmethanol	-	2	-	-	1.02	-	-	-	0.33		1.05	0.55	0.38	2.565	0.11
16.63	Phenylethanol	1.82	21.63	38.61	-	47.05	15.79	-	-	-	-	24.76	-	9.86	8.362	41.79
18.1	4-Methoxystyrene	29.24	-	3.42	3.47	-	-	17.07	-	-	-	-	-	-	1.637	-
18.57	Benzyl acetate	-	0.51	-	-	-	-	-	-	-	-	-	-	0.14	-	-
21.58	Phenethyl acetate	2.27	11.94	25.38	-	7.16	-	-	-	-	-	1.77	-	5.79	-	4.23
21.76	3,5-Dimethoxybezene	50.25	0.26	7.29	87.29	0.87	9.26	57.54	27.21	0.32	47.47	-	60.36	-	0.605	-
24.55	Eugenol	-	-	-	-	-	-	-	-	-	-	-	0.73	-	4.373	-
25.83	Methyleugenol	0.25	-	-	-	-	-	-	-	0.24	-	-	1.54	-	1.371	-
25.85	1,3,5-Trimethoxybezene	-	0.13	-	0.44	0.23	-	1.07	0.95	0.17	1.02	-	0.81	0.65	1.208	0.3

Supplemental Table 5. Emission amount of volatile compounds in modern roses.

		Emission amount (μg·g^{-1})														
Retention time	Volatiles	R45	R46	R47	R48	R49	R50	R51	R52	R53	R54	R55	R56	R57	R58	R59
Terpenoids																
10.108	β-Myrcene	-	0.4	-	-	-	0.8	-	-	-	-	-	-	-	-	-
14.04	β-Ocimene	-	-	-	-	-	-	2.5	-	-	-	-	-	-	-	-
15.98	Linalool	-	-	-	-	3.2	-	-	-	0.3	-	-	-	-	-	-
16.22	Perillene	-	-	-	-	-	-	-	-	-	-	0.1	-	-	-	-
18.18	Citronellal	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20.71	β-Citronellol	-	30.5	-	-	67.4	54.0	-	-	22.7	0.2	3.4	-	0.8	53.8	-
20.857	iso-Geraniol	-	-	-	-	-	-	-	-	0.8	-	-	-	-	1.2	-
21.11	Z-Citral	-	6.1	-	-	0.8	-	-	-	1.7	-	-	-	-	8.1	-
21.53	Geraniol	-	-	-	-	4.0	42.5	-	-	17.4	-	0.1	-	1.0	59.9	-
22.11	E-Citral	-	-	-	-	-	-	-	-	2.9	-	-	-	0.1	-	-
23.56	Methyl geranate	-	5.2	-	-	5.9	-	-	-	0.4	0.1	0.7	-	0.1	-	-
24.32	α-Cubebene	-	1.6	0.8	-	-	1.0	-	3.8	-	-	0.2	-	-	2.7	-
24.39	Citronellyl acetate	-	7.7	-	-	5.3	4.6	-	-	1.7	-	0.2	-	0.1	2.6	-
24.74	Neryl acetate	-	1.1	-	-	0.9	1.8	-	-	0.8	-	-	-	0.2	-	-
24.91	α-Copaene	-	4.0	1.2	-	-	2.1	-	10.5	-	-	0.4	-	-	-	-
25.26	Geranyl acetate	-	1.5	-	-	-	2.7	-	-	3.4	-	0.1	-	0.3	1.6	-
25.51	Elemene	-	-	-	-	-	-	-	-	-	-	0.1	-	-	-	-
26.35	β-Cubebene	-	-	-	-	-	-	-	-	-	-	0.1	-	-	-	-
26.26	*trans*-Caryophyllene	1.1	3.4	2.2	1.0	1.6	-	8.6	-	-	-	0.4	1.2	0.3	5.6	0.2
26.43	α-Ionone	-	-	-	-	-	-	-	-	-	0.1	-	4.9	-	-	-
26.57	Dihydro-β-ionone	-	-	2.3	13.9	-	-	-	8.2	0.9	-	-	1.2	0.1	-	-
26.78	Dihydro-β-ionol	-	-	5.3	12.7	-	-	-	10.7	6.2	-	-	3.8	-	-	-
27.17	α-Humlene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
27.76	Germacrene D	0.1	61.1	26.7	1.2	0.9	21.6	0.2	195.7	0.2	-	3.9	-	0.2	32.2	-
27.61	α-Amorphene	-	2.7	1.8	-	-	-	-	6.5	-	-	0.6	-	-	-	-
27.96	β-Ionone	-	-	-	-	-	-	-	-	-	-	-	10.6	-	-	-
28.17	α-Ylange	-	-	-	-	-	-	-	-	-	-	-	-	-	2.3	-
28.5	α-Farnesene	-	4.1	5.3	-	1.2	1.3	-	-	-	-	0.2	-	-	1.0	-
28.75	δ-Cadinene	-	8.0	3.4	-	-	-	-	24.7	-	-	0.9	-	-	5.2	-
Fatty acid derivatives																
4.23	3-Hexanone	-	-	1.7	-	-	-	0.9	-	-	-	-	-	-	-	0.1
4.46	2-Hexanol	0.1	1.0	2.0	-	1.4	-	-	-	-	-	0.1	-	-	2.6	-
6.17	3-Hexen-1-ol	-	-	-	-	2.3	-	-	-	-	-	0.1	-	-	-	-
6.6	1-Hexanol	-	-	-	-	12.5	4.1	-	-	-	-	0.7	-	-	-	-
11.96	*cis*-3-Hexenyl acetate	0.3	14.2	13.1	-	16.9	5.3	0.5	17.0	-	-	0.2	0.8	-	0.6	-
12.41	Acetic acid, hexyl ester	0.2	14.5	17.3	-	23.7	63.0	-	5.2	0.9	-	0.3	-	0.7	5.8	-
16.57	*trans*-Rose oxide	-	-	-	-	1.7	-	-	-	-	-	-	-	-	-	-
17.19	*cis*-Rose oxide	-	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-
Benzenoids/phenylpropanoids																
11.26	Benzyl methyl ether	-	4.6	-	-	2.0	-	-	-	0.1	-	0.1	0.6	0.1	-	-
13.35	Phenylmethanol	-	7.1	-	-	4.2	-	-	-	0.3	-	0.3	1.2	0.1	8.0	-
16.63	Phenylethanol	2.0	77.1	245.0	-	193.4	57.1	-	-	-	-	8.1	-	1.6	26.2	7.9
18.1	4-Methoxystyrene	31.9	-	21.7	33.3	-	-	34.5	-	-	-	-	-	-	5.1	-
18.57	Benzyl acetate	-	1.8	-	-	-	-	-	-	-	-	-	-	-	-	-
21.58	Benzenepropanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
21.76	phenethyl acetate	2.5	42.6	161.1	-	29.4	-	-	-	-	-	0.6	-	0.9	-	0.8
21.76	3,5-Dimethoxybezene	54.9	0.9	46.3	837.0	3.6	33.5	116.3	139.8	0.2	9.2	-	134.3	-	1.9	
24.55	Eugenol	-	-	-	-	-	-	-	-	-	-	-	1.6	-	13.7	-
25.83	Methyleugenol	0.3	-	-	-	-	-	-	-	0.2	-	-	3.4	-	4.3	-
25.85	1,3,5-Trimethoxybezene	-	0.5	-	4.2	0.9	-	2.2	4.9	0.1	0.2	-	1.8	0.1	3.8	0.10