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A high-resolution Orbitrap Mass spectral library for trace volatile compounds in fruit wines

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The overall aroma is an important factor of the sensory quality of fruit wines, which attributed to hundreds of volatile compounds. However, the qualitative determination of trace volatile compounds is considered to be very challenging work. GC-Orbitrap-MS with high resolution and high sensitivity provided more possibilities for the determination of volatile compounds, but without the high-resolution mass spectral library. For accuracy of qualitative determination in fruit wines by GC-Orbitrap-MS, a high-resolution mass spectral library, including 76 volatile compounds, was developed in this study. Not only the HRMS spectrum but also the exact ion fragment, relative abundance, retention indices (RI), CAS number, chemical structure diagram, aroma description and aroma threshold (ortho-nasally) were provided and were shown in a database website (Food Flavor Laboratory, http://foodflavorlab.cn/). HRMS library was used to successfully identify the volatile compounds mentioned above in 16 fruit wines (5 blueberry wines, 6 goji berry wines and 5 hawthorn wines). The library was developed as an important basis for further understanding of trace volatile compounds in fruit wines.

Background & Summary

Among the hundreds of volatile compounds detected in fruit wines, only a small percentage of them could play key roles in the contribution of characteristic aroma[1]. Currently, the gas chromatograph-mass spectrometer has been widely used for the identification and quantification of aroma compounds. The quadrupole mass spectrometer (qMS) could be the most common mass spectrometer for analysis[2–6]. However, some trace analytes were difficult to be detected using qMS due to their low resolution and sensitivity[4,7–12]. These trace compounds needed to be identified by other detectors. The aldehydes and ketones could be detected in Syrah wines[13] and model wine solution by flame ionization detector (FID)[14,15]. The flame photometry (FPD) was used to identify sulfur compounds in Cabernet Sauvignon wines[16,17]. Besides, sulphur chemiluminescence (SCD)[13,18,19] and pulsed flame photometry (PFPD)[20,21] also could be used for the analysis of sulfur compounds in grape wines. The pyrazines could be identified in wines[22] and oak woods[23] by nitrogen-phosphorous detection (NPD). The triple-quadrupole mass spectrometer (QqQ-MS) in selected-reaction-monitoring (SRM) could identify lactones[24], terpenes[25] and sulfur compounds[26] in wines. Thus, multiple methods had to be used for the detection of various aroma compounds[14,16]. Meanwhile, the use of multiple instruments is time-consuming and costly. And it is also difficult to have so many instruments in a same laboratory. And it is an urgent challenge to identify trace aroma volatile compounds mentioned above simply and effectively in fruit wines.

In recent years, high-resolution mass spectrometry, such as quadrupole-time-of-flight-MS (Q-TOF), could improve the accuracy of identification[22,23,27]. Since Orbitrap-MS technology invented by Alexander Makarov was first commercially available in 2005, this new technique of high resolution and high sensitivity mass spectrometry has been shown great advantages for qualitative and quantitative analysis of compounds[28–30], and therefore many studies have been focused on metabolomics using liquid chromatography coupling[31–34]. After GC was coupled with Orbitrap-MS in 2015, its resolution could reach 60,000 (219 m/z, FWHM), mass accuracy could reach 1 ppm, and sensitivity could reach femtogram level, which provided more possibilities to advance the

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Compounds	CAS No.	Purity	Manufacturer	Formula	RI	Content[h]/μg.L^{-1}
Ester						
Ethyl butanoate	105-54-4	≥99.5%	Aladdin[b]	$C_6H_{12}O_2$	1065	10020
Ethyl 2-methylbutanoate	7452-79-1	>98.0%	Aladdin	$C_7H_{14}O_2$	1077	5030
Ethyl isovalerate	108-64-5	>99.0%	Adamas[c]	$C_7H_{14}O_2$	1093	11050
Isoamyl acetate	123-92-2	≥99.5%	Macklin	$C_7H_{14}O_2$	1139	11390
Methyl caproate	106-70-7	>99.0%	Macklin	$C_7H_{14}O_2$	1200	5120
Ethyl hexanoate	123-66-0	>99.0%	Aladdin	$C_8H_{16}O_2$	1243	30300
Ethyl heptanoate	106-30-9	≥99.5%	Macklin	$C_9H_{18}O_2$	1340	5050
Ethyl lactate	97-64-3	≥99.0%	Macklin	$C_5H_{10}O_3$	1350	50810
Heptyl acetate	112-06-1	≥98.0%	TCI	$C_9H_{18}O_2$	1380	3280
Methyl octanoate	111-11-5	≥99.0%	Adamas	$C_9H_{18}O_2$	1394	2000
Ethyl caprylate	106-32-1	>99.0%	Aladdin	$C_{10}H_{20}O_2$	1439	29670
Ethyl 3-hydroxybutyrate	5405-41-4	>99.0%	Macklin	$C_6H_{12}O_3$	1511	15170
Ethyl nonanoate	123-29-5	≥95.0%	Macklin	$C_{11}H_{22}O_2$	1521	7250
Ethyl 2-hydroxy-4-methylpentanoate	10348-47-7	≥98.0%	Aladdin	$C_8H_{16}O_3$	1525	10180
Ethyl caprate	110-38-3	>99.0%	Macklin	$C_{12}H_{24}O_2$	1572	20980
Ethyl succinate	123-25-1	≥99.5%	Macklin	$C_8H_{14}O_4$	1592	50360
Methyl salicylate	119-36-8	≥99.5%	Macklin	$C_8H_8O_3$	1675	4760
Ethyl benzeneacetate	101-97-3	≥99.5%	Aladdin	$C_{10}H_{12}O_2$	1689	1940
Ethyl salicylate	118-61-6	>99.0%	Aladdin	$C_9H_{10}O_3$	1710	5480
Ethyl hydrocinnamate	2021-28-5	>98.0%	TCI[d]	$C_{11}H_{14}O_2$	1785	12040
Ethyl cinnamate	103-36-6	>98.0%	Adamas	$C_{11}H_{12}O_2$	2031	5040
Monoethyl succinate	1070-34-4	>95.0%	Aladdin	$C_6H_{10}O_4$	2308	11020
Carbonyl compounds						
(*E*)-2-Hexenal	6728-26-3	>98.0%	Aladdin	$C_6H_{10}O$	1329	7120
(*E*)-2-Heptenal	18829-55-5	>95.0%	Aladdin	$C_7H_{12}O$	1362	6530
(*E*)-2-Octenal	2548-87-0	>95.0%	Macklin	$C_8H_{14}O$	1432	1900
(*E*,*E*)-2,4-Heptadienal	4313-03-5	>90.0%	Macklin	$C_7H_{10}O$	1498	10220
(*E*,*Z*)-2,6-Nonadienal	557-48-2	≥95.0%	Aladdin	$C_9H_{14}O$	1545	4160
Benzeneacetaldehyde	122-78-1	>95.0%	Macklin	C_8H_8O	1574	5720
High alcohols						
Isobutanol	78-83-1	≥99.5%	Aladdin	$C_4H_{10}O$	1112	20620
Isoamylol	123-51-3	≥99.5%	Aladdin	$C_5H_{12}O$	1217	78820
1-Pentanol	71-41-0	≥99.5%	Macklin	$C_5H_{12}O$	1259	6340
2-Heptanol	543-49-7	>98.0%	Aladdin	$C_7H_{16}O$	1327	8700
3-Octenol	3391-86-4	>98.0%	Aladdin	$C_8H_{16}O$	1456	3220
1-Heptanol	111-70-6	>95.0%	Macklin	$C_7H_{16}O$	1460	5490
2-Nonanol	628-99-9	≥98.0%	Aladdin	$C_9H_{20}O$	1511	3240
1-Octanol	111-87-5	≥99.5%	Macklin	$C_8H_{18}O$	1532	9060
2-Phenylethanol	60-12-8	≥99.5%	Aladdin	$C_8H_{10}O$	1817	50690
2-Phenoxyethanol	122-99-6	≥99.5%	Macklin	$C_8H_{10}O_2$	2043	9900
Lactone						
γ-Octalactone	104-50-7	>98.0%	Sigma-Aldrich	$C_{11}H_{20}O_2$	1814	4140
δ-Octalactone	698-76-0	>98.0%	Sigma-Aldrich	$C_8H_{14}O_2$	1862	3480
γ-Nonalactone	104-61-0	>98.0%	Sigma-Aldrich	$C_8H_{14}O_2$	1925	3260
Pantolactone	599-04-2	>99.0%	Sigma-Aldrich	$C_6H_{10}O_3$	1935	19860
γ-Decalactone	706-14-9	>98.0%	Sigma-Aldrich	$C_{10}H_{18}O_2$	2041	3700
Sotolon	28664-35-9	>97.0%	Sigma-Aldrich	$C_6H_8O_3$	2108	4980
γ-Undecalactone	104-67-6	>98.0%	Sigma-Aldrich	$C_{11}H_{20}O_2$	2161	3520
Acid						
Butanoic acid	107-92-6	≥99.5%	Sigma-Aldrich	$C_4H_8O_2$	1574	30960
Hexanoic acid	142-62-1	≥99.5%	Macklin	$C_6H_{12}O_2$	1762	25780
Ethylhexanoic acid	149-57-5	≥99.9%	Aladdin	$C_8H_{16}O_2$	1860	10090
Octanoic acid	124-07-2	≥99.5%	Aladdin	$C_8H_{16}O_2$	1973	56880
Decanoic acid	334-48-5	>99.0%	Aladdin	$C_{10}H_{20}O_2$	2190	20170
Benzoic acid	65-85-0	≥99.9%	Aladdin	$C_7H_6O_2$	2378	11630

Continued

Compounds	CAS No.	Purity	Manufacturer	Formula	RI	Content[h]/μg.L^{-1}
Pyrazine						
3-Isopropyl-2-methoxypyrazine	25773-40-4	>97.0%	Sigma-Aldrich	$C_8H_{12}ON_2$	1435	1280
2-sec-Butyl-3-Methoxypyrazine	24168-70-5	>99.0%	Sigma-Aldrich	$C_9H_{14}ON_2$	1453	980
5-Ethyl-2,3-dimethylpyrazine	15707-34-3	>98.0%	Sigma-Aldrich	$C_8H_{12}N_2$	1459	2230
2-Isobutyl-3-methoxypyrazine	24683-00-9	>99.0%	Sigma-Aldrich	$C_9H_{14}ON_2$	1513	1490
Acetylpyrazine	22047-25-2	>97.0%	Sigma-Aldrich	$C_6H_6N_2O$	1565	2010
Furan						
Furfural	98-01-1	>99.0%	Sigma-Aldrich	$C_5H_4O_2$	1472	5250
Acetylfuran	1192-62-7	>99.0%	Sigma-Aldrich	$C_6H_6O_2$	1505	9840
5-Methylfurfural	620-02-0	>99.0%	Sigma-Aldrich	$C_6H_6O_2$	1540	1740
Ethyl 2-furoate	614-99-3	>99.0%	Sigma-Aldrich	$C_7H_8O_3$	1565	4250
Furfuryl alcohol	98-00-0	>98.0%	Sigma-Aldrich	$C_5H_6O_2$	1585	10820
5-Hydroxymethylfurfural	67-47-0	>99.0%	Sigma-Aldrich	$C_6H_6O_3$	2415	20050
Terpenes						
D-Limonene	5989-27-5	≥99.0%	TCI	$C_{10}H_{16}$	1203	1860
Terpinolene	586-62-9	>90.0%	TCI	$C_{10}H_{16}$	1284	2330
β-Linalool	78-70-6	>98.0%	Macklin	$C_{10}H_{18}O$	1527	2410
Citronellyl acetate	150-84-5	≥95.0%	Aladdin	$C_{12}H_{22}O_2$	1583	3180
β-Ionone	14901-07-6	>97.0%	Aladdin	$C_{13}H_{20}O$	1833	1560
Benzene						
o-Xylene	95-47-6	≥99.0%	Macklin	C_8H_{10}	1192	1520
Styrene	100-42-5	≥99.5%	Macklin	C_8H_8	1264	2190
p-Cymene	99-87-6	≥99.5%	Macklin	$C_{10}H_{14}$	1273	2900
Naphthalene	91-20-3	≥99.5%	Macklin	$C_{10}H_8$	1635	2070
Volatile phenol						
4-Methylguaiacol	93-51-6	>99.0%	Sigma-Aldrich	$C_8H_{10}O_2$	1860	2820
o-Cresol	95-48-7	>99.0%	Sigma-Aldrich	C_7H_7O	1913	4980
4-Propylguaiacol	2785-87-7	>99.0%	Sigma-Aldrich	$C_{10}H_{14}O_2$	2011	5370
4-Vinylphenol	2628-17-3	>95.0%	Sigma-Aldrich	C_8H_8O	2306	2540
Sulfide						
3-(Methylthio)propanol	505-10-2	≥99.0%	Macklin	$C_4H_{10}OS$	1618	6600
Internal standard						
4-Methyl-2-pentanol	108-11-2	≥98.0%	CNW[f]	$C_6H_{14}O$	1065	1000

Table 1. The information of standards used in this study. [a]Shanghai Macklin Biochemical Co., Ltd (Shanghai, China). [b]Aladdin Bio-Chem Technology (Shanghai, China). [c]Adamas Reagent, Co., Ltd. (Shanghai, China). [d]TCI Development Co., Ltd. (Shanghai, China). [e]Sigma-Aldrich (St. Louis, MO, USA). [f]CNW Technologies GmbH (Duesseldorf, Germany). [g]Bide Pharmatech Ltd. (Shanghai, China). [h]The contents of spiked standard mixtures used in direct liquid introduction method.

depth and breadth of GC-MS technology[35,36]. At present, GC-Orbitrap-MS began to be used to detect pesticide residues[37], nitrosamines in children's products[38], persistent organic pollutants in the environment[39], soluble and extractable substances in package materials[40], stimulants and banned substances in urine[41] and metabonomics[42]. GC-Orbitrap-MS can provide accurate qualitative quantification of benzene compounds in chili peppers[43]. In summary, the GC-Orbitrap-MS could be a potential technique for the determination of aroma volatile compounds in fruit wines due to its high resolution and high sensitivity.

At present, the NIST library is widely used for the identification of aroma volatile compounds analyzed by gas chromatography-mass spectrometry[7,8,44,45]. However, the mass spectrums in the NIST library were mostly obtained by low-resolution mass spectrometry. There were differences in ion fragments and ion abundance between high-resolution mass spectrums obtained by GC-Orbitrap-MS and low-resolution mass spectrums obtained by GC-Quadrupole-MS[46], which led to the qualitative inaccuracy. The high-resolution mass spectrometry (HRMS) spectrums of aroma compounds analyzed by GC-Orbitrap-MS need to be established for accurate identification. In addition, the basic information of aroma compounds, such as CAS number, chemical structure diagram, aroma description and aroma threshold (ortho-nasally), need to be acquired by a large collection of literature. Thus, there is an urgent need to establish a library of HRMS spectrum and basic information to facilitate analyzing and consulting by scholars all over the world.

Compounds	Precursor ions			Quantifier ions			Qualifier ions		
	Exact mass (m/z)	Molecular formula	Error mass (ppm[a])	Exact mass (m/z)	Molecular formula	Error mass (ppm)	Exact mass (m/z)	Molecular formula	Error mass (ppm)
Ester									
Ethyl butanoate				43.05422	C_3H_7	−0.99526	88.05202	$C_4H_8O_2$	0.7668
Ethyl 2-methylbutanoate				74.03639	$C_3H_6O_2$	0.2198	102.0677	$C_5H_{10}O_2$	0.41588
Ethyl isovalerate				57.06997	C_4H_9	0.34743	61.0285	$C_2H_5O_2$	0.15943
Isoamyl acetate				43.01782	C_2H_3O	−1.06298	55.05433	C_4H_9	0.6148
Methyl caproate				43.01782	C_2H_3O	−0.70828	74.03639	$C_3H_6O_2$	0.52895
Ethyl hexanoate				43.05422	C_3H_7	−0.99526	73.02851	$C_3H_5O_2$	0.70783
Ethyl heptanoate				73.02854	$C_3H_5O_2$	0.49889	88.05192	$C_4H_8O_2$	0.42009
Ethyl lactate				45.03354	C_2H_5O	1.30819	56.0621	C_4H_8	0.9174
Heptyl acetate				43.01778	C_2H_3O	−0.17621	70.07773	C_5H_{10}	0.8118
Methyl octanoate				43.01782	C_2H_3O	−0.70828	74.03639	$C_3H_6O_2$	0.73505
Ethyl caprylate				73.02845	$C_3H_5O_2$	−0.44136	101.05977	$C_5H_9O_2$	−0.43741
Ethyl 3-hydroxybutyrate				43.01778	C_2H_3O	−0.6196	71.01285	$C_3H_3O_2$	1.29569
Ethyl nonanoate				73.02845	$C_3H_5O_2$	−0.54583	101.05977	$C_5H_9O_2$	−0.51291
Ethyl 2-hydroxy-4-methylpentanoate				69.06999	C_5H_9	0.12138	45.03355	C_2H_5O	1.22348
Ethyl caprate				73.02853	$C_3H_5O_2$	0.39441	61.0285	$C_2H_5O_2$	0.28445
Ethyl succinate				101.02348	$C_4H_5O_3$	0.02484	73.02853	$C_3H_5O_2$	0.60336
Methyl salicylate	152.04683	$C_8H_8O_3$	0.22088	120.02077	$C_7H_4O_2$	0.28082	92.02578	C_6H_4O	0.15454
Ethyl benzeneacetate	164.08322	$C_{10}H_{12}O_2$	0.24546	91.05439	C_7H_7	−0.13544	136.05219	$C_8H_8O_2$	0.66442
Ethyl salicylate	166.06245	$C_9H_{10}O_3$	0.05133	120.02077	$C_7H_4O_2$	0.40795	92.02578	C_6H_4O	0.15454
Ethyl hydrocinnamate	178.09898	$C_{11}H_{14}O_2$	0.85652	104.06216	C_8H_8	0.34761	105.06997	C_8H_9	0.15241
Ethyl cinnamate	176.08331	$C_{11}H_{12}O_2$	0.96579	131.04938	C_9H_7O	0.98604	103.05436	C_8H_7	0.62066
Monoethyl succinate				101.02348	$C_4H_5O_3$	0.10036	73.02853	$C_3H_5O_2$	0.60336
Carbonyl compounds									
(*E*)-2-Hexenal				83.04919	C_5H_7O	0.17795	69.03339	C_6H_9O	0.46658
(*E*)-2-Heptenal				83.04919	C_5H_7O	0.54542	41.03839	C_3H_5	−3.22212
(*E*)-2-Octenal				83.04919	C_5H_7O	0.17795	41.03839	C_3H_5	−4.80235
(*E*,*E*)-2,4-Heptadienal				81.03347	C_5H_5O	−0.26157	109.0647	C_7H_9O	0.11559
(*E*,*Z*)-2,6-Nonadienal				41.03839	C_3H_5	−4.33758	70.04136	C_4H_6O	−0.48152
Benzeneacetaldehyde	120.05711	C_8H_8O	1.14129	91.05439	C_7H_7	0.61866	92.06208	C_7H_8	0.31004
High alcohols									
Isobutanol				41.0384	C_3H_5	−4.52349	45.0336	C_2H_5O	2.32468
Isoamylol				57.0699	C_4H_9	0.41428	70.07784	C_5H_{10}	0.37632
1-Pentanol				57.06991	C_4H_9	0.54796	70.07784	C_5H_{10}	0.59406
2-Heptanol				45.03354	C_2H_5O	0.88465	83.08566	C_6H_{11}	0.5339
3-Octenol				57.03355	C_3H_5O	0.49786	85.06478	C_5H_9O	0.50696
1-Heptanol				43.05422	C_2H_3O	−1.06298	70.07338	C_5H_{10}	0.48519
2-Nonanol				105.03364	C_7H_5O	0.74249	122.03642	$C_7H_6O_2$	0.75852
1-Octanol				69.06999	C_5H_9	0.23184	55.05433	C_4H_7	0.3996
2-Phenylethanol	122.07275	$C_8H_{10}O$	1.06311	91.05439	C_7H_7	0.95382	92.06208	C_7H_8	−0.51868
2-Phenoxyethanol				108.05687	C_7H_8O	−0.89706	94.04132	C_6H_6O	0.04701
Lactone									
γ-Undecalactone				85.02853	$C_4H_5O_2$	0.69766	95.0493	C_6H_7O	0.95817
δ-Octalactone				99.04407	$C_5H_7O_2$	−0.11627	71.04915	C_4H_7O	0.74492
γ-Octalactone				85.02851	$C_4H_5O_2$	−0.10989	57.03359	C_3H_5O	0.49786
Pantolactone				71.04915	C_4H_7O	0.10063	43.05414	C_3H_7	−2.23569
γ-Decalactone				85.02853	$C_4H_5O_2$	0.1593	95.0493	C_6H_7O	0.47656
Sotolon	128.04693	$C_6H_8O_3$	0.18604	83.04919	C_5H_7O	0.08357	55.05427	C_4H_7	0.81287
γ-Nonalactone				85.02851	$C_4H_5O_2$	−0.02016	57.03359	C_3H_5O	0.36409
Acid									
Butanoic acid				60.02063	$C_2H_4O_2$	0.56154	73.02845	$C_3H_5O_2$	0.39441
Hexanoic acid				73.02853	$C_3H_5O_2$	0.18547	60.02069	$C_2H_4O_2$	0.39361
Ethylhexanoic acid				73.02853	$C_3H_5O_2$	0.18547	87.04422	$C_4H_7O_2$	0.48125
Octanoic acid				73.02853	$C_3H_5O_2$	0.18547	101.05988	$C_5H_9O_2$	0.6195
Decanoic acid				73.02844	$C_3H_5O_2$	0.49889	101.05976	$C_5H_9O_2$	0.54401

Continued

Compounds	Precursor ions			Quantifier ions			Qualifier ions		
	Exact mass (m/z)	Molecular formula	Error mass (ppm[a])	Exact mass (m/z)	Molecular formula	Error mass (ppm)	Exact mass (m/z)	Molecular formula	Error mass (ppm)
Benzoic acid	122.03632	$C_7H_6O_2$	0.75852	105.03364	C_7H_5O	0.66985	122.03642	$C_7H_6O_2$	0.75852
Pyrazine									
3-Isopropyl-2-methoxypyrazine	152.09455	$C_8H_{12}ON_2$	0.50811	137.071	$C_7H_9ON_2$	0.50114	124.06324	$C_6H_8ON_2$	0.86187
2-sec-Butyl-3-Methoxypyrazine	166.10973	$C_9H_{14}ON_2$	−1.99624	138.07886	$C_7H_{10}ON_2$	0.56568	124.06321	$C_6H_8ON_2$	0.75882
5-Ethyl-2,3-dimethylpyrazine	136.0996	$C_8H_{12}N_2$	0.64728	135.0918	$C_8H_{11}N_2$	0.714	121.07612	$C_7H_9N_2$	−0.02603
2-Isobutyl-3-methoxypyrazine	166.11008	$C_9H_{14}ON_2$	0.08705	124.0632	$C_6H_8ON_2$	0.58057	95.06044	$C_5H_7N_2$	−0.08289
Acetylpyrazine	122.04759	$C_6H_6ON_2$	0.53454	94.0526	$C_5H_6N_2$	0.35341	80.03695	$C_4H_4N_2$	0.43185
Furan									
Furfural	96.02053	$C_5H_4O_2$	−0.84083	95.01279	$C_5H_3O_2$	0.16541	39.02277	C_3H_3	−3.43066
Acetylfuran	110.03637	$C_6H_6O_2$	0.42523	95.01281	$C_5H_3O_2$	0.64721	43.01782	C_2H_3O	−0.41717
5-Methylfurfural	110.03625	$C_6H_6O_2$	−0.47613	109.02855	$C_6H_5O_2$	0.68404	53.03864	C_4H_5	1.24689
Ethyl 2-furoate	140.04697	$C_7H_8O_3$	0.56667	95.01279	$C_5H_3O_2$	−0.07548	112.01554	$C_5H_4O_3$	−0.07007
Furfuryl alcohol	98.03629	$C_5H_6O_2$	0.01035	97.02851	$C_5H_5O_2$	0.29686	81.0336	C_5H_5O	0.11503
5-Hydroxymethylfurfural	126.03131	$C_6H_6O_3$	0.34424	97.02849	$C_5H_5O_2$	0.29686	69.03357	C_4H_5O	0.5771
Terpenes									
D-Limonene	136.1252	$C_{10}H_{16}$	1.65914	93.07005	C_7H_9	1.89353	121.10146	C_9H_{13}	1.60836
Terpinolene	136.12471	$C_{10}H_{16}$	0.4261	121.10132	C_9H_{13}	0.22236	93.06999	C_7H_9	0.25403
β-Linalool				93.07005	C_7H_9	0.41798	69.03339	C_5H_9	0.3423
Citronellyl acetate				81.06996	C_6H_9	0.00931	95.08559	C_7H_{11}	−0.17538
β-Ionone				177.12753	$C_{12}H_{17}O$	0.28057	178.13091	$C_{12}H_{17}O$	−2.13518
Benzene									
o-Xylene	106.07779	C_8H_{10}	−0.11101	91.05439	C_7H_7	0.03214	103.05429	C_8H_7	0.62066
Styrene	104.0621	C_8H_8	−0.09229	104.0621	C_8H_8	−0.09229	78.04652	C_6H_6	0.78457
p-Cymene	134.10954	$C_{10}H_{14}$	0.39181	119.0857	C_9H_{11}	0.05216	115.0543	C_9H_7	0.68855
Naphthalene	128.06218	$C_{10}H_8$	0.04416	128.06218	$C_{10}H_8$	0.04416	129.06557	$C_{10}H_8$	−3.16989
Volatile phenol									
4-Methylguaiacol	138.06754	$C_8H_{10}O_2$	0.04814	138.06754	$C_8H_{10}O_2$	0.04814	123.04407	$C_7H_7O_2$	−0.00386
o-Cresol	107.04918	C_7H_7O	0.20933	107.04918	C_7H_7O	0.20933	79.05427	C_6H_7	0.42305
4-Propylguaiacol	166.09877	$C_{10}H_{14}O_2$	−0.18399	137.05968	$C_8H_9O_2$	0.01147	122.03631	$C_7H_6O_2$	0.19587
4-Vinylphenol	120.057	C_8H_8O	0.14583	120.057	C_8H_8O	0.14583	91.05425	C_7H_7	0.19972
Sulfide									
3-(Methylthio)propanol	106.04483	C_7H_6O	3.52157	106.04483	C_7H_6O	3.52157	88.03425	C_7H_4	3.50426
Internal standard									
4-Methyl-2-pentanol				45.03355	C_2H_5O	0.79994			

Table 2. The qualitative and quantitative information of target volatile compounds. [a]ppm means parts per million mass error.

Methods

Overview of the experimental design. *Materials and methods*. Chemical and reagentsThe information of standards was shown in Table 1. The individual stock solution of each standard is dissolved in ethanol and stored at −20 °C.

Wine Samples collectionThree kinds of commercial fruit wines (blueberry wine, B, goji berry wine, G and hawthorn wine, H) purchased from retail stores in China were used for the establishment of HRMS library. All blueberry samples were with an alcohol content of 12% v/v (percent by volume). Three blueberry wines were received from Beiyushidai, including blueberry dry wine produced in 2019 (B1) and 2017 (B2) and blueberry semi-dry wine produced in 2019 (B3). A blueberry dry wine (B4) was produced by Shenghua in 2019. Another blueberry dry wine (B5) produced in 2019 was provided by Yicunshanye. Goji berry semi-dry wine (G1) was produced by Ningxiahong in 2019, with an alcohol content of 7% v/v. Four batches of goji berry dry wine (G2-G5) produced by Senmiao in 2017 were with an alcohol content of 11% v/v. G6 was made by our laboratory in 2016 with an alcohol content of 11% v/v. All hawthorn wine samples were semi-dry wines from Shengbali. H1 and H2 produced in 2019 were with an alcohol content of 12% v/v. The other H3-H5 were produced in 2020 with an alcohol content of 13% v/v from Shengbali.

Preparation of the spiked mixtureThe direct liquid introduction method was used to determine the mass spectral information of the target compound. The standard mixtures (Mixture 1 with 24 esters, Mixture 2 with 6 carbonyl compounds and 8 lactones and 6 acids, Mixture 3 with10 high alcohols and 6 furans and 5 pyrazines, Mixture 4 with 5 terpenes and 4 benzenes and 4 volatile phenols and 1 sulfide) were prepared to extract. The mother solution of each compound was dissolved in ethanol at higher concentration. Each standard mixtures were mixed by the mother solution of compounds according to the concentrations (Table 1).The standard

Compounds	B1	B2	B3	B4	B5	G1	G2	G3	G4	G5	G6	H1	H2	H3	H4	H5
Ester																
Ethyl butanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl 2-methylbutanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl isovalerate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Isoamyl acetate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Methyl caproate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl hexanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl heptanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl lactate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Heptyl acetate	√	√	√	√	√	√	√	√	√	√	nd	√	nd	nd	nd	nd
Methyl octanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl caprylate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl 3-hydroxybutyrate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl nonanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl 2-hydroxy-4-methylpentanoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl caprate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl succinate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Methyl salicylate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	nd	√
Ethyl benzeneacetate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl salicylate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl hydrocinnamate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl cinnamate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Monoethyl succinate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Carbonyl compounds																
(*E*)-2-Hexenal	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
(*E*)-2-Heptenal	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
(*E*)-2-Octenal	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
(*E*,*E*)-2,4-Heptadienal	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
(*E*,*Z*)-2,6-Nonadienal	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Benzeneacetaldehyde	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
High Alcohols																
Isobutanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Isoamylol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
1-Pentanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
2-Heptanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
3-Octenol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
1-Heptanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
2-Nonanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
1-Octanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
2-Phenylethanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
2-Phenoxyethanol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Lactone																
γ-Undecalactone	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
δ-Octalactone	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
γ-Octalactone	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Pantolactone	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
γ-Decalactone	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Sotolon	√	√	√	√	nd	nd	√	nd	nd	√	nd	nd	nd	nd	nd	nd
γ-Nonalactone	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Acid																
Butanoic acid	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Hexanoic acid	nd	√	nd	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethylhexanoic acid	nd	√	nd	√	√	√	√	√	√	√	√	√	√	√	√	√
Octanoic acid	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Decanoic acid	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Benzoic acid	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Pyrazine																

Continued

Compounds	B1	B2	B3	B4	B5	G1	G2	G3	G4	G5	G6	H1	H2	H3	H4	H5
3-Isopropyl-2-methoxypyrazine	√	√	√	√	√	√	√	√	√	nd	√	√	√	√	nd	√
2-sec-Butyl-3-Methoxypyrazine	√	√	√	√	nd	√	√	nd	√	nd	nd	√	√	nd	√	√
5-Ethyl-2,3-dimethylpyrazine	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
2-Isobutyl-3-methoxypyrazine	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Acetylpyrazine	nd	nd	√	√	nd	nd	√	√	√	nd	nd	√	√	√	√	√
Furan																
Furfural	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Acetylfuran	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
5-Methylfurfural	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Ethyl 2-furoate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Furfuryl alcohol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
5-Hydroxymethylfurfural	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Terpenes																
D-Limonene	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Terpinolene	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	nd
β-Linalool	√	√	√	√	nd	nd	√	√	√	√	nd	nd	nd	nd	√	nd
Citronellyl acetate	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
β-Ionone	√	√	√	nd	√	√	√	√	√	√	√	√	nd	√	nd	√
Benzene																
o-Xylene	nd	nd	nd	nd	nd	nd	nd	nd	√	nd	nd	nd	nd	√	√	√
Styrene	√	√	√	√	√	√	√	√	√	√	√	√	nd	√	√	√
p-Cymene	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Naphthalene	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
Volatile phenol																
4-Methylguaiacol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
o-Cresol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
4-Propylguaiacol	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√
4-Vinylphenol	√	√	√	√	√	nd	√	√	√	√	√	nd	nd	nd	nd	nd
Sulfide																
3-(Methylthio)propanol	√	√	√	nd	√	√	√	√	√	√	√	√	√	√	√	√

Table 3. The qualitative determination of target volatile compounds in goji berry wines, blueberry wines and hawthorn wines. 'B' represent blueberry wine, 'G' represent goji berry wine, 'H' represent hawthorn wine.

mixtures were diluted with dichloromethane to volume in a 10-mL volumetric flask. 1 μL of each mixture was injected. The split mode was applied with a split ratio of 10:1. The liquid injection was performed using the TriPlus RSH autosampler (Thermo Fisher Scientific, Bremen, Germany).

Extraction of volatile compounds in wine samplesHeadspace solid-phase microextraction (HS-SPME) was used to extract the volatile compounds from fruit wines. 5 mL of wine samples mixed with 1.00 g NaCl and 10 μL of internal standard (1.077 g/L 4-methyl-2-pentanol) were prepared in a 20 mL glass vial. The sample vials were stirred and heated at 60 °C for 30 min. Then the preconditioned fiber (50/30 μm Divinylbenzene/Carboxen/Polydimethylsiloxane (DVB/CAR/PDMS)) was used to absorb the volatile compounds in the headspace of the sample via for 30 min at 60 °C. After absorption, the fiber was inserted into the GC injection port for desorbing at 250 °C for 10 min. Two technical replicates were performed for each sample. Automatic headspace solid-phase microextraction was performed on the TriPlus RSH autosampler.

GC-Orbitrap-MS analysisA Thermo Scientific Trace 1300 gas chromatography equipped with a Thermo Scientific Q-Exactive Orbitrap mass spectrometer (GC-Orbitrap MS, Thermo Scientific, Bremen, Germany) was used for detection. The spiked mixture was performed under the following GC-Orbitrap-MS conditions. A TG-WAXMS 30 m × 0.25 mm × 0.25 μm (Thermo Scientific, Bremen, Germany) was used to separate analytes. Helium was used as the carrier gas (1.2 mL/min). The oven temperature program was set as follows: 40 °C held for 5 min, then heated to 180 °C at 3 °C/min, finally increased from 180 °C to 240 °C at 30 °C/min and hold 15 min. The wine samples were performed under the following GC-Orbitrap-MS conditions. A DB-WAX 30 m × 0.25 mm × 0.25 μm (J&W Scientific, Folsom, CA, USA) was used to separate the volatile compounds under a 1.2 mL/min flow rate of helium (carrier gas).The oven temperature program was set as follows: 40°C held for 5 min, then heated to 180°C at 3 °C /min, finally increased from 180 °C to 250 °C at 30 °C/min and hold 10 min.

The Orbitrap-MS operated in full-scan MS acquisition mode (m/z 33–350). The ion source was maintained at 280 °C with an MSD transfer line temperature of 230 °C. Positive ion-electron ionization (EI) was used at 70 electron volts (eV) in Orbitrap-MS.

Identification of the compoundsRetention indices (RI) were calculated from the retention times of C6-C24 n-alkanes under the same chromatographic and mass spectrometric conditions. The high-solution mass spectrums of volatile compounds were collected in different standard mixtures. Then, the qualitative determination

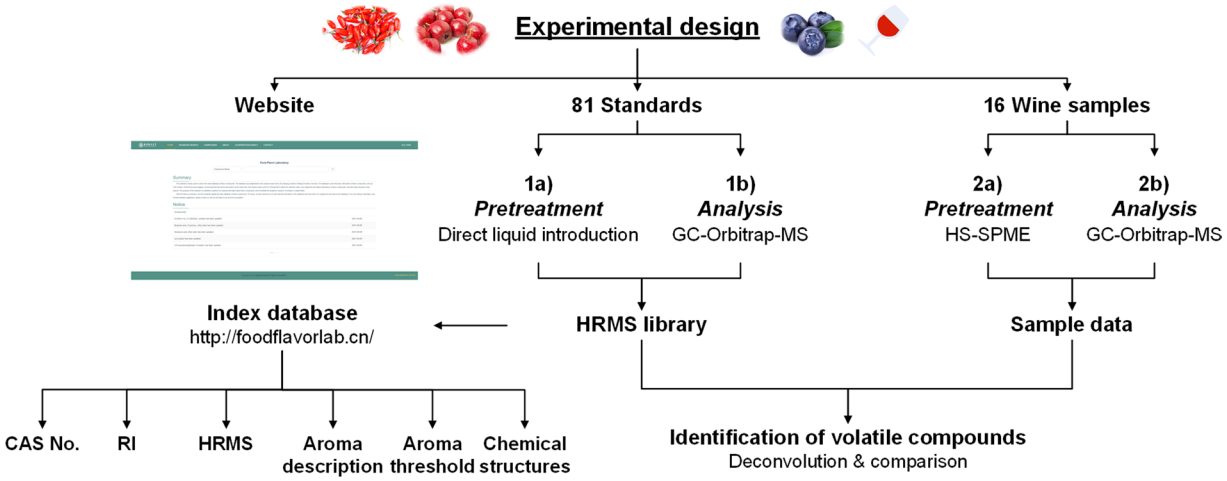

Fig. 1 Flowchart of the experimental design.

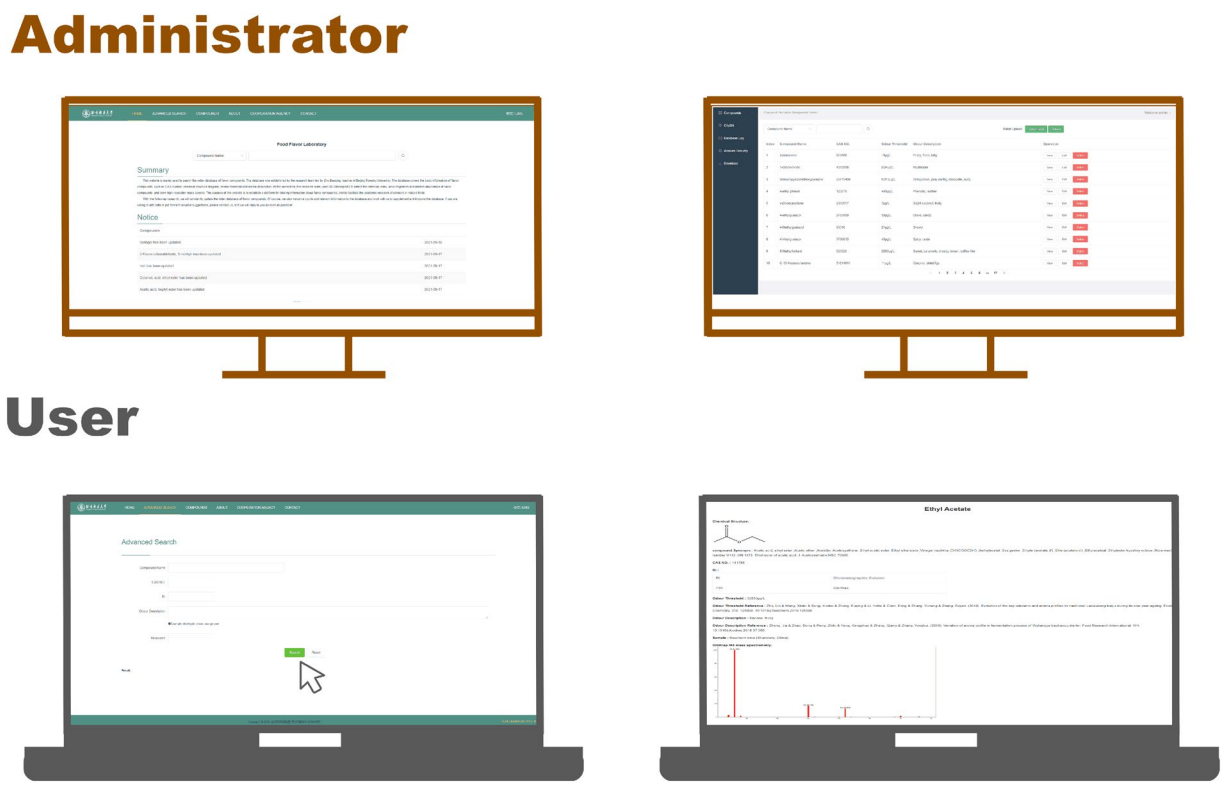

Fig. 2 The web page of the database website (http://foodflavorlab.cn/) including the home page, upload page, search page and result page.

of target compounds in fruit wines was performed by the match of the retention time and ion fragments in samples and standards.The experimental design and analysis pipeline are shown in Fig. 1.

Data Records

A total of 36 original data files were stored in MetaboLights[47], including 4 standard mixtures and 32 wine samples (two technical replicates).

Technical Validation

Two technical replicates were performed on each wine sample. The qualitative determination of target volatile compounds in fruit wines was shown in Table 3.

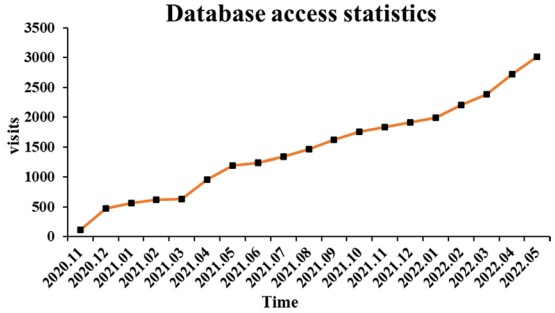

Fig. 3 The page view (PV) of database website (http://foodflavorlab.cn/).

Usage Notes

The HRMS library of volatile compounds was shown on the database website (http://foodflavorlab.cn/), including HRMS spectrum, exact ion fragment, relative abundance, RI, CAS number, chemical structure diagram, aroma description and aroma threshold (ortho-nasally). Table 1 showed CAS No., formula and RI of each target volatile compound. The information of standards and contents of spiked mixtures were shown in Table 1. Table 2 showed elemental composition judgments, exact ion fragments and error mass of each target volatile compound. Table 3 showed the qualitative determination of target volatile compounds in blueberry wine, goji berry wine and hawthorn wine. Figure 2 showed the web page of the database website (http://foodflavorlab.cn/) including the home page, upload page, search page and result page. Figure 3 showed the page view (PV) of the database website (http://foodflavorlab.cn/) from Nov. 2020 to May. 2022.

Code availability

The Processing setup, Quan browser and Qual browser (Thermo Fisher Scientific, Les Ulis, France) in Xcalibur version 4.1 and Thermo Scientific TraceFinder (version 4.1) were used for collecting the HRMS library of volatile compounds. The structures of the volatile compounds were drawn using ChemDraw Professional 17.0 (Cambridgesoft, USA). High-resolution mass spectrums are plotted using Python (version 3.7).

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Author contributions
Y.R.L. designed the experiments and wrote the manuscript. N.L. collected the basic information of volatile compounds. X.Y.L. build the database website. W.C.Q. and J.N.L. analyzed the data of GC-Orbitrap-MS. Q.Y.S. and Y.X.C. performed the GC-Orbitrap-MS experiment. B.L.Z., B.Q.Z. and J.X.C. review the manuscript. B.Q.Z. and J.X.C. supported the funding acquisition. B.Q.Z. designed the experiments. J.X.C. supervised the study.

Competing interests
The authors declare no competing interests.

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