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DATA DESCRIPTOR

OPEN 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 highresolution 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 aroma¹. 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 analysis²⁻⁶. 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 wines¹³ 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 wines²² and oak woods²³ by nitrogen-phosphorous detection (NPD). The triple-quadrupole mass spectrometer (QqQ-MS) in selected-reaction-monitoring (SRM) could identify lactones²⁴, terpenes²⁵ and sulfur compounds²⁶ 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 compounds²⁸⁻³⁰, and therefore many studies have been focused on metabolomics using liquid chromatography coupling³¹⁻³⁴. 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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SeriesJandboxJandboxJandboxJandboxJandboxEhylamethylamethyl1263-2429308AdadanCH,0103130130Ehylamethylamethyl1264-2429308AdamaCH,0130130130Mathylangeta1264-0429308MaklanCH,0130130130Ehylphenanat1264-0729308MaklanCH,0130300Ehylphenanat1264-0729308MaklanCH,0130300Ehylphenanat1114-1529038MaklanCH,0130300Ehylphenanat1114-1529038MaklanCH,0130200Ehylphenanat1114-1529038MaklanCH,0130200Ehylphenanat1114-1529038MaklanCH,0130200Ehylphenanat1114-1529038MaklanCH,0130200Ehylphenanat1114-1529038MaklanCH,0130200Ehylphenanat1114-1529038MaklanCH,0130200Ehylphenanat1114-1529138MaklanCH,0130200Ehylphenanat1124-1529138MaklanCH,0130200Ehylphenanat1124-1529138MaklanCH,0130200Ehylphenanat1124-1529138MaklanCH,0130200Ehylphenanat1124-1529138MaklanCH,	Compounds	CAS No.	Purity	Manufacturer	Formula	RI	Content ^h /µg.L ⁻¹
BindBi	Ester						
Birly 1-ouclybanoate192.9-71>98.0%AdaráC, H, Q, 107010701030Edhy 1-ouclyate108.4-1.5>99.0%AdaráC, H, Q, 113011301300Borny 1-actia102.3-22-2>99.0%MachinC, H, Q, 11401201300Ehyl heranoate106.3-0>99.0%MachinC, H, Q, 113013003000Ehyl heranoate106.3-0>99.0%MachinC, H, Q, 113013003000Ehyl heranoate112.0-1>99.0%MachinC, H, Q, 113013003000Ehyl actar107.2-0>99.0%MachinC, H, Q, 113013003000Ehyl actar101.2-0-1>99.0%MachinC, H, Q, 113013003000Ehyl actar101.2-0-1>99.0%MachinC, H, Q, 113013103000Ehyl actar101.3-3>99.0%MachinC, H, Q, 115013101370Ehyl actar103.3-3>99.0%MachinC, H, Q, 115013101300Ehyl actar103.3-3>99.0%MachinC, H, Q, 110013001300Ehyl actar103.3-6>99.0%MachinC, H, Q, 110013001300Ehyl actar103.3-6>99.0%MachinC, H, Q, 110013001300Ehyl actar103.3-6>99.0%MachinC, H, Q, 110013001300Ehyl actar103.3-6>99.0%MachinC, H, Q, 11001300 <td< td=""><td>Ethyl butanoate</td><td>105-54-4</td><td>≥99.5%</td><td>Aladdin^b</td><td>C₆H₁₂O₂</td><td>1065</td><td>10020</td></td<>	Ethyl butanoate	105-54-4	≥99.5%	Aladdin ^b	C ₆ H ₁₂ O ₂	1065	10020
Birly isocalarate08.45.4>90.96.AdamaséC, H, Q, 10031090Isoamy acctate123-92-2>99.95.6MacklinC, H, Q, 1203120Birly Incenante126-60>90.06.AladinC, H, Q, 13031300Birly Incenante126-60>99.06.MacklinC, H, Q, 13041300Birly Incenante127-61≥90.06.MacklinC, H, Q, 13041300Birly Incenante112-61≥90.06.MacklinC, H, Q, 13041300Birly Incenante112-15≥90.06.MacklinC, H, Q, 13021301Birly Incenante106-32-1>90.06.MacklinC, H, Q, 15111517Birly Incenante103-84.7≥90.06.MacklinC, H, Q, 1522152310180Birly Incenante103-84.7≥90.56.MacklinC, H, Q, 1572152010180Birly Incenante103-84.≥90.56.MacklinC, H, Q, 1575150210180Birly Incenante102-35.≥90.56.MacklinC, H, Q, 1575150210180Birly Inscrinte103-36.6>98.06.AladinC, H, Q, 170513021020Birly Inscrinte103-35.6>98.06.AladinC, H, Q, 17013021020Birly Inscrinte103-36.6>98.06.AladinC, H, Q, 17013021020Birly Inscrinte103-36.6>98.06.MacklinC, H, Q, 17013021302Birly	Ethyl 2-methylbutanoate	7452-79-1	>98.0%	Aladdin	$C_7H_{14}O_2$	1077	5030
isoamplaceate123-22>99.9%MachinC, H_u,O,113911390Methylogroate106-70.7>99.0%MachinC, H_u,O,12.030.00Ehyl heanoate103-30-9>99.0%MachinC, H_u,O,13.030.00Ehyl paraoate107-64-3>99.0%MachinC, H_u,O,13.030.00Ehyl actate97.64-3>99.0%MachinC, H_u,O,13.030.00Ehyl actotatoate111-15>99.0%MachinC, H_u,O,13.020.00Ehyl actotanoate110-15.2>99.0%MachinC, H_u,O,13.020.00Ehyl actotanoate103-32-1>99.0%MachinC, H_u,O,15.015.0Ehyl actotanoate103-83-1>99.0%MachinC, H_u,O,15.22080Ehyl actotanoate103-83-1>99.0%MachinC, H_u,O,15.210.80Ehyl actotanoate103-83-1>99.0%MachinC, H_u,O,15.210.80Ehyl actotanoate103-85-1>90.0%MachinC, H_u,O,15.010.00Ehyl actotanoate103-36-1>90.0%MachinC, H_u,O,15.010.00Ehyl actotanoate103-36-1>90.0%MachinC, H_u,O,15.010.00Ehyl actotanoate103-36-1>90.0%MachinC, H_u,O,15.010.00Ehyl actotanoate103-36-1>90.0%MachinC, H_u,O,15.010.00Ehyl actotanoate118-15-0	Ethyl isovalerate	108-64-5	>99.0%	Adamas ^c	$C_7H_{14}O_2$	1093	11050
Methylepanethyle1924667>990%MaklainC,H,O, C,HO,12001300Ehylhepanoate106-3092995%MachinC,H,O, C,H,O,1300050Ehylhatain076-412995%MachinC,H,O, C,H,O,1300050Ehylactain111-15290%MachinC,H,O, C,H,O,1301200Ehylactain101-152290%MachinC,H,O, C,H,O,1512200Ehylachylathyl106-32-1290.%MachinC,H,O, C,H,O,152200Ehylachylathylath103-84-7290.%MachinC,H,O, C,H,O,152200Ehylachydray-4methylpentanon103-84-7290.%MachinC,H,O, C,H,O,152200Ehylachydray-4methylpentanot103-83- 202-5290.%MachinC,H,O, C,H,O,150200Ehylachydray-4methylpentanot110-38- 202-5290.%MachinC,H,O, C,H,O,150200Ehylachydray-4methylpentanot110-37- 202-5290.%MachinC,H,O, C,H,O,150200Ehylachydray-4methylpentanot110-37- 202-5290.%MachinC,H,O, C,H,O,150200Ehylachydray-4methylpentanot110-37- 202-5290.%MachinC,H,O, C,H,O,150200Ehylachydray-4methylpentanot110-37- 202-5290.%MachinC,H,O, C,H,O,150200Ehylachylpentanot110-37- 202-5290.%MachinC,H,O, C,H,	Isoamyl acetate	123-92-2	≥99.5%	Macklin	$C_7H_{14}O_2$	1139	11390
BindDependencionD	Methyl caproate	106-70-7	>99.0%	Macklin	$C_7H_{14}O_2$	1200	5120
Bhylpspanote106.09.0299.0%MacklinC,H,,O,130050810Bhyllactate97.64.3290.0%MacklinC,H,,O,13043280Methyloctanoate111-11.5290.0%ManassC,H,O,13142000Ehyl aprytate160.32.1>90.0%MacklinC,H,O,1111570Ehyl aprytatoxybutyrate530.54.1.4>90.0%MacklinC,H,O,112.11570Ehyl aprytatoxybutyrate103.49.7.7298.0%MacklinC,H,O,152.210300Ehyl apratox110.38.3>90.0%MacklinC,H,O,152.20300Ehyl saccinter110.37.6.8>90.0%MacklinC,H,O,167.22080Ehyl saccinter110.75.3>99.5%MacklinC,H,O,167.21600Ehyl barcencetate110.75.3>99.5%MacklinC,H,O,170.21600Ehyl barcencetate110.75.3>99.5%MacklinC,H,O,170.21600Ehyl barcencetate101.97.3>99.5%MacklinC,H,O,180.21020Ehyl barcencetate101.97.3>99.5%MacklinC,H,O,180.21020Ehyl saccinter103.64>98.0%MadinC,H,O,180.21020Ehyl saccinter137.64>98.0%MadinC,H,O,180.21020Corburg672.92.5>98.0%MadinC,H,O,180.21020Ehyl saccinter672.92.5>98.0%Macklin <t< td=""><td>Ethyl hexanoate</td><td>123-66-0</td><td>>99.0%</td><td>Aladdin</td><td>$C_8H_{16}O_2$</td><td>1243</td><td>30300</td></t<>	Ethyl hexanoate	123-66-0	>99.0%	Aladdin	$C_8H_{16}O_2$	1243	30300
Bitylactaré97-64-3>290,%IacklinC,H,G,O1309810Ilepti actate112-01-0>290,%AdamasC,H,G,O134200Ehyl-aprylate106-32-1>990,%IadalinC,H,G,O1311570Ehyl-aprylate160-32-1>990,%MacklinC,H,G,O1511570Ehyl-aprylate103-84-17>990,%MacklinC,H,G,O1527250Ehyl-aprylate110-38-3>990,%MacklinC,H,G,O15210180Ehyl-aprylate110-38-3>990,%MacklinC,H,G,O1521020Ehyl-aprylate110-37-3>995,%MacklinC,H,G,O1631400Ehyl-aprylate110-37-3>995,%MacklinC,H,G,O1781400Ehyl-aprylate103-36-6>990,%AdadinC,H,G,O1781200Ehyl-aprylate103-36-6>980,%AdadinC,H,G,O132100Ehyl-aprylate103-36-6>980,%AdadinC,H,G,O132100Ehyl-aprylate103-36-6>980,%AdadinC,H,G,O132100Ehyl-aprylate103-36-6>980,%AdadinC,H,G,O132100Ehyl-aprylate103-36-6>980,%MaddinC,H,G,O132100Ehyl-aprylate123-51>950,%MaddinC,H,G,O132100Ehyl-aprylate123-51>950,%MaddinC,H,G,O132100Ehyl-apryla	Ethyl heptanoate	106-30-9	≥99.5%	Macklin	$C_9H_{18}O_2$	1340	5050
Hepplacetate112-06-1298.0%CICIC,H,G,G13982800Methyl octanoate1111-15299.0%AdamaC,H,G,G13942007Ehlyl arylata106-32-1>990.0%MaddinC,H,G,G1511517Ehlyl arydroxybutyrate5405-41-4>990.0%MaddinC,H,G,G152720Ehlyl arydroxy-methylpentanoate10348-7.7298.0%MaddinC,H,G,G1521018Ehlyl arydroxy-methylpentanoate10348-7.7298.0%MaddinC,H,G,G15722098.0%Ehlyl skrichate113-36.8299.5%MaddinC,H,G,G15784760Ehlyl skrichate119-37.8299.5%MaddinC,H,G,G15784760Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G1581340Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G132504Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G132150Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G132150Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G132150Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G132150Ehlyl skrichate118-16.5>98.0%AladinC,H,G,G132150Ehlyl skrichate118-26.5>95.0%MacklinC,H,G,G132150Ejl-24-tengtal1828567.5 <t< td=""><td>Ethyl lactate</td><td>97-64-3</td><td>≥99.0%</td><td>Macklin</td><td>$C_5H_{10}O_3$</td><td>1350</td><td>50810</td></t<>	Ethyl lactate	97-64-3	≥99.0%	Macklin	$C_5H_{10}O_3$	1350	50810
MethyNumber of the standNumber of the stand	Heptyl acetate	112-06-1	≥98.0%	TCI	$C_9H_{18}O_2$	1380	3280
Bity capyiesNormal <t< td=""><td>Methyl octanoate</td><td>111-11-5</td><td>≥99.0%</td><td>Adamas</td><td>$\mathrm{C_9H_{18}O_2}$</td><td>1394</td><td>2000</td></t<>	Methyl octanoate	111-11-5	≥99.0%	Adamas	$\mathrm{C_9H_{18}O_2}$	1394	2000
BirlyBirlySequenceSequenceSequenceSequenceSequenceSequenceBirly10434742800AddinCH_u01521103041Birly10434742800AddinCH_u01521103041Birly10734329030MakinCH_u01523103041Birly10734329030MakinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429030AddinCH_u01520163041Birly10745429130AddinCH_u01520163041Birly10745429130Addin<	Ethyl caprylate	106-32-1	>99.0%	Aladdin	$C_{10}H_{20}O_2$	1439	29670
BityEndSequence <th< td=""><td>Ethyl 3-hydroxybutyrate</td><td>5405-41-4</td><td>>99.0%</td><td>Macklin</td><td>$C_6H_{12}O_3$</td><td>1511</td><td>15170</td></th<>	Ethyl 3-hydroxybutyrate	5405-41-4	>99.0%	Macklin	$C_6H_{12}O_3$	1511	15170
Bindle sharesSequenceSequenceSequenceSequenceSequenceSequenceBindle shares123-23SequenceSequenceSequenceSequenceSequenceBindle shares123-24SequenceSequenceSequenceSequenceSequenceSequenceBindle shares123-24Sequence	Ethyl nonanoate	123-29-5	≥95.0%	Macklin	$C_{11}H_{22}O_2$	1521	7250
Bhyl caprate110-38-3990%MackinC, H, Q, C, H, Q, C, H, Q, C, B90802080Bhyl succinate123-25-1995%MackinC, H, Q, C, C, H, Q,16701670Bhyl benzenactate101-97-399.5%AladinC, H, Q, C, H, W,16801690Bhyl benzenactate118-61-6>99.0%AladinC, H, Q, C, H, W,17001680Bhyl hyndroinnanate103-36-6>98.0%AladinC, H, Q, C, H, W,1031040Bhyl chanata103-36-6>98.0%AladinC, H, Q, C, H, W,1031040Monochly laucinate1070-34-0>95.0%AladinC, H, Q, C, H, W,1031040Chrourcomcut1070-34-0>98.0%AladinC, H, Q, C, H, W,1031020Chrourcomcut1282-55>95.0%AladinC, H, Q, C, H, Q,12801020Ch2-2-Cytenal1882-55>95.0%AladinC, H, Q, C, H, Q,12401020Ch2-2-Al-Eptadienal131-03-0>90.0%MackinC, H, Q, C, H, Q,12401020Ch2-2-Al-Eptadienal57.4%>95.0%AladinC, H, Q, C, H, Q,12401250Ch2-2-Al-Eptadienal57.4%>95.0%AladinC, H, Q, C, H, Q,12401260Ch2-2-Al-Eptadienal137.6%28.0%AladinC, H, Q, C, H, Q,12401260Ch2-2-Al-Eptadienal137.6%28.0%AladinC, H, Q, C, H, Q,1	Ethyl 2-hydroxy-4-methylpentanoate	10348-47-7	≥98.0%	Aladdin	$C_8H_{16}O_3$	1525	10180
Ehyl succinate123-25-1299.5%MackinC,H,Q, C,H,Q,O159230300Methyl silcylate101-97-8299.5%AladinC,H,Q, C,H,Q,O17001400Ehyl salcylate118-61-6>99.0%AladinC,H,Q,O C,H,Q,O17005480Ehyl salcylate103-36-6>98.0%AladinC,H,Q,O C,H,Q,O17005480Ehyl sucinate1070-34-4>98.0%AladinC,H,Q,O C,H,Q,O17001000Chronetometo1070-34-4>98.0%AladinC,H,Q,O13201020Chronetometo1070-34-4>95.0%AladinC,H,Q,O13201020Chronetometo128-26-5>95.0%AladinC,H,Q,O13201020(£)-2-Hexnal6728-26-3>95.0%MackinC,H,Q,O14201020(£)-2-Arendacinal5748-2>95.0%MackinC,H,Q,O14501020(£)-2-Arendacinal127-81>99.5%AladinC,H,Q,O11212020Boatonol127-81>99.5%AladinC,H,Q,O11212020129-24-Nonaderal129-51295.5%AladinC,H,Q,O12129630Boatonol124-51>99.5%AladinC,H,Q,O12129630129-129-120129-51301-62301-62301-62301-62301-62129-129-120129-51AladinC,H,Q,O11239600129-129-120301-86AladinC,H,Q,O120	Ethyl caprate	110-38-3	>99.0%	Macklin	$C_{12}H_{24}O_2$	1572	20980
Methylaiskylate119-36-8299.5%MackinC4,H,Q. C,H1Q.16754760Ehly bancyclate118-61-6>990.5%AladinC,H2Q. C,H1Q.18801204Ehly langrance2021-28-5>98.0%AladinC,H2Q. C,H1Q.12031204Ehly langrance1070-34-0>98.0%AladinC,H2Q. C,H2Q.12031204Monoethyl succinate1070-34-0>98.0%AladinC,H2Q. C,H2Q.13021204Carbonyl compondsCarbonyl Componds59.0%AladinC,H2Q. C,H2Q.13226530(E)-2-Hexenal18829-55-5>95.0%MackinC,H2Q. C,H2Q.13231000(E)-2-Cotenal2548-87-0>95.0%MackinC,H2Q. C,H2Q.15481202(E)-2-Cotenal4131-03-5>90.0%MackinC,H2Q.15481202(E)-2-Cotenal257.48-2>95.0%MackinC,H2Q.15481202(E)-2-A-Enptadienal121-27.81->95.0%MackinC,H2Q.15481202(E)-2-A-Enptadienal121-27.81->95.0%MackinC,H2Q.15481202(E)-2-A-Enptadienal121-27.81->95.0%MackinC,H2Q.12727302(E)-2-A-Enptadienal123-78-1>90.0%MackinC,H2Q.12727302(E)-2-A-Enptadienal123-51-3≥95.5%MackinC,H2Q.127263401-Pentanol71-41-0≥95.5%MackinC,H2Q.1272 <td>Ethyl succinate</td> <td>123-25-1</td> <td>\geq99.5%</td> <td>Macklin</td> <td>$\mathrm{C_8H_{14}O_4}$</td> <td>1592</td> <td>50360</td>	Ethyl succinate	123-25-1	\geq 99.5%	Macklin	$\mathrm{C_8H_{14}O_4}$	1592	50360
Ehyl benzeneacetate101-97-3≥99.5%Aladdin $C_{01}H_{12}O_{1}$ 16891940Ethyl salcylate118-61-6>990.0%Aladain $C_{11}H_{10}O_{1}$ 17005400Ethyl shydrocinnamte103-36-6>98.0%Aladain $C_{11}H_{10}O_{1}$ 20315040Monoethyl succinate1070-34-4>95.0%Aladain $C_{4}H_{10}O_{1}$ 20301020Carbourd compounds728-26-3>98.0%Aladdin $C_{4}H_{10}O_{1}$ 13206530(E)-2-Heptanl18829-55->95.0%Aladdin $C_{4}H_{10}O_{1}$ 14321900(E)-2-Heptanl18829-55->95.0%Aladdin $C_{4}H_{10}O_{1}$ 14321900(E)-2-Heptanl18829-55->95.0%Aladdin $C_{4}H_{10}O_{1}$ 14321900(E)-2-Heptanlenal4313-03-5>90.0%Macklin $C_{4}H_{10}O_{1}$ 15451620(E)-2-Heptanlenal4313-03-5>90.0%Macklin $C_{4}H_{10}O_{1}$ 15451620(E)-2-Al-Heptadienal4313-03-5>90.0%Macklin $C_{4}H_{10}O_{1}$ 15451620(E)-2-Al-Heptadienal257.48>95.0%Macklin $C_{4}H_{10}O_{1}$ 15451620(E)-2-Al-Heptadienal257.48>95.0%Macklin $C_{4}H_{10}O_{1}$ 15451620(E)-2-Al-Heptadienal2548-87.0>98.0%Aladin $C_{4}H_{10}O_{1}$ 1545162010-2-178.1259.5%Macklin $C_{4}H_{10}O_{1}$ 152063041	Methyl salicylate	119-36-8	≥99.5%	Macklin	C ₈ H ₈ O ₃	1675	4760
Ehyl sakcylate118-61-6>99.0%Aladdin $C_{\mu}H_{\alpha}O_{1}$ 17.105480Ethyl phyl cinamate2021-28-5>98.0%TCl ⁴ $C_{11}H_{\alpha}O_{2}$ 2015040Bhyl cinamate103-36-6>98.0%Aladdin $C_{11}H_{\alpha}O_{2}$ 2015040Monoethyl succinate1070-34-4>95.0%Aladdin $C_{11}H_{\alpha}O_{1}$ 1321120Carbony compounds(J2-12-berenal6728-26-3>95.0%Aladdin $C_{11}H_{\alpha}O_{1}$ 132120(J2-2-Heptenal8829-55->95.0%Aladdin $C_{11}H_{\alpha}O_{1}$ 132120(J2-2-Heptenal431-03-5>95.0%Macklin $C_{11}H_{\alpha}O_{1}$ 132120(J2-2-Art-Heptadienal431-03-5>95.0%Macklin $C_{11}H_{\alpha}O_{1}$ 134120(J2-2-Art-Heptadienal431-03-5>95.0%Macklin $C_{11}H_{\alpha}O_{1}$ 134120Benzenezetaldehyde123-51-3≥95.0%Macklin $C_{11}H_{\alpha}O_{1}$ 1377882Botimation74-10≥95.5%Macklin $C_{11}H_{\alpha}O_{1}$ 1366301-Pentand71-41-0≥95.5%Macklin $C_{11}H_{\alpha}O_{1}$ 1326302-Pentony133-9>98.0%Macklin $C_{11}H_{\alpha}O_{1}$ 1326302-Pentony131-0595.5%Macklin $C_{11}G_{\alpha}$ 1529602-Pentony <t< td=""><td>Ethyl benzeneacetate</td><td>101-97-3</td><td>\geq99.5%</td><td>Aladdin</td><td>$C_{10}H_{12}O_2$</td><td>1689</td><td>1940</td></t<>	Ethyl benzeneacetate	101-97-3	\geq 99.5%	Aladdin	$C_{10}H_{12}O_2$	1689	1940
Ehyl hydrocinnamate2021-28-5>98.0%TCl ⁴ C ₁ H ₁ ,Q17851240Ethyl innamate103-36-6>98.0%AdamasC ₁ H ₄ ,Q20315040Monoethyl sucinate1070-34-4>95.0%AladinC ₄ H ₄ ,Q13021020Carbony Compounds6728-26-3>98.0%AladinC ₄ H ₁₀ O13226530(E)-2-Hexenal18829-55->95.0%AladdinC ₄ H ₁₀ O132265306530(E)-2-Octenal2548-87-0>95.0%AladkinC ₄ H ₄₀ O14321020(E)-2-A-Heptadienal413-03-5>90.0%MacklinC ₄ H ₄₀ O14321020(E)-2-A-Heptadienal557-48-2≥95.0%AladdinC ₄ H ₄₀ O14541020Benzeneacetaldehyde122-78-1>95.0%AladdinC ₄ H ₄₀ O14125020(E)-2-4-Heptadienal78-83-1≥95.5%AladdinC ₄ H ₄₀ O11278820Boarnylo123-51-3≥95.5%AladdinC ₄ H ₄₀ O132787001-Pentanol114-0≥95.5%AladdinC ₄ H ₄₀ O13206402-Heptanol133-18-64>98.0%AladdinC ₄ H ₄₀ O13206402-Heptanol111-87-5≥99.5%AladdinC ₄ H ₄₀ O13206402-Heptanol111-87-5≥99.5%MacklinC ₄ H ₄₀ O14105402-Heptanol111-87-5≥99.5%MacklinC ₄ H ₄₀ O1320650	Ethyl salicylate	118-61-6	>99.0%	Aladdin	$C_9H_{10}O_3$	1710	5480
Ethyl cinnamate103·36-6>98.0%Adamas $C_{11}H_{12}O_{2}$ 2015040Monechyl succinate1070-34-4>95.0%Aladdin $C_{4}H_{12}O_{2}$ 2081102 Carbonyt compounds 572-8-6-3>98.0%Aladdin $C_{4}H_{10}O_{2}$ 13297120(<i>B</i>)-2-Heptenal18829-55-5>95.0%Aladdin $C_{4}H_{10}O_{2}$ 13206530(<i>B</i>)-2-At-Heptadienal4313-03-5>90.0%Macklin $C_{4}H_{10}O_{2}$ 14321000(<i>E</i> , <i>C</i>)-2,4-Heptadienal557-48-2≥95.0%Aladdin $C_{4}H_{10}O_{2}$ 14321202(<i>E</i> , <i>C</i>)-2,6-Nonadienal557-48-2≥95.0%Aladdin $C_{4}H_{10}O_{2}$ 152372Benzenze-cateldehyde122-78-1≥95.0%Aladdin $C_{4}H_{10}O_{2}$ 1122620Isoamylol122-51.3≥95.5%Aladdin $C_{4}H_{10}O_{2}$ 1217820Isoamylol123-51.3≥95.5%Aladdin $C_{4}H_{10}O_{2}$ 132178201-Pentanol71-41-0≥95.5%Aladin $C_{4}H_{10}O_{2}$ 13213602-Heptanol11170-6>95.0%Macklin $C_{4}H_{10}O_{2}$ 13213602-Heptanol11170-6≥95.5%Aladin $C_{4}H_{10}O_{2}$ 1313602-Heptanol612-8>95.0%Aladin $C_{4}H_{10}O_{2}$ 13213602-Heptanol612-8>95.5%Aladin $C_{4}H_{10}O_{2}$ 1513242-Heptanol612-8>95.0	Ethyl hydrocinnamate	2021-28-5	>98.0%	TCI ^d	$C_{11}H_{14}O_2$	1785	12040
Monoethyl succinateIn70-34-4>95.0%AladinC ₈ H ₁₀ O ₄ 23.0811020Carboury compoundsUSE Set	Ethyl cinnamate	103-36-6	>98.0%	Adamas	$\mathrm{C}_{11}\mathrm{H}_{12}\mathrm{O}_2$	2031	5040
Carbony conspan="4">Carbony conspan="	Monoethyl succinate	1070-34-4	>95.0%	Aladdin	$\mathrm{C_6H_{10}O_4}$	2308	11020
(£)-2-Hexenal6728-26-3>98.0%AladdinC ₄ H ₁₀ O13297120(£)-2-14pptenal18829-55-5>95.0%AladdinC ₄ H ₁₀ O14321600(£)-2-Ctenal2548-87-0>95.0%MacklinC ₆ H ₁₀ O143810220(£,2)-2,6-Heptadienal4313-03-5>90.0%MacklinC ₆ H ₁₀ O149810220(£,2)-2,6-Nonadienal557-48-2>95.0%MacklinC ₆ H ₁₀ O14544160Benzeneacetaldehyde122-78-1>95.0%AladdinC ₆ H ₁₀ O11122020High alcohols78-83-1≥95.5%AladdinC ₆ H ₁₀ O11127820Isoanylol123-51-3≥95.5%AladdinC ₆ H ₁₀ O12778201-Pentanol71-41-0≥95.5%MacklinC ₆ H ₁₀ O132778002-Heytanol3391-86-4>98.0%AladdinC ₇ H ₁₀ O132454002-Heytanol111-70-6>95.0%MacklinC ₇ H ₁₀ O15132402-Heytanol111-70-6>95.0%MacklinC ₇ H ₁₀ O15132402-Heytanol111-70-6>95.0%MacklinC ₇ H ₁₀ O15132402-Heytanol111-70-6>95.0%MacklinC ₇ H ₁₀ O18145402-Heytanol111-70-6>95.0%MacklinC ₇ H ₁₀ O18145402-Heytanol111-87-5≥95.5%MacklinC ₈ H ₁₀ O18145502-Henoxyethanol628-99-9≥95.0%<	Carbonyl compounds						
(E)-2-Heptenal18829-55-3>95.0%AladdinC,H12O13626530(E)-2-Otenal2548-87-0>95.0%MacklinC,H14O14321900(E,E)-2,4-Heptadienal4313-03-5>90.0%MacklinC,H40149810220(E,Z)-2,6-Nonadienal557-48-2>95.0%AladdinC,H4015454160Benzeneaccaldehyde122-78-1>95.0%MacklinC,H4011212020High alcoholJest colspan="4">Jest colsp	(E)-2-Hexenal	6728-26-3	>98.0%	Aladdin	$C_6H_{10}O$	1329	7120
(E) -2-Octenal2548-87-0>95.0%Macklin C_8H_1O 14321900 (E,E) -2,4-Heptadienal4313-03-5>90.0%Macklin C_7H_0O 149810220 (E,C) -2,6-Nonadienal557-48-2>95.0%Aladdin C_9H_1O 15454160Benzeneacetaldehyde122-78-1>95.0%Macklin C_8H_0O 15745720 High alcohols 527-88-2>95.5%Aladdin C_8H_0O 111220620Isoamylol123-51-3>99.5%Aladdin C_8H_1O 125963401-Pentanol71-41-0>99.5%Macklin C_8H_1O 132787002-Nethanol543-49-7>98.0%Aladdin C_8H_1O 132787003-Octenol3391-86-4>98.0%Aladdin C_8H_1O 146054902-Nonanol628-99-9>98.0%Aladdin C_8H_1O 151332402-Nonanol612-8>99.5%Macklin C_8H_1O 151330602-Nonanol111-87-5>99.5%Macklin C_8H_1O 151330402-Nonanol104-50-7>98.0%Macklin C_8H_1O 151330402-Nonanol104-50-7>98.0%Sigma-Aldrich $C_8H_1O_2$ 181441408-Octalactone698-76-0>98.0%Sigma-Aldrich $C_8H_1O_2$ 1863480-y-Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8H_1O_2$ 1864340-y-Decalactone599-04-2>9	(E)-2-Heptenal	18829-55-5	>95.0%	Aladdin	$C_7H_{12}O$	1362	6530
(E,E) -2,4-Heptadienal4313-03-5>90.0%Macklin $C_r H_{10}$ 149810220 (E,Z) -2,6-Nonadienal557-48-2≥95.0%Aladdin $C_r H_{10}$ 15454160Beneneacetaldehyde122-78-1>95.0%Macklin $C_r H_{10}$ 15745720High alcohols78-83-1≥99.5%Aladdin $C_4 H_{10}$ 111220620Isoamylol123-51-3≥99.5%Aladdin $C_2 H_{10}$ 1277788201-Pentanol71-41-0≥99.5%Macklin $C_3 H_{10}$ 132787002-Heptanol543-49-7>98.0%Aladdin $C_8 H_{10}$ 145632203-Octenol3391-86-4>98.0%Aladdin $C_8 H_{10}$ 145632201-Heptanol111-70-6>95.0%Macklin $C_8 H_{10}$ 151132402-Nonanol628-99.9Aladdin $C_8 H_{10}$ 151132401-Octanol111-87-5≥99.5%Aladdin $C_8 H_{10}$ 1512506902-Phenylethanol60-12-8≥99.5%Aladdin $C_8 H_{10}$ 181441402-Phenylethanol104-50-7>98.0%Sigma-Aldrich $C_8 H_{10}$ 181236692-Phenylethanol104-61-0>98.0%Sigma-Aldrich $C_8 H_{10}$ 18441408-Octalactone698-76-0>98.0%Sigma-Aldrich $C_8 H_{10}$ 184037009-Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8 H_{10}$ 1860360 <t< td=""><td>(E)-2-Octenal</td><td>2548-87-0</td><td>>95.0%</td><td>Macklin</td><td>$C_8H_{14}O$</td><td>1432</td><td>1900</td></t<>	(E)-2-Octenal	2548-87-0	>95.0%	Macklin	$C_8H_{14}O$	1432	1900
(E,Z) -2,6-Nonadienal $557-48-2$ $\geq 95.0\%$ Aladdin $C_9H_{14}O$ 1545 4160 Benzeneacetaldehyde $122-78-1$ $>95.0\%$ Macklin C_8H_8O 1574 5720 Highachols 295.5% Aladdin C_8H_1O 1112 20620 Isoamylol $123-51-3$ $\geq 99.5\%$ Aladdin $C_9H_{12}O$ 1217 78820 1-Pentanol $71-41-0$ $\geq 99.5\%$ Macklin $C_9H_{12}O$ 1259 6340 2-Heptanol $543-49-7$ $>88.0\%$ Aladdin $C_9H_{10}O$ 1327 8700 3-Octenol $3391-86-4$ $>98.0\%$ Aladdin $C_9H_{10}O$ 1456 3220 1-Heptanol $111-70-6$ $>95.0\%$ Macklin $C_9H_{10}O$ 1511 3240 2-Nonanol $628-99-9$ $\geq 98.0\%$ Aladdin $C_9H_{10}O$ 1512 9060 2-Nonanol $118-75$ $\geq 99.5\%$ Macklin $C_8H_{10}O$ 1817 50690 2-Nensylethanol $60-12-8$ $\geq 99.5\%$ Macklin $C_8H_{10}O$ 1817 50690 2-Nensylethanol $104-50-7$ $>98.0\%$ Sigma-Aldrich $C_8H_{10}O$ 1817 50690 2-Nensylethanol $104-50-7$ $>98.0\%$ Sigma-Aldrich $C_1H_{20}O_2$ 1814 4140 $A_O Catalactone698-76-0>98.0\%Sigma-AldrichC_8H_{10}O_21840\gamma-Nonalactone104-61-0>98.0\%Sigma-AldrichC_8H_{10}O_21840\gamma-Dacalactone599-$	(E,E)-2,4-Heptadienal	4313-03-5	>90.0%	Macklin	$C_7H_{10}O$	1498	10220
Benzeneacetaldehyde122-78-1>95.0%Macklin $C_a H_0 O$ 15745720High alcoholsJisobutanol78-83-1 $\geq 99.5\%$ Aladdin $C_a H_1 O$ 111220620Isomylol123-51-3 $\geq 99.5\%$ Aladdin $C_a H_1 O$ 1127788201-Pentanol71-41-0 $\geq 99.5\%$ Macklin $C_3 H_1 O$ 1277788202-Heptanol543-49-7 $\geq 99.5\%$ Macklin $C_a H_1 O$ 132787003-Octenol3391-86-4 $\geq 98.0\%$ Aladdin $C_a H_1 O$ 152832201-Heptanol111-70-6 $\geq 95.0\%$ Macklin $C_a H_1 O$ 154032402-Nonanol628-90 $\geq 98.0\%$ Aladdin $C_a H_1 O$ 153290002-Nonanol111-87-5 $\geq 99.5\%$ Macklin $C_a H_1 O$ 153290002-Nonanol112-87-6 $\geq 99.5\%$ Macklin $C_a H_1 O$ 1817506902-Nehythanol102-89-6 $\geq 99.5\%$ Macklin $C_a H_1 O$ 181441402-Nehythanol104-50-7 $\geq 98.0\%$ Sigma-Aldrich $C_1 H_{20}$ 18441402-Nonalactone698-76-0 $\geq 98.0\%$ Sigma-Aldrich $C_a H_1 O_2$ 18203600 γ -Otalactone104-61-0 $\geq 98.0\%$ Sigma-Aldrich $C_a H_1 O_2$ 18203600 γ -Decalactone209-04-2 $\geq 99.0\%$ Sigma-Aldrich $C_a H_a O_3$ 193519860 γ -Decalactone206-43-59 $\geq 99.0\%$ Sigma-Aldrich<	(E,Z)-2,6-Nonadienal	557-48-2	≥95.0%	Aladdin	$C_9H_{14}O$	1545	4160
High alcoholsIsobutanol $78.83.1$ $\geq 99.5\%$ Aladin $C_4H_{10}O$ 112 20620 Isoamylol $123.51.3$ $\geq 99.5\%$ Aladin $C_5H_{1.0}O$ 1217 78820 1.Pentanol $71.41.0$ $\geq 99.5\%$ Macklin $C_5H_{1.0}O$ 1327 8700 2.Heptanol $543.49.7$ $\geq 98.0\%$ Aladin $C_8H_{10}O$ 1456 3220 3.Octenol $3391.86.4$ $\geq 98.0\%$ Aladin $C_8H_{10}O$ 1400 5490 1.Heptanol $111.70.6$ $\geq 95.0\%$ Macklin $C_9H_{20}O$ 1511 3240 2.Nonanol $628.99.9$ $\geq 98.0\%$ Aladin $C_8H_{10}O$ 1512 3000 2.Nonanol $111.87.5$ $\geq 99.5\%$ Macklin $C_9H_{10}O$ 1512 3000 2.Phenylethanol 012.8 $\geq 99.5\%$ Aladin $C_8H_{10}O$ 1812 9000 2.Phenylethanol $122.99.6$ $\geq 99.5\%$ Macklin $C_9H_{10}O$ 1812 3400 2.Phenoxylethanol $104.50.7$ $\geq 98.0\%$ Sigma-Aldrich $C_8H_{10}O$ 1814 4140 δ -Octalactone $104.50.7$ $\geq 98.0\%$ Sigma-Aldrich $C_1H_{20}O$ 1814 4140 δ -Octalactone $104.50.7$ $\geq 98.0\%$ Sigma-Aldrich $C_1H_{10}O$ 1852 3260 γ -Nonalactone $104.51.7$ $\geq 98.0\%$ Sigma-Aldrich $C_1H_{10}O$ 1852 3260 γ -Nonalactone $104.51.7$ $\geq 98.0\%$ Sigma-Aldrich $C_1H_{0}O$	Benzeneacetaldehyde	122-78-1	>95.0%	Macklin	C ₈ H ₈ O	1574	5720
Isobutanol $78-83-1$ $\geq 99.5\%$ Aladdin $C_4H_{10}O$ 11220620Isoamylol123-51-3 $\geq 99.5\%$ Aladdin $C_5H_{12}O$ 1217788201-Pentanol71-41-0 $\geq 99.5\%$ Macklin $C_5H_{12}O$ 125963402-Heptanol543-49-7 $>98.0\%$ Aladdin $C_7H_{16}O$ 132787003-Octenol3391-86-4 $>98.0\%$ Aladdin $C_8H_{10}O$ 146054201-Heptanol111-70-6 $>95.0\%$ Macklin $C_8H_{10}O$ 151132402-Nonanol628-99-9 $\geq 98.0\%$ Aladdin $C_8H_{10}O$ 151290602-Nonanol122-99-6 $\geq 99.5\%$ Macklin $C_8H_{10}O$ 1817506902-Phenylethanol60-12-8 $\geq 99.5\%$ Macklin $C_8H_{10}O$ 181441402-Phenylethanol104-50-7 $>98.0\%$ Sigma-Aldrich $C_8H_{10}O_2$ 184234802-Nonalactone104-61-0 $>98.0\%$ Sigma-Aldrich $C_8H_{10}O_2$ 18423480 γ -Notalactone104-61-0 $>98.0\%$ Sigma-Aldrich $C_8H_{10}O_2$ 1980320 γ -Decalactone104-61-0 $>98.0\%$ Sigma-Aldrich $C_8H_{10}O_2$ 1980320 γ -Indecalactone104-61-0 $>98.0\%$ Sigma-Aldrich $C_8H_{10}O_2$ 1980320 γ -Decalactone104-61-0 $>98.0\%$ Sigma-Aldrich $C_8H_{0}O_3$ 198320 γ -Decalactone104-61-6 $>98.0\%$ Sigma-Aldrich </td <td>High alcohols</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	High alcohols						
Isoamylol123-51-3 $\geq 99.5\%$ Aladdin $C_5H_{12}O$ 1217788201-Pentanol71-41-0 $\geq 99.5\%$ Macklin $C_5H_{12}O$ 125963402-Heptanol543-49-7>>8.0%Aladdin $C_7H_{16}O$ 132787003-Octenol3391-86-4>>8.0%Aladdin $C_8H_{10}O$ 145632201-Heptanol111-70-6>>50.0%Macklin $C_{11}H_{20}O$ 151132402-Nonanol628-99-9 $\geq 98.0\%$ Aladdin $C_9H_{20}O$ 151132401-Octanol111-87-5 $\geq 99.5\%$ Macklin $C_8H_{10}O$ 1817506902-Phenylethanol60-12-8 $\geq 99.5\%$ Macklin $C_8H_{10}O$ 1817506902-Phenylethanol102-99-6 $\geq 99.5\%$ Macklin $C_8H_{10}O$ 181441408-Octalactone104-50-7>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 181441408-Octalactone104-61-0>98.0%Sigma-Aldrich $C_8H_{10}O_2$ 182032609-Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8H_{10}O_2$ 192532609-Decalactone599-04-2>99.0%Sigma-Aldrich $C_8H_{10}O_2$ 193198609-Decalactone28664-35-9>97.0%Sigma-Aldrich $C_{10}H_{10}O_2$ 10437009-Decalactone28664-35-9>97.0%Sigma-Aldrich $C_8H_8O_3$ 210435209-Decalactone106-76>98.0%Sigma-Aldrich C_8H_8O	Isobutanol	78-83-1	≥99.5%	Aladdin	$C_4H_{10}O$	1112	20620
1-Pentanol 71-41-0 $\geq 95.\%$ Macklin $C_{g}H_{12}O$ 1259 6340 2-Heptanol 543-49-7 >98.0% Aladdin $C_{r}H_{16}O$ 1327 8700 3-Octenol 3391-86-4 >98.0% Aladdin $C_{g}H_{16}O$ 1456 3220 1-Heptanol 111-70-6 >95.0% Macklin $C_{g}H_{10}O$ 1511 3240 2-Nonanol 628-99-9 ≥98.0% Aladdin $C_{g}H_{10}O$ 1512 3240 1-Octanol 111-87-5 ≥99.5% Macklin $C_{g}H_{10}O$ 1817 50690 2-Phenylethanol 60-12-8 ≥99.5% Macklin $C_{g}H_{10}O$ 1817 50690 2-Phenoxyethanol 122-99-6 ≥99.5% Macklin $C_{g}H_{10}O$ 1817 50690 2-Phenoxyethanol 104-50-7 >98.0% Sigma-Aldrich $C_{11}H_{20}O_2$ 1814 4140 6-Octalactone 698-76-0 >98.0% Sigma-Aldrich $C_{g}H_{16}O_2$ 1925 3260 9-No	Isoamylol	123-51-3	≥99.5%	Aladdin	C ₅ H ₁₂ O	1217	78820
2-Heptanol543-49-7>98.0%Aladdin $C_7H_{16}O$ 132787003-Octenol3391-86-4>98.0%Aladdin $C_8H_{16}O$ 145632201-Heptanol111-70-6>95.0%Macklin $C_7H_{16}O$ 146054902-Nonanol628-99-9≥98.0%Aladdin $C_9H_{20}O$ 151132401-Octanol111-87-5≥99.5%Macklin $C_8H_{16}O$ 153290602-Phenylethanol60-12-8≥99.5%Macklin $C_8H_{10}O$ 1817506902-Phenoxyethanol122-99-6≥99.5%Macklin $C_8H_{10}O_2$ 18144140 γ -Octalactone104-50-7>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 18144140 δ -Octalactone698-76-0>98.0%Sigma-Aldrich $C_8H_{10}O_2$ 18123260 γ -Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 18623480 γ -Decalactone599-04-2>99.0%Sigma-Aldrich $C_8H_{14}O_2$ 19253260Pantolactone599-04-2>99.0%Sigma-Aldrich $C_{10}H_{10}O_2$ 193519860 γ -Decalactone706-14-9>98.0%Sigma-Aldrich $C_{10}H_{10}O_2$ 20413700Sotolon2864-35-9>97.0%Sigma-Aldrich $C_{10}H_{10}O_2$ 21613520 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 16143520Actid107-92-6≥95.%Sigma-Aldrich <td>1-Pentanol</td> <td>71-41-0</td> <td>≥99.5%</td> <td>Macklin</td> <td>C₅H₁₂O</td> <td>1259</td> <td>6340</td>	1-Pentanol	71-41-0	≥99.5%	Macklin	C ₅ H ₁₂ O	1259	6340
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 \geq 98.0% Aladdin $C_9H_{20}O$ 1511 3240 1-Octanol 111-87-5 \geq 99.5% Macklin $C_8H_{18}O$ 1532 9060 2-Phenylethanol 60-12-8 \geq 99.5% Aladdin $C_9H_{10}O_2$ 2043 9900 2-Phenyyethanol 122-99-6 \geq 99.5% Macklin $C_8H_{10}O_2$ 2043 9900 Lactone 104-50-7 \geq 99.5% Macklin $C_1H_{20}O_2$ 1814 4140 \diamond -Octalactone 104-61-0 \geq 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 $C_8H_{16}O_3$ 1935 19860 γ -Decalactone 706-14-9 $>$ 98.0% Sigma-Aldrich $C_1H_{19}O_2$	2-Heptanol	543-49-7	>98.0%	Aladdin	C ₇ H ₁₆ O	1327	8700
1-Heptanol111-70-6>95.0%Macklin $C_7H_{16}O$ 146054902-Nonanol628-99-9 $\geq 98.0\%$ Aladdin $C_9H_{12}O$ 151132401-Octanol111-87-5 $\geq 99.5\%$ Macklin $C_8H_{18}O$ 153290602-Phenylethanol60-12-8 $\geq 99.5\%$ Aladdin $C_8H_{10}O$ 1817506902-Phenoxyethanol122-99-6 $\geq 99.5\%$ Macklin $C_8H_{10}O_2$ 20439900 Lactone γ -Octalactone104-50-7 $\geq 98.0\%$ Sigma-Aldrich $C_{11}H_{20}O_2$ 18144140 δ -Octalactone698-76-0 $\geq 98.0\%$ Sigma-Aldrich $C_8H_{14}O_2$ 18623480 γ -Nonalactone104-61-0 $\geq 98.0\%$ Sigma-Aldrich $C_8H_{14}O_2$ 19253260Pantolactone599-04-2 $\geq 99.0\%$ Sigma-Aldrich $C_1H_{10}O_3$ 193519860 γ -Decalactone706-14-9 $\geq 98.0\%$ Sigma-Aldrich $C_1H_{10}O_2$ 1043700Sotolon28664-35-9 $\geq 97.0\%$ Sigma-Aldrich $C_1H_{00}O_3$ 193519860 γ -Undecalactone104-67-6 $\geq 98.0\%$ Sigma-Aldrich $C_1H_{20}O_2$ 1613520Acid Σ -Undecalactone104-67-6 $\geq 99.5\%$ Sigma-Aldrich $C_1H_{20}O_2$ 1613520Acid Σ -Undecalactone107-92-6 $\geq 99.5\%$ Sigma-Aldrich $C_1H_{20}O_2$ 1613520Acid Σ -Undecalacton107-92-6 $\geq 99.5\%$ Mack	3-Octenol	3391-86-4	>98.0%	Aladdin	$C_8H_{16}O$	1456	3220
2-Nonanol $628-99-9$ $\geq 98.0\%$ Aladdin $C_9H_{20}O$ 1511 3240 1-Octanol111-87-5 $\geq 99.5\%$ Macklin $C_8H_{16}O$ 1532 9060 2-Phenylethanol $60-12-8$ $\geq 99.5\%$ Aladdin $C_8H_{10}O$ 1817 50690 2-Phenoxyethanol $122-99-6$ $\geq 99.5\%$ 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 $C_8H_{10}O_3$ 1935 19860 γ -Docalactone $706-14-9$ $>98.0\%$ Sigma-Aldrich $C_{10}H_{18}O_2$ 2041 3700 Sotolon $28664-35-9$ $>97.0\%$ Sigma-Aldrich $C_{10}H_{18}O_2$ 2041 3700 γ -Undecalactone $104-67-6$ $>98.0\%$ Sigma-Aldrich $C_{10}H_{10}O_3$ 1935 19860 γ -Undecalactone $104-67-6$ $>98.0\%$ Sigma-Aldrich $C_{10}H_{10}O_2$ 2161 3520 γ -Undecalactone $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_{1}H_{20}O_2$ 161 3520 Hatanoic acid $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_8H_{10}O_2$ 1574 30960 <td>1-Heptanol</td> <td>111-70-6</td> <td>>95.0%</td> <td>Macklin</td> <td>C₇H₁₆O</td> <td>1460</td> <td>5490</td>	1-Heptanol	111-70-6	>95.0%	Macklin	C ₇ H ₁₆ O	1460	5490
1-Octanol111-87-5 $\geq 99.5\%$ Macklin $C_8H_{18}O$ 153290602-Phenylethanol60-12-8 $\geq 99.5\%$ Aladdin $C_8H_{10}O$ 1817506902-Phenoxyethanol122-99-6 $\geq 99.5\%$ Macklin $C_8H_{10}O_2$ 20439900Lactone γ -Octalactone104-50-7 $>98.0\%$ Sigma-Aldrich $C_{11}H_{20}O_2$ 18144140 δ -Octalactone698-76-0 $>98.0\%$ Sigma-Aldrich $C_8H_{14}O_2$ 18623480 γ -Nonalactone104-61-0 $>98.0\%$ Sigma-Aldrich $C_8H_{14}O_2$ 19253260Pantolactone599-04-2 $>99.0\%$ Sigma-Aldrich $C_8H_{10}O_3$ 193519860 γ -Decalactone706-14-9 $>98.0\%$ Sigma-Aldrich $C_{6}H_{10}O_3$ 193519860 γ -Duckcalactone706-14-9 $>98.0\%$ Sigma-Aldrich $C_{10}H_{18}O_2$ 20413700Sotolon28664-35-9 $>97.0\%$ Sigma-Aldrich $C_{10}H_{8}O_3$ 21084980 γ -Undecalactone104-67-6 $>98.0\%$ Sigma-Aldrich $C_1H_{20}O_2$ 1613520Acid $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_{4}H_{8}O_2$ 157430960Hexanoic acid107-92-6 $\geq 99.5\%$ Macklin $C_6H_{12}O_2$ 176225780Ethylhexanoic acid142-62-1 $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 197356880Octanoic acid124-07-2 $\geq 99.5\%$ Aladdin	2-Nonanol	628-99-9	≥98.0%	Aladdin	C ₉ H ₂₀ O	1511	3240
2-Phenylethanol $60-12-8$ $\geq 99.5\%$ Aladdin $C_8H_{10}O$ 1817 50690 2-Phenoxyethanol $122-99-6$ $\geq 99.5\%$ 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 $C_8H_{14}O_2$ 1862 3480 Pantolactone $599-04-2$ $>99.0\%$ Sigma-Aldrich $C_6H_{10}O_3$ 1935 19860 γ -Nonalactone $599-04-2$ $>99.0\%$ Sigma-Aldrich $C_6H_{10}O_3$ 1935 19860 γ -Decalactone $706-14-9$ $>98.0\%$ Sigma-Aldrich $C_10H_{18}O_2$ 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 $C_1H_{20}O_2$ 2161 3520 Acid $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_4H_8O_2$ 1574 30960 Hexanoic acid $107-92-6$ $\geq 99.5\%$ Macklin $C_6H_{12}O_2$ 1762 25780 Ethylhexanoic acid $142-62-1$ $\geq 99.5\%$ Macklin $C_8H_{16}O_2$ 1973 56880 Octanoic acid $124-07-2$ $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 1973 56880 Decanoic acid <td>1-Octanol</td> <td>111-87-5</td> <td>≥99.5%</td> <td>Macklin</td> <td>C₈H₁₈O</td> <td>1532</td> <td>9060</td>	1-Octanol	111-87-5	≥99.5%	Macklin	C ₈ H ₁₈ O	1532	9060
2-Phenoxyethanol122-99-6≥99.5%Macklin $C_8 H_{10} O_2$ 20439900Lactone γ -Octalactone104-50-7>98.0%Sigma-Aldrich $C_{11} H_{20} O_2$ 18144140δ-Octalactone698-76-0>98.0%Sigma-Aldrich $C_8 H_{14} O_2$ 18623480 γ -Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8 H_{14} O_2$ 19253260Pantolactone599-04-2>99.0%Sigma-Aldrich $C_6 H_{10} O_3$ 193519860 γ -Decalactone706-14-9>98.0%Sigma-Aldrich $C_{10} H_{10} O_2$ 20413700Sotolon28664-35-9>97.0%Sigma-Aldrich $C_6 H_8 O_3$ 21084980 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_1 H_{20} O_2$ 21613520AcidButanoic acid107-92-6≥99.5%Sigma-Aldrich $C_4 H_8 O_2$ 157430960Hexanoic acid142-62-1≥99.5%Macklin $C_6 H_{12} O_2$ 176225780Ethylhexanoic acid149-57-5≥99.9%Aladdin $C_8 H_{16} O_2$ 197356880Octanoic acid124-07-2≥99.5%Aladdin $C_8 H_{16} O_2$ 197356880	2-Phenylethanol	60-12-8	≥99.5%	Aladdin	C ₈ H ₁₀ O	1817	50690
Lactone γ -Octalactone104-50-7>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 18144140δ-Octalactone698-76-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 18623480 γ -Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 19253260Pantolactone599-04-2>99.0%Sigma-Aldrich $C_6H_{10}O_3$ 193519860 γ -Decalactone706-14-9>98.0%Sigma-Aldrich $C_{0}H_{10}O_3$ 20413700Sotolon28664-35-9>97.0%Sigma-Aldrich $C_{10}H_{18}O_2$ 20413520 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_1H_{20}O_2$ 21613520AcidButanoic acid107-92-6≥99.5%Sigma-Aldrich $C_4H_8O_2$ 157430960Hexanoic acid142-62-1≥99.5%Aladdin $C_8H_{10}O_2$ 160010090Octanoic acid124-07-2≥99.5%Aladdin $C_8H_{10}O_2$ 197356880Decanoic acid334-48-5>99.0%Aladdin $C_{n}H_{m}O_2$ 219020170	2-Phenoxyethanol	122-99-6	≥99.5%	Macklin	$C_8H_{10}O_2$	2043	9900
γ -Octalactone104-50-7>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 18144140 δ -Octalactone698-76-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 18623480 γ -Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 19253260Pantolactone599-04-2>99.0%Sigma-Aldrich $C_6H_{10}O_3$ 193519860 γ -Decalactone706-14-9>98.0%Sigma-Aldrich $C_10H_{18}O_2$ 20413700Sotolon28664-35-9>97.0%Sigma-Aldrich $C_10H_{18}O_2$ 21613520 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_1H_{20}O_2$ 21613520AcidButanoic acid107-92-6≥99.5%Sigma-Aldrich $C_4H_8O_2$ 157430960Hexanoic acid142-62-1≥99.5%Aladdin $C_8H_{10}O_2$ 166010090Octanoic acid124-07-2≥99.5%Aladdin $C_8H_{10}O_2$ 197356880Decanoic acid334-48-5>99.0%Aladdin $C_{n}H_{m}O_2$ 219020170	Lactone		22.22/		0 11 0		
6-Octalactone698-76-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 18623480 γ -Nonalactone104-61-0>98.0%Sigma-Aldrich $C_8H_{14}O_2$ 19253260Pantolactone599-04-2>99.0%Sigma-Aldrich $C_6H_{10}O_3$ 193519860 γ -Decalactone706-14-9>98.0%Sigma-Aldrich $C_{10}H_{18}O_2$ 20413700Sotolon28664-35-9>97.0%Sigma-Aldrich $C_6H_8O_3$ 21084980 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_1H_{20}O_2$ 21613520AcidButanoic acid107-92-6≥99.5%Sigma-Aldrich $C_6H_8O_3$ 157430960Hexanoic acid142-62-1≥99.5%Macklin $C_6H_{12}O_2$ 176225780Ethylhexanoic acid124-07-2≥99.5%Aladdin $C_8H_{16}O_2$ 197356880Decanoic acid334-48-5>99.0%Aladdin $C_{10}H_{20}O_2$ 210020170	γ-Octalactone	104-50-7	>98.0%	Sigma-Aldrich	$C_{11}H_{20}O_2$	1814	4140
γ -Nonlactone $104-61-0$ >98.0%Sigma-Aldrich $C_8H_{14}O_2$ 1925 3260 Pantolactone $599-04-2$ >99.0%Sigma-Aldrich $C_8H_{10}O_3$ 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 $C_1H_{20}O_2$ 2161 3520 AcidHexanoic acid $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_4H_8O_2$ 1574 30960 Hexanoic acid $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_6H_{12}O_2$ 1762 25780 Ethylhexanoic acid $149-57-5$ $\geq 99.9\%$ Aladdin $C_8H_{16}O_2$ 1860 10090 Octanoic acid $124-07-2$ $\geq 99.5\%$ Aladdin $C_8H_{10}O_2$ 1973 56880 Decanoic acid $334-48-5$ $>90.0\%$ Aladdin $C_{10}H_{20}O_2$ 2100 20170	8-Octalactone	698-76-0	>98.0%	Sigma-Aldrich	C ₈ H ₁₄ O ₂	1862	3480
Pantolactone599-04-2>99.0%Sigma-Aldrich $C_{e}H_{10}O_{3}$ 193519860 γ -Decalactone706-14-9>98.0%Sigma-Aldrich $C_{10}H_{18}O_{2}$ 20413700Sotolon28664-35-9>97.0%Sigma-Aldrich $C_{6}H_{8}O_{3}$ 21084980 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_{11}H_{20}O_{2}$ 21613520AcidButanoic acid107-92-6≥99.5%Sigma-Aldrich $C_{4}H_{8}O_{2}$ 157430960Hexanoic acid142-62-1≥99.5%Macklin $C_{6}H_{12}O_{2}$ 176225780Ethylhexanoic acid149-57-5≥99.9%Aladdin $C_{8}H_{16}O_{2}$ 186010090Octanoic acid124-07-2≥99.5%Aladdin $C_{8}H_{16}O_{2}$ 197356880Decanoic acid334-48-5>99.0%Aladdin $C_{10}H_{20}O_{2}$ 210020170	γ-Nonalactone	104-61-0	>98.0%	Sigma-Aldrich	C ₈ H ₁₄ O ₂	1925	3260
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 $C_8H_8O_3$ 2108 4980 γ -Undecalactone $104-67-6$ >98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 2161 3520 AcidButanoic acid $107-92-6$ $\geq 99.5\%$ Sigma-Aldrich $C_4H_8O_2$ 1574 30960 Hexanoic acid $142-62-1$ $\geq 99.5\%$ Macklin $C_6H_{12}O_2$ 1762 25780 Ethylhexanoic acid $149-57-5$ $\geq 99.9\%$ Aladdin $C_8H_{16}O_2$ 1860 10090 Octanoic acid $124-07-2$ $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 1973 56880 Decanoic acid $334-48-5$ $>90.0\%$ Aladdin $C_{10}H_{20}O_2$ 2190 20170	Pantolactone	599-04-2	>99.0%	Sigma-Aldrich	$C_6H_{10}O_3$	1935	19860
Solion $2864-35-9$ >97.0%Sigma-Aldrich $C_6H_8O_3$ 2108 4980 γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 21613520AcidButanoic acid107-92-6 $\geq 99.5\%$ Sigma-Aldrich $C_4H_8O_2$ 157430960Hexanoic acid142-62-1 $\geq 99.5\%$ Macklin $C_6H_{12}O_2$ 176225780Ethylhexanoic acid149-57-5 $\geq 99.9\%$ Aladdin $C_8H_{16}O_2$ 186010090Octanoic acid124-07-2 $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 197356880Decanoic acid334-48-5>99.0%Aladdin $C_{10}H_{20}O_2$ 210020170	γ-Decalactone	706-14-9	>98.0%	Sigma-Aldrich	$C_{10}H_{18}O_2$	2041	3700
γ -Undecalactone104-67-6>98.0%Sigma-Aldrich $C_{11}H_{20}O_2$ 21613520AcidButanoic acid107-92-6 \geq 99.5%Sigma-Aldrich $C_4H_8O_2$ 157430960Hexanoic acid142-62-1 \geq 99.5%Macklin $C_6H_{12}O_2$ 176225780Ethylhexanoic acid149-57-5 \geq 99.9%Aladdin $C_8H_{16}O_2$ 186010090Octanoic acid124-07-2 \geq 99.5%Aladdin $C_8H_{16}O_2$ 197356880Decanoic acid334-48-5>99.0%Aladdin $C_{10}H_{20}O_2$ 219020170	Sotolon	28664-35-9	>97.0%	Sigma-Aldrich	C ₆ H ₈ O ₃	2108	4980
ArticleButanoic acid107-92-6 $\geq 99.5\%$ Sigma-Aldrich $C_4H_8O_2$ 157430960Hexanoic acid142-62-1 $\geq 99.5\%$ Macklin $C_6H_{12}O_2$ 176225780Ethylhexanoic acid149-57-5 $\geq 99.9\%$ Aladdin $C_8H_{16}O_2$ 186010090Octanoic acid124-07-2 $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 197356880Decanoic acid334-48-5 $>99.0\%$ Aladdin $C_{10}H_{20}O_2$ 219020170	Acid	104-07-0	≫98.0%	Sigilia-Aldrich	$C_{11}\Pi_{20}O_2$	2101	3320
Butanoic actu 107-92-0 $\leq 99.5\%$ Sigma-Aldrich $C_4 H_8 O_2$ 1574 30960 Hexanoic acid 142-62-1 $\geq 99.5\%$ Macklin $C_6 H_{12} O_2$ 1762 25780 Ethylhexanoic acid 149-57-5 $\geq 99.9\%$ Aladdin $C_8 H_{16} O_2$ 1860 10090 Octanoic acid 124-07-2 $\geq 99.5\%$ Aladdin $C_8 H_{16} O_2$ 1973 56880 Decanoic acid 334-48-5 $>99.0\%$ Aladdin $C_{10} H_{20} O_2$ 2190 20170	Rutanoic acid	107.02.6	>00 E0/	Sigma Aldrich	CHO	1574	20060
Itexation actu I42-02-1 $\leq 99.5\%$ Macklin $C_6H_{12}O_2$ 1762 $25/80$ Ethylhexanoic acid 149-57-5 $\geq 99.9\%$ Aladdin $C_8H_{16}O_2$ 1860 10090 Octanoic acid 124-07-2 $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 1973 56880 Decanoic acid 334-48-5 $>99.0\%$ Aladdin $C_{10}H_{20}O_2$ 2190 20170	Herenoic acid	107-92-0	299.3%	Sigilia-Aldrich Modelin		17/4	25780
Litty in Cxanoc acid 149-57-5 $\geq 99.5\%$ Ataddin $C_8H_{16}O_2$ 1800 10090 Octanoic acid 124-07-2 $\geq 99.5\%$ Aladdin $C_8H_{16}O_2$ 1973 56880 Decanoic acid 334-48-5 $> 99.0\%$ Aladdin $C_{1n}H_{2n}O_2$ 2190 20170	Ethylbevanoic acid	142-02-1	≥99.3% >00.00/	Aladdin	CHO	1/02	10090
Decanoic acid 334-48-5 >99.0% Aladdin $C_{1n}H_{2n}O_2$ 19/3 50680	Octanoic acid	124-07 2	>90 50%	Aladdin	CH 0	1073	56880
Decanoic acia 354-40-5 235.070 Alduulli C ₁₀ 11 ₂₀ O ₂ 2170 20170	Decanoic acid	334-48-5	<u>~ 77.370</u>	Aladdin	С Н О	2190	20170
Benzoic acid 65-85-0 >99.9% Aladdin CHO 2378 11630	Benzoic acid	65-85-0	>99.9%	Aladdin	C-H-O	2378	11630
Continued	Continued				5/1602	2070	

Compounds	CAS No.	Purity	Manufacturer	Formula	RI	$Content^{h}/\mu g.L^{-1}$
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	$\mathrm{C_9H_{14}ON_2}$	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 ₆ H ₆ O ₃	2415	20050
Terpenes						
D-Limonene	5989-27-5	≥99.0%	TCI	C10H16	1203	1860
Terpinolene	586-62-9	>90.0%	TCI	C10H16	1284	2330
β-Linalool	78-70-6	>98.0%	Macklin	C10H18O	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	C13H20	1833	1560
Benzene						
o-Xylene	95-47-6	≥99.0%	Macklin	C_8H_{10}	1192	1520
Styrene	100-42-5	≥99.5%	Macklin	C ₈ H ₈	1264	2190
<i>p</i> -Cymene	99-87-6	≥99.5%	Macklin	C10H14	1273	2900
Naphthalene	91-20-3	\geq 99.5%	Macklin	C10H8	1635	2070
Volatile phenol						
4-Methylguaiacol	93-51-6	>99.0%	Sigma-Aldrich	$\mathrm{C_8H_{10}O_2}$	1860	2820
o-Cresol	95-48-7	>99.0%	Sigma-Aldrich	C ₇ H ₇ O	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 ₈ H ₈ O	2306	2540
Sulfide						
3-(Methylthio)propanol	505-10-2	≥99.0%	Macklin	C ₄ H ₁₀ OS	1618	6600
Internal standard						
4-Methyl-2-pentanol	108-11-2	≥98.0%	CNW ^f	C ₆ H ₁₄ O	1065	1000

Table 1. The information of standards used in this study. ^aShanghai Macklin Biochemical Co., Ltd (Shanghai, China). ^bAladdin Bio-Chem Technology (Shanghai, China). ^cAdamas Reagent, Co., Ltd. (Shanghai, China). ^dTCI Development Co., Ltd. (Shanghai, China). ^eSigma-Aldrich (St. Louis, MO, USA). ^fCNW Technologies GmbH (Duesseldorf, Germany). ^gBide Pharmatech Ltd. (Shanghai, China). ^hThe 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 residues³⁷, nitrosamines in children's products³⁸, persistent organic pollutants in the environment³⁹, soluble and extractable substances in package materials⁴⁰, stimulants and banned substances in urine⁴¹ and metabonomics⁴². GC-Orbitrap-MS can provide accurate qualitative quantification of benzene compounds in chili peppers⁴³. 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 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.

ImageImageImageImageImageImageImageImageImageImageEuroEuroEuroInten<		Precursor ions			Quantifier io	ns		Qualifier ions				
Non-NormalName <td>Compounds</td> <td>Exact mass</td> <td>Molecular</td> <td>Error mass</td> <td>Exact mass</td> <td>Molecular</td> <td>Error mass</td> <td>Exact mass</td> <td>Molecular</td> <td>Error mass</td>	Compounds	Exact mass	Molecular	Error mass	Exact mass	Molecular	Error mass	Exact mass	Molecular	Error mass		
matrixmatr	Ester	(111/2)	Iormuta	(ppm)	(111/2)	Toriniula	(PPm)	(111/2)	Iormula	(PPIII)		
matrix indipind	Ethyl butanoate				43 05422	C ₂ H ₂	-0.99526	88 05202	C.H.O.	0 7668		
market and anomaly and a strengt of the strengt o	Ethyl 2-methylbutanoate				74 03639	C ₂ H ₂ O ₂	0.2198	102.0677	C ₄ H ₈ O ₂	0.41588		
any sectorany sectorany sectorany sectorany sectorany sectorany sectorbeingy lacenationany sectorany sector <td< td=""><td>Ethyl isovalerate</td><td></td><td></td><td></td><td>57.06997</td><td>C.H.</td><td>0.2190</td><td>61 0285</td><td>C.H.O.</td><td>0.11900</td></td<>	Ethyl isovalerate				57.06997	C.H.	0.2190	61 0285	C.H.O.	0.11900		
andandandandandandandandandandandandBahy hermanateII </td <td>Isoamyl acetate</td> <td></td> <td></td> <td></td> <td>43 01782</td> <td>C.H.O</td> <td>-1.06298</td> <td>55 05433</td> <td>C.H.</td> <td>0.6148</td>	Isoamyl acetate				43 01782	C.H.O	-1.06298	55 05433	C.H.	0.6148		
many power	Methyl caproate				43 01782	C.H.O	-0.70828	74 03639	C.H.O.	0.52895		
mathy heptanomeindi	Ethyl hexanoate				43 05422	C ₂ H ₂	-0.99526	73 02851	C ₂ H ₂ O ₂	0.70783		
InductionImage	Ethyl heptanoate				73 02854	CaH-Oa	0 49889	88 05192	C.H.O.	0.42009		
math math <th< td=""><td>Ethyl lactate</td><td></td><td></td><td></td><td>45 03354</td><td>C₂H₂O</td><td>1 30819</td><td>56.0621</td><td>C.H.</td><td>0.9174</td></th<>	Ethyl lactate				45 03354	C ₂ H ₂ O	1 30819	56.0621	C.H.	0.9174		
modely modely<	Heptyl acetate				43 01778	C ₂ H ₂ O	-0.17621	70.07773	C ₂ H ₁₀	0.8118		
Barly appriate Image	Methyl octanoate				43 01782	C ₂ H ₂ O	-0.70828	74 03639	C ₂ H ₂ O ₂	0.73505		
Bayly - Mydroxphurytate Image Bayly - Mydroxphurytate Image Bayly - Mydroxphurytate Image	Ethyl caprylate				73.02845	C ₂ H ₂ O ₂	-0.44136	101.05977	CrH ₂ O ₂	-0.43741		
International basis International basis <thinternatecona basis<="" th=""> Internatecona basis</thinternatecona>	Ethyl 3-hydroxybutyrate				43 01778	C ₂ H ₂ O	-0.6196	71.01285	C ₂ H ₂ O ₂	1 29569		
Birly 1-Markan Birly	Ethyl nonanoate				73.02845	C ₂ H ₂ O ₂	-0.54583	101.05977	C ₂ H ₂ O ₂	-0.51291		
Intry capacity Intry capacity <thintry capacity<="" th=""> Intry c</thintry>	Ethyl 2-hydroxy-4-methylpentanoate				69.06999	C ₂ H ₀	0.12138	45.03355	C_H_O	1.22348		
http://product	Ethyl caprate				73.02853	C ₂ H ₂ O ₂	0.39441	61.0285	C ₂ H ₂ O ₂	0.28445		
L L <thl< th=""> L <thl< th=""> <thl< th=""></thl<></thl<></thl<>	Ethyl succinate				101.02348	C ₄ H ₂ O ₂	0.02484	73.02853	C ₂ H ₂ O ₂	0.60336		
Detay Detay <t< td=""><td>Methyl salicylate</td><td>152.04683</td><td>C₀H₀O₂</td><td>0.22088</td><td>120.02077</td><td>C₄H₂O₂</td><td>0.28082</td><td>92.02578</td><td>C.H.O</td><td>0.15454</td></t<>	Methyl salicylate	152.04683	C ₀ H ₀ O ₂	0.22088	120.02077	C ₄ H ₂ O ₂	0.28082	92.02578	C.H.O	0.15454		
Index <th< td=""><td>Ethyl benzeneacetate</td><td>164.08322</td><td>C₁₀H₁₂O₂</td><td>0.24546</td><td>91.05439</td><td>C₂H₂</td><td>-0.13544</td><td>136.05219</td><td>C₀H₀O₂</td><td>0.66442</td></th<>	Ethyl benzeneacetate	164.08322	C ₁₀ H ₁₂ O ₂	0.24546	91.05439	C ₂ H ₂	-0.13544	136.05219	C ₀ H ₀ O ₂	0.66442		
Instruction Instruction <thinstruction< th=""> <thinstruction< th=""></thinstruction<></thinstruction<>	Ethyl salicylate	166.06245	C ₀ H ₁₀ O ₂	0.05133	120.02077	C-H.O	0.40795	92.02578	C.H.O	0.15454		
IndexIndexIndexIndexIndexIndexIndexIndexIndexIndexIndexIndexIndexEthyl cinnante176.0831 C_{11L_DQ} 0.96579131.04938 $C_{41,Q}$ 0.9030773.02853 $C_{41,Q}$ 0.60336Monoethyl succinate11111110.03348 $C_{41,Q}$ 0.1003673.02853 $C_{41,Q}$ 0.60336CH-Pertual111110.1779569.03339 $C_{41,Q}$ 0.46658(b)-2-Chenal1183.04919 $C_{41,Q}$ 0.1779541.03839 $C_{41,Q}$ -4.80253(b)-2-Chenal1111114.0389 $C_{41,Q}$ 11-4.80253(b)-2-Chenal1111111111111-4.8025311 <td>Ethyl hydrocinnamate</td> <td>178.09898</td> <td>CuHuO</td> <td>0.85652</td> <td>104.06216</td> <td>C₀H₀</td> <td>0.34761</td> <td>105.06997</td> <td>C₀H₀</td> <td>0.15241</td>	Ethyl hydrocinnamate	178.09898	CuHuO	0.85652	104.06216	C ₀ H ₀	0.34761	105.06997	C ₀ H ₀	0.15241		
honoethyl succinatehonoethyl su	Ethyl cinnamate	176.08331	C ₁₁ H ₁₂ O ₂	0.96579	131.04938	C ₀ H ₂ O	0.98604	103.05436	C ₀ H ₇	0.62066		
Carbony compoundsCarbony compoundsCarbony compounds(E)-2-HexenalII83.04919 C_3H_2O 0.1779569.03339 C_6H_9O 0.46658(E)-2-HeptenalI83.04919 C_3H_2O 0.5454241.03839 C_4H_5 -3.22212 (E)-2-OctenalII83.04919 C_3H_2O 0.1779541.03839 C_3H_5 -3.22212 (E)-2-OctenalII81.03377 C_3H_3O 0.26157109.0647 C_1H_9O 0.11559(E,2)-2,4-HeptadienalII11.112991.05439 C_3H_5 -4.33758 70.04136 C_1H_9O 0.41862Benzenecactaldehyde120.05711 C_8H_9O 1.1412991.05439 C_3H_5 -4.52349 45.03366 C_7H_9O 2.32468IsobutanolIII1.0384 C_3H_5 -4.52349 45.03366 C_2H_9O 2.32468IsobutanolIIIIIIIIIIII-PetnanolIII	Monoethyl succinate		01112 0 2		101.02348	C ₄ H ₂ O ₂	0.10036	73.02853	C ₂ H ₂ O ₂	0.60336		
Barbon Market	Carbonyl compounds					-433			03502			
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	(E)-2-Hexenal				83.04919	CrH-O	0.17795	69.03339	C.H.O	0.46658		
(b) 1 or primin (c) 1	(E)-2-Heptenal				83 04919	C-H-O	0 54542	41 03839	C _o H _c	-3 22212		
(c) Forthal(c) Forth	(E)-2-Octenal				83 04919	C-H-O	0.17795	41 03839	C ₂ H ₂	-4 80235		
(c))((E, F)-2.4-Heptadienal				81 03347	C-H-O	-0.26157	109.0647	C_H_O	0 11559		
(A)((<i>E</i> , <i>Z</i>)-2.6-Nonadienal				41.03839	C ₂ H ₂	-4.33758	70.04136	C.H.O	-0.48152		
High alcohols High alcohols High alcohols January and allow allows January allows Galaxy allows	Benzeneacetaldehyde	120.05711	C ₀ H ₀ O	1.14129	91.05439	C ₂ H ₂	0.61866	92.06208	C ₇ H ₀	0.31004		
δ 41.0384 C ₃ H ₅ -4.52349 45.0336 C ₂ H ₃ O 2.32468 Isoamylol I 6 57.0699 C ₄ H ₉ 0.41428 70.07784 C ₃ H ₁₀ 0.37632 1-Pentanol I 6 57.0699 C ₄ H ₉ 0.54796 70.07784 C ₃ H ₁₀ 0.59406 2-Heptanol I 6 57.06991 C ₄ H ₉ 0.88465 83.08566 C ₆ H ₁₁ 0.5339 3-Octenol I I 6 57.03555 C ₃ H ₃ O 0.49786 85.06478 C ₅ H ₉ O 0.5096 1-Heptanol I I 6 57.03355 C ₃ H ₃ O 0.49786 85.06478 C ₅ H ₉ O 0.5096 1-Heptanol I I 6 57.03355 C ₃ H ₃ O 1.06288 70.07384 C ₅ H ₉ O 0.50896 1-Heptanol I I 105.03364 C ₇ H ₃ O 1.04819 I.04910 I.20.0542 C ₇ H ₆ O 0.50896 2-Nonanol I I I <td>High alcohols</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	High alcohols											
Isoamylol <td>Isobutanol</td> <td></td> <td></td> <td></td> <td>41.0384</td> <td>C₂H₅</td> <td>-4.52349</td> <td>45.0336</td> <td>C₂H₅O</td> <td>2.32468</td>	Isobutanol				41.0384	C ₂ H ₅	-4.52349	45.0336	C ₂ H ₅ O	2.32468		
1-PentanolImage: Constraint of the second seco	Isoamvlol				57.0699	C ₄ H ₀	0.41428	70.07784	C _r H ₁₀	0.37632		
2-HeptanolImage: Constraint of the section of the secti	1-Pentanol				57.06991	C ₄ H _o	0.54796	70.07784	C ₅ H ₁₀	0.59406		
AAA <th< td=""><td>2-Heptanol</td><td></td><td></td><td></td><td>45.03354</td><td>C₂H₅O</td><td>0.88465</td><td>83.08566</td><td>C₆H₁₁</td><td>0.5339</td></th<>	2-Heptanol				45.03354	C ₂ H₅O	0.88465	83.08566	C ₆ H ₁₁	0.5339		
1-HeptanolImage: Market M	3-Octenol				57.03355	C ₃ H ₅ O	0.49786	85.06478	C₅H₀O	0.50696		
2-NonanolImage: constraint of the second secon	1-Heptanol				43.05422	C ₂ H ₃ O	-1.06298	70.07338	C ₅ H ₁₀	0.48519		
1-OctanolImage: constraint of the second secon	2-Nonanol				105.03364	C ₇ H ₅ O	0.74249	122.03642	C ₇ H ₆ O ₂	0.75852		
2-Phenylethanol122.07275 $C_8H_{10}O$ 1.0631191.05439 C_7H_7 0.9538292.06208 C_7H_8 -0.51868 2-PhenoxyethanolIII08.05687 C_7H_8O -0.89706 94.04132 C_6H_6O 0.04701Lactone γ -UndecalactoneII	1-Octanol				69.06999	C ₅ H ₉	0.23184	55.05433	C ₄ H ₇	0.3996		
2-Phenoxyethanol 108.05687 C ₇ H ₈ O -0.89706 94.04132 C ₆ H ₆ O 0.04701 Lactone 94.04132 C ₆ H ₆ O 0.04701 γ-Undecalactone 85.02853 C ₄ H ₅ O ₂ 0.69766 95.0493 C ₆ H ₇ O 0.95817 δ-Octalactone 99.04407 C ₅ H ₇ O ₂ -0.11627 71.04915 C ₄ H ₇ O 0.74492 γ-Octalactone 85.02851 C ₄ H ₅ O ₂ -0.10989 57.03359 C ₃ H ₅ O 0.49786	2-Phenylethanol	122.07275	C ₈ H ₁₀ O	1.06311	91.05439	C ₇ H ₇	0.95382	92.06208	C ₇ H ₈	-0.51868		
Lactone Solution	2-Phenoxyethanol				108.05687	C ₇ H ₈ O	-0.89706	94.04132	C ₆ H ₆ O	0.04701		
γ-Undecalactone 85.02853 C ₄ H ₅ O ₂ 0.69766 95.0493 C ₆ H ₇ O 0.95817 δ-Octalactone 99.04407 C ₅ H ₇ O ₂ -0.11627 71.04915 C ₄ H ₇ O 0.74492 γ-Octalactone 85.02851 C ₄ H ₅ O ₂ -0.10899 57.03359 C ₃ H ₅ O 0.49786	Lactone					, .		1				
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	γ-Undecalactone				85.02853	C ₄ H ₅ O ₂	0.69766	95.0493	C ₆ H ₇ O	0.95817		
γ-Octalactone 85.02851 C ₄ H ₅ O ₂ -0.10989 57.03359 C ₃ H ₅ O 0.49786	δ-Octalactone				99.04407	C ₅ H ₇ O ₂	-0.11627	71.04915	C ₄ H ₇ O	0.74492		
	γ-Octalactone				85.02851	C ₄ H ₅ O ₂	-0.10989	57.03359	C ₃ H ₅ O	0.49786		
Pantolactone 71.04915 C_4H_7O 0.10063 43.05414 C_3H_7 -2.23569	Pantolactone				71.04915	C ₄ H ₇ O	0.10063	43.05414	C ₃ H ₇	-2.23569		
γ-Decalactone 85.02853 C ₄ H ₅ O ₂ 0.1593 95.0493 C ₆ H ₇ O 0.47656	γ-Decalactone				85.02853	C ₄ H ₅ O ₂	0.1593	95.0493	C ₆ H ₇ O	0.47656		
Sotolon 128.04693 C ₆ H ₈ O ₃ 0.18604 83.04919 C ₅ H ₇ O 0.08357 55.05427 C ₄ H ₇ 0.81287	Sotolon	128.04693	C ₆ H ₈ O ₃	0.18604	83.04919	C ₅ H ₇ O	0.08357	55.05427	C ₄ H ₇	0.81287		
γ-Nonalactone 85.02851 C ₄ H ₅ O ₂ -0.02016 57.03359 C ₃ H ₅ O 0.36409	γ-Nonalactone				85.02851	C ₄ H ₅ O ₂	-0.02016	57.03359	C ₃ H ₅ O	0.36409		
Acid	Acid	1	1	1	1		1	1		1		
Butanoic acid 60.02063 C ₂ H ₄ O ₂ 0.56154 73.02845 C ₃ H ₅ O ₂ 0.39441	Butanoic acid				60.02063	C ₂ H ₄ O ₂	0.56154	73.02845	C ₃ H ₅ O ₂	0.39441		
Hexanoic acid 73.02853 C ₃ H ₅ O ₂ 0.18547 60.02069 C ₃ H ₄ O ₂ 0.39361	Hexanoic acid				73.02853	C ₃ H ₅ O ₂	0.18547	60.02069	C ₂ H ₄ O ₂	0.39361		
Ethylhexanoic acid 73.02853 C ₃ H ₅ O ₂ 0.18547 87.04422 C ₄ H ₇ O ₂ 0.48125	Ethylhexanoic acid				73.02853	C ₃ H ₅ O ₂	0.18547	87.04422	C ₄ H ₇ O ₂	0.48125		
Octanoic acid 73.02853 C ₃ H ₅ O ₂ 0.18547 101.05988 C ₅ H ₆ O ₂ 0.6195	Octanoic acid				73.02853	C ₃ H ₅ O ₂	0.18547	101.05988	C ₅ H ₉ O ₂	0.6195		
Decanoic acid 73.02844 C ₃ H ₅ O ₂ 0.49889 101.05976 C ₅ H ₉ O ₂ 0.54401	Decanoic acid				73.02844	C ₃ H ₅ O ₂	0.49889	101.05976	C ₅ H ₉ O ₂	0.54401		
Continued	Continued	1	1	1	1		1	1	1			

	Precursor ion	15		Quantifier io	ns		Qualifier ions					
Compounds	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 ₇ H ₆ O ₂	0.75852	105.03364	C ₇ H ₅ O	0.66985	122.03642	C ₇ H ₆ O ₂	0.75852			
Pyrazine												
3-Isopropyl-2-methoxypyrazine	152.09455	C ₈ H ₁₂ ON ₂	0.50811	137.071	C ₇ H ₉ ON ₂	0.50114	124.06324	C ₆ H ₈ ON ₂	0.86187			
2-sec-Butyl-3-Methoxypyrazine	166.10973	C ₉ H ₁₄ ON ₂	-1.99624	138.07886	C ₇ H ₁₀ ON ₂	0.56568	124.06321	C ₆ H ₈ ON ₂	0.75882			
5-Ethyl-2,3-dimethylpyrazine	136.0996	C ₈ H 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 ₉ H ₁₄ ON ₂	0.08705	124.0632	C ₆ H ₈ ON ₂	0.58057	95.06044	C ₅ H ₇ N ₂	-0.08289			
Acetylpyrazine	122.04759	C ₆ H ₆ ON 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 ₃ H ₃	-3.43066			
Acetylfuran	110.03637	C ₆ H ₆ O ₂	0.42523	95.01281	$C_5H_3O_2$	0.64721	43.01782	C ₂ H ₃ O	-0.41717			
5-Methylfurfural	110.03625	C ₆ H ₆ O ₂	-0.47613	109.02855	$C_6H_5O_2$	0.68404	53.03864	C ₄ H ₅	1.24689			
Ethyl 2-furoate	140.04697	C ₇ H ₈ O ₃	0.56667	95.01279	$C_5H_3O_2$	-0.07548	112.01554	$C_5H_4O_3$	-0.07007			
Furfuryl alcohol	98.03629	C ₅ H ₆ O ₂	0.01035	97.02851	$C_5H_5O_2$	0.29686	81.0336	C ₅ H ₅ O	0.11503			
5-Hydroxymethylfurfural	126.03131	C ₆ H ₆ O ₃	0.34424	97.02849	C ₅ H ₅ O ₂	0.29686	69.03357	C ₄ H ₅ O	0.5771			
Terpenes												
D-Limonene	136.1252	C ₁₀ H ₁₆	1.65914	93.07005	C ₇ H ₉	1.89353	121.10146	C ₉ H ₁₃	1.60836			
Terpinolene	136.12471	C ₁₀ H ₁₆	0.4261	121.10132	C ₉ H ₁₃	0.22236	93.06999	C ₇ H ₉	0.25403			
β-Linalool				93.07005	C ₇ H ₉	0.41798	69.03339	C ₅ H ₉	0.3423			
Citronellyl acetate				81.06996	C ₆ H ₉	0.00931	95.08559	C ₇ H 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	C8H10	-0.11101	91.05439	C ₇ H ₇	0.03214	103.05429	C ₈ H ₇	0.62066			
Styrene	104.0621	C ₈ H ₈	-0.09229	104.0621	C ₈ H ₈	-0.09229	78.04652	C ₆ H ₆	0.78457			
<i>p</i> -Cymene	134.10954	C ₁₀ H ₁₄	0.39181	119.0857	C ₉ H ₁₁	0.05216	115.0543	C ₉ H ₇	0.68855			
Naphthalene	128.06218	C10H8	0.04416	128.06218	$C_{10}H_{8}$	0.04416	129.06557	C10H8	-3.16989			
Volatile phenol												
4-Methylguaiacol	138.06754	$C_8 H_{10} O_2$	0.04814	138.06754	$C_8 H_{10} O_2$	0.04814	123.04407	$C_7H_7O_2$	-0.00386			
o-Cresol	107.04918	C ₇ H ₇ O	0.20933	107.04918	C ₇ H ₇ O	0.20933	79.05427	C ₆ H 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 ₈ H ₈ O	0.14583	120.057	C ₈ H ₈ O	0.14583	91.05425	C ₇ H ₇	0.19972			
Sulfide												
3-(Methylthio)propanol	106.04483	C ₇ H ₆ O	3.52157	106.04483	C ₇ H ₆ O	3.52157	88.03425	C_7H_4	3.50426			
Internal standard												
4-Methyl-2-pentanol				45.03355	C ₂ H ₅ O	0.79994						

 Table 2.
 The qualitative and quantitative information of target volatile compounds. ^appm means parts per million mass error.

Methods

Overview of the experimental design. *Materials and methods*. Chemical and reagents The 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	\checkmark			\checkmark	\checkmark	\checkmark	\checkmark				\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	
Ethyl 2-methylbutanoate	\checkmark			\checkmark	\checkmark	\checkmark			\checkmark							
Ethyl isovalerate	\checkmark			\checkmark	\checkmark	\checkmark			\checkmark							
Isoamyl acetate				\checkmark	\checkmark	\checkmark										
Methyl caproate																
Ethyl hexanoate																
Ethyl heptanoate				\checkmark	\checkmark											
Ethyl lactate		\checkmark	\checkmark	\checkmark	\checkmark	\checkmark		\checkmark		\checkmark						\checkmark
Heptyl acetate	\checkmark		nd	\checkmark	nd	nd	nd	nd								
Methyl octanoate	\checkmark		\checkmark													
Ethyl caprylate	\checkmark															
Ethyl 3-hydroxybutyrate	\checkmark															
Ethyl nonanoate	\checkmark		\checkmark													
Ethyl 2-hydroxy-4-methylpentanoate	\checkmark	\bigvee	\checkmark													
Ethyl caprate	\checkmark															
Ethyl succinate	\checkmark		\checkmark													
Methyl salicylate	\checkmark		\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	nd	\checkmark						
Ethyl benzeneacetate	\checkmark															
Ethyl salicylate	\checkmark															
Ethyl hydrocinnamate	\checkmark															
Ethyl cinnamate	\checkmark															
Monoethyl succinate	\checkmark															
Carbonyl compounds																
(E)-2-Hexenal	\checkmark			\checkmark	\checkmark	\checkmark					\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
(E)-2-Heptenal	\checkmark															
(E)-2-Octenal	\checkmark															
(E,E)-2,4-Heptadienal	\checkmark		\checkmark													
(E,Z)-2,6-Nonadienal	\checkmark															
Benzeneacetaldehyde	\checkmark															
High Alcohols																
Isobutanol	\checkmark		\checkmark													
Isoamylol	\checkmark															
1-Pentanol	\checkmark		\checkmark	\checkmark	\checkmark	\checkmark		\checkmark								
2-Heptanol	\checkmark															
3-Octenol	\checkmark															
1-Heptanol	\checkmark															
2-Nonanol		\checkmark														
1-Octanol		\checkmark														
2-Phenylethanol		\checkmark														
2-Phenoxyethanol	\checkmark		\checkmark													
Lactone																
γ-Undecalactone	\checkmark		\checkmark													
δ-Octalactone	\checkmark		\checkmark													
γ-Octalactone	\checkmark															
Pantolactone	\checkmark															
γ-Decalactone	\checkmark															
Sotolon	\checkmark	\checkmark	\checkmark	\checkmark	nd	nd	\checkmark	nd	nd	\checkmark	nd	nd	nd	nd	nd	nd
γ-Nonalactone	\checkmark															
Acid																
Butanoic acid	\checkmark		\checkmark													
Hexanoic acid	nd	\checkmark	nd	\checkmark	\checkmark	\checkmark										\checkmark
Ethylhexanoic acid	nd	\checkmark	nd	\checkmark	\checkmark	\checkmark			\checkmark							
Octanoic acid	\checkmark	\checkmark		\checkmark	\checkmark	\checkmark			\checkmark							
Decanoic acid	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			\checkmark							
Benzoic acid	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark			\checkmark							
Pyrazine																
Continued																

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

 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. $1 \mu L$ 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 samples Headspace 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 μ L 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 μ m 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 $30 \text{ m} \times 0.25 \text{ mm} \times 0.25 \text{ µm}$ (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 $30 \text{ m} \times 0.25 \text{ µm}$ (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.

Administrator







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 MetaboLights⁴⁷, 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.

Additional information

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