International Food Research Journal 31(2): 276 - 305 (April 2024)
Journal homepage: *http://www.ifrj.upm.edu.my*

Review

A comprehensive review of quantified flavour components in Chinese *baijiu*

Xue, F. H., Zhou, J. Q. and *Yang, L. X.

College of Food and Chemical Engineering, Shaoyang University,
No. 28, Lane 3, Shaoshui West Road, Shaoyang 422000, Hunan, China

Article history

Received:
10 April 2023
Received in revised form:
22 January 2024
Accepted:
29 January 2024

Keywords

baijiu,
components,
quantification,
flavour compounds

Abstract

Baijiu, a Chinese distilled liquor, plays an essential role in Chinese life and culture. The intricate flavour profile and distinguished quality of *baijiu* are closely linked to its organic components, which encompass an array of elements such as esters, acids, alcohols, aldehydes, phenols, pyrazines, terpenes, and others. Consequently, the analysis of these components has emerged as a fundamental cornerstone for the study and comprehension of *baijiu*. In the present review, we succinctly encapsulate the latest research endeavours aimed at the identification and precise quantification of pivotal components within a diverse array of Chinese *baijiu* exhibiting varying aroma profiles. The culmination of this collective effort has yielded an impressive compendium comprising 397 quantified components, each with meticulously determined concentrations within *baijiu*. These components are categorised into major, medium, minor, and trace components, based on their respective concentration levels in *baijiu*. Furthermore, the focal attention on trace components, with concentrations below 1 mg L^{-1} threshold, is deliberately underscored. This emphasis is ascribed to the pivotal roles of these trace elements in shaping the nuanced flavour and overall quality of *baijiu*. As a result, the present review not only provides the most comprehensive reference compendium of quantified *baijiu* components to date, but also furnishes invaluable insights into the multifaceted study of Chinese *baijiu*.

DOI
https://doi.org/10.47836/ifrj.31.2.02

Introduction

Baijiu, a venerable traditional Chinese liquor with a rich historical legacy spanning over two millennia, has evolved to claim its place among the six principal distilled liquors globally, alongside well-known counterparts such as brandy, whiskey, vodka, gin, and rum (Jia *et al*., 2020). Renowned for its cultural significance, this liquor stands as an enduring symbol of felicity and good fortune within the Chinese tradition (Duan *et al*., 2022). Remarkably intricate in its craft, *baijiu* production traverses a complex process encompassing cooking, saccharification, fermentation, distillation, storage, and blending, as detailed by scholars such as Zheng and Han (2016), Jia *et al*. (2020), Zhao *et al*. (2021), and Duan *et al*. (2022). The outcome of this elaborate process yields four fundamental types of *baijiu*, each distinguished by its production methodology and unique flavour profile: strong-aroma, light-aroma, soy-sauce-aroma, and rice-aroma *baijiu*. Beyond its cultural significance, *baijiu* holds an indispensable role within the fabric of Chinese culture and the gastronomic landscape. In 2020, *baijiu*'s ubiquity was evident in its astonishing output, reaching 7.4 million kilolitres, generating a substantial profit amounting to 158.5 billion yuan (equivalent to approximately 24.9 billion US dollars), and exhibiting a steady upward trajectory (Duan *et al*., 2022). Given the prodigious consumption of *baijiu* and its profound impact on human health, it has emerged as a pivotal focal point within the realm of food science research in China (Sun *et al*., 2021). The burgeoning volume of research underscores the pivotal position that *baijiu* occupies in contemporary food science, attesting to its enduring importance in both cultural and scientific spheres.

The intricate weave of organic compounds within *baijiu*, ranging from esters, acids, alcohols, aldehydes, pyrazines, and others, forms the bedrock of its flavour and quality (Dung, 2013). Consequently, the analysis of these constituents has become the foundational pillar of *baijiu* research. This task is formidable given *baijiu*'s complex matrix,

*Corresponding author.
Email: y366001031@126.com

teeming with diverse organic compounds distinguished by varying structures and concentrations, thus making the identification and quantification of these components a challenging endeavour (Liu *et al*., 2022). Historically, up until the turn of the millennium, only the principal components with substantial concentrations (> 10 mg L^{-1}) were routinely detected in *baijiu*, owing to inefficacious pretreatment methods and restricted access to selective detectors such as mass spectrometers (MS). However, recent strides have been accomplished with the advent of highly efficient pretreatment methodologies such as solid-phase micro-extraction (SPME) and the proliferation of cutting-edge instrumentation, such as comprehensive two-dimensional gas chromatography combined with time-of-flight mass spectrometry (GC × GC-TOF-MS). These advancements have facilitated the identification and quantification of numerous trace compounds, with concentrations plunging as low as 0.1 μg L^{-1} or even lower, exemplified by terpenes (Wang *et al*., 2015) and pyrazines (Wu and Xu, 2013). Despite their relatively low concentrations, these trace compounds wield substantial influence over the flavour profile of *baijiu*, underscoring their pivotal role within its intricate sensory landscape. This emphasis on trace compounds not only elucidates the nuanced nature of *baijiu* production, but also underscores the critical importance of these elements in shaping its distinctive flavour.

The present review comprehensively and systematically compiles the natural compounds quantified in *baijiu*, aimed at furnishing valuable references and insights for the analysis of this revered Chinese liquor. The constituents are categorised into four distinct groups based on their concentrations within *baijiu*: major components (> 100 mg L^{-1}), medium components (10 - 100 mg L^{-1}), minor components (1 - 10 mg L^{-1}), and trace components (< 1 mg L^{-1}). It is important to note that components which are only qualitatively detected using MS but remain unquantified with standards have been deliberately excluded from the present review. This exclusion is predicated on the understanding that unquantified components provide limited insight into their functional role within *baijiu*, compounded by the high false positive rates associated with qualitative analysis using MS. Additionally, exogenous substances such as phthalates, pesticides, and heavy metals have been purposefully omitted from the purview of this paper. The rationale for this omission stems from the understanding that these substances can be mitigated through the use of appropriate raw materials and containers, and thus, do not fall within the principal domain of this specific analysis. By providing a meticulous focus on quantified natural compounds and carefully delineating the parameters of the review, this paper aims to enhance the understanding of *baijiu* composition and analysis, while deliberately steering clear of elements that fall outside the primary purview of this study.

Major components

Based on literature, 14 major components, excluding water and ethanol, are consistently detected at concentrations exceeding 100 mg L^{-1} (Table 1). These components are four esters (ethyl acetate, ethyl hexanoate, ethyl lactate, and ethyl butyrate), four acids (acetic acid, hexanoic acid, lactic acid, and butyric acid), four alcohols (methanol, propanol, isobutanol, and isoamylol), along with acetaldehyde and diethoxyethane. Owing to their substantial levels, these major components can be directly analysed using gas chromatography coupled with flame ionisation detector (GC-FID) without prior treatment (Xu, 2019). Crucial to the overarching *baijiu* flavour, these major components lead to a framework for its distinct taste spectrum. Given that the primary acids can react with abundant ethanol to produce the corresponding esters, and vice versa (Reactions 1 - 4), it is evident that esterification and hydrolysis play a central role in the complex reactions within *baijiu*. Additionally, it is suggested that these esters might also serve as by-products of microbial metabolism during fermentation (Yu *et al*., 2022). With a typically pleasant fruity aroma, esters significantly contribute to the overall fragrance of *baijiu*. Notably, ethyl hexanoate, due to its high concentration and low odour threshold (Table 1), exerts a dominant influence on the flavour profile of strong-aroma *baijiu*. Indeed, the content of ethyl hexanoate and its ratio to other major ethyl esters play a defining role in shaping the quality and style of strong-aroma *baijiu* (Shao *et al*., 2005). To achieve an optimal flavour in high-quality strong-aroma *baijiu*, the ideal ratio of ethyl hexanoate to ethyl lactate, ethyl acetate, and ethyl butyrate should be approximately 1:(0.6 - 0.8):(0.5 - 0.6):0.1 (Shao *et al*., 2005). Conversely, in light-aroma *baijiu*, ethyl acetate serves as the primary ester, with a moderate presence of ethyl lactate. Importantly, esters are not solely responsible for the

Table 1. Major components in *baijiu*.

No.	Name	CAS No.	Odour description[a]	Content (mg L^{-1})	Threshold[b] (mg L^{-1})	OAV [c]
1	Ethyl acetate	141-78-6	Fruity	1438 (Xu, 2019), 1076 (Cao, 2014), 985 (Dong, 2020), 2628 (Ma, 2014), 183 (Sha, 2017), 2444 (Ma, 2019)	32.6	44.8
2	Ethyl hexanoate	123-66-0	Fruity	398 (Cao, 2014), 149 (Zheng, 2017), 1487 (Dong, 2020), 626 (Sha, 2017), 130 (Ma, 2019)	0.055	10145
3	Ethyl lactate	97-64-3	Fruity	2263 (Xu, 2019), 1565 (Cao, 2014), 509 (Zheng, 2017), 4250 (Ma, 2014), 1464 (Sha, 2017)	128	15.7
4	Ethyl butyrate	105-54-4	Fruity	450 (Xu, 2019), 526 (Cao, 2014), 218 (Dong, 2020), 578 (Sha, 2017)	0.082	5402
5	Acetic acid	64-19-7	Vinegar	556 (Xu, 2019), 276 (Cao, 2014), 79 (Zheng, 2017), 993 (Ma, 2014), 280 (Sha, 2017)	200	2.2
6	Hexanoic acid	142-62-1	Sweaty, cheesy	362 (Xu, 2019), 45.1 (Cao, 2014), 90.4 (Zheng, 2017), 343 (Dong, 2020), 317 (Liu, 2008)	2.52	91.9
7	Lactic acid	50-21-5	-	242 (Xu, 2019), 432.7 (Ma, 2014), 446 (Fan and Xu, 2000), 636 (Yang, 2017)	-	-
8	Butanoic acid	107-92-6	Rancid, cheesy	367 (Xu, 2019), 78.6 (Dong, 2020), 78.3 (Sha, 2017), 122 (Ma, 2019), 246 (Liu, 2008)	0.96	186
9	Methanol	67-56-1	Alcoholic	161 (Ma, 2014), 168 (Fan and Xu, 2000), 181.6 (Wang, 2020a)	-	-
10	Propanol	71-23-8	Alcoholic	204 (Xu, 2019), 134 (Ma, 2014), 350 (Sha, 2017)	53.9	4.3
11	Isobutanol	78-83-1	Fruity, apple	114 (Xu, 2019), 187 (Cao, 2014), 105 (Ma, 2014), 234 (Sha, 2017), 508 (Ma, 2019), 174.8 (Wang, 2020a)	40 [d]	5.5
12	Isoamylol	123-51-3	Fruity	384 (Xu, 2019), 435 (Cao, 2014), 474 (Zheng, 2017), 142 (Dong, 2020), 417 (Ma, 2014), 126 (Sha, 2017)	179	1.8
13	Acetaldehyde	75-07-0	Green	106 (Xu, 2019), 192.2 (Ma, 2014), 293 (Fan and Xu, 2000), 111 (Ma, 2019)	110	1.6
14	1,1-Diethoxyethane	105-57-7	Creamy, fruity	414 (Xu, 2019), 475 (Cao, 2014), 389 (Fan and Xu, 2000), 481 (Wang, 2020a), 290 (Wang, 2020b)	1	410

([a]) Odour description taken from www.thegoodscentscompany.com. ([b]) Odour thresholds taken from Xu (2019) who collected the data from various sources. ([c]) OAV calculated using average concentration.

aroma of *baijiu*, but can also contribute to its pungency. For instance, based on the results of two-alternative forced-choice tests, ethyl hexanoate and ethyl acetate have been identified as the primary contributors to the pungency of *baijiu* (He *et al*., 2022).

Acids primarily manifest as microbial metabolites, wherein lactic acid, for instance, is predominantly generated by lactic acid bacteria. These acids, pivotal to the composite profile of *baijiu*, serve as crucial precursors to esters, elevating both the flavour and lingering aftertaste of the liquor. Notably, lactic acid, a key taste component influencing the acidity and astringency of *baijiu*, has garnered extensive attention within *baijiu* research. As a chiral compound, both D- and L-lactic acids, despite their differing optical properties, exhibit no variance in their chemical properties (Jiang *et al*., 2019). The concentration of lactic acid diverges across various *baijiu* types. Reports indicate an ascending order of lactic acid content: strong-aroma *baijiu* < light-aroma *baijiu* < soy-sauce-aroma *baijiu*, with some soy-sauce-flavour *baijiu* samples surpassing 1000 mg L^{-1} (Yang, 2017). While alcohols possess a relatively limited direct aroma contribution with odour activity value (OAV) < 10, they serve as the primary flavouring agents in *baijiu*, and also act as precursors of esters. Among these, methanol, a

toxic substance, presents concerns due to its potential accumulation in the body and its potential harm to the retinal nerve. The regulated upper limit of methanol content in *baijiu* is set at 400 mg L^{-1} for those brewed from grains. Furthermore, the aldehyde acetaldehyde is prevalent in *baijiu*. A portion of acetaldehyde evaporates during *baijiu* storage, while another fraction reacts with ethanol, forming diethoxyethane *via* the acetal reaction (Reaction 5). Diethoxyethane, with high OAVs ranging from 8,882 to 17,366, emerges as a significant contributor to the aroma of Kongfujia *baijiu* (Cao, 2014). Despite their relatively lower concentrations compared to esters and acids, both acetaldehyde and diethoxyethane play essential roles in imparting *baijiu* with a soft and nuanced flavour (Cao, 2014). Moreover, alcohols beyond ethanol, particularly isoamylol, significantly influence the aroma profile of Qingke *baijiu*, a renowned Tibetan alcoholic beverage crafted from a hull-less highland barley (Qian *et al*., 2019). However, excessive levels of isoamylol may induce high turbidity in *baijiu*, and potentially harm the central nervous system (Sun, 2012). The reactions are as follows:

$$CH_3COOH + CH_3CH_2OH \rightarrow CH_3COOCH_2CH_3 + H_2O \quad (1)$$

$$CH_3CH_2CH_2COOH + CH_3CH_2OH \rightarrow CH_3CH_2CH_2COOCH_2CH_3 + H_2O \quad (2)$$

$$CH_3CH(OH)COOH + CH_3CH_2OH \rightarrow CH_3CH(OH)COOCH_2CH_3 + H_2O \quad (3)$$

$$CH_3[CH_2]_4COOH + CH_3CH_2OH \rightarrow CH_3[CH_2]_4COOCH_2CH_3 + H_2O \quad (4)$$

$$CH_3CHO + 2CH_3CH_2OH \rightarrow CH_3CH_2O)_2CHCH_3 + H_2O \quad (5)$$

Medium components

Twenty-eight medium components with average concentration ranging from 10 to 100 mg L^{-1} are frequently detected in *baijiu* (Table 2). Unlike the major components, their relatively low concentration renders direct detection using GC-FID impractical, necessitating a straightforward pretreatment technique such as liquid-liquid extraction (LLE) to concentrate the sample for accurate assessment. Five monohydric alcohols including butanol, 2-butanol, 2-methylbutanol, pentanol, and hexanol, are among the medium components. Song *et al*. (2020) reported that butanol had the highest variable importance in strong-aroma *baijiu*, and contributed a banana-like odour to the overall aroma, making it not only an aroma contributor but also a marker compound for the discrimination of *baijiu* from different geographical origins. Polyalcohols such as 1,2-propanediol and 2,3-butanediol are also frequently detected with relatively high concertation. Five acids including formic acid, propionic acid, pentanoic acid, isovaleric acid, and pyruvic acid are among the medium components. Although acids have similar contents and varieties with those of alcohols, the former have relatively higher OAVs than the latter. This suggests that acids would have more direct contribution to the aroma of *baijiu*. Ten esters including ethyl formate, ethyl propionate, ethyl isobutyrate, ethyl valerate, ethyl isovalerate, ethyl heptanoate, ethyl octanoate, ethyl linoleate, ethyl oleate, and isoamyl butyrate are among the medium components in *baijiu*. Actually, all esters (except isoamyl butyrate) are ethyl esters due to the excessive amount of ethanol. Easters of both the major and medium components have much higher OAVs than those of alcohols and acids (Tables 1 and 2), making esters the main aroma substances in *baijiu* (Xu *et al*., 2022). It is worth noting that ethyl valerate, ethyl isovalerate, and ethyl octanoate have extraordinarily high OAVs of more than 1,000 due to their extremely low odour thresholds, and they should be among the key aroma substances in *baijiu*. Ethyl oleate and ethyl linoleate are the only long-chain compounds that are detected with concentration higher than 10 mg L^{-1}. It has been reported that these long-chain esters at high concentration would cause turbidity of *baijiu*, and affect its quality. Consequently, *baijiu* manufacturers usually take strict control on their content in order to keep the transparency of *baijiu* (Liu *et al*., 2016). Two aldehydes (isobutyraldehyde and isovaleraldehyde) and three ketones (acetone, 2-pentanone, and acetoin) are among the medium components. In the study by Gao *et al*. (2014), isovaleraldehyde was quantified with a high concentration of 200 mg L^{-1} in the Qingke *baijiu*, resulting in its high OAV of over 10,000. As both the concentration and OAV of isovaleraldehyde were much higher in Qingke *baijiu* than those of other *baijiu*, it was considered a marker component of Qingke *baijiu*. Furfural is the only heterocyclic compound that is detected with such a high concentration, which will be discussed in detail later.

Table 2. Medium components in *baijiu*.

No.	Name	CAS No.	Odour description[a]	Content (mg L^{-1})	Threshold[b] (mg L^{-1})	OAV [c]
1	Butanol	71-36-3	Alcoholic	41.8 (Dong, 2020), 88 (Xu, 2019), 5.57 (Ma, 2014), 60.6 (Wang, 2020a)	2.7	18.1
2	2-Butanol	78-92-2	Fruity	21.9 (Xu, 2019), 277 (Ma, 2019), 84.7 (Wang, 2020a), 70 (Liu, 2008)	50	2.3
3	2-Methylbutanol	137-32-6	Fruity	84.5 (Xu, 2019)	0.18	469
4	Pentanol	71-41-0	Fruity	29.9 (Ma, 2019), 5.97 (Xu, 2019), 10.7 (Wang, 2020a), 20 (Liu, 2008)	4	4.2
5	Hexanol	111-27-3	Green	13.9 (Sha, 2017), 53.6 (Xu, 2019), 30 (Dong, 2020), 77.1 (Ma, 2019), 23.2 (Wang, 2020a)	8	4.9
6	1,2-Propanediol	57-55-6	Alcoholic	132.4 (Wang, 2020a), 22.5 (Xu, 2019)	-	-
7	2,3-Butanediol	513-85-9	Fruity	97.7 (Xu, 2019), 18.9 (Ma, 2014), 64.2 (Wang, 2020a)	-	-
8	Formic acid	64-18-6	Acidic	27 (Fan and Xu, 2000), 23.8 (Xu, 2019), 13.1 (Song *et al*., 2019)	-	-
9	Propionic acid	79-09-4	Acidic	11.8 (Xu, 2019), 4.54 (Cao, 2014), 14.2 (Zheng, 2017), 1.94 (Dong, 2020)	20	0.4
10	Pentanoic acid	109-52-4	Cheesy	19.4 (Xu, 2019), 36.8 (Cao, 2014), 17.9 (Zheng, 2017), 13.7 (Dong, 2020), 11.6 (Sha, 2017)	0.39	51
11	Isovaleric acid	503-74-2	Acidic	94.1 (Zheng, 2017), 17.3 (Xu, 2019), 4.2 (Cao, 2014), 47.4 (Sha, 2017), 26 (Liu, 2008)	1	37.8
12	Pyruvic acid	127-17-3	Sour	20.2 (Song *et al*., 2019), 15.6 (Xu, 2019),	-	-
13	Ethyl formate	109-94-4	Ethereal	14.8 (Xu, 2019), 8.93 (Ma, 2014), 54.8 (Wang, 2020a)	-	-
14	Ethyl propionate	105-37-3	Fruity	14.8 (Cao, 2014), 11.2 (Xu, 2019), 27.5 (Sha, 2017), 19.6 (Liu, 2008)	19	1
15	Ethyl isobutyrate	97-62-1	Fruity	34.5 (Sha, 2017), 9.8 (Liu, 2008), 9.8 (Liu, 2020)	0.057	316
16	Ethyl valerate	539-82-2	Fruity	8.27 (Xu, 2019), 55.2 (Cao, 2014), 27.3 (Zheng, 2017), 44.8 (Dong, 2020), 26.9 (Sha, 2017)	0.027	1203
17	Ethyl isovalerate	108-64-5	Fruity	6.9 (Cao, 2014), 10.2 (Zheng, 2017), 22.8 (Sha, 2017), 6.48 (Wang, 2020b), 19.3 (Wang, 2020a)	0.007	1877
18	Ethyl heptanoate	106-30-9	Fruity	34.7 (Xu, 2019), 43.3 (Cao, 2014), 5.8 (Dong, 2020), 9.8 (Sha, 2017)	13.2	1.8
19	Ethyl octanoate	106-32-1	Banana	70.1 (Cao, 2014), 10.1 (Zheng, 2017), 7.71 (Ma, 2014), 98.1 (Sha, 2017), 23.8 (Ma, 2019)	0.013	3228
20	Ethyl linoleate	544-35-4	Fatty	25.8 (Xu, 2019), 34.5 (Ma, 2014)	-	-
21	Ethyl oleate	111-62-6	Fatty	26.2 (Ma, 2014), 19.9 (Xu, 2019), 11.9 (Dong, 2020)	-	-
22	Isoamyl butyrate	106-27-4	Fruity	38 (Zhou, 2015)	0.093	409
23	Isobutyraldehyde	78-84-2	Green	11.4 (Xu, 2019), 23.2 (Cao, 2014), 5.19 (Ma, 2014), 20.1 (Wang, 2020a)	-	-
24	Isovaleraldehyde	590-86-3	Malty	56.9 (Cao, 2014), 9.48 (Ma, 2014), 22.7 (Sha, 2017), 62.5 (Wang, 2020a)	0.18	211
25	Furfural	98-01-1	Sweet	62.3 (Xu, 2019), 62.7 (Cao, 2014), 81.6 (Zheng, 2017), 6.05 (Ma, 2014), 109 (Sha, 2017), 177 (Ma, 2019)	44	1.9
26	Acetone	67-64-1	Apple	41.1 (Wang, 2020a)	500	0.1
27	2-Pentanone	107-87-9	Fruity	61.4 (Xu, 2019), 32.6 (Cao, 2014), 12 (Wang, 2020a), 35 (Liu, 2008)	13.8	2.6
28	Acetoin	513-86-0	Buttery	14.5 (Ma, 2014), 18.2 (Xu, 2019), 29.2 (Cao, 2014), 91 (Wang, 2020a)	0.014	2730

([a]) Odour description taken from www.thegoodscentscompany.com. ([b]) Odour thresholds taken from Xu (2019), Wang (2020a), Wang *et al*. (2022c), Duan *et al*. (2022), and Zheng (2017), who collected the data from various sources. ([c]) OAV calculated using average concentration

Minor components

Fifty-three minor components with average concentration ranging from 1 to 10 mg L^{-1} are frequently detected in *baijiu* (Table 3). Due to the low content of minor components and matrix effect of ethanol, high efficient pretreatment methods such as solid phase extraction (SPE) should be applied for the separation and concentration of the target components (Misnawi and Ariza, 2011). Compared with LLE, SPE has advantages of simple operation, low operating cost, and good repeatability in quantification, which is very suitable for the analysis of *baijiu* (Jia *et al*., 2020). Six alcohols, namely 2-pentanol, octanol, dodecanol, benzyl alcohol, phenethyl alcohol, and furfuryl alcohol are among the minor components in *baijiu*. Octanol and dodecanol belong to the family of long-chain fat alcohols, and benzyl alcohol and phenethyl alcohol belong to the family of aromatic alcohols. These components represent the highest contents of their families in *baijiu*. Due to the abundance of furfural and ethanol, 2-furaldehyde diethylacetal can be easily formed *via* the acetal reaction. There are ten acids belonging to the minor components, among which lauric acid, linoleic acid, and oleic acid are natural long-chain aliphatic acids, and are usually found in crops. Linoleic acid and oleic acid are also precursor of ethyl linoleate and ethyl oleate which are relatively abundant in *baijiu*. Phenylacetic acid, furoic acid, and maleic acid are the only aromatic acid, heterocyclic acid, and dicarboxylic acid that are detected with such a relatively high concentration, respectively. Esters have the most numerous species (27) of minor components in *baijiu*, among which ethyl phenylacetate and ethyl 3-phenylpropionate are aromatic esters, and ethyl nonanoate, ethyl caprate, ethyl palmitate, ethyl stearate, ethyl *trans*-4-decenoate, and 3-methylbutyl dodecanoate are long-chain fatty esters. Besides ethyl esters, other esters such as butyl esters, isobutyl esters, isoamyl esters, propyl esters, and diethyl esters are also determined with concentration higher than 1 mg L^{-1} (Table 3). Compared with alcohols and acids, esters usually have high OAVs due to their low odour thresholds. For example, ethyl isobutyrate, ethyl 2-methylbutyrate, and ethyl 4-methylpentanoate have OAVs of as high as 81.8, 106.4, and 1,380 with low odour thresholds of 0.057, 0.018, and 0.006 mg L^{-1}, respectively, and are the main aroma compounds in *baijiu*. Two ketones (2-butanone and 2-heptanone) and six aldehydes (2-methyl butyraldehyde, propionaldehyde, valeraldehyde, hexaldehyde, benzaldehyde, and phenyl acetaldehyde) are among the minor components in *baijiu*. Due to their low odour thresholds, 2-methyl butyraldehyde and phenyl acetaldehyde have high VOA values of 360 and 787, respectively, which are even higher than those of most of the major and medium components in *baijiu*. Four acetals including 1,1-diethoxypropane, 1,1-diethoxy-2-methylbutane, 1,1-diethoxypentane, and 1,1-diethoxyisopentane are among the minor components, and they can be formed *via* the acetal reactions between ethanol and the corresponding aldehydes.

Trace components

Organic components, except ethanol, make up only 1 - 2% of *baijiu*. Among these organic components, more than 99% of flavour compounds, in terms of mass content, have been identified and quantified. Yet, the key flavour compounds (markers) of some *baijiu*, such as soy-sauce-aroma *baijiu*, still have not been identified, and remain a puzzle (Duan *et al*., 2022). This suggests that the remaining < 1% of the organic components, which generally have concentration of lower than 1 mg L^{-1}, namely trace components, largely determine the flavour of *baijiu*. Consequently, much has been done on identification and quantification of the key trace compounds in *baijiu* (Duan *et al*., 2022). As far as can be collected, 302 trace components including 13 alcohols, 42 acids, 37 esters, 26 carbonyl compounds, 23 phenols, 26 pyrazines, 57 terpenes, 11 furans, 14 sugars and sugar alcohols, 37 sulphur-containing compounds, 12 biogenic amines, and 14 other uncategorised components have been reportedly quantified with standards (Table 4). It is worth noting that the trace components, with a lot more to be discovered, make up more than 76% of the total organic components in terms of number of species, while make up only 0.5% of the total organic components in terms of mass content (Figure 1), which implies the importance of the trace components. Although the key flavour compounds for *baijiu* of many aroma types are still unknown, many important discoveries and progress have been made in identification and quantification of trace components in *baijiu* (Jia *et al*., 2020; Duan *et al*., 2022; Wang *et al*., 2022c).

Table 3. Minor components in *baijiu*.

No.	Name	CAS No.	Odour description[a]	Content (mg L^{-1})	Threshold[b] (mg L^{-1})	OAV[c]
1	2-Pentanol	6032-29-7	Alcoholic, fruity	7.6 (Xu, 2019), 7.1 (Wang, 2020a)	-	-
2	Octanol	111-87-5	Waxy, green	1.68 (Liu, 2008), 0.69 (Xu, 2019), 2.3 (Cao, 2014)	1.1	1.4
3	Dodecanol	112-53-8	Earthy	1.75 (Xu, 2019)	-	-
4	Benzyl alcohol	100-51-6	Floral	2.93 (Liu, 2020), 2.28 (Xu, 2019)	41	0.1
5	Phenethyl alcohol	60-12-8	Rosy	1.3 (Dong, 2020), 1.68 (Xu, 2019), 4 (Cao, 2014), 7.42 (Ma, 2014), 3.03 (Sha, 2017)	28.9	0.1
6	Furfuryl alcohol	98-00-0	Burnt sugar	3.18 (Zheng, 2017), 3.9 (Wang, 2020a), 0.4 (Yao, 2018)	-	-
7	2-Furaldehyde diethylacetal	13529-27-6	Fruity, earthy	8.77 (Zheng, 2017), 1.61 (Yao, 2018)	-	-
8	Isobutyric acid	79-31-2	Cheesy, acidic	3.85 (Cao, 2014), 3.88 (Dong, 2020), 4.7 (Wang, 2020a)	1.58	2.6
9	Heptanoic acid	111-14-8	Sweaty	8.2 (Xu, 2019), 2.8 (Zheng, 2017), 5.38 (Dong, 2020), 1.1 (Wang, 2020a)	13	0.3
10	Octanoic acid	124-07-2	Sweaty, cheesy	2.42 (Zheng, 2017), 5.53 (Dong, 2020), 1.9 (Wang, 2020a)	2.7	1.2
11	Phenylacetic acid	103-82-2	Honey, floral	3.95 (Zheng, 2017), 0.42 (Dong, 2020), 1.4 (Yang, 2017)	1.43	1.3
12	Lauric acid	143-07-7	Fatty	1.7 (Yang, 2017), 4.52 (Wang *et al*., 2022a)	-	-
13	Linoleic acid	60-33-3	Faint fatty	3.9 (Yang, 2017), 2.4 (Wang *et al*., 2022a)	-	-
14	Oleic acid	112-80-1	Faint fatty	2 (Yang, 2017), 1.12 (Wang *et al*., 2022a)	-	-
15	Ethyl 4-methylpentanoate	25415-67-2	Fruity	8.28 (Xu, 2019)	0.006	1,380
16	Ethyl phenylacetate	101-97-3	Honey, floral	6.97 (Xu, 2019), 0.56 (Cao, 2014), 1.42 (Zheng, 2017), 1 (Dong, 2020), 5.01 (Sha, 2017)	0.41	7.3
17	Ethyl nonanoate	123-29-5	Waxy	1.8 (Cao, 2014), 1.63 (Sha, 2017), 5.86 (Zhou, 2015)	-	-
18	Ethyl isobutyrate	97-62-1	Fruity	4.33 (Xu, 2019), 8.8 (Dong, 2020), 0.85 (Liu, 2008)	0.057	81.8
19	Ethyl 2-methylbutyrate	7452-79-1	Fruity	1.7 (Cao, 2014), 1.03 (Xu, 2019), 3.88 (Zheng, 2017), 0.82 (Dong, 2020), 2.15 (Sha, 2017)	0.018	106.4
20	Ethyl 2-hydroxyhexanoate	52089-55-1	Fruity	6.84 (Liu, 2008)	-	-
21	Ethyl caprate	110-38-3	Green, fruity	2.89 (Xu, 2019), 1.59 (Cao, 2014), 5.3 (Ma, 2014), 1.1 (Sha, 2017)	1.12	2.4
22	Ethyl palmitate	628-97-7	Waxy	0.6 (Dong, 2020), 2.74 (Ma, 2014), 1.9 (Ma, 2019)	-	-
23	Ethyl stearate	111-61-5	Waxy	5.01 (Xu, 2019)	-	-
24	Hexyl hexanoate	6378-65-0	Apple	1.14 (Cao, 2014), 0.71 (Sha, 2017), 8.39 (Liu, 2008)	1.89	1.8
25	Ethyl *trans*-4-decenoate	76649-16-6	Green, fruity	3.3 (Zhou, 2015)	-	-
26	ethyl 2-hydroxy-3-methylbutanoate	2441-06-7	Fruity	3.47 (Zheng, 2017)	-	-
27	Ethyl 2-hydroxy-4-methylvalerate	10348-47-7	-	6.7 (Dong, 2020)	-	-
28	Butyl hexanoate	626-82-4	Fruity	3.22 (Cao, 2014), 5.92 (Liu, 2008)	-	-

29	Isopentyl hexanoate	2198-61-0	Fruity	9.98 (Ma, 2014), 9.7 (Xu, 2019), 1.96 (Cao, 2014), 2.7 (Sha, 2017)	1.4	4.3
30	Isoamyl dodecanoate	6309-51-9	Wine, waxy	9.31 (Xu, 2019)	-	-
31	Isoamyl lactate	19329-89-6	-	8.69 (Xu, 2019)	-	-
32	Diethyl succinate	123-25-1	Fruity	1.72 (Dong, 2020), 6.95 (Xu, 2019), 1.04 (Cao, 2014), 10.6 (Ma, 2014), 2.6 (Wang, 2020a)	35.3	0.1
33	Ethyl 3-phenylpropionate	2021-28-5	Floral, honey	0.66 (Sha, 2017), 6.8 (Xu, 2019), 2.7 (Cao, 2014),	0.13	26.1
34	Isoamyl acetate	123-92-2	Banana	6.49 (Sha, 2017), 5.91 (Xu, 2019), 6.2 (Wang, 2020a)	0.094	66.0
35	Hexyl acetate	142-92-7	Apple, banana	71.3 (Cao, 2014), 2.13 (Xu, 2019), 1.99 (Liu, 2008)	-	-
36	Isobutyl hexanoate	105-79-3	Apple	2 (Xu, 2019), 1.63 (Sha, 2017), 6.47 (Zhou, 2015)	5.25	0.6
37	Propyl hexanoate	626-77-7	Fruity	2.5 (Cao, 2014), 1.78 (Xu, 2019), 2.52 (Sha, 2017)	12.8	0.2
38	Butyl lactate	138-22-7	Green, fruity	1 (Xu, 2019)	-	-
39	Propyl acetate	109-60-4	Celery, fruity	3.8 (Liu, 2020), 0.52 (Xu, 2019)	4.7	-
40	Isoamyl butyrate	106-27-4	Fruity	4.02 (Sha, 2017), 3.14 (Liu, 2008), 0.29 (Liu, 2020)	0.02	124.2
41	Butyl acetate	123-86-4	Fruity	1.46 (Liu, 2008)	-	-
42	2-Methyl butyraldehyde	96-17-3	Green	15.6 (Cao, 2014), 1.51 (Wang, 2020b), 0.17 (Liu, 2020)	0.016	360
43	Phenyl acetaldehyde	122-78-1	Clove	1.5 (Dong, 2020), 0.63 (Cao, 2014), 0.23 (Yao, 2018)	0.001	787
44	Valeraldehyde	110-62-3	Fermented	4.55 (Cao, 2014)	-	-
45	Hexaldehyde	66-25-1	Green grass	2 (Fan and Xu, 2000), 2.06 (Cao, 2014), 1.2 (Liu, 2008)	0.026	67.4
46	Benzaldehyde	100-52-7	Almond, fruity	2.42 (Xu, 2019), 1.6 (Cao, 2014), 17.4 (Ma, 2014), 0.42 (Sha, 2017), 3 (Wang, 2020a)	2	2.5
47	Propionaldehyde	123-38-6	Earthy	0.28 (Xu, 2019), 2.3 (Cao, 2014), 32 (Fan and Xu, 2000), 2.2 (Wang, 2020a)	-	-
48	2-Butanone	78-93-3	Ethereal, fruity	4.9 (Cao, 2014)	-	-
49	2-Heptanone	110-43-0	Fruity, spicy	1.03 (Cao, 2014), 1.17 (Liu, 2020)	-	-
50	1,1-Diethoxy-2-methylbutane	3658-94-4	Fruity	6.3 (Wang, 2020a)	-	-
51	1,1-Diethoxypentane	3658-79-5	-	3.16 (Zheng, 2017)	-	-
52	1,1-Diethoxypropane	4744-08-5	-	6.73 (Xu, 2019)	-	-
53	1,1-Diethoxyisopentane	3842-03-3	Fruity	6.57 (Ma, 2014)	-	-

([a]) Odour description taken from www.thegoodscentscompany.com. ([b]) Odour thresholds taken from Xu (2019), Wang (2020a), Wang *et al*. (2022c), Duan *et al*. (2022), and Zheng (2017), who collected the data from various sources. ([c]) OAV calculated using average concentration.

Table 4. Trace components in *baijiu*.

No.	Name	CAS No.	Odour description[a]	Content (mg L^{-1})	Threshold[b] (mg L^{-1})	OAV [c]
			Alcohol			
1	3-Phenylpropanol	122-97-4	Sweet spicy	0.27 (Xu, 2019)	-	-
2	2-Heptanol	543-49-7	Lemon	0.3 (Cao, 2014), 0.27 (Zhang, 2013), 0.37 (Liu, 2020)	-	-
3	1-Nonanol	143-08-8	Fatty	0.17 (Xu, 2019), 0.23 (Cao, 2014), 0.26 (Liu, 2008)	-	-
4	Mushroom alcohol	3391-86-4	Mushroom	0.11 (Zhang, 2013), 0.17 (Wang, 2020b), 0.045 (Yao, 2018)	0.006	20
5	*trans*-2-Octen-1-ol	18409-17-1	Green	0.12 (Zhang, 2013)	-	-
6	2-Ethylhexanol	104-76-7	Citrus	0.2 (Liu, 2008)	-	-
7	Heptanol	111-70-6	Musty, leafy	0.34 (Liu, 2020)	-	-
8	Diisobutylcarbinol	108-82-7	Ethereal	0.56 (Yao, 2018)	-	-
9	2-Octanol	123-96-6	Green woody	0.03 (Xu, 2019)	-	-
10	3-Octanol	20296-29-1	-	0.04 (Xu, 2019), 0.075 (Zhang, 2013)	-	-
11	Decyl alcohol	112-30-1	Fatty, waxy	0.02 (Xu, 2019), 0.019 (Zhou, 2015)	-	-
12	Inositol	87-89-8	-	0.048 (Yang, 2017)	-	-
13	2-Nonanol	628-99-9	Waxy, green	0.066 (Liu, 2020)	-	-
			Acid			
14	benzoic acid	65-85-0	Floral, urine	0.87 (Zheng, 2017), 0.72 (Yang, 2017), 0.74 (Wang *et al*., 2022a)	-	-
15	Phenylpropionic acid	501-52-0	Floral	0.89 (Zheng, 2017), 0.47 (Dong, 2020), 0.86 (Yang, 2017), 0.15 (Wang *et al*., 2022a)	0.42	1.4
16	Glycolic acid	79-14-1	Buttery	0.33 (Yang, 2017), 0.18 (Wang *et al*., 2022a)	-	-
17	2-Hydroxy-Butanoic acid	600-15-7	-	0.12 (Yang, 2017), 0.25 (Wang *et al*., 2022a)	-	-
18	3-Hydroxy-Propanoic acid	503-66-2	-	0.58 (Yang, 2017)	-	-
19	3-Hydroxybutyric acid	625-71-8	-	0.44 (Yang, 2017), 0.086 (Wang *et al*., 2022a)	-	-
20	2-Hydroxy-3-methylbutyric acid	4026-18-0	-	0.16 (Yang, 2017), 0.051 (Wang *et al*., 2022a)	-	-
21	2-Hydroxy-2-methylbutyric acid	3739-30-8	-	0.2 (Wang *et al*., 2022a)	-	-
22	3-Hydroxyisovaleric acid	625-08-1	Amber, woody	0.31 (Wang *et al*., 2022a)	-	-
23	2-Hydroxy-4-methyl-pentanoic acid	498-36-2	-	0.56 (Wang *et al*., 2022a)	-	-
24	Maleic acid	110-16-7	-	0.05 (Wang *et al*., 2022a)	-	-
25	2,3-Dihydroxypropanoic acid	6000-40-4	-	0.11 (Wang *et al*., 2022a)	-	-
26	Adipic acid	124-04-9	Odourless	0.07 (Wang *et al*., 2022a)	-	-
27	Heptanedioic acid	111-16-0	-	0.52 (Song *et al*., 2019), 0.097 (Wang *et al*., 2022a)	-	-
28	Oxalic acid	144-62-7	Caramellic	0.84 (Song *et al*., 2019)	-	-
29	Ethyl hydrogen malonate	1071-46-1	-	0.43 (Wang *et al*., 2022a)	-	-
30	Succinic acid	110-15-6	Odourless	0.82 (Yang, 2017), 0.12 (Wang *et al*., 2022a)	-	-
31	Glutaric acid	110-94-1	Odourless	0.033 (Wang *et al*., 2022a)	-	-
32	Glyceric acid	473-81-4	-	0.16 (Yang, 2017)	-	-
33	Fumaric acid	110-17-8	Odourless	0.26 (Yang, 2017), 0.024 (Wang *et al*., 2022a)	-	-

34	Malic acid	97-67-6	Odourless	0.76 (Yang, 2017), 0.14 (Wang *et al*., 2022a)	-	-
35	2-Hydroxy-3-phenylpropionic acid	7326-19-4	-	0.094 (Wang *et al*., 2022a)	-	-
36	Cinnamic acid	621-82-9	-	0.044 (Wang *et al*., 2022a)	-	-
37	4-Hydroxybenzoic acid	99-96-7	Nutty	0.065 (Wang *et al*., 2022a)	-	-
38	3-Phenyllactic acid	20312-36-1	-	0.56 (Yang, 2017)	-	-
39	Myristic acid	544-63-8	Coconut	0.98 (Yang, 2017), 0.23 (Wang *et al*., 2022a)	-	-
40	Palmitoleic acid	373-49-9	-	0.1 (Yang, 2017), 0.18 (Wang *et al*., 2022a)	-	-
41	Pyroglutamic acid	98-79-3	Sweet	0.75 (Yang, 2017)	-	-
42	Nonanoic acid	112-05-0	Fatty	0.11 (Liu, 2020)	3.6	0.03
43	Decanoic acid	334-48-5	Rancid, sour	0.19 (Liu, 2020), 0.37 (Yao, 2018)	-	-
44	4-Methylpentanoic acid	646-07-1	Sweaty	0.3 (Dong, 2020), 0.66 (Wang, 2020b)	0.14	3.4
45	Tartaric acid	526-83-0	Acidic	0.045 (Yang, 2017), 0.069 (Wang *et al*., 2022a)	-	-
46	Citric acid	77-92-9	Strong acidic	0.008 (Wang *et al*., 2022a)	-	-
47	Vanillic acid	121-34-6	Milky	0.042 (Wang *et al*., 2022a)	-	-
48	Suberic acid	505-48-6	-	0.021 (Wang *et al*., 2022a)	-	-
49	Azelaic acid	123-99-9	-	0.098 (Yang, 2017), 0.062 (Wang *et al*., 2022a)	-	-
50	Palmitic acid	57-10-3	Fatty	0.02 (Yang, 2017), 1.6 (Wang *et al*., 2022a)	-	-
51	Stearic acid	57-11-4	Fatty	0.099 (Wang *et al*., 2022a)	-	-
52	Elaidic acid	112-79-8	-	0.093 (Wang *et al*., 2022a)	-	-
53	Alanine	56-41-7	Sweet	0.036 (Yang, 2017)	-	-
54	Hydroxyproline	51-35-4	-	0.008 (Yang, 2017)	-	-
55	Serine	302-84-1	-	0.01 (Yang, 2017)	-	-
			Ester			
56	Ethyl myristate	124-06-1	Sweet, violet	0.3 (Dong, 2020), 0.7 (Liu, 2020)	-	-
57	2-Phenylethyl hexanoate	6290-37-5	Fruity	0.079 (Sha, 2017), 1.02 (Liu, 2008), 0.51 (Zhou, 2015)	0.91	0.6
58	Ethyl benzoate	93-89-0	Floral	1.25 (Xu, 2019), 0.12 (Cao, 2014), 0.24 (Zheng, 2017), 0.062 (Dong, 2020), 0.14 (Sha, 2017)	1.43	0.3
59	Amyl hexanoate	540-07-8	Pineapple	0.99 (Xu, 2019), 0.43 (Zhou, 2015)	-	-
60	Ethyl suberate	2050-23-9	-	0.88 (Xu, 2019)	-	-
61	Ethyl laurate	106-33-2	Floral	0.84 (Xu, 2019), 0.31 (Cao, 2014), 0.52 (Sha, 2017), 0.048 (Ma, 2019)	-	-
62	Phenethyl acetate	103-45-7	Honey, rose	0.81 (Xu, 2019), 0.12 (Cao, 2014), 0.027 (Zheng, 2017), 0.061 (Dong, 2020), 2.07 (Sha, 2017), 0.024 (Ma, 2019)	0.41	1.3
63	Isobutyl acetate	110-19-0	Fruity, banana	0.57 (Xu, 2019), 0.54 (Liu, 2020)	-	-
64	Ethyl 3-hydroxyhexanoate	2305-25-1	Fruity, grape	0.51 (Xu, 2019)	-	-
65	Isoamyl caprylate	2035-99-6	Fruity, coconut	0.48 (Xu, 2019), 0.054 (Sha, 2017), 0.12 (Zhou, 2015)	-	-
66	1,9-Diethyl nonanedioate	624-17-9	-	0.48 (Xu, 2019)	-	-
67	Isopentyl formate	110-45-2	Fruity ,fatty	0.45 (Xu, 2019)	-	-
68	Butyl octanoate	589-75-3	Butter, ether	0.39 (Xu, 2019)	-	-
69	Ethyl vanillate	617-05-0	Sweet creamy	0.25 (Xu, 2019)	-	-
70	Diethyl pimelate	2050-20-6	-	0.19 (Xu, 2019)	-	-
71	Phenethyl butyrate	103-52-6	Fruity, floral	0.06 (Xu, 2019), 0.53 (Sha, 2017)	-	-
72	Ethyl acrylate	140-88-5	Plastic, fruity	0.45 (Zheng, 2017), 0.64 (Dong, 2020)	0.0002	2,725

73	Ethyl 2-hydroxybutanoate	52089-54-0	-	0.4 (Zheng, 2017)	-	-
74	Ethyl 4-methylpentanoate	25415-67-2	Fruity	0.48 (Zheng, 2017), 0.61 (Dong, 2020), 0.17 (Dong, 2020)	0.006	70
75	Hexyl butyrate	2639-63-6	Green	0.23 (Dong, 2020)	8.6	0.03
76	Ethyl 3-hexenoate	2396-83-0	Fruity,	0.11 (Dong, 2020)	-	-
77	3-Methylbutyl octanoate	2035-99-6	Fruity	0.14 (Dong, 2020)	-	-
78	Monoethyl succinate	1070-34-4	-	0.64 (Yang, 2017), 0.21 (Wang *et al*., 2022a)	-	-
79	Butyl butyrate	109-21-7	Fruity	0.21 (Liu, 2020)	0.11	2
80	Ethyl pentadecanoate	41114-00-5	Honey	0.54 (Liu, 2020)	-	-
81	Isobutyl butyrate	539-90-2	Fruity	0.13 (Xu, 2019)	-	-
82	Nonanolactone	104-61-0	Sweet	0.14 (Wang, 2020b), 0.67 (Xu, 2019), 0.06 (Dong, 2020), 0.2 (Zhou, 2015), 0.084 (Sun *et al*., 2022)	0.09	2.6
83	Dodecalactone	2305-05-7	Fatty	0.08 (Xu, 2019)	0.06	1
84	Decalactone	706-14-9	Fruity	0.05 (Xu, 2019)	0.01	5
85	Sotolon	28664-35-9	Caramel	0.022 (Wang, 2020b), 1.2 (Sun *et al*., 2022)	-	-
86	γ-Octanoic lactone	104-50-7	Coconut	0.02 (Xu, 2019)	2.8	0.01
87	γ-Butyrolactone	96-48-0	Caramel	0.18 (Wang, 2020b), 0.45 (Sun *et al*., 2022)	-	-
88	Nonyl acetate	143-13-5	Fruity	0.03 (Xu, 2019)	-	-
89	Ethylundecanoat	627-90-7	Coconut	0.02 (Cao, 2014), 0.03 (Xu, 2019), 0.08 (Zhou, 2015)	-	-
90	Ethyl cinnamate	103-36-6	Fruity	0.02 (Xu, 2019)	0.001	20
91	Decyl acetate	112-17-4	Fatty, citrus	0.002 (Xu, 2019)	-	-
92	Ethyl nicotinoate	614-18-6	-	0.009 (Dong, 2020)	-	-
			Carbonyl compound			
93	Butyraldehyde	123-72-8	Fruity, floral	0.47 (Xu, 2019)	2.9	0.2
94	Decanal	112-31-2	Citrus	0.13 (Cao, 2014), 0.2 (Zheng, 2017), 0.55 (Liu, 2008)	-	-
95	Nonyl aldehyde	124-19-6	Soapy	0.41 (Xu, 2019), 0.17 (Cao, 2014), 0.01 (Sha, 2017), 0.91 (Wang, 2020b)	0.12	3
96	2-Phenyl-2-butenal	4411-89-6	Floral	0.1 (Cao, 2014)	-	-
97	Heptaldehyde	111-71-7	Cilantro	0.093 (Cao, 2014)	0.0028	33
98	Octanal	124-13-0	Green	0.022 (Cao, 2014)	0.015	1.5
99	Undecanal	112-44-7	Waxy, floral	0.004 (Cao, 2014)	-	-
100	*trans*-2-Pentenal	1576-87-0	Fruity	0.018 (Cao, 2014)	-	-
101	*trans*-2-Hexenal	6728-26-3	Banana	0.0078 (Cao, 2014)	-	-
102	*trans*-2-Heptenal	18829-55-5	Fruity	0.0089 (Cao, 2014)	-	-
103	*trans*-2-Octenal	2548-87-0	Fruity	0.011 (Cao, 2014)	-	-
104	*trans*-2-Nonenal	18829-56-6	Soapy	0.064 (Zhang, 2013), 0.013 (Cao, 2014), 0.26 (Wang, 2020b)	0.0001	1,123
105	*trans*-2-Decenal	3913-81-3	Cilantro	0.03 (Liu, 2020), 0.0055 (Cao, 2014)	-	-
106	*trans,cis*-2,6-Nonadienal	557-48-2	Green	0.47 (Wang, 2020b), 0.0098 (Cao, 2014)	-	-
107	*trans,trans*-2,4-Heptadienal	5910-85-0	Fruity	0.0018 (Cao, 2014)	-	-
108	*trans,trans*-2,4-Decadienal	25152-84-5	Fatty	0.01 (Wang, 2020b), 0.001 (Cao, 2014)	0.0001	55
109	p-Anisaldehyde	123-11-5	Typical	0.0015 (Cao, 2014)	-	-
110	Cinnamaldehyde	104-55-2	Spicy	0.024 (Cao, 2014)	-	-
111	2-Nonanone	821-55-6	Cheesy	0.03 (Xu, 2019), 0.092 (Cao, 2014), 0.23 (Sha, 2017), 0.19 (Liu, 2008)	-	-
112	2-Octanone	111-13-7	Green, herbal	0.28 (Wang, 2020b), 0.11 (Cao, 2014),	0.4	0.9

				0.94 (Liu, 2008), 0.13 (Liu, 2020)		
113	Acetophenone	98-86-2	Hawthorn	0.3 (Liu, 2008), 0.098 (Cao, 2014)	-	-
114	2,3-Butanedione	431-03-8	Butter,	0.18 (Wang, 2020b), 0.25 (Cao, 2014)	-	-
115	2-Hexanone	591-78-6	Fruity	0.079 (Cao, 2014)	-	-
116	2-Decanone	693-54-9	Orange	0.005 (Cao, 2014)	-	-
117	2-Undecanone	112-12-9	Fruity	0.011 (Sha, 2017)	-	-
118	Amyl vinylketone	4312-99-6	Herbal	0.14 (Zhang, 2013), 0.014 (Wang, 2020b)	-	-
			Phenol			
119	Phenol	108-95-2	Phenol	1.08 (Xu, 2019), 0.046 (Cao, 2014), 0.16 (Zheng, 2017), 0.33 (Zhang, 2013), 1.53 (Liu, 2008)	18	0.03
120	2-Methylphenol	95-48-7	Phenolic	0.028 (Li *et al*., 2017)	-	-
121	3-Methylphenol	108-39-4	Medicinal	0.22 (Li *et al*., 2017)	-	-
122	4-Methylphenol	106-44-5	Animal	0.16 (Zheng, 2017), 0.57 (Dong, 2020), 0.043 (Ma, 2019), 0.47 (Zhang, 2013), 0.12 (Wang, 2020b)	0.17	1.6
123	4-Ethylphenol	123-07-9	Smoky	0.03 (Xu, 2019), 0.049 (Dong, 2020), 0.078 (Sha, 2017), 0.01 (Ma, 2019), 0.11 (Zhang, 2013)	0.62	0.1
124	4-Ethenylphenol	2628-17-3	Phenolic	0.034 (Zhang, 2013)	-	-
125	2,4-Di-*tert*-butylphenol	96-76-4	Phenolic	0.12 (Liu, 2020)	-	-
126	Guaiacol	90-05-1	Phenolic	0.15 (Xu, 2019), 0.015 (Zheng, 2017), 0.066 (Zhang, 2013), 0.012 (Yao, 2018)	0.014	4
127	4-Methylguaiacol	93-51-6	Smoky	0.2 (Cao, 2014), 0.43 (Dong, 2020), 0.002 (Zhang, 2013), 0.75 (Liu, 2008)	0.31	1.1
128	4-Ethylguaiacol	2785-89-9	Clove	0.046 (Zheng, 2017), 0.13 (Dong, 2020), 0.096 (Zhang, 2013)	0.12	0.8
129	4-Vinyl guaiacoll	7786-61-0	Clove	0.012 (Dong, 2020), 0.002 (Zhang, 2013), 0.31 (Zhou, 2015)	0.31	0.3
130	Eugenol	97-53-0	Sweet, spicy	0.01 (Xu, 2019)	-	-
131	Vanillin	121-33-5	Vanilla	0.011 (Dong, 2020), 0.85 (Sun *et al*., 2022)	0.44	1
			Pyrazine			
132	Pyrazine	290-37-9	Pungent, sweet	0.035 (Fan *et al*., 2007)	-	-
133	2-Methylpyrazine	109-08-0	Nutty	0.25 (Fan and Xu, 2000), 0.013 (Ma, 2019), 0.125 (Fan *et al*., 2007)	121	0.001
134	2,3-Dimethylpyrazine	5910-89-4	Coffee	0.079 (Fan *et al*., 2007)	-	-
135	2,5-Dimethyl pyrazine	123-32-0	Roasted	0.1 (Fan and Xu, 2000), 0.056 (Fan *et al*., 2007)	0.008	10
136	2,6-Dimethylpyrazine	108-50-9	Cocoa	0.54 (Zhou, 2015), 0.395 (Fan *et al*., 2007)	0.8	1
137	2-Ethylpyrazine	13925-00-3	Nutty, cocoa	0.06 (Fan *et al*., 2007)	-	-
138	2-Ethyl-3-methylpyrazine	15707-23-0	Nutty, peanut	0.047 (Fan *et al*., 2007)	-	-
139	2-Ethyl-5-methylpyrazine	13360-64-0	Coffee	0.0067 (Zhou, 2015), 0.087 (Fan *et al*., 2007)	0.0016	29
140	2-Ethyl-6-methylpyrazine	13925-03-6	Roasted	0.32 (Zheng, 2017), 0.73 (Fan and Xu, 2000), 0.64 (Fan *et al*., 2007)	0.04	14
141	2,6-Diethylpyrazine	13067-27-1	Nutty	0.084 (Fan *et al*., 2007)	-	-
142	2,5-Dimethyl-3-ethylpyrazine	13360-65-1	Hazelnut	0.17 (Fan *et al*., 2007)	-	-
143	2-Ethyl-3,5-dimethylpyrazine	27043-05-6	Burnt coffee	0.09 (Zheng, 2017), 0.55 (Fan *et al*., 2007)	0.0075	43

144	2,3-Dimethyl-5-ethylpyrazine	15707-34-3	Burnt popcorn	0.013 (Fan *et al*., 2007)	-	-
145	Trimethyl-pyrazine	14667-55-1	Nutty	0.12 (Zheng, 2017), 0.021 (Ma, 2019), 0.53 (Fan and Xu, 2000), 0.056 (Yao, 2018), 0.47 (Fan *et al*., 2007)	0.73	0.3
146	3,5-Diethyl-2-methylpyrazine	18138-05-1	Green, nutty	0.046 (Fan *et al*., 2007)	-	-
147	Tetramethylpyrazine	1124-11-4	Nutty	0.23 (Fan and Xu, 2000), 0.089 (Yao, 2018), 0.44 (Fan *et al*., 2007)	80	0.003
148	2,3,5-Trimethyl-6-ethylpyrazine	17398-16-2	-	0.051 (Fan *et al*., 2007)	-	-
149	3-Isobutyl-2,5-dimethylpyrazin	32736-94-0	-	0.025 (Fan *et al*., 2007)	-	-
150	2-Methyl-6-vinylpyrazin	13925-09-2	Hazelnut	0.0085 (Fan *et al*., 2007)	-	-
151	2-Acetyl-3-methylpyrazine	23787-80-6	Baked potato	0.13 (Fan *et al*., 2007)	-	-
152	2-Butyl-3,5-dimethylpyrazine	50888-63-6	Sweet, earthy	0.066 (Fan *et al*., 2007)	-	-
153	2-Acetyl-6-methylpyrazine	22047-26-3	Coffee, cocoa	0.91 (Fan *et al*., 2007)	-	-
154	2-Methyl-6-propenylpyrazine	104638-11-1	-	0.042 (Fan *et al*., 2007)	-	-
155	2-Acetyl-3,5-dimethylpyrazine	54300-08-2	Nutty	0.34 (Fan *et al*., 2007)	-	-
156	2,5-Dimethyl-3-pentylpyrazine	56617-69-7	-	0.062 (Fan *et al*., 2007)	-	-
157	2-Hydroxymethyl-3,6-diethyl-5-methylpyrazine	-	-	0.51 (Zhao *et al*., 2018)	-	-
			Terpene			
158	D-limonene	95327-98-3	-	0.007 (Wang *et al*., 2015), 0.13 (Fan *et al*., 2012a)	-	-
159	*p*-Cymene	99-87-6	Citrus	0.066 (Fan *et al*., 2012a)	-	-
160	*β*-Patchoulene	514-51-2	-	0.031 (Fan *et al*., 2012a)	-	-
161	Clovene	469-92-1	-	0.049 (Fan *et al*., 2012a)	-	-
162	D-camphor	21368-68-3	-	0.038 (Fan *et al*., 2012a)	-	-
163	*α*-Gurjunene	-	-	0.0065 (Wang *et al*., 2015), 0.13 (Fan *et al*., 2012a)	-	-
164	Linalool	126-90-9	Sweet	0.032 (Wang *et al*., 2015), 0.087 (Fan *et al*., 2012a)	-	-
165	α-Cedrene	11028-42-5	Woody	0.031 (Zhou, 2015), 0.068 (Fan *et al*., 2012a), 0.0327 (Wang *et al*., 2015)	-	-
166	Longifolene	475-20-7	Sweet, woody	0.0071 (Wang *et al*., 2015), 0.017 (Fan *et al*., 2012a)	-	-
167	*β*-Caryophyllene	87-44-5	Sweet, clove	0.0217 (Wang *et al*., 2015), 0.015 (Fan *et al*., 2012a)	-	-
168	*β*-Elemene	33880-83-0	Herbal, waxy	0.012 (Fan *et al*., 2012a)	-	-
169	Terpineol	10482-56-1	Lilac, floral	0.005 (Zhou, 2015)	-	-
170	Calarene	-	-	0.0035 (Wang *et al*., 2015), 0.237 (Fan *et al*., 2012a)	-	-
171	Aromadendrene	489-39-4	Wood	0.032 (Fan *et al*., 2012a), 0.0031 (Wang *et al*., 2015)	-	-
172	Alloaromadendrene	25246-27-9	Woody	0.0039 (Wang *et al*., 2015),	-	-

				0.108 (Fan *et al*., 2012a)		
173	*γ*-Gurjunene	-	-	0.086 (Fan *et al*., 2012a)	-	-
174	*γ*-Selinene	515-17-3	Woody	0.096 (Fan *et al*., 2012a)	-	-
175	*α*-Humulene	6753-98-6	Woody	0.097 (Fan *et al*., 2012a)	-	-
176	*α*-Terpineol	8000-41-7	Woody-	0.0262 (Wang *et al*., 2015), 0.029 (Fan *et al*., 2012a)	-	-
177	Borneol	507-70-0	Pine, camphor	0.003 (Fan *et al*., 2012a)	-	-
178	*γ*-Muurolene	-	-	0.0038 (Wang *et al*., 2015), 0.028 (Fan *et al*., 2012a)	-	-
179	Valencene	24741-64-8	-	0.036 (Fan *et al*., 2012a)	-	-
180	*α*-Muurolene	10208-80-7	Woody	0.0039 (Wang *et al*., 2015), 0.065 (Fan *et al*., 2012a)	-	-
181	*α*-Selinene	473-13-2	Amber	0.0068 (Wang *et al*., 2015), 0.029 (Fan *et al*., 2012a)	-	-
182	*δ*-Cadinene	-	-	0.091 (Fan *et al*., 2012a), 0.0104 (Wang *et al*., 2015)	-	-
183	*γ*-Cadinene	-	-	0.0032 (Wang *et al*., 2015), 0.06 (Fan *et al*., 2012a),	-	-
184	*α*-Curcumene	644-30-4	Herbal	0.032 (Fan *et al*., 2012a)	-	-
185	*α*-Cadinene	523-47-7	Green woody	0.018 (Fan *et al*., 2012a)	-	-
186	*β*-Damascenone	23726-93-4	Honey	0.011 (Yao, 2018), 0.02 (Fan *et al*., 2012a), 0.018 (Wang, 2020b), 0.0118 (Wang *et al*., 2015)	0.00012	127
187	Anethole	4180-23-8	Sweet, anise	0.598 (Fan *et al*., 2012a)	-	-
188	Calamenene	483-77-2	Herb, spicy	0.0045 (Wang *et al*., 2015), 0.074 (Fan *et al*., 2012a)	-	-
189	Geranylacetone	689-67-8	Magnolia, rose	0.001 (Cao, 2014), 0.02 (Fan *et al*., 2012a), 0.078 (Wang *et al*., 2015)	-	-
190	*α*-Calacorene	-	-	0.052 (Fan *et al*., 2012a)	-	-
191	*β*-Ionone	-	-	0.0017 (Wang *et al*., 2015), 0.011 (Fan *et al*., 2012a),	-	-
192	E-nerolidol	40716-66-3	Citrus, woody	0.06 (Xu, 2019), 0.022 (Fan *et al*., 2012a), 0.0507 (Wang *et al*., 2015),	-	-
193	*p*-Anisaldehyde	123-11-5	Sweet, balsam	0.454 (Fan *et al*., 2012a)	-	-
194	*α*-Cedrol	77-53-2	Cedarwood	0.066 (Fan *et al*., 2012a), 0.0131 (Wang *et al*., 2015)	-	-
195	*α*-Cadinol	-	-	0.025 (Fan *et al*., 2012a), 0.0043 (Wang *et al*., 2015)	-	-
196	*β*-Eudesmol	473-15-4	Woody	0.349 (Fan *et al*., 2012a), 0.0037 (Wang *et al*., 2015)	-	-
197	Farnesol	4602-84-0	Sweet	0.233 (Fan *et al*., 2012a), 0.0337 (Wang *et al*., 2015)	-	-
198	Citral	5392-40-5	Sweet, lemon	0.025 (Wang *et al*., 2015)	-	-
199	Nerol	106-25-2	Sweet	0.0068 (Wang *et al*., 2015)	-	-
200	*β*-Citronellol	106-22-9	Leather, rose	0.016 (Wang *et al*., 2015)	-	-
201	Geraniol	106-24-1	Sweet, rose	0.0078 (Wang *et al*., 2015)	-	-
202	Eremophilene	10219-75-7	-	0.001 (Wang *et al*., 2015)	-	-
203	*β*-Cedrene	-	-	0.004 (Wang *et al*., 2015)	-	-
204	*γ*-Elemene	33880-83-0	Herbal, waxy	0.0103 (Wang *et al*., 2015)	-	-
205	*β*-Bisabolene	495-62-5	Balsamic	0.0039 (Wang *et al*., 2015)	-	-

206	*α*-Chamigrene	18431-82-8	-	0.0149 (Wang *et al*., 2015)	-	-
207	Globulol	51371-47-2	Floral rose	0.0047 (Wang *et al*., 2015)	-	-
208	*β*-Guaiene	87745-31-1	-	0.0036 (Wang *et al*., 2015)	-	-
209	*α*-Calacorenee	-	-	0.0076 (Wang *et al*., 2015)	-	-
210	Ledol	577-27-5	-	0.0044 (Wang *et al*., 2015)	-	-
211	*α*-Bergamotene	18252-46-5	-	0.012 (Wang *et al*., 2015)	-	-
212	*α*-Ionone	8013-90-9	Sweet, woody	0.0041 (Wang *et al*., 2015)	-	-
213	Theaspirane	36431-72-8	Herbal	0.0008 (Wang *et al*., 2015)	-	-
214	Isophorone	78-59-1	Sweet	0.014 (Wang *et al*., 2015)	-	-
			Furan			
215	Furoic acid	88-14-2	Odourless	0.62 (Yang, 2017), 0.12 (Wang *et al*., 2022a)	-	-
216	Ethyl furoate	614-99-3	Balsamic	0.17 (Liu, 2020), 0.57 (Zhou, 2015), 0.29 (Zheng, 2017)	132	0.003
217	5-Methyl furfural	620-02-0	Caramel	0.065 (Cao, 2014), 0.2 (Zheng, 2017)	466	0.0003
218	Furylacrolein	623-30-3	Grassy, spicy	0.23 (Zheng, 2017)	-	-
219	2-Acetyl-5-methylfuran	1193-79-9	Nutty	0.06 (Xu, 2019), 0.3 (Zheng, 2017)	40	0.005
220	2-Acetylfuran	1192-62-7	Caramel	0.87 (Zhou, 2015), 0.34 (Zheng, 2017)	58	0.01
221	2,3-Dihydrobenzofuran	496-16-2	-	0.027 (Li *et al*., 2017)	-	-
222	2-Pentylfuran	3777-69-3	Beany	0.16 (Cao, 2014)	-	-
223	Difurfuryl ether	4437-22-3	Coffee	0.36 (Zheng, 2017)	-	-
224	Furfuryl acetate	623-17-6	Caramel	0.013 (Dong, 2020)	26	0.001
225	Furfuryl hexanoate	39252-02-3	Waxy	0.044 (Zhou, 2015)	-	-
			Sugars and sugar alcohol			
226	Glycerol	56-81-5	Odourless	0.22 (Han *et al*., 2013), 1.03 (Wang et la., 2021), 0.62 (Xiang, 2021)	-	-
227	Erythritol	149-32-6	Odourless	0.34 (Yang, 2017), 0.017 (Han *et al*., 2013)	-	-
228	Arabinose	147-81-9	-	0.16 (Yang, 2017)	-	-
229	Arabinitol	488-82-4	-	0.44 (Yang, 2017), 0.014 (Han *et al*., 2013), 0.45 (Xiang, 2021)	-	-
230	D-Xylopyranose	58-86-6	Woody	0.047 (Yang, 2017), 0.13 (Xiang, 2021)	-	-
231	Xylitol	87-99-0	Odourless	0.031 (Yang, 2017), 0.27 (Xiang, 2021)	-	-
232	Glucose	50-99-7	-	0.22 (Yang, 2017), 0.5 (Xiang, 2021)	-	-
233	D-Sorbitol	50-70-4	Sweet	0.03 (Yang, 2017), 0.033 (Han *et al*., 2013), 0.00002 (Wang et la., 2021)	-	-
234	D-Mannitol	69-65-8	Odourless	0.1 (Yang, 2017)	-	-
235	Fructopyranose	7660-25-5	-	0.055 (Yang, 2017), 0.28 (Wang *et al*., 2021)	-	-
236	Galactose	59-23-4	-	0.027 (Yang, 2017)	-	-
237	Galactitol	608-66-2	-	0.006 (Han *et al*., 2013)	-	-
238	Sucrose	57-50-1	Sweet	0.067 (Yang, 2017)	-	-
239	Trehalose	99-20-7	-	0.005 (Yang, 2017), 0.01 (Han *et al*., 2013), 0.000026 (Wang et la., 2021)	-	-
			Sulphur-containing compound			
240	Dimethyl disulphide	624-92-0	Cabbage	0.12 (Sha, 2017), 0.23 (Fan and Xu, 2000), 0.087 (Wang, 2020b), 0.032 (Song *et al*., 2019)	0.009	15
241	Ethyl disulphide	110-81-6	Ripe onion	0.0015 (Sha, 2017)	-	-
242	Dimethyl trisulfide	3658-80-8	Cooked onion	0.15 (Xu, 2019), 0.14 (Zheng, 2017), 0.026 (Dong, 2020), 0.079 (Sha, 2017), 0.05 (Fan and Xu, 2000), 0.2 (Wang, 2020b), 0.06 (Song *et al*., 2019)	0.00036	280

243	3-Methylthiopropanol	505-10-2	Meaty	0.97 (Zheng, 2017), 0.21 (Dong, 2020), 0.84 (Zhou, 2015)	2.1	0.3
244	Methanethiol	74-93-1	Decomposing cabbage; garlic	0.18 (Wang, 2020b), 0.33 (Zhou, 2015), 0.44 (Yan *et al*., 2020)	-	-
245	Dimethyl sulphide	75-18-3	Sulphury; onion; sweet corn	0.24 (Sha, 2017)	0.0011	218
246	2-Furfurylthiol	98-02-2	Sulphury; coffee; oily	0.023 (Wang, 2020b), 0.011 (Song *et al*., 2019), 0.0064 (Song *et al*., 2020)	0.00001	1,000
247	1-Heptylthiol	1639-09-4	Sulphury; onion	0.072 (Sha, 2017)	-	-
248	Hexyl mercaptan	111-31-9	Sulphury; fatty; garlic	0.052 (Sha, 2017)	-	-
249	Ethanethiol	75-08-1	Sulphury; fruity	0.088 (Sha, 2017)	-	-
250	Ethyl 3-methylthiopropionate	13327-56-5	Sulphury	0.05 (Xu, 2019), 0.31 (Dong, 2020), 0.057 (Sha, 2017)	3.1	0.04
251	Methyl thioacetate	1534-08-3	Sulphury; eggy; dairy	0.27 (Sha, 2017)	-	-
252	Ethyl 3-methylthiopropionate	13327-56-5	Sulphury; metallic; pineapple	0.05 (Xu, 2019), 0.31 (Dong, 2020), 0.057 (Sha, 2017), 0.052 (Zhou, 2015)	-	-
253	Ethyl thioacetate	625-60-5	Sulphury, garlic	0.091 (Sha, 2017)	-	-
254	Ethyl (methylthio)acetate	4455-13-4	Sulphury	0.01 (Sha, 2017)	-	-
255	Methional	3268-49-3	Cooked potato	0.12 (Zheng, 2017), 0.37 (Dong, 2020), 0.19 (Wang, 2020b), 0.0017 (Song *et al*., 2019)	0.007	24
256	Allylmercaptan	870-23-5	Alliaceous	0.013 (Song *et al*., 2019)	-	-
257	Dipropyl disulphide	629-19-6	Sulphury	0.035 (Song *et al*., 2019)	-	-
258	Allyl propyl disulphide	2179-59-1	Alliaceous	0.024 (Song *et al*., 2019)	-	-
259	Diallyldisulphide	2179-57-9	Alliaceous	0.0014 (Song *et al*., 2019)	-	-
260	Furfuryl methyl sulphide	1438-91-1	Sulphury	0.011 (Song *et al*., 2019)	-	-
261	Benzenemethanethiol	100-53-8	Onion	0.0049 (Song *et al*., 2019), 0.001 (Li *et al*., 2019)	0.0001	30
262	Methyl furfuryl disulphide	57500-00-2	Sulphury, meaty	0.0077 (Yan *et al*., 2020)	-	-
263	Diallyl trisulfide	2050-87-5	Garlic, metallic	0.051 (Song *et al*., 2019)	-	-
264	2-Methyl-3-furanthiol	28588-74-1	Sulphury	0.005 (Wang, 2020b), 0.00065 (Song *et al*., 2020)	0.000005	565
265	2-Methyl-3-furyl disulphide	28588-75-2	Sulphury	0.0034 (Wang, 2020b)	-	-
266	Methyl 2-methyl-3-furyl disulphide	65505-17-1	Sulphury	0.0056 (Wang, 2020b)	-	-
267	2-Methyl-5-(methylthio)-furan	13678-59-6	Sulphury, garlic	0.0065 (Yan *et al*., 2020)	-	-
268	Methyl thiobutyrate	2432-51-1	Sulphury	0.0003 (Yan *et al*., 2020)	-	-
269	3-Methylthiophene	616-44-4	Fatty, winey	0.13 (Sha, 2017), 0.13 (Yan *et al*., 2020)	-	-
270	Thiophene	110-02-1	Alliaceous	0.0021 (Yan *et al*., 2020)	-	-
271	2-Thenaldehyde	98-03-3	Sulphury	0.011 (Dong, 2020), 0.0061 (Yan *et al*., 2020)	-	-
272	5-Methly-2-thiophenecarboxaldehyde	13679-70-4	Sweet, woody	0.0053 (Yan *et al*., 2020)	-	-
273	3-Phenylthiophene	2404-87-7	-	0.0066 (Yan *et al*., 2020)	-	-
274	Thiazole	288-47-1	Nutty, meaty	0.39 (Fan and Xu, 2000), 0.022 (Yan *et al*., 2020)	-	-

275	Benzothiazole	95-16-9	Beefy	0.003 (Yan *et al*., 2020)	-	-
276	4-Methyl-5-vinylthiazole	1759-28-0	Musty	0.0003 (Yan *et al*., 2020)	-	-
			Biogenic amine			
277	Aminomethane	74-89-5	-	0.048 (Wen *et al*., 2013)	-	-
278	Ethylamine	75-04-7	Ammoniacal, fishy	0.043 (Wen *et al*., 2013)	-	-
279	Pyrrolidine	123-75-1	Ammoniacal	0.29 (Wen *et al*., 2013)	-	-
280	1,4-Butanediamine	110-60-1	Rotting fish	0.053 (Wen *et al*., 2013), 0.06 (Liu *et al*., 2020)	-	-
281	1,5-Diaminopentane	462-94-2	-	0.02 (Wen *et al*., 2013), 0.19 (Liu *et al*., 2020)	-	-
282	Tryptamine	61-54-1	-	0.15 (Liu *et al*., 2020)	-	-
283	Phenethylamine	64-04-0	Ammoniacal	0.61 (Liu *et al*., 2020)	-	-
284	Pyridoxamine dihydrochloride	524-36-7	-	0.72 (Liu *et al*., 2020)	-	-
285	Histamine	51-45-6	-	0.09 (Liu *et al*., 2020)	-	-
286	Tyramine	51-67-2	Sweet	0.21 (Liu *et al*., 2020)	-	-
287	Spermidine	124-20-9	-	0.04 (Liu *et al*., 2020)	-	-
288	Spermine	71-44-3	-	0.3 (Liu *et al*., 2020)	-	-
			Other			
289	2-Acetylpyridine	1122-62-9	Cornmeal	0.8 (Cao, 2014)	-	-
290	Naphthalene	91-20-3	Pungent	0.56 (Sha, 2017), 0.06 (Liu, 2008), 0.3 (Zhou, 2015)	-	-
291	2,4,5-Trimethyl-1,3-oxazole	20662-84-4	Roasted wasabi	0.22 (Fan and Xu, 2000)	-	-
292	Pyridine	110-86-1	Sickening sour	0.42 (Fan and Xu, 2000)	-	-
293	Phenylethylene	100-42-5	Sweet, balsam	0.04 (Liu, 2020)	-	-
294	Diethoxymethane	462-95-3	-	0.061 (Xu, 2019)	-	-
295	Oxytetracycline	79-57-2	-	0.01 (Zhang, 2013), 0.0024 (Wang, 2020b)	-	-
296	Cyanides	-	-	0.023 (Zhang *et al*., 2014a), 0.17 (Zhang *et al*., 2016a)	-	-
297	Ethyl carbamate	51-79-6	Honey	0.01 (Sun *et al*., 2015), 0.26 (Zhang, 2014b)	-	-
298	Ochratoxin A	303-47-9	-	0.00017 (Zhu, 2017)	-	-
299	Geosmin	19700-21-1	Musty soil	0.0055 (Du *et al*., 2011)	-	-
300	3-Methylindole	83-34-1	Mud	0.14 (Dong, 2020)	0.006	23
301	6-(2-Formyl-5-methyl-1H-pyrrol-1-yl) hexanoic Acid	-	-	0.22 (Zhao, 2019)	-	-
302	Lichenysin	-	-	0.056 (Zhang, 2014a)	-	-

([a]) Odour description taken from www.thegoodscentscompany.com. ([b]) Odour thresholds taken from Xu (2019), Wang (2020a), Wang *et al*. (2022c), Duan *et al*. (2022), and Zheng (2017), who collected the data from various sources. ([c]) OAV calculated using average concentration

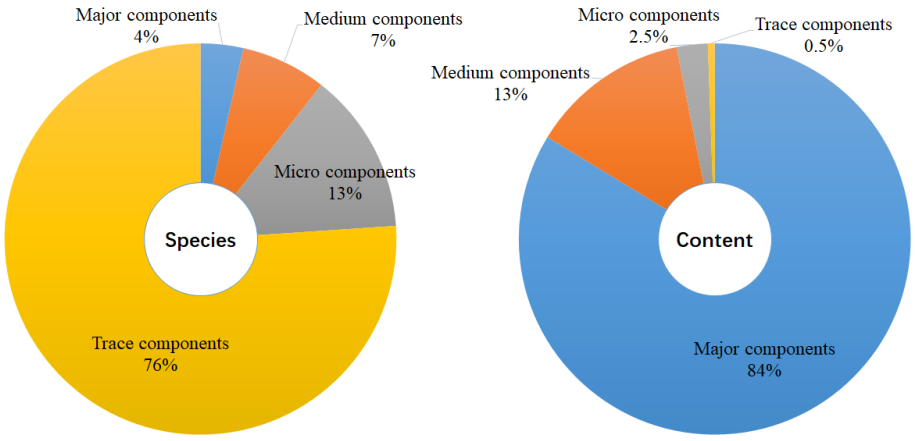

Figure 1. Percentages of number of species and mass content of the four component groups in *baijiu* (calculated from Tables 1 - 4).

Higher alcohols

With an unpleasant smell and a bitter and irritating taste, higher alcohols have various contents in *baijiu*. For example, isobutanol and isoamylol have concentration higher than 100 mg L^{-1}; butanol, pentanol, octanol, *etc*. have concentration ranging from 1 to 100 mg L^{-1}; however, the great majority of alcohols, in terms of number of species, have concentrations lower than 1 mg L^{-1} (Table 4). For example, mushroom alcohol was quantified with a low concentration of 0.11 mg L^{-1} using SPME-GC-MS (Zhang, 2013), but it became one of the main aroma contributors in medicine-aroma *baijiu* due to its low odour threshold. In the same study, another higher alcohol, namely 2-heptanol, made important contribution to the aroma of strong-aroma *baijiu*. There should be proper content of higher alcohols in *baijiu*. When the content of higher alcohols is too low, the generation of esters will be inhibited, resulting in the slight aroma and poor taste of *baijiu*; however, when the content of higher alcohols is too high, *baijiu* will taste bitter and irritating, and be harmful to the human body. Therefore, it is important to precisely control the content of higher alcohols within a reasonable range. Higher alcohols mainly come from the metabolism of yeasts (Eden *et al*., 2001). Based on the source of their precursors, higher alcohols are produced *via* two pathways, namely amino acid catabolic pathway (Ehrlich pathway) (Derrick and Large, 1993) and sugar metabolic pathway (Harris pathway) (Mangas *et al*., 1994). Since higher alcohols have slow metabolism and long retention time in the body, they have higher toxicity and anaesthetic effect than that of lower alcohols, and their toxicity increases with the increase in carbon chain, and decreases with primary, secondary, and tertiary alcohols with the same carbon chain (Cui *et al*., 2018). The high level of higher alcohols in *baijiu* could make the nervous system congested, causing symptoms of dizziness and pain (Wallgren, 1960).

Fatty acids

Fatty acids have great impacts on the flavour of *baijiu*, and they are the precursors of esters. Fatty acids have various contents in *baijiu*, ranging from several hundred milligrams per litre, such as those of butanoic acid and hexanoic acid, to as low as several micrograms per litre (Table 4). Based on the difference of boiling points, there are two types of fatty acids: volatile fatty acid and non-volatile fatty acid. Volatile fatty acids such as butanoic acid, isobutyric acid, isovaleric acid, hexanoic acid, *etc*., are mostly short-chain acids, and due to their high volatility and contents, these acids dominate the sour smell of *baijiu*. Non-volatile fatty acids such as palmitoleic acid, decanoic acid, malic acid, *etc*., however, are mostly long-chain acids, and they contribute mostly to tastes of *baijiu* due to their non-volatility and low contents. Wang *et al*. (2022a) developed a novel derivatisation method to systematically analyse non-volatile organic acids in Laobaigan *baijiu*, and quantified 37 species using GC-MS. Wang *et al*. (2022b) found out that the odour of the reconstituted samples that contained both odour-active volatiles and non-volatile organic acids was more similar to that of the original *baijiu* samples, than the samples that only contained odour-active volatiles. This proved that non-volatile organic acids could have strong impacts on the odour-active volatiles, and are indispensable for the overall aroma profile of *baijiu*. The flavoromics strategy based on the contents of non-volatile organic acids can be used

as a powerful tool for the differentiation of *baijiu* of various types (Wang *et al*., 2022b). Hu *et al*. (1994) quantified 20 fatty acids in Maotai, Wuliangye, Gujinggong, Jiananchun, Site, and Jingzhi *baijiu* using GC-MS, and the results showed that the total amount of odd-carbon fatty acids was much lower than that of even-carbon fatty acids. There should be a proper content of fatty acids in high-quality *baijiu*, which makes it mellow and have long aftertaste. Acids of low content may lead to bitterness and uncleanness of *baijiu*, while acids of high content may override the aroma of esters, and cause the coarseness and astringency of *baijiu* (Zhang *et al*., 2016b). Most of acids in *baijiu* come from *daqu*, fermented grains and pit mud in the brewing process. They are produced by microorganism as the by-products during its growth and reproduction process by using sugars and proteins as raw materials (Yang, 2017).

Trace esters

Esters are the main aroma compounds in *baijiu*. Although the trace esters have much lower contents than those of major esters, the former have much more diverse species than the latter. Some trace esters even have extremely low odour thresholds, leading to their strong smell in *baijiu* at relatively low concentration. For example, decalactone has a low odour threshold of 10 μg L^{-1}, so its OVA reached five at a concentration of 50 μg L^{-1} (Xu, 2019). Ethyl cinnamate also has a low odour threshold of 1 μg L^{-1}, and its OAV could reach as high as 20 at a concentration of 20 μg L^{-1} (Xu, 2019). Ethyl acrylate has an even lower odour threshold of 0.2 μg L^{-1}, resulting in its OAV as high as 2,250 at a concentration of 450 μg L^{-1} (Zheng, 2017). This shows that some trace esters have higher OAVs than those of many major esters. Sun *et al*. (2022) determined three lactones, namely γ-nonanolactone, γ-butyrolactone, and sotolon with concentrations ranging from 0.084 to 1.19 mg L^{-1} in *baijiu* using SPME-GC-MS. The lactones are largely the reaction products of sugars and amino acids under conditions of low temperature and short heating time, and their contents are various depending on factors such as aging time, glucose fraction, and oxygen content. Since sotolon, which smells like caramel, and naturally exists in many fruits, has a very low odour threshold of 9 μg L^{-1}, its OAV could reach as high as 133, making it a marker component of aged Xiaoqu *baijiu* (Sun *et al*., 2022). The production of sotolon was probably related to the Maillard reaction. It is also reported that the condensation reaction between 2-ketobutyric acid and acetaldehyde would lead to the formation of sotolon (Takahashi *et al*., 1976). However, the exact mechanism for the sotolon formation still remains a complex one. Ren (2016) identified six esters namely ethyl octanoate, ethyl nonanoate, ethyl benzoate, ethyl 2-yl isovalerate, isoamyl lactate, and diethyl succinate as the characteristic aroma substances that could be used to differentiate the Fen *baijiu* with different storage times.

Trace carbonyl compounds

Both aldehydes and ketones contain carbonyl group, so they are collectively referred to as carbonyl compounds. Carbonyl compounds generally have low odour thresholds, so they could exert great influence on the flavour of *baijiu*. Due to the low content and high solubility of carbonyl compounds in *baijiu*, it is not easy to obtain an ideal separation of carbonyl compounds. Therefore, derivatisation should be applied before detection using GC-MS. Carbonyl derivatising agents react specifically with carbonyl compounds, and the derivatives can effectively remove the influence of matrix, and change the solubility of carbonyl compounds, making them easier to be extracted. Derivatising agents usually have large molecular weights, and so will be the derivatives, thus significantly improving the detection sensitivity. Based on the derivatisation technique combined with SPME-GC-MS, Cao (2014) quantified 53 carbonyl compounds, including ten straight-chain saturated aliphatic aldehydes, three branched-chain saturated aliphatic aldehydes, eight saturated aliphatic ketones, 14 unsaturated aliphatic aldehydes, six aromatic carbonyl compounds, four furan carbonyl compounds, and five other carbonyl compounds in *baijiu* of different aroma types. The content of carbonyl compounds varies significantly in different *baijiu*, among which the soy-sauce-aroma *baijiu* has the highest total content of carbonyl compounds. Wang *et al*. (2020c) analysed 12 carbonyl compounds in soy-sauce-aroma *baijiu* using GC-O combined with GC×GC-MS, among which *trans*-2-nonenal and *trans*,*trans*-2,4-decadienal had an extremely low odour threshold of 0.1 μg L^{-1}, and contributed greatly to the "pickle-like" off-odour of *baijiu*. *trans*-2-Nonenal was also identified as the key marker for the Chixiang *baijiu* based on the results of omission experiments (Fan *et al*., 2015). In another

research, methional was quantified with a high concentration of 0.57 mg L^{-1}, resulting in a high flavour dilution (FD) factor of 1,024 and a high OAV of 17 (Zheng *et al*., 2016). When methional was removed in the omission experiments, the "roast" intensity significantly decreased, which confirmed that methional played a key role in typical roasting and burning flavour of sesame-aroma *baijiu*.

Phenols

As natural antioxidants, phenols are ubiquitous in foods and drinks, and have been widely concerned due to their various biological activities. There are various kinds of phenols in *baijiu*, and most of them are important aroma contributors. For example, benzenol smells like sour and burnt, and guaiacol and its derivatives make *baijiu* smell like clove. Zhang (2013) detected ten phenols in *baijiu* using SPME combined with GC-MS, and some phenols such as 4-methylphenol and 4-methylguaiacol had concentrations of as high as over 1 mg L^{-1}. Dong (2020) quantified six phenols, namely 4-methylphenol, 4-ethylphenol, 4-methylguaiacol, 4-ethylguaiacol, 4-vinylguaiacol, and vanillin using LLE-GC-MS with concentrations below 0.6 mg L^{-1} in all samples. He *et al*. (2021) identified 4-ethylguaiacol as the aroma marker for the classification of *baijiu* from different distillation stages by temperature-programmed HS-GC-IMS and GC-OF-MS combined with chemometric strategies. Sun *et al*. (2022) identified and quantified vanillin as a characteristic compound of Xiaoqu *baijiu*. It had a high concentration of 0.85 mg L^{-1} in the aged *baijiu*, resulting in its high OAV of 33. Phenols are mostly produced by microorganisms in the *daqu*-making process, and can also be chemically generated from amino acids or tannins (Guo *et al*., 2020). Besides being aroma compounds, many phenolic substances in *baijiu* have health-care effects on human body. Zhao (2019) found out that the antioxidant activity of *baijiu* was positively correlated with the contents of vanillin, 4-methylguaiacol, and 4-ethylguaiacol. Phenols could also help cells resist oxidative stress, which in turn prevents or delays the development of stress-related degenerative diseases (Lingua *et al*., 2016). However, some phenols such as benzenol with high concentration could also be harmful to human body; so, adsorbents can be applied to remove them in *baijiu* production (Bukowska and Kowalska, 2004). Increasing the content of functional phenolic substances can improve the quality of *baijiu*, but toxic phenolic substances should be avoided.

Pyrazines

Pyrazines, which widely exist in natural food, are heterocyclic compounds containing two hetero-nitrogen atoms in the first and fourth positions of the benzene ring. Many studies have confirmed pyrazines as important flavouring substances in *baijiu*.

For example, Zhao *et al*. (2018) discovered and identified a key retronasal burnt flavour compound, namely 2-hydroxymethyl-3,6-diethyl-5-methylpyrazine, in soy-sauce-aroma type *baijiu* with sensory-guided isolation assisted by multivariate data analysis. Fan *et al*. (2007) detected 27 pyrazines in *baijiu* of different types using LLE-GC-MS, and found out that the content of pyrazine in soy-sauce-aroma *baijiu* was the highest, followed by strong-aroma *baijiu* and light-aroma *baijiu*. Wu (2013) analysed the contents of pyrazines in *baijiu* of different types and studied the variation of tetramethylpyrazine in different stages of *daqu*-making such as stacking, fermentation, and distillation, and found out that tetramethylpyrazine was mainly produced by bacteria in the *daqu*-making process. Then the author investigated the synthesis of tetramethylpyrazine by the reactions among glucose, hydroxybutanone, amino acid, and ammonium salt in simulated fermentation process, and finally proposed a mechanism of two-stage enzymatic/thermodynamic combined reaction synthesis of tetramethylpyrazine (Wu and Xu, 2013). Many pyrazines in *baijiu*, such as 2-methylpyrazine, 2,3-dimethylpyrazine, and 2,3,5-trimethylpyrazine are salutary components, and have antioxidant ability (Guo *et al*., 2020). It has been proved that tetramethylpyrazine, which is a main ingredient of Chuanqiong, a Chinese traditional medicine, has the ability to inhibit tumour (Fu *et al*., 2008) and treat diabetes (Kang *et al*., 2009). Due to the importance of tetramethylpyrazine in improving the flavour and quality of *baijiu*, many methods such as increasing oxygen content and adding functional bacteria have been tried to increase its content in *baijiu* (Guo *et al*., 2020).

Terpenes

Terpenes are a group of naturally occurring hydrocarbons that are widely found in plants. There are two categories of terpenes: one is hydrocarbons without oxygen; the other is oxygen-containing

terpene alcohols, terpene aldehydes, and terpene esters. Since terpenes have very low content in *baijiu*, with some even lower than 1 μg L^{-1}, high efficient concentration pretreatments, such as dispersible liquid-liquid microextraction (DLLME), solid-phase micro-extraction (SPME), stir-bar sorptive extraction (SBSE), and supercritical fluid extraction (SFE) should be applied before detection using GC-MS (Jia *et al*., 2020). For instance, Fan *et al*. (2012a) used HS-SPME combined with GC-MS to analyse terpenes in medicine-aroma *baijiu*, and quantified 41 volatile terpenes with linear correlation coefficients (R^2) all higher than 0.99. Wang *et al*. (2015) also identified 55 terpenes in soy-sauce-aroma *baijiu* using SPME-GC-MS. There are generally two sources of terpene substances. One is from brewing materials such as sorghum, wheat, corn, *etc*. These materials contain a large number of terpene substances such as β-caryophyllene, β-eudesmol, and geranyl acetone, which can be brought into the *baijiu* during fermentation. The other source is from the metabolism of microorganisms, such as actinomycetes (Guo *et al*., 2020). Although terpenes generally have low concentrations in *baijiu*, they are important aroma contributors due to the low odour thresholds. For example, β-damascenone and β-ionone have an extremely low odour threshold of 0.002 and 0.007 μg L^{-1} (Buttery *et al*., 1990), and their OAVs could reach as high as 9,905 and 1,589 (Fan *et al*., 2012a), respectively. Due to their high OAVs and strong aroma, many terpenes have been identified as the important flavour marker of *baijiu* (Zeller and Rychlik, 2006; Fan *et al*., 2012a). Gao *et al*. (2014) identified and quantified β-damascenone as the key odorant of light-aroma *baijiu* using GC-O-MS. Besides being aroma contributors, some terpenes such as β-caryophyllene, elemene, and β-eudesmol have physiological properties such as anti-oxidation (Dahham *et al*., 2015) and anti-cancer (Wang *et al*., 2015).

Furans

Furans are important aroma contributors of *baijiu*. Zheng (2017) detected eight furans, namely furfural, furfuryl alcohol, 2-furaldehyde diethyl acetal, 5-methyl furfural, furylacrolein, 2-acetyl-5-methylfuran, 2-acetylfuran, and difurfuryl ether in commercial sesame-aroma *baijiu* using SPME-GC-MS. Cao (2014) quantified furfural, 5-methyl furfural, and 2-pentylfuran with concentrations of 62.7, 0.065, and 0.16 mg L^{-1}, respectively, in soy-sauce-aroma *baijiu*. Furfural is the most important furan in *baijiu*, and has the highest contents among the furan ring family. It has been confirmed that the content of furfural in *baijiu* of different types followed the order of soy-sauce-aroma > strong-aroma > light-aroma (Xu, 2002). Since the content of furfural in soy-sauce-aroma *baijiu* is significantly higher than that in other *baijiu*, it has been regarded as a marker component of soy-sauce-aroma *baijiu*. Furfural is mainly formed *via* the dehydration of pentose or pentosan in raw materials. There is a positive correlation between the content of furfural with the length of fermentation time and fermentation temperature (Xu, 2002). When grain husks, corn cobs, and brans are used as auxiliary materials, the distilled *baijiu* usually contains a high level of furfural. High furfural content makes *baijiu* mellow, but excessive furfural could cause harm to human body (Zhang *et al*., 2021). Other furans could also make important contribution to the aroma of *baijiu* considering their extremely low odour thresholds. For example, 2-methyl-3-furanthiol and 2-furfurylthiol have low odour thresholds of 0.0057 and 0.1 μg L^{-1}, respectively, and they could be used as the marker for the differentiation of light-aroma, strong-aroma, and soy-sauce-aroma *baijiu* based on the results of hierarchical cluster analysis and partial least squares discriminant analysis (Song *et al*., 2020). In another research, Yan *et al*. (2020) quantified two furans, namely 2-methyl-3-(methyldisulfanyl) furan and furfuryl methyl disulphide, both of which give a cooked meat-like aroma, with concentrations ranging from 2.7 to 8.7 μg L^{-1}. The formation of 2-methyl-3-(methyldisulfanyl) furan is probably caused by the Maillard reaction with glutathione and xylose, but the exact mechanism still remains unclear (Yang *et al*., 2012).

Sugars and sugar alcohols

Sugars and sugar alcohols are important sweet substances and contribute to the natural mellowness of *baijiu*. As Table 4 shows, 14 sugars and sugar alcohols are frequently detected in Chinese *baijiu*. Han *et al*. (2013) quantified six sugar alcohols (glycerol, erythritol, arabinitol, sorbitol, galactitol, and mannitol) in light-aroma *baijiu* using ion chromatograph (IC). Glycerol, which is the simplest sugar alcohol, had the highest concentration (0.62 mg L^{-1}) among the selected sugar alcohols in *baijiu*. Wang *et al*. (2021) detected seven sugars and sugar alcohols in Laobaigan *baijiu* using GC-MS, with the

concentrations of glycerol and glucose being much higher than other sugars and sugar alcohols. Yu *et al*. (2019) established a method for the determination of sorbitol in *baijiu* using liquid chromatography-mass spectrometry (LC-MS). The regression coefficient (R^2) of the method could reach as high as 0.998, and the relative error was lower than 5%, which renders it a proper method for the determination of sorbitol in *baijiu*. Since sugars and sugar alcohols have high boiling points, and are not volatile, they are difficult to detect and analyse using GC-based methods. Therefore, many other methods, such as IC and LC-based methods, are used to detect these substances in *baijiu* (Wang *et al*., 2021).

Sulphur-containing compounds

All sulphur-containing compounds detected have concentrations lower than 1 mg L^{-1}, and most of them, actually, have concentrations lower than 0.1 mg L^{-1} (Table 4). Although sulphur-containing compounds are present at low levels, they are important aroma contributors in *baijiu* due to their extremely low odour thresholds. Therefore, many previous studies have been reported on the key role of sulphur-containing compounds in affecting the flavour of *baijiu* (Zheng *et al*., 2016; Chen *et al*., 2017; Sha *et al*., 2017; Li *et al*., 2019; Song *et al*., 2019; Wang *et al*., 2020c). For example, benzene methanethiol, dimethyl trisulfide, 2-methyl-3-furanthiol, and 2-furfurylthiol have low odour thresholds of 0.01, 0.32, 0.0057, and 0.1 μg L^{-1}, resulting in their OAVs of as high as 487, 188, 135, and 107, respectively (Song *et al*., 2019). Chen *et al*. (2017) identified and quantified 13 sulphur-containing compounds in Moutai *baijiu*. The aroma contribution of these sulphur-containing compounds was evaluated by their OAVs, with the result that seven of 13 sulphur-containing compounds had OAVs > 1. In particular, 2-furfurylthiol, methanethiol, dimethyl trisulfide, ethanethiol, and methional had relatively high OAVs, and could be the key aroma contributors to the famous Moutai *baijiu*. Due to the great aroma contribution and low content of sulphur-containing compounds, much effort has been made to analyse sulphur-containing compounds using various efficient pretreatment methods and detectors. For instance, Fan and Xu (2013) used pretreatment method of LLE combined with fractionation using silica-agarose gel, and detected 21 sulphur-containing compounds using GC-MS. Zheng *et al*. (2016) applied SPME-GC-MS to analyse dimethyl trisulfide and methional in the sesame-aroma *baijiu*, and obtained limits of detection (LOD) of 2.18 and 76.4 μg L^{-1}, respectively. Song *et al*. (2019) identified 12 key sulphur-containing compounds in Laobaigan *baijiu* using GC-O and GC × GC coupled with sulphur chemiluminescence detector, resulting in an extremely low LOD of 0.05 - 1.53 ng L^{-1}. Li *et al*. (2019) identified benzene methanethiol, which had a high FD value of 191,863, as the key contributor to the sesame aroma of Guojing *baijiu*. Sulphur-containing compounds usually have unpleasant smell. Wang *et al*. (2020b) found out that eight sulphur-containing compounds, namely 2-methyl-3-furanthiol, methional, methyl 2-methyl-3-furyl disulphide, dimethyl trisulfide, 2-furfurylthiol, methanethiol, dimethyl disulphide, and bis (2-methyl-3-furyl) disulphide, were responsible for the pickle-like off-odour in soy-sauce-aroma *baijiu*. Most of sulphur-containing compounds are derived from sulphur-containing amino acids such as methionine, cystine, and cysteine in raw materials. The species of sulphur-containing compounds are various in different *baijiu* due to the different ingredients, production processes, distillation temperatures, and time (Fan and Xu, 2013).

Cyanides

Cyanides are compounds with cyanide group (CN), all of which are highly toxic. Cyanides poisoning is mainly caused by taking orally, for it can be fully absorbed by oral mucosa and digestive tract. Cyanides can be hydrolysed into cyanide ion (CN^-), which inhibits the activity of enzymes in tissue cells, leading to central respiratory failure and even death (Xu, 2017). According to the National Standards of Food Safety for Distilled Spirits (GB 2757-2012), the limits of cyanides in *baijiu* must be ≤ 8.0 mg L^{-1} (by HCN). Many methods such as GC-FID, GC-MS, LC-MS, IC, and spectrophotometry have been applied for the detection of cyanides in *baijiu*. For instance, Zhang *et al*. (2014a) developed a method of headspace combined with GC-MS for the detection of cyanides in *baijiu*. Low toxic KSCN was used as substitute for the high toxic KCN to react with chloramine-T to produce cyanide chloride. Relative standard deviation (RSD) of 5.4%, recovery rate of 120%, and LOD of 0.0025 μg L^{-1} were obtained after five repeated experiments under the safe conditions. Zhang *et al*. (2016a) used a method of purge and trap combined with GC-MS for the detection of cyanides in *baijiu*, and the concentration of cyanides in the

selected samples reached as high as 0.48 mg L^{-1}. Their method has merits of high recovery rates, accurate results, and low interference, and can quickly conduct quantitative analysis of cyanides in *baijiu*. Luo *et al*. (2020) established a method of IC-ECD for the cyanides detection in *baijiu*, which had a low LOD of 0.8 μg L^{-1}. The whole analysis process could be completed within ten minutes by direct injection without pretreatment. The main source for cyanides in *baijiu* is from the raw materials such as cassava, which is much cheaper than other cereals. However, the outer surface of cassava root contains large amount of hydrocyanic acid that leads to production of cyanides (Xu, 2017). Other sources of cyanides include use of cyanide-polluted water and low-quality edible ethanol during the production of *baijiu*.

Ethyl carbamate

Ethyl carbamate, also known as urane, is an ethyl ester of carbamate, which can be naturally produced in liquors of different types such as whisky, brandy, *baijiu*, *etc*., with content ranging from ng L^{-1} to mg L^{-1} (Zhang, 2014b). Since ethyl carbamate is genotoxic and carcinogenic to many animals of different species, it has been listed as a class 2A carcinogen by the International Agency for Research on Cancer. Due to its low content, many pretreatment methods such as LLE (Woo *et al*., 2011) and SPE (Jagerdeo *et al*., 2002) have been applied before the detection of ethyl carbamate using GC-MS. However, LLE has a relatively low extraction efficiency, and SPE is time-consuming and laborious, and the use of organic solvents has a certain degree of toxicity to human. Compared with LLE and SPE, HS-SPME has advantages of automatic extraction and simple and fast operation. Sample pretreatment can be completed within five minutes. Moreover, the extraction process does not need organic solvents (Jia *et al*., 2020). Zhang (2014b) used HS-SPME-GC-MS to evaluate the content changing of ethyl carbamate during the distillation and storage of Chinese *baijiu*, and the results showed that the ethyl carbamate content increased slowly from 59.04 to 117.39 μg L^{-1} in the first eight minutes during the distillation process. Then the ethyl carbamate content increased rapidly in the following two minutes, and reached as high as 261.00 μg L^{-1} after ten minutes. Fan *et al*. (2012b) also used the HS-SPME-GC-MS to detect ethyl carbamate, and the concentration of ethyl carbamate could reach 130 μg kg^{-1} in the fermented grains during the fermentation process of *baijiu*. Using propyl carbamate as internal standard, Li *et al*. (2014) applied SPE-GC-MS to determine ethyl carbamate in *baijiu*. The recovery rates ranged from 82 to 99%, and the ROS was less than 5%. The method had good precision and reproducibility, which met requirements for daily detection and analysis of ethyl carbamate in *baijiu*. Zhang (2016c) developed an HPLC-MS-MS method to investigate the behaviour of ethyl carbamate in *baijiu*, and the results indicated that the formation of ethyl carbamate was positively related to the content of cyanides, which confirmed the formation of ethyl carbamate *via* the reaction between ethanol and cyanides (Jia *et al*., 2020). Another pathway for the formation of ethyl carbamate was *via* the reaction between ethanol and the precursor substances such as urea, citrulline, and carbamoyl. The study by Fan *et al*. (2012b) proved that the formation of ethyl carbamate was also positively related to the content of urea.

Biogenic amines

Biogenic amines, which widely exist in fermented food such as *baijiu*, are a class of nitrogen-containing bioactive compounds. They can be regarded as the substances generated after the hydrogen atom(s) of ammonia molecule are replaced by alkyl or aryl group. Biogenic amines can be generated by microbial decarboxylation of the corresponding amino acids. Biogenic amines at low concentration are beneficial to human body, and the precursors of bioactive substances such as hormones, alkaloids, and proteins (Zhang *et al*., 2019). Biological amines at high concentration are harmful to human body, causing symptoms such as headaches, brain bleeding, and even heart failure (Zhou *et al*., 2020). HPLC based methods are commonly used for the detection of biogenic amines in *baijiu* due to their high boiling points and instability at high temperature. Since biogenic amines have few chromogenic functional groups, they must be derivatised before the detection. Common derivatising agents such as phthalaldehyde and benzoyl chloride are nucleophilic so that they can substitute the active hydrogen atom of the amine group. Wen *et al*. (2013) used dansyl chloride as derivatising agent to determine five biogenic amines, namely aminomethane, ethylamine, pyrrolidine, 1,4-butanediamine, and 1,5-diaminopentane in *baijiu*. The concentration of the five biogenic amines ranged from 0 to 1.4 mg L^{-1}, and the soy-sauce-aroma *baijiu*

had higher biogenic amines concentration than those of strong-aroma and light-aroma *baijiu*. Liu *et al*. (2020) also detected nine biogenic amines in *baijiu* using precolumn derivatisation combined with HPLC. The method had good linear correlation (R^2 > 0.998) at concentrations ranging from 0.5 to 50 mg L^{-1}, which is satisfactory for the detection of biogenic amines in *baijiu*.

Mycotoxins

Mycotoxins are secondary metabolites of moulds that come from raw materials, *jiuqu*, and the production environment. Most mycotoxins have high biological toxicity, and could cause reproductive disorder, kidney injury, and immune inhibition. Screening methods such as thin layer chromatography, enzyme-linked immunosorbent assay, immunobiosensor technique, and molecular imprinting technology are usually applied before the instrumental analysis (Liu *et al*., 2021). For example, Li *et al*. (2015) used enzyme-linked immunosorbent assay combined with HPLC for quantitative analysis of mycotoxins in various samples during the *baijiu* production. The results showed that the content of aflatoxin B_1 in *daqu*, fermented grains, and yellow water reached 2.55, 1.75, and 2.25 μg kg^{-1}, respectively. The content of aflatoxin B_1 in base *baijiu* and finished *baijiu* did not reach the detection limits. Zhu (2017) developed a method of SPE-HPLC-FLD for the detection of ochratoxin A in *baijiu*. The SPE column of a novel inverting/strong anion mixture was used to screen mycotoxins for the first time. The recovery rates ranged from 81.6 to 100.8%, and the LOD was 0.006 μg L^{-1}. The positive rates of ochratoxin A from 76 *baijiu* samples was 11.8%, and the highest concentration reached 0.17 μg L^{-1}. This indicates that safety risks of ochratoxin A in *baijiu* exist, and it is necessary to conduct routine monitoring of ochratoxin A in *baijiu* considering its high toxicity.

Other trace compounds

Besides the categorised trace compounds as discussed earlier, many still remain to be discovered. Much has been done on analysing the trace compounds that have low odour thresholds but high contribution to the off-odour or aroma of *baijiu*. For example, Du *et al*. (2011) identified and quantified geosmin (*trans*-1,10-dimethyl-*trans*-9-decalol) as the main contributor for the earthy and mouldy odour of *baijiu*. The concentration of geosmin ranged from 1.10 to 9.90 μg L^{-1} for all *baijiu* samples, except for the strong-aroma *baijiu*. As geosmin was not detected in steamed or non-steamed rice husk, this proved that rice husk was not the origin of earthy and mouldy odour of *baijiu*. Geosmin is also an important odour contributor in light-aroma *baijiu* (Gao *et al*., 2014). To find the origin of geosmin that causes the earthy odour of light-aroma *baijiu*, Du and Xu (2012) carried out microbial analysis of *daqu* containing geosmin. The results showed that geosmin appeared in all fermented sorghums at different fermentation periods, and about 57% of geosmin in the fermented sorghums was distilled into *baijiu*. They concluded that microorganisms developing in *daqu* were responsible for the presence of geosmin in *baijiu*. In another study, 3-methylindole was found to be responsible for the "mud-like" off-odour of strong-aroma *baijiu* (Dong *et al*., 2018). With the threshold of 3-methylindole determined using three-alternative forced-choice procedure, the OAV of 3-methylindole reached as high as 23, which confirmed its important contribution to the "mud-like" odour of *baijiu*. Zhao *et al*. (2019) discovered a complex acid, 6-(2-formyl-5-methyl-1H-pyrrol-1-yl) hexanoic acid, as an important retronasal burnt aroma compound in the soy-sauce-aroma *baijiu* using high-resolution mass spectrometry and 1D/2D nuclear magnetic resonance (NMR). Quantitative analysis showed that the concentration of the targeted compound ranged from below the limit of quantitation (3.8 μg L^{-1}) to 224.2 μg L^{-1} in all selected *baijiu* samples. In another research, Zhang *et al*. (2014d) isolated and identified a new cyclic lipopeptide, namely lichenysin, in *baijiu* using HPLC-TOF-MS and NMR. Lichenysin was quantified with concentration ranging from 0.01 to 111.74 μg L^{-1}, with the highest concentration determined in Dong *baijiu*, among the 14 selected commercial *baijiu* samples. Lichenysin was found to have selective effect on aroma volatility in strong-aroma *baijiu*. Interaction between lichenysin and volatile phenolic compounds was characterised using HS-SPME-GC-MS, and the results indicated that lichenysin suppressed the volatility of phenolic compounds by 36 - 48% (p < 0.05) (Zhang *et al*., 2014c).

Conclusion

The present review discusses recent research on the identification and quantification of components in various aroma types of Chinese *baijiu*,

systematically detailing 397 quantified components, many of which fall within the category of trace components with precise concentrations. This compendium represents the most extensive reference material for quantified *baijiu* components to date, providing invaluable insights into *baijiu* analysis. Despite this advancement, several critical areas within *baijiu* research remain open for further exploration. For instance, identifying the specific markers for soy-sauce-aroma *baijiu*, isolating the components responsible for common symptoms such as dizziness and headache, and establishing means to assess *baijiu* quality based on its chemical composition all necessitate deeper investigation. These questions underscore the need for continued and in-depth research endeavours to unravel the complexities and mysteries inherent in *baijiu* production and its overall impact.

Acknowledgement

The present work was financially supported by the Natural Science Foundation of Hunan Province (grant no.: 2022JJ50227), Postgraduate Research and Innovation Project of Shaoyang University (grant no.: CX2022SY085), and Aid Program for Science and Technology Innovative Research Team in Higher Educational Institutions of Hunan Province (grant no.: Xiangjiaotong [2023] NO. 233).

References

Bukowska, B. and Kowalska, S. 2004. Phenol and catechol induce prehemolytic and hemolytic changes in human erythrocytes. Toxicology Letters 152(1): 73-84.

Buttery, R. G., Teranishi, R., Ling, L. C. and Turnbaugh, J. G. 1990. Quantitative and sensory studies on tomato paste volatiles. Journal of Agricultural and Food Chemistry 38: 336-340.

Cao, C. 2014. Flavor compounds of Chinese Kongfujia liquor. China: Jiangnan University, MSc thesis.

Chen, S., Sha, S., Qian, M. and Xu, Y. 2017. Characterization of volatile sulfur compounds in Moutai liquors by headspace solid-phase microextraction gas chromatography-pulsed flame photometric detection and odour activity value. Journal of Food Science 82(12): 2816-2822.

Cui, D. Y., Zhang, Y., Xu, J., Zhang, C. Y., Li, W. and Xiao, D. G. 2018. PGK1 promoter library for the regulation of acetate ester production in saccharomyces cerevisiae during Chinese *baijiu* fermentation. Journal of Agricultural and Food Chemistry 66(28): 7417-7427.

Dahham, S. S., Tabana, Y. M., Iqbal, M. A., Ahamed, M. B., Ezzat, M. O., Majid, A. S. and Majid, A. M. 2015. The anticancer, antioxidant and antimicrobial properties of the sesquiterpene beta-caryophyllene from the essential oil of *Aquilaria crassna*. Molecules 20(7): 11808-11829.

Derrick, S. and Large, P. J. 1993. Activities of the enzymes of the Ehrlich pathway and formation of branched-chain alcohols in *Saccharomyces cerevisiae* and *Candida utilis* grown in continuous culture on valine or ammonium as sole nitrogen source. Journal of General Microbiology 139: 2783-2792.

Dong, W. 2020. The studies of the key odourants causing Jiao-aroma and their formation pathways in the strong-aroma types of *baijiu*. China: South China University of Technology, MSc thesis.

Dong, W., Shi, K., Liu, M., Shen, C., Li, A., Sun, X., ... and Huang, M. 2018. Characterization of 3-methylindole as a source of a "mud"-like off-odour in strong-aroma types of base *baijiu*. Journal of Agricultural and Food Chemistry 66(48): 12765-12772.

Du, H. and Xu, Y. 2012. Determination of the microbial origin of geosmin in Chinese liquor. Journal of Agricultural and Food Chemistry 60(9): 2288-2292.

Du, H., Fan, W. and Xu, Y. 2011. Characterization of geosmin as source of earthy odour in different aroma type Chinese liquors. Journal of Agricultural and Food Chemistry 59(15): 8331-8337.

Duan, J., Yang, S., Li, H., Qin, D., Shen, Y., Li, H., ... and Sun, B. 2022. Why the key aroma compound of soy sauce aroma type *baijiu* has not been revealed yet? LWT – Food Science and Technology 154: 112735.

Dung, N. T. P. 2013. Vietnamese rice-based alcoholic beverages. International Food Research Journal 20(3): 1035-1041.

Eden, A., Van Nedervelde, L., Drukker, M., Benvenisty, N. and Debourg, A. 2001. Involvement of branched-chain amino acid

aminotransferases in the production of fusel alcohols during fermentation in yeast. Applied Microbiology and Biotechnology 55(3): 296-300.

Fan, H., Fan, W. and Xu, Y. 2015. Characterization of key odourants in Chinese Chixiang aroma-type liquor by gas chromatography-olfactometry, quantitative measurements, aroma recombination, and omission studies. Journal of Agricultural and Food Chemistry 63(14): 3660-3668.

Fan, W. and Xu, Y. 2000. A comparison of flavor characteristics between Chinese strong aromatic liquors (Daqu). Liquor-Making Science and Technology 101: 92-94.

Fan, W. and Xu, Y. 2013. Identification of volatile compounds of Fenjiu and Langjiu by liquid-liquid extraction coupled with normal phase liquid chromatography. Liquor-Making Science and Technology 225: 17-27.

Fan, W., Hu, G. and Xu, Y. 2012a. Quantification of volatile terpenoids in Chinese medicinal liquor using headspace-solid phase microextraction coupled with gas chromatography-mass spectrometry. Food Science 33(14): 110-116.

Fan, W., Xu, Y. and Shi, B. 2012b. Evolvement of ethyl carbamate and urea from fermented grains in the fermentation process of Chinese liquor. Science and Technology of Food Industry 33(23): 171-174.

Fan, W., Xu, Y. and Zhang, Y. 2007. Characterization of pyrazines in some Chinese liquors and their approximate concentrations. Journal of Agricultural and Food Chemistry 55: 9956-9962.

Fu, Y., Lin, Y., Chou, S., Tsai, T., Kao, L., Hsu, S., ... and Wang, J. 2008. Tetramethylpyrazine inhibits activities of glioma cells and glutamate neuroexcitotoxicity: Potential therapeutic application for treatment of gliomas. Neuro-Oncology 10(2): 139-152.

Gao, W., Fan, W. and Xu, Y. 2014. Characterization of the key odourants in light aroma type Chinese liquor by gas chromatography-olfactometry, quantitative measurements, aroma recombination, and omission studies. Journal of Agricultural and Food Chemistry 62(25): 5796-5804.

Guo, X., Fan, E., Ma, B., Li, Z., Zhang, Y., Zhang, Z., ... and Xiao, D. 2020. Recent progress in micro components of Chinese *baijiu*. Food Science 41(11): 267-276.

Han, X., Wang, Y., Wei, J., Wang, D., Tang, K. and Zhao, C. 2013. Analysis of polyhydric alcohols in Qing-flavor liquor. Liquor-Making Science and Technology 8: 44-49.

He, F., Duan, J., Zhao, J., Li, H., Sun, J., Huang, M. and Sun, B. 2021. Different distillation stages *baijiu* classification by temperature-programmed headspace-gas chromatography-ion mobility spectrometry and gas chromatography-olfactometry-mass spectrometry combined with chemometric strategies. Food Chemistry 365: 130430.

He, Y., Tang, K., Yu, X., Chen, S. and Xu, Y. 2022. Identification of compounds contributing to trigeminal pungency of *baijiu* by sensory evaluation, quantitative measurements, correlation analysis, and sensory verification testing. Journal of Agricultural and Food Chemistry 70(2): 598-606.

Hu, G., Cheng, J. and Zhu, Y. 1994. Quantitative determination of free organic acids in Chinese liquors. Chinese Journal of Chromatography, 12(4): 265-267.

Jagerdeo, E., Dugar, S., Foster, G. D. and Schenck, H. 2002. Analysis of ethyl carbamate in wines using solid-phase extraction and multidimensional gas chromatography/mass spectrometry. Journal of Agricultural and Food Chemistry 50(21): 5797-5802.

Jia, W., Fan, Z., Du, A., Li, Y., Zhang, R., Shi, Q., ... and Chu, X. 2020. Recent advances in *baijiu* analysis by chromatography based technology - A review. Food Chemistry 324: 126899.

Jiang, F., Zhao, Z., Nie, Y., Li, Q., Liu, S. and Wang, H. 2019. Chiral separation and determination of L- and D-lactic acid in *baijiu* by high-performance liquid chromatography. Liquor-Making Science and Technology 9: 93-97.

Kang, Y., Hu, M., Zhu, Y., Gao, X. and Wang, M. W. 2009. Antioxidative effect of the herbal remedy Qin Huo Yi Hao and its active component tetramethylpyrazine on high glucose-treated endothelial cells. Life Science 84(13-14): 428-436.

Li, A., Liu, G., Tang, Y., Zhang, Y., Gao, J., Jiang, L. and Zhang, P. 2014. Determination of ethyl carbamate in liquor by SPE combined with GC-MS. Liquor-Making Technology 12: 99-101.

Li, H., Qin, D., Wu, Z., Sun, B., Sun, X., Huang, M., ... and Zheng, F. 2019. Characterization of key aroma compounds in Chinese Guojing sesame-flavor *baijiu* by means of molecular sensory science. Food Chemistry 284: 100-107.

Li, J., Du, N., Yuan, X., Pang, H., Guo, X. and Zhang, Y. 2017. Determination of volatile phenols in Jiangxiang *baijiu* by GC-MS. Liquor-making Science and Technology 1: 98-101.

Li, M., Deng, J., Yang, Y., Ye, G., Wei, C., Yang, X., ... and Luo, H. 2015. Safety testing of mycotoxins in Luzhou-flavor liquor production. China Brewing 34: 129-133.

Lingua, M. S., Fabani, M. P., Wunderlin, D. A. and Baroni, M. V. 2016. *In vivo* antioxidant activity of grape, pomace and wine from three red varieties grown in Argentina: Its relationship to phenolic profile. Journal of Functional Foods 20: 332-345.

Liu, H., Zhao, Y., Zhang, Y., Tang, J. and Wang, J. 2020. Determination of biogenic amines in *baijiu* and Chinese rice by high performance liquid chromatography. Journal of Chinese Institute of Food Science and Technology 20: 248-254.

Liu, J. 2008. Studies on aroma compounds of Chinese "Kouzijiao" and "Jiannanchun" liquors. China: Jiangnan University, MSc thesis.

Liu, K., Wang, Q., Chen, Z., Mao, D. M. and Liang, Z. W. 2022. Correlation analysis between amino acids and bacterial communities of Wuliangye-flavour liquor fermentation in aged fermentation pit. International Food Research Journal 29(4): 892-899.

Liu, X., Zhang, H., Shen, J. and Wu, T. 2021. Detection of mycotoxins in fermented grains of *Baijiu*. China Brewing 40: 180-185.

Liu, Y. 2020. Study on key aroma components of Langjiu. China: Shanghai Institute of Technology, MSc thesis.

Liu, Y., Lian, Z., Liang, L., Yin, B. and Zhou, H. 2016. Determination of ethyl palmitate, ethyl oleate and ethyl linoleate in liquor by gas chromatography-mass spectrometry (GC-MS). Forensic Science and Technology 41(2): 111-115.

Luo, W., Shen, Y., Zhou, Y., He, S., Shi, Y., Chen, Z. and Xu, Y. 2020. Detection of cyanides in *baijiu* by ion chromatography-electrochemical detector. Liquor-Making Science and Technology 1: 71-74.

Ma, Y. 2014. Research and application of the relationship between liquor composition and its quality. China: Shanxi University, PhD thesis.

Ma, Y. 2019. Study on the key components of soy sauce aroma *baijiu* and their characteristics based on the strategy of flavor omics. China: Guizhou University, MSc thesis.

Mangas, J. J., Cabranes, C., Moreno, J. and Gomis, D. B. 1994. Influence of cider-making technology on cider taste. LWT – Food Science and Technology 27(6): 583-586.

Misnawi and Ariza, B. T. S. 2011. Use of gas chromatography-olfactometry in combination with solid phase micro extraction for cocoa liquor aroma analysis. International Food Research Journal 18: 829-835.

Qian, Y. L., An, Y., Chen, S. and Qian, M. C. 2019. Characterization of Qingke liquor aroma from Tibet. Journal of Agricultural and Food Chemistry 67(50): 13870-13881.

Ren, H. 2016. Research on Fenjiu aroma components and aging behaviors. China: Shanxi University, MSc thesis.

Sha, S. 2017. Characterization and flavor impact of volatile sulfur compounds in Chinese liquors. China: Jiangnan University, MSc thesis.

Sha, S., Chen, S., Qian, M., Wang, C. and Xu, Y. 2017. Characterization of the typical potent odourants in Chinese roasted sesame-like flavor type liquor by headspace solid phase microextraction-aroma extract dilution analysis, with special emphasis on sulfur-containing odourants. Journal of Agricultural and Food Chemistry 65(1): 123-131.

Shao, C., Li, G., Li, L. and Zhang, K. 2005. Investigation on liquor flavor types and flavoring components. Liquor-Making Science and Technology 8: 92-92.

Song, X., Zhu, L., Jing, S., Li, Q., Ji, J., Zheng, F., ... and Sun, B. 2020. Insights into the role of 2-methyl-3-furanthiol and 2-furfurylthiol as markers for the differentiation of Chinese light, strong, and soy sauce aroma types of *baijiu*. Journal of Agricultural and Food Chemistry 68(30): 7946-7954.

Song, X., Zhu, L., Wang, X., Zheng, F., Zhao, M., Liu, Y., … and Chen, F. 2019. Characterization of key aroma-active sulfur-containing compounds in Chinese Laobaigan *Baijiu* by gas chromatography-olfactometry and

comprehensive two-dimensional gas chromatography coupled with sulfur chemiluminescence detection. Food Chemistry 297: 124959.

Sun, J. 2012. Methods for isoamyl alcohol control in wine. Modern Food Science and Technology 28(11): 1541-1544.

Sun, J., Ning, Z., Ning, G., Yin, B. and Li, S. 2015. Change in ethyl carbamate content during fermentation and storage of Chongming rice wine and sample pretreatment optimization for ethyl carbamate (EC) detection. Food Science 36(18): 193-198.

Sun, J., Wang, Z. and Sun, B. 2021. Low quantity but critical contribution to flavor: Review of the current understanding of volatile sulfur-containing compounds in *baijiu*. Journal of Food Composition and Analysis 103: 104079.

Sun, X., Qian, Q., Xiong, Y., Xie, Q., Yue, X., Liu, J., ... and Yang, Q. 2022. Characterization of the key aroma compounds in aged Chinese Xiaoqu *Baijiu* by means of the sensomics approach. Food Chemistry 384: 132452.

Takahashi, K., Tadenuma, M. and Sato, S. 1976. 3-Hydroxy-4:5-dimethyl-2(5H)-furanone, a burnt flavoring compound from aged Sake. Agricultural and Biological Chemistry 40(2): 325-330.

Wallgren, H. 1960. Relative intoxicating effects on rats of ethyl, propyl and butyl alcohols. Acta Pharmacologica et Toxicologica 16(3): 217-222.

Wang, D. 2020a. Study on minor component and main flavor in DQ Jiang-flavour Chinese spirits. China: Hebei University of Engineering, MSc thesis.

Wang, G., Jing, S., Song, X., Zhu, L., Zheng, F. and Sun, B. 2022a. Reconstitution of the flavor signature of Laobaigan-type *baijiu* based on the natural concentrations of its odour-active compounds and nonvolatile organic acids. Journal of Agricultural and Food Chemistry 70(3): 837-846.

Wang, G., Song, X., Zhu, L., Li, Q., Zheng, F., Geng, X., ... and Sun, B. 2022b. A flavoromics strategy for the differentiation of different types of *baijiu* according to the non-volatile organic acids. Food Chemistry 374: 131641.

Wang, J., Chen, H., Wu, Y. and Zhao, D. 2022c. Uncover the flavor code of strong-aroma *baijiu*: Research progress on the revelation of aroma compounds in strong-aroma *baijiu* by means of modern separation technology and molecular sensory evaluation. Journal of Food Composition and Analysis 109: 104499.

Wang, L. 2020b. Characterization of potent odourants causing a “pickle-like” off-odour in soy sauce-aroma type *baijiu*. China: Jiangnan University, MSc thesis.

Wang, L., Fan, S., Yan, Y., Yang, L., Chen, S. and Xu, Y. 2020c. Characterization of potent odourants causing a pickle-like off-odour in Moutai-aroma type *baijiu* by comparative aroma extract dilution analysis, quantitative measurements, aroma addition, and omission studies. Journal of Agricultural and Food Chemistry 68(6): 1666-1677.

Wang, L., Hu, G., Lei, L., Lin, L., Wang, D. and Wu, J. 2015. Identification and aroma impact of volatile terpenes in Moutai liquor. International Journal of Food Properties 19(6): 1335-1352.

Wang, X., Xiang, Y., Yin, L., Zhang, F., Han, C., Jiang, D. and Zhang, Y. 2021. Sugars and sugar alcohols of the Laobaigan *baijiu*. China Brewing 40: 70-74.

Wen, Y., Fan, W., Xu, Y. and Nie, Y. 2013. Quantification for 5 selected biogenic amines in Chinese liquor by HPLC. Science and Technology of Food Industry 34: 305-308.

Woo, I. S., Kim, I. H., Yun, U. J., Chung, S. K., Rhee, I. K., Choi, S. W. and Park, H. D. 2011. An improved method for determination of ethyl carbamate in Korean traditional rice wine. Journal of Industrial Microbiology and Biotechnology 26: 363-368

Wu, J. 2013. Study on the biosynthesis mechanism of tetra-methylpyrazine during the Chinese liquor brewing. China: Jiangnan University, PhD thesis.

Wu, J. F. and Xu, Y. 2013. Comparison of pyrazine compounds in seven Chinese liquors using headspace solid-phase micro-extraction and GC-nitrogen phosphorus detection. Food Science and Biotechnology 22(5): 1-6.

Xiang, Y. 2021. Analysis of sugar and sugar alcohols in liquor. China: Guizhou University, MSc thesis.

Xu, H. 2002. Study on relativity between furfural content and fragrance style of Chinese liquor. Liquor Making 29(5): 37-38.

Xu, J. 2019. Study on aroma components of strong-aroma Zhijiang *baijiu*. China: Huazhong Agriculture University, PhD thesis.

Xu, X. 2017. Source and treatments of cyanide in *baijiu*. Liquor-Making Science and Technology 10: 90-91.

Xu, Y., Zhao, J., Liu, X., Zhang, C., Zhao, Z., Li, X. and Sun, B. 2022. Flavor mystery of Chinese traditional fermented *baijiu*: The great contribution of ester compounds. Food Chemistry 369: 130920.

Yan, Y., Chen, S., Nie, Y. and Xu, Y. 2020. Characterization of volatile sulfur compounds in soy sauce aroma type *baijiu* and changes during fermentation by GC×GC-TOFMS, organoleptic impact evaluation, and multivariate data analysis. Food Research International 131: 109043.

Yang, C., Song, H. L. and Chen, F. 2012. Response surface methodology for meat-like odourants from Maillard reaction with glutathione I: The optimization analysis and the general pathway exploration. Journal of Food Science 77(9): C966-C974.

Yang, H. 2017. Characterization of non-volatile gustatory organic acids and polyhydroxy compounds in Chinese liquors. China: Jiangnan University, MSc thesis.

Yao, Z. 2018. Study on key aroma compounds and sensory evaluation of synergism among odourants in light aroma-type liquors. China: Shanghai Institute of Technology, MSc thesis.

Yu, Y., Chen, S., Nie, Y. and Xu, Y. 2022. Optimization of an intra-oral solid-phase microextraction (SPME) combined with comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry (GC×GC-TOFMS) method for oral aroma compounds monitoring of *baijiu*. Food Chemistry 385: 132502.

Yu, Y., Liu, Y. and Zhou, Y. 2019. Determination of sorbitol content in *baijiu* by LC-ESI-MS/MS. Liquor-Making Science and Technology 296: 117-120.

Zeller, A. and Rychlik, M. 2006. Character impact odourants of fennel fruits and fennel tea. Journal of Agricultural and Food Chemistry 54: 3686-3692.

Zhang, C. 2013. Investigation of off-flavor compounds in Chinese liquors. China: Jiangnan University, MSc thesis.

Zhang, F., Zhang, S., Su, Z., Huang, T., Ding, H., Wang, C., ... and Luo, J. 2016b. Research progress in the effects of organic acids on the quality of Nongxiang *baijiu* and its production process. Liquor-Making Science and Technology 259: 94-98.

Zhang, J., Su, L., Li, K., Huang, J., Tian, Z., Zhan, S., … and Li, X. 2014a. GC-MS qualitative/HS-20 headspace coupled with GC quantitative detection of trace cyanide content in liquor. Liquor-Making Science and Technology 7: 105-108.

Zhang, R., Wu, Q. and Xu, Y. 2014c. Lichenysin, a cyclooctapeptide occurring in Chinese liquor jiannanchun reduced the headspace concentration of phenolic off-flavors *via* hydrogen-bond interactions. Journal of Agricultural and Food Chemistry 62(33): 8302-8307.

Zhang, R., Wu, Q., Xu, Y. and Qian, M. C. 2014d. Isolation, identification, and quantification of lichenysin, a novel nonvolatile compound in Chinese distilled spirits. Journal of Food Science 79(10): C1907-1915.

Zhang, S. 2016c. Research of ethyl carbamate formation in Chinese liquor from the cyanide way. China: Jiangnan University, MSc thesis.

Zhang, X., Zhu, J., Peng, L., Xie, A. and Zhu, F. 2016a. Analysis of cyanide in liquor by purge and trap-gas chromatography-mass spectrometry. Chinese Journal of Food Hygiene 28: 344-347.

Zhang, X.-J., Meng, L.-J., Lu, Z.-M., Chai, L.-J., Wang, S.-T., Shi, J.-S., ... and Xu, Z.-H. 2021. Identification of age-markers based on profiling of *baijiu* volatiles over a two-year maturation period: Case study of Lu-flavor *baijiu*. LWT – Food Science and Technology 141: 110913.

Zhang, Y. J., Zhang, Y., Zhou, Y., Li, G. H., Yang, W. Z. and Feng, X. S. 2019. A review of pretreatment and analytical methods of biogenic amines in food and biological samples since 2010. Journal of Chromatography A 1605: 360361.

Zhang, Z. 2014b. Research of ethyl carbamate during the distillation and storage of Chinese liquors. China: Jiangnan University, MSc thesis.

Zhao, D. 2019. Research on the aroma compounds of Gujinggong Chinese *baijiu* and evaluation of the antioxidant and anti-inflammatory effects

of phenolic aroma compounds. China: South China University of Technology.

Zhao, T., Chen, S., Li, H. and Xu, Y. 2018. Identification of 2-hydroxymethyl-3,6-diethyl-5-methylpyrazine as a key retronasal burnt flavor compound in soy sauce aroma type *baijiu* using sensory-guided isolation assisted by multivariate data analysis. Journal of Agricultural and Food Chemistry 66(40): 10496-10505.

Zhao, T., Ni, D., Hu, G., Wang, L., Chen, S. and Xu, Y. 2019. 6-(2-Formyl-5-methyl-1H-pyrrol-1-yl) hexanoic acid as a novel retronasal burnt aroma compound in soy sauce aroma-type Chinese *baijiu*. Journal of Agricultural and Food Chemistry 67(28): 7916-7925.

Zhao, Z., Sugimachi, M., Yoshizaki, Y., Yin, X., Han, X., Okutsu, K., … and Takamine, K. 2021. Correlation between key aroma and manufacturing processes of rice-flavor *baijiu* and awamori, Chinese and Japanese traditional liquors. Food Bioscience 44: 101375.

Zheng, X. and Han, Z. 2016. *Baijiu* (白酒), Chinese liquor: History, classification and manufacture. Journal of Ethnic Foods 3: 19-25.

Zheng, Y. 2017. Characterization of the key odourants in Chinese Zhima aroma-type *baijiu* studies. China: South China University of Technology, PhD thesis.

Zheng, Y., Sun, B., Zhao, M., Zheng, F., Huang, M., Sun, J., ... and Li, H. 2016. Characterization of the key odourants in Chinese Zhima aroma-type *baijiu* by gas chromatography-olfactometry, quantitative measurements, aroma recombination, and omission studies. Journal of Agricultural and Food Chemistry 64(26): 5367-5374.

Zhou, J., Ao, Z., Shao, Y., Song, Y., Yao, Y. and Xu, C. 2020. Research progress in biogenic amine in traditional Chinese alcoholic drinks. Liquor-Making Science and Technology 7: 58-65.

Zhou, Q. 2015. Odour profile of Chinese roasted-sesame-like aroma type liquor. China: Jiangnan University, MSc thesis.

Zhu, W. 2017. The distribution of ochratoxin A in Daqu and its producing microorganisms. China: Jiangnan University, MSc thesis.