

Table S1. Volatile organic compounds in Chi-aroma Baijiu.

Substance	RI HP-Innowax	Identification	Concentration (mg/L)
Ethyl acetate	889	RI、MS、Std	221.5
Ethyl lactate	1327	RI、MS、Std	178.4
Ethyl butyrate	1030	RI、MS、Std	11.78
3-methylbutyrate ethyl	1065	RI、MS、Std	1.64
2-methylpropionate ethyl	964	RI、MS、Std	25.08
Isoamyl acetate	1120	RI、MS、Std	6.12
Ethyl valerate	910	RI、MS、Std	7.16
Ethyl caproate	1230	RI、MS、Std	40.51
Ethyl enanthate	1330	RI、MS、Std	32.26
Isobutane	925	RI、MS、Std	61.62
1-1-Diethoxypentane	813	RI、MS、Std	21.16
Dimethyl ether	510	RI、MS、Std	83.07
Diethylene glycol hexyl ether	1420	RI、MS、Std	4.02
Hexanoic acid	1830	RI、MS、Std	59.44
2-Undecylenic acid	1470	RI、MS、Std	23.06
N-butanol	1140	RI、MS、Std	115.38
Cyclohexyl ethyl alcohol	1550	RI、MS、Std	58.28
Isobutanol	1210	RI、MS、Std	97.25
Dodecyl thioglycol	2325	RI、MS、Std	20.88
β -phenyl ethanol	1928	RI、MS、Std	150.26
Diethylacetal	705	RI、MS、Std	1.31
Acetaldehyde	535	RI、MS、Std	28.38
Heptanal	920	RI、MS、Std	2.75
Octanal	1010	RI、MS、Std	1.64
Benzaldehyde	1528	RI、MS、Std	5.94
Ethyl caprylate	1433	RI、MS、Std	60.8

Table S1. Volatile organic compounds in Chi-aroma Baijiu (Cont).

Substance	RI	Identify	Concentration (mg/L)
	HP-Innowax		
Ethyl 2-hydroxybutyrate	914	RI、MS、Std	22.18
2-Heptanone	950	RI、MS、Std	0.88
Ethylene glycol	910	RI、MS、Std	7.72
Nonanone	1162	RI、MS、Std	6.55
Ethyl nonanoate	1288	RI、MS、Std	6.13
Ethyl caprate	1628	RI、MS、Std	44.7
Ethyl benzoate	1242	RI、MS、Std	46.5
Diethyl succinate	1671	RI、MS、Std	6.16
Ethyl myristate	2050	RI、MS、Std	6.96
Ethyl 2,3-epoxybutyrate	1040	RI、MS、Std	3.65
Diethyl azelaate	1950	RI、MS、Std	4.12

Table S2. Statistical analysis between peptides and volatile substances.

PLS-DA analysis	VIP Value	Spearman analysis	Correlation coefficient ($P < 0.05$)
2-Hydroxy4-methylpentanoic acid	1.382	Acetaldehyde	0.974
Ethyl nonanoate	1.281	Benzaldehyde	0.951
2-methylpropionate ethyl	1.255	Dimethyl ether	0.919
Diethyl ether	1.196	Isoamyl acetate	0.893
3-methylbutyrate ethyl	1.186	Diethyl succinate	0.882
Heptanal	1.161	Ethyl enanthate	0.856
Ethyl butyrate	1.142	Isobutanol	0.853
Nonanone	1.117	2-Heptanone	0.727
Butyl caprylate	1.076	Ethyl caproate	0.726
Octanal	1.069	Octanal	0.699
Ethyl lactate	1.063	Diethylacetal	0.624
Cyclo hexylethanol	1.062	Ethyl caprylate	0.577
Diethyl azelaate	1.040	Ethyl benzoate	0.561
Ethyl sunmate	1.022	Ethyl nonanoate	0.443
Diethyl lacetal	1.018	Ethylene glycol	-0.874
		Dodecyl thioglycol	-0.771
		Butanol	-0.582
		2-Undecylenic acid	-0.424
		Ethyl 2,3-epoxy butyrate	-0.37