

Comparison of Aroma and Taste Profiles of Kiwi Wine Fermented with/without Peel by Combining Intelligent Sensory, Gas Chromatography-Mass Spectrometry, and Proton Nuclear Magnetic Resonance

Bingde Zhou ¹, Xiaochen Liu ¹, Qiuyu Lan ^{1,2}, Fang Wan ¹, Zhibo Yang ^{1,3}, Xin Nie ⁴, Zijian Cai ¹, Bin Hu ³, Junni Tang ¹, Chenglin Zhu ^{1,*} and Luca Laghi ^{2,*}

Supporting Materials

Table S1. Relative content based on GC-MS characterization (Mean \pm SD).

Compound Name	Cas	RT	SI	RSI	Relative content	
					PKW	UKW
Esters						
Phenethyl acetate	103-45-7	31.77	787	908	$1.07 \times 10^{-3} \pm 1.62 \times 10^{-4}$	$9.24 \times 10^{-4} \pm 3.10 \times 10^{-4}$
Ethyl 2-hydroxy-4-methyl valerate	10348-47-7	21.87	646	900	$5.13 \times 10^{-4} \pm 2.39 \times 10^{-4}$	ND
Ethyl propanoate	105-37-3	3.80	626	944	$5.41 \times 10^{-4} \pm 1.79 \times 10^{-4}$	$6.03 \times 10^{-4} \pm 5.52 \times 10^{-5}$
Ethyl butanoate	105-54-4	5.24	665	919	$5.50 \times 10^{-3} \pm 8.26 \times 10^{-4}$	$5.81 \times 10^{-3} \pm 1.08 \times 10^{-3}$
Isobutyl hexanoate	105-79-3	13.74	819	901	$5.81 \times 10^{-4} \pm 1.10 \times 10^{-4}$	$5.60 \times 10^{-4} \pm 1.14 \times 10^{-4}$
Ethyl heptanoate	106-30-9	13.23	878	917	$1.23 \times 10^{-3} \pm 2.28 \times 10^{-4}$	$1.99 \times 10^{-3} \pm 3.52 \times 10^{-4}$
Ethyl caprylate	106-32-1	16.53	920	920	$0.49 \pm 6.04 \times 10^{-2}$	$0.50 \pm 3.97 \times 10^{-2}$
Ethyl laurate	106-33-2	32.16	884	885	$1.73 \times 10^{-3} \pm 2.99 \times 10^{-4}$	$5.56 \times 10^{-3} \pm 4.38 \times 10^{-3}$
Methyl hexoate	106-70-7	9.07	827	861	$1.62 \times 10^{-3} \pm 3.09 \times 10^{-4}$	$2.15 \times 10^{-3} \pm 3.79 \times 10^{-4}$

Ethyl isovalerate	108-64-5	5.98	760	878	$2.65 \times 10^{-4} \pm 9.10 \times 10^{-5}$	$2.79 \times 10^{-4} \pm 5.41 \times 10^{-5}$
Isobutyl acetate	110-19-0	4.73	894	923	$8.57 \times 10^{-4} \pm 8.58 \times 10^{-5}$	$8.79 \times 10^{-4} \pm 1.20 \times 10^{-4}$
Ethyl caprate	110-38-3	28.01	932	932	$7.50 \times 10^{-2} \pm 1.14 \times 10^{-2}$	$8.56 \times 10^{-2} \pm 2.82 \times 10^{-2}$
Methyl Caprate	110-42-9	25.46	861	908	$6.46 \times 10^{-4} \pm 1.68 \times 10^{-4}$	$9.27 \times 10^{-4} \pm 1.60 \times 10^{-4}$
Methyl octylate	111-11-5	14.79	898	921	$6.71 \times 10^{-3} \pm 2.34 \times 10^{-3}$	$1.14 \times 10^{-2} \pm 9.22 \times 10^{-4}$
Diethyl succinate	123-25-1	29.28	867	885	$7.42 \times 10^{-4} \pm 2.49 \times 10^{-4}$	$6.91 \times 10^{-4} \pm 1.73 \times 10^{-4}$
Ethyl nonanoate	123-29-5	21.25	897	908	$2.02 \times 10^{-3} \pm 3.92 \times 10^{-4}$	$3.48 \times 10^{-3} \pm 1.97 \times 10^{-3}$
Ethyl hexanoate	123-66-0	10.45	924	924	$0.11 \pm 1.33 \times 10^{-2}$	$0.13 \pm 2.71 \times 10^{-2}$
Isoamyl acetate	123-92-2	7.27	926	926	$5.09 \times 10^{-2} \pm 8.79 \times 10^{-3}$	$4.07 \times 10^{-2} \pm 5.60 \times 10^{-3}$
Ethyl tetradecanoate	124-06-1	34.44	770	844	$3.31 \times 10^{-4} \pm 1.16 \times 10^{-4}$	$7.57 \times 10^{-4} \pm 5.75 \times 10^{-4}$
Ethyl Acetate	141-78-6	2.84	891	966	$1.20 \times 10^{-2} \pm 2.00 \times 10^{-3}$	$1.22 \times 10^{-2} \pm 2.62 \times 10^{-3}$
Hexyl acetate	142-92-7	11.56	933	938	$3.84 \times 10^{-3} \pm 7.99 \times 10^{-4}$	$2.40 \times 10^{-3} \pm 7.42 \times 10^{-4}$
Isopentyl octanoate	2035-99-6	28.61	895	898	$2.83 \times 10^{-3} \pm 7.06 \times 10^{-4}$	$4.62 \times 10^{-3} \pm 8.77 \times 10^{-4}$
Isopentyl hexanoate	2198-61-0	17.29	869	883	$1.64 \times 10^{-3} \pm 1.47 \times 10^{-4}$	$1.98 \times 10^{-3} \pm 5.70 \times 10^{-4}$
Isoamyl decanoate	2306-91-4	32.40	913	920	$6.11 \times 10^{-4} \pm 2.34 \times 10^{-4}$	$1.06 \times 10^{-3} \pm 2.81 \times 10^{-4}$
Isobutyl octanoate	5461-06-3	22.29	765	834	$1.29 \times 10^{-3} \pm 1.90 \times 10^{-4}$	$1.07 \times 10^{-3} \pm 2.08 \times 10^{-4}$
Ethyl palmitate	628-97-7	36.22	770	802	$4.10 \times 10^{-4} \pm 6.65 \times 10^{-5}$	$1.55 \times 10^{-3} \pm 9.76 \times 10^{-4}$
Ethyl 9-decenoate	67233-91-4	29.50	843	935	$3.78 \times 10^{-3} \pm 2.31 \times 10^{-3}$	ND
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	32.57	848	923	ND	$3.65 \times 10^{-4} \pm 9.75 \times 10^{-5}$
Ethyl (E)-4-decenoate	76649-16-6	29.47	840	841	ND	$2.46 \times 10^{-3} \pm 1.31 \times 10^{-3}$
Hex-2-enoic acid ethyl ester	1552-67-6	13.55	826	864	$4.48 \times 10^{-4} \pm 9.63 \times 10^{-5}$	$7.22 \times 10^{-4} \pm 4.26 \times 10^{-4}$
Ethyl 2-methylpropanoate	97-62-1	3.87	857	905	$3.95 \times 10^{-4} \pm 2.05 \times 10^{-4}$	$2.69 \times 10^{-4} \pm 5.00 \times 10^{-5}$
Alcohols						
2-Ethylhexanol	104-76-7	18.87	887	915	$6.16 \times 10^{-4} \pm 5.70 \times 10^{-5}$	$7.06 \times 10^{-4} \pm 1.65 \times 10^{-4}$

1-Hexanol	111-27-3	13.88	939	943	$1.87 \times 10^{-2} \pm 3.06 \times 10^{-3}$	$2.89 \times 10^{-2} \pm 1.20 \times 10^{-2}$
D-Citronellol	1117-61-9	31.07	728	872	$4.31 \times 10^{-4} \pm 1.78 \times 10^{-4}$	$1.37 \times 10^{-3} \pm 2.69 \times 10^{-4}$
1-Decanol	112-30-1	30.97	780	853	ND	$2.72 \times 10^{-4} \pm 5.87 \times 10^{-5}$
3-Methyl-1-butanol	123-51-3	10.00	915	915	ND	$9.56 \times 10^{-2} \pm 1.48 \times 10^{-2}$
1-Nonanol	143-08-8	28.81	723	856	$2.48 \times 10^{-4} \pm 3.57 \times 10^{-5}$	$9.63 \times 10^{-4} \pm 7.34 \times 10^{-4}$
5-Methyl-3-heptanol	18720-65-5	15.04	773	933	ND	$4.37 \times 10^{-3} \pm 3.11 \times 10^{-3}$
1-Octen-3-ol	3391-86-4	17.08	688	839	ND	$4.77 \times 10^{-4} \pm 1.12 \times 10^{-4}$
methionol	505-10-2	30.10	768	833	$5.93 \times 10^{-4} \pm 6.04 \times 10^{-4}$	$5.37 \times 10^{-4} \pm 4.65 \times 10^{-4}$
3-Hexen-1-ol	544-12-7	14.16	868	931	$7.47 \times 10^{-4} \pm 1.46 \times 10^{-4}$	$1.30 \times 10^{-3} \pm 4.75 \times 10^{-4}$
Phenethyl alcohol	60-12-8	33.06	954	963	$2.16 \times 10^{-2} \pm 1.58 \times 10^{-2}$	$2.12 \times 10^{-2} \pm 9.54 \times 10^{-3}$
1-Pentanol	71-41-0	9.93	911	927	$0.11 \pm 2.44 \times 10^{-2}$	ND
Linalool	78-70-6	22.30	843	865	ND	$1.63 \times 10^{-3} \pm 6.83 \times 10^{-4}$
trans-2-Hexenol	928-95-0	15.48	719	919	ND	$4.37 \times 10^{-4} \pm 1.73 \times 10^{-4}$
Ketones						
Cyclohexanone	108-94-1	11.93	873	911	$9.06 \times 10^{-4} \pm 2.65 \times 10^{-4}$	ND
2-Hydroxy-5-methylacetophenone	1450-72-2	35.89	701	870	$2.82 \times 10^{-4} \pm 3.24 \times 10^{-5}$	ND
1-(4-Hydroxy-3-methylphenyl)ethanone	876-02-8	35.88	653	779	ND	$3.29 \times 10^{-4} \pm 3.03 \times 10^{-5}$
3-Pentanone	96-22-0	4.12	820	867	$3.03 \times 10^{-4} \pm 8.33 \times 10^{-5}$	$3.59 \times 10^{-4} \pm 1.34 \times 10^{-4}$
Aldehydes						
Decanal	112-31-2	19.22	826	890	$1.63 \times 10^{-3} \pm 5.46 \times 10^{-4}$	$2.12 \times 10^{-3} \pm 9.79 \times 10^{-4}$
Undecanal	112-44-7	26.22	629	801	$3.89 \times 10^{-4} \pm 1.23 \times 10^{-4}$	ND
Dodecanal	112-54-9	29.90	885	939	$8.89 \times 10^{-4} \pm 6.58 \times 10^{-4}$	$6.44 \times 10^{-4} \pm 3.62 \times 10^{-4}$
Octanal	124-13-0	12.07	866	950	$1.73 \times 10^{-3} \pm 3.52 \times 10^{-4}$	ND
Nonanal	124-19-6	15.01	931	936	$1.59 \times 10^{-2} \pm 4.84 \times 10^{-3}$	$1.18 \times 10^{-2} \pm 9.43 \times 10^{-3}$

2-Undecenal	2463-77-6	30.66	872	910	$1.22 \times 10^{-3} \pm 7.62 \times 10^{-4}$	ND
2,5-Dimethylbenzaldehyde	5779-94-2	31.67	828	922	ND	$7.91 \times 10^{-4} \pm 2.40 \times 10^{-4}$
Hexanal	66-25-1	6.29	772	841	$4.87 \times 10^{-4} \pm 1.04 \times 10^{-4}$	ND
Acids						
Nonanoic acid	112-05-0	35.53	913	915	$1.11 \times 10^{-2} \pm 1.31 \times 10^{-2}$	$5.77 \times 10^{-3} \pm 6.91 \times 10^{-3}$
Octanoic acid	124-07-2	34.58	918	923	$4.00 \times 10^{-3} \pm 1.76 \times 10^{-3}$	$3.45 \times 10^{-3} \pm 1.66 \times 10^{-3}$
Hexanoic acid	142-62-1	32.25	899	924	$2.18 \times 10^{-3} \pm 7.99 \times 10^{-4}$	$2.75 \times 10^{-3} \pm 2.40 \times 10^{-4}$
Lauric acid	143-07-7	38.72	689	828	$3.38 \times 10^{-4} \pm 8.23 \times 10^{-5}$	ND
Decanoic acid	334-48-5	36.42	908	936	$3.02 \times 10^{-3} \pm 2.27 \times 10^{-3}$	$2.36 \times 10^{-3} \pm 2.44 \times 10^{-3}$
Ethylboronic acid	4433-63-0	6.88	800	822	$2.86 \times 10^{-3} \pm 4.56 \times 10^{-4}$	$2.41 \times 10^{-3} \pm 4.57 \times 10^{-4}$
2-Methylhexanoic acid	4536-23-6	29.09	684	748	$6.18 \times 10^{-4} \pm 3.65 \times 10^{-4}$	$3.13 \times 10^{-4} \pm 6.02 \times 10^{-5}$
Others						
Propylbenzene	103-65-1	9.49	873	913	$4.33 \times 10^{-4} \pm 7.38 \times 10^{-5}$	$4.85 \times 10^{-4} \pm 1.55 \times 10^{-4}$
<i>p</i> -Xylene	106-42-3	8.83	892	921	$4.21 \times 10^{-4} \pm 6.79 \times 10^{-5}$	$6.16 \times 10^{-4} \pm 1.25 \times 10^{-4}$
4-Ethyltoluene	622-96-8	10.96	888	909	ND	$8.10 \times 10^{-4} \pm 4.97 \times 10^{-4}$
2,4,5-Trichlorotoluene	6639-30-1	30.73	847	905	$9.08 \times 10^{-4} \pm 2.10 \times 10^{-4}$	$6.02 \times 10^{-4} \pm 9.21 \times 10^{-5}$
2,3,4-Trichlorotoluene	7359-72-0	32.05	867	899	$7.20 \times 10^{-4} \pm 1.09 \times 10^{-4}$	$8.41 \times 10^{-4} \pm 1.80 \times 10^{-4}$
1,2,4-Trimethylbenzene	95-63-6	11.02	783	798	$1.28 \times 10^{-3} \pm 1.64 \times 10^{-4}$	$2.19 \times 10^{-3} \pm 1.21 \times 10^{-3}$
Hemimellitene	526-73-8	10.89	750	841	ND	$1.00 \times 10^{-3} \pm 7.51 \times 10^{-4}$
Pentylcyclopropan	2511-91-3	22.96	840	902	$8.78 \times 10^{-4} \pm 8.17 \times 10^{-5}$	$9.98 \times 10^{-4} \pm 2.68 \times 10^{-4}$
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15, 15-	19095-24-0	34.15	736	794	$5.80 \times 10^{-4} \pm 1.00 \times 10^{-4}$	$7.46 \times 10^{-4} \pm 1.32 \times 10^{-4}$
Hexadecamethyloctasiloxane						
Tetradecamethyl Cycloheptasiloxane	107-50-6	25.90	771	792	$1.68 \times 10^{-3} \pm 3.04 \times 10^{-4}$	$2.32 \times 10^{-3} \pm 7.47 \times 10^{-4}$

Dodecamethylcyclohexasiloxane	540-97-6	14.83	736	787	$6.42 \times 10^{-3} \pm 3.80 \times 10^{-3}$	$1.24 \times 10^{-2} \pm 6.28 \times 10^{-3}$
Decamethylcyclopentasiloxane	541-02-6	9.83	842	916	ND	$2.89 \times 10^{-3} \pm 1.71 \times 10^{-3}$
Hexamethylcyclotrisiloxane	541-05-9	2.56	941	950	$4.22 \times 10^{-3} \pm 1.21 \times 10^{-3}$	$4.48 \times 10^{-3} \pm 1.14 \times 10^{-3}$
Octamethylcyclotetrasiloxane	556-67-2	5.06	941	962	$3.96 \times 10^{-3} \pm 6.51 \times 10^{-4}$	$4.65 \times 10^{-3} \pm 2.17 \times 10^{-3}$
Hexadecamethylcyclooctasiloxane	556-68-3	30.83	838	870	$1.92 \times 10^{-3} \pm 3.42 \times 10^{-4}$	$2.23 \times 10^{-3} \pm 4.06 \times 10^{-4}$
Octadecamethylcyclononasiloxane	556-71-8	32.73	853	869	$1.26 \times 10^{-3} \pm 2.43 \times 10^{-4}$	$1.24 \times 10^{-3} \pm 4.10 \times 10^{-4}$
2,4-Di-tert-butylphenol	96-76-4	36.77	926	934	$4.26 \times 10^{-3} \pm 1.18 \times 10^{-3}$	$4.27 \times 10^{-3} \pm 1.19 \times 10^{-3}$
2,4-Di-tert-butyl-6-nitrophenol	20039-94-5	34.84	763	867	$3.76 \times 10^{-4} \pm 1.41 \times 10^{-4}$	ND
Rose oxide	16409-43-1	13.64	696	835	$2.68 \times 10^{-4} \pm 6.75 \times 10^{-5}$	$8.51 \times 10^{-4} \pm 2.64 \times 10^{-4}$
2-Chlorohydrocinnamitrile	7315-17-5	40.32	620	813	$7.49 \times 10^{-4} \pm 7.60 \times 10^{-5}$	$9.11 \times 10^{-4} \pm 2.14 \times 10^{-4}$
Bornylene	464-17-5	19.88	696	851	$3.59 \times 10^{-4} \pm 5.73 \times 10^{-5}$	$6.11 \times 10^{-4} \pm 1.10 \times 10^{-4}$
Coumaran	496-16-2	37.76	798	854	$5.05 \times 10^{-4} \pm 2.02 \times 10^{-4}$	$5.43 \times 10^{-4} \pm 1.74 \times 10^{-4}$

"ND" indicates that the substance was not detected.

The relative odor activity values (ROAV) of VOCs in KW were calculated using the following formula [1].

$$ROAV = 100 \times \frac{C_A}{C_{stan}} \times \frac{T_{stan}}{T_A}$$

C_A : The relative content of VOCs in the KW sample.

C_{stan} : The relative content of VOCs that contribute most to the overall flavor.

T_{stan} : The odor threshold of VOCs that contribute most to the overall flavor.

T_A : The odor threshold of VOCs in the KW sample.

Table S2. ROAV of VOCs in KW with/without peel.

Compound Name	Cas	Descriptor	Aroma threshold (µg/L)	ROAV	
				PKW	UKW
Phenethyl acetate	103-45-7	rose	250	0.225317	0.178642
Ethyl 2-hydroxy-4-methyl valerate	10348-47-7	blackberry	10.12	2.530065	-
Ethyl butanoate	105-54-4	sweet	82	3.434718	3.50991
Ethyl heptanoate	106-30-9	pineapple	13153	0.004672	0.007545
Ethyl caprylate	106-32-1	apricot, banana, pear	250	100	100
Ethyl laurate	106-33-2	fruity, floral	400	0.217636	0.69472
Ethyl isovalerate	108-64-5	fruity	7	2.194651	2.126694
Isobutyl acetate	110-19-0	apple, banana, glue, pear	2100	0.021947	0.021267
Diethyl succinate	123-25-1	wine, fruity	353193	0.000101	0.000098
Ethyl nonanoate	123-29-5	grape	3151	0.032503	0.055119
Ethyl hexanoate	123-66-0	apple, raw banana, pineapple, floral	210	27.09175	30.26995
Isoamyl acetate	123-92-2	banana	94	27.72887	21.48565
Ethyl tetradecanoate	124-06-1	sweet	180	0.085348	0.220546
Ethyl acetate	141-78-6	pineapple	32551	0.018878	0.018598
Hexyl acetate	142-92-7	apple, banana, grass, herb, pear	670	0.290436	0.177754

Ethyl palmitate	628-97-7	apple, sweet	1000	0.020483	0.074434
Ethyl 9-decenoate	67233-91-4	fruity	100	1.945924	-
1-Hexanol	111-27-3	banana, floral, grass	1300	0.736615	1.103154
1-Decanol	112-30-1	floral	400	-	0.037217
3-Methyl-1-butanol	123-51-3	whisky, malt, burnt	50000	-	0.094879
1-Nonanol	143-08-8	/	5000	0.002048	0.009925
1-Octen-3-ol	3391-86-4	fresh mushroom	6.12	-	4.054156
Phenethyl alcohol	60-12-8	rose	14000	0.079007	0.075143
1-Pentanol	71-41-0	bitter almond, fatty	80000	0.07118	-
Linalool	78-70-6	floral	5300	-	0.01498
Decanal	112-31-2	oil, soap, orange peel	1.25	65.54691	83.36642
Octanal	124-13-0	citrus, grassy	39	2.232166	-
Nonanal	124-19-6	melon	122	6.673897	4.799589
Octanoic acid	124-07-2	cheese, fatty	2701	0.075836	0.064302
Hexanoic acid	142-62-1	barbecue, cheese	8500	0.013254	0.015763
Lauric acid	143-07-7	metal	9154	0.001678	-
Decanoic acid	334-48-5	rancid, fatty	13737	0.011183	0.00867
2,4-Di-tert-butylphenol	96-76-4	/	200	1.100983	1.066892
Rose oxide	16409-43-1	rose	0.2	76.81278	223.3029

"-" indicates that the substance was not detected. "/" indicates that no information on the substance was sought.

Table S3. Molecular concentrations based on ¹H-NMR characterization (Mean ± SD).

Compound Name	Molecular concentration	
	PKW	UKW
Amino acids, peptides, and analogs		
Tryptophan	$6.05 \times 10^{-2} \pm 2.92 \times 10^{-2}$	$3.99 \times 10^{-2} \pm 2.45 \times 10^{-2}$
Phenylalanine	$0.23 \pm 6.77 \times 10^{-2}$	$0.17 \pm 6.29 \times 10^{-2}$
Tyrosine	$0.19 \pm 2.14 \times 10^{-2}$	$0.18 \pm 2.48 \times 10^{-2}$
Ornithine	$3.32 \times 10^{-2} \pm 9.86 \times 10^{-3}$	$3.26 \times 10^{-2} \pm 1.06 \times 10^{-2}$
Creatine	$4.38 \times 10^{-2} \pm 4.73 \times 10^{-3}$	$4.54 \times 10^{-2} \pm 6.94 \times 10^{-3}$
Creatinine	$0.17 \pm 1.25 \times 10^{-2}$	$0.16 \pm 4.28 \times 10^{-2}$
Aspartate	$0.19 \pm 1.84 \times 10^{-2}$	$0.18 \pm 2.90 \times 10^{-2}$
Alanine	1.01 ± 0.15	0.86 ± 0.19
Sarcosine	$4.03 \times 10^{-2} \pm 3.21 \times 10^{-3}$	$3.82 \times 10^{-2} \pm 5.67 \times 10^{-3}$
Valine	$0.18 \pm 3.63 \times 10^{-2}$	$0.13 \pm 3.62 \times 10^{-2}$
Isoleucine	$0.16 \pm 4.68 \times 10^{-2}$	$0.13 \pm 3.51 \times 10^{-2}$
Leucine	0.38 ± 0.12	0.28 ± 0.10
N, N-Dimethylglycine	$3.07 \times 10^{-2} \pm 1.02 \times 10^{-3}$	$3.28 \times 10^{-2} \pm 2.64 \times 10^{-3}$
N-Acetylglycine	$1.70 \pm 9.69 \times 10^{-2}$	2.17 ± 0.15
Carbohydrates and derivatives		
Galactose	0.68 ± 0.32	0.39 ± 0.30
Glucose	$0.25 \pm 4.17 \times 10^{-2}$	0.28 ± 0.11
Lactose	$0.10 \pm 5.33 \times 10^{-2}$	$6.42 \times 10^{-2} \pm 3.64 \times 10^{-2}$
Xylose	1.25 ± 0.70	0.72 ± 0.61
Fucose	$0.25 \pm 6.00 \times 10^{-2}$	$0.20 \pm 3.75 \times 10^{-2}$
Arabinose	0.87 ± 0.12	0.70 ± 0.35
Lactulose	$0.29 \pm 3.49 \times 10^{-2}$	$0.26 \pm 5.07 \times 10^{-2}$

1,6-Anhydro- β -D-glucose	$1.34 \times 10^{-2} \pm 2.43 \times 10^{-3}$	$1.64 \times 10^{-2} \pm 9.13 \times 10^{-3}$
Fructose	1.88 ± 0.11	1.43 ± 0.42
Organic acids and derivatives		
Formate	$9.29 \times 10^{-2} \pm 9.07 \times 10^{-3}$	$0.10 \pm 2.58 \times 10^{-2}$
Acetate	4.87 ± 1.73	3.67 ± 1.18
Butyrate	$0.40 \pm 5.00 \times 10^{-2}$	$0.36 \pm 6.48 \times 10^{-2}$
Fumarate	$1.24 \times 10^{-2} \pm 1.53 \times 10^{-3}$	$1.68 \times 10^{-2} \pm 2.20 \times 10^{-3}$
Tartrate	$3.49 \times 10^{-2} \pm 5.32 \times 10^{-3}$	$4.40 \times 10^{-2} \pm 5.63 \times 10^{-3}$
Pantothenate	$0.40 \pm 9.79 \times 10^{-2}$	0.42 ± 0.22
Malonate	$2.39 \times 10^{-2} \pm 5.19 \times 10^{-3}$	$1.71 \times 10^{-2} \pm 4.65 \times 10^{-3}$
Malate	$1.28 \pm 8.92 \times 10^{-2}$	1.46 ± 0.40
Pyroglutamate	$5.89 \times 10^{-2} \pm 3.03 \times 10^{-2}$	$5.25 \times 10^{-2} \pm 1.51 \times 10^{-2}$
Succinate	5.36 ± 0.51	5.11 ± 0.20
Isocaproate	$1.36 \pm 9.19 \times 10^{-2}$	1.21 ± 0.22
2-Hydroxyisovalerate	$5.70 \times 10^{-2} \pm 9.18 \times 10^{-3}$	$4.23 \times 10^{-2} \pm 1.24 \times 10^{-2}$
4-Aminobutyrate	0.54 ± 0.13	0.51 ± 0.14
Lactate	1.05 ± 0.63	0.88 ± 0.61
Indole-3-acetate	$3.49 \times 10^{-2} \pm 1.77 \times 10^{-2}$	$3.67 \times 10^{-2} \pm 1.79 \times 10^{-2}$
4-Hydroxyphenyllactate	$0.27 \pm 1.39 \times 10^{-2}$	$0.26 \pm 1.42 \times 10^{-2}$
trans-Aconitate	$4.72 \times 10^{-2} \pm 3.61 \times 10^{-3}$	$4.59 \times 10^{-2} \pm 6.19 \times 10^{-3}$
Epicatechin	$1.99 \times 10^{-2} \pm 6.40 \times 10^{-3}$	$2.73 \times 10^{-2} \pm 6.75 \times 10^{-3}$
5-Aminolevulinate	$0.19 \pm 1.85 \times 10^{-2}$	$0.19 \pm 3.17 \times 10^{-2}$
Galactonate	1.03 ± 0.18	1.13 ± 0.27
Galactarate	$0.17 \pm 6.93 \times 10^{-3}$	$0.22 \pm 5.05 \times 10^{-2}$
2-Oxoglutarate	0.67 ± 0.12	$0.63 \pm 9.63 \times 10^{-2}$
2-Methylglutarate	$0.14 \pm 1.55 \times 10^{-2}$	$0.14 \pm 2.36 \times 10^{-2}$

Methionine	$0.12 \pm 2.25 \times 10^{-2}$	$9.83 \times 10^{-2} \pm 3.00 \times 10^{-2}$
4-Hydroxy-3-methoxymandelate	$5.65 \times 10^{-2} \pm 7.17 \times 10^{-3}$	$7.98 \times 10^{-2} \pm 1.10 \times 10^{-2}$
Syringate	$0.11 \pm 1.81 \times 10^{-2}$	$0.12 \pm 1.21 \times 10^{-2}$
Nucleosides, nucleotides, and analogs		
Guanosine	$2.03 \times 10^{-2} \pm 8.67 \times 10^{-3}$	$2.43 \times 10^{-2} \pm 3.26 \times 10^{-2}$
Cytidine	$3.01 \times 10^{-2} \pm 3.77 \times 10^{-3}$	$2.41 \times 10^{-2} \pm 9.58 \times 10^{-3}$
Uridine	$0.13 \pm 2.01 \times 10^{-2}$	$0.11 \pm 4.32 \times 10^{-2}$
Uracil	$8.93 \times 10^{-2} \pm 3.76 \times 10^{-2}$	$7.66 \times 10^{-2} \pm 2.76 \times 10^{-2}$
Thymine	$0.34 \pm 2.86 \times 10^{-2}$	$0.31 \pm 4.38 \times 10^{-2}$
Alcohols		
Oxypurinol	$4.39 \times 10^{-2} \pm 1.16 \times 10^{-2}$	$2.93 \times 10^{-2} \pm 6.52 \times 10^{-3}$
Methanol	10.20 ± 0.69	12.00 ± 1.7
Ethanol	1166.00 ± 51.00	1177.49 ± 271.00
Propylene glycol	3.08 ± 0.24	3.05 ± 1.11
myo-Inositol	8.05 ± 0.31	7.81 ± 0.54
Glycerol	32.30 ± 2.05	33.10 ± 6.12
Others		
Hypoxanthine	$3.58 \times 10^{-2} \pm 1.59 \times 10^{-2}$	$2.70 \times 10^{-2} \pm 8.92 \times 10^{-3}$
Xanthine	$5.26 \times 10^{-2} \pm 6.33 \times 10^{-3}$	$4.23 \times 10^{-2} \pm 1.11 \times 10^{-2}$
N-Acetylserotonin	$2.71 \times 10^{-2} \pm 6.00 \times 10^{-3}$	$3.97 \times 10^{-2} \pm 9.00 \times 10^{-3}$
N-Acetylglucosamine	$0.60 \pm 8.25 \times 10^{-2}$	0.77 ± 0.14
1,3-Dihydroxyacetone	$0.40 \pm 5.38 \times 10^{-2}$	0.42 ± 0.20
Choline	$0.45 \pm 4.24 \times 10^{-2}$	$0.42 \pm 5.70 \times 10^{-2}$
Dimethyl sulfone	$2.69 \times 10^{-2} \pm 1.62 \times 10^{-3}$	$2.63 \times 10^{-2} \pm 2.76 \times 10^{-3}$
Ethanolamine	$0.19 \pm 1.50 \times 10^{-2}$	$0.18 \pm 1.01 \times 10^{-2}$
Asparagine	$8.82 \times 10^{-2} \pm 1.36 \times 10^{-2}$	$8.59 \times 10^{-2} \pm 2.25 \times 10^{-2}$

Methylamine	$1.50 \times 10^{-2} \pm 2.05 \times 10^{-3}$	$1.60 \times 10^{-2} \pm 1.01 \times 10^{-3}$
Pyridoxine	$2.10 \times 10^{-2} \pm 6.12 \times 10^{-3}$	$1.90 \times 10^{-2} \pm 5.16 \times 10^{-3}$
Acetone	$8.10 \times 10^{-2} \pm 9.22 \times 10^{-2}$	0.12 ± 0.11
Acetoin	0.11 ± 0.17	0.17 ± 0.18
Hydroxy acetone	$3.93 \times 10^{-2} \pm 3.65 \times 10^{-3}$	$3.92 \times 10^{-2} \pm 5.35 \times 10^{-3}$

Reference

1. Li, P.; Jia, Y.; Cai, D.; Wang, X.; Liu, J.; Zhu, R.; Wang, Z.; He, Y.; Wen, L. Study on the Relationship between Flavor Components and Quality of Ice Wine during Freezing and Brewing of "beibinghong" Grapes. *Food Chem X* **2023**, *20*, 101016, doi:10.1016/J.FOCHX.2023.101016.