

Table. Schedule A. Quantitative parameters of 92 Compounds in Meilanchun Sesame Flavor Style Baijiu

count	compound	Quantified ion	IS ^a	n ^b	Standard Curve		R ^{2c}	Linear Range	Recovery (%)
					Slope	Intercept			
esters									
1	ethyl acetate*	88	IS3	6	0.04286	0.004634	0.9991	253.0-2024.0	91.6
2	ethyl 2-methylpropanoate*	116	IS4	6	0.2136	-2.9323	0.9905	0.3960-19.80	95.8
3	ethyl butanoate*	88	IS4	10	0.4433	0.5658	0.9982	0.2550-510.0	105.6
4	ethyl 2-methylbutanoate*	102	IS4	9	0.8488	0.03224	0.999	0.2466-32.89	108.7
5	ethyl 3-methylbutanoate*	88	IS4	9	0.5734	0.01608	0.9992	0.2600-34.67	106.4
6	ethyl pentanoate*	85	IS4	8	0.5565	0.2597	0.9986	0.4300-86.00	105.9
7	ethyl hexanoate*	88	IS3	6	0.6329	-0.07126	0.9986	201.0-1612	112.0
8	ethyl lactate*	75	IS3	6	0.09667	0.006092	0.9992	250.50-2004	104.1
9	diethyl butanedioate*	129	IS5	6	2.3950	0.009055	0.9993	0.6897-34.48	106.5
10	ethyl propanoate	102	IS5-2	6	0.00486	0.000693	0.9969	5.300-1060	94.7
11	ethyl 4-methylpentanoate	115	IS5-2	5	0.01138	0.002001	0.9961	5.300-106.0	98.4
alcohols									
1	2-methyl-1-propanol*	74	IS4	6	0.2860	-0.0469	0.9932	5.400-216.0	92.9
2	1-butanol*	56	IS4	6	0.5037	0.5131	0.9902	2.500-200.0	98.6
3	3-methyl-1-butanol*	55	IS4	6	0.4596	0.8167	0.9984	5.400-216.0	106.3
4	1-hexanol*	56	IS4	6	4.2145	1.1466	0.9937	0.4200-84.00	102.5
carboxylic acids									
1	acetic acid*	60	IS2	7	0.4980	0.05804	0.9953	151.5-1212	104.5
2	butyric acid*	60	IS1	6	20.4174	-23.7704	0.9987	15.15-242.4	94.5
3	3-methylbutanoic acid*	60	IS1	6	13.6220	-0.6983	0.9958	0.9103-45.52	98.2
4	pentanoic acid*	60	IS1	6	22.6466	-8.2068	0.9974	2.612-104.5	93.1
5	hexanoic acid*	60	IS1	8	18.3250	-17.4996	0.9983	8.621-215.5	94.1
6	octanoic acid*	60	IS1	5	8.3997	-3.0989	0.9987	0.8828-22.07	106
7	decanoic acid	60	IS5-2	5	0.1902	-0.9641	0.9982	192.0-12200	115.2
aldehydes									
1	3-methylbutanal*	58	IS4	5	0.8719	0.0074	0.9957	0.7888-39.40	97.4

Table.continued

count	compound	Quantified ion	IS ^a	n ^b	Standard Curve		R ^{2c}	Linear Range	Recovery (%)
					Slope	Intercept			
aromatic compounds									
1	phenethyl alcohol*	91	IS5	5	3.3110	-0.05813	0.9979	1.690-33.79	102.5
2	phenyl acetaldehyde	91	IS5	8	3.2001	0.05065	0.9978	37.90-1897	96.2
3	ethyl phenylacetate	91	IS5	5	6.2687	-0.08484	0.9985	16.67-1655	92.2
4	ethyl 3-phenylpropanoate	104	IS5	5	2.5192	0.06822	0.9987	57.20-2862	93
5	vanillin	151	IS5-2	6	0.0251	-0.0890	0.9986	24.00-960.0	100.2
pyrazines									
1	2,6-dimethyl pyrazine	108	IS5-2	6	0.4198	-0.04714	0.9963	5.100-255.0	95.3
2	2,3,5-trimethyl pyrazine	122	IS5-2	7	0.4162	-0.1054	0.9968	25.25-1010	93.2
3	2,3-diethyl-5-methyl pyrazine	-	-	-	-	-	-	-	-
phenols									
1	guaiacol	109	IS5-2	4	0.1625	0.001154	0.999	8.200-82.00	84.6
2	4-methylphenol	107	IS5	7	3.0546	-0.1018	0.9991	47.10-4710	97.8
3	4-ethyl guaiacol	137	IS5-2	7	3.3199	-1.9108	0.9969	6.100-610.0	89.3
sulfides									
1	dimethyl trisulfide	126	IS5	9	0.5026	0.001597	0.9989	7.060-2355.6	93.4
2	methional	104	ES ^b	7	71.3171	785.6467	0.9991	8.1875-1637.5	96.9
3	3-methylthiopropanol	106	ES ^b	7	202.8130	871.8886	0.9957	8.1875-1637.5	104.7
other odorants									
1	1,1-diethoxyethane*	103	IS4	6	0.0225	-0.0086	0.9912	1.520-760.0	99.8
2	ethyl nicotinate	106	IS5-2	4	0.04108	-0.00991	0.9916	25.25-252.5	94.6
3	3-phenylpyridine	155	IS5-2	6	0.01724	0.03957	0.9984	42.50-850.0	104.1
4	isobutyraldehyde diethyl acetal	103	IS4	5	0.4650	0.0576	0.9945	1.670-100.0	98.6
5	2,4,6-trimethyl-1,3-dioxane	-	-	-	-	-	-	-	-
6	2-methoxy-1,3-dioxolane	73	IS3	5	0.7851	1.6305	0.9956	1.530-112.0	99.2
7	ethyl acrylate	55	IS4	5	0.6834	0.8765	0.9978	2.650-109.0	99.4

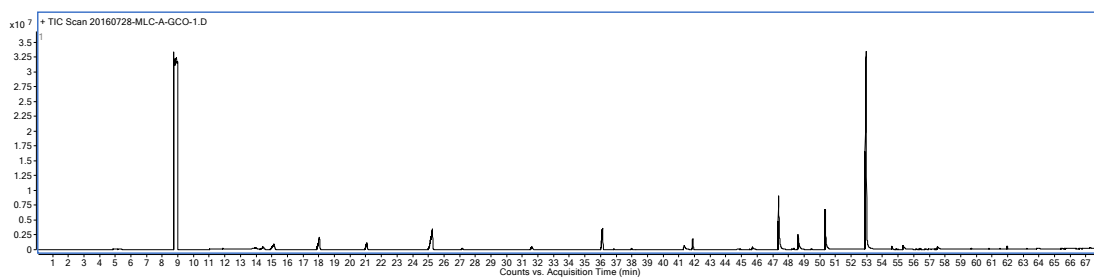
Table.continued

count	compound	Quantified ion	IS ^a	n ^b	Standard Curve		R ^{2c}	Linear Range	Recovery (%)
					Slope	Intercept			
8	2,3-butanedione	43	IS4	5	0.7145	0.3648	0.9967	1.000-80.00	98.6
9	uk1-M	-	-	-	-	-	-	-	-
10	uk2-M	-	-	-	-	-	-	-	-
Odourless compounds in Meilanchun									
1	ethyl octanoate*	88	IS5	7	2.1350	0.01491	0.999	0.1780-17.80	94.7
2	hexyl acetate	84	IS4	8	0.2643	-0.00412	0.9984	60.00-10000	95.3
3	propyl hexanoate	99	IS5-2	6	0.1983	-0.03213	0.9951	28.25-1130	96.3
4	butyl hexanoate	99	IS5-2	7	0.08215	-0.08905	0.9965	119.0-5950	94.8
5	hexyl hexanoate	117	IS5-2	5	0.1738	-0.06129	0.9993	300.0-3000	102.2
6	ethyl nonanoate	88	IS5	8	1.3991	0.007299	0.9991	11.33-1889	94
7	ethyl decanoate	88	IS5-2	5	0.1857	-0.1652	0.9966	80.00-2000	103.9
8	pentylhexanoate	117	IS5-2	5	0.0790	-0.01912	0.9957	27.75-555.0	95.9
9	ethyl 2-hydroxy-4-methylvalerate*	69	IS5	6	2.0564	-6.5044	0.9968	2.182-85.50	99.4
10	ethyl heptanoate*	88	IS4	10	1.0638	-0.04603	0.9996	0.0525-52.50	99.5
11	isobutyl hexanoate	99	IS4	6	1.2132	-0.03109	0.9981	105.0-5250	97.9
12	isopentylhexanoate	70	IS5	7	1.7385	0.01753	0.9984	51.50-5150	94.3
13	ethyl dodecanoate	88	IS5-2	5	0.1330	0.06638	0.9978	51.50-1030	95
14	ethyl myristate	157	IS5	5	0.1394	-0.00356	0.9978	35.70-1427.6	97.7
15	butyl butyrate	71	IS4-2	5	9.5710	-24.8454	0.9815	49.00-1960	101.3
16	hexyl butyrate	71	IS5-2	5	6.0533	-3.9544	0.9957	17.70-422.5	113.9
17	diethyl octanedioate	143	IS5-2	5	2.2679	-0.0986	0.9879	1.000-50.00	102
18	ethyl hexadecanoate	88	IS5-2	5	16.8518	-3.4432	0.9926	10.00-200.0	90
19	1-propanol*	60	IS4	7	0.1313	1.9691	0.9967	4.310-431.0	102.5
20	1- heptanol	70	IS5-2	6	3.9459	1.0434	0.9972	1.940-194.0	105.3
21	1-octanol	56	IS5-2	5	9.1395	-10.6868	0.9998	20.60-515.0	112.5
22	propionic acid*	60	IS1	5	7.9079	0.9813	0.9992	9.386-82.40	99.4
23	pentanoic acid*	60	IS1	5	6.3750	1.0321	0.9993	4.316-120.0	98.4

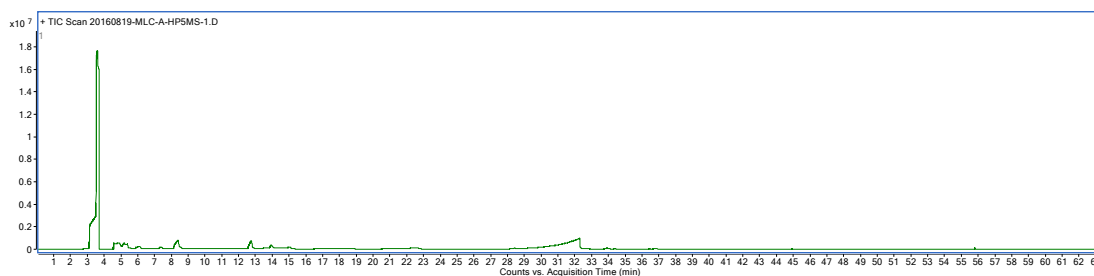
Table.continued

count	compound	Quantified ion	IS ^a	n ^b	Standard Curve		R ^{2c}	Linear Range	Recovery (%)
					Slope	Intercept			
24	heptanoic acid*	73	IS1	5	7.6811	-2.2568	0.9989	0.7172-17.93	91.3
25	nonanoic acid	60	IS5-2	5	1.3852	-18.4863	0.9976	201.6-10080	98.8
26	4-methyl pentanoic acid*	57	IS1	5	7.8408	-2.4683	0.9985	0.7054-17.59	103.6
27	acetoin*	88	IS4	6	0.1297	-0.04051	0.9994	6.667-66.67	100.3
28	ethyl benzoate	105	IS5-2	5	1.3111	0.1215	0.9918	3.025-121.0	89.4
29	benzyl alcohol	108	IS5-2	5	0.03576	0.000345	0.999	3.850-192.5	99.3
30	acetophenone	95	IS5-2	6	0.6204	-0.01412	0.9987	4.700-235.0	99.6
31	benzaldehyde*	106	IS5	8	2.1952	-0.01901	0.9988	0.3066-30.67	90.5
32	2-phenylethyl acetate	104	IS5	5	4.4663	0.03227	0.9989	19.30-386.2	105.2
33	2-furfural*	96	IS5	7	1.7522	1.6069	0.9989	4.310-434.5	97.3
34	furfuryl alcohol	98	IS5-2	5	0.00904	-0.00375	0.991	11.20-280.0	90.3
35	2-acetylfuran	95	IS5-2	6	0.6204	-0.01412	0.9987	4.700-235.0	99.6
36	5-methylfurfural	110	IS5-2	6	0.3358	-0.05285	0.9938	5.200-520.0	93.5
37	2-acetyl-5-methylfuran	109	IS5-2	5	0.2658	0.002283	0.9971	2.652-105.0	97.9
38	tetramethylpyrazine	136	IS5-2	4	0.2479	-0.06537	0.9972	24.75-247.5	101.7
39	phenol	94	IS5-2	7	2.5804	-2.7461	0.9987	9.500-475.0	110.2
40	4-ethylphenol	107	IS5	5	4.8707	-0.1337	0.9991	26.20-1310	99.4
41	2,4-di-tert-butylphenol	191	IS5-2	5	2.5595	-0.3855	0.9998	15.75-630.0	100.6
42	ethyl 3-methylthiopropionate	148	IS5-2	4	0.5326	-0.1275	0.9950	9.700-97.00	97.5
43	1,1,3-triethoxypropane	103	IS4	8	0.5660	-0.01308	0.9987	45.30-7555	96.8
44	γ -valerolactone	85	IS5	8	0.7155	-0.00257	0.9983	58.00-9667	97.2
45	3-(2-furyl)-2-propenal	122	IS5	5	0.7628	-0.00937	0.9978	28.25-1130	92.8
46	α -terpenol	121	IS5-2	6	0.3788	-0.0068	0.9977	2.925-117.0	94.7
47	nonanal	57	IS5-2	5	4.4211	-1.7001	0.9939	8.190-163.8	108.7
48	ethyl 2-furoate	95	IS5-2	6	19.2009	-33.684	0.9999	2.594-648.5	102.5
49	lactic acid*	-	ES ^d	5	0.06000	1.1196	0.9992	219.7-4394	102.01

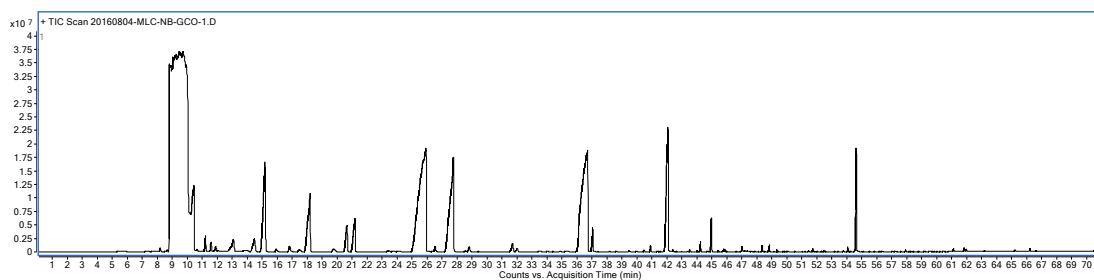
^a The method of quantitation for the compound was internal standard except special label. IS1(pivalic acid), IS2(2- ethyl butyric acid), IS3(methyl octanoate), IS4(methyl hexanoate), IS5(octyl propionate) as internal standard substance. IS5-2 and IS4-2 mean different concentration from IS5 and IS4, respectively. ^bThe number of point to be establish the standard curve. ^c Coefficient of determination. ^d The method of quantitation for the compound was external standard. *The unit of concentration was mg/L, the unit of other compounds was µg/L.



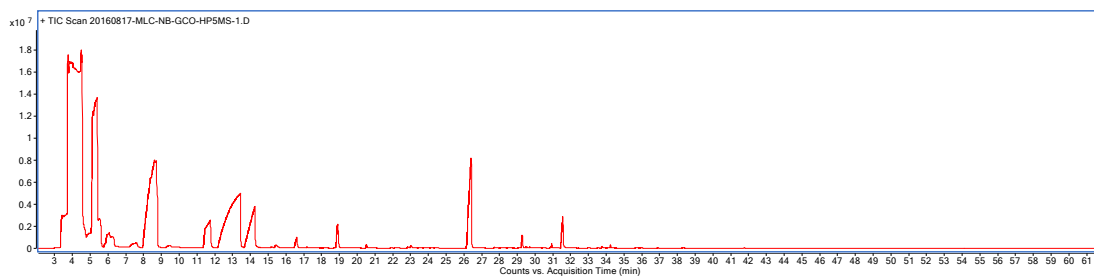
a



b



c



d

Fig Total ion current chromatogram of meilanchun (a. acidic fraction in DB-WAX fused silica capillary; b. acidic fraction in HP-5MS fused silica capillary; c. neutral/basic fraction in DB-WAX fused silica capillary; d. neutral/basic fraction in HP-5MS fused silica capillary.)