

Table.1 The concentrations of organic acids in standard solution mixture and their selected ions.

No.	Organic acids	t_R (min)	Concentration ($\mu\text{g mL}^{-1}$)	Precursor-product ions (m/z)
1	Acetic acid	7.54	79.74	60→55,43
2	Propionic acid	8.95	37.63	74→55,45
3	Isobutyric acid	9.53	36.10	73→55,43
4	Butyric acid	11.09	36.52	73→55,43
5	2-methyl butyric acid	12.38	106.73	87→59,45
6	Pentanoic acid	14.72	35.71	73→55,43
7	Caproic acid	18.41	33.11	87→59,45
8	Heptanoic acid	22.03	36.42	101→55,45
9	Octanoic acid	25.51	34.62	115→73,45
10	Pelargonic acid	27.51	33.43	129→59,55
11	Decylic acid	28.74	38.11	143→87,59
12	Benzoic acid	29.57	52.32	122→105,77
13	2-furan formic acid	30.26	179.93	112→95,55
14	Dodecanoic acid	30.82	35.90	171→101,86
15	Myristic acid	33.82	170.11	228→185,115
16	Palmitic acid	37.20	613.80	157→129,115
17	Stearic acid	41.31	608.03	199→143,129
18	Oleic acid	42.02	440.61	111→83,55
19	Linoleic acid	43.46	692.61	163→150,109
20	Linolenic acid	45.71	237.93	278→171,129

Table.2. Method performance data: calibration curve, correlation coefficient (R^2), linear range and limit of detection (LOD)

Organic acids	Calibration curve ($\mu\text{g mL}^{-1}$)	R^2	Linear range ($\mu\text{g mL}^{-1}$)	LOD ($\mu\text{g mL}^{-1}$) ^a
Acetic acid	$Y=2.62\text{E-}07\cdot X-1.0741$	0.9985	0.33-7.97	0.01
Propionic acid	$Y=6.80\text{E-}07\cdot X+0.0016$	0.9998	0.31-3.76	0.01
Isobutyric acid	$Y=3.12\text{E-}07\cdot X-0.00001$	0.9998	0.30-3.61	0.01
Butyric acid	$Y=4.27\text{E-}07\cdot X+0.1000$	0.9988	0.30-3.65	0.01
2-methyl butyric acid	$Y=1.86\text{E-}07\cdot X+0.0456$	0.9995	0.89-10.67	0.01
Pentanoic acid	$Y=3.21\text{E-}07\cdot X+0.0680$	0.9997	0.29-3.57	0.01
Caproic acid	$Y=4.84\text{E-}07\cdot X+0.0795$	0.9995	0.27-3.31	0.01
Heptanoic acid	$Y=1.57\text{E-}06\cdot X+0.0731$	0.9999	0.30-3.64	0.01
Octanoic acid	$Y=1.57\text{E-}06\cdot X+0.0512$	0.9986	0.29-3.46	0.01
Pelargonic acid	$Y=2.67\text{E-}07\cdot X+0.0305$	0.9975	0.28-3.34	0.01
Decylic acid	$Y=9.34\text{E-}07\cdot X+0.0930$	0.9991	0.31-3.80	0.01
Benzoic acid	$Y=3.82\text{E-}08\cdot X+0.0843$	0.9987	0.29-5.23	0.01
2-furan formic acid	$Y=8.72\text{E-}06\cdot X-0.0989$	0.9986	0.30-17.99	0.01
Dodecanoic acid	$Y=1.42\text{E-}06\cdot X+0.0926$	0.9991	0.30-3.59	0.01
Myristic acid	$Y=3.96\text{E-}05\cdot X-0.3719$	0.9997	0.26-17.01	0.01
Palmitic acid	$Y=2.30\text{E-}06\cdot X-0.4025$	0.9973	2.67-61.38	0.02
Stearic acid	$Y=6.21\text{E-}06\cdot X-0.4700$	0.9999	7.87-60.80	0.06
Oleic acid	$Y=6.85\text{E-}06\cdot X-0.0612$	0.9992	0.88-44.06	0.01
Linoleic acid	$Y=4.79\text{E-}05\cdot X+0.5632$	0.9998	2.66-69.26	0.02
Linolenic acid	$Y=5.85\text{E-}06\cdot X-0.0412$	0.9988	1.52-23.79	0.02

^aLOD: was estimated by determining tobacco samples with estimated LOQ values added concentration of analytes for seven times repeatability and calculated as 3 times the standard deviation of the peak response.

Table.3. Recovery and relative standard deviation (RSD) of organic acids.

Organic acids	Added ($\mu\text{g mL}^{-1}$)	Detected ($\mu\text{g mL}^{-1}$)	$\pm\text{SD}$ ($\mu\text{g mL}^{-1}$)	Recovery (%) ^a	RSD (%) ^b
Acetic acid	0.00	5.12	0.15	--	2.87
	1.99	6.56	0.60	72.36	9.64
Propionic acid	0.00	0.58	0.03	--	5.17
	0.47	0.99	0.03	87.37	3.03
Isobutyric acid	0.00	1.04	0.02	--	1.44
	0.45	1.44	0.05	88.45	3.26
Butyric acid	0.00	0.33	0.01	--	1.52
	0.46	0.76	0.04	95.92	4.87
2-methyl butyric acid	0.00	7.53	0.11	--	1.51
	1.79	9.31	0.20	99.34	2.13
Pentanoic acid	0.00	0.49	0.01	--	2.04
	0.45	0.85	0.08	80.56	9.29
Caproic acid	0.00	0.52	0.01	--	2.12
	0.41	0.86	0.10	80.90	11.28
Heptanoic acid	0.00	0.27	0.01	--	1.85
	0.23	0.47	0.04	87.95	9.15
Octanoic acid	0.00	0.37	0.01	--	3.78
	0.23	0.57	0.08	86.68	13.33
Pelargonic acid	0.00	0.28	0.01	--	5.00
	0.22	0.48	0.05	89.20	10.63
Decylic acid	0.00	0.20	0.00	--	2.00
	0.23	0.39	0.05	82.51	11.54
Benzoic acid	0.00	3.79	0.03	--	0.71
	1.31	5.02	0.12	93.87	2.47
2-furan formic acid	0.00	12.48	0.25	--	2.03
	1.35	13.62	0.78	84.85	5.71
Dodecanoic acid	0.00	0.46	0.01	--	1.96
	0.85	1.25	0.06	92.48	4.96
Myristic acid	0.00	6.91	0.12	--	1.77
	1.16	7.99	0.14	93.43	1.69
Palmitic acid	0.00	52.55	1.66	--	3.16
	5.34	58.50	2.52	111.47	4.31
Stearic acid	0.00	55.58	0.54	--	0.96
	3.73	59.28	1.44	99.05	2.43
Oleic acid	0.00	6.95	0.71	--	10.27
	5.00	12.28	0.46	106.64	3.71
Linoleic acid	0.00	47.87	1.25	--	2.61
	5.33	53.69	1.75	109.24	3.25
Linolenic acid	0.00	11.84	0.71	--	5.97
	3.00	14.49	0.48	88.42	2.87

^aRecovery were calculated by $(C_{\text{spiked}} - C_{\text{unspiked}}) \times 100\% / C_{\text{addition}}$; ^bRSD is relative standard deviation (n=5).

Table.4. Concentration and standard deviation (SD) of organic acids in flue-cured tobacco samples

Organic acids	ShaoyangB ₂ F ($\mu\text{g g}^{-1}$) ^a	ChenzhouB ₂ F ($\mu\text{g g}^{-1}$) ^a	LonghuiB ₂ F ($\mu\text{g g}^{-1}$) ^a
Acetic acid	109.13 $\pm$ 18.64	153.40 $\pm$ 27.35	179.67 $\pm$ 28.26
Propionic acid	63.87 $\pm$ 12.87	71.59 $\pm$ 13.62	64.36 $\pm$ 13.04
Isobutyric acid	6.93 $\pm$ 0.13	6.13 $\pm$ 0.47	4.47 $\pm$ 0.96
Butyric acid	2.20 $\pm$ 0.44	2.28 $\pm$ 0.37	1.71 $\pm$ 0.28
2-methyl butyric acid	50.20 $\pm$ 5.97	63.87 $\pm$ 5.66	44.15 $\pm$ 4.83
Pentanoic acid	3.27 $\pm$ 0.36	4.09 $\pm$ 0.45	3.61 $\pm$ 0.54
Caproic acid	3.47 $\pm$ 0.07	5.66 $\pm$ 0.31	3.59 $\pm$ 0.09
Heptanoic acid	1.80 $\pm$ 0.05	2.54 $\pm$ 0.03	1.83 $\pm$ 0.06
Octanoic acid	2.47 $\pm$ 0.11	7.63 $\pm$ 0.34	3.57 $\pm$ 0.16
Pelargonic acid	1.87 $\pm$ 0.12	6.79 $\pm$ 0.74	2.45 $\pm$ 0.02
Decylic acid	1.33 $\pm$ 0.11	2.67 $\pm$ 0.13	1.31 $\pm$ 0.76
Benzoic acid	25.27 $\pm$ 4.22	49.62 $\pm$ 4.63	30.50 $\pm$ 3.91
2-furan formic acid	83.20 $\pm$ 11.87	107.20 $\pm$ 14.26	99.13 $\pm$ 11.68
Dodecanoic acid	3.07 $\pm$ 0.32	7.54 $\pm$ 1.47	3.42 $\pm$ 0.03
Myristic acid	46.07 $\pm$ 6.08	56.36 $\pm$ 8.66	44.91 $\pm$ 8.20
Palmitic acid	370.33 $\pm$ 38.24	642.23 $\pm$ 40.06	550.36 $\pm$ 39.32
Stearic acid	350.53 $\pm$ 8.08	533.32 $\pm$ 9.37	406.16 $\pm$ 9.01
Oleic acid	46.33 $\pm$ 10.02	54.38 $\pm$ 9.33	60.87 $\pm$ 9.81
Linoleic acid	319.13 $\pm$ 37.32	623.52 $\pm$ 48.01	539.57 $\pm$ 48.13
Linolenic acid	78.93 $\pm$ 12.21	127.21 $\pm$ 12.16	110.00 $\pm$ 11.93

a. All values are mean $\pm$ SD obtained by five analyses.