

GC–MS Combined with Fast GC E-Nose for the Analysis of Volatile Components of Chamomile (*Matricaria chamomilla* L.)

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Table S1. The formula, and sensory description of flavor components in chamomile by fast GC e-nose.

MXT-5		MXT-1701		CAS	Formula	Nmae	Score	Sensory descriptors
RT	RI	RT	RI					
15.94	418	14.50	576	107-01-7	C ₄ H ₈	2-Butene	86.81	Aromatic
16.96	439	14.50	576	107-02-8	C ₃ H ₄ O	Propenal	75.19	Almond; Cherry
18.16	463	14.54	577	64-17-5	C ₂ H ₆ O	Ethanol	95.25	Spicy; Ethanol
22.64	552	18.12	694	71-23-8	C ₃ H ₈ O	1-Propanol	86.95	Spicy; Ethanol
26.10	621	15.18	598	110-54-3	C ₆ H ₁₄	Hexane	90.58	Gasoline; Alkane
26.98	639	16.34	636	96-37-7	C ₆ H ₁₂	methylcyclopentane	81.25	Gasoline; Gasoline
37.08	761	25.72	834	623-43-8	C ₅ H ₈ O ₂	Methyl crotonate	95.03	Fruity; Green
39.32	781	27.16	853	105-54-4	C ₆ H ₁₂ O ₂	Ethyl butyrate	83.57	Fruity; Sweety
41.90	804	30.26	895	6789-80-6	C ₆ H ₁₀ O	(Z)-3-hexenal	87.58	Fruity; Oak
47.04	855	32.28	919	7452-79-1	C ₇ H ₁₄ O ₂	Butanoic acid	96.01	Fruity; Apple
52.52	911	44.24	1066	109-52-4	C ₅ H ₁₀ O ₂	Pentanoic acid	72.63	Spicy; Sweety
54.16	932	38.06	985	7785-26-4	C ₁₀ H ₁₆	<i>a</i> -pinene	83.14	Resin; Terpenoids
55.74	951	48.72	1130	620-02-0	C ₆ H ₆ O ₂	5-Methylfurfural	83.93	Spicy; Almond
57.04	967	39.82	1006	127-91-3	C ₁₀ H ₁₆	β -Pinene	95.16	Resin; Wooden
58.69	987	33.47	932	123-35-3	C ₁₀ H ₁₆	Myrcene	91.60	Fruity; Lemon
59.16	993	47.16	1106	124-13-0	C ₈ H ₁₆ O	Octanal	88.77	Fruity; Orange
59.74	1000	42.00	1036	99-83-2	C ₁₀ H ₁₆	<i>a</i> -Phellandrene	79.98	Spicy; Orange
62.45	1041	56.66	1263	19322-27-1	C ₅ H ₆ O ₃	norfuraneol	70.04	Sweety; Caramel
63.19	1055	47.70	1115	99-85-4	C ₁₀ H ₁₆	γ -Terpinene	91.29	Fruity; Orange
64.42	1070	51.32	1170	925-78-0	C ₉ H ₁₈ O	3-Nonanone	93.95	Fruity; Vegetable

¹ RT, MXT-5 and RT, MXT-1701: Retention time measured in column MXT-5 or MXT-1701; RI, MXT-5 and RI, MXT-1701: Retention index measured by n-alkanes in column MXT-5 or MXT-1701; CAS: Chemical Abstracts Service registry number.

[illegible]

Spathulenol	25.2 1	15921568	6750- 60-3	0.00	0.48	0.15	0.27	0.23	0.14	0.19	0.18	0.25	0.23	0.55	0.49	0.59	0.36	0.68	0.08	0.06	0.06
γ -Eudesmol	25.9 0	16221630	1209- 71-8	0.00	0.10	0.00	0.10	0.09	0.09	0.10	0.12	0.08	0.08	0.10	0.07	0.09	0.08	0.15	0.05	0.03	0.04
β -Bisabolol	26.2 9	16401758	15352- 77-9	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.03	0.04	0.04	0.00	0.06	0.00	0.00	0.00
γ -Cadinol	26.4 9	16491639	5937- 11-1	0.00	0.05	0.06	0.00	0.00	0.00	0.03	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
α -Bisabolol oxide B	26.8 2	16631644	26184- 88-3	0.67	2.92	0.70	2.34	2.82	2.62	2.30	2.62	3.36	2.63	1.51	1.40	1.44	0.88	2.04	1.17	1.26	0.83
Bisabolol oxide B	26.8 6	16651666	55399- 12-7	0.00	0.21	0.14	0.15	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.04	0.06
α -Bisabolone oxide A	27.3 7	16881670	22567- 38-0	0.39	1.31	0.60	1.41	0.98	1.04	1.47	1.31	2.14	1.76	1.21	1.07	1.22	0.72	1.38	0.45	0.54	0.31
α -Bisabolol	27.5 3	16951684	515-69- 5	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00
Chamazulene	28.4 2	17371707	529-05- 5	0.09	1.08	0.17	1.28	0.93	0.57	1.92	2.05	3.79	2.37	0.52	0.51	0.57	0.17	0.47	0.18	0.31	0.17
α -Bisabolol oxide A	28.9 0	17591758	22567- 36-8	0.61	0.31	0.85	0.32	0.23	0.25	0.39	0.40	0.44	0.42	0.25	0.26	0.21	0.13	0.25	0.25	0.32	0.21
(Z)-ene-yne- Dicycloether	31.0 0	18551849	4575- 53-5	0.07	0.08	0.08	0.06	0.12	0.06	0.07	0.08	0.16	0.09	0.07	0.07	0.05	0.02	0.08	0.00	0.00	0.00
(Z)-18- Octadec-9- enolide	36.4 7	21572158	74992- 69-1	0.04	0.04	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.05	0.05	0.07	0.05	0.06	0.12	0.15	0.10
Heptacosane	42.2 9	25022500	593-49- 7	0.07	0.07	0.08	0.07	0.07	0.07	0.08	0.07	0.10	0.05	0.14	0.14	0.20	0.16	0.14	0.10	0.03	0.06
Essential oil (%)				0.75 %	0.90 %	1.00 %	0.77 %	0.92 %	0.91 %	1.20 %	1.10 %	0.86 %	1.00 %	0.63 %	0.55 %	0.52 %	0.44 %	0.43 %	0.66 %	1.05 %	0.93 %

² RT: relative retention time in GC-MS; RI-m: the actual retention index calculated by n-alkanes; RI-r: the theoretical retention index in the NIST 14 library; CAS: Chemical Abstracts Service registry number; S1~S18: the content of each sample compared with the internal standard($\mu\text{g/mL}$).

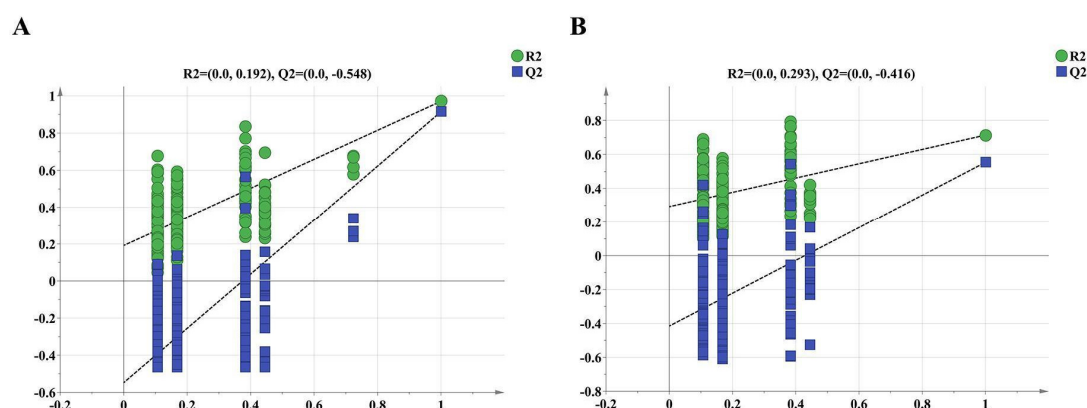
Table S3. Electronic nose raw data.

ID	S1	S2	S3	S4	S5	S6	S7	S8	S9
2-Butene	759.73	65103.6 3	1926.23	913.93	1101.27	1098.17	17751.00	1334.97	22260.4 0
Propenal	0.00	1874.43	0.00	2095.53	1734.67	2144.97	3113.40	1542.33	2181.33
Ethanol	0.00	0.00	0.00	0.00	0.00	0.00	1331.93	1345.47	1215.23
1-Propanol	0.00	1812.70	0.00	0.00	0.00	1086.30	0.00	0.00	1039.83
Hexane	1413.77	1442.03	0.00	1842.60	1701.47	2573.47	1375.23	2227.33	1316.00
Methylcyclopentane	1101.57	1025.63	0.00	1141.00	1544.90	1630.97	0.00	1506.77	0.00
Ethylbutyrate	1288.90	1442.63	2349.67	1655.70	2217.40	2232.27	0.00	1999.20	2163.43
(Z)-3-hexenal	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Butanoicacid	39825.9 0	36090.4 0	64121.77	47016.9 3	52171.7 3	63605.33	30753.70	85530.10	87087.0 7
Pentanoicacid	1541.80	2946.93	2015.40	1996.03	3305.83	3454.83	1886.03	3532.13	3321.63
α -pinene	3964.10	12011.3 3	5066.50	9059.00	11462.0 7	6641.10	12468.67	16600.90	12740.5 3
5-Methylfurfural	10386.5 7	10242.2 7	16823.20	10652.5 0	12929.7 0	14065.03	9431.53	18276.87	17622.1 7

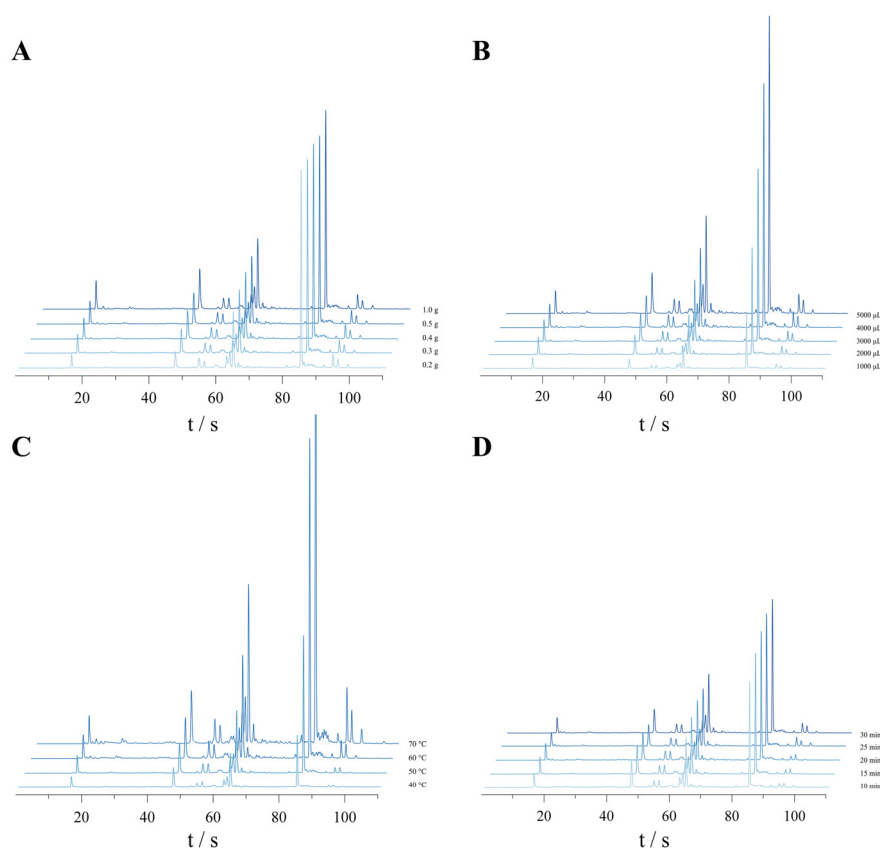
β-Pinene	2825.27	0.00	3759.80	0.00	0.00	0.00	0.00	0.00	0.00
Myrcene	0.00	0.00	0.00	0.00	0.00	1411.57	0.00	0.00	0.00
Octanal	5071.87	5695.73	8308.40	3830.50	4472.23	4511.77	5300.87	8600.37	6826.03
α-Phellandrene	0.00	4068.90	0.00	2417.53	2901.03	3362.17	3352.40	4638.93	3901.97
Norfuraneol	13087.6	29475.4	26534.43	12418.7	15652.1	19603.53	14096.07	23196.83	22225.1
	0	0		7	0				7
γ-Terpinene	3934.27	15148.4	6726.33	12691.2	19262.8	11272.73	22346.10	30543.47	21975.9
		3		7	0				7
3-Nonanone	19686.6	53662.3	31473.97	44372.2	54650.0	58637.87	58901.03	81433.23	75145.1
	3	7		7	0				3
p-Cymenene	1686.13	4190.17	2799.60	3223.77	4061.13	4378.00	5590.67	7329.37	5053.70
n-nonanal	1560.13	1899.97	2609.00	1967.13	1848.50	2787.47	2879.03	4546.57	2688.83
1,3,8para-Menthatriene	0.00	0.00	1088.83	0.00	1237.03	0.00	2007.83	2998.63	1786.87
camphor	0.00	0.00	0.00	974.83	0.00	1373.33	1576.70	2549.07	1742.67
Cymen-8-ol	1108.40	0.00	1104.30	0.00	0.00	0.00	0.00	0.00	0.00
2,6-dimethoxy-phenol	1438.27	1109.00	1981.37	0.00	0.00	0.00	0.00	0.00	0.00
trans-Carveol	0.00	0.00	1761.77	0.00	0.00	0.00	0.00	0.00	0.00
(Z)-3-Hexenylhexanoate	0.00	0.00	0.00	0.00	1431.77	1001.40	2276.87	3302.57	0.00
N-hexyl-hexanoate	0.00	0.00	0.00	0.00	1064.13	885.43	0.00	1270.37	0.00
(E)-Cinnamicacid	0.00	0.00	1596.70	0.00	0.00	1066.33	0.00	1034.03	0.00
Geosmin	55573.7	60881.9	112647.8	53439.8	89852.3	112605.7	114816.7	129848.1	40686.5
	3	0	0	7	0	7	0	7	0
β-Caryophyllene	0.00	3165.20	1211.83	3023.50	2076.07	3725.37	4616.73	5347.63	1834.57
α-Selinene	0.00	1076.03	1023.40	920.90	1422.33	1468.30	1794.07	2091.00	976.57
Methyldodecanoate	1141.80	1871.83	1953.47	2264.87	2651.07	3926.50	3601.00	5437.80	1375.33
8-methylpentadecane	0.00	1386.10	3178.50	1246.83	1850.03	2136.53	3247.63	4391.73	1331.03
Rheosmin	1580.07	1732.53	0.00	1565.50	2461.57	2460.23	3832.57	5646.20	1310.87
1-Tridecanol	0.00	1235.83	1502.37	1177.00	1655.07	1926.73	2619.20	3772.20	1025.37
Tetradecanal	0.00	1214.87	1275.77	0.00	2401.50	1869.07	2514.83	2116.43	1598.35
2-Pentadecanone	2512.53	2492.53	3742.90	1322.43	9398.00	5122.23	8470.77	7775.10	8841.70
Methyltetradecanoate	2041.27	2530.77	2690.80	2151.07	4356.57	4535.70	7265.13	5108.70	6779.10
Tetradecylacetate	2114.10	0.00	3467.87	0.00	1709.83	0.00	2113.90	0.00	0.00
ID	S10	S11	S12	S13	S14	S15	S16	S17	S18
2-Butene	15453.9	413.00	326.94	541.57	437.23	361.97	69229.50	73239.37	11689.1
	0								3
Propenal	1687.17	1656.57	0.00	0.00	0.00	1196.13	2680.07	1976.20	3484.53
Ethanol	1307.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-Propanol	1260.07	0.00	0.00	1079.27	0.00	2470.63	2685.50	3379.37	1027.57
Hexane	1062.37	1305.40	1275.99	0.00	0.00	1103.63	0.00	0.00	0.00
Methylcyclopentane	0.00	1241.27	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylbutyrate	2113.10	0.00	0.00	0.00	1057.57	0.00	0.00	0.00	0.00

(Z)-3-hexenal	0.00	1720.70	0.00	0.00	0.00	2890.20	3723.83	0.00	2307.57
Butanoicacid	91001.3 3	7112.23	3888.48	5250.17	20890.0 7	13121.03	0.00	0.00	0.00
Pentanoicacid	2813.30	1172.67	0.00	1295.67	1381.90	1494.97	0.00	0.00	0.00
α -pinene	10498.7 3	3970.93	1658.28	1774.40	4717.53	4330.73	0.00	0.00	0.00
5-Methylfurfural	16116.1 0	1809.30	840.39	1142.87	4081.90	3074.50	0.00	0.00	0.00
β -Pinene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Myrcene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Octanal	5815.93	0.00	0.00	0.00	0.00	0.00	1254.50	1946.27	2810.00
α -Phellandrene	3433.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Norfuraneol	18564.7 0	1271.47	553.15	623.50	1925.73	1635.27	3386.67	6801.70	0.00
γ -Terpinene	17006.9 7	4203.13	2975.24	2987.33	5673.67	5740.60	0.00	1350.00	0.00
3-Nonanone	60307.1 7	11423.8 7	5198.19	6392.27	21668.4 7	18359.43	4088.63	4111.10	2843.93
p-Cymenene	4424.33	901.27	0.00	0.00	1764.83	1468.80	0.00	0.00	0.00
n-nonanal	2093.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,3,8para-Menthatriene	1481.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
camphor	1343.37	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cymen-8-ol	0.00	0.00	0.00	0.00	0.00	0.00	1399.50	0.00	1290.00
2,6-dimethoxy-phenol	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
trans-Carveol	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
(Z)-3-Hexenylhexanoate	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-hexyl-hexanoate	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
(E)-Cinnamicacid	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Geosmin	44809.7 0	10433.4 0	19981.88	6580.30	8910.20	8476.73	30665.90	82372.40	25840.8 0
β -Caryophyllene	2881.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
α -Selinene	763.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methyldodecanoate	1754.87	0.00	1237.49	0.00	0.00	0.00	0.00	1416.80	0.00
8-methylpentadecane	1399.57	0.00	1268.35	0.00	0.00	0.00	1463.33	4185.30	0.00
Rheosmin	1362.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2156.43
1-Tridecanol	1034.13	0.00	0.00	0.00	0.00	0.00	0.00	1094.47	0.00
Tetradecanal	0.00	0.00	1525.54	1368.37	870.03	1571.03	0.00	0.00	0.00
2-Pentadecanone	2631.07	1457.70	1502.56	1718.83	1054.37	2089.23	3408.67	5812.40	4252.50
Methyltetradecanoate	3956.00	2571.93	3466.89	3800.03	1721.23	3065.97	1468.40	2271.27	1852.00
Tetradecylacetate	0.00	0.00	1103.28	0.00	0.00	0.00	1027.77	2104.77	1017.13

³ ID: S1-S18 represent different chamomile samples; the leftmost column lists the name of identified compounds for each peak; the data represent the signal peak areas analysed by the Rapid Gas Chromatography Electronic Nose.

Figure S1. Results of Permutation.

⁴ A: PLSDA Permutation result of GC-MS; B: PLSDA Permutation result of electronic nose.

Figure S2. Results of Single-Factor Investigations

⁵ A: Chromatograms of Sample Quantity; B: Chromatograms of Injection Volume; C: Chromatograms of Incubation Temperature; D: Chromatograms of Incubation Time.