Table S1. Identification of 87 nonvolatile compounds in this study.

No.	Compounds	RT (min)	Formula	Theoretical mass ([M–H]⁻)	Experimental mass ([M–H]⁻)	Relative concentration (mg/kg)				Ref
						Maofeng	Congou	Xiangluo	Jinzhen	
C1	D-(-)-quinic acid*	1.46	C7H12O6	191.0561	191.0549	751.62±118.45	1003.10±201.58	445.94±120.59	631.42±85.39	[1]
C2	Caffeic acid hexoside	1.48	C12H22O11	341.1089	341.1081	1.83±0.27	1.57±0.41	1.66±0.34	1.47±0.27	[1]
C3	(E)GC-(E)GC-1	5.29	C30H26O14	609.1250	609.1263	2.72±1.24	2.60±1.01	1.43±0.51	1.23±0.44	[1]
C4	β-glucogallin*	5.42	C13H16O10	331.0671	331.0671	25.02±6.67	18.25±4.12	18.58±7.80	22.29±7.51	[1]
C5	Galloyl acid*	5.42	C7H6O5	169.0142	169.0131	1125.48±183.99	1040.99±150.95	1139.19±133.71	1054.82±186.17	[1]
C6	3-O-Galloylquinic acid*	6.63	C14H16O10	343.0671	343.0667	300.59±38.99	245.34±28.14	250.56±32.36	238.60±46.12	[1]
C7	(E)GC-(E)GC-2	7.49	C30H26O14	609.1250	609.1232	0.08±0.07	0.08±0.05	0.02±0.03	0.04±0.03	[1]
C8	Gallocatechin-glucoside	8.93	C21H24O12	467.1195	467.1186	0.36±0.13	0.28±0.06	0.11±0.05	0.16±0.04	[1]
C9	GC*	9.8	C15H14O7	305.0667	305.0666	1.60±0.68	1.51±0.67	0.84±0.36	1.13±0.55	[1]
C10	(E)GC-(E)GC-4	10.35	C30H26O14	609.1250	609.1236	0.21±0.10	0.20±0.08	0.05±0.04	0.10±0.03	[1]
C11	3-Caffeoylquinic acid	11.65	C16H18O9	353.0878	353.0880	1.57±0.71	1.36±0.53	0.51±0.17	0.64±0.62	[1]
C12	Theasinensin B	13.31	C37H30O18	761.1359	761.1361	21.47±6.93	19.30±4.81	10.73±2.88	13.32±3.19	[2]
C13	3-p-coumaroylquinic acid	14.25	C16H18O8	337.0929	337.0931	55.87±15.15	64.86±24.58	38.91±9.87	34.02±7.72	[1]
C14	Theacitrin A	14.39	C37H28O18	759.1203	759.1201	8.77±1.69	8.37±2.74	4.63±1.18	4.87±1.25	[2]
C15	3-p-coumaroylquinic acid isomer	14.83	C16H18O8	337.0929	337.0931	54.58±11.18	62.44±18.20	35.45±7.47	33.86±7.18	[1]
C16	proanthocyanidin B1*	15.28	C30H26O12	577.1351	577.1355	0.65±0.85	1.13±0.71	0.64±0.58	0.48±0.42	[1]
C17	proanthocyanidin B3*	15.55	C30H26O12	577.1351	577.1357	0.61±0.99	1.18±0.77	0.67±0.58	0.71±0.63	[1]
C18	EGC*	15.76	C15H14O7	305.0667	305.0665	26.90±11.83	25.66±9.52	16.34±3.87	19.64±10.78	[1]
C19	C*	17.11	C15H14O6	289.0718	289.0719	16.03±6.78	13.26±8.73	8.81±5.78	8.58±6.77	[1]
C20	chlorogenic acid	17.38	C16H18O9	353.0878	353.0881	6.13±2.46	4.91±1.77	2.64±0.75	3.37±3.09	[1]
C21	digalloyl glucose	19.16	C20H20O14	483.0780	483.0779	144.57±48.78	78.47±32.92	73.57±36.36	95.26±41.92	[1]
C22	4-caffeoylquinic acid	19.51	C16H18O9	353.0878	353.0878	4.68±1.82	4.47±1.36	1.90±0.57	2.23±1.05	[1]

C23	5-*p*-coumaroylquinic acid	21.92	C16H18O8	577.1351	577.1353	3.87 ±3.01	2.83 ±1.89	1.78 ±1.48	1.82 ±1.66	[1]
C24	proanthocyanidin B4*	21.95	C30H26O12	337.0929	337.0932	197.47 ±37.19	185.35 ±40.60	155.80 ±30.14	128.84 ±29.69	[1]
C25	strictinin	22.47	C27H22O18	633.0733	633.0732	142.14 ±41.77	99.06 ±29.44	62.77 ±25.16	108.26 ±46.29	[1]
C26	proanthocyanidin B2*	25.85	C30H26O12	577.1351	577.1355	1.69 ±0.80	1.40 ±0.67	0.72 ±0.50	0.79 ±0.55	[1]
C27	4-*p*-coumaroylquinic acid	26.22	C16H18O8	337.0929	337.0931	232.79 ±50.55	237.51 ±61.25	225.64 ±54.38	155.43 ±32.57	[1]
C28	EC-EGCG	26.80	C37H30O17	745.1410	745.1414	0.16 ±0.06	0.16 ±0.12	0.03 ±0.03	0.10 ±0.07	[1]
C29	cis-5-*p*-coumaroylquinic acid	27.27	C16H18O8	337.0929	337.0929	368.55 ±46.92	350.70 ±49.77	345.02 ±55.82	266.53 ±40.54	[1]
C30	EC*	27.70	C15H14O6	289.0718	289.0719	44.59 ±12.27	40.51 ±13.66	34.63 ±14.45	33.53 ±15.59	[1]
C31	EGC-ECG-1	28.24	C37H30O17	745.1410	745.1423	0.15 ±0.06	0.17 ±0.10	0.06 ±0.04	0.12 ±0.08	[1]
C32	EGCG*	28.45	C22H18O11	457.0776	457.0780	128.55 ±29.32	115.08 ±19.76	91.33 ±17.98	100.60 ±30.25	[1]
C33	GCG*	31.96	C22H18O11	457.0776	457.0776	1.19 ±0.67	1.54 ±0.52	0.75 ±0.35	1.31 ±0.60	[1]
C34	EC-EC-EC	32.24	C45H38O18	865.1985	865.1979	0.77 ±0.29	0.58 ±0.24	0.21 ±0.12	0.30 ±0.16	[1]
C35	Procyanidin C1	32.25	C45H38O18	865.1985	865.1981	0.78 ±0.29	0.57 ±0.23	0.22 ±0.12	0.30 ±0.15	[3]
C36	Epiafzelechin	33.17	C15H14O5	273.0768	273.0771	16.38 ±3.20	14.25 ±3.35	19.49 ±4.34	15.10 ±2.22	[1]
C37	EC-ECG	33.19	C37H30O16	729.1461	729.1465	3.93 ±1.16	3.25 ±1.51	2.08 ±1.01	2.62 ±1.33	[1]
C38	Myricetin-3-*O*-galactosylrutinoside	33.39	C33H40O22	787.1938	787.1918	0.17 ±0.11	0.13 ±0.12	0.03 ±0.02	0.06 ±0.08	[1]
C39	Theacitrin A isomer1	33.63	C37H28O18	759.1203	759.1203	2.11 ±0.41	2.25 ±0.75	1.33 ±0.48	1.94 ±0.61	[3]
C40	Myricetin-3-*O*-glucosylrutinoside	33.72	C33H40O22	787.1938	787.1943	0.19 ±0.11	0.21 ±0.13	0.06 ±0.03	0.07 ±0.06	[1]
C41	Trigalloyl glucose	34.16	C27H24O18	635.0890	635.0892	105.45 ±33.52	68.64 ±22.40	54.68 ±23.40	73.70 ±23.12	[1]
C42	Myricetin-3-*O*-galactoside*	34.29	C21H20O13	479.0831	479.0831	6.49 ±2.42	6.86 ±2.52	3.24 ±1.05	4.33 ±1.76	[1]
C43	Myricetin-3-*O*-rutinoside	34.44	C27H30O17	625.1410	625.1411	0.56 ±0.28	0.51 ±0.23	0.16 ±0.12	0.32 ±0.11	[1]
C44	Isoorientin	34.55	C21H20O11	447.0933	447.0938	0.16 ±0.09	0.25 ±0.20	0.04 ±0.03	0.07 ±0.03	[1]
C45	Apigenin-6-C-glucosyl-8-C-arabinoside	34.65	C26H28O14	563.1406	563.1405	0.15 ±0.09	0.25 ±0.21	0.04 ±0.03	0.07 ±0.03	[1]
C46	Orientin	34.81	C26H28O14	563.1406	563.1407	13.41 ±4.53	15.59 ±6.23	7.98 ±2.27	9.63 ±2.34	[1]
C47	(−)-EGC-3-*O*-(4″-*O*-methyl)-gallate	34.93	C23H20O11	471.0933	471.0933	1.23 ±0.84	1.17 ±0.76	0.53 ±0.28	0.53 ±0.30	[1]
C48	Apigenin-6-C-arabinosyl-8-C-glucoside	35.67	C26H28O14	563.1406	563.1407	9.04 ±3.18	10.10 ±3.66	6.43 ±1.98	5.74 ±1.49	[1]

C49	Vitexin-4″-*O*-glucoside	35.71	C27H30O15	593.1511	593.1515	0.55 ±0.18	0.69 ±0.28	0.26 ±0.11	0.40 ±0.09	[1]
C50	Quercetin-3-*O*-galactosylrutinoside*	35.75	C33H40O21	771.1989	771.1987	1.27 ±0.47	1.87 ±0.96	0.87 ±0.31	0.91 ±0.30	[1]
C51	Quercetin-3-*O*-glucosylrutinoside	35.84	C33H40O21	771.1989	771.1987	7.16 ±2.28	7.99 ±2.83	5.88 ±2.61	5.57 ±1.72	[1]
C52	Theaflavin-3-*O*-(3-*O*-methyl)gallate-3-gallate isomer1	36.07	C44H34O20	881.1571	881.1565	3.20 ±0.42	2.79 ±0.55	2.05 ±0.52	3.15 ±0.76	[3]
C53	ECG*	36.19	C22H18O10	441.0827	441.0828	133.32 ±27.49	113.39 ±28.77	122.50 ±30.54	122.48 ±48.95	[1]
C54	vitexin*	36.22	C21H20O10	431.0984	431.0983	0.14 ±0.07	0.34 ±0.21	0.17 ±0.12	0.12 ±0.10	[1]
C55	Rhamnosylvitexin	36.42	C27H30O14	577.1563	577.1566	0.66 ±0.24	1.11 ±0.72	0.45 ±0.19	0.44 ±0.15	[1]
C56	Vitexin-2″-*O*-rhamnoside	36.42	C27H30O14	577.1563	577.1566	0.66 ±0.24	1.11 ±0.72	0.45 ±0.19	0.44 ±0.15	[1]
C57	Kaempferol-3-*O*-galactosylrutinoside	36.49	C33H40O20	755.2040	755.2039	6.55 ±2.52	5.63 ±1.45	3.87 ±2.03	6.08 ±2.39	[1]
C58	Rutin*	36.49	C27H30O16	609.1461	609.1464	37.60 ±5.08	35.02 ±4.91	32.51 ±6.22	33.81 ±3.30	[1]
C59	Isovitexin	36.51	C21H20O10	431.0984	431.0985	0.43 ±0.16	0.65 ±0.38	0.29 ±0.11	0.29 ±0.11	[1]
C60	Quercetin-3-*O*-galactoside	36.6	C21H20O12	463.0882	463.0887	19.76 ±4.97	19.12 ±3.52	16.20 ±6.60	15.94 ±4.11	[1]
C61	CG*	36.76	C22H18O10	441.0827	441.0827	0.01 ±0.00	0.33 ±0.11	0.23 ±0.12	0.30 ±0.22	[1]
C62	Quercetin-3-*O*-glucoside	36.93	C21H20O12	463.0882	463.0888	5.56 ±1.90	5.95 ±1.78	4.50 ±2.72	4.63 ±1.55	[1]
C63	Luteolin-7-*O*-glucoside	37.08	C21H20O11	447.0933	447.0947	0.07 ±0.03	0.07 ±0.03	0.01 ±0.02	0.04 ±0.02	[1]
C64	Kaempferol-3-*O*-glucosylrutinoside	37.21	C33H40O20	755.2040	755.2048	44.71 ±6.79	44.25 ±7.34	37.80 ±9.29	38.93 ±4.48	[1]
C65	Kaempferol-3-*O*-rutinoside isomer	37.28	C27H30O15	593.1512	593.1518	6.40 ±1.92	5.55 ±1.38	4.61 ±1.44	5.29 ±1.17	[1]
C66	Kaempferol-3-*O*-galactoside	37.87	C21H20O11	447.0933	447.0934	36.64 ±6.15	35.91 ±6.92	34.92 ±10.01	36.29 ±4.76	[1]
C67	Kaempferol-3-*O*-rutinoside	37.94	C27H30O15	593.1512	593.1516	11.29 ±3.29	10.18 ±2.52	8.91 ±4.11	9.84 ±2.25	[1]
C68	Kaempferol-3-*O*-glucoside	38.44	C21H20O11	447.0933	447.0936	16.50 ±4.43	16.35 ±4.53	14.47 ±6.16	14.56 ±3.19	[1]
C69	Epicatechin-3-*O*-(4″-*O*-methyl)-gallate	38.58	C23H20O10	455.0984	455.0987	1.23 ±0.81	1.46 ±0.91	0.92 ±0.39	0.71 ±0.37	[1]
C70	Theacitrin A isomer2	38.59	C37H28O18	759.1203	759.1202	0.68 ±0.24	0.86 ±0.30	0.45 ±0.22	0.56 ±0.17	[3]
C71	Epiafzelechin gallate	38.66	C22H18O9	425.0878	425.0883	101.62 ±22.23	91.69 ±18.89	95.12 ±19.56	90.60 ±25.78	[1]
C72	Theaflavin-3-*O*-(3-*O*-methyl)gallate-3-gallate isomer 2	39.35	C44H34O20	881.1571	881.1571	1.37 ±0.46	1.36 ±0.38	0.72 ±0.27	1.12 ±0.58	[3]
C73	Myricetin*	39.46	C15H10O8	317.0303	317.0298	2.25 ±0.89	2.77 ±0.88	1.49 ±0.59	2.37 ±0.94	[1]
C74	Kaempferol-7-*O*-glucoside	39.66	C21H20O11	447.0933	447.0933	0.18 ±0.08	0.24 ±0.10	0.10 ±0.07	0.15 ±0.05	[1]

C75	Theaflavin isomer1	39.78	C29H24O12	563.1195	563.1198	0.80 ±0.21	0.73 ±0.14	0.57 ±0.08	0.40 ±0.10	[3]
C76	Theaflavin-3-*O*-(3-*O*-methyl)gallate-3-gallate isomer 3	40.04	C44H34O20	881.1571	881.1571	2.07 ±0.51	1.89 ±0.72	1.03 ±0.47	1.60 ±0.73	[3]
C77	Theaflavin isomer2	40.59	C29H24O12	563.1195	563.1197	0.48 ±0.15	0.47 ±0.09	0.32 ±0.08	0.24 ±0.05	[3]
C78	Theaflavin*	41.85	C29H24O12	563.1195	563.1195	15.47 ±3.71	14.66 ±2.05	12.41 ±2.04	8.74 ±1.61	[3]
C79	Theaflavin-3-gallate*	42.56	C36H28O16	715.1304	715.1311	47.97 ±6.58	42.27 ±3.97	38.83 ±4.03	34.22 ±3.89	[3]
C80	Quercetin*	42.71	C15H10O7	301.0353	301.0349	7.77 ±2.60	10.39 ±3.12	8.68 ±3.89	8.15 ±1.41	[1]
C81	Theaflavin-3,3'-di-*O*-gallate*	42.96	C43H32O20	867.1414	867.1402	131.53 ±10.43	110.69 ±13.53	89.34 ±11.63	105.58 ±10.16	[3]
C82	Theaflavin-3'-Gallate*	43.03	C36H28O16	715.1304	715.1310	11.50 ±1.40	10.85 ±1.21	9.27 ±1.44	8.74 ±0.85	[2]
C83	Theaflavin-3-*O*-(3-*O*-methyl)gallate-3-gallate	43.86	C44H34O20	881.1571	881.1578	4.19 ±1.51	3.33 ±1.08	2.47 ±1.05	2.46 ±0.88	[3]
C84	Kaempferol	45.38	C15H10O6	285.0405	285.0403	29.50 ±8.45	34.57 ±6.57	38.02 ±9.22	37.81 ±4.75	[1]
C85	Kaempferol-3-*O*-di-*p*-coumaroylhexoside isomer1	45.78	C39H32O15	739.1668	739.1663	6.15 ±1.11	5.87 ±1.60	5.18 ±1.08	6.83 ±0.93	[1]
C86	Kaempferol-3-*O*-di-*p*-coumaroylhexoside isomer2	45.85	C39H32O15	739.1668	739.1671	6.16 ±1.11	5.88 ±1.60	5.53 ±0.94	6.83 ±0.92	[1]
C87	Kaempferol-3-*O*-di-*p*-coumaroylhexoside	45.92	C39H32O15	739.1668	739.1669	6.15 ±1.12	5.83 ±1.67	5.59 ±0.84	6.83 ±0.93	[1]

[1] Zhuang et al., (2020) Evaluation of astringent taste of green tea through mass spectrometry-based targeted metabolic profiling of polyphenols. *Food Chemistry*, 305, 125507.

[2] Huang et al., (2021) Targeted and nontargeted metabolomics analysis for determining the effect of storage time on the metabolites and taste quality of keemun black tea. *Food Chemistry*, 359, 129950.

[3] Liu et al., (2022) Dynamic changes in flavonoids content during congou black tea processing. *LWT*, 170, 114073.

Compounds labeled with * mean that their identification are based on authentic standard.