ELECTRONIC SUPPLEMENTARY INFORMATION (E.S.I.)

In Quest for Chemomarkers to Classify Taiwanese Teas

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ADDITIONAL TABLES

Tab. S1 The list of all tea samples. More details on the samples (only for scientific purposes) can be obtained on request. This table is in a separate Excel file.

Tab. S2 LC-MS method parameters and performance data for selected compounds analyzed in tea samples.

Analyte	Chemical formula	Retention time / min	Precursor ion *m/z* / u e^{-1}	Fragment ion *m/z* / u e^{-1}	Est. limit of quantification* / µg L^{-1}
caffeine (Caf)	$C_8H_{10}N_4O_2$	23.4	194.9	138.1	1.1
catechin (C)	$C_{15}H_{14}O_6$	20.4 or 25.7	291.0	123.1, 138.9, 164.9	6.8×10^3
epicatechin (EC)	$C_{15}H_{14}O_6$	20.4 or 25.7	291.0	123.1, 138.9, 164.9	6.8×10^3
epigallocatechin (EGC)	$C_{15}H_{14}O_7$	20.0	307.1	139.0, 150.9	-
gallocatechin (GaC)	$C_{15}H_{14}O_7$	13.9	307.1	139.0, 150.9, 289.0	0.23×10^3
epicatechin 3-gallate (ECG)	$C_{22}H_{18}O_{10}$	30.0 or 32.0	443.1	273.0, 123.0, 151.0	23×10^3
catechin 3-gallate (CG)	$C_{22}H_{18}O_{10}$	30.0 or 32.0	443.1	273.0, 123.0, 151.0	23×10^3
epigallocatechin 3-gallate (EGCG)	$C_{22}H_{28}O_{11}$	24.9 or 27.8	459.1	289.0, 139.0	30×10^3
gallocatechin 3-gallate (GCG)	$C_{22}H_{28}O_{11}$	24.9 or 27.9	459.3	289.0, 139.0	30×10^3

* Limits of quantification estimated based on the $S/N = 10$ criterion. The S/N values are estimated for the peaks in mass spectra.

Tab. S3 Quantitation of selected compounds in representative tea samples by LC-MS.

Analyte	Concentration / mg g^{-1} DW		
	Green tea (#1)*	**Oolong tea (#2)***	**Black tea (#15)***
caffeine (Caf)	4.97 ± 0.91	5.41 ± 1.57	6.41 ± 0.36
catechin (C)	0.90 ± 0.90	0.88 ± 4.23	0.98 ± 0.35
epicatechin (EC)	6.60 ± 4.06	2.96 ± 14.27	2.43 ± 1.24
epigallocatechin (EGC)**	13.16 ± 5.18	3.82 ± 2.00	1.38 ± 0.49
gallocatechin (GaC)	2.01 ± 1.43	0.96 ± 0.53	0.30 ± 0.12
epicatechin 3-gallate (ECG)	7.96 ± 5.22	16.85 ± 4.95	10.53 ± 3.04
catechin 3-gallate (CG)	0.22 ± 0.07	0.58 ± 0.18	0.24 ± 0.27
epigallocatechin 3-gallate (EGCG)	18.47 ± 8.87	9.50 ± 3.03	9.06 ± 2.00
gallocatechin 3-gallate (GCG)	0.85 ± 0.83	0.39 ± 0.59	0.26 ± 0.02

* Randomly selected samples (sample ID).

** Values calculated in relation to the standard of GaC.

ADDITIONAL FIGURES

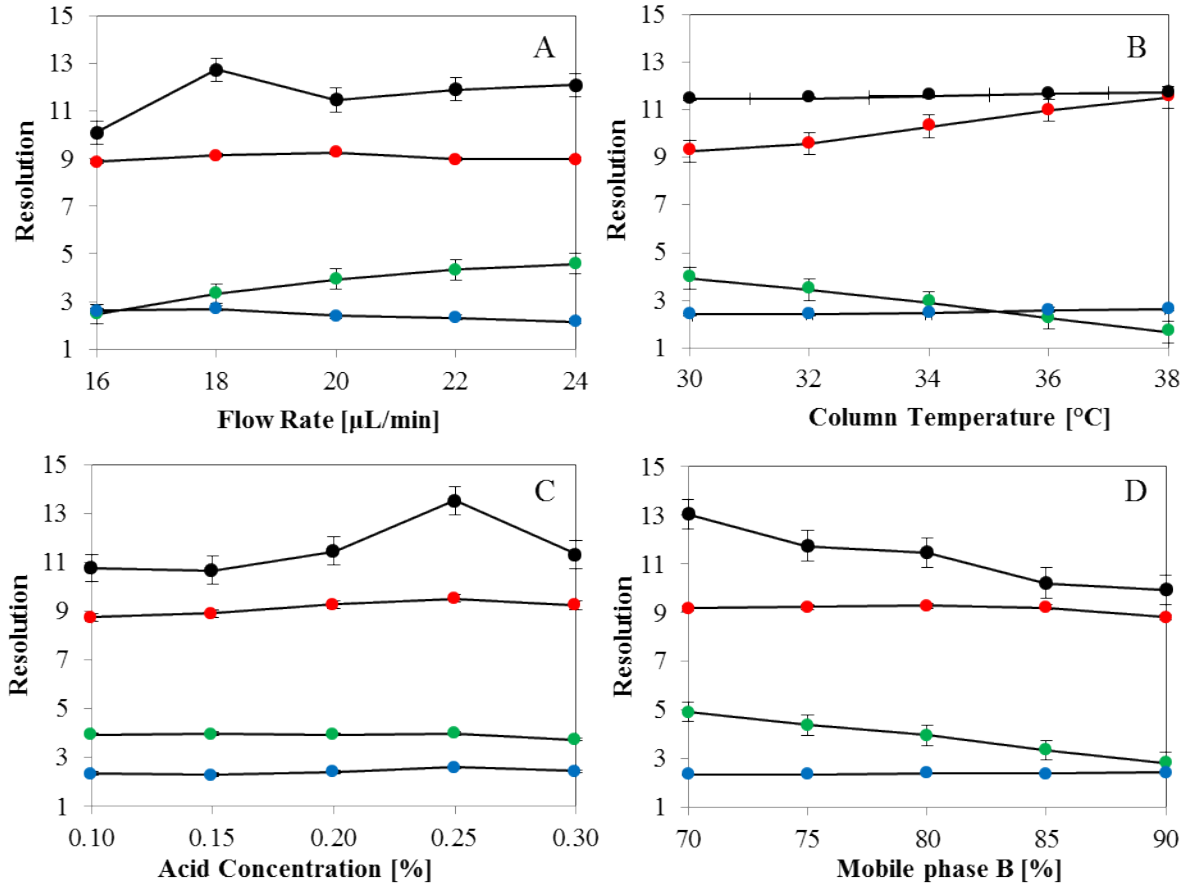

Fig. S1 Robustness of chromatographic conditions. Resolution between catechin compounds caffeine/EGC (red markers), (EGCG/GCG)/caffeine (green markers), (C/EC)/(EGCG/GCG) (blue markers), and (ECG/CG)/(C/EC) (black markers) was not significantly affected by small but deliberate changes of separation parameters: flow rate (A), column temperature (B), acetic acid concentration (C), or mobile phase composition (D).

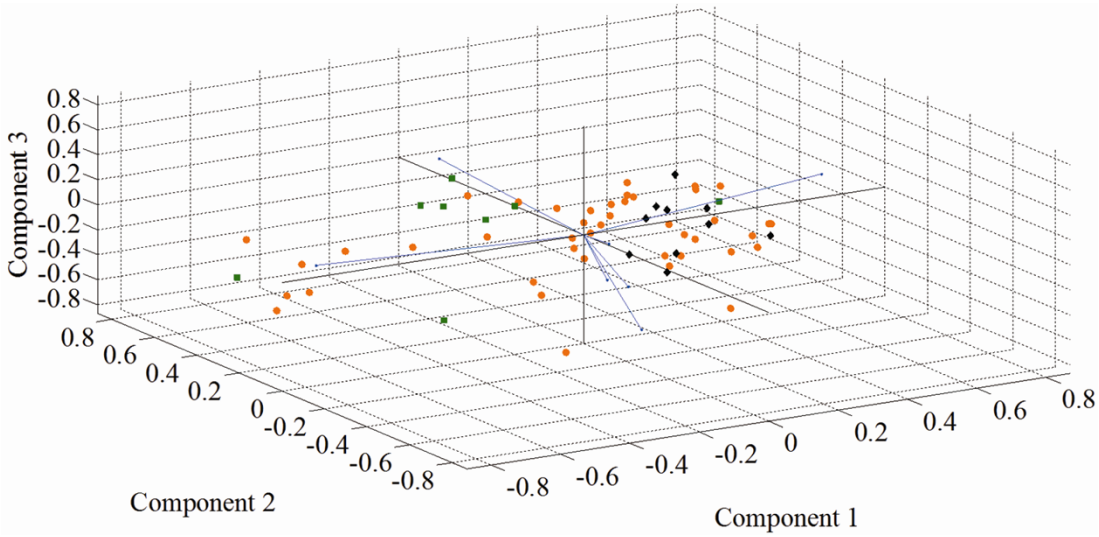

Fig. S2 3D PCA scores plots of Taiwanese tea: general bucketing. The data used to make this plot are the same as those in **Fig. 3C**. Markers: orange – oolong tea; green – green tea; black – black tea.

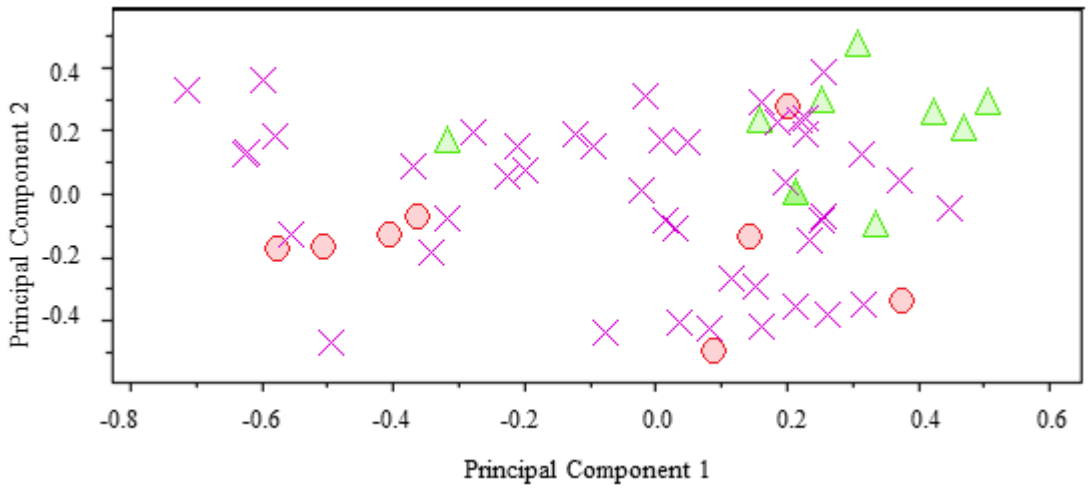

Fig. S3 PCA analysis of row data obtained by general bucketing (i) using a commercial metabolomics software package. Pink markers – oolong tea (n = 46), green markers – black tea (n = 10), red markers – green tea (n = 8).

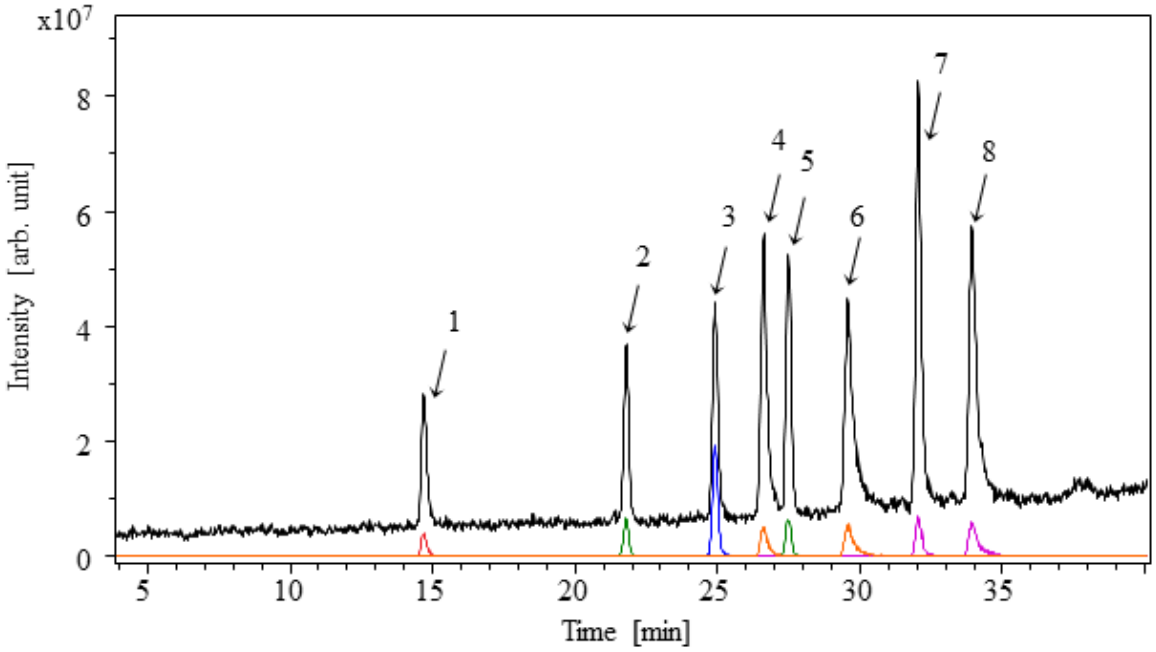

Fig. S4 Total ion current (black line) and extracted ion currents of the standard mixture. Peaks: (1) – gallocatechin, (2/5) – epi/catechin, (3) – caffeine, (4/6) – epi/gallocatechin 3-gallate, (7/8) – epi/catechin 3-gallate.