SUPPORTING INFORMATION

Comparison of Metabolomics Approaches for Evaluating the Variability of Complex Botanical Preparations: Green Tea (*Camellia sinensis*) as a Case Study

Joshua J. Kellogg, [†] Tyler N. Graf, [†] Mary F. Paine, [‡] Jeannine S. McCune, [§] Olav M. Kvalheim, [⊥] Nicholas H. Oberlies, [†] and Nadja B. Cech[†*]

[†] Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, North Carolina 27412, United States

[‡] College of Pharmacy, Washington State University, Spokane, Washington 99202, United States

[§] Department of Pharmaceutics, University of Washington, Seattle, Washington 99202, United States

[⊥] Department of Chemistry, University of Bergen, Bergen 5020, Norway

CONTENTS

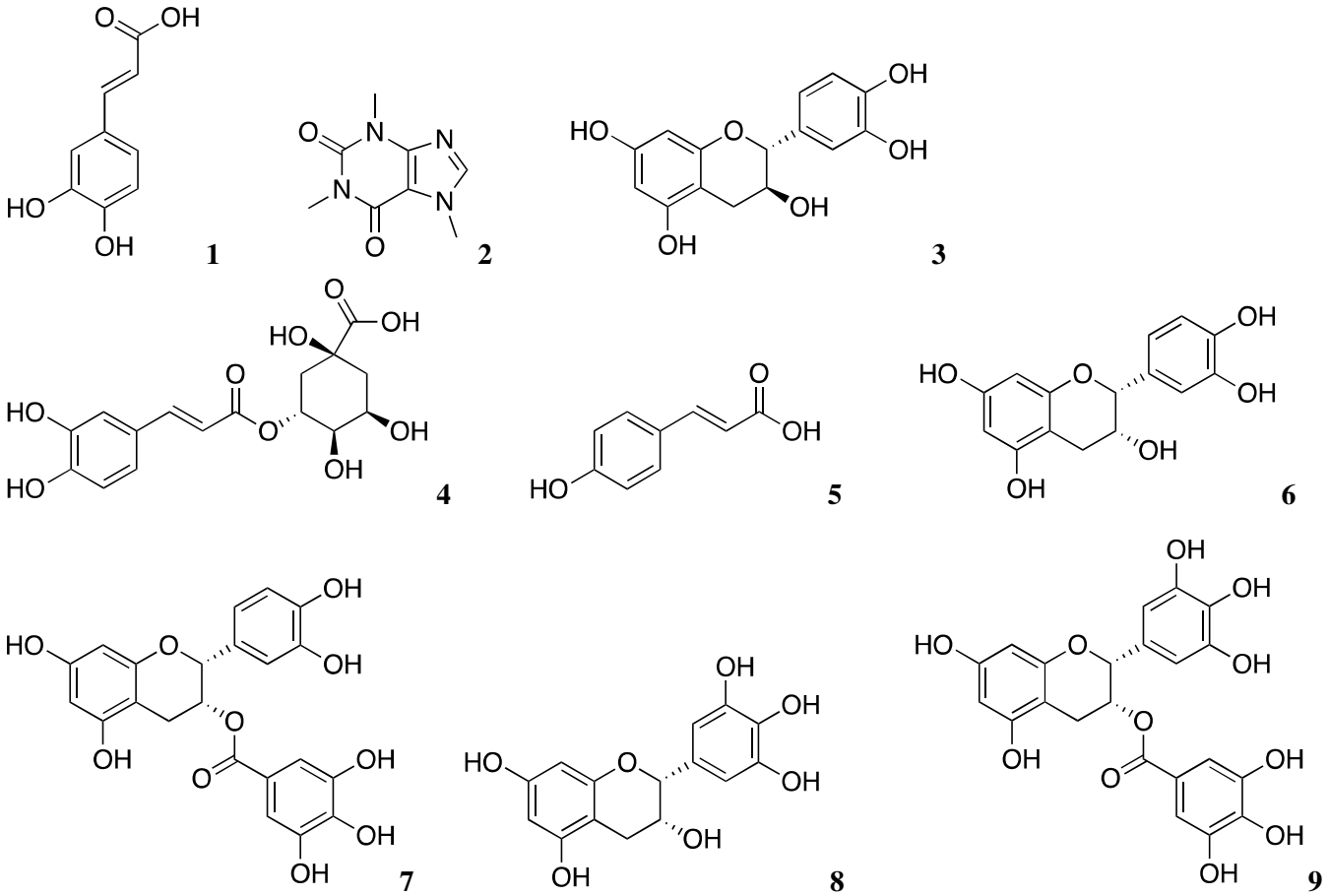
Table S1. Selection and coding of commercial green tea products under investigation.

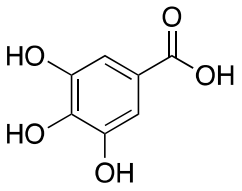
code	product form	selection criteria[a]
T01	leaf tea	consumer sales[36]
T02	leaf tea	quality report[37]
T03	leaf tea	consumer sales[36]
T04	leaf tea	quality report[37]
T05	leaf tea	quality report[37]
T06	leaf tea	quality report[37]
T07	leaf tea	quality report[37]
T08	leaf tea	quality report[37]
T09	leaf tea	quality report[37]
T10	leaf tea	quality report[37]
T11	powdered tea	consumer sales[36]
T12	powdered tea	quality report[37]
T13	leaf tea	quality report[37]
T14	leaf tea	quality report[37]
T15	tea supplement	extract report[38]
T16	leaf tea	quality report[37]
T17	leaf tea	quality report[37]
T18	leaf tea	quality report[37]
T19	tea supplement	extract report[38]
T20	leaf tea	quality report[37]
T21	leaf tea	quality report[37]
T22	powdered tea	quality report[37]
T23 [b]	leaf tea	non-green tea
T24 [c]	leaf tea	consumer sales[36]
T25	tea supplement	extract report[38]
T26 [d]	leaf tea	NIST standard
T27 [d]	tea supplement	NIST standard
T28	tea supplement	extract report[38]
T29	tea supplement	extract report[38]
T30	powdered tea	consumer sales[36]
T31	powdered tea	consumer sales[36]
T32	powdered tea	consumer sales[36]
T33	leaf tea	quality report[37]
T34	leaf tea	quality report[37]
T35	tea supplement	extract report[38]
T36	tea supplement	extract report[38]
T37 [d]	tea supplement	NIST standard
T38 [c]	leaf tea	consumer sales[36]

[a] Selection criteria represent the basis for which the product was included in the dataset (quality report[37], green tea extract consumer report,[38] consumer sales report,[36]). [b] Non-green tea negative control. [c] Green teas with botanical additives that served as partial negative controls. [d] NIST standard reference materials positive controls.

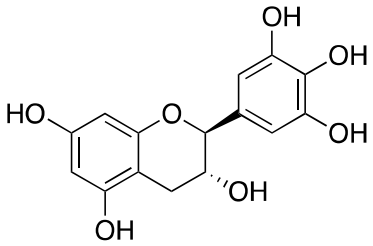
Table S1. Green tea standards used in the quantification of green tea samples described in Table 1.

	standard	compound class	formula	$[M+H]^+$	$[M-H]^-$	calibration equation	R^2
1	caffeic acid	phenolic acid	$C_9H_8O_4$	181.0501	179.0344	$y=2.36\times10^8x+4.5\times10^5$	0.9988
2	caffeine	purine alkaloid	$C_8H_{10}N_4O_2$	195.0883	193.0726	$y=3.03\times10^8x+6.4\times10^5$	0.9973
3	(+)-catechin	catechin	$C_{15}H_{14}O_6$	291.0869	289.0712	$y=6.50\times10^7x+3.5\times10^5$	0.9925
4	chlorogenic acid	phenolic acid	$C_{16}H_{18}O_9$	355.1029	353.0872	$y=1.31\times10^8x+5.4\times10^5$	0.9999
5	coumaric acid	phenolic acid	$C_9H_8O_3$	165.0552	163.0395	$y=8.44\times10^7x+2.1\times10^5$	0.9969
6	(-)-epicatechin	catechin	$C_{15}H_{14}O_6$	291.0869	289.0712	$y=7.48\times10^7x+1.6\times10^5$	0.9971
7	(-)-epicatechin gallate	catechin	$C_{22}H_{18}O_{10}$	443.0978	441.0821	$y=5.75\times10^7x+1.6\times10^5$	0.9951
8	(-)-epigallocatechin	catechin	$C_{15}H_{14}O_7$	307.0818	305.0661	$y=6.55\times10^7x+1.9\times10^5$	0.9945
9	(-)-epigallocatechin gallate	catechin	$C_{22}H_{18}O_{11}$	459.0927	457.077	$y=5.46\times10^7x+2.8\times10^5$	0.9998
10	gallic acid	phenolic acid	$C_7H_6O_5$	171.0294	169.0137	$y=1.64\times10^8x+4.2\times10^5$	0.9960
11	(-)-gallocatechin	catechin	$C_{15}H_{14}O_7$	307.0818	305.0661	$y=8.50\times10^7x+5.2\times10^5$	0.9977
12	kaempferol	flavonol	$C_{15}H_{14}O_7$	287.0556	285.0399	$y=1.59\times10^8x+4.3\times10^5$	0.9957
13	myricetin	flavonol	$C_{22}H_{18}O_{11}$	319.0454	317.0297	$y=2.78\times10^7x+8.8\times10^5$	0.9949
14	quercetin	flavonol	$C_{15}H_{10}O_6$	303.0505	301.0348	$y=4.43\times10^7x+1.5\times10^5$	0.9970
15	rutin	flavonol	$C_{15}H_{10}O_8$	611.1612	609.1455	$y=8.69\times10^6x+2.0\times10^5$	0.9966
16	theanine	amino acid	$C_{15}H_{10}O_7$	175.1083	173.0926	$y=3.05\times10^8x+1.0\times10^5$	0.9992

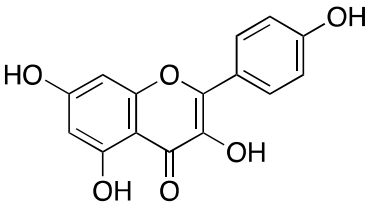




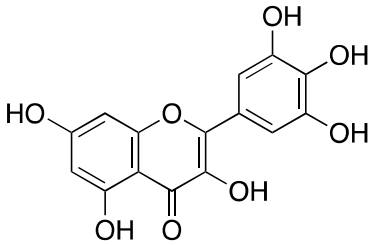
10



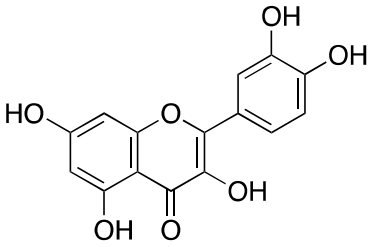
11



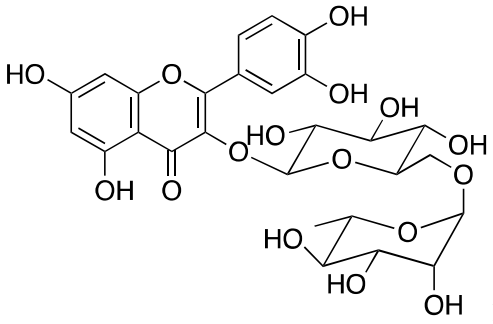
12



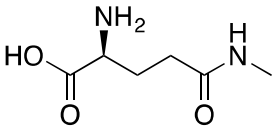
13



14



15



16

Table S2. Quantification of green tea standards in green tea methanol extract samples. Values given in µg/mL extract and represent the mean ± SD of triplicate extractions. ND, not detected; [#] non-green tea negative control; [‡] NIST, standard reference material positive controls; [§] green teas with botanical additives.

sample	caffeic acid	caffeine	catechin	chlorogenic acid	coumaric acid	epicatechin	epicatechin gallate	epigallocatechin
T01	0.0358 ± 0.0069	50.5 ± 1.2	0.966 ± 0.013	1.171 ± 0.036	0.0126 ± 0.0011	18.74 ± 0.49	28.10 ± 0.73	81.8 ± 1.6
T02	0.0185 ± 0.0042	61.5 ± 1.0	0.641 ± 0.021	0.27 ± 0.12	0.0959 ± 0.0037	9.66 ± 0.13	26.92 ± 0.38	38.4 ± 1.0
T03	0.0144 ± 0.0032	78.6 ± 5.1	1.481 ± 0.074	37.9 ± 1.9	0.0398 ± 0.0022	11.10 ± 0.65	50.76 ± 2.16	57.1 ± 4.2
T04	0.04515 ± 0.00052	73.5 ± 1.1	0.745 ± 0.022	17.66 ± 0.26	0.0637 ± 0.0054	12.98 ± 0.31	41.39 ± 0.36	56.33 ± 0.77
T05	0.0568 ± 0.0024	73.00 ± 0.43	0.676 ± 0.018	31.19 ± 0.88	0.0421 ± 0.0060	10.65 ± 0.64	55.21 ± 0.44	55.6 ± 1.5
T06	0.0133 ± 0.0033	53.4 ± 1.8	1.228 ± 0.012	0.338 ± 0.012	0.1152 ± 0.0063	6.40 ± 0.21	19.44 ± 0.22	27.49 ± 0.88
T07	0.0298 ± 0.0039	17.70 ± 0.28	1.275 ± 0.023	0.11 ± 0.41	0.07642 ± 0.00094	13.547 ± 0.049	35.10 ± 0.35	45.3 ± 1.6
T08	0.01813 ± 0.00069	65.01 ± 0.56	1.42 ± 0.17	0.06 ± 0.16	0.08277 ± 0.00091	10.813 ± 0.054	35.44 ± 0.19	48.02 ± 0.43
T09	0.03006 ± 0.00099	58.6 ± 1.1	1.357 ± 0.079	0.024 ± 0.092	0.0079 ± 0.0015	17.06 ± 0.96	33.57 ± 0.76	72.0 ± 1.9
T10	0.0301 ± 0.0041	67.1 ± 1.7	1.198 ± 0.043	0.578 ± 0.059	0.0142 ± 0.0027	14.81 ± 0.74	32.32 ± 0.76	64.52 ± 0.42
T11	0.02323 ± 0.00084	53.622 ± 0.062	0.997 ± 0.052	0.446 ± 0.042	0.0228 ± 0.0022	13.485 ± 0.021	30.04 ± 0.16	56.91 ± 0.79
T12	0.02452 ± 0.00084	66.6 ± 2.1	1.109 ± 0.065	0.32 ± 0.13	0.0164 ± 0.0022	9.46 ± 0.17	31.97 ± 0.92	44.07 ± 0.77
T13	0.0641 ± 0.0052	91.39 ± 2.74	1.298 ± 0.031	1.19 ± 0.20	0.1386 ± 0.0081	7.47 ± 0.71	32.86 ± 1.90	39.2 ± 2.9
T14	0.0139 ± 0.0023	18.20 ± 0.64	1.025 ± 0.064	0.617 ± 0.086	0.0843 ± 0.0028	7.45 ± 0.22	20.43 ± 0.40	27.6 ± 1.0
T15	0.01378 ± 0.0022	7.364 ± 0.083	1.3548 ± 0.0054	1.368 ± 0.035	0.2851 ± 0.0041	10.46 ± 0.11	67.90 ± 0.48	53.22 ± 0.42
T16	0.01866 ± 0.00084	57.27 ± 0.61	1.0816 ± 0.0053	0.026 ± 0.088	0.0499 ± 0.0023	13.89 ± 0.29	31.73 ± 0.59	48.32 ± 0.62
T17	0.0373 ± 0.0053	74.3 ± 1.7	1.706 ± 0.096	1.71 ± 0.10	0.1228 ± 0.0039	13.603 ± 0.089	30.50 ± 0.50	61.82 ± 0.95
T18	0.0192 ± 0.0039	88.92 ± 0.82	1.3479 ± 0.0024	1.80 ± 0.054	0.0865 ± 0.0028	6.76 ± 0.18	45.03 ± 0.81	37.39 ± 0.59
T19	0.046 ± 0.011	75.4 ± 1.1	0.946 ± 0.016	0.744 ± 0.075	0.168 ± 0.020	16.32 ± 0.29	25.67 ± 0.51	75.0 ± 1.2
T20	0.0275 ± 0.0011	66.2 ± 1.4	0.747 ± 0.071	0.077 ± 0.082	0.0323 ± 0.0017	14.62 ± 0.26	36.63 ± 0.55	58.84 ± 0.54
T21	0.03393 ± 0.00051	72.6 ± 2.0	1.046 ± 0.011	1.62 ± 0.17	0.06052 ± 0.00072	12.30 ± 0.10	36.09 ± 1.38	55.18 ± 0.60
T22	0.0256 ± 0.0012	65.84 ± 0.70	1.632 ± 0.029	1.141 ± 0.015	0.02691 ± 0.00037	10.65 ± 0.13	33.79 ± 0.77	43.93 ± 1.92
T23	0.028 ± 0.011	0.037 ± 0.011	1.365 ± 0.041	4.62 ± 0.92	1.27 ± 0.19	1.4169 ± 0.0045	1.6334 ± 0.0073	1.4127 ± 0.0033
T24	0.0638 ± 0.0053	41.9 ± 1.9	1.065 ± 0.013	12.57 ± 0.85	0.446 ± 0.020	9.4 ± 1.0	27.1 ± 1.0	14.97 ± 0.97
T25	0.04754 ± 0.00037	93.8 ± 1.5	0.94 ± 0.10	2.929 ± 0.098	0.093 ± 0.011	11.45 ± 0.10	21.95 ± 0.55	66.19 ± 0.36
T26	0.02867 ± 0.00027	69.48 ± 0.52	1.145 ± 0.012	0.090 ± 0.051	0.0762 ± 0.0033	12.75 ± 0.20	35.56 ± 0.35	44.7 ± 1.1
T27	0.028 ± 0.014	39.67 ± 0.62	1.411 ± 0.021	1.5843 ± 0.0089	0.2674 ± 0.0020	14.11 ± 0.21	63.7 ± 1.9	41.6 ± 9.5
T28	0.0516 ± 0.0022	41.33 ± 15.88	0.989 ± 0.025	3.26 ± 0.18	0.338 ± 0.011	11.1 ± 4.8	25 ± 13	39 ± 15
T29	0.0386 ± 0.0081	51.5 ± 4.4	1.08 ± 0.11	4.7 ± 1.8	0.0551 ± 0.0093	14.2 ± 1.6	14.8 ± 2.8	54.1 ± 3.8
T30	0.0201 ± 0.0028	58.9 ± 2.9	1.50 ± 0.11	0.64 ± 0.38	0.0400 ± 0.0054	9.89 ± 0.25	23.08 ± 0.79	44.49 ± 0.21
T31	0.0226 ± 0.0034	58.1 ± 6.4	1.129 ± 0.021	0.88 ± 0.66	0.0460 ± 0.0107	9.73 ± 0.41	25.42 ± 0.93	39.65 ± 3.45
T32	0.0230 ± 0.0052	38.5 ± 2.8	0.881 ± 0.036	0.17 ± 1.1	0.0280 ± 0.0107	11.0 ± 1.1	27.6 ± 3.4	38.6 ± 9.9
T33	0.0313 ± 0.0029	31.6 ± 7.9	0.676 ± 0.018	1.67 ± 0.83	0.0469 ± 0.0075	13.57 ± 0.79	33.72 ± 0.65	60.1 ± 1.7
T34	0.046 ± 0.010	59 ± 14	1.632 ± 0.029	3.3 ± 1.2	0.044 ± 0.020	15.0 ± 1.1	34.85 ± 1.47	49.6 ± 9.2
T35	0.0636 ± 0.0053	90 ± 18	1.462 ± 0.026	10.7 ± 3.8	0.096 ± 0.012	11.98 ± 0.43	38.13 ± 1.37	26.5 ± 1.5
T36	0.028 ± 0.011	62 ± 14	1.11 ± 0.48	2.1 ± 1.3	0.1123 ± 0.0030	11.29 ± 0.21	38.32 ± 1.40	27.1 ± 5.3
T37	0.0376 ± 0.0021	77 ± 19	0.973 ± 0.041	16 ± 14	0.1013 ± 0.0076	9.97 ± 0.50	28.8 ± 5.0	30.9 ± 4.8
T38	0.0423 ± 0.0058	28.94 ± 0.95	1.0812 ± 0.0053	51.9 ± 1.4	0.0941 ± 0.0026	8.81 ± 0.36	17.2 ± 1.1	23.2 ± 2.8

Table S2 (con't)

sample	epigallocatechin gallate	gallic acid	gallocatechin	kaempferol	myrecetin	quercetin	rutin	theanine
T01	59.91 ± 0.26	0.1537 ± 0.0057	7.22 ± 0.38	0.00201 ± 0.00056	0.858 ± 0.034	0.434 ± 0.011	6.34 ± 0.19	12.11 ± 0.38
T02	52.48 ± 0.42	1.96 ± 0.33	3.42 ± 0.31	0.0597 ± 0.0047	0.109 ± 0.048	1.025 ± 0.063	4.98 ± 0.12	9.77 ± 0.31
T03	73.72 ± 3.38	0.87 ± 0.10	5.06 ± 0.45	0.0142 ± 0.0017	0.513 ± 0.232	0.86 ± 0.119	10.59 ± 0.76	9.27 ± 0.45
T04	67.02 ± 0.43	1.365 ± 0.041	4.99 ± 0.40	0.0459 ± 0.0034	0.506 ± 0.071	0.917 ± 0.018	14.131 ± 0.030	14.35 ± 0.40
T05	80.34 ± 1.13	0.54 ± 0.31	4.92 ± 0.10	0.0138 ± 0.0016	0.205 ± 0.058	0.883 ± 0.035	5.72 ± 0.61	9.66 ± 0.10
T06	43.56 ± 0.58	1.834 ± 0.034	2.47 ± 0.06	0.06730 ± 0.00049	0.18 ± 0.05	1.012 ± 0.013	3.26 ± 0.18	5.184 ± 0.056
T07	59.9 ± 2.4	1.416 ± 0.058	4.50 ± 0.47	0.03786 ± 0.00059	0.606 ± 0.066	0.629 ± 0.003	9.02 ± 0.12	12.84 ± 0.47
T08	66.32 ± 0.54	1.288 ± 0.039	4.26 ± 0.49	0.0258 ± 0.0010	0.654 ± 0.019	1.106 ± 0.009	4.85 ± 0.21	3.50 ± 0.49
T09	60.96 ± 0.92	0.221 ± 0.024	6.37 ± 0.11	0.00230 ± 0.00073	0.166 ± 0.057	0.602 ± 0.018	2.64 ± 0.19	4.42 ± 0.11
T10	60.76 ± 0.56	0.3905 ± 0.0024	5.713 ± 0.072	0.0419 ± 0.0062	0.19 ± 0.082	0.365 ± 0.012	4.253 ± 0.087	5.181 ± 0.072
T11	57.95 ± 0.24	0.2281 ± 0.0042	5.042 ± 0.099	0.00510 ± 0.00066	0.321 ± 0.167	0.385 ± 0.004	5.94 ± 0.11	10.040 ± 0.099
T12	58.7 ± 1.1	0.594 ± 0.029	3.92 ± 0.26	0.0119 ± 0.0013	0.097 ± 0.021	0.457 ± 0.018	2.80 ± 0.14	8.61 ± 0.26
T13	63.5 ± 1.2	3.05 ± 0.30	3.49 ± 0.69	0.0440 ± 0.0029	0.207 ± 0.048	1.228 ± 0.064	3.97 ± 0.30	8.11 ± 0.69
T14	42.47 ± 0.61	1.613 ± 0.027	2.48 ± 0.16	0.0391 ± 0.0015	0.184 ± 0.044	0.637 ± 0.009	6.78 ± 0.36	4.05 ± 0.16
T15	98.7 ± 1.4	5.541 ± 0.047	5.0959 ± 0.0089	0.438 ± 0.013	0.205 ± 0.01	5.206 ± 0.136	0.225 ± 0.025	0.0502 ± 0.0010
T16	54.22 ± 0.65	0.937 ± 0.017	4.291 ± 0.045	0.0204 ± 0.0015	0.211 ± 0.013	0.61 ± 0.11	12.27 ± 0.31	5.966 ± 0.045
T17	64.35 ± 0.76	0.818 ± 0.029	5.47 ± 0.33	0.0383 ± 0.0022	0.18 ± 0.068	0.983 ± 0.025	2.276 ± 0.088	13.07 ± 0.33
T18	76.44 ± 2.25	1.469 ± 0.076	3.3 ± 1.2	0.0569 ± 0.0022	0.104 ± 0.069	0.597 ± 0.013	3.55 ± 0.11	11.0 ± 1.2
T19	66.2 ± 1.4	1.38 ± 0.37	6.625 ± 0.091	0.0948 ± 0.0047	0.189 ± 0.114	2.30 ± 0.10	2.20 ± 0.10	2.828 ± 0.092
T20	63.45 ± 0.47	0.5472 ± 0.0054	5.21 ± 0.32	0.01642 ± 0.00065	0.452 ± 0.101	0.617 ± 0.016	6.22 ± 0.14	11.76 ± 0.32
T21	64.96 ± 0.85	0.946 ± 0.028	4.89 ± 0.18	0.0399 ± 0.0062	0.232 ± 0.092	0.49 ± 0.14	6.84 ± 0.13	8.38 ± 0.18
T22	61.1 ± 1.4	0.490 ± 0.022	4.56 ± 0.18	0.01320 ± 0.00084	0.723 ± 0.023	0.0069 ± 0.0021	3.68 ± 0.16	6.98 ± 0.18
T23	1.363 ± 0.016	0.00139 ± 0.0045	0.0610 ± 0.0013	ND	ND	ND	ND	0.01568 ± 0.00096
T24	33.5 ± 1.5	3.55 ± 0.27	1.372 ± 0.16	0.0132 ± 0.0014	0.089 ± 0.02	0.1949 ± 0.0062	5.89 ± 0.55	1.39 ± 0.16
T25	68.36 ± 0.56	2.21 ± 0.49	5.8538 ± 0.0083	0.2518 ± 0.0040	0.904 ± 0.129	2.647 ± 0.041	9.87 ± 0.25	0.7459 ± 0.0082
T26	60.83 ± 0.62	2.609 ± 0.047	3.997 ± 0.010	0.0203 ± 0.0011	0.896 ± 0.056	0.5190 ± 0.0054	4.140 ± 0.084	0.242 ± 0.013
T27	107.8 ± 1.4	2.8064 ± 0.0023	5.1826 ± 0.0023	0.2929 ± 0.0014	0.473 ± 0.042	2.88 ± 0.57	0.440 ± 0.015	0.1453 ± 0.0019
T28	55 ± 24	3.83 ± 0.33	3.49 ± 0.33	2.21 ± 0.49	0.211 ± 0.013	1.79 ± 0.33	1.834 ± 0.034	1.357 ± 0.079
T29	49.47 ± 0.40	3.1 ± 1.1	4.8 ± 1.2	0.192 ± 0.065	0.049 ± 1.158	0.602 ± 0.018	2.8 ± 1.2	1.198 ± 0.043
T30	49.2 ± 1.2	1.086 ± 0.043	3.989 ± 0.090	0.0220 ± 0.0019	0.089 ± 0.09	0.365 ± 0.012	0.201 ± 0.090	6.3 ± 1.8
T31	49.2 ± 1.5	1.02 ± 0.32	4.03 ± 0.32	0.0142 ± 0.0033	0.084 ± 0.315	0.6368 ± 0.0091	0.73 ± 0.32	8.0 ± 1.3
T32	49.4 ± 6.9	0.59 ± 0.33	4.1 ± 0.33	0.0085 ± 0.0039	0.05 ± 0.325	0.983 ± 0.025	1.91 ± 0.33	1.091 ± 0.040
T33	61.4 ± 2.5	0.7 ± 1.2	5.3 ± 1.2	0.0155 ± 0.0039	0.029 ± 1.158	0.6371 ± 0.0091	0.40 ± 0.21	1.02 ± 0.18
T34	60.6 ± 5.2	0.964 ± 0.052	4.403 ± 0.092	0.019 ± 0.012	0.063 ± 0.09	1.025 ± 0.063	0.792 ± 0.090	0.14 ± 0.12
T35	75.1 ± 2.3	2.12 ± 0.32	2.5 ± 0.32	0.079 ± 0.027	0.044 ± 0.003	1.55 ± 0.32	0.41 ± 0.12	2.26 ± 0.26
T36	74.5 ± 4.3	5.8 ± 4.5	3.36 ± 0.50	0.165 ± 0.017	0.087 ± 0.036	2.95 ± 0.16	1.49 ± 0.34	1.35 ± 0.50
T37	53.1 ± 8.5	12.7 ± 4.4	3.49 ± 0.69	0.152 ± 0.053	0.093 ± 0.019	2.61 ± 0.56	2.84 ± 0.75	3.13 ± 0.69
T38	34.0 ± 2.4	1.220 ± 0.018	2.63 ± 0.12	0.01452 ± 0.00089	0.099 ± 0.005	1.105 ± 0.051	5.02 ± 0.18	5.03 ± 0.12

Table S3. Quantified constituents from NIST green tea leaf reference material (no. 3254)[a]

standard	methanol extract (mg/g dry tea)	NIST CoA[b] (mg/g dry tea)
(-)-epicatechin	6.25 ± 0.05	9.0 ± 1.6
(-)-epicatechin gallate	12.36 ± 0.13	12.7 ± 1.2
(-)-epigallocatechin	18.43 ± 0.82	25.2 ± 4.5
(-)-epigallocatechin gallate	24.69 ± 0.29	52.0 ± 2.2
(-)-gallocatechin	3.40 ± 0.12	2.4 ± 1.1
gallic acid	1.06 ± 0.02	1.12 ± 0.61

[a] values are calculated as average of triplicate runs ± standard deviation (SD)
[b] values obtained from the provided NIST Certificate of Analysis[38]

Table S4. Correlation matrix for green tea samples. Correlation was based upon the averaged metabolomic profile for each sample, and calculated from the reproduced correlation coefficient matrix comprised of a four principal component model.

	T01	T02	T03	T04	T05	T06	T07	T08	T09	T10	T11	T12	T13	T14	T15	T16	T17	T18	T19	T20	T21	T22	T23	T24	T25	T26	T27	T28	T29	T30	T31	T32	T33	T34	T35	T36	T37	T38
T01	1.000	0.465	-0.196	0.062	-0.236	0.086	0.513	0.891	0.987	0.944	0.991	0.934	0.615	0.244	-0.772	0.841	0.762	0.438	-0.642	0.978	0.591	0.723	-0.374	-0.283	-0.649	0.676	-0.860	-0.767	-0.450	0.533	0.609	0.793	0.581	0.683	-0.936	-0.608	-0.662	0.147
T02	0.465	1.000	0.595	0.739	0.569	0.901	0.919	0.815	0.372	0.707	0.583	0.730	0.948	0.896	-0.059	0.834	-0.208	0.571	-0.952	0.523	0.841	0.872	-0.007	0.461	-0.916	0.974	-0.426	-0.891	-1.000	-0.436	-0.355	-0.074	-0.440	-0.317	-0.736	-0.983	-0.954	0.544
T03	-0.196	0.595	1.000	0.966	0.999	0.608	0.725	0.192	-0.192	0.128	-0.090	-0.001	0.610	0.398	0.737	0.099	-0.567	0.714	-0.321	-0.016	0.675	0.527	-0.325	0.164	-0.223	0.585	0.451	-0.187	-0.615	-0.910	-0.877	-0.752	-0.817	-0.775	-0.023	-0.451	-0.333	-0.110
T04	0.062	0.739	0.966	1.000	0.955	0.657	0.875	0.435	0.060	0.380	0.170	0.250	0.787	0.487	0.543	0.331	-0.388	0.834	-0.508	0.238	0.842	0.728	-0.412	0.112	-0.411	0.774	0.225	-0.403	-0.755	-0.791	-0.736	-0.558	-0.687	-0.616	-0.275	-0.629	-0.524	-0.053
T05	-0.236	0.569	0.999	0.955	1.000	0.597	0.696	0.153	-0.231	0.088	-0.130	-0.041	0.578	0.382	0.763	0.061	-0.593	0.691	-0.290	-0.056	0.644	0.492	-0.308	0.172	-0.192	0.551	0.484	-0.152	-0.589	-0.924	-0.894	-0.778	-0.833	-0.795	0.017	-0.420	-0.301	-0.118
T06	0.086	0.901	0.608	0.657	0.597	1.000	0.709	0.511	-0.039	0.347	0.219	0.432	0.725	0.967	0.148	0.603	-0.580	0.269	-0.817	0.116	0.567	0.578	0.348	0.776	-0.798	0.590	-0.212	-0.700	-0.903	-0.632	-0.578	-0.343	-0.702	-0.608	-0.431	-0.837	-0.804	0.715
T07	0.513	0.919	0.725	0.875	0.696	0.709	1.000	0.816	0.480	0.767	0.613	0.687	0.986	0.652	0.070	0.737	-0.050	0.848	-0.817	0.635	0.983	0.963	-0.393	0.108	-0.747	0.977	-0.269	-0.775	-0.924	-0.452	-0.368	-0.110	-0.371	-0.255	-0.705	-0.892	-0.835	0.172
T08	0.891	0.815	0.192	0.435	0.153	0.511	0.816	1.000	0.839	0.982	0.945	0.980	0.893	0.607	-0.520	0.970	0.394	0.600	-0.901	0.911	0.830	0.927	-0.272	0.033	-0.884	0.899	-0.766	-0.951	-0.806	0.116	0.207	0.471	0.150	0.280	-0.985	-0.898	-0.915	0.352
T09	0.987	0.372	-0.192	0.060	-0.231	-0.039	0.480	0.839	1.000	0.919	0.963	0.873	0.566	0.103	-0.726	0.754	0.830	0.495	-0.535	0.983	0.584	0.698	-0.505	-0.434	-0.531	0.655	-0.780	-0.670	-0.359	0.557	0.629	0.786	0.634	0.726	-0.878	-0.513	-0.559	-0.015
T10	0.944	0.707	0.128	0.380	0.088	0.347	0.767	0.982	0.919	1.000	0.976	0.966	0.840	0.445	-0.556	0.918	0.543	0.644	-0.802	0.972	0.816	0.910	-0.416	-0.155	-0.781	0.879	-0.754	-0.878	-0.698	0.224	0.313	0.552	0.288	0.409	-0.974	-0.803	-0.823	0.192
T11	0.991	0.583	-0.090	0.170	-0.130	0.219	0.613	0.945	0.963	0.976	1.000	0.971	0.711	0.364	-0.720	0.903	0.667	0.488	-0.738	0.979	0.672	0.798	-0.342	-0.186	-0.739	0.755	-0.858	-0.844	-0.569	0.423	0.505	0.718	0.465	0.578	-0.974	-0.711	-0.756	0.222
T12	0.934	0.730	-0.001	0.250	-0.041	0.432	0.687	0.980	0.873	0.966	0.971	1.000	0.792	0.574	-0.676	0.979	0.484	0.446	-0.872	0.914	0.703	0.835	-0.171	0.046	-0.877	0.794	-0.878	-0.946	-0.716	0.284	0.370	0.618	0.292	0.417	-0.999	-0.841	-0.883	0.422
T13	0.615	0.948	0.610	0.787	0.578	0.725	0.986	0.893	0.566	0.840	0.711	0.792	1.000	0.710	-0.086	0.839	0.025	0.780	-0.894	0.708	0.965	0.981	-0.318	0.154	-0.838	0.983	-0.423	-0.868	-0.949	-0.336	-0.247	0.027	-0.277	-0.151	-0.805	-0.946	-0.909	0.283
T14	0.244	0.896	0.398	0.487	0.382	0.967	0.652	0.607	0.103	0.445	0.364	0.574	0.710	1.000	-0.103	0.729	-0.426	0.155	-0.892	0.229	0.513	0.577	0.438	0.797	-0.896	0.571	-0.439	-0.807	-0.891	-0.416	-0.357	-0.109	-0.514	-0.410	-0.566	-0.876	-0.875	0.843
T15	-0.772	-0.059	0.737	0.543	0.763	0.148	0.070	-0.520	-0.726	-0.556	-0.720	-0.676	-0.086	-0.103	1.000	-0.591	-0.737	0.231	0.358	-0.625	0.025	-0.174	-0.135	0.078	0.434	-0.104	0.928	0.504	0.035	-0.859	-0.892	-0.969	-0.793	-0.846	0.658	0.240	0.356	-0.377
T16	0.841	0.834	0.099	0.331	0.061	0.603	0.737	0.970	0.754	0.918	0.903	0.979	0.839	0.729	-0.591	1.000	0.297	0.411	-0.952	0.821	0.715	0.841	-0.033	0.238	-0.957	0.806	-0.843	-0.992	-0.821	0.133	0.220	0.489	0.115	0.246	-0.976	-0.921	-0.957	0.564
T17	0.762	-0.208	-0.567	-0.388	-0.593	-0.580	-0.050	0.394	0.830	0.543	0.667	0.484	0.025	-0.426	-0.737	0.297	1.000	0.170	0.006	0.721	0.105	0.209	-0.519	-0.728	-0.014	0.161	-0.573	-0.174	0.222	0.855	0.881	0.878	0.936	0.958	-0.485	0.049	-0.018	-0.334
T18	0.438	0.571	0.714	0.834	0.691	0.269	0.848	0.600	0.495	0.644	0.488	0.446	0.780	0.155	0.231	0.411	0.170	1.000	-0.421	0.615	0.916	0.834	-0.810	-0.393	-0.322	0.861	0.017	-0.413	-0.582	-0.361	-0.295	-0.138	-0.186	-0.111	-0.475	-0.536	-0.455	-0.375
T19	-0.642	-0.952	-0.321	-0.508	-0.290	-0.817	-0.817	-0.901	-0.535	-0.802	-0.738	-0.872	-0.894	-0.892	0.358	-0.952	0.006	-0.421	1.000	-0.644	-0.749	-0.841	-0.088	-0.455	0.994	-0.821	0.680	0.983	0.944	0.156	0.072	-0.213	0.191	0.061	0.871	0.989	0.999	-0.664
T20	0.978	0.523	-0.016	0.238	-0.056	0.116	0.635	0.911	0.983	0.972	0.979	0.914	0.708	0.229	-0.625	0.821	0.721	0.615	-0.644	1.000	0.722	0.818	-0.528	-0.359	-0.626	0.783	-0.745	-0.754	-0.512	0.396	0.477	0.670	0.480	0.586	-0.923	-0.641	-0.669	0.024
T21	0.591	0.841	0.675	0.842	0.644	0.567	0.983	0.830	0.584	0.816	0.672	0.703	0.965	0.513	0.025	0.715	0.105	0.916	-0.749	0.722	1.000	0.978	-0.547	-0.076	-0.673	0.990	-0.277	-0.733	-0.846	-0.348	-0.263	-0.022	-0.237	-0.124	-0.724	-0.829	-0.773	0.023
T22	0.723	0.872	0.527	0.728	0.492	0.578	0.963	0.927	0.698	0.910	0.798	0.835	0.981	0.577	-0.174	0.841	0.209	0.834	-0.841	0.818	0.978	1.000	-0.460	-0.029	-0.784	0.997	-0.470	-0.847	-0.871	-0.196	-0.105	0.155	-0.110	0.014	-0.850	-0.893	-0.862	0.154
T23	-0.374	-0.007	-0.325	-0.412	-0.308	0.348	-0.393	-0.272	-0.505	-0.416	-0.342	-0.171	-0.318	0.438	-0.135	-0.033	-0.519	-0.810	-0.088	-0.528	-0.547	-0.460	1.000	0.855	-0.173	-0.478	-0.146	-0.024	0.017	-0.034	-0.065	-0.075	-0.247	-0.263	0.200	0.012	-0.047	0.800
T24	-0.283	0.461	0.164	0.112	0.172	0.776	0.108	0.033	-0.434	-0.155	-0.186	0.046	0.154	0.797	0.078	0.238	-0.728	-0.393	-0.455	-0.359	-0.076	-0.029	0.855	1.000	-0.496	-0.029	-0.125	-0.336	-0.458	-0.433	-0.430	-0.321	-0.610	-0.577	-0.028	-0.408	-0.420	0.888
T25	-0.649	-0.916	-0.223	-0.411	-0.192	-0.798	-0.747	-0.884	-0.531	-0.781	-0.739	-0.877	-0.838	-0.896	0.434	-0.957	-0.014	-0.322	0.994	-0.626	-0.673	-0.784	-0.173	-0.496	1.000	-0.758	0.738	0.984	0.906	0.083	0.002	-0.276	0.138	0.010	0.872	0.966	0.989	-0.728
T26	0.676	0.974	0.585	0.774	0.551	0.590	0.977	0.899	0.655	0.879	0.755	0.794	0.983	0.571	-0.104	0.806	0.161	0.861	-0.821	0.783	0.990	0.997	-0.478	-0.029	-0.758	1.000	-0.407	-0.818	-0.875	-0.258	-0.168	0.089	-0.165	-0.044	-0.811	-0.883	-0.843	0.124
T27	-0.860	-0.426	0.451	0.225	0.484	-0.212	-0.269	-0.766	-0.780	-0.754	-0.858	-0.878	-0.423	-0.439	0.928	-0.843	-0.573	0.017	0.680	-0.745	-0.277	-0.470	-0.146	-0.125	0.738	-0.407	1.000	0.788	0.404	-0.611	-0.671	-0.845	-0.545	-0.638	0.863	0.583	0.678	-0.565
T28	-0.767	-0.891	-0.187	-0.403	-0.152	-0.700	-0.775	-0.951	-0.670	-0.878	-0.844	-0.946	-0.868	-0.807	0.504	-0.992	-0.174	-0.413	0.983	-0.754	-0.733	-0.847	-0.024	-0.336	0.984	-0.818	0.788	1.000	0.880	-0.017	-0.104	-0.382	0.010	-0.122	0.944	0.959	0.985	-0.617
T29	-0.450	-1.000	-0.615	-0.755	-0.589	-0.903	-0.924	-0.806	-0.359	-0.698	-0.569	-0.716	-0.949	-0.891	0.035	-0.821	0.222	-0.582	0.944	-0.512	-0.846	-0.871	0.017	-0.458	0.906	-0.875	0.404	0.880	1.000	0.456	0.376	0.096	0.458	0.335	0.723	0.978	0.946	-0.531
T30	0.533	-0.436	-0.910	-0.791	-0.924	-0.632	-0.452	0.116	0.557	0.224	0.423	0.284	-0.336	-0.416	-0.859	0.133	0.855	-0.361	0.156	0.396	-0.348	-0.196	-0.034	-0.433	0.083	-0.258	-0.611	-0.017	0.456	1.000	0.996	0.929	0.977	0.967	-0.269	0.262	0.152	-0.052
T31	0.609	-0.355	-0.877	-0.736	-0.894	-0.578	-0.368	0.207	0.629	0.313	0.505	0.370	-0.247	-0.357	-0.892	0.220	0.881	-0.295	0.072	0.477	-0.263	-0.105	-0.065	-0.430	0.002	-0.168	-0.671	-0.104	0.376	0.996	1.000	0.958	0.977	0.980	-0.356	0.176	0.067	-0.025
T32	0.793	-0.074	-0.752	-0.558	-0.778	-0.343	-0.110	0.471	0.786	0.552	0.718	0.618	0.027	-0.109	-0.969	0.489	0.878	-0.138	-0.213	0.670	-0.022	0.155	-0.075	-0.321	-0.276	0.089	-0.845	-0.382	0.096	0.929	0.958	1.000	0.909	0.949	-0.605	-0.112	-0.220	0.137
T33	0.581	-0.440	-0.817	-0.687	-0.833	-0.702	-0.371	0.150	0.634	0.288	0.465	0.292	-0.277	-0.514	-0.793	0.115	0.936	-0.186	0.191	0.480	-0.237	-0.110	-0.247	-0.610	0.138	-0.165	-0.545	0.010	0.458	0.977	0.977	0.909	1.000	0.991	-0.284	0.272	0.179	-0.234
T34	0.683	-0.317	-0.775	-0.616	-0.795	-0.608	-0.255	0.280	0.726	0.409	0.578	0.417	-0.151	-0.410	-0.846	0.246	0.958	-0.111	0.061	0.586	-0.124	0.014	-0.263	-0.577	0.010	-0.044	-0.638	-0.122	0.335	0.967	0.980	0.949	0.991	1.000	-0.409	0.142	0.047	-0.168
T35	-0.936	-0.736	-0.023	-0.275	0.017	-0.431	-0.705	-0.985	-0.878	-0.974	-0.974	-0.999	-0.805	-0.566	0.658	-0.976	-0.485	-0.475	0.871	-0.923	-0.724	-0.850	0.200	-0.028	0.872	-0.811	0.863	0.944	0.723	-0.269	-0.356	-0.605	-0.284	-0.409	1.000	0.844	0.883	-0.399
T36	-0.608	-0.983	-0.451	-0.629	-0.420	-0.837	-0.892	-0.898	-0.513	-0.803	-0.711	-0.841	-0.946	-0.876	0.240	-0.921	0.049	-0.536	0.989	-0.641	-0.829	-0.893	0.012	-0.408	0.966	-0.883	0.583	0.959	0.978	0.262	0.176	-0.112	0.272	0.142	0.844	1.000	0.992	-0.575
T37	-0.662	-0.954	-0.333	-0.524	-0.301	-0.804	-0.835	-0.915	-0.559	-0.823	-0.756	-0.883	-0.909	-0.875	0.356	-0.957	-0.018	-0.455	0.999	-0.669	-0.773	-0.862	-0.047	-0.420	0.989	-0.843	0.678	0.985	0.946	0.152	0.067	-0.220	0.179	0.047	0.883	0.992	1.000	-0.633
T38	0.147	0.544	-0.110	-0.053	-0.118	0.715	0.172	0.352	-0.015	0.192	0.222	0.422	0.283	0.843	-0.377	0.564	-0.334	-0.375	-0.664	0.024	0.023	0.154	0.800	0.888	-0.728	0.124	-0.565	-0.617	-0.531	-0.052	-0.025	0.137	-0.234	-0.168	-0.399	-0.575	-0.633	1.000

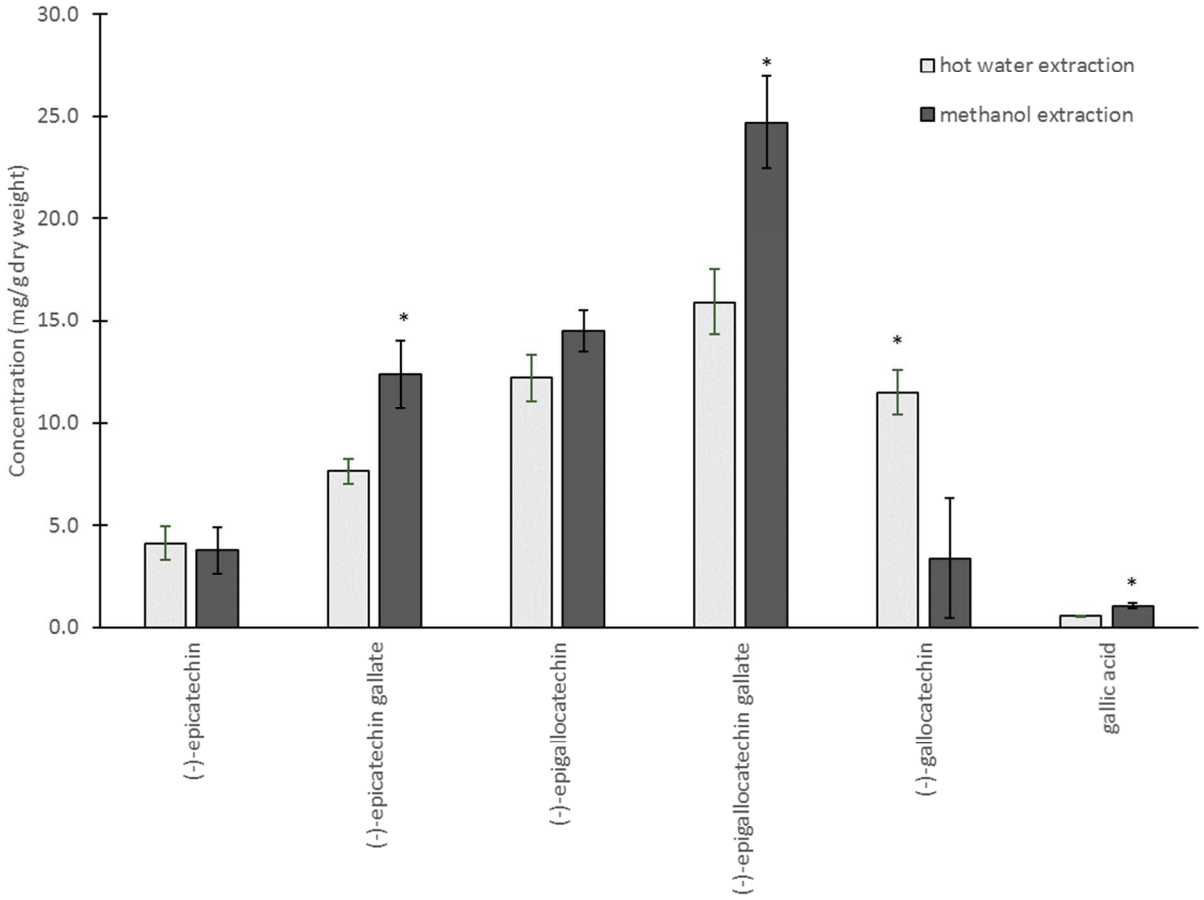


Figure S1. Comparison of quantities of selected green tea constituents extracted in hot water versus methanol. Triplicate extractions were conducted on a sample of green tea from the NIST (no. 3254). The mean concentration among triplicate extracts as determined by linear regression of the relevant calibration curve is reported. Error bars represent standard deviation(SD). * indicates significantly differing concentrations, as determined by the student's t-test, with $p < 0.05$.

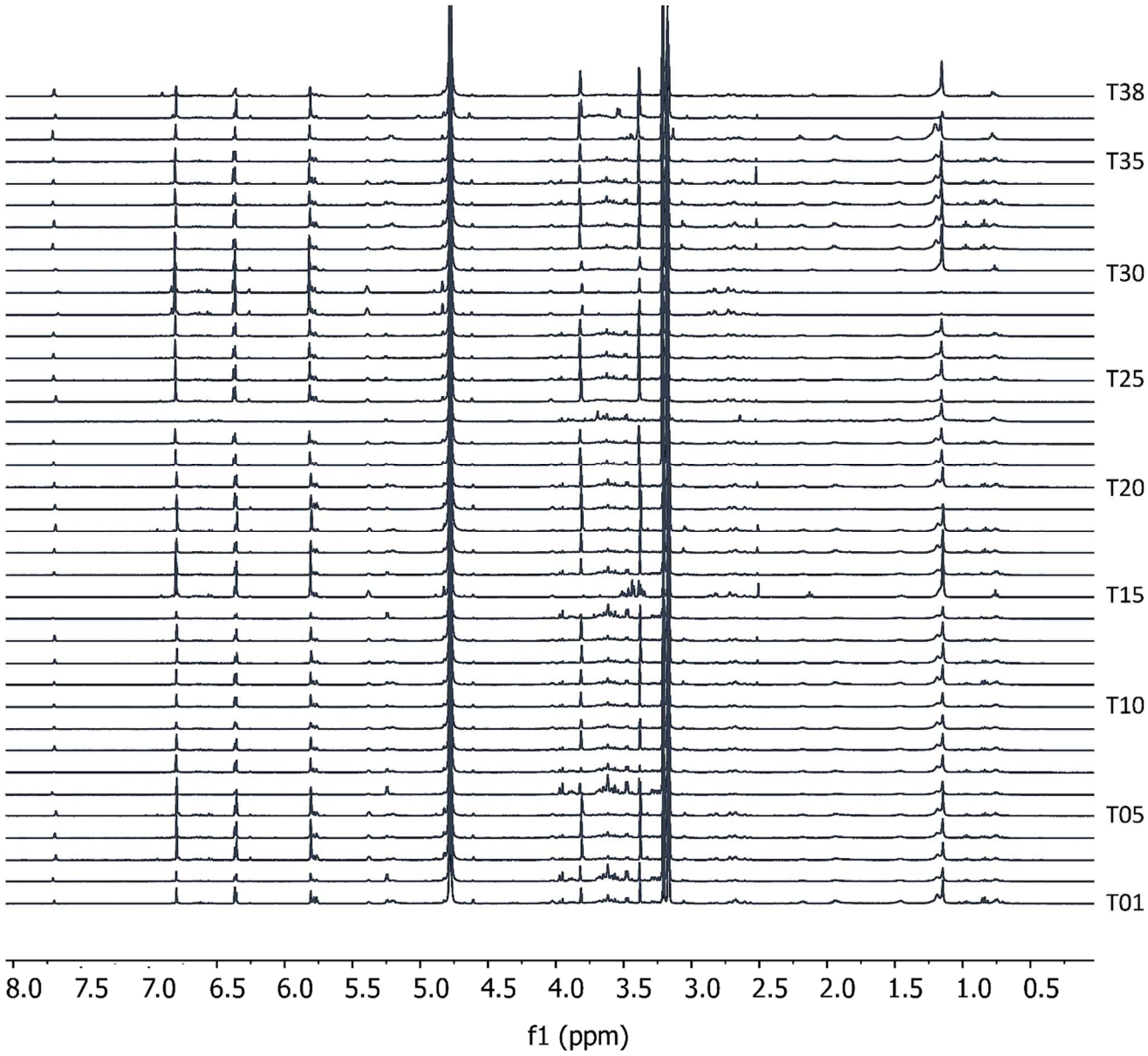


Figure S2. Untargeted ^{1}H-NMR spectra for all 38 tea samples. Spectra were acquired in CD_3OD at a concentration of 10 mg/mL.