SUPPORTING INFORMATION

Interlaboratory Comparison of Untargeted Mass Spectrometry Data Uncovers Underlying Causes for Variability

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CONTENTS

Note S1.

Gradient selection was designed to identify conditions that balanced separation of the standard compounds (Supplementary Table S2) against overall acquisition time. Three gradients were chosen for testing:

1) A gradient of (A) H2O + 0.1% FA to (B) ACN + 0.1% FA at a flow rate of 500 µL/min and 45°C for 7.6 min (5% ACN, 0-0.3 min; 5-90% ACN, 0.3-4.7 min; 90-98% ACN, 4.7-5.5 min; 98% ACN, 5.5-5.8 min; 5% ACN, 5.81-7.6 min).

2) A gradient of (A) H2O + 0.1% FA to (B) ACN + 0.1% FA at a flow rate of 500 µL/min and 45°C for 12.8 min (5% ACN, 0-0.3 min; 5-90% ACN, 0.3-9.1 min; 90-98% ACN, 9.1-10.7 min; 98% ACN, 10.7-11 min; 5% ACN, 11.01-12.8 min).

3) A gradient of (A) H2O + 0.1% FA to (B) ACN + 0.1% FA at a flow rate of 500 µL/min and 45°C for 17.8 min (5% ACN, 0-0.3 min; 5-90% ACN, 0.3-14 min; 90-98% ACN, 14-15.6 min; 98% ACN, 15.6-15.9 min; 5% ACN, 15.91-17.8 min).

Gradient 2 was the shortest gradient that achieved separation of the standards; gradient 2 was therefore selected for this study.

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

code	product form	selection criteria
GT 1	leaf tea	consumer sales[1]
GT 2	leaf tea	quality report[2]
GT 3	leaf tea	consumer sales[1]
GT 4	leaf tea	quality report[2]
GT 5	leaf tea	quality report[2]
GT 6	leaf tea	quality report[2]
GT 7	leaf tea	quality report[2]
GT 8	leaf tea	quality report[2]
GT 9	leaf tea	quality report[2]
GT 10	leaf tea	quality report[2]
GT 11	powdered tea	consumer sales[1]
GT 12	powdered tea	quality report[2]
GT 13	leaf tea	quality report[2]
GT 14	leaf tea	quality report[2]
GT 15	tea supplement	quality report[2]
GT 16	leaf tea	quality report[2]
GT 17	leaf tea	quality report[2]
GT 18	leaf tea	quality report[2]
GT 19	tea supplement	quality report[2]
GT 20	leaf tea	quality report[2]
GT 21	leaf tea	quality report[2]
GT 22	powdered tea	quality report[2]
GT 23	leaf tea	non-green tea
GT 24	leaf tea	consumer sales[1]
GT 25	tea supplement	extract report[3]
GT 26	leaf tea	NIST standard
GT 27	tea supplement	NIST standard
GT 28	tea supplement	extract report[3]
GT 29	tea supplement	extract report[3]
GT 30	powdered tea	consumer sales[1]
GT 31	powdered tea	consumer sales[1]
GT 32	powdered tea	consumer sales[1]
GT 33	leaf tea	quality report[2]
GT 34	leaf tea	quality report[2]
GT 35	tea supplement	extract report[3]
GT 36	tea supplement	extract report[3]
GT 37	tea supplement	NIST standard
GT 38	leaf tea	consumer sales[1]

Table S2. Green tea reference compounds used as quality control checks for green tea samples from Table S1

	reference compounds	formula	$[M+H]^+$	RT* in lab A	RT in lab B
1	caffeic acid	$C_9H_8O_4$	181.0501	2.30	2.48
2	caffeine	$C_8H_{10}N_4O_2$	195.0883	2.18	2.32
3	chlorogenic acid	$C_{16}H_{18}O_9$	355.1029	1.99	2.17
4	coumaric acid	$C_9H_8O_3$	165.0552	2.80	2.96
5	(-)-epicatechin	$C_{15}H_{14}O_6$	291.0869	2.37	2.52
6	(-)-epicatechin gallate	$C_{22}H_{18}O_{10}$	443.0978	2.90	3.03
7	(-)-epigallocatechin	$C_{15}H_{14}O_7$	307.0818	1.90	2.05
8	gallic acid	$C_7H_6O_5$	171.0294	1.10	1.27
9	(-)-gallocatechin	$C_{15}H_{14}O_7$	307.0818	1.54	1.70
10	(-)-gallocatechin gallate	$C_{22}H_{18}O_{11}$	459.0927	2.51	2.62
11	kaempferol	$C_{15}H_{10}O_6$	287.0556	4.58	4.73
12	myricetin	$C_{15}H_{10}O_8$	319.0454	3.45	3.59
13	quercetin	$C_{15}H_{10}O_7$	303.0505	4.03	4.20
14	rutin	$C_{27}H_{30}O_{16}$	611.1612	2.80	2.94
15	theanine	$C_7H_{14}N_2O_3$	175.1083	0.52	0.59

*RT = retention time (min)

Table S3. Presence of reference compounds detected in Green tea samples

		Standards															
		caffeic acid	caffeine	chlorogenic acid	coumaric acid	epicatechin	catechin	epicatechin gallate	epigallocatechin	gallic acid	gallocatechin	gallocatechin gallate	kaempferol	myricetin	quercetin	rutin	theanine
Lab A	GT 1 R1	+	+	-	-	+	-	+	+	-	+	+	+	-	-	+	+
	GT 1 R2	+	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 1 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 2 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 2 R2	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 2 R3	+	-	-	-	-	+	+	+	-	+	+	+	+	+	+	+
	GT 3 R1	+	+	+	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 3 R2	+	+	+	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 3 R3	-	-	+	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 4 R1	+	+	-	-	+	-	+	+	-	+	+	+	+	+	+	+
	GT 4 R2	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 4 R3	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 5 R1	+	+	+	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 5 R2	+	+	-	-	+	+	+	+	-	+	+	-	+	+	+	+
	GT 5 R3	+	+	+	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 6 R1	+	-	-	-	-	+	+	+	+	+	+	+	+	+	+	+
	GT 6 R2	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 6 R3	-	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 7 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 7 R2	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 7 R3	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 8 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 8 R2	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 8 R3	+	+	-	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 9 R1	-	-	-	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 9 R2	-	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 9 R3	-	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 10 R1	+	-	-	-	+	+	+	+	+	+	+	+	-	-	+	+
	GT 10 R2	+	+	-	-	+	-	+	+	+	+	+	+	-	-	+	+
	GT 10 R3	+	+	-	-	+	+	+	+	+	+	+	+	-	-	+	+
	GT 11 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 11 R2	+	-	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 11 R3	+	-	-	-	+	+	+	+	-	+	+	-	-	-	+	+
	GT 12 R1	+	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 12 R2	+	-	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 12 R3	-	+	-	-	+	-	+	+	-	+	+	+	+	-	+	+
	GT 13 R1	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 13 R2	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 13 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 14 R1	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 14 R2	+	+	-	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 14 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 15 R1	+	+	-	-	-	+	+	+	+	+	+	+	+	+	-	-
	GT 15 R2	+	+	-	-	+	+	+	+	+	+	+	+	+	+	-	-
	GT 15 R3	+	-	-	-	+	+	+	+	+	+	+	+	+	+	-	-
	GT 16 R1	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 16 R2	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 16 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 17 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 17 R2	+	-	-	-	-	+	+	+	-	+	+	+	+	+	-	+
	GT 17 R3	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 18 R1	-	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 18 R2	+	-	-	-	+	+	+	+	-	-	+	+	+	+	+	+
	GT 18 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	+	-	+
	GT 19 R1	-	-	-	-	-	-	+	+	-	+	+	-	-	-	-	-
	GT 19 R2	-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 19 R3	-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 20 R1	+	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 20 R2	+	+	-	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 20 R3	-	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 21 R1	+	+	-	-	+	+	+	+	-	+	+	+	-	+	-	+
	GT 21 R2	-	-	-	-	+	+	+	+	-	+	+	+	+	+	-	+
	GT 21 R3	+	+	-	-	+	-	+	+	-	+	+	+	+	+	-	+
	GT 22 R1	+	+	-	-	+	+	+	+	-	+	+	+	-	-	-	+
	GT 22 R2	+	+	-	-	+	+	+	+	-	+	+	-	+	-	+	+
	GT 22 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 23 R1	-	+	-	-	-	-	-	-	-	-	-	-	-	-	+	-
	GT 23 R2	-	+	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	GT 23 R3	-	+	-	-	-	-	-	-	-	-	-	-	-	-	+	-
	GT 24 R1	+	-	-	-	+	+	+	+	-	+	+	-	-	-	+	-
	GT 24 R2	+	-	-	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 24 R3	+	-	-	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 25 R1	+	-	-	-	-	+	+	+	+	+	+	+	+	+	+	+

	GT 25 R2	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 25 R3	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 26 R1	+	-	-	-	+	-	+	+	-	+	+	+	+	+	-	+
	GT 26 R2	+	+	-	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 26 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	+	-	+
	GT 27 R1	+	+	-	-	+	+	+	+	+	+	-	+	+	+	-	+
	GT 27 R2	-	-	-	+	+	+	+	+	+	+	-	+	+	+	-	-
	GT 27 R3	+	+	-	+	+	+	+	+	+	+	-	+	+	+	-	+
	GT 28 R1	+	+	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 28 R2	+	-	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 28 R3	+	+	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 29 R1	-	-	+	-	+	+	+	+	+	+	+	+	+	+	+	-
	GT 29 R2	-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	-
	GT 29 R3	-	-	+	-	-	+	+	+	+	+	+	+	+	+	+	-
	GT 30 R1	+	+	-	-	-	-	+	+	+	+	+	+	-	-	-	+
	GT 30 R2	+	+	-	-	-	-	+	+	+	+	+	+	-	-	+	+
	GT 30 R3	+	+	-	-	-	-	+	+	+	+	+	+	-	-	+	+
	GT 31 R1	+	+	-	-	-	-	+	+	-	+	+	-	-	-	-	+
	GT 31 R2	-	+	-	-	+	+	+	+	-	+	+	+	-	-	-	+
	GT 31 R3	+	+	-	-	+	+	+	+	-	+	+	+	-	-	-	+
	GT 32 R1	+	+	-	-	+	+	+	+	-	+	+	-	+	-	-	+
	GT 32 R2	+	-	-	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 32 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	-	-	+
	GT 33 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	-	+	+
	GT 33 R2	+	-	-	-	-	+	+	+	-	+	+	+	+	+	+	+
	GT 33 R3	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 34 R1	+	+	-	-	+	+	+	+	-	+	+	+	-	-	+	+
	GT 34 R2	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 34 R3	+	+	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 35 R1	+	+	+	-	+	+	+	+	-	+	+	+	+	+	-	-
	GT 35 R2	+	+	+	-	+	+	+	+	+	+	+	+	+	+	-	-
	GT 35 R3	+	+	+	-	+	+	+	+	+	+	+	+	+	+	-	-
	GT 36 R1	+	-	-	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 36 R2	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	-
	GT 36 R3	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+
	GT 37 R1	+	+	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 37 R2	+	-	-	-	-	+	+	+	+	+	+	+	+	+	-	+
	GT 37 R3	+	+	-	-	+	+	+	+	+	+	+	+	+	+	-	+
	GT 38 R1	-	-	+	-	+	+	+	+	-	+	+	+	+	+	+	+
	GT 38 R2	+	-	+	-	+	-	+	+	-	+	+	+	+	+	+	+
	GT 38 R3	+	-	+	-	+	+	+	+	-	+	+	+	+	+	+	+
Lab B	GT 1 R1	+	+	+	-	+	+	-	+	-	-	+	+	+	+	+	+
	GT 1 R2	+	+	+	-	+	+	-	+	-	-	+	-	+	+	+	+
	GT 1 R3	+	+	+	-	+	+	-	+	-	-	+	+	+	+	+	+
	GT 2 R1	+	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
	GT 2 R2	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
	GT 2 R3	-	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
	GT 3 R1	+	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 3 R2	+	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
	GT 3 R3	+	+	+	-	+	+	-	+	-	+	+	-	-	+	+	+
	GT 4 R1	-	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 4 R2	-	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 4 R3	-	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 5 R1	+	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 5 R2	+	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 5 R3	+	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 6 R1	-	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 6 R2	-	+	+	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 6 R3	-	+	+	-	+	+	+	+	-	+	+	-	-	+	+	+
	GT 7 R1	+	+	+	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 7 R2	+	+	+	-	+	+	+	+	-	+	+	+	-	+	+	+
	GT 7 R3	+	+	+	-	+	+	+	+	-	+	+	-	-	+	+	+
	GT 8 R1	+	+	+	-	+	+	+	+	-	+	+	-	+	+	+	+
	GT 8 R2	+	+	+	-	+	+	+	+	-	+	+	-	+	+	+	+
	GT 8 R3	+	+	+	-	+	+	+	+	-	+	+	-	-	+	+	+
	GT 9 R1	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 9 R2	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 9 R3	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 10 R1	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 10 R2	+	+	+	-	-	+	+	+	-	-	+	-	-	-	+	+
	GT 10 R3	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 11 R1	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 11 R2	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 11 R3	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
	GT 12 R1	+	+	+	-	+	+	+	+	-	-	+	-	-	+	+	+
	GT 12 R2	+	+	+	-	+	+	+	+	-	-	+	+	-	+	+	+
	GT 12 R3	-	+	+	-	+	+	+	+	-	-	+	+	-	+	+	+
	GT 13 R1	-	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 13 R2	-	+	+	-	+	+	-	+	-	-	+	+	-	+	+	+
	GT 13 R3	-	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
	GT 14 R1	-	+	+	-	+	+	-	+	-	-	+	+	-	+	+	+

GT 14 R2	-	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 14 R3	-	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 15 R1	-	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 15 R2	-	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 15 R3	-	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 16 R1	-	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 16 R2	-	-	+	-	+	+	-	-	-	-	+	+	-	+	+	+
GT 16 R3	-	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 17 R1	+	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 17 R2	+	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 17 R3	-	-	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 18 R1	-	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 18 R2	-	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 18 R3	-	-	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 19 R1	+	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 19 R2	+	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 19 R3	+	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 20 R1	+	+	+	+	+	+	+	+	-	-	+	-	+	+	+	+
GT 20 R2	+	+	+	+	+	+	+	+	-	-	+	-	+	+	+	+
GT 20 R3	+	+	+	+	+	+	+	+	-	-	+	-	+	+	+	+
GT 21 R1	+	+	+	+	+	+	+	+	-	-	+	-	-	+	+	+
GT 21 R2	+	+	+	+	+	+	+	+	-	-	+	-	-	+	+	+
GT 21 R3	+	+	+	+	+	+	+	+	-	-	+	-	-	+	+	+
GT 22 R1	+	+	+	-	+	+	+	+	-	+	+	-	-	+	+	+
GT 22 R2	+	+	+	-	+	+	+	+	-	+	+	-	-	+	+	+
GT 22 R3	+	+	+	-	+	+	+	+	-	+	+	-	-	+	+	+
GT 23 R1	-	+	-	-	-	-	-	-	-	-	-	-	-	-	-	+
GT 23 R2	-	+	-	-	-	-	-	-	-	-	-	-	-	-	-	+
GT 23 R3	-	+	-	-	-	-	-	-	-	-	-	-	-	-	-	+
GT 24 R1	-	+	+	-	-	+	-	+	-	+	+	-	-	-	+	+
GT 24 R2	-	+	+	-	+	+	-	+	-	+	+	-	-	+	+	+
GT 24 R3	-	+	+	-	+	+	-	+	-	+	+	-	-	+	+	+
GT 25 R1	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 25 R2	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 25 R3	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 26 R1	-	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 26 R2	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 26 R3	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 27 R1	+	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 27 R2	+	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 27 R3	-	-	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 28 R1	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 28 R2	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 28 R3	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 29 R1	+	+	+	-	+	+	+	+	-	+	+	+	+	+	+	+
GT 29 R2	+	+	+	-	+	+	+	+	-	+	+	+	+	+	+	+
GT 29 R3	+	+	+	-	+	+	+	+	-	+	+	+	+	+	+	+
GT 30 R1	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
GT 30 R2	+	+	+	+	+	+	+	+	-	-	+	-	-	-	+	+
GT 30 R3	+	+	+	+	+	+	+	+	-	-	+	-	-	-	+	+
GT 31 R1	+	+	+	+	+	+	+	+	-	-	+	-	-	-	+	+
GT 31 R2	+	+	+	+	+	+	+	+	-	-	+	-	-	-	+	+
GT 31 R3	+	+	+	-	+	+	+	+	-	-	+	-	-	-	+	+
GT 32 R1	+	+	+	-	-	+	+	+	-	-	+	-	-	-	+	+
GT 32 R2	-	+	+	-	-	+	+	+	-	-	+	-	-	-	+	+
GT 32 R3	+	+	+	-	-	+	-	+	-	-	+	-	-	-	+	+
GT 33 R1	+	+	+	-	+	+	-	+	-	-	+	+	-	+	+	+
GT 33 R2	+	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 33 R3	+	+	+	-	+	+	-	+	-	+	+	+	-	+	+	+
GT 34 R1	+	+	+	-	+	+	-	+	-	+	+	-	-	+	+	+
GT 34 R2	+	+	+	-	+	+	-	+	-	-	+	-	-	+	+	+
GT 34 R3	+	+	+	-	+	+	-	+	-	+	+	-	-	+	+	+
GT 35 R1	-	+	+	-	-	+	-	+	-	+	+	+	-	+	+	+
GT 35 R2	-	+	+	-	-	+	-	+	-	+	+	+	-	+	+	+
GT 35 R3	-	+	+	-	-	+	-	+	-	+	+	+	-	+	+	+
GT 36 R1	-	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 36 R2	-	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 36 R3	-	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 37 R1	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 37 R2	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 37 R3	+	+	+	-	+	+	-	+	-	+	+	+	+	+	+	+
GT 38 R1	-	-	+	-	-	+	-	+	-	+	+	-	-	+	+	+
GT 38 R2	-	-	+	-	-	+	-	+	-	+	+	-	-	+	+	+
GT 38 R3	-	-	+	-	-	+	-	+	-	+	+	-	-	+	+	+

Figure S1. Butterfly plots for MS^2 spectra from reference compounds

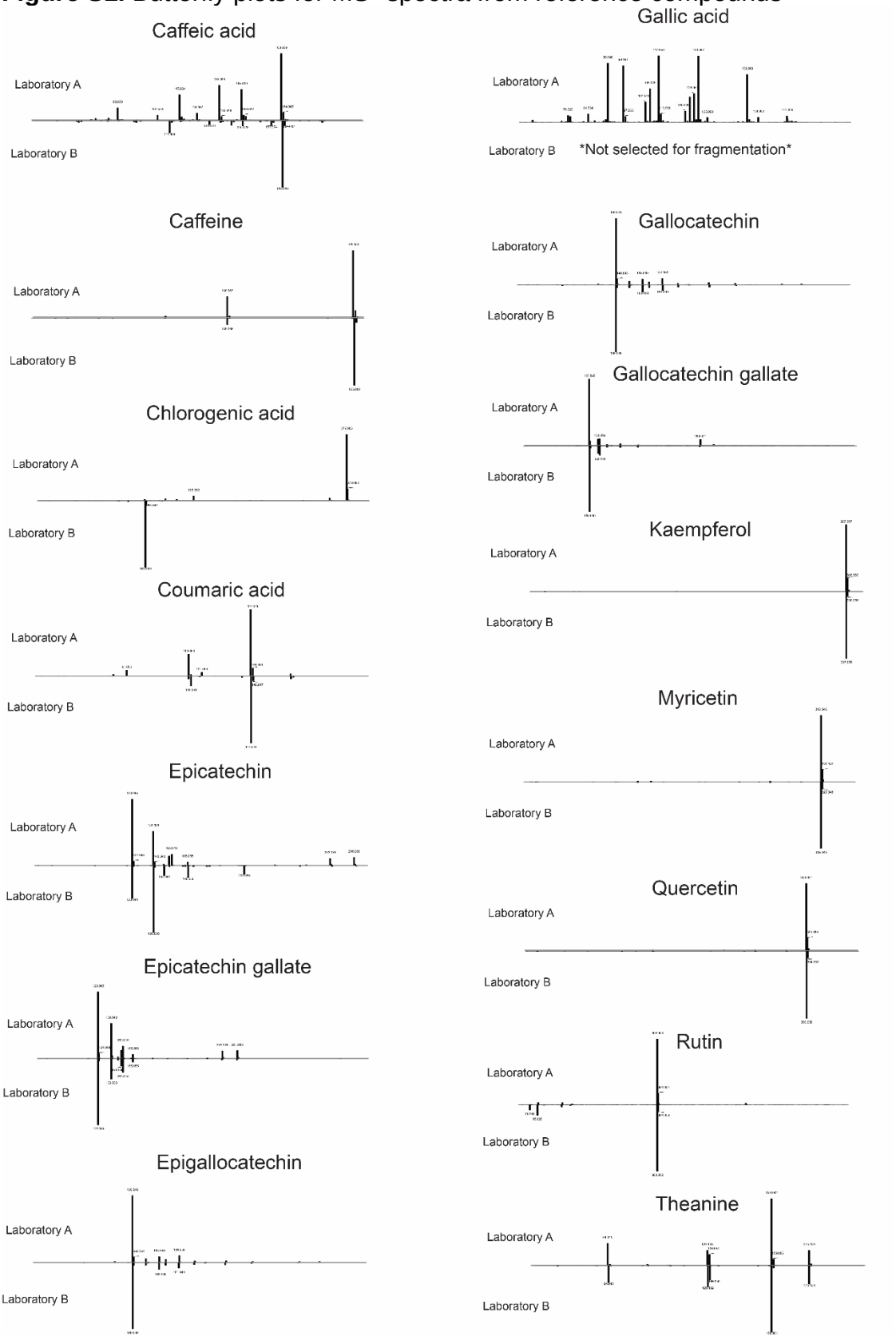


***Table S4a**:* Detailed annotations of the reference compounds and associated features for Laboratory A used for Figure 5

m/z	retention time (min)	annotation
181.0503	2.32	Caffeic acid: $[M+H]^+$
233.9608	2.30	Caffeic acid: unknown feature
251.9715	2.30	Caffeic acid: unknown feature
275.9945	2.32	Caffeic acid: unknown feature
331.9382	2.32	Caffeic acid: unknown feature
415.0102	2.32	Caffeic acid: unknown feature
194.0804	2.16	Caffeine: $[M\cdot]^+$
195.0887	2.12	Caffeine: $[M+H]^+$
195.2075	2.16	Caffeine: unknown feature
197.0928	2.16	Caffeine: unknown feature
214.0613	2.16	Caffeine: unknown feature
214.5629	2.16	Caffeine: unknown feature
223.0668	2.16	Caffeine: unknown feature
234.5747	2.16	Caffeine: unknown feature
255.0665	2.16	Caffeine: unknown feature
267.0178	2.16	Caffeine: unknown feature
295.013	2.16	Caffeine: unknown feature
311.1016	2.17	Caffeine: unknown feature
311.6031	2.16	Caffeine: unknown feature
312.0145	2.16	Caffeine: unknown feature
331.0123	2.17	Caffeine: unknown feature
346.9845	2.17	Caffeine: unknown feature
506.0959	2.16	Caffeine: unknown feature
706.0835	2.16	Caffeine: unknown feature
163.0397	1.99	Chlorogenic acid: $[M+H-C_7H_{12}O_6]^+$
354.0932	1.98	Chlorogenic acid: $[M\cdot]^+$
355.1029	1.99	Chlorogenic acid: $[M+H]^+$
337.0923	1.99	Chlorogenic acid: $[M+H-H_2O]^+$
361.1105	1.99	Chlorogenic acid: $[M+Li]^+$
377.0845	1.99	Chlorogenic acid: $[M+Na]^+$
197.0286	1.99	Chlorogenic acid: unknown feature
217.5419	1.99	Chlorogenic acid: unknown feature
228.9808	1.99	Chlorogenic acid: unknown feature
257.9851	1.99	Chlorogenic acid: unknown feature
270.0055	1.99	Chlorogenic acid: unknown feature
374.0756	1.99	Chlorogenic acid: unknown feature
393.0557	1.99	Chlorogenic acid: unknown feature
408.0139	1.99	Chlorogenic acid: unknown feature
409.0191	1.82	Chlorogenic acid: unknown feature
439.0534	1.99	Chlorogenic acid: unknown feature
449.0404	1.99	Chlorogenic acid: unknown feature

454.0193	1.99	Chlorogenic acid: unknown feature
165.0554	2.79	Coumaric acid & rutin: $[M+H]^+$
611.1606	2.79	Coumaric acid & rutin: $[M+H]^+$
303.0503	2.77	Coumaric acid & rutin: $[M+H-(C_{12}H_{22}O_{10}-H_2O)]^+$
285.0391	2.79	Coumaric acid & rutin: $[M+H-(C_{12}H_{22}O_{10}-H_2O)-H_2O]^+$
325.0577	2.79	Coumaric acid & rutin: $[M+H-(C_{12}H_{22}O_{10}-H_2O)-H_2O+ACN]^+$
257.0443	2.79	Coumaric acid & rutin: $[M+H-(C_{12}H_{22}O_{10}-H_2O)-H_2O-CO]^+$
465.1028	2.79	Coumaric acid & rutin: $[M+H-(C_6H_{12}O_5-H_2O)]^+$
449.1076	2.79	Coumaric acid & rutin: $[M+H-(C_6H_{12}O_6-H_2O)]^+$
617.1688	2.79	Coumaric acid & rutin: $[M+Li]^+$
633.1419	2.79	Coumaric acid & rutin: $[M+Na]^+$
325.5595	2.79	Coumaric acid & rutin: unknown feature
382.0142	2.79	Coumaric acid & rutin: unknown feature
397.9959	2.79	Coumaric acid & rutin: unknown feature
407.0808	2.79	Coumaric acid & rutin: unknown feature
518.0143	2.79	Coumaric acid & rutin: unknown feature
546.6025	2.79	Coumaric acid & rutin: unknown feature
631.1339	2.79	Coumaric acid & rutin: unknown feature
635.1448	2.79	Coumaric acid & rutin: unknown feature
665.0782	2.79	Coumaric acid & rutin: unknown feature
291.0865	2.37	Epicatechin: $[M+H]^+$
165.0554	2.37	Epicatechin: $[M+H-C_6H_6O_3]^+$
313.0683	2.37	Epicatechin: $[M+Na]^+$
169.0504	2.37	Epicatechin: unknown feature
174.0266	2.37	Epicatechin: unknown feature
248.0007	2.37	Epicatechin: unknown feature
249.0763	2.37	Epicatechin: unknown feature
343.9981	2.37	Epicatechin: unknown feature
345.005	2.37	Epicatechin: unknown feature
385.0248	2.37	Epicatechin: unknown feature
393.2086	2.34	Epicatechin: unknown feature
399.0382	2.32	Epicatechin: unknown feature
443.0978	2.91	Epicatechin gallate: [M+H]+
291.0867	2.90	Epicatechin gallate: $[M+H-(C_7H_6O_5-H_2O)]^+$
273.0758	2.91	Epicatechin gallate : $[M+H-(C_7H_6O_5-H_2O)-H_2O]^+$
250.0024	2.90	Epicatechin gallate: unknown feature
272.0678	2.90	Epicatechin gallate: unknown feature
345.0056	2.91	Epicatechin gallate: unknown feature
496.0085	2.89	Epicatechin gallate: unknown feature
537.0357	2.89	Epicatechin gallate: unknown feature
579.0211	2.90	Epicatechin gallate: unknown feature
938.0975	2.91	Epicatechin gallate: unknown feature
307.0816	1.92	Epigallocatechin: $[M+H]^+$
181.0502	1.92	Epigallocatechin: $[M+H-C_6H_6O_3]^+$

173.0186	1.92	Epigallocatechin: unknown feature
206.9966	1.92	Epigallocatechin: unknown feature
349.0499	1.92	Epigallocatechin: unknown feature
401.0193	1.92	Epigallocatechin: unknown feature
171.0294	1.09	Gallic acid: $[M+H]^+$
250.0027	1.09	Gallic acid: unknown feature
262.9723	1.08	Gallic acid: unknown feature
264.9673	1.09	Gallic acid: unknown feature
265.973	1.09	Gallic acid: unknown feature
266.9751	1.09	Gallic acid: unknown feature
301.9548	1.09	Gallic acid: unknown feature
321.9175	1.09	Gallic acid: unknown feature
322.9235	1.09	Gallic acid: unknown feature
394.9682	1.09	Gallic acid: unknown feature
307.0815	1.55	Gallocatechin: $[M+H]^+$
289.0705	1.55	Gallocatechin: $[M+H-H_2O]^+$
169.0505	1.54	Gallocatechin: unknown feature
173.5201	1.55	Gallocatechin: unknown feature
349.05	1.55	Gallocatechin: unknown feature
359.9924	1.55	Gallocatechin: unknown feature
399.0215	1.55	Gallocatechin: unknown feature
401.0192	1.55	Gallocatechin: unknown feature
457.9694	1.55	Gallocatechin: unknown feature
666.066	1.54	Gallocatechin: unknown feature
459.0924	2.50	Gallocatechin gallate: $[M+H]^+$
289.035	2.48	Gallocatechin gallate: $[M+H-C_8H_8O_4-2H^{app}]^+$
481.074	2.52	Gallocatechin gallate: $[M+Na]^+$
361.0004	2.51	Gallocatechin gallate: unknown feature
512.0035	2.50	Gallocatechin gallate: unknown feature
553.0305	2.52	Gallocatechin gallate: unknown feature
286.0468	4.55	Kaempferol: $[M\cdot]^+$
259.0588	4.56	Kaempferol: $[M.-CO]^+$
287.0554	4.55	Kaempferol: $[M+H]^+$
241.0499	4.56	Kaempferol: $[M+H-HCOOH]^+$
163.0049	4.58	Kaempferol: unknown feature
183.5184	4.55	Kaempferol: unknown feature
229.0503	4.55	Kaempferol: unknown feature
287.1998	4.55	Kaempferol: unknown feature
325.0021	4.56	Kaempferol: unknown feature
366.0286	4.56	Kaempferol: unknown feature
371.0074	4.57	Kaempferol: unknown feature
380.0038	4.58	Kaempferol: unknown feature
382.001	4.55	Kaempferol: unknown feature
384.0016	4.55	Kaempferol: unknown feature

387.9951	4.57	Kaempferol: unknown feature
422.9774	4.57	Kaempferol: unknown feature
438.9512	4.55	Kaempferol: unknown feature
611.0495	4.55	Kaempferol: unknown feature
626.014	4.55	Kaempferol: unknown feature
709.0239	4.55	Kaempferol: unknown feature
319.0454	3.45	Myricetin: $[M+H]^+$
178.9998	3.45	Myricetin: unknown feature
188.0057	3.45	Myricetin: unknown feature
199.5135	3.45	Myricetin: unknown feature
207.4997	3.45	Myricetin: unknown feature
322.0529	3.45	Myricetin: unknown feature
356.9911	3.45	Myricetin: unknown feature
389.9675	3.45	Myricetin: unknown feature
398.0178	3.45	Myricetin: unknown feature
413.9907	3.45	Myricetin: unknown feature
689.9933	3.45	Myricetin: unknown feature
303.0508	4.02	Quercetin: $[M+H]^+$
229.0502	4.02	Quercetin: $[M+H-CO-CO_2]^+$
285.0397	4.02	Quercetin: $[M+H-H_2O]^+$
257.0446	4.02	Quercetin: $[M+H-H_2O-CO]^+$
180.008	4.01	Quercetin: unknown feature
198.9982	4.02	Quercetin: unknown feature
200.0037	4.02	Quercetin: unknown feature
201.0552	4.02	Quercetin: unknown feature
303.1993	4.02	Quercetin: unknown feature
303.2879	4.02	Quercetin: unknown feature
305.0558	4.02	Quercetin: unknown feature
340.997	4.02	Quercetin: unknown feature
382.0232	4.02	Quercetin: unknown feature
397.9958	4.02	Quercetin: unknown feature
399.9975	4.02	Quercetin: unknown feature
454.9467	4.02	Quercetin: unknown feature
629.0511	4.02	Quercetin: unknown feature
643.0385	4.03	Quercetin: unknown feature
658.0037	4.02	Quercetin: unknown feature
755.9795	4.02	Quercetin: unknown feature
175.1086	0.49	Theanine: $[M+H]^+$
160.0867	0.49	Theanine: $[M+H-CH_3]^+$
306.0977	0.49	Theanine: unknown feature

Table S4b: Detailed annotations of the reference compounds and associated features for Laboratory B used for Figure 5

m/z	retention time (min)	annotation
181.0498	2.47	Caffeic acid: $[M+H]^+$
222.9983	2.47	Caffeic acid: $[M+H+2Na-2H]^+$
225.014	2.47	Caffeic acid: $[M+Na+Na-H]^+$
293.0001	2.47	Caffeic acid: $[M+Na+Na-H+NaCOOH]^+$
301.0484	2.47	Caffeic acid: unknown feature
304.995	2.47	Caffeic acid: unknown feature
306.0283	2.48	Caffeic acid: unknown feature
311.0079	2.47	Caffeic acid: unknown feature
316.014	2.48	Caffeic acid: unknown feature
317.0211	2.47	Caffeic acid: unknown feature
319.0215	2.48	Caffeic acid: unknown feature
319.0593	2.47	Caffeic acid: unknown feature
321.0165	2.48	Caffeic acid: unknown feature
328.0098	2.47	Caffeic acid: unknown feature
334.0236	2.47	Caffeic acid: unknown feature
342.0746	2.47	Caffeic acid: unknown feature
343.9815	2.47	Caffeic acid: unknown feature
345.9837	2.48	Caffeic acid: unknown feature
347.0542	2.47	Caffeic acid: unknown feature
354.971	2.47	Caffeic acid: unknown feature
370.9441	2.47	Caffeic acid: unknown feature
387.9475	2.47	Caffeic acid: unknown feature
422.9562	2.47	Caffeic acid: unknown feature
428.976	2.47	Caffeic acid: unknown feature
194.0793	2.33	Caffeine: $[M\cdot]^+$
195.0871	2.33	Caffeine: $[M+H]^+$
355.1012	2.17	Chlorogenic acid: $[M+H]^+$
372.1292	2.17	Chlorogenic acid: $[M+H+NH_3]^+$
353.0854	2.17	Chlorogenic acid: $[M+H-2H^{app}]^+$
370.1121	2.17	Chlorogenic acid: $[M+H-2H^{app}+NH_3]^+$
163.0386	2.17	Chlorogenic acid: $[M+H-C_7H_{12}O_6]^+$
377.0832	2.17	Chlorogenic acid: $[M+Na]^+$
399.0653	2.17	Chlorogenic acid: $[M+Na+Na-H]^+$
467.0544	2.17	Chlorogenic acid: $[M+Na+Na-H+NaCOOH]^+$
375.067	2.17	Chlorogenic acid: $[M+Na-2H^{app}]^+$
465.0363	2.17	Chlorogenic acid: $[M+Na-2H^{app}+Na-H+NaCOOH]^+$
378.0885	2.17	Chlorogenic acid: unknown feature
439.0548	2.17	Chlorogenic acid: unknown feature
454.0183	2.17	Chlorogenic acid: unknown feature
459.0226	2.18	Chlorogenic acid: unknown feature
472.0281	2.17	Chlorogenic acid: unknown feature

478.0669	2.18	Chlorogenic acid: unknown feature
480.0804	2.17	Chlorogenic acid: unknown feature
490.0646	2.16	Chlorogenic acid: unknown feature
493.0304	2.17	Chlorogenic acid: unknown feature
529.0245	2.17	Chlorogenic acid: unknown feature
533.0224	2.16	Chlorogenic acid: unknown feature
165.0543	2.96	Coumaric acid : $[M+H]^+$
209.018	2.97	Coumaric acid : $[M+Na+Na-H]^+$
277.0038	2.96	Coumaric acid : $[M+Na+Na-H+NaCOOH]^+$
318.0294	2.96	Coumaric acid : $[M+Na+Na-H+NaCOOH+ACN]^+$
244.0268	2.96	Coumaric acid : unknown feature
250.045	2.97	Coumaric acid : unknown feature
270.9889	2.97	Coumaric acid : unknown feature
285.0538	2.97	Coumaric acid : unknown feature
288.999	2.97	Coumaric acid : unknown feature
290.0336	2.97	Coumaric acid : unknown feature
295.0131	2.96	Coumaric acid : unknown feature
301.0256	2.97	Coumaric acid : unknown feature
303.0272	2.97	Coumaric acid : unknown feature
303.0647	2.96	Coumaric acid : unknown feature
304.9976	2.97	Coumaric acid : unknown feature
305.0228	2.96	Coumaric acid : unknown feature
308.0434	2.96	Coumaric acid : unknown feature
312.0141	2.97	Coumaric acid : unknown feature
326.0803	2.96	Coumaric acid : unknown feature
327.9871	2.96	Coumaric acid : unknown feature
329.9874	2.97	Coumaric acid : unknown feature
331.0589	2.97	Coumaric acid : unknown feature
338.9758	2.96	Coumaric acid : unknown feature
343.9573	2.97	Coumaric acid : unknown feature
344.9938	2.97	Coumaric acid : unknown feature
354.9486	2.96	Coumaric acid : unknown feature
406.9635	2.96	Coumaric acid : unknown feature
422.9358	2.96	Coumaric acid : unknown feature
423.0386	2.97	Coumaric acid : unknown feature
443.0959	3.04	Epicatechin gallate: $[M+H]^+$
578.0646	3.04	Epicatechin gallate: $[M+H+2xNaCOOH]^+$
273.0761	3.04	Epicatechin gallate: $[M+H-C_7H_5O_5-H_2O]^+$
487.0582	3.03	Epicatechin gallate: $[M+Na+Na-H]^+$
458.11	3.04	Epicatechin gallate: unknown feature
474.1017	3.05	Epicatechin gallate: unknown feature
492.1131	3.05	Epicatechin gallate: unknown feature
527.0505	3.04	Epicatechin gallate: unknown feature
533.0689	3.04	Epicatechin gallate: unknown feature

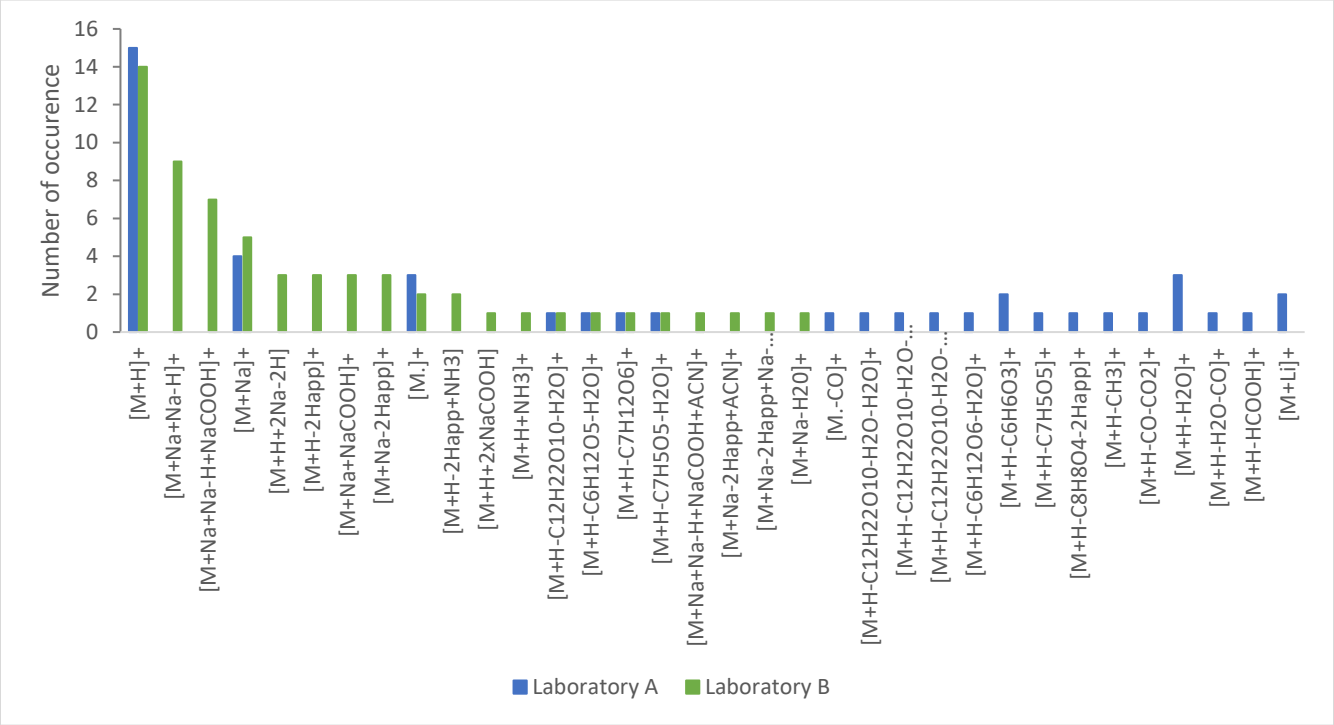
534.0683	3.05	Epicatechin gallate: unknown feature
537.0358	3.04	Epicatechin gallate: unknown feature
545.0618	3.04	Epicatechin gallate: unknown feature
549.0291	3.04	Epicatechin gallate: unknown feature
555.0506	3.04	Epicatechin gallate: unknown feature
556.0503	3.05	Epicatechin gallate: unknown feature
568.0738	3.04	Epicatechin gallate: unknown feature
590.0579	3.04	Epicatechin gallate: unknown feature
595.0367	3.03	Epicatechin gallate: unknown feature
605.0262	3.04	Epicatechin gallate: unknown feature
617.0186	3.04	Epicatechin gallate: unknown feature
623.0365	3.05	Epicatechin gallate: unknown feature
638.9989	3.04	Epicatechin gallate: unknown feature
291.0858	2.53	Epicatechin: $[M+H]^+$
289.071	2.53	Epicatechin: $[M+H-2H^{app}]^+$
306.0968	2.53	Epicatechin: $[M+H-2H^{app}+NH_3]^+$
381.055	2.52	Epicatechin: $[M+Na+NaCOOH]^+$
403.0371	2.52	Epicatechin: $[M+Na+Na-H+NaCOOH]^+$
311.052	2.53	Epicatechin: $[M+Na-2H^{app}]^+$
352.0777	2.53	Epicatechin: $[M+Na-2H^{app}+ACN]^+$
293.0907	2.53	Epicatechin: unknown feature
375.0393	2.53	Epicatechin: unknown feature
393.0479	2.53	Epicatechin: unknown feature
416.0632	2.53	Epicatechin: unknown feature
426.0502	2.52	Epicatechin: unknown feature
443.0251	2.53	Epicatechin: unknown feature
453.0109	2.53	Epicatechin: unknown feature
454.0184	2.53	Epicatechin: unknown feature
479.9709	2.52	Epicatechin: unknown feature
480.9795	2.52	Epicatechin: unknown feature
307.0819	2.05	Epigallocatechin: $[M+H]^+$
321.0603	2.05	Epigallocatechin: unknown feature
391.0342	2.05	Epigallocatechin: unknown feature
409.0427	2.06	Epigallocatechin: unknown feature
432.0596	2.05	Epigallocatechin: unknown feature
442.0452	2.05	Epigallocatechin: unknown feature
469.0086	2.05	Epigallocatechin: unknown feature
495.966	2.05	Epigallocatechin: unknown feature
329.063	2.05	Epigallocatechin: $[M+Na]^+$
397.0505	2.06	Epigallocatechin: $[M+Na+NaCOOH]^+$
419.0327	2.05	Epigallocatechin: $[M+Na+Na-H+NaCOOH]^+$
214.9924	1.26	Gallic acid: $[M+Na+Na-H]^+$
459.0929	2.64	Gallocatechin gallate: $[M+H]^+$
481.0746	2.64	Gallocatechin gallate: $[M+Na]^+$

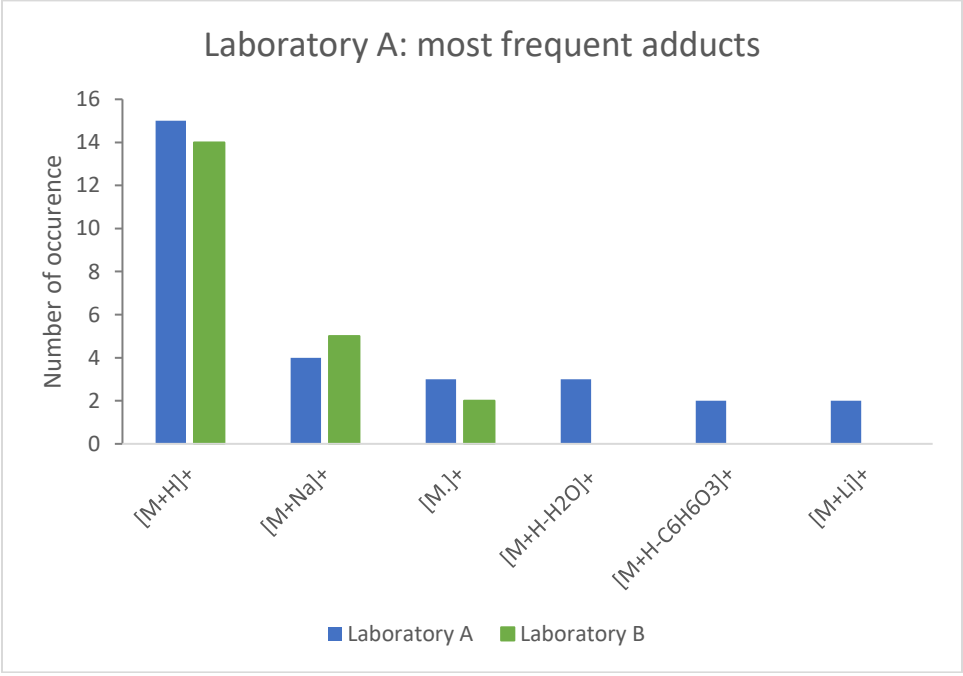
549.0601	2.63	Gallocatechin gallate: $[M+Na+NaCOOH]^+$
503.0544	2.64	Gallocatechin gallate: $[M+Na+Na-H]^+$
571.0452	2.64	Gallocatechin gallate: $[M+Na+Na-H+NaCOOH]^+$
303.0496	2.64	Gallocatechin gallate: unknown feature
461.0957	2.64	Gallocatechin gallate: unknown feature
492.1132	2.64	Gallocatechin gallate: unknown feature
508.1104	2.64	Gallocatechin gallate: unknown feature
553.0286	2.63	Gallocatechin gallate: unknown feature
584.0691	2.64	Gallocatechin gallate: unknown feature
594.0544	2.64	Gallocatechin gallate: unknown feature
595.0644	2.63	Gallocatechin gallate: unknown feature
606.0549	2.63	Gallocatechin gallate: unknown feature
307.0819	1.70	Gallocatechin: $[M+Na+Na-H+NaCOOH]^+$
286.0469	4.74	Kaempferol: $[M^{\cdot}]^+$
287.0543	4.73	Kaempferol: $[M+H]^+$
399.0044	4.74	Kaempferol: $[M+Na+Na-H+NaCOOH]^+$
407.0533	4.74	Kaempferol: unknown feature
224.5442	4.74	Kaempferol: unknown feature
289.0595	4.73	Kaempferol: unknown feature
366.0267	4.74	Kaempferol: unknown feature
384.039	4.74	Kaempferol: unknown feature
392.9885	4.74	Kaempferol: unknown feature
408.0596	4.74	Kaempferol: unknown feature
408.9602	4.74	Kaempferol: unknown feature
410.999	4.74	Kaempferol: unknown feature
412.0323	4.74	Kaempferol: unknown feature
423.0266	4.74	Kaempferol: unknown feature
425.0263	4.74	Kaempferol: unknown feature
425.0637	4.74	Kaempferol: unknown feature
425.9624	4.74	Kaempferol: unknown feature
426.9985	4.74	Kaempferol: unknown feature
427.0236	4.74	Kaempferol: unknown feature
434.0165	4.74	Kaempferol: unknown feature
435.0173	4.74	Kaempferol: unknown feature
448.082	4.74	Kaempferol: unknown feature
451.9886	4.73	Kaempferol: unknown feature
453.0612	4.75	Kaempferol: unknown feature
460.9783	4.73	Kaempferol: unknown feature
319.0459	3.60	Myricetin: $[M+H]^+$
360.9927	3.60	Myricetin: $[M+H+2Na-2H]^+$
317.0289	3.60	Myricetin: $[M+H-2H^{app}]^+$
363.0082	3.61	Myricetin: $[M+Na+Na-H]^+$
339.0115	3.60	Myricetin: $[M+Na-2H^{app}]^+$
321.0495	3.61	Myricetin: unknown feature

430.9929	3.60	Myricetin: unknown feature
439.0461	3.60	Myricetin: unknown feature
440.0469	3.61	Myricetin: unknown feature
454.0093	3.61	Myricetin: unknown feature
455.016	3.60	Myricetin: unknown feature
457.0194	3.61	Myricetin: unknown feature
457.0565	3.60	Myricetin: unknown feature
466.0037	3.61	Myricetin: unknown feature
492.9685	3.61	Myricetin: unknown feature
303.0497	4.19	Quercetin: $[M+H]^+$
347.0149	4.19	Quercetin: $[M+H+2Na-2H]^+$
382.022	4.19	Quercetin: unknown feature
397.9937	4.19	Quercetin: unknown feature
408.9835	4.19	Quercetin: unknown feature
414.9987	4.19	Quercetin: unknown feature
423.0514	4.19	Quercetin: unknown feature
424.0518	4.19	Quercetin: unknown feature
424.9556	4.19	Quercetin: unknown feature
428.0295	4.19	Quercetin: unknown feature
438.0134	4.19	Quercetin: unknown feature
439.0202	4.19	Quercetin: unknown feature
441.0243	4.19	Quercetin: unknown feature
442.994	4.19	Quercetin: unknown feature
450.0087	4.19	Quercetin: unknown feature
451.0151	4.19	Quercetin: unknown feature
464.0772	4.19	Quercetin: unknown feature
476.9734	4.19	Quercetin: unknown feature
611.1595	2.92	Rutin: $[M+H]^+$
303.0497	2.93	Rutin: $[M+H-(C_{12}H_{22}O_{10}-H_2O)]^+$
465.1029	2.92	Rutin: $[M+H-(C_6H_{12}O_5-H_2O)]^+$
633.142	2.92	Rutin: $[M+Na]^+$
655.1217	2.92	Rutin: $[M+Na+Na-H]^+$
301.0339	2.93	Rutin: unknown feature
626.1744	2.93	Rutin: unknown feature
631.1291	2.93	Rutin: unknown feature
665.0769	2.93	Rutin: unknown feature
695.116	2.93	Rutin: unknown feature
701.1252	2.92	Rutin: unknown feature
705.0952	2.92	Rutin: unknown feature
717.0972	2.92	Rutin: unknown feature
723.108	2.92	Rutin: unknown feature
393.1709	0.59	Theanine: $[2M+Na+Na-H]^+$
175.1079	0.59	Theanine: $[M+H]^+$
197.0894	0.59	Theanine: $[M+Na]^+$

219.0717	0.59	Theanine: $[M+Na+Na-H]^+$
179.0792	0.59	Theanine: $[M+Na-H_2O]^+$
168.1033	0.59	Theanine: unknown feature
176.1044	0.59	Theanine: unknown feature
177.1124	0.59	Theanine: unknown feature
189.1234	0.59	Theanine: unknown feature
208.1326	0.59	Theanine: unknown feature
231.0649	0.59	Theanine: unknown feature
254.081	0.59	Theanine: unknown feature
259.0598	0.59	Theanine: unknown feature
270.0526	0.60	Theanine: unknown feature
274.0244	0.59	Theanine: unknown feature
275.0318	0.59	Theanine: unknown feature
277.0324	0.59	Theanine: unknown feature
281.0415	0.59	Theanine: unknown feature
287.059	0.59	Theanine: unknown feature
342.0115	0.59	Theanine: unknown feature
409.1367	0.59	Theanine: unknown feature

Figure S2. Number of occurrences of adducts/fragments in the annotated features in the analyses of the mixture of reference compounds by laboratory A and laboratory B





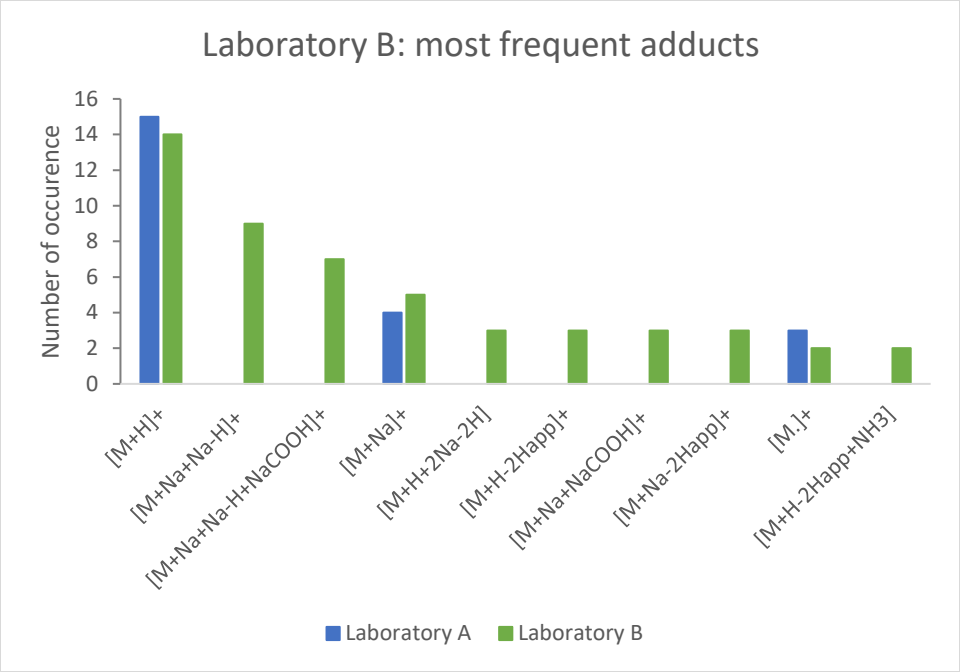

Laboratory B: most frequent adducts
Number of occurence
16
14
12
10
8
6
4
2
0
[M+H]+
[M+Na+Na-H]+
[M+Na+Na-H+NaCOOH]+
[M+Na]+
[M+H+2Na-2H]
[M+H-2Happ]+
[M+Na+NaCOOH]+
[M+Na-2Happ]+
[M.]+
[M+H-2Happ+NH3]
Laboratory A
Laboratory B

Table S5a: Reference list of charged adducts used for annotation

Charge carrier	Neutral mass	Formal annotation	Mass difference related to [M+H]+	Comment	References
H^+	NH_3-H_2O	$[M+H+NH_3-H_2O]^+$	-0.98456		4
Li^+		$[M+Li]^+$	6.00763		4
H^+	NH_3	$[M+H+NH_3]^+$	17.02600		5
H^+	H_2O	$[M+H+H_2O]^+$	18.01002		4
Na^+		$[M+Na]^+$	21.98140		5
H^+	CH_3OH	$[M+H+CH_3OH]^+$	32.02567	methanol	5
Na^+	NH_3	$[M+Na+NH_3]^+$	39.00795		6
Na^+	H_2O	$[M+Na+H_2O]^+$	39.99196		5
H^+	CH_3CN	$[M+H+CH_3CN]^+$	41.02600	acetonitrile	5
Na+	Na-H	$[M+Na+Na-H]^+$	43.96334		5
H^+	HCOOH	$[M+H+HCOOH]^+$	46.00493		7
K^+	NH_3	$[M+K+NH_3]^+$	54.98188		6
H^+	NaCl	$[M+H+NaCl]^+$	57.95807		6
Na^+	K-H	$[M+Na+K-H]^+$	59.93728		6
H^+	C_3H_8O	$[M+H+C_3H_8O]^+$	60.05697	isopropanol	5
Na^+	CH_3CN	$[M+Na+CH_3CN]^+$	63.00795	acetonitrile	5
H^+	NH_3+HCOOH	$[M+H+NH_3+HCOOH]^+$	63.03148		7
Na^+	2Na-2H	$[M+Na+2Na-2H]^+$	65.94529		5
Na^+	HCOOH	$[M+Na+HCOOH]^+$	67.98688		7
K^+	K-H	$[M+K+K-H]^+$	75.91122		5
K^+		$[M+K]^+$	37.95533		5
H^+	C_2H_6OS	$[M+H+C_2H_6OS]^+$	78.01339	DMSO	5
K^+	CH_3CN	$[M+K+CH_3CN]^+$	78.98188	acetonitrile	6
Na^+	NaCl	$[M+Na+NaCl]^+$	79.94002		6
H^+	2xCH_3CN	$[M+H+2xCH_3CN]^+$	82.05255	acetonitrile	5
H^+	C_3H_8O+Na	$[M+H+C_3H_8O+Na]^+$	83.04674	isopropanol	5
K^+	HCOOH	$[M+K+HCOOH]^+$	83.96081		7
Na^+	NaCOOH	$[M+Na+NaCOOH]^+$	89.96882		6
K^+	NaCl	$[M+K+NaCl]^+$	95.91396		6
K^+	NaCOOH	$[M+K+NaCOOH]^+$	105.94276		6
Na^+	Na-H+NaCOOH	$[M+Na+Na-H+NaCOOH]^+$	111.95077		Observed in Lab A dataset
H^+	Na-H+NaCOOH	$[M+H+Na-H+NaCOOH]^+$	89.96882		Observed in Lab A dataset
H^+	CH_3OH-H_2O	$[M+H+CH_3OH-H_2O]^+$	14.01510		4
H^+	H_2^{app}	$[M+H+H_2^{app}]^+$	-2.01620	oxidation-like process	4

Table S5b: Reference list of neutral losses used for annotation

Neutral losses			
Description	**Mass difference**	**Comments**	**Reference**
($C_6H_{12}O_5$-H_2O)	-146.05791	desoxy-hexose-H_2O / methyl-pentose-H_2O	8
($C_{12}H_{22}O_{10}$-H_2O)	-308.11074	rutinose-H_2O	8
2xH_2O	-36.02113		9
C_2H_6O	-46.04187		9
3xH_2O	-54.03170		9
CH_3-COOH	-60.02113		9
CO-CO_2	-74.00040		9
CH_3-CH_2-COOH-NH	-89.04768		9
2xCO_2-H_2O	-105.99023		9
2CO_2+2H_2O	-124.00079		9
$C_6H_8O_6$	-176.03209	glucuronic acid	4
NH_3	-17.02655	amine containing molecule	4
H_2O	-18.01057		4
H_2O-NH_3	-35.03711		4
C_2H_2O	-42.01057	deacetylation	4
2Na-2H	-43.96389		4
$C_9H_8O_3$-H_2O	-146.03678	coumaroyl	4
($C_6H_{12}O_6$-H_2O)	-162.05283	hexose-H2O	4
$C_6H_6O_3$	-126.03170	Hetero Cyclic Ring Fragmentation	10
$C_8H_8O_2$	-136.05243	Retro Diels Alder (ring B:1xOH)	10
$C_8H_8O_3$	-152.04735	Retro Diels Alder (ring B: 2xOH)	10
$C_8H_8O_4$	-168.04226	Retro Diels Alder (ring B: 3xOH)	10
$C_6H_6O_3$-H_2O	-144.04226	Hetero Cyclic Ring Fragmentation-H2O	10
$CH_3^{\bullet}$	-15.02348	demethylation	11
O	-15.99492		11
CHN	-27.01090		11
CO	-27.99492		11
CH_3OH	-32.02622	methanol	11
CO_2	-43.98983		11
COOH	-44.99766		11
HCOOH	-46.00548		11
2xCO	-55.98983		11
($C_7H_6O_5$-H_2O)	-152.01096	galloyl	12
NaCOOH	-67.98743		6
$C_7H_{12}O_6$	-192.06339	quinic acid	13

Table S5c: Reference list of neutral additions used for annotation

Neutral additions			
Description	**Mass difference**	**Comments**	**Reference**
NaCl	57.95862		[9]
Na+C_3H_8O	83.04729	sodium and isopropanol	[5]
KCOOH	83.96136		[9]
NaCOOH+Na-H	89.96937		[9]
2xNaCl	115.91725		[9]
2xNaCOOH	135.97485		[9]
Na-H	21.98195		[9]
K-H	37.95588		[9]
C_2H_3N	41.02655	acetonitrile	[9]
3Na-3H	65.94584		[9]
HCOOH+NaCOOH	113.99291		[9]
NaCl+NaCOOH	125.94605		[9]
CH_3OH	32.02622	methanol	[4]
HCOOH	46.00548		[4]
C_3H_8O	60.05752	isopropanol	[5]

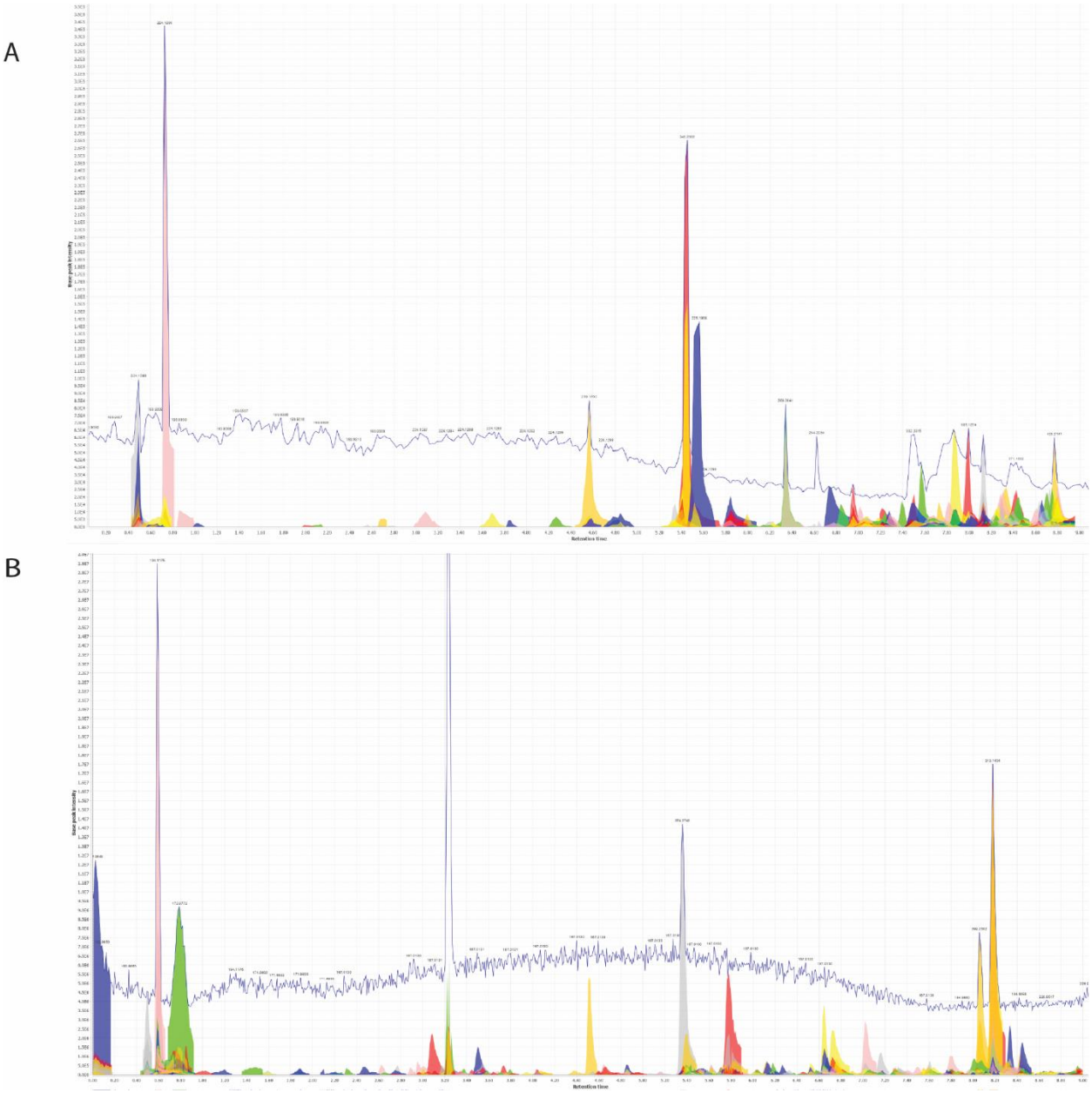


Figure S3. Blank traces for Laboratory A (**A**) and Laboratory B (**B**) showing TIC (above in blue line) and retained features after MZmine 2.0 processing (below).

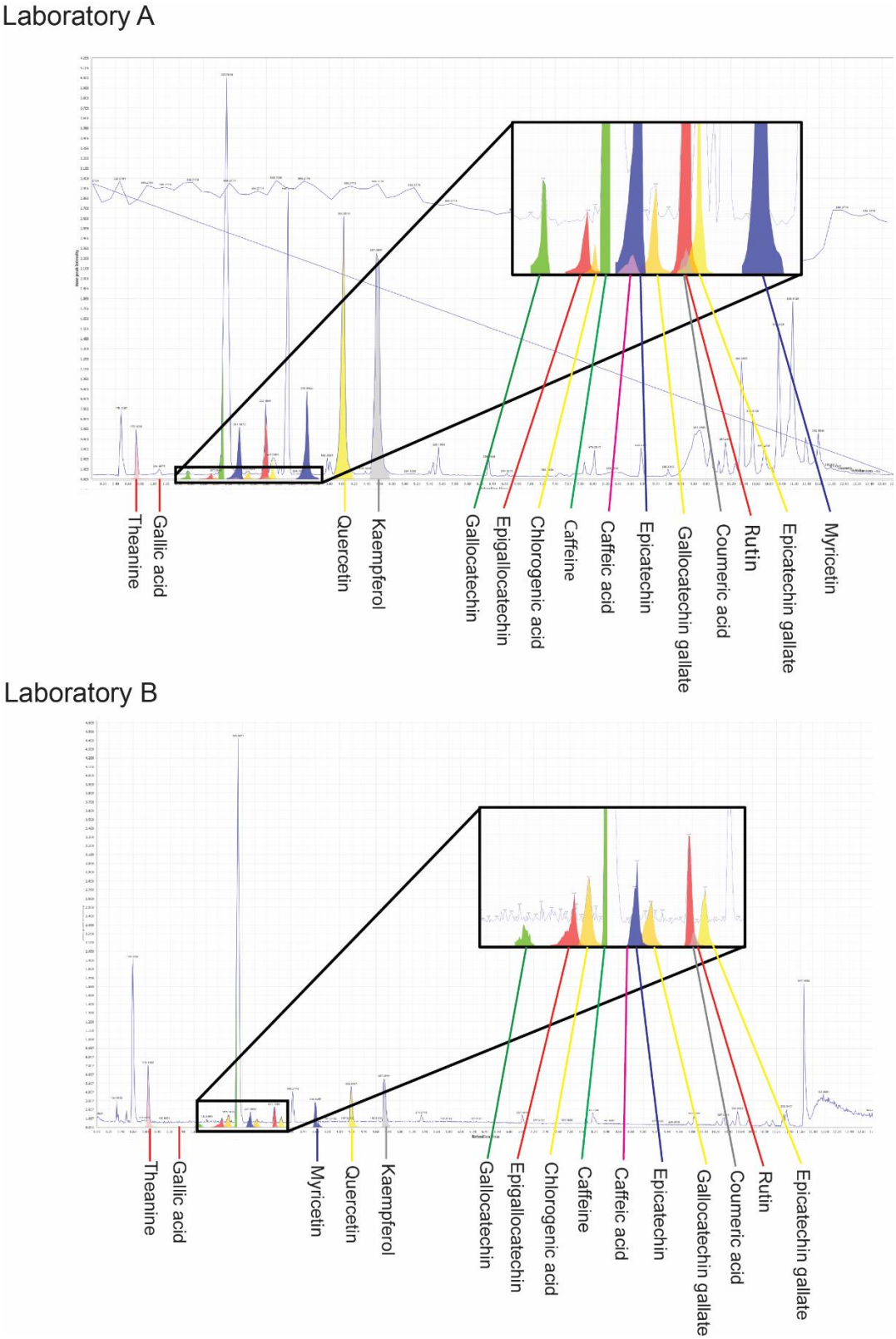


Figure S4. Standard mix injection traces for Laboratory A and Laboratory B after MZmine 2.0 processing and filtered for only the standards.

Table S6. Comparison of limits of detection for three representative green tea constituents between Laboratory A and Laboratory B.

Compound	Laboratory A[a]		Laboratory B[b]	
	LOD (µg/mL)[c]	LOQ (µg/mL)[d]	LOD (µg/mL)	LOQ (µg/mL)
(-)-epigallocatechin	0.57	1.9	0.078	0.26
rutin	0.091	0.30	0.044	0.15
kaempferol	0.25	0.84	0.061	0.20

a. Data for laboratory A were collected on a Waters SYNAPT G2-Si qTOF mass spectrometer.
b. Data for laboratory B were collected with a Thermo Fisher Q-Exactive Plus Orbitrap.
c. Limit of detection (LOD) was calculated from analyzing standards in triplicate at a range of concentrations between 0.2 and 100 µg/mL on each instrument. Only the linear portion of the calibration curve was used for the LOD determination. LOD was calculated by the equation $LOD = \frac{3s}{m}$, where m is the slope of the calibration curve and s = the standard deviation in peak area of three replicate injections of the standard at the lowest concentration within the linear range of the calibration curve.
d. Limit of Quantitation (LOQ) was calculated by the equation $LOD = \frac{10s}{m}$.

References

(1) Amazon.com, AmazonBest Sellers http://www.amazon.com/ Best-Sellers-Grocery-Gourmet-Food-Green-Tea-Beverages/zgbs/ grocery/16318471 (accessed Nov 11, 2015).

(2) Anonymous. *Consum. Rep*; 2003.

(3) Health, J. Green Tea Supplement Reviews.

(4) Damont, A.; Olivier, M.-F.; Warnet, A.; Lyan, B.; Pujos-Guillot, E.; Jamin, E. L.; Debrauwer, L.; Bernillon, S.; Junot, C.; Tabet, J.-C.; Fenaille, F. Proposal for a Chemically Consistent Way to Annotate Ions Arising from the Analysis of Reference Compounds under ESI Conditions: A Prerequisite to Proper Mass Spectral Database Constitution in Metabolomics. *J. Mass Spectrom.* **2019**, *54* (6), 567–582.

(5) Feihn Lab. Mass Spectrometry Adduct Calculator 2016 https://fiehnlab.ucdavis.edu/staff/kind/metabolomics/ms-adduct-calculator/ (accessed Jul 8, 2020).

(6) Uppal, K.; Walker, D. I.; Jones, D. P. XMSannotator: An R Package for Network-Based Annotation of High-Resolution Metabolomics Data. *Anal. Chem.* **2017**, *89* (2), 1063–1067.

(7) Kuhl, C.; Tautenhahn, R.; Böttcher, C.; R. Larson, T.; Neumann, S. CAMERA: An Integrated Strategy for Compound Spectra Extraction and Annotation of Liquid Chromatography/Mass Spectrometry Data Sets. *Anal. Chem.* **2011**, *84* (1), 283–289.

(8) Abrankó, L.; García-Reyes, J. F.; Molina-Díaz, A. In-Source Fragmentation and Accurate Mass Analysis of Multiclass Flavonoid Conjugates by Electrospray Ionization Time-of-Flight Mass Spectrometry. *J. Mass Spectrom.* **2011**, *46* (5), 478–488.

(9) Kachman, M.; Habra, H.; Duren, W.; Wigginton, J.; Sajjakulnukit, P.; Michailidis, G.; Burant, C.; Karnovsky, A. Deep Annotation of Untargeted LC-MS Metabolomics Data with Binner. *Bioinformatics* **2020**, *36* (6), 1801–1806.

(10) Li, H.-J.; Deinzer, M. L. Tandem Mass Spectrometry for Sequencing Proanthocyanidins. *Anal. Chem.* **2007**, *79* (4), 1739–1748.

(11) Levsen, K.; Schiebel, H.-M.; Terlouw, J. K.; Jobst, K. J.; Elend, M.; Preiß, A.; Thiele, H.; Ingendoh, A. Even-Electron Ions: A Systematic Study of the Neutral Species Lost in the Dissociation of Quasi-Molecular Ions. *J. Mass Spectrom.* **2007**, *42* (8), 1024–1044.

(12) Wyrepkowski, C. C.; Costa, D. L. M. G. da; Sinhorin, A. P.; Vilegas, W.; De Grandis, R. A.; Resende, F. A.; Varanda, E. A.; dos Santos, L. C. Characterization and Quantification of the Compounds of the Ethanolic Extract from Caesalpinia Ferrea Stem Bark and Evaluation of Their Mutagenic Activity. *Molecules* **2014**, *19* (10), 16039–16057.

(13) Xu, L.; Xu, Z.; Strashnov, I.; Liao, X. Use of Information Dependent Acquisition Mass Spectra and Sequential Window Acquisition of All Theoretical Fragment-Ion Mass Spectra for Fruit Juices Metabolomics and Authentication. *Metabolomics* **2020**, *16* (7), 81.