Supporting Information

Fast profiling of metabolite mixtures using chemometric analysis of a speeded-up 2D heteronuclear correlation NMR experiment

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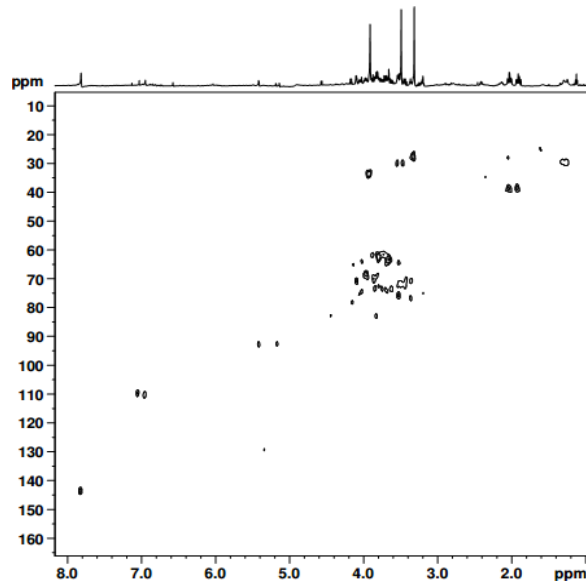
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ST1- List of metabolites identified and used for metabolite fingerprinting in tea samples.

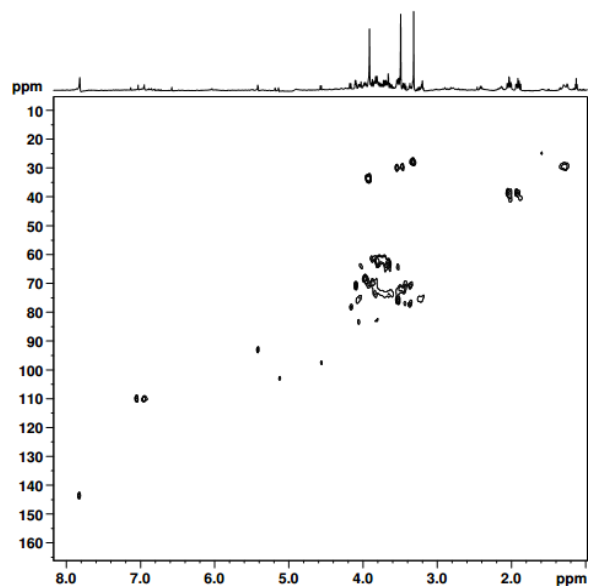| Metabolite	Chemical shift(ppm) (multiplicity, J in Hz)	Metabolite	Chemical shift(ppm) (multiplicity, J in Hz)
phytosterols	0.7(s), 2.02(m), 5.3(m)	malic acid	2.37(dd,15.3,9.8), 2.63(dd,15.3,2.7), 4.27(dd,10.1,2.7)
Lipids		citric acid	2.51(d,15.2), 2.67(d)
terminal methyl group	0.89(t,6.9), 0.95(t,6.9)	succinic acid	2.52(s)
$(CH_2)n$	1.27(m)	fumaric acid	6.51(s)
CH_2CH_2COOH(C3)	1.64(m)	**Carbohydrates**	
allylic protons of unsaturated fatty acids	2.03(m)	beta-glucose	4.54(d,7.9)
CH_2COOH(C2)	2.37(t,7.5)	alpha-glucose	5.16(d,3.1)
olefinic protons of unsaturated fatty acids	5.3(m)	sucrose	4.17(d,8.7), 5.4(d,3.8)
Amino acids		**Phenols and others**	
leucine	0.95(t,6), 1.7(m)	hesperidin	1.08(dd), 2.78(ddd), 5.48(m), 6.90(m), 6.94(m)
isoleucine	1.04, 1.98	rutin	1.12(d,6.2), 4.52(d,1.4), 5.11(d), 6.39(d,2.0), 7.62(d), 7.65(dd)
valine	0.98(d,7), 1.03(d,7), 2.29(m)	chlorogenic acid	2.02(m), 2.17(m), 5.33(m), 6.4(d,15.9), 6.89(d,8.2), 7.11(dd), 7.2(d,1.6), 7.65(d,15.9)
alanine	1.46(d,7.2)	naringenin	2.74(dd), 3.02(dd), 5.36(dd), 5.88(d), 5.89(d), 6.8(m), 7.30(m)
arginine	1.68(m), 1.90(m)	ferulic acid	3.89(s), 6.36(d,15.97), 7.04(d,8.10), 7.15(m), 7.28(d,15.97)
lysine	1.71(m), 1.87(m)	kaempferol/apigenin	6.2(d,2.1), 6.49(d,2.1), 6.9(m), 8.05(d,8.8)
glutamic acid	2.02(m), 2.12(m), 2.44(m)	caffeine	3.22(s), 3.38(s), 3.77(s), 7.63(s)
glutamine	2.12(m), 2.44(m)	gallic acid	7.07(s)
aspartic acid	2.75(dd,17.3,8.8), 2.85(dd,17.3,3.7)	theobromine	7.84
cysteine	3.06(m), 3.97(dd)	theanine	1.10, 2.13, 2.37, 3.19, 3.72
phenylalanine	3.19(m), 7.32(d,6.9), 7.37(m), 7.41(m)	choline	3.22(s)
serine	3.83, 3.95(m)	myoinositol	3.30
tyrosine	6.87(m), 7.19(m)	**Found in Green tea**	
histidine	7.09(d,0.8), 7.85(d,1.1)	epicatechin(EC)	2.74, 2.89, 4.26, 4.81
tryptophan	7.17(m), 7.24(m), 7.28(s), 7.53(d,8.1), 7.72(d,7.9)0.99(d,6.9)	epigallocatechin(EGC)	2.74, 2.89, 4.25, 4.87, 6.58
Organic acids		epicatechin-3-gallate(ECG)	2.89, 3.03, 5.09, 5.50, 6.03, 6.78, 6.88, 6.99
priopionic acid	1.04(t,7.6), 2.14(q,7.6)	epigallocatechin-3-gallate(EGCG)	2.89, 3.03, 5.03, 5.50, 6.03, 6.59, 6.95
lactic acid	1.31(d,6.8), 4.08(q,6.9)	**Found in Black tea**	
quinic acid	1.84(dd), 1.94(m), 2.05(m), 2.1(dddd), 3.54(dd,9.2,3.2), 4.04(ddd), 4.16(q,3.4),	theaflavin	2.74(d,17.1), 2.75(d,17), 2.86(dd,17,4.5), 2.87(dd,17.1,5.9), 4.21, 4.29, 5.41, 6.01-6.13, 6.86, 7.02,7.15
acetic acid	1.96(s)	thearubigin	1.88, 1.98, 2.05, 2.08, 3.54, 3.62, 4.02, 4.14, 6.04-6.13, 6.85, 7.03, 7.16

ST2-*Post-hoc* analysis showing the metabolites responsible for differentiation between green and black tea samples, given the *p* value threshold of 0.05.

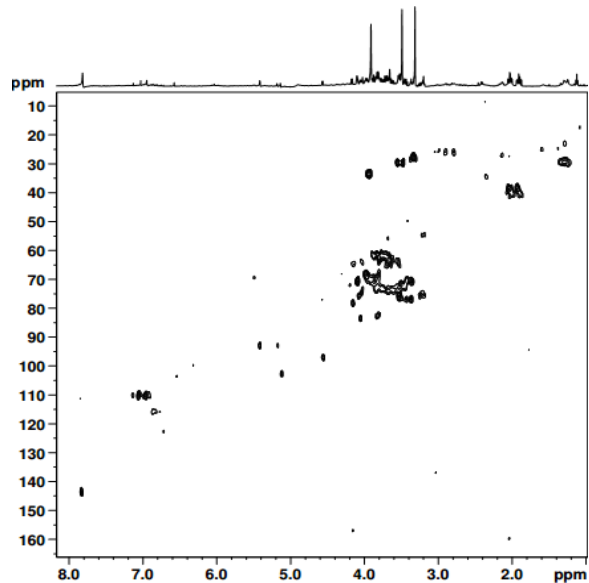| ppm	p-value	-log10(P)	FDR
theobromine	2.4296E-14	13.6148	2.8499E-12
EC	7.4349E-12	11.129	5.4771E-10
thearubigin	8.0795E-11	10.093	3.5711E-9
cysteine	1.2679E-10	9.8969	4.6702E-09
caffeine	4.54E-09	8.3429	9.12E-08
isoleucine	6.82E-09	8.166	1.26E-07
aspartate	2.31E-08	7.6362	3.19E-07
hesperidin	5.78E-08	7.2379	7.10E-07
ECG	1.18E-07	6.9297	1.30E-06
glucose	2.47E-07	6.607	2.37E-06
valine	1.48E-06	5.8291	1.08E-05
alanine	2.62E-06	5.5811	1.61E-05
sucrose	3.11E-05	4.5071	0.00015278
EGCG	3.43E-05	4.4644	0.00016141
lipids	0.0032136	2.49	0.0076514
theanine	0.0060433	2.2187	0.01272
theaflavin	0.02459	1.6092	0.0418
leucine	0.016211	1.79211	0.0288

S1- 2D ASAP-HSQC spectrum for green tea, number of scans = 1 and total experimental time = 49 sec.
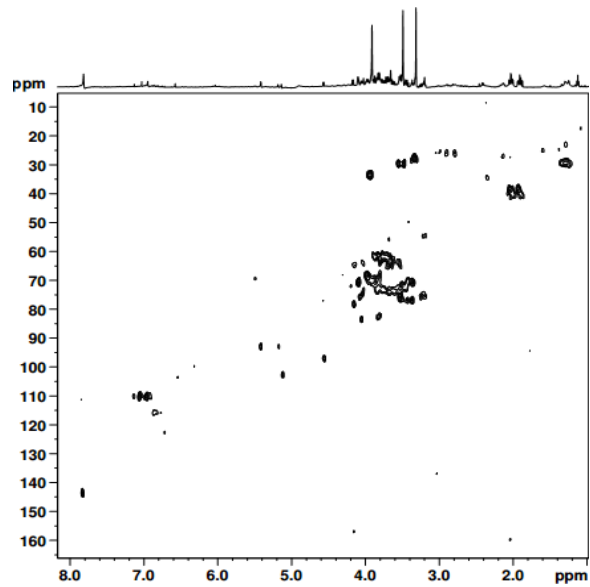
S2- 2D ASAP-HSQC spectrum for green tea, number of scans = 2 and total experimental time = 1 min 33 sec.
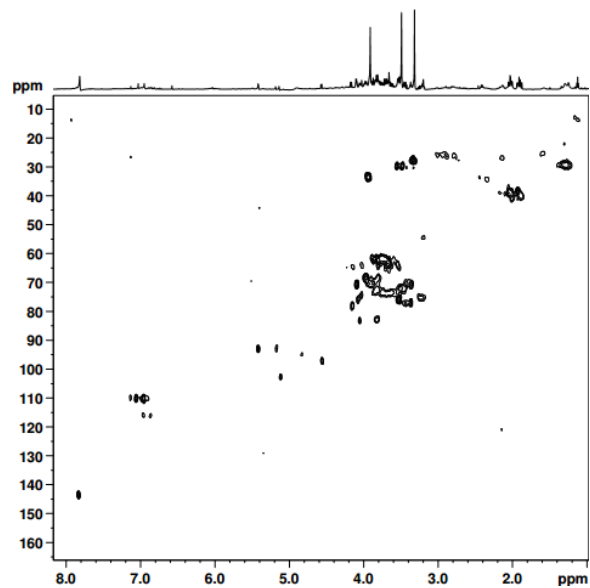

S3- 2D ASAP-HSQC spectrum for green tea, number of scans = 4 and total experimental time = 2 min 58 sec.
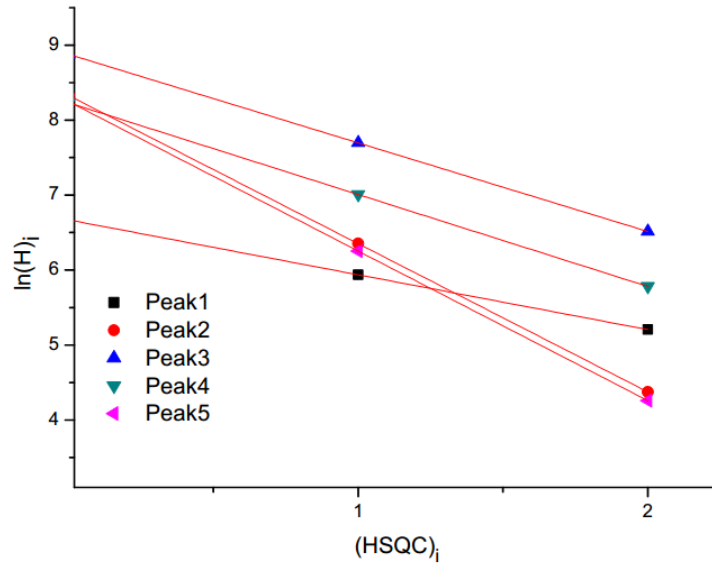
S4- 2D ASAP-HSQC spectrum for green tea, number of scans = 6 and total experimental time = 4 min 24 sec.

S5- 2D ASAP-HSQC spectrum for green tea, number of scans = 8 and total experimental time = 5 min 49 sec.

S6- Extrapolation of peak heights measured from 600 MHz 2D HSQC$_i$ (i=1,2) spectra for different peaks

S7- Extrapolation of peak heights measured from 600 MHz 2D ASAP-HSQC$_i$ (i=1,2) spectra for different peaks