

Table S1. Peak Assignment of Metabolites Identified on Zucchini extracts by ^1H -NMR

Compound ^a	Assignment ^b	^1H δ (ppm)	Multiplicity ^c	^{13}C δ (ppm)
<u>Organic acids</u>				
Acetic acid (AA)	CH ₃	1.92	s	25.98
Citric acid (CA)	α,γ -CH	2.67	d	44.77
	α',γ' -CH	2.71	d	44.77
Chlorogenic acid (CGA)	CH ₂ -2'	2.02,2.17	m	40.11
	CH-3'	5.33	m	40.14
	CH-4'	3.88	dd	75.43
	CH-5'	4.23	m	72.93
	CH-8	6.39	d	73.82
	CH-7	6.94	d	117.56
	CH-2	7.12	dd	118.90
	CH-5	7.19	d	117.81
	CH-6	7.65	d	149.59
Formic acid (FA)	CH	8.46	s	171.90
Fumaric acid (FumA)	CH=CH	6.51	s	137.94
Lactic acid (LA)	CH ₃	1.32	d	22.95
	CH	4.11	q	77.04
Malic acid (MA)	α - CH	4.31	dd	69.33
	β,β' - CH	2.38,2.69	dd	40.86
Neochlorogenic acid (nCGA)	CH ₂ -2'	1.92,2.09	m	40.11
	CH-3'	4.04	dd	75.43
	CH-4'	3.61	dd	72.93
	CH-5'	5.35	m	43.23
	CH ₂ -6'	2.09,2.23	m	40.14
	CH-8	6.43	d	115.95
	CH-7	7.66	d	117.56
	CH-2	7.22	d	118.90
	CH-5	6.96	dd	117.81

	CH-6	6.15	d	149.59
Succinic acid (SA)	2 CH ₂	2.39	s	36.31
<u>Amino acids</u>				
Alanine (Ala)	β-CH₃	1.49	d	19.05
	α- CH	3.80	q	53.56
Arginine (Arg)	γ- CH ₂	1.69	m	30.51
	β- CH ₂	1.95	m	43.27
	δ- CH₂	3.21	t	43.12
	α- CH ₂	3.78	t	57.32
Aspartic acid (Asp)	β'-CH	2.68	dd	39.31
	β-CH	2.72	dd	39.31
	α-CH	3.91	m	55.09
Asparagine (Asn)	β'-CH	2.86	dd	37.44
	β-CH	2.89	dd	37.44
	α-CH	4.01	m	54.09
Glutamate (Glu)	γ- CH ₂	2.07	m	29.25
	β,β-CH₂	2.35	m	37.12
	α-CH	3.78	m	58.01
Glutamine (Gln)	γ- CH ₂	2.11	m	29.31
	β,β-CH₂	2.45	m	34.02
	α-CH	3.81	m	57.19
Histidine (His)	CH-6	3.19	dd	30.25
	CH-7	3.99	dd	57.29
	CH-5	7.09	d	120.03
	CH-2	8.01	d	138.31
Isoleucine (Ile)	δ-CH ₃	0.95	t	13.85
	γ-CH₃	1.02	d	17.38
	γ'-CH	1.25	m	27.01
	γ''-CH	1.49	m	27.01
	β-CH	1.99	m	38.71
	α-CH	3.69	m	63.04
Leucine (Leu)	δ,δ'- CH₃	0.97	m	23.85, 24.59

	γ -CH	1.72	m	26.81
	β -CH ₂	1.73	m	42.60
	α -CH	3.74	m	56.21
γ-aminobutyric acid (GABA)	β-CH₂	1.95	t	26.38
	γ -CH ₂	2.30	m	37.06
	α -CH ₂	3.01	t	42.21
Phenylalanine (Phe)	CH-2,6	7.32	d	130.3
	CH-4	7.38	d	128.6
	CH-3,5	7.42	d	130.3
	β -CH ₂	3.27	m	37.1
	α -CH	3.98	dd	56.8
Threonine (Thr)	γ-CH₃	1.33	d	22.15
	α -CH	3.60	m	63.46
	β -CH	4.27	m	68.94
Tyrosine (Tyr)	CH-2,6	7.22	d	130.0
	CH-3,5	7.08	d	117.0
	β -CH ₂	3.15	dd	37.1
	α -CH	3.93	dd	56.8
Valine (Val)	γ -CH ₃	0.99	d	19.41
	γ'-CH₃	1.05	d	20.75
	β -CH	2.29	m	31.89
	α -CH	3.62	m	63.36
<u>Carbohydrates</u>				
α-Glucose (α-G)	CH-1	5.25	d	93.10
	CH-2	3.55	m	72.49
	CH-3	3.72	m	73.84
	CH-4	3.42	m	70.67
	CH-5	3.84	m	72.52
	CH ₂ -6	3.73, 3.90	m	96.97
β-Glucose (β-G)	CH-1	4.69	d	96.97
	CH-2	3.26	m	75.17
	CH-3	3.50	m	76.84
	CH-4	3.42	m	70.70

	CH-5	3.48	m	74.57
	CH ₂ -6	3.74, 3.91	m	61.80
α-Xylose (α-X)	CH-1	5.17	d	93.1
	CH-6	3.80	m	72.5
	CH-3	3.70	m	73.8
	CH-5	3.45	m	70.7
	CH-2	3.35	m	72.5
	CH ₂ -6	3.73-3.90	m	96.9
β-Xylose (β-X)	CH-1	4.56	d	97.0
	CH-5	3.87	m	74.6
	CH-3	3.69	m	76.8
	CH-4	3.36	m	70.7
	CH-2	3.18	m	75.2
Sucrose (S)	GLC CH-1	5.42	d	93.22
	CH-2	3.59	m	72.11
	CH-3	3.79	m	73.54
	CH-4	3.48	m	70.26
	CH-5	3.85	m	73.38
	CH ₂ -6	3.82	m	61.18
	FRU CH ₂ -1'	3.69	m	62.44
	C-2	\	\	104.85
	CH-3'	4.22	m	77.45
	CH-4'	4.06	m	75.04
	CH-5'	3.90	m	82.44
	CH ₂ -6	3.82	m	63.38
Raffinose (R)	CH-1 Glucose	5.45	d	96.41
	CH-2 G	3.55	dd	73.69
	CH-3 G	3.74	dd	75.34
	CH-4 G	3.53	dd	72.05
	CH-5 G	4.05	m	74.11
	CH ₂ -6 G	4.69-4.02	m	68.37
	CH-1 Galactose	5.01	d	101.08
	CH-2 g	3.82	dd	71.03
	CH-3 g	3.89	dd	72.04

	CH-4 g	3.98	dd	83.88
	CH-5 g	3.95	m	73.71
	CH2-6 g	3.73	m	63.72
	CH-1 Fructose	3.67	s	64.01
	C-2 F	/	/	104.88
	CH-3 F	4.22	d	79.00
	CH-4	4.05	dd	79.69
	CH-5	3.88	m	83.98
	CH2-6	3.77-3.82	m	65.05
<u>Lipids & Sterols</u>				
Stearic acid (SFA)	CH ₃	0.87	t	14.05
	n-CH ₂	1.26	m	29.32
	CH ₂ -CH ₂ -CO ₂ ⁻	1.62	m	24.61
	CH₂-CO₂⁻	2.30	t	33.52
Linoleic acid (ω-6)	CH ₃	0.86	t	14.06
	n-CH ₂	1.36	m	29.37
	CH ₂ -CH=CH	2.04	m	29.45
	CH=CH	5.37	m	130.29; 128.45
	=CH-CH₂-CH=	2.76	t	25.68
	CH ₂ -CH ₂ -CO ₂ ⁻	2.06	m	24.75
	CH ₂ -CO ₂ ⁻	2.31	t	34.05
β-Sitosterol (β-ST)	CH ₂ -1	1.08, 1.85	m	37.19
	CH ₂ -2	1.51, 1.84	m	31.50
	CHOH-3	3.52	m	71.81
	CH ₂ -4	2.28	m	42.37
	CH-6	5.34	m	121.79
	CH ₂ -7	1.52, 1.98	m	31.98
	CH-8	1.46	m	31.78
	CH-14	0.99	m	56.74
	CH ₂ -15	1.57	m	24.25
	CH ₂ -16	1.26, 1.85	m	28.37
	CH₃-18	0.68	s	12.20
	CH ₃ -25	1.01	s	19.12
Campsterol (Camp)	CH ₂ -1	1.08, 1.85	m	37.19

	CH ₂ -2	1.51, 1.84	m	31.50
	CHOH-3	3.52	m	71.81
	CH ₂ -4	2.28	m	42.37
	CH-6	5.34	m	121.79
	CH ₂ -7	1.52, 1.98	m	31.98
	CH-8	1.46	m	31.78
	CH-14	0.99	m	56.74
	CH ₂ -15	1.57	m	24.25
	CH ₂ -16	1.26, 1.85	m	28.37
	CH₃-18	0.70	s	12.21
	CH ₃ -25	1.01	s	19.12
<u>Miscellaneous Metabolites</u>				
Choline (Chn)	N(CH₃)₃	3.20	s	56.70
Betaine (Bet)	N-(CH₃)₃ CH ₂	3.26 3.84	s s	55.95 68.58
Trigonelline (Trg)	N-CH ₃ CH ₄ CH ₃ ,5 CH1	4.42 8.07 8.82 9.11	s m m s	51.1 130.4 148.5 148.1
Uracile (Ur)	CH-5 CH-6	5.92 7.85	d d	103.7 146.3
Nicotinamide adenine dinucleotide (NAD)	CH-2 CH-4 CH-6 CH-5	9.45 9.21 8.95 8.48	s dd dd m	151.42 153.25 138.89 126.84
Monoacylglycerol (MAG)	CH₂ CH ₂ CH	3.65-3,55 4.05-4.15 3.82	dd dd m	65.45 70.32 75.12
Phospholipids (PP)	CH 2CH₂	5.13-5.21 4.15-4.29	bm dd	77.45 68.23
Carotenoids (Crt)	CH ₂ -2,2' CH ₂ -3,3' CH ₂ -4,4' CH-7,7'	1.47 1.62 2.02 6.15	m m m d	39.62 19.27 33.18 126.68

	CH-8,8'	6.14	d	137.78
	CH-10,10'	6.14	d	130.88
	CH-11,11'	6.68	m	125.04
	CH-12,12'	6.35	d	137.26
	CH-14,14'	6.25	d	132.45
	CH-15,15'	6.63	m	130.02
	CH ₃ -16,16',17,17'	1.03	s	29.01
	CH ₃ -18,18'	1.72	s	21.77
	CH ₃ -19,19'	1.97	s	12.81
Total Chlorofylls	CH-5	9.57	s	137.6
	CH-10	9.22	s	108.2
	CH-20	8.41	s	93.4

In bold are evidenced the resonances chosen for metabolite quantification; s: singlet, d: doublet, t: triplet, q: quadruplet, dd: doublet of doublets, m: multiplet, bm: broad multiplet.