

Free Amino Acids, Fatty Acids, and Phenolic Compounds in Tartary Buckwheat of Different Hull Colour

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Electronic supplementary material (ESM)

Table S1. Chromatographic and MRM method parameters for free amino acids using UPLC–MS/MS

Amino acid	Labeled ion-pairs	Dwell (s)	Cone Volt	Collision Energy
Gly	132.1 > 76	0.05	15	10
Ala	146.1 > 44.3	0.05	15	16
β-Ala	146.1 > 72.2	0.05	15	13
GABA	160.1 > 87	0.05	15	15
Ser	162.1 > 60	0.05	15	10
Pro	172.1 > 70	0.05	15	10
Thr	176.1 > 74	0.05	15	15
Asn	189.1 > 144	0.05	15	10
Lys	203.1 > 84	0.05	15	20
His	212.1 > 110	0.05	15	10
Arg	231.2 > 70	0.05	15	30
Val	174.2 > 72	0.05	15	10
Ile	188.2 > 69	0.05	20	20
Leu	188.2 > 86	0.05	15	10
Met	206.1 > 104	0.05	15	10
Phe	222.2 > 120	0.05	15	10
Tyr	238.1 > 136	0.05	15	20
Asp	246.2 > 144	0.05	15	10
Glu	260.2 > 84	0.05	15	25
Trp	261.2 > 159	0.05	15	10

Table S2. Calibration linearity (R^2), limit of detection (LOD), and precision for fatty acids

No.	Abbreviation	Rt (min)	linear equation	R^2	Lr (mg/l)	RSD (%)	LOD (mg/l)
1	C4:0	3.665	$y = 0.428x + 0.0166$	0.998	0.4~80	2.01	0.032
2	C6:0	6.802	$y = 1.89x - 0.0166$	0.999	0.4~80	1.33	0.019
3	C8:0	9.904	$y = 2.82x - 0.0341$	0.999	0.4~80	1.42	0.024
4	C10:0	12.613	$y = 3.24x - 0.0399$	0.999	0.4~80	1.48	0.023
5	C11:0	13.847	$y = 3.37x - 0.0265$	0.998	0.2~40	1.94	0.013
6	C12:0	15.013	$y = 3.51x - 0.0554$	0.998	0.4~80	1.63	0.028
7	C13:0	16.110	$y = 3.5x - 0.0295$	0.998	0.2~40	1.58	0.014
8	C14:0	17.173	$y = 3.57x - 0.0538$	0.998	0.4~80	1.13	0.031
9	C14:1	17.567	$y = 1.32x - 0.00737$	0.998	0.2~40	5.00	0.040
10	C15:0	18.184	$y = 3.51x - 0.0292$	0.998	0.2~40	1.43	0.031
11	C15:1	18.578	$y = 1.40x - 0.0117$	0.998	0.2~40	2.17	0.024
12	C16:0	19.144	$y = 3.50x - 0.0446$	0.998	0.6~120	1.18	0.060
13	C16:1	19.418	$y = 1.49x - 0.0704$	0.996	0.2~40	7.89	0.870
14	C17:0	20.07	$y = 3.44x - 0.0162$	0.997	0.2~40	0.99	0.034
15	C17:1	20.344	$y = 1.21x - 0.00747$	0.996	0.2~40	1.67	0.041
16	C18:0	21.081	$y = 3.37x - 0.0345$	0.997	0.4~80	2.17	0.032
17	C18:1	21.338	$y = 0.806x + 0.03$	0.996	0.6~120	1.88	0.025
18	C18:2	21.904	$y = 1.16x - 0.0205$	0.997	0.6~120	1.84	0.028
19	C18:3n-6	22.315	$y = 1.15x - 0.0318$	0.996	0.2~40	2.10	0.111
20	C18:3n-3	22.795	$y = 1.12x - 0.0112$	0.996	0.2~40	2.00	0.019
21	C20:0	23.738	$y = 2.83x - 0.0574$	0.997	0.4~80	1.70	0.036
22	C20:1	24.132	$y = 1.17x - 0.00918$	0.997	0.2~40	5.25	0.030
23	C20:2	25.058	$y = 1.08x - 0.0120$	0.996	0.2~40	1.07	0.035
25	C21:0	25.606	$y = 2.59x - 0.0317$	0.996	0.2~40	2.28	0.019
26	C20:4n-6	26.189	$y = 0.717x - 0.00842$	0.996	0.2~40	1.83	0.043
27	C20:3n-3	26.498	$y = 0.988x - 0.0123$	0.996	0.2~40	2.02	0.032
28	C20:5n-3	27.869	$y = 8.66x - 0.0691$	0.997	0.2~40	1.34	0.018
29	C22:0	28.023	$y = 13.7x - 0.338$	0.996	0.4~80	1.90	0.042
30	C22:1n-9	28.675	$y = 1.17x - 0.183$	0.996	0.2~40	1.97	0.214
31	C22:2	30.252	$y = 1.01x - 0.0125$	0.996	0.2~40	2.63	0.023
32	C23:0	31.143	$y = 1.95x - 0.0435$	0.995	0.2~40	3.77	0.044
33	C24:0	35.257	$y = 1.78x - 0.0692$	0.996	0.4~80	2.61	0.074
34	C24:1	36.372	$y = 1.3x - 0.0334$	0.996	0.2~40	1.43	0.067
35	C22:6n-3	36.509	$y = 0.681x - 0.0172$	0.996	0.2~40	4.24	0.049

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Table S3. Concentration (in mg/100 g) of amino acid, fatty acid, and phenolic compounds in buckwheat flour

	Flour						
	gy1-f	mql-f	jq4-f	jq2-f	fh-f	xq1-f	yq1-f
C14:0	12.2 ± 0.5	11.3 ± 0.4	10.2 ± 0.4	12.4 ± 0.4	13.0 ± 0.5	10.9 ± 0.3	11.7 ± 0.3
C16:0	251.3 ± 8.1	184.2 ± 9.2	112.7 ± 5.1	327.9 ± 12.5	252.7 ± 8.9	163.5 ± 0.7	178.8 ± 0.5
C18:0	105.9 ± 4.1	66.5 ± 3.2	35.2 ± 1.3	135.6 ± 4.3	112.8 ± 4.2	64.9 ± 2.3	82.1 ± 3.9
C18:1	324.4 ± 16.2	285.8 ± 15.8	215.6 ± 14.3	262.0 ± 13.5	220.7 ± 11.1	243.9 ± 15.0	198 ± 9.8
C18:2n-6c	380.5 ± 14.3	246.5 ± 10.8	229.4 ± 8.9	308.6 ± 13.5	259.8 ± 15.2	269.3 ± 11.0	204.9 ± 8.9
C18:3n-3	29.9 ± 9.8	25.1 ± 1.2	16.7 ± 0.9	45.4 ± 2.1	20.0 ± 0.8	24.0 ± 1.0	23.3 ± 1.1
C20:0	16.9 ± 0.7	14.9 ± 0.6	14.4 ± 0.5	15.9 ± 0.5	14.8 ± 0.7	15.0 ± 0.6	14.2 ± 0.6
C20:1	12.7 ± 0.5	11.0 ± 0.4	5.4 ± 0.3	10.4 ± 0.7	4.7 ± 0.1	4.8 ± 0.2	4.6 ± 0.2
Ala	8.2 ± 0.3	3.6 ± 0.1	10.5 ± 0.5	5.1 ± 0.2	4.9 ± 0.3	4.8 ± 0.2	5.7 ± 0.3
Arg	127.1 ± 5.2	80.5 ± 3.5	287.7 ± 11.3	56.8 ± 2.8	114.5 ± 5.1	42.7 ± 2.1	19.1 ± 0.9
Asn	10.8 ± 0.4	4.9 ± 0.1	7.9 ± 0.2	4.6 ± 0.2	4.8 ± 0.2	3.3 ± 0.1	2.5 ± 0.1
Asp	37.3 ± 1.7	22.1 ± 1.2	42.3 ± 2.1	18.1 ± 0.8	18.9 ± 0.7	15.3 ± 0.6	10.4 ± 0.4
β-Ala	12.5 ± 1.0	5.2 ± 0.6	10.5 ± 0.9	5.8 ± 0.5	4.5 ± 0.4	4.2 ± 0.3	4.1 ± 0.5
GABA	72.6 ± 5.1	30.6 ± 1.6	77.3 ± 3.8	38.9 ± 1.8	42.2 ± 2.6	43.5 ± 2.3	46.4 ± 1.3
Glu	259.9 ± 10.2	129.1 ± 6.1	281.1 ± 12.0	110.6 ± 5.3	118.6 ± 4.8	90.1 ± 4.1	75.3 ± 3.1
Gly	7.0 ± 0.6	3.2 ± 0.3	5.0 ± 0.6	2.9 ± 0.3	3.8 ± 0.4	3.2 ± 0.3	4.3 ± 0.4
His	3.3 ± 0.2	1.5 ± 0.2	3.7 ± 0.2	2.5 ± 0.2	2.7 ± 0.3	1.3 ± 0.2	0.8 ± 0.1
Ile	nd	nd	nd	nd	nd	nd	nd
Leu	6.3 ± 0.4	2.4 ± 0.1	7.0 ± 0.5	3.1 ± 0.3	2.8 ± 0.2	2.4 ± 0.2	2.6 ± 0.1
Met	0.7 ± 0.06	0.3 ± 0.04	0.8 ± 0.07	0.50 ± 0.05	0.4 ± 0.05	0.5 ± 0.06	0.4 ± 0.05
Phe	7.0 ± 0.6	4.6 ± 0.4	7.2 ± 0.6	3.2 ± 0.3	2.3 ± 0.3	2.5 ± 0.3	3.0 ± 0.3
Pro	10.3 ± 0.8	3.7 ± 0.3	9.5 ± 0.8	4.6 ± 0.3	5.1 ± 0.4	6.8 ± 0.4	6.1 ± 0.5
Ser	2.5 ± 0.2	1.6 ± 0.1	3.3 ± 0.2	0.8 ± 0.6	1.5 ± 0.1	1.1 ± 0.1	1.4 ± 0.1
Thr	1.0 ± 0.1	0.4 ± 0.05	1.1 ± 0.09	0.6 ± 0.05	0.7 ± 0.06	0.6 ± 0.06	0.6 ± 0.05
Trp	5.6 ± 0.5	4.9 ± 0.4	4.7 ± 0.3	3.3 ± 0.4	3.2 ± 0.3	2.4 ± 0.2	2.7 ± 0.2
Tyr	3.5 ± 0.3	1.8 ± 0.2	2.1 ± 0.2	1.2 ± 0.1	1.4 ± 0.1	2.1 ± 0.2	2.3 ± 0.2
Val	3.6 ± 0.2	1.6 ± 0.2	4.1 ± 0.3	1.6 ± 0.2	1.5 ± 0.2	1.4 ± 0.2	1.6 ± 0.1
Lys	10.7 ± 0.8	2.0 ± 0.9	4.3 ± 0.4	2.2 ± 0.2	2.9 ± 0.3	2.6 ± 0.3	2.5 ± 0.2
Caffeic acid	54 ± 2	19 ± 1	42 ± 1	18 ± 0	21 ± 1	31 ± 0	30 ± 0
Vitexin	3 ± 0	1 ± 0	2 ± 0	1 ± 0	2 ± 0	2 ± 0	2 ± 0
Rutin	1337 ± 28	1033 ± 42	1063 ± 34	854 ± 8	972 ± 27	762 ± 43	875 ± 45
Quercitrin	69 ± 1	62 ± 3	58 ± 2	53 ± 1	57 ± 2	43 ± 1	52 ± 1
Quercetin	41 ± 4	29 ± 2	28 ± 3	23 ± 1	29 ± 2	25 ± 2	29 ± 4
Kaempferol	1 ± 0	1 ± 0	1 ± 0	1 ± 0	1 ± 0	1 ± 0	1 ± 0

nd – not detected

Table S4. Concentration (in mg/100 g) of amino acid, fatty acid, and phenolic compounds in buckwheat bran

	Bran						
	gy1-b	mql1-b	jq4-b	jq2-b	fh-b	xq1-b	yq1-b
C14:0	24.4 ± 1.1	22.6 ± 1.0	23.8 ± 0.9	23.0 ± 0.9	22.6 ± 1.0	22.4 ± 0.9	22.8 ± 0.8
C16:0	503.6 ± 20.1	380.4 ± 17.5	444.6 ± 18.4	375.2 ± 15.3	365.8 ± 16.2	384.6 ± 15.6	391.0 ± 15.1
C18:0	186.2 ± 8.6	148.4 ± 6.5	118.2 ± 5.4	93.6 ± 4.1	97.2 ± 4.5	100.2 ± 4.8	135.6 ± 6.1
C18:1	616.6 ± 20.1	440.0 ± 15.4	759 ± 21.2	631.2 ± 19.5	583.4 ± 16.2	671.8 ± 18.1	618.8 ± 15.1
C18:2n-6c	815.4 ± 21.3	456.8 ± 15.6	929.8 ± 23.1	861.6 ± 22.2	864.8 ± 20.7	879.8 ± 18.9	743.2 ± 17.6
C18:3n-3	46.4 ± 2.3	37.4 ± 2.1	44.6 ± 2.1	44.8 ± 1.9	39.0 ± 1.8	45.8 ± 2.3	43.0 ± 2.2
C20:0	33.0 ± 1.7	25.2 ± 1.6	35.8 ± 1.6	33.8 ± 1.8	33.0 ± 1.5	34.0 ± 1.6	32.4 ± 1.5
C20:1	25.6 ± 1.6	17.4 ± 1.0	27.0 ± 1.5	24.4 ± 1.1	25.4 ± 1.2	29.2 ± 1.0	22.6 ± 0.9
Ala	20.5 ± 1.8	9.5 ± 0.7	27.5 ± 1.9	24.1 ± 1.8	9.8 ± 0.6	21.7 ± 1.1	26.6 ± 1.3
Arg	531.7 ± 18.6	180.9 ± 9.8	466.7 ± 19.5	448.1 ± 18.7	329.6 ± 15.3	363.1 ± 14.6	225.3 ± 10.2
Asn	35.6 ± 2.3	12.2 ± 0.9	24.9 ± 1.8	23.8 ± 1.7	13.5 ± 0.9	22.0 ± 1.0	17.5 ± 1.2
Asp	121.4 ± 6.1	60.1 ± 3.2	124.0 ± 7.5	112.5 ± 6.3	62.6 ± 3.6	93.8 ± 5.6	93.9 ± 4.8
β-Ala	33.0 ± 1.6	12.2 ± 0.8	34.7 ± 2.1	24.0 ± 1.2	11.3 ± 0.7	23.3 ± 1.3	24.6 ± 1.1
GABA	127.5 ± 9.4	62.2 ± 4.1	272.5 ± 18.6	171.9 ± 1.2	60.6 ± 4.3	152.2 ± 9.5	157.3 ± 8.9
Glu	677.9 ± 31.2	389.9 ± 19.2	757.7 ± 30.3	640.7 ± 31.5	328.6 ± 17.8	476.0 ± 20.1	436.9 ± 18.9
Gly	16.3 ± 0.8	5.9 ± 0.5	11.3 ± 0.8	10.0 ± 0.7	5.4 ± 0.4	10.8 ± 0.6	11.0 ± 0.6
His	6.9 ± 0.5	4.2 ± 0.5	10.7 ± 0.7	7.3 ± 0.4	6.5 ± 0.5	5.8 ± 0.5	5.6 ± 0.5
Ile	0.2 ± 0.02	nd	0.1 ± 0.02	0.1 ± 0.02	nd	0.1 ± 0.01	0.1 ± 0.03
Leu	20.5 ± 1.2	5.3 ± 0.4	21.2 ± 1.8	13.9 ± 0.8	6.4 ± 0.4	11.8 ± 1.0	11.3 ± 0.9
Met	1.5 ± 0.1	0.5 ± 0.04	2.2 ± 0.2	1.7 ± 0.1	0.4 ± 0.03	1.2 ± 0.1	1.1 ± 0.1
Phe	19.3 ± 1.2	11.3 ± 0.1	20.0 ± 0.9	11.3 ± 0.6	5.6 ± 0.5	12.1 ± 0.7	14.5 ± 0.8
Pro	29.1 ± 1.8	8.9 ± 0.5	23.6 ± 1.4	21.3 ± 1.2	9.7 ± 0.6	17.1 ± 1.0	18.4 ± 0.9
Ser	5.4 ± 0.4	2.7 ± 0.2	7.2 ± 0.5	4.3 ± 0.2	1.8 ± 0.1	3.8 ± 0.2	3.0 ± 0.1
Thr	2.6 ± 0.2	0.9 ± 0.06	2.5 ± 0.1	2.4 ± 0.1	1.1 ± 0.2	1.8 ± 0.1	1.9 ± 0.2
Trp	17.1 ± 1.0	12.1 ± 0.7	12.3 ± 0.6	19.9 ± 0.8	7.6 ± 0.5	17.5 ± 1.1	9.5 ± 0.5
Tyr	39.8 ± 2.1	2.2 ± 0.1	62.0 ± 4.2	35.5 ± 2.1	2.5 ± 0.3	53.5 ± 3.1	86.7 ± 5.6
Val	11.3 ± 0.8	3.6 ± 0.2	9.5 ± 0.5	7.5 ± 0.6	3.3 ± 0.3	7.3 ± 0.5	7.7 ± 0.6
Lys	21.4 ± 1.0	3.5 ± 0.3	10.9 ± 0.5	9.1 ± 0.4	4.7 ± 0.3	6.5 ± 0.4	7.6 ± 0.5
Caffeic acid	140 ± 8	50 ± 4	125 ± 7	64 ± 4	87 ± 20	119 ± 3	110 ± 5
Vitexin	7 ± 0	3 ± 0	6 ± 0	4 ± 0	8 ± 4	5 ± 0	5 ± 0
Rutin	5212 ± 97	3554 ± 6	4160 ± 638	3622 ± 403	4376 ± 587	4320 ± 153	4676 ± 4.87
Quercitrin	287 ± 5	223 ± 12	263 ± 6	282 ± 15	274 ± 34	263 ± 5	296 ± 9
Ferulic acid	88 ± 6	54 ± 3	63 ± 3	67 ± 2	68 ± 1	75 ± 5	69 ± 5
Quercetin	4 ± 0	2 ± 0	3 ± 0	4 ± 1	5 ± 1	4 ± 1	4 ± 0

nd – not detected