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Biochemical profiling of steamed leaf extracts used in traditional food wrapping

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Supplementary Data

Supplementary Table S1 Multiple reactions monitoring (MRM) details for LC-MS/MS estimation of Phenolic acids

Compound	Formula/ Mass	t_R	Parent m/z	Cone Voltage	Daughters	Collision Energy	Ion Mode
Caffeic acid	180	6.61	178.90	30	135.05	16	ES-
2,4-Dihydroxybenzoic acid	154	6.50	152.90	28	65.20	18	ES-
Ferulic acid	194	9.36	192.90	26	134.02	14	ES-
Gallic acid	170	2.10	168.90	28	125.03	12	ES-
Gentisic acid	154	5.69	152.90	24	108.98	12	ES-
o-Coumaric acid	164	8.39	162.90	22	119.06	12	ES-
p-Coumaric acid	164	8.34	162.90	24	119.05	14	ES-
p-Hydroxybenzoic acid	138	5.69	136.90	26	93.01	12	ES-
Protocatecuic acid	154	4.24	152.90	26	109.05	16	ES-
Salicylic acid	138	12.70	136.90	28	93.10	14	ES-
t-Cinnamic acid	148	11.08	146.90	26	103.05	10	ES-
Vanillic acid	168	6.48	166.97	26	108.01	20	ES-
Benzoic acid	122	11.35	120.96	26	77.02	10	ES-
3-Hydroxy Benzoic acid	138	6.76	137.02	28	93.05	10	ES-
Sinapic acid	224	9.66	223.11	32	164.1	14	ES-
Ellagic acid	302	8.22	301.09	70	284.01	28	ES-

Supplementary Table S2 Multiple reactions monitoring (MRM) details for LC-MS/MS estimation of Flavonoids

Flavonoids	Formula/Mass	t_R	Parent m/z $[M+H]^-$	Cone Voltage (V)	Daughters	Collision Energy (CE)	Ion Mode
Apigenin	270	7.07	268.97	46	107.04	30	ES-
Catechin	290	1.15	289.03	38	245.15	12	ES-
Hesperetin	302	6.62	300.97	42	286.15	16	ES-
Leutoline	286	6.47	284.9	54	150.99	26	ES-
Myricetin	318	5.21	317.03	42	151.06	28	ES-
Naringenin	272	6.39	271.03	34	151	16	ES-
Quercetin	302	6.19	301.03	36	151.12	20	ES-
Rutin	610	4.66	609.10	60	300.20	42	ES-
Epicatechin	290	1.67	289.05	36	109.08	22	ES-
Epigallocatechin	458	0.79	305.05	34	164.7	18	ES-

Supplementary Table S3 Multiple reaction monitoring (MRM) details for LC-MS/MS estimation of organic acids

Water soluble organic acids	Formula/Mass	Parent m/z $[M+H]^+$	Daughters	Cone voltage (V)	Collision energy (CE)	Ion Mode
Citric acid	191.99	190.96	111.09	20	10	ES^-
Fumaric acid	116	114.84	70.99	20	8	ES^-
Maleic acid	116	114.84	70.98	20	12	ES^-
Malic acid	134	132.84	115.03	18	12	ES^-
Malonic acid	104	102.84	59.00	24	6	ES^-
Oxalic acid	90	88.78	44.98, 60.95	16, 20	8	ES^-
Oxaloacetic acid	132	130.84	87.02	20	8	ES^-
Pyruvic acid	88.03	86.87	43.02	12	6	ES^-
Shikimic acid	174.03	172.93	93.05	22	14	ES^-
Succinic acid	118	116.84	73.00	34	10	ES^-
Tartaric acid	150	148.84	87.01, 73.00 73.00	20, 22 22	10 12	ES^-

Supplementary Table S4 Multiple reaction monitoring (MRM) details for LC-MS/MS estimation of Water soluble vitamins

Sl. No.	Compounds	Formula/Mass	Parent ion (m/z) $[M+H]^+$	Daughters	Cone voltage (V)	Collision energy (eV)	Ion mode
			Water soluble vitamins				
1	Thiamine (B1)	264	265.03	122.06	20	16	ES+
			265.03	144.02	20	14	
2	Riboflavin (B2)	376	376.97	243.05	40	24	ES+
3	Niacin (B3)	123	123.9	80.523	34	20	ES+
			123.9	77.47	34	18	
4	Pantothenic acid (B5)	219.03	220.01	202.21	28	12	ES+
			220.01	124.16	28	20	
5	Pyridoxine (B6)	169	169.97	152.09	24	12	ES+
			169.97	134.04		20	ES+
6	Folic acid (B9)	441	442.1	295.16	24	16	ES+
7	Cyanocobalamin (B12)	677	678.29	147.18	38	68	ES+