

Supplementary material

Development and Validation of a LC-QTOF-MS/MS Method to Assess the Phenolic Profile of Pulse Flours

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Table S1. Granulometric composition of wheat, lupin, and chickpea flours from commercial and Lemnos sources.

Mean particle size (μm)	WFC (%)	WFL (%)	LFC (%)	LFL (%)	CFC (%)	CFL (%)	GSFC (%)	GSFL (%)	OSFC (%)	OSFL (%)
9	6.49	0.27	0.37	0.32	0.35	0.48	0.30	0.32	0.23	0.36
79.5	18.66	55.56	4.86	1.47	1.20	3.74	1.98	0.96	0.36	3.32
175	4.43	11.37	2.16	3.82	1.87	2.39	1.52	1.15	0.68	1.69
250	21.08	27.54	6.79	6.97	2.38	5.64	6.75	5.07	2.18	2.54
350	1.14	2.97	10.85	13.76	4.46	3.02	2.21	4.67	10.55	11.55
500	0.68	1.86	36.72	24.27	16.24	54.24	20.73	48.38	75.03	51.73
600	47.52	0.44	38.26	49.39	73.50	30.49	66.50	39.46	10.98	28.81

***WFC: wheat flour commercial; WFL: wheat flour Lemnos; LFC: lupin flour commercial; LFL: lupin flour Lemnos; CFC: chickpea flour commercial; CFL: chickpea flour Lemnos; GSFC: grape seed flour commercial; GSFL: grape seed flour Lemnos; OSFC: olive stone flour commercial; OSFL: olive stone flour Lemnos**

Table S2. Validation results

Compound	Equation y = (a ± Sa) + (b ± Sb)x Linearity range: LOQ – 5 mg/Kg	R ²	RE %	LOD (mg/Kg)	LOQ (mg/Kg)	Intra-day % RSD			Inter-day % RSD			% Matri x Effect
						(n = 6)			(n = 3 × 3)			
						Concentration Level (mg/Kg)			Concentration Level (mg/Kg)			
						LOQ	1	5	LOQ	1	5	
Apigenin	y = (55655224 ± 32522) x + (212649 ± 102221)	0.993 2	88.1	0.2	0.5	4.3	4.2	5.0	3.1	4.1	4.2	-9.1
Caffeic acid	y = (4689561 ± 15522) x + (135224 ± 30255)	0.992 5	82.4	0.2	0.8	2.1	3.3	2.7	3.5	3.1	4.1	-8.5
p-Coumaric acid	y = (2565452 ± 100224) x - (7950 ± 6552)	0.992 1	90.5	0.2	0.5	3.4	8.1	2.5	5.2	3.8	4.3	-10.6
Chrysin	y = (95221 ± 4235) x + (50321 ± 10214)	0.993 5	83.4	0.2	0.5	2.1	3.5	4.7	4.4	6.4	3.5	-12.5
Diosmin	y = (1865458 ± 19252) x + (215423 ± 53452)	0.999 5	92.7	0.2	0.5	3.2	2.9	2.6	2.9	5.1	3.2	-7.5
Ferulic acid	y = (1745523 ± 6325) x + (61563 ± 15654)	0.999 2	89.1	0.3	1.0	1.4	2.7	5.9	3.4	3.7	4.0	-9.9
Kaempferol	y = (178562 ± 10121) x + (32565 ± 18452)	0.997 1	88.7	0.3	0.9	2.2	2.1	5.1	5.4	5.8	3.2	-12.2
Luteolin	y = (10565853 ± 124563) x + (365452 ± 304523)	0.998 5	86.3	0.03	0.1	3.4	2.5	4.6	3.2	3.7	5.1	-6.5
Naringin	y = (22532241 ± 1235232) x + (12252324 ± 3020456)	0.993 2	92.4	0.2	0.8	2.3	1.8	1.9	4.1	2.4	5.0	-10.4
Quercetin	y = (11452568 ± 554562) x + (5032652 ± 1452565)	0.994 4	93.3	0.2	0.8	2.4	1.3	2.1	5.2	1.2	4.1	-8.8
Quercitrin	y = (2452326 ± 22352) x - (165251 ± 50451)	0.998 5	92.4	0.03	0.1	2.5	1.2	2.1	4.7	3.5	10.9	-11.4
Rutin	y = (16525844 ± 545625) x + (3565245 ± 1315425)	0.996 6	95.4	0.2	0.7	1.6	1.9	3.3	4.3	2.8	4.6	-5.6
Sinapic acid	y = (10645287 ± 9154630) x - (355456 ± 221145)	0.997 4	93.4	0.2	0.5	2.4	1.4	2.2	4.1	4.1	5.1	-9.5
Taxifolin	y = (9456544 ± 235006) x + (940632 ± 523248)	0.998 4	92.7	0.2	0.5	2.7	2.5	2.3	4.4	5.1	4.1	-8.2
Vanillin	y = (821065 ± 2224) x + (27556 ± 5652)	0.996 5	91.1	0.03	0.1	1.5	3.7	3.4	4.2	4.1	4.4	-11.5
Vanillic acid	y = (435651 ± 4108) x - (10454 ± 10335)	0.997 8	90.8	0.3	0.9	4.3	2.6	2.5	3.5	3.2	4.2	-14.7

Table S3. Target screening list of compounds

Compound	Molecular formula	Class
Apigenin	C ₁₅ H ₁₀ O ₅	Flavonoids
Caffeic acid	C ₉ H ₈ O ₄	Cinnamic acids and derivatives
Catechin	C ₁₅ H ₁₄ O ₆	Flavonoids
Chrysin	C ₁₅ H ₁₀ O ₄	Flavonoids
Cinammic acid	C ₁₄ H ₁₀ N ₂ O ₄ S	Cinnamic acids and derivatives
Coumaric acid	C ₉ H ₈ O ₃	Cinnamic acids and derivatives
Diosmin	C ₂₈ H ₃₂ O ₁₅	Flavonoids
Epicatechin	C ₁₅ H ₁₄ O ₆	Flavonoids
Epigallocatechin	C ₁₅ H ₁₄ O ₇	Flavonoids
Ferulic acid	C ₁₀ H ₁₀ O ₄	Hydroxycinnamic acid
Gallic acid	C ₇ H ₆ O ₅	Benzene and substituted derivatives
Epicatechin gallate	C ₂₂ H ₁₈ O ₁₀	Flavonoids
Hesperidin	C ₂₈ H ₃₄ O ₁₅	Flavonoids
Kaempferol	C ₁₅ H ₁₀ O ₆	Flavonoids
Luteolin	C ₁₅ H ₁₀ O ₆	Flavonoids
Myricetin	C ₁₅ H ₁₀ O ₈	Flavonoids
Myricitrin	C ₂₁ H ₂₀ O ₁₂	Flavonoids
Naringin	C ₂₇ H ₃₂ O ₁₄	Flavonoids
Quercetin	C ₁₅ H ₁₀ O ₇	Flavonoids
Quercitrin	C ₂₁ H ₂₀ O ₁₁	Flavonoids
Rosmarinic acid	C ₁₈ H ₁₆ O ₈	Cinnamic acids and derivatives
Protocatechuic acid	C ₇ H ₆ O ₄	hydroxybenzoic acid derivatives
Rutin	C ₂₇ H ₃₀ O ₁₆	Flavonoids
Sinapic acid	C ₁₁ H ₁₂ O ₅	Hydroxycinnamic acids
Syringaldehyde	C ₉ H ₁₀ O ₄	Phenols
Syringic acid	C ₉ H ₁₀ O ₅	Benzene and substituted derivatives
Taxifolin	C ₁₅ H ₁₂ O ₇	Flavonoids
Vanillic acid	C ₈ H ₈ O ₄	Benzene and substituted derivatives
Vanillin	C ₈ H ₈ O ₃	Phenols

Table S4. Suspect screening list for wheat flour

Compound	Molecular formula	Class
2,4-Dihydroxybenzoic acid	C ₇ H ₆ O ₄	Phenolic acids
3',4',5'-trihydroxy-3,7-dimethylflavone	C ₁₇ H ₁₄ O ₇	Flavonoids
4-Hydroxybenzoic acid	C ₇ H ₆ O ₃	Benzene and substituted derivatives
Cyanidin	C ₁₅ H ₁₁ O ₆ Cl	Flavonoids
Apigenin-6-C-arabinoside-8-C-hexoside	C ₂₆ H ₂₈ O ₁₄	Flavonoids (8-c-glycosides)
apigenin-7-O-neohesperidoside	C ₂₇ H ₃₀ O ₁₄	Flavonoids (O-glycosides)
Chlorogenic acid	C ₁₆ H ₁₈ O ₉	Phenolic acid
chrysoeriol-7-O-neosperidoside	C ₂₈ H ₃₂ O ₁₅	Flavonoids (O-glycosides)
Coumarin	C ₉ H ₆ O ₂	Coumarins
Cyanidin-3-glucoside	C ₂₁ H ₂₁ O ₁₁	Flavonoids
Cyanidin-3-glucoside (kuromanin)	C ₂₁ H ₂₁ O ₁₁ Cl	Flavonoids
Delphinidin-3-glucoside	C ₂₁ H ₂₁ O ₁₂	Hydroxyflavonoids
Dihydroferulic acid	C ₂₀ H ₁₈ O ₈	Phenylpropanoic acids
Ellagic acid	C ₁₄ H ₆ O ₈	Tannins
Formononetin	C ₂₃ H ₂₄ O ₉	Isoflavonoids
Hinokinin	C ₂₀ H ₁₈ O ₆	Lignan
Hydrocinnamic acid	C ₉ H ₁₀ O ₂	Phenylpropanoids
Hydroxytyrosol	C ₈ H ₁₀ O ₃	Phenolic alcohols
Isovitexin-2''-O-rhamnoside	C ₂₇ H ₃₀ O ₁₄	Flavonoids
kaempferol-7-O-neohesperidoside	C ₂₇ H ₃₀ O ₁₅	Flavonoids (O-glycosides)
kaempferol-7-O-sopheroside	C ₂₇ H ₃₀ O ₁₆	Flavonoids (O-glycosides)
Lucenin-1/3 (luteolin-6/8-C-xyloside-8/6-C-glucoside)	C ₂₆ H ₂₈ O ₁₅	Flavonoids (8-c-glycosides)
luteolin-7-O-neohesperidoside	C ₂₇ H ₃₀ O ₁₅	Flavonoids (O-glycosides)
Methylisoorientin-2''-O-rhamnoside	C ₂₈ H ₃₂ O ₁₅	Flavonoids
Nobiletin	C ₂₁ H ₂₂ O ₈	Flavonoids
Pelargonidin-3-glucoside (callistephin)	C ₂₁ H ₂₁ O ₁₀ Cl	Flavonoids
Phloridzin	C ₂₁ H ₂₄ O ₁₀	Flavonoids
Pinoresinol	C ₂₀ H ₂₂ O ₆	Lignan
Pinosylvin	C ₂₆ H ₃₂ O ₁₂	Stilbenes
Pinosylvin (double glycosylation)	C ₂₆ H ₃₂ O ₁₂	Stilbenes

Procatechuic acid	C ₇ H ₆ O ₄	Phenolic acids
Procyanidin B3	C ₃₀ H ₂₆ O ₁₂	Proanthocyanidins
Prodelphinidin B3	C ₃₀ H ₂₆ O ₁₄	Proanthocyanidins
Prunin	C ₂₁ H ₂₂ O ₁₀	Flavonoids
quercetin-3-O-rutinoside	C ₂₇ H ₃₀ O ₁₆	Flavonoids (O-glycosides)
Salicylic acid	C ₁₂ H ₁₆ O ₃	Benzene and substituted derivatives
trans-caffeic acid	C ₉ H ₈ O ₄	Phenolic acids
trans-p-coumaric acid	C ₉ H ₈ O ₃	Phenolic acids
Tricin	C ₁₇ H ₁₄ O ₇	Flavonoids
Vicenin-2 (apigenin-6,8-di-C-glucoside)	C ₂₇ H ₃₀ O ₁₅	Flavonoids (8-c-glycosides)
Vitexin/isovitexin	C ₂₁ H ₂₀ O ₁₀	Flavonoids

Table S5. Suspect screening list for lupin flour

Compound	Molecular formula	Class
1-(3'-methoxy-4'-hydroxy)-phenyl-6,7-dihydroxyisochroman	C ₁₆ H ₁₆ O ₅	Benzopyrans
1-phenyl-6,7-dihydroxy-isochroman	C ₁₅ H ₁₄ O ₃	Benzopyrans
2'-Hydroxygenistein 7-O-glucoside	C ₂₁ H ₂₁ O ₁₁	Flavonoids (O-glycosides)
2'-Hydroxygenistein O-glucoside malonylated (I)	C ₂₄ H ₂₃ O ₁₄	Flavonoids (O-glycosides)
Kaempferol-glucoside 3	C ₂₂ H ₂₃ O ₁₀	Flavonoids
2'-hydroxygenistein	C ₁₅ H ₁₀ O ₆	Flavonoids
4-Hydroxybenzoic acid	C ₇ H ₆ O ₃	Benzene and substituted derivatives
Abscisic acid	C ₁₅ H ₂₀ O ₄	Prenol lipids
Amentoflavone	C ₃₀ H ₁₈ O ₁₀	Flavonoids
Apigenin 4', 7-O-diglucosideb 3	C ₂₇ H ₃₁ O ₁₅	Flavonoids (O-glycosides)
Apigenin 7-neohesperidoside	C ₂₇ H ₃₀ O ₁₄	Flavonoids
Apigenin 7-O-β-apiofuranosyl-6,8-di-C-β-glucopyranoside	C ₃₂ H ₃₈ O ₂₁	Flavonoids (O-glycosides)
Apigenin O-rhamnosylglucoside	C ₂₇ H ₃₁ O ₁₄	Flavonoids (O-glycosides)
Apigenin-6,8-di-C-β-glucopyranoside	C ₂₇ H ₃₀ O ₁₅	Flavonoids
Apigenin-7-O-β-glucopyranoside	C ₂₁ H ₂₀ O ₁₀	Flavonoids (O-glycosides)
Apiin	C ₂₆ H ₂₈ O ₁₄	Naphthalenes
Azelaic acid	C ₉ H ₁₆ O ₉	Fatty Acyls

Baicalein	C ₁₅ H ₁₀ O ₅	Flavonoids
Calceolarioside	C ₂₃ H ₂₆ O ₁₁	Cinnamic acids and derivatives
Chlorogenic acid	C ₁₆ H ₁₈ O ₉	Organooxygen compounds
Chrysoeriol	C ₁₆ H ₁₂ O ₆	Flavonoids
Chrysoeriol glucoside–xylosylglucoside malonylated (III)b 2	C ₃₆ H ₄₃ O ₂₃	Flavonoids
Chrysoeriol O-glucoside	C ₂₂ H ₂₃ O ₁₁	Flavonoids (O-glycosides)
Chrysoeriol O-glucoside malonylated (I)	C ₂₅ H ₂₅ O ₁₄	Flavonoids (O-glycosides)
Chrysoeriol O-pentosylhexoside	C ₂₇ H ₃₀ O ₁₅	Flavonoids
Cichoriin	C ₁₅ H ₁₆ O ₁₀	Coumarins
Cinnamic acid glucoside	C ₁₅ H ₁₈ O ₈	Phenolic acids
DicaFFEoylquinic acid	C ₂₅ H ₂₄ O ₁₂	Phenolic acids
Eriodictyol	C ₁₅ H ₁₂ O ₆	Flavonoids
Esculin	C ₁₅ H ₁₆ O ₉	Coumarins and derivatives
Ferulic acid glucoside	C ₁₆ H ₂₀ O ₉	Organooxygen compounds
Genistein	C ₁₅ H ₁₀ O ₅	Isoflavonoids
Genistein 4', 7-O-diglucoside dimalonylated (I) 2	C ₃₃ H ₃₅ O ₂₁	Isoflavonoids
Genistein 6-C-glucoside 1	C ₂₁ H ₂₁ O ₁₀	Isoflavonoids
Genistein 7-O-glucoside malonylated	C ₂₄ H ₂₃ O ₁₃	Isoflavonoids
Genistein 8-C-glucoside 2	C ₂₁ H ₂₁ O ₁₀	Isoflavonoids
Genistein C-diglucoside 3	C ₂₇ H ₃₁ O ₁₅	Isoflavonoids
Genistein C-diglucoside–xyloside 3	C ₃₂ H ₃₉ O ₁₉	Isoflavonoids
Genistein O-diglucoside malonylated (II) 2	C ₃₀ H ₃₃ O ₁₈	Isoflavonoids
Isorhamnetin	C ₁₆ H ₁₂ O ₇	Flavonoids
Kaempferol 3-O-glucoside	C ₂₁ H ₂₁ O ₁₁	Flavonoids
Licodione	C ₁₅ H ₁₂ O ₅	Flavonoids
Ligstroside	C ₂₅ H ₃₂ O ₁₂	Prenol lipids
Ligstroside aglycone	C ₁₉ H ₂₂ O ₇	Prenol lipids
Luteolin 7-O-glucoside	C ₂₁ H ₂₀ O ₁₁	Flavonoids
Luteolin-4'-O-glucoside	C ₂₁ H ₂₀ O ₁₁	Flavonoids
Luteone	C ₂₀ H ₁₈ O ₆	Flavonoids
Naringenin	C ₁₅ H ₁₈ O ₈	Flavonoids
p-coumaric acid glucoside	C ₇ H ₆ O ₃	Organooxygen compounds
p-hydroxybenzoic acid	C ₁₅ H ₁₀ O ₇	Benzene and substituted derivatives
Quercetin	C ₂₇ H ₃₁ O ₁₆	Flavonoids
Quercetin rhamnosylglucoside 2	C ₇ H ₁₂ O ₆	Flavonoids
Quinic acid	C ₁₅ H ₁₈ O ₈	Organooxygen

		compounds
trans p-Coumaric acid	C ₂₇ H ₃₀ O ₁₅	Benzene and substituted derivatives
Vicenin 2	C ₂₁ H ₂₀ O ₁₀	Flavonoids
Vitexin	C ₂₀ H ₁₈ O ₅	Flavonoids
Wighteone	C ₁₆ H ₁₆ O ₅	Flavonoids

Table S6. Suspect screening list for chickpea flour

Compound	Molecular formula	Class
(Epi)afzelechin	C ₁₅ H ₁₄ O ₅	Flavonoids
Apigenin 7-O-neohesperidoside	C ₂₇ H ₃₀ O ₁₄	Flavonoids
Apigenin-6-C-glucoside	C ₂₁ H ₂₀ O ₁₀	Flavonoids
Aromadendrin-3-O-β-D-glucopyranoside	C ₂₁ H ₂₂ O ₁₁	Flavonoids
Benzoic acid	C ₇ H ₆ O ₂	Benzene and substituted derivatives
Biochanin A 7-O-β-D-glucopyranoside	C ₂₂ H ₂₂ O ₁₀	Isoflavonoids
Biochanin B	C ₁₆ H ₁₂ O ₄	Flavonoids
Caffeoylquinic acid I	C ₁₆ H ₁₈ O ₉	Organooxygen compounds
Caffeoylquinic acid I	C ₁₆ H ₁₈ O ₉	Organooxygen compounds
Caffeoylquinic acid IV	C ₁₆ H ₁₈ O ₉	Organooxygen compounds
Caffeoylquinic acid V	C ₁₆ H ₁₈ O ₉	Organooxygen compounds
Cyanidin	C ₁₅ H ₁₁ O ₆ ⁺	Flavonoids
Daidzein	C ₁₅ H ₁₀ O ₄	Flavonoids
Dalpanin I	C ₂₆ H ₃₀ O ₁₂	Lignan
Delphinidin	C ₁₅ H ₁₁ ClO ₇	Anthocyanins
Dihydrokaempferol [aromadendrin]	C ₁₅ H ₁₂ O ₆	Flavonoids
Dihydroxybenzoic acid hexoside	C ₁₃ H ₁₆ O ₉	Benzene and substituted derivatives
Dihydroxybenzoic acid hexoside deoxyhexoside	C ₁₉ H ₂₆ O ₁₃	Benzene and substituted derivatives
Dihydroxybenzoic acid hexoside pentoside I	C ₁₈ H ₂₄ O ₁₃	Benzene and substituted derivatives
Dihydroxybenzoic acid I	C ₇ H ₆ O ₄	Benzene and substituted derivatives
Dihydroxybenzoic acid malonyl hexoside I	C ₁₆ H ₁₈ O ₁₂	Benzene and substituted derivatives
Dihydroxybenzoic acid pentosided	C ₁₂ H ₁₄ O ₈	Benzene and substituted derivatives

Ferulic acid hexoside	C ₁₆ H ₂₀ O ₉	Organooxygen compounds
Gallic acid hexoside	C ₁₃ H ₁₆ O ₁₀	Benzene and substituted derivatives
Genistein	C ₁₅ H ₁₀ O ₅	Isoflavonoids
Hydroxybenzoic acid hexoside	C ₁₆ H ₁₆ O ₈	Phenolic acids
Hydroxybenzoic acid hexoside pentoside I	C ₁₈ H ₂₄ O ₁₂	Benzene and substituted derivatives
Isorhamentin 3-O-β-D-glucopyranoside	C ₂₂ H ₂₂ O ₁₂	Flavonoids
Kaempferide	C ₁₆ H ₁₂ O ₆	Flavonoids
Kaempferol 3,7-O-b-D-diglucopyranoside	C ₅₆ H ₁₀₀ O ₆	Flavonoids
Kaempferol 3,7-O-β-D-diglucopyranoside	C ₂₇ H ₃₀ O ₁₆	Flavonoids
Kaempferol 3-O-lathyroside-7-O-α-L-rhamnopyranoside	C ₃₂ H ₃₈ O ₁₉	Flavonoids
Kaempferol 3-O-rutinoseb	C ₂₇ H ₃₀ O ₁₅	Flavonoids
Kaempferol 3-O-β-D-diglucopyranoside	C ₂₇ H ₃₀ O ₁₆	Flavonoids
Kaempferol 3-O-β-d-glucopyarnoside	C ₂₁ H ₂₀ O ₁₁	Flavonoids
Kaempferol malonyl dihexoside I	C ₃₀ H ₃₂ O ₁₉	Flavonoids
Kaempferol malonyl dihexoside pentoside I	C ₃₅ H ₄₀ O ₂₃	Flavonoids
Kaempferol-3,4'-O-β-D-diglucopyranoside	C ₂₇ H ₃₀ O ₁₆	Flavonoids
Kaempferol-3-O-(6''-malonyl)-β-D-glucopyranoside	C ₂₄ H ₂₂ O ₁₄	Flavonoids
Kaempferol-3-O-rutinoside-7-O-β-D-glucopyranoside	C ₃₃ H ₄₀ O ₂₀	Flavonoids
Kaempferol-3-O-β-D-glucopyranoside-7-O-α-l-rhamnopyranside	C ₂₇ H ₃₀ O ₁₅	Flavonoids
Luteolin-3,7-di-O-glucoside	C ₂₇ H ₃₀ O ₁₆	Flavonoids
Malvidin	C ₁₇ H ₁₅ O ₇ ⁺	Flavonoids
Methoxy hydroxybenzoic acid hexoside pentosidee	C ₁₉ H ₂₆ O ₁₂	Benzene and substituted derivatives
Myricetin-3-O-rhamnoside	C ₂₁ H ₂₀ O ₁₂	Flavonoids
Myricetin-O-methyl ether hexoside deoxyhexoside	C ₂₈ H ₃₂ O ₁₇	Flavonoids
Myricetin-O-methyl ether hexoside deoxyhexoside pentoside	C ₃₃ H ₄₀ O ₂₁	Flavonoids
Naringenin dihexoside pentoside	C ₃₂ H ₄₀ O ₁₉	Flavonoids
Naringenin hexoside pentoside I	C ₂₆ H ₃₀ O ₁₄	Flavonoids
Orobol	C ₁₅ H ₁₀ O ₆	Isoflavonoids
p-Coumaric acid glucopyranoside	C ₁₅ H ₁₈ O ₈	Organooxygen compounds
Petunidin	C ₁₆ H ₁₃ O ₇ ⁺	Anthocyanins
p-hydroxybenzoic acid	C ₇ H ₆ O ₃	Benzene and substituted derivatives
Pratensein	C ₁₆ H ₁₂ O ₆	Flavonoids

Pratensein 7-O-β-D-glucopyranoside	C ₂₂ H ₂₂ O ₁₁	Isoflavonoids
Prunin [naringenin 7-O-β-D-glucopyranoside]	C ₂₁ H ₂₂ O ₁₀	Flavonoids
Quercetin 3-O-(6''-malonylneohesperidoside)	C ₃₀ H ₃₂ O ₁₉	Flavonoids
Quercetin 3-O-β-d-glucopyranosideb	C ₂₁ H ₂₀ O ₁₂	Flavonoids
Quercetin-3,7-O-di-glucopyranoside	C ₂₇ H ₃₀ O ₁₇	Flavonoids
Quercetin-3-O-galactoside	C ₂₁ H ₂₀ O ₁₂	Flavonoids
Quercetin-3-O-rhamnoside	C ₂₁ H ₂₀ O ₁₁	Flavonoids
Quercetin-3-O-rutinoside-7-O-α-L-rhamnopyranoside	C ₃₃ H ₄₀ O ₂₀	Flavonoids
Quercetin-3-O-β-D-glucopyranuronic acid	C ₂₁ H ₁₈ O ₁₃	Flavonoids
Sinapic acid hexoside I	C ₁₇ H ₂₂ O ₁₀	Hydroxycinammic acids
Vanillic acid hexoside pentoside	C ₁₉ H ₂₆ O ₁₃	Benzene and substituted derivatives
Vanillic acid hexoside pentoside I	C ₁₉ H ₂₆ O ₁₃	Benzene and substituted derivatives
Vanillic acid-4-O-b-D-glucopyranoside	C ₁₄ H ₁₈ O ₉	Benzene and substituted derivatives

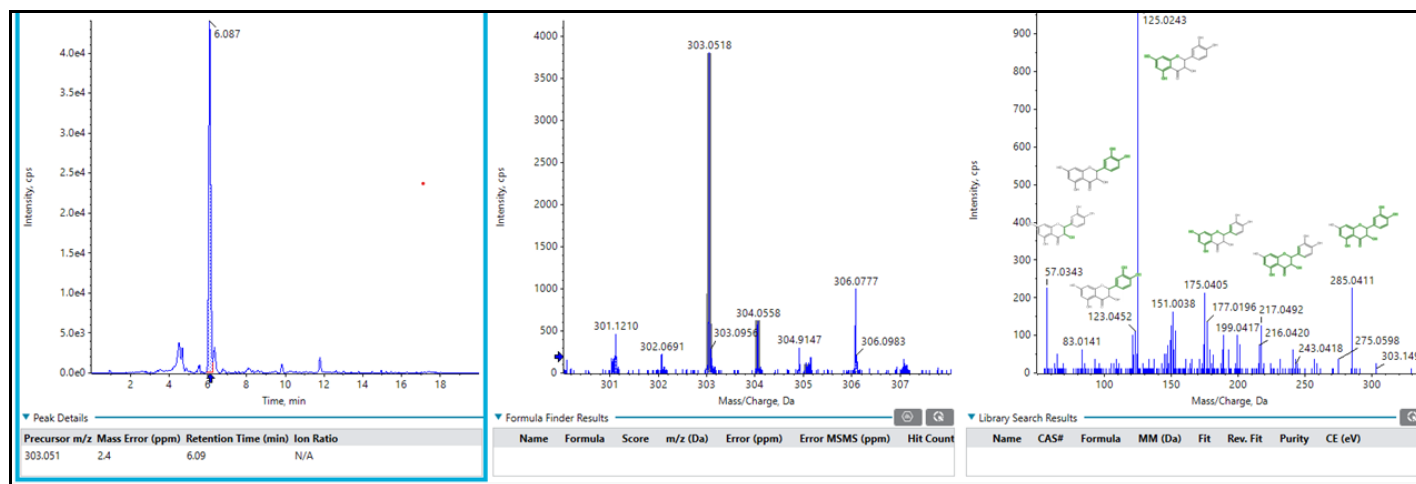


Figure S1. Extracted ion chromatogram, MS, and MS/MS spectra of taxifolin in LFL.

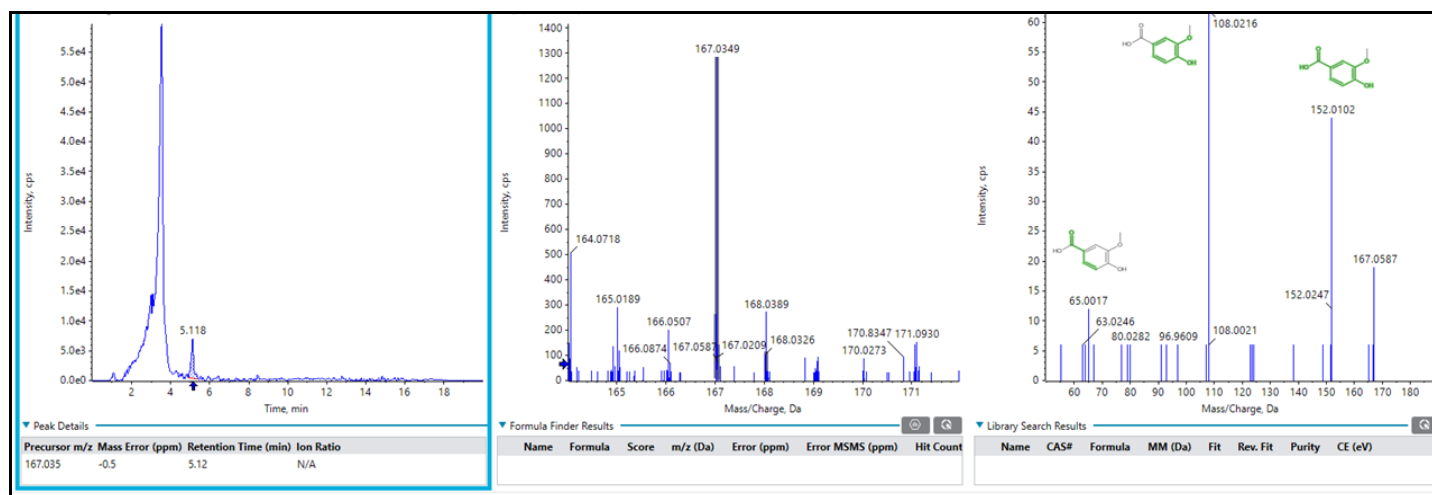


Figure S2. Extracted ion chromatogram, MS, and MS/MS spectra of vanillic acid in LFC.

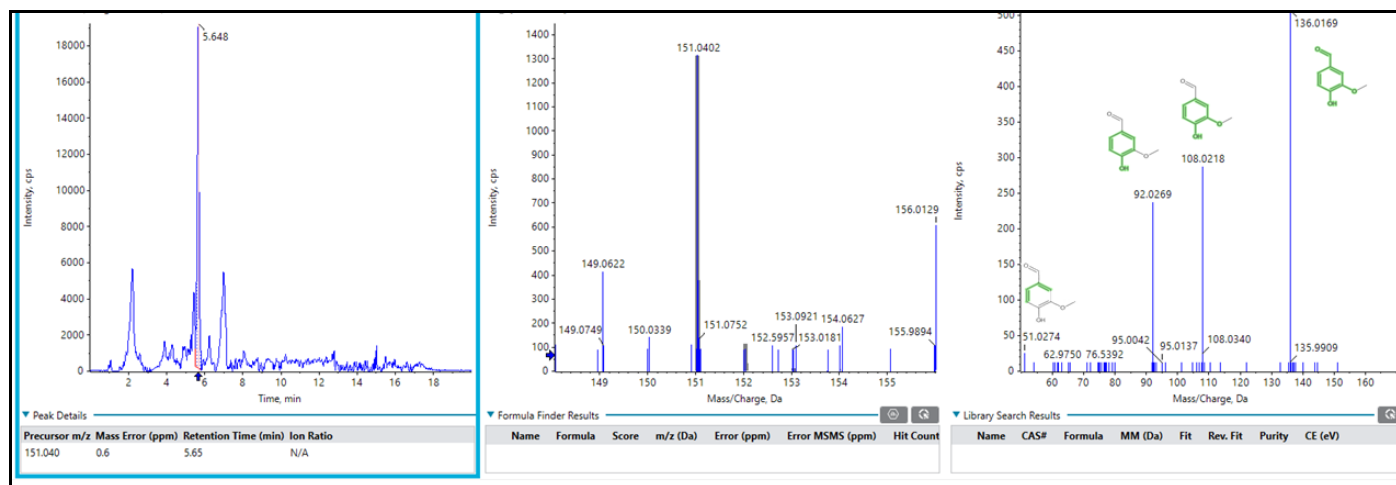


Figure S3. Extracted ion chromatogram, MS, and MS/MS spectra of vanillin in LFL.

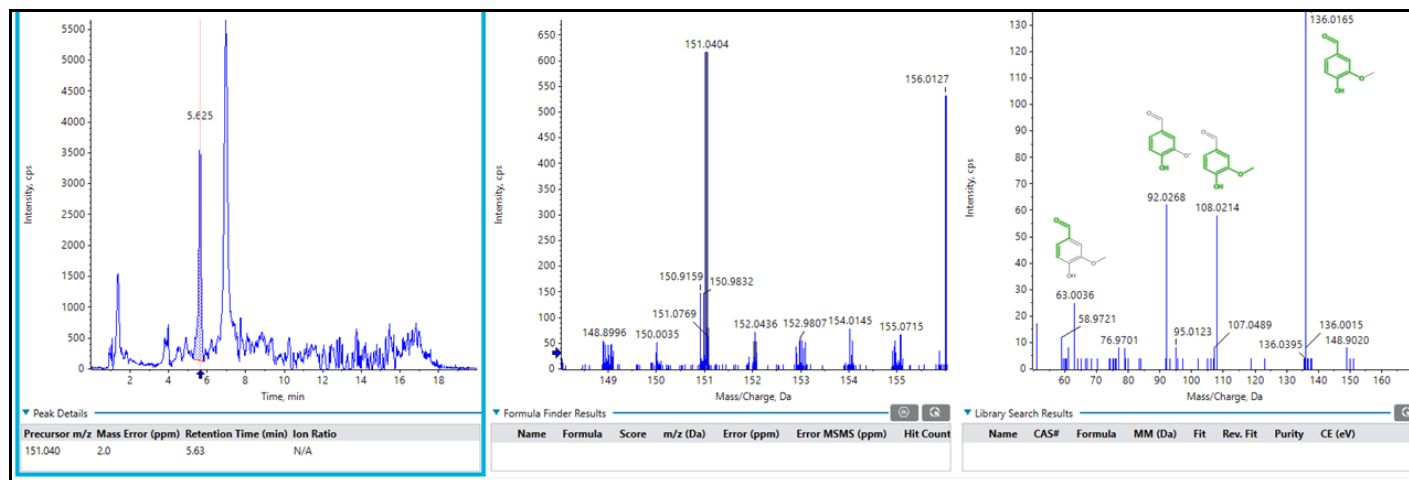


Figure S4. Extracted ion chromatogram, MS, and MS/MS spectra of vanillin in WFL.

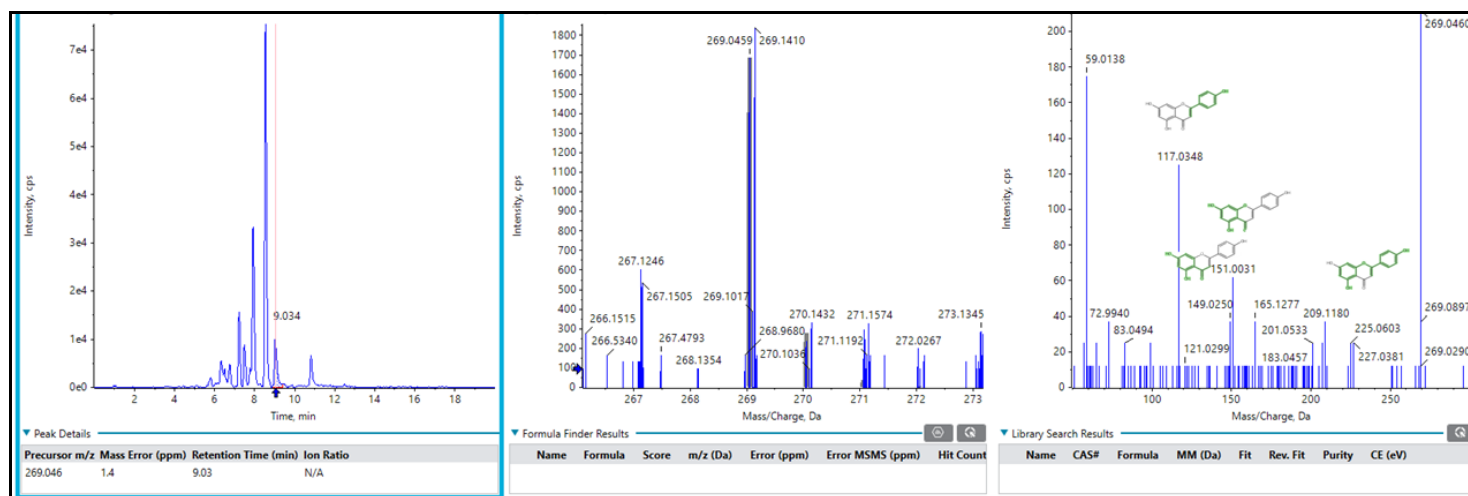


Figure S5. Extracted ion chromatogram, MS, and MS/MS spectra of apigenin in LFL.

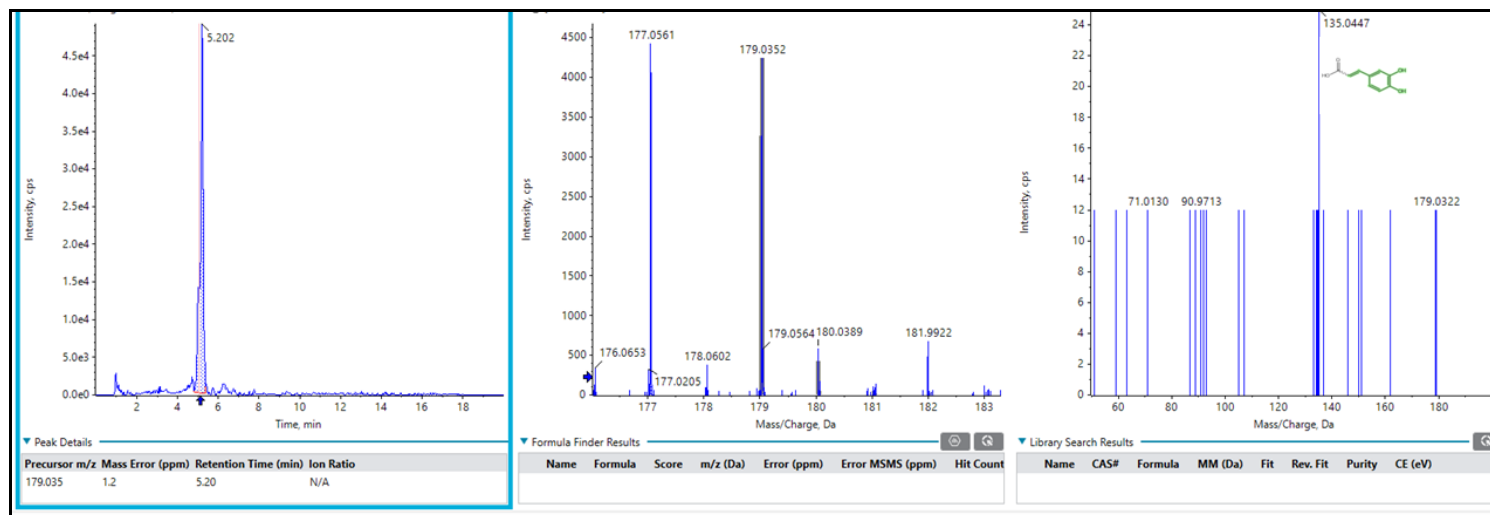


Figure S6. Extracted ion chromatogram, MS, and MS/MS spectra of caffeic acid in LFL.

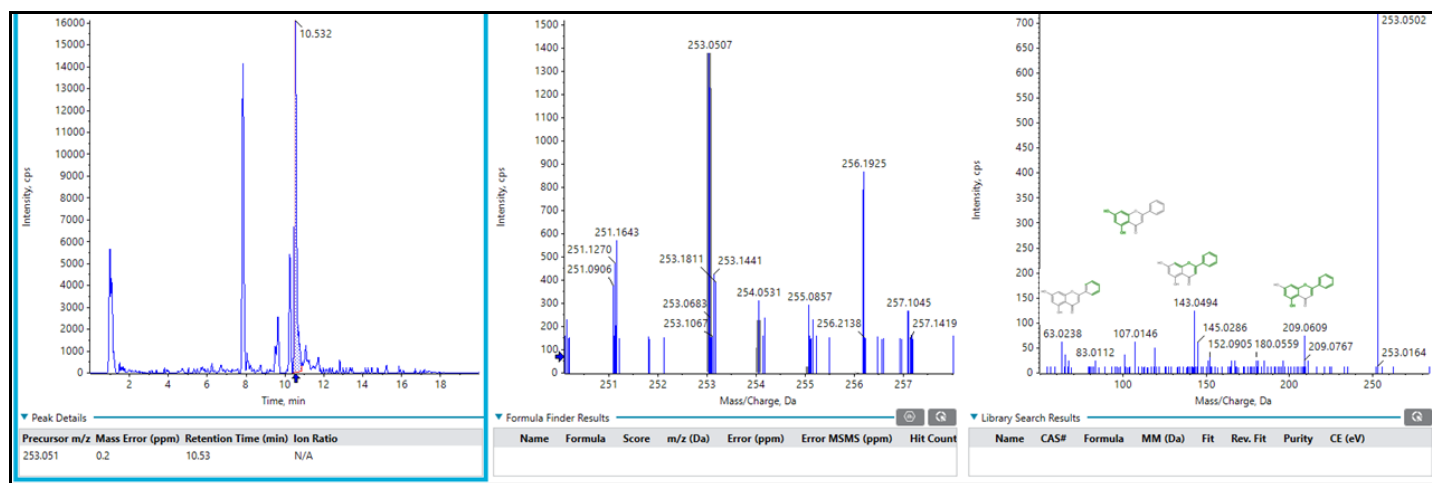


Figure S7. Extracted ion chromatogram, MS, and MS/MS spectra of chrysin in CFL.

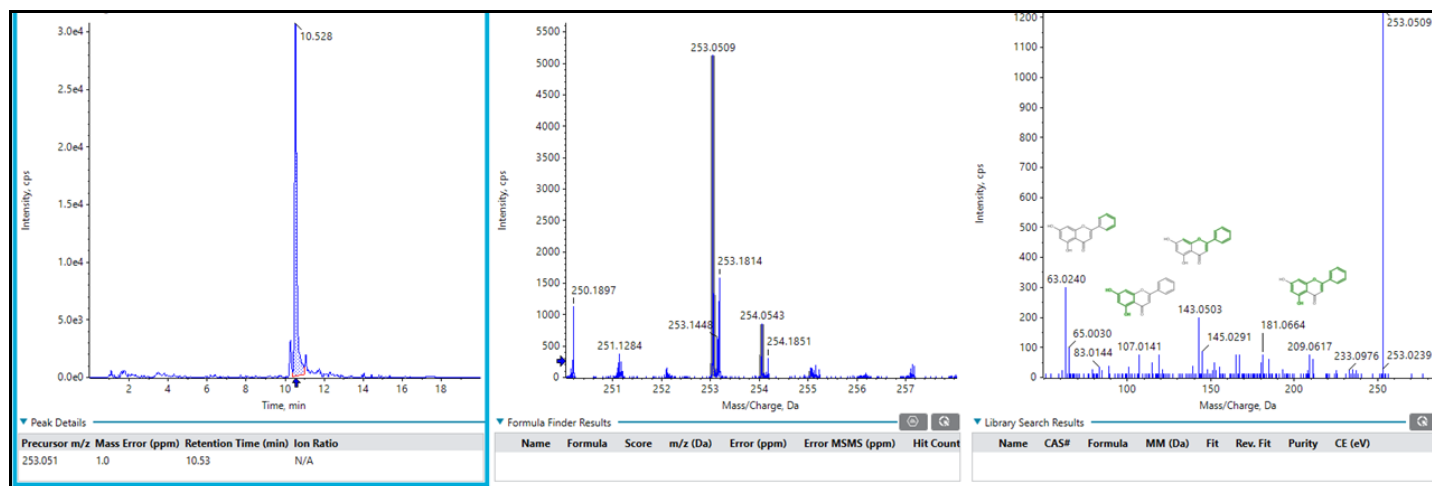


Figure S8. Extracted ion chromatogram, MS, and MS/MS spectra of chrysin in LFC.

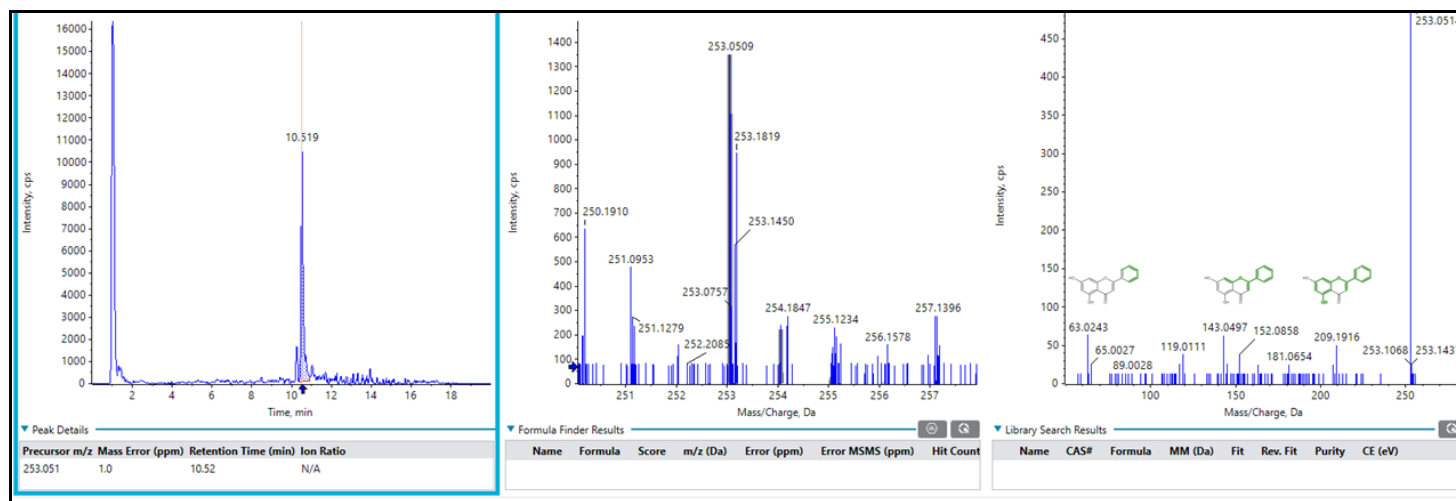


Figure S9. Extracted ion chromatogram, MS, and MS/MS spectra of chrysin in WFL.

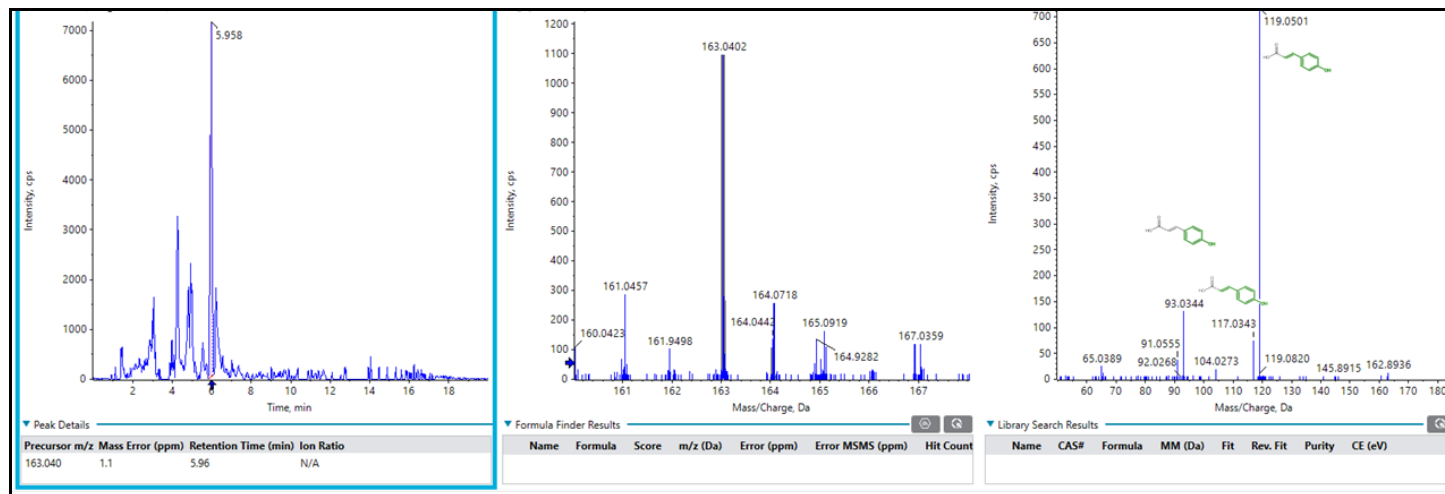


Figure S10. Extracted ion chromatogram, MS, and MS/MS spectra of coumaric acid in CFL.

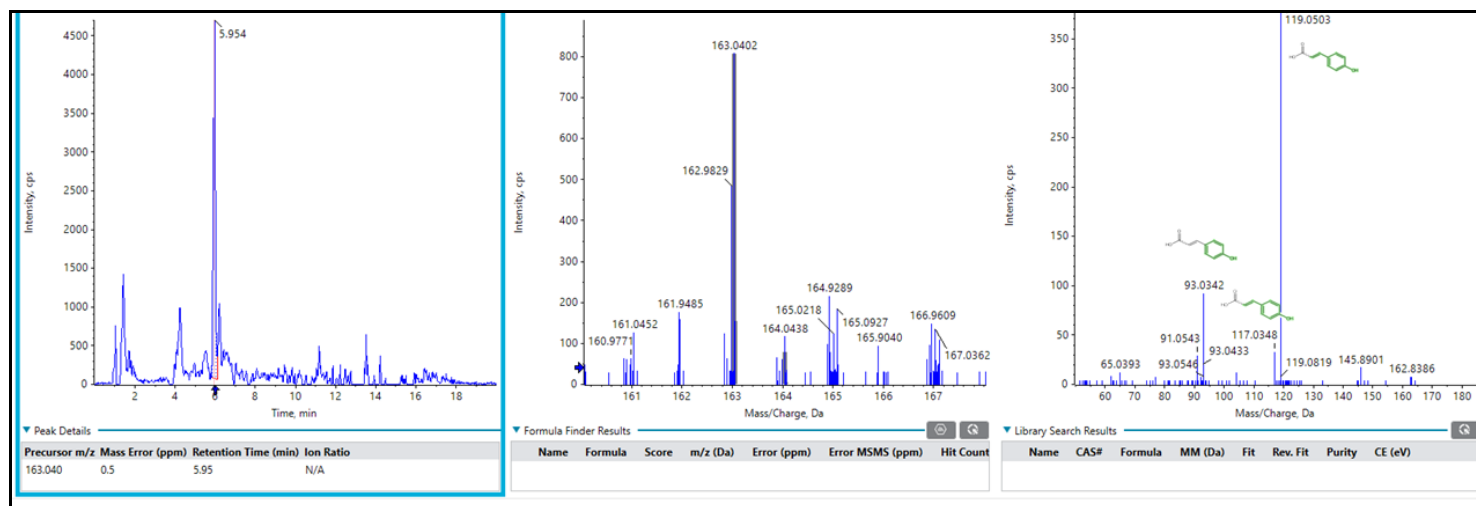


Figure S11. Extracted ion chromatogram, MS, and MS/MS spectra coumaric acid in WFL.

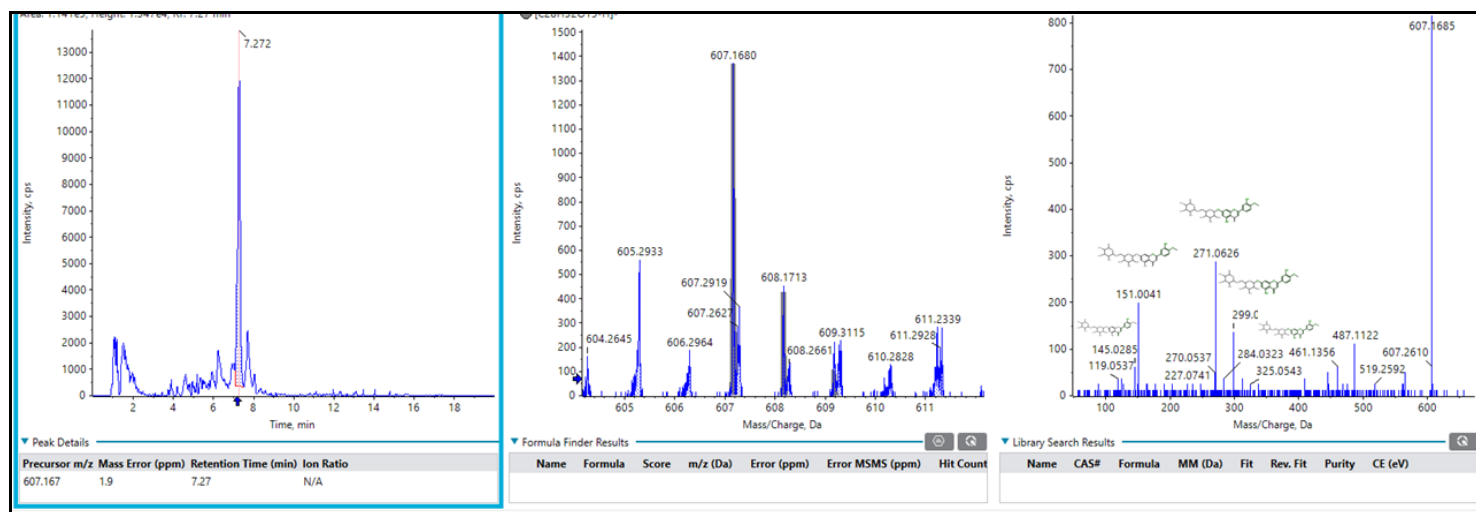


Figure S12. Extracted ion chromatogram, MS, and MS/MS spectra of diosmin in CFL.

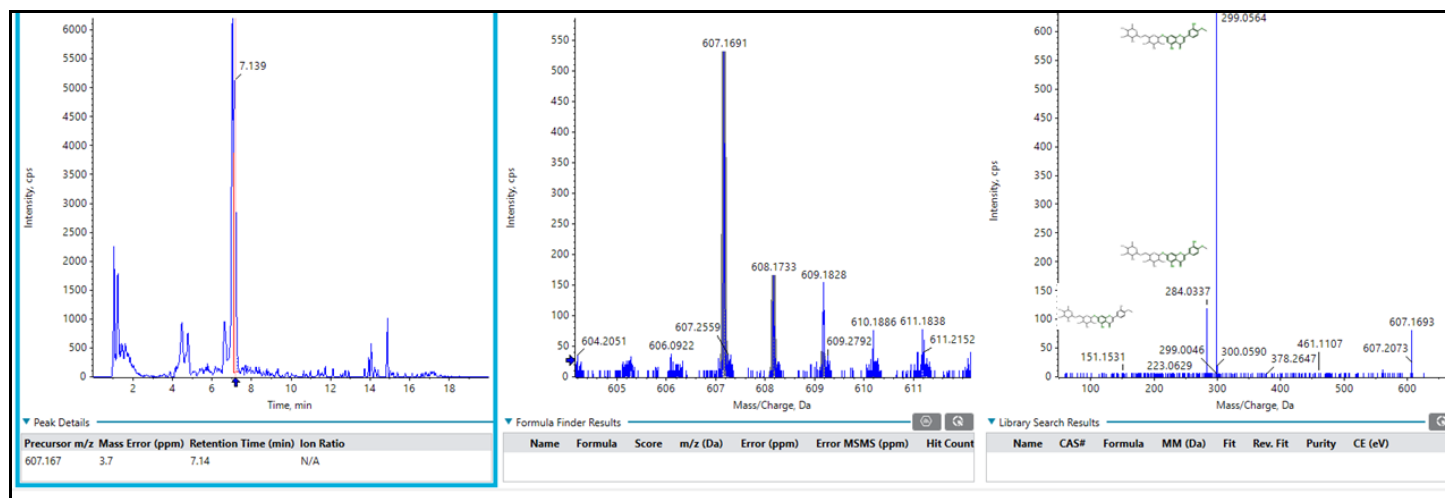


Figure S13. Extracted ion chromatogram, MS, and MS/MS spectra of diosmin in WFL.

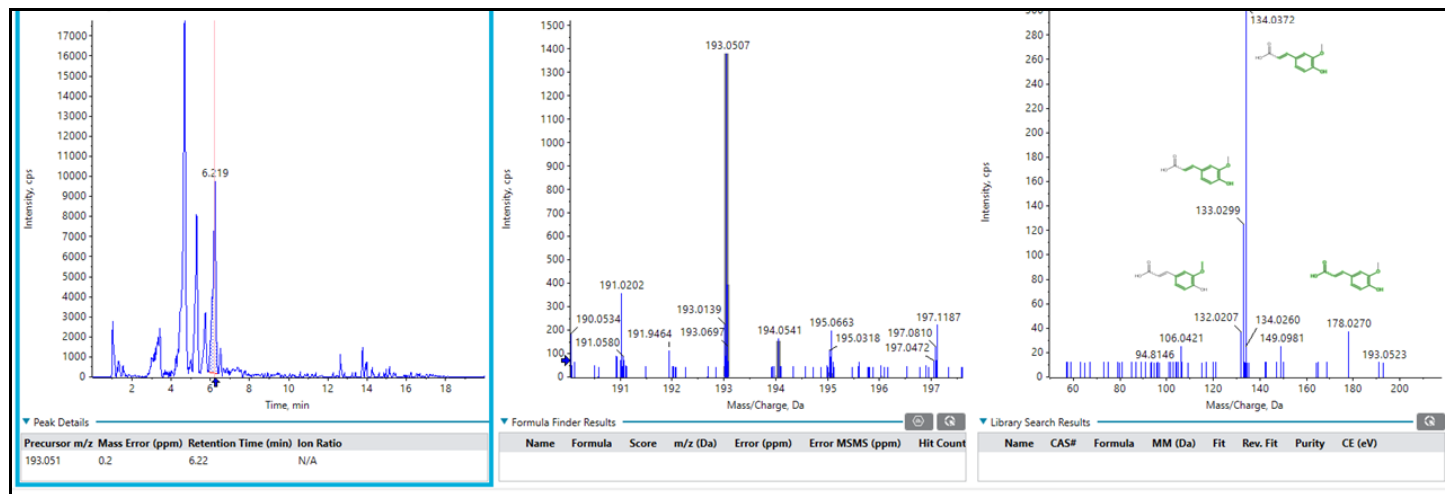


Figure S14. Extracted ion chromatogram, MS, and MS/MS spectra of ferulic acid in CFL.

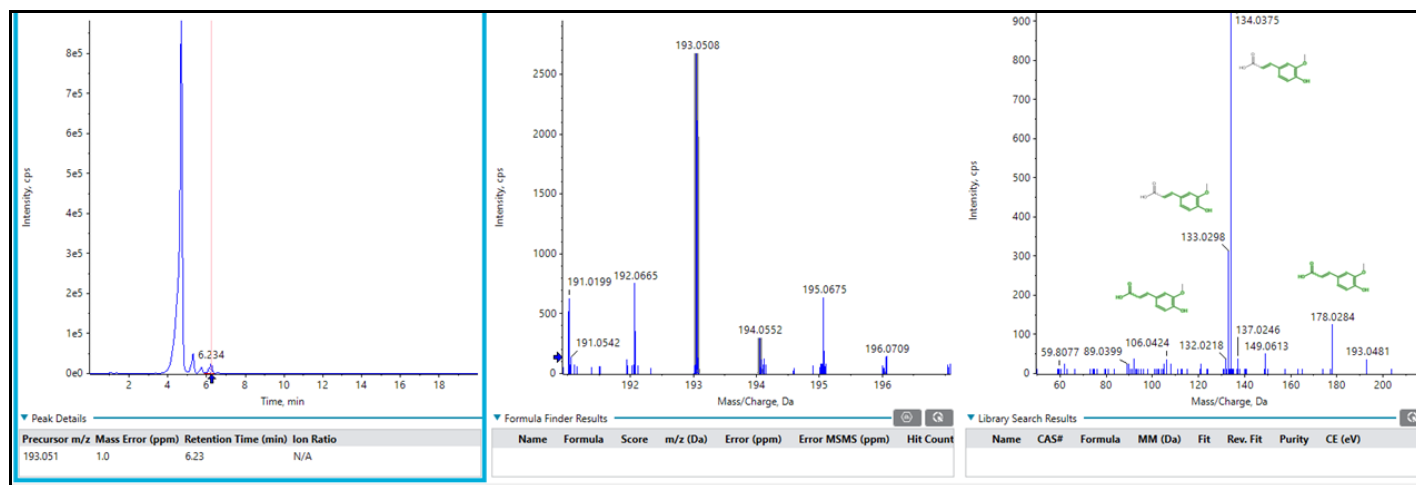


Figure S15. Extracted ion chromatogram, MS, and MS/MS spectra of ferulic acid in LFC.

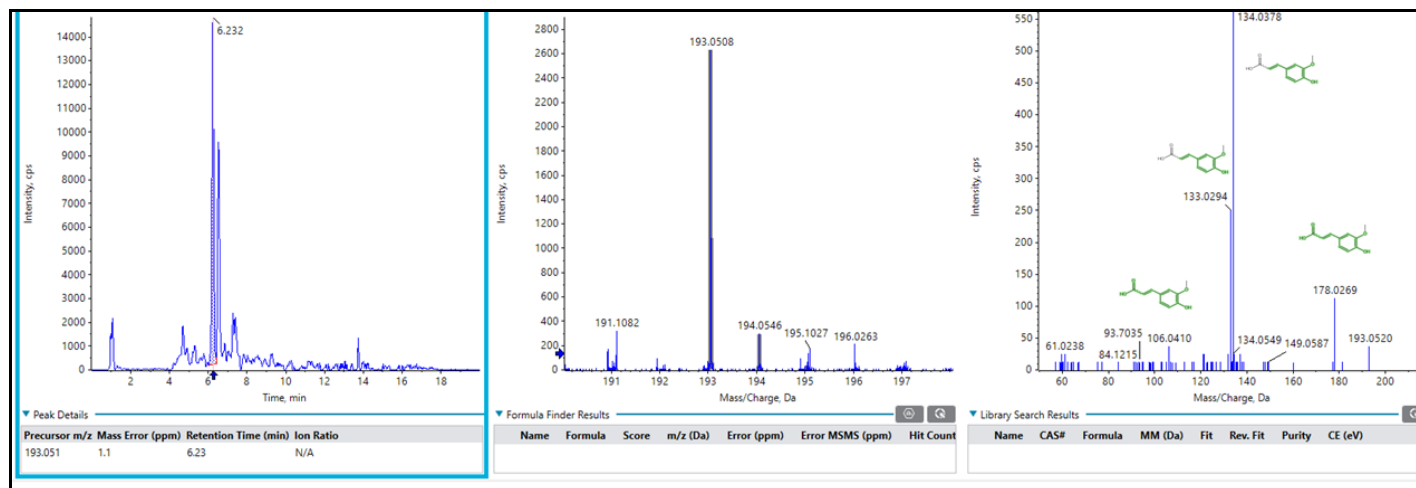


Figure S16. Extracted ion chromatogram, MS, and MS/MS spectra of ferulic acid in WFL.

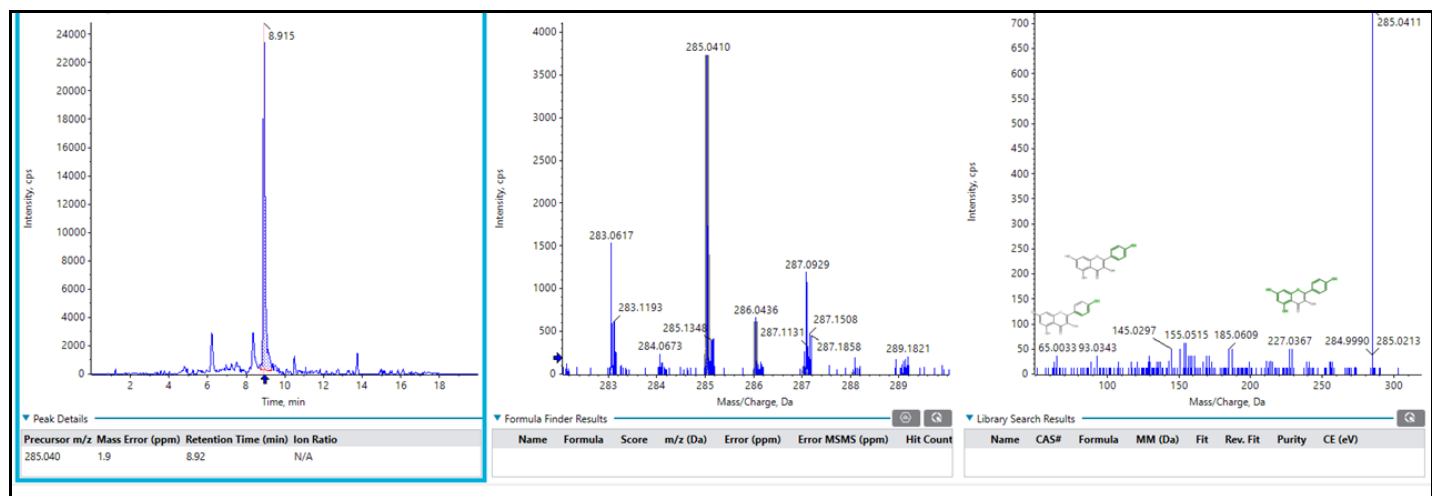


Figure S17. Extracted ion chromatogram, MS, and MS/MS spectra of kaempferol in CFL.

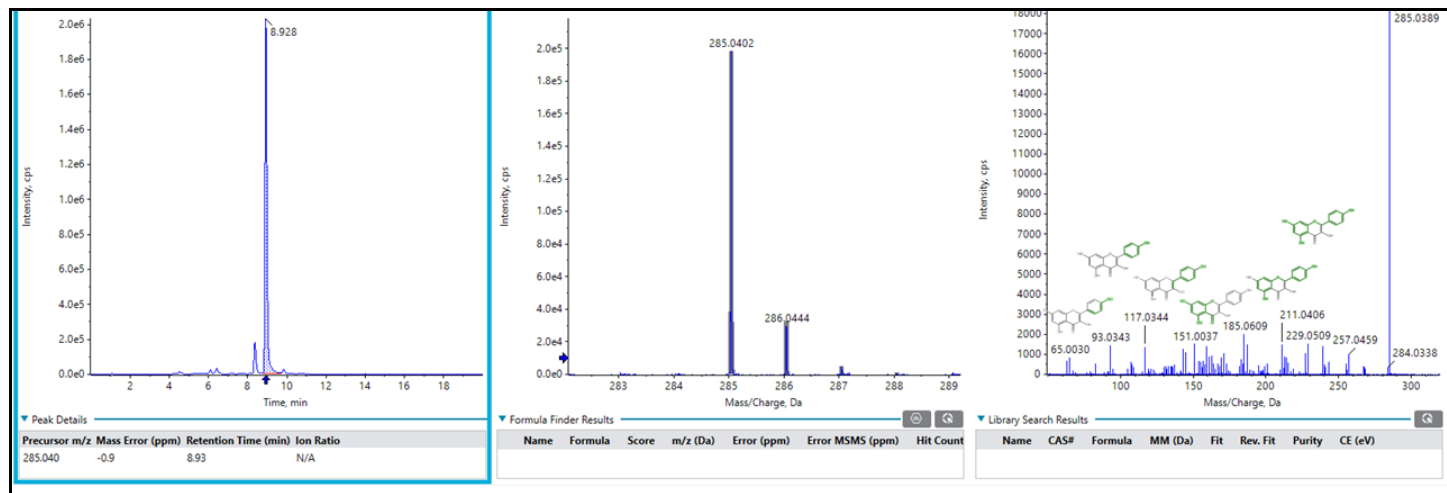


Figure S18. Extracted ion chromatogram, MS, and MS/MS spectra of kaempferol in CFC.

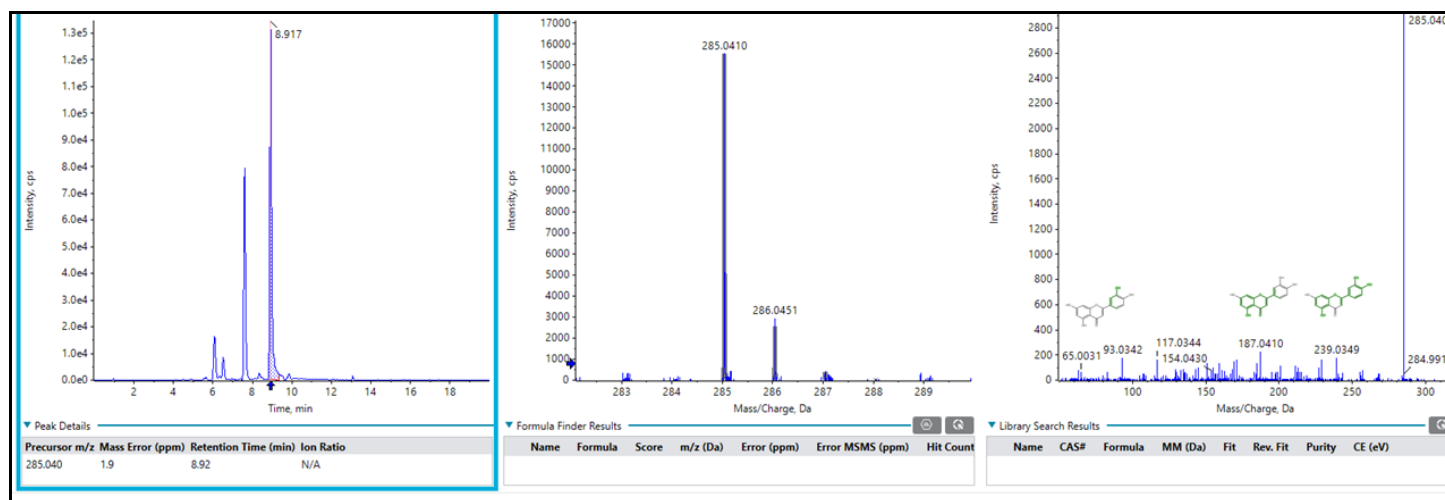


Figure S21. Extracted ion chromatogram, MS, and MS/MS spectra of luteolin in LFL.

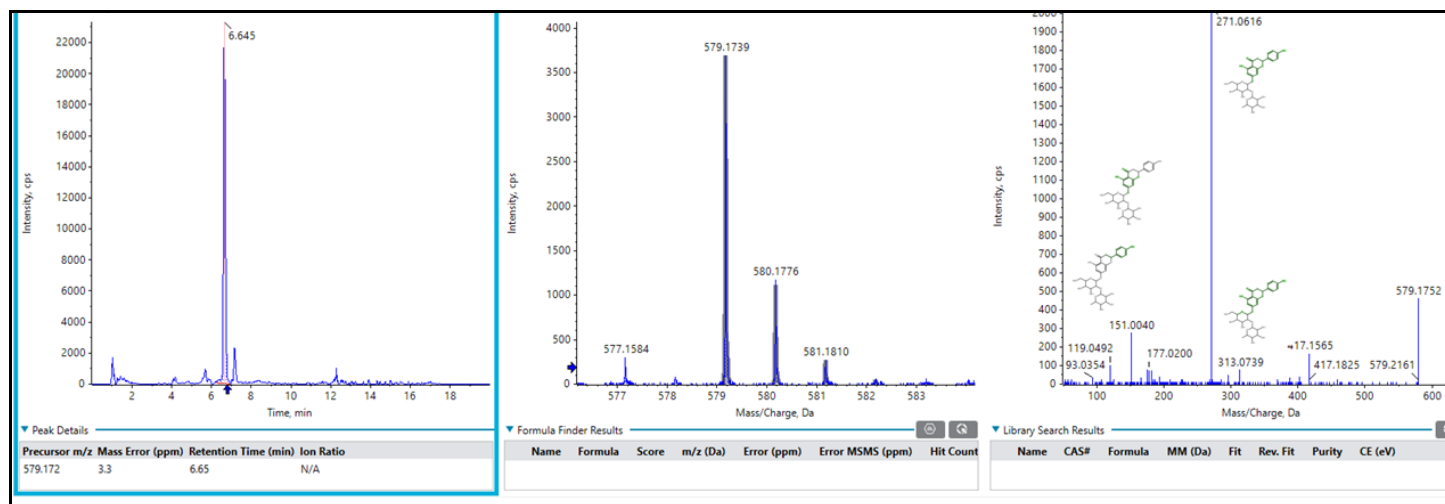


Figure S22. Extracted ion chromatogram, MS, and MS/MS spectra of naringin in WFC.

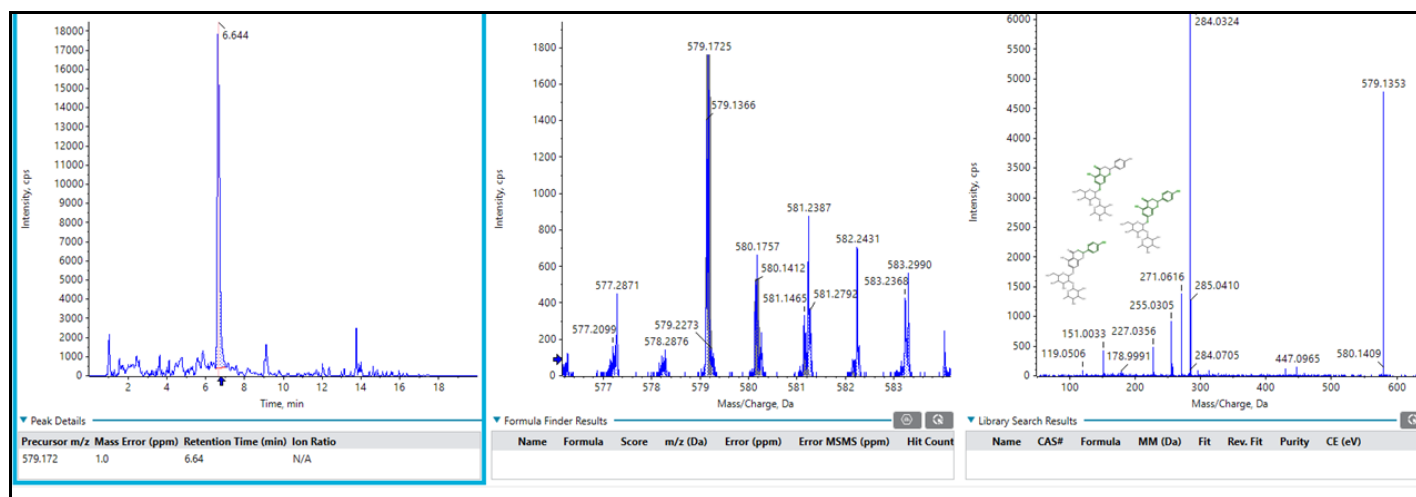


Figure S23. Extracted ion chromatogram, MS, and MS/MS spectra of naringin in CFL.

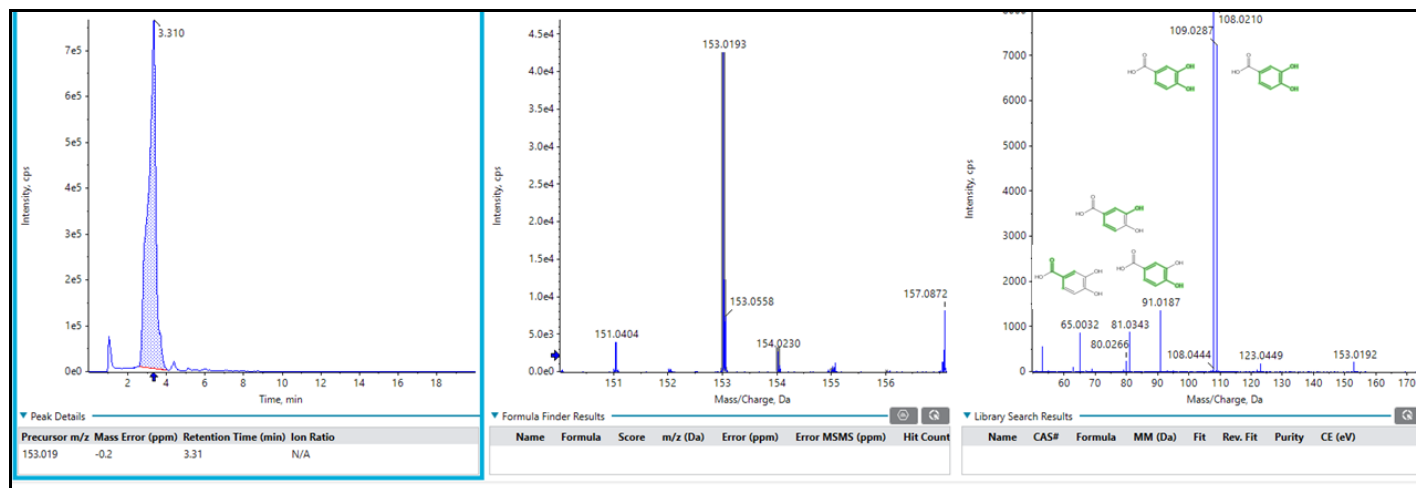


Figure S24. Extracted ion chromatogram, MS, and MS/MS spectra of procatechuic acid in CFL.

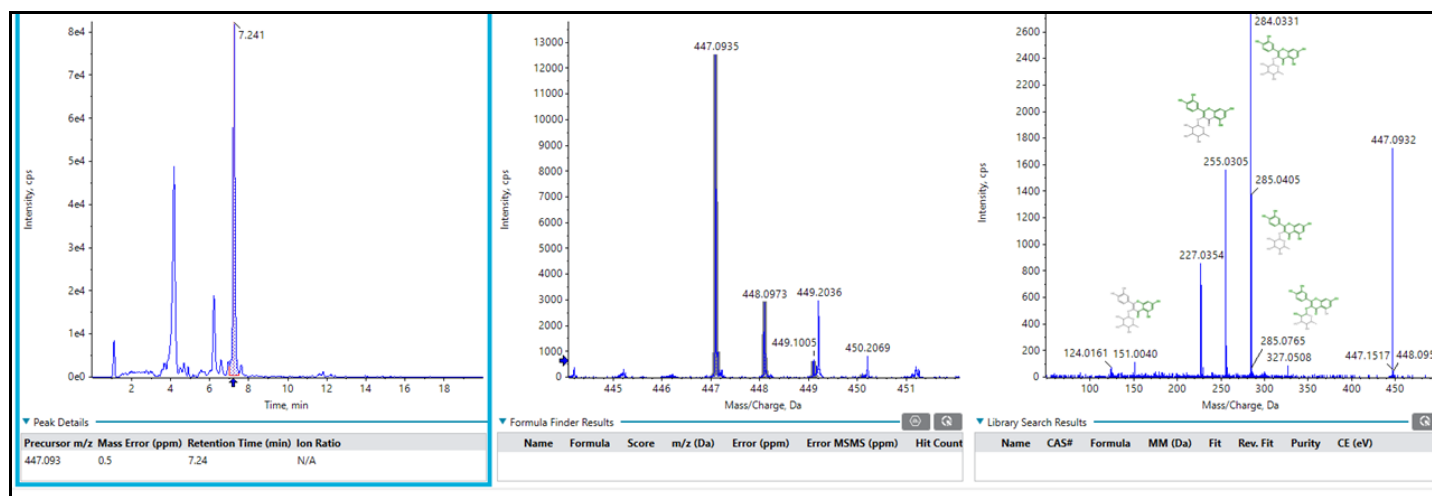


Figure S25. Extracted ion chromatogram, MS, and MS/MS spectra of quercitrin in CFL.

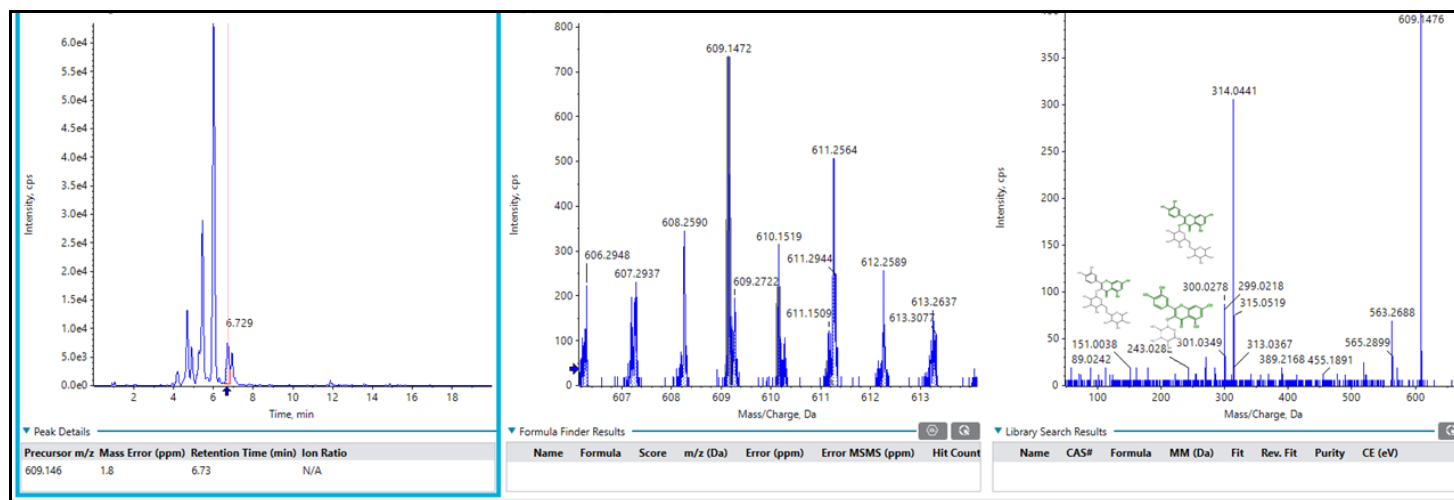


Figure S26. Extracted ion chromatogram, MS, and MS/MS spectra of rutin in CFL.

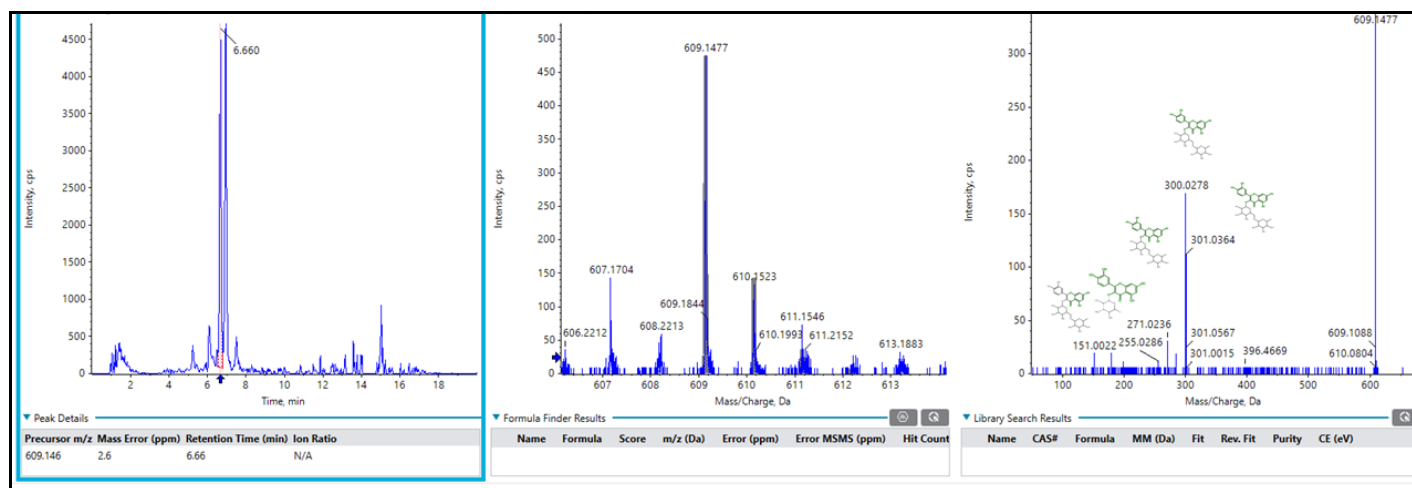


Figure S27. Extracted ion chromatogram, MS, and MS/MS spectra of rutin in WFC