

SUPPLEMENTARY INFORMATION

Exploring the chemical composition and coloring qualities of cacao fruit epicarp extracts

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Table S1. Flavonoids identified in MALDI-TOF spectra of yellow CHE extract using DCTB, CNPV-CH₃ y CNPV-OCH₃ matrices

Compound	DCTB	CNPV-CH ₃	CNPV-OCH ₃	Exp Mass	Mass accuracy	Isotopic pattern		S/N ratio
						Calc	Exp	
Phloretin	X	X	X	274.088	15	100:16.58:2.31	100:24.74:2.52	748
Methylgalangin	X	X	X	284.083	53	100:17.63:2.49	100:17.40	29
(+)-Catechin / (-)-epicatechin	X			290.068	37	100:16.61:2.53	100:14.28	83
Quercetin	X	X	X	302.063	70	100:16.61:2.73	100:17.63:7.73	375
Myricetin	X	X	X	318.030	22	100:16.64:2.94	100:24.62:2.77	648
Jaceosidin	X	X	X	330.049	72	100:18.81:3.11	100:20.94	222
Quercetin 3-O-arabinoside	X			434.071	30	100:22.26:4.62	100:23.63:5.02	41
Isorhamnetin 3-O-rutinoside	X			462.096	43	100:24.47:5.12	100:29.68:12	29
Luteolin 7-O-malonyl-glucoside	X			534.116	30	100:26.74:6.31	100:35.69	28
Procyanidin dimer B1	X			578.092	86	100:33.20:7.80	100:34.57:7.75	116

Table S2. Flavonoids identified in MALDI-TOF spectra of red CHE extract using DCTB, CNPV-CH₃ y CNPV-OCH₃ matrices

Compound	DCTB	CNPV- CH ₃	CNPV- OCH ₃	Exp Mass	Mass accuracy	Isotopic pattern		S/N ratio
						Calc	Exp	
Phloretin	X	X	X	274.088	22	100:16.58:2.31	100:18.80:1.45	1405
+) -Catechin / (-) -epicatechin	X			290.060	65	100:16.61:2.53	100:12.47	128
Quercetin	X	X	X	302.063	70	100:16.61:2.73	100:16.87	466
Myricetina	X	X	X	318.030	22	100:16.64:2.94	100:17.86:1.75	912
Jaceosidin	X	X	X	330.048	76	100:18.81:3.11	100:18.04	233
Quercetin-3-O- arabinoside	X			434.036	110	100:22.26:4.62	100:23.46:5.54	37
Luteolin 7-O- malonyl- glucoside	X			534.099	2	100:26.74:6.31	100:30.79	48
Procyanidin dimer B1	X			578.130	21	100:33.20:7.80	100:33.60:6.38	195
Luteolin 7-O- rutinoside	X			594.123	59	100:30.12:7.46	100:31.69	104
Apigenin 7-O- diglucuronide	X			622.160	69	100:30.15:7.88	100:41.25:15.5	50

Table S3. Flavonoids identified in MALDI-TOF spectra of purple CHE extract using DCTB, CNPV-CH₃ y CNPV-OCH₃ matrices

Compound	DCT B	CNPV -CH ₃	CNPV -OCH ₃	Exp Mass	Mass accurac y	Isotopic pattern		S/N rati o
						Calc	Exp	
Phloretin	X	X	X	274.08 2	15	100:16.58:2.3 1	100:13.72:1.1 7	721
Methylgalangin	X			284.08 6	63	100:17.63:2.4 9	100:16.80	34
Hispidulin	X			300.06 8	17	100:17.67:2.7 0	100:17.00	18
Quercetin	X	X	X	302.05 9	56	100:16.61:2.7 3	100:13.05	269
Myricetin	X	X	X	318.04 7	31	100:16.64:2.9 4	100:16.4:3.94	415
Jaceosidin	X	X		330.04 3	91	100:18.81:3.1 1	100:14.73	141
5,3',4'-Trihydroxy-3-methoxy-6:7-methylenedioxyflavone 4'-O-glucuronide			X	520.10 0	29	100:25.64:6.0 3	100:33.52	22
6''-O-Malonylglycitin			X	532.12 1	116	100:27.81:6.3 9	100:45.73	13
Procyanidin dimer B1	X			578.17 8	62	100:33.20:7.8 0	100:31.20	28

Figure S1. MALDI-TOF spectra of yellow CHE extract using DCTB, CNPV-CH₃ and CNPV-OCH₃ matrices

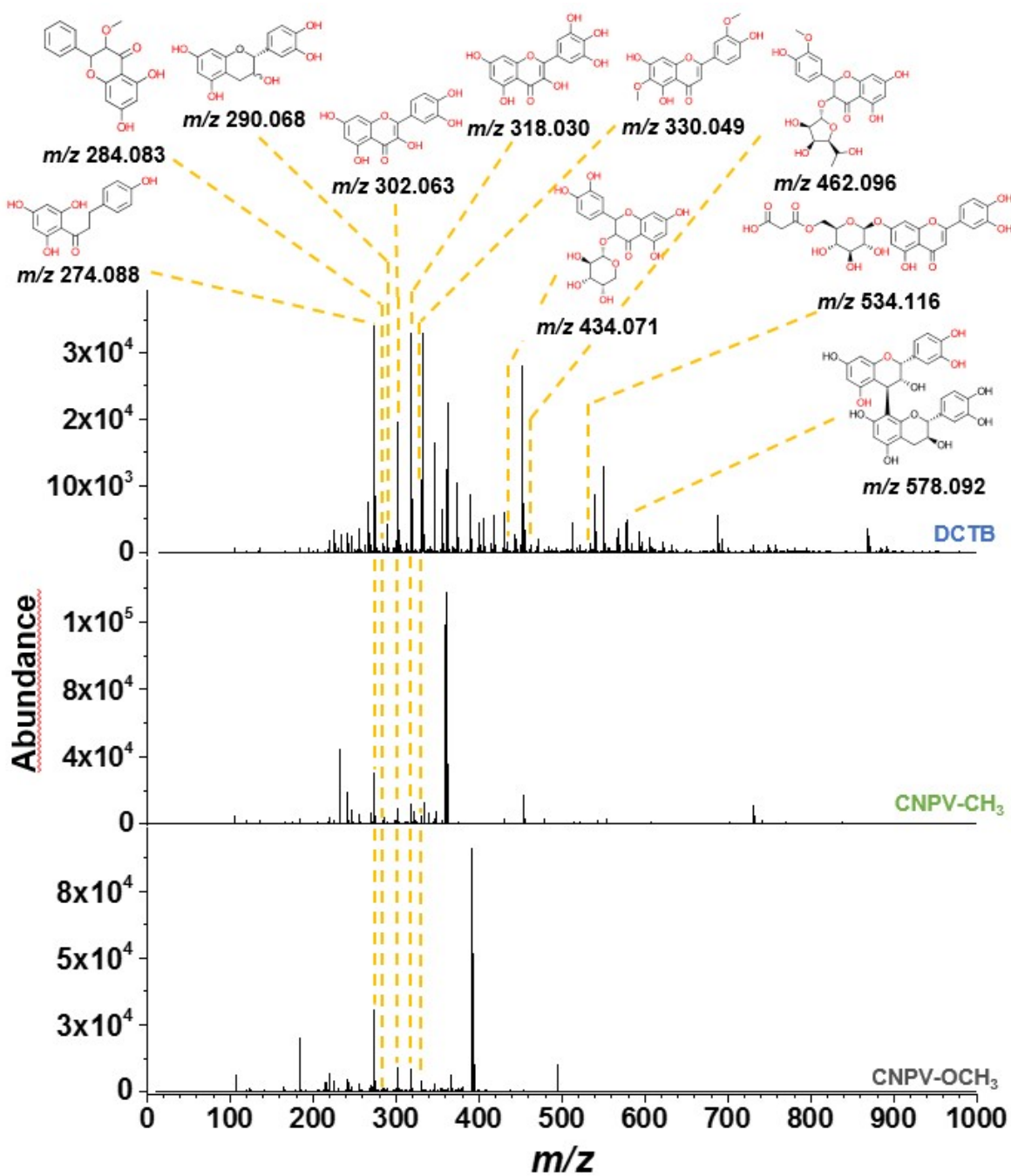


Figure S2. MALDI-TOF spectra of red CHE extract using DCTB, CNPV-CH₃ and CNPV-OCH₃ matrices

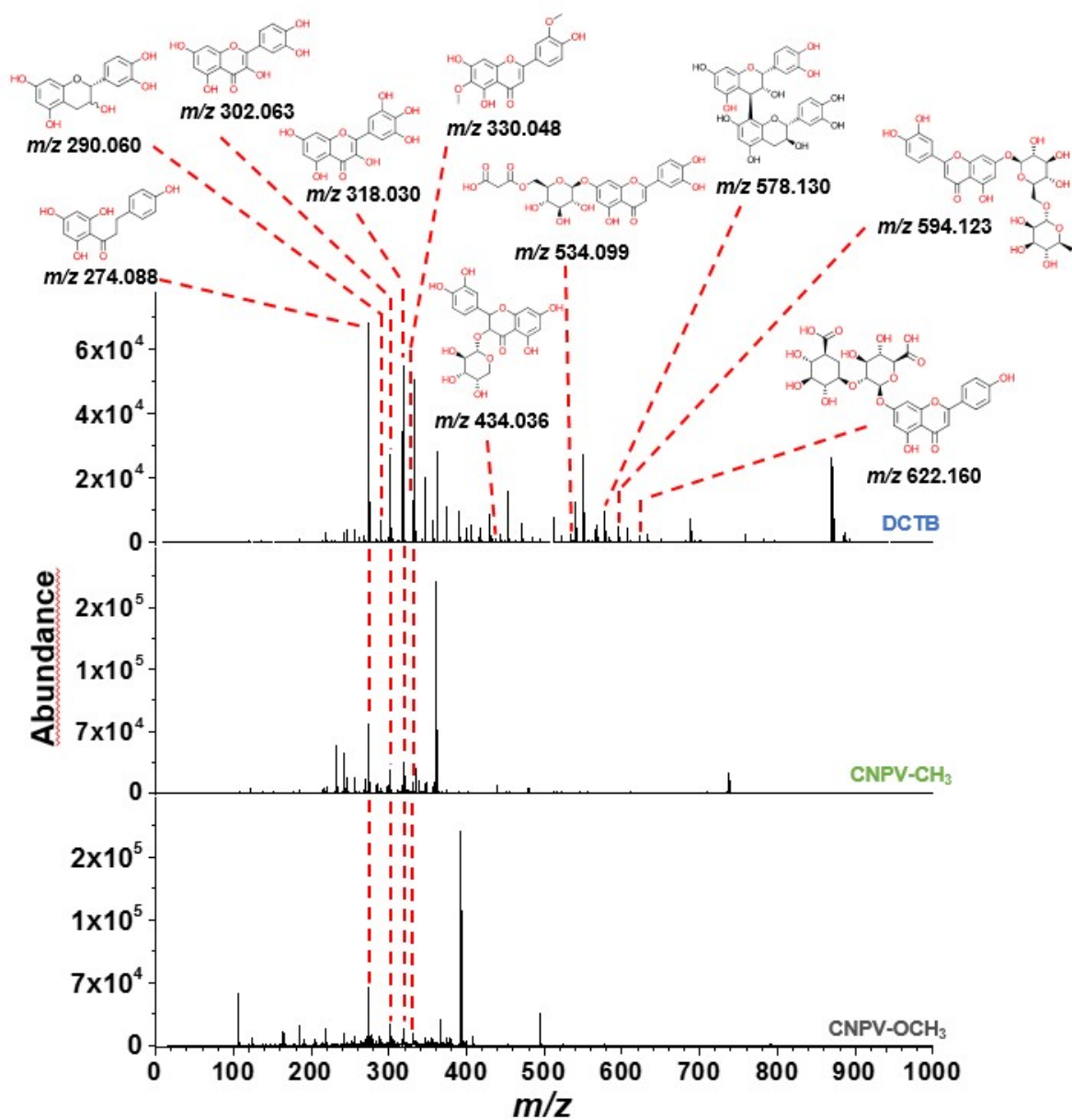


Figure S3. MALDI-TOF spectra of purple CHE extract using DCTB, CNPV-CH₃ and CNPV-OCH₃ matrices

