



Supplementary materials

Discrimination of Olive Oil and Extra-Virgin Olive Oil from Other Vegetable Oils by Targeted and Untargeted HRMS Profiling of Phenolic and Triterpenic Compounds Combined with Chemometrics

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Table S1. Phenolic compounds from different oil types (EVOO* - authentic extra virgin oils, EVOO – commercially available extra virgin oils, VOO – commercially available virgin olive oil, SF – sunflower oils, other vegetable oils including walnut, grape seed, pumpkin, linseed, soybean, sesame, palm, hemp and coconut oils) expressed as µg/g of oil.

Compounds	EVOO*	EVOO	VOO	SF	Vegetable oils
3,4-Dihydroxybenzoic acid	0.04±0.03 (n.d.-0.12)	0.03±0.02 (0.01-0.06)	0.03±0.02 (n.d. -0.06)	0.01±0.02 (n.d. -0.04)	0.01±0.00 (n.d. -0.02)
4-Hydroxybenzoic acid	0.07±0.03 (n.d.-0.13)	0.08±0.03 (0.04-0.12)	0.06±0.04 (n.d. -0.13)	0.03±0.05 (n.d. -0.12)	0.07±0.13 (n.d. -0.38)
t-Ferulic acid	0.11±0.07 (n.d.-0.30)	0.10±0.05 (0.05-0.18)	0.09±0.08 (0.01-0.24)	0.09±0.18 (n.d. -0.42)	0.22±0.27 (0.01-1.01)
Chlorogenic acid	n.d. (0.00-0.01)	n.d. (n.d. -0.01)	0.01±0.02 (n.d. -0.09)	0.02±0.03 (n.d. -0.08)	0.01±0.01 (n.d. -0.05)
Cinnamic acid	2.81±1.48 (n.d.-5.08)	2.78±0.83 (1.92-3.82)	2.34±1.42 (0.02-4.83)	0.33±0.66 (0.01-1.52)	0.10±0.11 (0.01-0.37)
p-Coumaric acid	0.31±0.20 (n.d.-0.81)	0.46±0.08 (0.37-0.54)	0.33±0.20 (0.01-0.71)	0.02±0.04 (0.01-0.09)	0.04±0.05 (0.01-0.18)
Ellagic acid	0.04±0.05 (n.d.-0.18)	0.02±0.01 (n.d. -0.04)	0.04±0.05 (n.d. -0.16)	0.06±0.06 (0.01-0.16)	0.17±0.21 (0.02-0.73)
Absciscic acid	0.01±0.01 (n.d.-0.04)	0.01±0.01 (n.d. -0.02)	0.01±0.01 (n.d. -0.03)	0.05±0.11 (0.00-0.24)	0.03±0.11 (n.d. -0.42)
Rutin	n.d. (n.d. -0.01)	n.d.	0.01±0.01 (n.d. -0.03)	0.01±0.00 (0.01-0.02)	0.02±0.00 (0.01-0.03)
Quercetin	n.d. (n.d. -0.02)	0.01±0.02 (n.d. -0.04)	0.01±0.02 (n.d. -0.06)	0.00±0.01 (n.d. -0.01)	0.01±0.01 (n.d. -0.05)
Isorhamnetin	0.01±0.01 (n.d. -0.04)	0.01±0.01 (n.d. -0.02)	0.01±0.01 (n.d. -0.05)	0.01±0.02 (n.d. -0.05)	0.02±0.01 (n.d. -0.04)
Kaempferol	n.d. (n.d. -0.01)	n.d.	0.00±0.00 (n.d. -0.02)	0.00±0.00 (n.d. -0.01)	0.02±0.02 (n.d. -0.05)
Apigenin	1.58±1.60 (n.d.-6.49)	1.03±0.34 (0.74-1.58)	1.03±0.67 (0.01-1.95)	0.01±0.01 (n.d.-0.02)	0.02±0.01 (0.01-0.05)
Pinocembrin	0.02±0.03 (n.d.-0.11)	0.11±0.05 (0.02-0.16)	0.07±0.09 (0.01-0.38)	0.01±0.02 (0.01-0.04)	0.01±0.00 (n.d. -0.02)
Chrysin	0.01±0.00 (n.d. -0.02)	0.01±0.00 (n.d. -0.01)	0.01±0.00 (0.00-0.02)	0.01±0.00 (n.d. -0.01)	0.01±0.01 (n.d. -0.04)
Hydroxytyrosol	5.44±8.11 (0.01-24.58)	3.66±4.61 (0.01-10.72)	0.87±1.57 (n.d.-5.38)	n.d.	n.d.
Tyrosol	0.53±0.88 (n.d.-2.55)	1.19±1.81 (n.d.-4.36)	1.89±2.73 (n.d.-10.39)	3.24±2.97 (0.39-7.32)	5.19±4.09 (n.d.-12.76)

Trigoneline	11.87±7.24 (0.83-22.51)	14.78±11.50 (5.77-34.06)	9.70±6.44 (2.07-26.99)	4.78±5.09 (1.01-13.58)	12.08±17.44 (n.d.-65.13)
Verbascoside	0.41±0.13 (0.31-0.76)	0.36±0.07 (0.30-0.47)	0.34±0.10 (0.29-0.77)	0.18±0.17 (n.d.-0.31)	0.28±0.08 (n.d.-0.31)
Oleuropein	9.75±5.56 (0.81-18.91)	14.04±7.44 (0.30-21.81)	10.44±7.94 (0.81-33.00)	4.63±4.93 (2.01-33.00)	7.66±8.18 (n.d.-32.10)
Maslinic_acid	2.58±1.55 (0.76-5.84)	4.31±5.59 (1.62-14.31)	5.52±5.32 (0.24-18.73)	0.11±0.08 (n.d.-0.22)	0.49±1.20 (n.d.-4.53)
Oleanolic_acid	0.17±0.17 (0.03-0.66)	2.05±2.30 (0.69-6.15)	2.96±4.53 (0.07-16.07)	0.65±0.25 (0.25-0.91)	1.28±4.11 (n.d.-15.45)

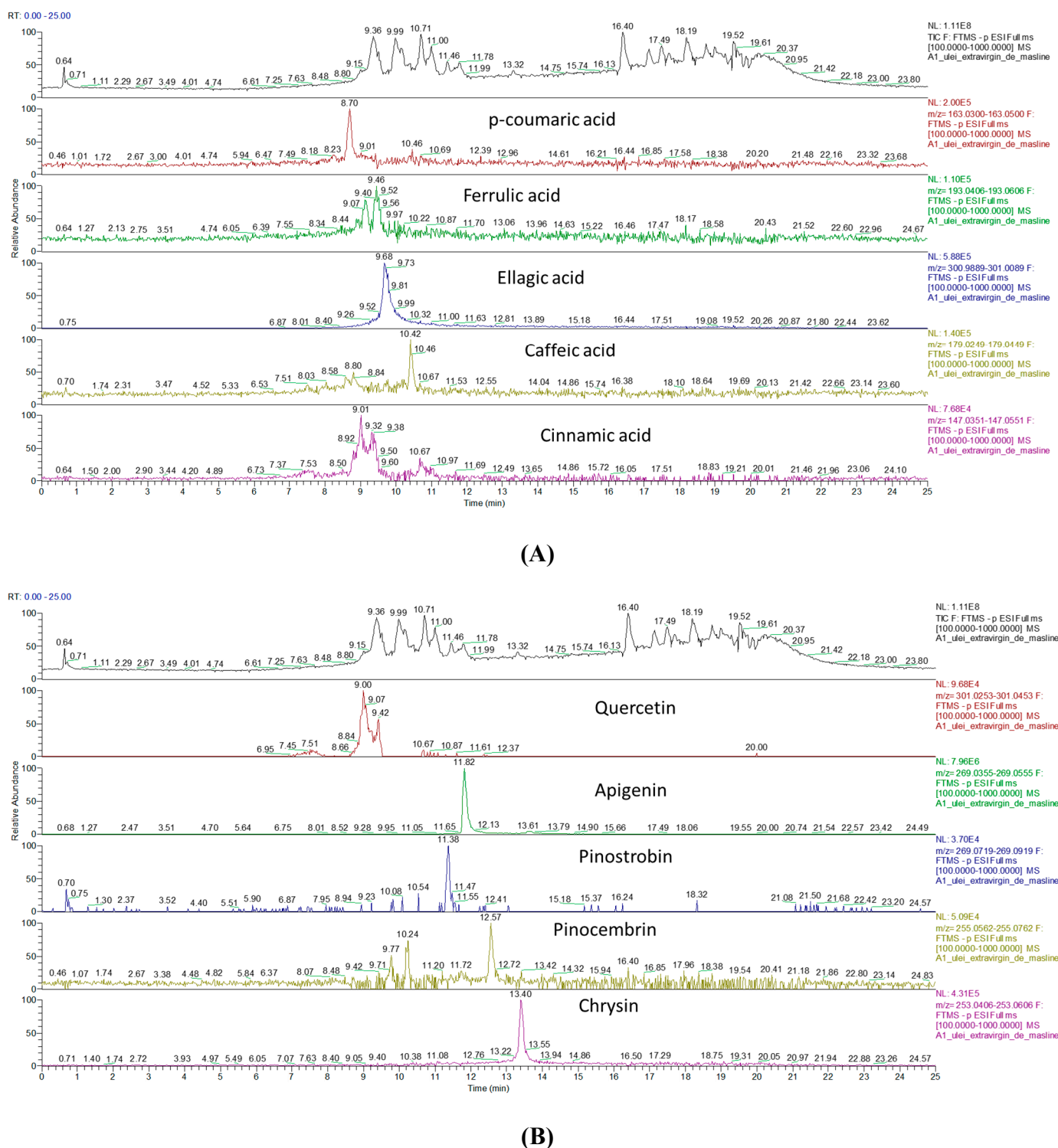


Figure S1. TIC and the extracted chromatograms of the minor phenolic compounds quantified in liquid extract of extra virgin olive oil (the chromatograms were extracted from TIC using a 5 ppm mass accuracy window; negative ion mode, full scan, base peak in the range 75–1000 m/z): (A) phenolic acids, (B) flavonoids

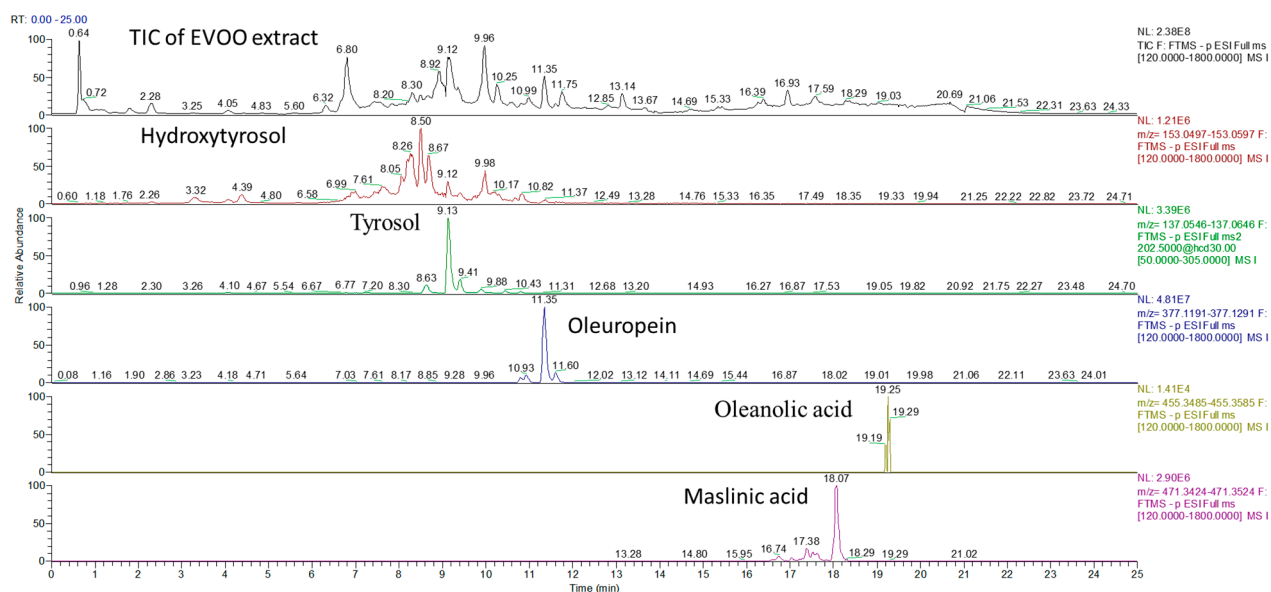


Figure S2. TIC and the extracted chromatograms of the phenolic and triterpenic compounds quantified in liquid extract of extra virgin olive oil (the chromatograms were extracted from TIC using a 5 ppm mass accuracy window; negative ion mode, full scan, base peak in the range 75-1000 m/z).

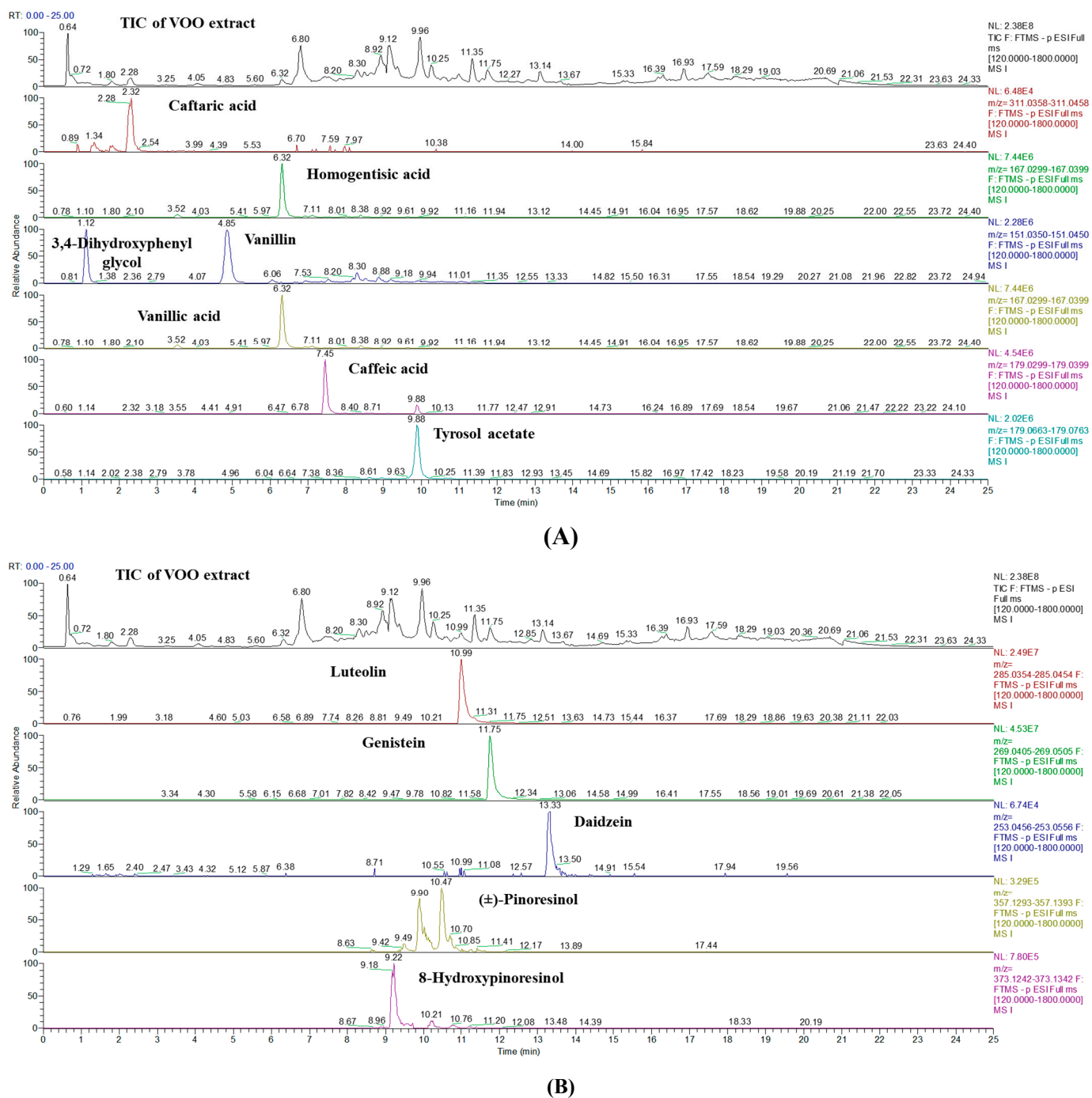


Figure S3. TIC and the extracted chromatograms of the specific compounds identified in VOO extract (the chromatograms were extracted from TIC using a 5 ppm mass accuracy window; negative ion mode, full scan, base peak in the range 75–1000 m/z): (A) simple phenols & derivatives and (B) flavonoids and lignans.

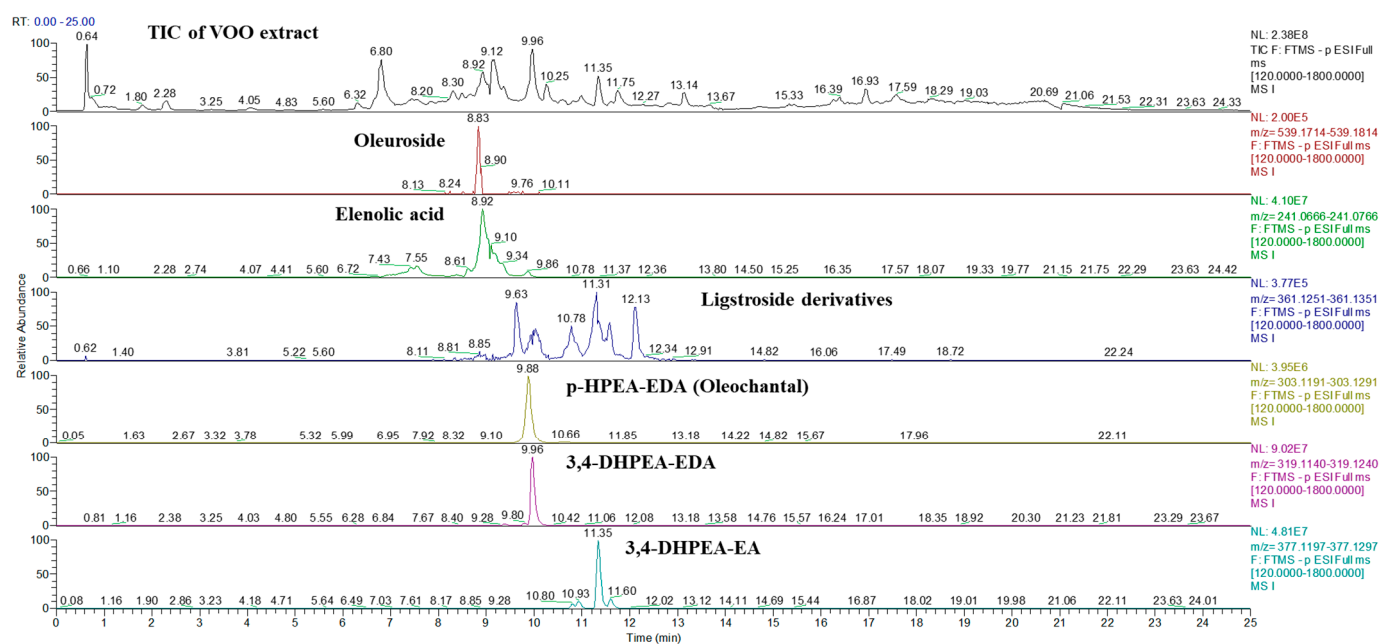


Figure S4. TIC and the extracted chromatograms of the secoiridoids and derivatives identified in VOO extract (the chromatograms were extracted from TIC using a 5 ppm mass accuracy window; negative ion mode, full scan, base peak in the range 75-1000 m/z).