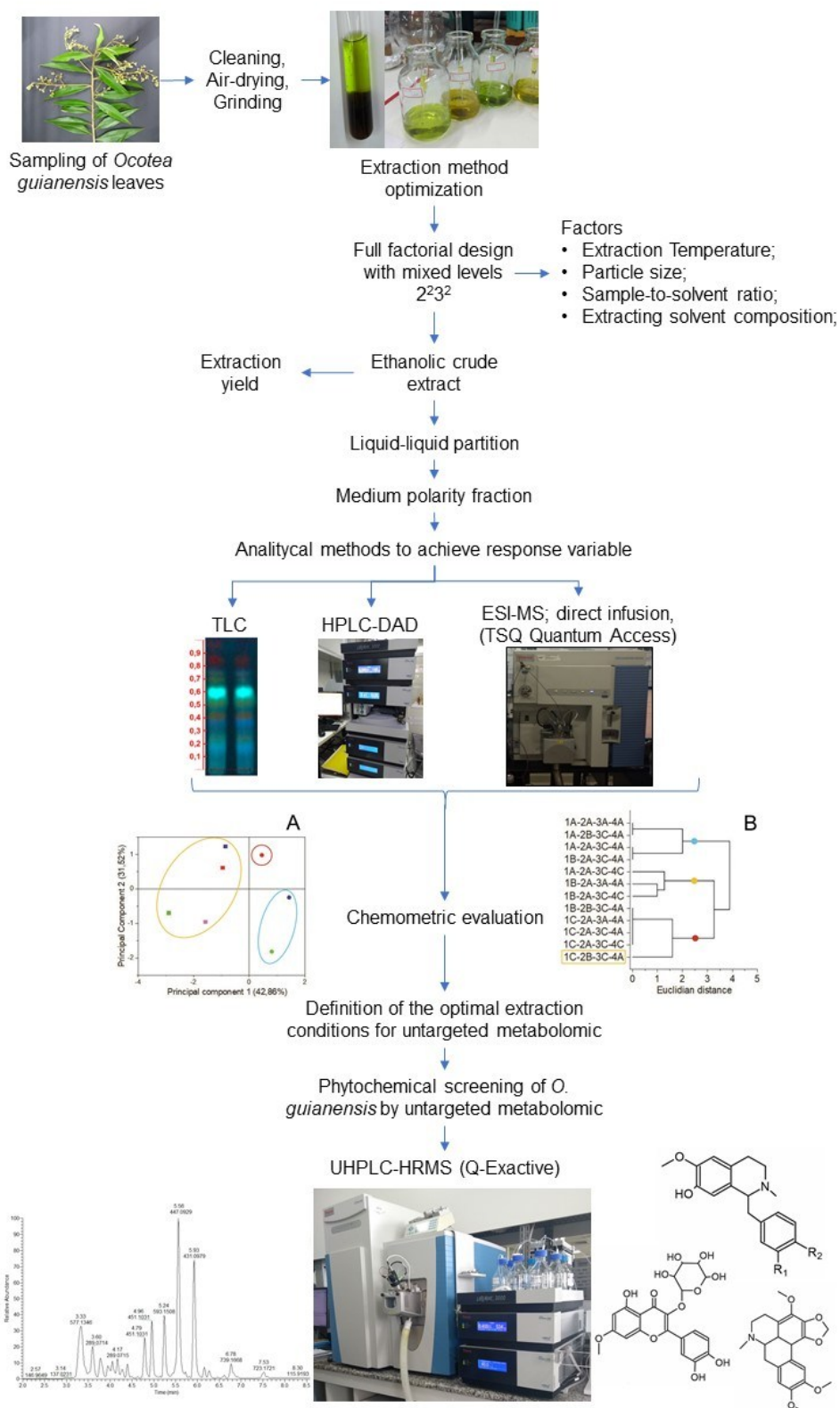


Supplementary material

Figure S1. Schematic chart of experimental section



Board S1. Instrumental details of high performance liquid chromatography tandem diode array detector analysis (used during the optimization of the extraction method)

Dionex Ultimate 3000 (Thermo Scientific, Bremen, Germany)		
Stationary phase	C18, 250 x 4.6 mm, 5.0 μ m Shim-Pack ODS(H) Shimadzu®	
Oven Temperature (°C)	40	
Injection system temperature (°C)	40	
Flow rate (mL min ⁻¹)	1.0	
Injection volume (μ L)	20	
Sample concentration (mg mL ⁻¹) in methanol	1.0	
Mobile phase	Solvent A: 0.05% formic acid Solvent B: 100% acetonitrile	
Elution gradient	Time (min.)	% of Solvent B
	0	5
	5	5
	32.5	70
	33.5	70
	43	100
	53	100
63	0	
DAD wavelength detection (nm)	300	

Board S2. Instrumental details of mass spectrometric analysis by direct injection in full scan mode (used during the optimization of the extraction method)

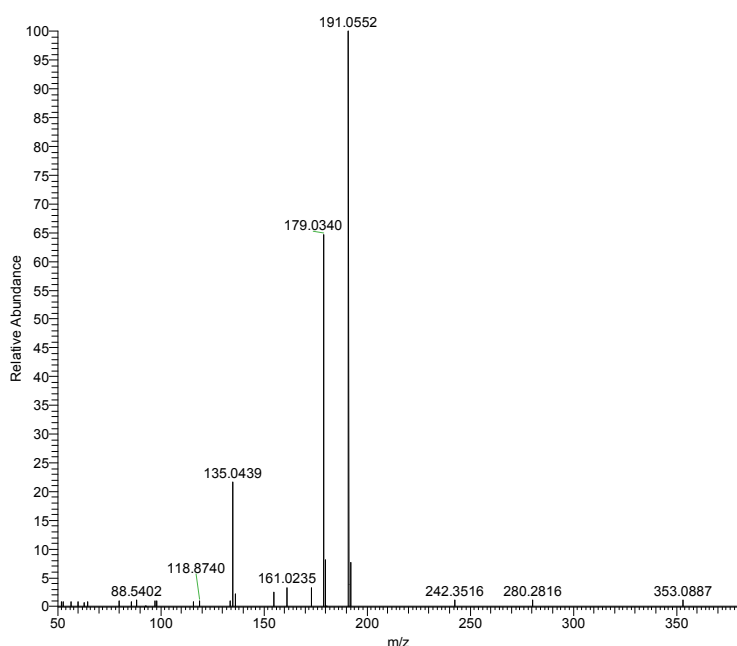
TSQ Quantum Access (Thermo Scientific, Bremen, Germany)	
Detector	Triple quadrupole
<i>m/z</i> range (Da)	100 - 1000
Acquisition mode	Full scan (MS ¹) Average of 10 scan
Isolation window	4.0
Resolution (FHWM)	75,000
Ionization source	ESI
Ionization modes	Positive and negative
Spray voltage (kV)	3.0 (negative mode) 4.5 (positive mode)
Sheath gas flow (arb)	35
Sweep gas flow (arb)	0.0
Auxiliary gas flow (arb)	15
Nebulizing gas flow (L min ⁻¹)	2.5
Nebulizing gas	N ₂
Capillary Temperature (°C)	350
Source temperature (°C)	250
Collision energy (eV)	30

Board S3. Instrumental details of ultra high performance liquid chromatography tandem high resolution mass spectrometry analysis (used in the phytochemical screening of *Ocotea delicata*)

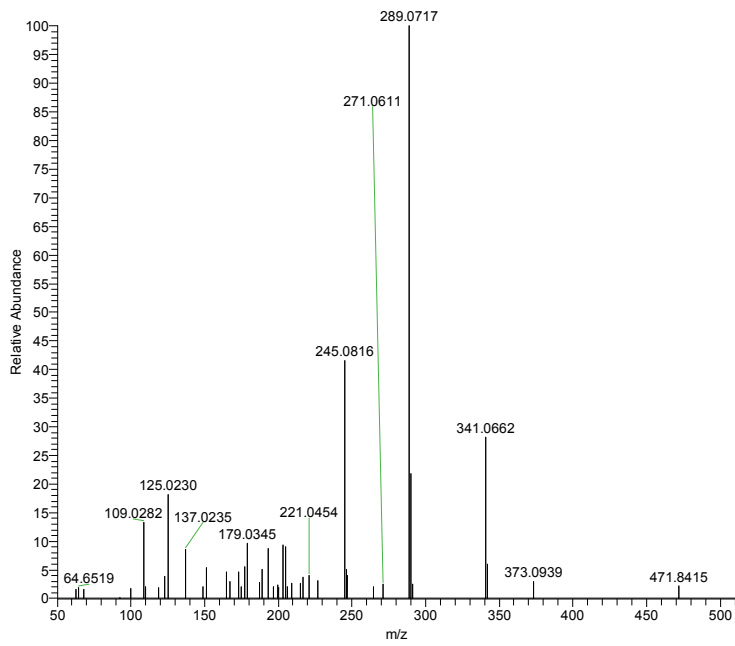
Liquid chromatograph	Dionex Ultimate 3000 (Thermo Scientific, Bremen, Germany)
Mass spectrometer	Q-Exactive (ThermoFisher Scientific, Bremen, Germany)
Detector	Hybrid quadrupole-orbitrap mass
Ionization source	ESI
Acquisition mode	MS ¹ and MS ² Data Dependent analysis (DDA) with “TopN” algorithm set to 5 precursors for MS ² experiments
<i>m/z</i> range (Da)	100 – 900
Ionization modes	Positive and negative
Spray voltage (kV)	2.9 (negative mode) 3.9 (positive mode)
Sheath gas flow (arb)	60
Sweep gas flow (arb)	0.0
Auxiliary gas flow (arb)	20
Capillary Temperature (°C)	380
Source temperature (°C)	250
Collision energy (eV)	30
Resolution (FWHM)	70,000
Mass error (ppm)	5.0
Isolation window	4.0
Mass spectrometer calibration	Xcalibur v3.0.63 Lock mass as “best” for polydimethylsiloxane

MS² data for the suggestive identification of substances in the article “Phytochemistry by design: a case study of the chemical composition of *Ocotea guianensis* optimized extracts focused on untargeted metabolomics analysis”

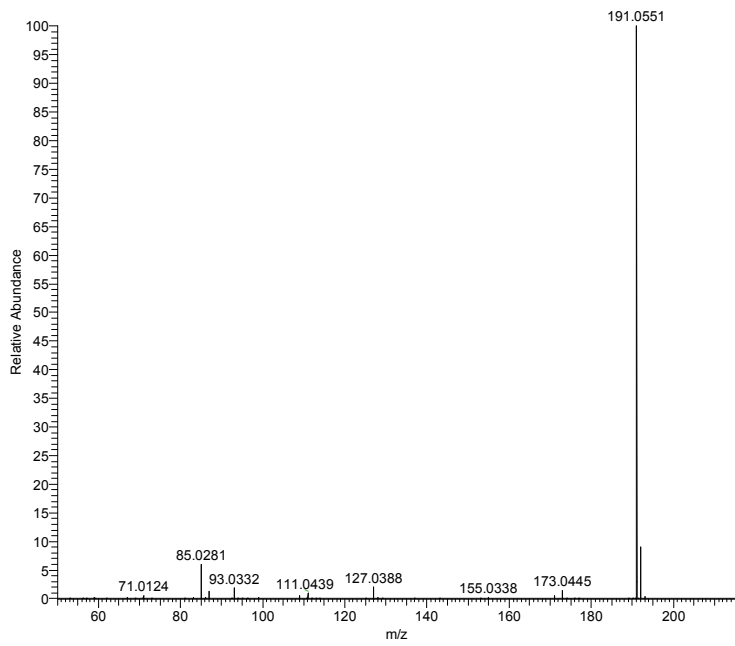
- Chlorogenic acid



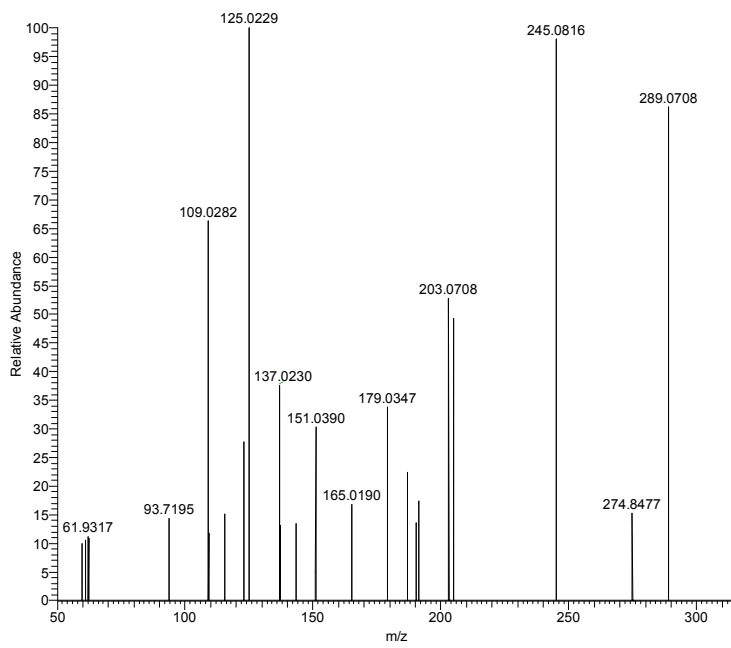
- Glycosylated derivative of catechin



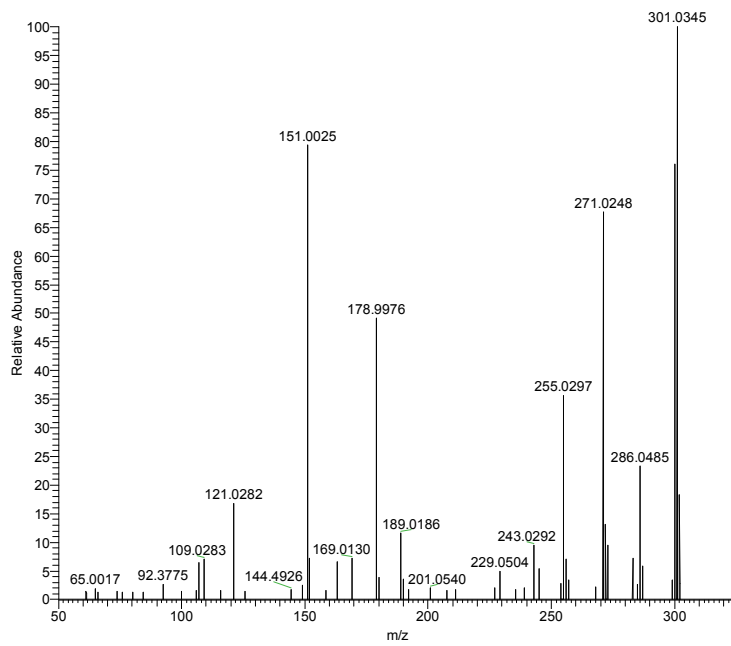
- Quinic acid



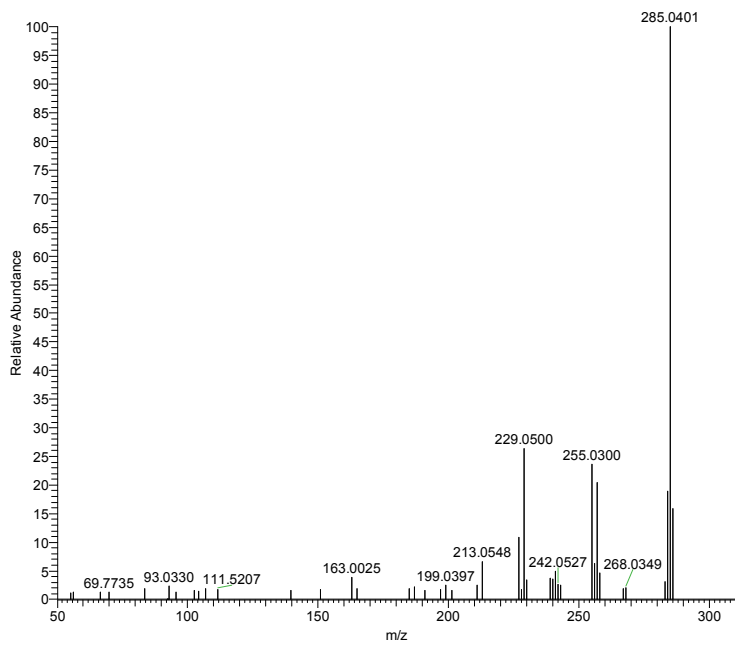
- Catechin



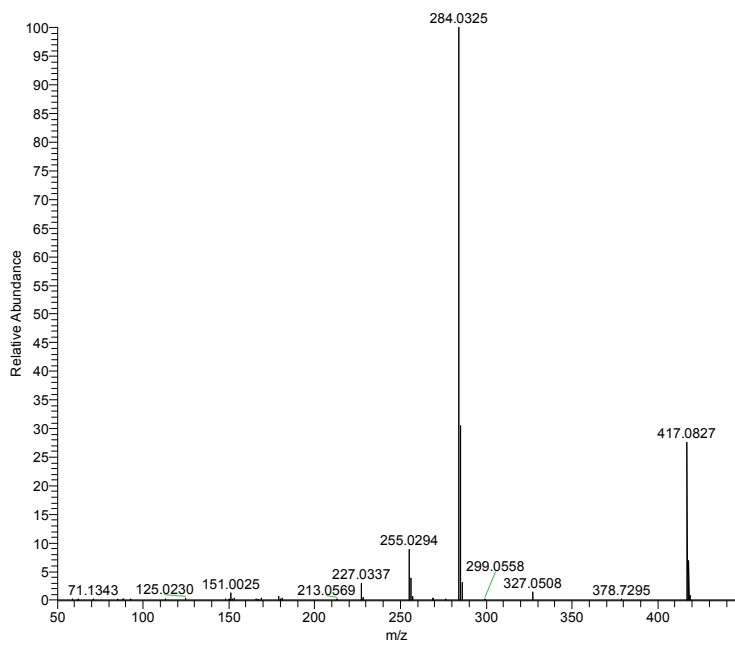
- Quercetin



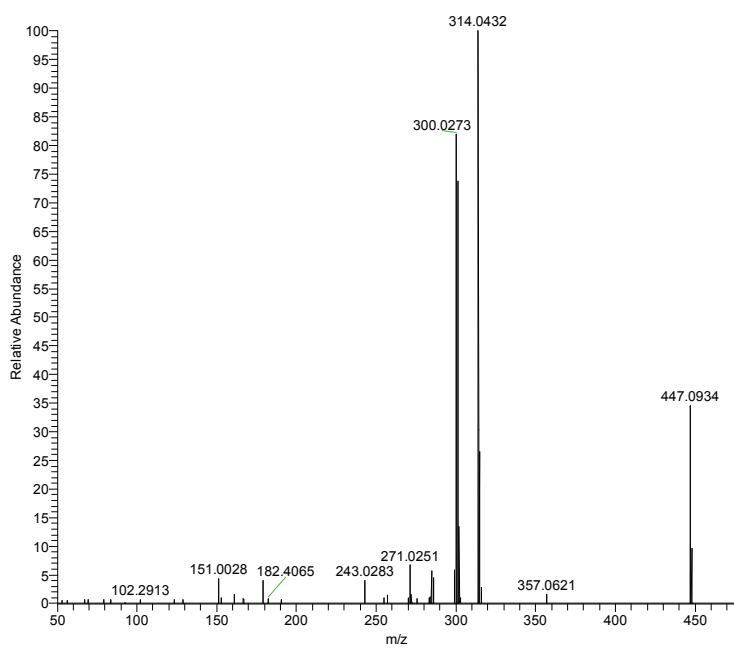
- Kaempferol



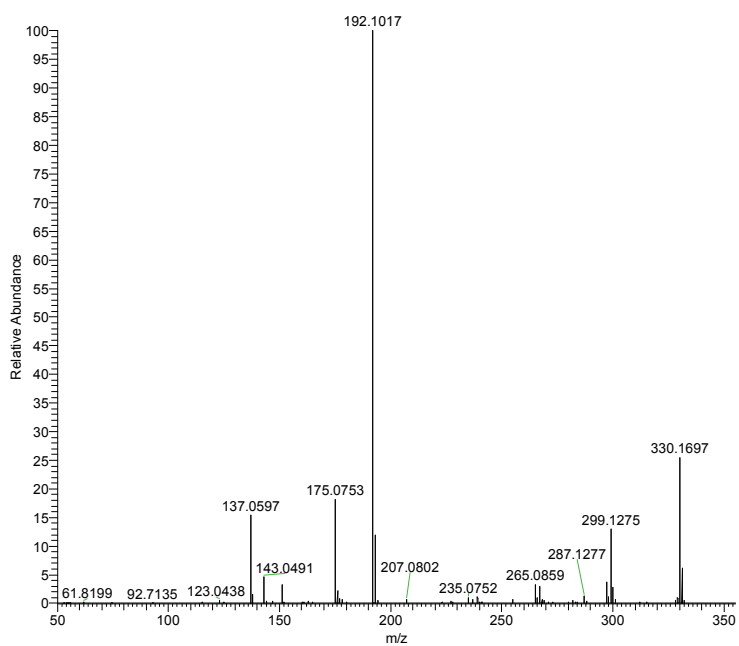
- Kaempferol-3-O-pentoside



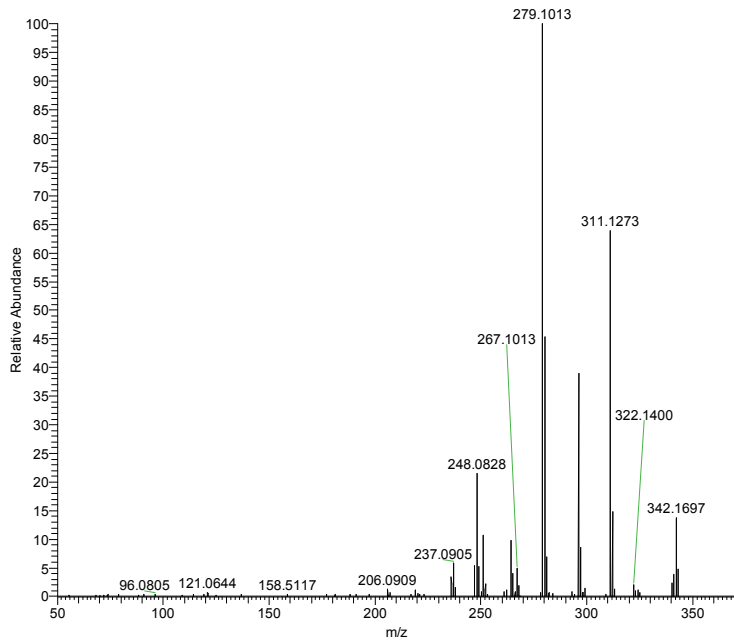
- Isorhamnetin derivate



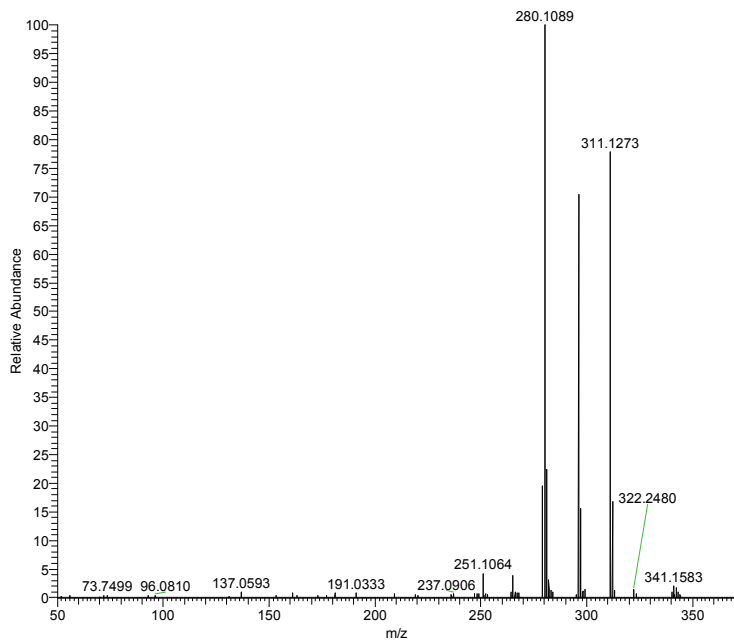
- Reticuline



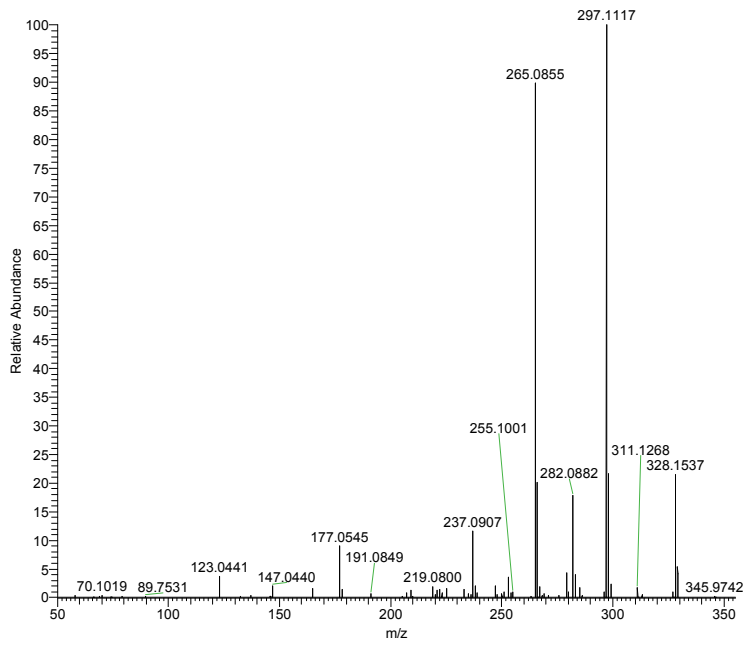
- Corydine/predicentrine
 - Retention time of 4.28 min



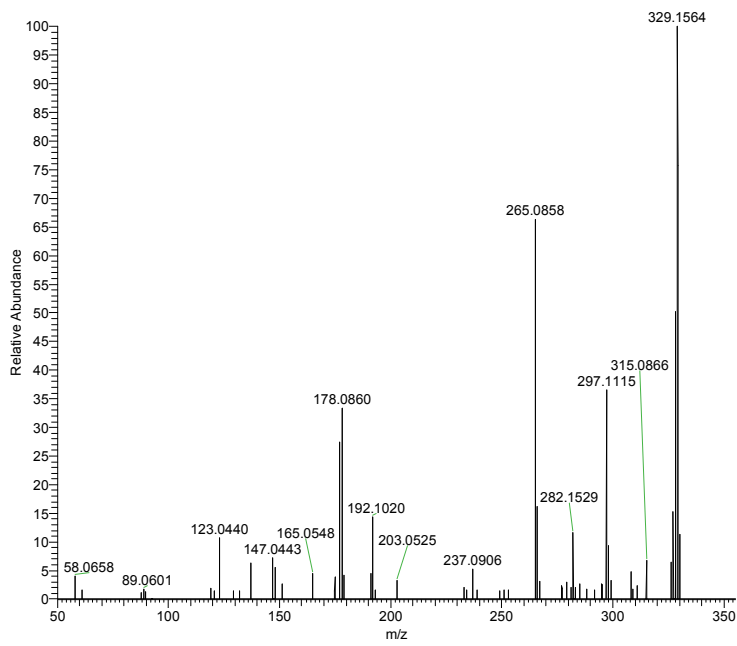
- Retention time of 4.56 min



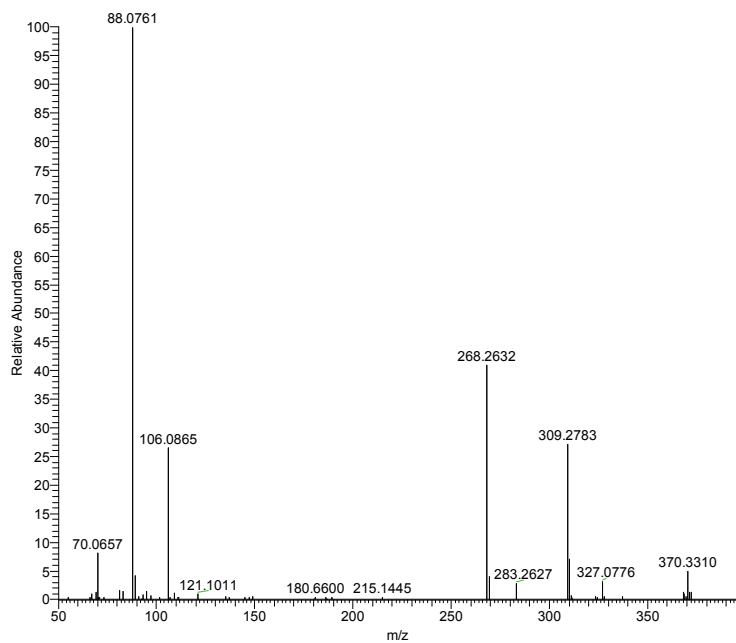
- Corytuberine/isoboldine
 - Retention time of 3.91 min



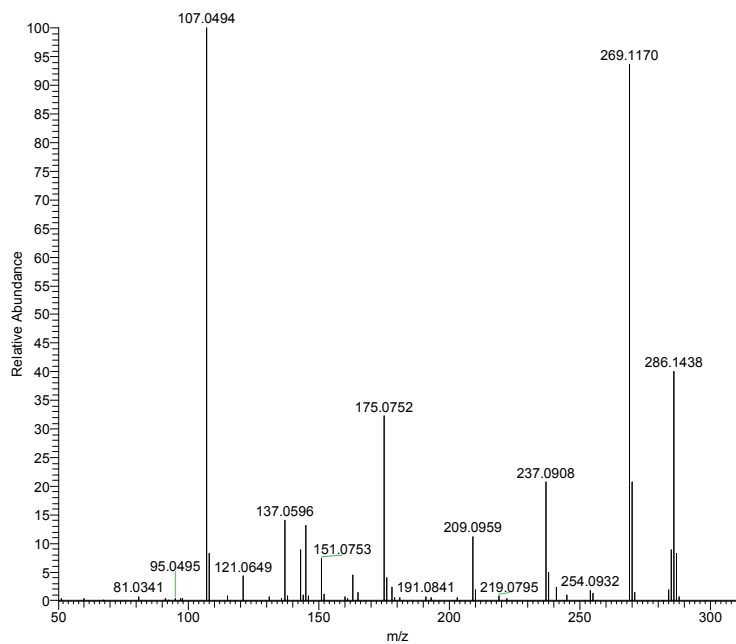
- Retention time of 4.27 min



• Ocoteine



• Coclaurine



• Norisoboldine

