Supplementary Materials: A New Alkamide with An Endoperoxide Structure from *Acmella ciliata* (Asteraceae) and Its *in Vitro* Antiplasmodial Activity

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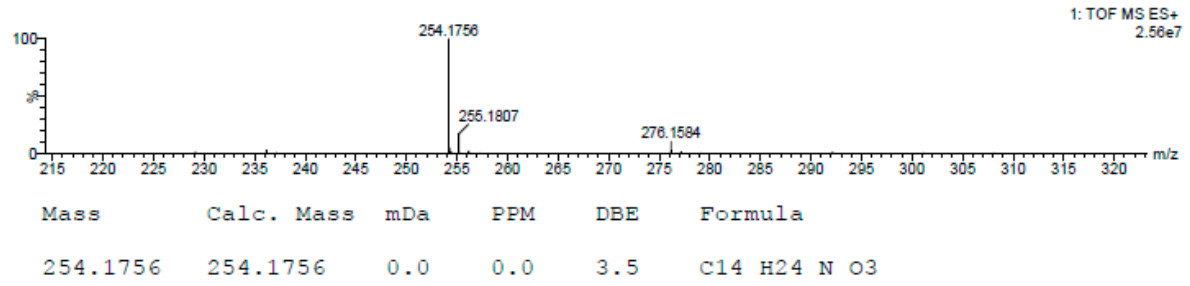

Mass	Calc. Mass	mDa	PPM	DBE	Formula
254.1756	254.1756	0.0	0.0	3.5	C14 H24 N O3

Figure S1. +ESI-QTOF mass spectrum of compound **3**.

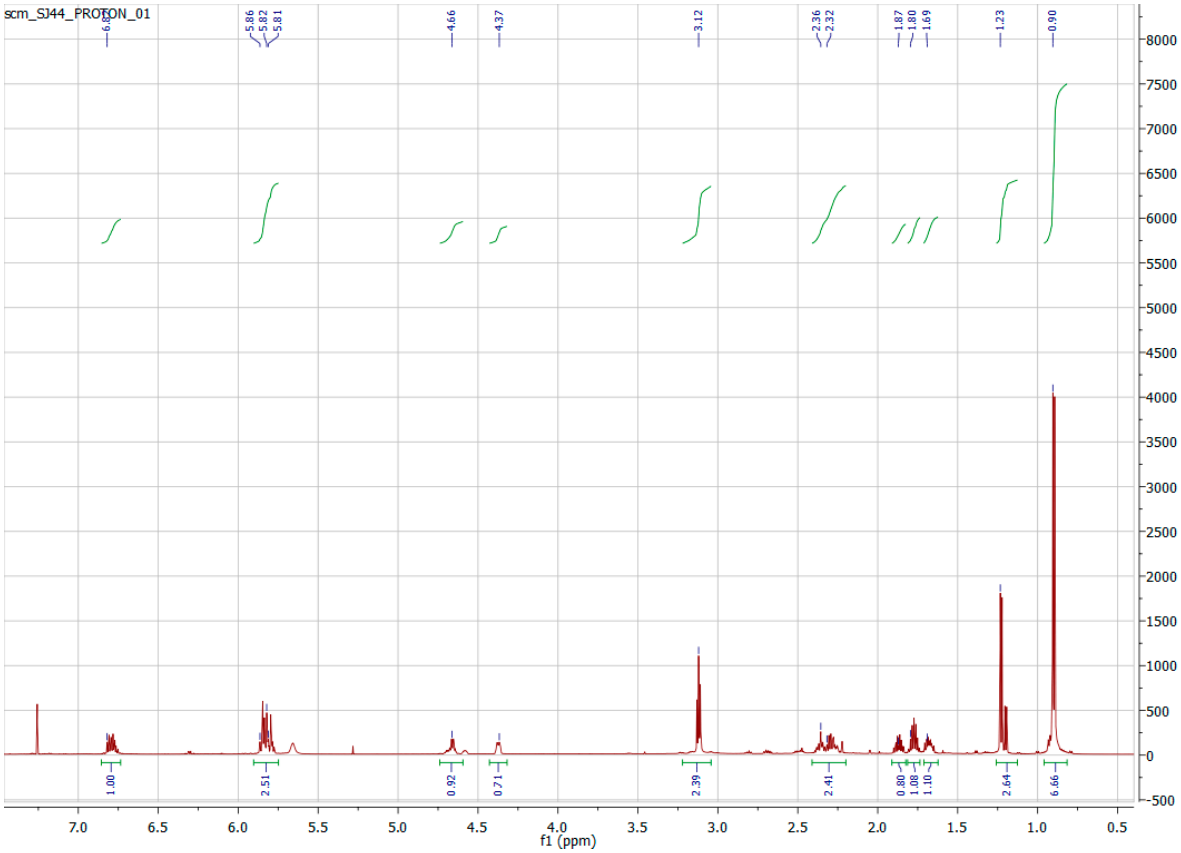

Figure S2. ^{1}H-NMR spectrum (600 MHz, $CDCl_3$) of compound **3**.

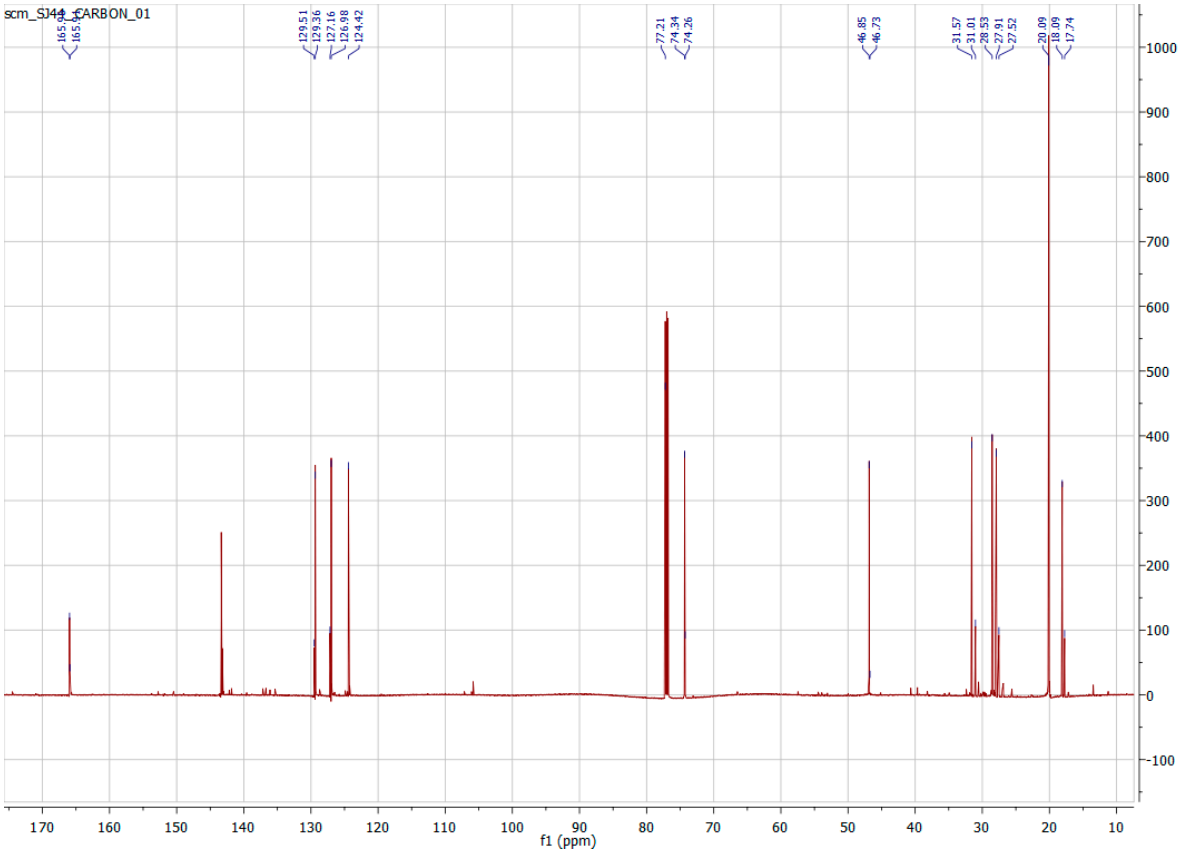

Figure S3. ^{13}C-NMR spectrum (150 MHz, $CDCl_3$) of compound **3**.

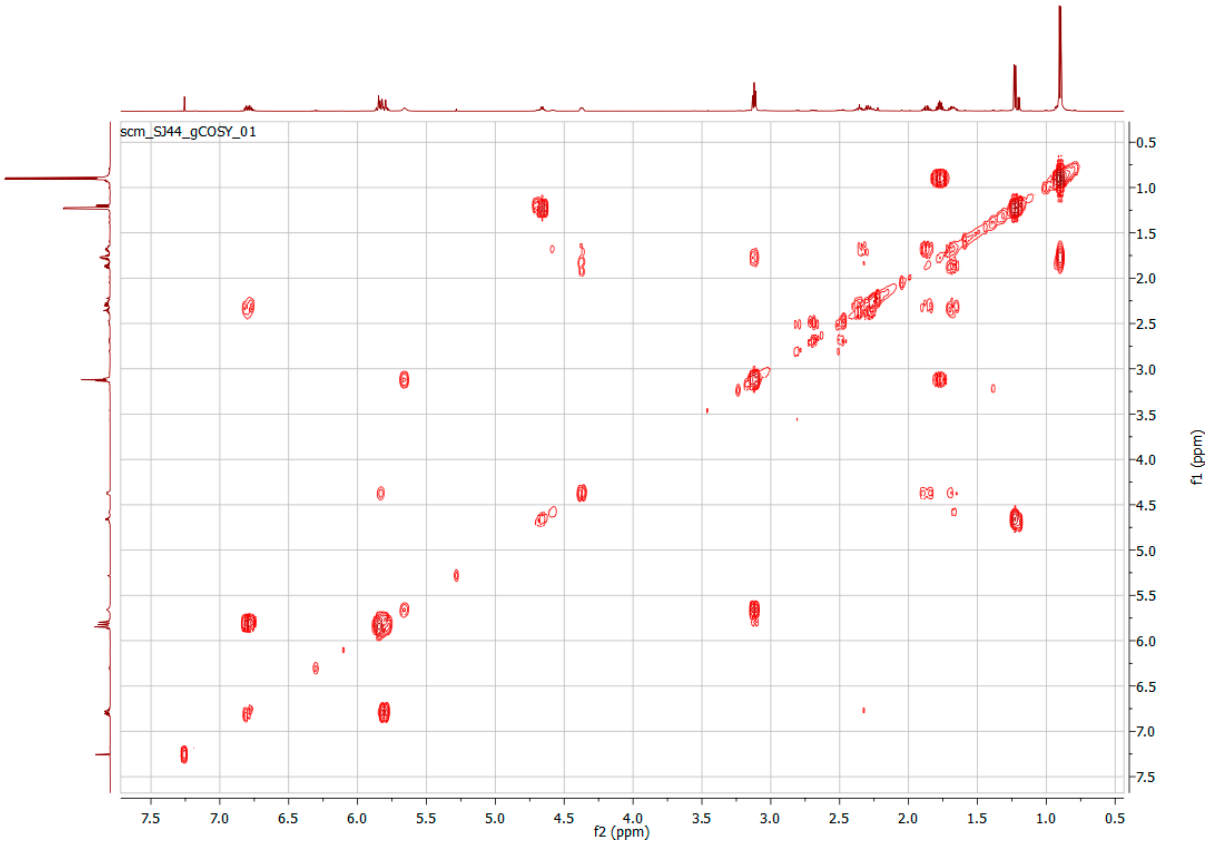

Figure S4. ^{1}H/^{1}H-COSY spectrum (600 MHz, $CDCl_3$) of compound **3**.

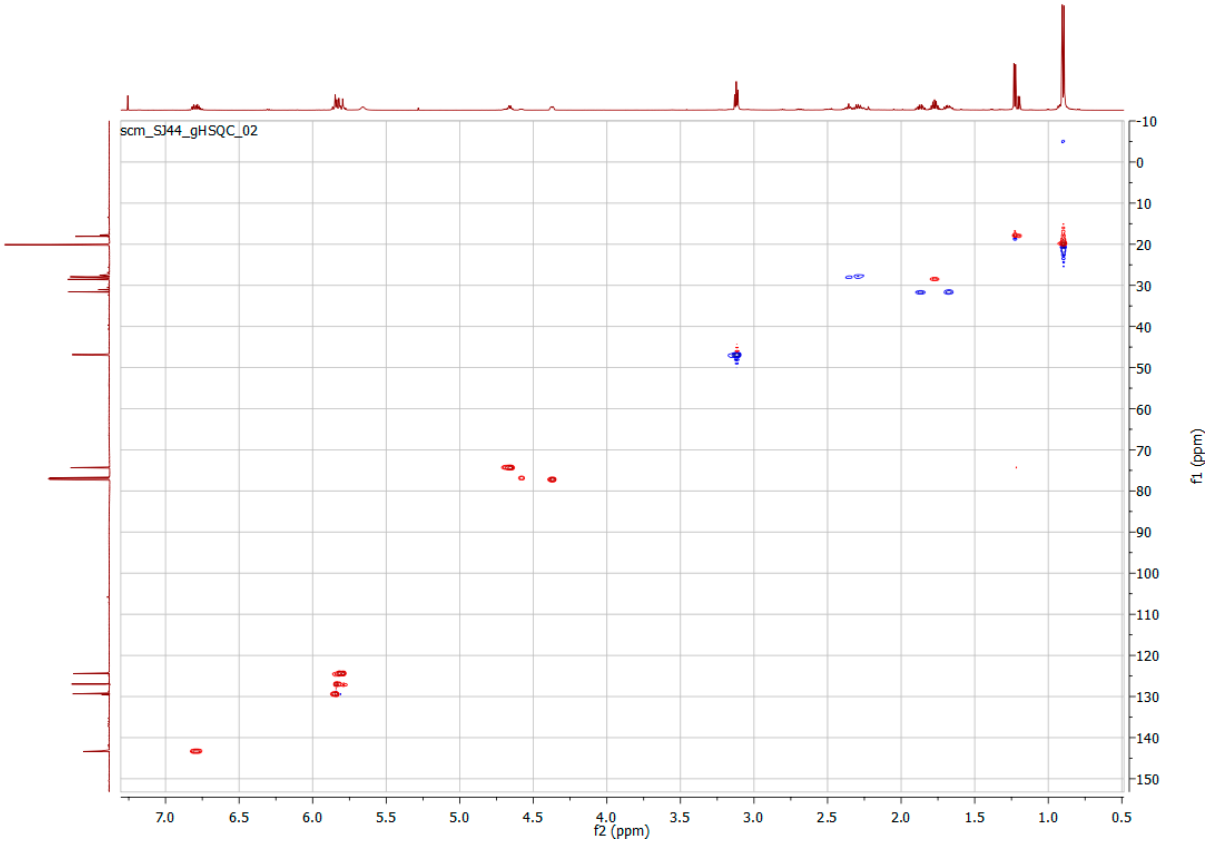

Figure S5. $^{1}H/^{13}C$-HSQC spectrum (600/150 MHz, $CDCl_3$) of compound **3**.

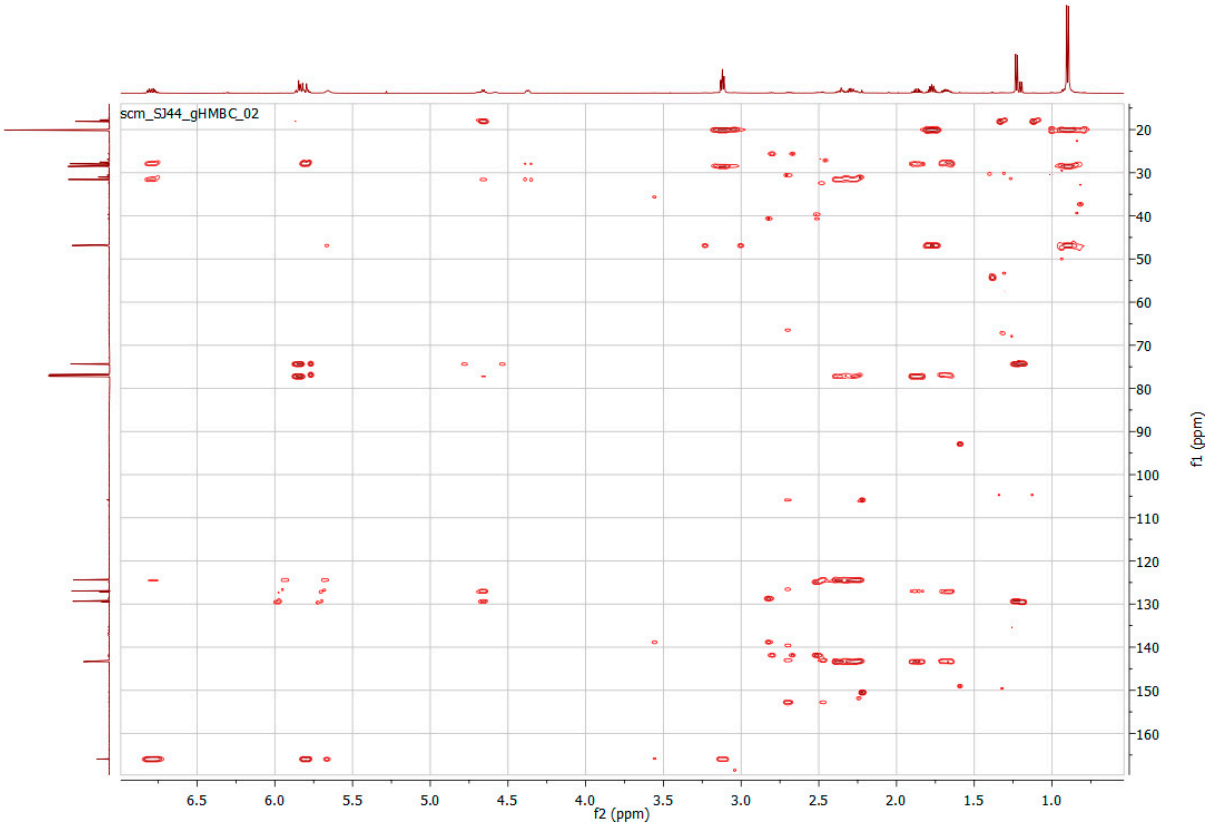

Figure S6. $^{1}H/^{13}C$-HMBC spectrum (600/150 MHz, $CDCl_3$) of compound **3**.

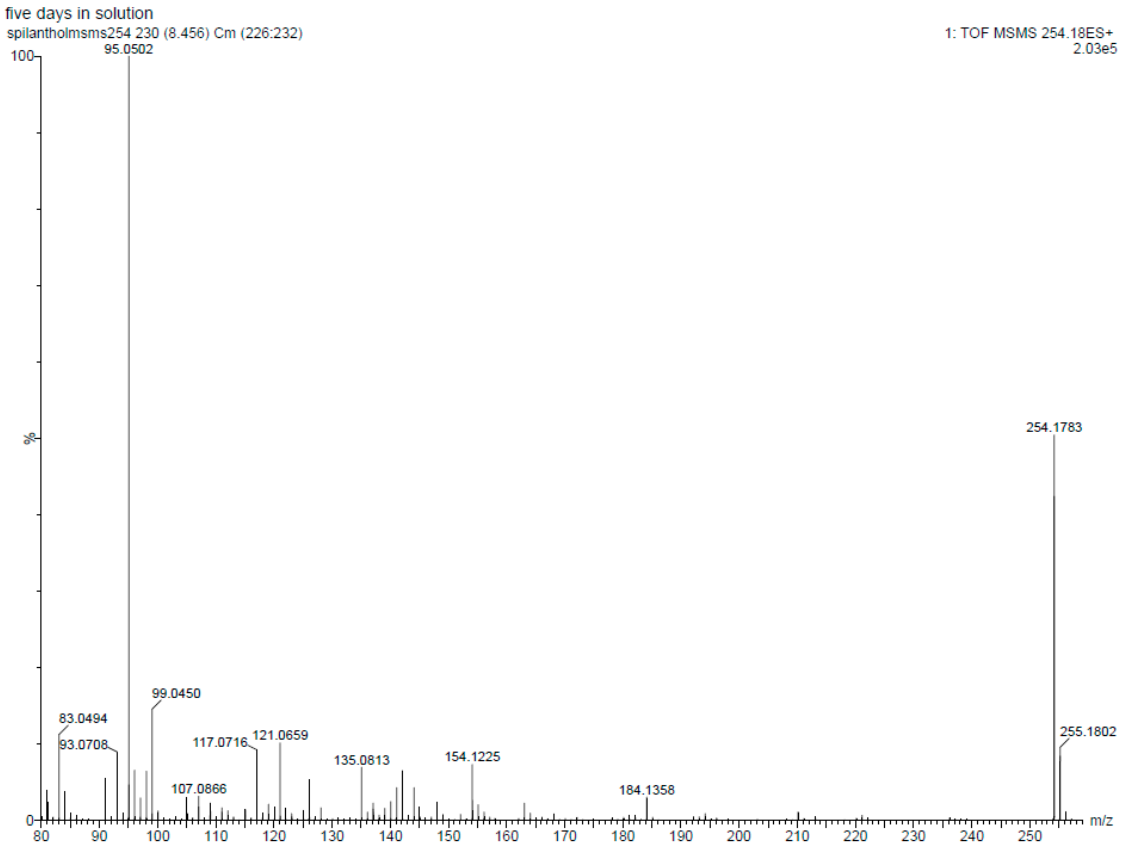

Figure S7. HR-ESI-MS/MS spectrum of the endoperoxide alkamide **3** (parent ion *m*/*z* 254).

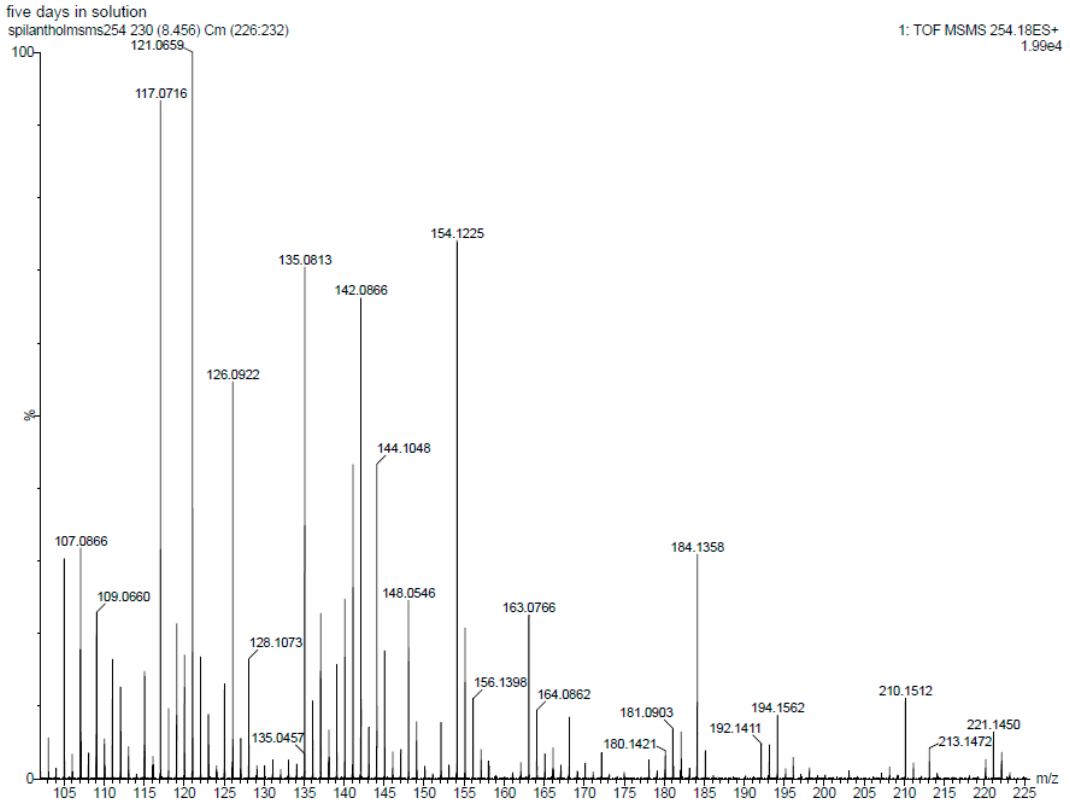

Figure S8. Magnified HR-ESI-MS/MS spectrum of the endoperoxide alkamide **3** (parent ion *m*/*z* 254).

LC-MS and LC-MS/MS Analyses

Pure compounds: Chromatograpic separation and check for purity was performed on a Dionex Ultimate 3000 RS Liquid Chromatography System on a Dionex Acclaim RSLC 120, C18 column (2.1 × 100 mm, 2.2 μm) with a binary gradient (A: water with 0.1% formic acid; B: acetonitrile with 0.1% formic acid) at 0.8 mL/min: 0 to 9.5 min: linear from 5% B to 100% B; 9.5 to 12.5 min: isocratic 100% B; 12.5 to 12.6 min: linear from 100% B to 5% B; 12.6 to 15 min: isocratic 5% B. The injection volume was 2 μL. Eluted compounds were detected using a Dionex Ultimate DAD-3000 RS over a wavelength range of 200–400 nm and a Bruker Daltonics micrOTOF-QII time-of-flight mass spectrometer equipped with an Apollo electrospray ionization source in positive mode at 5 Hz over a mass range of *m*/*z* 50–1,000 using the following instrument settings: nebulizer gas nitrogen, 5 bar; dry gas nitrogen, 9 L/min, 220 °C; capillary voltage 4,500 V; end plate offset −500 V; transfer time 70 μs; collision gas nitrogen; collision energy and collision RF settings were combined to each single spectrum of 1000 summations as follows: 250 summations with 20% base collision energy and 130 Vpp + 250 summations with 100% base collision energy and 500 Vpp + 250 summations with 20% base collision energy and 130 Vpp + 250 summations with 100% base collision energy and 500 Vpp. Base collision energy was 50 eV for precursor ions with a m/z less than 500 and then linearly interpolated against m/z up to a maximum of 70 eV for precursor ions with a *m*/*z* of up to 1000. Internal dataset calibration (HPC mode) was performed for each analysis using the mass spectrum of a 10 mM solution of sodium formiate in 50% isopropanol that was infused during LC re-equilibration using a divert valve equipped with a 20 μL sample loop. The sample concentration was 0.1 mg/mL in methanol.

CH_3Cl_3-extract: Chromatographic separation was performed on a BEH C18 column: 50 mm, 1.0 mm, particle size 1.7 μm (Waters) during 15 min. The temperature of the column and the sample tray temperature were respectively 40 °C and 20 °C. The gradient employed at flow rate of 0.3 mL/min, was 95% A (water/formic acid, 99.9/0.1 *v*/*v*) and 5% B (acetonitrile); 0–8 min, 60% of A; 8.1–8.5 min 40% of A; 8.5–10.9 min 10% of A; 10.9–15 min 95% of A. The injection volume of the sample was amounted to 5 μL. The analysis was recorded in ESI positive mode using the following instrument settings: nebulizer and desolvation gas: nitrogen; flow cone gas 10 L/h; flow desolvation gas 700 L/h; sampling cone 40 V; source offset 80 V; temperature cone 90 °C; temperature desolvation 200 °C; collision gas: argon; energy of collision: 25 eV; Lockspray reference sample: Leucine encephalin with the lock mass at *m*/*z* 556.2771 (ESI+).