Supporting Information

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A New Phloroglucinol Derivative Isolated from *Hypericum afrum*, a Plant Endemic to Algeria

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General

Melting points were determined on an Opti-Melt automated melting point system (Stanford Research Systems) and were uncorrected. IR spectra were recorded using an Agilent model Cary 630 FT-IR. Optical rotations were recorded using a Rudolph Research Analytical Autopol V Polarimeter. UV was obtained using a Perkin-Elmer Lambda 3B UV/vis-spectrophotometer. ^{1}H and ^{13}C NMR spectra were obtained on Bruker model AMX 500 NMR spectrometer with standard pulse sequences, operating at 400 MHz in ^{1}H and 100 MHz in ^{13}C. The chemical shift values were reported in parts per million units (ppm) from trimethylsilane (TMS) using known solvent chemical shifts. Coupling constants were recorded in Hertz (Hz). Standard pulse sequences were used for COSY, HMQC, HMBC, NOESY and DEPT. High-resolution mass spectra (HRMS) were measured on a Micromass Q-Tof Micro mass spectrometer with a lock spray source. Column chromatography was carried out on silica gel (70-230 mesh, Merck, Germany), C18 SPE and SPE columns (500 mg Bed, Thermo scientific, USA), Diaion HP-20 (Sorbetch technologies, Norcross, USA) and Sorbadex 20-LH (Sorbetch technologies, Norcross, USA). TLC (silica gel 60 F254) was used to monitor fractions from column chromatography. Preparative TLC was carried out on silica gel 60 PF254+366 plates (20 × 20 cm, 1 mm thick). Visualization of the TLC plates was achieved with a UV lamp (λ = 254 and 365 nm) and anisaldehyde/acid spray reagent (MeOH-acetic acid-anisaldehyde-sulfuric acid, 85:9:1:5).

In vitro MAO inhibition assays

The extracts and purified constituents were tested for inhibition of recombinant human MAO-A and B activities as described earlier [1]. Fixed substrate concentration and varying inhibitor concentrations were used to determine the IC_{50} value. The reactions were carried out in 0.1 M potassium phosphate buffer at pH 7.4. Incubations mixtures contained of MAO-A (5 µg/mL) or of MAO-B (10 µg/mL) in 200 µL reaction mixture. The extracts and test compounds were dissolved in DMSO or in buffer. The reaction mixtures were pre-incubated for 10 minutes at 37 °C followed by the addition of MAO-A/MAO-B to initiate the reactions. The formation of 4-hydroxyquinoline was determined fluorometrically by SpectraMax M5 fluorescence plate reader (Molecular Devices, Sunnyvale, CA) with an excitation and emission wavelength of 320 nm and 380 nm, respectively, using the SoftMax Pro program. IC_{50} values were determined by dose-response analysis using ExcelFit.

[1] V. Samoylenko, Md. M. Rahman, B. L. Tekwani, L. M. Tripathi, Y. H. Wang, S. I. Khan, L. S. Miller, V. C. Joshi and I. Muhammad (2010). *Banisteriopsis caapi*, a unique combination of MAO inhibitory and antioxidante constituents for the activities relevant to neurodegenerative disorders and Parkinson's disease, J. Ethnopharmacol. **127**, 357-367.

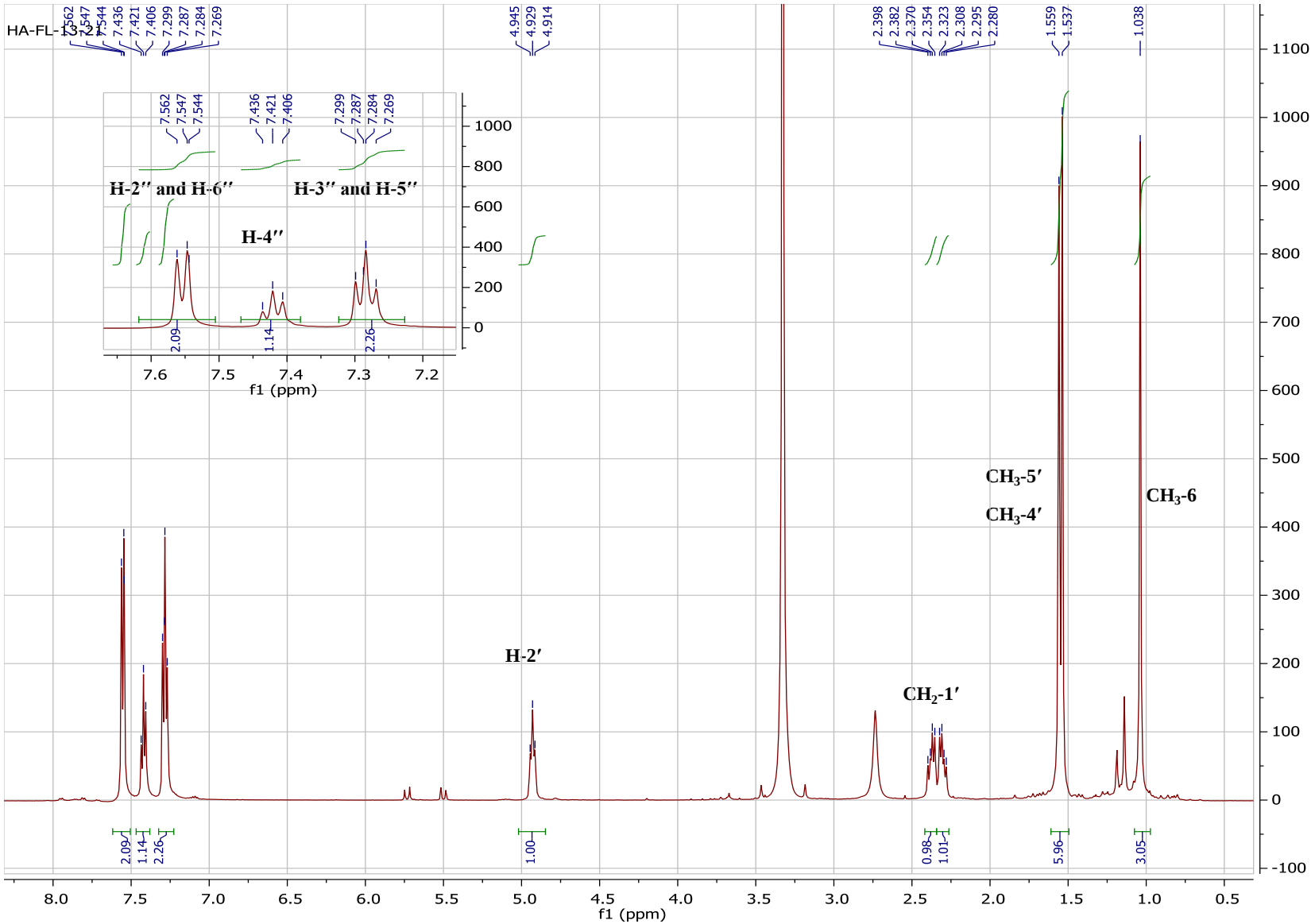

Figure S1. ^{1}H NMR spectrum of compound 1.

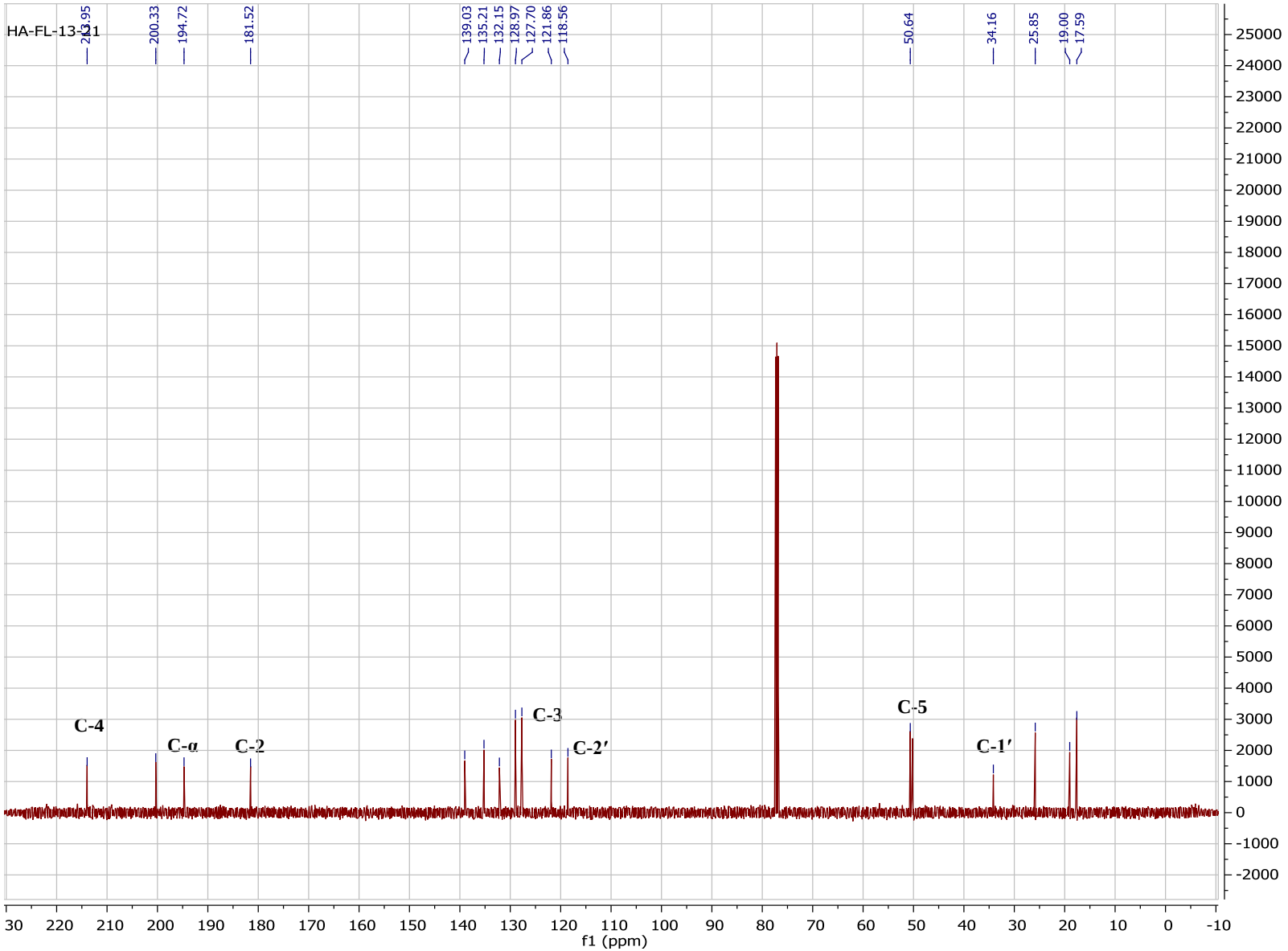

Figure S2. ^{13}C NMR spectrum of compound 1.

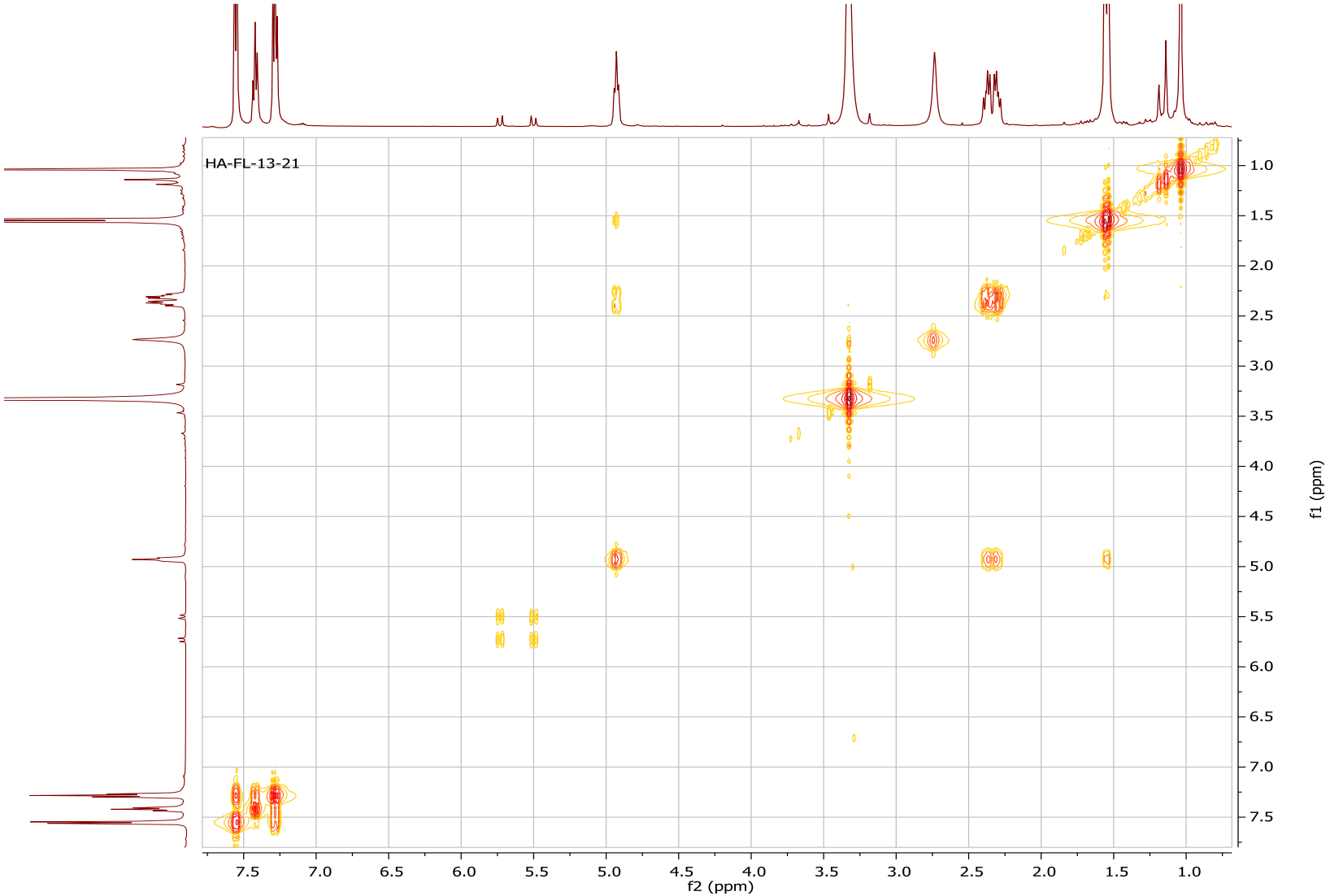

Figure S3. COSY experiment of compound 1.

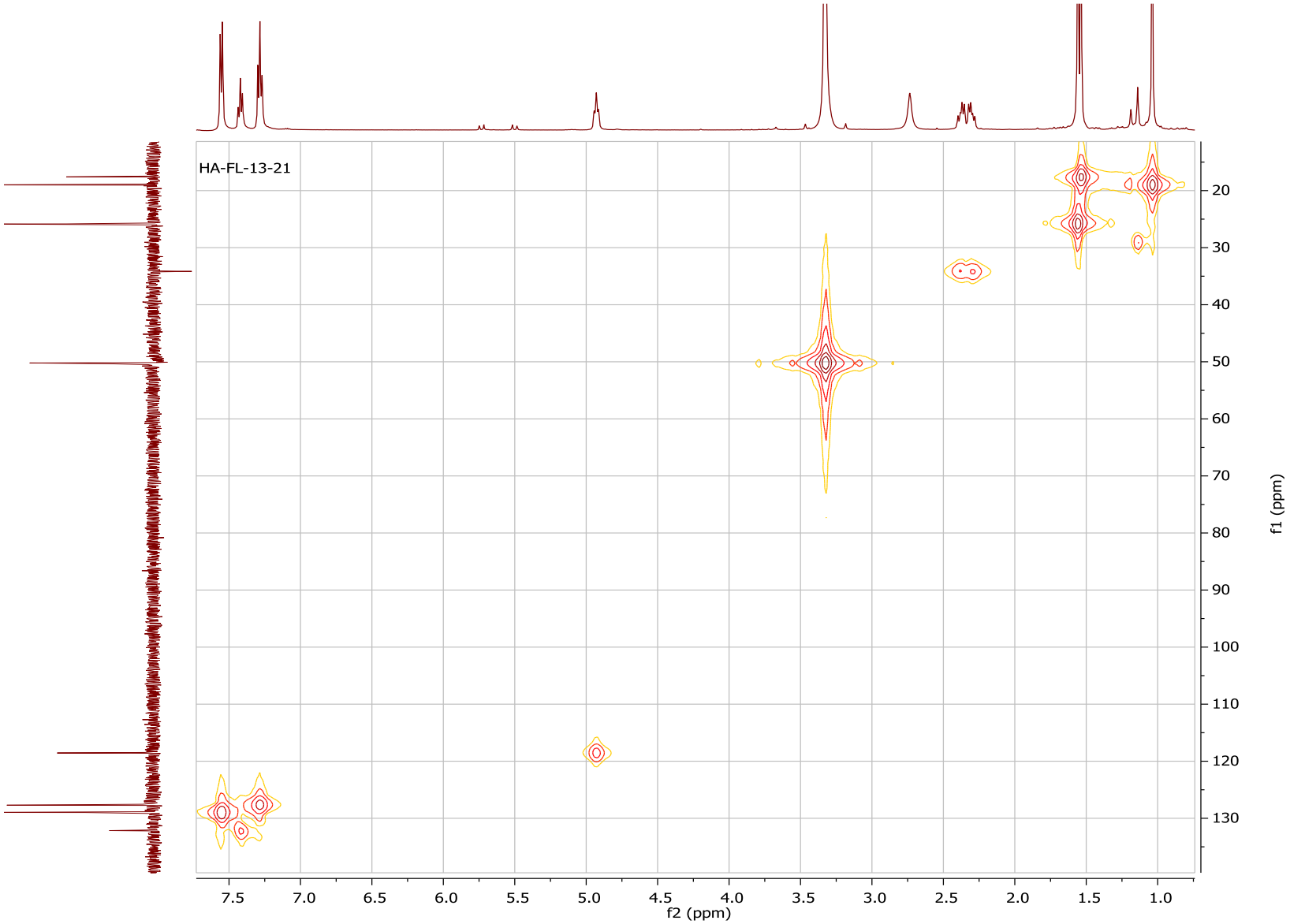

Figure S4. HSQC experiment of compound 1.

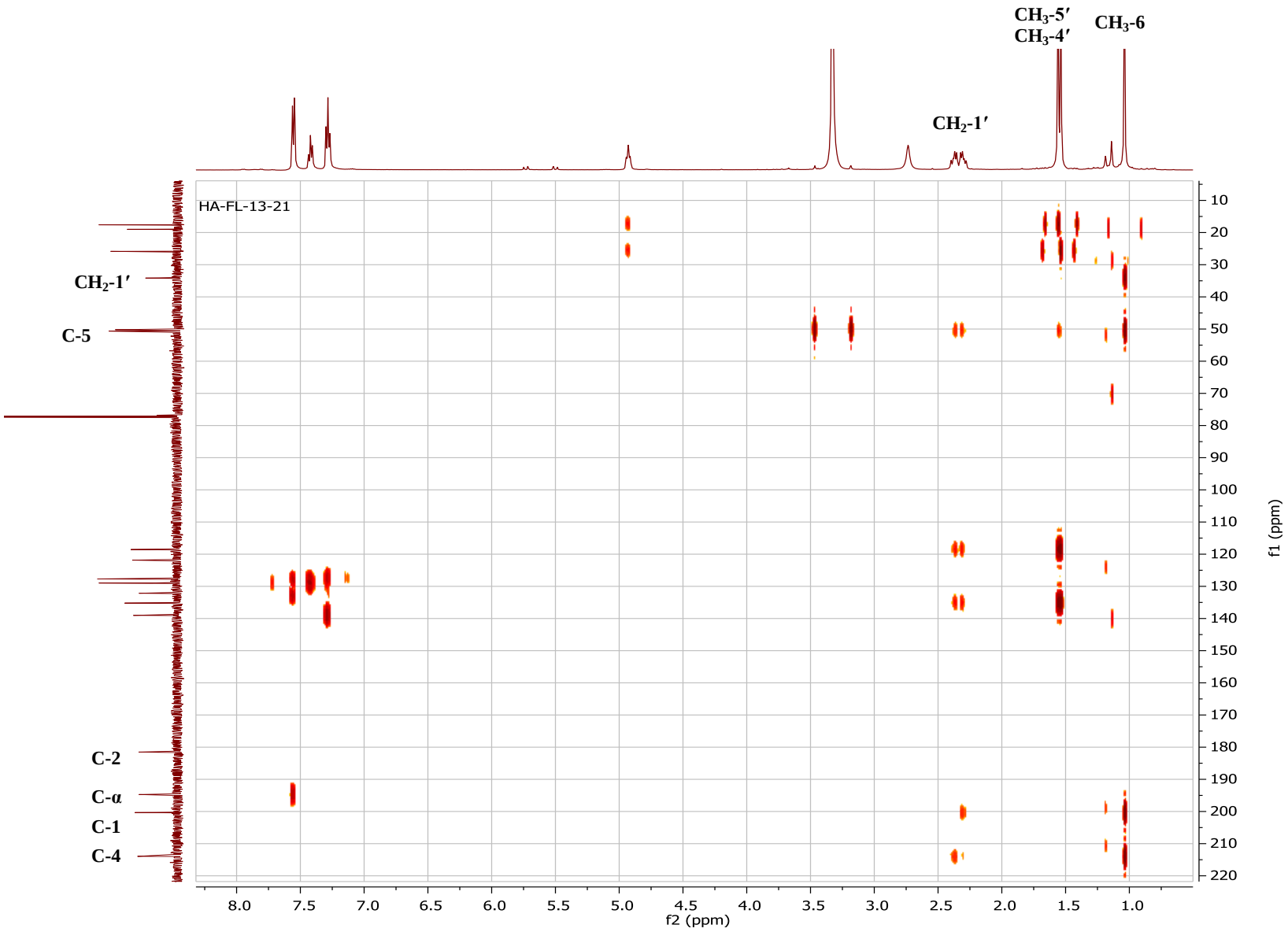

Figure S5. HMBC experiment of compound 1.

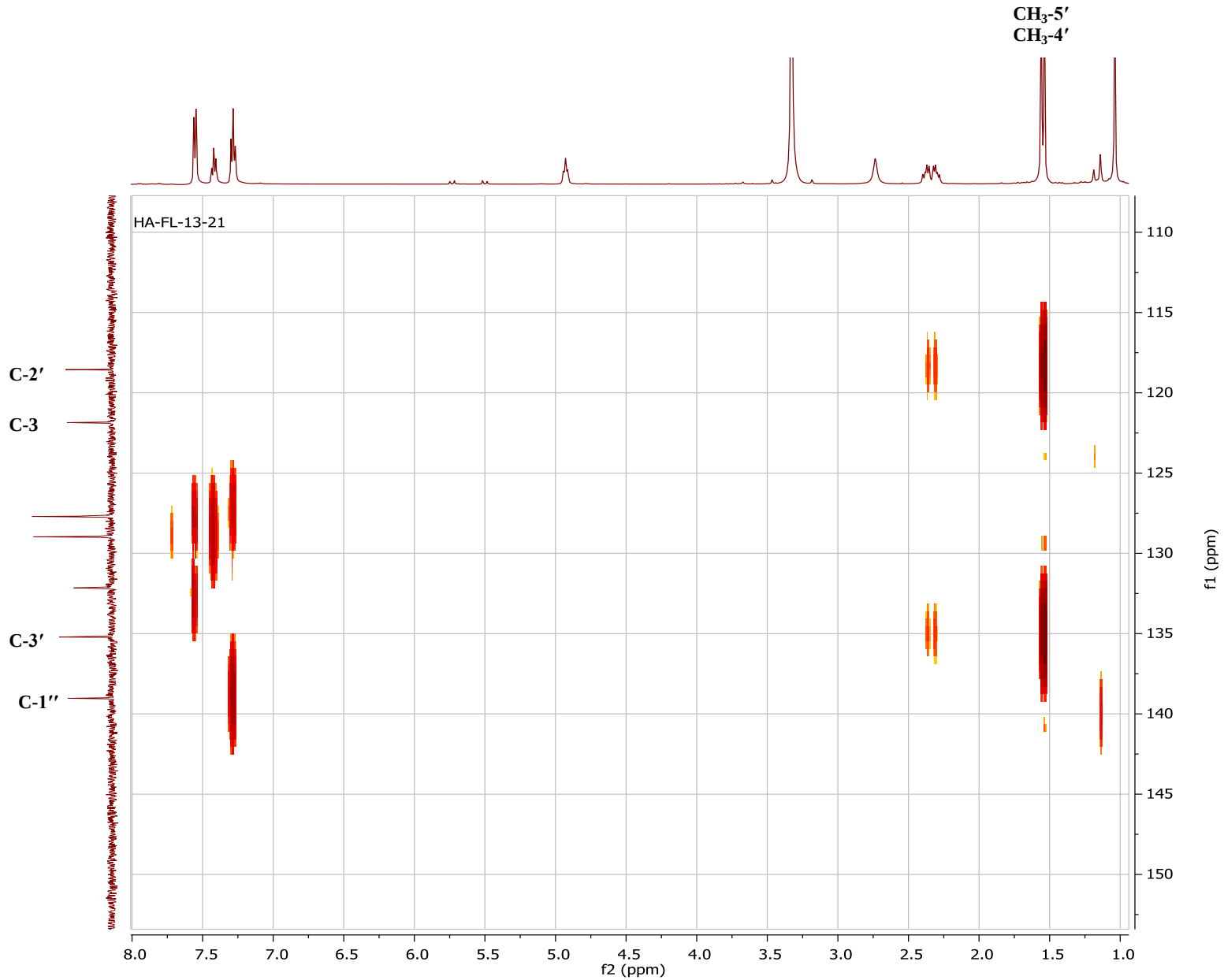

Figure S6. Enlargement HMBC experiment of compound 1.

	Formula	Calculated Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
1	C18 H17 O5	313.10705	10.5	0.16	-0.05	-0.16	0.932

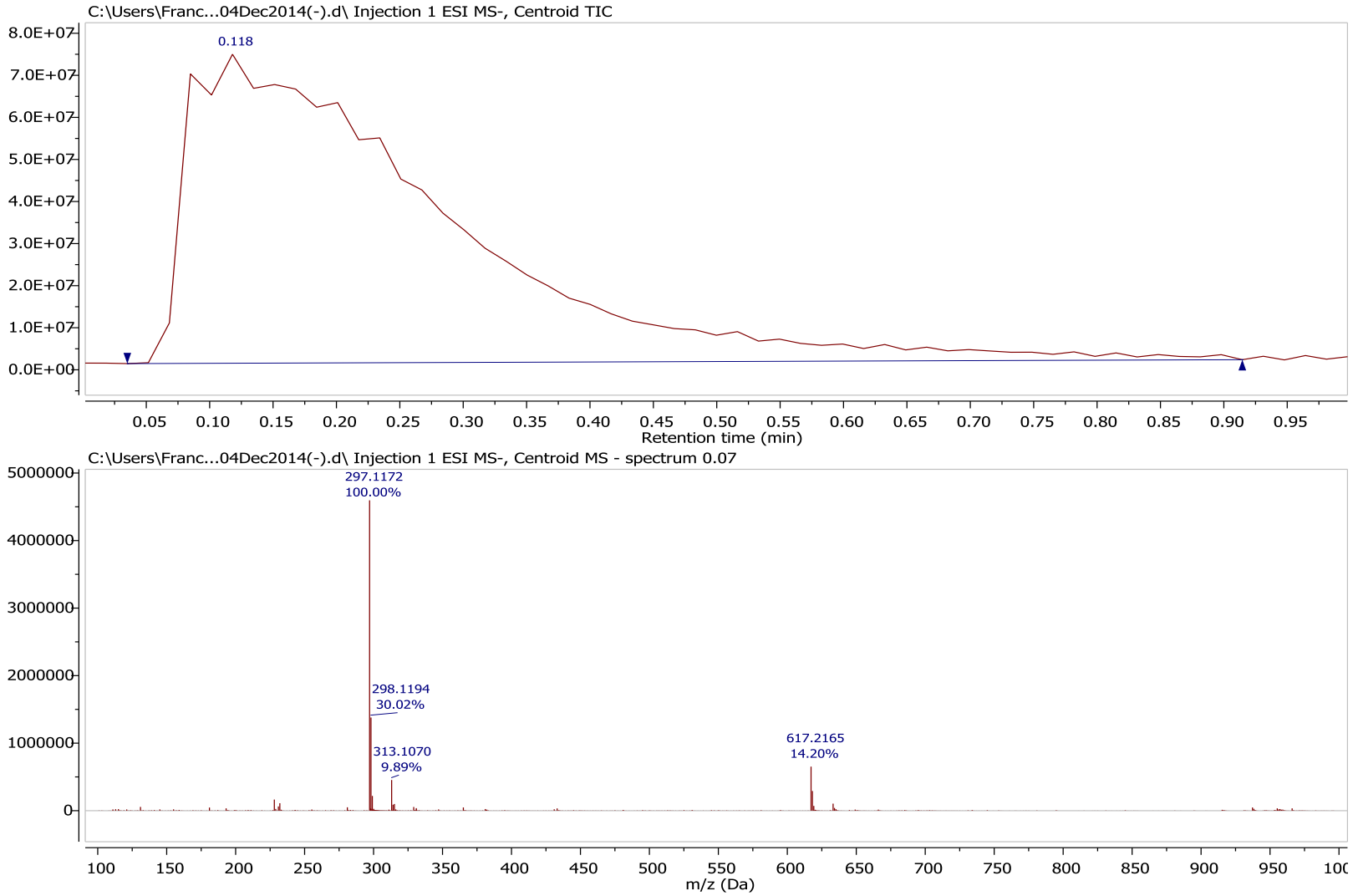

Figure S7. HRESIMS (-) for compound 1.