

Supplementary Materials

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General experimental procedures

Optical rotations were measured using a JASCO P-2000 polarimeter (JASCO, Easton, MD, USA). Ultraviolet spectra were acquired on an Agilent 8453 UV–visible spectrophotometer (Agilent Technologies, Santa Clara, CA, USA). Infrared spectra were recorded with a Bruker IFS-66/S FT-IR spectrometer (Bruker, Karlsruhe, Germany). NMR spectra were recorded with a Bruker AVANCE III HD 800 NMR spectrometer with a 5 mm TCI CryoProbe operating at 800 MHz (^1H) and 200 MHz (^{13}C), with chemical shifts given in ppm (δ) for ^1H and ^{13}C NMR analyses. All HRESIMS data were obtained with a Waters Xevo G2 QTOF mass spectrometer and Synapt G2 HDMS quadrupole time-of-flight (TOF) mass spectrometer (Waters). Preparative high-performance liquid chromatography (HPLC) was performed using a Waters 1525 Binary HPLC pump with a Waters 996 photodiode array detector (Waters Corporation, Milford, MA, USA) and an Agilent Eclipse C₁₈ column (250 × 21.2 mm, 5 μm ; flow rate: 5 mL/min; Agilent Technologies). Semipreparative HPLC was performed using a Shimadzu Prominence HPLC System with SPD-20A/20AV Series Prominence HPLC UV–vis detectors (Shimadzu, Tokyo, Japan) and a Phenomenex Luna C₁₈ column (250 × 10 mm, 5 μm ; flow rate: 2 mL/min; Phenomenex, Torrance, CA, USA). LC/MS analysis was performed on an Agilent 1200 Series HPLC system equipped with a diode array detector and 6130 Series ESI mass spectrometer using an analytical Kinetex C₁₈ 100 Å column (100 × 2.1 mm, 5 μm ; flow rate: 0.3 mL/min; Phenomenex). Silica gel 60 (230–400 mesh, Merck, Darmstadt, Germany) and RP-C₁₈ silica gel (Merck, 230–400 mesh) were used for column chromatography. The packing material for molecular sieve column chromatography was Sephadex LH-20 (Pharmacia, Uppsala, Sweden). Thin-layer chromatography (TLC) was performed with precoated silica gel F254 plates and RP-C₁₈ F254s plates (Merck), and spots were detected under UV light or by heating after spraying with anisaldehyde-sulfuric acid.

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

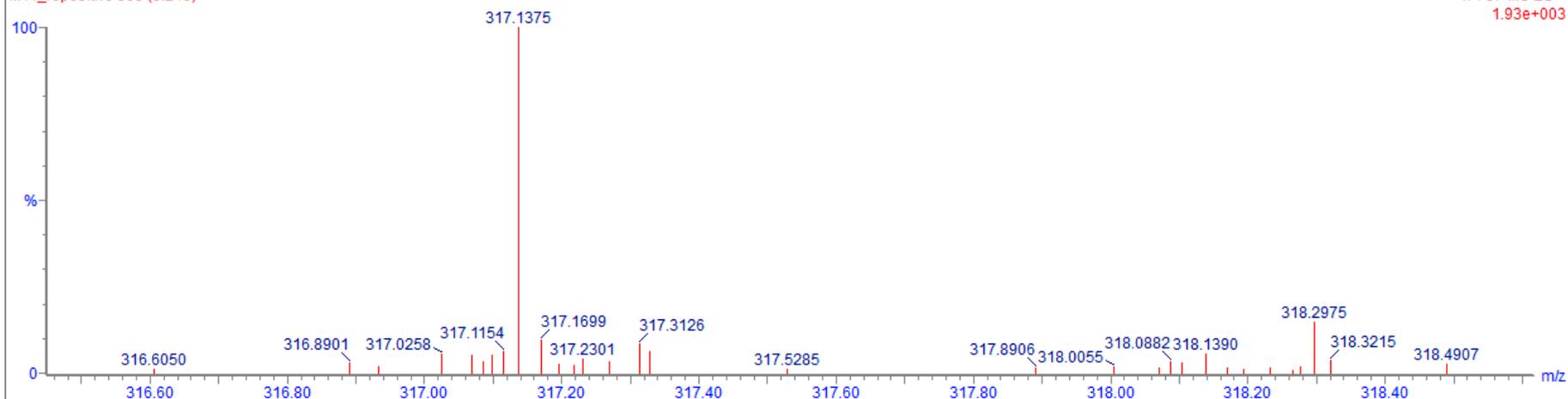
107 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
317.1375	317.1365	1.0	3.2	5.5	C16 H22 O5 Na	292.8	0.456	63.39	16	22	5	1
	317.1389	-1.4	-4.4	8.5	C18 H21 O5	293.5	1.140	31.99	18	21	5	
	317.1330	4.5	14.2	17.5	C25 H17	295.4	3.074	4.63	25	17		

IIH4_repositive

IIH4_repositive 565 (5.248)

1: TOF MS ES+
1.93e+003**Figure S1.** The HRESIMS data of compounds 1 and 2.

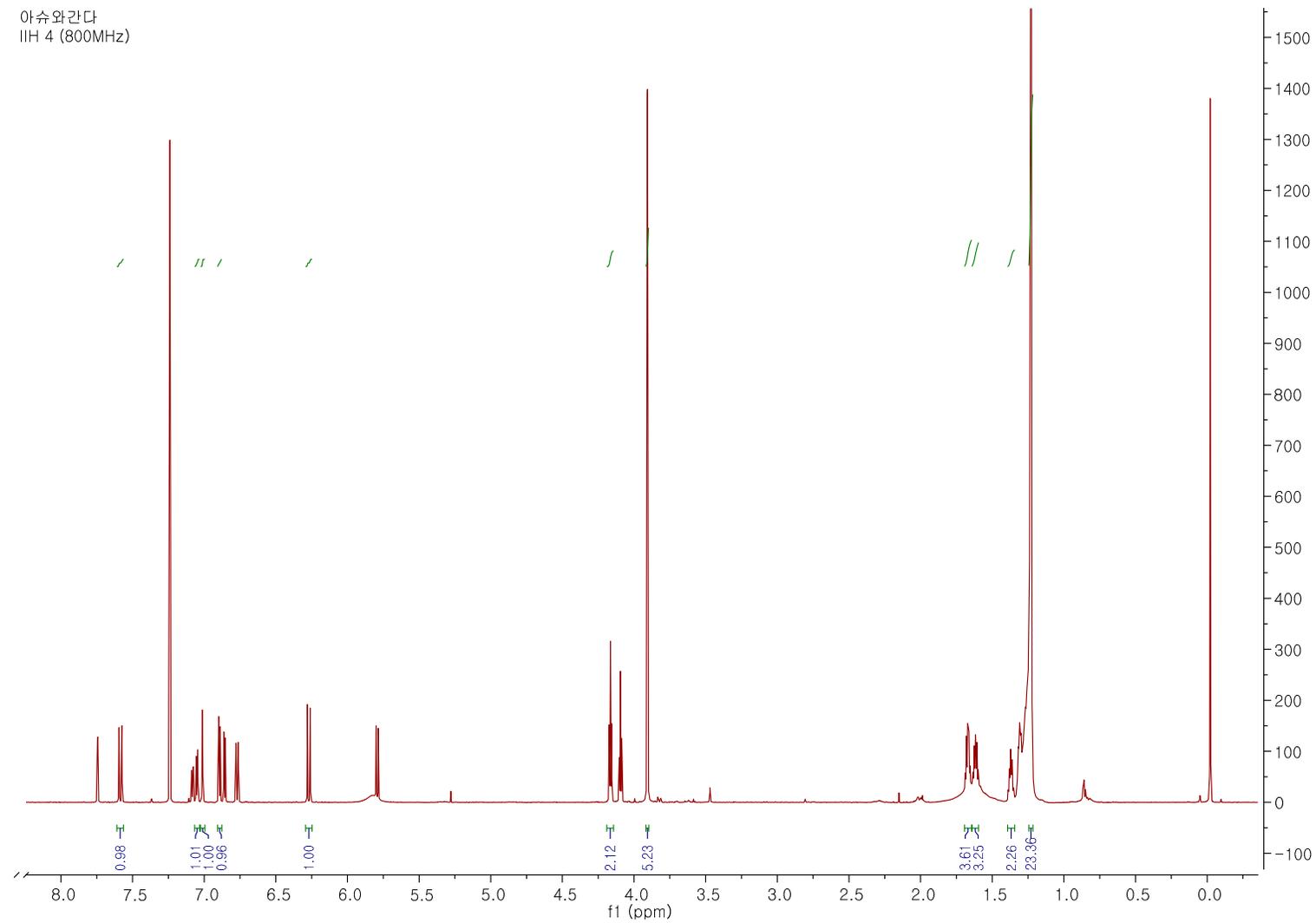


Figure S2. The ^1H NMR spectrum of compounds 1 and 2 (CD_3OD , 800 MHz).

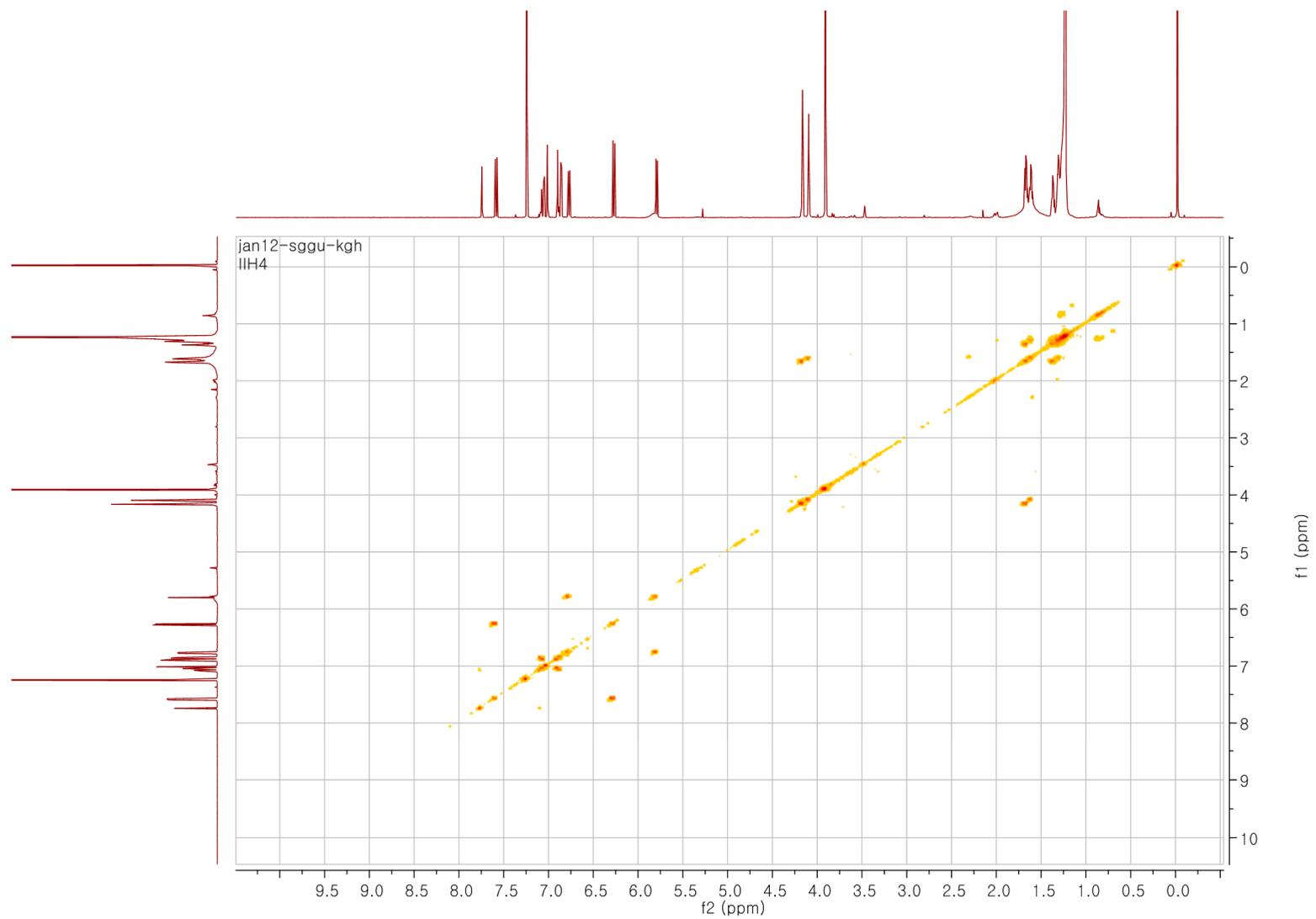


Figure S3. The ^1H - ^1H COSY spectrum of compounds **1** and **2**.

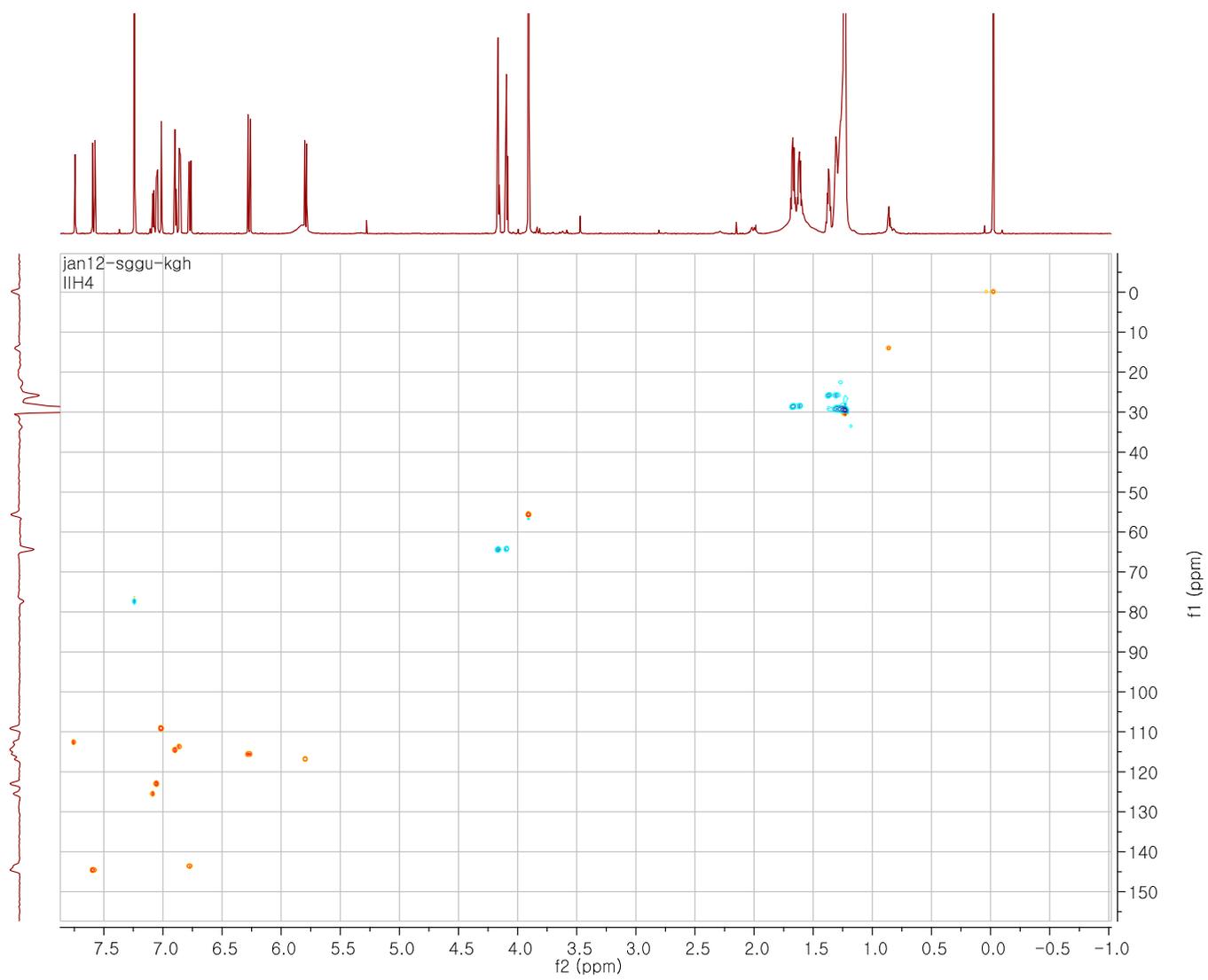


Figure S4. The HSQC spectrum of compounds **1** and **2**.

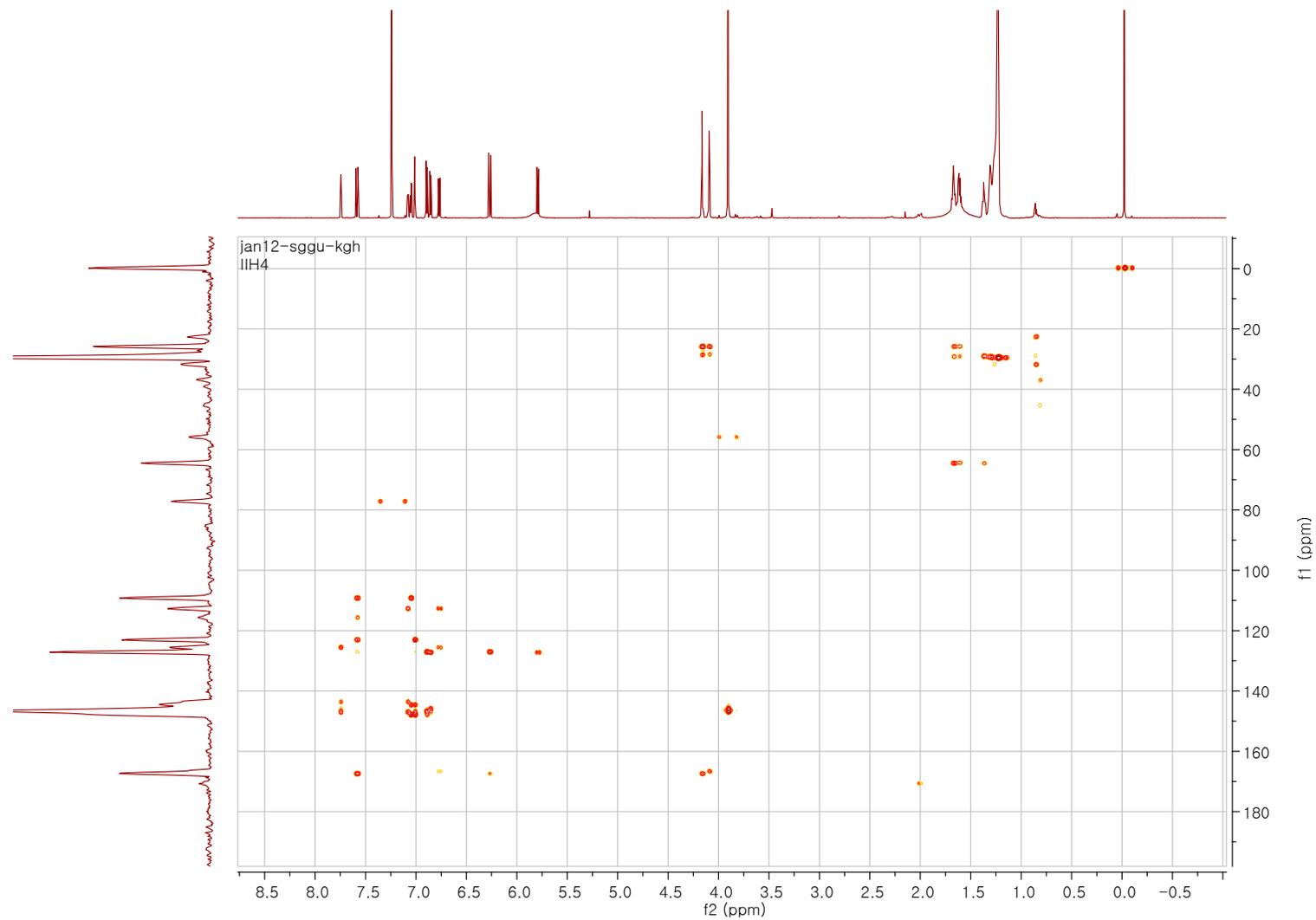


Figure S5. The HMBC spectrum of compounds 1 and 2.