Supporting Information

Structural Revision and Absolute Configuration of Burnettramic Acid A

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EXPERIMENTAL PROCEDURES

General Experimental Procedures. Optical rotations were measured using a Perkin-Elmer model 343 polarimeter. UV and ECD spectra were recorded on an Applied Photophysics Chirascan spectrometer. IR spectra were measured using a Nicolet 5700 FT-IR microscope spectrometer (FT-IR microscope transmission). 1D- and 2D-NMR spectra were acquired at 600 MHz for ^{1}H and 150 MHz for ^{13}C, respectively, on a Bruker AVANCE III HD 600 MHz spectrometer in CD_3OD, DMSO-d_6, and $CDCl_3$ using tetramethylsilane as an internal reference. LC-MS analysis was performed on an Agilent 1100 LC/MSD with a G1956**b** single quadrupole mass spectrometer. HRESIMS data were recorded using a Thermo LTQ Orbitrap XL mass spectrometer. Flash chromatography was performed on an Ez Purifier (Suzhou Lisure Science Co., Ltd.). TLC analysis was carried out using glass precoated silica gel GF254 plates. Detection was performed under UV light and visualized by 7% H_2SO_4 EtOH solution followed by heating. Preparative HPLC separation was performed with a Shimadzu LC-20AP binary pump equipped with an SPD-M20A diode array detector using a Shiseido Capcell PAK C18 MGII preparative (20 mm × 250 mm) or semi-preparative (10 mm × 250 mm) column.

Fungal material. Strains IMB17-055 and IMB18-208 were isolated from marine sediments collected from a mangrove swamp in Sanya, Hainan province, China (109°51'08.0"E, 18°24'09.0"N, –1 m in depth) and near Xieyang Island, Guanxi province, China, (109°16'01.0"E, 20°54'56.0"N, –20 m in depth), respectively. The fungi were identified based on their morphological characteristics and the ITS gene sequences (GenBank accession no. MN294468 and MN294469) analysis. The strains were deposited in the National Laboratory for Screening Microbial Drug, Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences.

Fermentation and Isolation. Each fungus was grown on potato dextrose agar (PDA) plates supplemented with 3% artificial sea salts (Engineering Technology Institute Co., Ltd., China National Salt Industry Group) plates at 28 °C for 7 days. One piece of mycelial agar plug (about 1 cm^2) was respectively inoculated into 500 mL Fernbach flasks containing 100 mL of the PDB medium (composed of 3 g of potato extract, 20 g of glucose, 30 g of artificial sea salt in 1L of H_2O) at 28 °C for 3 days to obtain the seed culture. The seed cultures of IMB17-055 and IMB18-208 were mixed at a ratio of 1 : 1 and then the mixed cultures (5 ml) were inoculated into 30 replicate 500 mL Fernbach flasks containing 100 mL of the PDB medium. The cultures were grown at 28 °C for 10 days on a rotary shaker at 200 rpm. Single control cultures of IMB17-055 and IMB18-208 were grown under identical conditions. After cultivation, the whole fermentation broth (30 L) was separated into the supernatant and the mycelia by filtration. The mycelia was extracted with acetone (3 × 2 L). The broth was concentrated to 5 L and partitioned five times with equal volumes of EtOAc. The organic solvents of the mycelia and the supernatant extracts were evaporated *in vacuo* and combined to yield 54 g of crude extract. The extract was applied to reversed-phase (RP) C18 flash chromatography with a stepwise gradient of MeOH-H_2O (10–100%) to give 14 fractions (F_1–F_{14}). Fraction F_{12} was chromatographed on a Sephadex LH-20 column eluting with CH_2Cl_2-MeOH (1 : 1) and further purified by preparative C18 HPLC (Capcell PAK C18 MGII 5 μM, 20 × 250 mm, 50% CH_3CN containing 0.1% formic acid) to give **1** (300 mg) and **3** (8.5 mg). Fraction F_{13} was separated by Sephadex LH-20 column chromatography in a similar manner and further purified by C18 HPLC (Capcell PAK C18 MGII 5 μM, 20 × 250 mm, 55% CH_3CN containing 0.1% formic acid) to yield **2** (5 mg), **4** (4 mg), and **5** (7 mg).

Burnettramic acid A (1): white amorphous powder; $[\alpha]^{20}_D$ –40.7 (*c* 1.01, MeOH); UV (MeOH) λ_{max} (logε) 225 (3.86), 282 (4.16) nm; ECD (*c* 6.5 × 10^{-4} M, MeOH) λ_{max} ($\Delta\varepsilon$) 212 (-20.04), 244 (+2.36), 285 (+2.86) nm; IR ν_{max} 3332, 1711, 1609, 1081 cm^{-1}; ^{1}H-NMR (CD_3OD and DMSO-d_6, 600 MHz), Table S1; ^{13}C NMR (CD_3OD and DMSO-d_6, 150 MHz), Table S2; HRESIMS: *m/z* 770.5055 [M + H]$^+$ (calcd. for $C_{41}H_{72}NO_{12}$, 770.5049), 792.4851 [M + Na]$^+$ (calcd. for $C_{41}H_{71}NO_{12}Na$, 792.4868).

Burnettramic acid C (2): white amorphous powder; $[\alpha]^{20}_D$ –35.7 (*c* 0.57, MeOH); UV (MeOH) λ_{max} (logε) 227 (3.64), 282 (3.91) nm; ECD (*c* 7.5× 10^{-4} M, MeOH) λ_{max} ($\Delta\varepsilon$) 215 (-13.28), 252 (+0.38), 291 (+1.74) nm; IR ν_{max} 3346, 1709, 1606, 1455, 1074 cm^{-1}; ^{1}H-NMR (CD_3OD, 600 MHz), Table S3; ^{13}C NMR (CD_3OD, 150 MHz), Table S3; HRESIMS: *m/z* 754.5102 [M + H]$^+$ (calcd for $C_{41}H_{72}NO_{11}$, 754.5100), 776.4898 [M + Na]$^+$ (calcd. for $C_{41}H_{71}NO_{11}Na$, 776.4919).

Burnettramic acid D (3): white amorphous powder; $[\alpha]^{20}_D$ –28.0 (*c* 0.27, MeOH); UV (MeOH) λ_{max} (logε) 231 (4.17), 282 (3.76) nm; ECD (*c* 6.5 × 10^{-4} M, MeOH) λ_{max} ($\Delta\varepsilon$) 219 (-9.53), 249 (+1.20), 289 (+2.58) nm; IR ν_{max} 3355, 1655, 1600, 1465, 1079 cm^{-1}; ^{1}H-NMR (CD_3OD, 600 MHz), Table S3; ^{13}C NMR (CD_3OD, 150 MHz), Table S3; HRESIMS: *m/z* 768.4890 [M + H]$^+$ (calcd for $C_{41}H_{70}NO_{12}$, 768.4893), 790.4727 [M + Na]$^+$ (calcd. For $C_{41}H_{69}NO_{12}Na$, 790.4712).

Burnettramic acid E (4): white amorphous powder; $[\alpha]^{20}_D$ – 42.5 (*c* 0.41, MeOH); UV (MeOH) λ_{max} (logε) 282 (4.09) nm; ECD (*c* 6.5 × 10^{-4} M, MeOH) λ_{max} ($\Delta\varepsilon$) 214 (-16.64), 247 (+2.46), 289 (+2.98) nm; IR ν_{max} 3331, 1602, 1466, 1082 cm^{-1}; ^{1}H-NMR (CD_3OD, 600 MHz), Table S3; ^{13}C NMR (CD_3OD, 150 MHz), Table S3; HRESIMS: *m/z* 772.5210 [M + H]$^+$ (calcd for $C_{41}H_{74}NO_{12}$, 772.5206), 794.5015 [M + Na]$^+$ (calcd. for $C_{41}H_{73}NO_{12}Na$, 794.5025).

Burnettramic acid A aglycone (5): white amorphous powder; $[\alpha]^{20}_D$ –18.0 (*c* 1.00, MeOH); UV (MeOH) λ_{max} (logε) 281 (4.12) nm; ECD (*c* 8.2 × 10^{-4} M, MeOH) λ_{max} ($\Delta\varepsilon$) 217 (-17.80), 249 (+0.41), 287 (+3.04) nm; IR ν_{max} 3334, 1690, 1604, 1465, 1080 cm^{-1}; ^{1}H-NMR (CD_3OD and $CDCl_3$, 600 MHz), Table S4; ^{13}C NMR (CD_3OD and $CDCl_3$, 150 MHz), Table S4; HRESIMS: *m/z* 608.4524 [M + Na]$^+$ (calcd. for $C_{35}H_{62}NO_7$, 608.4521), 630.4329 [M + Na]$^+$ (calcd. for $C_{35}H_{61}NO_7Na$, 630.4340).

Ozonolysis of 1 to Yield 6 and 7. A steam of ozone gas passed through a solution of **1** (40 mg) in 15 mL of anhydrous MeOH at –20°C. The reaction was monitored by TLC and LC-MS (Capcell PAK C18 MGII 3.0 × 150 mm, 0.5 mL/min, 210

and 230 nm, a gradient of 15% to 80% CH_3CN-5 mM NH_4Ac over 15 min, t_R **6** = 10.1 min, t_R **7** = 7.5 min). After 9 h the reaction was terminated and the solvent was removed under N_2. The residue was dissolved in MeOH and purified by RP-HPLC (C18, 20 mm × 250 mm, 10 mL/min, a gradient of 20% to 60% CH_3CN over 35 min) to afford compound **7** (7 mg, t_R 14.3 min) and a mixture containing **6** (t_R 26.0 min). The mixture was further purified by RP-HPLC (C18, 10 mm × 250 mm, 4 mL/min, 25% CH_3CN) to obtain compound **6** (2 mg, t_R 72 min). Compound **6**: white powder; $[\alpha]^{20}_D$ –18.0 (*c* 0.07, MeOH); UV (MeOH) λ_{max} (logε) 247 (3.78), 281 (3.96) nm; ECD (*c* 1.18 × 10^{-3} M, MeOH) λ_{max} ($\Delta\varepsilon$) 219 (-11.28), 250 (+0.72), 287 (+3.51) nm; ^{1}H NMR (CD_3OD, 600 MHz) and ^{13}C NMR (CD_3OD, 150 MHz), Table S5; HRESIMS: *m/z* 424.2677 $[M - H]^-$ (calcd. for $C_{23}H_{38}NO_6$, 424.2694); Compound **7**: white powder; ^{1}H NMR (CD_3OD, 600 MHz) and ^{13}C NMR (CD_3OD, 150 MHz) data, Table S5; HRESIMS: *m/z* 467.2830 $[M - H]^-$ (calcd. for $C_{22}H_{43}O_{10}$, 467.2851).

Enzymatic Hydrolysis of 7 to Yield 8. Compound **7** (7 mg) was dissolved in 5 mL of H_2O and treated with snailase (30 mg, Shanghai Sangon Biotech Co.) at 37 °C, with shaking for 36 h. The reaction mixture of **7** was then passed through a 2g C18 SPE column and successively eluted with H_2O and MeOH. The MeOH-eluting fraction was purified by RP-HPLC (C18, 10 mm × 250 mm, 4 mL/min, 23% CH_3CN) to yield **8** (4 mg, t_R = 24.7 min). Compound **8**: white powder; $[\alpha]^{20}_D$ –4.0 (*c* 0.5, MeOH); ^{1}H NMR (CD_3OD, 600 MHz) and ^{13}C NMR (CD_3OD, 150 MHz) data, Table S5; ESIMS: *m/z* 305.2 $[M–H]^-$, 365.2 $[M + CH_3COO]^-$; HRESIMS: *m/z* 305.2338 $[M–H]^-$ (calcd. for $C_{16}H_{33}O_5$, 305.2333), 365.2552 $[M + CH_3COO]^-$ (calcd. for $C_{18}H_{37}O_7$, 365.2545).

Enzymatic Hydrolysis of 1 to Yield the Aglycone (5). Compound **1** (30 mg) was dissolved in 30 mL of H_2O and then snailase (90 mg) was added. After incubation at 37 °C for 36 h, the reaction mixture was extracted with EtOAc (25 mL × 3). The EtOAc extract was separated by RP-HPLC (C18, 10 mm × 250 mm, 4 mL/min, 60% CH_3CN-0.1% formic acid) to afford the aglycone (16 mg, t_R = 49.0 min). The aglycone was determined to be identical with **5** by comparison of the UV, ^{1}H and ^{13}C NMR spectra, and LC-MS data.

Determination of the Absolute Configuration of the Mannose Residue in 1. Compound **1** (2 mg) was dissolved in 1 mL of 2 M HCl and heated at 110° for 4 h. The mixture was evaporated to dryness in vacuo and redisolved in 5 mL acetic acid. To the hydrolysate solution was added 4 mg of 2,3-naphthalenediamine and 1 mg of molecular iodine. The reaction mixture was stirred in open air at room temperature for 6 h to afford the fluorescent naphthimidazole derivative of mannose as previously reported.[1] Similarly, the standard D- and L-mannose were respectively derivatized to yield the corresponding the 2,3-naphthalenediamine derivatives. The fluorescent product was subjected to LC- MS analysis using a cyclodextrin-based chiral column (Capcell Chiral CD-ph 5 μM, 10 × 250 mm, 13% CH_3CN-0.1% formic acid, flow rate 2 mL/min, column temperature 30 °C, 254 nm). The D- and L-forms of mannose-naphthimidazole derivatives were enantioseparated with the retention times 15.71 and 17.25 min, respectively. The retention time of the mannose-naphthimidazole derivative of the hydrolysate of **1** was 15.77 min. Therefore, the mannose residue in **1** was determined to be the D-configuration.

Preparation of Tri-MTPA Ester of 8 (8a and 8b). To a solution of **8** (2 mg) in anhydrous CH_2Cl_2 (1 mL) was added pyridine (5 mL), dimethylaminopyridine (DMAP, 2 mg), and (*R*)-α-methoxy-α-(trifluoromethyl)phenylacetyl chloride (*R*-MTPA-Cl, 25 μL) in sequence. The reaction solution was stirred at room temperature under N_2. The progress of reaction was monitored at different time points (12, 36, 48, 72, and 96 h) by LC-MS (Capcell MGII C18, 3.0 × 150 mm, flow rate 0.5 mL/min, a linear gradient of 15% to 80% CH_3CN–5 mM NH_4Ac over 5 min, then a linear gradient to 100% over the next 20 min). Bis- and Tri-MTPA esters were distinguished by ESIMS data of *m/z* 756.4 and 972.4 $[M + NH_4]^+$, respectively. After incubation for 102 h, the reaction mixture was evaporated *in vacuo* and purified by RP-HPLC (Capcell MGII C18, 10 mm × 250 mm, 4 mL/min, a gradient of 30% to 90% CH_3CN over 10 min, then eluting with 90% CH_3CN for additional 30 min) to yield tri-(*S*)-MTPA ester **8a** (0.62 mg, 31.0 min). The identical condition was used to obtain the tri-(*R*)-MTPA ester **8b** (0.58 mg) with *S*-MTPA-Cl.

Tri-(*S*)-MTPA ester of 8 (8a): amphous powder; ^{1}H NMR data (600 MHz), see Table S6 in Supporting Information; ESIMS: *m/z* 972.4 $[M + NH_4]^+$, 977.4 $[M + Na]^+$, 1013.4 $[M + CH_3CN + NH_4]^+$; HRESIMS: *m/z* 977.3501 $[M + Na]^+$ (calcd. For $C_{46}H_{55}F_9O_{11}Na$, 977.3943).

Tri-(*R*)-MTPA ester of 8 (8b): amphous powder; ^{1}H NMR data (600 MHz), see Table S6 in Supporting Information; ESIMS: *m/z* 972.4 $[M + NH_4]^+$, 977.4 $[M + Na]^+$, 1013.4 $[M + CH_3CN + NH_4]^+$; HRESIMS: *m/z* 977.3508 $[M + Na]^+$ (calcd. For $C_{46}H_{55}F_9O_{11}Na$, 977.3943).

Marfey's analysis. A solution of compound **1** (0.5 mg) in 1 M HCl/EtOAc (1 mL) was heated at 110°C for 1 h and evaporated to dryness. The residue was dissolved in 0.5 M KOH and stirred for 2h at room temperature, followed by neutralization with 2 M HCl. The hydrolysate was dried in vacuo and redissolved in 0.1 M $NaHCO_3$ (200 μL) and divided into two portions. To each portion (100 μL) was added 50 μL of a 1% L-FDLA and 1% D-FDLA in acetone, respectively. The authentic *trans*-4-L- and *cis*-4-D-hydroxyproline were separately dissolved in 0.1 M $NaHCO_3$ (100 μL) and 50 μL of 1% L- or D-FDLA solution. Each mixture was heated at 55 °C for 30 min, cooled to room temperature, neutralized with 0.2 M HCl (50 μL), and diluted with CH_3CN (100 μL). The FDLA derivatives were analyzed by LC-MS (Capcell MG II C_{18} column 5 μm, 4.6 × 150 mm, flow rate, 1.0 mL/min; a linear gradient of 10%–50% CH_3CN–5 mM NH_4Ac over 60 minutes; UV detection at 340 nm; column temperature, 40 °C). The retention times (t_R, min) of the L- and D-FDLA derivatives (*m/z* 426.2) of *trans*-4-L-hydroxyproline were 16.3 and 18.3 min, respectively, while the retention times of the L- and D-FDLA derivatives (*m/z* 426.2) of *cis*-4-D-hydroxyproline were at 19.4 min and 25.0 min . The L-FDLA derivative from **1** gave two peaks (*m/z* 426.2) at 16.3 min and

25.0 min, respectively and the D-FDLA derivative from **1** showed two peaks (*m*/*z* 426.2) at 18.3 min and 19.4 min, respectively. Therefore, the absolute configuration of the *trans*-4-hydroxyproline moiety in **1** was assigned as 2′*S* and 4′*R*.

NMR Calculations. Conformational search for **6a**–**6d** was carried out by means of Spartan 14 software (Wavefunction Inc., Irine, CA, USA) using the molecular mechanics force field (MMFF94).[2] The conformers within 10 kcal/mol energy threshold were geometry optimized at the B3LYP/6-31+G (d, p) level in gas using the Gaussian 09 program.[3] The harmonic vibrational frequencies were calculated at the same level. The Boltzmann-weighted population was calculated based on their relative thermal free energy (ΔG) obtained from the geometry optimization. The conformations within 10 kJ/mol were subjected to NMR calculation using the Gauge-Independent Atomic Orbital (GIAO) method at the mPW1PW91/6-311+G(d,p) level in MeOH with the polarizable continuum model (PCM). The scaled chemical shift (δ_s) of each conformer was calculated according to the equation proposed by Sarotti et al..[4] The final chemical shifts were generated by averaging the data of all the conformers based on their Boltzmann distribution at 298.15 K. The DP4+ probability for each diastereoisomer was calculated according to the shielding tensor data using the Excel sheet provided by Sarotti et. al.[4]

ECD Calculations. The geometry optimized conformers within 10 kJ/mol for **6a** and **6b** were subjected to ECD calculation using the TDDFT methodology (NStates = 65) at the CAM-B3LYP/TZVP level in MeOH with the PCM model. ECD spectrum of each conformer was simulated by the SpecDis program[5] using a Gaussian function band width σ = 0.30 eV. Final ECD spectra for was generated by averaging the calculated data of the lowest energy conformers for each structure according to their Boltzmann distribution.

Antimicrobial Assay. Compounds **1**–**5** were tested against six fungi *Candida albicans*, *Curvularia lunata* (CPCC 400186), *Fusarium* sp. (CPCC 400381), *Fusarium* sp. (CPCC 400307), *Alternaria* sp. (CPCC 400323), *Aspergillus versicolor* IMB17-055, and *Aspergillus chevalieri* IMB18-208, Gram-positive bacteria *Bacillus subtilis* (ATCC 6633) and *Staphylococcus aureus* (ATCC 29213), and Gram-negative bacteria *Pseudomonas aeruginosa* (ATCC 27853) and *Klebsiella pneumonia* (ATCC 700603). The minimum inhibitory concentration (MIC) were determined in 96-well plates by two-fold dilution in Sabouraud medium (1% peptone, 4% glucose) for *C. albicans*, PDB medium (0.3 % potato extract, 2% glucose) for other fungi and Mueller-Hinton medium (0.6% beef extract, 1.75% acid hydrolysate of casein, 0.15% starch) for bacteria under the guidelines of Clinical and Laboratory Standards Institute (CLSI).[6-7] Negative controls were left blank. Nystatin and rifampicin were used as positive control for fungi and bacteria, respectively. Using a multi-channel pipet, 100 μL of the test strain cultures in the medium at a concentration of 3×10^4 CFU/mL were aliquoted in all the rows. To the first row, an additional 98 μL of the strain-medium cultures and 2 μL of compounds in DMSO were added and mixed before transferring 100 μL to the second. A two-fold dilution was done in the subsequent rows except the last row (H). After incubation at 28°C for 24 h, the lowest concentration without the visible growth of the microbes was determined as the MIC. The concentrations tested ranged from 64 to 0.5 μg/mL for fungi and from 128 to 0.0625 μg/mL for bacteria.

Cytotoxicity Assay. Cytotoxicity was assayed against the human pancreatic cancer MIA PaCa-2 cell line using the CCK colorimetric assay and compared to the controls as described previously.[8]

Genome Sequencing and Bioinformatic Analysis. Genomic DNA was extracted using the Omega Fungal DNA Kit D3390-02 according to the manufacturer's instructions. The genome was sequenced at the Shanghai Majorbio Company on an Illumina HiSeq X Ten instrument. The raw data were assembled by using SOAPdenovo v2.04. The putative biosynthetic gene clusters were detected and analyzed by AntiSMASH 5.0. Gene prediction and functional annotation was performed using the 2ndFind tool (available online: http://biosyn.nih.go.jp/2ndfind/) and compared with the *bua* gene cluster in *Aspergillus burnettii*. Protein similarity was calculated by the online BLAST program (http://blast.ncbi.nlm.nib.gov/). The annotated sequence of the putative burnettramic acid biosynthetic gene cluster in *A. versicolor* IMB17-055 was deposited in the GenBank with the accession number MN395477.

Table S1. ^{1}H NMR data for **1** and reported for burnettramic acid A (δ_H, mult., *J* in Hz)

No.	**1** (CD_3OD)[a]	**1** (DMSO-d_6)[a]	Burnettramic acid A (DMSO-d_6)[c,9]	Reassigned for burnettramic acid A
4	3.79, sextet (7.2)	3.65, m	3.62, brm	3.62, brm
4-Me	1.11, d (7.2)	1.00, d (6.6)	1.04,d (6.8)	1.04,d (6.8)
5	1.55, dt (12.6,6.6)	1.41, m	1.43, m	1.43, m
	1.37, m	1.30, m	1.35, m	1.35, m
6	1.43, m	1.36, m	1.36, m	1.36, m
6-Me	0.89, d (6.6)	0.81, d (6.6)	0.81, d (6.4)	0.81, d (6.4)
7	1.35, m; 1.08, m	1.26, m; 1.03, m	1.26, m; 1.03, m	1.26, m; 1.03, m
8	1.32, m; 1.24, m	1.25, m; 1.17, m	1.25, m; 1.16, m	1.25, m; 1.16, m
9	1.25-1.35	1.24, m	1.14-1.31, m	1.14-1.31, m
10	1.25-1.35	1.18-1.30, m	1.14-1.31, m	1.14-1.31, m
11	1.29, m	1.22, m	1.21, m	1.21, m
12	1.36, m	1.29, m	1.14-1.31, m	1.14-1.31, m
13	2.01, q (6.0)	1.94, m	1.14-1.31, m	1.93, dt (6.7, 6.0)
14	5.47, dt (15.0, 6.0)	5.36, dt (15.0, 5.4)	1.41-1.31, m	5.35, dt (15.4, 6.0)
15	5.45, dt (15.0, 6.6)	5.40, dt (15.0, 5.4)	1.93, dt (6.7, 6.0)	5.39, dt (15.4, 6.3)
16	2.15, m	2.02, m	5.35, dt (15.4, 6.0)	2.01, dd (6.3, 6.0)
17	3.55, m	3.38, m	5.39, dt (15.4, 6.3)	3.37, m
18	1.50, m; 1.36, m	1.33, m; 1.20, m	2.01, dd (6.3, 6.0)	1.33, m; 1.20, m
19	1.59, m; 1.36, m	1.47, m; 1.20, m	3.37, m	1.46, m; 1.20, m
20	1.45, m; 1.37, m	1.30, m; 1.21, m	1.33, m; 1.20, m	1.29, m; 1.21, m
21	3.51, m	3.33, m	1.46, m; 1.20, m	3.33, m
22	1.42, m; 1.37, m	1.30, m; 1.24, m	1.29, m; 1.21, m	1.30, m; 1.24, m
23	1.45, m; 1.34, m	1.35, m; 1.22, m	3.33, m	1.34, m; 1.23, m
24	1.33, m	1.23-1.36, m	1.30, m; 1.24, m	1.14-1.31, m
25	1.35, m	1.26, m	1.34, m; 1.23, m	1.41-1.31, m
26	1.39, m	1.28, m	1.27, m	1.27, m
27	1.61, m	1.50, m	1.49, p (6.9)	1.49, p (6.9)
28	3.91, dt (9.0, 6.6)	3.75, dt (11.4, 6.0)	3.74, dt (9.6, 6.9)	3.74, dt (9.6, 6.9)
	3.53, dt (9.0, 6.6)	3.39, dt (11.4, 6.0)	3.39, dt (9.6, 6.9)	3.39, dt (9.6, 6.9)
2'	4.25, dd (10.8, 6.0)	4.14, m	4.22, brs	4.22, brs
3'	2.11, dd (13.2, 6.0)	1.91, m	1.92, m	1.92, m
	1.60, m	1.55, m	1.59, brt (12.9)	1.59, brt (12.9)
4'	4.60, brt (4.8)	4.44, m	4.47, brt (4.9)	4.47, brt (4.9)
5'	3.88, dd, (12.0, 1.8)	3.74, m	3.76, brm	3.76, brm
	3.10, d (12.0)	2.92, brd (12.0)	2.96, brd (12.0)	2.96, brd (12.0)
1"	4.49, brs	4.33, s	4.32, d (0.7)	4.32, d (0.7)
2"	3.84, d (3.6)	3.60, d (3.0)	3.60, dd (3.1, 0.7)	3.60, dd (3.1, 0.7)
3"	3.44, dd (9.0, 3.0)	3.23, dd (9.0, 3.0)	3.23, dd (9.3, 3.1)	3.23, dd (9.3, 3.1)
4"	3.92, dd (9.0, 9.0)	3.28, dd (9.6, 9.0)	3.27, dd (9.3, 9.0)	3.27, dd (9.3, 9.0)
5"	3.20, ddd (9.0, 6.0, 2.4)	3.00, dd (9.6, 6.6)	2.99, ddd (9.0, 6.4, 2.3)	2.99, ddd (9.0, 6.4, 2.3)
6"	3.87, dd (12.0, 2.4)	3.67, brd (11.4)	3.67, dd (11.7, 2.3)	3.67, dd (11.7, 2.3)
	3.71, dd (12.0, 6.0)	3.44, dd (11.4, 6.6)	3.43, dd (11.7, 6.4)	3.43, dd (11.7, 6.4)

[a] ^{1}H NMR data were recorded at 600 MHz. The assignments were based on 2D NMR (^{1}H-^{1}H COSY, TOCSY, ROESY, HSQC, and HMBC) experiments. [c] Data taken from ref. [9].

Table S2. ^{13}C NMR data for **1** and reported for burnettramic acid A (δC, type)

No.	**1** (CD_3OD) [a]	**1** (DMSO-d_6) [a]	Burnettramic acid A (DMSO-d_6) [c, 9]	Reassigned for burnettramic acid A
1	178.0, C	not obs	not obs.	not obs.
2	103.8, C	102.0, C	not obs.	not obs.
3	196.4, C	not obs. [b]	190.8, C	190.8, C
4	35.7, CH	33.9, CH	32.8, CH	32.8, CH
4-Me	17.7, CH_3	17.0, CH_3	16.9, CH_3	16.9, CH_3
5	42.1, CH_2	40.3, CH_2	40.2, CH_2	40.2, CH_2
6	30.9, CH	30.0, CH	30.0, CH_3	30.0, CH_3
6-Me	20.2, CH_3	19.5, CH_3	19.4, CH_2	19.4, CH_2
7	37.8, CH_2	36.3, CH_2	36.11, CH_2	36.11, CH_2
8	28.0, CH_2	26.3, CH_2	26.2, CH_2	26.2, CH_2
9	31.0, CH_2	29.2, CH_2	28.8-29.2, CH_2	28.8-29.2, CH_2
10	30.7, CH_2	28.8, CH_2	28.8-29.2, CH_2	28.8-29.2, CH_2
11	30.3, CH_2	28.5, CH_2	28.5, CH_2	28.5, CH_2
12	30.8, CH_2	29.2, CH_2	28.8-29.2, CH_2	28.8-29.2, CH_2
13	33.8, CH_2	32.1, CH_2	28.8-29.2, CH_2	32.0, CH_2
14	134.0, CH	131.5, CH	28.8-29.2, CH_2	131.5, CH
15	127.6, CH	127.2, CH	32.0, CH_2	127.2, CH
16	41.8, CH_2	40.6, CH_2	131.5, CH	40.6, CH_2
17	72.5, CH	69.9, CH	127.2, CH	69.9, CH
18	37.6, CH_2	36.6, CH_2	40.6, CH_2	36.6, CH_2
19	22.9, CH_2	21.5, CH_2	69.9, CH	21.5, CH_2
20	38.4, CH_2	37.5, CH_2	36.6, CH_2	37.4, CH_2
21	72.4, CH	69.6, CH	21.5, CH_2	69.6, CH
22	38.5, CH_2	37.2, CH_2	37.4, CH_2	37.2, CH_2
23	26.9, CH_2	25.3, CH_2	69.6, CH	25.3, CH_2
24	30.7, CH_2	28.9, CH_2	37.2, CH_2	28.8-29.2, CH_2
25	30.7, CH_2	29.0, CH_2	25.3, CH_2	28.8-29.2, CH_2
26	27.2, CH_2	25.6, CH_2	25.6, CH_2	25.6, CH_2
27	30.9, CH_2	29.3, CH_2	29.3, CH_2	29.3, CH_2
28	70.6, CH_2	68.4, CH_2	68.4, CH_2	68.4, CH_2
1'	198.2, C	194.9, C	194.8, C	194.8, C
2'	67.5, CH	65.7, CH	not obs.	not obs.
3'	37.7, CH_2	36.4, CH_2	36.17, CH_2	36.17, CH_2
4'	74.3, CH	72.1, CH_2	72.1, CH	72.1, CH
5'	53.8, CH_2	52.7, CH_2	52.2, CH_2	52.2, CH_2
1"	101.7, CH	100.2, CH	100.2, CH	100.2, CH
2"	72.6, CH	70.6, CH	70.6, CH	70.6, CH
3"	75.2, CH	73.7, CH	73.7, CH	73.7, CH
4"	68.4, CH	67.2, CH	67.2, CH	67.2, CH
5"	78.2, CH	77.5, CH	77.5, CH	77.5, CH
6"	62.8, CH_2	61.4, CH_2	61.4, CH_2	61.4, CH_2

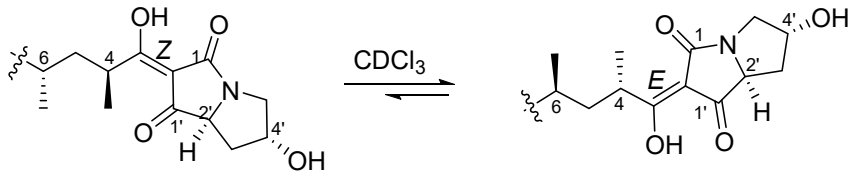
[a] ^{13}C NMR data were recorded at 150 MHz. The assignments were based on 2D NMR (^1H-^1H COSY, TOCSY, ROESY, HSQC, and HMBC) experiments. [b] not observed. [c] Data taken from ref. [9].

Table S3. ^{1}H and ^{13}C NMR data of compounds **2–4** in CD_3OD[a]

No.	**2**		**3**		**4**	
	δ_C, type	δ_H, mult. (*J* in Hz)	δ_C, type	δ_H, mult. (*J* in Hz)	δ_C, type	δ_H, mult. (*J* in Hz)
1	178.3, C		not obs.[b]		178.3, C	
2	103.8, C		103.9		103.7, C	
3	not obs.		not obs.		not obs.	
4	36.2, CH	3.79, m	38.8, CH	3.85, m	36.4, CH	3.79, m
4-Me	17.8, CH_3	1.09, d (7.2)	18.0, CH_3	1.00, d (6.6)	17.8, CH_3	1.08, d (7.2)
5	42.1, CH_2	1.54, m; 1.35, m	42.1, CH_2	1.51, m; 1.23, m	42.1, CH_2	1.54, m; 1.34, m
6	31.9, CH	1.42, m	31.9, CH	1.41, m	31.9, CH	1.42, m
6-Me	20.2, CH_3	0.88, d (6.6)	20.3, CH_3	0.86, d (6.6)	20.2, CH_3	0.88, d (6.0)
7	38.0, CH_2	1.34, m; 1.08, m	38.3, CH_2	1.34, m; 1.08, m	38.0, CH_2	1.35, m; 1.08, m
8	28.1, CH_2	1.32, m; 1.23, m	28.0, CH_2	1.31, m; 1.23, m	28.1, CH_2	1.31, m; 1.23, m
9	31.0, CH_2	1.25-1.35	30.6, CH_2	1.26, m	31.0, CH_2	1.25-1.35
10	30.7, CH_2	1.25-1.35	30.6, CH_2	1.36, m	30.8-31.0, CH_2	1.25-1.35
11	30.3, CH_2	1.28, m	33.7, CH_2	2.03, q (7.2)	30.8-31.0, CH_2	1.25-1.35
12	30.9, CH_2	1.35, m	133.8, CH	5.56, dt (15.0, 7.2)	30.8-31.0, CH_2	1.25-1.35
13	33.8, CH_2	2.00, m	131.8, CH	5.99, dd (15.0, 10.8)	30.8-31.0, CH_2	1.25-1.35
14	134.0, CH	5.46, dt (15.0, 5.4)	134.1, CH	6.04, dd (15.0, 10.8)	30.8-31.0, CH_2	1.25-1.35
15	127.7, CH	5.44, dt (15.0, 5.4)	129.1, CH	5.58, dt (15.0, 7.2)	26.8, CH_2	1.45, m; 1.33, m
16	41.7, CH_2	2.15, m	41.8, CH_2	2.20, m	37.9, CH_2	1.45, m; 1.37, m
17	72.5, CH	3.54, m	72.5, CH	3.59, m	72.4, CH	3.52, m
18	37.7, CH_2	1.49, m; 1.37, m	37.9, CH_2	1.49, m; 1.37, m	38.5, CH_2	1.48, m; 1.38, m
19	22.9, CH_2	1.59, m; 1.34, m	22.9, CH_2	1.59, m; 1.36, m	23.0, CH_2	1.59, m; 1.37, m
20	38.4, CH_2	1.47, m; 1.39, m	38.4, CH_2	1.45, m; 1.36, m	38.5, CH_2	1.45, m; 1.37, m
21	72.4, CH	3.52, m	72.4, CH	3.51, m	72.4, CH	3.52, m
22	38.5, CH_2	1.42, m; 1.36, m	38.5, CH_2	1.42, m; 1.37, m	38.0, CH_2	1.42, m; 1.37, m
23	26.8, CH_2	1.45, m; 1.34, m	26.8, CH_2	1.45, m; 1.37, m	26.9, CH_2	1.45, m; 1.33, m
24	30.6, CH_2	1.32, m	30.9, CH_2	1.33, m	30.8-30.9, CH_2	1.33, m
25	30.6, CH_2	1.34, m	30.6, CH_2	1.35, m	30.6, CH_2	1.33, m
26	27.2, CH_2	1.39, m	27.2, CH_2	1.38, m	27.2, CH_2	1.39, m
27	30.9, CH_2	1.60, m	30.8, CH_2	1.61, p (7.2)	30.8, CH_2	1.60, m
28	68.6, CH_2	3.90, m; 3.53, m	70.7, CH_2	3.91, m; 3.53, m	70.7, CH_2	3.91, m; 3.54, m
1'	198.4, C		not obs.		not obs.	
2'	68.9, CH	3.97, dd (9.0, 6.0)	67.0, CH	4.09, m	67.3, CH	4.22, dd (10.2, 6.0)
3'	28.2, CH_2	2.14, m	38.3, CH_2	2.09, m	37.9, CH_2	2.10, m
		1.46, m		1.53, m		1.58, m
4'	28.0, CH_2	2.11, m; 2.06, m	74.5, CH	4.53, m	74.3, CH	4.58, m
5'	44.3, CH_2	3.64, ddd (12.0, 7.8, 3.0)	54.0, CH_2	3.81, dd, (12.6, 5.4)	53.8, CH_2	3.86, m
		3.21, ddd (12.0, 6.0, 3.0)		3.03, brd (12.6)		3.08, d (12.6)
1"	101.7, CH	4.49, brs	101.8, CH	4.49, brs	101.8, CH	4.49, brs
2"	72.6, CH	3.84, d (3.0)	72.6, CH	3.84, d (3.0)	72.6, CH	3.84, d (3.6)
3"	75.4, CH	3.44, dd (9.6, 3.0)	75.4, CH	3.44, dd (9.6, 3.0)	75.4, CH	3.44, dd (9.6, 3.6)
4"	68.6, CH	3.56, dd (9.6, 9.6)	68.6, CH	3.56, dd (9.6, 9.6)	68.6, CH	3.56, dd (9.6, 9.0)
5"	78.2, CH	3.20, ddd (9.6, 6.0, 2.4)	78.3, CH	3.20, ddd (9.0, 6.0, 2.4)	78.3, CH	3.20, ddd (9.0, 6.0, 2.4)
6"	62.9, CH_2	3.87, dd (12.0, 2.4)	62.9, CH_2	3.86, dd (11.4, 2.4)	62.9, CH_2	3.86, dd (12.0, 2.4)
		3.71, dd (12.0, 6.0)		3.71, dd (11.4, 6.0)		3.71, dd (12.0, 6.0)

[a] ^{1}H and ^{13}C NMR data were recorded at 600 and 150 MHz, respectively. The assignments were based on 2D NMR (^{1}H-^{1}H COSY, TOCSY, ROESY, HSQC, and HMBC) experiments. [b] not observed.

Table S4. ^{1}H and ^{13}C NMR data of compound **5** [a]



Z form 2 : 1 *E* form

No.	CD_3OD		CD_3Cl [c]			
			Z form		*E* form	
	δ_C, type	δ_H, mult. (*J* in Hz)	δ_C, type	δ_H, mult. (*J* in Hz)	δ_C, type	δ_H, mult. (*J* in Hz)
1	not obs. [b]		177.2, C		170.4, C	
2	103.6, C		101.9, C		104.5, C	
3	not obs.		193.2, C		197.0, C	
4	36.2, CH	3.80, m	33.7, CH	3.72, m	34.2, C	3.78, m
4-Me	17.8, CH_3	1.07, d (7.2)	17.3, CH_3	1.14, d (7.2)	17.1, CH_3	1.17, d (7.2)
5	42.2, CH_2	1.54, m; 1.35, m	41.2, CH_2	1.56, m; 1.40, m	40.5, CH_2	1.54, m; 1.43, m
6	31.9, CH	1.42, m	30.6, CH	1.41, m	30.6, CH	1.41, m
6-Me	20.3, CH_3	0.88, d (6.0)	19.7, CH_3	0.88, d (6.0)	19.4, CH_3	0.89, d (6.0)
7	38.1, CH_2	1.35, m; 1.08, m	36.5, CH_2	1.34, m; 1.06, m	36.6, CH_2	1.34, m; 1.06, m
8	28.1, CH_2	1.31, m; 1.23, m	26.8, CH_2	1.26, m; 1.19, m	27.0, CH_2	1.26, m; 1.19, m
9	31.0, CH_2	1.25-1.35, m	29.3-29.6, CH_2	1.20-1.34, m	29.3-29.6, CH_2	1.20-1.34, m
10	30.7, CH_2	1.25-1.35, m	29.3-29.6, CH_2	1.20-1.34, m	29.3-29.6, CH_2	1.20-1.34, m
11	30.3, CH_2	1.28, m	29.2, CH_2	1.20-1.34, m	29.2, CH_2	1.20-1.34, m
12	30.9, CH_2	1.36, m	29.6, CH_2	1.35, m	29.6, CH_2	1.35, m
13	33.8, CH_2	2.00, q, (6.0)	32.6, CH_2	2.02, q (6.6)	32.6, CH_2	2.02, q (6.6)
14	134.1, CH	5.47, dt (15.0, 6.0)	135.0, CH	5.54, dt (15.0, 6.6)	135.0, CH	5.54, dt (15.0, 6.6)
15	127.7, CH	5.45, dt (15.0, 6.0)	125.6, CH	5.40, dt (15.0, 6.6)	125.6, CH	5.40, dt (15.0, 6.6)
16	41.7, CH_2	2.14, m	40.7, CH_2	2.24, m; 2.07, m	40.7, CH_2	2.24, m; 2.07, m
17	72.5, CH	3.55, m	70.8, CH	3.61, m	70.8, CH	3.61, m
18	37.7, CH_2	1.50, m; 1.36, m	36.4, CH_2	1.50, m; 1.45, m	36.4, CH_2	1.50, m; 1.45, m
19	22.9, CH	1.59, m; 1.35, m	21.6, CH_2	1.59, m; 1.41, m	21.6, CH_2	1.59, m; 1.41, m
20	38.4, CH_2	1.45, m; 1.37, m	37.3, CH_2	1.50, m; 1.42, m	37.3, CH_2	1.50, m; 1.42, m
21	72.4, CH	3.51, m	71.9, CH	3.61, m	71.9, CH	3.61, m
22	38.5, CH_2	1.42, m; 1.37, m	37.4, CH_2	1.50, m; 1.44, m	37.4, CH_2	1.50, m; 1.44, m
23	26.8, CH_2	1.45, m; 1.34, m	25.5, CH_2	1.43, m; 1.33, m	25.5, CH_2	1.43, m; 1.33, m
24	30.7, CH_2	1.33, m	29.3-29.6, CH_2	1.34, m	29.3-29.6, CH_2	1.34, m
25	30.7, CH_2	1.35, m	29.1, CH_2	1.35, m	29.1, CH_2	1.35, m
26	27.0, CH_2	1.39, m	25.6, CH_2	1.36, m	25.6, CH_2	1.36, m
27	33.7, CH_2	1.53, m	32.7, CH_2	1.57, m	32.7, CH_2	1.57, m
28	63.0, CH_2	3.54, t (6.6)	63.0, CH_2	3.64, t (6.6)	63.0, CH_2	3.64, t (6.6)
1'	not obs.		194.5, C		201.6, C	
2'	67.1, CH	4.19, m	67.0, CH	4.29, dd (10.8, 6.6)	63.9, CH	4.42, dd (10.8, 6.6)
3'	38.0, CH_2	2.09, dd (12.6, 6.0); 1.60, m	37.0, CH_2	2.20, dd (12.6, 6.0) 1.63, m	36.9, CH_2	2.20, dd (12.6, 6.0) 1.62, m
4'	74.4, CH	4.57, m	73.4, CH	4.71, m	73.8, CH	4.71, m
5'	53.9, CH_2	3.85, dd (12.0, 4.8) 3.07, d (12.0)	52.6, CH_2	3.98, dd (12.6, 4.8) 3.23, d(12.6)	52.8, CH_2	4.01, dd (12.6, 4.8) 3.15, d (12.6)

[a] ^{1}H and ^{13}C NMR data were recorded at 600 and 150 MHz, respectively. [b] not observed. [c] The NMR data recorded in $CDCl_3$ showed two sets of signals with a ratio of 2:1 corresponding to *Z* and *E* form, respectively.[10-11]

Table S5. ^{1}H and ^{13}C NMR data of compounds **6**–**8** in CD_3OD[a]

No.	**6**		**7**		**8**	
	δ_C	δ_H, mult. (*J* in Hz)	δ_C	δ_H, mult. (*J* in Hz)	δ_C	δ_H, mult. (*J* in Hz)
1	not obs.					
2	103.7, C					
3	not obs.					
4	not obs.	3.83, m				
4-Me	17.8, CH_3	1.09, d (7.2)				
5	42.2, CH_2	1.54, m; 1.34, m				
6	31.9, CH	1.42, m				
6-Me	20.2, CH_3	0.88, d (6.6)				
7	38.0, CH_2	1.36, m; 1.09, m				
8	28.0, CH_2	1.30, m; 1.24, m				
9	30.6-30.9, CH_2	1.26-1.33, m				
10	30.6-30.9, CH_2	1.26-1.33, m				
11	30.6-30.9, CH_2	1.26-1.33, m				
12	25.6, CH_2	1.32, m				
13	33.7, CH_2	1.56, m				
14	106.3, CH	4.35, t (6.0)				
15			104.3, CH	4.58, dd (7.8, 3.6)	104.3, CH	4.58, dd (7.8, 3.6)
16			41.4, CH_2	1.74, ddd (14.4, 7.8, 3.6)	41.4, CH_2	1.74, ddd (14.4, 7.8, 3.6)
				1.62, ddd (14.4, 9.6, 3.6)		1.61, ddd (14.4, 9.0, 3.6)
17			68.9, CH	3.66, m	68.9, CH	3.66, m
18			38.8, CH_2	1.48, m; 1.44, m	38.8, CH_2	1.48, m; 1.44, m
19			22.8, CH_2	1.58, m; 1.37, m	22.8, CH_2	1.58, m; 1.37, m
20			38.3, CH_2	1.45, m; 1.37, m	38.3, CH_2	1.45, m; 1.37, m
21			72.3, CH	3.51, m	72.3, CH	3.52, m
22			38.4, CH_2	1.42, m; 1.37, m	38.4, CH_2	1.42, m; 1.37, m
23			26.8, CH_2	1.45, m; 1.33, m	26.8, CH_2	1.45, m; 1.33, m
24			30.8, CH_2	1.30, m	30.8, CH_2	1.30-1.39, m
25			30.6, CH_2	1.35, m	30.6, CH_2	1.30-1.39, m
26			27.1, CH_2	1.39, m	26.9, CH_2	1.30-1.39, m
27			30.7, CH_2	1.61, m	33.7, CH_2	1.53, m
28			70.6, CH_2	3.91, dt (9.0, 6.6)	63.0, CH_2	3.54, t (6.6)
				3.53, dt (9.0, 6.6)		
1'	not obs.					
2'	67.5, CH	4.21, m				
3'	37.9, CH_2	2.10, m; 1.58, m				
4'	74.4, CH	4.58, m				
5'	53.8, CH_2	3.86, dd (12.0, 4.2)				
		3.09, d (12.0)				
1"			101.7, CH	4.49, brs		
2"			72.6, CH	3.84, d (3.0)		
3"			75.3, CH	3.44, dd (9.6, 3.0)		
4"			68.6, CH	3.56, dd (9.0, 9.0)		
5"			78.2, CH	3.20, ddd (9.0, 6.0, 2.4)		
6"			62.9, CH_2	3.86, dd (12.0, 2.4)		
				3.71, dd (11.4, 6.0)		
OMe	53.4, CH_3	3.34, s	53.9, CH_3	3.34, s	53.9, CH_3	3.34, s
			53.4, CH_3	3.32, s	53.4, CH_3	3.32, s

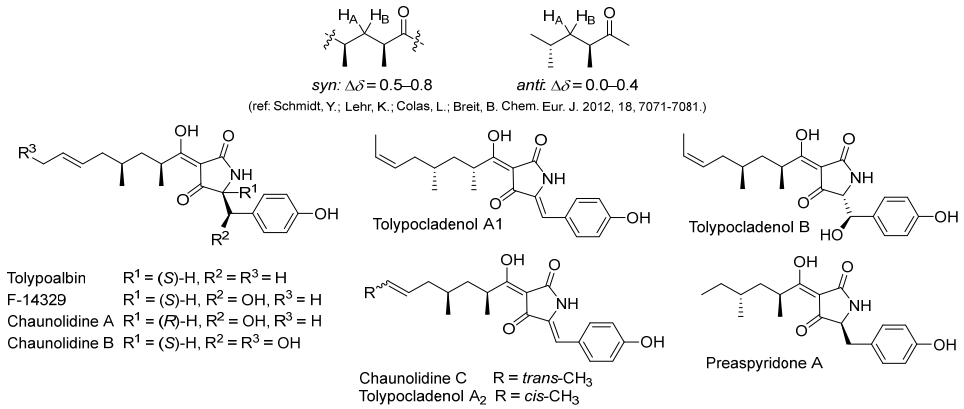
[a] ^{1}H and ^{13}C NMR data were recorded at 600 and 150 MHz, respectively. [b] not observed.

Table S6. ^{1}H NMR data of compounds **8a** and **8b** in CD_3OD (δ_H, mult. (J in Hz))[a]

no.	**8a**	**8b**	$\Delta\delta^{SR}$
15	4.14, dd (6.0, 4.8)	4.41, dd (6.6, 4.8)	–0.27
16	1.74, m	1.93, ddd (14.4, 7.8, 4.8)	–0.19
		1.86, ddd (14.4, 6.6, 4.8)	–0.12
17	5.06, m	5.16, m	–0.10
18	1.61, m	1.61, m	0.00
19	1.24, m	1.23, m	+0.01
	1.13, m	1.14, m	–0.01
20	1.59, m	1.55, m	+0.04
21	5.06, m	4.96, m	+0.10
22	1.59, m	1.45, m	+0.14
23	1.29, m	1.10, m	+0.19
24	1.29, m	1.20, m	+0.09
25	1.29, m	1.20, m	+0.09
26	1.29, m	1.26, m	+0.03
27	1.67, m	1.65, m	+0.02
28	4.34, dt (10.8, 6.6)	4.34, dt (10.8, 6.6)	0.00
	4.29, dt (10.8, 6.6)	4.29, dt (10.8, 6.6)	0.00
OMe	3.25, s	3.31, s	–0.06
	3.20, s	3.29, s	–0.09

[a] ^{1}H NMR data were recorded at 600 MHz. The assignments were based on 2D NMR (^{1}H-^{1}H COSY, TOCSY, ROESY, HSQC) experiments.

Table S7. The $\Delta\delta$ value of the germinal methylene protons of 3-acetyltetramic acids derivatives



Compound	Configuration of 1,3-dimethyl	$\Delta\delta$				Ref.
		CD_3OD	Acetone-d_6	DMSO-d_6	$CDCl_3$	
F-14329	*syn*	-	0.62	0.58	0.63	12-15
Tolypoalbin	*syn*	-		-	0.63	12
Tolypocladenols A1, A2, and B	*syn*	-	0.65-0.66	-	-	15
Chaunolidines A-C	*syn*	-		0.56-0.61	-	13
Preaspyridone A	*anti*	-		0.08	-	16
1	*anti*	0.19		0.11	-	
5	*anti*	0.19		-	0.16	

Table S8. Antimicrobial activity of compounds **1–5** (MIC, μg/mL)

Microorganism	Strain no.	**1**	**2**	**3**	**4**	**5**	rifampicin	nystatin
Fusarium sp.	CPCC 400381	16	64	>64	>64	>64	nt[a]	16
Fusarium sp.	CPCC 400307	64	>64	>64	>64	>64	nt	1
Alternaria sp.	CPCC 400323	32	32	32	>64	>64	nt	8
Curvularia lunata	CPCC 400186	4	16	32	32	>64	nt	<0.5
Aspergillus chevalieri	IMB18-208	4	4	8	8	>64	nt	2
Aspergillus versicolor	IMB17-055	>64	>64	>64	>64	>64	nt	32
Candida Albicans	ATCC 10231	1	4	2	0.5	>64	nt	>64
Pseudomonas aeruginosa	ATCC 27853	>128	>128	>128	>128	>128	16	nt
Klebsiella pneumoniae	ATCC 700603	>128	>128	>128	>128	>128	16	nt
Staphylococcus aureus	ATCC 29213	>128	>128	>128	>128	>128	<0.0625	nt
Bacillus subtilis	ATCC 6633	>128	>128	>128	>128	>128	<0.0625	nt

[a] nt: not tested.

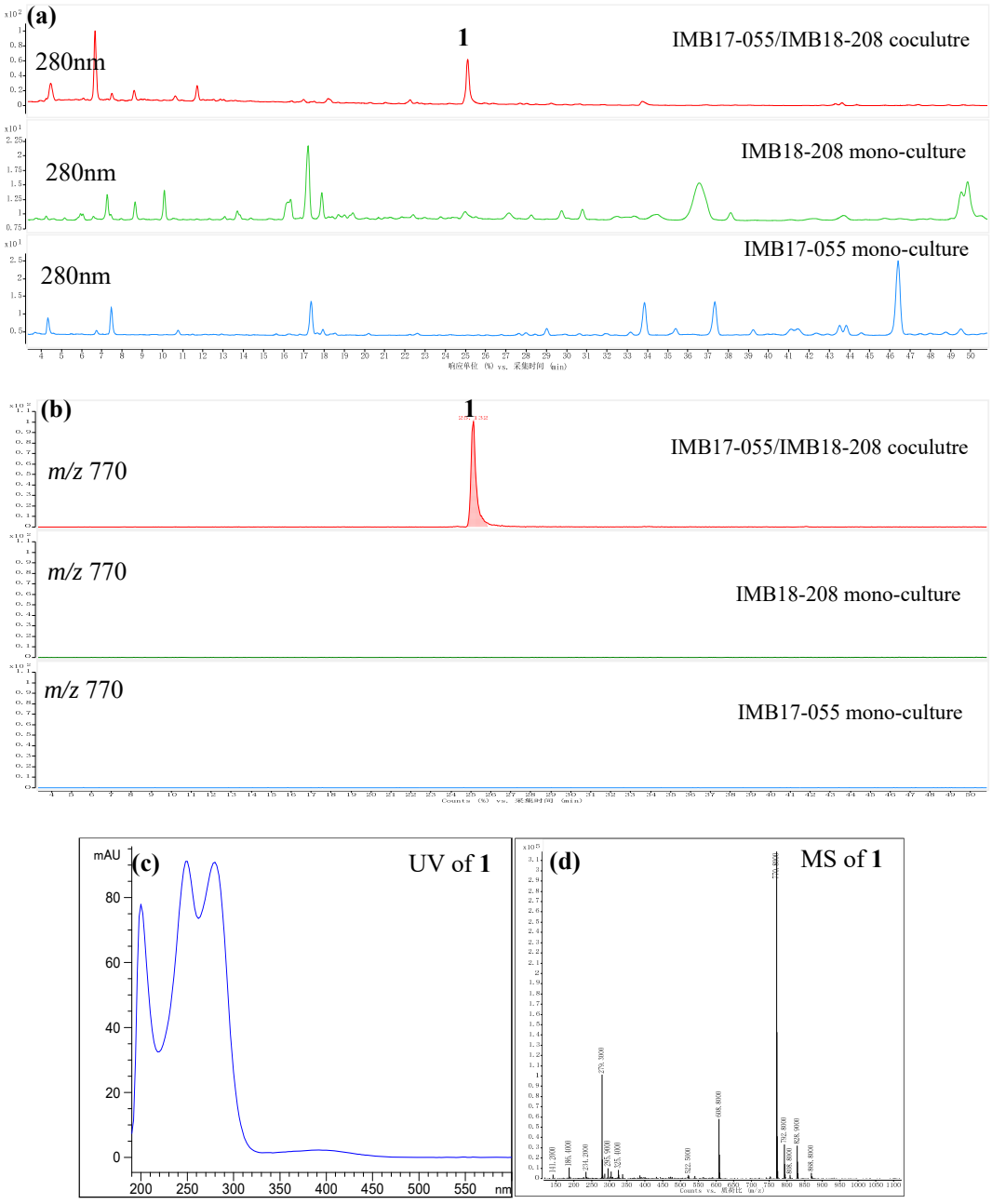


Figure S1. LC-MS profile of the coculture extract of *Aspergillus versicolor* IMB17-055 and *Aspergillus chevalieri* IMB18-208. (a) LC-DAD chromatogram at 280 nm; (b) Extracted ion chromatogram (*m/z* 770 $[M + H]^+$); (c) UV spectrum of **1** obtained by LC-DAD; (d) MS spectrum of **1**. (Conditions: Capcell MGII C18 4.6×150mm, flow rate 1 mL/min, a linear gradient of 10%–70% CH_3CN-5mM NH_4Ac over 50 min, then eluting with 95% CH_3CN for additional 10 min, detector 280 nm)

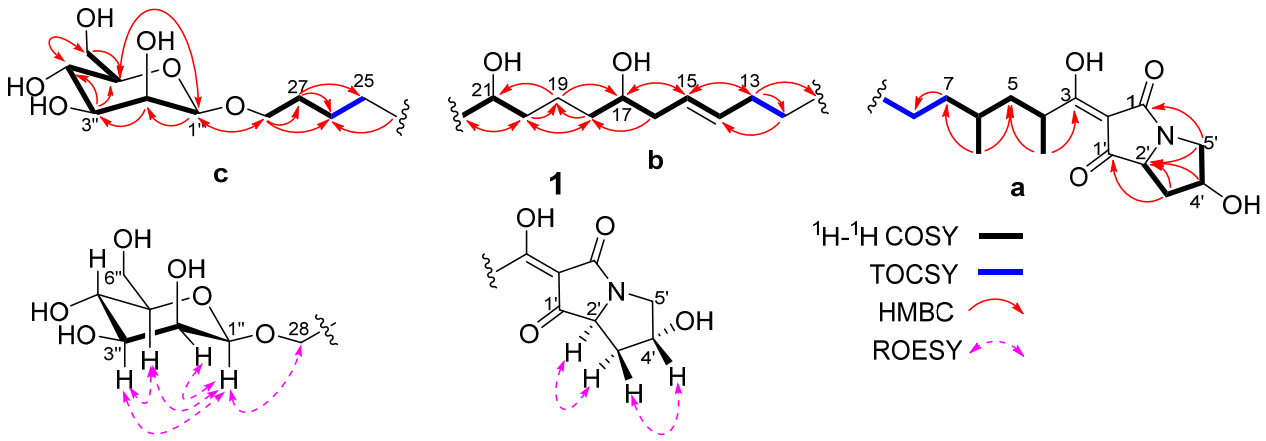


Figure S2. Substructure confirmed by 2D NMR data of **1**.

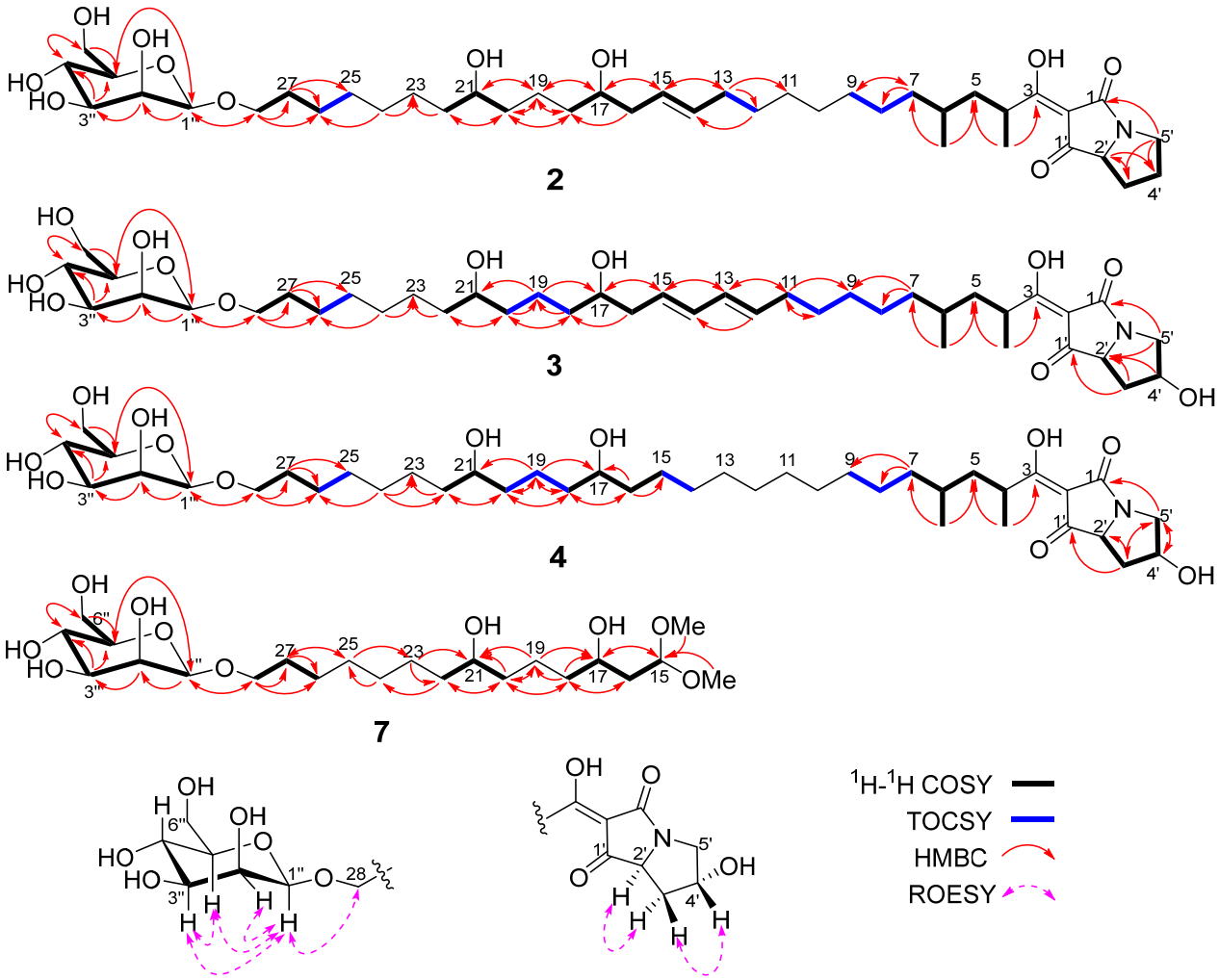


Figure S3. Key COSY, TOCSY, HMBC and ROESY correlations of compounds **2–4** and **7**.

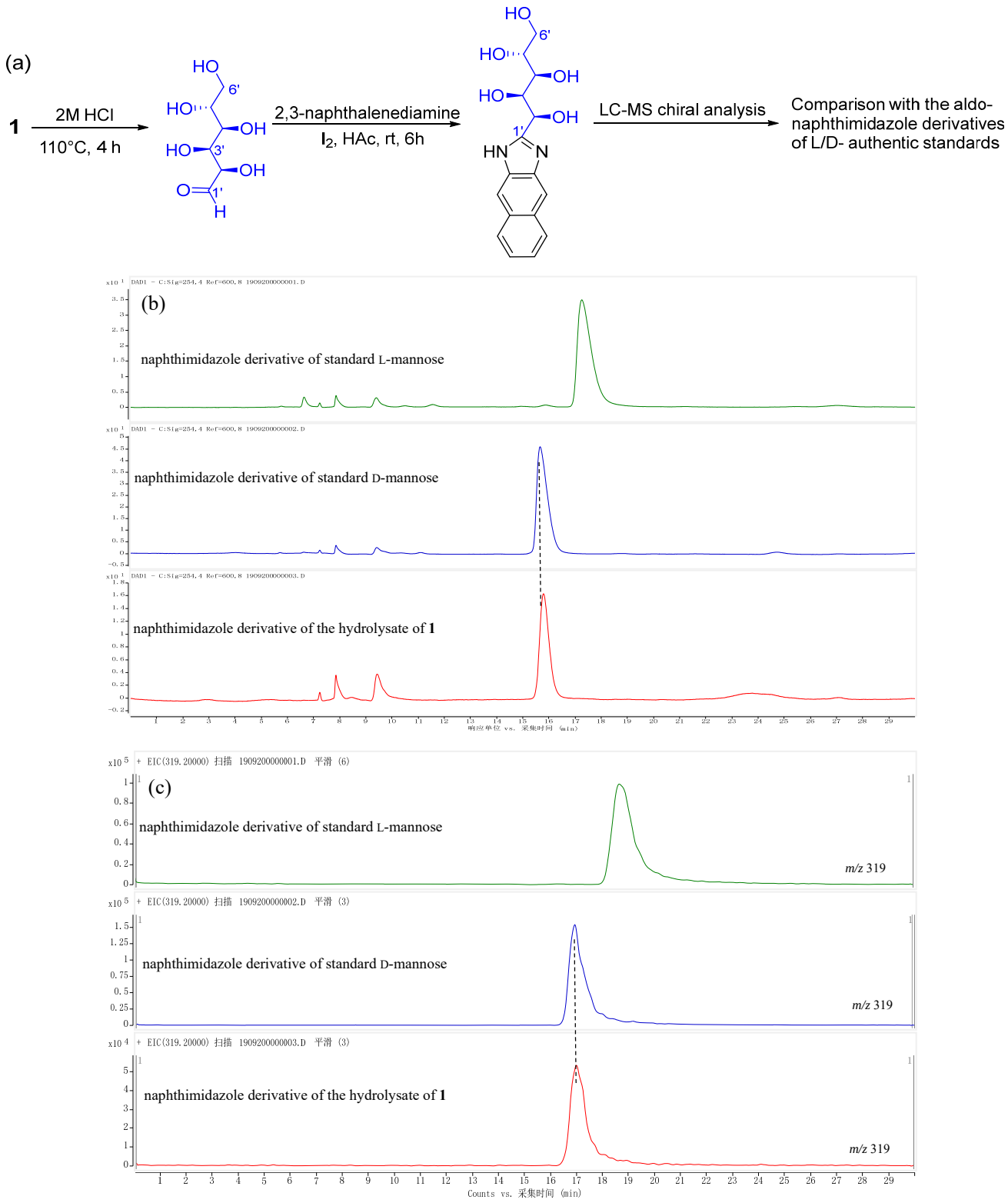


Figure S4. Chromatographic determination of the absolute configuration of the mannose residue in **1** by naphthimidazole derivatization. (a) Procedure for the chemical derivatization with 2,3-naphthalenediamine. (b) LC-MS analysis (UV chromatogram at 254 nm). (c) LC-MS analysis (extracted ion chromatogram at *m/z* 319).

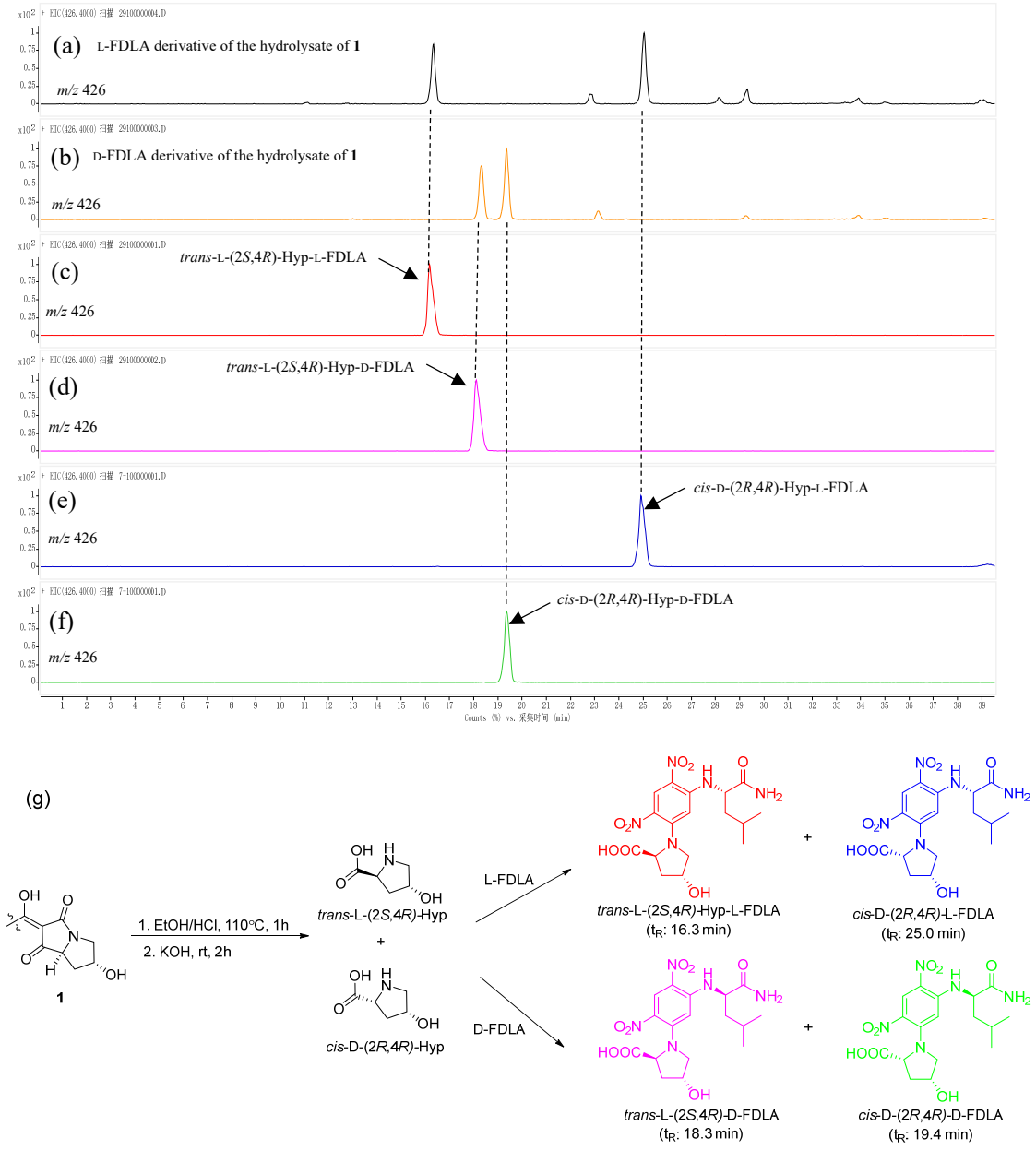


Figure S5. Marfey's analysis of **1**. Extracted ion chromatogram (*m/z* 426.0) of (a) L-FDLA derivative of the hydrolysate of **1**, (b) D-FDLA derivative of the hydrolysate of **1**, (c) L-FDLA derivative of standard *trans*-L-(2*S*,4*R*)-hydroxyproline, (d) D-FDLA derivative of standard *trans*-L-(2*S*,4*R*)-hydroxyproline, (e) L-FDLA derivative of standard *cis*-D-(2*R*,4*R*)-hydroxyproline, (f) D-FDLA derivative of standard *cis*-D-(2*R*,4*R*)-hydroxyproline, (g) Hydrolysis and derivatization of **1**.

Table S9. DP4+ analysis of **6a–6d**

	6a	6b	6c	6d
DP4+ (H data)	95.58%	0.03%	4.39%	0.00%
DP4+ (H data)	85.73%	0.84%	12.28%	1.15%
DP4+ (all data)	99.35%	0.00%	0.65%	0.00%

A	B	C	D	E	F	G	H
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311+G(d,p)		Shielding Tensors	
		DP4+	99.35%	0.00%	0.65%	0.00%	-
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	178.0	3.03	2.55	3.08	3.19	
C	x	103.8	78.20	79.13	77.88	78.19	
C	x	196.4	-13.83	-13.98	-13.75	-14.41	
C		35.9	150.27	149.23	149.09	147.33	
C		42.1	141.21	141.87	143.05	142.60	
C		30.9	153.06	151.10	152.97	156.83	
C		37.8	150.20	152.35	148.41	150.30	
C	x	198.4	-17.24	-17.04	-16.86	-17.46	
C		67.5	114.86	115.12	114.58	115.51	
C		37.7	146.97	145.20	148.61	147.75	
C		74.3	107.59	108.64	107.25	109.99	
C		53.8	131.99	132.69	130.69	132.78	
C		17.8	166.56	166.16	165.81	169.52	
C		20.2	166.76	166.62	169.30	168.48	
H		3.79	27.68	27.82	27.78	28.24	
H		1.56	29.86	29.73	29.91	29.75	
H		1.37	30.59	30.62	30.51	30.74	
H		1.43	30.59	30.77	30.51	30.49	
H		1.35	30.13	29.99	30.55	30.51	
H		1.08	31.01	31.22	30.66	30.72	
H		4.25	27.39	27.41	27.42	27.43	
H		2.11	29.75	29.51	30.14	29.90	
H		1.6	30.18	30.26	29.67	29.80	
H		4.6	27.07	26.95	26.96	27.28	
H		3.88	27.72	27.77	27.59	27.76	
H		3.11	28.59	28.65	28.66	28.66	
H		1.11	30.56	30.53	30.52	30.75	
H		0.89	30.94	30.82	30.90	30.39	

Table S10. Boltzmann populations of the identified conformers of **6a**

conformer	G (Hartree)	ΔG (KJ/mol)	P (%)
6a-C1	-1405.615451	1.0134	37.37%
6a-C2	-1405.612795	7.9868	2.24%
6a-C3	-1405.61281	7.9474	2.28%
6a-C4	-1405.615837	0.0000	56.25%
6a-C5	-1405.612624	8.4357	1.87%

Table S11. Boltzmann populations of the identified conformers of **6b**

conformer	G (Hartree)	ΔG (KJ/mol)	P (%)
6b-C1	-1405.61255	7.0232	3.57%
6b-C2	-1405.611619	9.4676	1.33%
6b-C3	-1405.615225	0.0000	60.77%
6b-C4	-1405.614244	2.5756	21.49%
6b-C5	-1405.611325	10.2395	0.97%
6b-C6	-1405.613463	4.6261	9.39%
6b-C7	-1405.612201	7.9395	2.47%

Table S12. Boltzmann populations of the identified conformers of **6c**

conformer	G (Hartree)	ΔG (KJ/mol)	P (%)
6c-C1	-1405.609354	7.5824	1.72%
6c-C2	-1405.611736	1.3285	21.47%
6c-C3	-1405.611576	1.7486	18.12%
6c-C4	-1405.609665	6.7659	2.39%
6c-C5	-1405.611294	2.4890	13.44%
6c-C6	-1405.609224	7.9238	1.50%
6c-C7	-1405.609541	7.0915	2.10%
6c-C8	-1405.609735	6.5821	2.58%
6c-C9	-1405.612242	0.0000	36.70%

Table S13. Boltzmann populations of the identified conformers of **6d**

conformer	G (Hartree)	ΔG (KJ/mol)	P (%)
6d-C1	-1405.612978	0.0000	48.40%
6d-C2	-1405.611597	3.6258	11.20%
6d-C3	-1405.612655	0.8480	34.37%
6d-C4	-1405.610036	7.7242	2.14%
6d-C5	-1405.609261	9.7590	0.94%
6d-C6	-1405.610334	6.9418	2.94%

Table S14. Calculated NMR data of **6a**[a]

atom	Shielding tensor						δs	δexp.
	6a-C1	**6a**-C2	**6a**-C3	**6a**-C4	**6a**-C5	average		
C-1	2.34	3.94	3.03	3.50	1.69	3.03	178.45	178.0
C-2	77.89	77.52	78.12	78.39	80.09	78.20	105.03	103.8
C-3	-13.82	-13.46	-12.60	-13.85	-15.27	-13.83	194.91	196.4
C-4	150.05	150.48	149.96	150.37	152.65	150.27	34.64	35.9
C-5	141.14	140.82	141.67	141.22	142.66	141.21	43.49	42.1
C-6	156.22	151.28	151.16	151.25	149.43	153.06	31.92	30.9
C-7	150.56	149.88	153.16	149.95	148.26	150.20	34.71	37.8
C-1'	-17.33	-17.57	-16.42	-17.22	-16.49	-17.24	198.24	198.4
C-2'	114.49	114.88	114.31	115.13	115.29	114.86	69.23	67.5
C-3'	147.56	147.68	149.01	146.51	146.52	146.97	37.87	37.7
C-4'	107.66	107.65	107.39	107.55	108.13	107.59	76.33	74.3
C-5'	130.63	131.41	130.30	132.98	132.89	131.99	52.49	53.8
$\underline{C}H_3$-4	166.55	167.21	166.50	166.66	164.02	166.56	18.73	17.8
$\underline{C}H_3$-6	167.56	165.67	166.12	166.23	169.66	166.76	18.54	20.2
H-4	27.74	27.71	27.73	27.63	27.82	27.68	3.94	3.79
H-5a	29.80	30.01	29.81	29.90	29.52	29.86	1.90	1.56
H-5b	30.62	30.56	30.58	30.59	30.25	30.59	1.21	1.37
H-6	30.54	30.71	30.69	30.63	30.21	30.59	1.21	1.43
H-7a	30.11	30.39	30.04	30.13	30.60	30.13	1.64	1.35
H-7b	30.88	31.01	31.25	31.10	30.93	31.01	0.81	1.08
H-2'	27.33	26.96	27.15	27.47	27.48	27.39	4.21	4.25
H-3'a	29.73	29.78	29.42	29.77	29.75	29.75	2.00	2.11
H-3'b	30.12	30.09	30.20	30.24	30.21	30.18	1.59	1.6
H-4'	27.26	27.25	26.96	26.95	26.93	27.07	4.52	4.6
H-5'a	27.76	27.67	27.82	27.70	27.64	27.72	3.90	3.88
H-5'b	28.57	28.64	28.74	28.60	28.54	28.59	3.09	3.11
C$\underline{H}_3$-4	30.71	30.71	30.77	30.64	30.76	30.56	1.24	1.11
C$\underline{H}_3$-6	31.05	31.01	30.91	30.92	31.00	30.94	0.88	0.89

[a] The scaled chemical shifts (δs) were obtained by GIAO NMR computation at the SCRF-PW1PW91/6-311+G(2d,p) level with PCM model in MeOH using the formula $\delta_s = (\delta_u - b)/-m$, where δ_u is the unscaled chemical shift relative to TMS according to $\delta_u = \sigma_0 - \sigma^x$; σ^x is the Boltzmann averaged isotropic shielding constant, σ_0 is the shielding tensor of TMS calculated at the same level of theory used for σ^x , m and b are the slope and intercept, respectively, obtained from a linear regression calculation on a plot of δ_u against δ_{exp}. δ_{exp} are the experimental chemical shift.

Table S15. Calculated NMR data of **6b**[a]

atom	Shielding tensor								δs	δexp
	6b-C1	**6b**-C2	**6b**-C3	**6b**-C4	**6b**-C5	**6b**-C6	**6b**-C7	average		
C-1	2.21	2.20	2.20	3.64	3.38	2.53	2.35	2.55	179.07	178.0
C-2	79.46	79.55	79.55	78.15	77.99	78.80	78.40	79.13	104.17	103.8
C-3	-13.87	-13.53	-13.53	-13.74	-13.56	-16.89	-16.84	-13.98	195.24	196.4
C-4	150.48	150.34	150.34	149.98	149.44	141.77	141.87	149.23	35.59	35.9
C-5	140.66	141.01	141.01	142.76	142.81	145.26	144.99	141.87	42.79	42.1
C-6	151.18	151.02	151.02	151.20	150.96	151.32	151.86	151.10	33.76	30.9
C-7	152.68	152.52	152.52	151.95	153.34	152.11	152.21	152.35	32.54	37.8
C-1'	-17.68	-17.24	-17.24	-17.26	-16.38	-15.54	-15.12	-17.04	198.23	198.4
C-2'	114.87	115.18	115.18	114.68	115.33	115.70	115.94	115.12	68.96	67.5
C-3'	145.03	144.26	144.26	147.09	148.50	146.54	146.61	145.20	39.54	37.7
C-4'	108.94	109.35	109.35	107.49	106.48	107.13	107.50	108.64	75.30	74.3
C-5'	132.48	132.56	132.56	133.30	130.92	132.51	132.59	132.69	51.78	53.8
$\underline{C}H_3$-4	165.80	165.80	165.80	164.79	165.41	170.96	170.32	166.16	19.03	17.8
$\underline{C}H_3$-6	166.91	166.85	166.85	166.17	166.26	166.27	166.46	166.62	18.58	20.2
H-4	27.61	27.61	27.69	27.61	27.64	28.91	29.28	27.82	3.81	3.79
H-5a	29.83	29.88	29.71	29.84	29.81	29.25	30.76	29.73	2.02	1.56
H-5b	30.57	30.58	30.60	30.67	30.66	30.75	30.66	30.62	1.17	1.37
H-6	30.81	30.81	30.78	30.71	30.86	30.69	31.22	30.77	1.04	1.43
H-7a	30.24	30.39	30.02	29.97	29.93	29.73	30.06	29.99	1.77	1.35
H-7b	31.26	31.29	31.25	31.28	31.33	31.26	29.76	31.22	0.61	1.08
H-2'	27.49	27.49	27.42	27.36	27.50	27.43	27.45	27.41	4.20	4.25
H-3'a	29.20	29.56	29.68	28.97	28.93	29.80	29.78	29.51	2.22	2.11
H-3'b	30.38	30.30	30.25	30.34	30.13	30.22	30.25	30.26	1.51	1.6
H-4'	27.01	26.97	26.94	26.99	27.21	26.91	26.88	26.95	4.63	4.6
H-5'a	27.64	27.56	27.77	27.83	27.75	27.71	27.73	27.77	3.86	3.88
H-5'b	28.73	28.72	28.66	28.60	28.65	28.61	28.93	28.65	3.04	3.11
C$\underline{H}_3$-4	30.51	30.51	30.56	30.55	30.58	30.45	30.28	30.53	1.26	1.11
C$\underline{H}_3$-6	31.06	31.04	30.96	30.87	30.93	30.94	26.29	30.82	0.99	0.89

[a] The scaled chemical shifts (δs) were obtained by GIAO NMR computation at the SCRF-PW1PW91/6-311+G(2d,p) level with PCM model in MeOH using the formula $\delta_s = (\delta_u - b)/-m$, where δ_u is the unscaled chemical shift relative to TMS according to $\delta_u = \sigma_0 - \sigma^x$; σ^x is the Boltzmann averaged isotropic shielding constant, σ_0 is the shielding tensor of TMS calculated at the same level of theory used for σ^x , m and b are the slope and intercept, respectively, obtained from a linear regression calculation on a plot of δ_u against δ_{exp}. δ_{exp} are the experimental chemical shift.

Table S16. Calculated NMR data of **6c**[a]

atom	Shielding tensor (σ)										δ_s	δ_{exp}
	6c-C1	**6c**-C2	**6c**-C3	**6c**-C4	**6c**-C5	**6c**-C6	**6c**-C7	**6c**-C8	**6c**-C9	average		
C-1	3.50	2.90	3.57	2.41	2.61	2.68	3.68	2.09	3.18	3.08	178.39	178.0
C-2	77.97	77.92	78.23	78.99	78.82	80.12	77.74	78.71	77.16	77.88	105.36	103.8
C-3	-14.61	-14.14	-13.45	-13.56	-13.62	-14.00	-13.31	-16.48	-13.51	-13.75	194.82	196.4
C-4	150.10	150.10	149.54	146.73	146.24	151.03	149.55	142.04	149.85	149.09	35.84	35.9
C-5	140.28	140.17	141.99	148.72	143.53	148.40	141.17	144.26	144.69	143.05	41.74	42.1
C-6	154.60	155.99	153.47	149.40	148.38	154.07	156.90	150.42	152.73	152.97	32.06	30.9
C-7	147.18	146.64	147.87	153.81	150.00	153.10	151.09	145.23	148.74	148.41	36.51	37.8
C-1'	-17.72	-17.36	-17.13	-17.00	-17.17	-17.11	-16.78	-15.45	-16.37	-16.86	197.86	198.4
C-2'	114.16	114.39	114.03	114.19	113.63	114.05	114.64	115.09	115.38	114.58	69.53	67.5
C-3'	149.67	149.09	149.25	148.80	149.24	149.54	146.41	148.83	147.83	148.61	36.31	37.7
C-4'	107.31	107.58	107.64	107.83	107.77	107.21	107.55	107.28	106.64	107.25	76.69	74.3
C-5'	130.61	130.22	130.57	130.25	130.61	130.60	133.01	129.98	131.03	130.69	53.81	53.8
$\underline{C}H_3$-4	166.14	167.18	165.72	163.82	163.40	170.27	166.68	170.34	165.55	165.81	19.52	17.8
$\underline{C}H_3$-6	168.72	170.77	168.76	165.94	165.99	165.91	171.21	169.93	170.20	169.30	16.11	20.2
H-4	27.69	27.67	27.61	28.02	27.88	27.91	27.67	28.99	27.80	27.78	3.85	3.79
H-5a	29.94	30.04	29.89	29.40	29.69	30.24	29.95	29.28	29.98	29.91	1.82	1.56
H-5b	30.54	30.57	30.51	30.57	30.40	30.48	30.56	30.70	30.50	30.51	1.25	1.37
H-6	30.68	30.59	30.72	30.01	30.49	29.92	30.57	30.65	30.41	30.51	1.25	1.43
H-7a	30.54	30.53	30.67	31.03	31.40	30.16	30.84	30.81	30.17	30.55	1.21	1.35
H-7b	30.74	30.57	30.88	30.45	30.42	30.40	30.29	30.70	30.74	30.66	1.11	1.08
H-2'	27.29	27.38	27.35	27.33	27.31	27.33	27.38	27.29	27.55	27.42	4.19	4.25
H-3'a	29.58	30.15	30.26	30.15	30.21	29.73	30.19	30.08	30.11	30.14	1.60	2.11
H-3'b	29.73	29.67	29.68	29.64	29.69	29.73	29.74	29.62	29.66	29.67	2.05	1.6
H-4'	27.00	27.00	26.99	26.51	26.39	26.95	26.93	26.98	27.17	26.96	4.63	4.6
H-5'a	27.93	27.43	27.26	27.77	27.83	27.80	27.76	27.90	27.70	27.59	4.03	3.88
H-5'b	28.65	28.68	28.75	28.67	28.66	28.66	28.63	28.67	28.60	28.66	3.01	3.11
C$\underline{H}_3$-4	30.64	30.62	30.59	30.80	30.76	30.72	30.61	30.75	30.52	30.52	1.24	1.11
C$\underline{H}_3$-6	31.53	31.46	31.46	30.88	31.18	30.83	31.63	31.39	31.02	30.90	0.88	0.89

[a] The scaled chemical shifts (δ_s) were obtained by GIAO NMR computation at the SCRF-PW1PW91/6-311+G(2d,p) level with PCM model in MeOH using the formula $\delta_s = (\delta_u - b)/-m$, where δ_u is the unscaled chemical shift relative to TMS according to $\delta_u = \sigma_0 - \sigma^x$; σ^x is the Boltzmann averaged isotropic shielding constant, σ_0 is the shielding tensor of TMS calculated at the same level of theory used for σ^x , m and b are the slope and intercept, respectively, obtained from a linear regression calculation on a plot of δ_u against δ_{exp}. δ_{exp} are the experimental chemical shift.

Table S17. Calculated NMR data of **6d**[a]

atom	Shielding tensor							δs	δexp.
	6d-C1	**6d**-C2	**6d**-C3	**6d**-C4	**6d**-C5	**6d**-C6	average		
C-1	3.16	5.43	2.48	2.46	3.68	3.85	3.19	178.12	178.0
C-2	76.55	77.20	80.43	80.61	78.62	80.51	78.19	105.55	103.8
C-3	-12.65	-12.56	-17.44	-16.97	-13.92	-13.49	-14.41	195.15	196.4
C-4	150.15	150.05	142.36	142.26	150.32	150.72	147.33	38.66	35.9
C-5	139.10	140.17	147.54	148.17	140.76	147.58	142.60	43.23	42.1
C-6	157.66	156.75	155.95	155.69	153.25	155.07	156.83	29.46	30.9
C-7	152.01	151.16	147.50	147.28	143.37	155.58	150.30	35.78	37.8
C-1'	-17.68	-17.21	-17.44	-15.73	-17.17	-16.31	-17.46	198.10	198.4
C-2'	114.89	115.47	116.35	116.73	114.21	114.96	115.51	69.44	67.5
C-3'	147.94	146.46	148.10	145.24	149.20	146.31	147.75	38.24	37.7
C-4'	107.94	107.65	113.77	110.94	107.51	108.08	109.99	74.78	74.3
C-5'	130.93	133.80	134.99	133.53	130.52	133.10	132.78	52.73	53.8
$\underline{C}H_3$-4	168.34	168.14	171.32	170.61	166.40	172.84	169.52	17.18	17.8
$\underline{C}H_3$-6	169.89	170.58	165.98	165.89	171.32	166.79	168.48	18.19	20.2
H-4	27.82	27.78	28.99	28.95	27.64	27.83	28.24	3.56	3.79
H-5a	30.14	30.09	29.08	28.98	29.91	30.31	29.75	1.99	1.56
H-5b	30.58	30.62	31.01	31.12	30.58	30.36	30.74	0.96	1.37
H-6	30.48	30.57	30.52	30.64	30.44	29.77	30.49	1.23	1.43
H-7a	30.43	30.40	30.62	30.66	30.50	30.78	30.51	1.20	1.35
H-7b	30.85	30.77	30.59	30.62	30.57	29.92	30.72	0.99	1.08
H-2'	27.35	27.49	27.51	27.61	27.35	27.46	27.43	4.40	4.25
H-3'a	30.10	30.09	29.50	30.19	30.18	30.22	29.90	1.84	2.11
H-3'b	29.75	29.73	29.88	29.74	29.65	29.81	29.80	1.94	1.6
H-4'	27.27	26.90	27.47	27.03	26.96	26.95	27.28	4.55	4.6
H-5'a	27.90	27.75	27.58	27.33	27.84	27.80	27.76	4.06	3.88
H-5'b	28.59	28.31	28.85	28.82	28.60	28.63	28.66	3.12	3.11
C$\underline{H}_3$-4	30.72	30.74	30.78	30.66	30.55	30.90	30.75	0.96	1.11
C$\underline{H}_3$-6	30.32	30.74	30.31	30.27	30.70	30.88	30.39	1.33	0.89

[a] The scaled chemical shifts (δs) were obtained by GIAO NMR computation at the SCRF-PW1PW91/6-311+G(2d,p) level with PCM model in MeOH using the formula $\delta_s = (\delta_u - b)/-m$, where δ_u is the unscaled chemical shift relative to TMS according to $\delta_u = \sigma_0 - \sigma^x$; σ^x is the Boltzmann averaged isotropic shielding constant, σ_0 is the shielding tensor of TMS calculated at the same level of theory used for σ^x , m and b are the slope and intercept, respectively, obtained from a linear regression calculation on a plot of δ_u against δ_{exp}. δ_{exp} are the experimental chemical shift.

Table S18. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6a** in vacuo

atom	**6a**-C1			**6a**-C2			**6a**-C3			**6a**-C4			**6a**-C5		
	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z
C	-1.46003	-1.60200	0.12618	-1.50888	-1.63761	-0.10751	-1.45632	1.63289	0.13556	-3.29184	0.34521	-0.00267	3.77690	-0.21743	0.34533
C	-0.81710	-1.31040	-1.15237	-0.68611	-1.03462	-1.15397	-0.19884	1.00358	0.52869	-2.34217	0.86211	0.97755	4.22844	0.19243	-0.97908
C	0.68855	-1.53426	-0.93000	0.76548	-1.42218	-0.82630	0.90205	1.70701	-0.28413	-2.01943	2.29967	0.53357	4.44120	1.71460	-0.89879
N	0.80045	-1.90946	0.49253	0.66248	-2.22032	0.40787	0.17127	2.66705	-1.13228	-2.77484	2.47904	-0.71555	4.03488	2.07247	0.46892
C	-0.42903	-2.04453	1.07165	-0.63491	-2.42661	0.77042	-1.15709	2.70635	-0.81724	-3.58798	1.41106	-0.96730	3.75990	0.96256	1.21605
C	1.37608	-2.70904	-1.64640	1.51346	-2.36906	-1.77983	1.89521	2.61163	0.46852	-2.53725	3.45969	1.40261	5.88253	2.25005	-0.96648
C	2.52105	-3.09292	-0.67482	2.49032	-3.12929	-0.84462	2.26003	3.67739	-0.58057	-2.73410	4.59604	0.37311	5.80453	3.54799	-0.13043
C	1.93018	-2.81711	0.73962	1.74135	-3.20737	0.52247	0.96961	3.85988	-1.42926	-3.15383	3.87990	-0.93373	4.75411	3.25062	0.96718
O	-0.64790	-2.50246	2.21392	-1.02738	-3.18167	1.68716	-1.98029	3.54471	-1.24330	-4.46511	1.35749	-1.85495	3.55545	0.94702	2.44857
O	-1.29969	-0.94497	-2.21845	-1.00627	-0.34458	-2.11543	0.01610	0.09911	1.32884	-1.85226	0.33300	1.96882	4.41882	-0.46691	-1.99521
H	1.21761	-0.59389	-1.12863	1.33700	-0.50484	-0.64078	1.44249	0.96701	-0.88455	-0.94084	2.39502	0.36193	3.80757	2.21099	-1.64314
C	-2.79213	-1.59050	0.49775	-2.87433	-1.60955	0.10421	-2.75090	1.42972	0.57805	-3.94382	-0.87164	-0.07978	3.46179	-1.46669	0.84984
C	-3.94110	-1.20630	-0.39434	-3.86797	-0.85173	-0.73422	-3.16933	0.39789	1.58882	-3.75584	-2.01811	0.87514	3.52191	-2.75181	0.07117
C	-4.76861	-0.04638	0.21660	-4.63831	0.19456	0.11385	-4.34433	-0.46930	1.07331	-3.33961	-3.31125	0.12986	2.24066	-3.61683	0.20237
C	-4.02665	1.29250	0.42204	-3.78116	1.29385	0.77687	-4.11848	-1.23953	-0.24579	-2.00897	-3.26200	-0.65250	0.97356	-3.16411	-0.56306
C	-3.63984	1.94121	-0.92538	-3.15337	2.25872	-0.25526	-2.96078	-2.25458	-0.13932	-0.79363	-3.08584	0.28318	0.33599	-1.88451	0.01829
C	-2.72498	3.17805	-0.85184	-1.88679	2.96981	0.24435	-2.58603	-2.94692	-1.46055	0.54540	-2.83534	-0.42725	-1.08801	-1.59192	-0.47986
C	-1.36241	2.91289	-0.19182	-1.25131	3.90240	-0.80241	-1.31409	-3.81129	-1.38291	1.69978	-2.56122	0.54687	-1.71384	-0.36562	0.20246
C	-0.33528	4.02476	-0.44973	0.22298	4.25186	-0.51981	-0.01436	-3.01636	-1.18724	3.04334	-2.30571	-0.14996	-3.10488	0.03253	-0.32209
C	0.99003	3.86379	0.31522	1.16594	3.06168	-0.74549	1.24617	-3.89321	-1.21575	4.19054	-2.02410	0.83126	-4.21739	-0.98463	-0.02251
C	1.70651	2.52741	0.06624	2.64937	3.35457	-0.47809	2.56093	-3.11674	-1.02535	5.57960	-1.87524	0.18257	-5.60804	-0.59268	-0.55279
C	3.12045	2.48972	0.65920	3.54728	2.10885	-0.64063	2.76890	-2.57576	0.39792	5.74197	-0.71169	-0.81070	-6.21836	0.64201	0.12442
C	-4.83595	-2.44146	-0.64697	-4.84749	-1.83733	-1.40940	-3.55268	1.10167	2.91209	-5.05916	-2.24512	1.67539	4.75796	-3.55079	0.55727
C	-4.88742	2.23295	1.28177	-4.61796	2.05177	1.82121	-5.43769	-1.90414	-0.67517	-1.88782	-4.52251	-1.52609	1.22065	-3.06643	-2.07918
O	-3.12516	-1.95995	1.72555	-3.38853	-2.29559	1.11521	-3.72267	2.20277	0.11715	-4.82541	-1.07483	-1.04713	3.13196	-1.58417	2.12641
O	3.72502	-2.38258	-0.91678	3.76988	-2.52454	-0.74479	3.34206	3.15213	-1.35685	-1.51002	5.28165	0.08961	5.29940	4.64874	-0.89313
C	3.74177	1.09545	0.67019	3.72234	1.27250	0.62622	4.07497	-1.79755	0.54570	5.55878	0.67762	-0.19962	-7.62048	0.97537	-0.38377
O	3.72145	0.44175	-0.60942	2.47462	0.90269	1.12867	3.91247	-0.55994	-0.12333	6.39312	0.94288	0.92034	-8.56714	-0.07499	-0.24179
C	4.46388	1.08129	-1.65583	2.50306	0.35723	2.44919	5.12945	0.15136	-0.34253	7.79878	0.87712	0.68680	-8.80262	-0.53223	1.08864
O	5.04456	1.21017	1.17603	4.44521	0.06118	0.35855	4.50104	-1.62146	1.88770	5.75408	1.61299	-1.24081	-8.03436	2.15356	0.27675
C	5.65599	-0.02707	1.54343	5.86583	0.16768	0.35840	3.55879	-1.01612	2.77330	5.36728	2.94357	-0.91220	-9.21250	2.74432	-0.26332
H	1.75684	-2.45484	-2.63706	2.04617	-1.85421	-2.58136	2.77734	2.07621	0.82109	-1.85313	3.73514	2.20931	6.23136	2.42608	-1.98731
H	0.67288	-3.54505	-1.74648	0.80469	-3.07380	-2.23162	1.40027	3.08755	1.32298	-3.50250	3.19042	1.84909	6.56834	1.53987	-0.48806
H	2.79048	-4.14700	-0.78151	2.69241	-4.13292	-1.22765	2.56356	4.62316	-0.11360	-3.49843	5.31385	0.69707	6.77546	3.81123	0.30836
H	1.56338	-3.72320	1.23322	1.30890	-4.19374	0.71890	0.40177	4.75475	-1.15284	-4.22886	3.93910	-1.12807	5.20328	3.01861	1.93747
H	2.68845	-2.36388	1.38492	2.42995	-2.96945	1.33918	1.21326	3.92628	-2.49534	-2.61896	4.32098	-1.77913	4.09353	4.11407	1.08316
H	-3.50849	-0.89650	-1.34798	-3.29479	-0.34639	-1.51471	-2.29454	-0.22659	1.78185	-2.97270	-1.71975	1.57529	3.68786	-2.48140	-0.97402
H	-5.63080	0.12195	-0.44360	-5.38068	0.66633	-0.54485	-4.58654	-1.18826	1.86834	-3.28159	-4.11344	0.87857	2.50857	-4.61539	-0.16603
H	-5.17366	-0.38472	1.17784	-5.20272	-0.33961	0.88794	-5.22339	0.17615	0.95890	-4.14901	-3.58485	-0.55746	2.00167	-3.73476	1.26611
H	-3.10553	1.08100	0.98355	-2.95745	0.79798	1.31255	-3.84965	-0.50799	-1.02323	-2.04160	-2.39336	-1.32824	0.24661	-3.97608	-0.40465
H	-3.13667	1.19799	-1.55542	-2.88079	1.70802	-1.16315	-2.07540	-1.74279	0.25166	-0.97566	-2.24564	0.96421	0.31098	-1.97106	1.11328
H	-4.56617	2.21423	-1.45254	-3.90894	2.99881	-0.55965	-3.22549	-3.01982	0.60706	-0.70657	-3.98147	0.91768	0.97317	-1.01810	-0.20622
H	-3.22868	4.00581	-0.33494	-1.16389	2.19666	0.53359	-2.44982	-2.18367	-2.24157	0.43655	-1.97774	-1.10778	-1.71298	-2.47877	-0.30760

H	-2.55542	3.52722	-1.87975	-2.09899	3.54379	1.15690	-3.41742	-3.57952	-1.79434	0.80953	-3.69435	-1.05780	-1.08090	-1.42560	-1.56548
H	-1.48879	2.78379	0.89235	-1.31167	3.42709	-1.79169	-1.42052	-4.54316	-0.56850	1.44526	-1.69609	1.17550	-1.77332	-0.54357	1.28624
H	-0.97115	1.96017	-0.57103	-1.84331	4.82483	-0.87022	-1.23250	-4.39826	-2.30847	1.80510	-3.41445	1.23287	-1.03540	0.48914	0.07451
H	-0.12590	4.06989	-1.52846	0.52809	5.08462	-1.16885	0.06362	-2.25993	-1.98283	3.30331	-3.17782	-0.76856	-3.37079	1.00274	0.11590
H	-0.77726	4.99548	-0.18543	0.32465	4.61563	0.51371	-0.05546	-2.46265	-0.24282	2.92681	-1.46394	-0.84637	-3.04834	0.19386	-1.40922
H	0.80498	3.97297	1.39367	1.05786	2.71880	-1.78453	1.28495	-4.42353	-2.17744	4.24281	-2.84909	1.55509	-4.27596	-1.14347	1.06488
H	1.65944	4.68969	0.03678	0.86239	2.22297	-0.11369	1.16810	-4.67219	-0.44278	3.95573	-1.12837	1.42178	-3.94927	-1.95551	-0.45714
H	1.11548	1.70962	0.49736	2.99407	4.13482	-1.16902	3.40235	-3.77762	-1.27666	6.32509	-1.77118	0.97999	-5.54459	-0.41817	-1.63675
H	1.75231	2.33206	-1.01324	2.77197	3.76957	0.53268	2.59889	-2.28307	-1.73813	5.82194	-2.80682	-0.34686	-6.29007	-1.44181	-0.42640
H	3.78667	3.17967	0.12738	3.14915	1.45461	-1.42594	1.93903	-1.92357	0.68941	6.73245	-0.75811	-1.27814	-6.25246	0.50601	1.21271
H	3.10120	2.82895	1.70191	4.55136	2.40751	-0.96386	2.79715	-3.41379	1.10623	5.02192	-0.79789	-1.63143	-5.60277	1.52992	-0.05292
H	-4.26471	-3.26347	-1.09007	-4.31484	-2.56986	-2.02434	-2.71743	1.68834	3.30735	-4.90359	-3.04481	2.40621	5.67391	-2.95687	0.47709
H	-5.28879	-2.79766	0.28313	-5.43966	-2.37789	-0.66506	-4.40911	1.76789	2.77022	-5.35422	-1.34307	2.22098	4.63815	-3.86355	1.59915
H	-5.63748	-2.17494	-1.34291	-5.53133	-1.28434	-2.06098	-3.82010	0.34945	3.66086	-5.88216	-2.53465	1.01516	4.88044	-4.44467	-0.06188
H	-5.13208	1.77289	2.24561	-4.97720	1.37912	2.60814	-6.24464	-1.16618	-0.74506	-2.75049	-4.62194	-2.19424	1.69824	-3.97758	-2.45862
H	-5.83192	2.46961	0.77481	-5.49470	2.51722	1.35272	-5.74475	-2.66704	0.05221	-1.84228	-5.42523	-0.90289	1.86969	-2.22067	-2.33295
H	-4.37663	3.17892	1.48778	-4.03846	2.84664	2.30235	-5.35162	-2.39053	-1.65124	-0.98919	-4.50314	-2.14965	0.28290	-2.93829	-2.62829
H	-2.28105	-2.25017	2.19814	-2.63219	-2.79210	1.56373	-3.30655	2.88544	-0.49893	-4.90169	-0.22070	-1.57883	3.20875	-0.67051	2.54911
H	3.60842	-1.42150	-0.77824	3.72578	-1.62096	-0.38040	3.58875	3.79255	-2.03701	-1.23631	5.77930	0.87145	5.94693	4.89136	-1.56816
H	3.14597	0.41482	1.29612	4.28469	1.83787	1.39344	4.91092	-2.35058	0.09129	4.54833	0.79794	0.21548	-7.60493	1.14520	-1.47105
H	3.95259	1.98382	-2.00956	3.10582	-0.55594	2.48958	5.64038	0.36760	0.60318	8.14550	-0.15715	0.56405	-7.96370	-1.12907	1.46988
H	5.47266	1.33908	-1.31960	2.90481	1.09180	3.16102	5.80712	-0.42716	-0.98763	8.08746	1.45967	-0.19543	-8.99070	0.30217	1.77380
H	4.52342	0.35982	-2.47266	1.47054	0.12446	2.71183	4.85962	1.08515	-0.83877	8.27326	1.30293	1.57360	-9.68991	-1.16706	1.03853
H	6.63646	0.22254	1.95249	6.22906	0.78836	-0.47044	3.11934	-0.11146	2.33982	5.52859	3.54622	-1.80836	-9.07312	2.99849	-1.32425
H	5.77550	-0.69270	0.68160	6.22821	0.58560	1.30809	2.75075	-1.70807	3.04043	4.30381	2.98645	-0.63502	-10.07828	2.07864	-0.16983
H	5.06332	-0.54020	2.31364	6.25329	-0.84550	0.23838	4.11543	-0.75528	3.67628	5.96494	3.34603	-0.08601	-9.39112	3.65967	0.30455

Table S19. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6b (6b**-C1–**6b-**C4**)** in vacuo

atom	**6b**-C1			**6b**-C2			**6b**-C3			**6b**-C4		
	x	y	z	x	y	z	x	y	z	x	y	z
C	-2.22235	-1.65958	0.38498	-2.28668	-1.64801	0.38826	-2.41491	-1.50139	0.47288	2.02258	1.60740	0.39269
C	-1.14398	-1.11401	1.19967	-1.22806	-1.14987	1.25771	-1.13983	-1.13706	1.08024	0.67895	1.22588	0.81087
C	0.11968	-1.86587	0.77347	0.04209	-1.89391	0.83323	-0.13019	-2.19599	0.60831	-0.25736	2.31251	0.26044
N	-0.35604	-2.92466	-0.13147	-0.41781	-2.91204	-0.12421	-0.92935	-3.14028	-0.18829	0.63728	3.26843	-0.41110
C	-1.66780	-2.72286	-0.46446	-1.71961	-2.68444	-0.48439	-2.20485	-2.68753	-0.36707	1.92350	2.81639	-0.43624
C	1.08618	-1.08186	-0.12989	1.02372	-1.06958	-0.01779	0.95593	-1.76059	-0.39105	-1.24207	1.93467	-0.85915
C	1.76743	-2.19099	-0.95974	1.70387	-2.12700	-0.91345	1.23570	-3.05866	-1.17933	-1.41457	3.27093	-1.61237
C	0.68939	-3.30086	-1.09701	0.64580	-3.25321	-1.08081	-0.12506	-3.79697	-1.22680	-0.03268	3.96091	-1.52005
O	-2.29399	-3.31549	-1.36829	-2.32404	-3.23577	-1.42766	-3.05326	-3.18095	-1.14028	2.86628	3.32644	-1.07890
O	-1.15275	-0.22634	2.04751	-1.25339	-0.29901	2.14127	-0.84718	-0.20132	1.81774	0.28988	0.26165	1.46390
H	0.63514	-2.28258	1.64516	0.53816	-2.34598	1.69828	0.31648	-2.69042	1.47883	-0.78692	2.78885	1.09417
C	-3.53302	-1.24896	0.23953	-3.58258	-1.20432	0.21025	-3.65442	-0.89033	0.52774	3.24862	1.00491	0.60854
C	-4.17671	-0.14103	1.02737	-4.22572	-0.09932	1.00212	-3.99542	0.29690	1.38660	3.48161	-0.18740	1.49618
C	-4.78043	0.94921	0.10798	-4.77583	1.02211	0.08623	-4.72051	1.41119	0.59486	4.35524	-1.26636	0.81583
C	-3.82014	1.68401	-0.85387	-3.77603	1.73455	-0.85214	-3.95831	2.04348	-0.58982	3.77224	-1.95068	-0.43994
C	-2.70623	2.45418	-0.10806	-2.64805	2.45971	-0.08249	-2.64952	2.72933	-0.14341	2.49497	-2.75550	-0.11494
C	-1.73509	3.22364	-1.02263	-1.63503	3.19879	-0.97669	-1.81013	3.32859	-1.28628	1.84881	-3.47293	-1.31253
C	-0.49151	3.79268	-0.31068	-0.39334	3.73778	-0.23845	-0.37762	3.72140	-0.87681	0.47421	-4.09429	-0.99966
C	0.59337	2.75281	0.01247	0.66290	2.67533	0.10559	0.54114	2.52063	-0.61096	-0.67405	-3.07826	-0.90499
C	1.85041	3.36782	0.64950	1.90554	3.26218	0.79424	1.99064	2.88959	-0.26602	-2.02317	-3.71834	-0.54233
C	2.98115	2.36583	0.95530	3.01633	2.24854	1.12997	2.84559	1.64642	0.01405	-3.23112	-2.77254	-0.65474
C	3.66678	1.79794	-0.29613	3.76912	1.69755	-0.09398	4.31483	1.94629	0.32832	-3.18186	-1.57329	0.30332
C	-5.26591	-0.73403	1.95157	-5.35588	-0.68436	1.88089	-4.86898	-0.18029	2.57276	4.14298	0.29727	2.81035
C	-4.64763	2.60028	-1.77311	-4.55832	2.68759	-1.77373	-4.89605	3.00887	-1.33492	4.86205	-2.82224	-1.08783
O	-4.31216	-1.85645	-0.64339	-4.34344	-1.76753	-0.71676	-4.65448	-1.38833	-0.18338	4.33149	1.52415	0.05125
O	2.88876	-2.74249	-0.27378	2.85659	-2.68374	-0.28788	2.14989	-3.91549	-0.48911	-2.34969	4.13211	-0.95512
C	4.81565	0.83706	-0.00538	4.97113	0.82961	0.28386	5.10818	0.69258	0.69558	-4.37018	-0.62995	0.12926
O	4.34720	-0.33620	0.68310	4.49499	-0.42872	0.76014	5.05595	-0.34430	-0.28410	-5.51024	-1.26658	0.66146
C	4.85917	-0.54070	2.00045	5.47389	-1.16832	1.50188	5.58176	-0.00927	-1.56850	-6.74505	-0.63180	0.34379
O	5.36895	0.46669	-1.23636	5.92896	0.66783	-0.74278	6.43133	1.09187	0.96922	-4.17041	0.66450	0.69242
C	6.56395	-0.30380	-1.15063	5.46431	0.11728	-1.97460	7.23206	0.09080	1.59189	-3.85394	0.69411	2.08886
H	1.80865	-0.48279	0.42335	1.74438	-0.50933	0.57847	1.85375	-1.35888	0.08332	-2.18907	1.53620	-0.48635
H	0.51256	-0.41858	-0.78859	0.46081	-0.36128	-0.63661	0.55505	-0.99412	-1.06533	-0.78457	1.19084	-1.52369
H	2.07839	-1.82110	-1.94613	1.97833	-1.70392	-1.89017	1.61049	-2.84945	-2.18964	-1.71563	3.11911	-2.65725
H	0.24908	-3.35722	-2.09609	0.21845	-3.30534	-2.08548	-0.63162	-3.70080	-2.19161	0.56222	3.84829	-2.43154
H	1.13297	-4.26903	-0.84958	1.10572	-4.21564	-0.84030	0.02735	-4.85835	-1.01330	-0.16523	5.02656	-1.31527
H	-3.39530	0.29104	1.65617	-3.45466	0.30193	1.66336	-3.05370	0.67180	1.79333	2.49826	-0.59256	1.74506
H	-5.58494	0.49245	-0.48096	-5.58505	0.60001	-0.52172	-5.67249	1.00905	0.22835	5.32081	-0.81452	0.56040
H	-5.25758	1.69199	0.76250	-5.23869	1.77274	0.74197	-4.97362	2.20336	1.31325	4.56335	-2.03873	1.56921
H	-3.33378	0.93041	-1.49283	-3.30593	0.97170	-1.49220	-3.68952	1.23775	-1.29069	3.50118	-1.16698	-1.16464
H	-3.17432	3.16664	0.58899	-3.10195	3.18483	0.61072	-2.89209	3.52515	0.57786	2.73811	-3.50485	0.65453
H	-2.13864	1.75266	0.51294	-2.11642	1.73538	0.54439	-2.03874	2.00269	0.40215	1.75714	-2.08343	0.33747
H	-2.27021	4.05326	-1.49926	-2.13653	4.04097	-1.46744	-2.31721	4.21289	-1.69045	2.51864	-4.26533	-1.66669

H	-1.40541	2.56661	-1.84196	-1.30578	2.53022	-1.78695	-1.75395	2.60532	-2.11414	1.74157	-2.76741	-2.15047
H	-0.04700	4.56835	-0.94975	0.08105	4.50575	-0.86515	0.06290	4.33611	-1.67410	0.22729	-4.82756	-1.77972
H	-0.80069	4.30209	0.61369	-0.71024	4.25110	0.68106	-0.41477	4.36158	0.01672	0.53996	-4.66258	-0.06009
H	0.19186	1.98571	0.68652	0.22580	1.90750	0.75602	0.13400	1.90982	0.20393	-0.42328	-2.30367	-0.17097
H	0.86399	2.23980	-0.92081	0.95717	2.16931	-0.82491	0.54366	1.87827	-1.50515	-0.76964	-2.56636	-1.87510
H	2.24041	4.16182	-0.00435	2.32718	4.06149	0.16673	2.43336	3.46705	-1.09086	-2.19735	-4.57945	-1.20253
H	1.56167	3.86110	1.58718	1.58870	3.74620	1.72767	2.00325	3.54947	0.61311	-1.97031	-4.12397	0.47830
H	2.57849	1.54656	1.56445	2.59532	1.41949	1.71218	2.79156	0.97191	-0.85002	-4.15199	-3.33680	-0.46746
H	3.73584	2.87080	1.57480	3.74541	2.74252	1.78696	2.40095	1.09667	0.85516	-3.29666	-2.40503	-1.69011
H	2.95182	1.26605	-0.93255	3.09437	1.12694	-0.74106	4.80172	2.45095	-0.51511	-3.15729	-1.93053	1.33977
H	4.07585	2.61733	-0.89986	4.15386	2.53590	-0.68849	4.38978	2.63263	1.18008	-2.26903	-0.99100	0.14299
H	-4.84789	-1.48866	2.62528	-4.97491	-1.45764	2.55532	-4.35774	-0.94959	3.15973	3.52822	1.05111	3.31182
H	-6.06824	-1.19695	1.36909	-6.14801	-1.12141	1.26537	-5.82163	-0.58793	2.22088	5.13087	0.72710	2.61797
H	-5.69861	0.06301	2.56437	-5.79228	0.11162	2.49241	-5.07821	0.66616	3.23430	4.26155	-0.55058	3.49217
H	-4.03507	3.06144	-2.55314	-3.91921	3.13551	-2.54000	-4.43134	3.41387	-2.23874	4.53091	-3.25577	-2.03591
H	-5.44444	2.03695	-2.27124	-5.36605	2.15647	-2.28929	-5.82003	2.50349	-1.63723	5.76326	-2.23351	-1.29170
H	-5.11971	3.40756	-1.19778	-5.01155	3.50455	-1.19699	-5.17330	3.85591	-0.69373	5.14675	-3.64901	-0.42378
H	-3.75285	-2.55057	-1.11630	-3.78367	-2.45799	-1.19294	-4.29633	-2.17172	-0.71010	4.04040	2.31468	-0.50705
H	3.50515	-2.01165	-0.08710	3.44159	-1.94438	-0.04285	3.00496	-3.46882	-0.41935	-3.20339	3.68130	-0.89757
H	5.58614	1.31035	0.62909	5.54354	1.31200	1.08783	4.67183	0.20987	1.58295	-4.53628	-0.40901	-0.93682
H	4.53110	0.24962	2.68637	5.77714	-0.60923	2.39632	6.56803	0.46045	-1.48740	-6.88523	-0.56884	-0.74526
H	5.95610	-0.58739	2.00100	6.35550	-1.38137	0.88864	4.90963	0.65902	-2.12234	-6.80073	0.37694	0.76887
H	4.46102	-1.49732	2.34507	5.00036	-2.10380	1.80558	5.67417	-0.94956	-2.11673	-7.53460	-1.25281	0.77155
H	6.38121	-1.27604	-0.67888	4.78986	0.80547	-2.49918	7.36355	-0.78293	0.94313	-2.82455	0.36503	2.27353
H	6.90701	-0.46033	-2.17462	6.35332	-0.03943	-2.58821	8.20326	0.54787	1.79099	-3.95811	1.73520	2.40240
H	7.34032	0.23600	-0.58848	4.96089	-0.84502	-1.82473	6.78389	-0.23458	2.54171	-4.54833	0.07330	2.66547

Table S20. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6b (6b**-C5–**6b-**C7**)** in vacuo

atom	**6b**-C5			**6b**-C6			**6b**-C7		
	x	y	z	x	y	z	x	y	z
C	1.76110	1.67945	0.49283	-3.48893	-0.28765	0.37846	-2.98434	-0.20401	0.33494
C	0.42367	1.16843	0.76866	-4.73766	0.43678	0.59182	-4.26394	0.43529	0.62411
C	-0.55362	2.23148	0.22968	-5.82361	-0.35378	-0.15699	-5.32317	-0.35245	-0.16489
N	0.31503	3.29851	-0.29655	-5.10047	-1.45815	-0.80023	-4.55772	-1.36491	-0.90333
C	1.63251	2.94281	-0.24232	-3.79462	-1.49174	-0.40741	-3.24408	-1.35925	-0.53612
C	-1.44879	1.89017	-0.97556	-6.88448	-1.09348	0.67765	-6.32677	-1.20869	0.62814
C	-1.64381	3.26389	-1.65953	-7.25497	-2.29157	-0.22622	-6.65395	-2.35257	-0.35884
C	-0.30388	4.01609	-1.42013	-5.94457	-2.64707	-0.96974	-5.34302	-2.58027	-1.15009
O	2.57742	3.57374	-0.76125	-2.99287	-2.41963	-0.65418	-2.40097	-2.22216	-0.86715
O	0.06404	0.13330	1.31947	-4.97323	1.46439	1.21808	-4.53892	1.39870	1.33105
H	-1.15374	2.59251	1.07748	-6.29905	0.29668	-0.90044	-5.84693	0.32652	-0.84791
C	3.01232	1.14920	0.75777	-2.19156	-0.07802	0.83257	-1.69025	0.03888	0.78191
C	3.27454	-0.10108	1.55272	-1.66950	1.06920	1.66404	-1.21046	1.14548	1.69035
C	4.27199	-1.04768	0.84386	-1.84162	2.44219	0.96911	-1.46603	2.55609	1.10520
C	3.82652	-1.62962	-0.51569	-1.15289	2.60877	-0.40415	-0.80985	2.86020	-0.26037
C	2.62514	-2.58757	-0.36422	0.38735	2.60407	-0.28775	0.72977	2.93896	-0.16257
C	1.98808	-3.04127	-1.68748	1.13785	2.51868	-1.62651	1.46262	2.96110	-1.51352
C	0.71636	-3.89359	-1.52253	2.67201	2.53452	-1.49992	2.99408	3.07356	-1.40758
C	-0.43770	-3.17223	-0.80983	3.28294	1.30159	-0.81732	3.69350	1.86861	-0.76006
C	-1.78239	-3.90614	-0.91425	4.81751	1.32008	-0.79873	5.22525	1.98297	-0.78982
C	-2.90493	-3.29114	-0.05930	5.43675	0.08956	-0.12257	5.97360	0.85755	-0.05555
C	-3.17611	-1.81343	-0.37266	6.96973	0.12548	-0.10522	5.79872	-0.53210	-0.68596
C	3.80534	0.30209	2.95072	-2.30162	1.06691	3.07390	-1.81233	1.00294	3.10623
C	5.02684	-2.30721	-1.19819	-1.67504	3.88990	-1.07774	-1.41519	4.15264	-0.83556
O	4.08852	1.79334	0.33646	-1.26621	-0.97368	0.53091	-0.72676	-0.78128	0.39627
O	-2.76829	3.98431	-1.15367	-8.21051	-1.93247	-1.22944	-7.64788	-1.96966	-1.31481
C	-4.42360	-1.25735	0.31167	7.60013	-1.07320	0.60167	6.66076	-1.60008	-0.01534
O	-4.45538	-1.42189	1.71854	7.23153	-2.33624	0.06575	6.15595	-1.80017	1.28915
C	-3.40829	-0.78623	2.45402	7.55552	-2.55524	-1.30593	6.99953	-2.57831	2.13220
O	-4.52746	0.10431	-0.07007	8.99944	-0.87868	0.58541	6.75099	-2.81523	-0.74446
C	-5.77661	0.70995	0.25210	9.72459	-1.77676	1.41989	5.51821	-3.47833	-1.02151
H	-2.40003	1.42505	-0.70790	-7.74754	-0.47201	0.92974	-7.21520	-0.65479	0.94205
H	-0.90902	1.21627	-1.65206	-6.43890	-1.45616	1.61226	-5.84351	-1.61722	1.52432
H	-1.85150	3.15923	-2.72655	-7.62636	-3.14447	0.35610	-6.96825	-3.26582	0.16238
H	0.36539	3.97927	-2.28608	-5.43495	-3.51764	-0.54634	-4.78044	-3.45257	-0.80447
H	-0.49468	5.06668	-1.18185	-6.16399	-2.84535	-2.02223	-5.57433	-2.70853	-2.21086
H	2.30992	-0.59487	1.68946	-0.60172	0.85705	1.77833	-0.13113	0.98137	1.77021
H	5.21855	-0.51085	0.71155	-2.91257	2.64495	0.87142	-2.54753	2.70884	1.03753
H	4.47925	-1.87843	1.53249	-1.44574	3.20186	1.65810	-1.09798	3.28160	1.84454
H	3.50927	-0.79292	-1.15763	-1.44412	1.75822	-1.04000	-1.06088	2.04095	-0.95203
H	2.94780	-3.47244	0.20656	0.70105	3.51482	0.24621	0.99882	3.83919	0.41196
H	1.85602	-2.09653	0.24088	0.69630	1.76020	0.33917	1.09657	2.08520	0.41804
H	2.71614	-3.61152	-2.27731	0.84018	3.35621	-2.26889	1.09954	3.80265	-2.11604

H	1.73961	-2.15145	-2.28565	0.82949	1.60368	-2.15340	1.20665	2.05014	-2.07436
H	0.37893	-4.20625	-2.52080	3.10277	2.62454	-2.50692	3.40244	3.21259	-2.41843
H	0.95984	-4.81961	-0.98141	2.98044	3.44041	-0.95722	3.25252	3.98564	-0.84938
H	-0.19280	-3.02564	0.24984	2.91642	1.22064	0.21453	3.36808	1.75845	0.28305
H	-0.53710	-2.16509	-1.23618	2.93742	0.39503	-1.33548	3.37455	0.95415	-1.27858
H	-2.09786	-3.93112	-1.96787	5.19130	1.39370	-1.83059	5.56540	2.02576	-1.83518
H	-1.64719	-4.95414	-0.61260	5.16291	2.22964	-0.28579	5.51386	2.94256	-0.33853
H	-2.65422	-3.39780	1.00352	5.09392	-0.82080	-0.63026	5.64764	0.81935	0.99096
H	-3.82588	-3.87035	-0.21123	5.06378	0.01655	0.90909	7.04447	1.10492	-0.03718
H	-2.31588	-1.19525	-0.09729	7.36720	0.19250	-1.12538	4.74954	-0.84136	-0.63385
H	-3.32403	-1.68077	-1.45226	7.31959	1.02415	0.41677	6.08128	-0.49876	-1.74625
H	3.10115	0.95862	3.47117	-2.16521	0.09854	3.56663	-1.61624	0.00852	3.52073
H	4.76742	0.81762	2.87220	-3.36811	1.29817	3.02773	-2.89000	1.18063	3.09609
H	3.94327	-0.59641	3.56009	-1.81003	1.82840	3.68824	-1.34753	1.74033	3.76890
H	4.77209	-2.68677	-2.19213	-1.25634	4.02900	-2.07891	-1.01313	4.39062	-1.82491
H	5.85939	-1.60495	-1.31677	-2.76573	3.86434	-1.17613	-2.50301	4.06733	-0.93224
H	5.38702	-3.15436	-0.59995	-1.41607	4.77464	-0.48167	-1.20623	5.00530	-0.17648
H	3.78002	2.60674	-0.17776	-1.71313	-1.72717	0.01540	-1.14568	-1.51575	-0.16789
H	-2.69565	4.07585	-0.19361	-9.05809	-1.74049	-0.80688	-8.49499	-1.85521	-0.86411
H	-5.32050	-1.80100	-0.02148	7.24624	-1.13607	1.64190	7.70896	-1.26889	0.04162
H	-3.39507	0.29541	2.27674	8.59806	-2.29371	-1.52001	7.98906	-2.10999	2.23744
H	-2.42017	-1.19174	2.21134	6.89682	-1.98822	-1.97668	7.12863	-3.59578	1.74562
H	-3.62646	-0.97694	3.50682	7.40482	-3.62172	-1.48656	6.51472	-2.61668	3.10989
H	-5.94910	0.72704	1.33450	9.60453	-2.81682	1.09542	4.94534	-2.96189	-1.80223
H	-5.73714	1.73153	-0.13166	10.77564	-1.48959	1.34834	5.78383	-4.47445	-1.38211
H	-6.60706	0.17498	-0.23072	9.39695	-1.69146	2.46631	4.89997	-3.57139	-0.12123

Table S21. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6c (6c**-C1–**6c-**C5**)** in vacuo

atom	**6c**-C1			**6c**-C2			**6c**-C3			**6c**-C4			**6c**-C5		
	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z
C	2.60601	0.58655	-0.06877	2.00681	-1.61471	0.48357	0.11086	-2.27853	0.61529	2.04271	-1.61950	0.45023	2.00525	-1.70699	0.22592
C	2.07342	1.33065	1.06983	2.14493	-2.07423	-0.89654	-0.30358	-3.11047	-0.51216	1.80536	-2.30610	-0.81636	1.48863	-2.08528	-1.08588
C	1.73378	2.73337	0.53836	0.87024	-2.87766	-1.20391	-1.83533	-2.99785	-0.57876	0.41500	-2.95322	-0.69193	0.11565	-2.72888	-0.82847
N	2.09215	2.68006	-0.89036	0.09547	-2.83533	0.04886	-2.18774	-2.10659	0.54013	-0.01559	-2.63768	0.68173	-0.03172	-2.70841	0.63765
C	2.49737	1.43302	-1.26322	0.69735	-2.04870	0.98615	-1.07972	-1.61627	1.16265	0.85638	-1.78530	1.29477	0.99297	-2.0325	1.23495
C	0.26284	3.18437	0.50315	-0.12241	-2.31243	-2.23501	-2.47709	-2.28968	-1.78449	-0.73281	-2.37688	-1.54165	-1.14476	-1.98371	-1.3019
C	0.24050	4.15835	-0.68648	-1.46994	-2.86859	-1.74414	-3.77982	-1.72867	-1.18832	-1.97749	-2.65231	-0.67911	-2.21112	-2.43885	-0.29051
C	1.24510	3.55589	-1.70662	-1.35379	-2.86779	-0.19657	-3.41219	-1.34140	0.27014	-1.47518	-2.53006	0.78773	-1.43691	-2.60409	1.04692
O	2.71134	1.05673	-2.43633	0.20078	-1.71376	2.08474	-1.06639	-0.72066	2.03744	0.66098	-1.20473	2.38575	1.04872	-1.71118	2.44207
O	1.90357	0.98429	2.23425	3.05285	-1.90513	-1.70226	0.36385	-3.79082	-1.28260	2.51157	-2.39511	-1.81406	1.98325	-1.95878	-2.20034
H	2.34927	3.47087	1.06782	1.14597	-3.90698	-1.46175	-2.27425	-3.99343	-0.44221	0.50109	-4.03564	-0.84101	0.12072	-3.75648	-1.21023
C	3.08115	-0.70779	-0.17172	2.82214	-0.80784	1.25468	1.36510	-2.01487	1.13225	3.09287	-0.82172	0.86747	3.18273	-1.07936	0.58975
C	3.27592	-1.66185	0.97601	4.15116	-0.24533	0.82569	2.64650	-2.64347	0.65583	4.36956	-0.60272	0.10244	4.30994	-0.76453	-0.35422
C	2.50598	-2.98654	0.74694	4.10241	1.30602	0.80204	3.75253	-1.59147	0.40092	4.80456	0.88298	0.01738	4.93663	0.63745	-0.16077
C	0.96850	-2.86980	0.69689	3.12793	1.91680	-0.22879	3.41224	-0.46867	-0.59923	4.11669	1.73733	-1.07127	4.1737	1.83952	-0.76423
C	0.34461	-4.20398	0.22504	2.79669	3.37902	0.14103	4.57744	0.54663	-0.69497	2.60389	1.98053	-0.85539	2.89424	2.19437	0.02594
C	-1.11953	-4.10957	-0.24628	1.67336	4.04153	-0.68107	4.14038	1.96161	-1.12370	2.21617	2.85490	0.35033	2.03261	3.30382	-0.59997
C	-1.27924	-3.48584	-1.64340	0.35092	3.26032	-0.65604	3.59220	2.79915	0.04591	0.70712	2.85407	0.65719	0.8142	3.72119	0.24302
C	-2.73890	-3.23676	-2.06700	-0.84900	4.02547	-1.23472	2.88120	4.10001	-0.37192	-0.17354	3.46804	-0.44274	-0.32856	2.69715	0.32465
C	-3.46110	-2.09301	-1.32830	-2.09462	3.14704	-1.45490	1.48331	3.91469	-0.99359	-1.67132	3.53554	-0.09596	-1.50791	3.21588	1.16246
C	-2.87979	-0.69908	-1.61800	-2.62533	2.46808	-0.18378	0.42514	3.39639	-0.00836	-2.35642	2.16570	0.02583	-2.71718	2.27188	1.27067
C	-3.67674	0.46947	-1.01553	-3.81701	1.53693	-0.44341	-0.95480	3.20266	-0.65112	-3.86612	2.27553	0.27152	-3.46668	2.05504	-0.05395
C	4.78705	-1.93098	1.16509	5.26749	-0.75042	1.76563	3.11667	-3.68862	1.69591	5.47442	-1.45670	0.77703	5.38689	-1.86767	-0.17647
C	0.39163	-2.43222	2.05474	3.66750	1.79084	-1.66352	3.05163	-1.01617	-1.99132	4.88309	3.05859	-1.26164	5.13705	3.03725	-0.86351
O	3.43731	-1.17329	-1.36004	2.43153	-0.47077	2.47555	1.48424	-1.17213	2.14915	3.02698	-0.23496	2.05317	3.39562	-0.78768	1.86379
O	0.68030	5.42858	-0.19374	-1.58760	-4.19171	-2.27773	-4.74406	-2.78604	-1.24151	-2.40773	-3.98520	-0.98541	-2.72202	-3.69035	-0.77016
C	-3.65661	0.56246	0.50916	-4.26006	0.76707	0.79882	-1.97591	2.60813	0.31704	-4.55275	0.92501	0.46533	-4.82389	1.37986	0.13265
O	-2.33384	0.75850	0.91972	-5.41202	-0.03718	0.54596	-2.28168	3.59034	1.27974	-5.91680	1.17825	0.71351	-5.66469	1.43059	-1.00689
C	-2.14254	0.72659	2.33527	-6.65400	0.62779	0.71228	-2.98813	3.09996	2.41823	-6.65146	0.05080	1.18085	-5.14699	0.86026	-2.20813
O	-4.43617	1.66983	0.96159	-3.21408	-0.07747	1.17984	-3.15080	2.10670	-0.32446	-4.36923	0.00899	-0.61294	-4.59844	0.04784	0.56391
C	-5.80356	1.38154	1.20431	-3.35975	-0.67491	2.46930	-3.90913	3.05845	-1.07053	-4.85798	0.43858	-1.88500	-5.77012	-0.60857	1.04323
H	-0.40031	2.33526	0.30697	-0.13162	-1.21766	-2.18806	-1.83740	-1.46688	-2.12287	-0.59897	-1.29636	-1.66658	-0.99254	-0.90134	-1.2214
H	-0.06108	3.67626	1.42168	0.09129	-2.62099	-3.25947	-2.67431	-2.95505	-2.62638	-0.81840	-2.83756	-2.52702	-1.43379	-2.2248	-2.32605
H	-0.76252	4.25047	-1.12143	-2.31617	-2.25362	-2.07441	-4.14511	-0.85667	-1.74408	-2.78424	-1.93764	-0.87376	-3.02213	-1.70975	-0.18803
H	0.75103	2.96457	-2.48555	-1.82717	-1.98746	0.24945	-3.21855	-0.26968	0.37087	-1.73550	-1.56980	1.24432	-1.56086	-1.74377	1.71293
H	1.82965	4.34334	-2.19457	-1.81385	-3.76592	0.22978	-4.21643	-1.61843	0.96079	-1.89237	-3.33114	1.40714	-1.76779	-3.50171	1.58059
H	2.90023	-1.16101	1.87098	4.34300	-0.62281	-0.18153	2.41072	-3.17270	-0.27032	4.20638	-0.99645	-0.90531	3.90716	-0.85142	-1.36784
H	2.86880	-3.43651	-0.18474	3.84051	1.65242	1.80902	4.02904	-1.13828	1.36036	4.70339	1.35201	1.00302	5.12422	0.81319	0.90612
H	2.78540	-3.67418	1.55730	5.11993	1.66764	0.60065	4.63864	-2.13456	0.04328	5.87916	0.87909	-0.20405	5.92205	0.59726	-0.64078
H	0.71522	-2.09865	-0.04513	2.19142	1.34593	-0.16999	2.53638	0.06824	-0.20621	4.20296	1.17455	-2.01271	3.87427	1.56381	-1.78742
H	0.41805	-4.92978	1.04764	3.71054	3.98565	0.05865	5.32427	0.15412	-1.39875	2.09457	1.01179	-0.77005	3.18423	2.49423	1.04434
H	0.94739	-4.61461	-0.59727	2.50492	3.40793	1.20040	5.08581	0.61958	0.27662	2.21212	2.43680	-1.77375	2.27951	1.29411	0.13773
H	-1.70610	-3.54539	0.48920	1.99255	4.18610	-1.72183	3.38902	1.88370	-1.92042	2.54726	3.88857	0.18231	1.69612	2.98567	-1.59789

H	-1.55590	-5.11764	-0.26505	1.50455	5.04939	-0.27694	4.99123	2.49551	-1.56739	2.74378	2.50330	1.24504	2.64807	4.1969	-0.75751
H	-0.71653	-2.54619	-1.70220	0.46904	2.32305	-1.21697	2.91175	2.18752	0.65188	0.39175	1.82193	0.85918	1.15117	3.96767	1.26063
H	-0.81064	-4.15739	-2.37575	0.13562	2.96755	0.38000	4.43087	3.04933	0.70965	0.53768	3.40996	1.59028	0.4076	4.65347	-0.17318
H	-2.76323	-3.02129	-3.14437	-1.10029	4.86610	-0.57172	2.78533	4.75281	0.50660	0.18545	4.48565	-0.65216	-0.6631	2.46062	-0.69523
H	-3.31096	-4.16530	-1.93055	-0.56250	4.47201	-2.19706	3.52047	4.64148	-1.08322	-0.05430	2.90516	-1.37852	0.03306	1.75604	0.7607
H	-4.51925	-2.10290	-1.62660	-2.89125	3.75629	-1.90434	1.14801	4.88004	-1.39711	-1.80363	4.09320	0.84264	-1.14425	3.43155	2.17628
H	-3.45169	-2.28816	-0.24815	-1.85054	2.37125	-2.19579	1.54425	3.23479	-1.85500	-2.18673	4.11910	-0.87160	-1.84414	4.17922	0.75106
H	-1.84628	-0.63602	-1.26200	-1.83098	1.87847	0.28322	0.75050	2.43860	0.41810	-2.17341	1.58769	-0.88978	-2.40115	1.30314	1.67638
H	-2.84160	-0.55811	-2.70706	-2.91170	3.23914	0.54722	0.33446	4.09420	0.83303	-1.90149	1.59314	0.84433	-3.41759	2.69543	2.00403
H	-3.28670	1.42314	-1.39019	-4.67299	2.10941	-0.82261	-1.32780	4.16268	-1.02799	-4.05800	2.86119	1.17838	-3.65471	3.02397	-0.53429
H	-4.72510	0.40811	-1.33526	-3.56366	0.79546	-1.21149	-0.87441	2.52171	-1.50824	-4.35534	2.81568	-0.54821	-2.85855	1.46228	-0.74582
H	5.34018	-1.00111	1.33160	5.30702	-1.84429	1.78655	2.35968	-4.46340	1.85188	5.17870	-2.50797	0.84836	4.96135	-2.86618	-0.3148
H	5.21097	-2.43244	0.28996	5.11553	-0.39235	2.78815	3.33437	-3.21595	2.65870	5.69286	-1.08902	1.78453	5.8378	-1.81704	0.8197
H	4.93607	-2.57336	2.03858	6.23618	-0.38477	1.41104	4.02871	-4.17536	1.33625	6.39071	-1.40254	0.18141	6.17593	-1.72961	-0.92187
H	0.65677	-3.15956	2.83353	4.59454	2.36800	-1.77717	3.87714	-1.61846	-2.39227	4.92181	3.64120	-0.33413	5.45935	3.36218	0.13432
H	-0.70023	-2.36505	2.02348	2.95036	2.17056	-2.39865	2.86454	-0.20219	-2.70011	4.40903	3.68311	-2.02768	4.68057	3.8966	-1.36243
H	0.76648	-1.45287	2.36477	3.87857	0.75041	-1.92774	2.15931	-1.64876	-1.97524	5.91601	2.87147	-1.57602	6.03495	2.77002	-1.43171
H	3.24517	-0.45306	-2.04206	1.51164	-0.86094	2.62061	0.56586	-0.80968	2.35385	2.12887	-0.46365	2.45751	2.57229	-1.05992	2.38114
H	0.66412	6.07506	-0.91146	-2.42378	-4.57945	-1.98796	-5.57758	-2.47849	-0.86196	-3.23777	-4.16366	-0.52476	-3.4206	-3.9978	-0.17821
H	-4.06050	-0.35272	0.98208	-4.50100	1.46130	1.62827	-1.56768	1.71623	0.81259	-4.11151	0.38855	1.31906	-5.40914	1.91248	0.89679
H	-2.66591	1.55621	2.82113	-6.74842	1.05755	1.72113	-3.99372	2.75583	2.14831	-7.66508	0.40151	1.38410	-4.76364	-0.15315	-2.04137
H	-2.50172	-0.22497	2.75309	-6.80040	1.42830	-0.02681	-2.44332	2.27250	2.89174	-6.68402	-0.74918	0.43194	-5.98427	0.81633	-2.90755
H	-1.06883	0.81067	2.50962	-7.43417	-0.12341	0.57176	-3.06549	3.93394	3.11873	-6.21366	-0.34538	2.10856	-4.3549	1.48132	-2.64478
H	-6.24803	2.29076	1.61476	-2.43138	-1.21428	2.66474	-4.86249	2.57829	-1.30332	-5.88562	0.81079	-1.81311	-5.4607	-1.59899	1.38469
H	-6.34184	1.11185	0.28439	-3.49767	0.09796	3.23911	-4.09541	3.96685	-0.48690	-4.22140	1.21774	-2.32284	-6.20702	-0.05995	1.88936
H	-5.92016	0.56515	1.93310	-4.21170	-1.36330	2.49092	-3.41045	3.32782	-2.01036	-4.83555	-0.43983	-2.53365	-6.52533	-0.70971	0.25597

Table S22. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6c (6c**-C6–**6c-**C9**)** in vacuo

atom	**6c**-C6			**6c**-C7			**6c**-C8			**6c**-C9		
	x	y	z	x	y	z	x	y	z	x	y	z
C	-1.41717	-2.10755	-0.09610	2.21247	0.29746	0.98055	2.78263	-0.31453	0.37840	4.35551	0.48009	0.53224
C	-0.98986	-1.81153	1.26974	3.45238	0.65766	0.29836	2.86182	0.00625	-1.04431	5.06176	0.43602	-0.74337
C	0.34098	-2.55572	1.46767	4.07996	-0.66933	-0.16266	2.80288	1.53965	-1.14277	6.05655	-0.73539	-0.63301
N	0.56771	-3.24850	0.18654	3.16144	-1.70472	0.33596	2.64642	1.99296	0.24845	5.87763	-1.24754	0.73613
C	-0.37527	-2.91386	-0.74145	2.04405	-1.15807	0.89431	2.74665	0.94996	1.12403	4.83522	-0.62577	1.36748
C	1.63111	-1.73414	1.63890	4.12518	-0.96730	-1.67169	4.06651	2.28946	-1.60203	5.81756	-1.98592	-1.49759
C	2.70540	-2.67058	1.06191	4.05755	-2.51127	-1.71608	3.93281	3.64513	-0.88726	6.41974	-3.12399	-0.63956
C	1.99553	-3.40981	-0.10651	3.17137	-2.90459	-0.50920	3.26181	3.30611	0.47318	6.14999	-2.68894	0.82939
O	-0.34184	-3.21345	-1.95480	1.02183	-1.78741	1.24535	2.82583	1.06361	2.36754	4.34635	-0.96700	2.46423
O	-1.52430	-1.13117	2.13817	3.95873	1.75467	0.09409	2.95577	-0.72291	-2.02495	4.95651	1.14150	-1.73931
H	0.23028	-3.27451	2.28826	5.07566	-0.77582	0.28367	1.94025	1.82957	-1.75352	7.07019	-0.33712	-0.78072
C	-2.53207	-1.70106	-0.80493	1.23443	1.08285	1.56149	2.81543	-1.51878	1.07290	3.33629	1.30365	0.97645
C	-3.63764	-0.84874	-0.25194	1.28809	2.57945	1.69906	2.86413	-2.91834	0.50858	2.77372	2.47441	0.21839
C	-3.70500	0.50265	-1.02054	0.03804	3.25080	1.07748	1.64202	-3.24707	-0.38364	1.23547	2.37479	0.06950
C	-4.34821	1.65813	-0.22071	-0.18517	3.01073	-0.43088	0.25655	-3.11481	0.28489	0.71693	1.16122	-0.73135
C	-3.48109	2.13582	0.97062	-1.58266	3.53356	-0.83280	-0.84776	-3.23376	-0.78741	-0.80712	0.96667	-0.54021
C	-2.14715	2.81313	0.61316	-2.03272	3.23888	-2.27742	-2.26645	-2.89105	-0.30842	-1.70851	2.11211	-1.03150
C	-1.25048	3.02594	1.84235	-2.14838	1.74996	-2.65418	-3.29146	-2.87301	-1.45204	-3.21537	1.81363	-0.92245
C	0.06681	3.76788	1.55835	-3.26566	0.98393	-1.92912	-4.74282	-2.60629	-1.01189	-3.74082	1.68649	0.51668
C	0.98616	3.07671	0.53853	-3.29176	-0.51046	-2.28421	-5.00077	-1.25419	-0.32046	-5.27050	1.56539	0.62865
C	2.37611	3.72582	0.46247	-4.52021	-1.28569	-1.77373	-4.69237	-0.02976	-1.19680	-5.85684	0.27345	0.04003
C	3.30559	3.22348	-0.65616	-4.75695	-1.27124	-0.25365	-5.11832	1.31854	-0.58985	-7.37257	0.16654	0.24764
C	-4.97992	-1.61004	-0.30217	1.42668	2.95451	3.19308	4.19347	-3.17215	-0.23697	3.17277	3.78453	0.93807
C	-4.71907	2.81395	-1.16622	0.93121	3.63889	-1.28260	0.06428	-4.12856	1.42563	1.11856	1.22423	-2.21599
O	-2.66611	-2.06251	-2.07325	0.15485	0.50148	2.06583	2.80946	-1.48375	2.39552	2.80727	1.09212	2.17127
O	3.08477	-3.56876	2.11057	5.33778	-3.11105	-1.49567	3.09576	4.46275	-1.70916	7.80588	-3.34177	-0.90023
C	3.81774	1.78982	-0.49489	-3.62872	-1.85498	0.59442	-4.34784	1.72229	0.66751	-7.98584	-1.08849	-0.37106
O	2.85355	0.76326	-0.71342	-3.97654	-1.84858	1.98039	-3.00009	1.92589	0.29569	-7.42316	-2.30924	0.08972
C	2.26287	0.72089	-2.01469	-3.67251	-0.64855	2.67199	-2.10479	2.07817	1.39375	-7.52095	-2.55584	1.49123
O	4.92734	1.65019	-1.35936	-3.42315	-3.17733	0.19786	-4.89521	2.85239	1.33398	-9.37864	-1.02771	-0.14417
C	5.68084	0.45885	-1.16603	-2.31949	-3.82241	0.83344	-4.99124	4.05443	0.57222	-10.13309	-1.99191	-0.87228
H	1.58924	-0.81774	1.04086	3.24249	-0.54136	-2.16447	4.96309	1.76719	-1.24888	4.73986	-2.14448	-1.62399
H	1.84416	-1.47446	2.67716	5.01620	-0.56998	-2.16438	4.13211	2.41130	-2.68418	6.27775	-1.93413	-2.48595
H	3.58004	-2.11353	0.70529	3.63011	-2.87536	-2.65895	4.90577	4.13127	-0.73982	5.95207	-4.08619	-0.85881
H	2.22036	-2.96775	-1.08311	2.14597	-3.15566	-0.79625	3.98275	3.23524	1.29486	5.28413	-3.19301	1.27086
H	2.28443	-4.46619	-0.13500	3.61334	-3.76252	0.00441	2.51488	4.06189	0.73901	7.02154	-2.90297	1.45564
H	-3.37875	-0.65774	0.79175	2.18879	2.91159	1.17811	2.84743	-3.56805	1.38944	3.24455	2.46819	-0.76735
H	-2.69627	0.80232	-1.32918	-0.84505	2.91076	1.63170	1.68514	-2.61216	-1.27392	0.79135	2.36566	1.07244
H	-4.26510	0.34282	-1.94988	0.12432	4.33106	1.25866	1.77138	-4.28142	-0.73262	0.90139	3.30130	-0.41398
H	-5.28752	1.28234	0.21066	-0.17203	1.92421	-0.59985	0.18005	-2.10330	0.71355	1.18375	0.25993	-0.30611
H	-3.27107	1.28372	1.62905	-1.60164	4.62279	-0.68039	-0.83755	-4.25338	-1.20211	-0.99481	0.78701	0.52625
H	-4.08128	2.83448	1.57037	-2.32283	3.12212	-0.13408	-0.59314	-2.56473	-1.62101	-1.10139	0.04393	-1.06120
H	-2.33275	3.78130	0.12749	-1.34698	3.72885	-2.97968	-2.24350	-1.90969	0.18474	-1.47807	2.33225	-2.08139

H	-1.60625	2.20197	-0.11917	-3.00911	3.71805	-2.43482	-2.59650	-3.61109	0.45244	-1.48891	3.03037	-0.46950
H	-1.81234	3.58579	2.60320	-2.32421	1.67863	-3.73643	-2.98508	-2.12817	-2.19876	-3.76802	2.62095	-1.42399
H	-1.02539	2.04730	2.28831	-1.18894	1.24420	-2.47696	-3.26213	-3.84252	-1.96869	-3.43654	0.89694	-1.48575
H	-0.15307	4.78834	1.21073	-3.15286	1.10162	-0.84404	-5.39411	-2.67936	-1.89427	-3.27970	0.82106	1.01128
H	0.61120	3.88225	2.50646	-4.23438	1.43861	-2.18578	-5.05930	-3.41107	-0.33354	-3.41788	2.57044	1.08495
H	1.08620	2.01464	0.79301	-3.25959	-0.61381	-3.37803	-6.05761	-1.21868	-0.02002	-5.55052	1.62694	1.68961
H	0.52280	3.11159	-0.45656	-2.37213	-0.98493	-1.91462	-4.42336	-1.20618	0.61138	-5.73893	2.43296	0.14083
H	2.24948	4.80811	0.32278	-5.41845	-0.87649	-2.25671	-3.62251	0.01442	-1.42787	-5.63867	0.21799	-1.03450
H	2.88319	3.60870	1.43153	-4.43860	-2.32776	-2.10151	-5.21251	-0.14789	-2.15757	-5.35963	-0.59348	0.49421
H	2.82489	3.33420	-1.63545	-4.94384	-0.24777	0.09293	-4.98449	2.10309	-1.34313	-7.62077	0.20097	1.31558
H	4.19866	3.85709	-0.68445	-5.65651	-1.85225	-0.01987	-6.18398	1.29413	-0.32853	-7.87667	1.02663	-0.20917
H	-4.93833	-2.52777	0.29331	2.31935	2.50223	3.63650	5.05408	-2.95504	0.40440	4.25957	3.87191	1.03507
H	-5.24129	-1.87689	-1.33046	0.55293	2.62780	3.76491	4.25939	-2.56520	-1.14260	2.73110	3.83528	1.93785
H	-5.77910	-0.98431	0.10592	1.51612	4.04106	3.28877	4.24675	-4.22736	-0.52444	2.81610	4.64119	0.35795
H	-5.45415	2.49100	-1.91190	0.93606	4.73055	-1.16475	0.12321	-5.15601	1.04275	0.74530	2.13642	-2.69581
H	-3.84335	3.18868	-1.70850	0.79435	3.42332	-2.34691	-0.90949	-4.00964	1.91012	0.70745	0.36917	-2.76523
H	-5.15132	3.65465	-0.61125	1.92144	3.26812	-1.00219	0.82437	-4.01651	2.20496	2.20492	1.20697	-2.34540
H	-1.83948	-2.57627	-2.33434	0.23103	-0.48933	1.88548	2.81995	-0.51044	2.68508	3.25132	0.27696	2.56629
H	3.76443	-4.17384	1.78603	5.90980	-2.92803	-2.25273	2.98402	5.32913	-1.29646	8.30924	-2.53872	-0.70706
H	4.13463	1.61214	0.54442	-2.68936	-1.27976	0.48139	-4.40325	0.94006	1.43702	-7.78679	-1.12049	-1.45303
H	3.01844	0.82873	-2.80025	-4.29676	0.19303	2.33812	-2.33674	2.97365	1.98161	-7.24292	-3.60213	1.63514
H	1.78562	-0.25730	-2.10564	-3.87719	-0.83478	3.72875	-2.14183	1.20119	2.05595	-6.82985	-1.92554	2.06608
H	1.49833	1.49710	-2.13723	-2.61491	-0.36974	2.55580	-1.10188	2.16643	0.97147	-8.54152	-2.39701	1.85762
H	6.53996	0.52068	-1.83693	-2.21099	-4.79435	0.34757	-5.19917	4.85187	1.28916	-11.18386	-1.80449	-0.64212
H	5.09446	-0.43612	-1.40636	-1.39409	-3.24389	0.70431	-4.05426	4.27461	0.04744	-9.97426	-1.87854	-1.95462
H	6.03746	0.38334	-0.12823	-2.50869	-3.96515	1.90220	-5.81226	4.01217	-0.15490	-9.86973	-3.01532	-0.58131

Table S23. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6d (6d**-C1–**6d-**C3**)** in vacuo

atom	**6d**-C1			**6d**-C2			**6d**-C3		
	x	y	z	x	y	z	x	y	z
C	1.35197	-1.75672	-0.30675	0.94901	-1.76858	-0.53470	-2.36100	-1.64836	-0.06336
C	0.81041	-1.71152	1.04910	0.88136	-2.62146	0.64854	-1.68007	-1.53624	1.22238
C	-0.71718	-1.78577	0.89396	-0.61162	-2.72295	1.00660	-0.39677	-2.38198	1.10516
N	-0.93609	-1.90673	-0.55983	-1.28492	-1.89436	0.00021	-0.39815	-2.85520	-0.28887
C	0.24179	-1.97239	-1.24270	-0.42237	-1.43171	-0.94163	-1.46635	-2.36501	-0.98374
C	-1.48562	-2.99112	1.45628	-1.33100	-4.07350	0.84762	0.97891	-1.69348	1.29769
C	-2.71060	-3.07876	0.51229	-2.78973	-3.64779	0.55117	1.70900	-1.82364	-0.07370
C	-2.13956	-2.68709	-0.87958	-2.66894	-2.31349	-0.22774	0.95924	-2.95430	-0.81266
O	0.36425	-2.20518	-2.46517	-0.73516	-0.83094	-1.99445	-1.64934	-2.49185	-2.21487
O	1.38142	-1.61318	2.12928	1.77260	-3.17023	1.28691	-1.98935	-0.92639	2.24019
H	-1.14382	-0.84592	1.26735	-0.76577	-2.32092	2.01575	-0.50536	-3.22747	1.79652
C	2.65226	-1.67897	-0.76946	2.02877	-1.31002	-1.26417	-3.58627	-1.18017	-0.52419
C	3.86780	-1.43297	0.08203	3.47419	-1.53188	-0.91258	-4.67194	-0.47876	0.25780
C	4.36839	0.02786	-0.11673	4.16788	-0.17415	-0.61761	-4.27121	0.96164	0.67243
C	3.51380	1.12243	0.56044	3.57628	0.64395	0.55054	-3.98869	1.95040	-0.47913
C	3.82503	2.49556	-0.07395	4.13066	2.08473	0.51814	-3.45168	3.29584	0.06487
C	3.04309	3.69831	0.48917	3.48508	3.07965	1.50386	-2.06689	3.26869	0.73704
C	1.50739	3.60470	0.41453	1.96437	3.28058	1.35463	-0.90632	2.94482	-0.21469
C	0.93726	3.56991	-1.01246	1.53067	3.85987	-0.00097	0.45134	2.84917	0.49311
C	-0.59858	3.64273	-1.08455	0.02189	4.13263	-0.13386	1.60100	2.45597	-0.44456
C	-1.33056	2.37379	-0.61863	-0.85746	2.87240	-0.16732	2.90447	2.12671	0.29403
C	-2.85563	2.52803	-0.68836	-2.32686	3.18838	-0.47394	4.02324	1.64356	-0.64020
C	4.97820	-2.45095	-0.24615	4.19718	-2.28449	-2.04994	-5.12515	-1.30787	1.47757
C	3.72363	1.12460	2.08413	3.82281	-0.03722	1.90765	-5.23608	2.20472	-1.34322
O	2.88367	-1.79956	-2.06851	1.81344	-0.58644	-2.35393	-3.89732	-1.37800	-1.79523
O	-3.78306	-2.24187	0.91936	-3.51957	-3.36211	1.74915	3.07760	-2.16482	0.02295
C	-3.63248	1.23525	-0.45371	-3.20735	1.94661	-0.60578	5.24836	1.12945	0.11280
O	-3.31704	0.57821	0.78553	-3.24550	1.11942	0.55207	4.86826	-0.07926	0.76952
C	-3.60290	1.31840	1.97934	-3.71291	1.73592	1.75037	5.82027	-0.56085	1.72317
O	-4.99834	1.54094	-0.54581	-4.49796	2.39294	-0.97399	6.40013	0.95140	-0.68174
C	-5.86249	0.40990	-0.66643	-5.37698	1.35711	-1.39861	6.26706	0.09504	-1.81886
H	-0.87551	-3.89860	1.36891	-0.91894	-4.61759	-0.01118	0.86500	-0.65406	1.61792
H	-1.78673	-2.87130	2.49829	-1.25119	-4.71476	1.72919	1.56892	-2.21358	2.05694
H	-3.12854	-4.08864	0.49210	-3.32235	-4.40580	-0.03737	1.58808	-0.89090	-0.64344
H	-1.86015	-3.55846	-1.48219	-2.84032	-2.43136	-1.30202	0.95066	-2.84797	-1.89852
H	-2.87226	-2.10462	-1.44563	-3.37654	-1.58012	0.16804	1.41126	-3.91806	-0.55185
H	3.55653	-1.56467	1.12124	3.48898	-2.15679	-0.01672	-5.51344	-0.42043	-0.43959
H	5.39076	0.08236	0.28119	5.22664	-0.38452	-0.41270	-5.10034	1.35913	1.27532
H	4.44690	0.22139	-1.19384	4.13907	0.42751	-1.53411	-3.40938	0.89071	1.34153
H	2.45678	0.89452	0.36490	2.49013	0.70424	0.39521	-3.21958	1.51440	-1.13233
H	4.89939	2.70040	0.04505	5.21197	2.05045	0.71735	-3.41984	4.01503	-0.76582
H	3.65312	2.42491	-1.15630	4.02731	2.47530	-0.50251	-4.18648	3.69473	0.77943
H	3.33259	3.86174	1.53455	3.69893	2.76737	2.53378	-1.88586	4.25191	1.19280

H	3.36630	4.59823	-0.05269	3.98245	4.05167	1.37853	-2.06237	2.55067	1.56713
H	1.16382	2.72870	0.97918	1.44761	2.33030	1.53820	-1.09859	1.99102	-0.72377
H	1.08772	4.47877	0.93269	1.62800	3.96129	2.14962	-0.85942	3.70747	-1.00602
H	1.35276	4.41960	-1.57198	2.07525	4.80019	-0.16740	0.68436	3.80510	0.98364
H	1.27793	2.66647	-1.53652	1.83534	3.18545	-0.81263	0.37606	2.10532	1.29941
H	-0.94536	4.50233	-0.49202	-0.30569	4.78715	0.68752	1.29565	1.57713	-1.03149
H	-0.89528	3.85087	-2.12161	-0.14747	4.70057	-1.05918	1.77662	3.25893	-1.17457
H	-1.01798	1.52892	-1.24812	-0.47301	2.18504	-0.93371	3.24780	3.00971	0.85132
H	-1.03377	2.11741	0.40514	-0.79018	2.33380	0.78518	2.70412	1.35036	1.04266
H	-3.20205	3.29006	0.02033	-2.74977	3.85623	0.28674	3.64238	0.84542	-1.28954
H	-3.14931	2.88493	-1.68278	-2.40030	3.72733	-1.42603	4.35154	2.46051	-1.29392
H	5.81575	-2.31098	0.44410	5.23565	-2.47424	-1.76089	-5.41138	-2.32243	1.18137
H	4.62135	-3.48064	-0.14009	3.72255	-3.24991	-2.25324	-4.33878	-1.36636	2.23309
H	5.34601	-2.32245	-1.26802	4.19684	-1.69930	-2.97425	-6.00103	-0.83106	1.92969
H	3.51875	0.14241	2.51897	3.42036	-1.05400	1.93611	-5.60879	1.29026	-1.81394
H	4.75683	1.40342	2.32999	4.89896	-0.09442	2.11821	-6.04835	2.63000	-0.73923
H	3.05963	1.83632	2.58398	3.35545	0.51806	2.72702	-5.01355	2.91607	-2.14625
H	2.00028	-1.98543	-2.52170	0.81414	-0.52184	-2.48519	-3.10631	-1.83293	-2.24429
H	-3.53366	-1.29751	0.87049	-3.65308	-4.18302	2.24112	3.61217	-1.37913	0.24604
H	-3.35728	0.47884	-1.20306	-2.80822	1.27215	-1.37637	5.56993	1.85510	0.87280
H	-2.87537	2.12433	2.12898	-2.96514	2.41839	2.17520	6.78372	-0.76924	1.24769
H	-3.52546	0.60946	2.80582	-3.89160	0.92524	2.46023	5.96233	0.17406	2.52644
H	-4.61348	1.73672	1.94947	-4.64664	2.28476	1.58271	5.40714	-1.48076	2.14027
H	-6.87295	0.80573	-0.78184	-6.30506	1.84204	-1.70872	5.81718	-0.86709	-1.54941
H	-5.81803	-0.23329	0.21890	-5.58867	0.64841	-0.58889	5.67386	0.56595	-2.61213
H	-5.60324	-0.18555	-1.55264	-4.95369	0.80742	-2.25177	7.28036	-0.07177	-2.18881

Table S24. Cartesian coordinates of the optimized low-energy conformers calculated at B3LYP/6-31G+(d,p) level of **6d (6d**-C4–**6d-**C6**)** in vacuo

atom	**6d**-C4			**6d**-C5			**6d**-C6		
	x	y	z	x	y	z	x	y	z
C	-2.43085	-1.64724	0.07170	-1.81517	-1.27627	0.41476	-3.60435	0.53207	-0.21200
C	-1.61104	-1.36633	1.24539	-2.12728	-1.93123	-0.85348	-2.91202	-0.72958	0.02476
C	-0.25404	-2.04276	0.98979	-0.94414	-2.86932	-1.14753	-4.01049	-1.76169	0.33347
N	-0.44176	-2.78253	-0.26266	-0.01856	-2.65466	-0.02262	-5.26092	-0.98766	0.31229
C	-1.62709	-2.45785	-0.85601	-0.55350	-1.82802	0.92124	-5.04868	0.29490	-0.10579
C	0.91905	-1.09537	0.66126	-1.17772	-4.38997	-1.10245	-4.28507	-2.86216	-0.70709
C	1.75025	-1.83198	-0.43133	0.20216	-4.92984	-0.68671	-5.78638	-3.16483	-0.49573
C	0.82615	-2.96334	-0.96790	0.77338	-3.85092	0.27647	-6.41063	-1.80933	-0.08374
O	-1.96997	-2.78172	-2.01488	-0.06622	-1.60194	2.05058	-5.93865	1.12544	-0.38647
O	-1.85673	-0.72023	2.25888	-3.09759	-1.80960	-1.59177	-1.71551	-0.99748	0.00856
H	-0.00933	-2.71641	1.81884	-0.48274	-2.57995	-2.09895	-3.83176	-2.19919	1.32269
C	-3.70726	-1.24289	-0.30056	-2.52828	-0.35343	1.15681	-3.12386	1.77649	-0.57888
C	-4.69234	-0.41667	0.49260	-3.84284	0.25571	0.75309	-1.67111	2.13327	-0.72811
C	-4.20993	1.03746	0.73596	-3.75728	1.80272	0.70631	-1.25751	3.03377	0.47096
C	-3.92089	1.88982	-0.51899	-2.72927	2.40173	-0.27748	0.23413	3.42893	0.52856
C	-3.37193	3.28309	-0.12510	-2.65116	3.92947	-0.06071	1.20971	2.22729	0.53672
C	-1.97507	3.32658	0.52252	-1.56184	4.71486	-0.81999	1.05149	1.22599	1.69321
C	-0.82275	2.97281	-0.42952	-0.10212	4.42103	-0.40637	2.13883	0.13545	1.72807
C	0.54888	2.93870	0.25950	0.59844	3.29088	-1.17801	2.11810	-0.82477	0.52730
C	1.68795	2.49279	-0.66991	2.02724	3.01917	-0.68695	3.03710	-2.05061	0.68212
C	2.98331	2.13134	0.07187	2.69420	1.84018	-1.41041	4.54480	-1.76416	0.80999
C	4.05267	1.53356	-0.85124	4.14359	1.54527	-0.98769	5.16126	-1.09143	-0.42438
C	-5.06550	-1.11048	1.82053	-4.95063	-0.20158	1.72943	-1.41476	2.79662	-2.09637
C	-5.16700	2.05958	-1.40555	-3.05854	2.04857	-1.73744	0.46701	4.37779	1.71824
O	-4.16584	-1.61582	-1.48461	-2.05396	0.04212	2.32965	-3.98057	2.75887	-0.81051
O	2.93927	-2.42640	0.06722	0.97561	-5.04415	-1.88379	-6.00446	-4.06451	0.59569
C	5.22071	0.88833	-0.11509	4.31041	1.16974	0.48555	6.66806	-0.87841	-0.31549
O	4.74886	-0.22173	0.66753	3.53540	0.01785	0.72957	7.28486	-2.13175	-0.29750
C	5.09453	-0.21327	2.05316	3.37026	-0.30307	2.11031	8.68658	-2.10190	-0.04917
O	6.13225	0.45551	-1.08490	5.66743	1.00266	0.88063	7.18128	-0.14466	-1.42800
C	7.34353	-0.09456	-0.57896	6.40934	-0.00567	0.19899	7.13463	1.26472	-1.28745
H	0.52419	-0.15511	0.26306	-1.92210	-4.63397	-0.33591	-4.12322	-2.46955	-1.71862
H	1.53075	-0.86324	1.53487	-1.50129	-4.81046	-2.05574	-3.65470	-3.74586	-0.57904
H	2.00094	-1.13430	-1.24076	0.13023	-5.90644	-0.19080	-6.25614	-3.55952	-1.40567
H	0.65099	-2.92119	-2.04494	0.64797	-4.11753	1.33166	-6.94363	-1.31699	-0.90256
H	1.27956	-3.92792	-0.71951	1.83981	-3.68492	0.08908	-7.10625	-1.96530	0.74517
H	-5.58920	-0.38818	-0.13397	-4.07904	-0.13394	-0.23939	-1.11661	1.19331	-0.67039
H	-4.99981	1.53478	1.31725	-4.75856	2.17395	0.44705	-1.86128	3.94930	0.43829
H	-3.32922	0.99730	1.38237	-3.54103	2.16594	1.71830	-1.52695	2.51931	1.40230
H	-3.15557	1.37645	-1.11911	-1.74848	1.97340	-0.02995	0.46109	4.00496	-0.37946
H	-3.35551	3.91462	-1.02465	-3.63014	4.35806	-0.32348	1.12181	1.69239	-0.41686
H	-4.09523	3.75277	0.55735	-2.51681	4.12193	1.01332	2.23289	2.63085	0.55719
H	-1.80851	4.33918	0.91507	-1.67251	4.57520	-1.90360	1.07402	1.76501	2.64902

H	-1.94001	2.65992	1.39381	-1.76239	5.77896	-0.64093	0.07091	0.73716	1.63222
H	-1.00703	1.98945	-0.88335	0.49270	5.33535	-0.53772	3.12389	0.61610	1.81405
H	-0.80326	3.69105	-1.26231	-0.07146	4.19891	0.67055	2.00815	-0.45338	2.64727
H	0.77848	3.92657	0.68351	0.01963	2.36254	-1.10230	1.08984	-1.17974	0.38154
H	0.49324	2.24899	1.11377	0.62203	3.54697	-2.24737	2.38038	-0.28335	-0.39084
H	1.35661	1.61135	-1.23793	2.63794	3.92563	-0.81315	2.71671	-2.61759	1.56751
H	1.88766	3.27200	-1.41869	1.99166	2.82115	0.39260	2.87986	-2.71748	-0.17704
H	3.38069	3.02036	0.58201	2.09387	0.93602	-1.25578	4.73156	-1.14172	1.69644
H	2.74211	1.40434	0.85690	2.68868	2.03819	-2.49109	5.06758	-2.71078	0.98632
H	3.61180	0.75811	-1.49014	4.52713	0.72543	-1.60550	4.98279	-1.69619	-1.32209
H	4.45975	2.29797	-1.52272	4.78147	2.41845	-1.17527	4.69713	-0.11358	-0.59823
H	-5.42517	-2.12977	1.64551	-5.91367	0.20381	1.40374	-1.77449	2.16278	-2.91348
H	-4.21199	-1.14584	2.50105	-5.03545	-1.29275	1.75288	-1.91983	3.76411	-2.16936
H	-5.87087	-0.54893	2.30551	-4.75209	0.15180	2.74567	-0.34340	2.95253	-2.24666
H	-5.54441	1.10306	-1.77848	-3.09609	0.96820	-1.90412	-0.14510	5.28179	1.62356
H	-5.97702	2.54957	-0.84931	-4.03439	2.46434	-2.02115	0.20923	3.90612	2.67306
H	-4.94081	2.68291	-2.27774	-2.31348	2.45693	-2.42678	1.51649	4.68920	1.77199
H	-3.43240	-2.14328	-1.95257	-1.20632	-0.47269	2.50791	-4.91280	2.38624	-0.70357
H	3.60859	-1.72612	0.17934	1.86156	-5.36313	-1.66742	-5.66461	-4.93802	0.36051
H	5.71148	1.59672	0.57556	3.97231	1.98494	1.13987	6.92491	-0.32058	0.60826
H	4.64293	0.64122	2.57281	3.03707	0.57776	2.67735	9.22243	-1.58805	-0.85399
H	4.69965	-1.13798	2.47902	2.59645	-1.07041	2.16596	8.90476	-1.60554	0.90852
H	6.18175	-0.18921	2.19763	4.30481	-0.67033	2.55100	9.01391	-3.14205	0.00438
H	7.85421	0.61834	0.08577	6.69898	0.31152	-0.81119	7.66644	1.59781	-0.38277
H	7.16276	-1.03232	-0.04127	5.84748	-0.94501	0.13569	7.62956	1.68502	-2.16574
H	7.97872	-0.29435	-1.44357	7.31526	-0.16690	0.78787	6.10419	1.64631	-1.24938

Table S25. The deduced functions of ORFs in the burnettramic acid biosynthetic gene cluster from A. versicolor IMB17-055

ORF	*A. burnettii* FRR 5400[a]	Accession no.	Identity/Similarity (%)	Proposed function
1	BuaA	QBE85649	76/86	PKS-NRPS
2	Orf2	QBE85648	71/81	Hypothetical protein
3	BuaG	QBE85647	74/84	Cytochrome P450
4	BuaF	QBE85646	75/83	Hypothetical protein
5	BuaE	QBE85645	72/80	Proline hydroxylase
6	Orf1	QBE85644	52/62	Ankyrin repeat domain-containing protein
7	BuaD	QBE85643	76/83	Cytochrome P450
8	BuaC	QBE85642	86/91	Enoyl_reductase
9	BuaB	QBE85641	69/80	Glycosyltransferase

[a] The strain containing the Bua biosynthetic gene cluster in GenBank database was described as *Aspergillus* sp. CLMG-2019a FRR 5400, but *A. burnettii* FRR5400 in ref. [9]

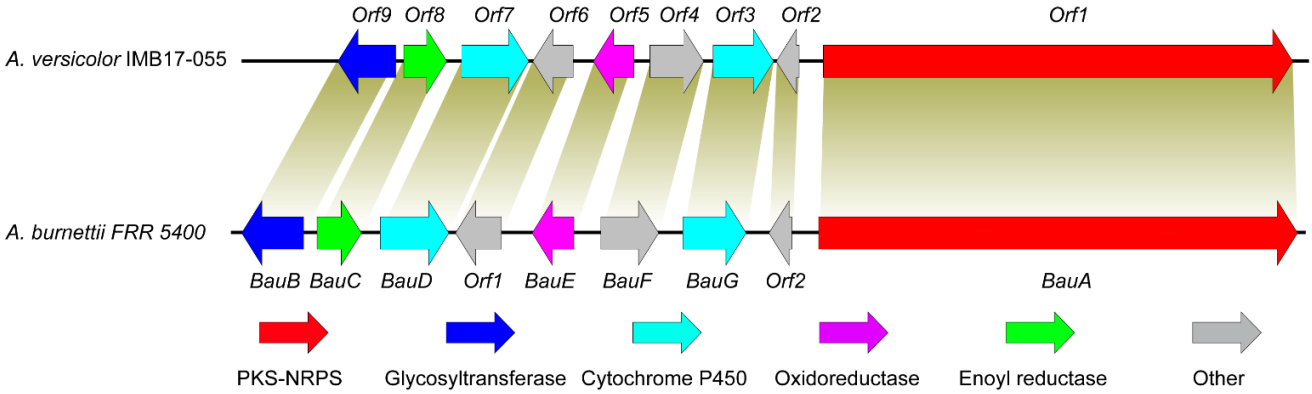


Figure S6. Graphical comparison of the burnettramic acid biosynthetic gene clusters from *A. versicolor* IMB17-055 and *A. burnettii* FRR 5400

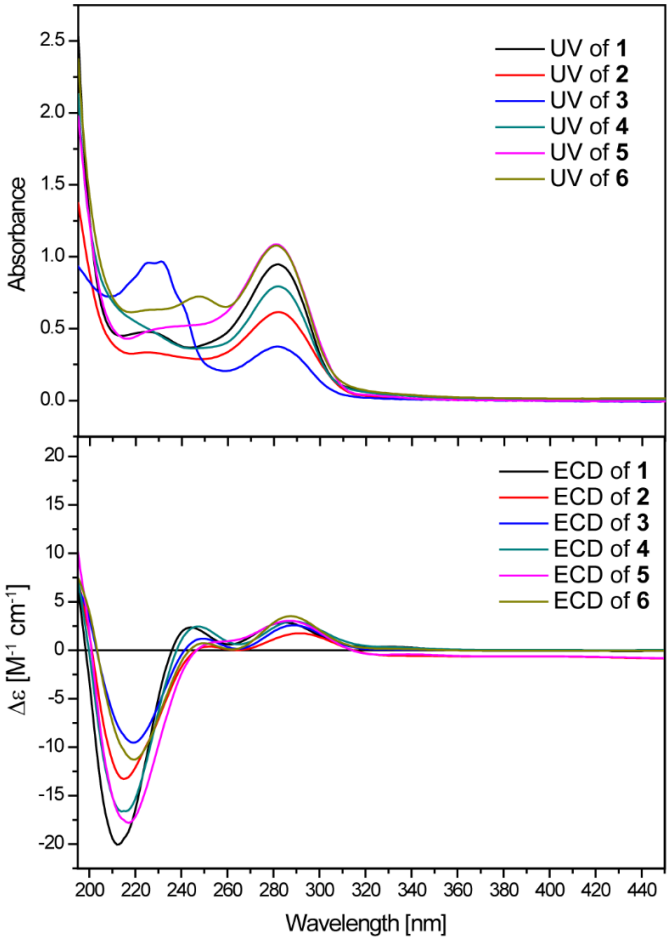


Figure S7. Experimental UV and ECD spectra of compounds **1–6.**

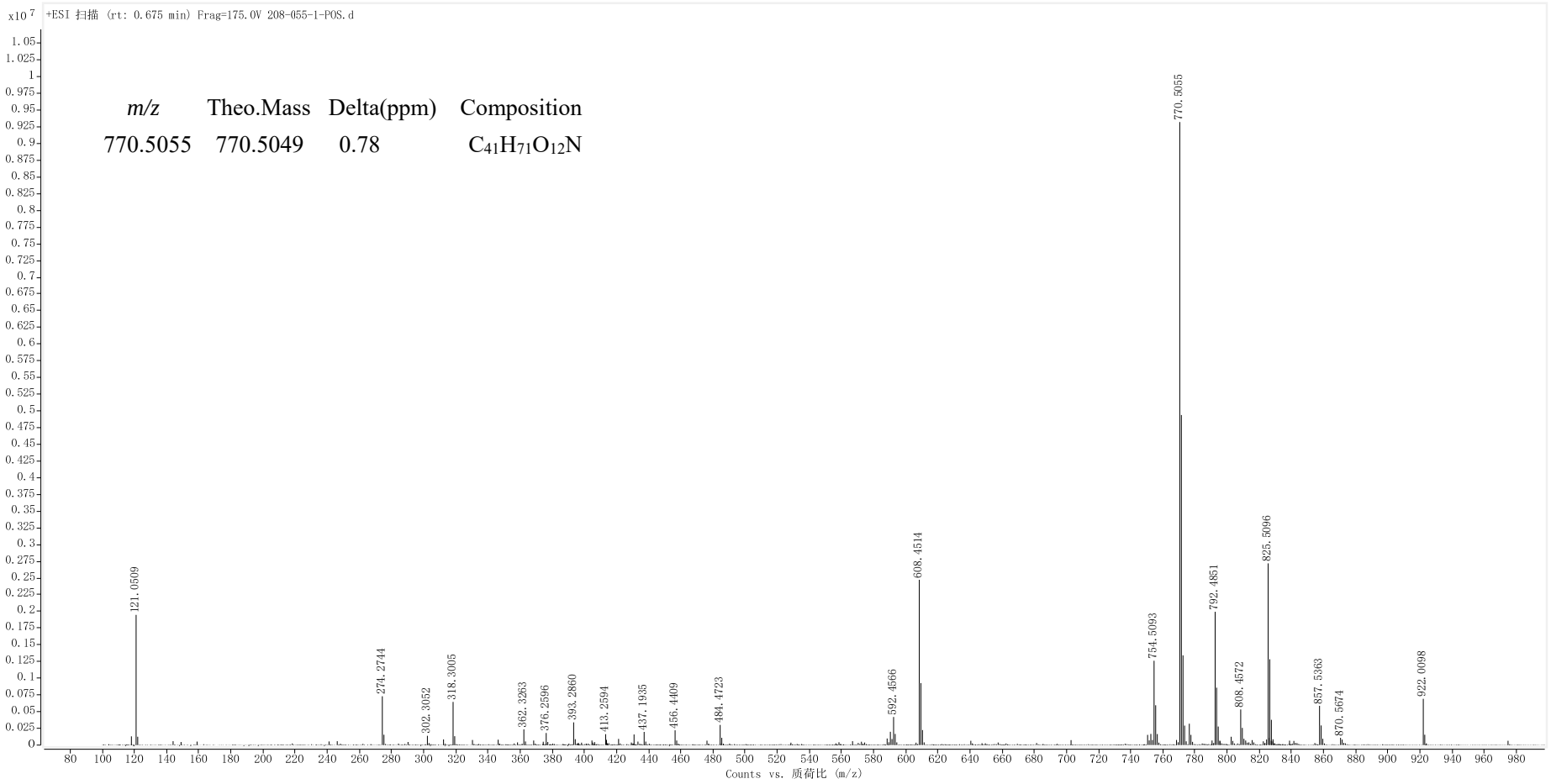


Figure S8. The (+)-HRESIMS spectrum of compound **1**.

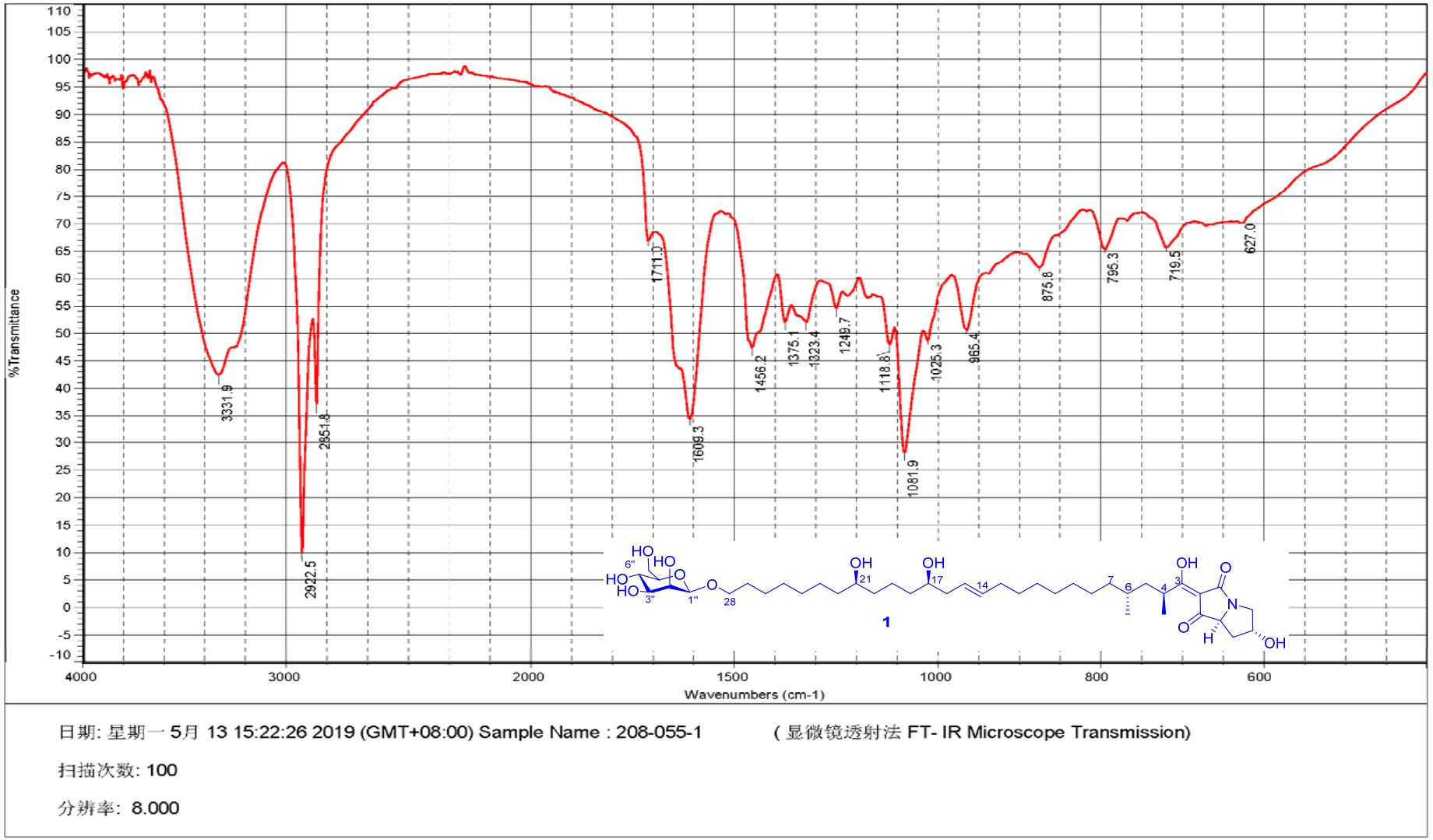


Figure S9. The IR spectrum of compound **1**.

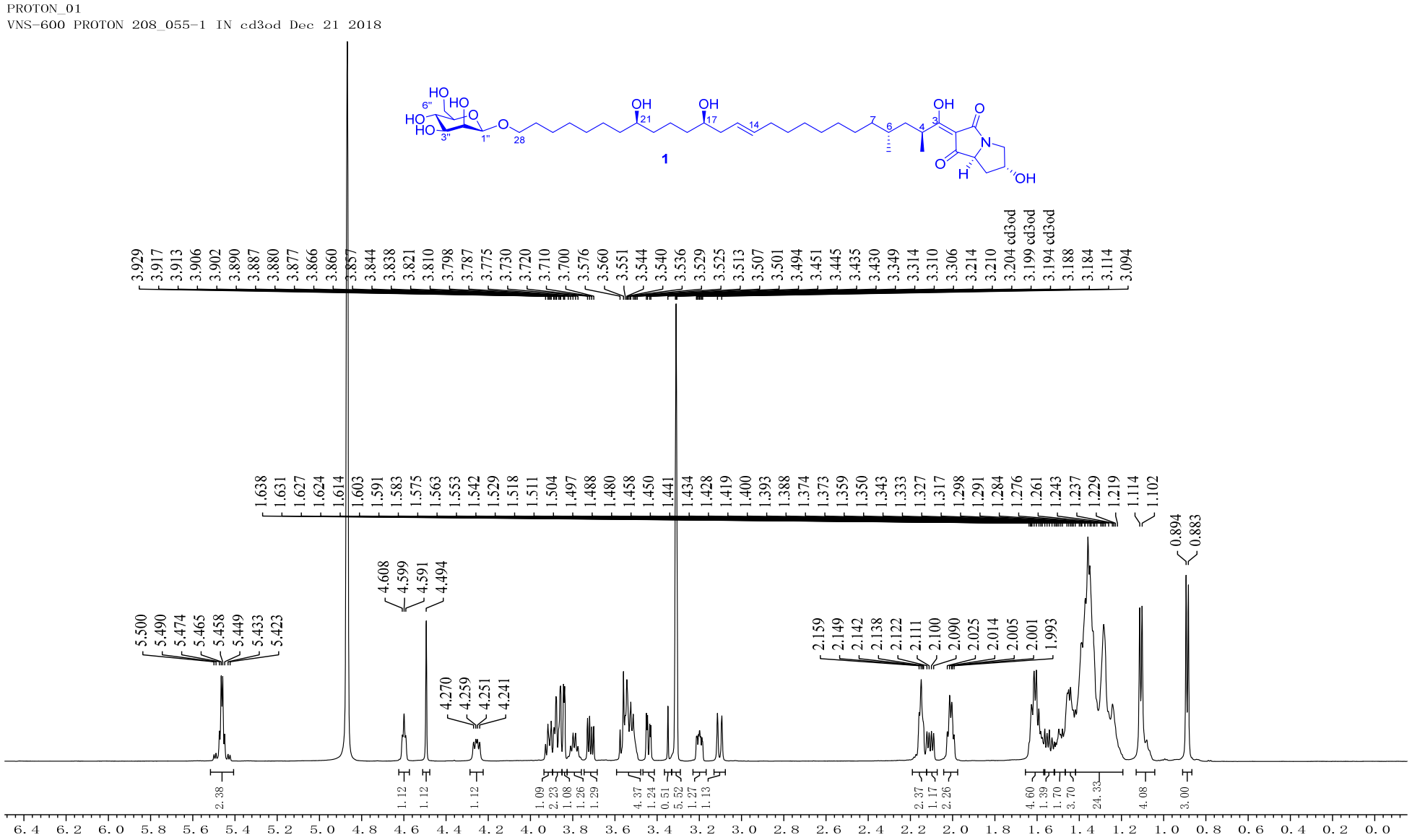


Figure S10. The ^{1}H NMR spectrum of compound **1** in CD_3OD (600 MHz).

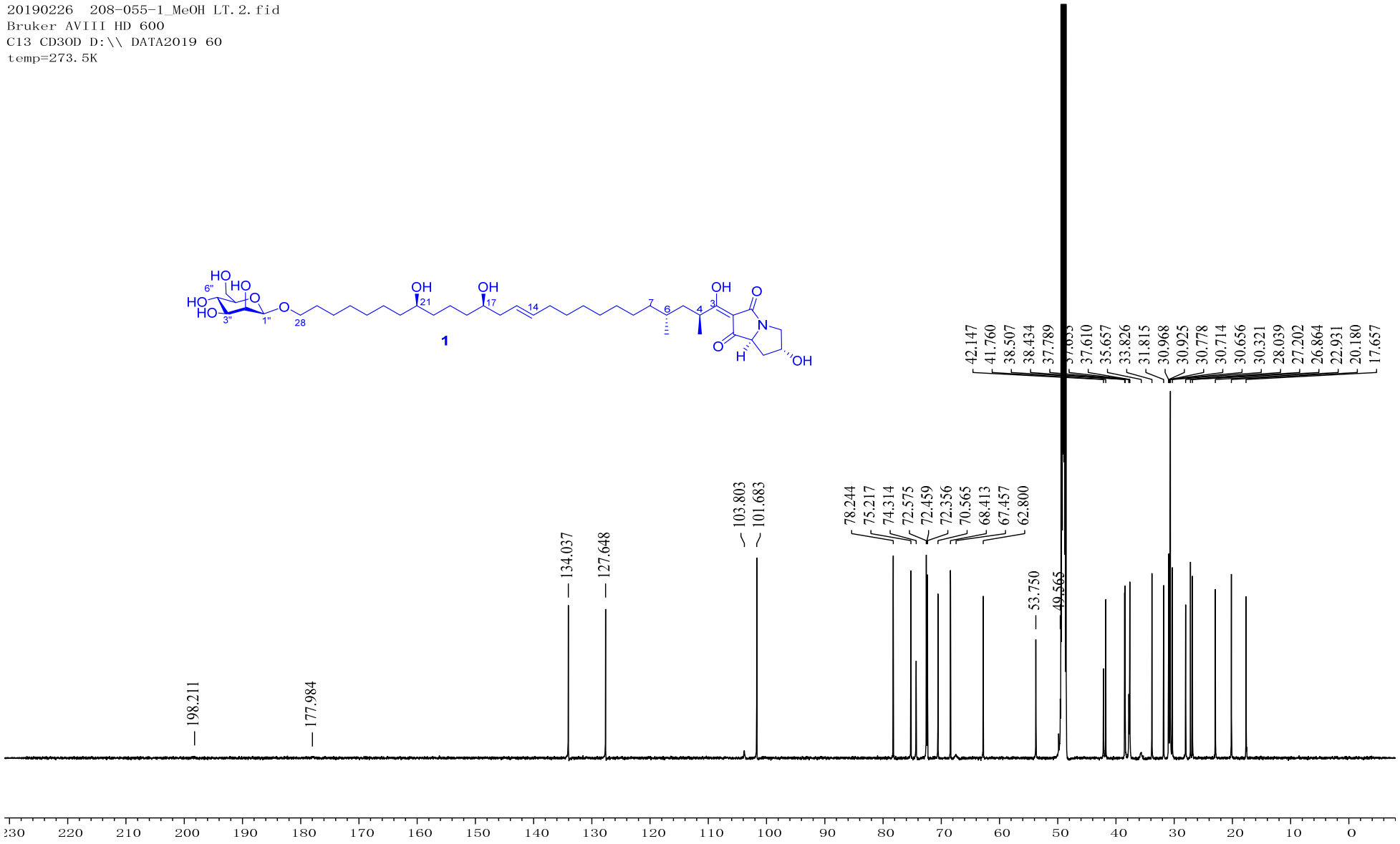


Figure S11. The ^{13}C NMR spectrum of compound **1** in CD_3OD (150 MHz).

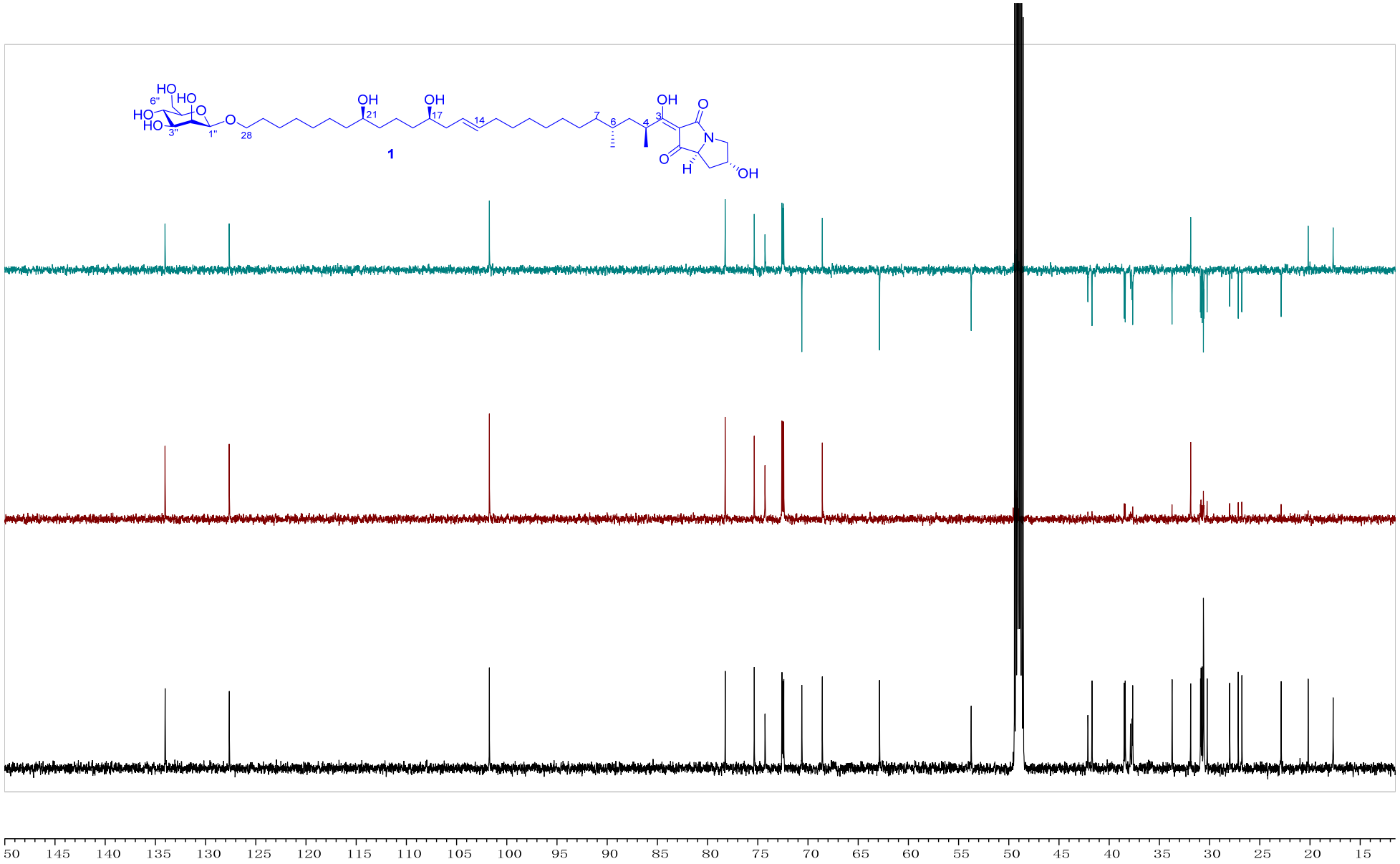


Figure S12. The DEPT spectrum of compound **1** in CD_3OD (150 MHz).

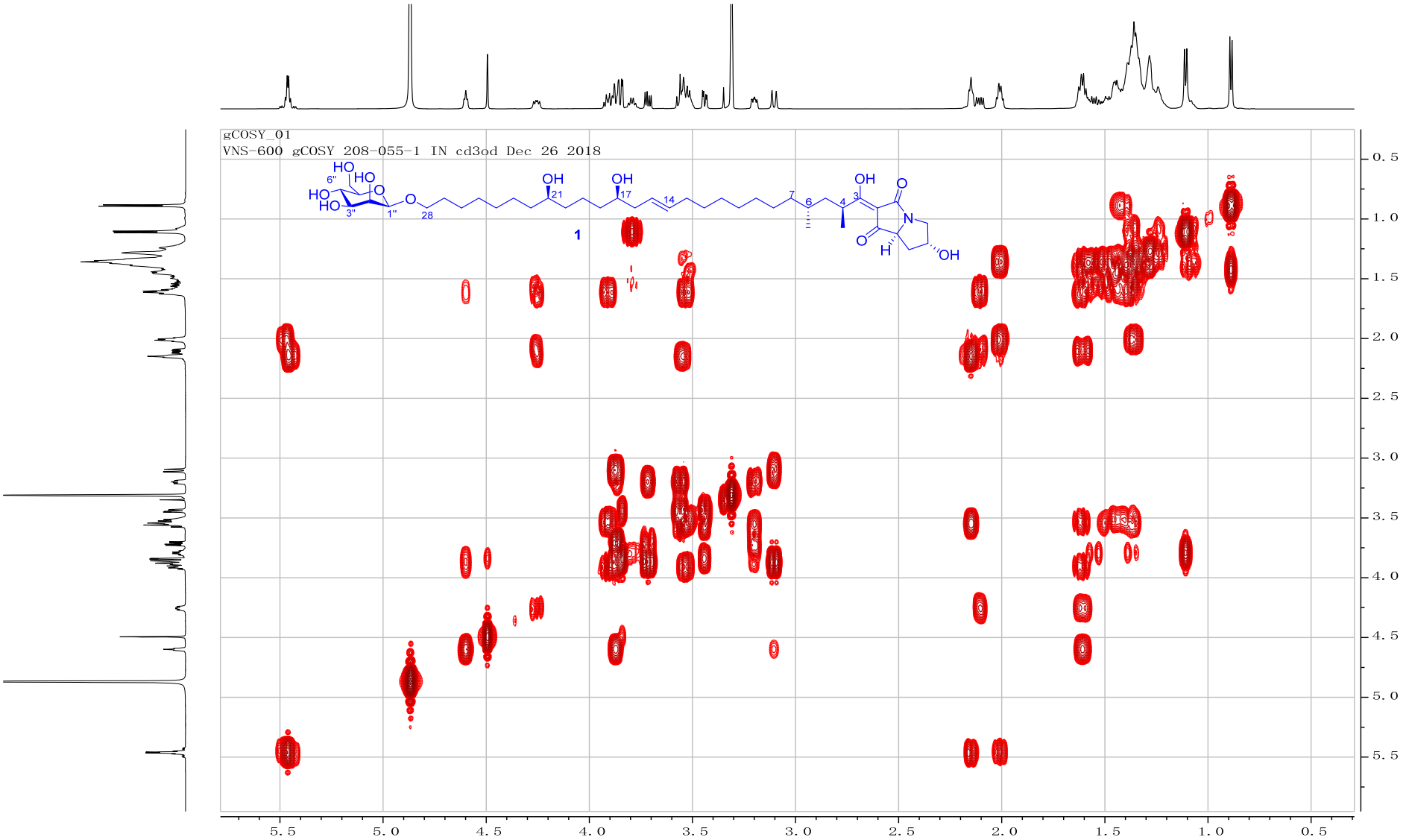


Figure S13. The ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD (600 MHz).

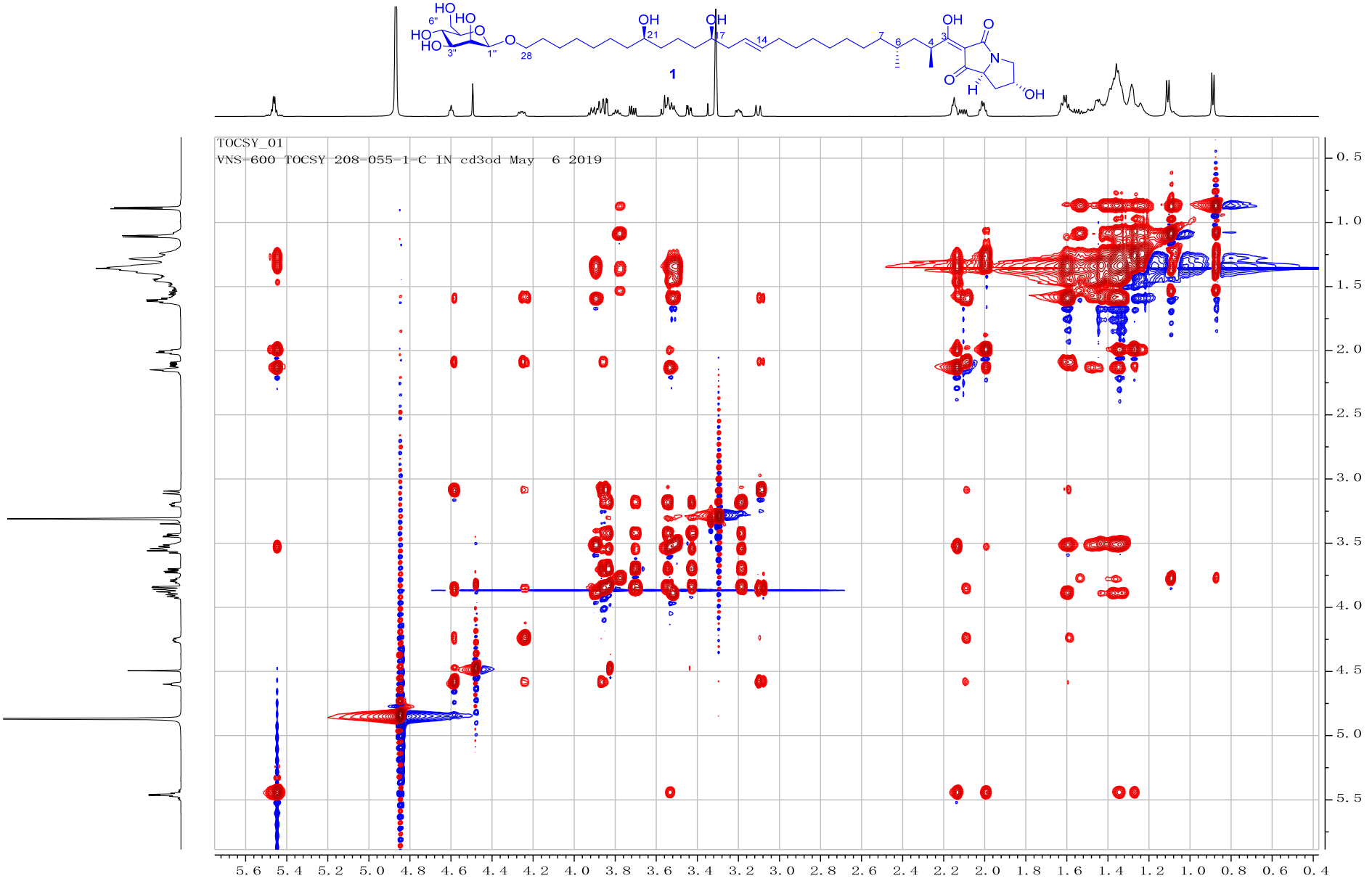


Figure S14. The TOCSY spectrum of compound **1** in CD_3OD (600 MHz).

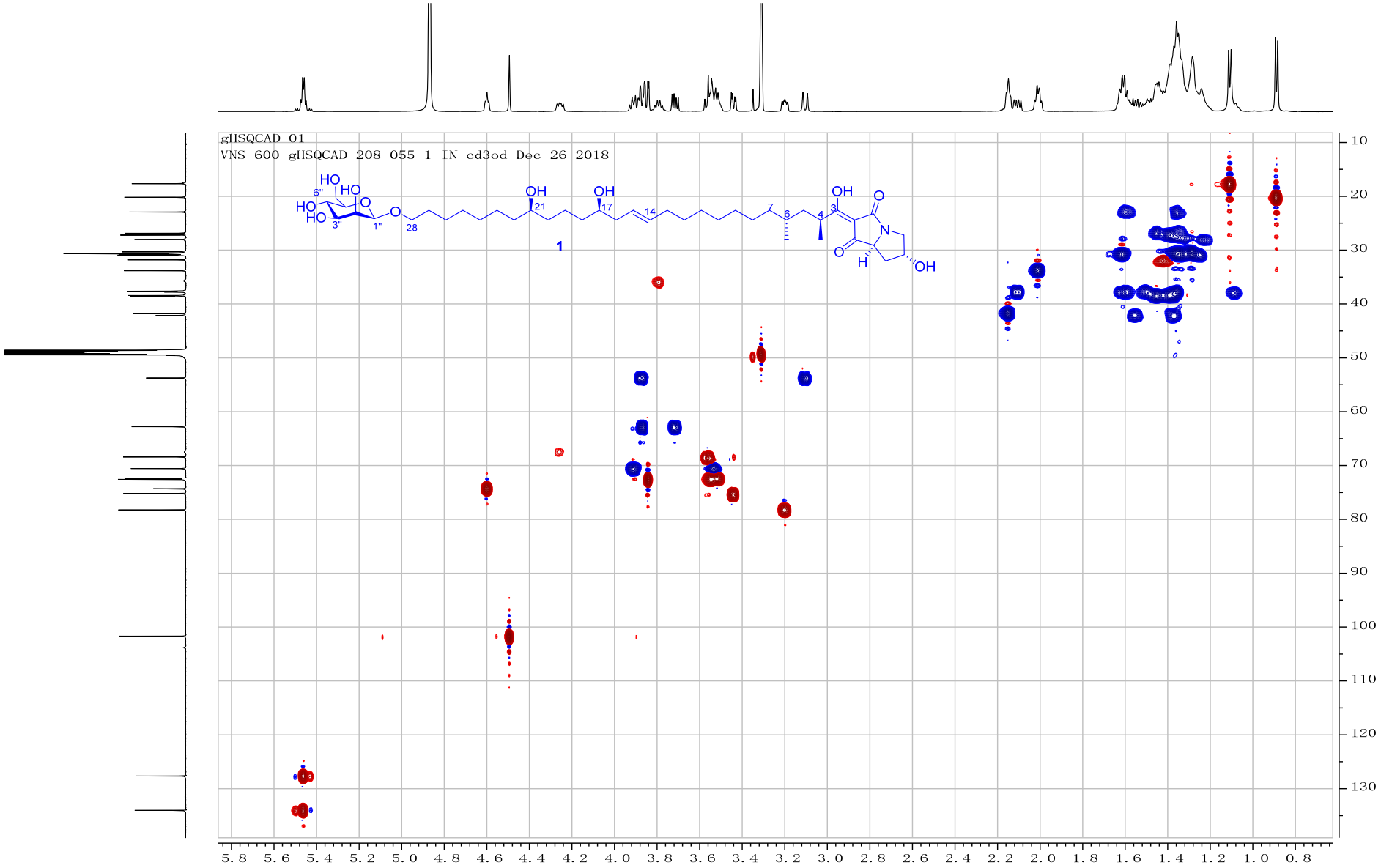


Figure S15. The HSQC spectrum of compound **1** in CD_3OD (600 MHz).

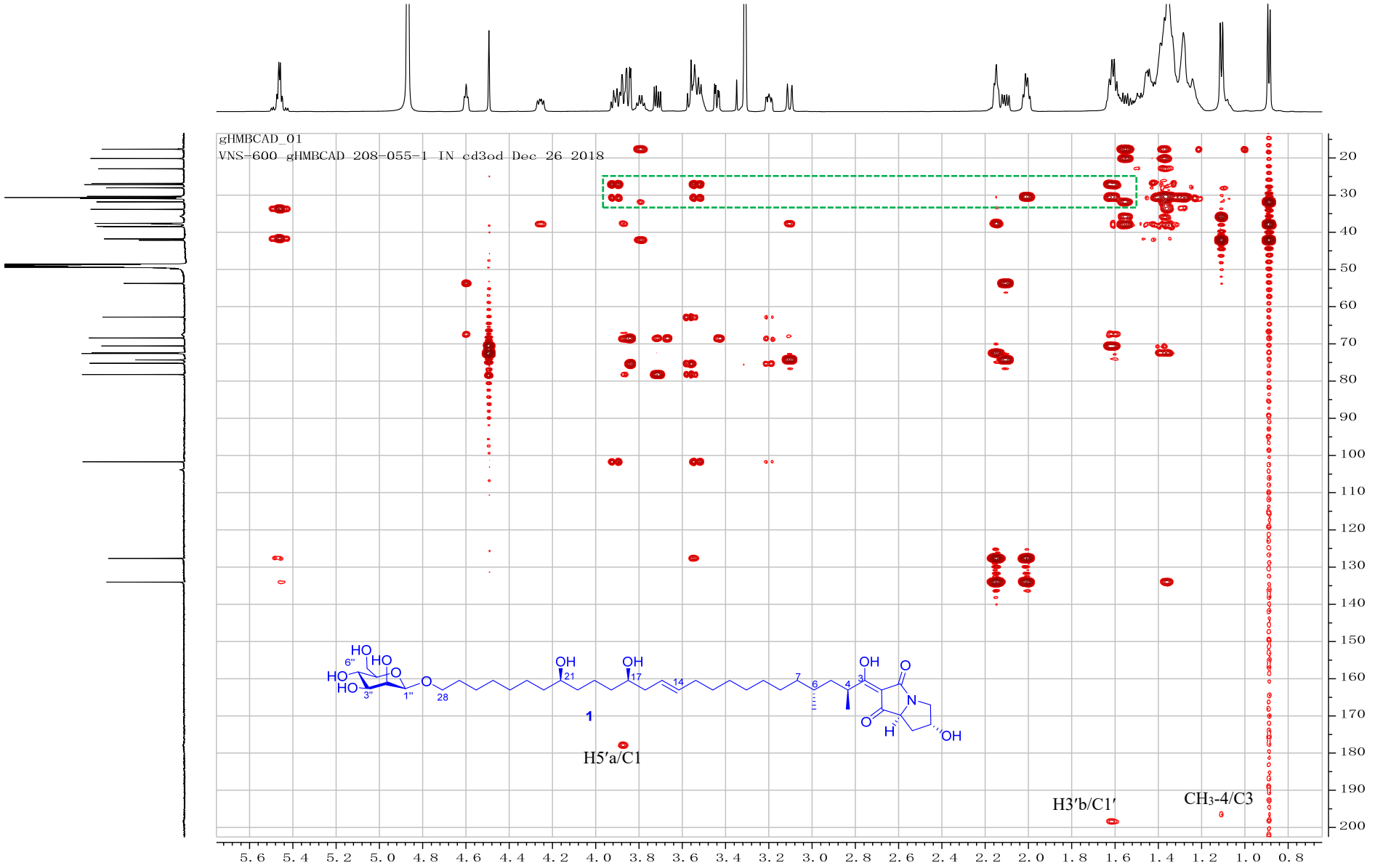


Figure S16. The HMBC spectrum of compound **1** in CD_3OD (600 MHz).

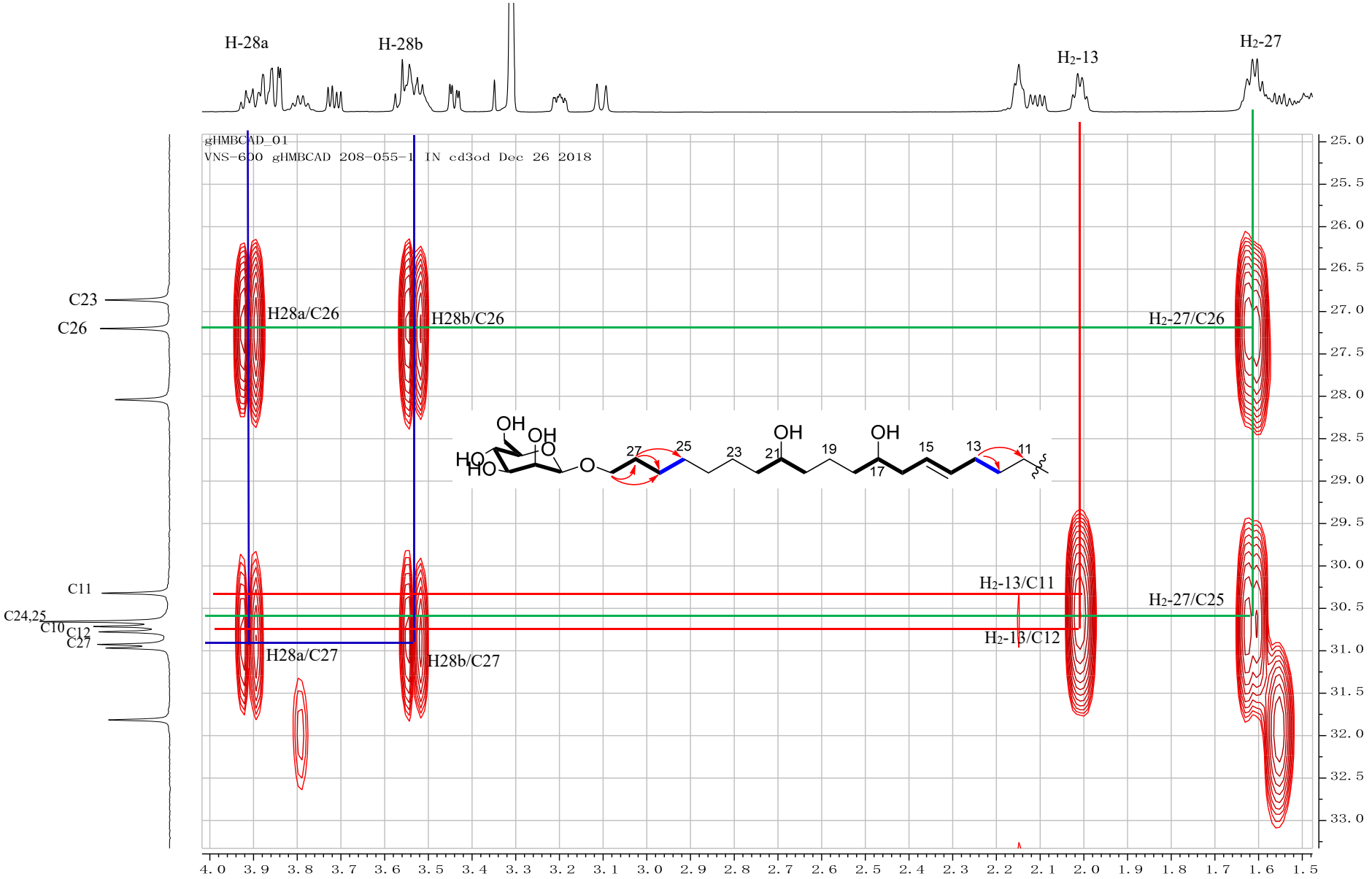


Figure S17. The enlarged HMBC spectrum of compound **1** in CD_3OD (600 MHz).

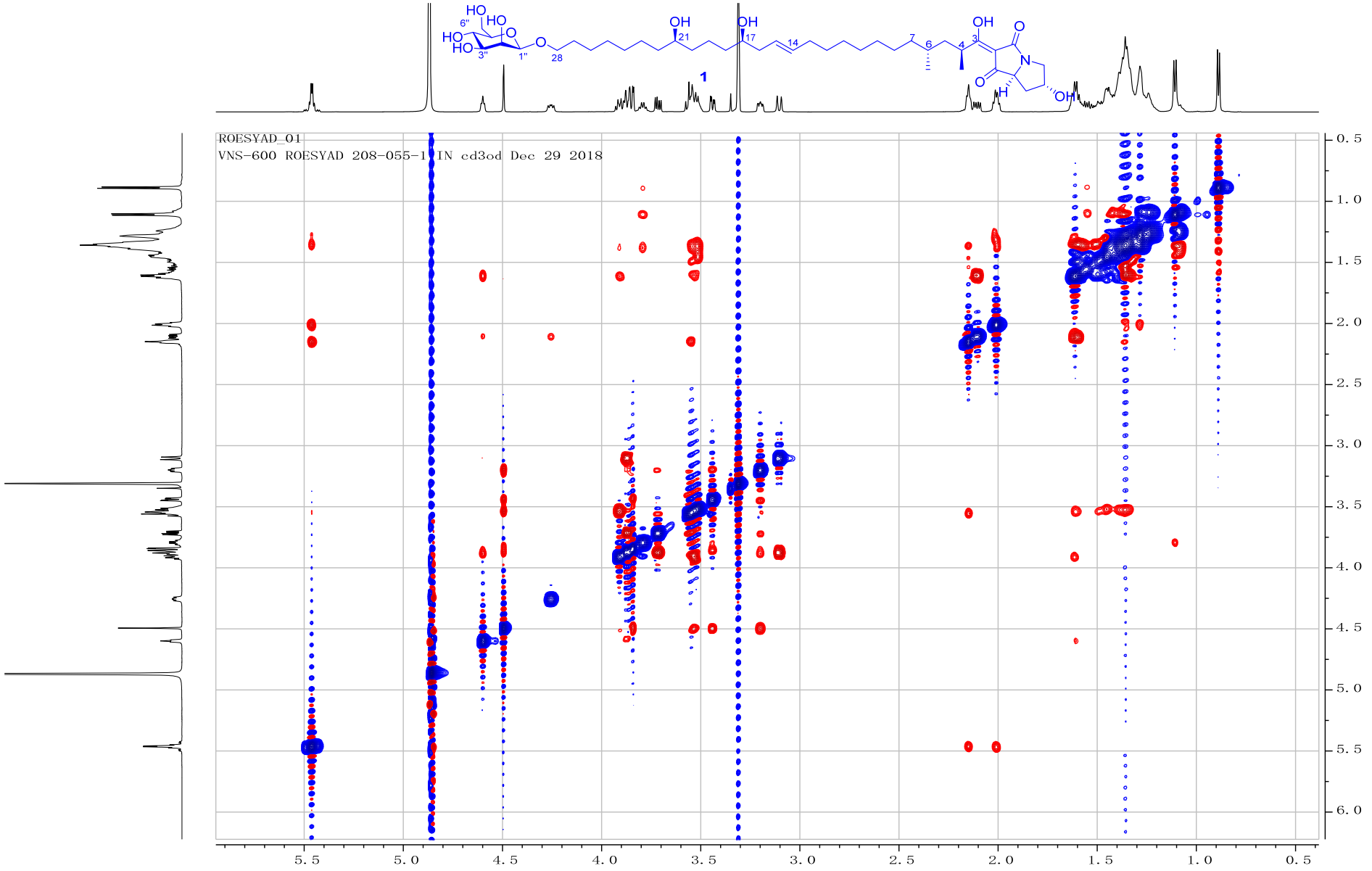


Figure S18. The ROESY spectrum of compound **1** in CD_3OD (600 MHz).

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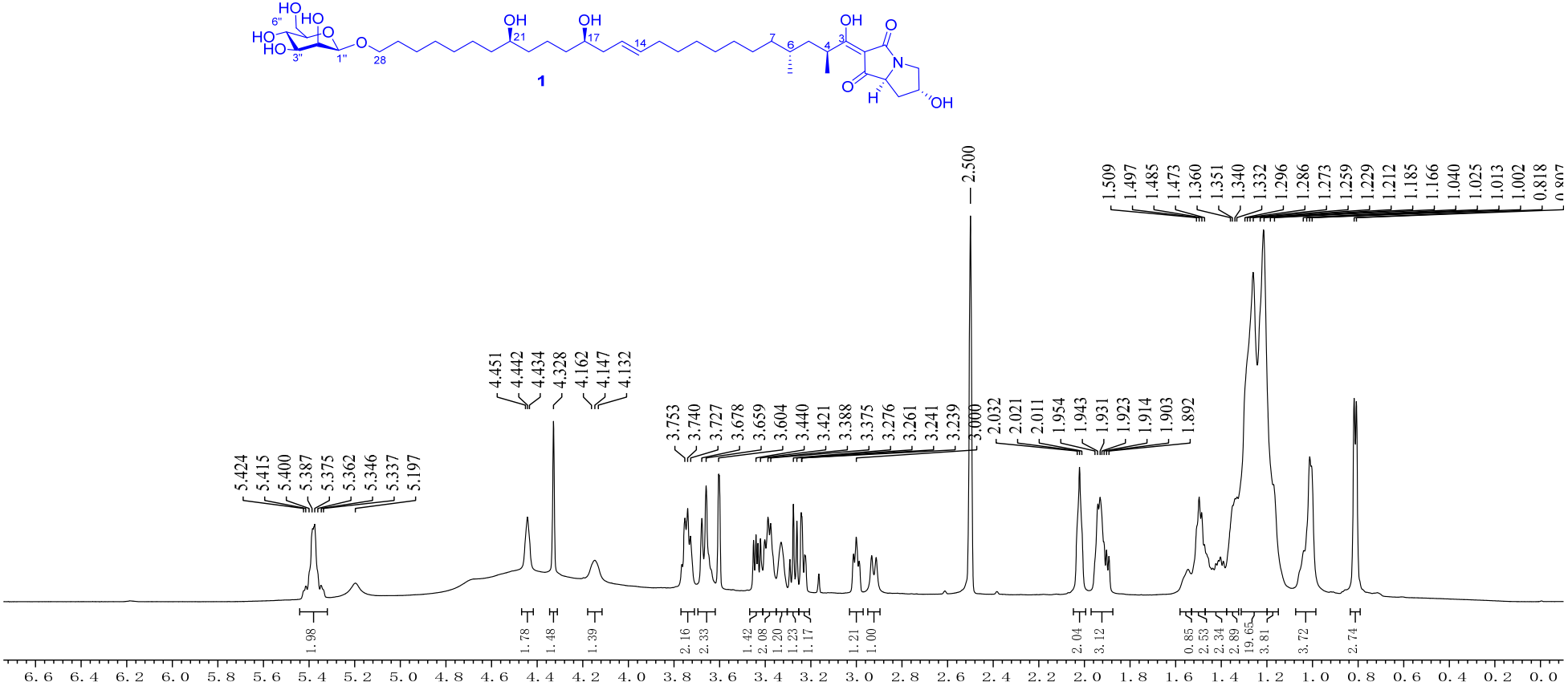

Figure S19. The ^{1}H NMR spectrum of compound **1** in DMSO-d_6 (600 MHz).

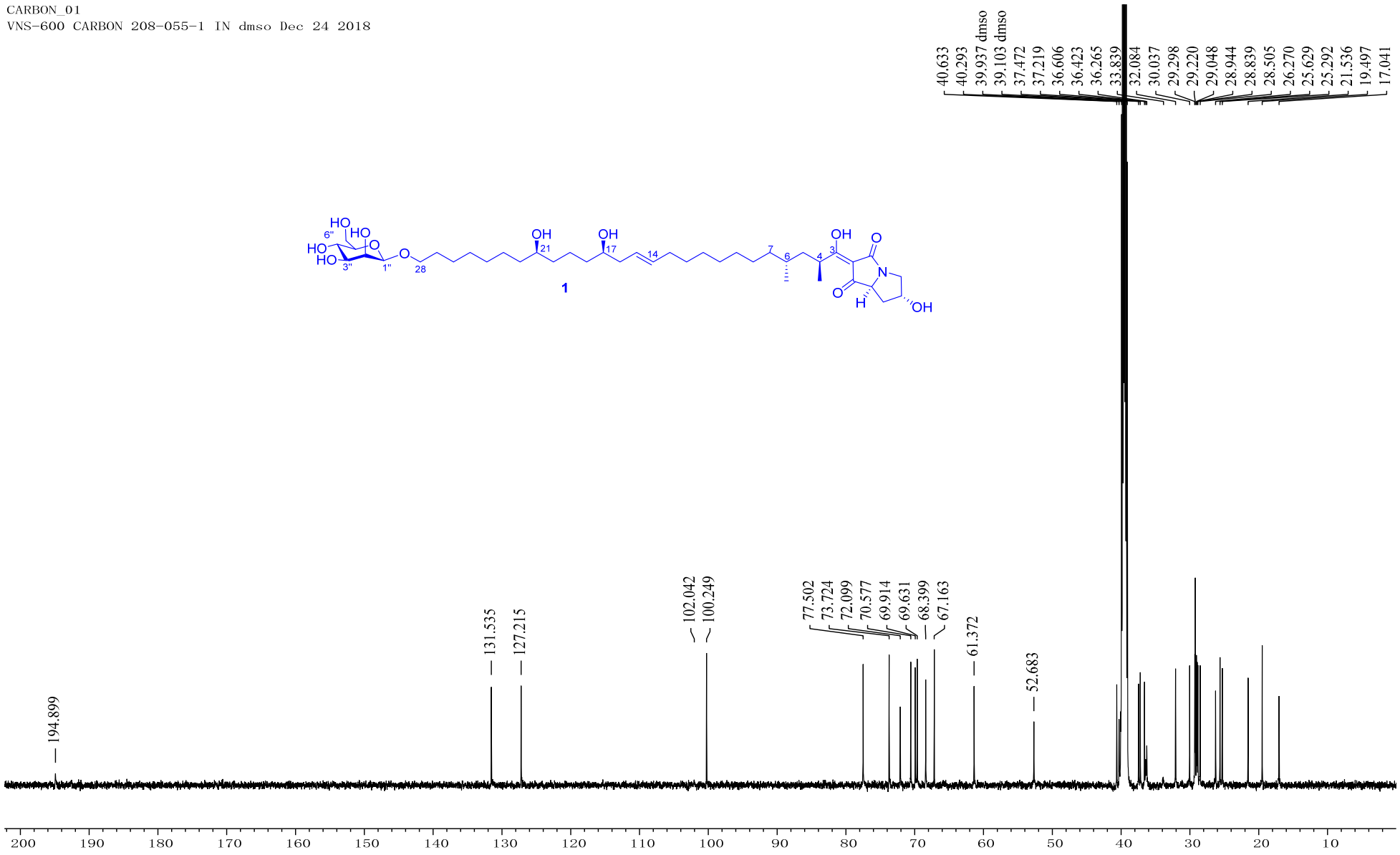

Figure S20. The ^{13}C NMR spectrum of compound **1** in DMSO-d_6 (150 MHz).

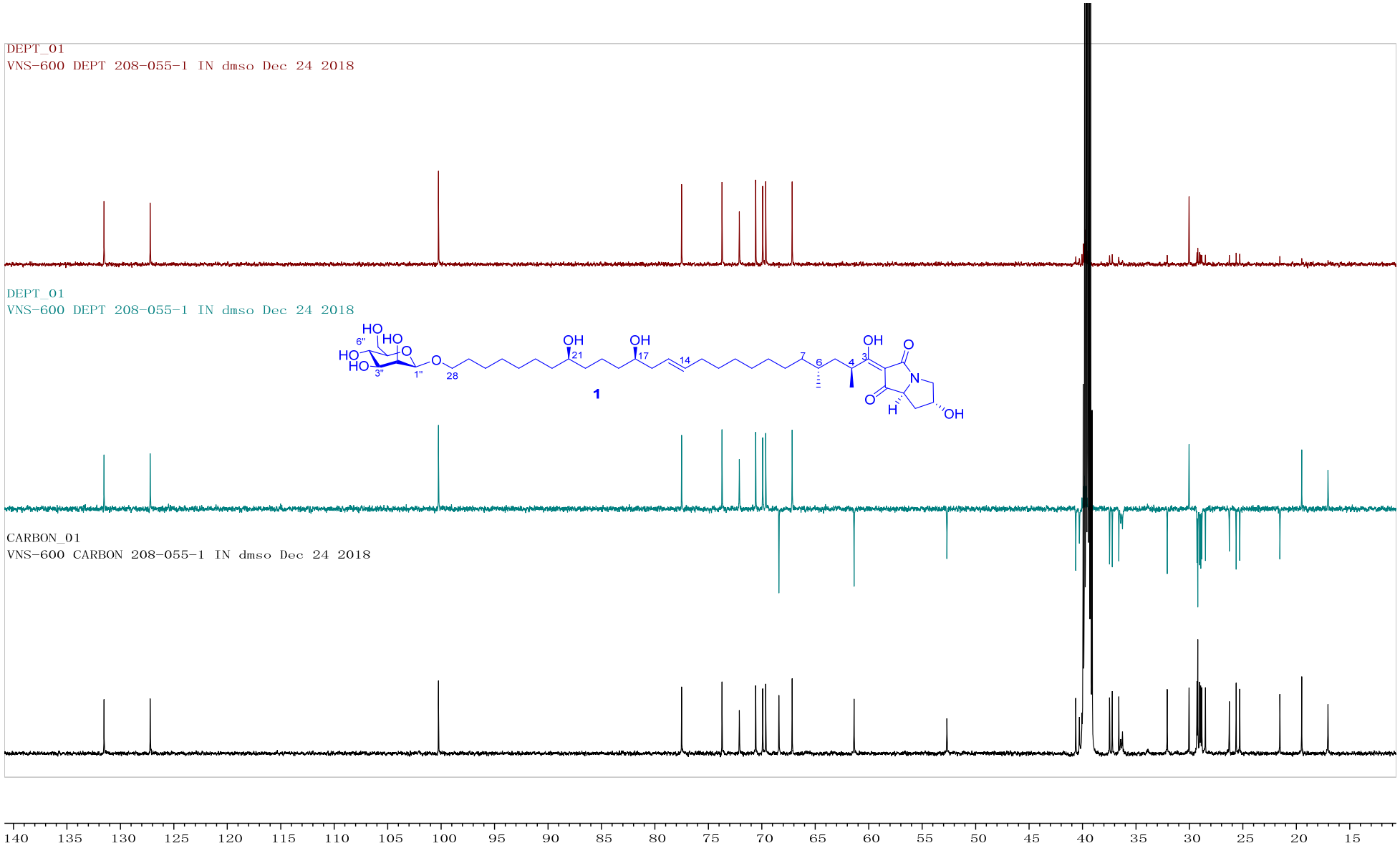

Figure S21. The DEPT spectrum of compound **1** in DMSO-d_6 (150 MHz).

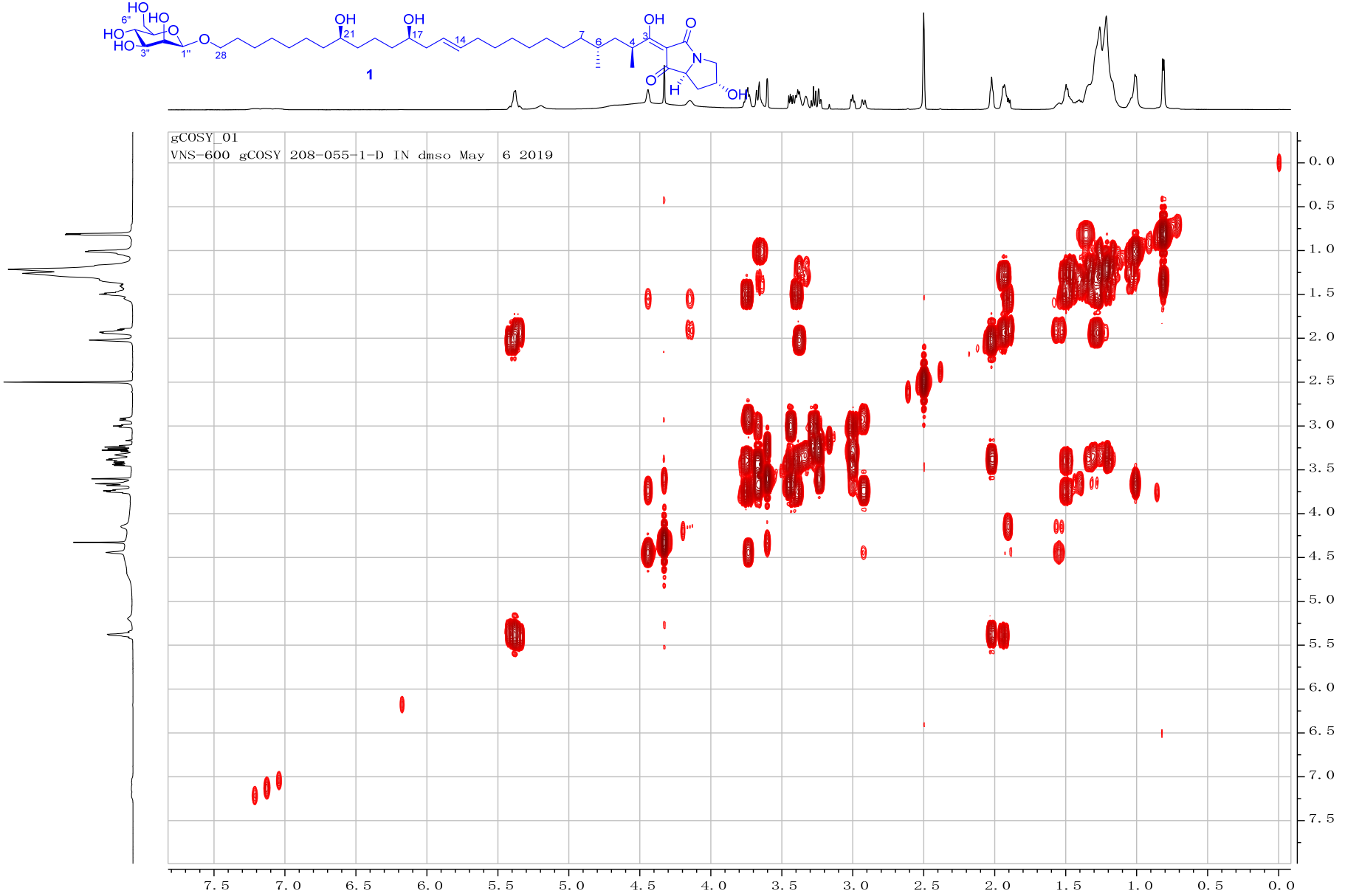

Figure S22. The ^{1}H-^{1}H COSY spectrum of compound **1** in DMSO-d_6 (600 MHz).

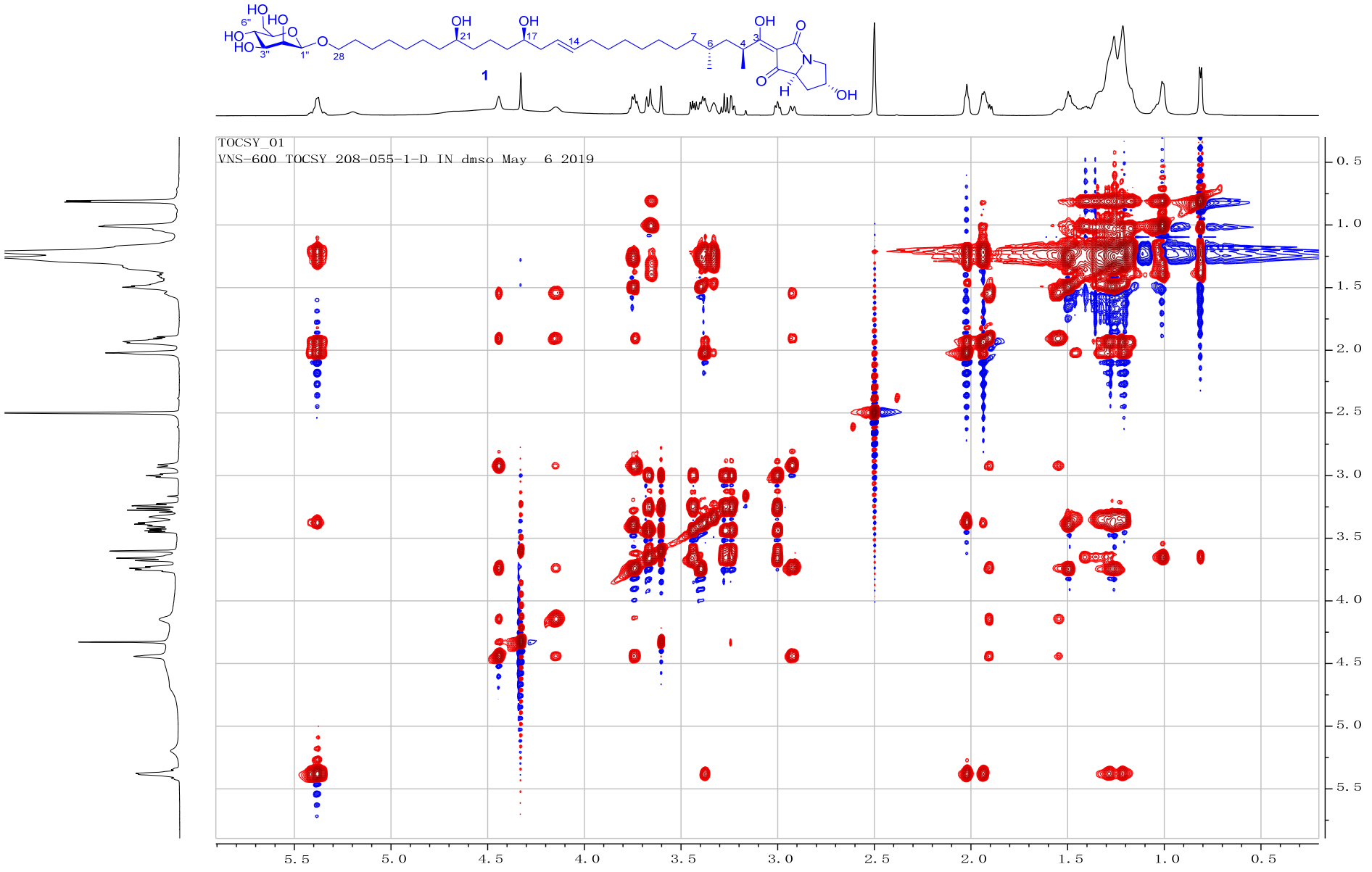

Figure S23. The TOCSY spectrum of compound **1** in DMSO-d_6 (600 MHz).

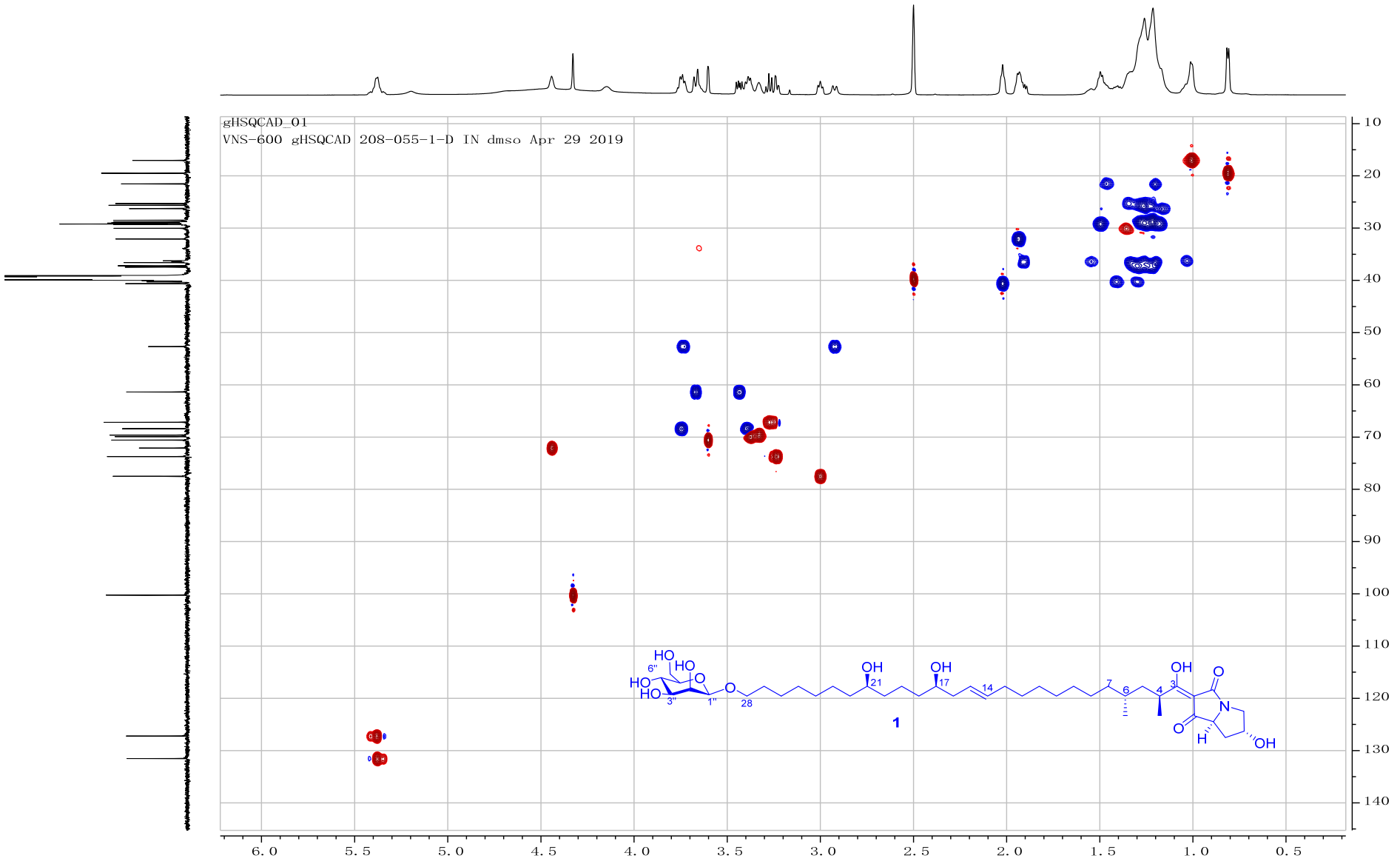

Figure S24. The HSQC spectrum of compound **1** in DMSO-d_6 (600 MHz).

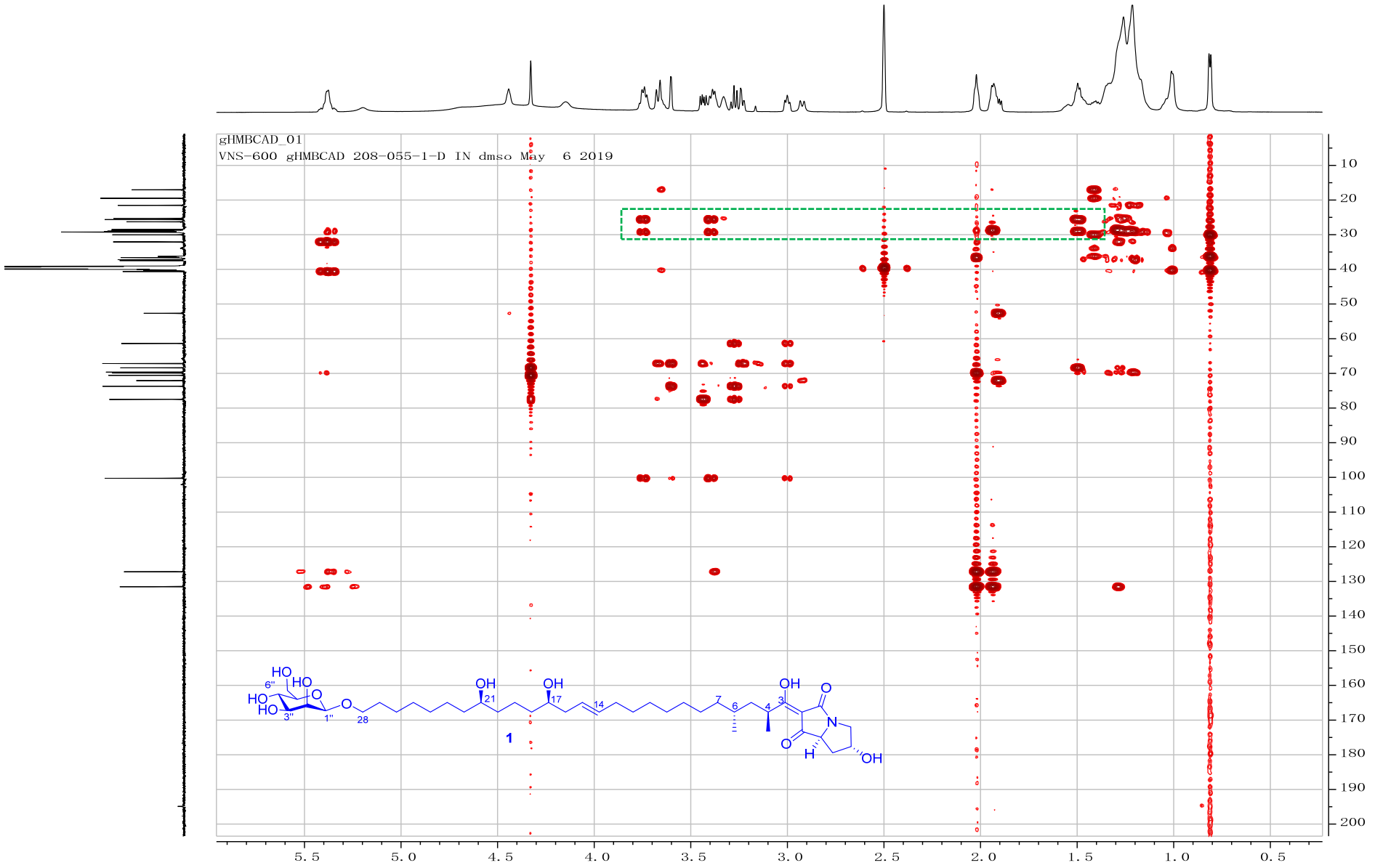

Figure S25. The HMBC spectrum of compound **1** in DMSO-d_6 (600 MHz).

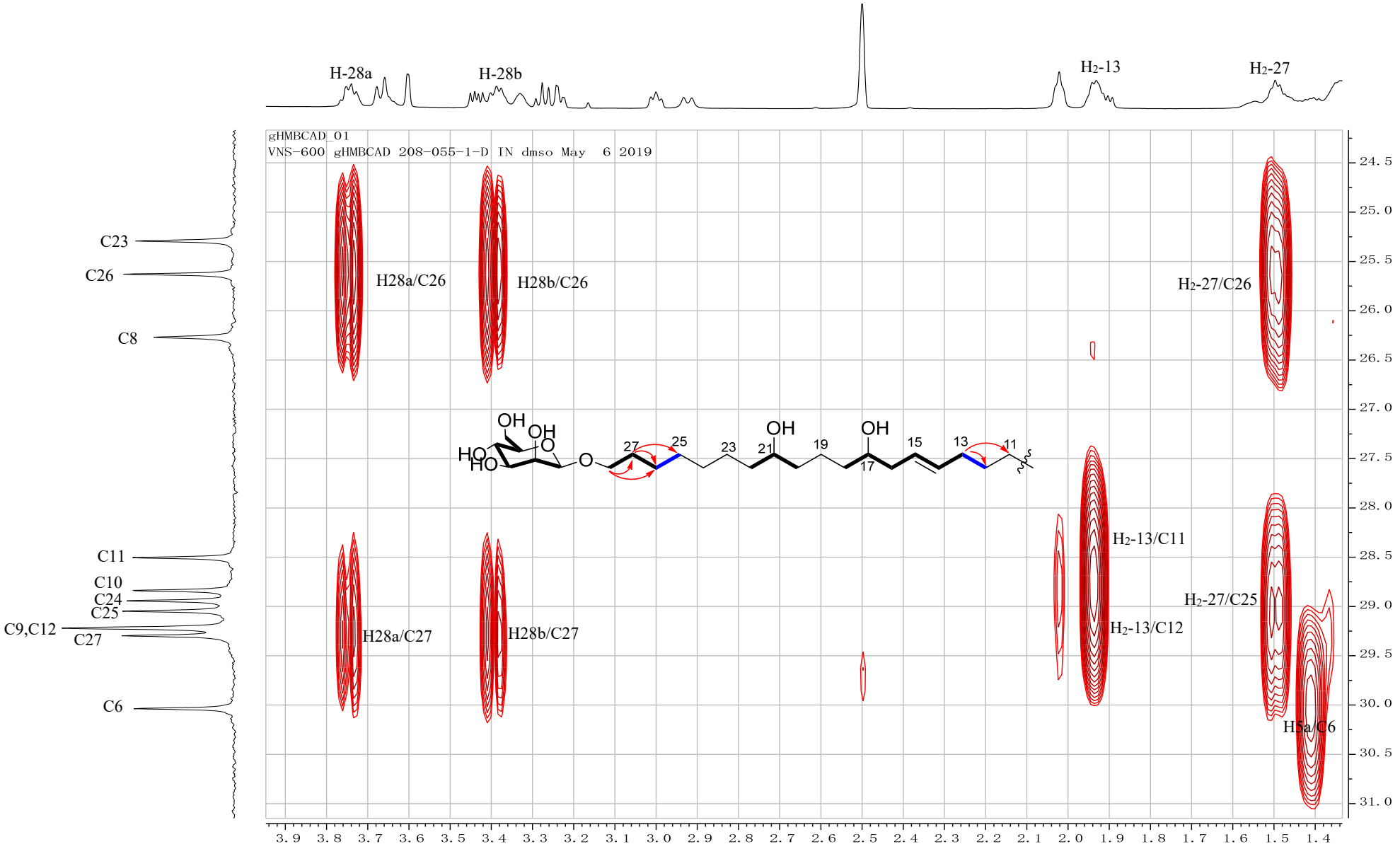

Figure S26. The enlarged HMBC spectrum of compound **1** in DMSO-d_6 (600 MHz).

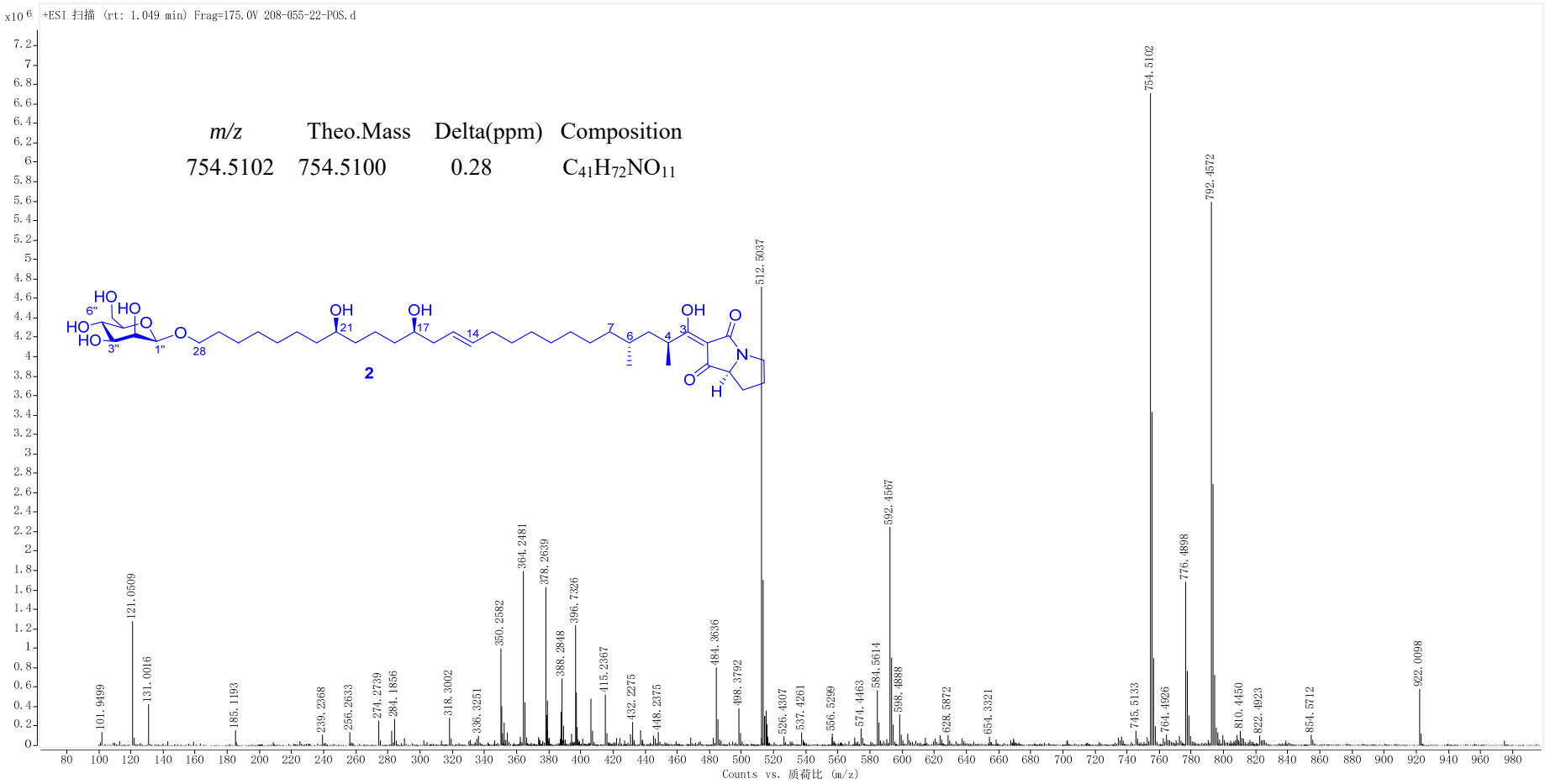

Figure S27. The (+)-HRESIMS spectrum of compound **2**.

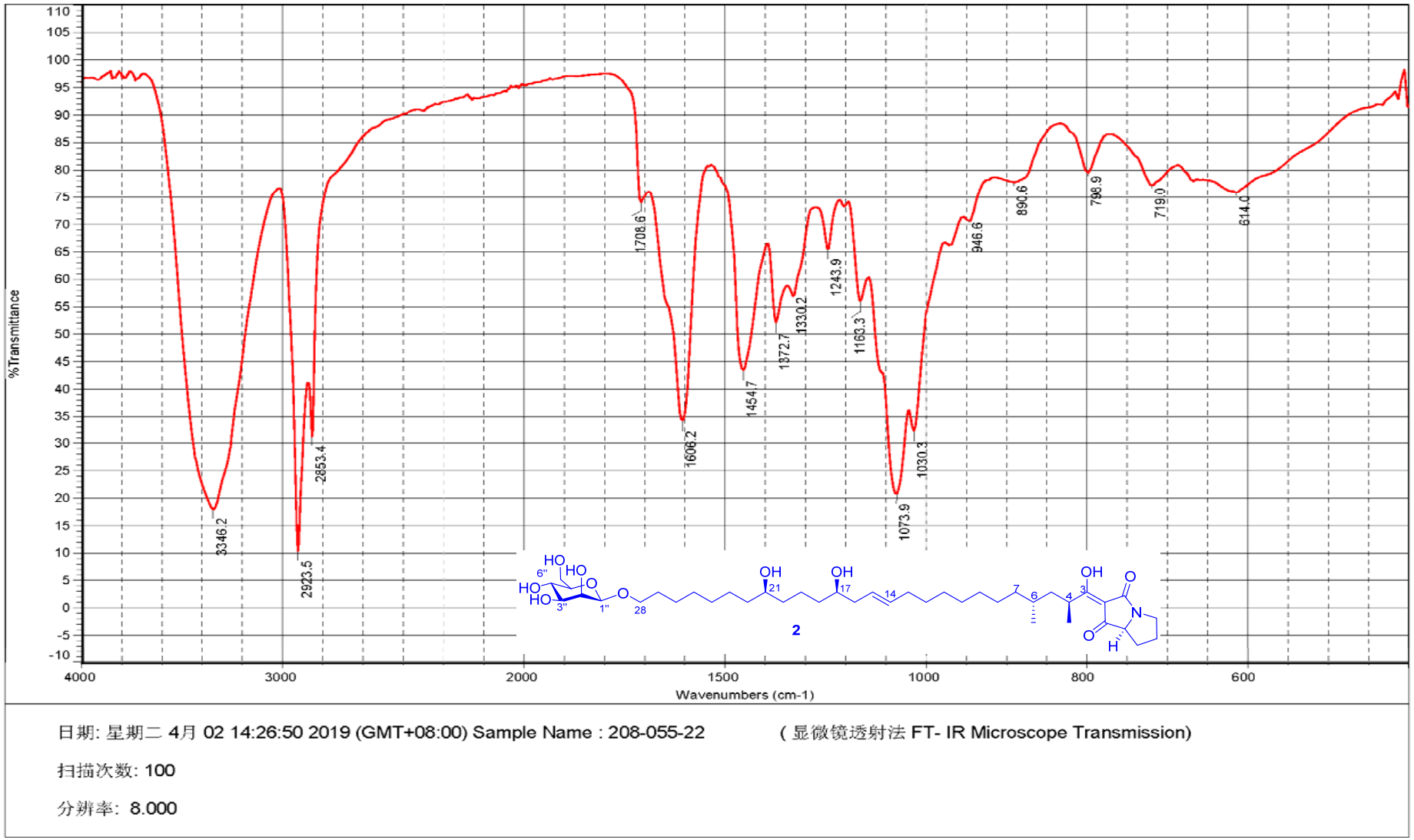

Figure S28. The IR spectrum of compound **2**.

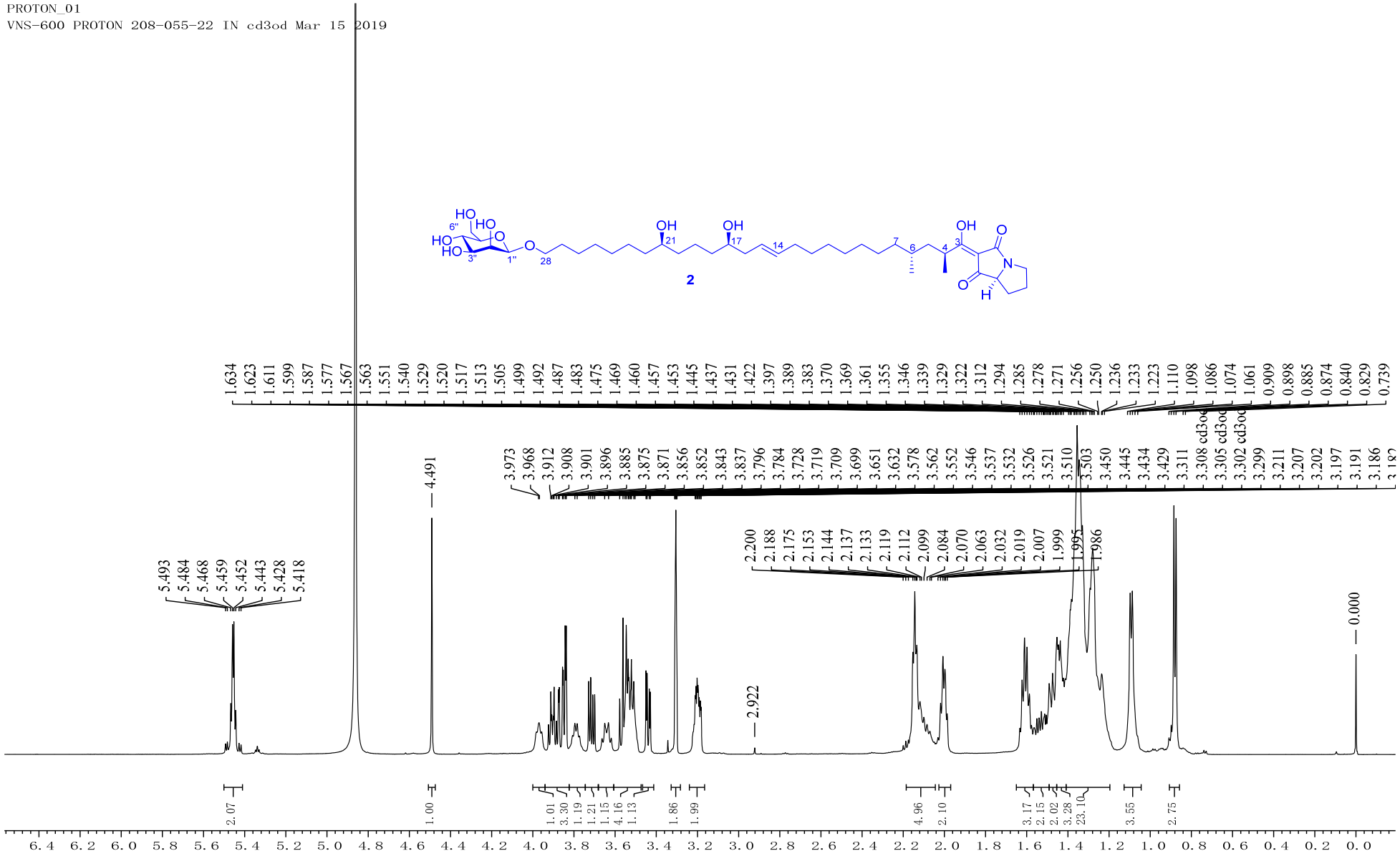

Figure S29. The ^{1}H NMR spectrum of compound **2** in CD_3OD (600 MHz).

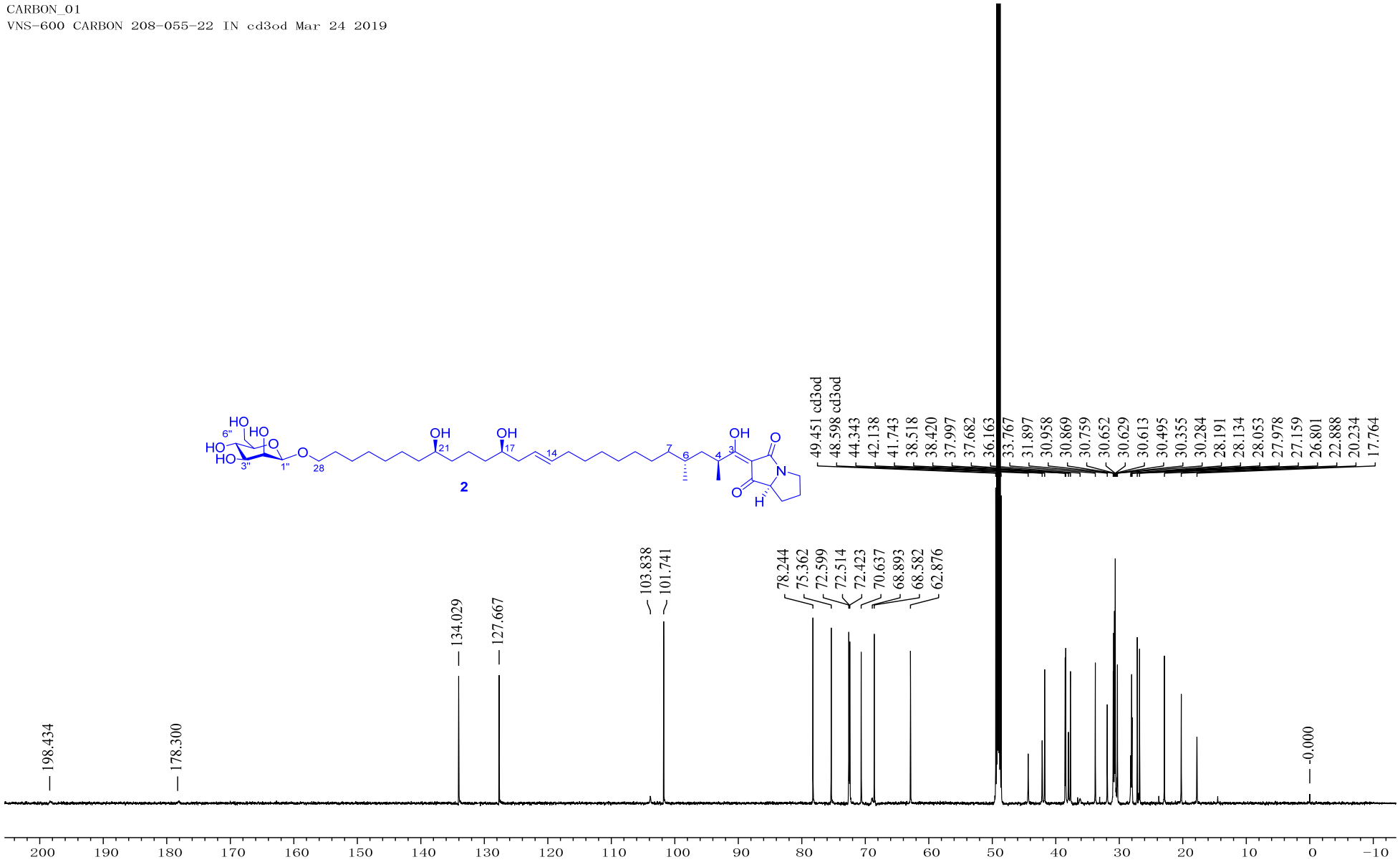

Figure S30. The ^{13}C NMR spectrum of compound **2** in CD_3OD (150 MHz).

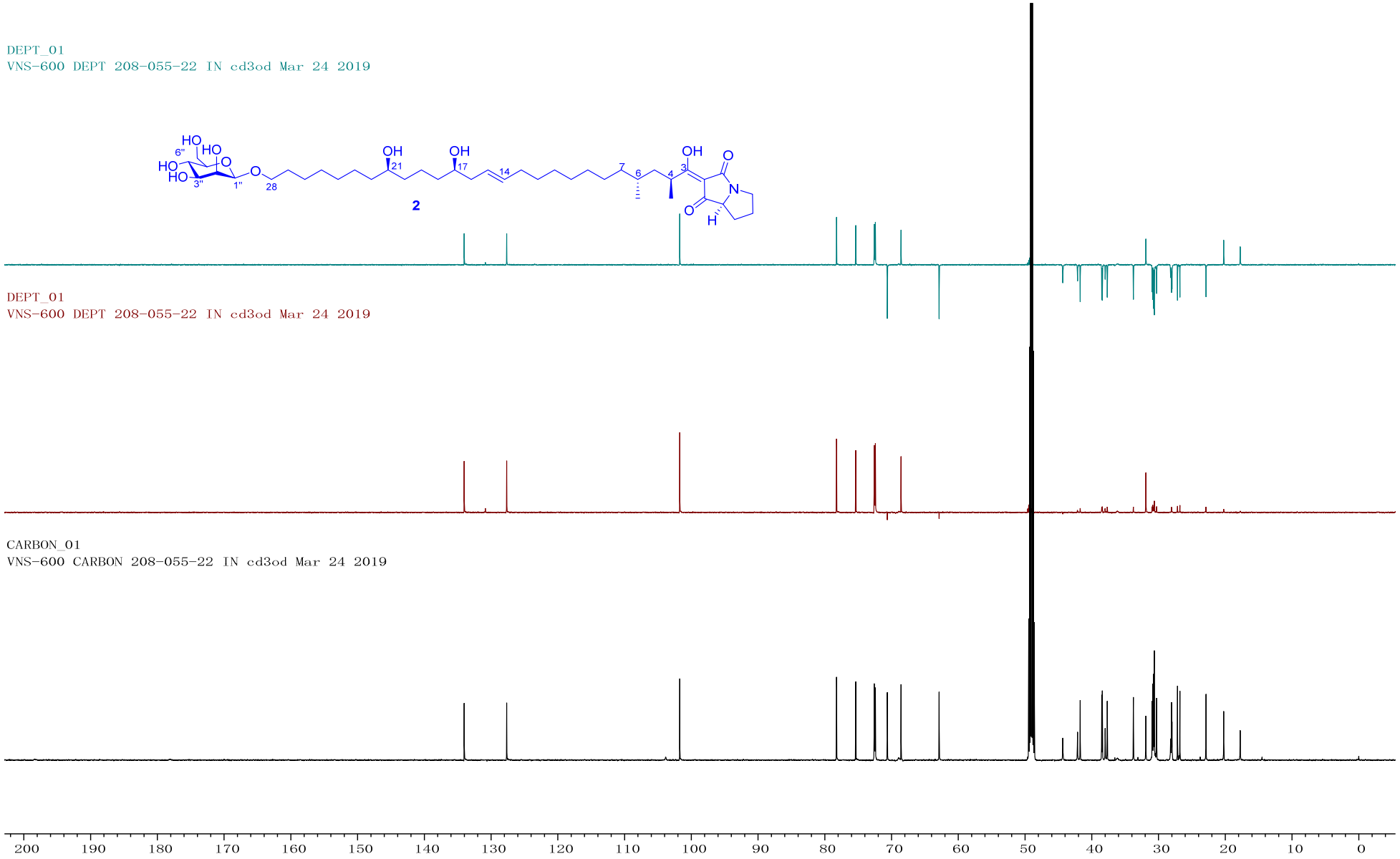

Figure S31. The DEPT spectrum of compound **2** in CD_3OD (150 MHz).

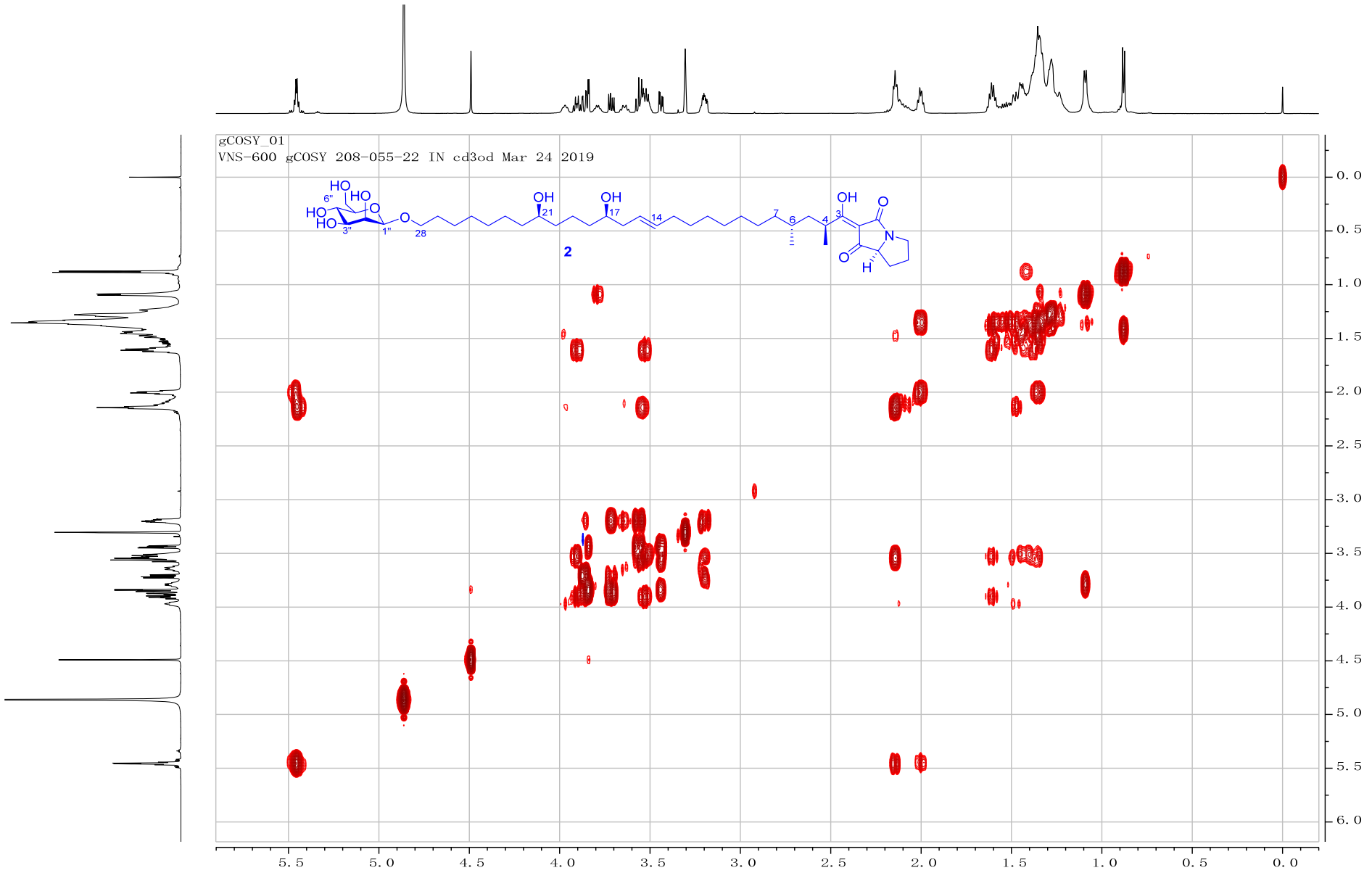

Figure S32. The ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD (600 MHz).

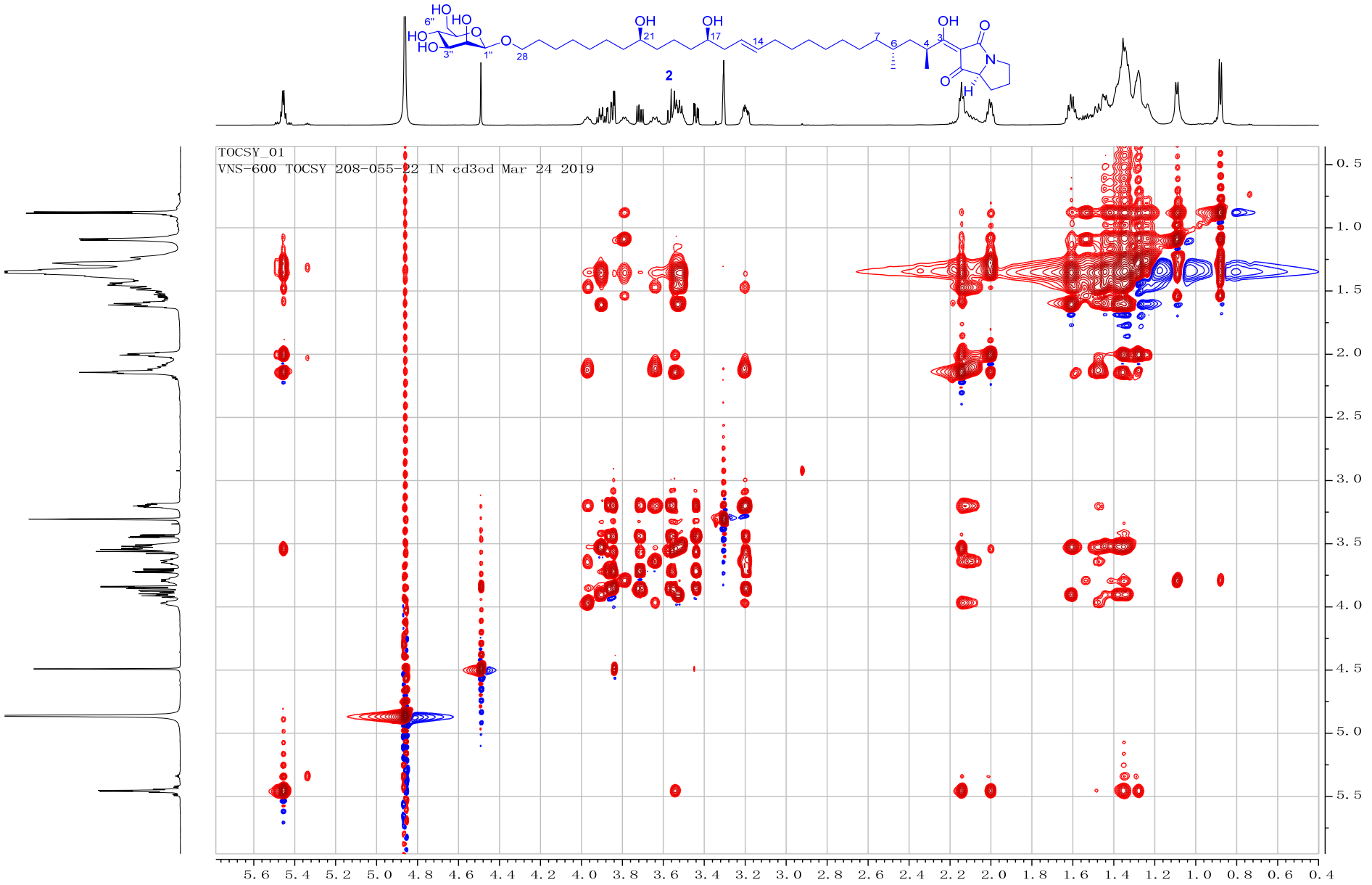

Figure S33. The TOCSY spectrum of compound **2** in CD_3OD (600 MHz).

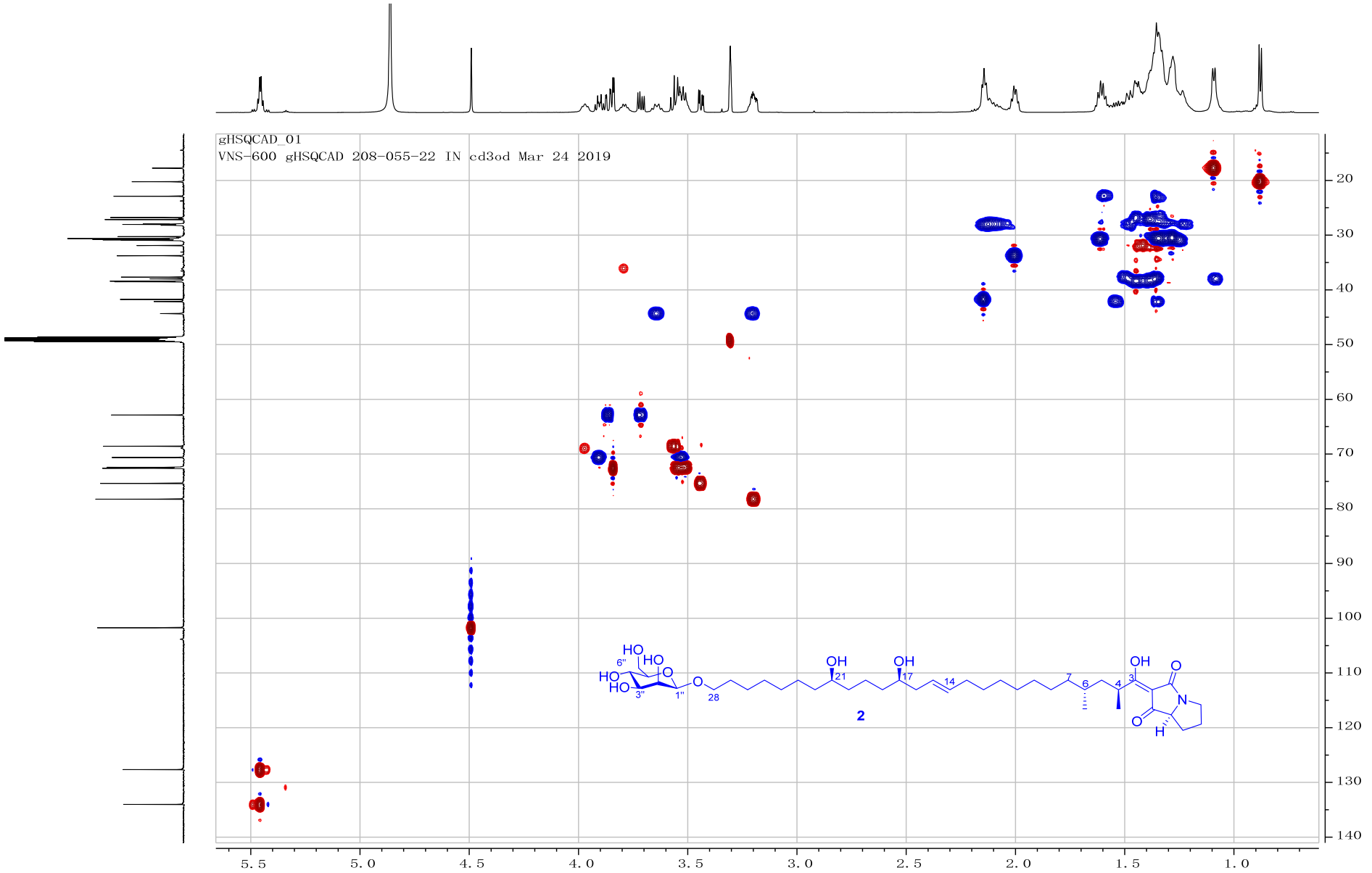

Figure S34. The HSQC spectrum of compound **2** in CD_3OD (600 MHz).

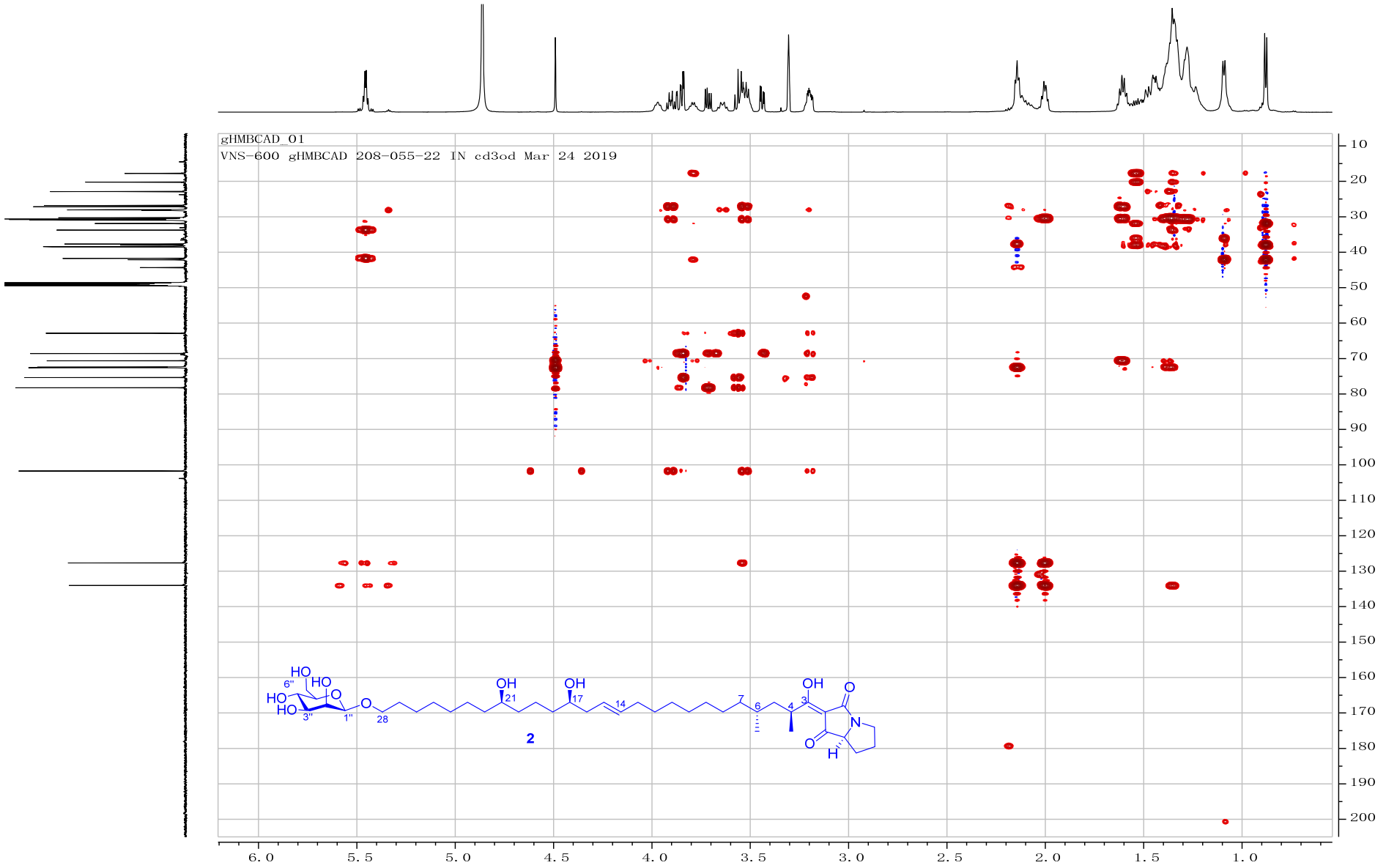

Figure S35. The HMBC spectrum of compound **2** in CD_3OD (600 MHz).

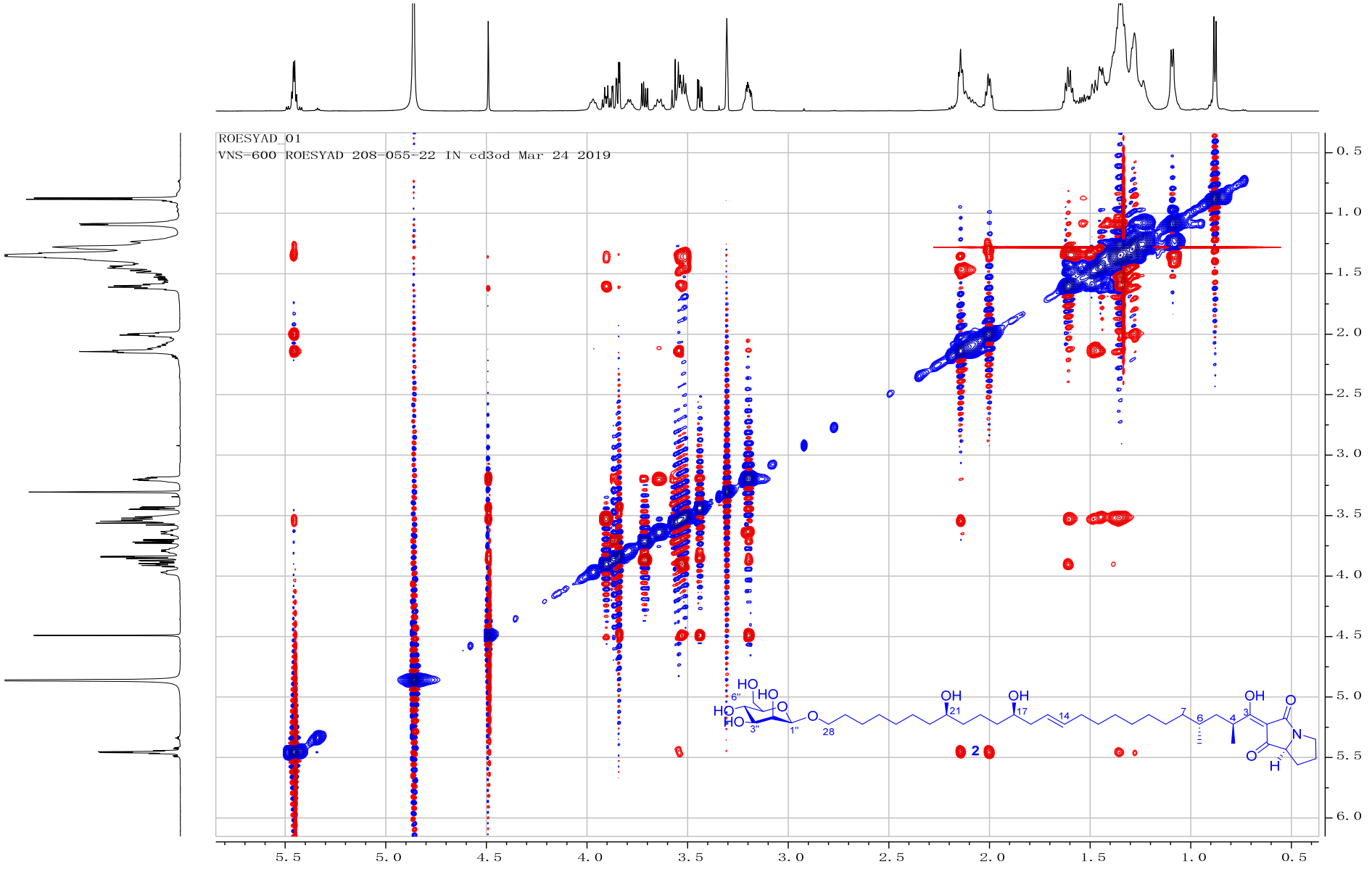

Figure S36. The ROESY spectrum of compound **2** in CD_3OD (600 MHz).

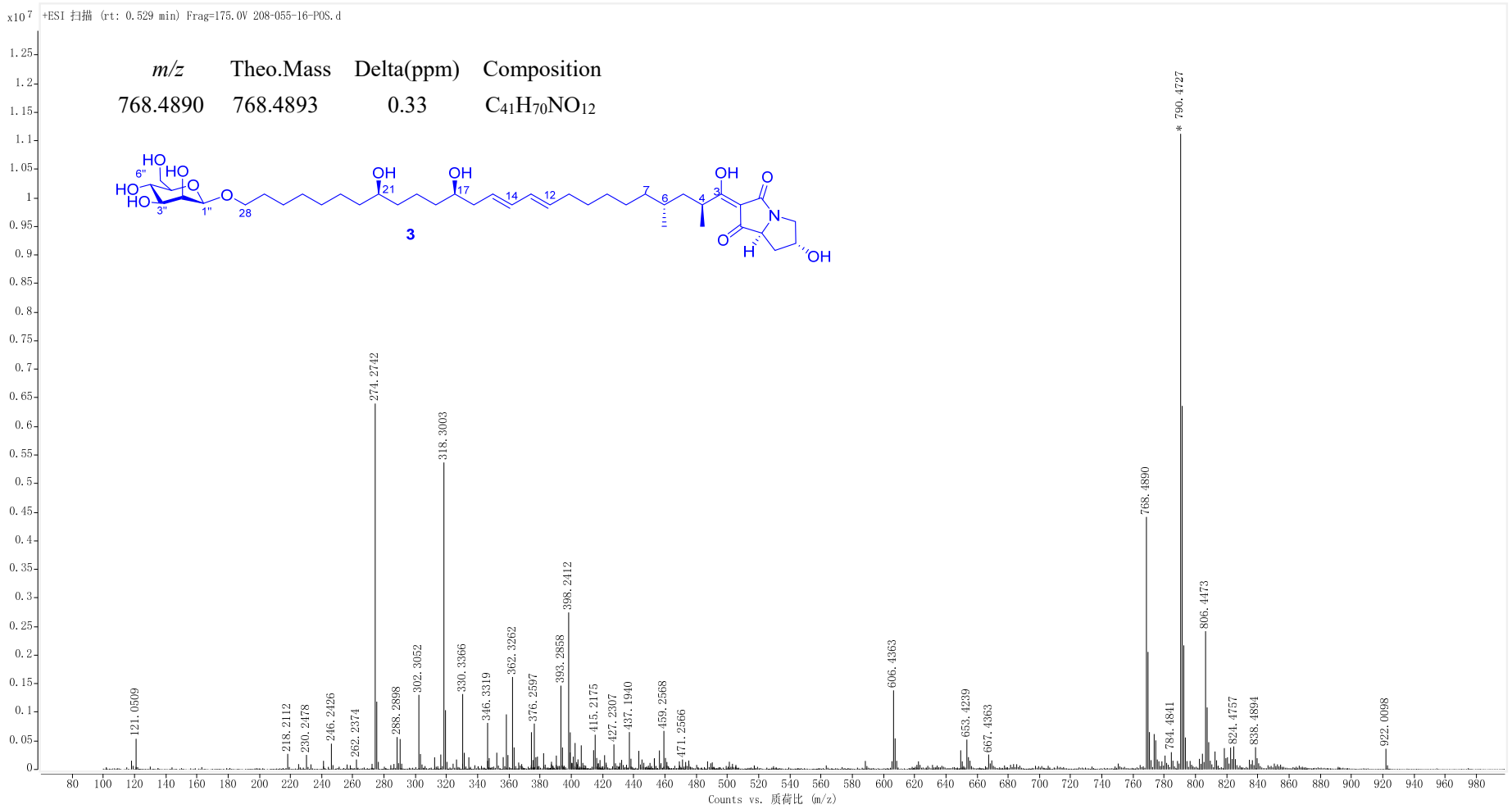

Figure S37. The (+)-HRESIMS spectrum of compound **3**

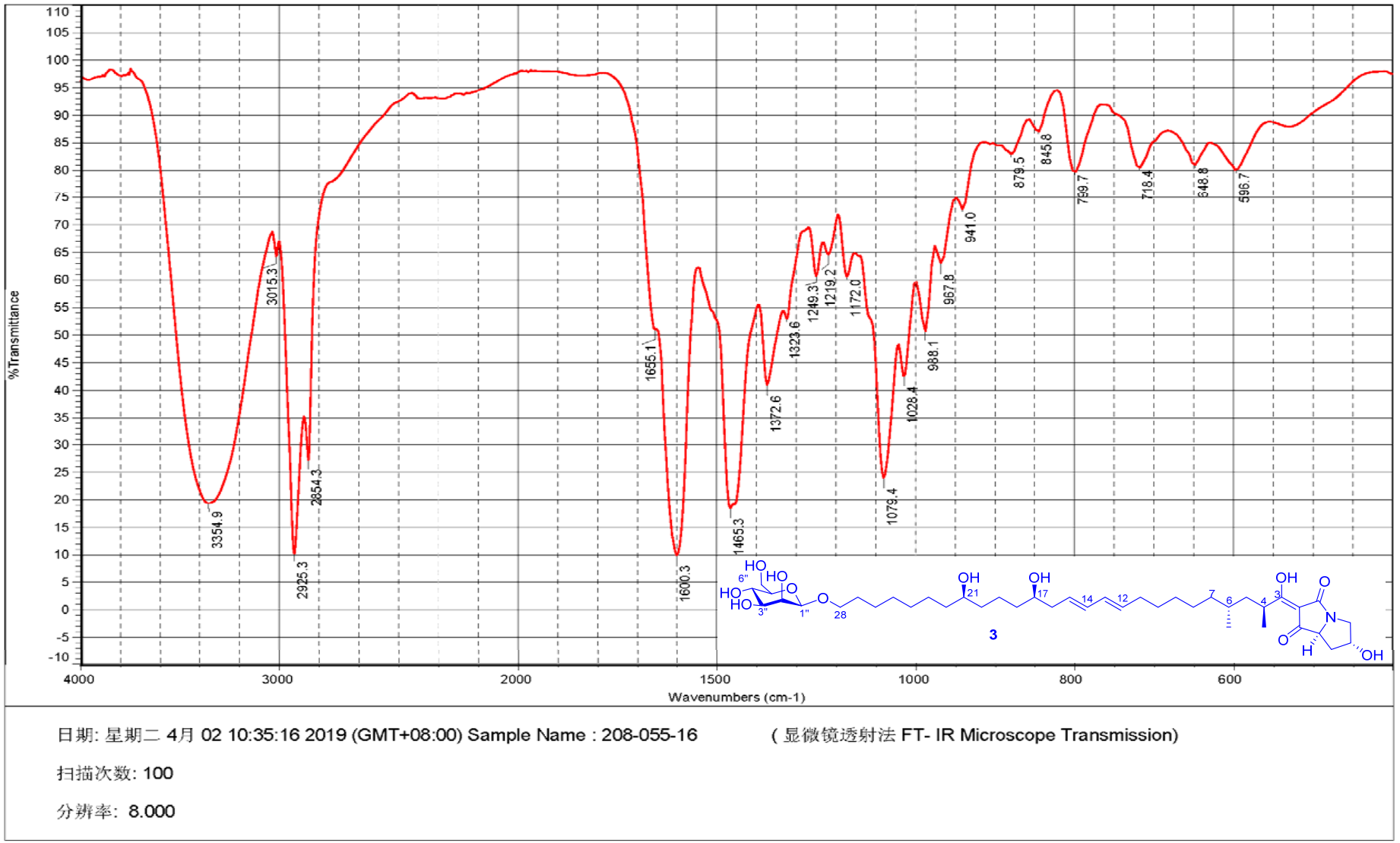

Figure S38. The IR spectrum of compound **3**.

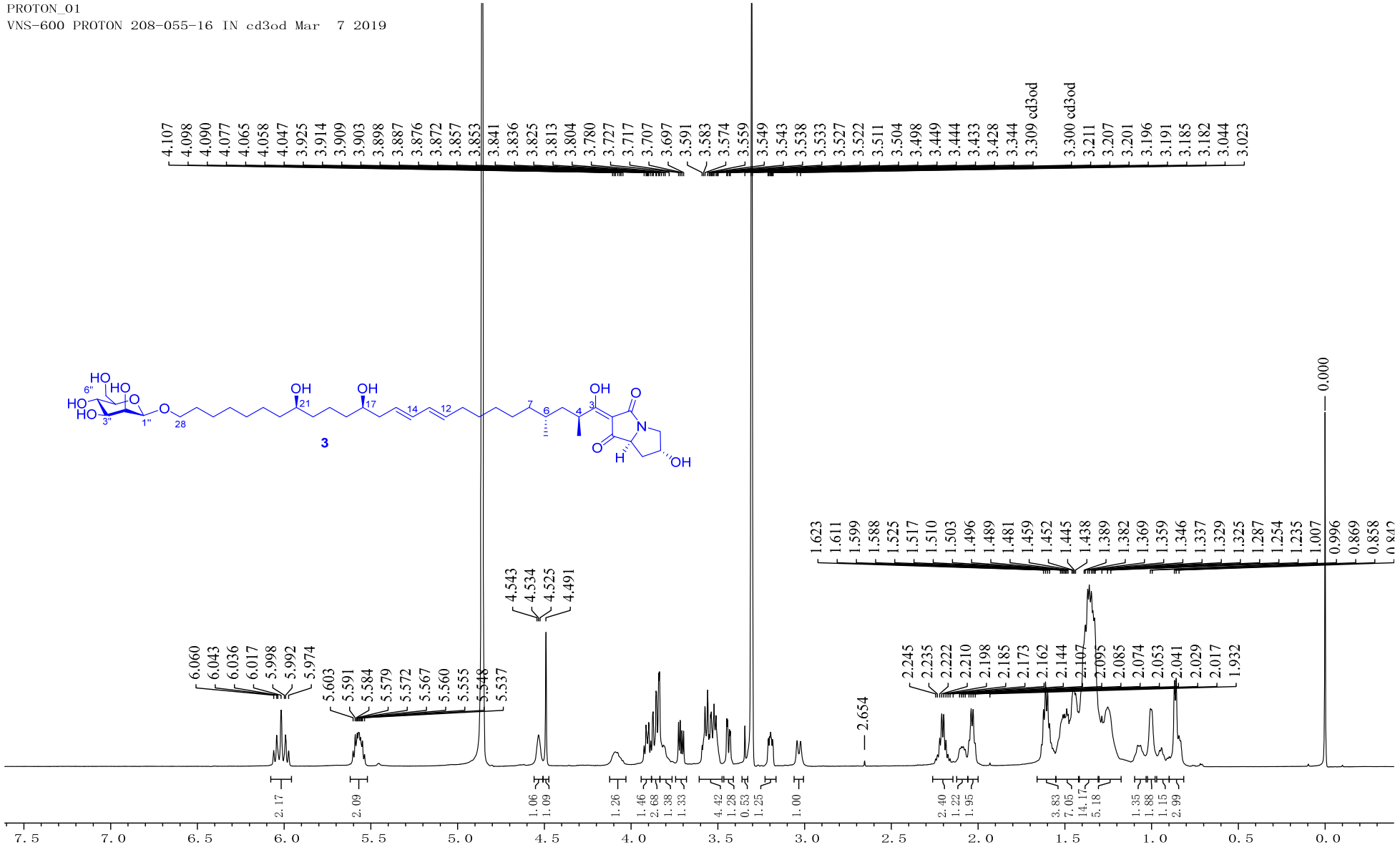

Figure S39. The ^{1}H NMR spectrum of compound **3** in CD_3OD (600 MHz).

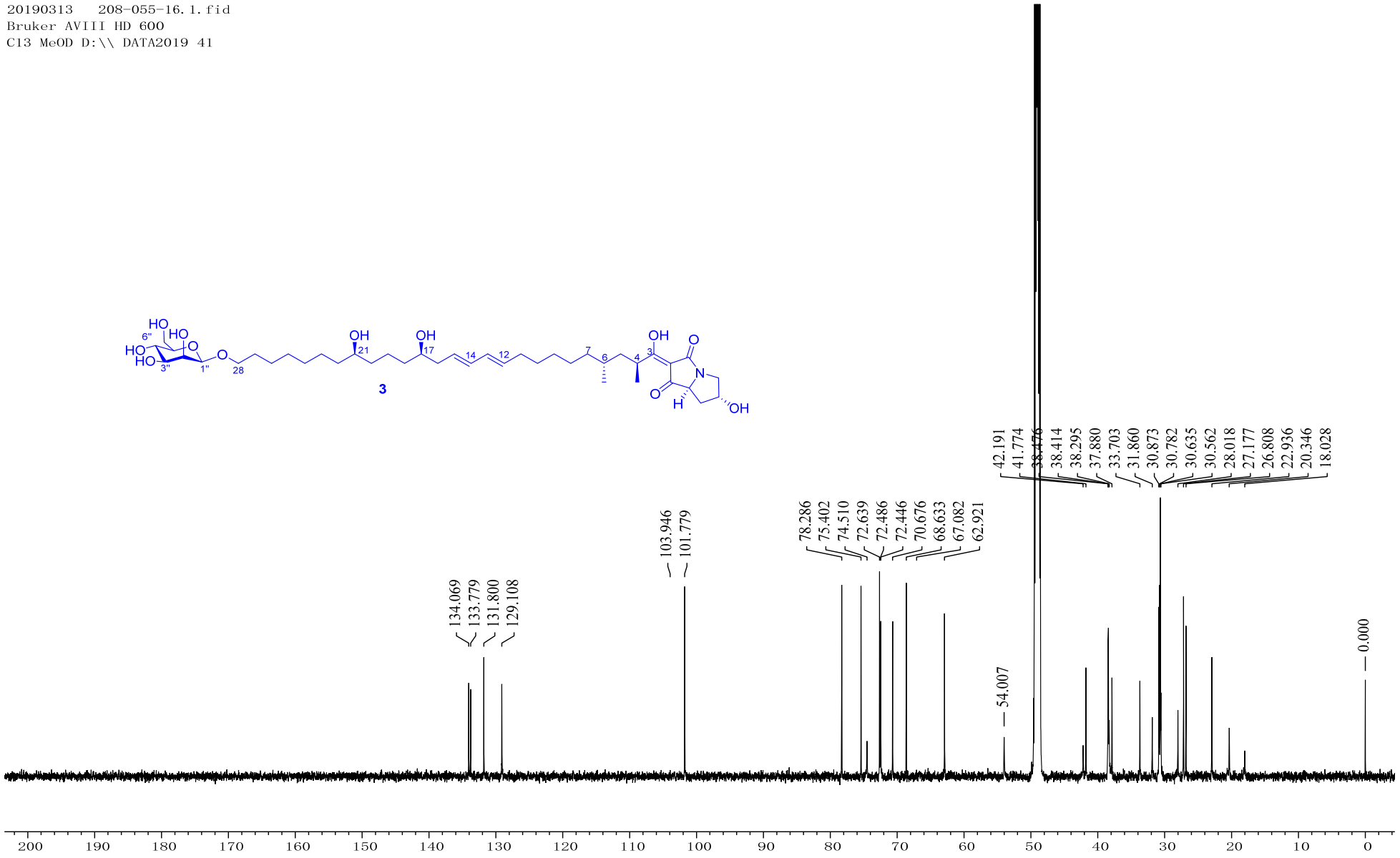

Figure S40. The ^{13}C NMR spectrum of compound **3** in CD_3OD (150 MHz).

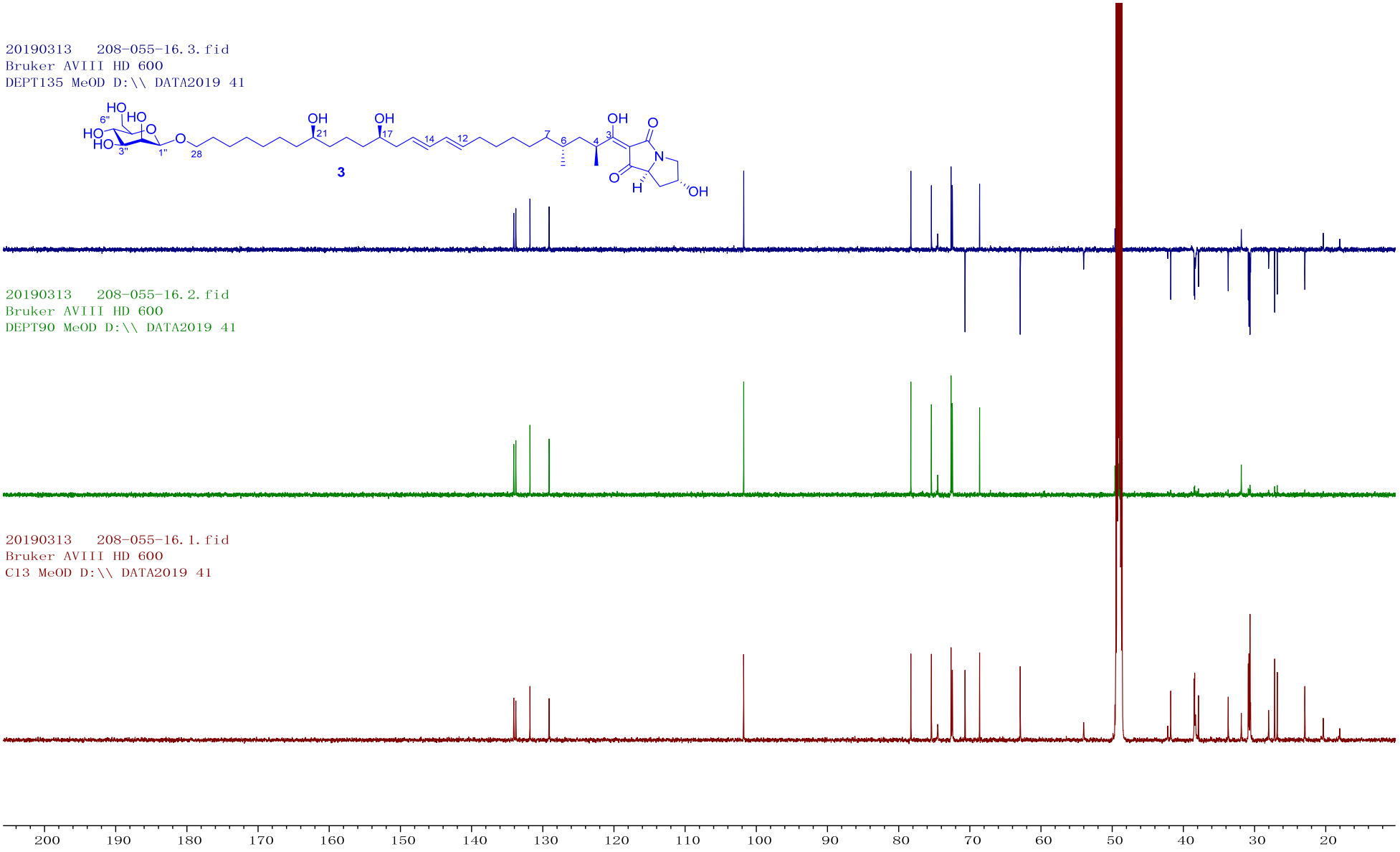

Figure S41. The DEPT spectrum of compound **3** in CD_3OD (150 MHz).

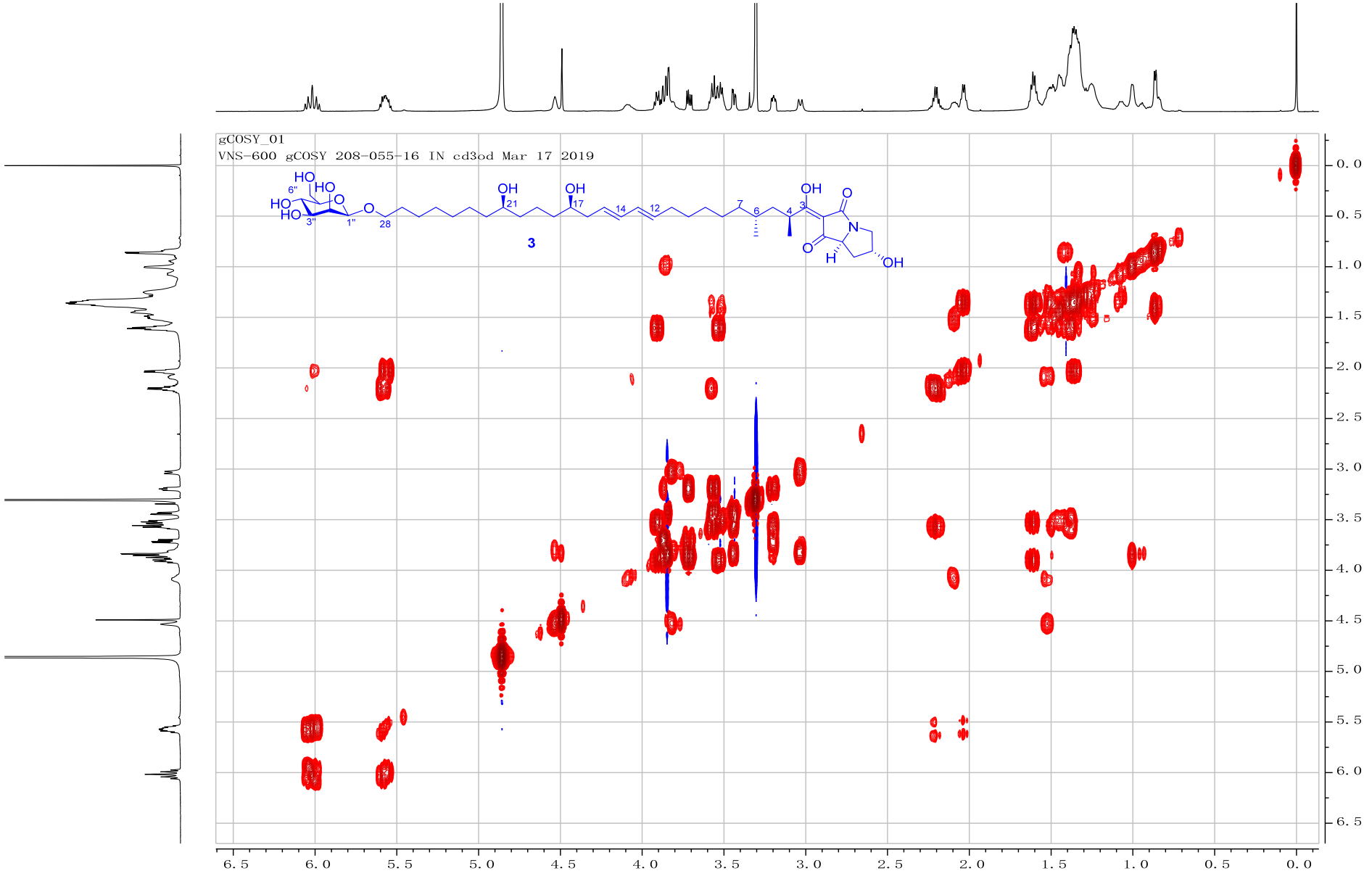

Figure S42. The ^{1}H-^{1}H COSY spectrum of compound **3** in CD_3OD (600 MHz).

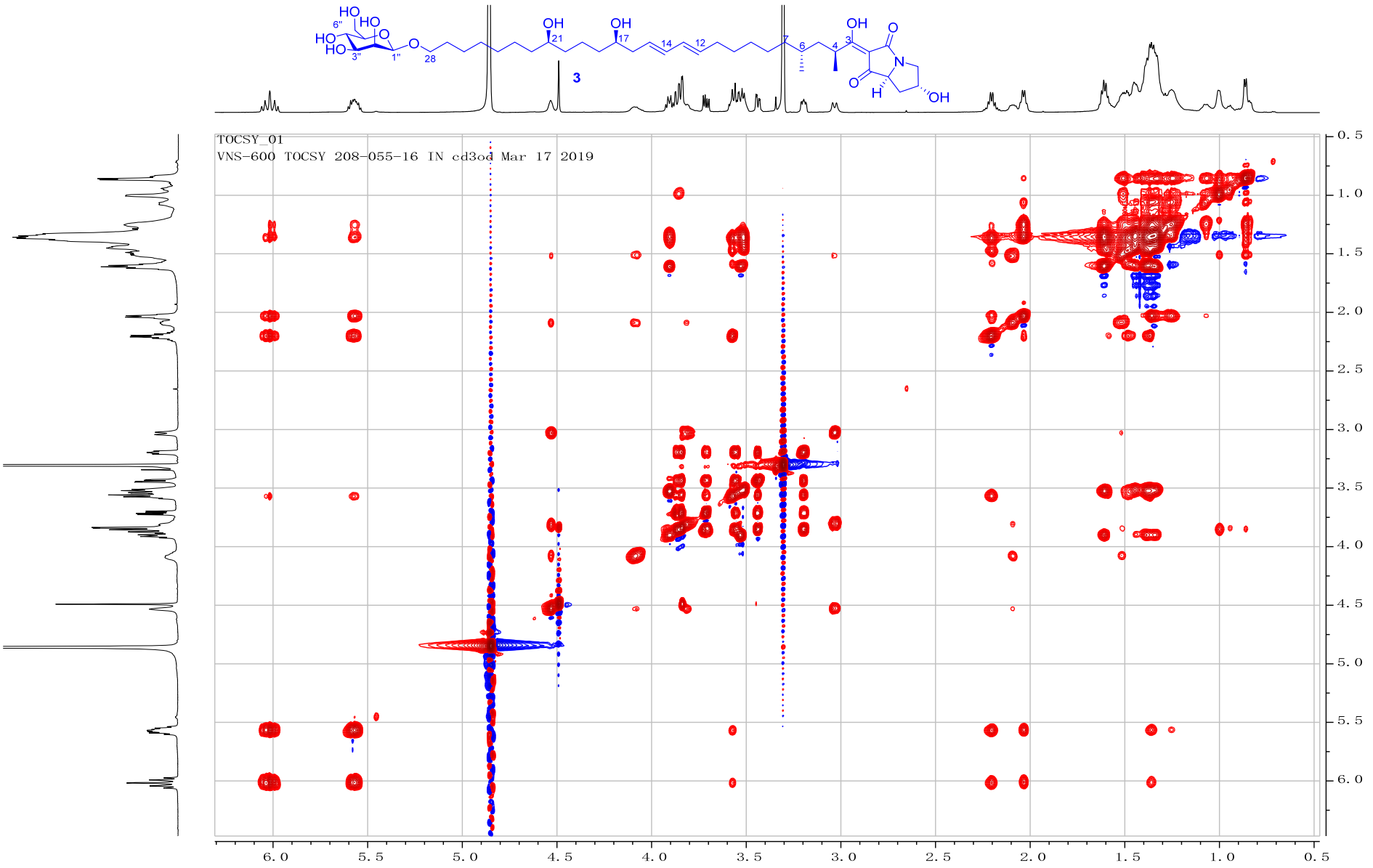

Figure S43. The TOCSY spectrum of compound **3** in CD_3OD (600 MHz).

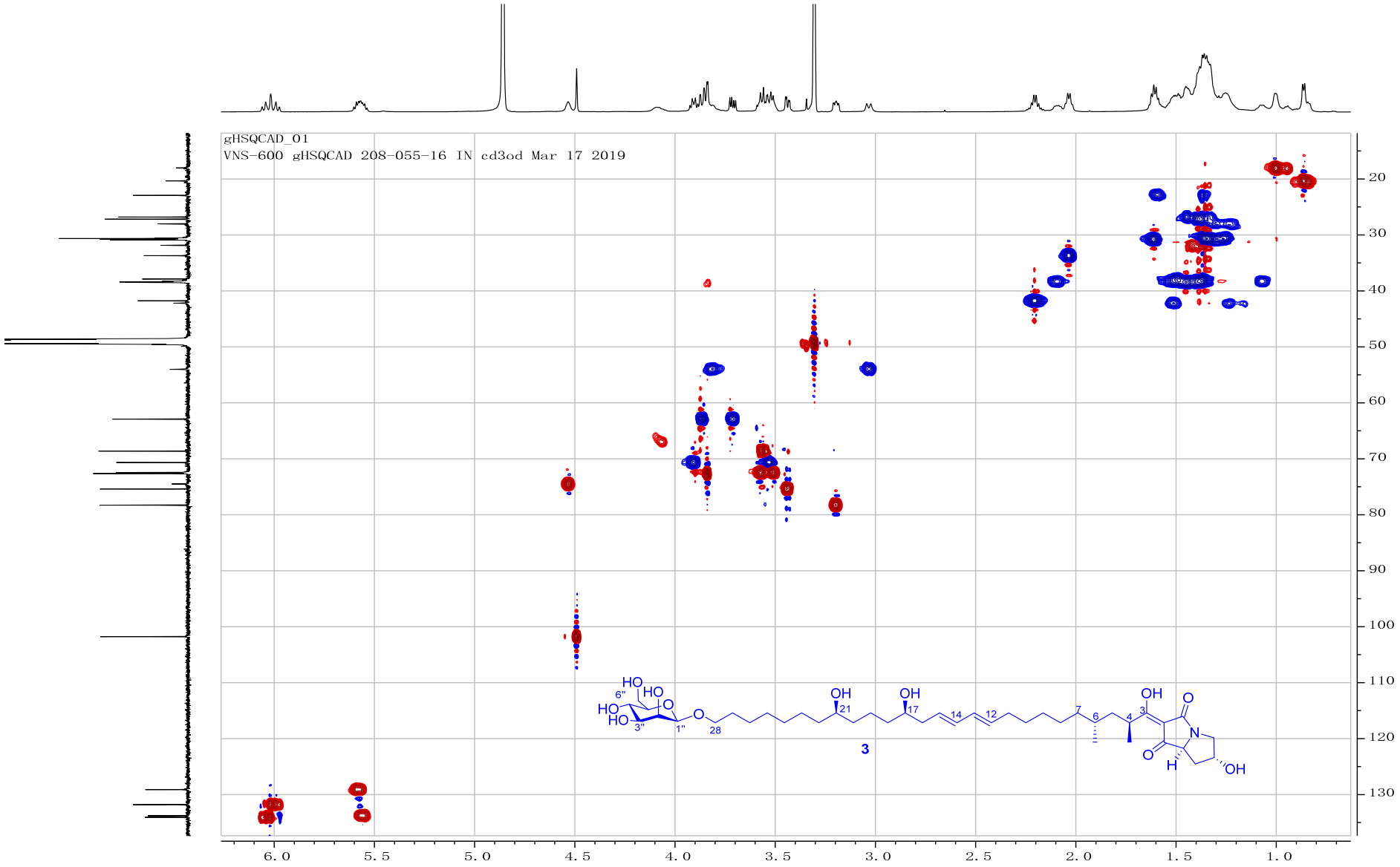

Figure S44. The HSQC spectrum of compound **3** in CD_3OD (600 MHz).

Figure S45. The HMBC spectrum of compound **3** in CD_3OD (600 MHz).

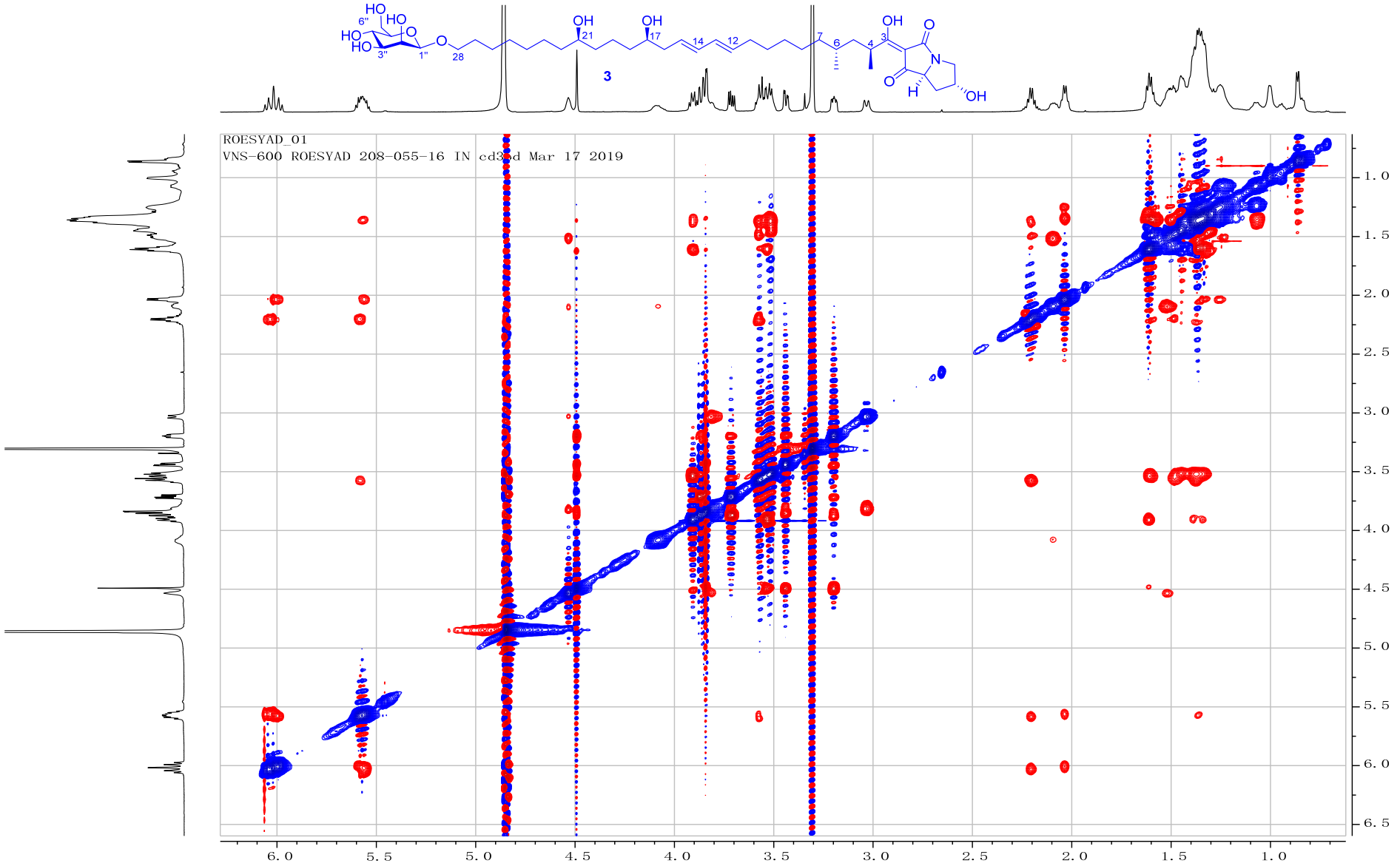

Figure S46. The ROESY spectrum of compound **3** in CD_3OD (600 MHz).

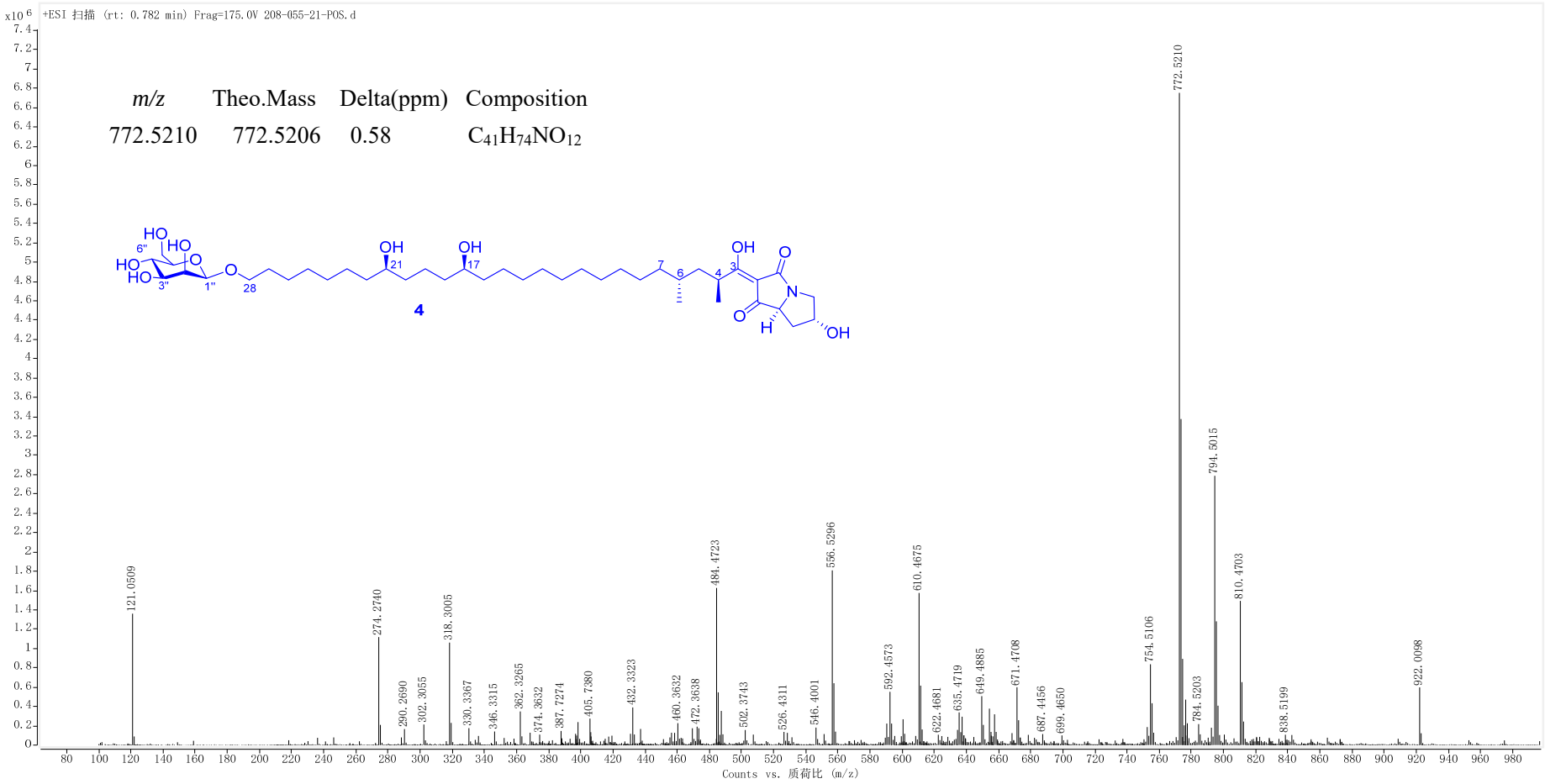

Figure S47. The (+)-HRESIMS spectrum of compound **4**.

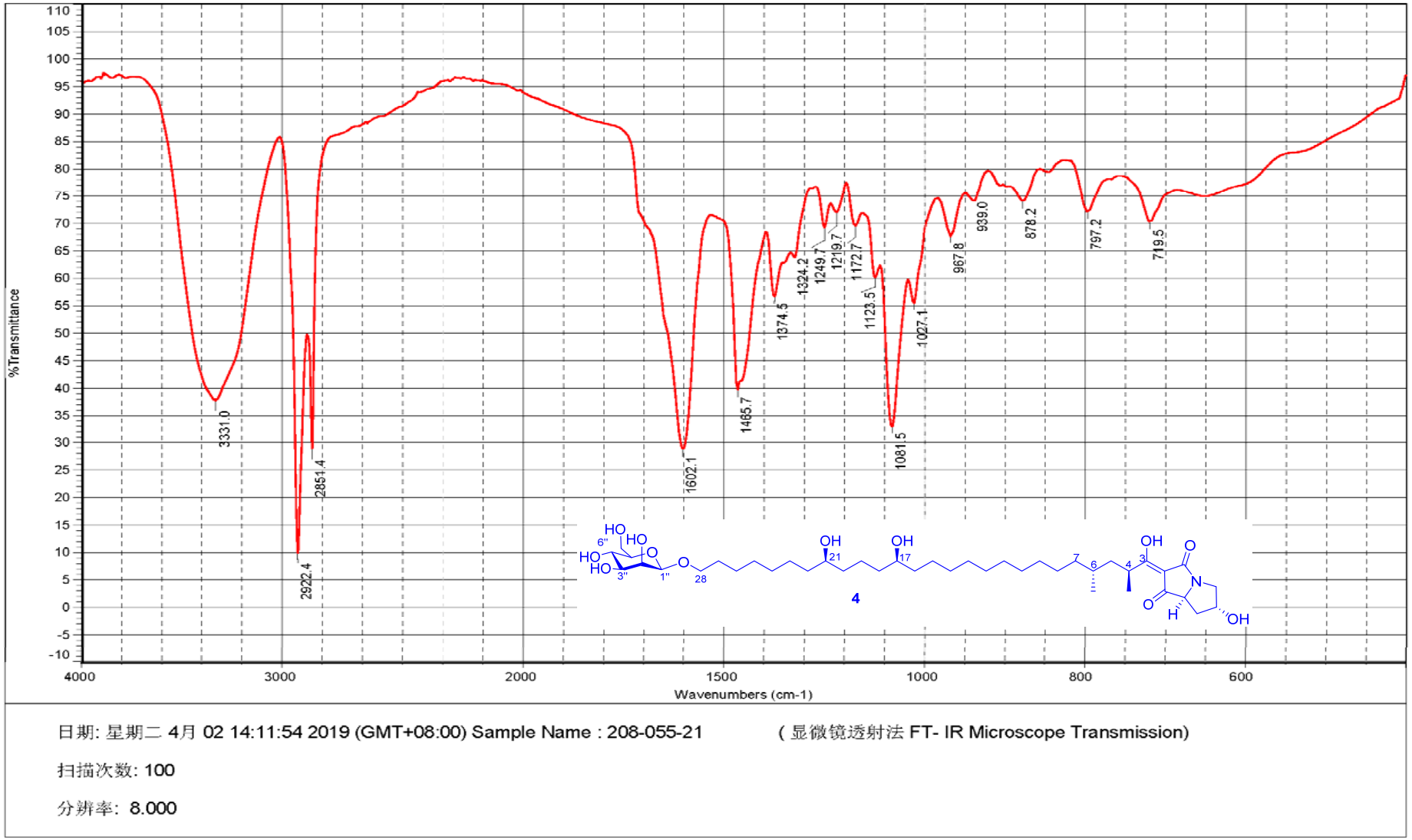

Figure S48. The IR spectrum of compound **4**.

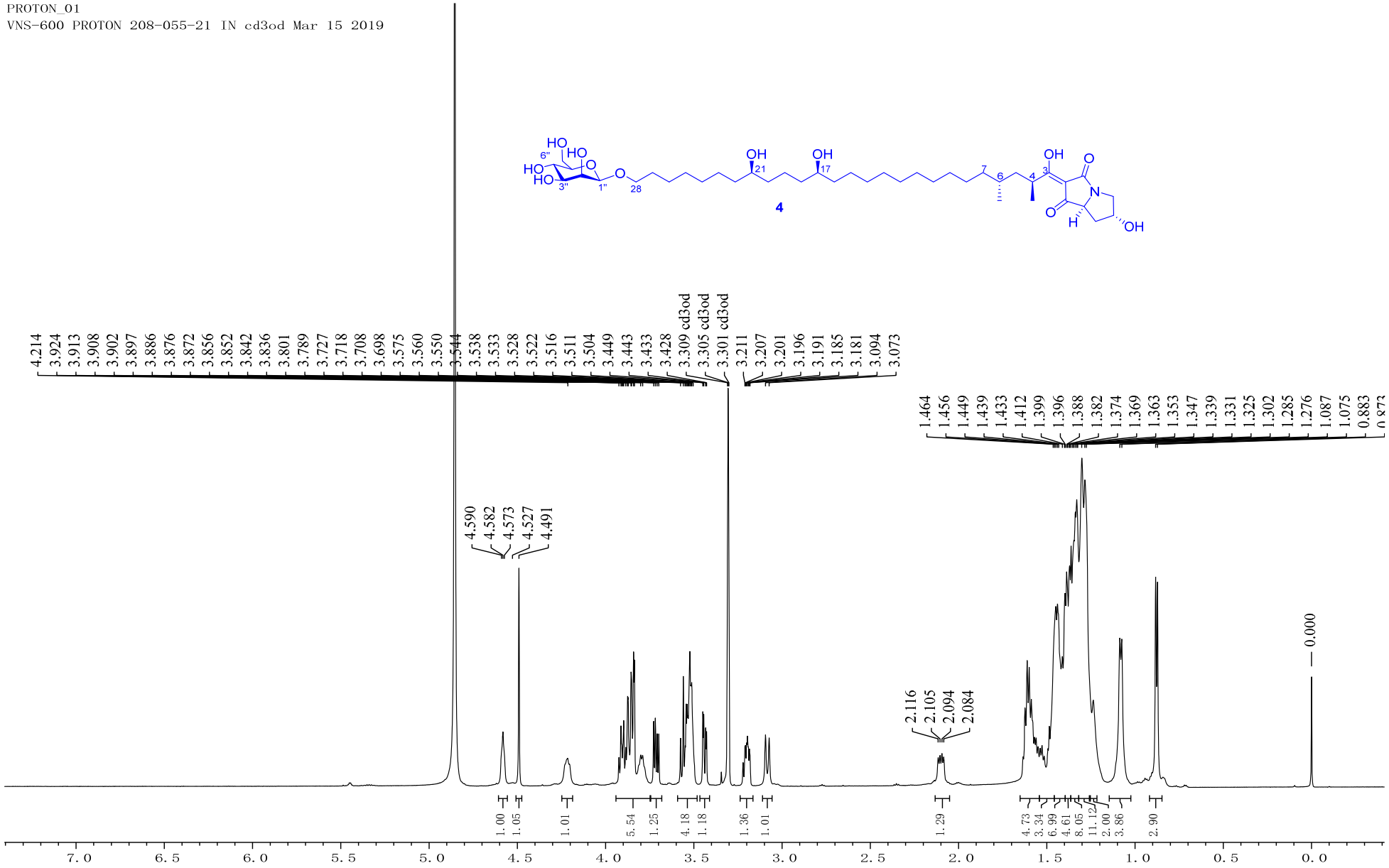

Figure S49. The ^{1}H NMR spectrum of compound **4** in CD_3OD (600 MHz).

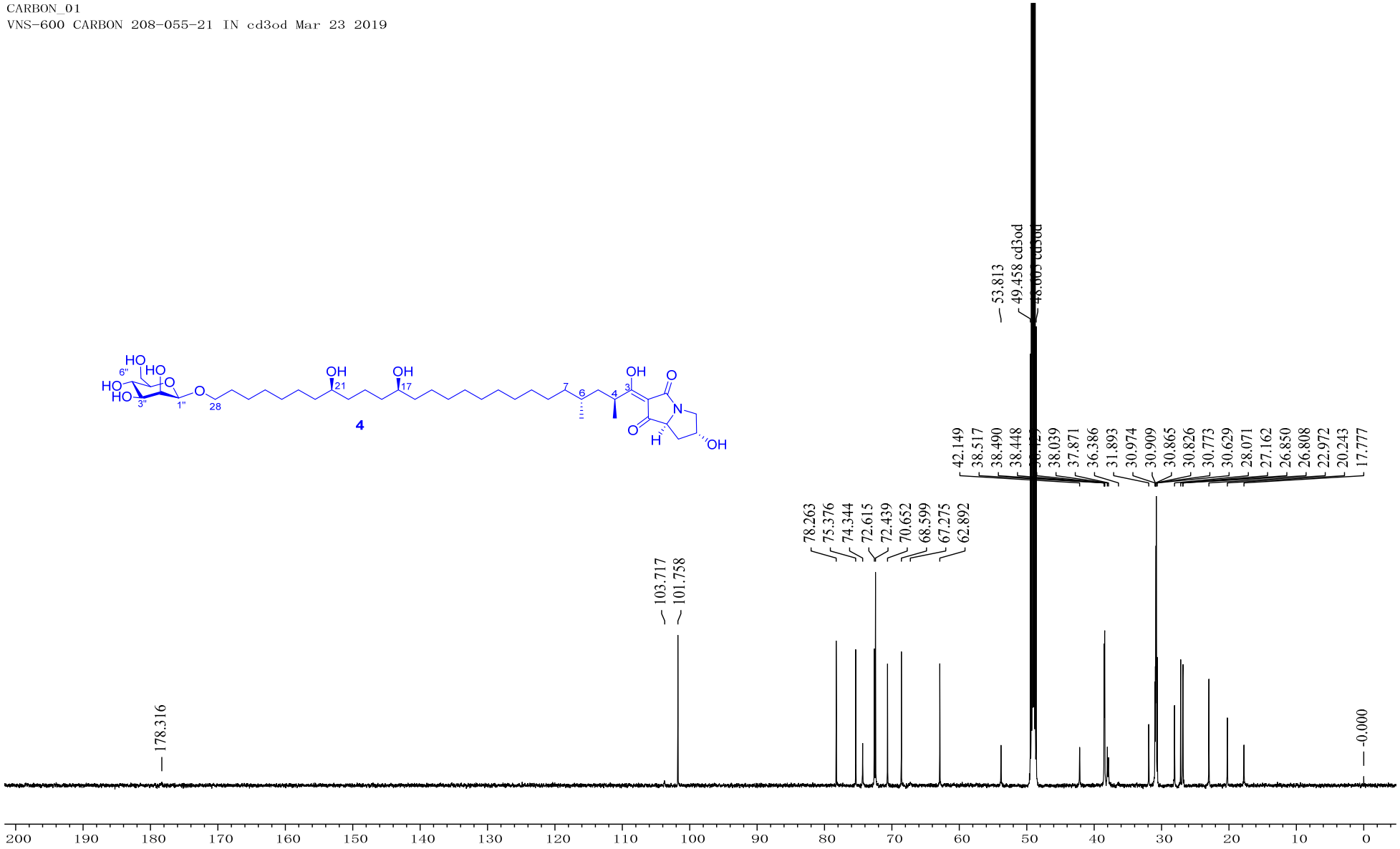

Figure S50. The ^{13}C NMR spectrum of compound **4** in CD_3OD (150 MHz).

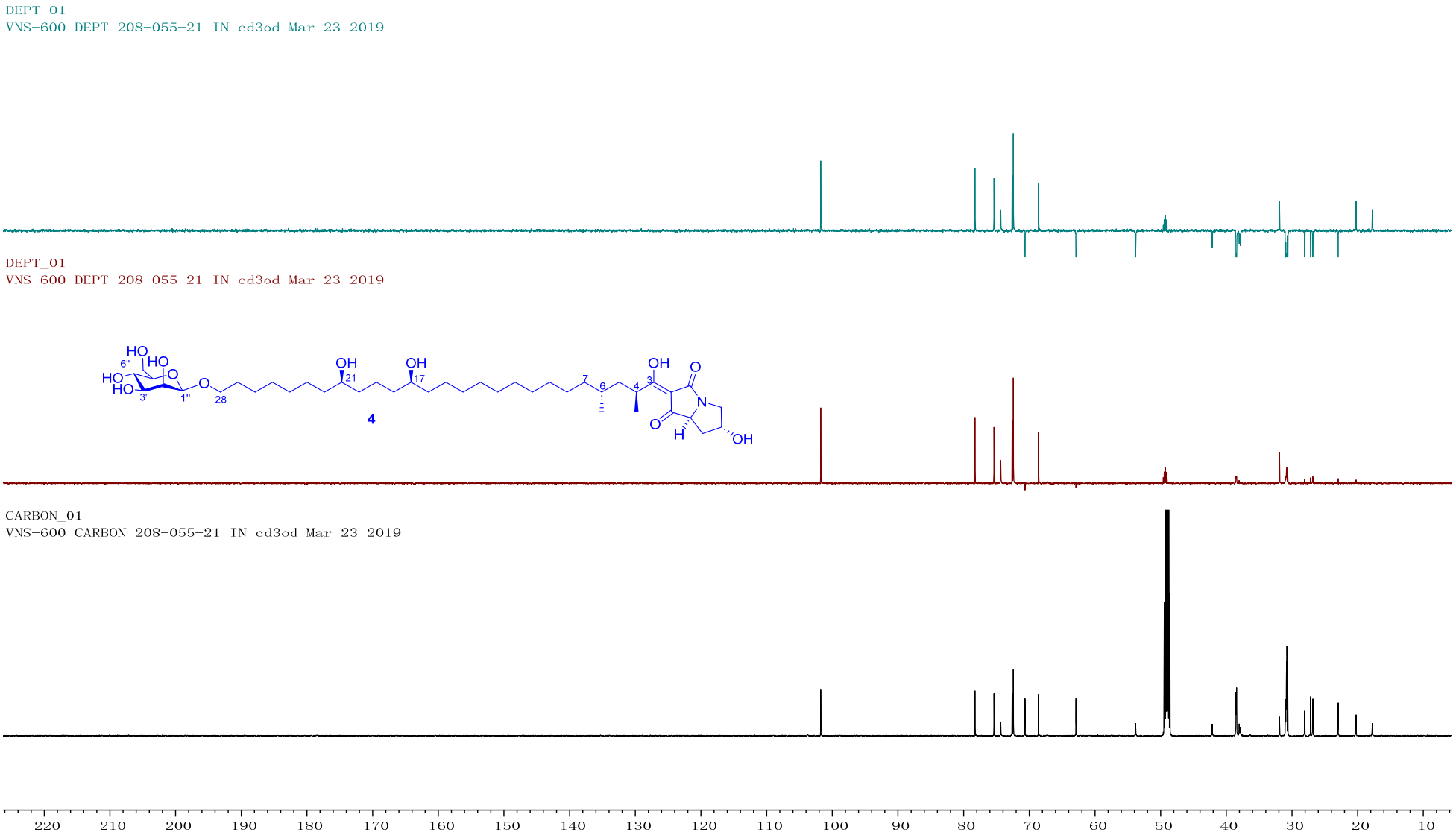

Figure S51. The DEPT spectrum of compound **4** in CD_3OD (150 MHz).

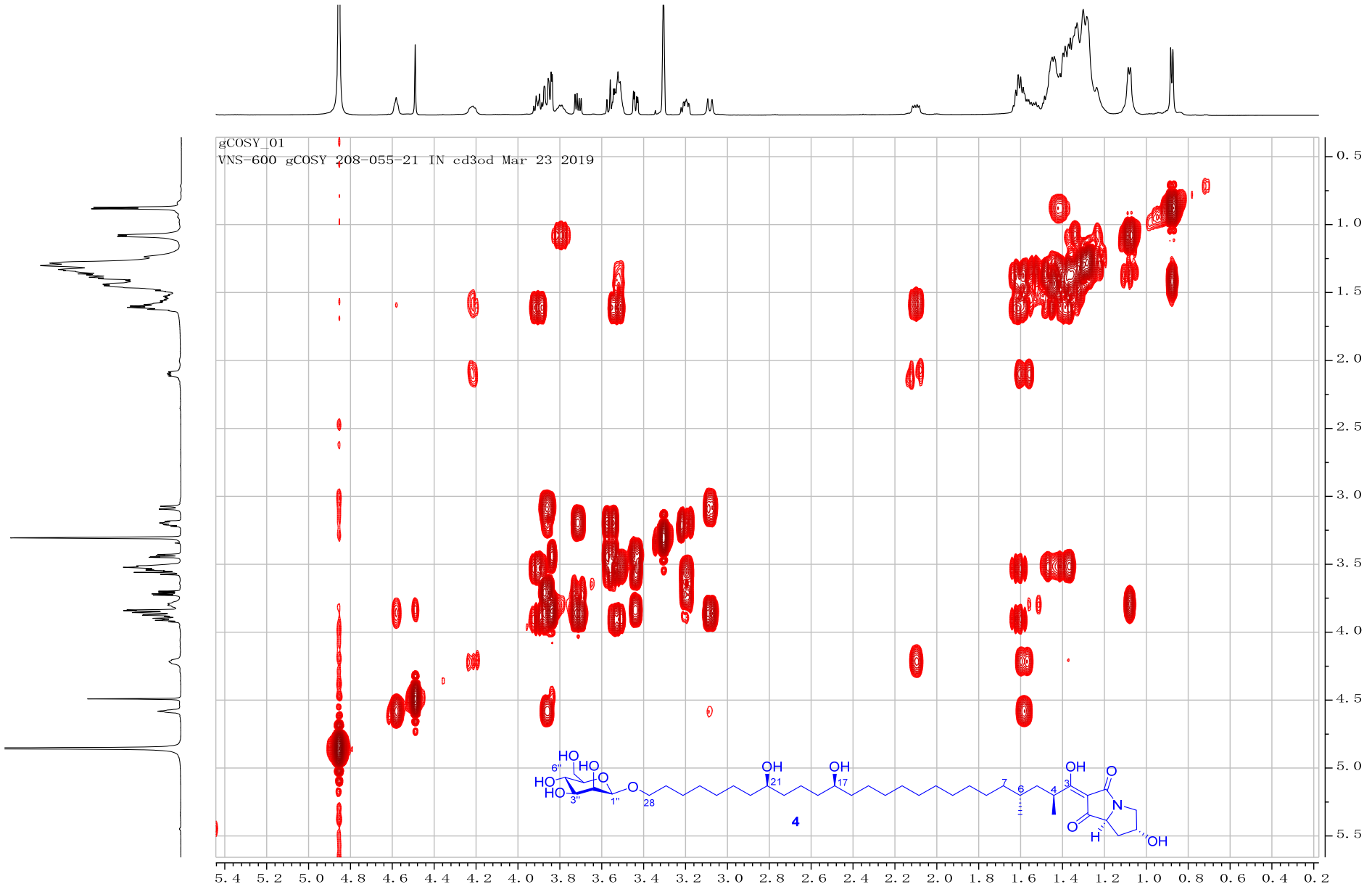

Figure S52. The ^{1}H-^{1}H COSY spectrum of compound **4** in CD_3OD (600 MHz).

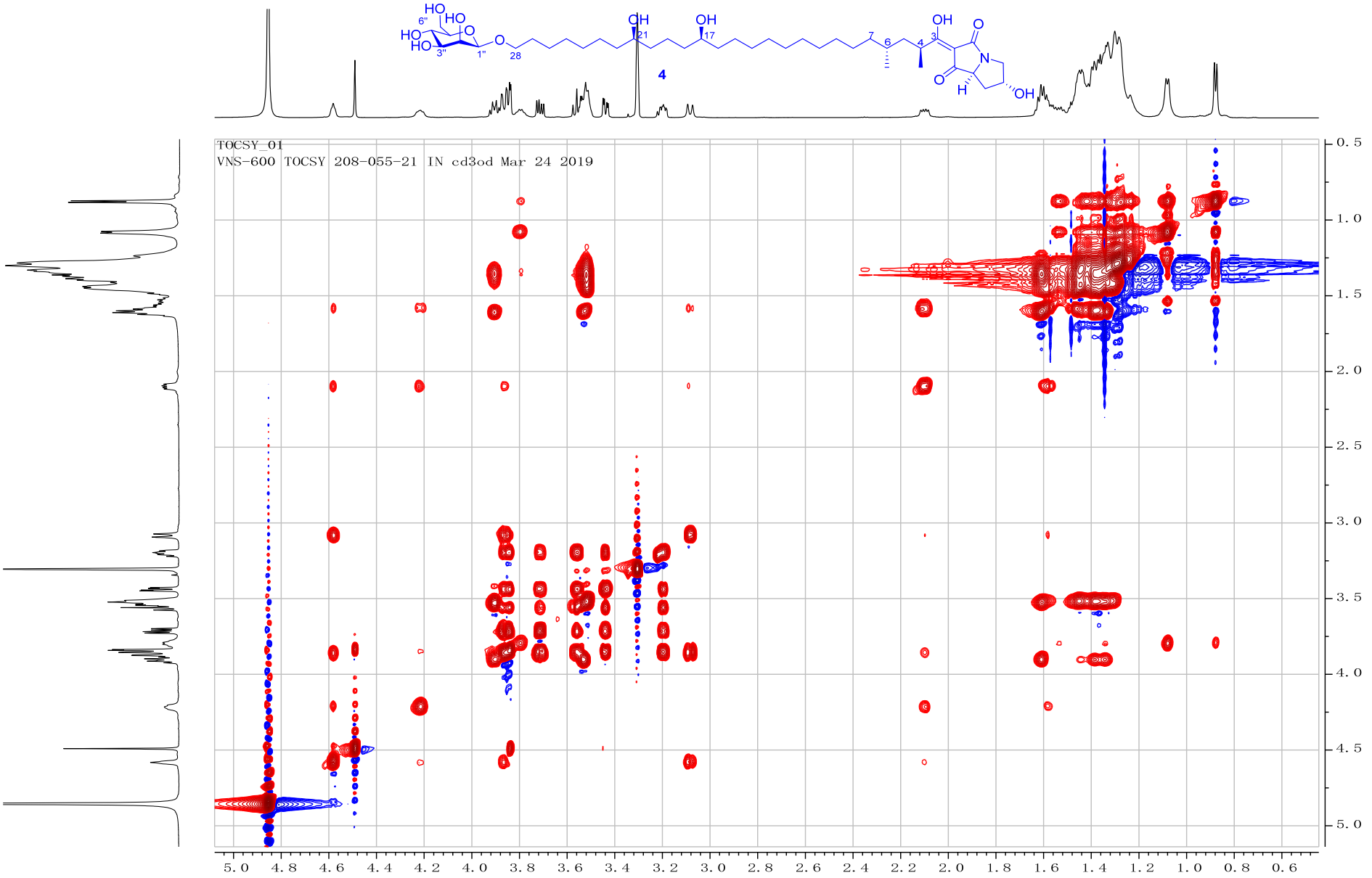

Figure S53. The TOCSY spectrum of compound **4** in CD_3OD (600 MHz).

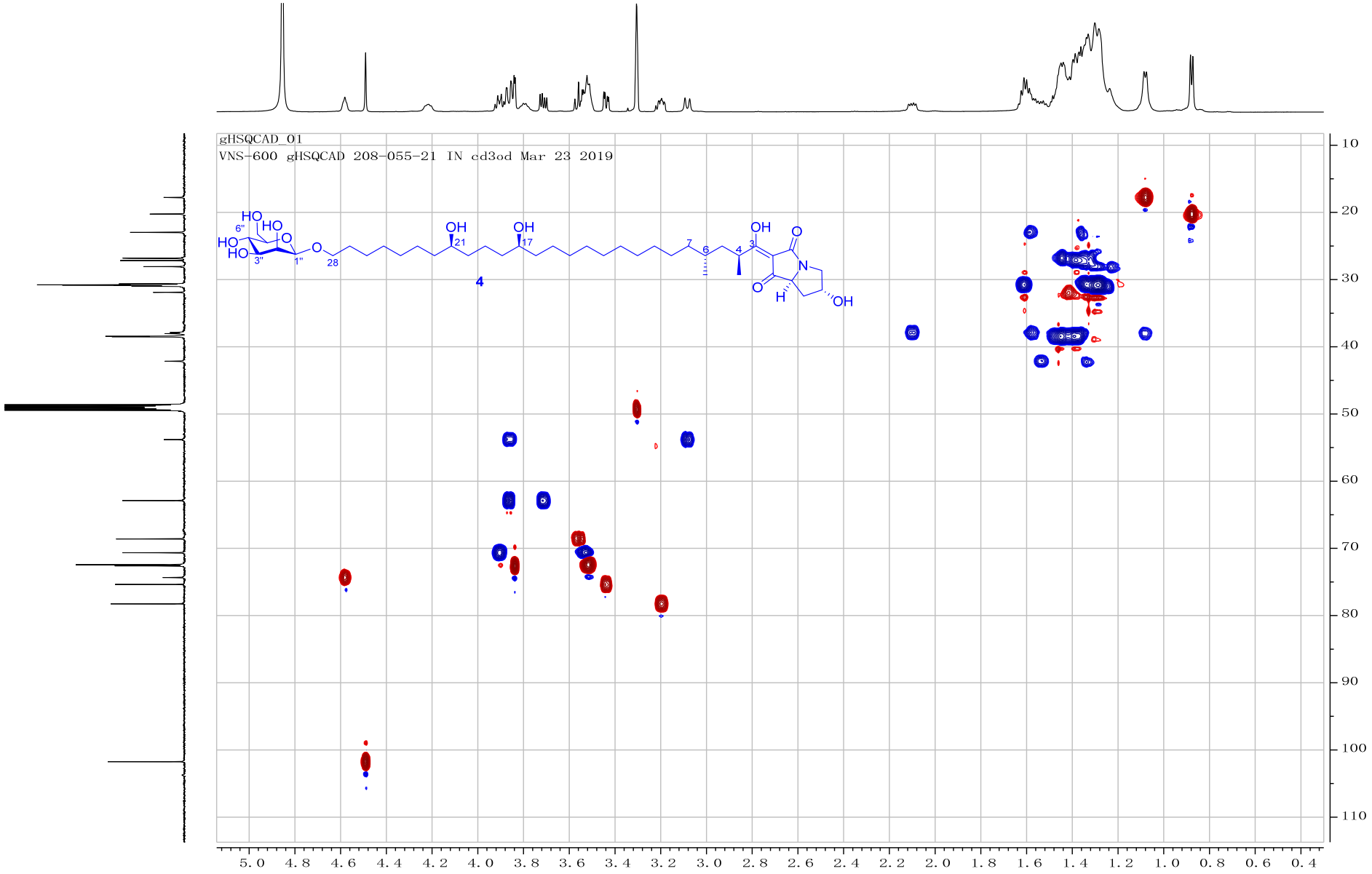

Figure S54. The HSQC spectrum of compound **4** in CD_3OD (600 MHz).

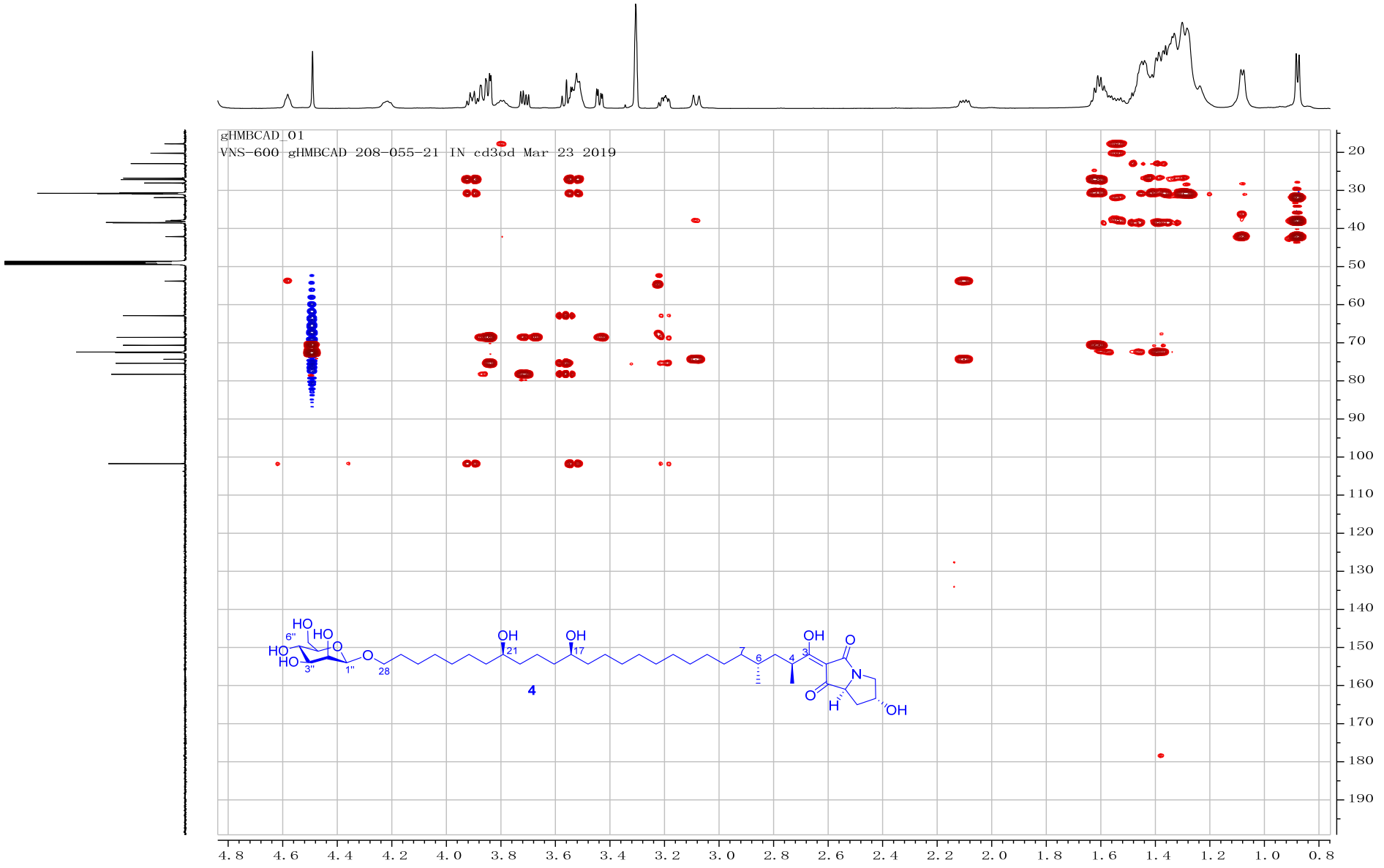

Figure S55. The HMBC spectrum of compound **4** in CD_3OD (600 MHz).

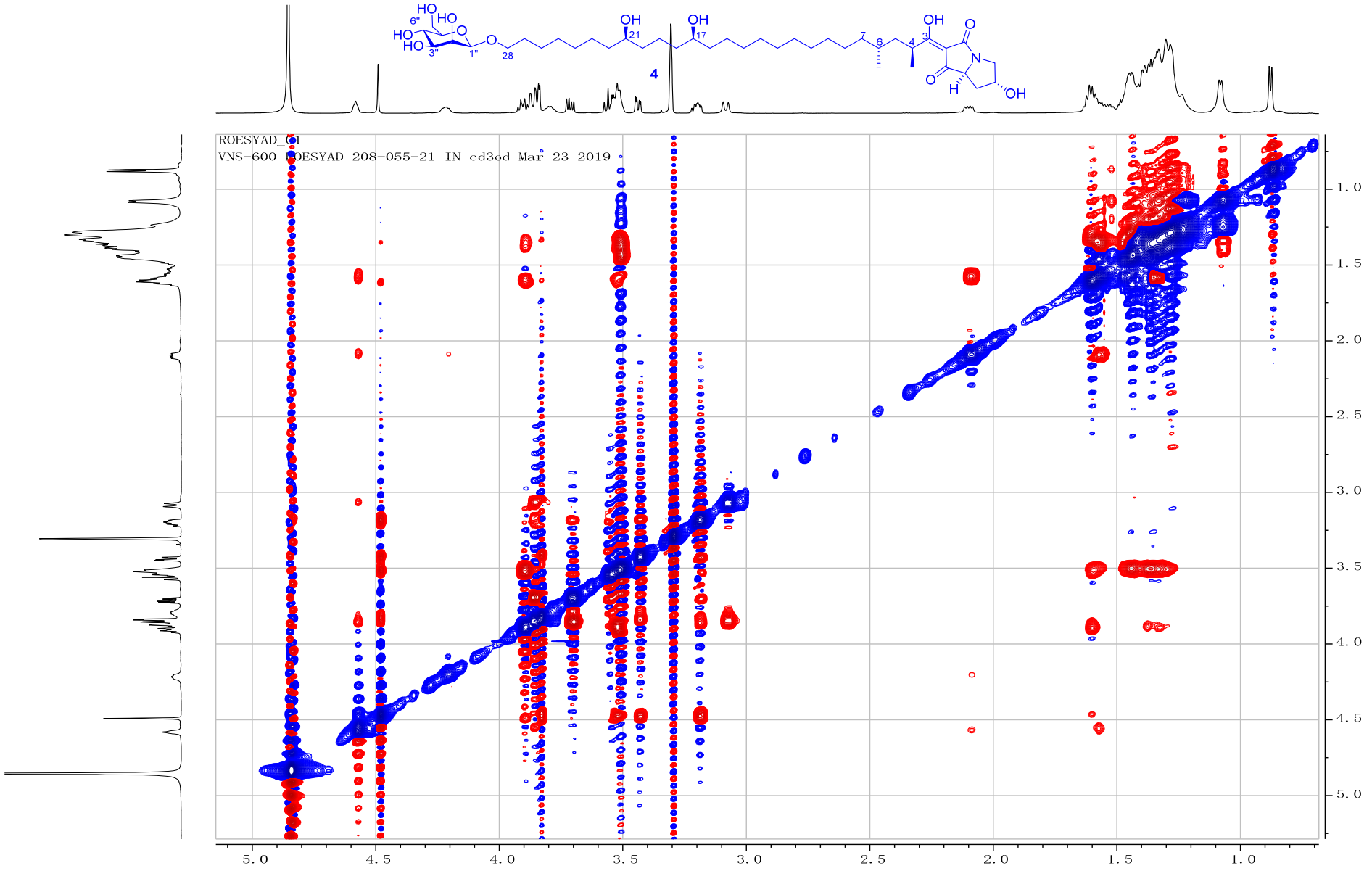

Figure S56. The ROESY spectrum of compound **4** in CD_3OD (600 MHz).

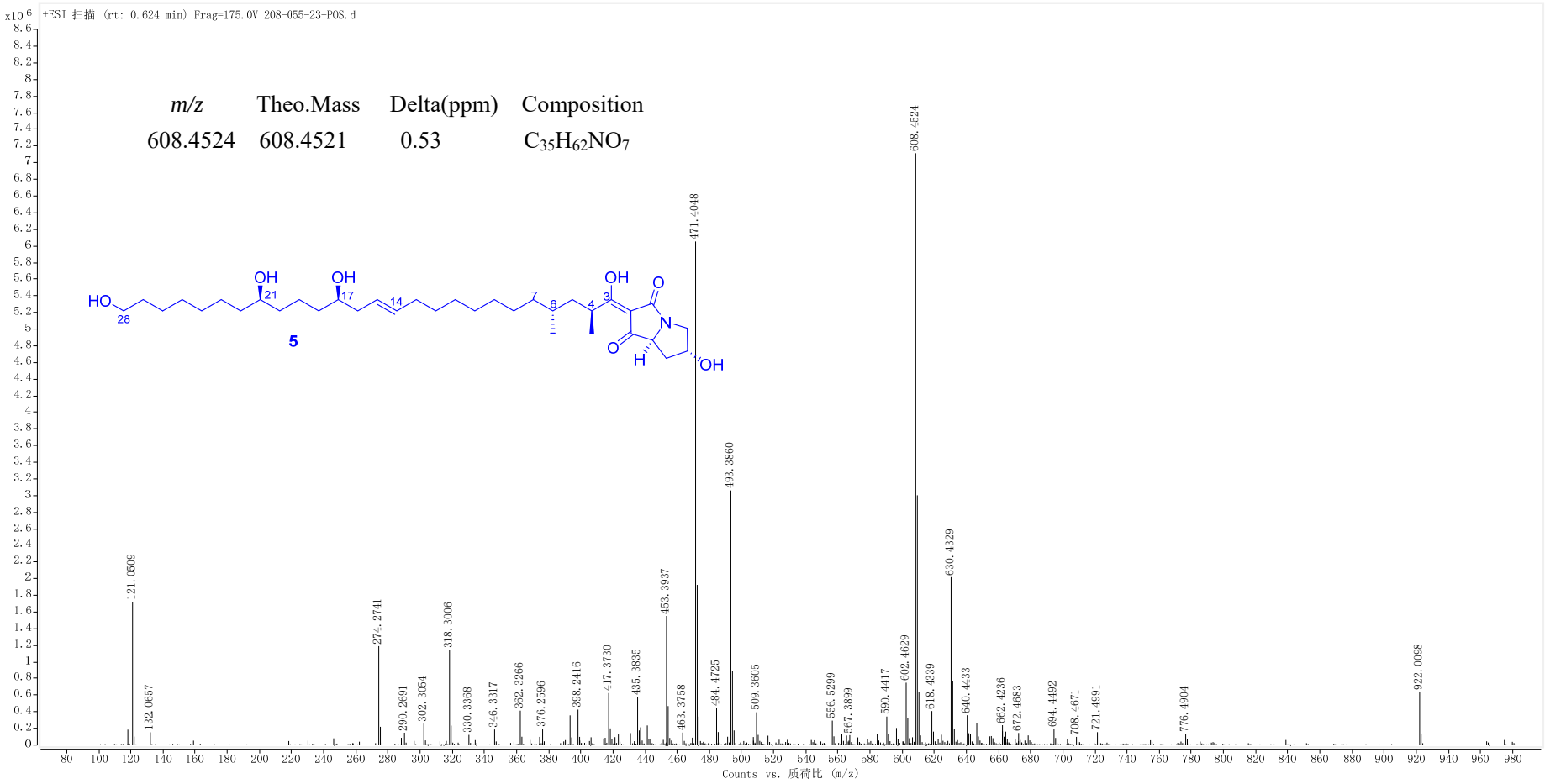

Figure S57. The (+)-HRESIMS spectrum of compound **5**.

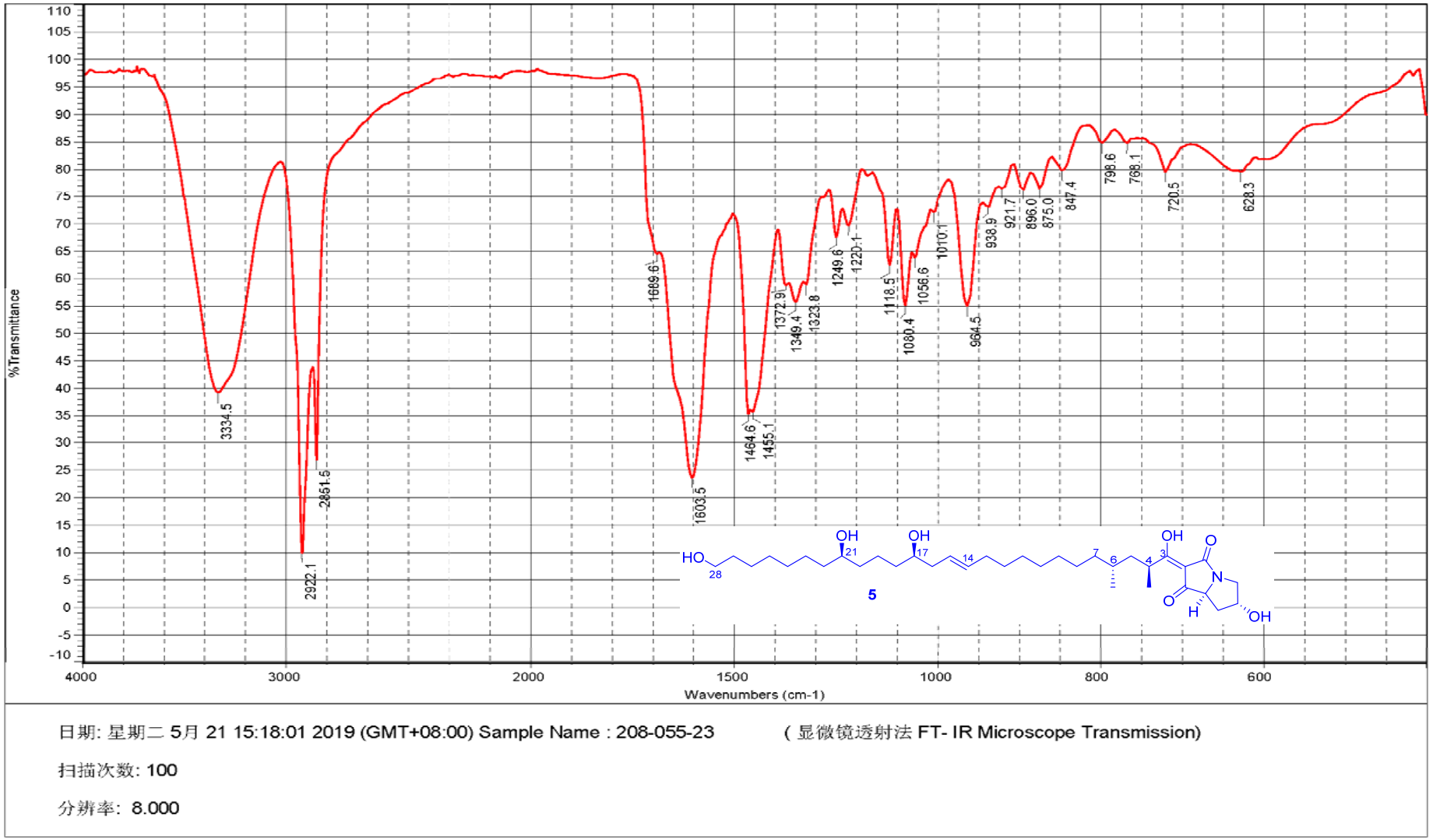

Figure S58. The IR spectrum of compound **5**.

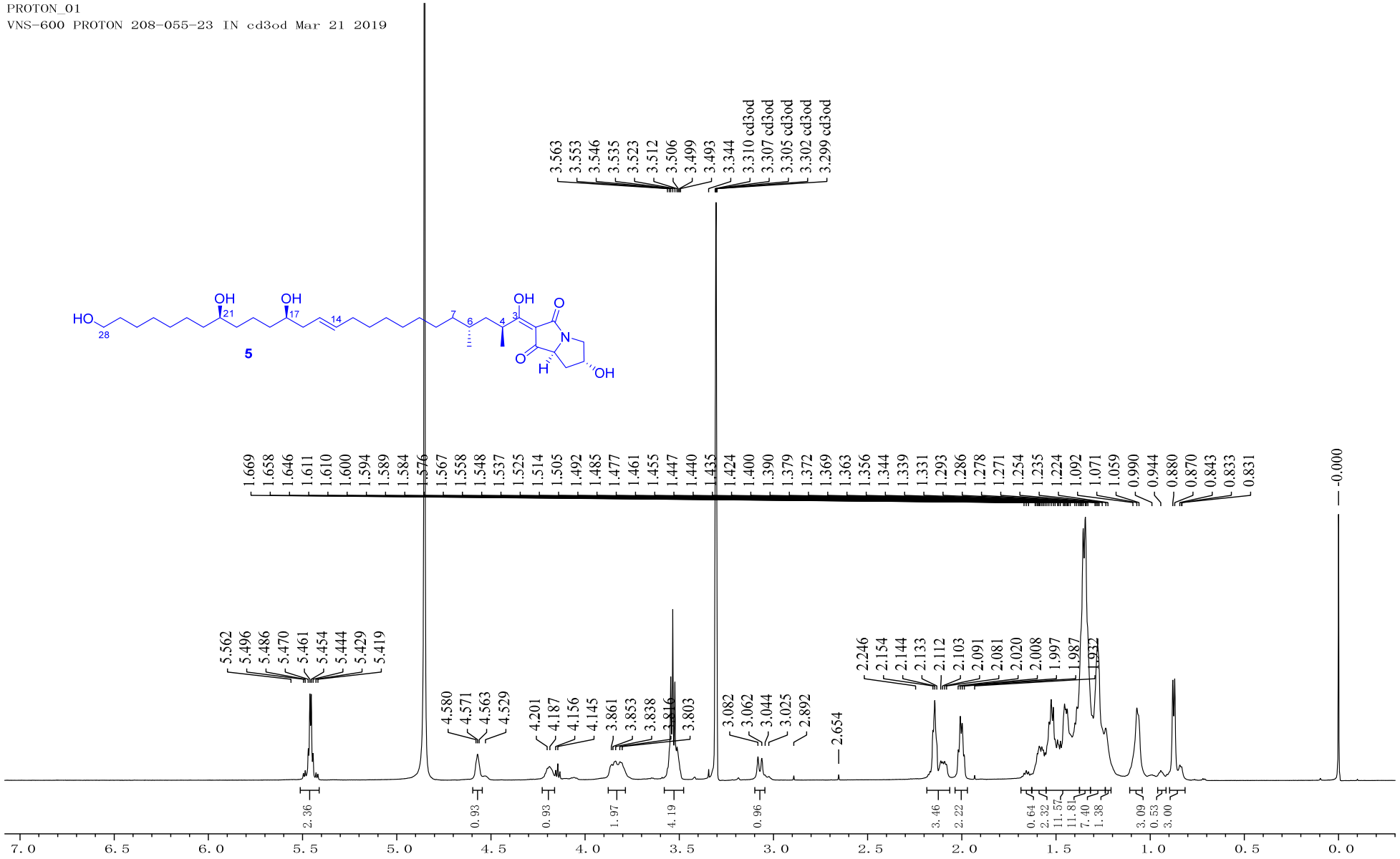

Figure S59. The ^{1}H NMR spectrum of compound **5** in CD_3OD (600 MHz).

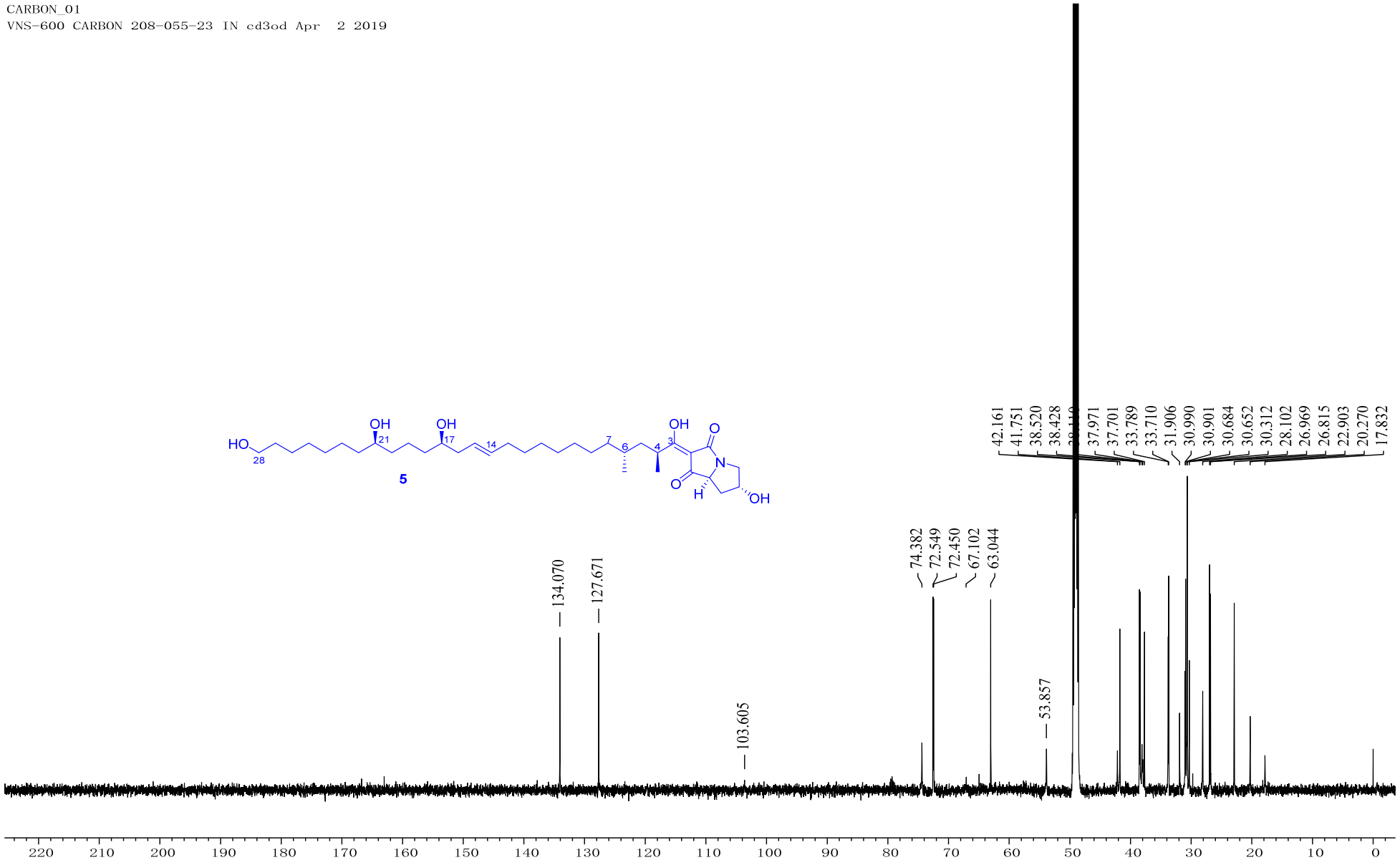

Figure S60. The ^{13}C NMR spectrum of compound **5** in CD_3OD (150 MHz).

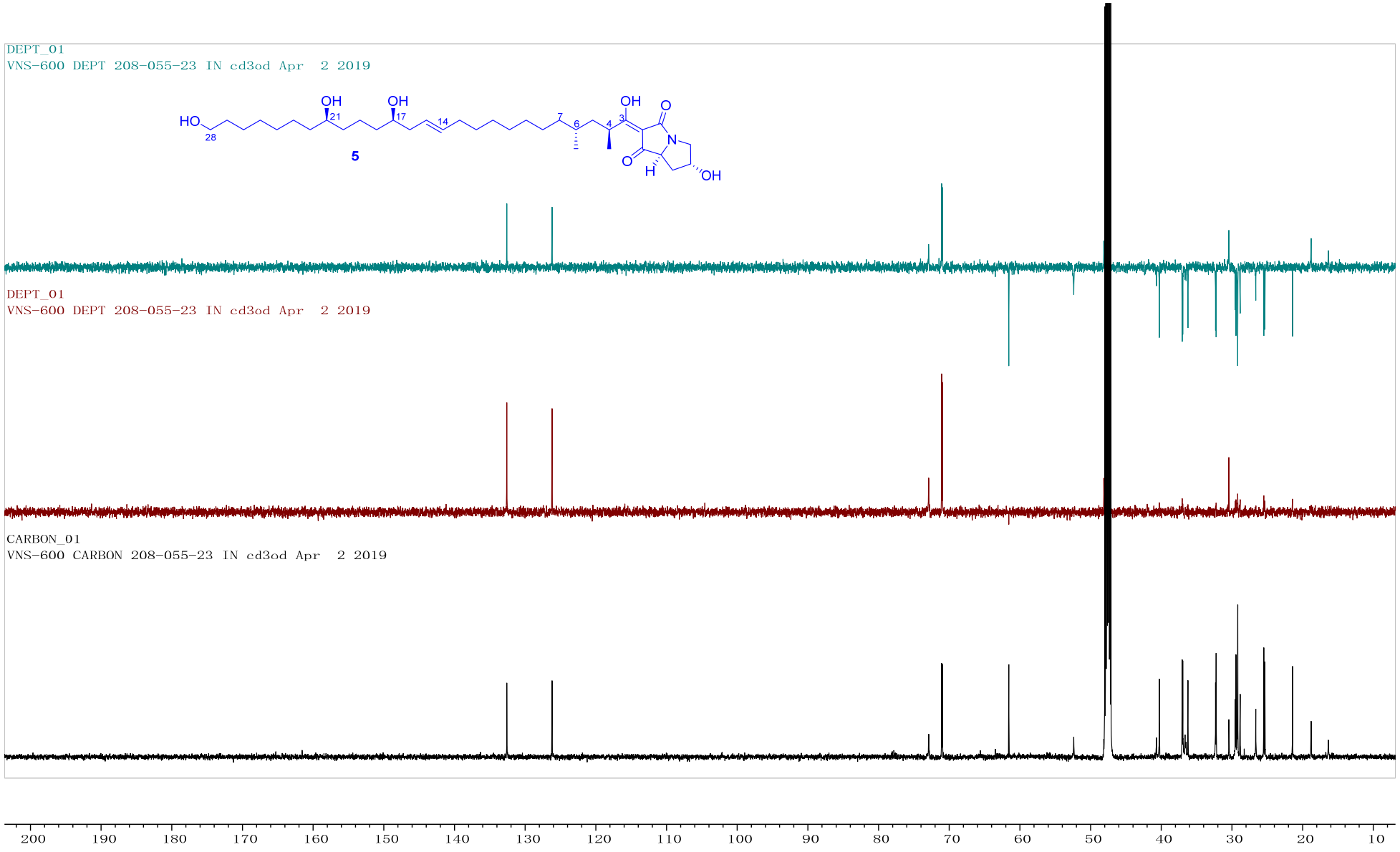

Figure S61. The DEPT spectrum of compound **5** in CD_3OD (150 MHz).

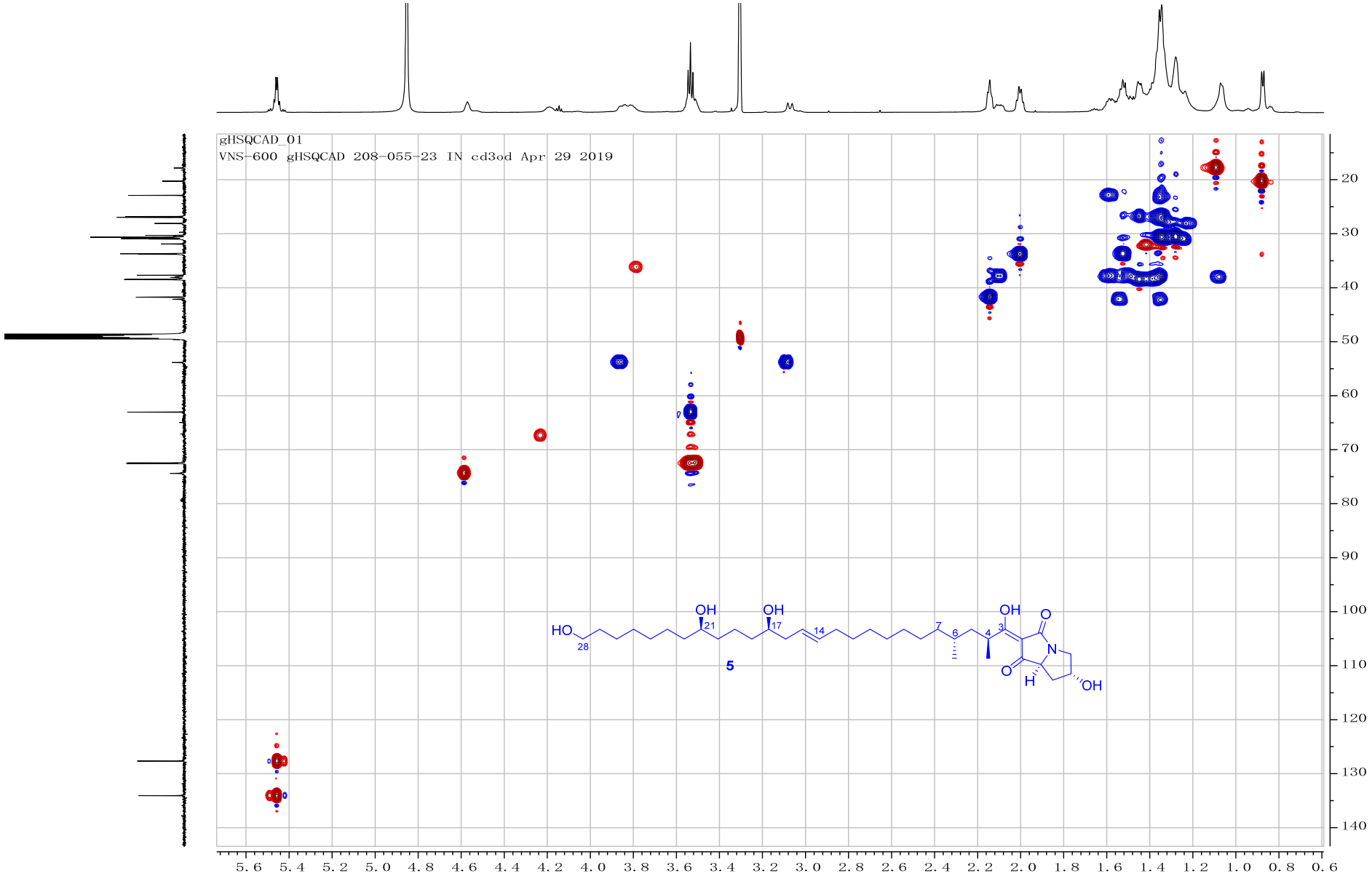

Figure S62. The HSQC spectrum of compound **5** in CD_3OD (600 MHz).

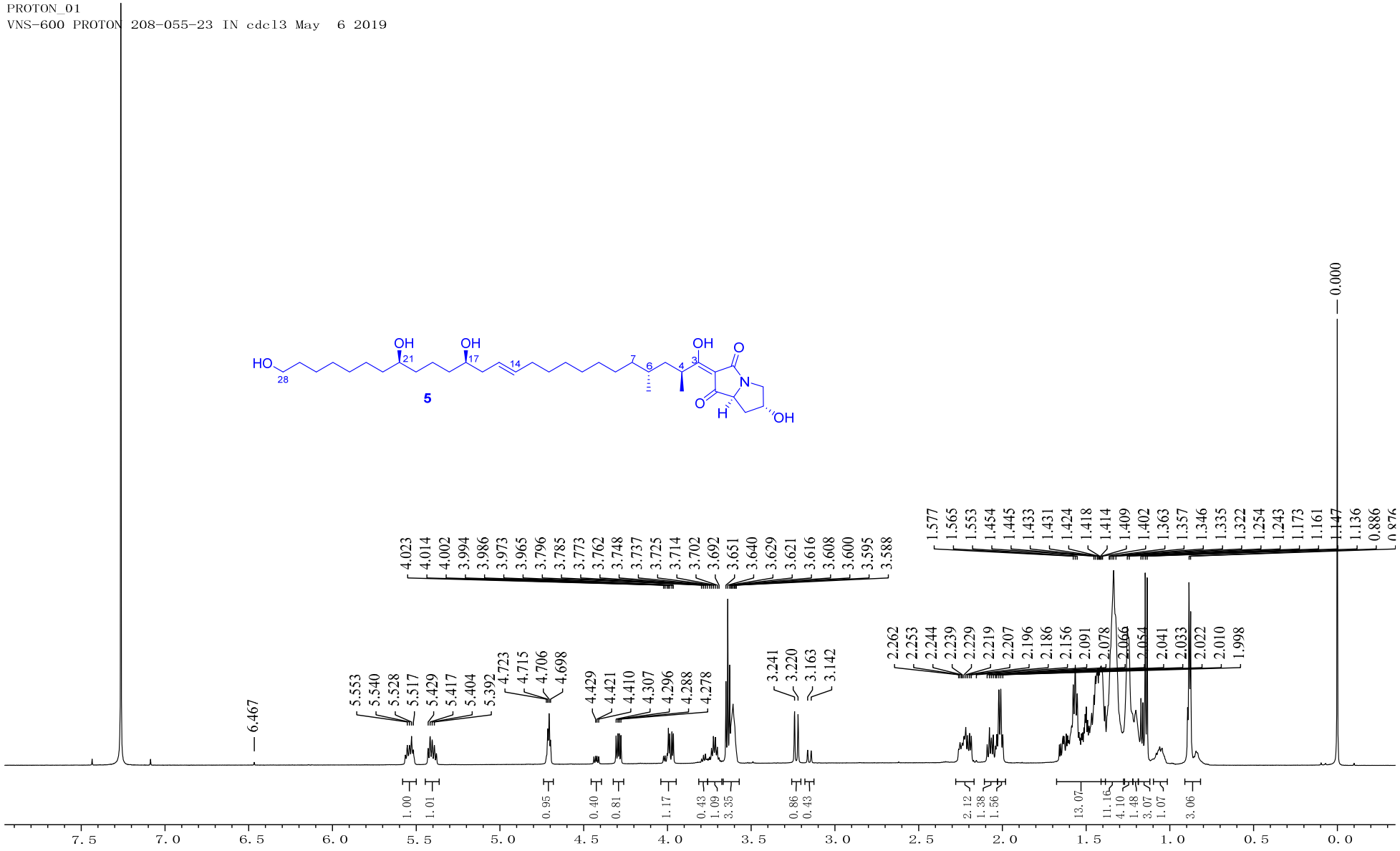

Figure S63. The ^{1}H NMR spectrum of compound **5** in $CDCl_3$ (600 MHz).

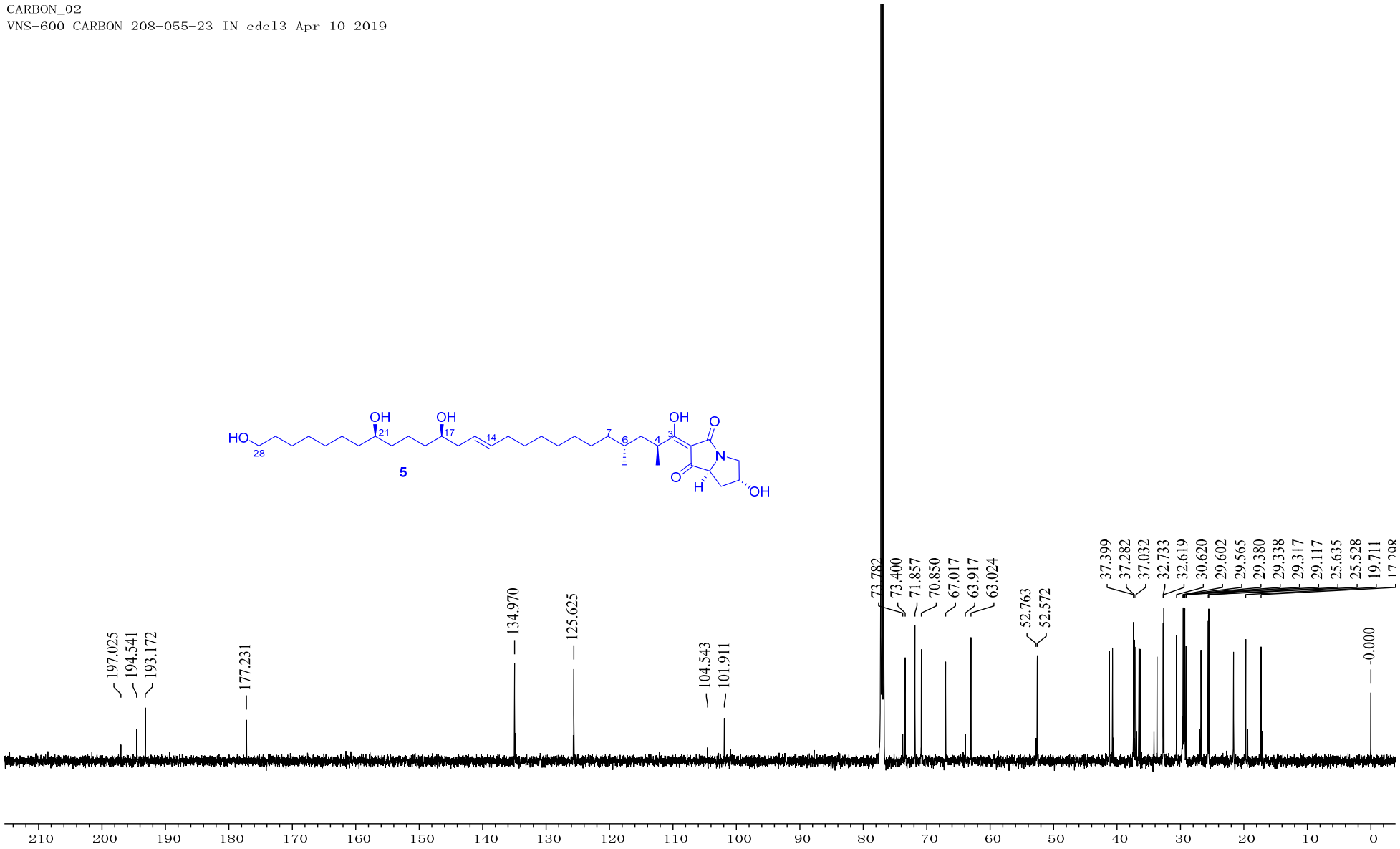

Figure S64. The ^{13}C NMR spectrum of compound **5** in $CDCl_3$ (150 MHz).

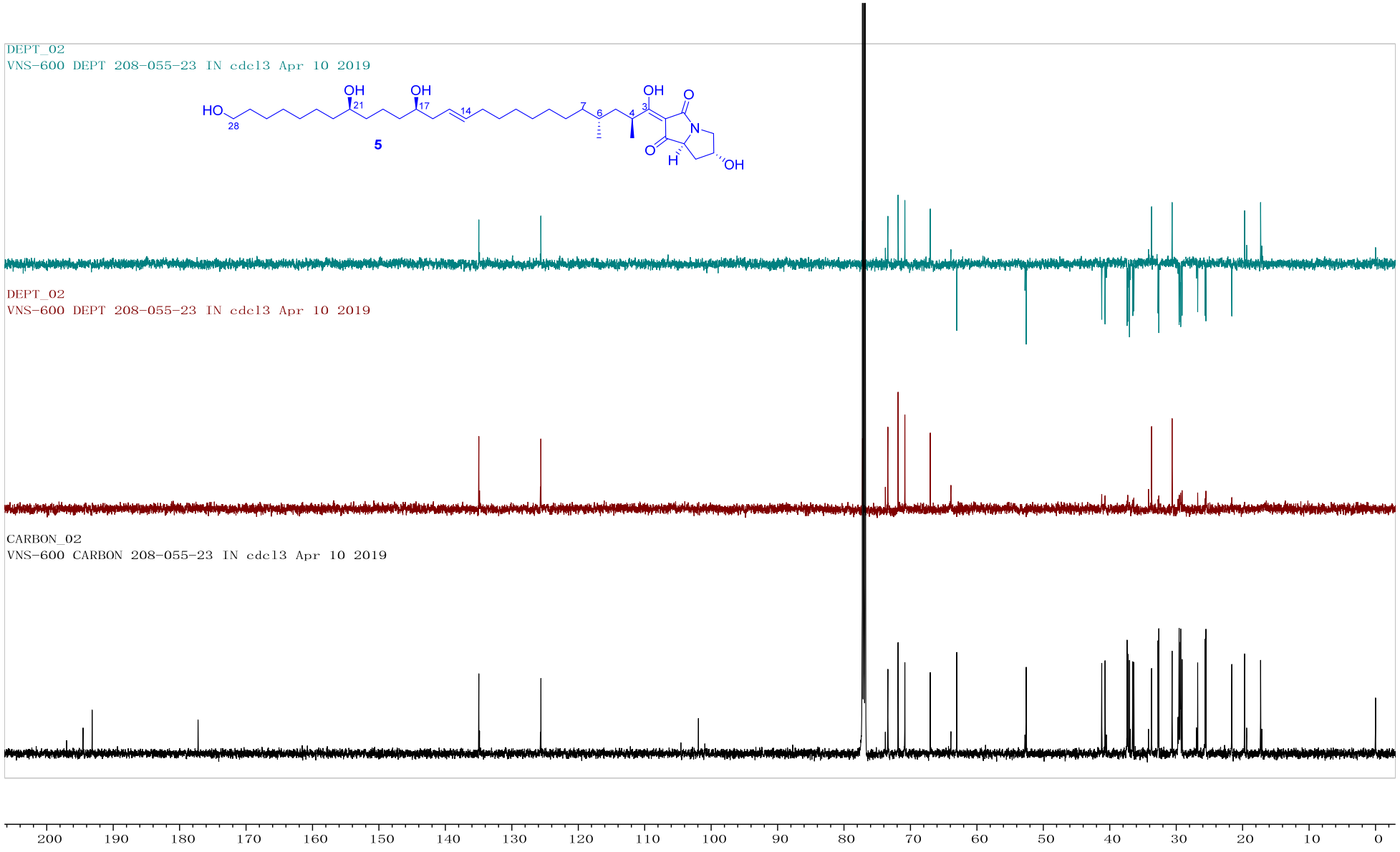

Figure S65. The DEPT spectrum of compound **5** in $CDCl_3$ (150 MHz).

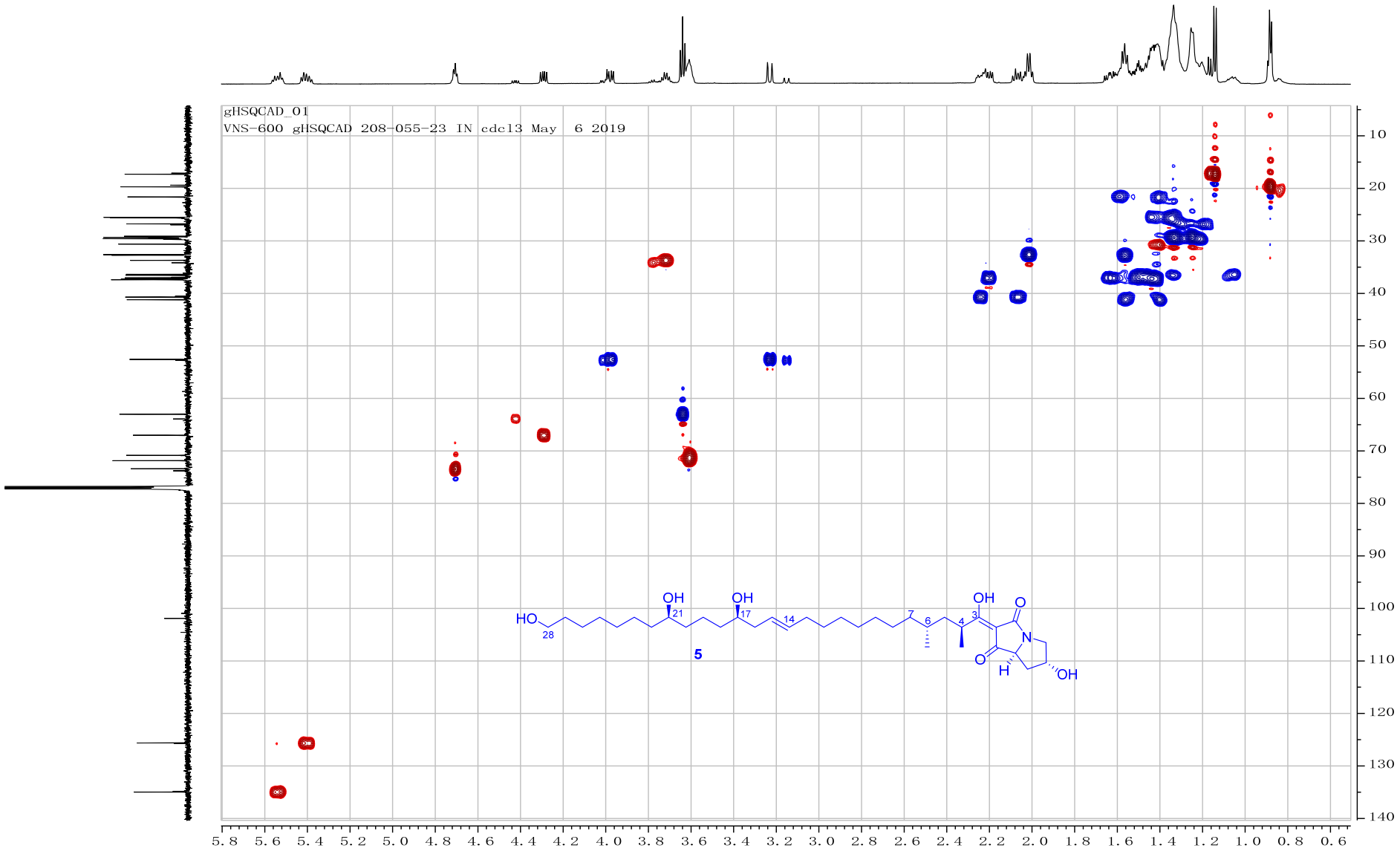

Figure S66. The HSQC spectrum of compound **5** in $CDCl_3$ (600 MHz).

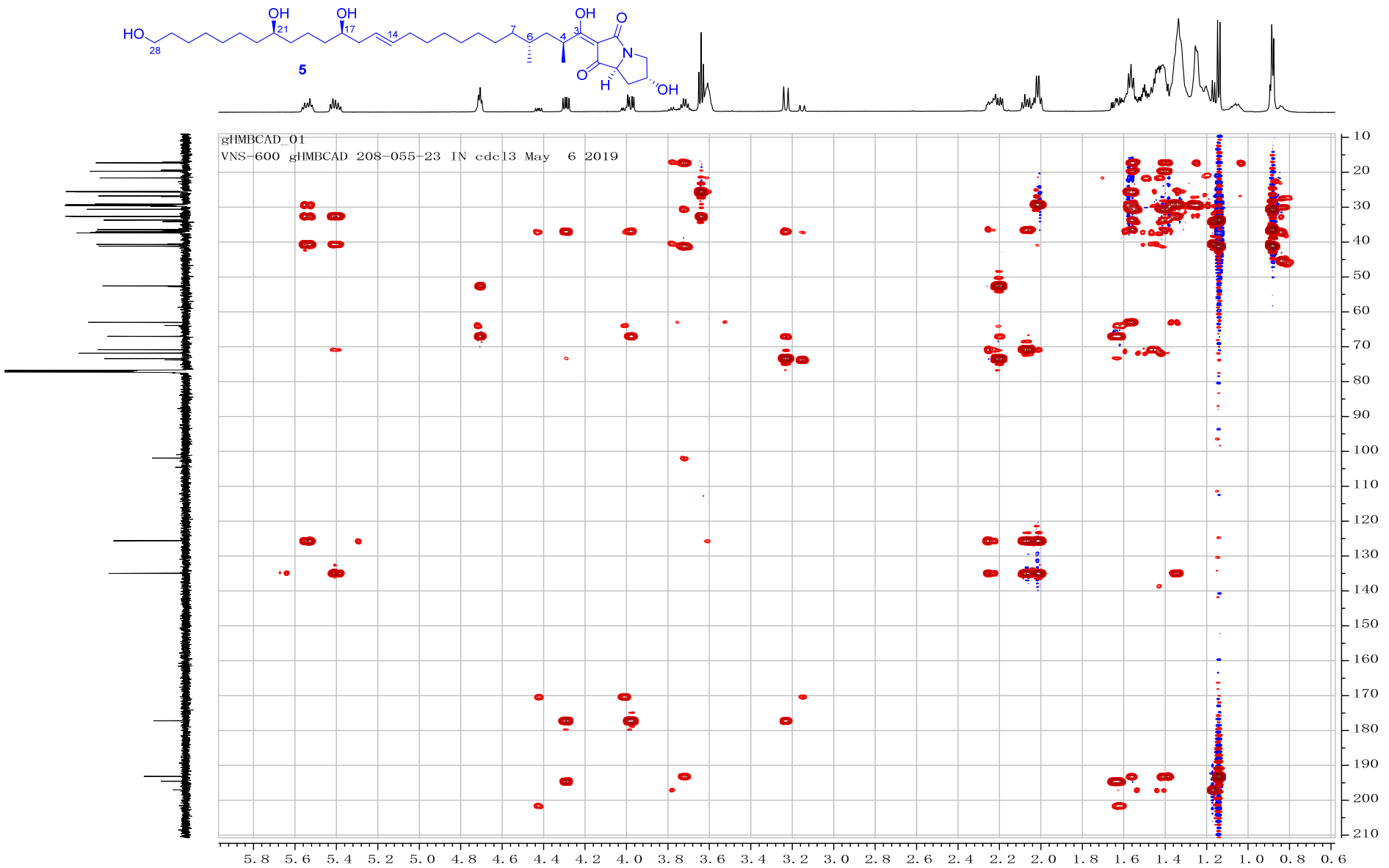

Figure S67. The HMBC spectrum of compound **5** in $CDCl_3$ (600 MHz).

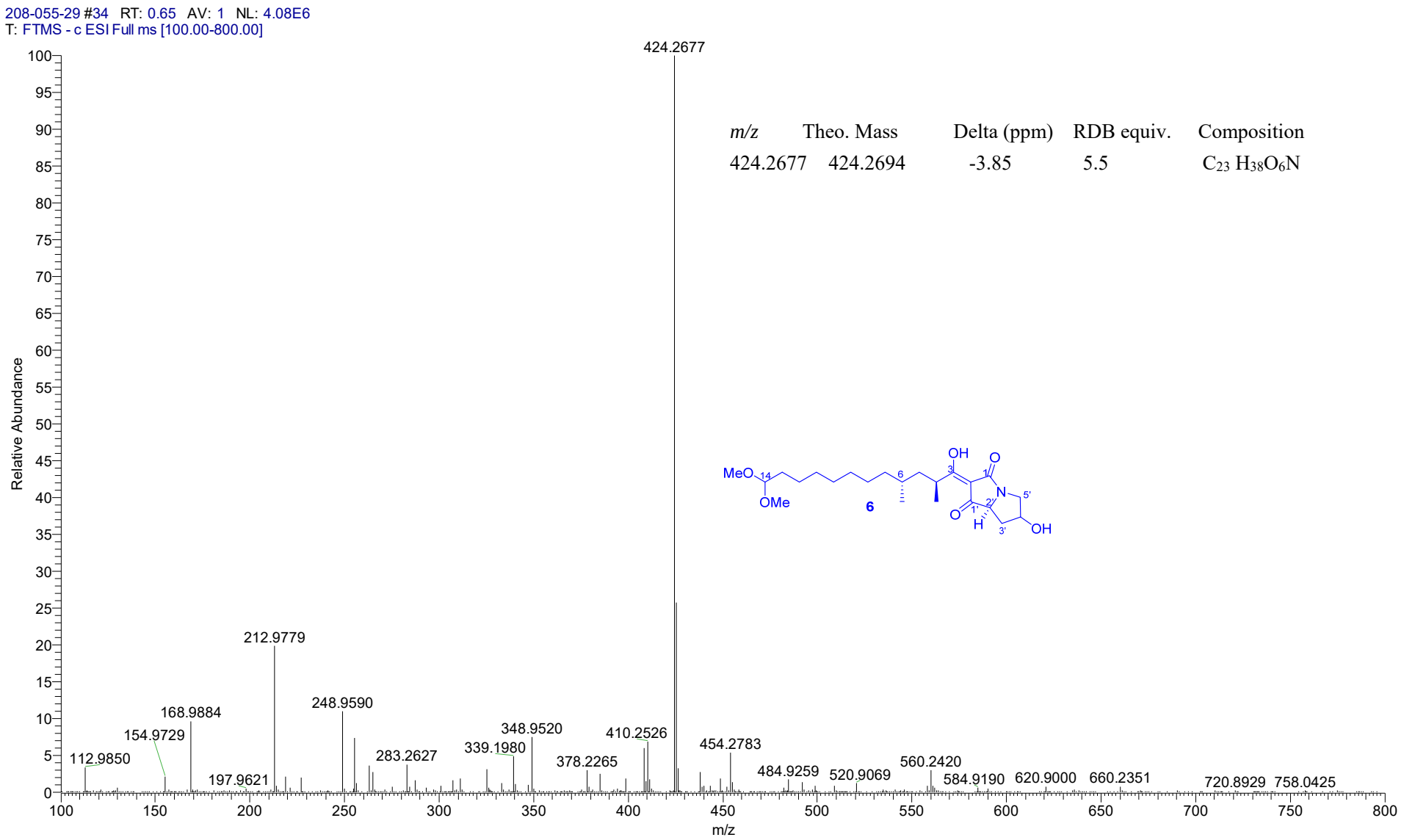

Figure S68. The (–)-HRESIMS spectrum of compound **6**.

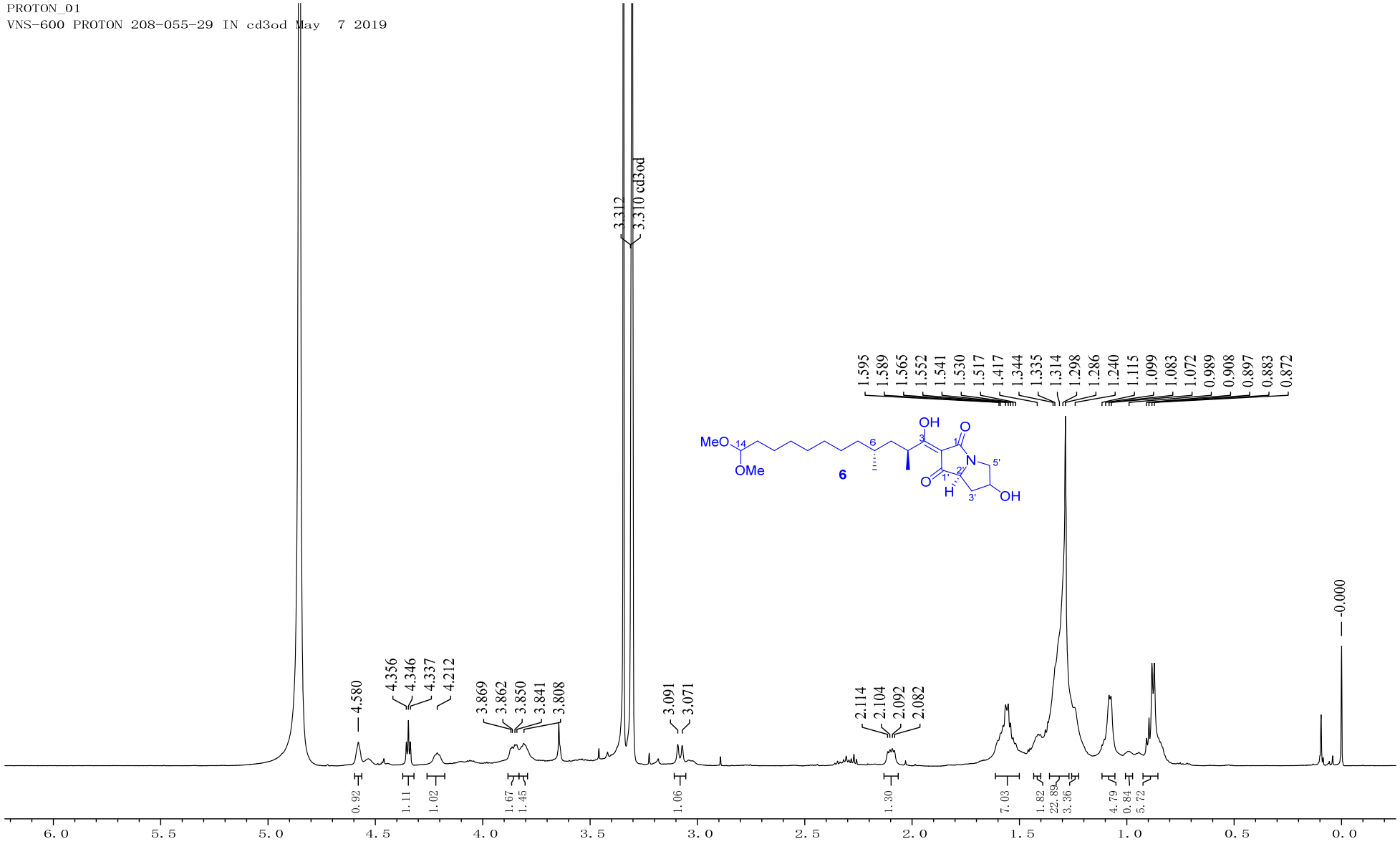

Figure S69. The ^{1}H NMR spectrum of compound **6** in CD_3OD (600 MHz).

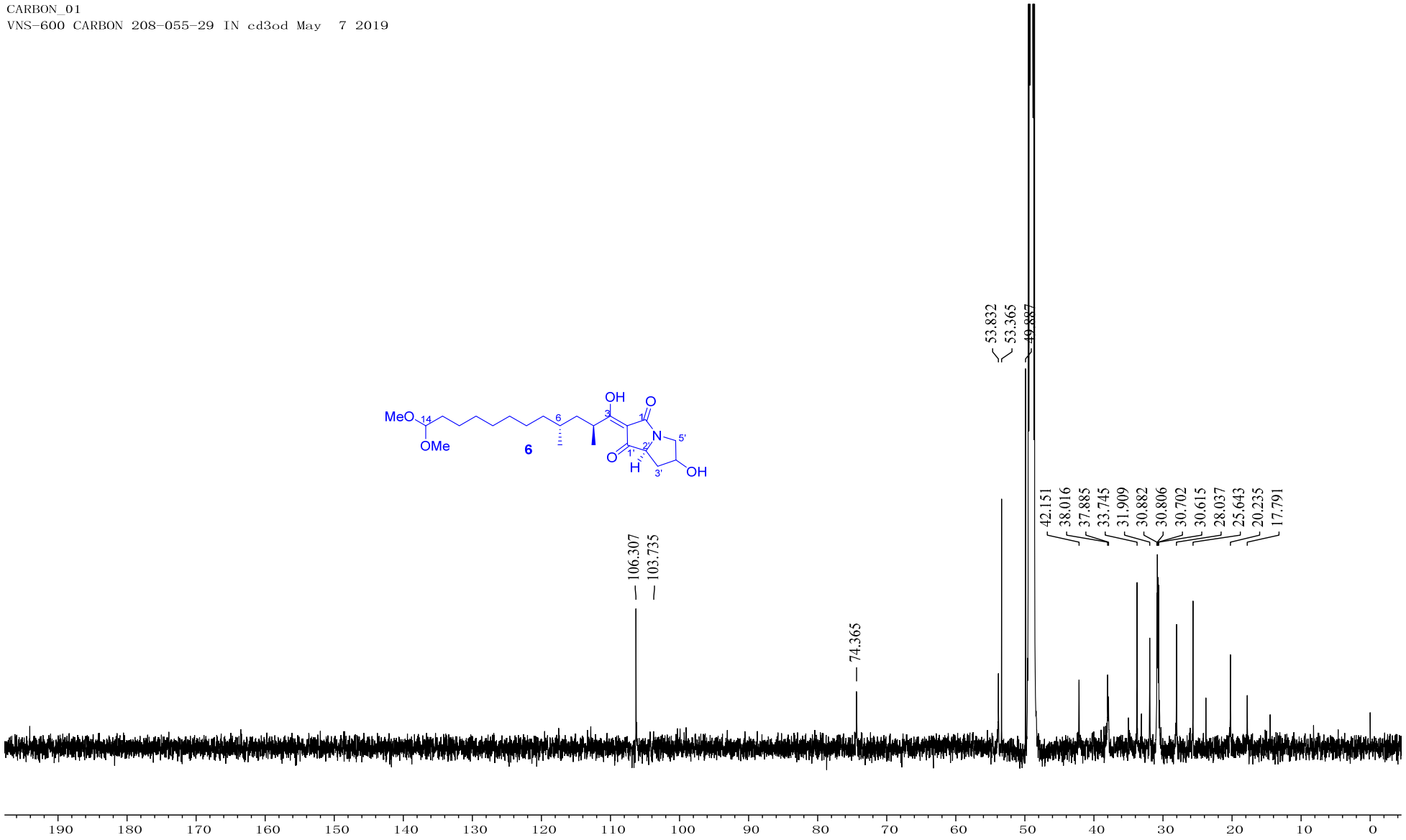

Figure S70. The ^{13}C NMR spectrum of compound **6** in CD_3OD (150 MHz).

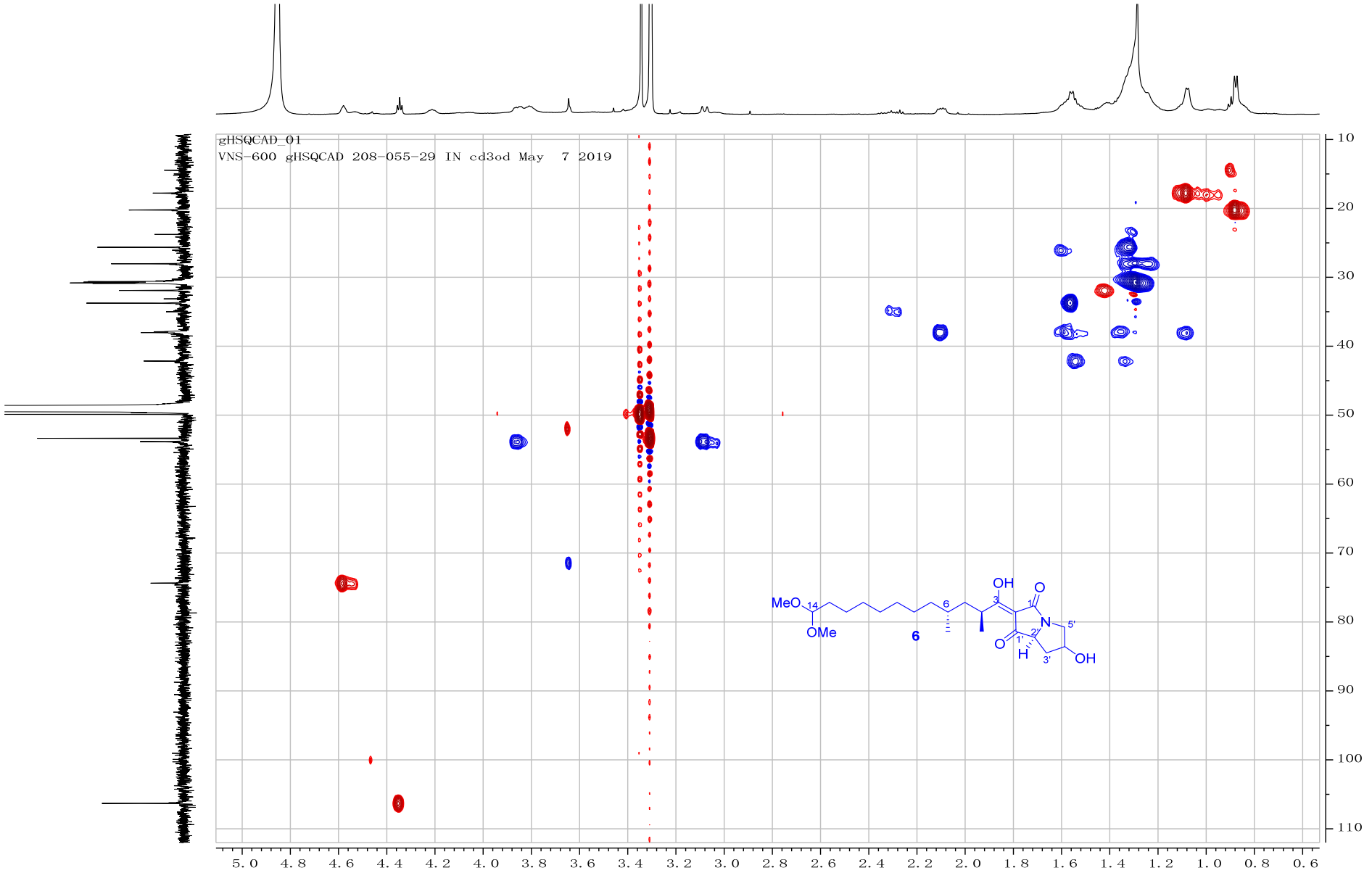

Figure S71. The HSQC spectrum of compound **6** in CD_3OD (600 MHz).

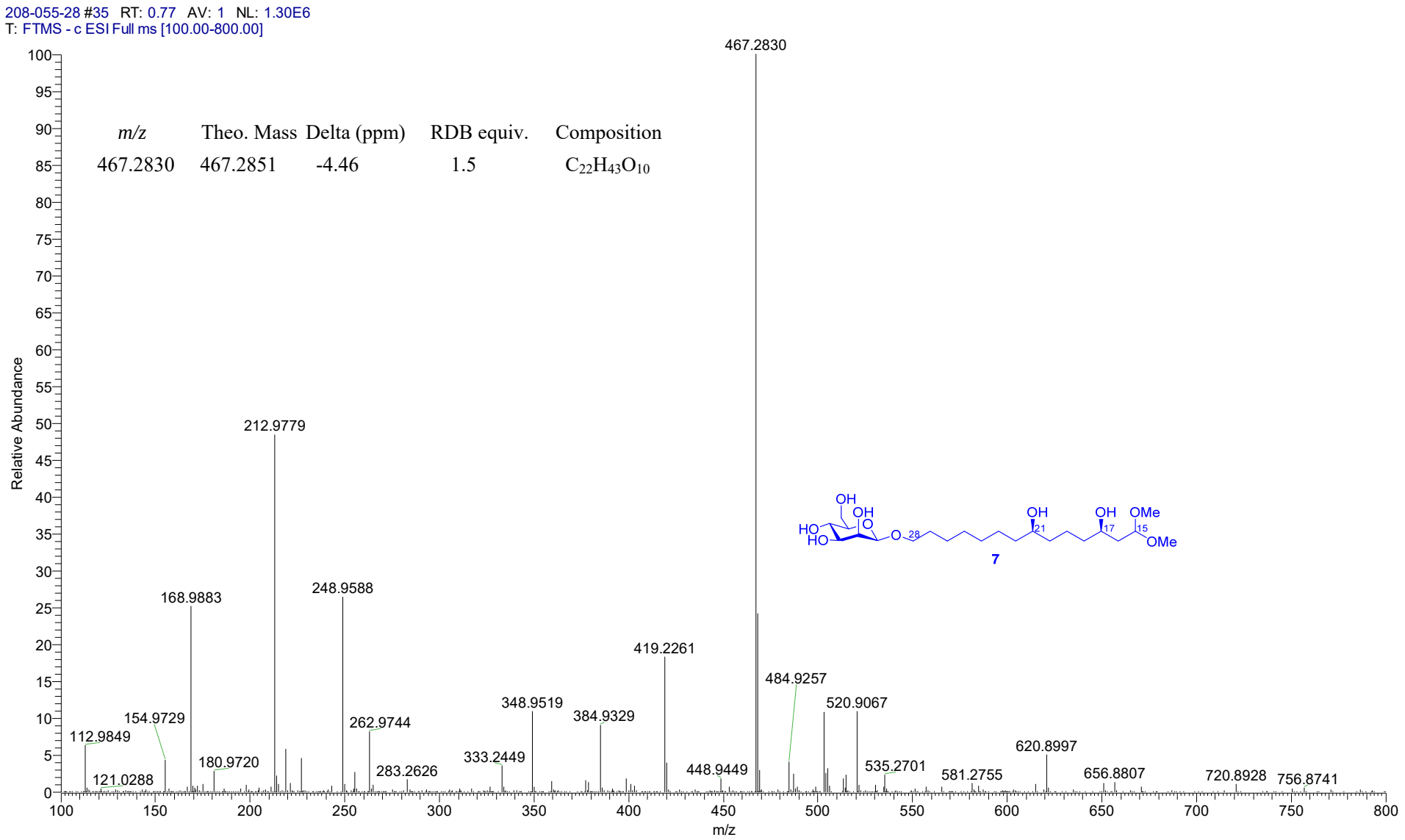

Figure S72. The (–)-HRESIMS spectrum of compound **7**.

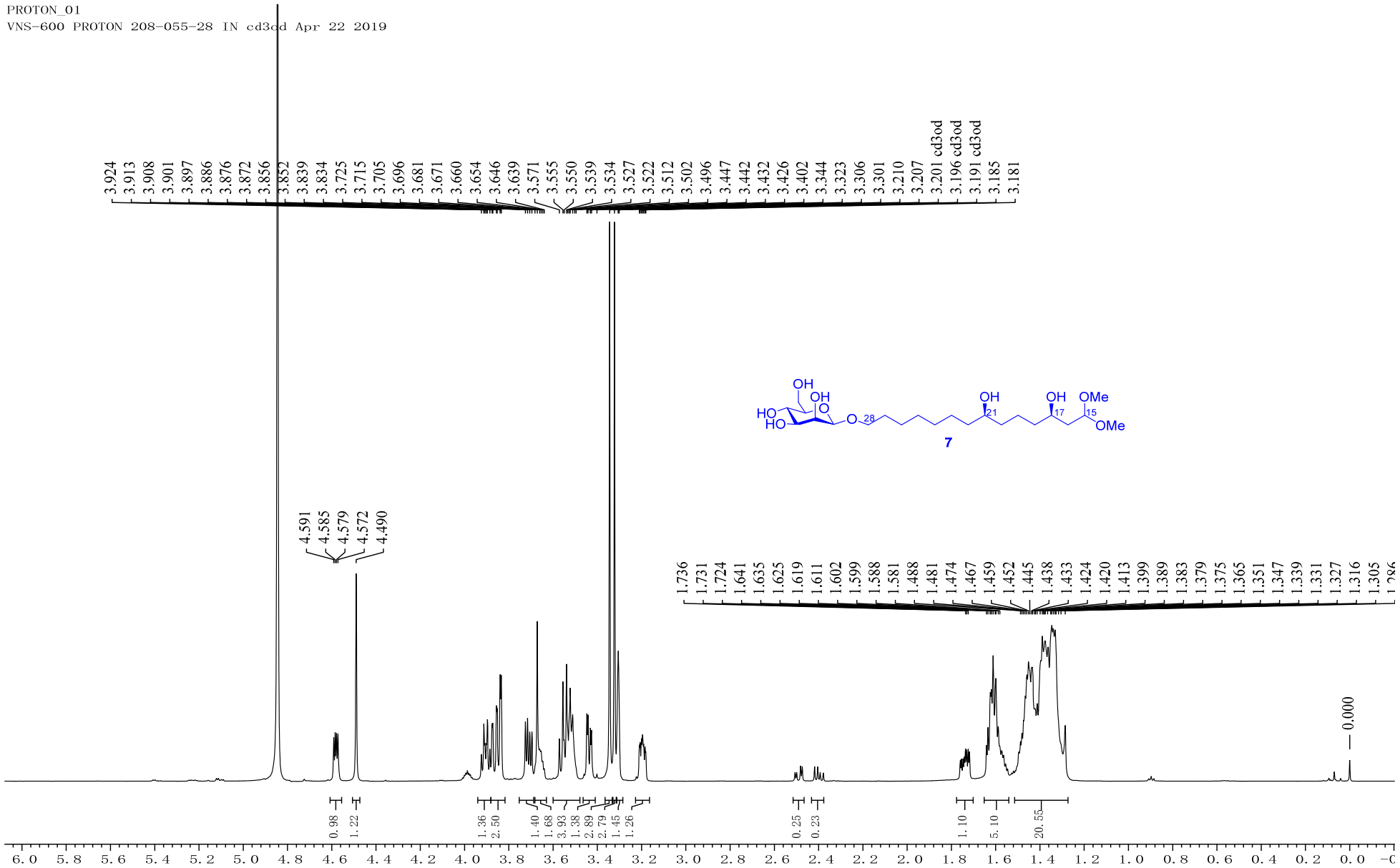

Figure S73. The ^{1}H NMR spectrum of compound **7** in CD_3OD (600 MHz).

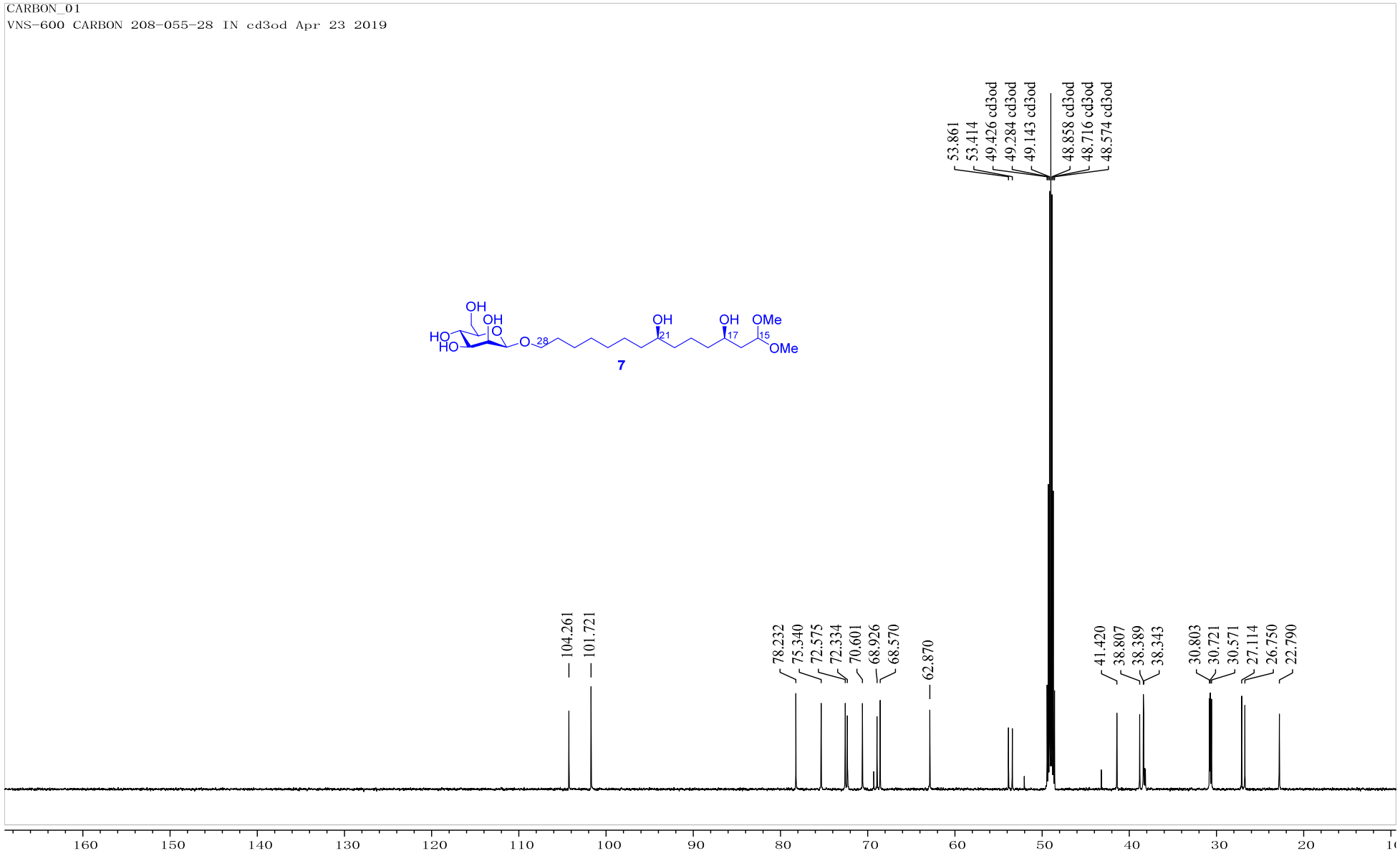

Figure S75. The ^{13}C NMR spectrum of compound **7** in CD_3OD (150 MHz).

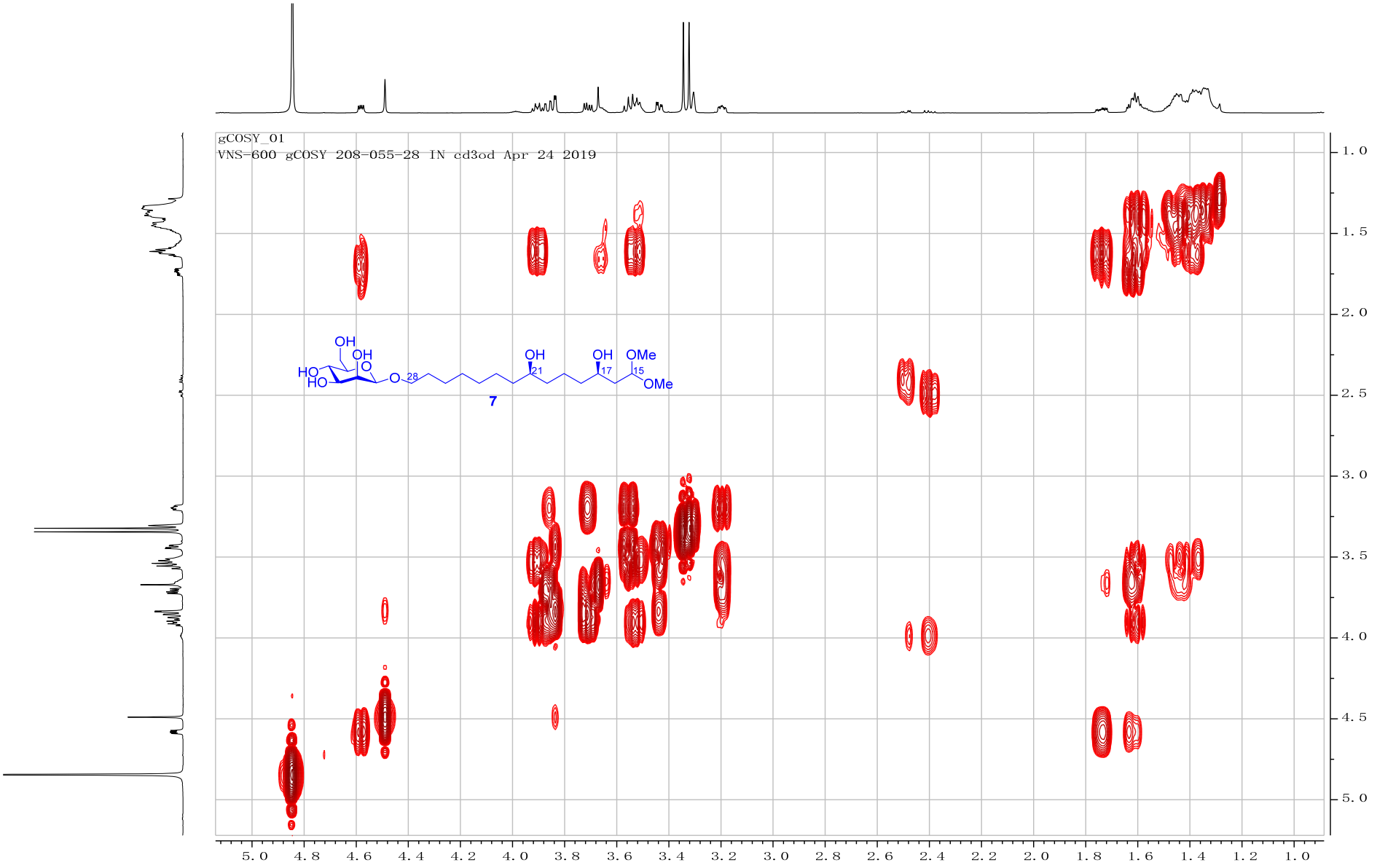

Figure S76. The ^{1}H-^{1}H COSY spectrum of compound **7** in CD_3OD (600 MHz).

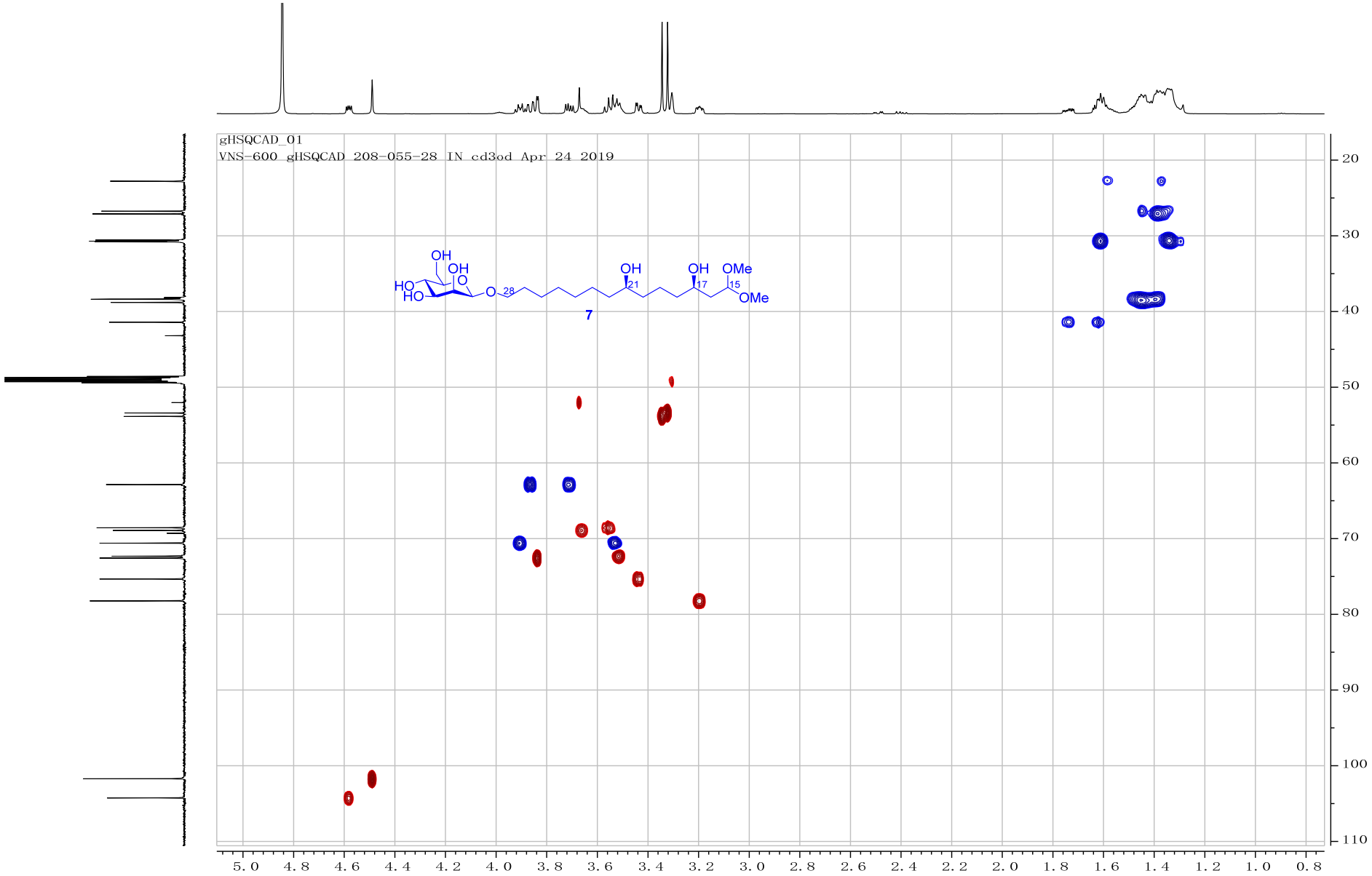

Figure S77. The HSQC spectrum of compound **7** in CD_3OD (600 MHz).

Figure S78. The HMBC spectrum of compound **7** in CD_3OD (600 MHz).

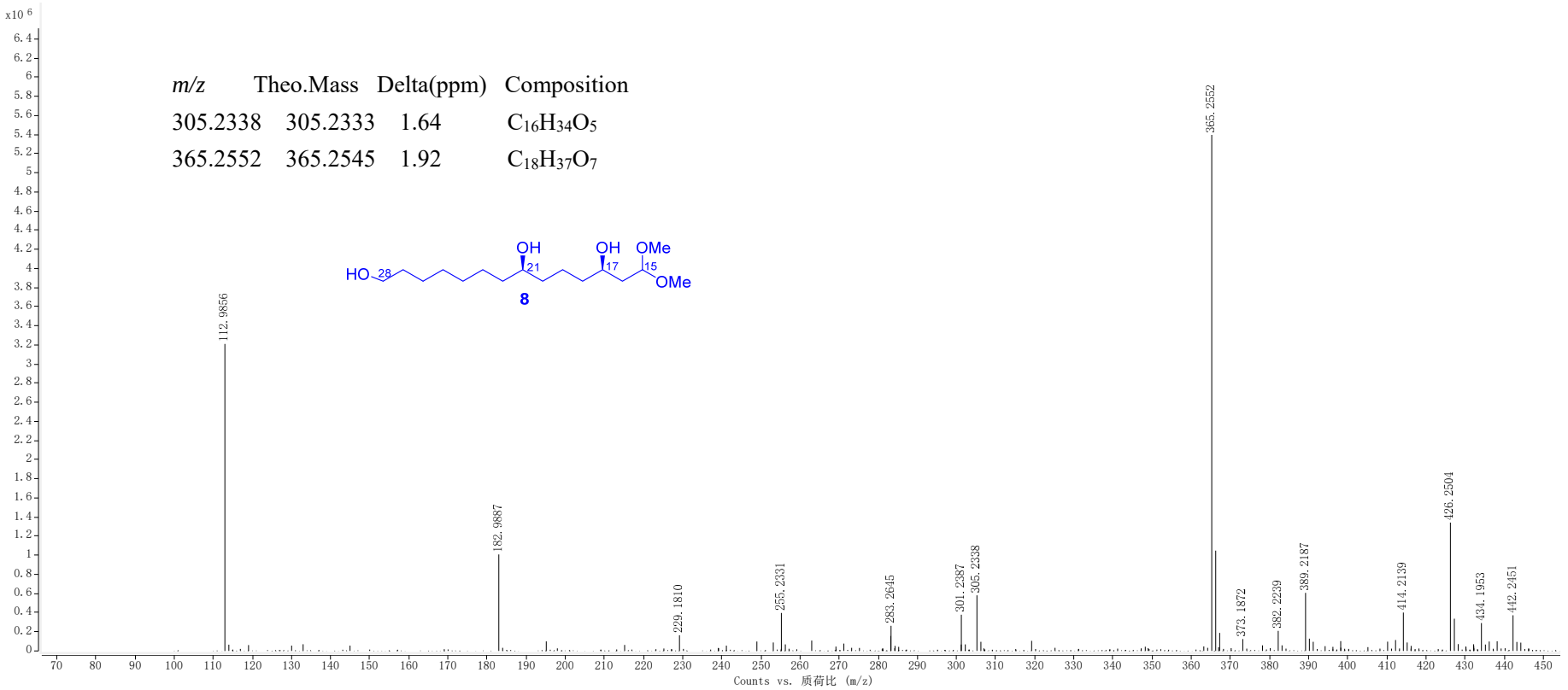

Figure S79. The (–)-HRESIMS spectrum of compound **8**.

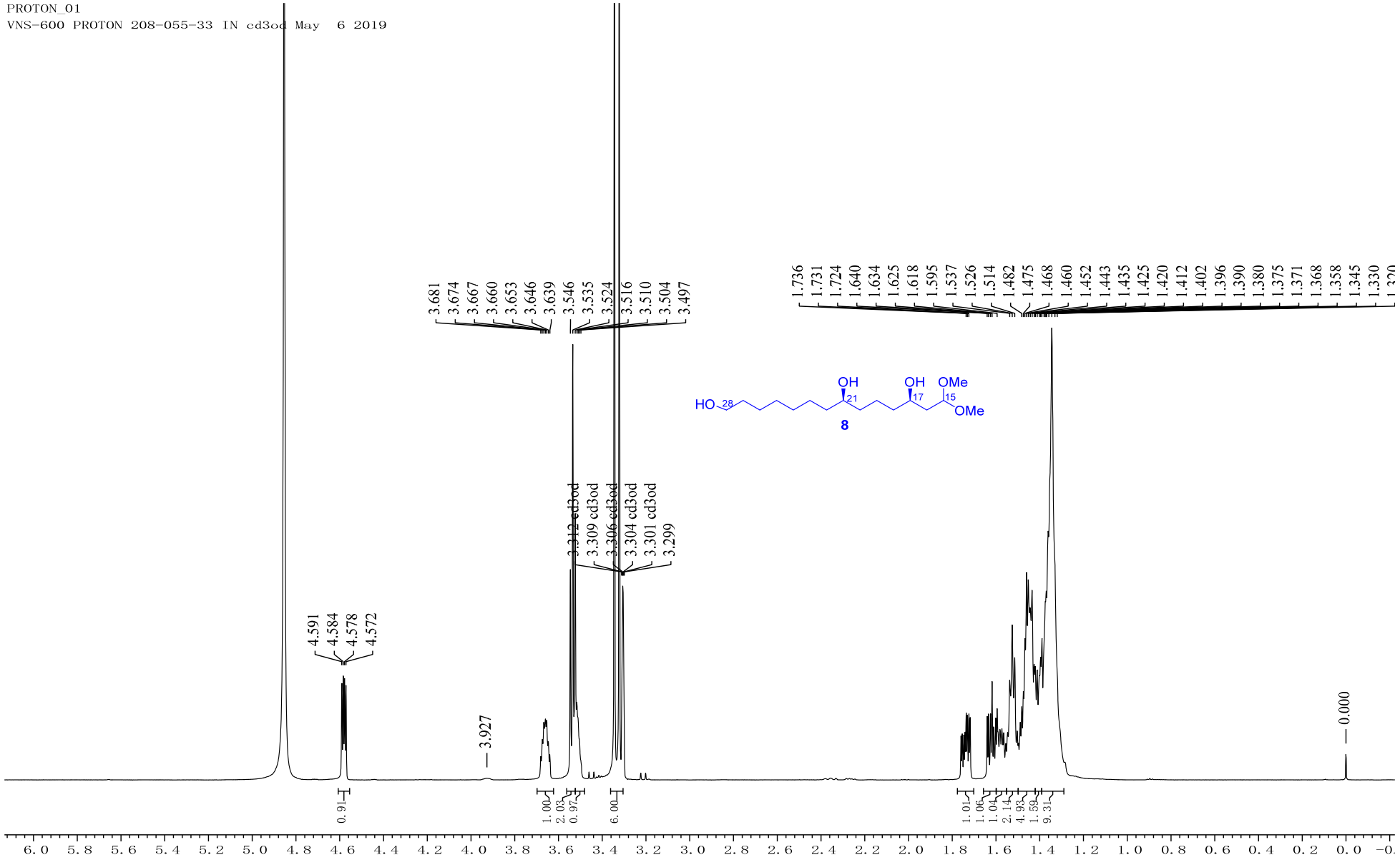

Figure S80. The ^{1}H NMR spectrum of compound **8** in CD_3OD (600 MHz).

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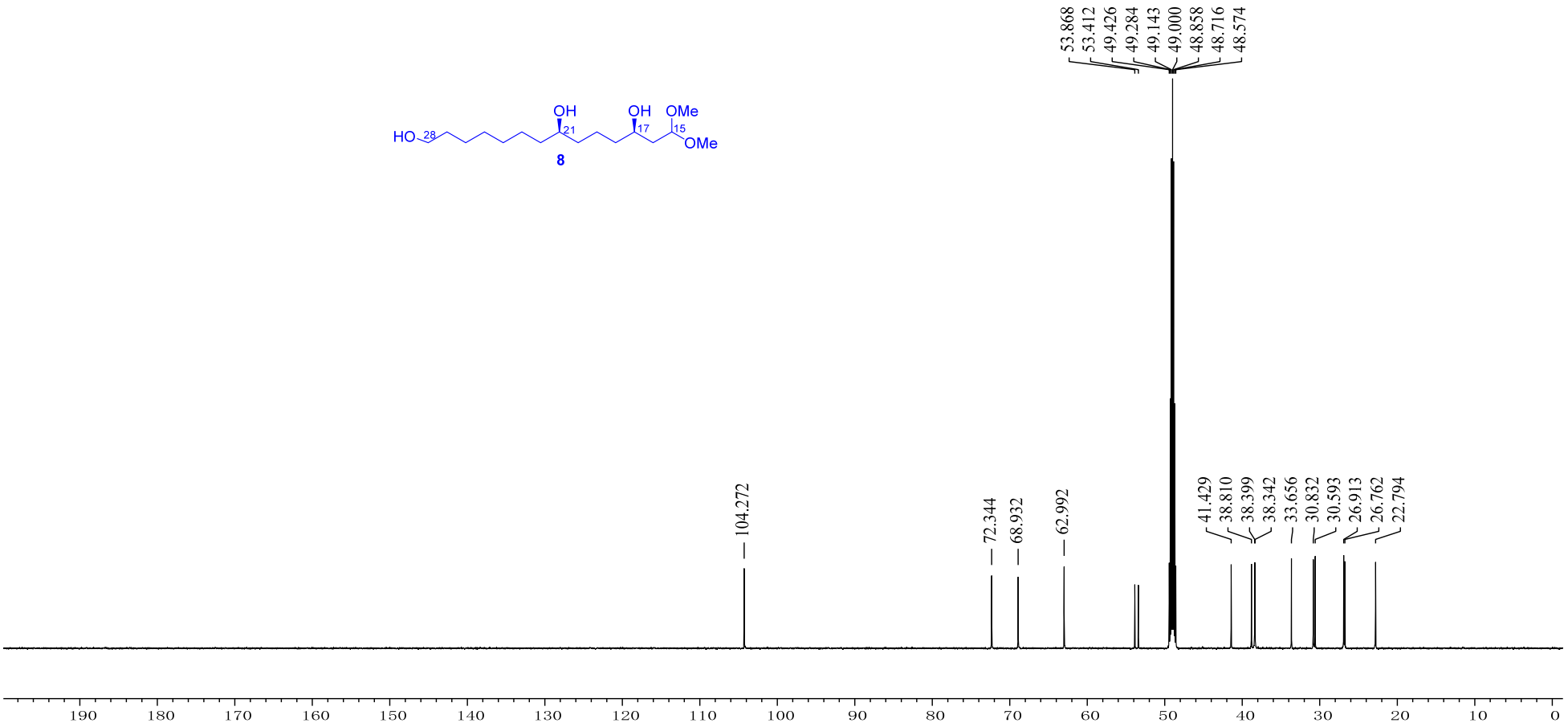

Figure S81. The ^{13}C NMR spectrum of compound **8** in CD_3OD (150 MHz).

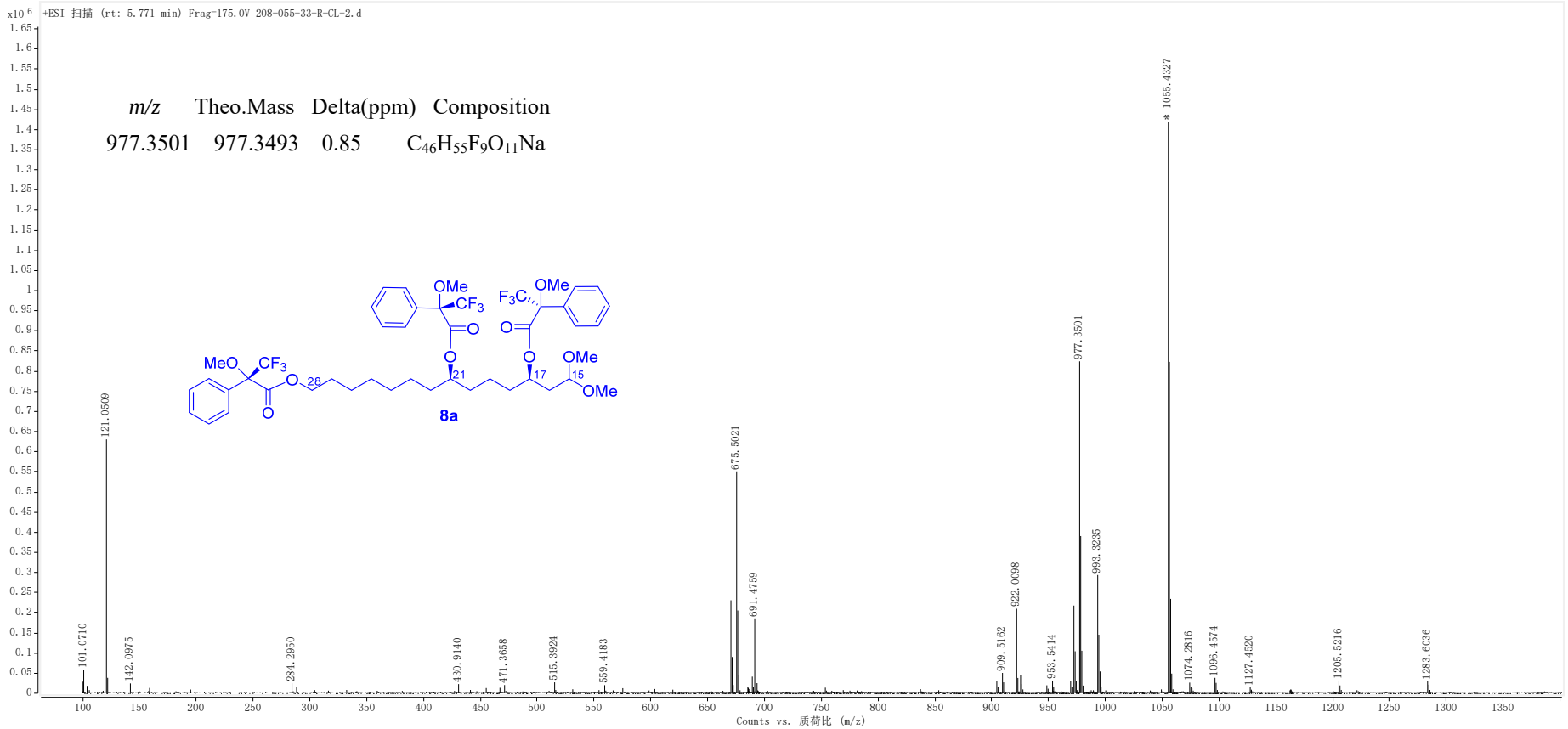

Figure S82. The (+)-HRESIMS spectrum of compound **8a**.

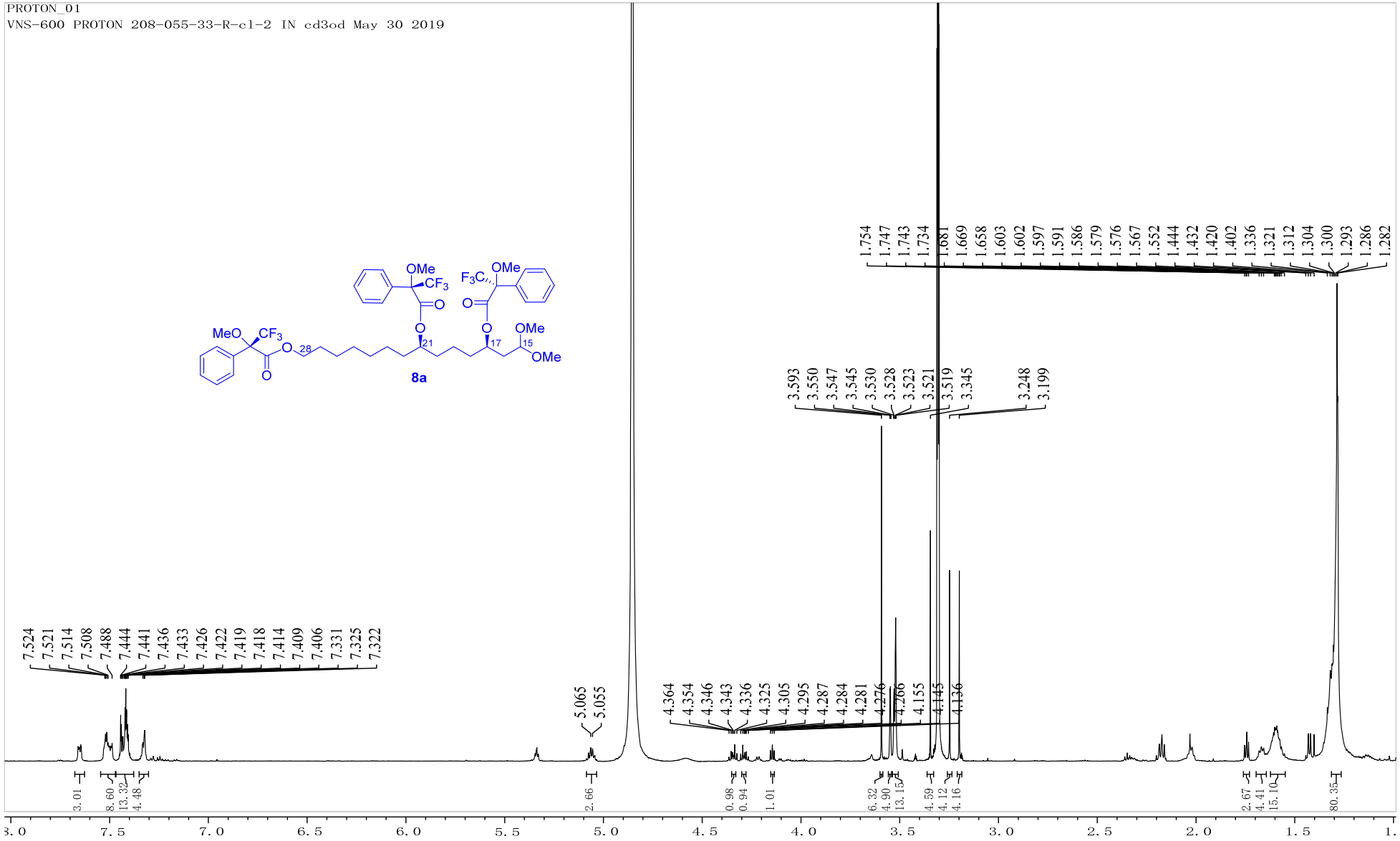

Figure S83. The ^{1}H NMR spectrum of compound **8a** in CD_3OD (600 MHz).

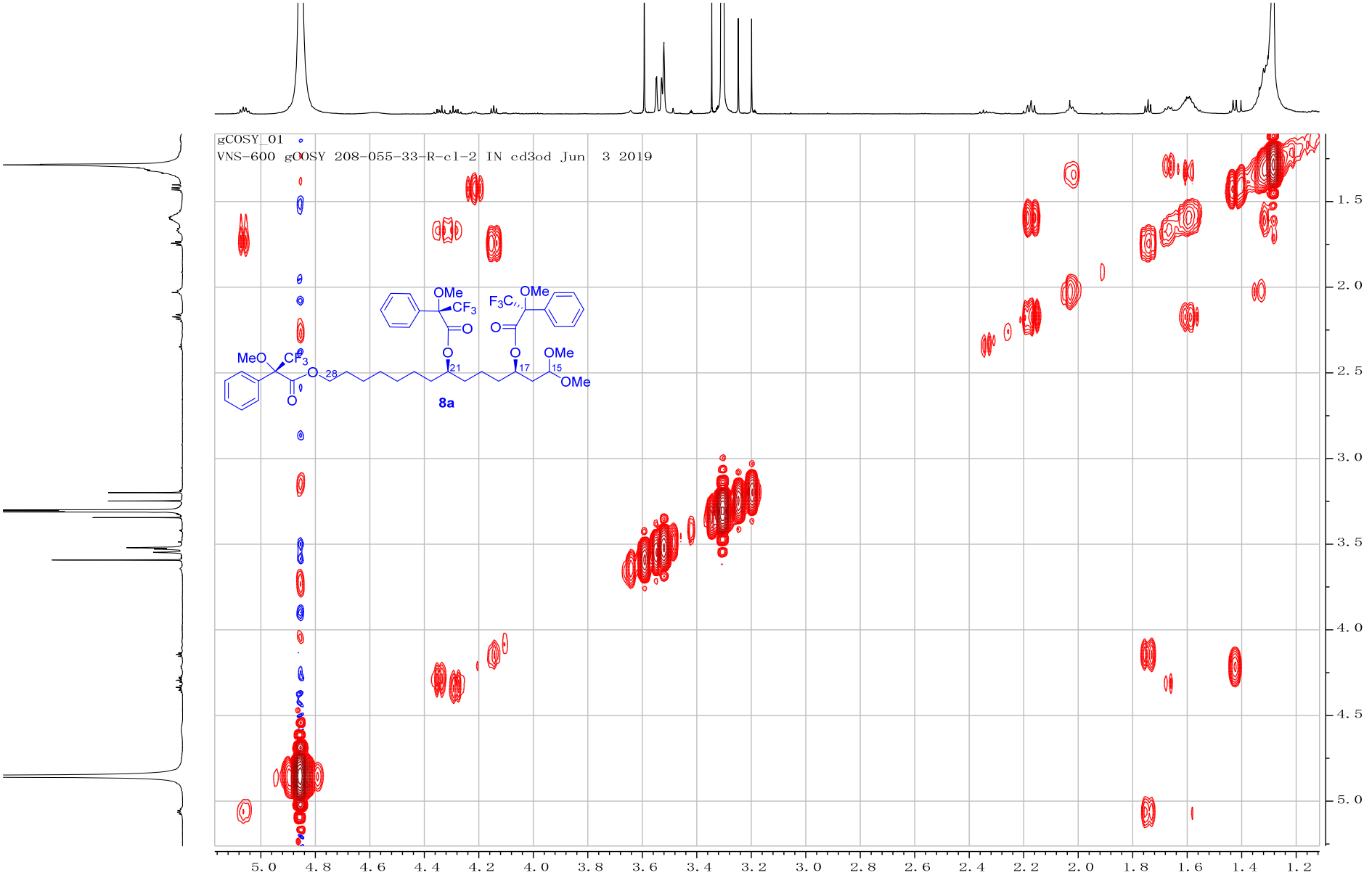

Figure S84. The ^{1}H-^{1}H COSY spectrum of compound **8a** in CD_3OD (600 MHz).

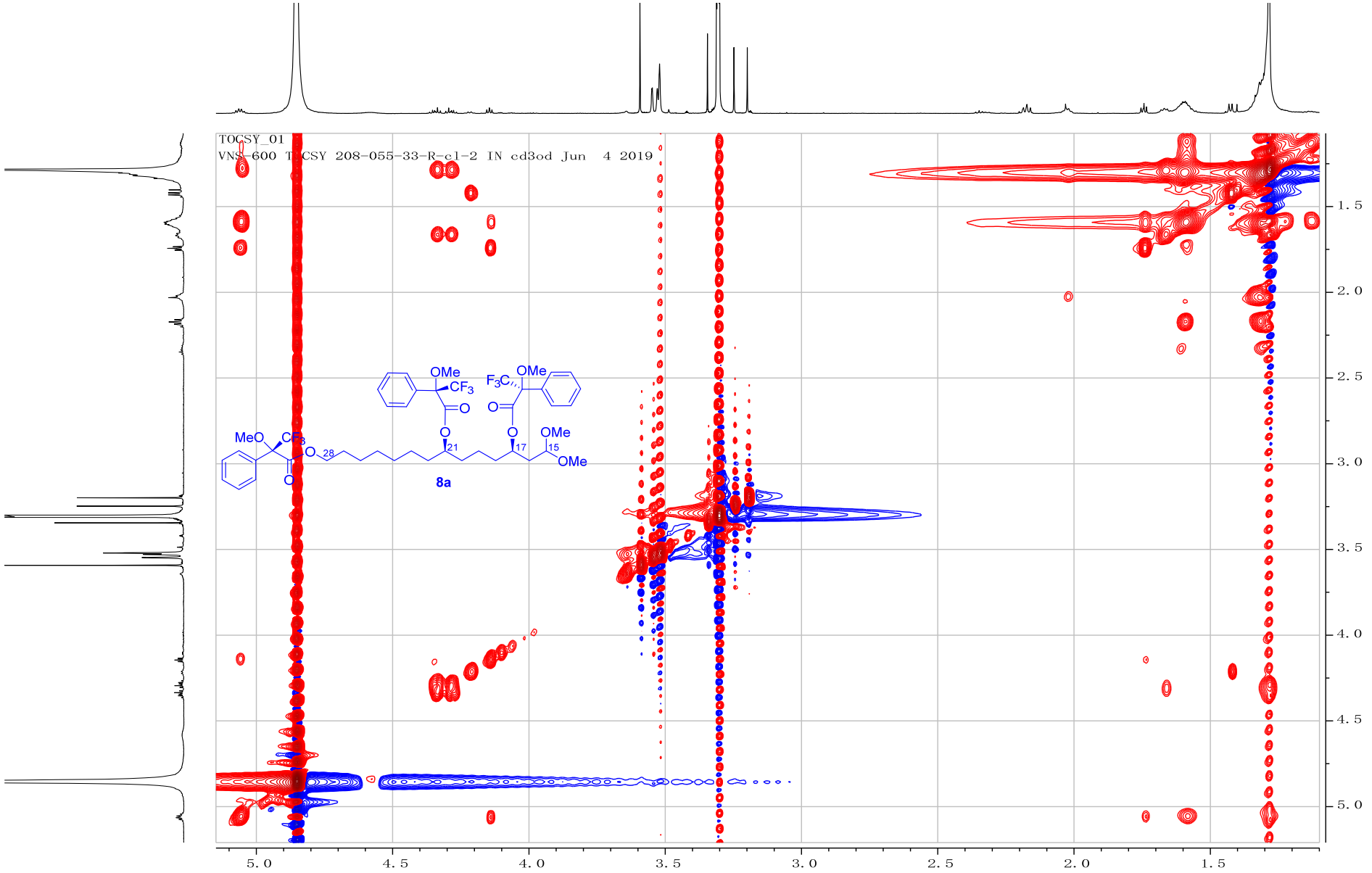

Figure S85. The TOCSY spectrum of compound **8a** in CD_3OD (600 MHz).

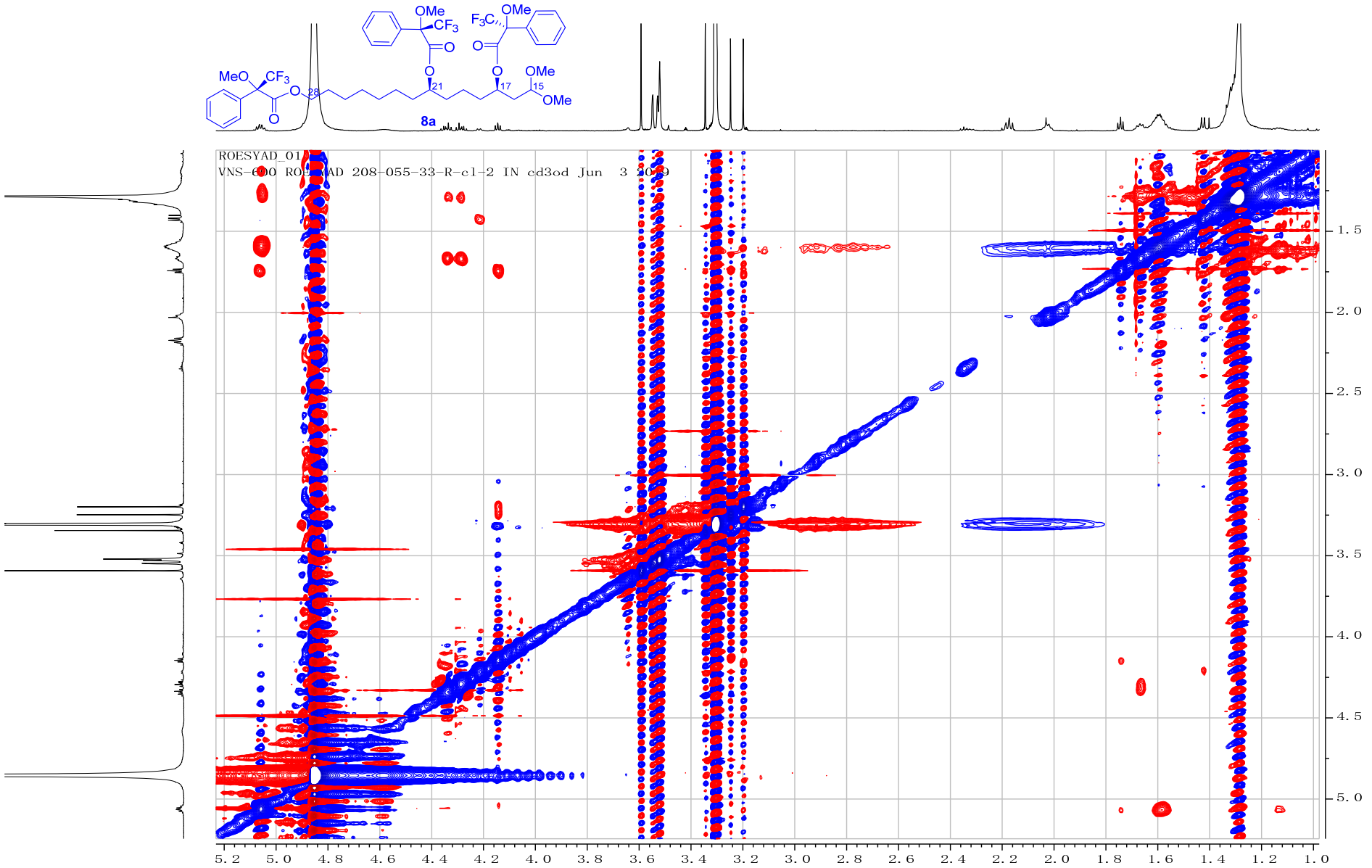

Figure S86. The ROESY spectrum of compound **8a** in CD_3OD (600 MHz).

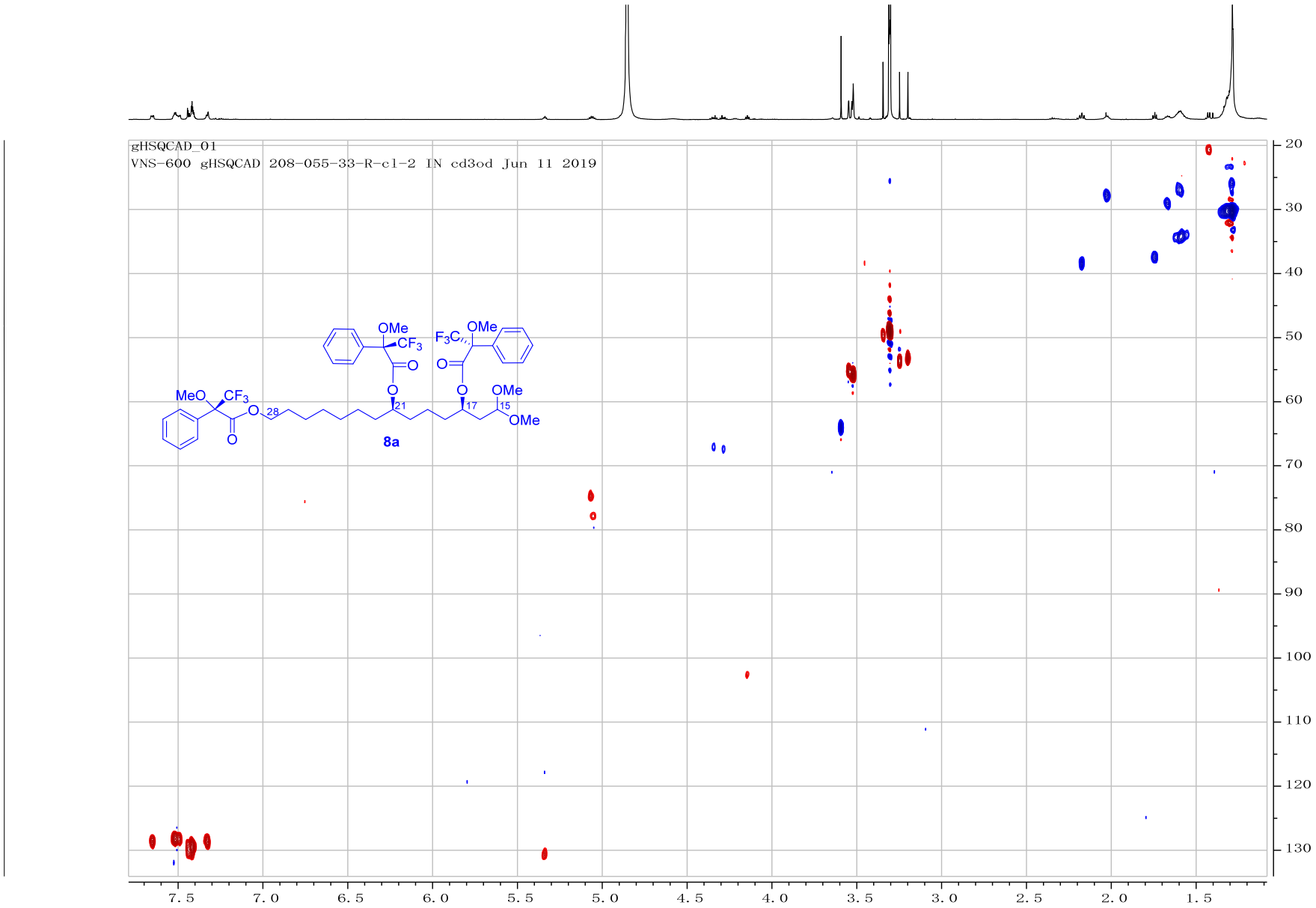

Figure S87. The HSQC spectrum of compound **8a** in CD_3OD (600 MHz).

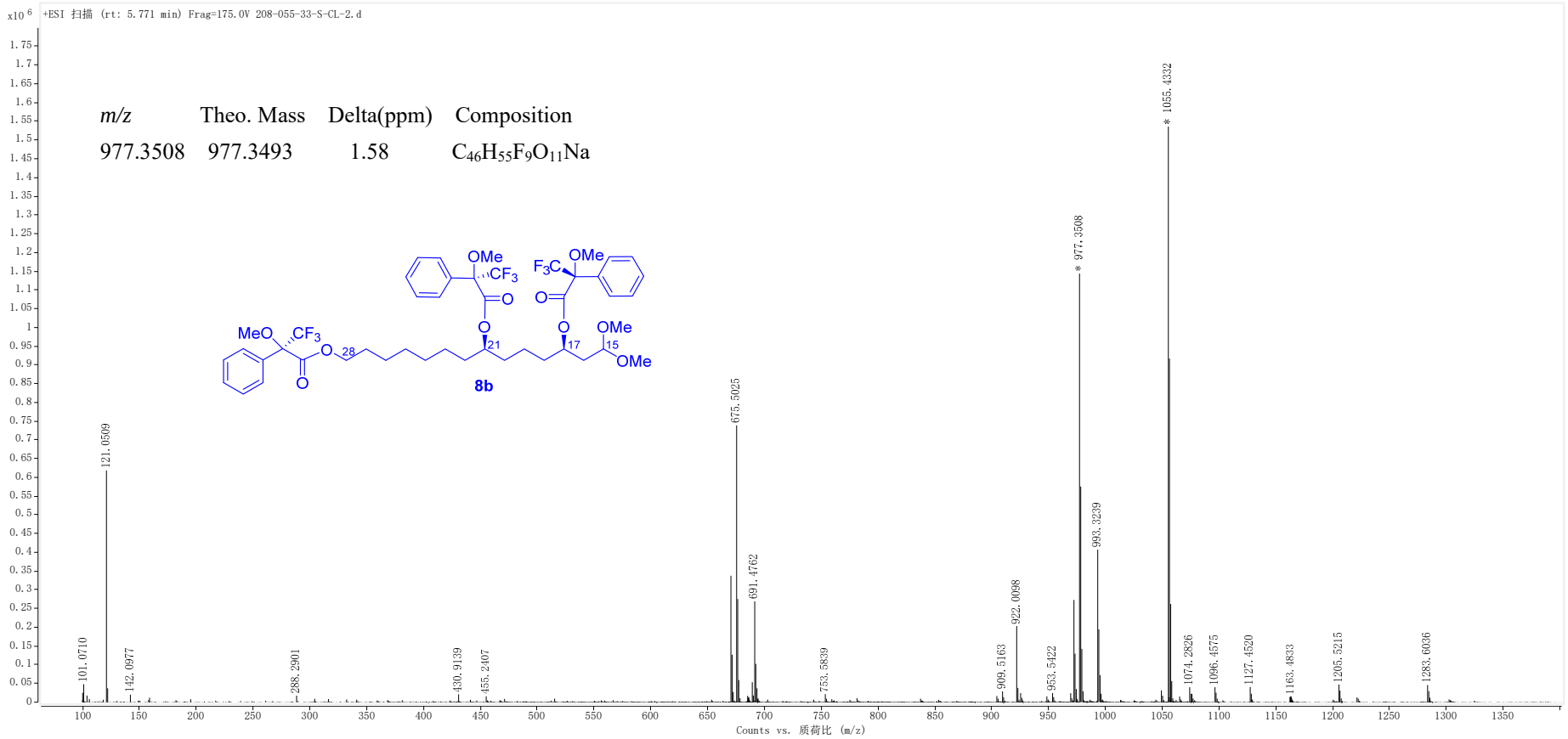

Figure S88. The (+)-HRESIMS spectrum of compound **8b**.

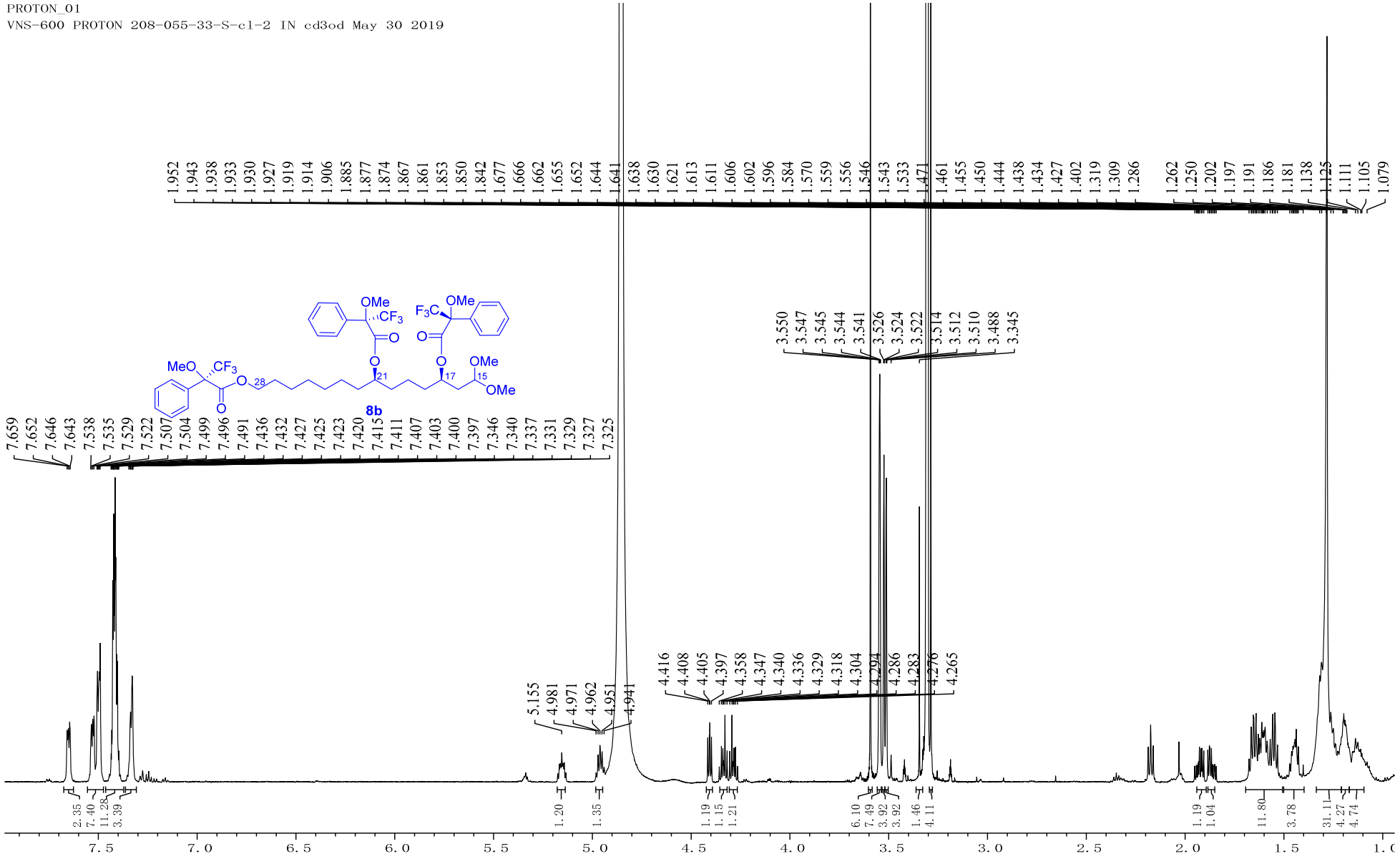

Figure S89. The ^{1}H NMR spectrum of compound **8b** in CD_3OD (600 MHz).

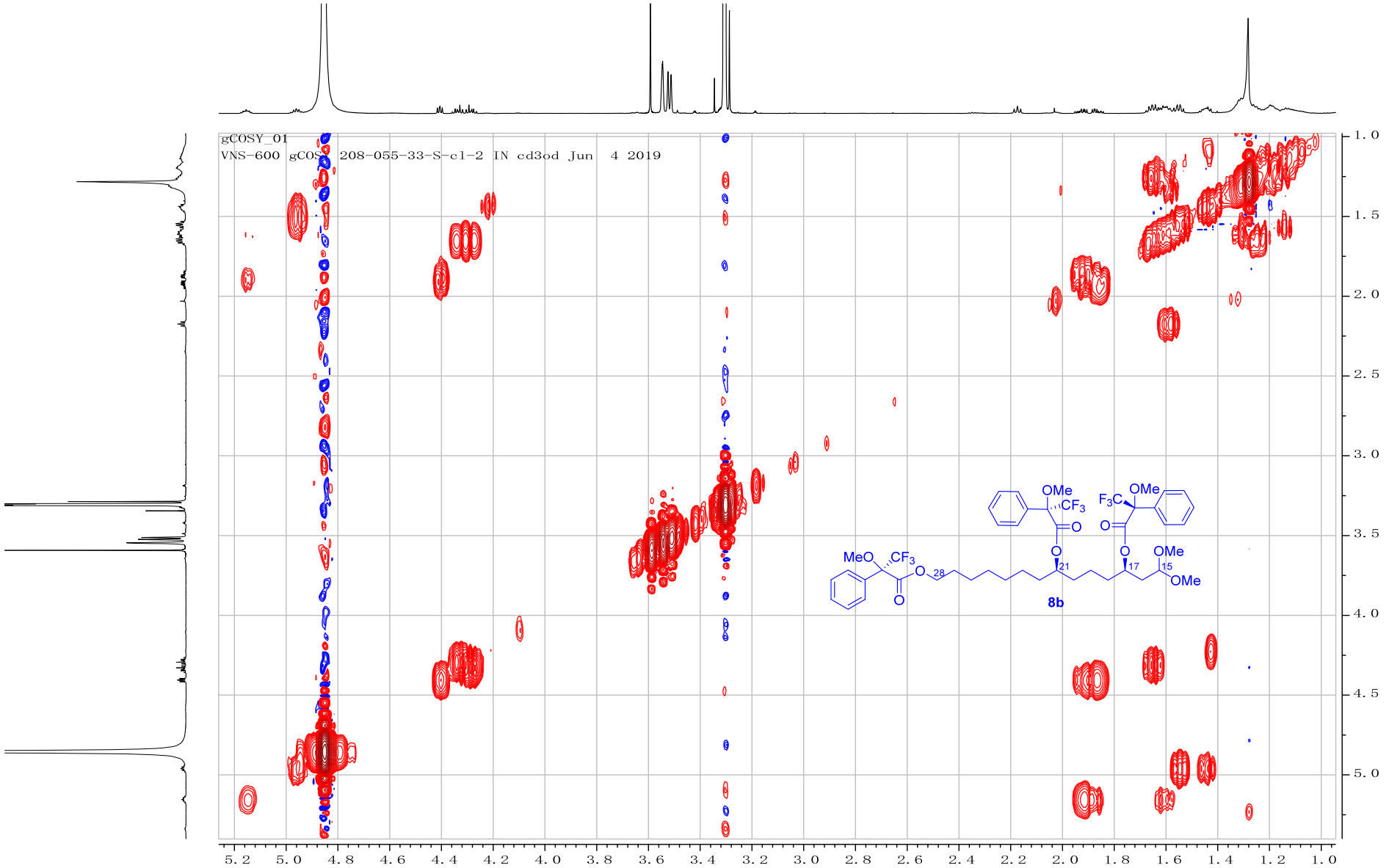

Figure S90. The ^{1}H-^{1}H COSY spectrum of compound **8b** in CD_3OD (600 MHz).

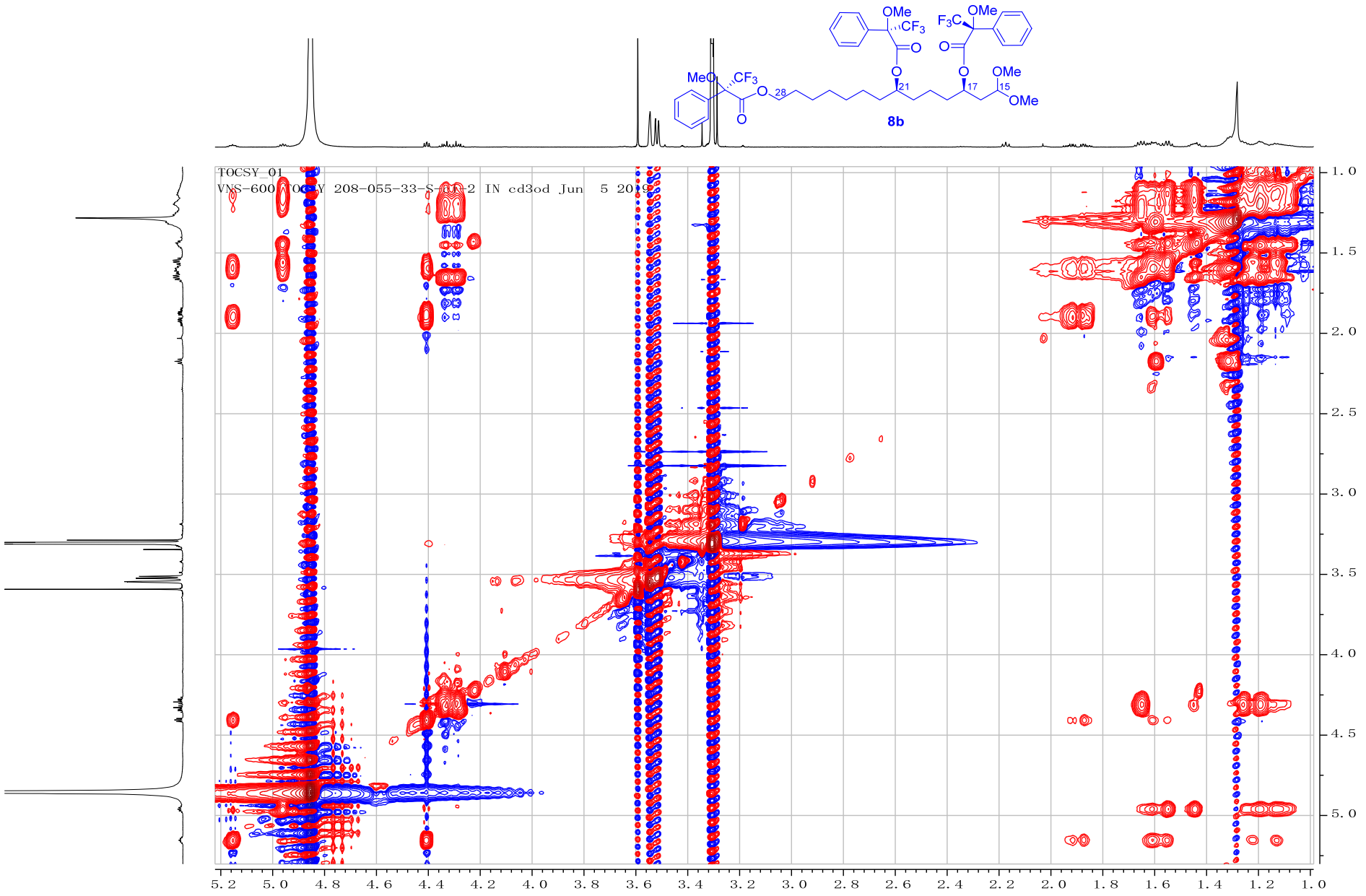

Figure S91. The TOCSY spectrum of compound **8b** in CD_3OD (600 MHz).

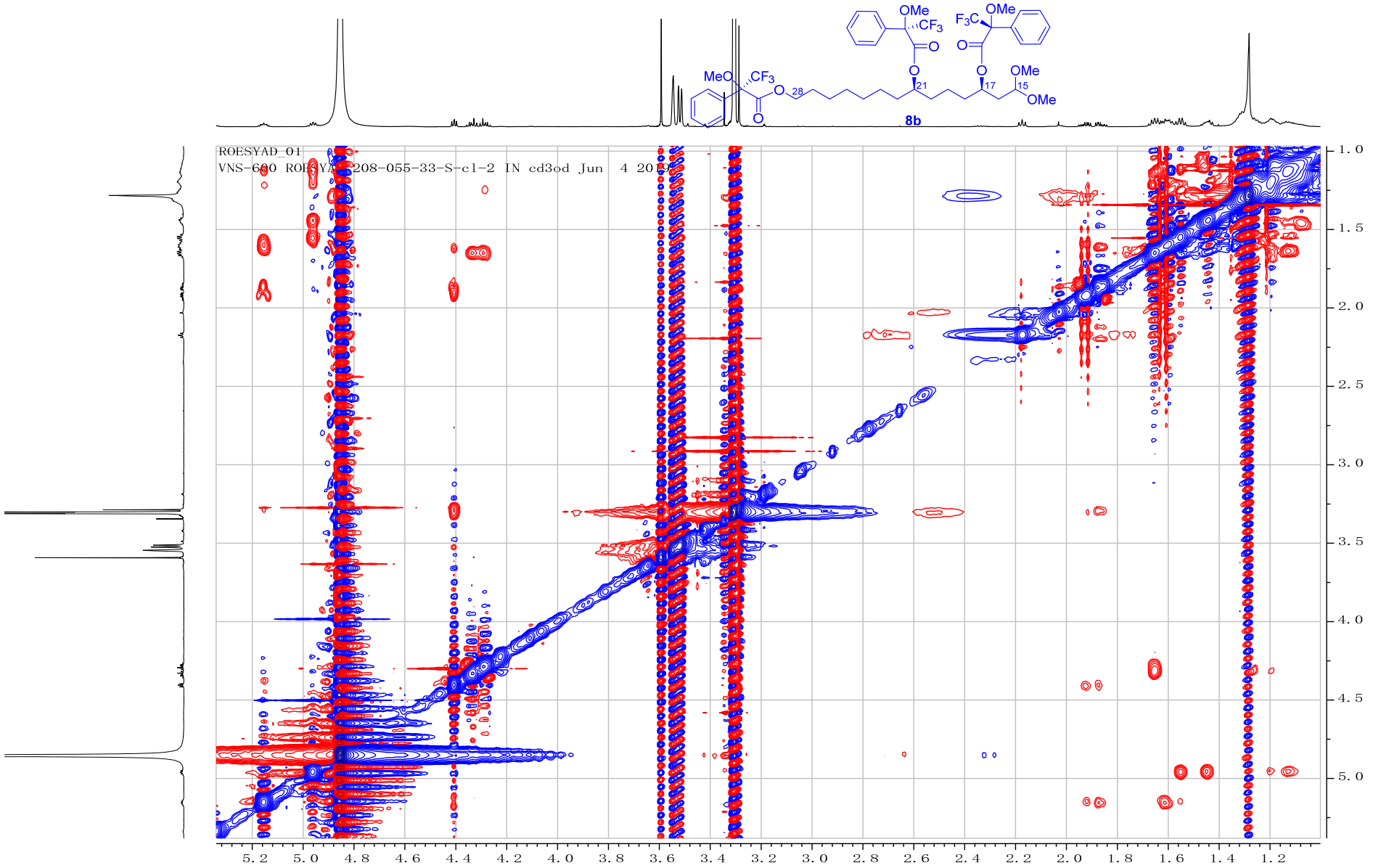

Figure S92. The ROESY spectrum of compound **8b** in CD_3OD (600 MHz).

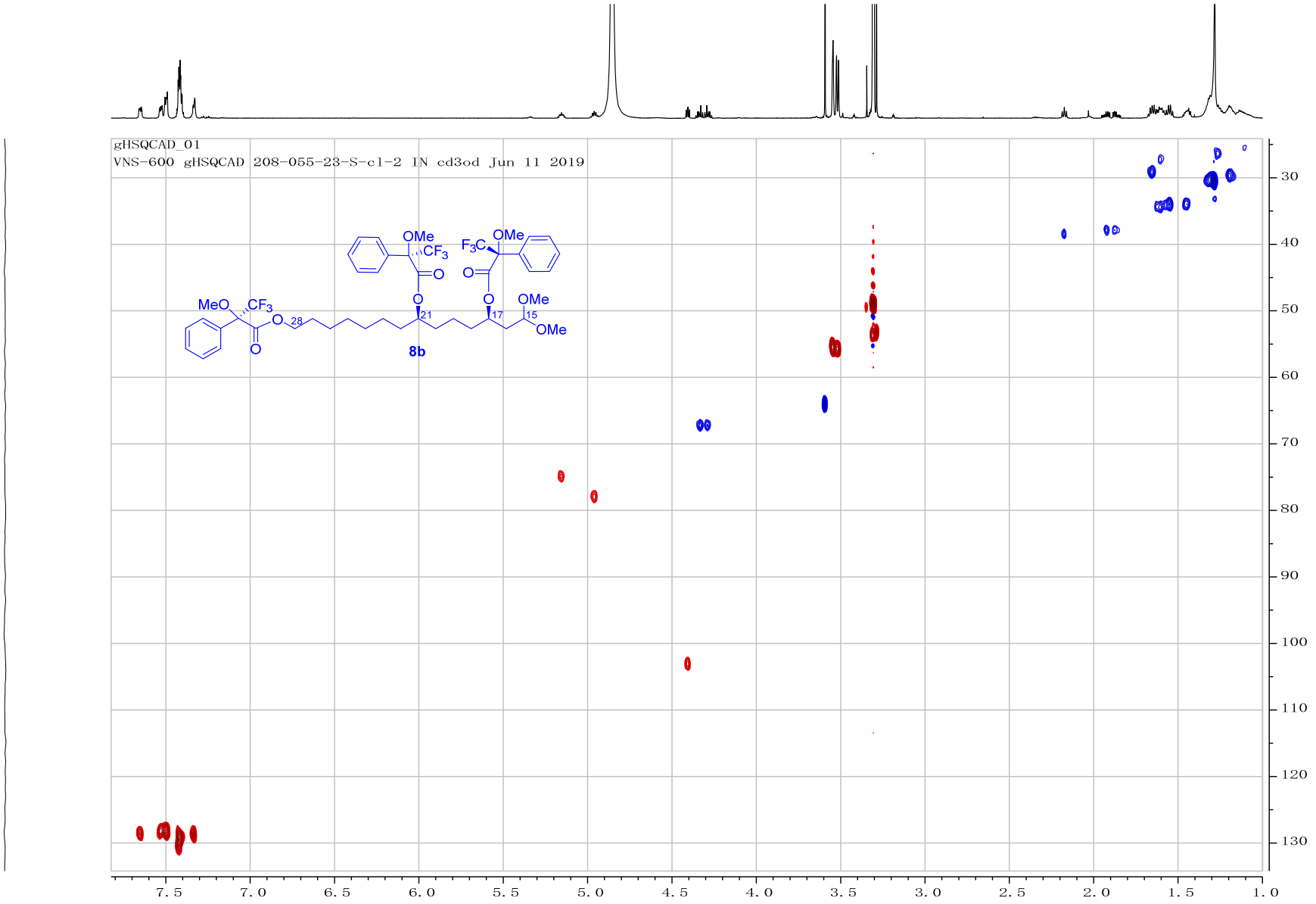

Figure S93. The HSQC spectrum of compound **8b** in CD_3OD (600 MHz).

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