Supplementary Material

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1. **Experimental data**
   1. **General consideration**

All reagents and organic solvents used in the synthesis were obtained from Aldrich, TCI (South Korea) and used without further purification. Flash chromatography was carried out on silica gel (230-400 mesh) followed by determination of 1H and 13C NMR spectra using a Bruker Avance 400 MHz spectrometer. Mass spectra were obtained using a maXis-HD (Bruker). UV absorption spectroscopy measurements were carried out on V-730 UV-Visible Spectrophotometer (Jasco) at room temperature. Fluorescence emission spectra were obtained using an F-7000 Fluorescence Spectrophotometer (Hitachi High-Tech).

* 1. **Synthesis process**



Scheme S1. Synthesis process of R1IR2.

* + 1. Synthesis **DBr**: 2,4-Dibromotoluene (3.0 g, 2 mmol) was added in 50 mL CH3CN including NBS (2.3 g – 12.9 mmol). The mixture was stirred and irradiated under white lamp 25W during 30 min. The reaction solution was evaporated and purified by column chromatography on silica gel using n-hexane as eluent to obtain yellow oil as pure product (yield ~ 95 %). 1H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 2.0 Hz, 1H), 7.41 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 4.52 (s, 2H). 13C NMR (101 MHz, CHLOROFORM-*D*) δ 136.61, 136.16, 132.67, 131.65, 125.52, 123.46, 32.82.



Scheme S2. Synthesis of **DBr** and **CBr**.

* + 1. Synthesis **CBr:** A mixture of carbazole (5.0 g), benzene (15 mL), 1,4 dichlorobutane (10 eq.), benzyltriethylammonium chloride (phase transfer catalyst) and aqueous sodium hydroxide (15 mL, 50%) was stirred overnight. The obtained solution was acidified with HCl to pH around 3, extracted with chloroform, and then dried over anhydrous Na2SO4. After evaporation, the viscous liquid was purified by column chromatography on silica gel using n-hexane-DCM (9/1) as eluent to obtain brown powder as pure product (yield ~ 65%). 1H NMR (400 MHz, Chloroform-*d*) δ 8.10 (dq, *J* = 7.7, 1.1 Hz, 2H), 7.46 (ddt, *J* = 8.2, 7.1, 1.3 Hz, 2H), 7.36 (s, 2H), 7.28 – 7.19 (m, 2H), 4.29 (td, *J* = 7.0, 1.3 Hz, 2H), 3.33 (t, *J* = 6.5 Hz, 2H), 2.08 – 1.96 (m, 2H), 1.93 – 1.81 (m, 2H); 13C NMR (101 MHz, Chloroform-*d*) δ 140.43, 125.89, 123.04, 120.59, 119.11, 108.70, 42.26, 33.32, 30.37, 27.78; ESI HRMS m/z = 302.0534 [M+H]+, calc. for C16H16BrN = 301.05.
    2. Synthesis of **I**: A mixture of 2,4-diaminonaphthalene (2.0 g) and formic acid (20 mL) was refluxed at 100 °C for 24 h. The obtained solution was added NaOH solution (50%) to pH 9, extracted with chloroform, and then dried over anhydrous Na2SO4. After evaporation, the crude product was purified by column chromatography on silica gel using n-hexane-Methanol (95/5) as eluent to obtain white powder as pure product (yield ~ 75%). 1H NMR (400 MHz, Acetone-*d*6) δ 8.43 (s, 1H), 8.15 (s, 2H), 7.99 (dt, *J* = 6.0, 3.0 Hz, 2H), 7.42 – 7.34 (m, 2H). 13C NMR (101 MHz, DMSO-*D*6) δ 147.08, 130.33, 128.42, 123.98. ESI HRMS m/z = 169.0761 [M+H]+, calc. for C11H8N2 = 168.07.
    3. Synthesis of **R1I**: NaH (200 mg) was added to the mixture of **I** (1.0 g, 5.95 mmol) and tetrahydrofuran (20 mL) under ice bath, and the mixture was stirred for 30 min. Then, **R­1Br** or **R2Br** (6.0 mmol) was added, and ice bath was removed. The mixture was refluxed under N2 overnight. After solvent evaporation, water was added and washed with MC. Organic phase was collected, dried over anhydrous Na2SO4, then evaporation. The crude product was purified by column chromatography on silica gel using n-hexane-Ethyl acetate (9/1) as eluent to obtain brown powder as pure product (yield ~ 50%).
       1. **BI**: 1H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 8.12 (s, 1H), 8.04 – 7.96 (m, 1H), 7.91 – 7.83 (m, 1H), 7.70 – 7.59 (m, 2H), 7.45 – 7.34 (m, 2H), 7.23 – 7.12 (m, 2H), 6.87 – 6.78 (m, 1H), 5.50 (s, 2H); 13C NMR (101 MHz, CHLOROFORM-*D*) δ 147.43, 143.93, 134.68, 134.46, 133.37, 130.75, 130.33, 129.95, 128.70, 128.63, 128.15, 127.59, 124.79, 123.82, 122.98, 117.83, 105.93, 49.10; ESI HRMS m/z = 337.0339 [M+H]+, calc. for C18H13BrN2 = 336.03.
       2. **CI**: 1H NMR (400 MHz, Chloroform-*d*) δ 8.25 (s, 1H), 8.09 (dt, *J* = 7.7, 1.0 Hz, 2H), 8.01 – 7.95 (m, 1H), 7.91 – 7.79 (m, 2H), 7.60 (s, 1H), 7.46 – 7.36 (m, 4H), 7.33 (dt, *J* = 8.2, 0.9 Hz, 2H), 7.23 (ddd, *J* = 7.9, 7.1, 1.0 Hz, 3H), 4.33 (d, *J* = 5.8 Hz, 2H), 4.05 (d, *J* = 5.8 Hz, 2H), 3.47 (s, 2H); 13C NMR (101 MHz, CHLOROFORM-*D*) δ 140.31, 130.55, 130.16, 128.67, 127.53, 125.94, 124.68, 123.69, 123.03, 120.64, 119.25, 117.62, 108.58, 105.41, 50.92, 44.95, 42.46, 27.48, 26.37; ESI HRMS m/z = 390.1967 [M+H]+, calc. for C27H23N3 = 389.19.
       3. **DI:** 1H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 8.12 (s, 1H), 8.04 – 7.96 (m, 1H), 7.91 – 7.84 (m, 1H), 7.81 (d, *J* = 2.0 Hz, 1H), 7.63 (s, 1H), 7.46 – 7.35 (m, 2H), 7.30 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.69 – 6.62 (m, 1H), 5.44 (s, 2H). 13C NMR (101 MHz, CHLOROFORM-*D*) δ 147.25, 143.81, 135.73, 134.22, 133.82, 131.33, 130.79, 130.39, 129.58, 128.72, 127.56, 124.95, 123.95, 123.38, 122.80, 118.00, 105.83, 48.66. ESI HRMS m/z = 414.9443 [M+H]+, calc. for C18H12Br2N2 = 413.94.
    4. Synthesis of **R1IR2**: A mixture of **R1I** (1.0 mmol) and **R2Br** or **CH3I** (1.2 mmol) in CH3CN were refluxed overnight. After cooled to room temperature, solvents were removed, then residue was dissolved in methanol (1 mL). Hexane (15-25 mL) was added to the solution, vibrate in Ultrasonic Cleaner and the precipitate was collected by filter to obtain the product as white solid (yield ~ 90%).
       1. **BIB**: 1H NMR (400 MHz, DMSO-d6) δ 10.03 (s, 1H), 8.61 (s, 2H), 8.22 – 8.13 (m, 2H), 7.79 (dd, J = 7.8, 1.4 Hz, 2H), 7.70 – 7.62 (m, 2H), 7.47 – 7.35 (m, 6H), 5.95 (s, 4H). 13C NMR (101 MHz, DMSO-D6) δ 148.43, 133.86, 133.19, 131.64, 131.46, 130.81, 130.71, 129.01, 128.84, 127.52, 123.43, 112.08, 51.24. ESI HRMS m/z = 504.9909 [M]+, calc. for C25H19Br2N2 = 504.99.
       2. **BIM**: 1H NMR (400 MHz, DMSO-d6) δ 9.91 (s, 1H), 8.68 (s, 1H), 8.55 (s, 1H), 8.28 – 8.21 (m, 1H), 8.21 – 8.14 (m, 1H), 7.80 (dd, J = 7.8, 1.6 Hz, 1H), 7.73 – 7.62 (m, 2H), 7.47 – 7.34 (m, 3H), 5.90 (s, 2H), 4.20 (s, 3H). 13C NMR (101 MHz, DMSO-D6) δ 147.92, 133.81, 133.28, 131.66, 131.55, 131.50, 131.44, 130.80, 130.68, 128.97, 128.84, 128.81, 127.31, 123.48, 111.87, 111.47, 50.87, 34.13. ESI HRMS m/z = 504.9909 [M]+, calc. for C25H19Br2N2 = 504.99. ESI HRMS m/z = 351.0497 [M]+, calc. for C19H16BrN2 = 351.05.
       3. **CIB**: 1H NMR (400 MHz, DMSO-*d*6) δ 9.93 (s, 1H), 8.68 (s, 1H), 8.52 (s, 1H), 8.23 – 8.09 (m, 4H), 7.74 (ddd, *J* = 7.1, 2.8, 1.6 Hz, 1H), 7.72 – 7.64 (m, 2H), 7.61 (dt, *J* = 8.2, 0.9 Hz, 2H), 7.41 (ddd, *J* = 8.3, 7.1, 1.2 Hz, 2H), 7.39 – 7.32 (m, 3H), 7.18 (ddd, *J* = 7.9, 7.2, 0.9 Hz, 2H), 5.84 (s, 2H), 4.64 (t, *J* = 7.0 Hz, 2H), 4.48 (t, *J* = 6.9 Hz, 2H), 2.07 (q, *J* = 7.4 Hz, 2H), 1.91 (dq, *J* = 14.5, 7.0 Hz, 2H). 13C NMR (101 MHz, DMSO-D6) δ 147.56, 140.50, 133.90, 133.20, 131.64, 131.58, 131.52, 131.02, 130.84, 130.75, 129.03, 128.90, 127.45, 126.27, 123.54, 122.67, 120.91, 119.36, 112.03, 111.75, 109.86, 51.13, 47.44, 42.26, 31.55, 26.53, 26.13, 22.66, 14.56. ESI HRMS m/z = 558.1539 [M]+, calc. for C34H29BrN3 = 558.15.
       4. **CIC**: 1H NMR (600 MHz, DMSO-*d*6) δ 9.82 (s, 1H), 8.55 (d, *J* = 2.3 Hz, 2H), 8.14 (dt, *J* = 5.7, 2.7 Hz, 2H), 8.10 (d, *J* = 7.7 Hz, 4H), 7.69 (dt, *J* = 5.8, 2.6 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 4H), 7.39 (t, *J* = 7.8 Hz, 4H), 7.16 (t, *J* = 7.3 Hz, 4H), 4.51 (t, *J* = 7.2 Hz, 4H), 4.43 (t, *J* = 7.2 Hz, 4H), 2.01 (p, *J* = 7.6 Hz, 4H), 1.87 (p, *J* = 7.3 Hz, 4H). 13C NMR (101 MHz, DMSO-*D*6) δ 146.60, 140.40, 131.41, 130.67, 128.78, 127.17, 126.18, 122.58, 120.84, 119.29, 111.50, 109.74, 47.14, 42.16, 26.34, 26.00. ESI HRMS m/z = 611.3169 [M]+, calc. for C43H39N3 = 611.32.
       5. **CID**: 1H NMR (600 MHz, DMSO-*d*6) δ 9.87 (s, 1H), 8.68 (s, 1H), 8.53 (s, 1H), 8.17 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 2H), 8.12 (dt, *J* = 7.7, 0.9 Hz, 2H), 8.01 (d, *J* = 2.0 Hz, 1H), 7.73 – 7.65 (m, 2H), 7.64 – 7.57 (m, 3H), 7.41 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.18 (ddd, *J* = 7.9, 7.1, 0.9 Hz, 2H), 5.79 (s, 2H), 4.62 (t, *J* = 7.1 Hz, 2H), 4.47 (t, *J* = 7.1 Hz, 2H), 2.06 (p, *J* = 7.1 Hz, 2H), 1.89 (p, *J* = 7.3 Hz, 2H). 13C NMR (101 MHz, DMSO-*D*6) δ 146.66, 139.65, 134.93, 131.91, 131.77, 131.12, 130.81, 129.89, 128.06, 126.63, 125.43, 123.77, 122.63, 121.83, 120.09, 118.53, 111.19, 110.90, 109.02, 49.80, 46.63, 41.44, 25.70, 25.31. ESI HRMS m/z = 636.0654 [M]+, calc. for C34H28Br2N3 = 636.06.
       6. **CIM**: 1H NMR (400 MHz, DMSO-*d*6) δ 9.81 (s, 1H), 8.59 (d, *J* = 2.6 Hz, 2H), 8.25 – 8.19 (m, 1H), 8.19 – 8.15 (m, 1H), 8.15 – 8.08 (m, 2H), 7.70 (dt, *J* = 6.0, 3.4 Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.43 (ddd, *J* = 8.3, 7.1, 1.2 Hz, 2H), 7.23 – 7.14 (m, 2H), 4.58 (t, *J* = 7.0 Hz, 2H), 4.49 (t, *J* = 6.8 Hz, 2H), 4.09 (s, 3H), 3.39 (s, 5H), 2.06 (dd, *J* = 17.1, 8.6 Hz, 2H), 1.94 (t, *J* = 7.7 Hz, 2H). 13C NMR (101 MHz, DMSO-*D*6) δ 147.24, 140.44, 131.57, 131.40, 130.57, 128.81, 128.77, 127.15, 127.12, 126.20, 122.58, 120.83, 119.29, 111.44, 111.30, 109.80, 47.07, 42.24, 33.88, 26.56, 26.07. ESI HRMS m/z = 404.2121 [M]+, calc. for C28H26N3 = 404.21.
       7. **DIB**: 1H NMR (400 MHz, DMSO-*d*6) δ 10.01 (s, 1H), 8.62 (d, *J* = 6.5 Hz, 2H), 8.18 (dt, *J* = 7.4, 3.1 Hz, 2H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.80 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.72 – 7.63 (m, 3H), 7.48 – 7.30 (m, 4H), 5.93 (d, *J* = 10.0 Hz, 4H). 13C NMR (101 MHz, DMSO-*D*6) δ 148.44, 135.74, 133.86, 133.17, 132.72, 132.34, 131.95, 131.66, 131.44, 130.79, 130.76, 130.61, 129.00, 128.85, 127.54, 124.51, 123.39, 112.08, 51.24, 50.79. ESI HRMS m/z = 582.9015 [M]+, calc. for C25H18Br3N2 = 582.90.
       8. **DID**: 1H NMR (400 MHz, DMSO-*d*6) δ 9.97 (s, 1H), 8.61 (s, 2H), 8.22 – 8.14 (m, 2H), 8.08 (d, *J* = 2.0 Hz, 2H), 7.72 – 7.62 (m, 4H), 7.31 (d, *J* = 8.3 Hz, 2H), 5.90 (s, 4H). 13C NMR (101 MHz, DMSO-*D*6) δ 135.74, 132.73, 132.25, 131.95, 131.69, 130.76, 128.89, 127.59, 124.47, 123.36, 112.09, 50.80. ESI HRMS m/z = 660.8120 [M]+, calc. for C25H17Br4N2 = 660.81.
       9. **DIM**: 1H NMR (400 MHz, DMSO-*d*6) δ 9.87 (s, 1H), 8.69 (s, 1H), 8.56 (s, 1H), 8.28 – 8.22 (m, 1H), 8.22 – 8.15 (m, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.74 – 7.63 (m, 3H), 7.34 (d, *J* = 8.3 Hz, 1H), 5.87 (s, 2H), 4.19 (s, 3H). 13C NMR (101 MHz, DMSO-*D*6) δ 135.71, 132.41, 131.91, 131.65, 128.87, 127.35, 124.57, 123.38, 111.88, 111.49, 50.42, 34.10. ESI HRMS m/z = 428.9596 [M]+, calc. for C19H15Br2N2 = 428.96.
  1. **Fluorescence quantum yield measurements**

The photoluminescence quantum yield (ՓF) was determined according to following equation:

Where the subscripts *ref* and *s* denote reference and test respectively, Փ is the fluorescence quantum yield, A is absorbance of test solution, I is integrated fluorescence intensity, and η the refractive index of the solvent. 9,10-Diphenylanthracene (ՓF = 0.90 in Cyclohexane) was used as a reference.1

* 1. **Generation of ROS/RNS**

H2O2 was diluted from a 28 % solution in water, and tert-butyl hydroperoxide was diluted from a 70 % solution in water. ROO· was generated from 2,2’- azobis(2-amidinopropane)dihydrochloride, NO· was generated from SNP (sodium nitroferricyanide(III)dihydrate), and ·OH was generated from the reaction of iron(II) chloride with H2O2. ONOO− was prepared according to previous literature, and the concentration was determined by the absorbance at 302 nm.2 NaClO was obtained by dilution of 5 % of the solution in water. The above ROS or reactive nitrogen species (RNS) was incubated with the probe in a PBS (pH 7.4)/THF (5/5) mixture for 15 min.

* 1. **LOD calculation**

The limit of detection was calculated according to the literature procedure. 3 The linear calibration cure was assumed that the response y is linearly related to the concentration x for a limited range of concentration and expressed as y = a + bx. This model was used to determine the sensitivity (b) and the LOD value. The limit of detection (LOD) was calculated using the following equation: LOD=3×Sa/b, where Sa is the standard deviation of the response and b as the slope of calibration cure.

* 1. **Reaction of DSM with ClO-:**

0.1 mL of NaClO solution (5%) was added slowly to the solution of **DSM** (100 mg) in CH3CN (25 mL) under stirring 30 min. The solvent was removed under reduced pressure, the residue was purified by silica gel column chromatography, using MC/MeOH (from 9/1) as eluent to get a white solid as the main product (**DSM’**) (yield ~ 91 %) which assigned **DIM**. 1H NMR (400 MHz, DMSO-*d*6) δ 9.90 – 9.85 (m, 1H), 8.68 (d, *J* = 1.1 Hz, 1H), 8.55 (d, *J* = 1.0 Hz, 1H), 8.27 – 8.21 (m, 1H), 8.21 – 8.14 (m, 1H), 8.08 (d, *J* = 2.0 Hz, 1H), 7.73 – 7.62 (m, 3H), 7.33 (d, *J* = 8.3 Hz, 1H), 5.86 (s, 2H), 4.21 – 4.16 (m, 3H); 13C NMR (101 MHz, DMSO-*D*6) δ 147.38, 135.14, 132.27, 131.86, 131.35, 131.10, 131.01, 130.96, 130.07, 128.31, 128.27, 126.78, 124.01, 122.83, 111.33, 110.93, 49.87, 40.13, 33.59; ESI HRMS m/z = 428.9602 [M]+, calc. for C19H15Br2N2 = 428.96.

* 1. **Computational details**

The DFT calculations of the molecules were performed using the Gaussian 09 program package. Geometry optimizations of the molecule were performed using the B3LYP hybrid functional with 6-31+G(2d,p) basis set.4-5 After optimizing structures, vibrational frequencies were computed to ensure that there are no imaginary frequencies. Optical excitation energies were calculated with various functionals using time-dependent DFT (TD-DFT) with the 6-31+G(2d,p), def-2-TZVP and cc-PVTZ basis sets in ACN solvent.6 The solvent was modeled by the polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM) as implemented in Gaussian 09. Our calculated excitation energies using the Cam-B3LYP functional with Def2-TZVP for **R1IR2** and TPSSTPSS functional with 6-31+G(2d,p) for **R1SR2** were nearest to the experimental data (Table S2). Natural transition-orbital (NTO) analysis was done to characterize the nature of different molecular excited states.7

* 1. **Bacterial experiments**

Three strains of gram-negative bacteria (*E. Coli, ESBL EC, EC GFP*) and two strains of gram-positive bacteria (*S. Aureus, MRSA*) were procured from the Korean Collection for Type Cultures (KCTC) at the Korea Research Institute of Bioscience and Biotechnology (KRIBB). Three isolated colonies were transferred to 3 mL LB broth and grown overnight at 37 °C in a shaking incubator at 250 rpm. The final test concentration of bacterial suspension was adjusted to 2×105 CFU/mL in LB broth. **R1IR2** and **R1SR2** were dissolved in DMSO. The obtained solution was diluted with sterilized LB broth to give a stock solution of 256 µM in 1% DMSO (stock solution). The stock solution was diluted two-fold serially in the LB in microplates to a final volume of 100 μL in each well. The same volume (100 μL) of bacterial suspension was added in each well making concentration range of 1, 2 to 128 µM for each test compound. The microplates were then incubated at 37 °C for 18 h, and the absorbance at 600 nm was measured using a FilterMax™ F5 Multi-Mode Microplate Reader (Molecular Devices, USA). CFU rate (%) was calculated by ratio of CFU value between bacteria treated with/without reagents. To compare the antibacterial activity between couple of **R1IR2** and **R1SR2,** we calculated the concentration (µM) (CFU50­), at which the CFU rate equals 50 %; and the between a couple of imidazolium salt and imidazoline-2-thiones. The CFU50 of imidazoline-2-thiones­ are higher than 128 µM.

1. **Results**
   1. **NMR and Mass spectra**

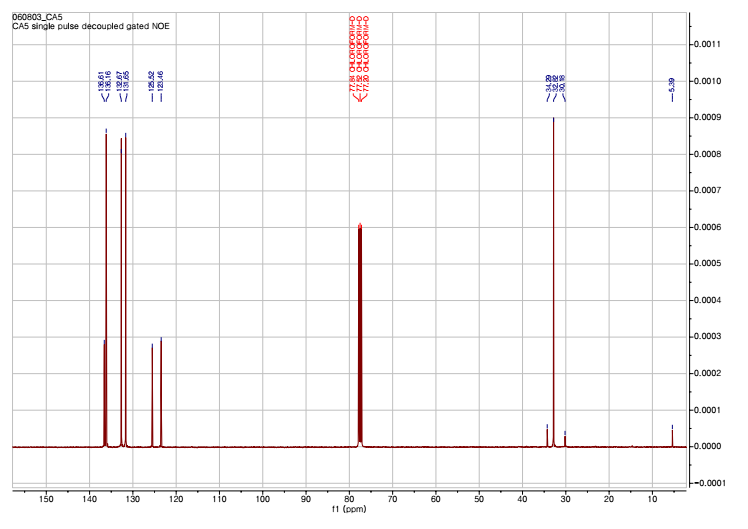
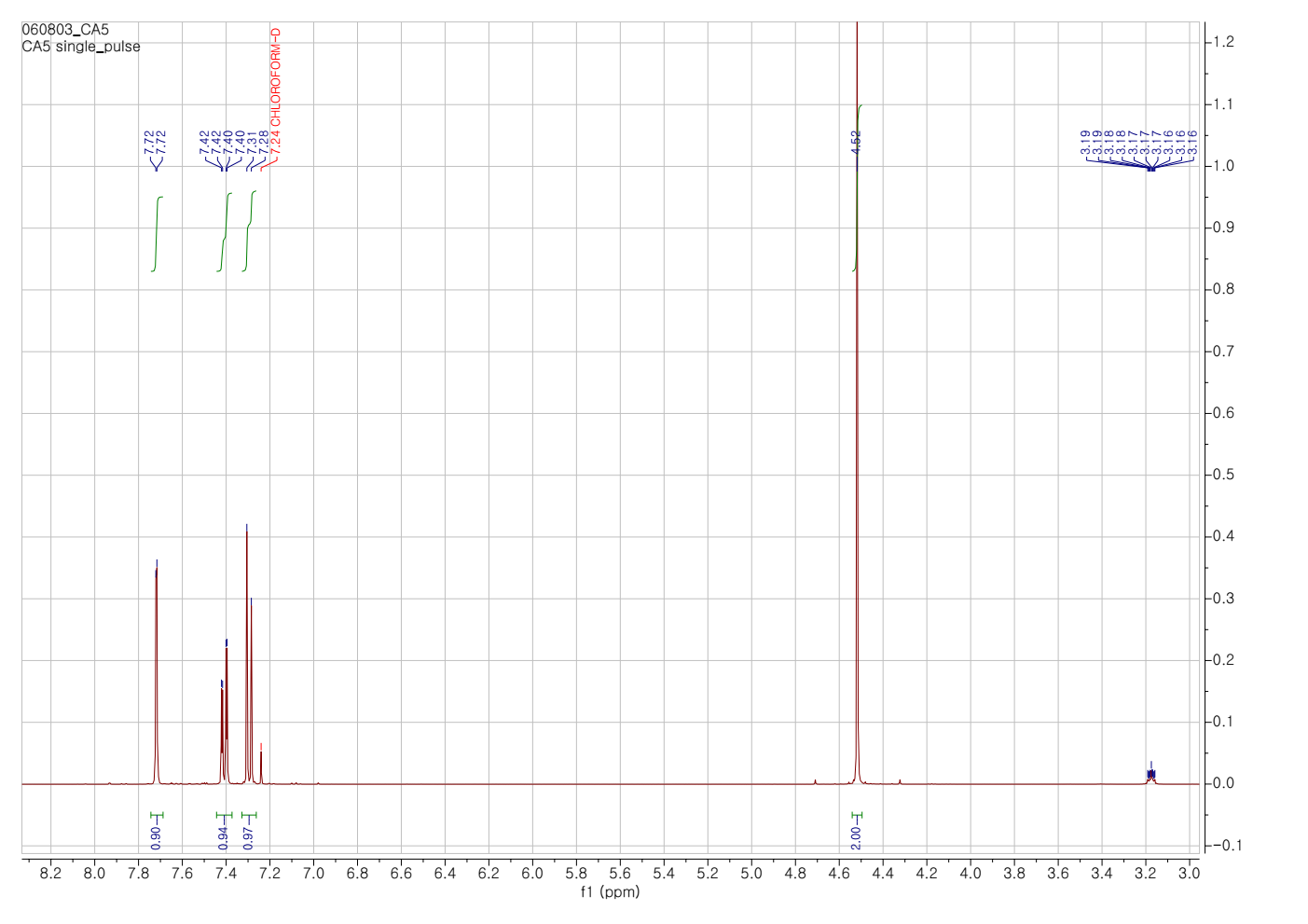


Figure S1. 1H-NMR and 13C-NMR spectra of **DBr** in CDCl3

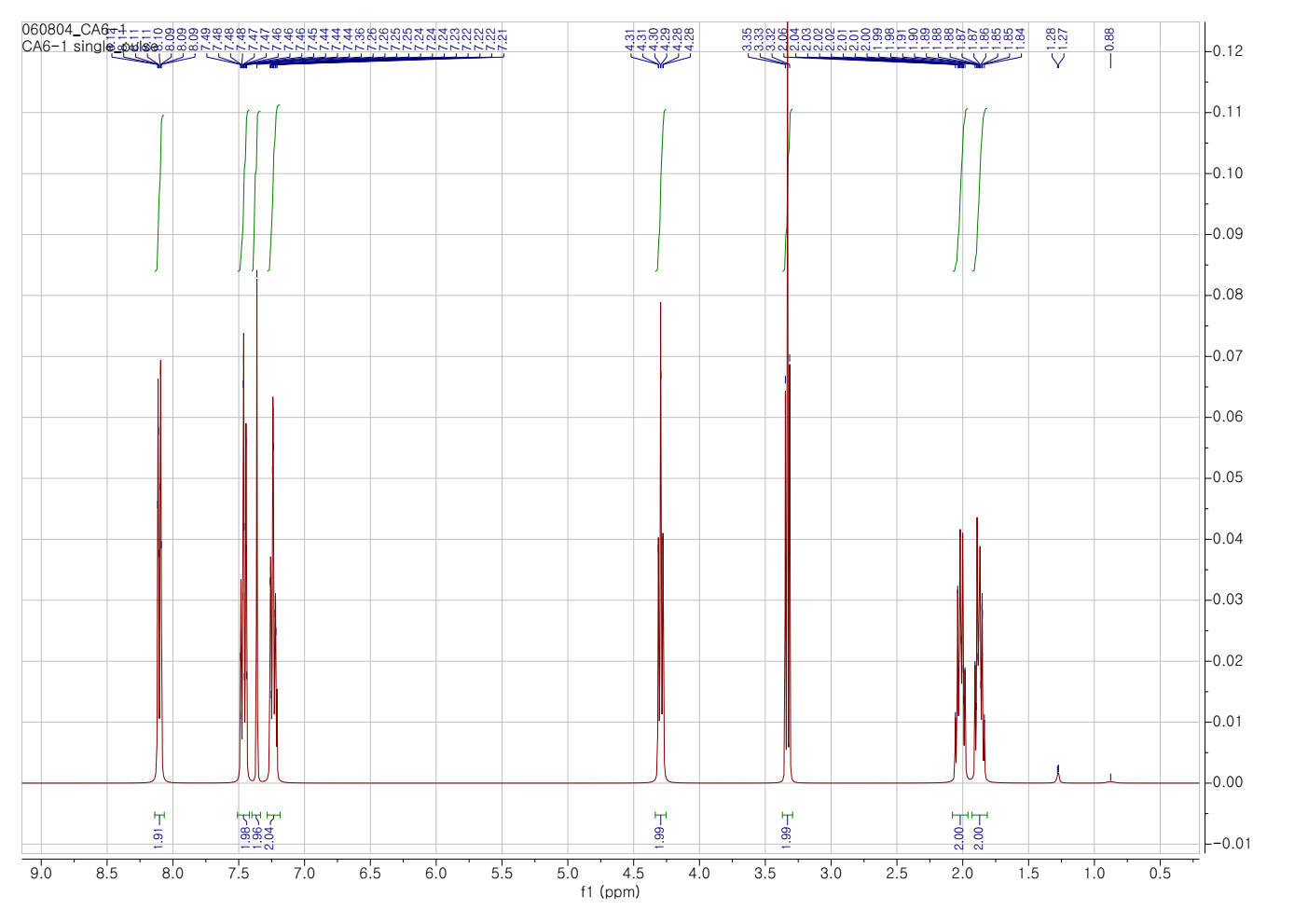
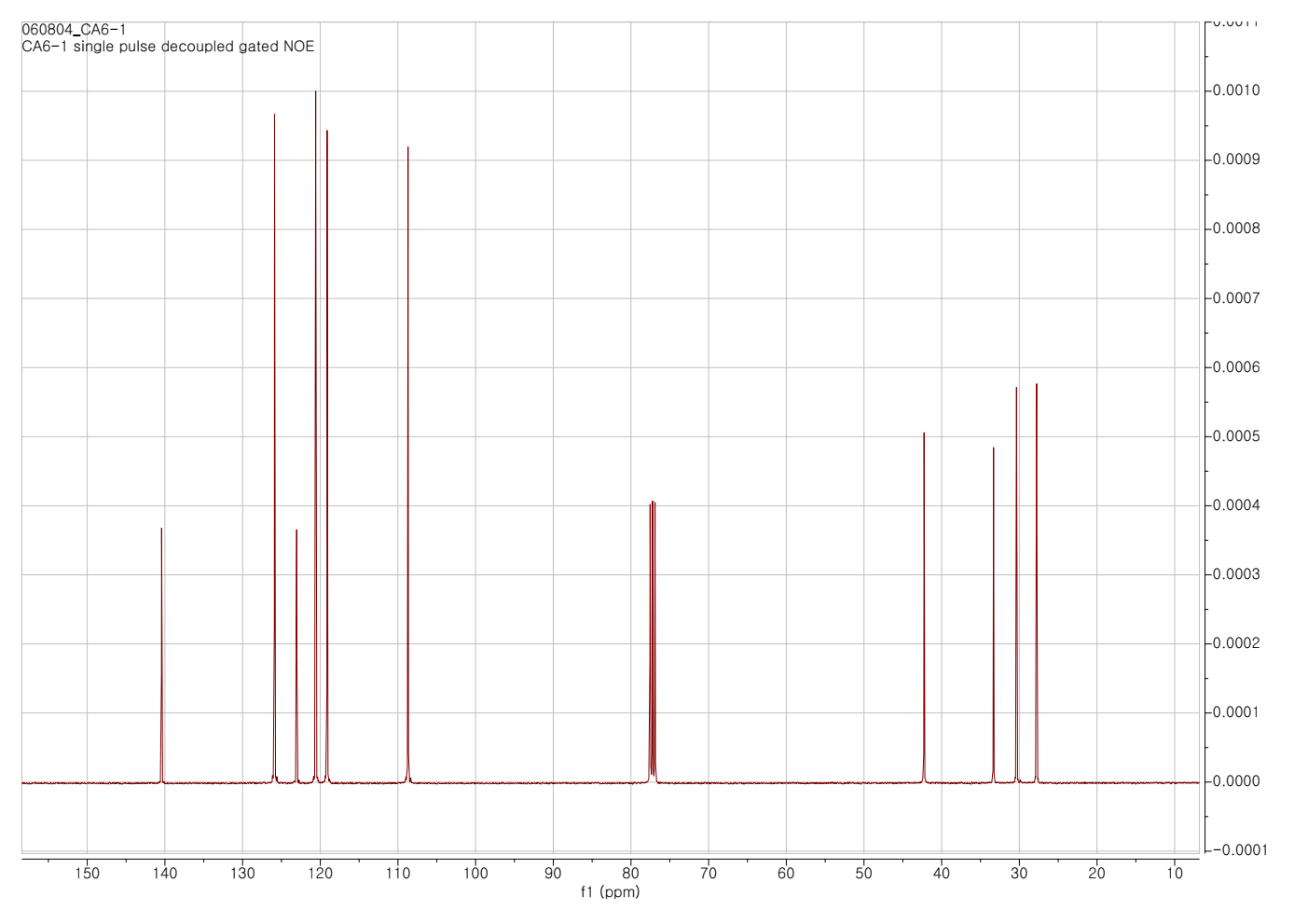
 

Figure S2. 1H-NMR and 13C-NMR spectra of **CBr** in CDCl3

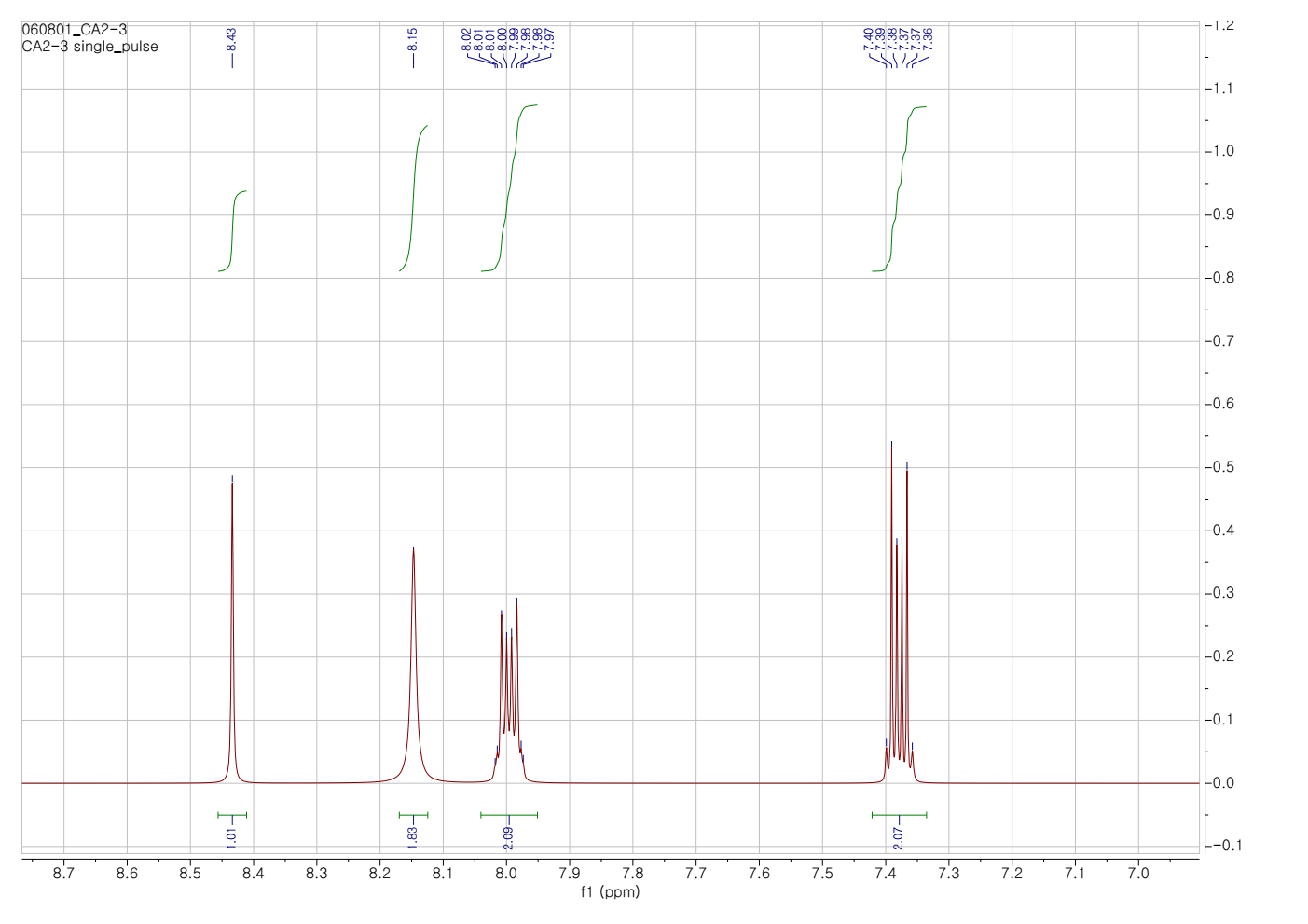
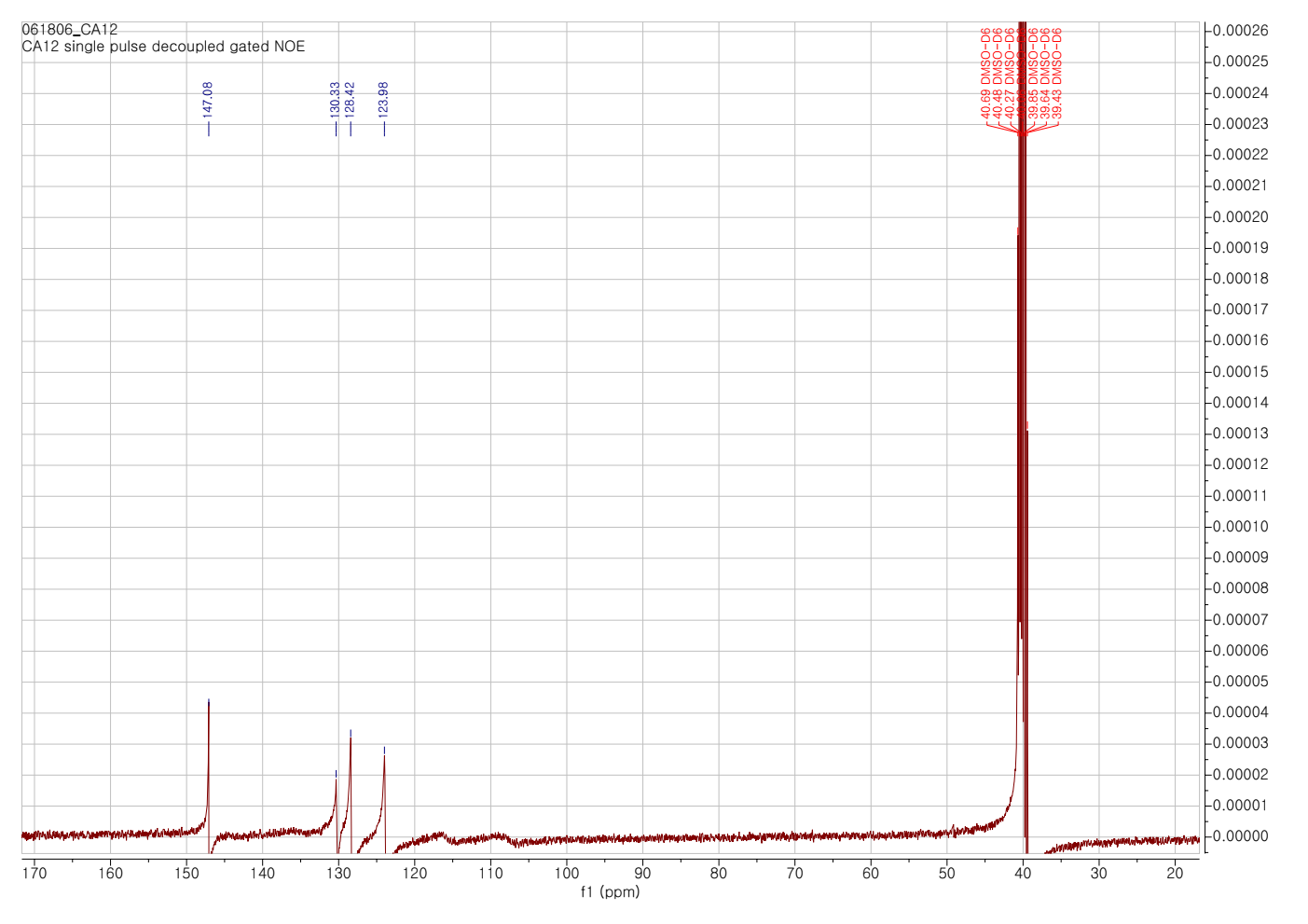
 

Figure S3. 1H-NMR and 13C-NMR spectra of **I** in DMSO

|  |  |
| --- | --- |
| a) Mass spectra of **CBr** | b) Mass spectra of **I** |

Figure S4. Mass spectra of **CBr** and **I**.

|  |  |
| --- | --- |
| a) Mass spectra of **BI** | b) Mass spectra of **CI** |

Figue S5. Mass spectra of (a) **BI** and (b) **CI**.

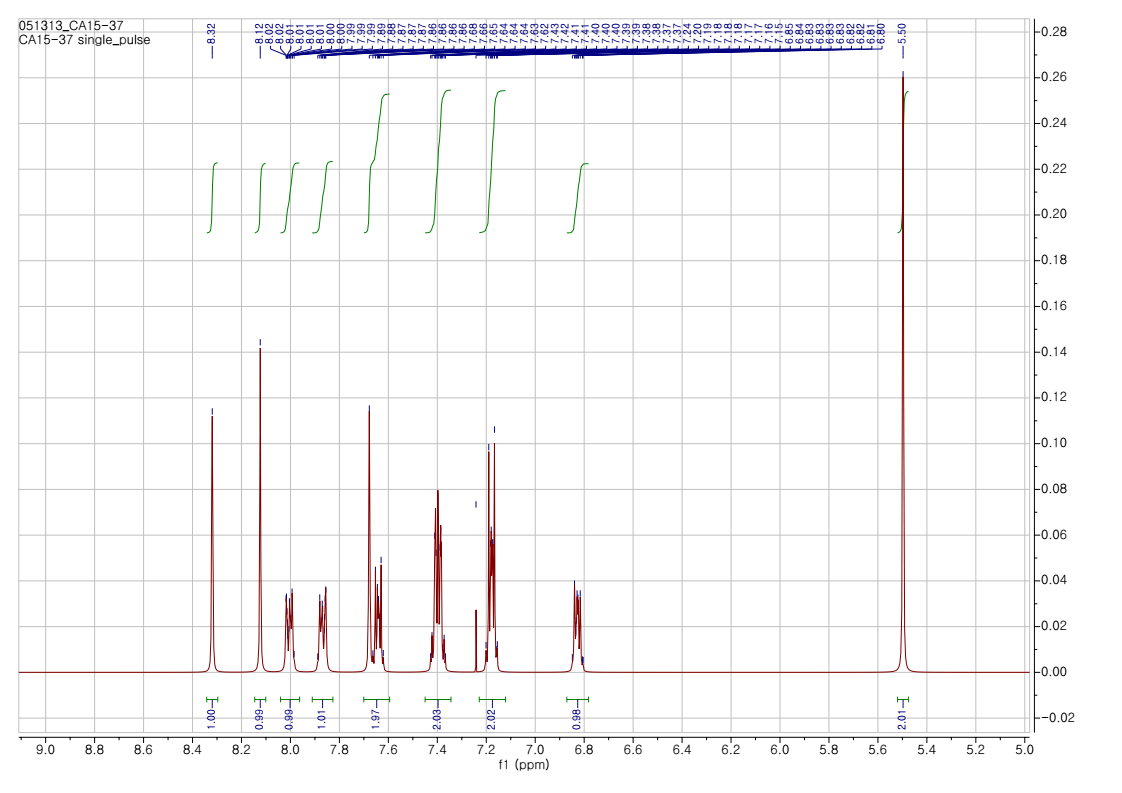
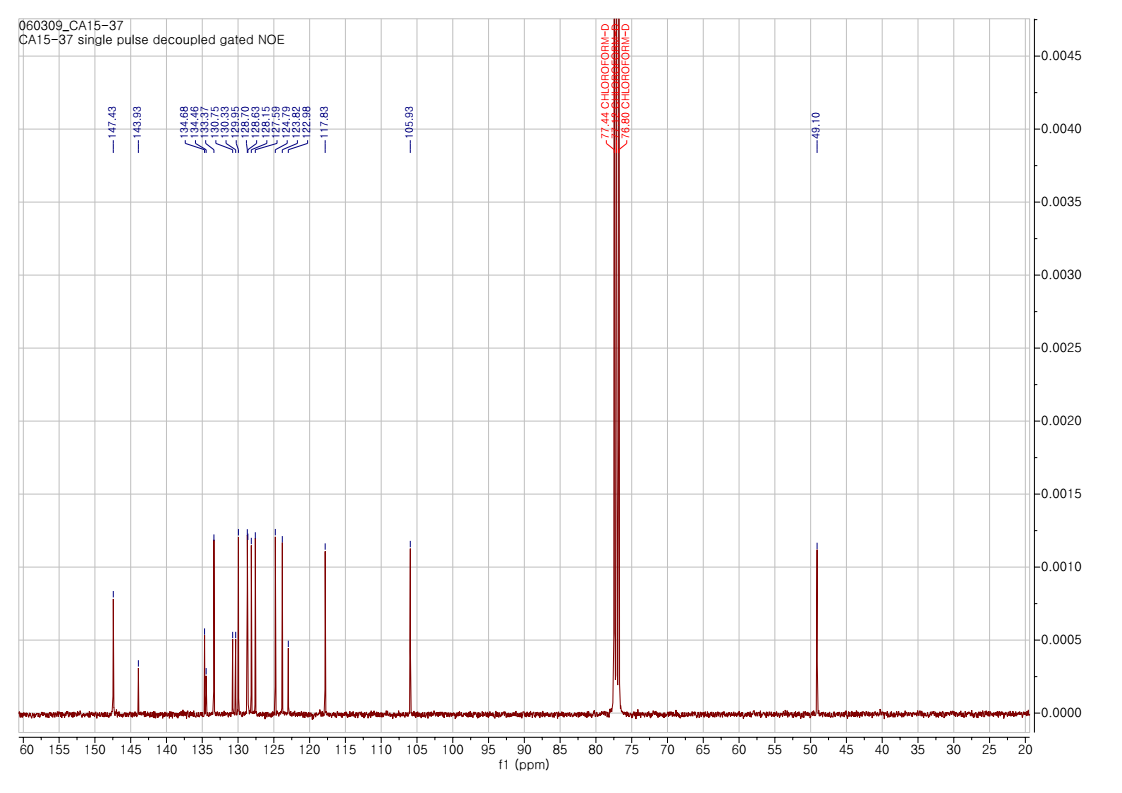
 

Figure S6. 1H-NMR and 13C-NMR spectra of **BI** in CDCl3

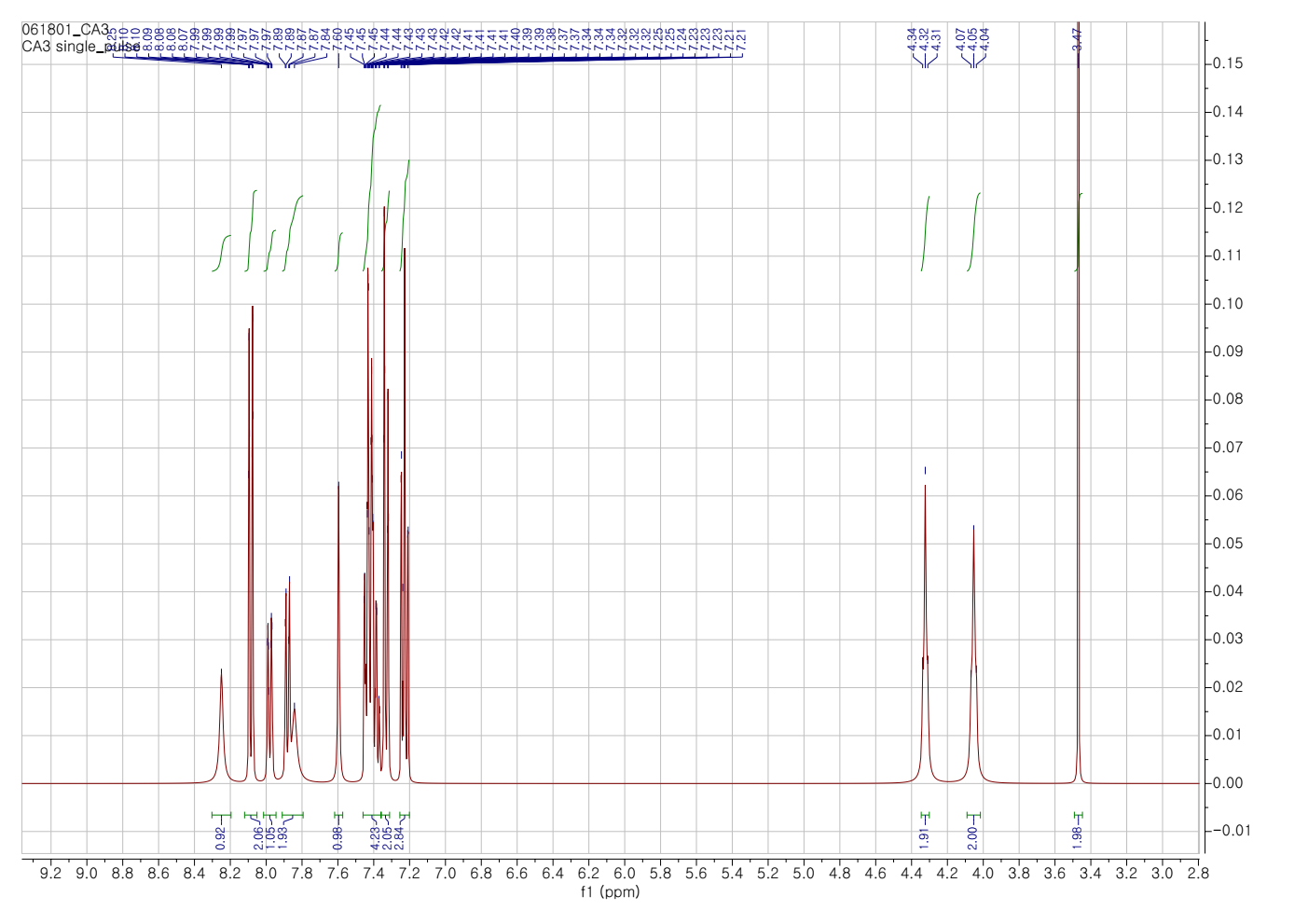
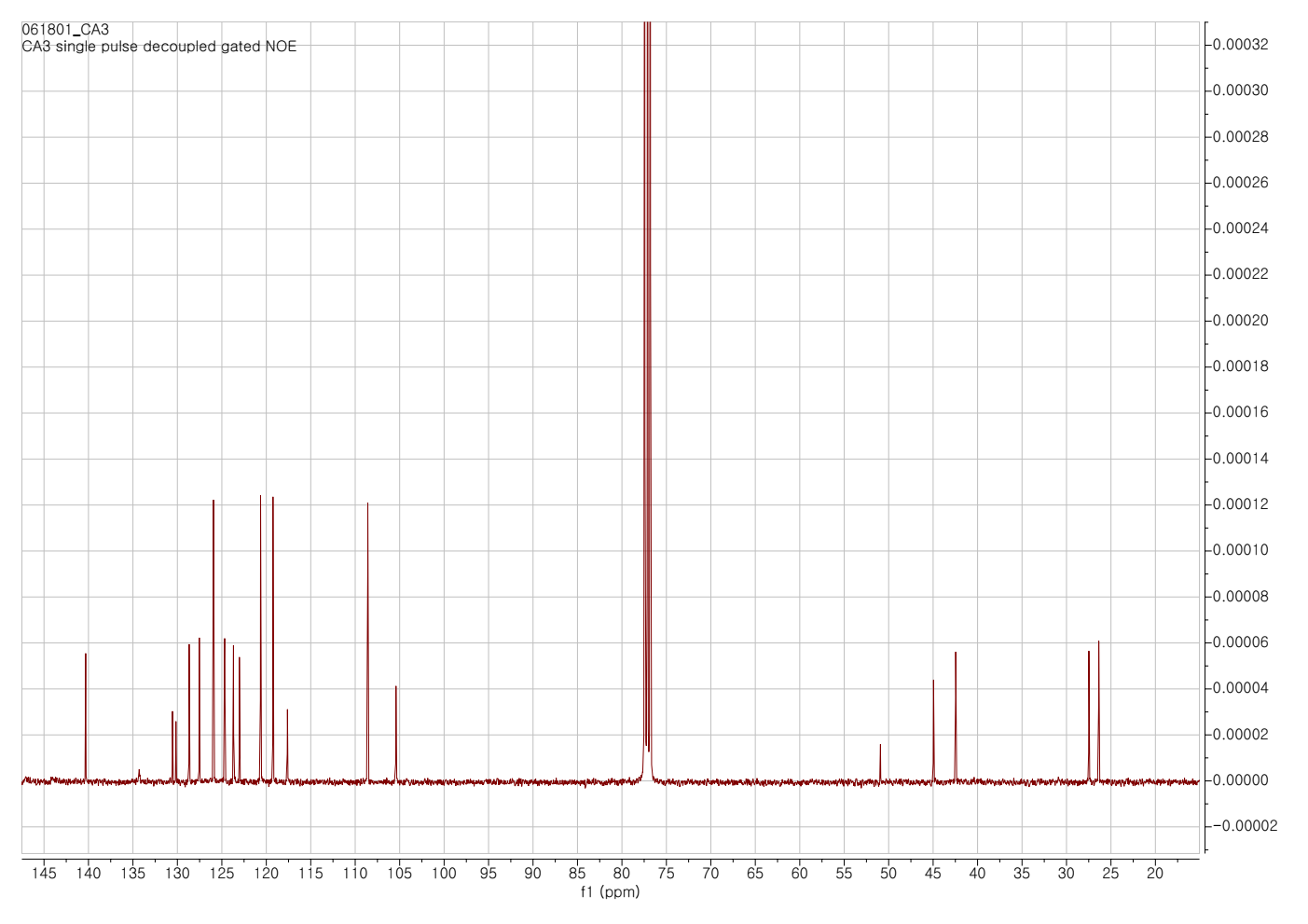
 

Figure S7. 1H-NMR and 13C-NMR spectra of **CI** in CDCl3

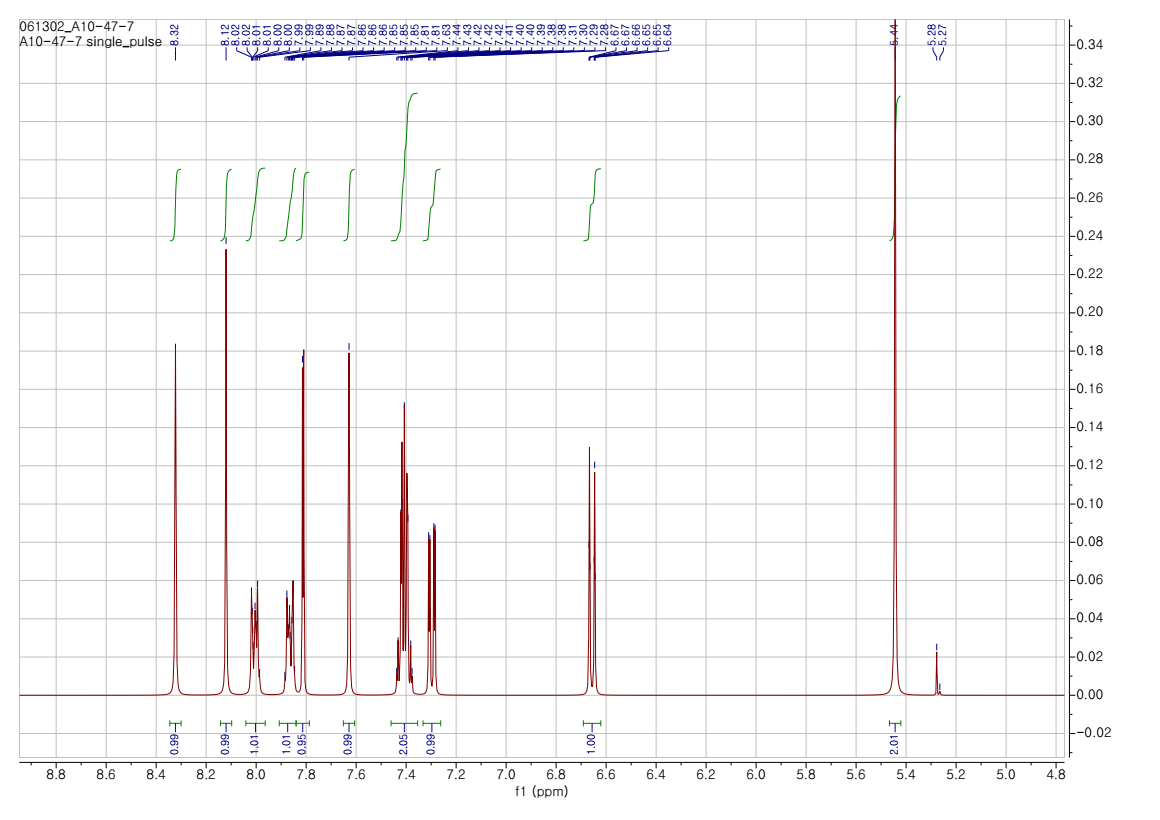
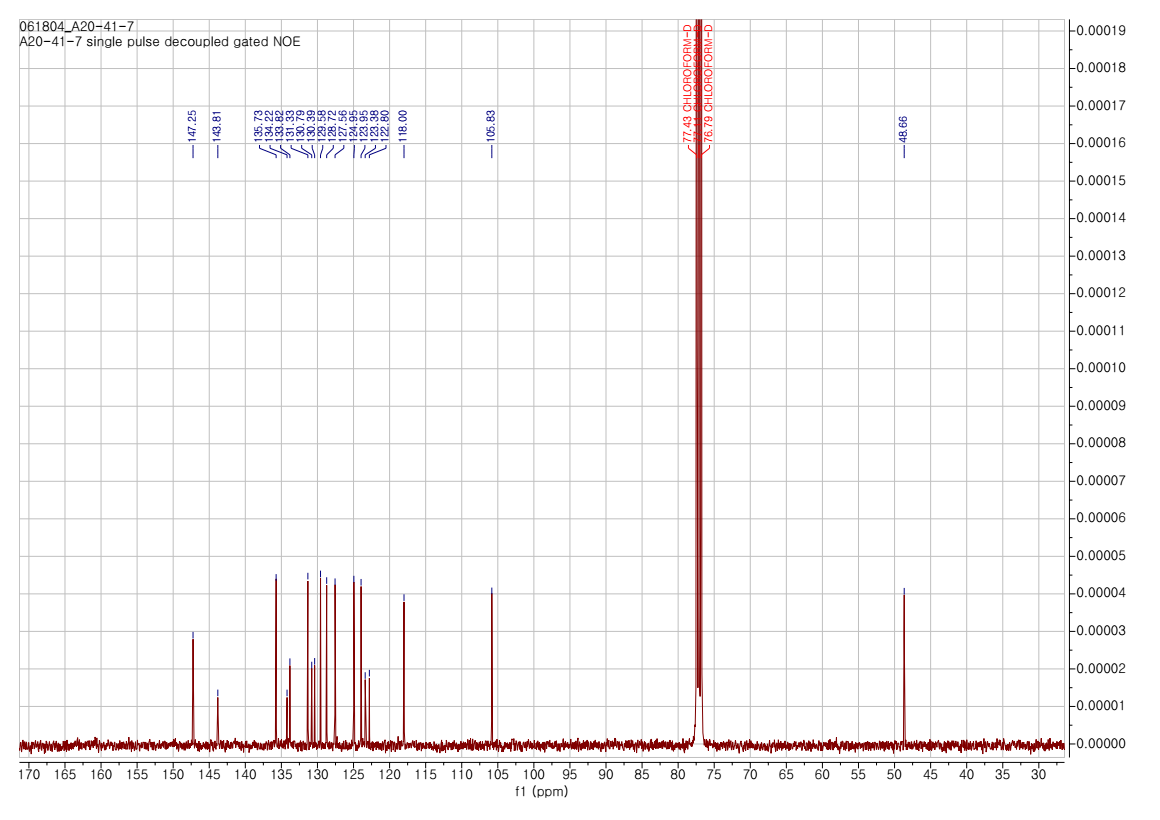
 

Figure S8. 1H-NMR and 13C-NMR spectra of **DI** in CDCl3

|  |  |
| --- | --- |
| a) Mass spectra of **DI** | a) Mass spectra of **BIB** |

Figue S9. Mass spectra of (a) **DI** and (b) **BIB**

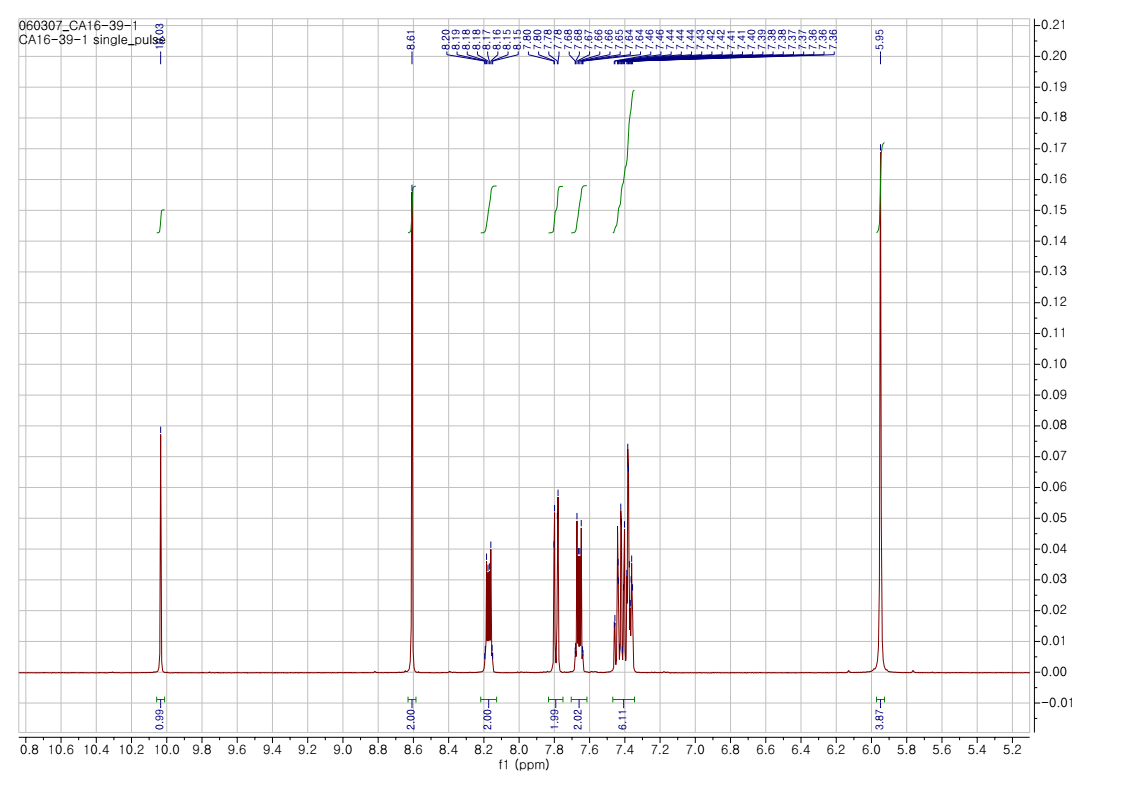
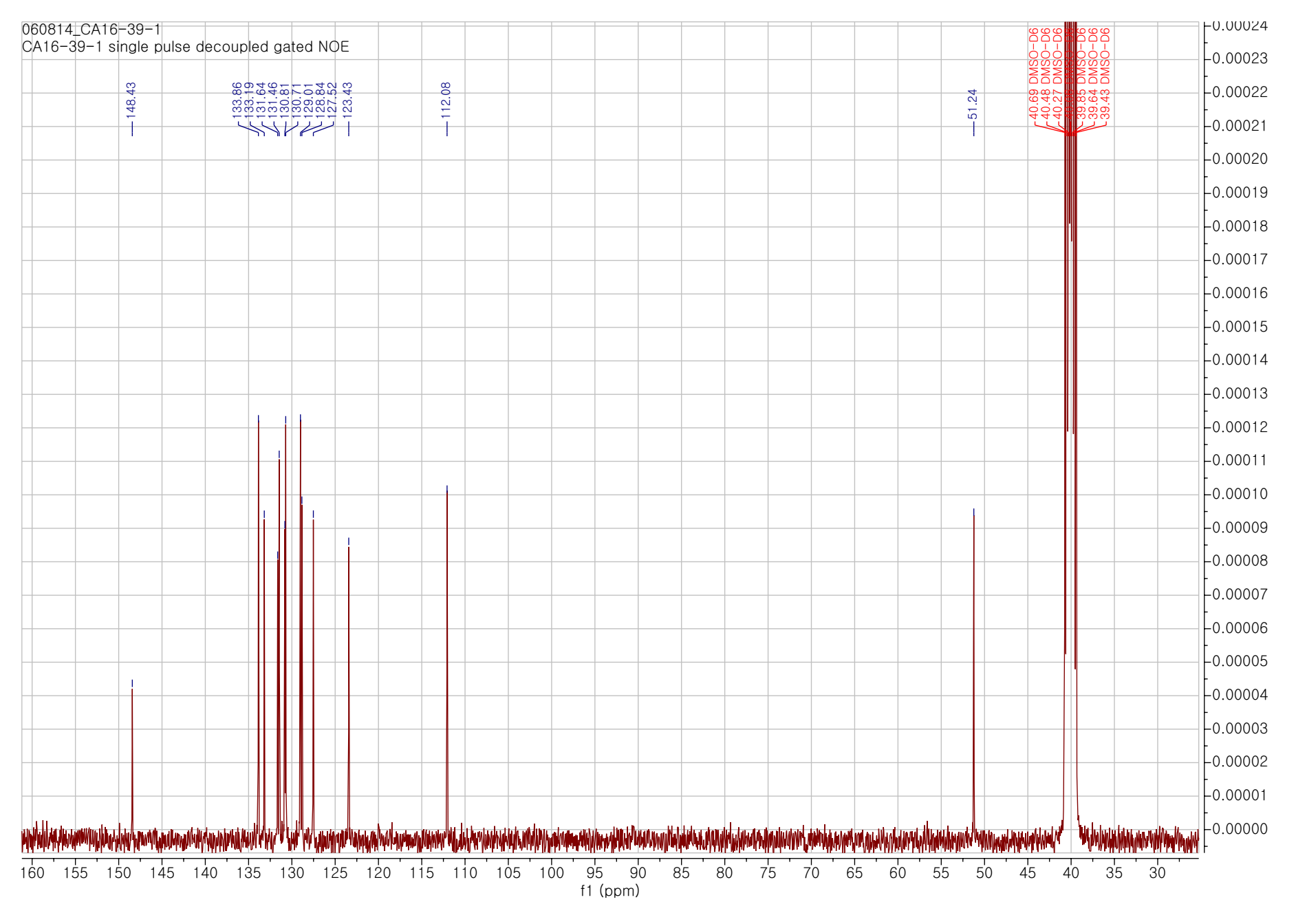
 

Figure S10. 1H-NMR and 13C-NMR spectra of **BIB** in DMSO

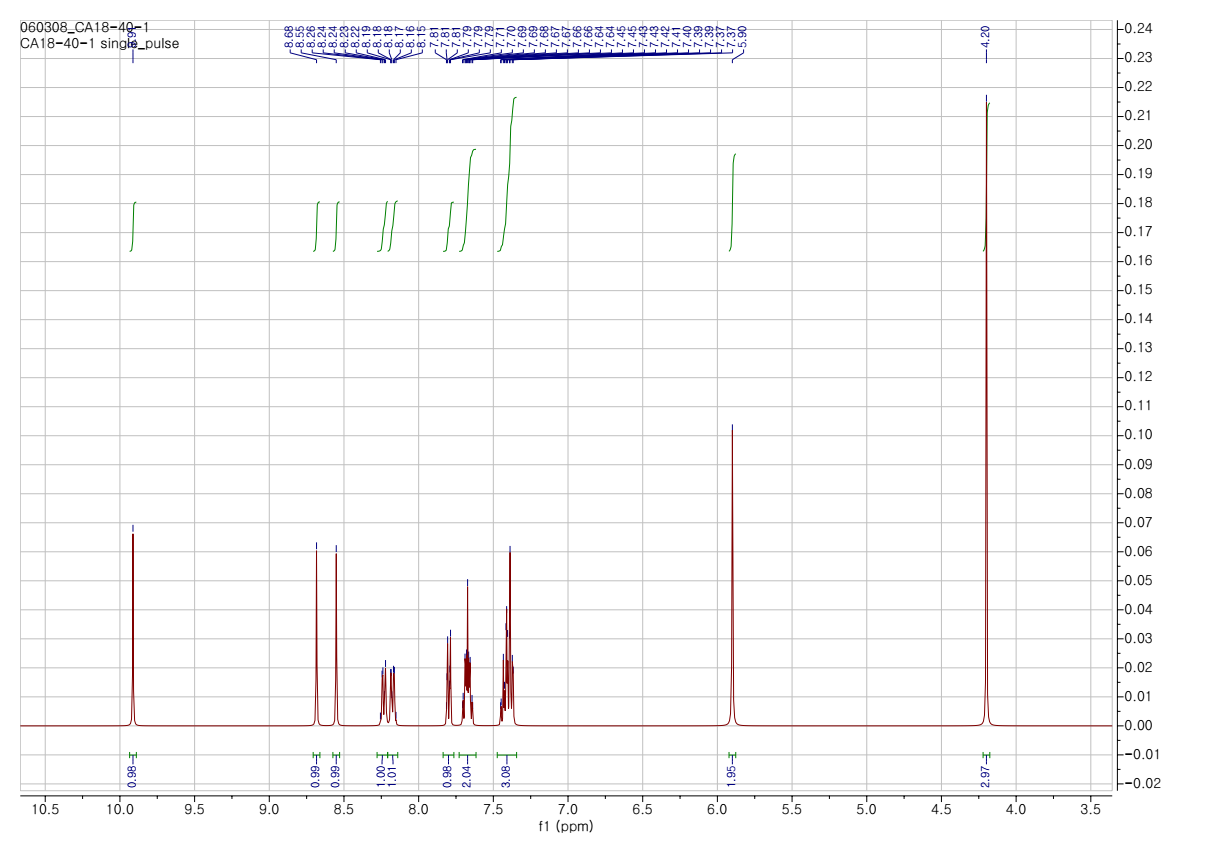
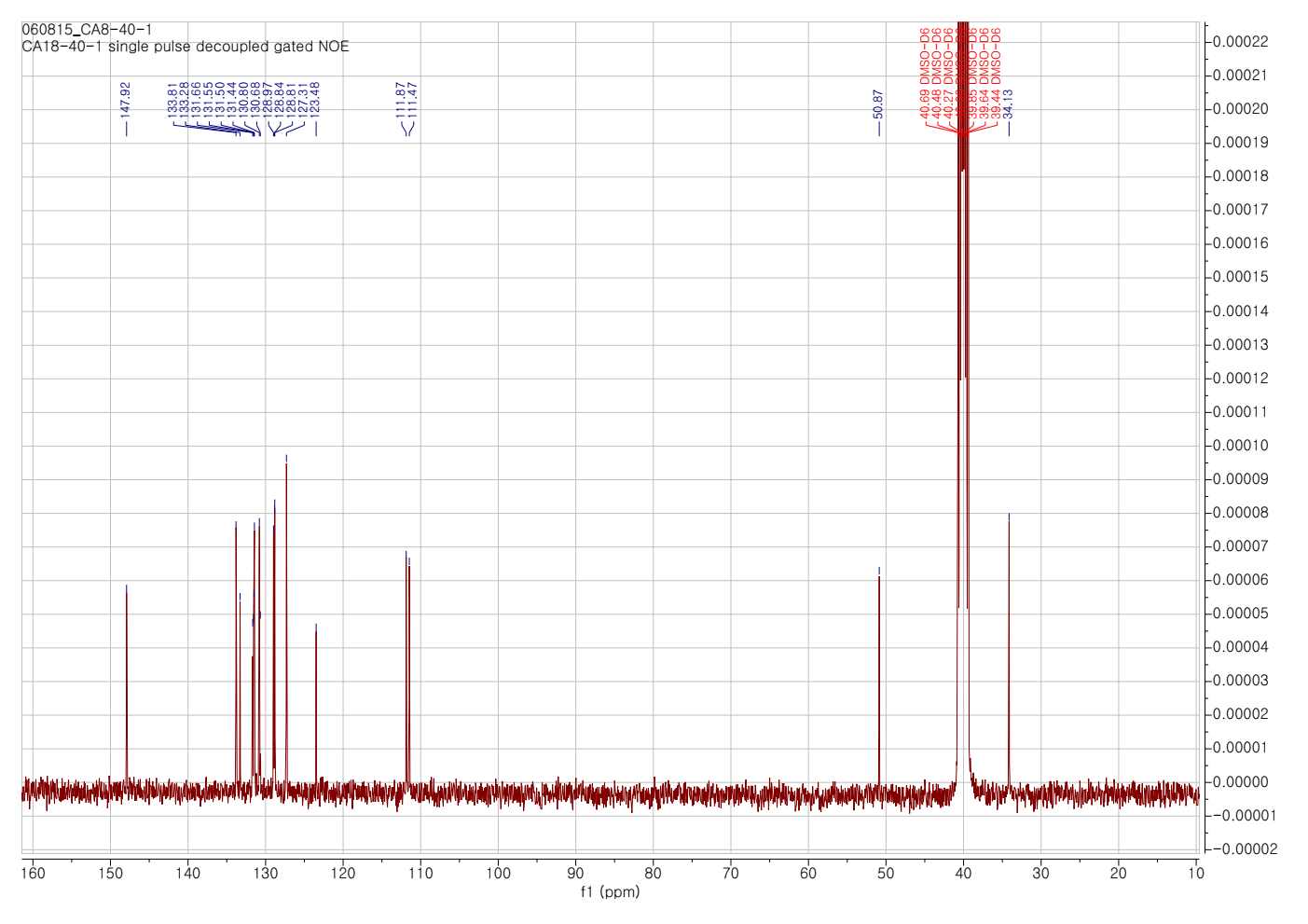
 

Figure S11. 1H-NMR and 13C-NMR spectra of **BIM** in DMSO

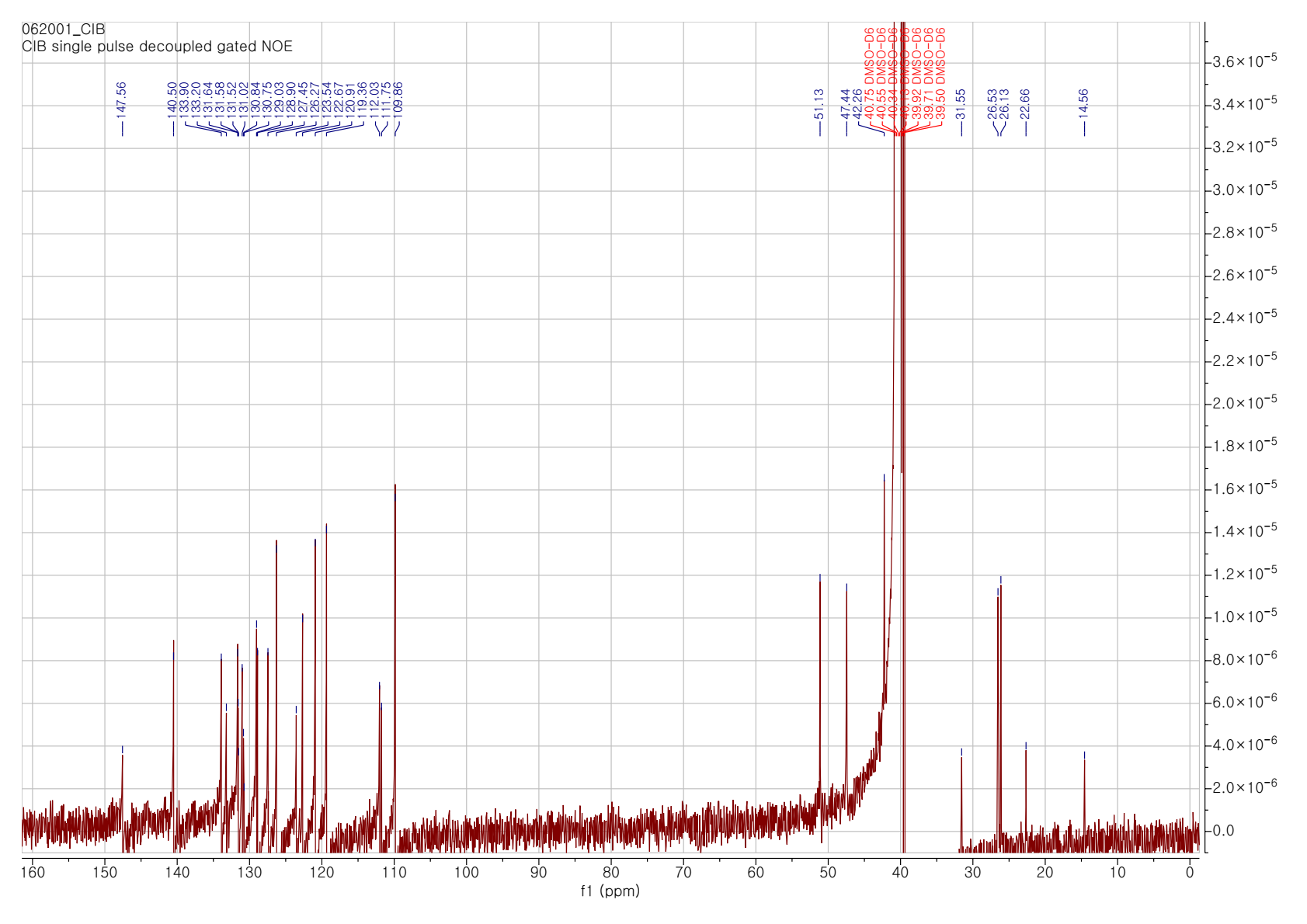
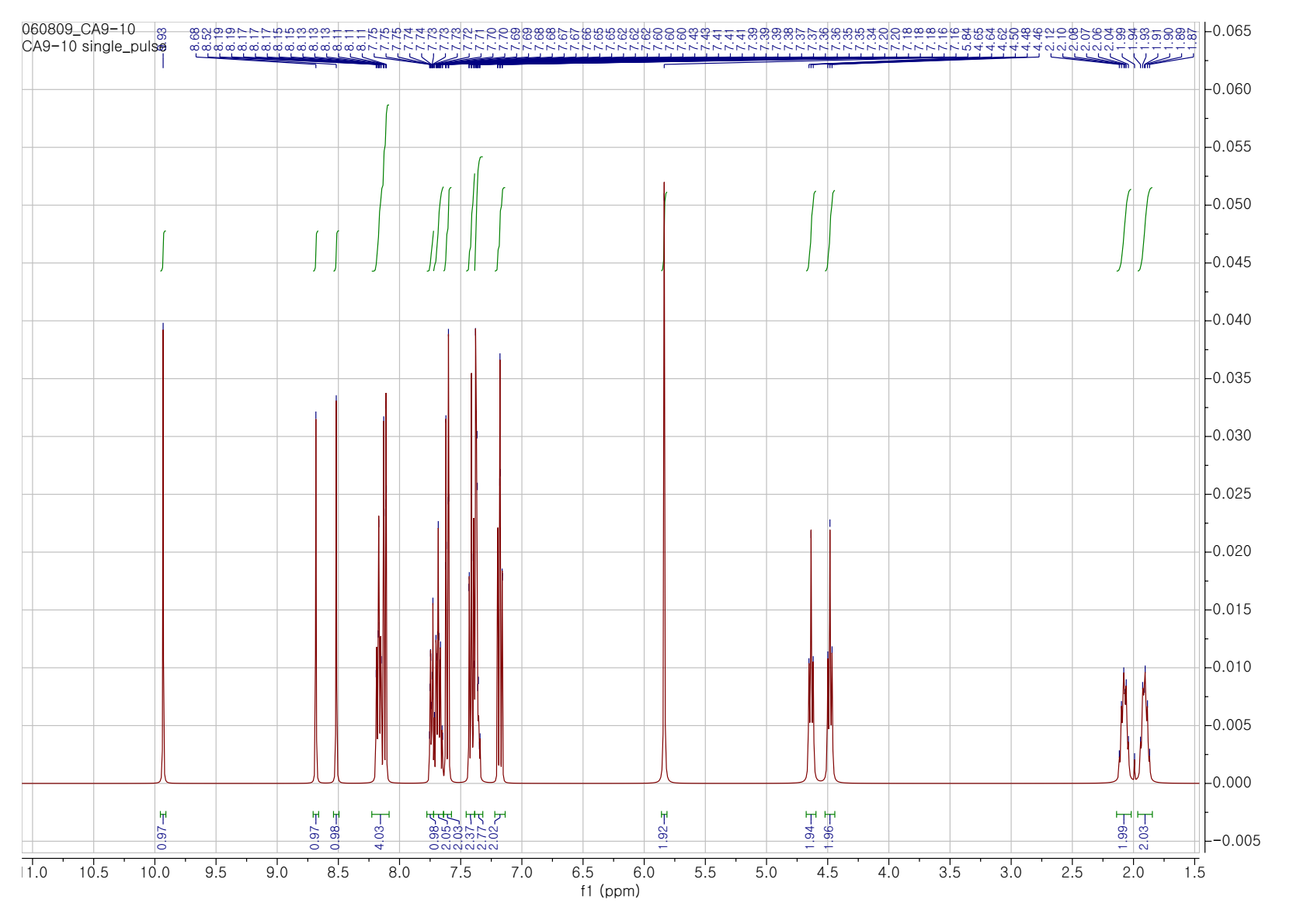


Figure S12. 1H-NMR and 13C-NMR spectra of **CIB** in DMSO

|  |  |
| --- | --- |
| a) Mass spectra of **BIM** | b) Mass spectra of **CIB** |

Figue S13. Mass spectra of (a) **BIM** and (b) **CIB**

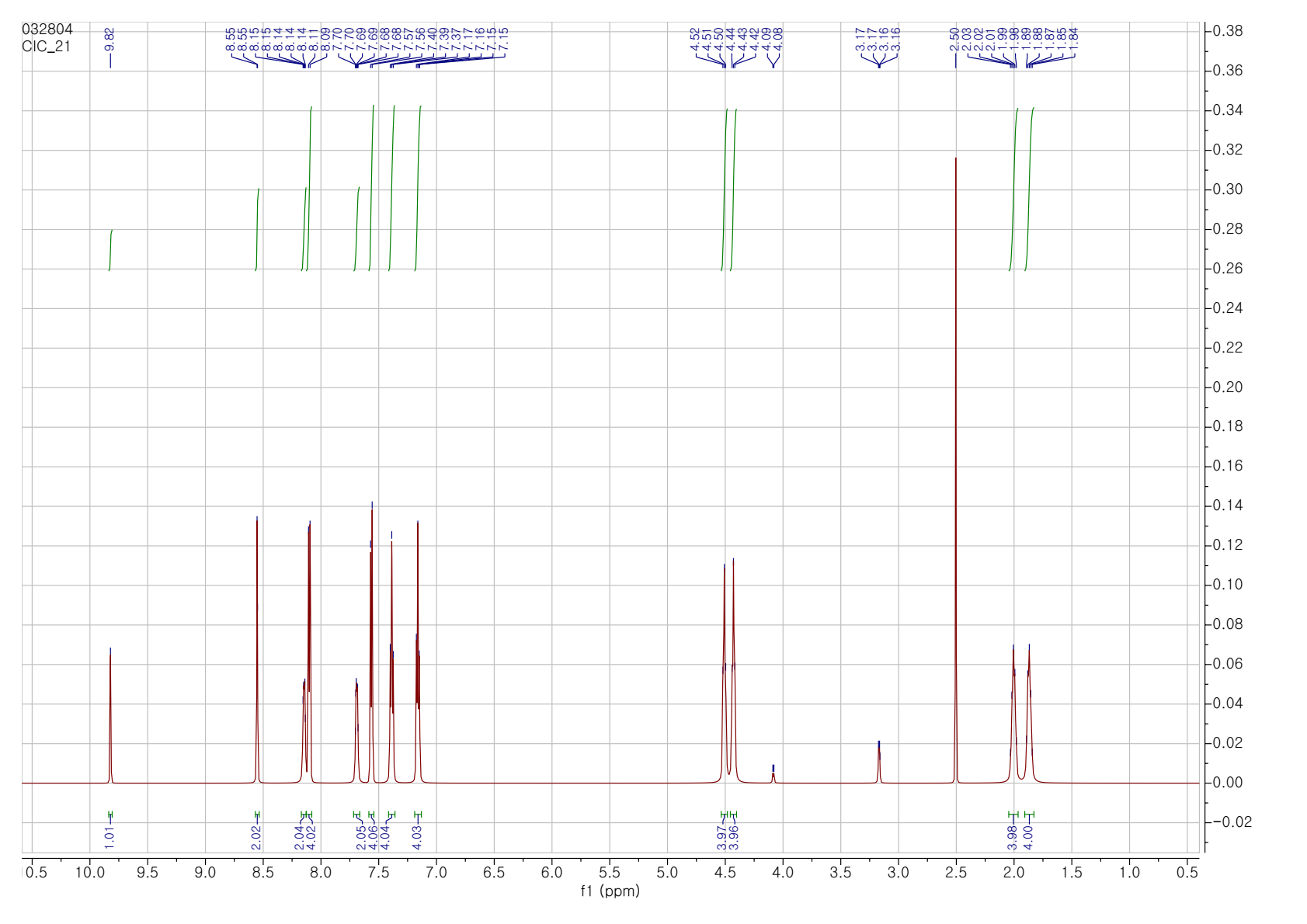
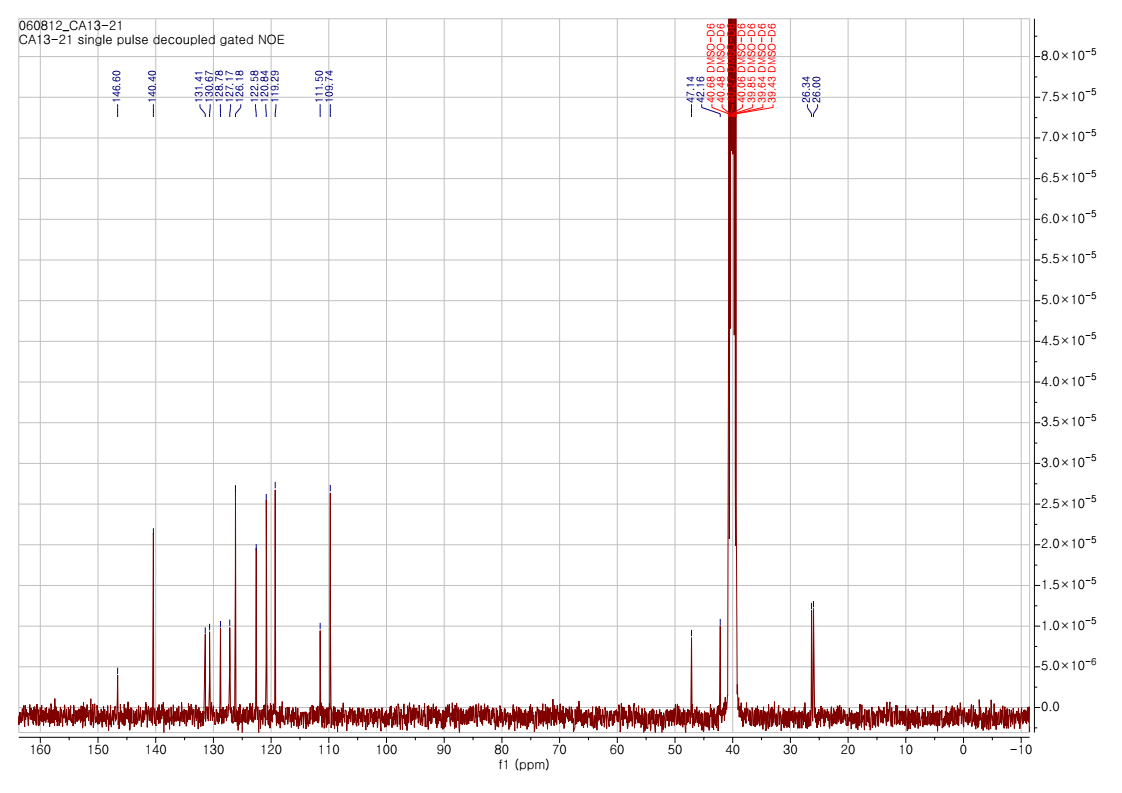
 

Figure S14. 1H-NMR and 13C-NMR spectra of **CIC** in DMSO

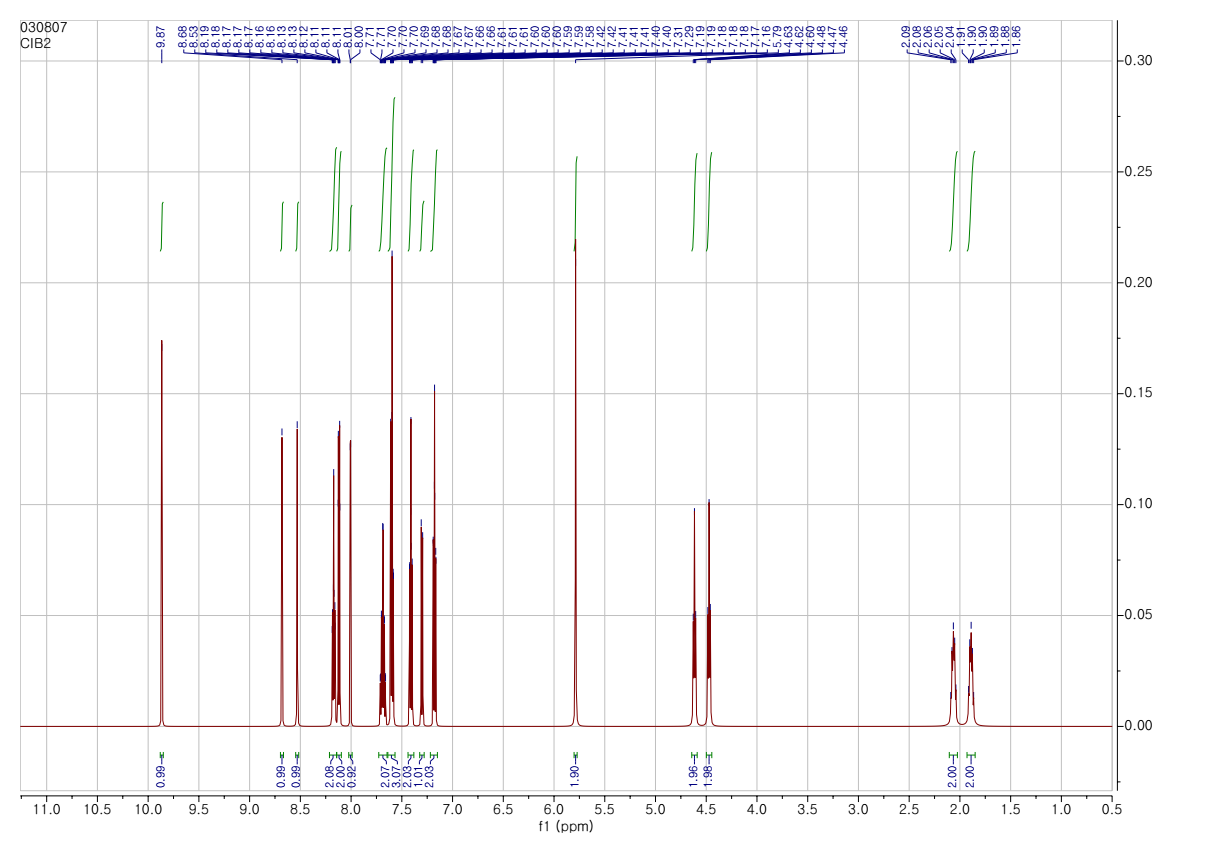
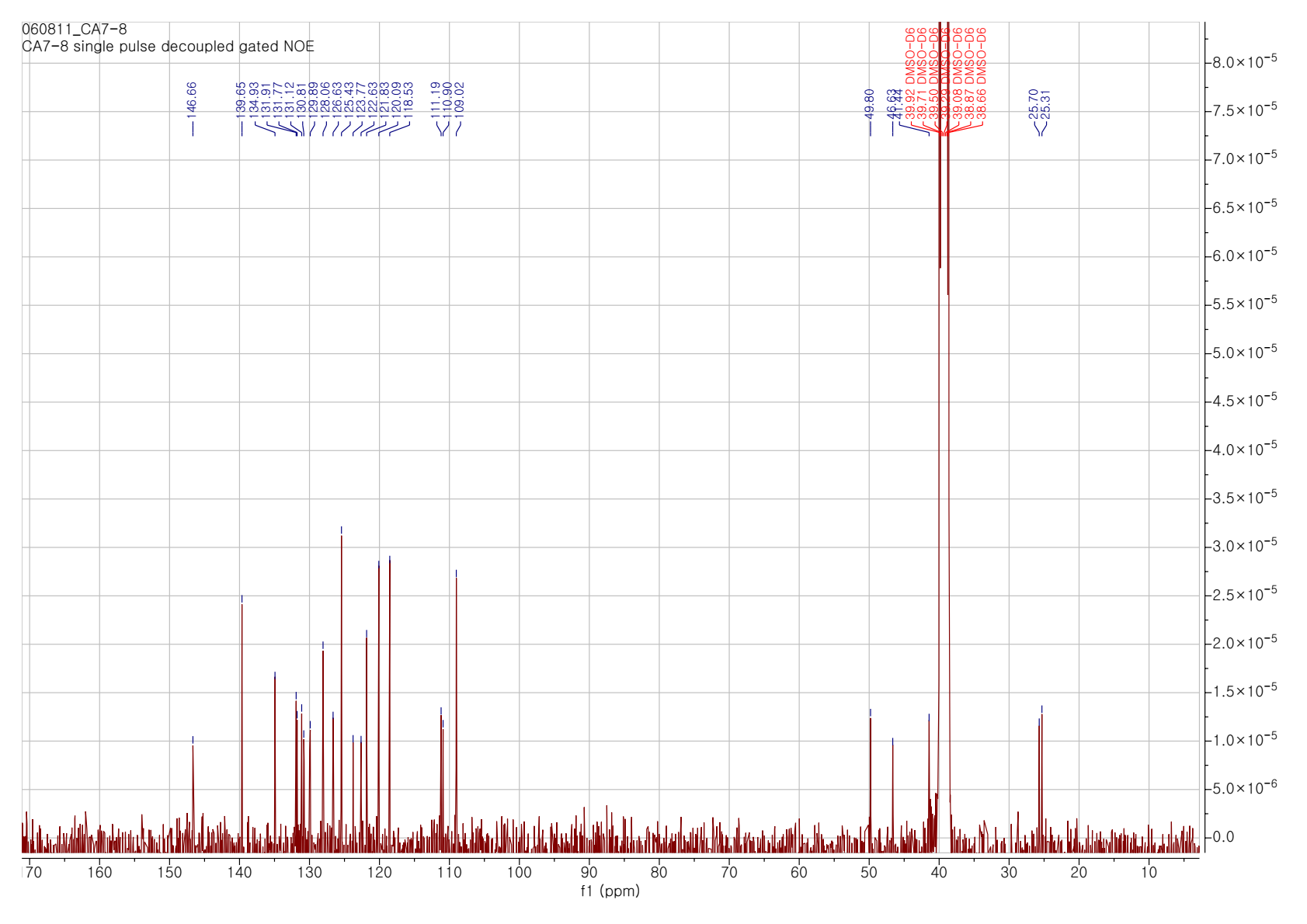
 

Figure S15. 1H-NMR and 13C-NMR spectra of **CID** in DMSO

|  |  |
| --- | --- |
| a) Mass spectra of **CIC** | b) Mass spectra of **CID** |
| c) Mass spectra of **CIM** | d) Mass spectra of **DIB** |

Figue S16. Mass spectra of (a) **CIC**, (b) **CIB,** (c) **CIM** and (d) **DIB.**

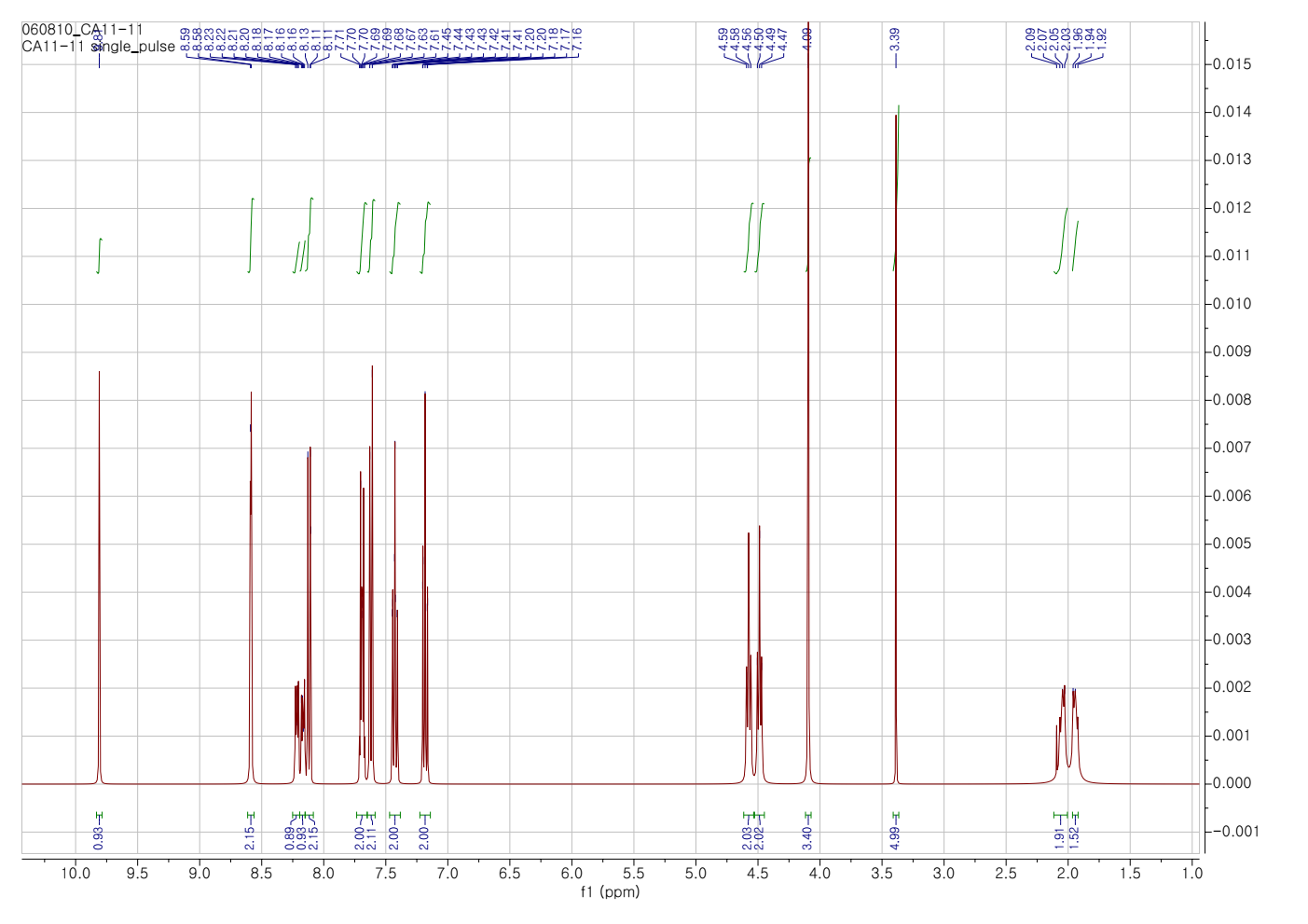
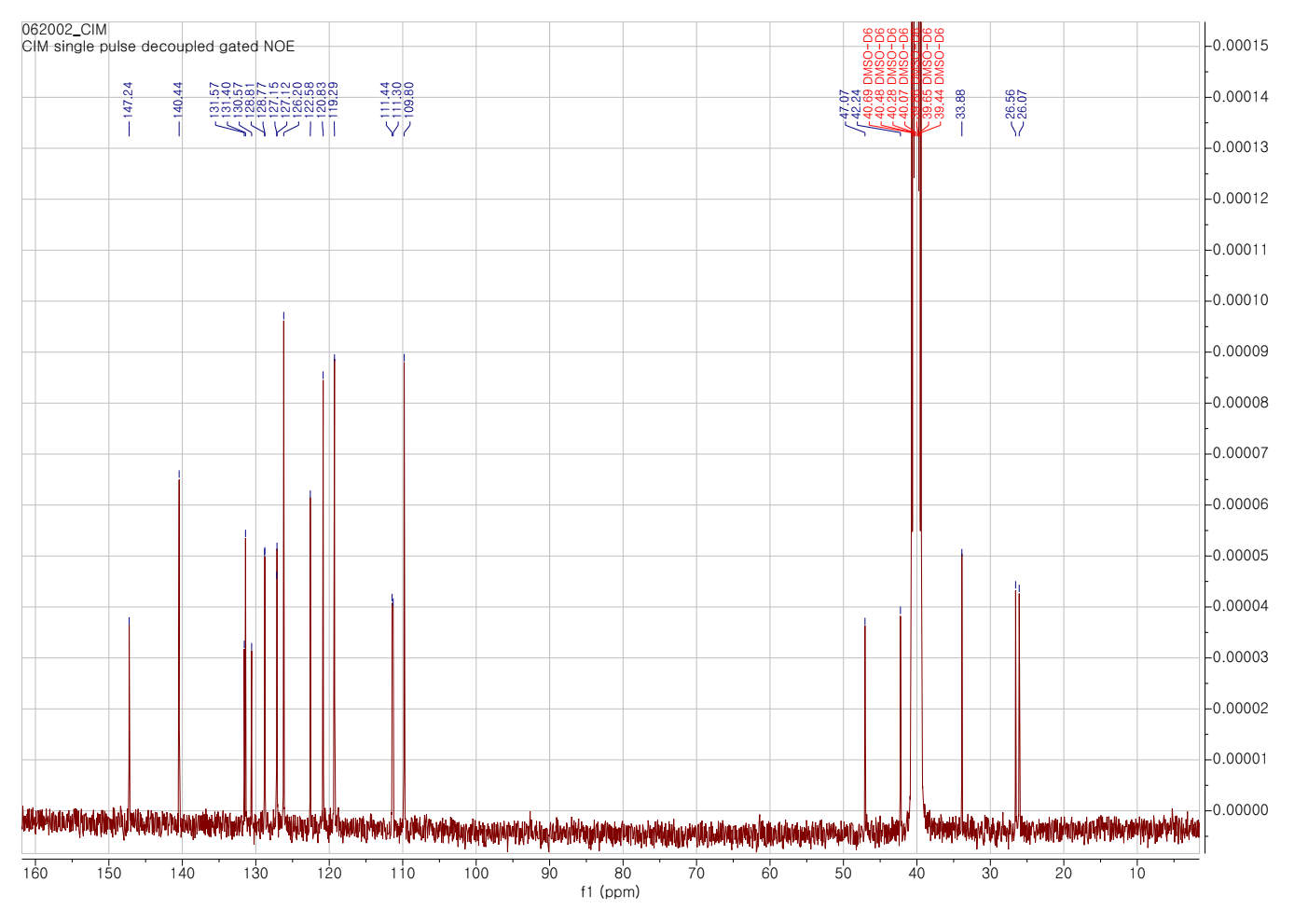
 

Figure S17. 1H-NMR and 13C-NMR spectra of **CIM** in DMSO

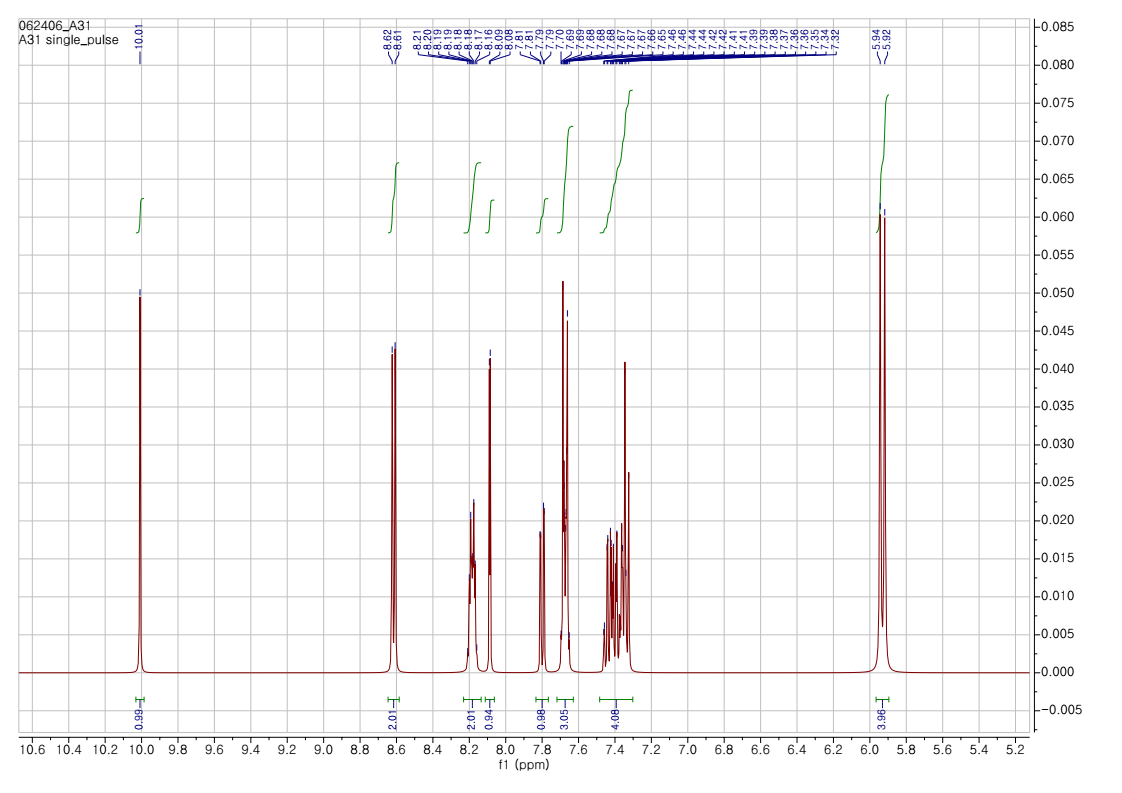
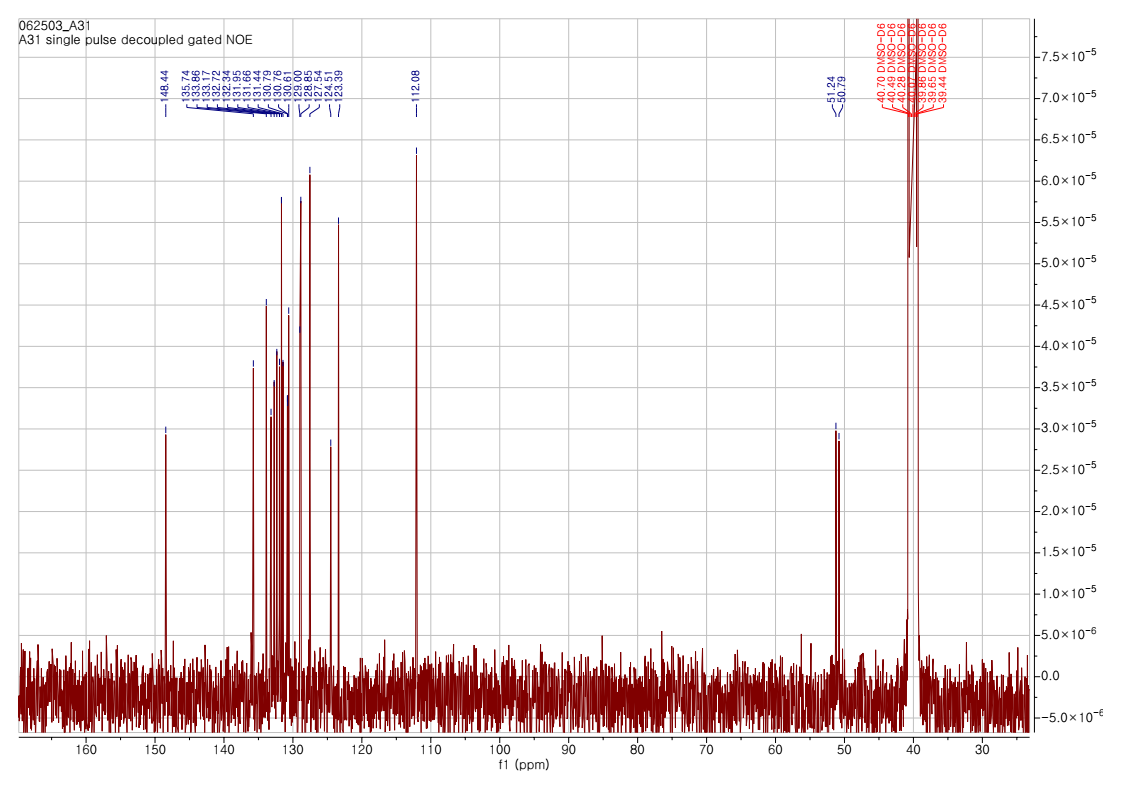
 

Figure S18. 1H-NMR and 13C-NMR spectra of **DIB** in DMSO

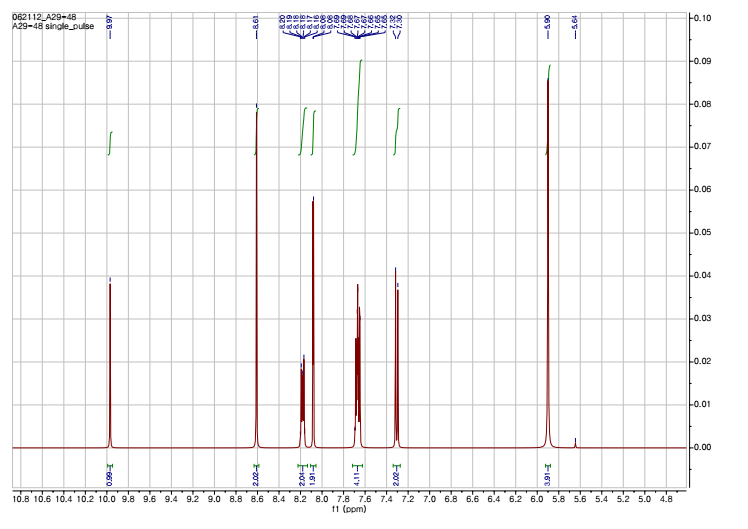
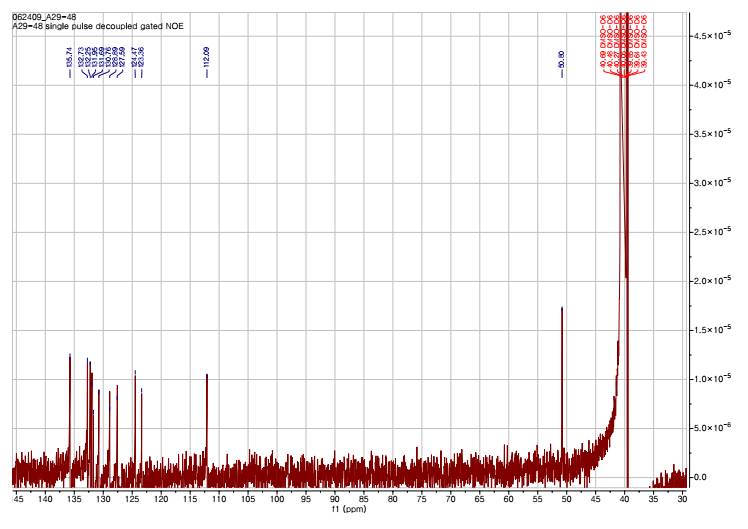
 

Figure S19. 1H-NMR and 13C-NMR spectra of **DID** in DMSO

|  |  |
| --- | --- |
| a) Mass spectra of **DID** | b) Mass spectra of **DIM** |

Figure S20. Mass spectra of (a) **DID** and (b) **DIM**.

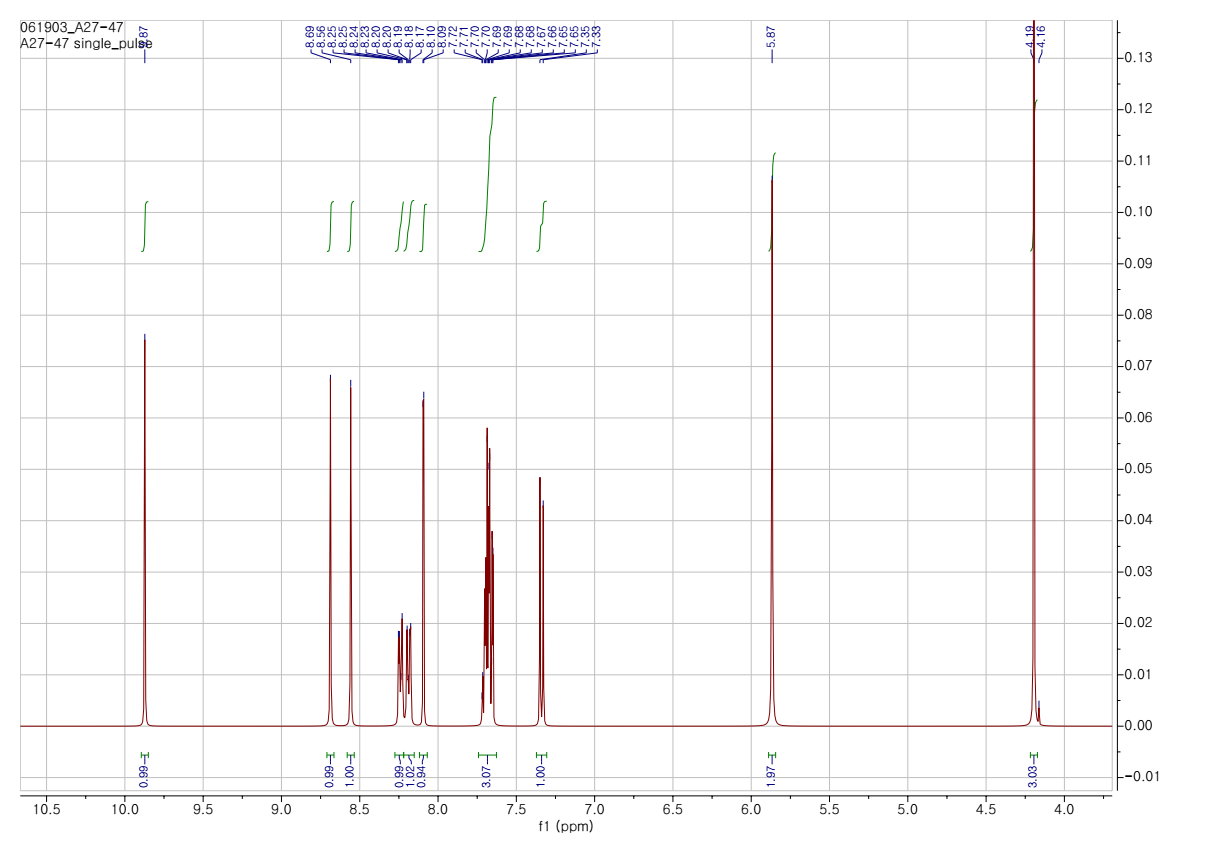
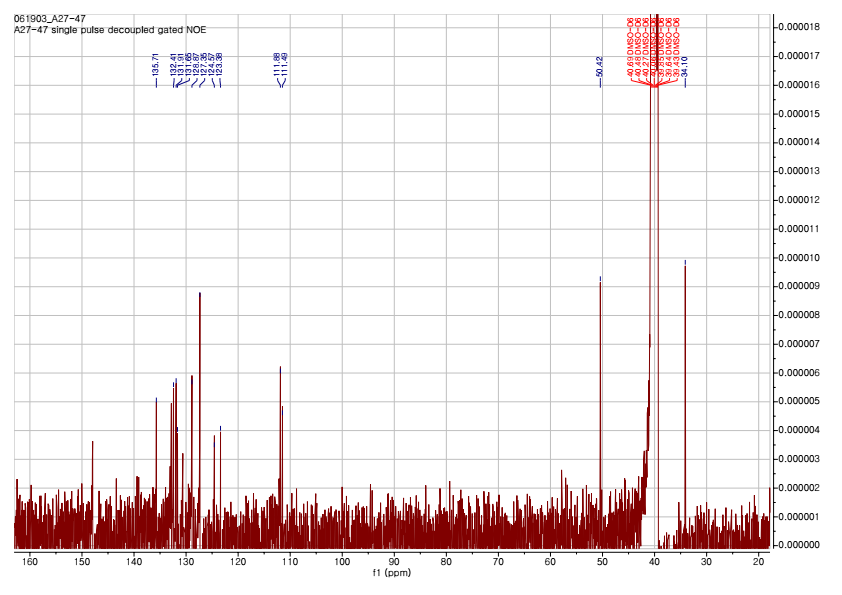
 

Figure S21. 1H-NMR and 13C-NMR spectra of **DIM** in DMSO

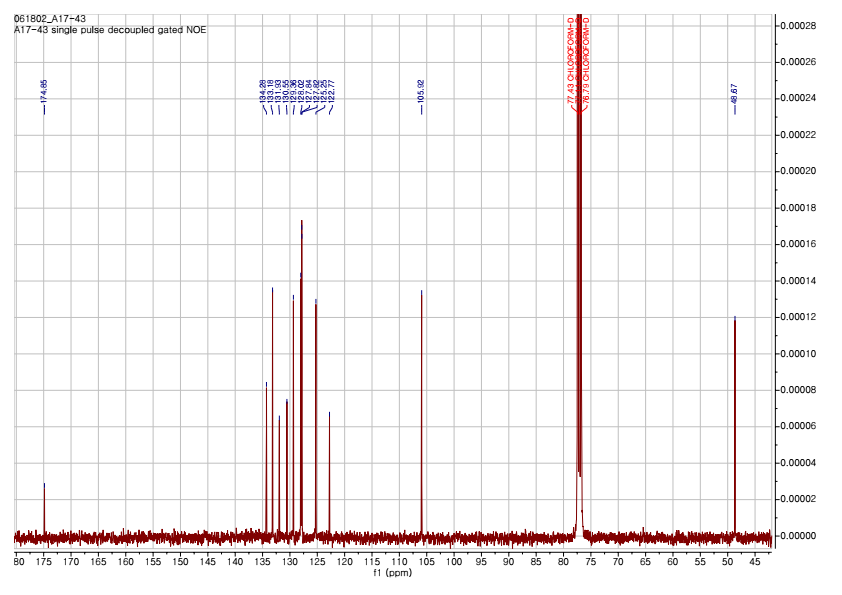
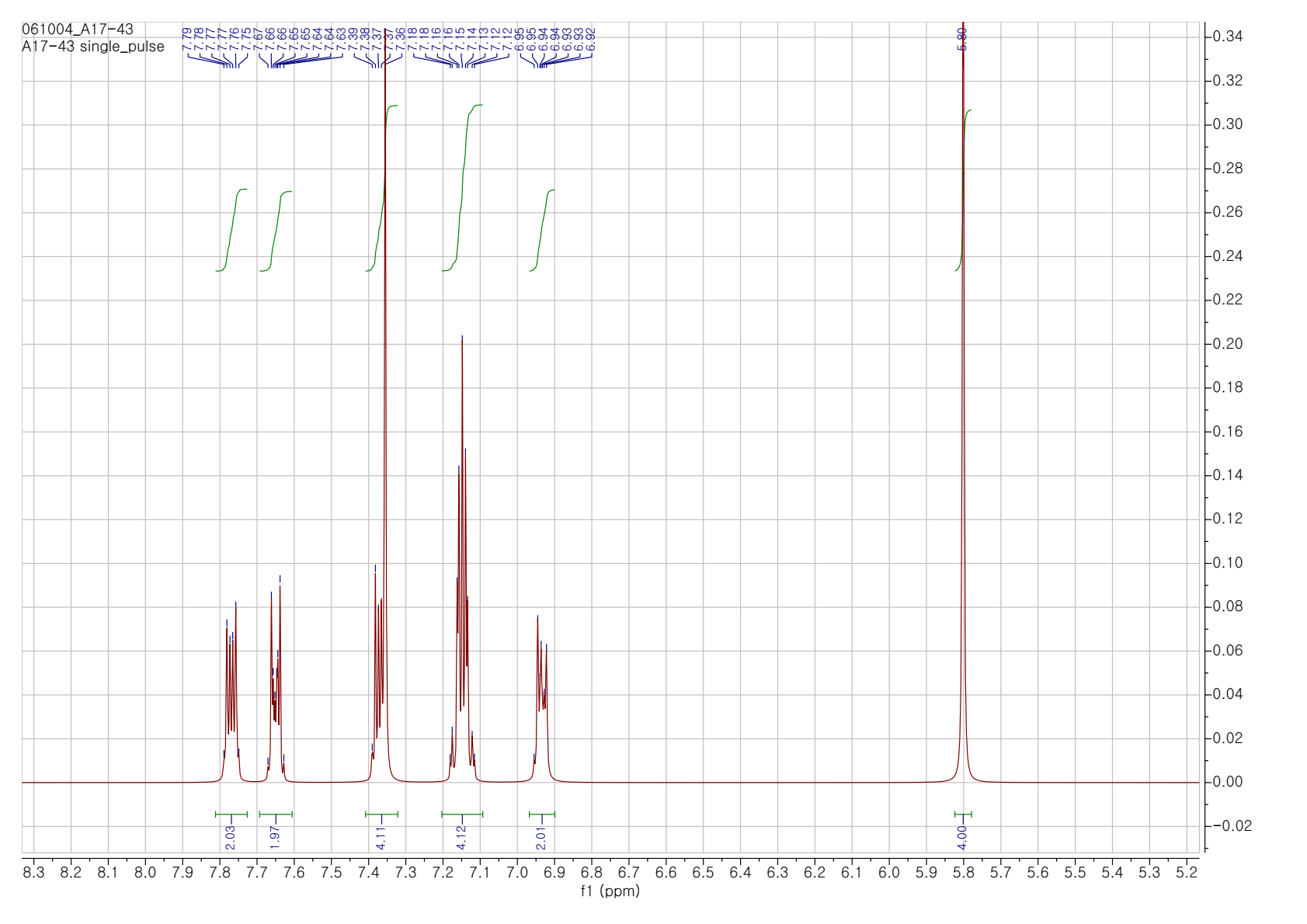


Figure S22. 1H-NMR and 13C-NMR spectra of **BSB** in CHCl3

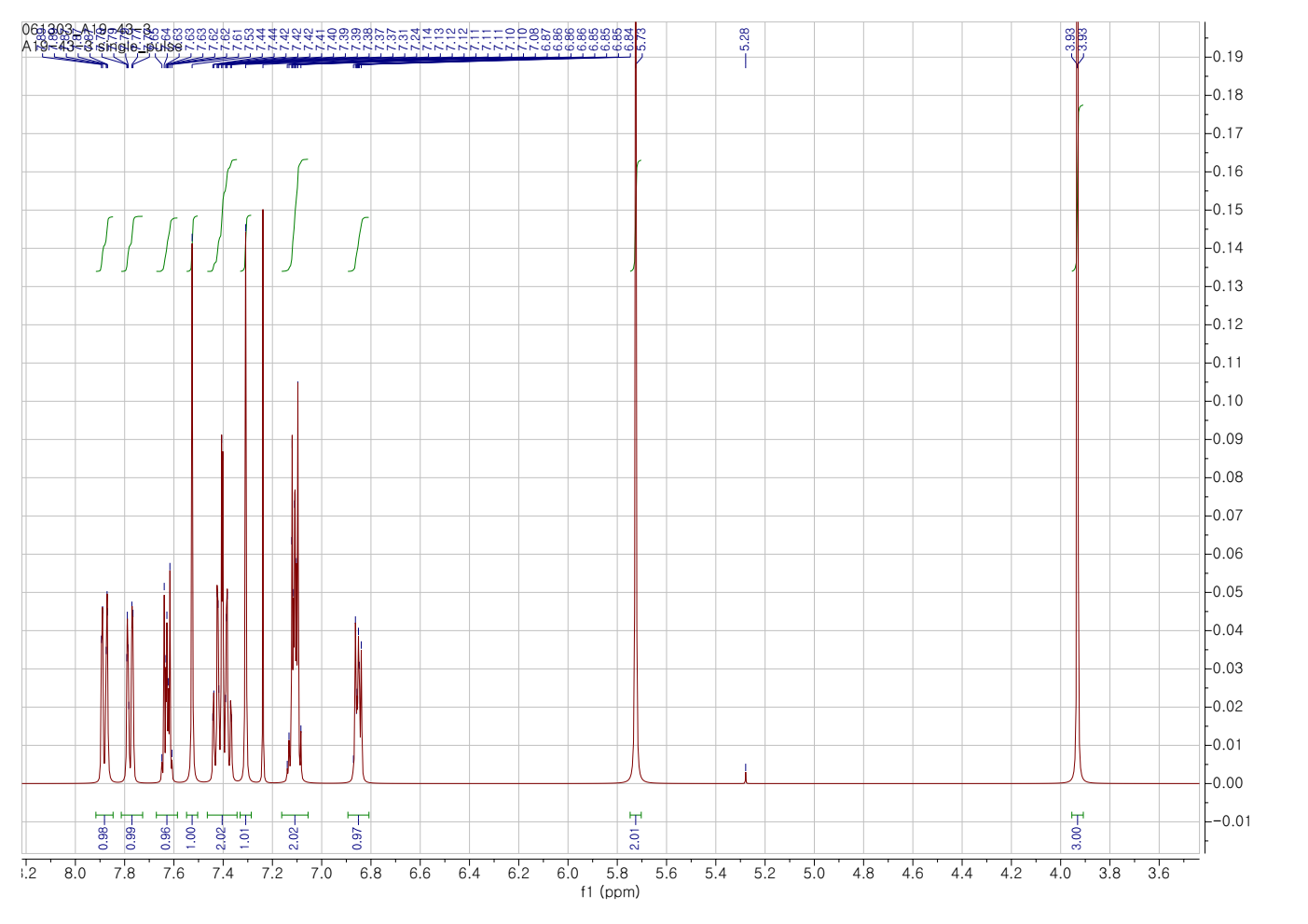
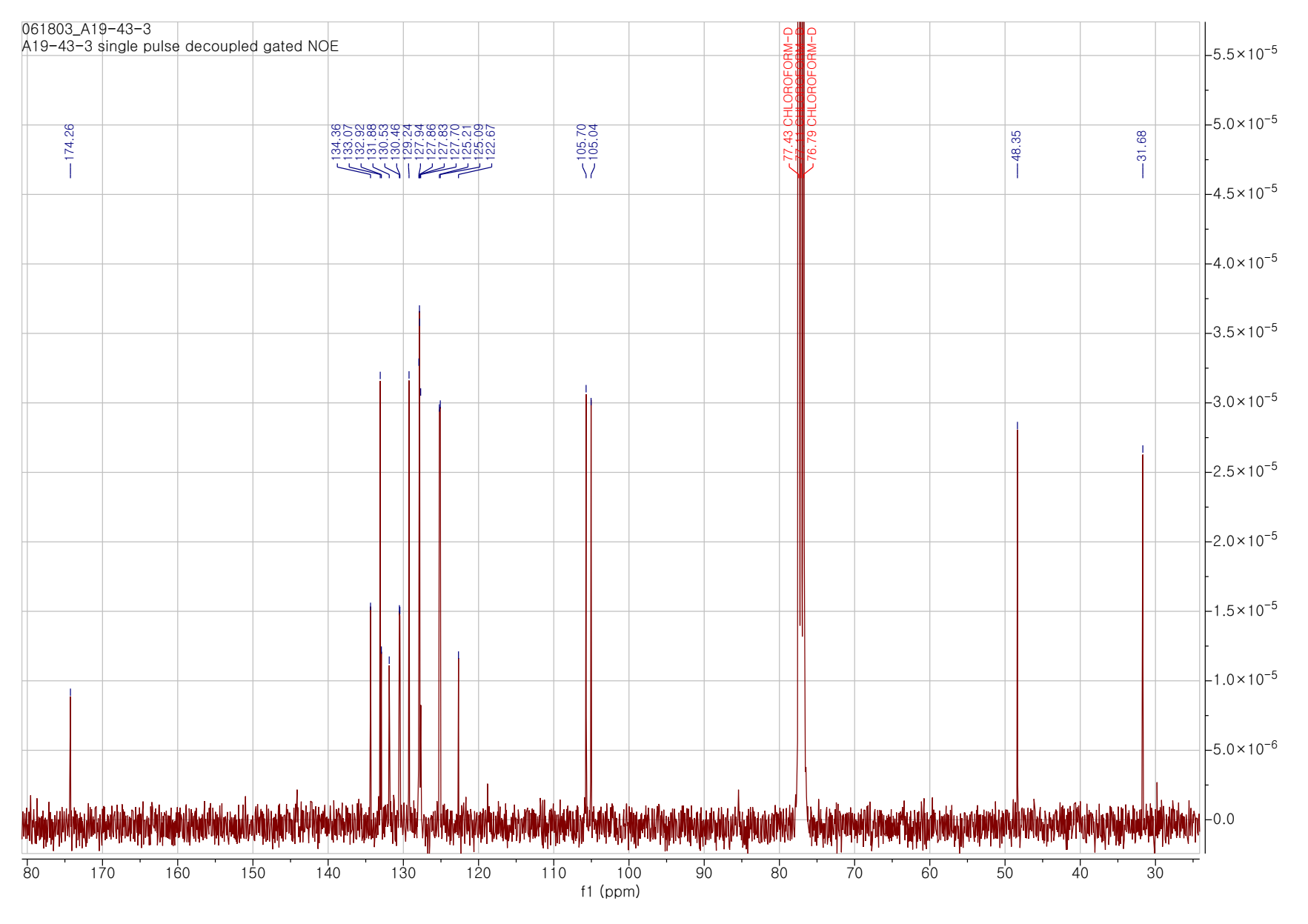
 

Figure S23. 1H-NMR and 13C-NMR spectra of **BSM** in CHCl3

|  |  |
| --- | --- |
| a) Mass spectra of **BSB** | b) Mass spectra of **BSM** |

Figure S24. Mass spectra of (a) **BSB** and (b) **BSM**.

|  |  |
| --- | --- |
| a) Mass spectra of **CSB** | b) Mass spectra of **CSC** |

Figure S25. Mass spectra of (a) **CSB** and (b) **CSC**.

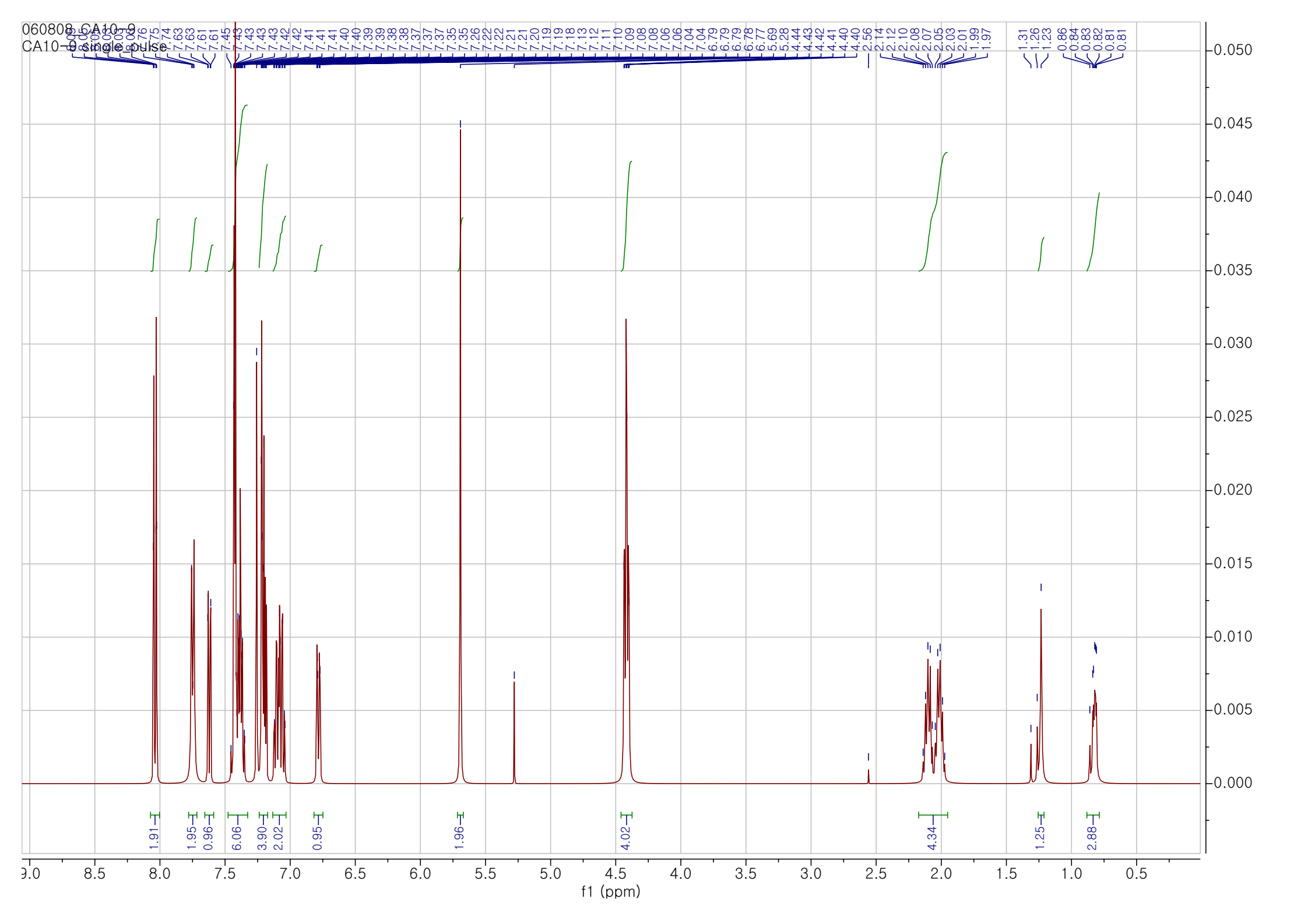
 

Figure S26. 1H-NMR and 13C-NMR spectra of **CSB** in CHCl3

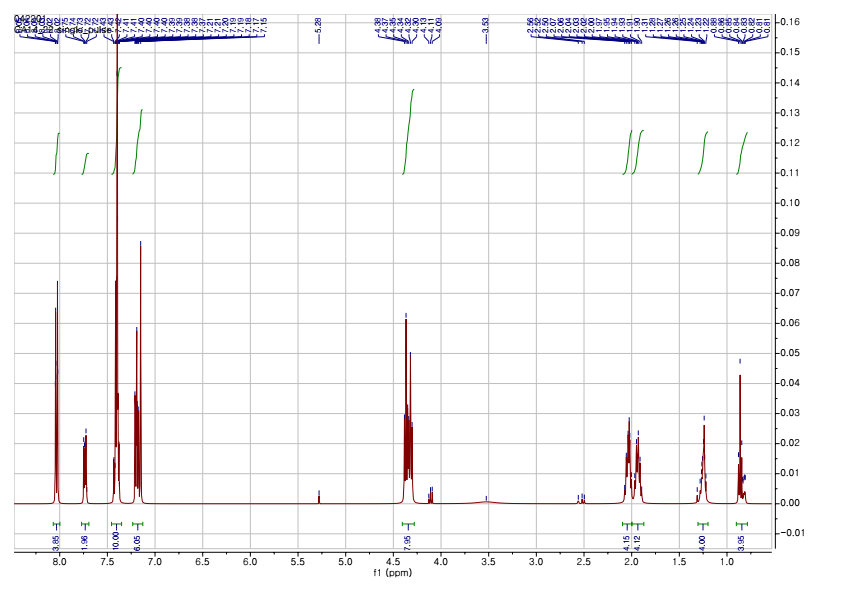
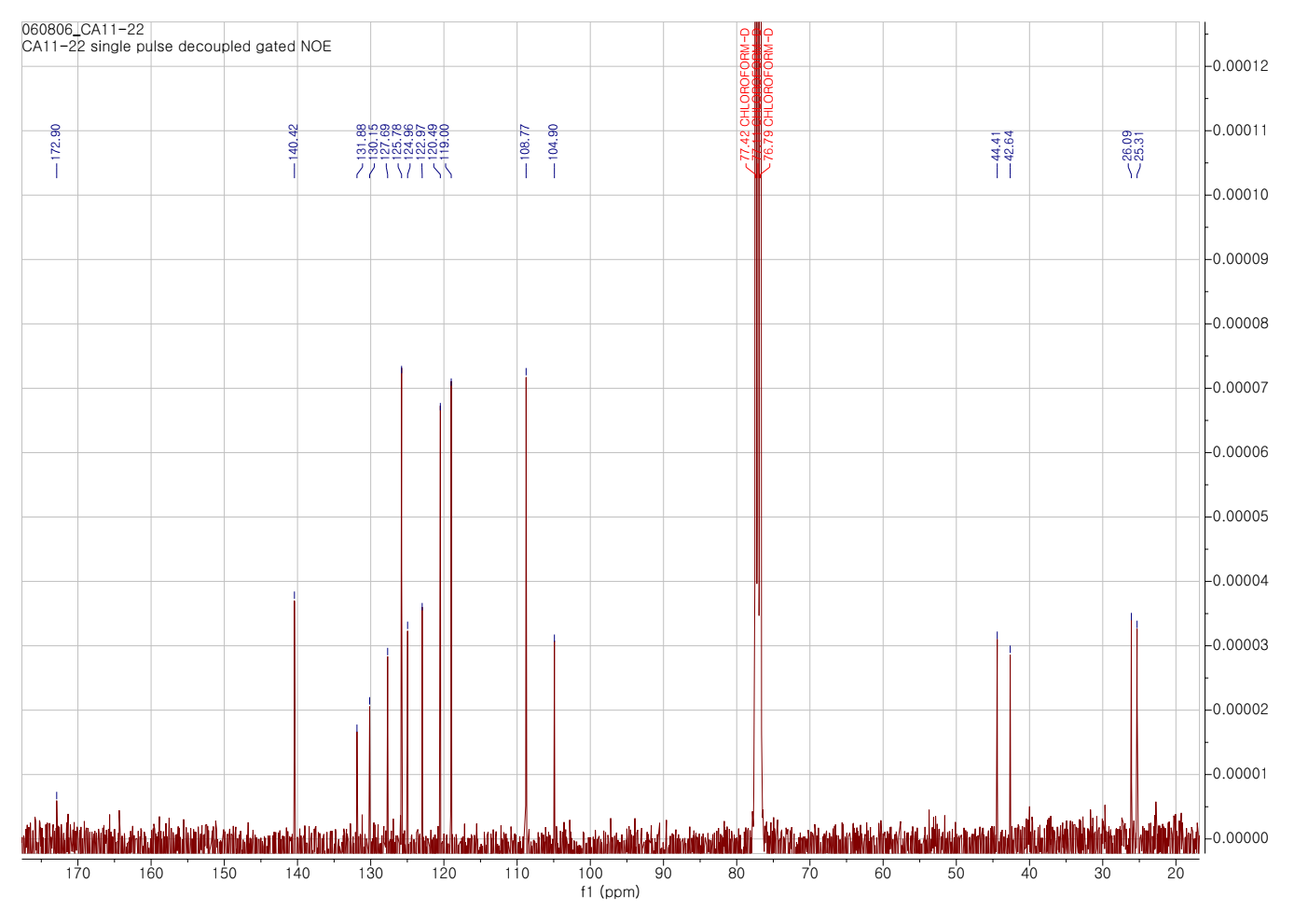
 

Figure S27. 1H-NMR and 13C-NMR spectra of **CSC** in CHCl3

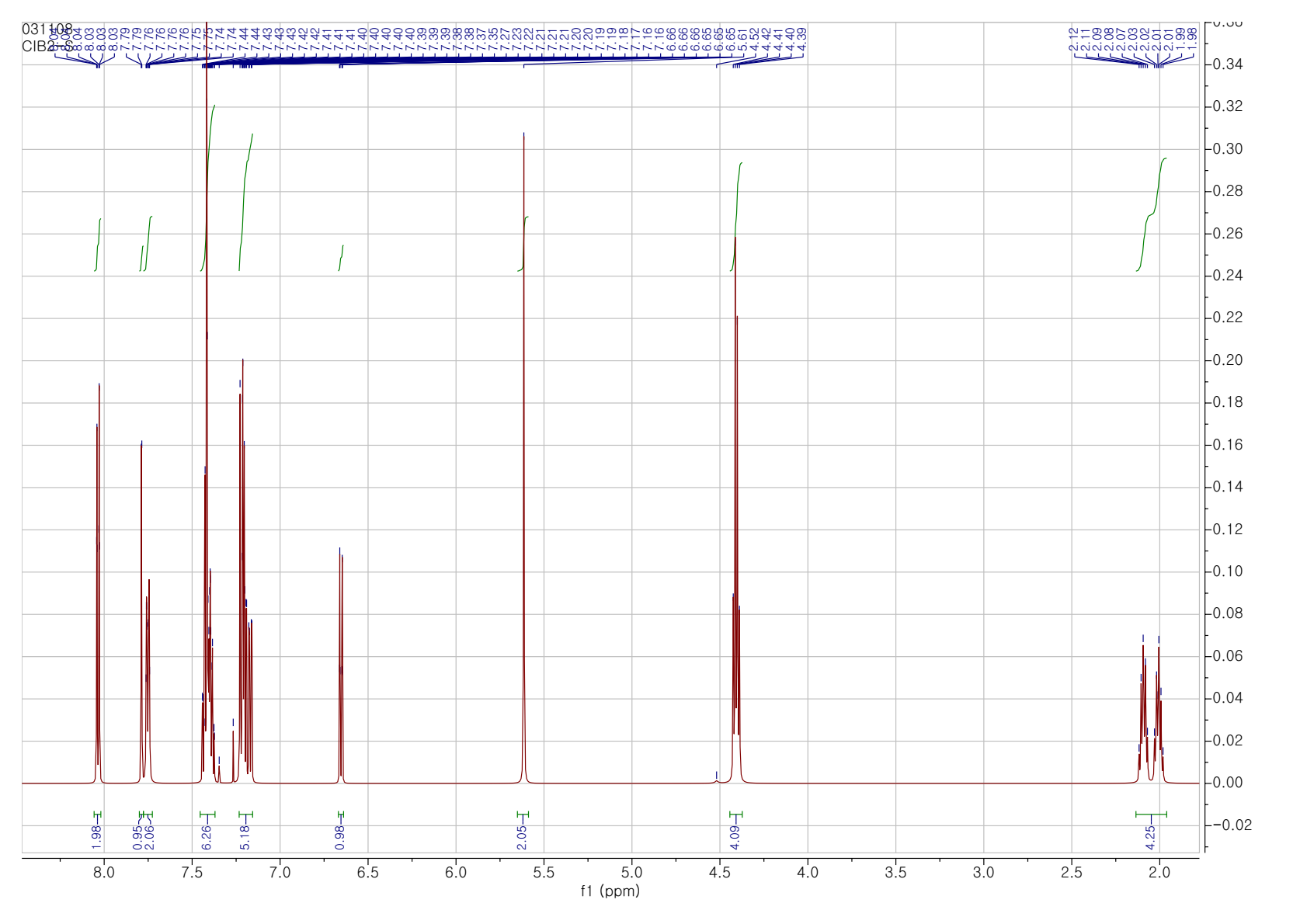
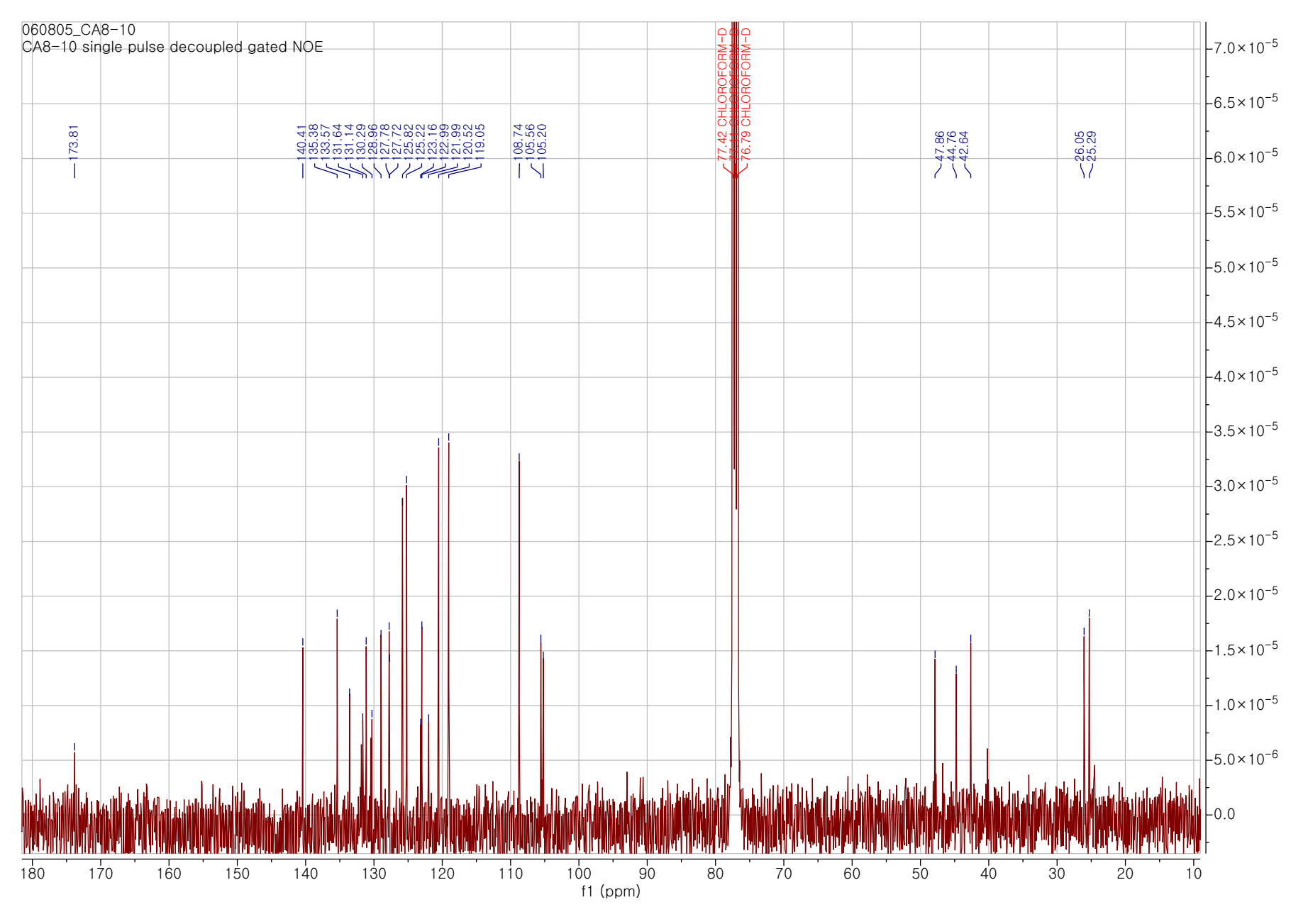
 

Figure S28. 1H-NMR and 13C-NMR spectra of **CSD** in CHCl3

|  |  |
| --- | --- |
| a) Mass spectra of **CSD** | b) Mass spectra of **CSM** |

Figure S29. Mass spectra of (a) **CSD** and (b) **CSM**.

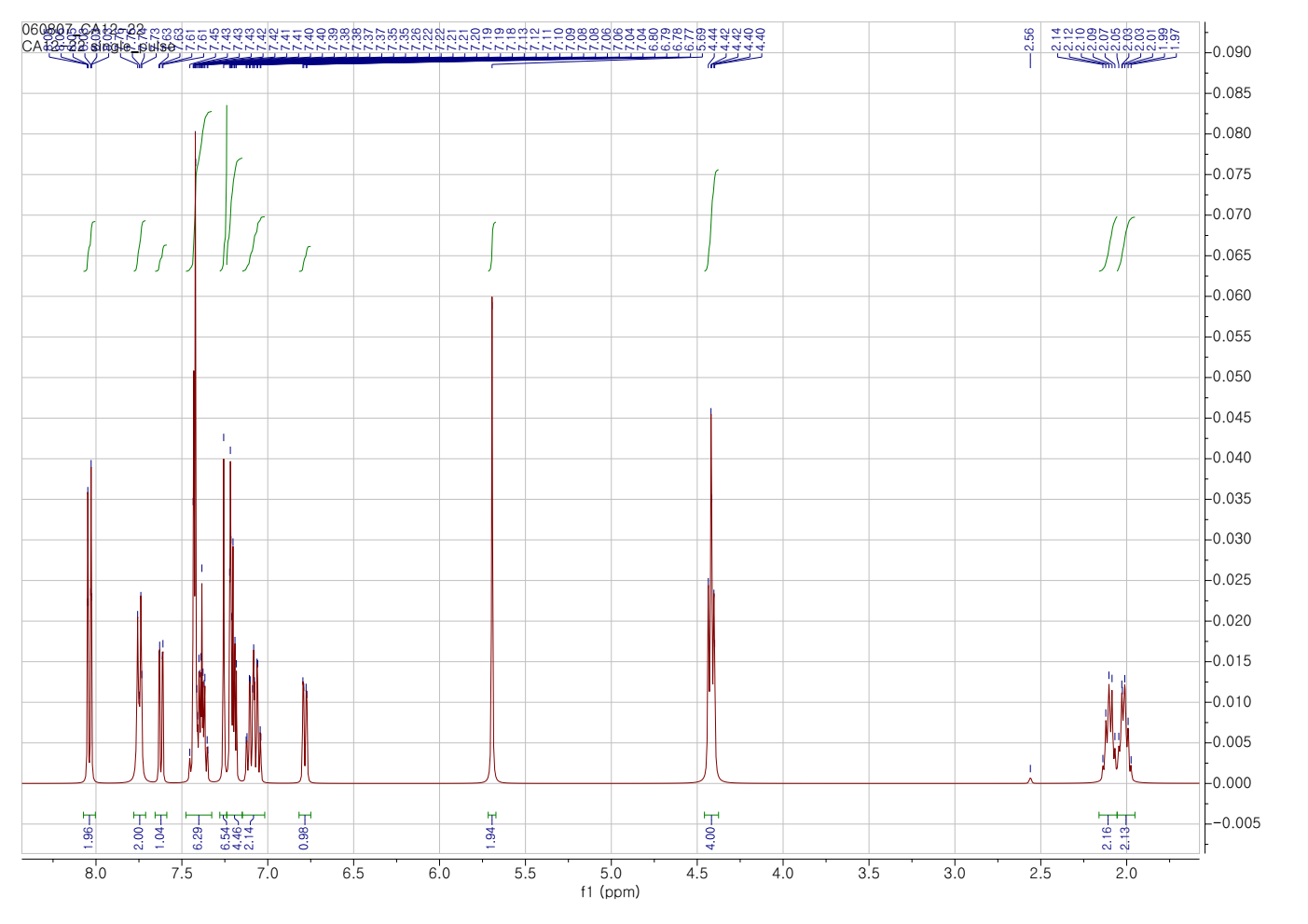
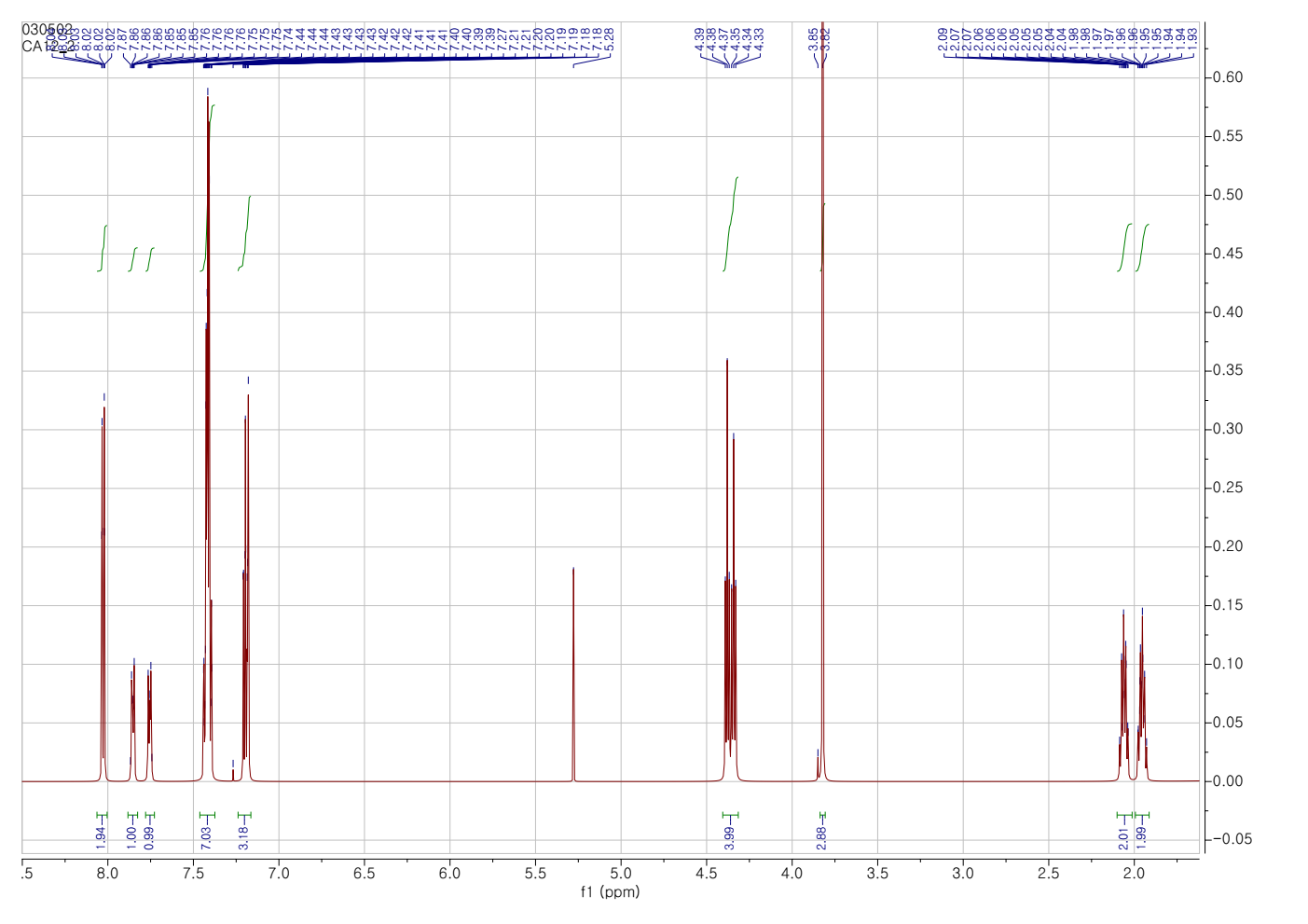
 

Figure S30. 1H-NMR and 13C-NMR spectra of **CSM** in CHCl3

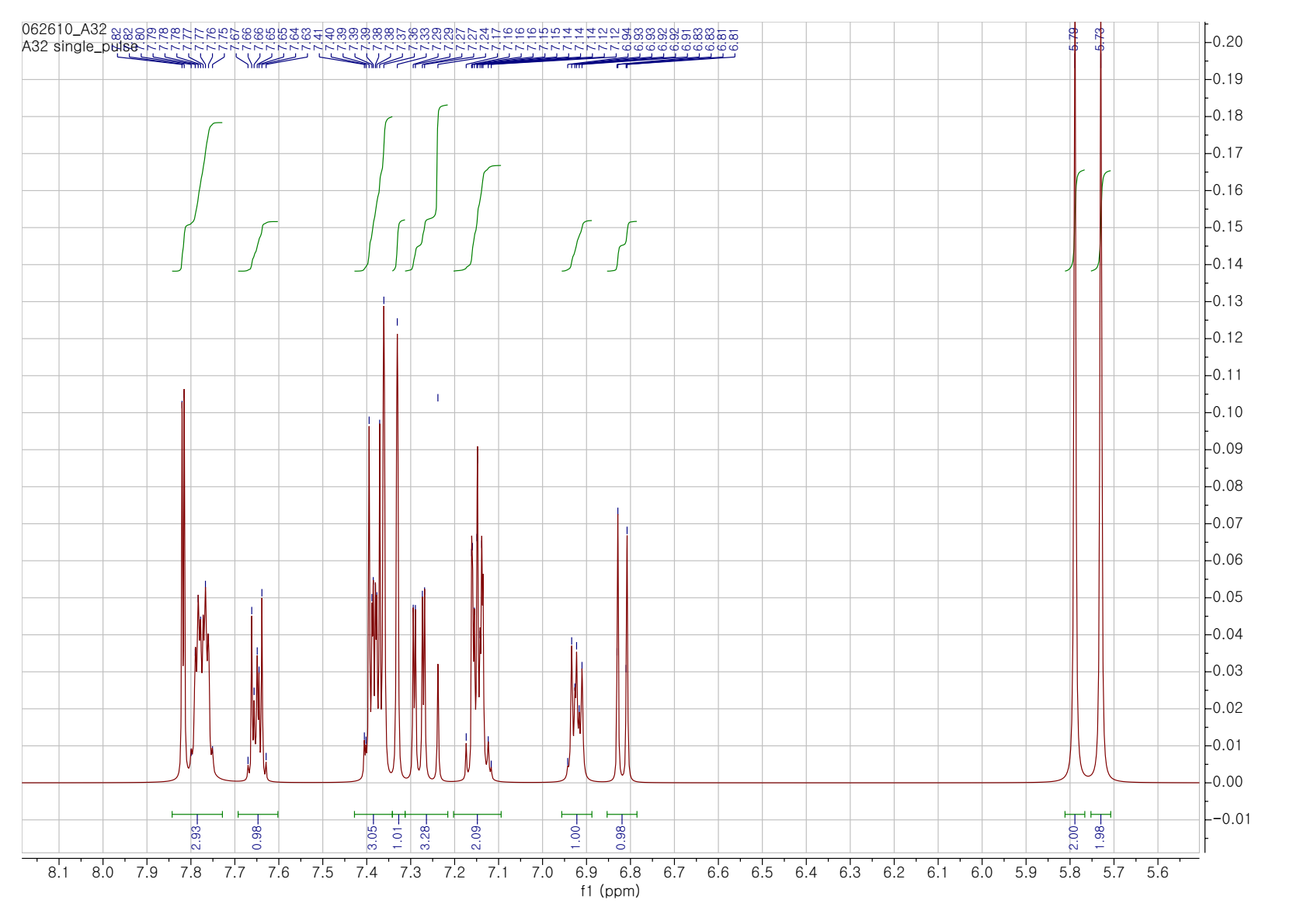
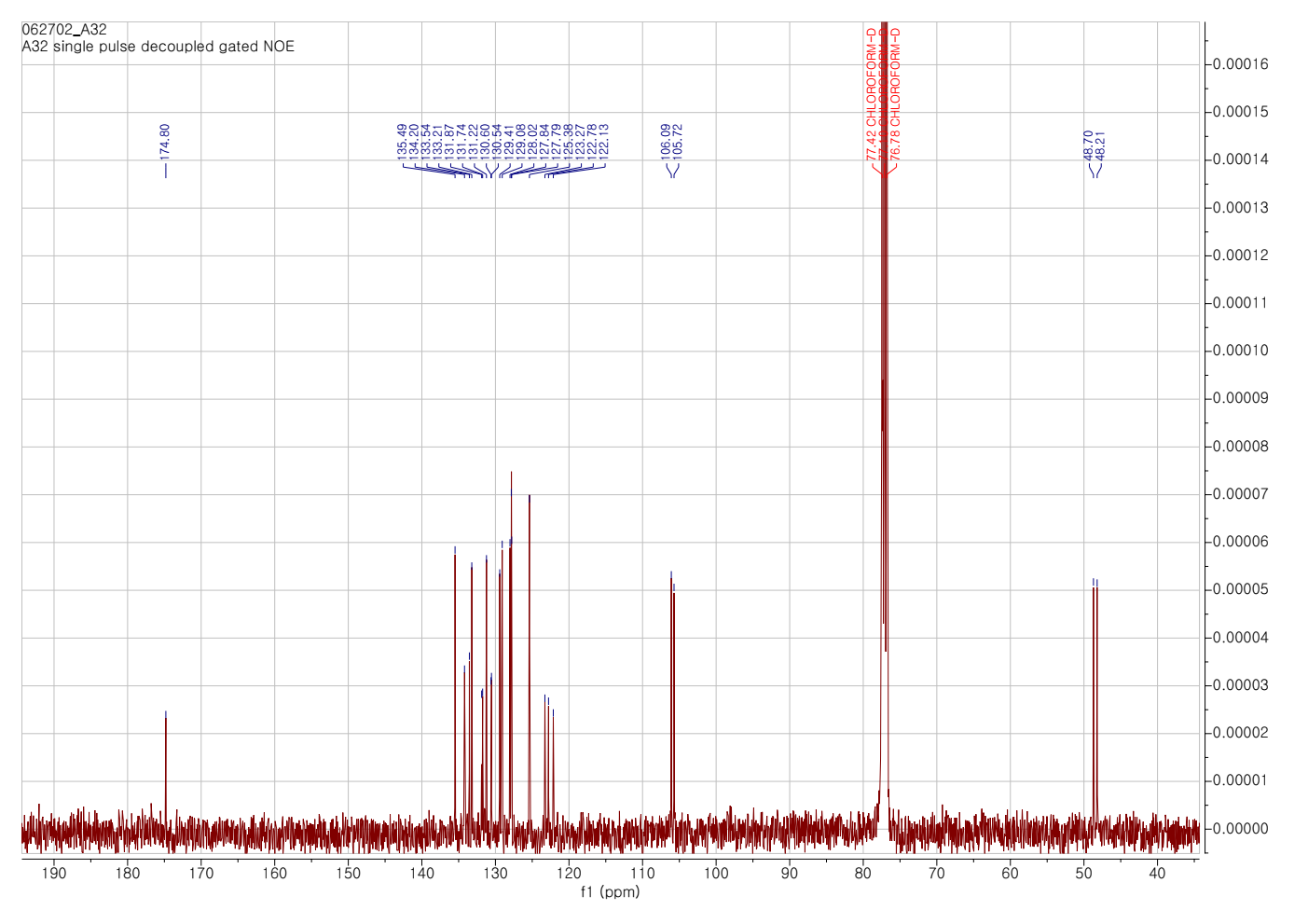
 

Figure S31. 1H-NMR and 13C-NMR spectra of **DSB** in CHCl3

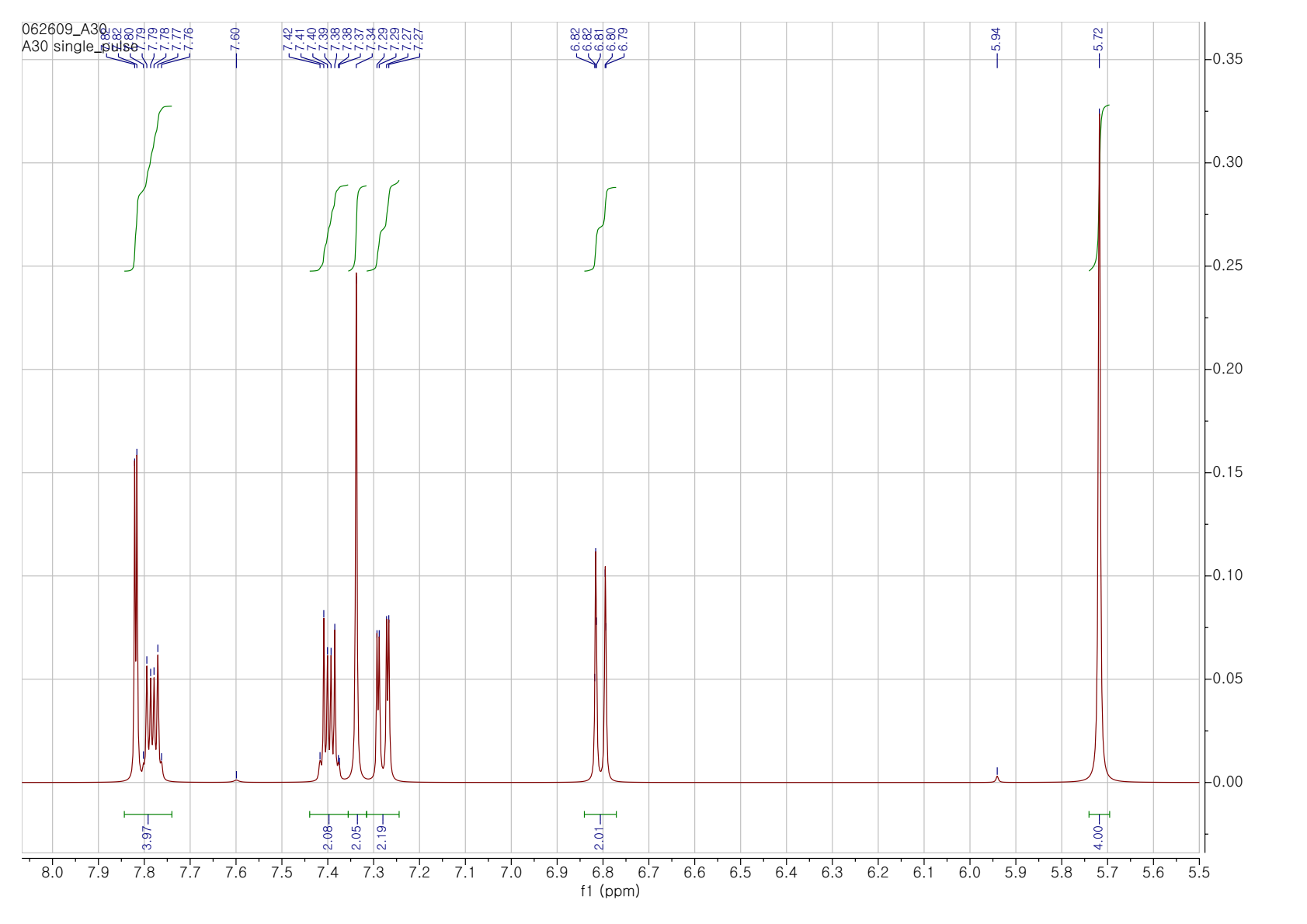
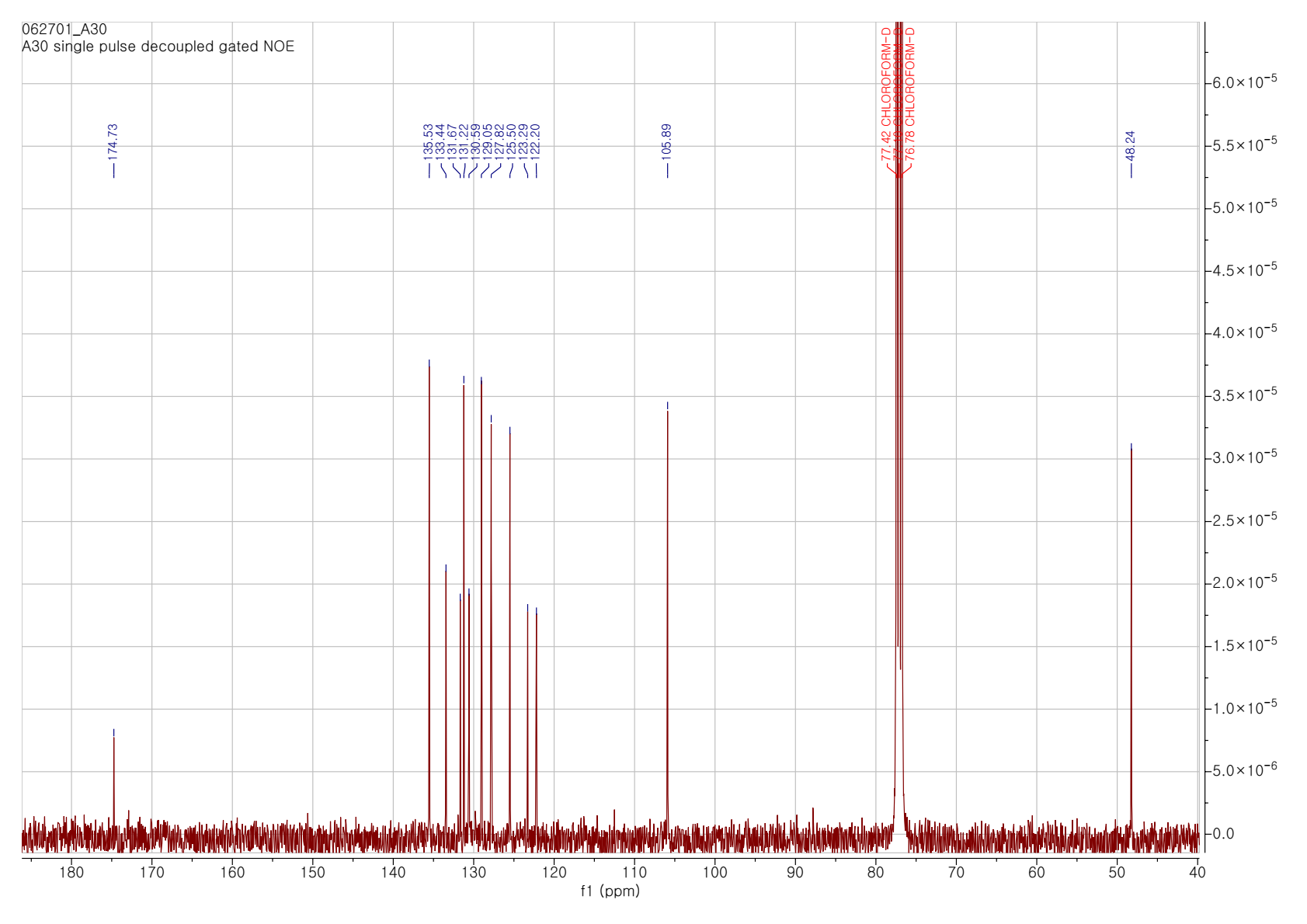
 

Figure S32. 1H-NMR and 13C-NMR spectra of **DSD** in CHCl3

|  |  |
| --- | --- |
| a) Mass spectra of **DSB** | b) Mass spectra of **DSD** |

Figure S33. Mass spectra of (a) **DSB** and (b) **DSD**.

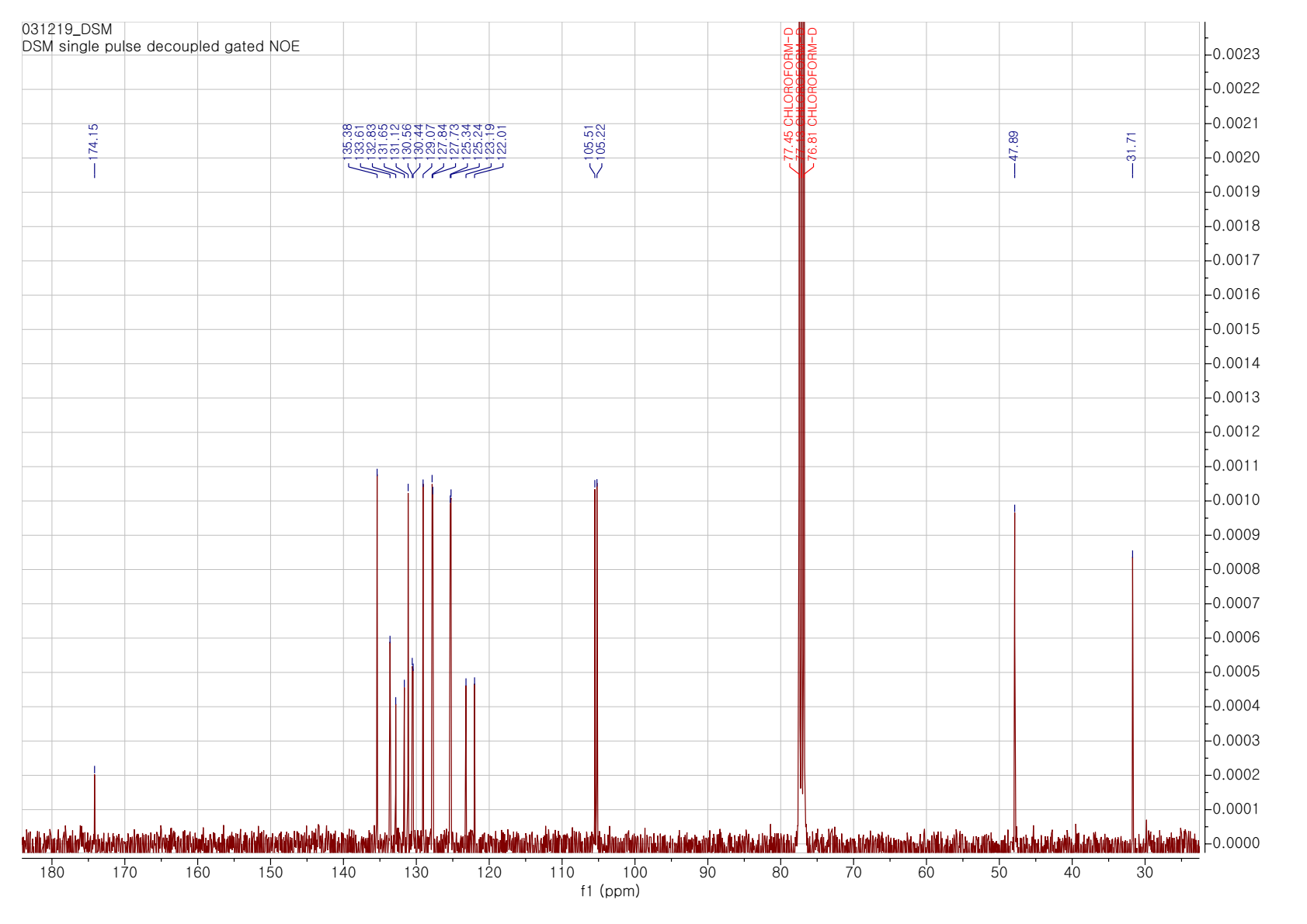
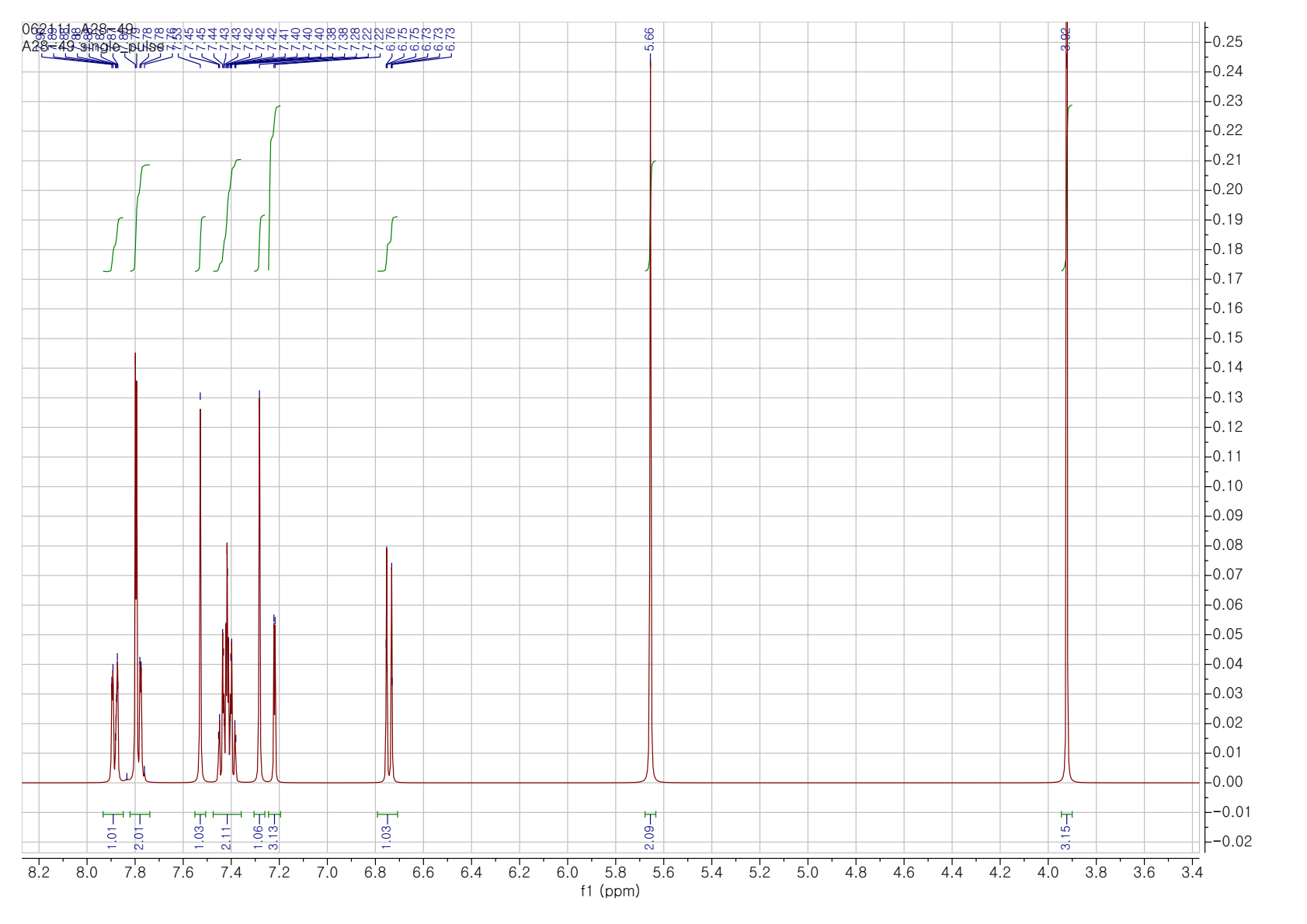


Figure S34. 1H-NMR and 13C-NMR spectra of **DSM** in CHCl3

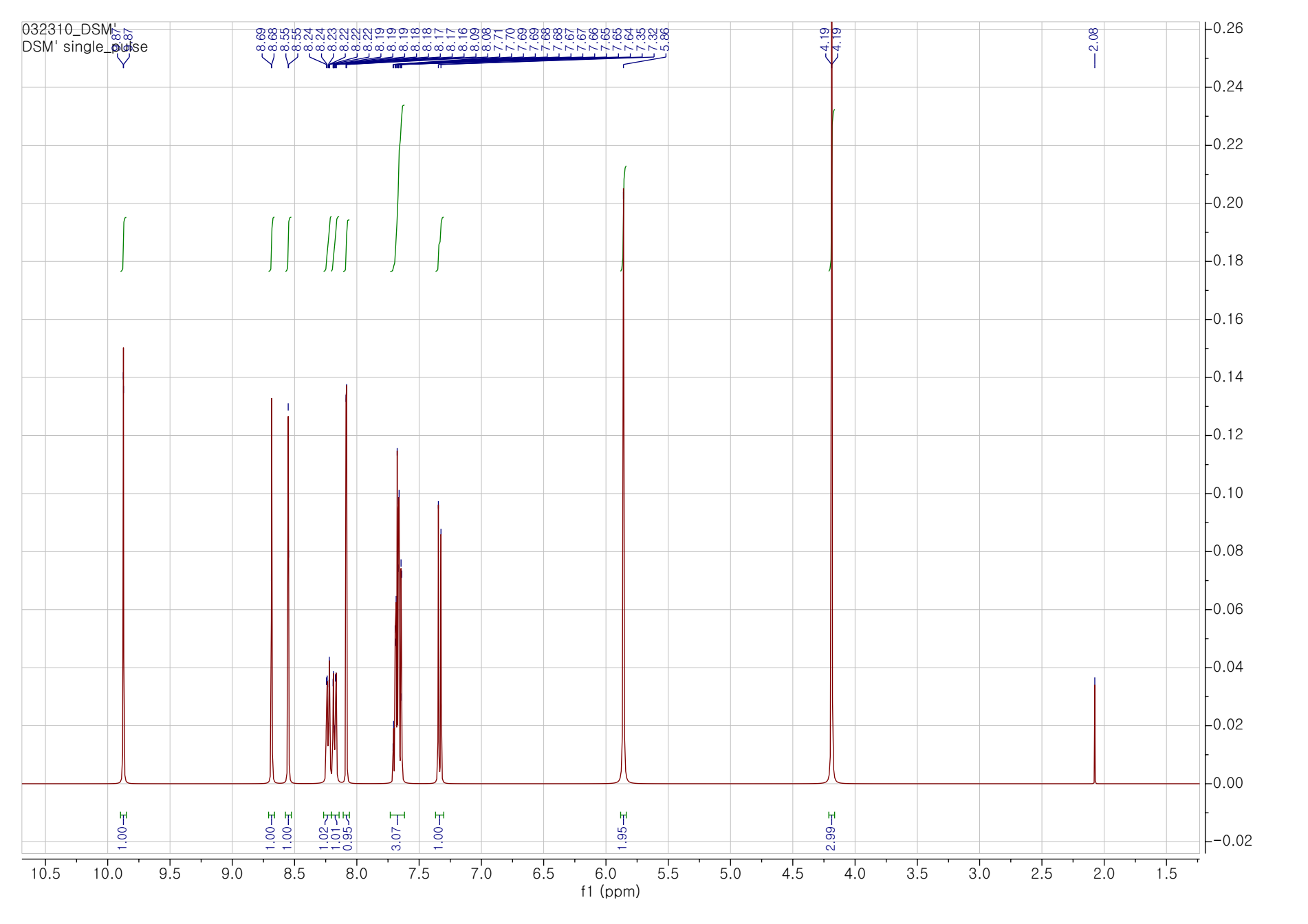
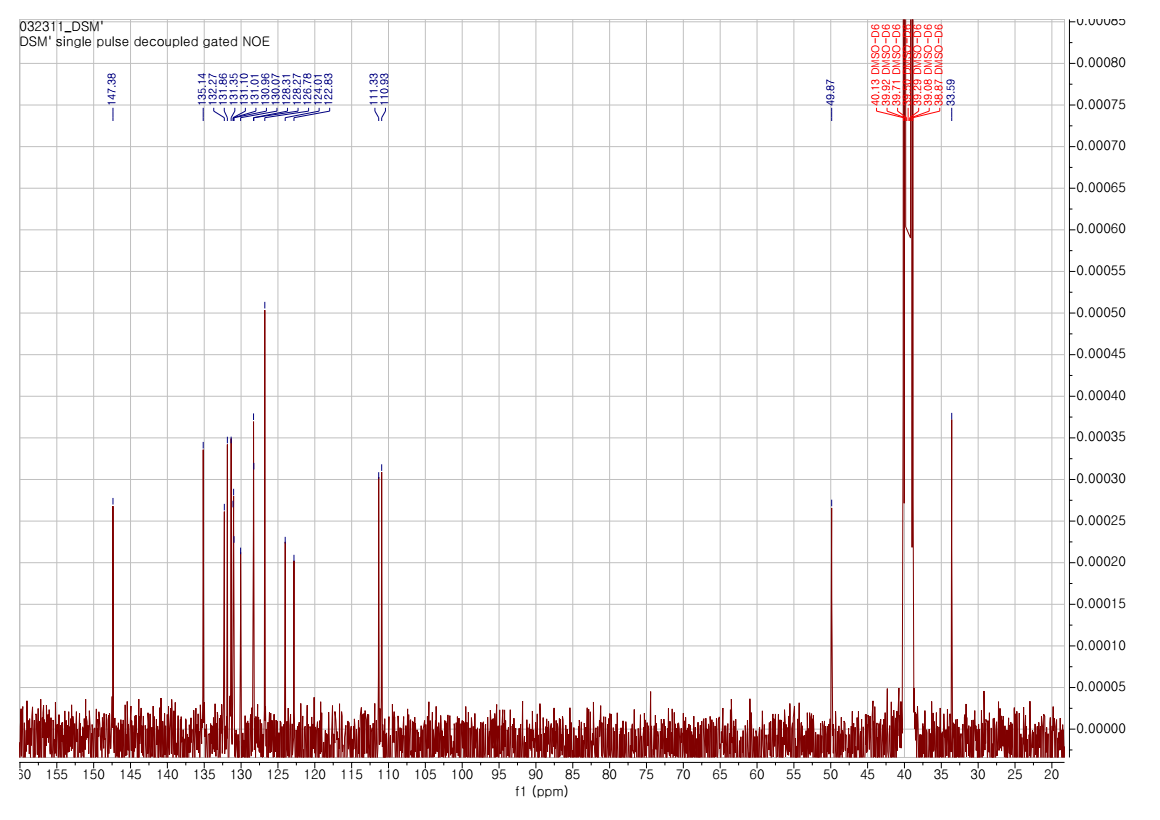
 

Figure S35. 1H-NMR and 13C-NMR spectra of **DSM’ (DIM)** in DMSO

|  |  |
| --- | --- |
| a) Mass spectra of **DSM** | b) Mass spectra of **DSM’ (DIM)** |

Figure S36. Mass spectra of (a) **DSM** and (b) **DSM’ (DIM)**.

* 1. **Crystallization data**

Table S1. Crystal data of **CIM** and **CIC**.

|  |  |  |
| --- | --- | --- |
|  | **CIM** | **CIC** |
| Empirical formula | C29 H30 I N3 O | C45 H47 Br N4 O2 |
| Formula weight | 563.46 | 755.77 |
| Temperature | 173(2) K | 171(2) K |
| Wavelength | 0.700 Å | 0.650 Å |
| Crystal system | Monoclinic | Triclinic |
| Space group | P2**1** | P-1 |
| Unit cell dimensions | a = 10.308(2) Å = 90°.  b = 7.8540(16) Å = 102.96(3)°.  c = 16.040(3) Å  = 90°. | a = 8.4980(17) Å = 84.53(3)°.  b = 10.255(2) Å = 86.87(3)°.  c = 23.313(5) Å  = 72.93(3)°. |
| Volume | 1265.5(5) Å3 | 1932.5(7) Å3 |
| Z | 2 | 2 |
| Density (calculated) | 1.479 Mg/m3 | 1.299 Mg/m3 |
| Absorption coefficient | 1.225 mm-1 | 0.880 mm-1 |
| F(000) | 572 | 792 |
| Crystal size | 0.120 x 0.053 x 0.044 mm3 | 0.120 x 0.080 x 0.070 mm3 |
| Theta range for data collection | 2.118 to 27.996°. | 1.606 to 30.000°. |
| Index ranges | -13<=h<=13, -10<=k<=10, -21<=l<=21 | -13<=h<=13, -15<=k<=15, -35<=l<=35 |
| Reflections collected | 11493 | 29303 |
| Independent reflections | 6350 [R(int) = 0.0633] | 14668 [R(int) = 0.0192] |
| Completeness to theta = | (24.835°) 99.3 % | (22.955°**)** 99.8 % |
| Absorption correction | Empirical | Empirical |
| Max. and min. transmission | 1.000 and 0.882 | 1.000 and 0.934 |
| Refinement method | Full-matrix least-squares on F2 | Full-matrix least-squares on F2 |
| Data / restraints / parameters | 6350 / 1 / 310 | 14668 / 0 / 474 |
| Goodness-of-fit on F2 | 1.096 | 1.151 |
| Final R indices [I>2sigma(I)] | R1 = 0.0394, wR2 = 0.1146 | R1 = 0.0624, wR2 = 0.1884 |
| R indices (all data) | R1 = 0.0410, wR2 = 0.1156 | R1 = 0.0760, wR2 = 0.1963 |
| Absolute structure parameter | -0.006(8) |  |
| Extinction coefficient | n/a | n/a |
| Largest diff. peak and hole | 1.533 and -0.765 e.Å-3 | 2.352 and -1.296 e.Å-3 |
| CCDC deposition number | 2084935 | 2084931 |

|  |  |
| --- | --- |
| a) | b) |

Figure S37. Crystal structure of (a) CIM and (b) CIC

|  |  |
| --- | --- |
| c) | d) |

Figure S38. Crystal structure of (a) CSM and (b) CSC

Table S2. Crystal data of **CSM** and **CSC**.

|  |  |  |
| --- | --- | --- |
|  | **CSM** | **CSC** |
| Empirical formula | C28 H25 N3 S | C43 H38 N4 S |
| Formula weight | 435.57 | 642.83 |
| Temperature | 173(2) K | 173(2) K |
| Wavelength | 0.650 Å | 0.800 Å |
| Crystal system | Monoclinic | Triclinic |
| Space group | P2**1**/n | P-1 |
| Unit cell dimensions | a = 9.6770(19) Å = 90°  b = 14.016(3) Å = 90.67(3)°  c = 16.317(3) Å  = 90° | a = 9.3930(19) Å = 89.06(3)°.  b = 15.420(3) Å = 86.63(3)°.  c = 23.453(5) Å  = 84.27(3)°. |
| Volume | 2213.0(8) Å3 | 3373.9(12) Å3 |
| Z | 4 | 4 |
| Density (calculated) | 1.307 Mg/m3 | 1.266 Mg/m3 |
| Absorption coefficient | 0.133 mm-1 | 0.177 mm-1 |
| F(000) | 920 | 1360 |
| Crystal size | 0.300 x 0.120 x 0.100 mm3 | 0.110 x 0.020 x 0.019 mm3 |
| Theta range for data collection | 2.226 to 25.998°. | 1.494 to 28.000°. |
| Index ranges | -13<=h<=13, -18<=k<=18, -21<=l<=22 | -11<=h<=11, -18<=k<=18, -27<=l<=27 |
| Reflections collected | 18790 | 22674 |
| Independent reflections | 5588 [R(int) = 0.1117] | 11358 [R(int) = 0.0400] |
| Completeness to theta | 22.955° - 98.0 % | 28.000° - 99.6 % |
| Absorption correction | Empirical | Empirical |
| Max. and min. transmission | 1.000 and 0.923 | 1.000 and 0.859 |
| Refinement method | Full-matrix least-squares on F2 | Full-matrix least-squares on F2 |
| Data / restraints / parameters | 5588 / 0 / 290 | 11358 / 825 / 1009 |
| Goodness-of-fit on F2 | 1.065 | 1.724 |
| Final R indices [I>2sigma(I)] | R1 = 0.0776, wR2 = 0.2205 | R1 = 0.1376, wR2 = 0.4293 |
| R indices (all data) | R1 = 0.0835, wR2 = 0.2291 | R1 = 0.1672, wR2 = 0.4424 |
| Extinction coefficient | n/a | 0.017(4) |
| Largest diff. peak and hole | 1.023 and -0.422 e.Å-3 | 0.549 and -0.817 e.Å-3 |
| CCDC deposition number | 2084934 | 2084933 |

* 1. **Photophysical results**

|  |  |
| --- | --- |
| a) | b) |

Figure S39. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **BIB** (80 µM, λex = 325 nm) and (b) **BSB** (20 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S40. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **BIM** (80 µM, λex = 325 nm) and (b) **BSM** (10 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S41. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **CIB** (80 µM, λex = 325 nm) and (b) **CSB** (10 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S42. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **CIC** (80 µM, λex = 325 nm) and (b) **CSC** (10 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S43. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **CID** (80 µM, λex = 325 nm) and (b) **CSD** (20 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S44. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **CIM** (80 µM, λex = 325 nm) and (b) **CSM** (20 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S45. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **DIB** (80 µM, λex = 325 nm) and (b) **DSB** (10 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S46. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **DID** (80 µM, λex = 325 nm) and (b) **DSD** (20 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S47. UV-Vis (dot line) and Fluorescence emission (dash dot line) spectra of (a) **DIM** (80 µM, λex = 325 nm) and (b) **DSM** (10 µM, λex = 350 nm) in several solvent.

|  |  |
| --- | --- |
| a) | b) |

Figure S48. (a) The fluorescence emission spectra of **DIM** (5 µM) in DMF/pH 7.4 PBS buffer (0 - 99.5%); (b) the emission under UV-365 nm irradiation **DIM** (5 µM) in DMF/pH 7.4 PBS buffer and DMF/Tol (0 - 99.5%).

|  |  |
| --- | --- |
| a) | b) |
| c) | d) |

Figure S49. The fluorescence emission spectra of **DID** (5 µM) in (a) DMF/pH 7.4 PBS buffer and (b) DMF/Tol (0 - 99.5%); (c) the fluorescence emission intensity and (d) the emission under UV-365 nm irradiation of **DID** (5 µM) in DMF/ pH 7.4 PBS buffer and DMF/Tol (0 - 99.5%).

|  |  |
| --- | --- |
| a) | b) |

Figure S50. (a) Fluorescence emission spectra (λex = 325 nm; slit 5/5) of **DSD** (5 µM) upon the treatment of ClO- (0 - 80 µM) in pH 7.4 PBS buffer (0.05 % DMF); (b) Plot of fluorescence intensity of **DSM** (5 µM) upon the treatment of ClO- (0 - 55 µM) in pH 7.4 PBS buffer (0.05 % DMF).

|  |  |
| --- | --- |
| a) | b) |

Figure S51. (a) UV-vis absorbance and (b) fluorescence emission (λex = 325 nm, slit 5/5) spectra of **DSM** (5 µM) upon the treatment of ClO- (50 µM); ROO• (1 mM); NO• (1 mM), H2O2 (1 mM), TBHP (1 mM), ONOO- (200 µM) and •OH (200 µM) in pH 7.4 PBS buffer (0.05 % DMF).

* 1. **Computational calculation results**

Table S1. Molecular orbital and energies of **BIB** and **BSB**, **BIM** and **BSM**, **CIB** and **CSB**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **BIB** | **BSB** | **BIM** | **BSM** |
| LUMO+2 | -3.88 eV | -0.90 eV | -3.83 eV | -0.83 eV |
| LUMO+1 | -3.91 eV | -0.94 eV | -4.04 eV | -0.89 eV |
| LUMO | -5.09 eV | -1.75 eV | -5.34 eV | -1.72 eV |
| HOMO | -8.95 eV | -5.87 eV | -9.13 eV | -5.80 eV |
| HOMO-1 | -9.75 eV | -6.05 eV | -9.90 eV | -6.02 eV |
| HOMO-2 | -9.78 eV | -6.20 eV | -10.04 eV | -6.14 eV |

Table S2. Molecular orbital and energies of **CIB** and **CSB**, **CID** and C**SD.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **CIB** | **CSB** | **CID** | **CSD** |
| LUMO+2 | -3.82 eV | -0.93 eV | -4.03 eV | -1.15 eV |
| LUMO+1 | -4.03 eV | 1.11 eV | -4.20 eV | -1.23 eV |
| LUMO | -5.29 eV | -1.79 eV | -5.35 eV | -1.86 eV |
| HOMO | -7.30 eV | -5.63 eV | -7.31 eV | -5.65 eV |
| HOMO-1 | -7.59 eV | -5.88 eV | -7.60 eV | -5.96 eV |
| HOMO-2 | -8.64 eV | -5.98 eV | -8.65 eV | -6.00 eV |

Table S3. Molecular orbital and energies of **CIC** and **CSC**

|  |  |  |
| --- | --- | --- |
|  | **CIC** | **CSC** |
| LUMO+2 | -3.72 eV | -1.12 eV |
| LUMO+1 | -3.96 eV | -1.13 eV |
| LUMO | -5.50 eV | -1.82 eV |
| HOMO | -7.35 eV | -5.63 eV |
| HOMO-1 | -7.36 eV | -5.64 eV |
| HOMO-2 | -7.64 eV | -5.89 eV |

Table S4. Molecular orbital and energies of **CIM** and **CSM**, **DIB** and **DSB**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **CIM** | **CSM** | **DIB** | **DSB** |
| LUMO+2 | -3.79 eV | -0.58 eV | -3.95 eV | -1.15 eV |
| LUMO+1 | -4.00 eV | -1.09 eV | -4.10 eV | -1.22 eV |
| LUMO | -5.57 eV | -1.75 eV | -5.14 eV | -1.82 eV |
| HOMO | -7.37 eV | -5.61 eV | -9.00 eV | -5.95 eV |
| HOMO-1 | -7.65 eV | -5.81 eV | -9.67 eV | -6.13 eV |
| HOMO-2 | -8.70 eV | -5.97 eV | -9.80 eV | -6.29 eV |

Table S5. Molecular orbital and energies of **DID** and **DSD**, **DIM** and **DSM**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **DID** | **DSD** | **DIM** | **DSM** |
| LUMO+2 | -4.11 eV | -1.25 eV | -4.04 eV | -1.11 eV |
| LUMO+1 | -4.15 eV | -1.28 eV | -4.22 eV | -1.19 eV |
| LUMO | -5.19 eV | -1.90 eV | -5.40 eV | -1.80 eV |
| HOMO | -9.04 eV | -6.04 eV | -9.17 eV | -5.89 eV |
| HOMO-1 | -9.69 eV | -6.21 eV | -9.77 eV | -6.10 eV |
| HOMO-2 | -9.70 eV | -6.38 eV | -10.09 eV | -6.23 eV |

Table S6. Excitation energy (eV) with significant oscillator strength (f) for the **R1IR2**molecules predicted using different DFT functionals with 6-31+G(2d,p) basis set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BIB** | **BIM** | **CIB** | **CIC** | **CID** |
| Expt. | 3.7754 eV | 3.8267 eV | 3.8149 eV | 3.7800 eV | 3.8126 eV |
| LSDA | 3.1504 eV  f=0.0485 | 3.9721 eV  f=0.0846 | 3.1343 eV  f=0.0528 | 3.1308 eV  f=0.0611 | 3.1255 eV  f=0.0556 |
| BVP86 | 3.1723 eV  f=0.0495 | 3.9822 eV  f=0.0742 | 3.1572 eV  f=0.0547 | 3.1508 eV  f=0.0628 | 3.1454 eV  f=0.0542 |
| B3LYP | 4.1823 eV  f=0.1082 | 4.1948 eV  f=0.0982 | 4.1895 eV  f=0.0910 | 3.5262 eV  f=0.0977 | 3.5244 eV  f=0.0843 |
| **CAM-B3LYP** | **3.9624 eV**  **f=0.1178** | **3.9625 eV**  **f=0.1229** | **3.9506 eV**  **f=0.1351** | **3.9413 eV**  **f=0.1577** | **3.9443 eV**  **f=0.1357** |
| B3PW91 | 4.2083 eV  f=0.1034 | 4.2223 eV  f=0.0935 | 3.2169 eV  f=0.0870 | 3.5597 eV  f=0.0984 | 3.5556 eV  f=0.0847 |
| MPW1PW91 | 4.2762 eV  f=0.1076 | 4.2830 eV  f=0.0941 | 3.6512 eV  f=0.0922 | 3.6449 eV  f=0.1054 | 4.2758 eV  f=0.0935 |
| PBEPBE | 3.1751 eV  f=0.0485 | 3.9796 eV  f=0.0762 | 3.1570 eV  f=0.0541 | 3.1477 eV  f=0.0627 | 3.1458 eV  f=0.0551 |
| HSEH1PBE | 4.2404 eV  f=0.1012 | 4.2560 eV  f=0.0944 | 3.5955 eV  f=0.0873 | 3.5895 eV  f=0.1021 | 3.5855 eV  f=0.0870 |
| HCTH | 3.9148 eV  f=0.0495 | 4.0018 eV  f=0.0527 | 3.1738 eV  f=0.0553 | 3.1553 eV  f=0.0615 | 3.1797 eV  f=0.0696 |
| TPSSTPSS | 4.0006 eV  f=0.0583 | 4.0127 eV  f=0.0546 | 3.2565 eV  f=0.0628 | 3.2418 eV  f=0.0677 | 3.2409 eV  f=0.0628 |
| 𝞈B97XD | 3.9935 eV  f=0.1211 | 3.9985 eV  f=0.1262 | 3.9872 eV  f=0.1391 | 3.9827 eV  f=0.1619 | 3.9817 eV  f=0.1397 |
| APFD | 4.2527 eV  f=0.1077 | 4.2619 eV  f=0.0940 | 3.6181 eV  f=0.0892 | 3.6123 eV  f=0.1028 | 4.2544 eV  f=0.0929 |
| BhandHLYP | 4.0075 eV  f=0.1180 | 4.0062 eV  f=0.1230 | 3.9942 eV  f=0.1346 | 3.9836 eV  f=0.1561 | 3.9872 eV  f=0.1351 |
| LC-𝞈PBE | 4.2624 eV  f=0.1483 | 4.2636 eV  f=0.1541 | 4.2545 eV  f=0.1696 | 4.2483 eV  f=0.1974 | 4.2503 eV  f=0.1706 |
| M06-2X | 3.9941 eV  f=0.1170 | 4.0009 eV  f=0.1224 | 3.9849 eV  f=0.1363 | 3.9797 eV  f=0.1613 | 3.9781 eV  f=0.1369 |
| M06 | 4.1486 eV  f=0.1229 | 4.1562 eV  f=0.1066 | 4.1498 eV  f=0.1008 | 3.8882 eV  f=0.1005 | 4.1465 eV  f=0.1073 |
| M06L | 4.0808 eV  f=0.1175 | 4.0964 eV  f=0.1095 | 3.3206 eV  f=0.0670 | 3.3179 eV  f=0.0724 | 3.3022 eV  f=0.0621 |
| M06HF | 4.3954 eV  f=0.1650 | 4.3953 eV  f=0.1725 | 4.3780 eV  f=0.2021 | 4.3627 eV  f=0.2455 | 4.3738 eV  f=0.2030 |
|  | **CIM** | **DIB** | **DID** | **DIM** | **MAD\*** |
| Expt. | 3.8196 eV | 3.8172 eV | 3.8172 eV | 3.8267 eV |  |
| LSDA | 3.4456 eV  f=0.0274 | 3.1432 eV  f=0.0470 | 3.1297 eV  f=0.0441 | 3.9456 eV  f=0.0956 | 0.5157 |
| BVP86 | 3.1677 eV  f=0.0585 | 3.1627 eV  f=0.0464 | 3.1555 eV  f=0.0461 | 3.9468 eV  f=0.0879 | 0.5334 |
| B3LYP | 4.3534 eV  f=0.1438 | 4.1803 eV  f=0.1187 | 4.1831 eV  f=0.1230 | 4.1939 eV  f=0.1054 | 0.3691 |
| **CAM-B3LYP** | **3.9538 eV**  **f=0.1413** | **3.9607 eV**  **f=0.1171** | **3.9556 eV**  **f=0.1160** | **3.9573 eV**  **f=0.1237** | **0.1442** |
| B3PW91 | 4.3954 eV  f=0.1388 | 4.2063 eV  f=0.1138 | 4.2099 eV  f=0.1186 | 4.2218 eV  f=0.1005 | 0.7396 |
| MPW1PW91 | 4.4556 eV  f=0.1642 | 4.2738 eV  f=0.1148 | 4.2737 eV  f=0.1178 | 4.2812 eV  f=0.0997 | 0.4136 |
| PBEPBE | 3.1661 eV  f=0.0578 | 3.1731 eV  f=0.0493 | 3.1613 eV  f=0.0469 | 3.9473 eV  f=0.0905 | 0.5316 |
| HSEH1PBE | 4.4204 eV  f=0.1466 | 4.2380 eV  f=0.1123 | 4.2411 eV  f=0.1171 | 4.2550 eV  f=0.1015 | 0.3783 |
| HCTH | 3.1724 eV  f=0.0570 | 3.1996 eV  f=0.0520 | 3.1924 eV  f=0.0522 | 3.9540 eV  f=0.1019 | 0.47 |
| TPSSTPSS | 3.2570 eV  f=0.0627 | 3.2679 eV  f=0.0566 | 3.2476 eV  f=0.0487 | 4.0281 eV  f=0.0934 | 0.4403 |
| 𝞈B97XD | 3.9948 eV  f=0.1451 | 3.9917 eV  f=0.1204 | 3.9873 eV  f=0.1195 | 3.9939 eV  f=0.1272 | 0.1801 |
| APFD | 4.4347 eV  f=0.1538 | 4.2501 eV  f=0.1155 | 4.2508 eV  f=0.1183 | 4.2603 eV  f=0.0997 | 0.4038 |
| BhandHLYP | 3.9962 eV  f=0.1409 | 4.0054 eV  f=0.1173 | 4.4946 eV  f=0.1165 | 4.0005 eV  f=0.1238 | 0.2428 |
| LC-𝞈PBE | 4.2580 eV  f=0.1768 | 4.2617 eV  f=0.1477 | 4.2588 eV  f=0.1467 | 4.2603 eV  f=0.1554 | 0.4475 |
| M06-2X | 3.9958 eV  f=0.1429 | 3.9918 eV  f=0.1162 | 3.9854 eV  f=0.1148 | 3.9956 eV  f=0.1234 | 0.1796 |
| M06 | 4.2891 eV  f=0.1702 | 4.1455 eV  f=0.1325 | 4.1440 eV  f=0.1367 | 4.1537 eV  f=0.1133 | 0.3257 |
| M06L | 3.3338 eV  f=0.0669 | 3.3120 eV  f=0.0554 | 3.3074 eV  f=0.0565 | 4.1046 eV  f=0.1429 | 0.4245 |
| M06HF | 4.3807 eV  f=0.2115 | 4.3954 eV  f=0.1639 | 4.3910 eV  f=0.1628 | 4.3920 eV  f=0.1741 | 0.5749 |

\*Mean absolute deviations,

Table S7. Excitation energy (eV) with significant oscillator strength (f) for the **R1IR2** molecules predicted using different DFT functionals with def2-TZVP basis set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BIB** | **BIM** | **CIB** | **CIC** | **CID** |
| Expt. | 3.7754 eV | 3.8267 eV | 3.8149 eV | 3.7800 eV | 3.8126 eV |
| LSDA | 3.1420 eV  f=0.0447 | 3.9675 eV  f=0.0817 | 3.1342 eV  f=0.0547 | 3.1281 eV  f=0.0607 | 3.1191 eV  f=0.0519 |
| BVP86 | 3.8884 eV  f=0.0477 | 3.9804 eV  f=0.0690 | 3.1554 eV  f=0.0556 | 3.1493 eV  f=0.0629 | 3.1429 eV  f=0.0546 |
| B3LYP | 4.1747 eV  f=0.1045 | 4.1890 eV  f=0.0948 | 4.1834 eV  f=0.0889 | 3.5240 eV  f=0.0972 | 3.5225 eV  f=0.0841 |
| **CAM-B3LYP** | **3.9542 eV**  **f=0.1171** | **3.9549 eV**  **f=0.1207** | **3.9422 eV**  **f=0.1338** | **3.9325 eV**  **f=0.1550** | **3.9360 eV**  **f=0.1343** |
| B3PW91 | 4.2005 eV  f=0.1008 | 4.2159 eV  f=0.0914 | 4.2104 eV  f=0.0853 | 3.5557 eV  f=0.0982 | 3.5515 eV  f=0.0849 |
| MPW1PW91 | 4.2712 eV  f=0.1072 | 4.2791 eV  f=0.0925 | 3.6493 eV  f=0.0922 | 3.6436 eV  f=0.1051 | 4.2718 eV  f=0.0926 |
| PBEPBE | 3.1703 eV  f=0.0459 | 3.1738 eV  f=0.0486 | 3.1574 eV  f=0.0554 | 3.1479 eV  f=0.0621 | 3.1456 eV  f=0.0540 |
| HSEH1PBE | 4.2327 eV  f=0.0975 | 4.2503 eV  f=0.0917 | 3.5925 eV  f=0.0875 | 3.5868 eV  f=0.1018 | 3.5827 eV  f=0.0873 |
| HCTH | 3.9099 eV  f=0.0560 | 3.1851 eV  f=0.0484 | 3.1725 eV  f=0.0550 | 3.1550 eV  f=0.0623 | 3.1583 eV  f=0.0545 |
| TPSSTPSS | 4.0004 eV  f=0.0691 | 4.0149 eV  f=0.0611 | 3.2532 eV  f=0.0595 | 3.2448 eV  f=0.0684 | 3.2396 eV  f=0.0596 |
| 𝞈B97XD | 3.9837 eV  f=0.1210 | 3.9885 eV  f=0.1249 | 3.9769 eV  f=0.1379 | 3.9721 eV  f=0.1603 | 3.9717 eV  f=0.1390 |
| APFD | 4.2461 eV  f=0.1066 | 4.2561 eV  f=0.0923 | 3.6141 eV  f=0.0893 | 3.6085 eV  f=0.1025 | 4.2488 eV  f=0.0922 |
| BhandHLYP | 4.0007 eV  f=0.1174 | 4.0007 eV  f=0.1215 | 3.9877 eV  f=0.1337 | 3.9773 eV  f=0.1542 | 3.9809 eV  f=0.1341 |
| LC-𝞈PBE | 4.2458 eV  f=0.1463 | 4.2469 eV  f=0.1509 | 4.2376 eV  f=0.1668 | 4.2312 eV  f=0.1932 | 4.2336 eV  f=0.1679 |
| M06-2X | 3.9920 eV  f=0.1161 | 4.0000 eV  f=0.1206 | 3.9834 eV  f=0.1351 | 3.9791 eV  f=0.1593 | 3.9769 eV  f=0.1357 |
| M06 | 4.1346 eV  f=0.1212 | 4.1438 eV  f=0.1035 | 4.1368 eV  f=0.0994 | 3.5255 eV  f=0.0991 | 4.1341 eV  f=0.1063 |
| M06L | 4.0694 eV  f=0.0968 | 4.0809 eV  f=0.1100 | 3.3077 eV  f=0.0643 | 3.3102 eV  f=0.0738 | 3.2964 eV  f=0.0635 |
| M06HF | 4.3782 eV  f=0.1596 | 4.3789 eV  f=0.1655 | 4.3609 eV  f=0.1886 | 4.3461 eV  f=0.2251 | 4.3566 eV  f=0.1901 |
|  | **CIM** | **DIB** | **DID** | **DIM** | **MAD\*** |
| Expt. | 3.8196 eV | 3.8172 eV | 3.8172 eV | 3.8267 eV |  |
| LSDA | 3.1507 eV  f=0.0566 | 3.1362 eV  f=0.0439 | 3.1248 eV  f=0.0424 | 3.9419 eV  f=0.1031 | 0.5509 |
| BVP86 | 3.1681 eV  f=0.0587 | 3.1586 eV  f=0.0456 | 3.1462 eV  f=0.0438 | 3.9458 eV  f=0.1094 | 0.4808 |
| B3LYP | 4.3656 eV  f=0.1423 | 4.1728 eV  f=0.1158 | 4.1760 eV  f=0.1209 | 4.1883 eV  f=0.1025 | 0.3665 |
| **CAM-B3LYP** | **3.9455 eV**  **f=0.1381** | **3.9526 eV**  **f=0.1163** | **3.9472 eV**  **f=0.1153** | **3.9499 eV**  **f=0.1216** | **0.1361** |
| B3PW91 | 4.3994 eV  f=0.1391 | 4.1987 eV  f=0.1121 | 4.2025 eV  f=0.1175 | 4.2156 eV  f=0.0986 | 0.3812 |
| MPW1PW91 | 4.4678 eV  f=0.1637 | 4.2688 eV  f=0.1143 | 4.2687 eV  f=0.1177 | 4.2774 eV  f=0.0984 | 0.4124 |
| PBEPBE | 3.1668 eV  f=0.0575 | 3.1660 eV  f=0.0451 | 3.1533 eV  f=0.0431 | 3.9480 eV  f=0.1063 | 0.5893 |
| HSEH1PBE | 4.4280 eV  f=0.1459 | 4.2305 eV  f=0.1101 | 4.2338 eV  f=0.1156 | 4.2495 eV  f=0.0995 | 0.3764 |
| HCTH | 3.1698 eV  f=0.0561 | 3.1884 eV  f=0.0462 | 3.1761 eV  f=0.0442 | 3.9516 eV  f=0.1111 | 0.5269 |
| TPSSTPSS | 3.2607 eV  f=0.0627 | 3.2594 eV  f=0.0497 | 3.2465 eV  f=0.0475 | 4.0313 eV  f=0.1047 | 0.4417 |
| 𝞈B97XD | 3.9843 eV  f=0.1427 | 3.9822 eV  f=0.1204 | 3.9776 eV  f=0.1194 | 3.9843 eV  f=0.1259 | 0.1701 |
| APFD | 4.4413 eV  f=0.1536 | 4.2436 eV  f=0.1145 | 4.2443 eV  f=0.1177 | 4.2546 eV  f=0.0980 | 0.4013 |
| BhandHLYP | 3.9904 eV  f=0.1382 | 3.9988 eV  f=0.1168 | 3.9926 eV  f=0.1157 | 3.9952 eV  f=0.1221 | 0.1816 |
| LC-𝞈PBE | 4.2407 eV  f=0.1719 | 4.2452 eV  f=0.1458 | 4.2421 eV  f=0.1449 | 4.2437 eV  f=0.1522 | 0.4307 |
| M06-2X | 3.9952 eV  f=0.1403 | 3.9895 eV  f=0.1153 | 3.9830 eV  f=0.1142 | 3.9948 eV  f=0.1215 | 0.1782 |
| M06 | 4.3208 eV  f=0.1715 | 4.1315 eV  f=0.1309 | 4.1308 eV  f=0.1350 | 4.1417 eV  f=0.1107 | 0.3354 |
| M06L | 3.3262 eV  f=0.0664 | 3.3043 eV  f=0.0541 | 3.2931 eV  f=0.0525 | 4.0925 eV  f=0.1400 | 0.4264 |
| M06HF | 4.3642 eV  f=0.1950 | 4.3777 eV  f=0.1588 | 4.3737 eV  f=0.1578 | 4.3758 eV  f=0.1672 | 0.558 |

\*Mean absolute deviations,

Table S8. Excitation energy (eV) with significant oscillator strength (f) for the **R1IR2** molecules predicted using different DFT functionals with cc-PVTZ basis set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BIB** | **BIM** | **CIB** | **CIC** | **CID** |
| Expt. | 3.7754 eV | 3.8267 eV | 3.8149 eV | 3.7800 eV | 3.8126 eV |
| LSDA | 3.1488 eV  f=0.0451 | 3.9763 eV  f=0.0773 | 3.1380 eV  f=0.0533 | 3.1323 eV  f=0.0611 | 3.1253 eV  f=0.0521 |
| BVP86 | 3.8937 eV  f=0.0487 | 3.9901 eV  f=0.0630 | 3.1586 eV  f=0.0547 | 3.1523 eV  f=0.0628 | 3.1465 eV  f=0.0545 |
| B3LYP | 4.1823 eV  f=0.1053 | 4.1966 eV  f=0.0950 | 4.1905 eV  f=0.0894 | 3.5307 eV  f=0.0975 | 3.5299 eV  f=0.0848 |
| **CAM-B3LYP** | **3.9633 eV**  **f=0.1182** | **3.9647 eV**  **f=0.1212** | **3.9513 eV**  **f=0.1345** | **3.9414 eV**  **f=0.1555** | **3.9450 eV**  **f=0.1351** |
| B3PW91 | 4.2066 eV  f=0.1013 | 4.2219 eV  f=0.0916 | 3.5664 eV  f=0.0857 | 3.5608 eV  f=0.0986 | 3.5570 eV  f=0.0856 |
| MPW1PW91 | 4.2774 eV  f=0.1076 | 4.2857 eV  f=0.0927 | 3.6559 eV  f=0.0932 | 3.6501 eV  f=0.1059 | 3.6468 eV  f=0.0932 |
| PBEPBE | 3.8979 eV  f=0.0470 | 3.9931 eV  f=0.0625 | 3.1625 eV  f=0.0545 | 3.1524 eV  f=0.0627 | 3.1500 eV  f=0.0532 |
| HSEH1PBE | 4.2401 eV  f=0.0986 | 4.2576 eV  f=0.0922 | 3.5997 eV  f=0.0882 | 3.5931 eV  f=0.1022 | 3.5898 eV  f=0.0881 |
| HCTH | 3.9179 eV  f=0.0569 | 3.1925 eV  f=0.0487 | 3.1780 eV  f=0.0546 | 3.1589 eV  f=0.0615 | 3.1645 eV  f=0.0539 |
| TPSSTPSS | 4.0084 eV  f=0.0744 | 4.0231 eV  f=0.0669 | 3.2580 eV  f=0.0597 | 3.2495 eV  f=0.0685 | 3.2447 eV  f=0.0588 |
| 𝞈B97XD | 3.9912 eV  f=0.1220 | 3.9966 eV  f=0.1254 | 3.9844 eV  f=0.1388 | 3.9794 eV  f=0.1606 | 3.9790 eV  f=0.1397 |
| APFD | 4.2527 eV  f=0.1069 | 4.2629 eV  f=0.0924 | 4.2568 eV  f=0.0875 | 3.6145 eV  f=0.1030 | 4.2550 eV  f=0.0930 |
| BhandHLYP | 4.0102 eV  f=0.1185 | 4.0111 eV  f=0.1223 | 3.9974 eV  f=0.1347 | 3.9867 eV  f=0.1549 | 3.9905 eV  f=0.1352 |
| LC-𝞈PBE | 4.2525 eV  f=0.1475 | 4.2541 eV  f=0.1515 | 4.2444 eV  f=0.1676 | 4.2378 eV  f=0.1935 | 4.2403 eV  f=0.1687 |
| M06-2X | 3.9931 eV  f=0.1179 | 4.0021 eV  f=0.1218 | 3.9850 eV  f=0.1363 | 3.9809 eV  f=0.1598 | 3.9785 eV  f=0.1369 |
| M06 | 4.1338 eV  f=0.1146 | 4.1429 eV  f=0.0977 | 4.3412 eV  f=0.1646 | 3.5388 eV  f=0.0996 | 4.1332 eV  f=0.1006 |
| M06L | 4.0528 eV  f=0.0583 | 4.0818 eV  f=0.1047 | 3.3169 eV  f=0.0648 | 3.3211 eV  f=0.0735 | 3.3056 eV  f=0.0642 |
| M06HF | 4.3629 eV  f=0.1621 | 4.3649 eV  f=0.1670 | 4.3463 eV  f=0.1885 | 4.3318 eV  f=0.2221 | 4.3421 eV  f=0.1900 |
|  | **CIM** | **DIB** | **DID** | **DIM** | **MAD\*** |
| Expt. | 3.8196 eV | 3.8172 eV | 3.8172 eV | 3.8267 eV |  |
| LSDA | 3.1555 eV  f=0.0559 | 3.1428 eV  f=0.0440 | 3.1293 eV  f=0.0424 | 3.9480 eV  f=0.1017 | 0.5484 |
| BVP86 | 3.1707 eV  f=0.0577 | 3.1630 eV  f=0.0458 | 3.1508 eV  f=0.0439 | 3.9512 eV  f=0.1084 | 0.4806 |
| B3LYP | 4.3869 eV  f=0.1386 | 4.1803 eV  f=0.1164 | 4.1834 eV  f=0.1216 | 4.1959 eV  f=0.1027 | 0.3722 |
| **CAM-B3LYP** | **3.9552 eV**  **f=0.1384** | **3.9615 eV**  **f=0.1173** | **3.9560 eV**  **f=0.1164** | **3.9596 eV**  **f=0.1222** | **0.1453** |
| B3PW91 | 4.4161 eV  f=0.1356 | 4.2048 eV  f=0.1124 | 4.2085 eV  f=0.1179 | 4.2216 eV  f=0.0989 | 0.3689 |
| MPW1PW91 | 4.4859 eV  f=0.1600 | 4.2750 eV  f=0.1147 | 4.2747 eV  f=0.1182 | 4.2839 eV  f=0.0986 | 0.3838 |
| PBEPBE | 3.1713 eV  f=0.0569 | 3.1714 eV  f=0.0457 | 3.1585 eV  f=0.0440 | 3.9545 eV  f=0.1062 | 0.4791 |
| HSEH1PBE | 3.6087 eV  f=0.0920 | 4.2379 eV  f=0.1110 | 4.2413 eV  f=0.1168 | 4.2569 eV  f=0.1002 | 0.334 |
| HCTH | 3.1759 eV  f=0.0553 | 3.1942 eV  f=0.0462 | 3.1817 eV  f=0.0447 | 3.9592 eV  f=0.1119 | 0.5242 |
| TPSSTPSS | 3.2667 eV  f=0.0630 | 3.2638 eV  f=0.0501 | 3.2502 eV  f=0.0478 | 4.0378 eV  f=0.1052 | 0.441 |
| 𝞈B97XD | 3.9924 eV  f=0.1428 | 3.9895 eV  f=0.1214 | 3.9847 eV  f=0.1204 | 3.9922 eV  f=0.1264 | 0.1777 |
| APFD | 4.4595 eV  f=0.1498 | 4.2502 eV  f=0.1148 | 4.2508 eV  f=0.1181 | 4.2613 eV  f=0.0983 | 0.4338 |
| BhandHLYP | 4.0008 eV  f=0.1388 | 4.0081 eV  f=0.1179 | 4.0018 eV  f=0.1170 | 4.0054 eV  f=0.1230 | 0.1913 |
| LC-𝞈PBE | 4.2480 eV  f=0.1721 | 4.2517 eV  f=0.1470 | 4.2486 eV  f=0.1462 | 4.2509 eV  f=0.1528 | 0.4376 |
| M06-2X | 3.9978 eV  f=0.1409 | 3.9905 eV  f=0.1171 | 3.9840 eV  f=0.1160 | 3.9970 eV  f=0.1227 | 0.1798 |
| M06 | 4.3416 eV  f=0.1674 | 4.1308 eV  f=0.1235 | 4.1296 eV  f=0.1277 | 4.1409 eV  f=0.1044 | 0.3583 |
| M06L | 3.3382 eV  f=0.0675 | 3.3107 eV  f=0.0551 | 3.2989 eV  f=0.0537 | 4.0932 eV  f=0.1343 | 0.4188 |
| M06HF | 4.3506 eV  f=0.1936 | 4.3624 eV  f=0.1615 | 4.3583 eV  f=0.1607 | 4.3618 eV  f=0.1687 | 0.5434 |

\*Mean absolute deviations,

Table S9. Excitation energy (eV) with significant oscillator strength (f) for the **R1SR2** molecules predicted using different DFT functionals with 6-31+G(2d,p) basis set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BSB** | **BSM** | **CSB** | **CSC** | **CSD** |
| Expt. | 3.5751 eV | 3.5689 eV | 3.5123 eV | 3.5587 eV | 3.5648 eV |
| LSDA | 3.4135 eV  f=0.3907 | 3.3816 eV  f=0.4068 | 3.3919 eV  f=0.3553 | 3.3786 eV  f=0.3739 | 3.3874 eV  f=0.2782 |
| BVP86 | 3.4440 eV  f=0.3972 | 3.4133 eV  f=0.3722 | 3.4182 eV  f=0.2726 | 3.4095 eV  f=0.3078 | 3.4145 eV  f=0.2423 |
| B3LYP | 3.7942 eV  f=0.4352 | 3.7789 eV  f=0.4017 | 3.7705 eV  f=0.3558 | 3.7563 eV  f=0.3683 | 3.7721 eV  f=0.3456 |
| CAM-B3LYP | 4.0883 eV  f=0.5032 | 4.0751 eV  f=0.5497 | 4.0726 eV  f=0.4805 | 4.0613 eV  f=0.4746 | 4.0749 eV  f=0.4763 |
| B3PW91 | 3.8154 eV  f=0.4318 | 3.7994 eV  f=0.3948 | 3.7908 eV  f=0.3514 | 3.7760 eV  f=0.3666 | 3.7925 eV  f=0.3414 |
| MPW1PW91 | 3.8985 eV  f=0.4842 | 3.8790 eV  f=0.4222 | 3.8942 eV  f=0.3336 | 3.8508 eV  f=0.4234 | 3.8952 eV  f=0.3381 |
| PBEPBE | 3.4367 eV  f=0.3949 | 3.4068 eV  f=0.3872 | 3.4134 eV  f=0.3084 | 3.4024 eV  f=0.3706 | 3.4100 eV  f=0.2727 |
| HSEH1PBE | 3.8498 eV  f=0.4569 | 3.8319 eV  f=0.4107 | 3.8226 eV  f=0.3642 | 3.8082 eV  f=0.4181 | 3.8243 eV  f=0.3520 |
| HCTH | 3.4589 eV  f=0.4081 | 3.4303 eV  f=0.3852 | 3.4340 eV  f=0.3228 | 3.4206 eV  f=0.3534 | 3.4329 eV  f=0.2867 |
| TPSSTPSS | **3.5516 eV**  **f=0.3909** | **3.5387 eV**  **f=0.2849** | **3.5380 eV**  **f=0.2760** | **3.5193 eV**  **f=0.3039** | **3.5401 eV**  **f=0.2707** |
| 𝞈B97XD | 4.1226 eV  f=0.4883 | 4.1095 eV  f=0.5310 | 4.1078 eV  f=0.4652 | 4.0977 eV  f=0.4600 | 4.1102 eV  f=0.4612 |
| APFD | 3.8659 eV  f=0.4688 | 3.8474 eV  f=0.4193 | 3.8483 eV  f=0.3685 | 3.7994 eV  f=0.2237 | 3.8492 eV  f=0.3569 |
| BhandHLYP | 4.2197 eV  f=0.5256 | 4.2006 eV  f=0.4951 | 4.1953 eV  f=0.3976 | 4.1902 eV  f=0.4940 | 4.1966 eV  f=0.3901 |
| LC-𝞈PBE | 4.2368 eV  f=0.4508 | 4.2261 eV  f=0.4905 | 4.2255 eV  f=0.4353 | 4.2157 eV  f=0.4221 | 4.2278 eV  f=0.4322 |
| M06-2X | 4.0734 eV  f=0.5182 | 4.0640 eV  f=0.5880 | 4.0587 eV  f=0.5026 | 4.0469 eV  f=0.4953 | 4.0614 eV  f=0.4969 |
| M06 | 3.8296 eV  f=0.4312 | 3.7892 eV  f=0.1459 | 3.8158 eV  f=0.3435 | 3.7869 eV  f=0.4096 | 3.7790 eV  f=0.1607 |
| **M06L** | **3.6964 eV**  **f=0.4004** | **3.6764 eV**  **f=0.3974** | **3.6818 eV**  **f=0.2131** | **3.6693 eV**  **f=0.3549** | **3.6873 eV**  **f=0.2065** |
| M06HF | 4.1608 eV  f=0.3477 | 4.1806 eV  f=0.6170 | 4.1654 eV  f=0.4520 | 4.1659 eV  f=0.4904 | 4.1659 eV  f=0.4311 |
|  | **CSM** | **DSB** | **DSD** | **DSM** | **MAD\*** |
| Expt. | 3.5587 eV | 3.5283 eV | 3.5772 eV | 3.5730 eV |  |
| LSDA | 3.3686 eV  f=0.4228 | 3.4086 eV  f=0.3414 | 3.4103 eV  f=0.3106 | 3.3758 eV  f=0.3578 | 0.1667 |
| BVP86 | 3.4007 eV  f=0.3977 | 3.4413 eV  f=0.3322 | 3.4417 eV  f=0.3215 | 3.4080 eV  f=0.3322 | 0.1362 |
| B3LYP | 3.7695 eV  f=0.4818 | 3.7963 eV  f=0.4173 | 3.7982 eV  f=0.4161 | 3.7796 eV  f=0.3780 | 0.2221 |
| CAM-B3LYP | 4.0637 eV  f=0.5336 | 4.0906 eV  f=0.4997 | 4.0927 eV  f=0.4941 | 4.0775 eV  f=0.5462 | 0.52 |
| B3PW91 | 3.7897 eV  f=0.4761 | 3.8176 eV  f=0.4132 | 3.8195 eV  f=0.4122 | 3.8000 eV  f=0.3723 | 0.2427 |
| MPW1PW91 | 3.8749 eV  f=0.3341 | 3.9007 eV  f=0.4580 | 3.9031 eV  f=0.4683 | 3.8798 eV  f=0.4026 | 0.3288 |
| PBEPBE | 3.3953 eV  f=0.4019 | 3.4312 eV  f=0.1806 | 3.4361 eV  f=0.3284 | 3.4032 eV  f=0.3476 | 0.1424 |
| HSEH1PBE | 3.8207 eV  f=0.4861 | 3.8519 eV  f=0.4198 | 3.8541 eV  f=0.4378 | 3.8325 eV  f=0.3867 | 0.2754 |
| HCTH | 3.4160 eV  f=0.3245 | 3.4584 eV  f=0.3392 | 3.4610 eV  f=0.3579 | 3.4291 eV  f=0.3551 | 0.1195 |
| **TPSSTPSS** | **3.5020 eV**  **f=0.2911** | **3.5500 eV**  **f=0.3605** | **3.5528 eV**  **f=0.3145** | **3.5411 eV**  **f=0.2505** | **0.0309** |
| 𝞈B97XD | 4.0992 eV  f=0.5162 | 4.1250 eV  f=0.4848 | 4.1270 eV  f=0.4795 | 4.1117 eV  f=0.5279 | 0.5549 |
| APFD | 3.8416 eV  f=0.4370 | 3.8682 eV  f=0.4473 | 3.8704 eV  f=0.4514 | 3.8482 eV  f=0.3983 | 0.2913 |
| BhandHLYP | 4.1929 eV  f=0.5428 | 4.2219 eV  f=0.5174 | 4.2243 eV  f=0.5175 | 4.2017 eV  f=0.4812 | 0.6474 |
| LC-𝞈PBE | 4.2164 eV  f=0.4722 | 4.2391 eV  f=0.4477 | 4.2406 eV  f=0.4437 | 4.2285 eV  f=0.4881 | 0.6711 |
| M06-2X | 4.0526 eV  f=0.5668 | 4.0755 eV  f=0.5124 | 4.0769 eV  f=0.5007 | 4.0672 eV  f=0.5828 | 0.5066 |
| M06 | 3.8009 eV  f=0.5001 | 3.8316 eV  f=0.4216 | 3.8328 eV  f=0.4083 | 3.8275 eV  f=0.4249 | 0.2529 |
| **M06L** | **3.6233 eV**  **f=0.1348** | **3.6954 eV**  **f=0.3830** | **3.6994 eV**  **f=0.3385** | **3.6796 eV**  **f=0.3564** | **0.1213** |
| M06HF | 4.1760 eV  f=0.5996 | 4.1599 eV  f=0.3211 | 4.2392 eV  f=0.3379 | 4.1832 eV  f=0.6014 | 0.62 |

\*Mean absolute deviations,

Table S10. Excitation energy (eV) with significant oscillator strength (f) for the **R1SR2** molecules predicted using different DFT functionals with def2-TZVP basis set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BSB** | **BSM** | **CSB** | **CSC** | **CSD** |
| Expt. | 3.5751 eV | 3.5689 eV | 3.5123 eV | 3.5587 eV | 3.5648 eV |
| LSDA | 3.3939 eV  f=0.3686 | 3.3666 eV  f=0.3916 | 3.3751 eV  f=0.3464 | 3.3786 eV  f=0.3739 | 3.3689 eV  f=0.3029 |
| BVP86 | 3.4282 eV  f=0.3731 | 3.4032 eV  f=0.3861 | 3.4081 eV  f=0.3365 | 3.3963 eV  f=0.3615 | 3.4041 eV  f=0.2984 |
| B3LYP | 3.7859 eV  f=0.3185 | 3.7841 eV  f=0.4473 | 3.7650 eV  f=0.2847 | 3.7502 eV  f=0.2474 | 3.7672 eV  f=0.2857 |
| CAM-B3LYP | 4.0931 eV  f=0.4605 | 4.0837 eV  f=0.5003 | 4.0787 eV  f=0.4377 | 4.0690 eV  f=0.4308 | 4.0807 eV  f=0.4342 |
| B3PW91 | 3.8063 eV  f=0.3454 | 3.8006 eV  f=0.4266 | 3.7842 eV  f=0.3019 | 3.7688 eV  f=0.2754 | 3.7863 eV  f=0.3010 |
| MPW1PW91 | 3.8982 eV  f=0.4321 | 3.8850 eV  f=0.4247 | 3.8568 eV  f=0.2458 | 3.8554 eV  f=0.3986 | 3.9015 eV  f=0.2439 |
| PBEPBE | 3.4258 eV  f=0.3760 | 3.4006 eV  f=0.3895 | 3.4053 eV  f=0.3146 | 3.3932 eV  f=0.3594 | 3.4018 eV  f=0.3063 |
| HSEH1PBE | 3.8429 eV  f=0.3705 | 3.8352 eV  f=0.4420 | 3.8186 eV  f=0.3304 | 3.8026 eV  f=0.3389 | 3.8208 eV  f=0.3263 |
| HCTH | 3.4524 eV  f=0.3760 | 3.4293 eV  f=0.3881 | 3.4310 eV  f=0.3472 | 3.4166 eV  f=0.3605 | 3.4294 eV  f=0.3189 |
| **TPSSTPSS** | **3.5455 eV**  **f=0.3864** | **3.5112 eV**  **f=0.3093** | **3.5130 eV**  **f=0.1587** | **3.5118 eV**  **f=0.3177** | **3.5358 eV**  **f=0.1838** |
| 𝞈B97XD | 4.1246 eV  f=0.4518 | 4.1146 eV  f=0.4871 | 4.1110 eV  f=0.4273 | 4.1025 eV  f=0.4208 | 4.1130 eV  f=0.4245 |
| APFD | 3.8616 eV  f=0.4055 | 3.8507 eV  f=0.4290 | 3.8483 eV  f=0.3030 | 3.8105 eV  f=0.3202 | 3.8490 eV  f=0.3083 |
| BhandHLYP | 4.2267 eV  f=0.4856 | 4.2102 eV  f=0.4379 | 4.2027 eV  f=0.3504 | 4.1998 eV  f=0.4523 | 4.2038 eV  f=0.3456 |
| LC-𝞈PBE | 4.2362 eV  f=0.4223 | 4.2279 eV  f=0.4554 | 4.2259 eV  f=0.4056 | 4.2173 eV  f=0.3913 | 4.2279 eV  f=0.4028 |
| M06-2X | 4.0819 eV  f=0.4645 | 4.0771 eV  f=0.5373 | 4.0690 eV  f=0.4545 | 4.0596 eV  f=0.4497 | 4.0713 eV  f=0.4494 |
| M06 | 3.8194 eV  f=0.3610 | 3.8055 eV  f=0.2505 | 3.7908 eV  f=0.2589 | 3.7836 eV  f=0.3452 | 3.7923 eV  f=0.2520 |
| M06L | **3.6814 eV**  **f=0.4041** | **3.6252 eV**  **f=0.1464** | **3.6706 eV**  **f=0.3807** | **3.6574 eV**  **f=0.3682** | **3.6729 eV**  **f=0.3627** |
| M06HF | 4.1931 eV  f=0.2820 | 4.2211 eV  f=0.5809 | 4.2044 eV  f=0.4178 | 4.2102 eV  f=0.4661 | 4.2040 eV  f=0.3933 |
|  | **CSM** | **DSB** | **DSD** | **DSM** | **MAD\*** |
| Expt. | 3.5587 eV | 3.5283 eV | 3.5772 eV | 3.5730 eV |  |
| LSDA | 3.3543 eV  f=0.4035 | 3.3893 eV  f=0.3353 | 3.3902 eV  f=0.3049 | 3.3603 eV  f=0.3406 | 0.1822 |
| BVP86 | 3.3914 eV  f=0.4056 | 3.4250 eV  f=0.3398 | 3.4272 eV  f=0.3161 | 3.3986 eV  f=0.3456 | 0.1483 |
| B3LYP | 3.7680 eV  f=0.2861 | 3.7880 eV  f=0.3143 | 3.7890 eV  f=0.3059 | 3.7852 eV  f=0.4271 | 0.2184 |
| CAM-B3LYP | 4.0732 eV  f=0.4818 | 4.0951 eV  f=0.4567 | 4.0968 eV  f=0.4515 | 4.0858 eV  f=0.4978 | 0.5266 |
| B3PW91 | 3.7866 eV  f=0.3359 | 3.8086 eV  f=0.3407 | 3.8096 eV  f=0.3296 | 3.8015 eV  f=0.4024 | 0.2373 |
| MPW1PW91 | 3.8634 eV  f=0.2932 | 3.9004 eV  f=0.4243 | 3.9020 eV  f=0.4149 | 3.8858 eV  f=0.4060 | 0.3257 |
| PBEPBE | 3.3883 eV  f=0.4049 | 3.4221 eV  f=0.3441 | 3.4242 eV  f=0.3176 | 3.3960 eV  f=0.3494 | 0.1511 |
| HSEH1PBE | 3.8187 eV  f=0.3681 | 3.8453 eV  f=0.3654 | 3.8465 eV  f=0.3535 | 3.8361 eV  f=0.4182 | 0.2722 |
| HCTH | 3.4143 eV  f=0.3978 | 3.4509 eV  f=0.3534 | 3.4540 eV  f=0.3323 | 3.4270 eV  f=0.3583 | 0.1236 |
| **TPSSTPSS** | **3.5038 eV**  **f=0.3916** | **3.5438 eV**  **f=0.3550** | **3.5462 eV**  **f=0.3222** | **3.5074 eV**  **f=0.2836** | **0.0368** |
| 𝞈B97XD | 4.1054 eV  f=0.4697 | 4.1267 eV  f=0.4488 | 4.1284 eV  f=0.4445 | 4.1165 eV  f=0.4845 | 0.5584 |
| APFD | 3.8462 eV  f=0.3534 | 3.8638 eV  f=0.3992 | 3.8652 eV  f=0.3877 | 3.8516 eV  f=0.4089 | 0.2922 |
| BhandHLYP | 4.2036 eV  f=0.4727 | 4.2287 eV  f=0.4774 | 4.2309 eV  f=0.4787 | 4.2110 eV  f=0.4266 | 0.6556 |
| LC-𝞈PBE | 4.2190 eV  f=0.4355 | 4.2383 eV  f=0.4196 | 4.2396 eV  f=0.4163 | 4.2300 eV  f=0.4536 | 0.6717 |
| M06-2X | 4.0668 eV  f=0.5156 | 4.0835 eV  f=0.4576 | 4.0840 eV  f=0.4422 | 4.0799 eV  f=0.5333 | 0.5173 |
| M06 | 3.8034 eV  f=0.3571 | 3.8203 eV  f=0.2951 | 3.8215 eV  f=0.3374 | 3.8057 eV  f=0.2470 | 0.2473 |
| **M06L** | **3.6240 eV**  **f=0.1466** | **3.6811 eV**  **f=0.3942** | **3.6850 eV**  **f=0.3671** | **3.6696 eV**  **f=0.3400** | **0.1056** |
| M06HF | 4.2201 eV  f=0.5684 | 4.2695 eV  f=0.3264 | 4.1799 eV  f=0.2007 | 4.2226 eV  f=0.5604 | 0.6564 |

\*Mean absolute deviations,

Table S11. Excitation energy (eV) with significant oscillator strength (f) for the **R1SR2** molecules predicted using different DFT functionals with cc-PVTZ basis set.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BSB** | **BSM** | **CSB** | **CSC** | **CSD** |
| Expt. | 3.5751 eV | 3.5689 eV | 3.5123 eV | 3.5587 eV | 3.5648 eV |
| LSDA | 3.4046 eV  f=0.3650 | 3.3780 eV  f=0.3904 | 3.3861 eV  f=0.3460 | 3.3786 eV  f=0.3739 | 3.3804 eV  f=0.3030 |
| BVP86 | 3.4395 eV  f=0.3717 | 3.4142 eV  f=0.3811 | 3.4195 eV  f=0.3313 | 3.4077 eV  f=0.3498 | 3.4153 eV  f=0.2917 |
| B3LYP | 3.8023 eV  f=0.3420 | 3.7981 eV  f=0.4320 | 3.7810 eV  f=0.3016 | 3.7661 eV  f=0.2791 | 3.7830 eV  f=0.3005 |
| **CAM-B3LYP** | 4.1075 eV  f=0.4597 | 4.0975 eV  f=0.4957 | 4.0924 eV  f=0.4346 | 4.0820 eV  f=0.4268 | 4.0945 eV  f=0.4313 |
| B3PW91 | 3.8204 eV  f=0.3656 | 3.8121 eV  f=0.4074 | 3.7977 eV  f=0.3140 | 3.7825 eV  f=0.2996 | 3.7997 eV  f=0.3108 |
| MPW1PW91 | 3.9119 eV  f=0.4410 | 3.8968 eV  f=0.4063 | 3.9112 eV  f=0.2631 | 3.8675 eV  f=0.3961 | 3.9126 eV  f=0.2750 |
| PBEPBE | 3.4375 eV  f=0.3694 | 3.4131 eV  f=0.3848 | 3.4182 eV  f=0.3394 | 3.4056 eV  f=0.3510 | 3.4143 eV  f=0.3015 |
| HSEH1PBE | 3.8581 eV  f=0.3896 | 3.8481 eV  f=0.4249 | 3.8332 eV  f=0.3375 | 3.8178 eV  f=0.3542 | 3.8352 eV  f=0.3316 |
| HCTH | 3.4657 eV  f=0.3711 | 3.4431 eV  f=0.3831 | 3.4447 eV  f=0.3430 | 3.4299 eV  f=0.3232 | 3.4425 eV  f=0.3110 |
| **TPSSTPSS** | **3.5564 eV**  **f=0.3785** | **3.5231 eV**  **f=0.3027** | **3.5468 eV**  **f=0.2635** | **3.5248 eV**  **f=0.3545** | **3.5483 eV**  **f=0.2347** |
| 𝞈B97XD | 4.1372 eV  f=0.4480 | 4.1265 eV  f=0.4795 | 4.1229 eV  f=0.4217 | 4.1137 eV  f=0.4143 | 4.1249 eV  f=0.4190 |
| APFD | 3.8756 eV  f=0.4176 | 3.8627 eV  f=0.4124 | 3.8607 eV  f=0.3229 | 3.8195 eV  f=0.2780 | 3.8615 eV  f=0.3221 |
| BhandHLYP | 4.2414 eV  f=0.4838 | 4.2240 eV  f=0.4234 | 4.2161 eV  f=0.3363 | 4.2131 eV  f=0.4477 | 4.2171 eV  f=0.3321 |
| LC-𝞈PBE | 4.2485 eV  f=0.4197 | 4.2395 eV  f=0.4503 | 4.2374 eV  f=0.4014 | 4.2280 eV  f=0.3862 | 4.2395 eV  f=0.3987 |
| M06-2X | 4.0965 eV  f=0.4723 | 4.0909 eV  f=0.5441 | 4.0824 eV  f=0.4593 | 4.0719 eV  f=0.4535 | 4.0847 eV  f=0.4542 |
| M06 | 3.8365 eV  f=0.3970 | 3.8177 eV  f=0.2605 | 3.8051 eV  f=0.2427 | 3.8009 eV  f=0.3712 | 3.8062 eV  f=0.2356 |
| **M06L** | **3.6835 eV**  **f=0.3951** | **3.6692 eV**  **f=0.3373** | **3.6732 eV**  **f=0.3683** | **3.6599 eV**  **f=0.3549** | **3.6753 eV**  **f=0.3510** |
| M06HF | 4.2852 eV  f=0.4149 | 4.2392 eV  f=0.5358 | 4.2163 eV  f=0.3506 | 4.2246 eV  f=0.4421 | 4.2150 eV  f=0.3199 |
|  | **CSM** | **DSB** | **DSD** | **DSM** | **MAD\*** |
| Expt. | 3.5587 eV | 3.5283 eV | 3.5772 eV | 3.5730 eV |  |
| LSDA | 3.3654 eV  f=0.3977 | 3.4004 eV  f=0.3335 | 3.4007 eV  f=0.3016 | 3.3713 eV  f=0.3380 | 0.1724 |
| BVP86 | 3.4025 eV  f=0.3952 | 3.4361 eV  f=0.3360 | 3.4379 eV  f=0.3129 | 3.4095 eV  f=0.3402 | 0.1372 |
| B3LYP | 3.7830 eV  f=0.3245 | 3.8046 eV  f=0.3379 | 3.8054 eV  f=0.3279 | 3.7989 eV  f=0.4076 | 0.2339 |
| CAM-B3LYP | 4.0862 eV  f=0.4763 | 4.1097 eV  f=0.4566 | 4.1112 eV  f=0.4520 | 4.0995 eV  f=0.4932 | 0.5404 |
| B3PW91 | 3.7991 eV  f=0.3660 | 3.8229 eV  f=0.3608 | 3.8238 eV  f=0.3499 | 3.8127 eV  f=0.3842 | 0.2504 |
| MPW1PW91 | 3.8928 eV  f=0.2910 | 3.9142 eV  f=0.4312 | 3.9158 eV  f=0.4253 | 3.8975 eV  f=0.3883 | 0.3448 |
| PBEPBE | 3.4007 eV  f=0.3952 | 3.4347 eV  f=0.3409 | 3.4361 eV  f=0.3137 | 3.4086 eV  f=0.3452 | 0.1387 |
| HSEH1PBE | 3.8327 eV  f=0.3869 | 3.8606 eV  f=0.3843 | 3.8617 eV  f=0.3726 | 3.8696 eV  f=0.1380 | 0.2889 |
| HCTH | 3.4283 eV  f=0.3640 | 3.4643 eV  f=0.3479 | 3.4670 eV  f=0.3276 | 3.4405 eV  f=0.3522 | 0.1101 |
| **TPSSTPSS** | **3.5159 eV**  **f=0.3871** | **3.5557 eV**  **f=0.3504** | **3.5575 eV**  **f=0.3175** | **3.5191 eV**  **f=0.2776** | **0.0326** |
| 𝞈B97XD | 4.1165 eV  f=0.4611 | 4.1393 eV  f=0.4455 | 4.1410 eV  f=0.4418 | 4.1283 eV  f=0.4775 | 0.5704 |
| APFD | 3.8572 eV  f=0.3753 | 3.8780 eV  f=0.4107 | 3.8793 eV  f=0.4014 | 3.8635 eV  f=0.3928 | 0.3046 |
| BhandHLYP | 4.2170 eV  f=0.4565 | 4.2435 eV  f=0.4725 | 4.2455 eV  f=0.4772 | 4.2247 eV  f=0.4126 | 0.6695 |
| LC-𝞈PBE | 4.2298 eV  f=0.4296 | 4.2507 eV  f=0.4173 | 4.2519 eV  f=0.4145 | 4.2416 eV  f=0.4487 | 0.6833 |
| M06-2X | 4.0794 eV  f=0.5201 | 4.0982 eV  f=0.4658 | 4.0986 eV  f=0.4488 | 4.0936 eV  f=0.5403 | 0.531 |
| M06 | 3.8152 eV  f=0.3733 | 3.8389 eV  f=0.3522 | 3.8394 eV  f=0.3784 | 3.8180 eV  f=0.2551 | 0.2623 |
| M06L | **3.6533 eV**  **f=0.3174** | **3.6833 eV**  **f=0.3873** | **3.6874 eV**  **f=0.3601** | **3.6728 eV**  **f=0.3132** | **0.1157** |
| M06HF | 4.2380 eV  f=0.5696 | 4.2861 eV  f=0.4312 | 4.2863 eV  f=0.4657 | 4.2398 eV  f=0.4831 | 0.6904 |

\*Mean absolute deviations,

Table S12. Calculated electronic transition with significant oscillator strength (*f*) of **R1IR2** (CAM-B3LYP/Def-2-TZVP).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BIB** | **BIM** | **CIB** | **CIC** | **CID** |
| **S1** | **3.9542 eV; f=0.1171** | **3.9549 eV; f=0.1207**  [H]→[L]: 96.4% | **3.9422 eV; f=0.1338**  [H]→[L]: 95.9% | **3.9325 eV; f=0.1550**  [H-5] → [L+3]: 2.7%  [H-4] → [L]: 95.5% | **3.9360 eV; f=0.1343**  [H-3] → [L+4]: 2.3%  [H-2] → [L]: 95.8% |
| **S2** | 4.3794 eV; f=0.0870 | 4.3819 eV; f=0.0768 | 4.1921 eV; f=0.0623 | 4.1919 eV; f=0.1110 | 4.1916 eV; f=0.0624 |
|  | **CIM** | **DIB** | **DID** | **DIM** |  |
| **S1** | **3.9455 eV; f=0.1381**  [H-3] → [L+2]: 2.8%  [H-2] → [L]: 96.0% | **3.9526 eV; f=0.1163**  [H]→[L]: 96.2% | **3.9472 eV; f=0.1153**  [H]→[L]: 96.1% | **3.9499 eV; f=0.1216**  [H-1] → [L+3]: 2.2%  [H]→[L]: 96.3% |  |
| **S2** | 4.1923 eV; f=0.0613 | 4.3787 eV; f=0.0922 | 4.3779 eV; f=0.0958 | 4.3806 eV; f=0.0815 |  |

Table S13. Calculated electronic transition with significant oscillator strength (*f*) of **R1IR2** (TPSSTPSS/6-31+G(2d,p)).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BSB** | **BSM** | **CSB** | **CSC** | **CSD** |
| **S1** | 3.4480 eV; f=0.0379 | 3.4359 eV; f=0.0100 | 2.7423 eV; f=0.0011 | 2.7811 eV; f=0.0012 | 2.7313 eV; f=0.0011 |
| **S2** | 3.5150 eV; f=0.0636 | 3.5064 eV; f=0.2238 | 3.2048 eV; f=0.0000 | 2.7837 eV; f=0.0009 | 3.1943 eV; f=0.0000 |
| **S3** | **3.5516 eV; f=0.3909**  [H-2] → [L]:13.5%  [H-1] → [L]:75.5%  [H] → [L+1]:2.5%  [H] → [L+6]:3.3% | **3.5387 eV; f=0.2849**  [H-2] → [L]:9.5%  [H-1] → [L]:81.9%  [H] → [L+3]:3.9% | 3.4190 eV; f=0.0563 | 3.2454 eV; f=0.0000 | 3.2845 eV; f=0.0000 |
| **S4** | 3.9183 eV; f=0.0001 | 3.8746 eV; f=0.0099 | 3.5034 eV; f=0.0861 | 3.2454 eV; f=0.0000 | 3.3404 eV; f=0.0000 |
| **S5** |  |  | 3.5278 eV; f=0.0581 | 3.2821 eV; f=0.0000 | 3.4250 eV; f=0.0604 |
| **S6** |  |  | **3.5380 eV; f=0.2761**  [H-4] → [L]: 13.6%  [H-2] → [L]: 60.1%  [H-1] → [L]:2.0%  [H-1] → [L+4]: 2.8%  [H] → [L+2]: 13.8% | 3.2821 eV; f=0.0000 | 3.4597 eV; f=0.0007 |
| **S7** |  |  | 3.5432 eV; f=0.0490 | 3.3894 eV; f=0.0614 | 3.5011 eV; f=0.0894 |
| **S8** |  |  |  | 3.4972 eV; f=0.0746 | 3.5300 eV; f=0.0647 |
| **S9** |  |  |  | 3.5142 eV; f=0.0633 | **3.5401 eV; f=0.2707**  [H-4] → [L]:15.1%  [H-2] → [L]:66.7%  [H-2] → [L+2]:2.6%  [H-1] → [L+5]:4.8%  [H] → [L+1]:3.0% |
| **S10** |  |  |  | 3.5147 eV; f=0.0259 | 3.6199 eV; f=0.0218 |
| **S11** |  |  |  | **3.5193 eV; f=0.3039**  [H-6] → [L]:21.5%  [H-3] → [L]:61.0%  [H-2] → [L+2]:3.1%  [H-2] → [L+3]:4.8%  [H-1] → [L+1]:2.6%  [H] → [L+2]:2.5% |  |
| **S12** |  |  |  | 3.5641 eV; f=0.0002 |  |
|  | **CSM** | **DSB** | **DSD** | **DSM** |  |
| **S1** | 2.7856 eV; f=0.0011 | 3.4523 eV; f=0.0393 | 3.4570 eV; f=0.0464 | 3.4413 eV; f=0.0103 |  |
| **S2** | 3.2493 eV; f=0.0000 | 3.5063 eV; f=0.0599 | 3.5053 eV; f=0.0597 | 3.5023 eV; f=0.2185 |  |
| **S3** | 3.4044 eV; f=0.0243 | **3.5500 eV; f=0.3605**  [H-2] → [L]:13.4%  [H-1] → [L]: 71.7%  [H] → [L+1]:3.7%  [H-2] → [L+7]:2.3% | **3.5528 eV; f=0.3145**  [H-2] → [L]:16.5%  [H-1] → [L]: 64.3%  [H-1] → [L+2]:2.2%  [H] → [L+1]:9.4%  [H] → [L+7]:9.4% | **3.5411 eV; f=0.2505**  [H-2] → [L]:10.7%  [H-1] → [L]: 76.9%  [H] → [L+4]:5.1% |  |
| **S4** | **3.5020 eV; f=0.2911**  [H-2] → [L]:32.1%  [H-2] → [L+2]:2.3%  [H-1] → [L]:56.5%  [H-1] → [L+2]:2.4%  [H] → [L+1]:2.6% | 3.6781 eV; f=0.0346 | 3.6855 eV; f=0.0750 | 3.6219 eV; f=0.0176 |  |
| **S5** | 3.5144 eV; f=0.0239 |  |  |  |  |

Table S14. Calculated natural orbitals (NTOs) of **R1SR2** for most excitation channels.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **BSB** | **BSM** | **CSB** | **CSC** | **CSD** |
| LUTO |  |  |  |  |  |
| HOTO |  |  |  |  |  |
|  | S0 → S3 | S0 → S3 | S0 → S6 | S0 → S11 | S0 → S9 |
|  | **CSM** |  | **DSB** | **DSD** | **DSM** |
| LUTO |  |  |  |  |  |
| HOTO |  |  |  |  |  |
|  | S0 → S4 |  | S0 → S3 | S0 → S3 | S0 → S3 |

* 1. **Bacterial experiments results**

|  |  |
| --- | --- |
| a) | b) |

Figure S52. The CFU percentage of bacteria in the presence of (a) **BIB** and (b) **BSB** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S53. The CFU percentage of bacteria in the presence of (a) **BIM** and (b) **BSM** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S54. The CFU percentage of bacteria in the presence of (a) **CIB** and (b) **CSB** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S55. The CFU percentage of bacteria in the presence of (a) **CIC** and (b) **CSC** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S56. The CFU percentage of bacteria in the presence of (a) **CID** and (b) **CSD** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S57. The CFU percentage of bacteria in the presence of (a) **CIM** and (b) **CSM** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S58. The CFU percentage of bacteria in the presence of (a) **DIB** and (b) **DSB** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S59. The CFU percentage of bacteria in the presence of (a) **DID** and (b) **DSD** (1 – 128 µM).

|  |  |
| --- | --- |
| a) | b) |

Figure S60. The CFU percentage of bacteria in the presence of (a) **DIM** and (b) **DSM** (1 – 128 µM).

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