Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supporting Information

Enhancing the binding of calix[5]arene containers for ferrocenes by fluorophobic effect through the release of high-energy perfluoro-1-iodoalkanes

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General experimental details

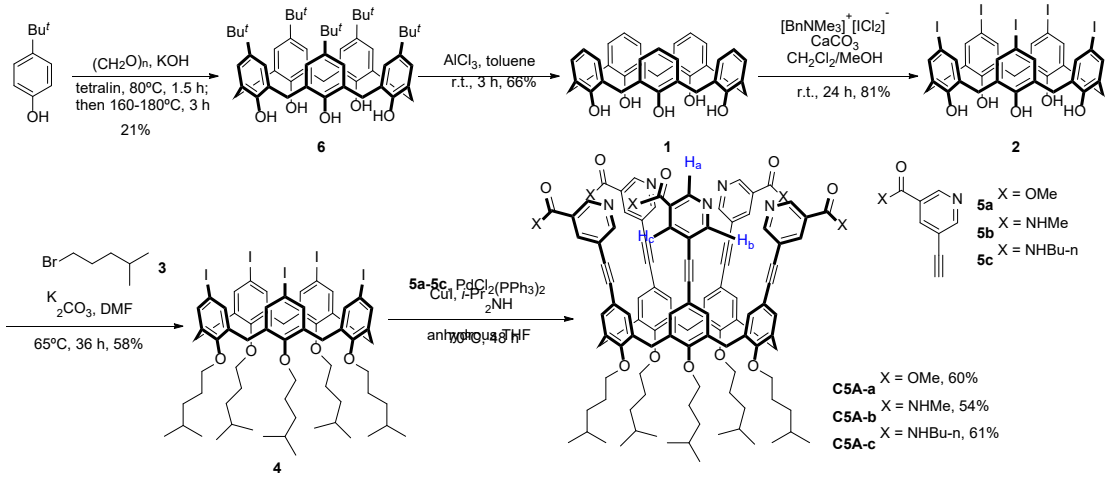
Materials

Chemical reagents and most solvents were purchased from commercial sources and were directly used without further pretreatment. Perfluoro-1-iodohexane (PFIH), perfluoro-1-iodobutane (PFIB) and perfluoro-1-iodooctane (PFIO) are treated with anhydrous sodium sulfite to remove iodine in the solvent, and then dried with anhydrous sodium sulfate.

Methods

Nuclear magnetic resonance (NMR) spectra were recorded using Bruker AVANCE III 400 spectrometer and Bruker AVANCE III HD 500 MHz spectrometer. High-resolution mass spectra (HRMS) were recorded on Fourier transform ion cyclotron resonance mass spectrometry. Single crystal suitable for X-ray diffraction was obtained by slow vapor diffusion of methanol into the DMF solution of **C5A-a**. Single-crystal X-ray diffraction data were collected at low temperature (173 K) on a Bruker D8 VENTURE Metaljet liquid metal X-ray source system (GaKα, λ = 1.34138 Å). The theoretical studies of **C5A-c** and **C5A-c•G-a** by PM6D3 computations were carried out using Gaussian 09 software package.[S1,S2] The solvent model SMD (chloroform) was used in geometry optimization and frequency calculations. The fluorescence experiments were performed on Agilent Cary Eclipse Fluorescence Spectrophotometer. The binding constant K_a was fitted using Bindfit software.[S3]

Synthesis procedure



Scheme S1. Synthesis of Compound **C5A-a~c**.

Compound **6**:

4-tert-butylphenol (25.0 g, 166.4 mmol) and paraformaldehyde (16.7 g, 556.1 mmol) were placed in a 3-necked round bottom flask that connected with thermometer, condenser and a Dean-Stark receiver (In this experiment, it is best to use flask heating sleeve for heating and the temperature here refers to the internal temperature). 1,2,3,4-tetrahydronaphthalene (350 mL) was added. Then LiOH aqueous solution (1.2 g, 50.4 mmol in 10 mL H_2O) was added under the protection of nitrogen, and reacted at 80°C for 1.5h, the solution became light brown. Rapidly raised the temperature to 180°C, and kept the system at this temperature for 10 minutes (Water was collected with the Dean-Stark receiver. In the meanwhile, nitrogen gas was injected to remove as much excess water as possible). Then the temperature in the bottle was lowered to 160°C, and the mixture was stirred at this temperature for 3 hours. After cooling to room

temperature, the mixture was filtered and collected the filtrate. The liquid was removed under reduced pressure, 90 mL of chloroform and 45 mL of 1 M hydrochloric acid solution were added, and the mixture was stirred for half an hour. The organic phase was extracted with separatory funnel, washed with water three times and dried with anhydrous sodium sulfate. The liquid was removed in vacuo, then the solid was dispersed in 100 mL ethanol and stirred for 1 hour to remove the remaining 1,2,3,4-tetrahydronaphthalene. The mixture was cooled in the refrigerator, and filtered the solid after precipitation. The resulting solid was dried to remove ethanol. Then 160 mL acetone was added to reflux for 30 min, and the insoluble impurities were removed by hot filtration. The filtrate was concentrated to about 70 mL and then placed in a refrigerator for cooling and crystallization. The resulting solids are filtered, and the filtrate is further concentrated and placed in the refrigerator for recrystallization, repeating this step three times. The solid were dried under high vacuum and a white powder is obtained (5.7 g, 21%).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (s, 5H), 7.20 (s, 10H), 3.82 (s, 10H), 1.18 (s, 45H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.60, 144.01, 126.27, 125.66, 33.90, 31.58, 31.45. The data was consistent with the reported values.[S4]

Compound **1**:

Compound **6** (4.1 g, 5.1 mmol) was dissolved in 80 mL of anhydrous toluene. $AlCl_3$ (6.6 g., 49.6 mmol) was added in portions under the nitrogen atmosphere. The mixture was stirred for 3 h at room temperature. Then the solution was quenched with water (150 mL) and stirred for 20 min. The organic phase was extracted, washed with water and dried with anhydrous Na_2SO_4. After that, the solvent was removed at reduced pressure. The residue was dispersed in ether and stirred for half an hour, filtered to obtain the solid. Then the solid was dispersed in acetone and refluxed for 1 h. After cooling to room temperature, a white powder (1.7 g, 66%) was obtained after filtering and drying. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (s, 5H), 7.11 (d, J = 7.5 Hz, 10H), 6.70 (t, J = 7.5 Hz, 5H), 3.84 (s, 10H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.01, 129.19, 126.72, 121.60, 31.31. The data as consistent with the reported values.[S5]

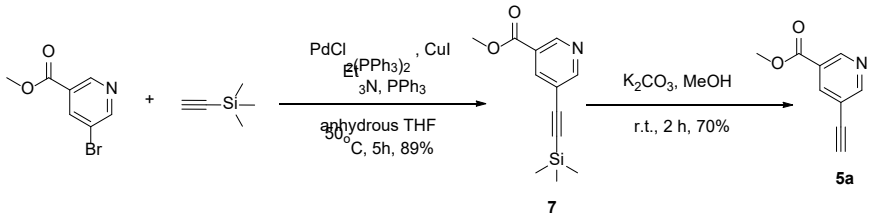
Compound **2**:

Compound **1** (300 mg, 0.6 mmol) and benzyltrimethylammonium dichloroiodate (1082 mg, 3.2 mmol) were dissolved in 30 mL of CH_2Cl_2 under a nitrogen atmosphere. The mixture was stirred for 30 min at room temperature. 12 mL of MeOH was added and continued to stir for 30 min. Then $CaCO_3$ (584 mg, 5.8 mmol) was added and the suspension was stirred for 24 h. Then 2 mL of 12 M hydrochloric acid, 60 mL of MeOH and 40 mL of 5% $NaHSO_3$ aqueous solution were added and the mixture was stirred for 30 min. The solid was filtered then washed with H_2O and MeOH. The product was vacuum-dried and obtained as yellow solid (532.8 mg, 81%). The reaction can be monitored by TLC ($CHCl_3$: Hexane = 1 : 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 5H), 7.50 (s, 10H), 3.74 (s, 10H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.01, 138.02, 128.30, 84.15, 30.50. HR ESI-MS: Calculated for $C_{35}H_{25}O_5I_5Na^+$ [M + Na^+]: 1182.6823, found: 1182.6820.

Compound **4**:

Compound **2** (300 mg, 0.3 mmol) and 1-bromo-4-methylpentane (854 mg, 5.2 mmol) were dissolved in 15 mL of DMF. K_2CO_3 (1073 mg, 7.8 mmol) was added under a nitrogen atmosphere. The mixture was stirred at 65°C for 36 h (The reaction can be monitored by TLC (DCM : Hexane = 1: 1). Appropriate amount of hydrochloric acid was added to neutralize K_2CO_3. The solvent was removed at reduced pressure. Then 80 mL of DCM was added. The mixture was washed with H_2O (20 mL × 3) and saturated NH_4Cl aqueous solution before being dried over anhydrous $MgSO_4$. The crude product was separated by column chromatography (DCM : Hexane = 1 : 5) and the product was obtained as white solid (236 mg,

58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (s, 10H), 4.39 (d, *J* = 14.4 Hz, 5H), 3.72 (t, *J* = 7.6 Hz, 10H), 3.24 (d, *J* = 12.0 Hz, 5H), 1.80 (m, 10H), 1.64–1.56 (m, 5H), 1.28–1.22 (m, 10H), 0.93 (d, *J* = 6.5 Hz, 30H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.00, 137.48, 135.95, 87.33, 74.03, 35.02, 29.56, 28.01, 27.92, 22.63. HR ESI-MS: Calculated for $C_{65}H_{85}O_5I_5Na^+$ [M + Na^+]: 1603.1519, found: 1603.1523.



Scheme S2. Synthesis of **5a**.

Compound **7**:

Methyl 5-bromonicotinate (2.5 g, 11.6 mmol), $PdCl_2(PPh_3)_2$ (39 mg, 0.056 mmol) and PPh_3 (30 mg, 0.11 mmol) were dissolved in 25 mL of anhydrous THF and 13 mL of NEt_3 under a nitrogen atmosphere. Then CuI (22 mg, 0.12 mmol) and trimethylsilylacetylene (1.8 mL, 12.7 mmol) were added. The mixture was stirred at 50°C for 5 h. After cooling to the room temperature, the mixture was filtered with diatomaceous earth. The filtrate was concentrated and separated by column chromatography (Hexane : EA = 100 : 1). The product was obtained as white solid (2.4 g, 89%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.05 (d, *J* = 2.0 Hz, 1H), 8.88 (d, *J* = 2.0 Hz, 1H), 8.27 (q, *J* = 2.1 Hz, 1H), 3.90 (s, 3H), 0.27 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.76, 155.74, 149.58, 139.47, 125.75, 119.76, 100.85, 99.84, 53.04, 0.00. The data was consistent with the reported values.[S6]

Compound **5a**:

Compound **7** (1.9 g, 7.9 mmol) was dissolved in 15 mL of MeOH. Then K_2CO_3 (1.1 g, 7.9 mmol) was added under a nitrogen atmosphere. The mixture was stirred at room temperature for 2 h and filtered. The filtrate was concentrated and separated by column chromatography (Hexane : EA = 10 : 1). The product was obtained as white solid (0.9 g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (d, *J* = 2.0 Hz, 1H), 8.88 (d, *J* = 2.1 Hz, 1H), 8.42 (t, *J* = 2.0 Hz, 1H), 4.00 (s, 3H), 3.32 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.89, 155.84, 149.83, 140.10, 125.62, 119.36, 81.79, 79.20, 52.63. The data as consistent with the reported values.[S6]

Compound **5b**:

Compound **5a** (300 mg, 1.86 mmol) was dissolved in 20 mL of methylamine solution (2.0 M in methanol) under a nitrogen atmosphere. The mixture was stirred at room temperature for 3 h. Then the solvent was removed by rotary evaporation. The product was separated by column chromatography (DCM : MeOH = 20 : 1) and obtained as white solid (275 mg, 92%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.97 (d, *J* = 2.0 Hz, 1H), 8.80 (d, *J* = 1.9 Hz, 1H), 8.71 (s, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 4.54 (s, 1H), 2.81 (d, *J* = 4.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.40, 154.71, 147.02, 138.02, 129.81, 119.48, 81.83, 79.40, 26.97. HR APGC-MS: Calculated for $C_9H_9N_2O^+$ [M + H^+]:161.0715, found: 161.0711.

Compound **5c**:

Compound **5a** (200 mg, 1.86 mmol) was dissolved in 10 mL of *n*-butylamine solution (2.0 M in methanol) under a nitrogen atmosphere. The mixture was stirred at room temperature for 3 h. Then the solvent was removed by rotary evaporation. The product was separated by column chromatography (Hexane : EA = 5 : 1) and obtained as white solid (223 mg, 89%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (d, *J* = 2.1 Hz, 1H), 8.82 (d, *J* = 2.0 Hz, 1H), 8.22 (d, *J* = 2.1 Hz, 1H), 6.25 (s, 1H), 3.51 (td, *J* = 7.2, 5.6 Hz, 2H), 3.31 (s, 1H), 1.72–1.58 (m, 2H), 1.50–1.41 (m, 2H), 1.00 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 164.69, 154.54, 147.01, 138.07, 130.07, 119.46, 81.83, 79.40, 40.04, 31.59, 20.13, 13.73. HR APGC-MS: Calculated for $C_{12}H_{15}N_2O^+$ [M + H$^+$]: 203.1184, found: 203.1182.

Compound **C5A-a**:

Compound **4** (100.0 mg, 0.06 mmol) and $PdCl_2(PPh_3)_2$ (22.3 mg, 0.03 mmol) were dissolved in 5 mL of anhydrous THF and 5 mL of *i*-Pr_2NH under a nitrogen atmosphere. The mixture was degassed with nitrogen for 30 min. After that, CuI (6.1 mg, 0.03 mmol) was added. Then compound **5a** (76 mg, 0.47 mmol in 5 mL of anhydrous THF) was added with constant pressure drop funnel. The mixture was stirred at 70°C for 48 h. After cooling to the room temperature, the mixture was filtered. The filtrate was concentrated and separated by column chromatography (CH_2Cl_2 : MeOH = 50 : 1). The product was obtained as yellow solid (66.5 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (brs, 5H), 8.76 (brs, 5H), 8.18 (s, 5H), 7.19 (s, 10H), 4.57 (d, *J* = 12.0 Hz, 5H), 3.91 (s, 15H), 3.83 (t, *J* = 7.6 Hz, 10H), 3.37 (d, *J* = 14.5 Hz, 5H), 1.93–1.82 (m, 10H), 1.68–1.56 (m, 5H), 1.35–1.26 (m, 10H), 0.96 (d, *J* = 6.6 Hz, 30H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.14, 156.23, 155.20, 148.78, 138.89, 134.24, 132.31, 125.58, 120.83, 116.75, 93.95, 84.17, 74.25, 52.47, 35.12, 30.06, 28.09, 22.70. HR ESI-MS: Calculated for $C_{110}H_{116}N_5O_{15}^+$ [M + H$^+$]: 1746.8468, found: 1746.8480.

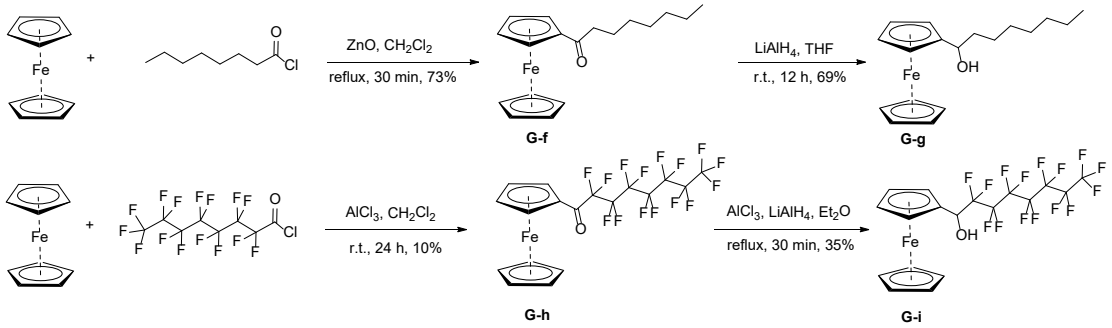
Compound **C5A-b**:

Compound **4** (100.0 mg, 0.06 mmol) and $PdCl_2(PPh_3)_2$ (22.3 mg, 0.03 mmol) were dissolved in 5 mL of anhydrous THF and 5 mL of *i*-Pr_2NH under a nitrogen atmosphere. The mixture was degassed with nitrogen for 30 min. After that, CuI (6.1 mg, 0.03 mmol) was added. Then compound **5b** (76 mg, 0.47 mmol in 5 mL of anhydrous THF) was added with constant pressure drop funnel. The mixture was stirred at 70°C for 48 h. After cooling to the room temperature, the mixture was filtered. The filtrate was concentrated and separated by column chromatography (CH_2Cl_2 : MeOH = 20 : 1). The product was obtained as white solid (60.0 mg, 54%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (brs, 5H), 8.63 (brs, 5H), 8.26 (brs, 5H), 7.20 (brs, 10H), 4.57 (d, *J* = 12.0 Hz, 5H), 3.87 (s, 10H), 3.41 (s, 5H), 2.90 (brs, 15H), 1.91 (CH_2 was covered by water), 1.67–1.60 (m, 5H), 1.36–1.28 (m, 10H), 0.97 (d, *J* = 6.5 Hz, 30H). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.77 (d, *J* = 2.1 Hz, 5H), 8.65 (d, *J* = 2.0 Hz, 5H), 8.50 (q, *J* = 4.5 Hz, 5H), 8.12 (t, *J* = 2.1 Hz, 5H), 7.27 (s, 10H), 4.44 (d, *J* = 12.0 Hz, 5H), 3.82 (t, *J* = 7.3 Hz, 10H), 3.52 (d, *J* = 14.2 Hz, 5H), 2.73 (d, *J* = 4.5 Hz, 15H), 1.91–1.81 (m, 10H), 1.65-1.54 (m, 5H), 1.35–1.27 (m, 10H), 0.92 (d, *J* = 6.5 Hz, 30H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.50, 156.38, 153.45, 147.69, 136.91, 134.90, 132.52, 129.58, 119.50, 116.59, 93.51, 85.35, 74.36, 35.12, 29.28, 28.06, 26.62, 22.96. HR ESI-MS: Calculated for $C_{110}H_{121}N_{10}O_{10}^+$ [M + H$^+$]: 1741.9268, found: 1741.9264.

Compound **C5A-c**:

Compound **4** (100 mg, 0.06 mmol) and $PdCl_2(PPh_3)_2$ (22.3 mg, 0.03 mmol) were dissolved in 5 mL of anhydrous THF and 5 mL of *i*-Pr_2NH under a nitrogen atmosphere. The mixture was degassed with nitrogen for 30 min. After that, CuI (6.1 mg, 0.03 mmol) was added. Then compound **5c** (95.9 mg, 0.47 mmol in 5 mL of anhydrous THF) was added with constant pressure drop funnel. The mixture was stirred at 70°C for 48 h. After cooling to the room temperature, the mixture was filtered. The filtrate was concentrated and separated by column chromatography (CH_2Cl_2 : MeOH = 50 : 1). The product was obtained as yellow solid (75.6 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 5H), 8.64 (s, 5H), 7.96 (s, 5H), 7.17 (s, 10H), 6.91 (s, 5H), 4.57 (d, *J* = 12.0 Hz, 5H), 3.84 (t, *J* = 7.6 Hz, 10H), 3.47–3.37 (m, 15H), 1.92–1.83 (m, 10H), 1.65–1.59 (m, 15H), 1.46–1.38 (m, 10H), 1.37–1.28 (m, 10H), 0.98–0.95 (m, 45H). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.77 (s, 5H), 8.62 (s, 5H), 8.46 (t, *J* = 5.5 Hz, 5H), 8.14 (s, 5H), 7.26 (s, 10H), 4.43 (d, *J* = 12.0 Hz, 5H), 3.80 (t, *J* = 7.5 Hz, 10H), 3.50 (d, *J* = 14.0 Hz, 5H), 3.18 (q, *J* = 5.5 Hz, 10H), 1.92–1.79 (m, 10H), 1.64–1.53 (m, 5H), 1.47–1.38 (m, 10H), 1.32–1.22 (m, 20H), 0.91 (d,

J = 6.6 Hz, 30H), 0.80 (t, J = 7.3 Hz, 15H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.86, 156.33, 153.32, 147.80, 136.86, 134.88, 132.48, 129.63, 119.35, 116.55, 93.43, 85.37, 74.34, 35.07, 31.33, 29.18, 28.04, 28.01, 22.93, 20.00, 14.02. HR ESI-MS: Calculated for $C_{125}H_{151}N_{10}O_{10}^+$ [M + H$^+$]: 1952.1615, found: 1952.1610.



Scheme S3. Synthesis of **G-f~i**.

Compound **G-f**:

A solution of ferrocene (0.47 g, 2.5 mmol) in CH_2Cl_2 (5 mL) was added in a suspension of ZnO (0.25 g, 3.0 mmol) in CH_2Cl_2 (5 mL). The mixture was stirred and refluxed. Octanoyl chloride (1.30 g, 8.0 mmol) was added dropwise and reacted for 30 min. The resulting solution was poured into ice water. Organic layer was separated, aqueous phase was extracted with CH_2Cl_2. Organic fractions were combined and dried over $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified by column chromatography (hexane : EA = 20 : 1) to afford brown liquid (0.57 g, 73%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.77 (s, 2H), 4.53 (s, 2H), 4.20 (s, 5H), 2.70 (t, J = 7.2 Hz, 2H), 1.62–1.43 (m, 4H), 1.34–1.17 (m, 6H), 0.85 (t, J = 6.2 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 203.85, 79.64, 72.42, 69.95, 69.51, 39.19, 31.71, 29.26, 29.11, 24.45, 22.55, 14.43. The data was consistent with the reported values.[S7]

Compound **G-g**:

A suspension of $LiAlH_4$ (0.15 g, 3.8 mmol) in anhydrous THF (5 mL) was cooled to -78℃. A solution of compound **G-f** (1.50 g, 5.0 mmol) in anhydrous THF (15 mL) was added dropwise and reacted at room temperature for 1 h. Then the solution was cooled to -78 ºC and more $LiAlH_4$ (0.055 g, 1.5 mmol) was added. The mixture was stirred at room temperature for 12 h. The resulting solution was poured into ice water. Organic layer was separated, aqueous phase was extracted with CH_2Cl_2. Organic fractions were combined and dried over $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified by column chromatography (hexane : EA = 20 : 1) to afford yellow liquid (1.04 g, 69%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.48 (d, J = 5.8 Hz, 1H), 4.28–4.22 (m, 1H), 4.18–4.15 (m, 1H), 4.12 (s, 4H), 4.10–4.08 (m, 1H), 4.06–4.03 (m, 2H), 1.66–1.54 (m, 1H), 1.54–1.36 (m, 2H), 1.36–1.18 (m, 10H), 0.85 (t, J = 6.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 94.49, 68.71, 68.43, 67.27, 67.23, 66.90, 66.15, 38.43, 31.77, 29.49, 29.28, 26.14, 22.59, 14.45. The data was consistent with the reported values.[S8]

Compound **G-h**:

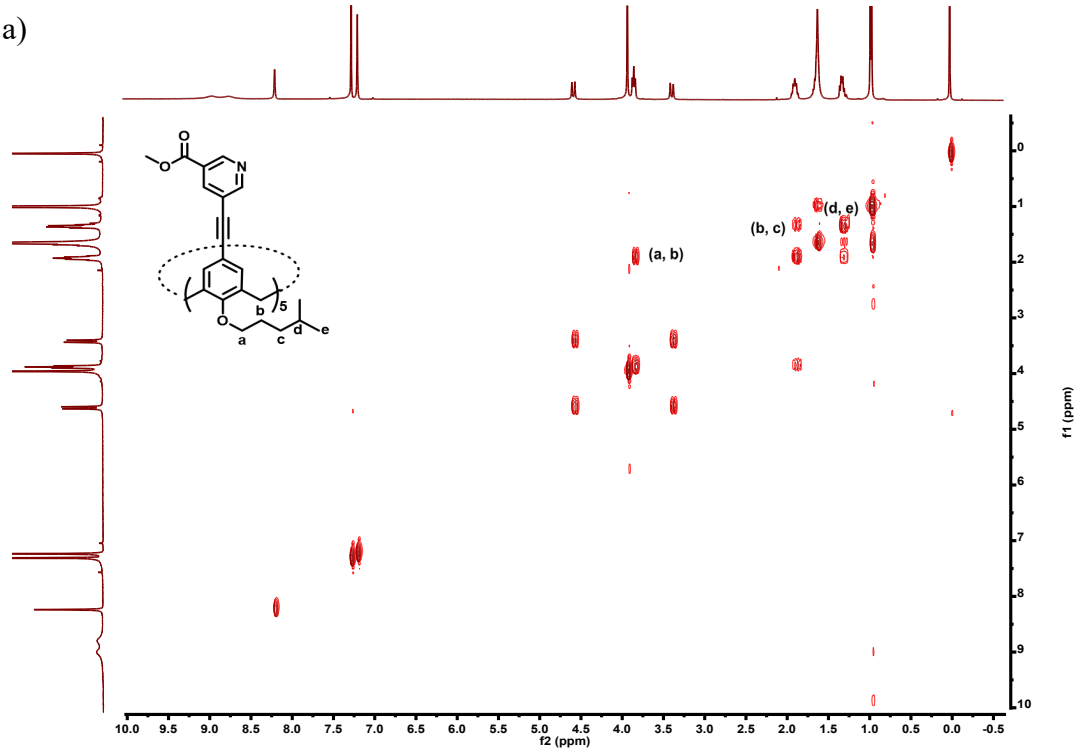
A solution of pentadecafluorooctanoyl chloride (2.32 g, 5.37 mmol) in CH_2Cl_2 (5 mL) was added in portions to a suspension of $AlCl_3$ (716.7 mg, 5.37 mmol) in CH_2Cl_2 (5 mL). The mixture was stirred at 0ºC for 10 min under a nitrogen atmosphere. Then ferrocene (1.0 g, 5.37 mmol) was added in portions. The reaction mixture was stirred at room temperature for 24 h. The resulting solution was quenched with water. Organic layer was separated, aqueous phase was extracted with hexane. Organic fractions were combined and dried over $MgSO_4$. The solvent was removed under reduced pressure and the residue was

purified by column chromatography (hexane : CH_2Cl_2 = 10 : 1) to afford red liquid (324 mg, 10%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.01 (brs, 2H), 4.79 (t, *J* = 2.0 Hz, 2H), 4.33 (s, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.49, 121.45, 118.59, 115.72, 113.38, 111.03, 110.70, 108.22, 74.54, 72.56, 70.99, 70.62. ^{19}F NMR (376 MHz, $CDCl_3$) δ –80.85 (t, *J* = 7.5 Hz, 3F), –113.72 (t, *J* = 13.1 Hz, 2F), –121.02 ~ –121.33 (m, 4F), –122.00 (brs, 2F), –122.72 (brs, 2F), –126.09 ~ –126.24 (m, 2F). HR ESI-MS: Calculated for $C_{18}H_{10}F_{15}FeO^+$ [M + H$^+$]:582.9842, found: 582.9842.

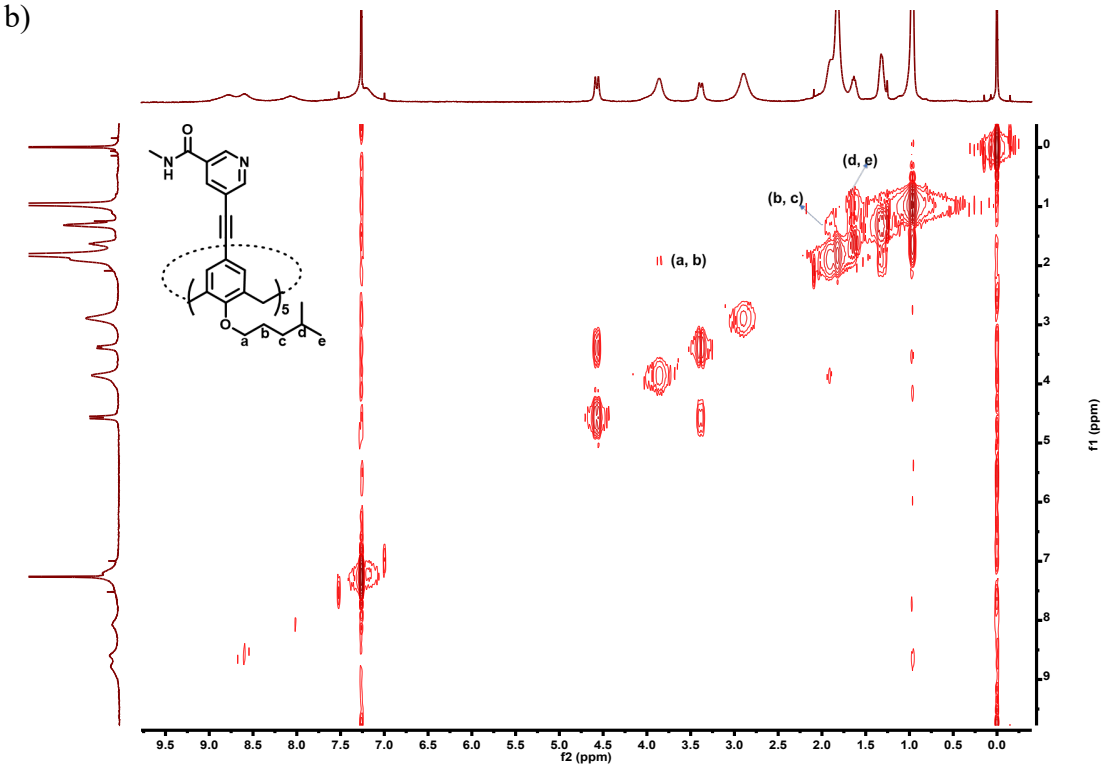
Compound **G-i**:

$AlCl_3$ (99.6 mg, 0.75 mmol) was added to a stirred suspension of $LiAlH_4$ (28.4 mg, 0.75 mmol) in 6 mL of dry Et_2O. The mixture was stirred for 10 min. A solution of compound **G-h** (217.4 mg, 0.37 mmol) in 4 mL of dry Et_2O was added dropwise. The reaction mixture was refluxed for 30 min, and 2 mL of ice water and 2 mL of ice 3 M HCl were added. The mixture was extracted with Et_2O, organic fractions were collected, washed with water, and dried over $MgSO_4$. The product was separated by column chromatography (Hexane : CH_2Cl_2 = 10 : 1) and obtained as yellow solid (76.9 mg, 35%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.51 (d, *J* = 8.2 Hz, 1H), 5.00–4.92 (m, 1H), 4.36 (s, 1H), 4.31 (s, 1H), 4.23 (s, 5H), 4.20–4.16 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 69.21, 68.77, 68.27, 66.96. ^{19}F NMR (376 MHz, DMSO-d_6) δ –80.17 (t, *J* = 9.8 Hz, 3F), –120.00 (AB, J_{AB} = 270.7 Hz, 2F), –120.16 ~ –121.74 (m, 6F), –124.11 (AB, J_{AB} = 90.2 Hz, 4F). HR ESI-MS: Calculated for $C_{18}H_{11}F_{15}FeO^+$ [M$^+$]: 583.9920, found: 583.9920.

a)



b)



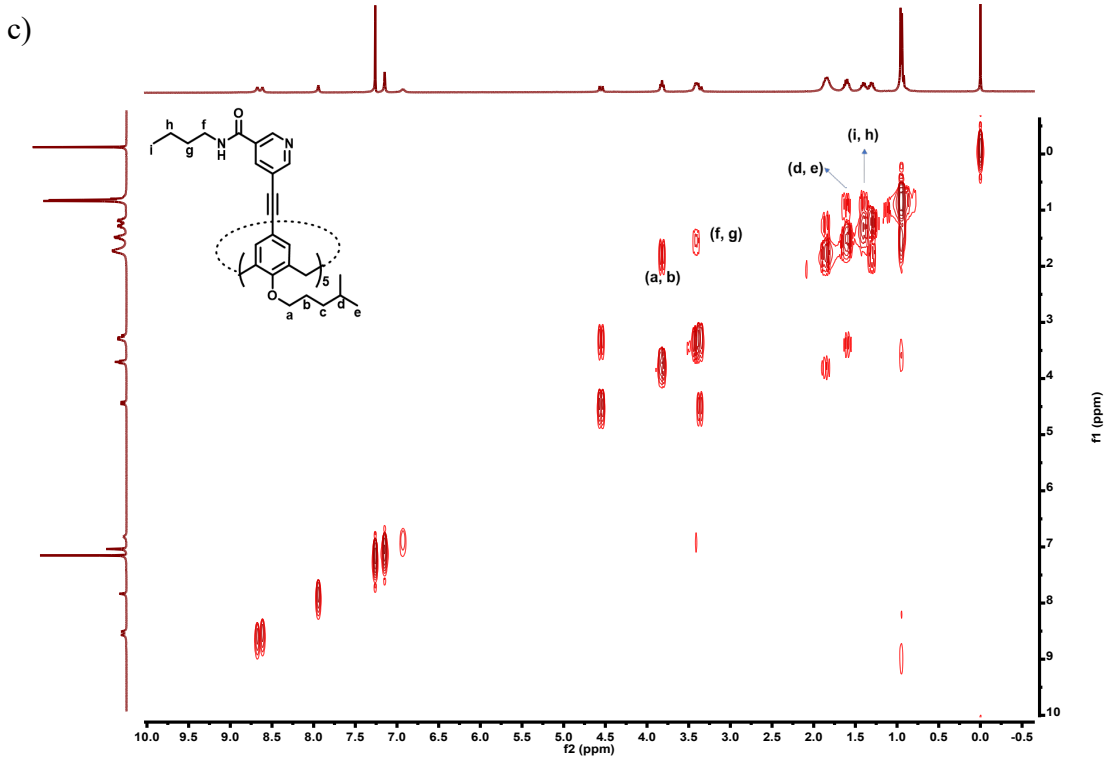


Fig. S1 2D ^{1}H COSY spectrum (400 MHz, $CDCl_3$, 298 K) of a) **C5A-a**, b) **C5A-b** and c) **C5A-c**.

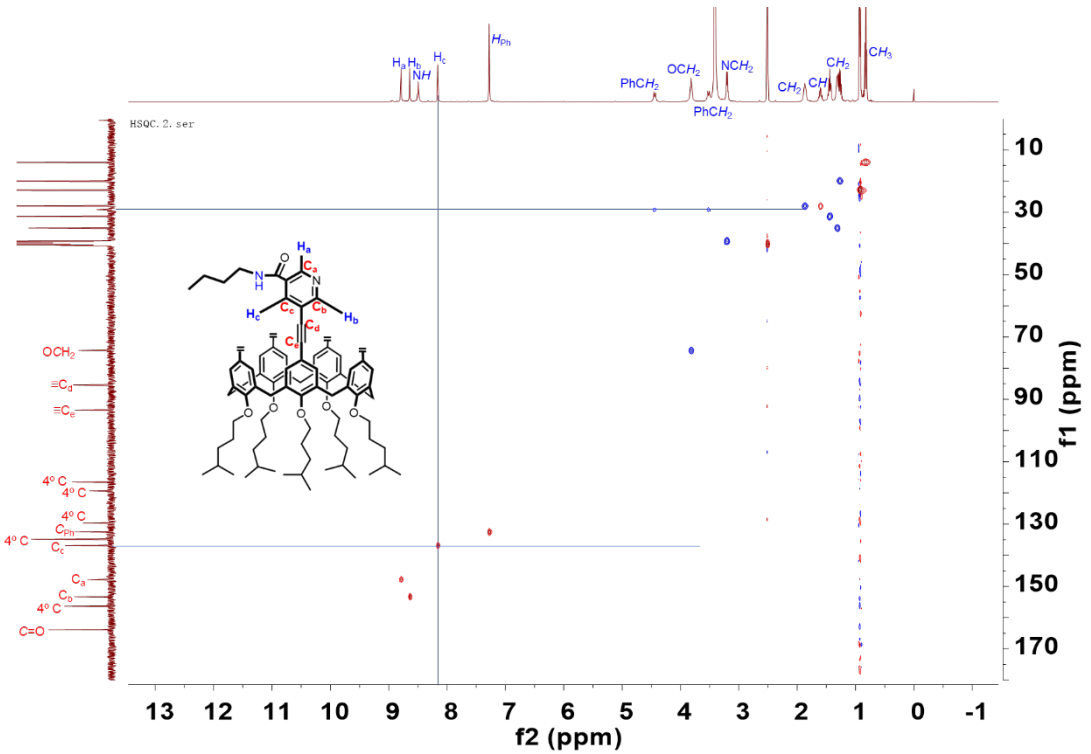


Fig. S2 HSQC spectrum (500 MHz, DMSO-d_6, 298 K) of **C5A-c**.

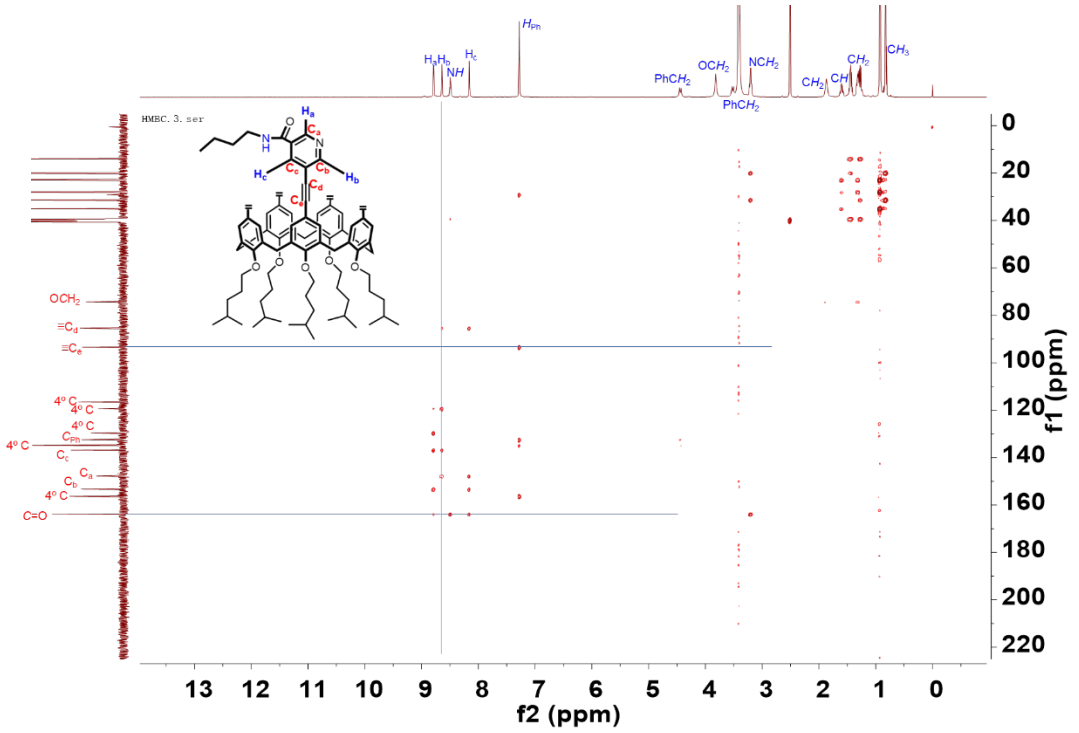


Fig. S3 HMBC spectrum (500 MHz, DMSO-d_6, 298 K) of **C5A-c**.

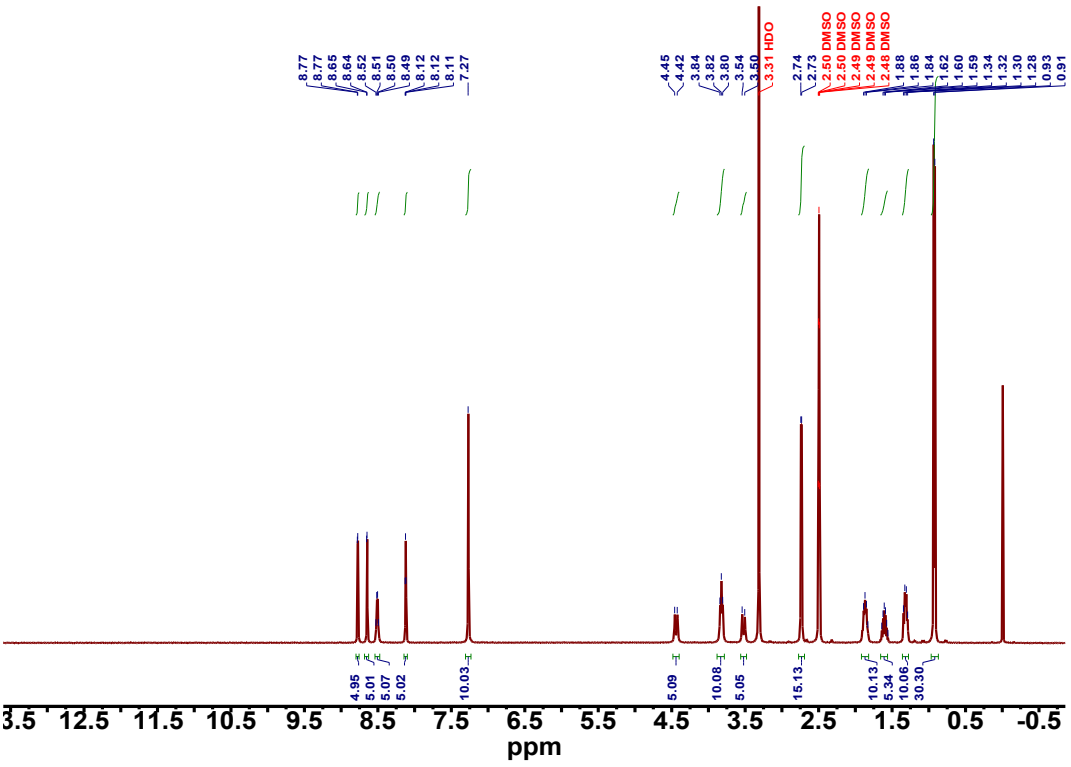


Fig. S4 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **C5A-b**.

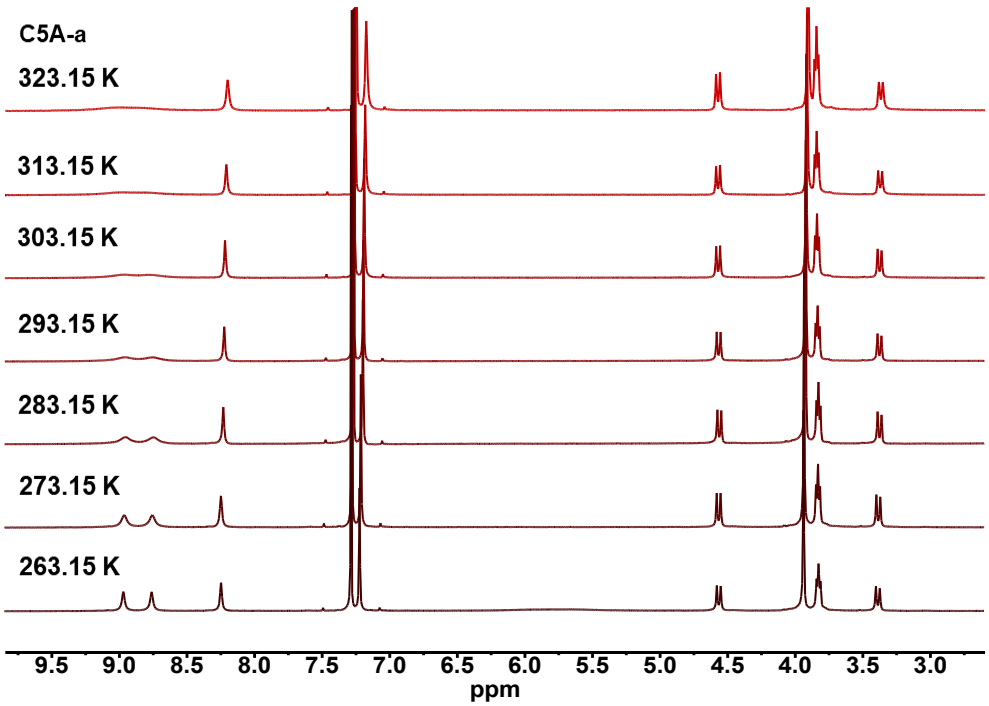


Fig. S5 Downfield region of the ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **C5A-a** at different temperatures ([**C5A-a**] = 1.0 mM).

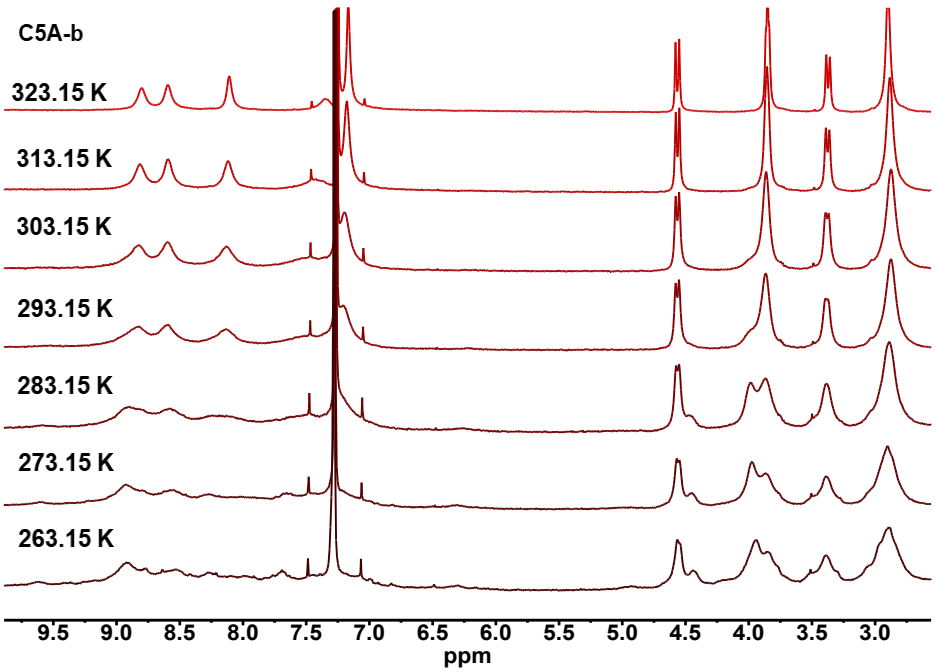


Fig. S6 Downfield region of the ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **C5A-b** at different temperatures ([**C5A-b**] = 1.0 mM).

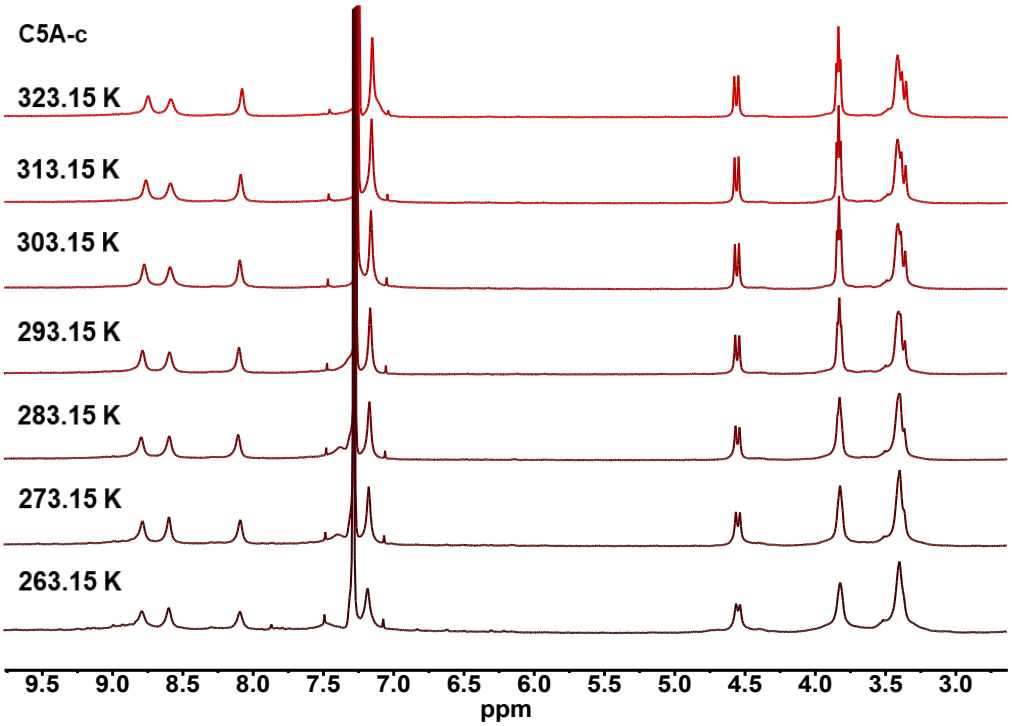


Fig. S7 Downfield region of the ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **C5A-c** at different temperatures ([**C5A-c**] = 1.0 mM).

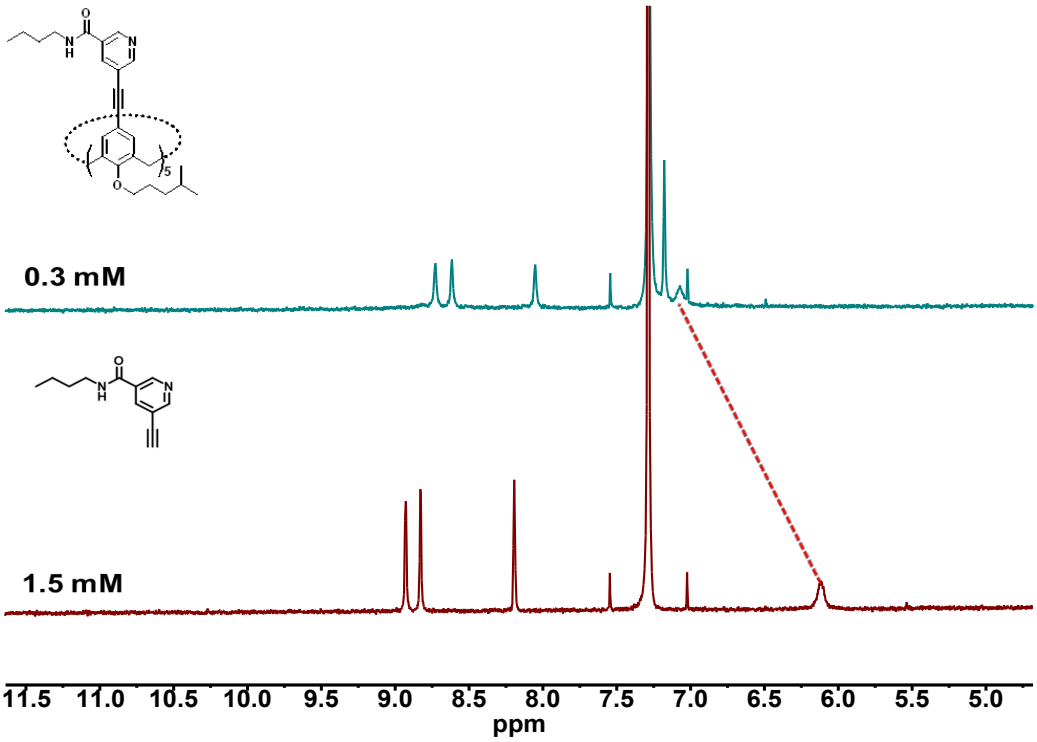


Fig. S8 The ^{1}H NMR spectra (400 MHz, $CDCl_3$, 298 K) of **C5A-c** ([**C5A-c**] = 0.3 mM) and **5c** ([**5c**] = 5[**C5A-c**]).

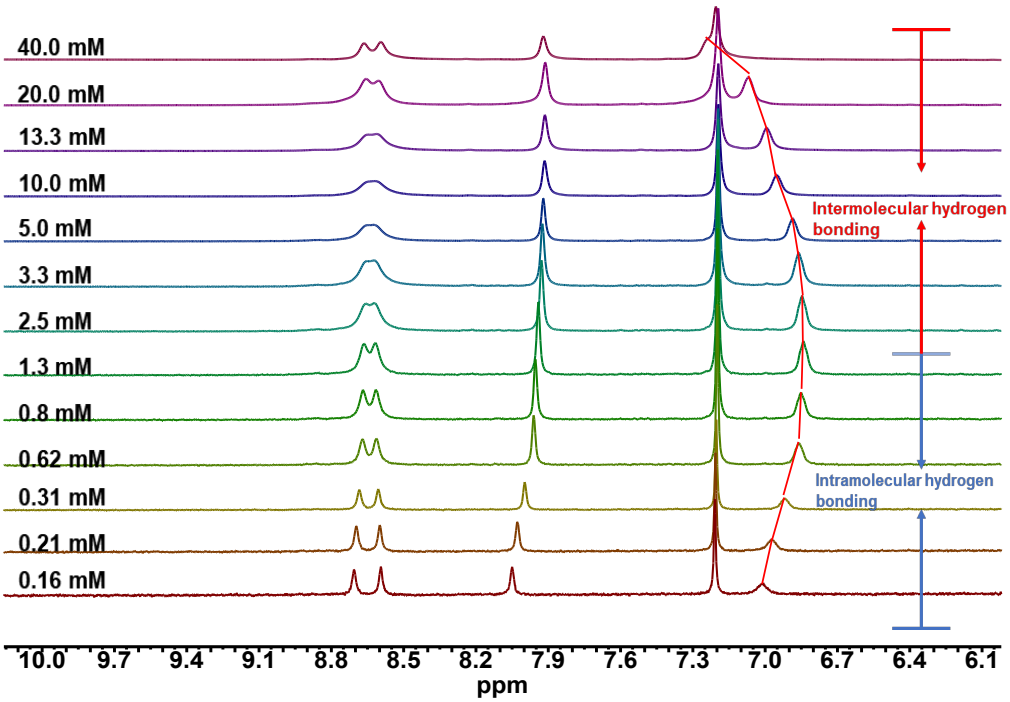


Fig. S9 Downfield region of the ^{1}H NMR spectra (400 MHz, CD_2Cl_2, 298 K) of **C5A-c** at different concentrations.

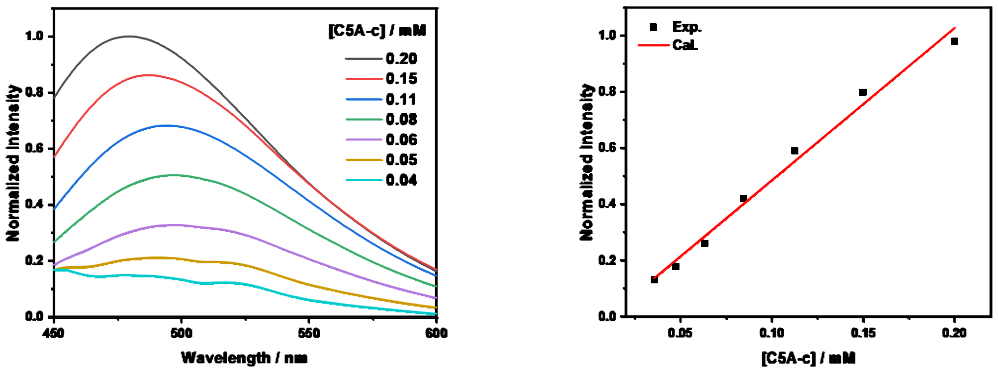


Fig. S10 Fluorescence spectra of **C5A-c** (λ_{ex} = 380 nm) at different concentrations in 90v% PFHI. And the dilution curve at λ_{em} = 470 nm was fitted according to linear regression.

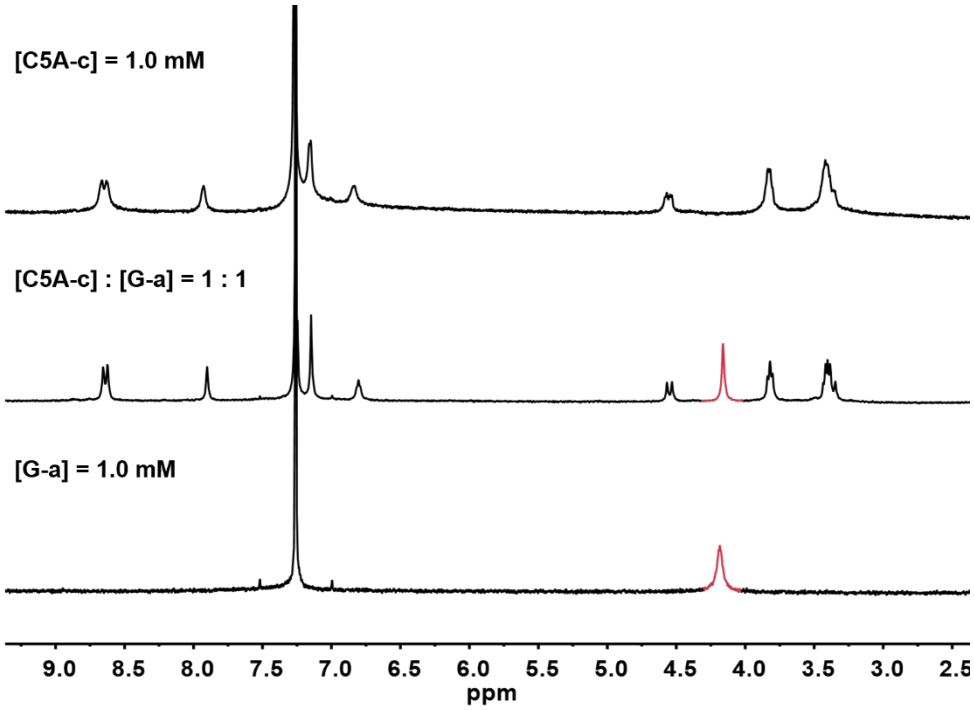


Fig. S11 The ^{1}H NMR spectra (400 MHz, 298 K) of **C5A-c**, **G-a** and their complex in $CDCl_3$ ([**C5A-c**] = [**G-a**] = 1.0 mM). The red peak indicates the resonance of **G-a**.

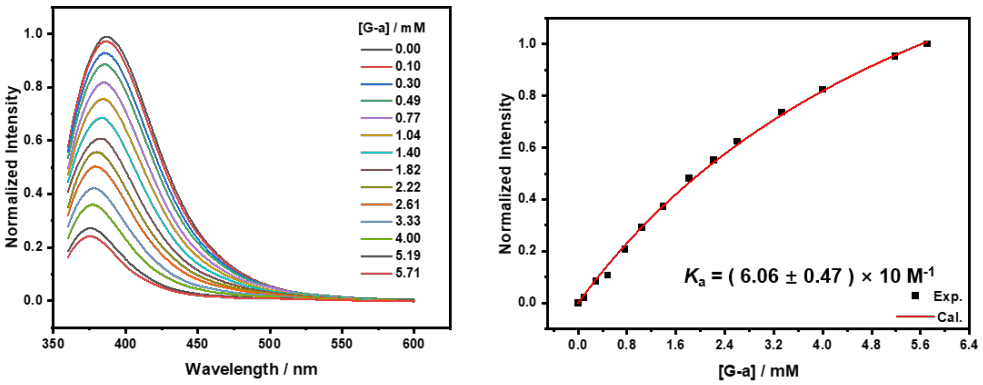


Fig. S12 Fluorescence spectra (λ_{ex} = 350 nm) of **C5A-b** (0.2 mM) with different concentrations of **G-a** in $CHCl_3$, and the associated titration curve at λ_{em} = 480 nm was fitted according to a 1:1 binding stoichiometry.

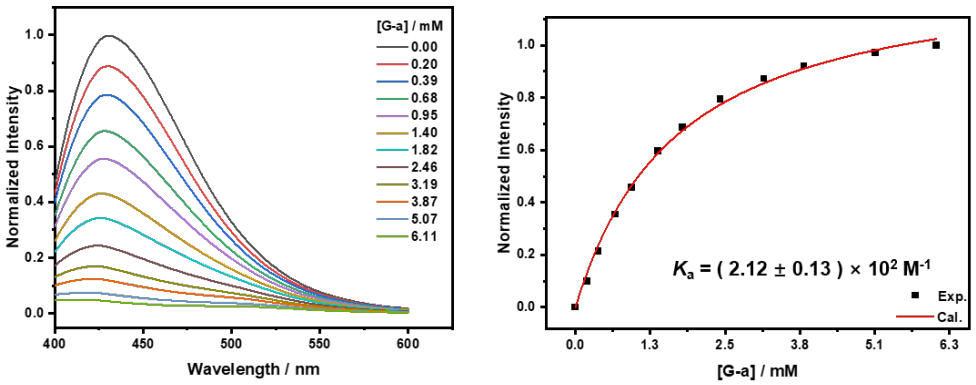


Fig. S13 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-a** in $CHCl_3$, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

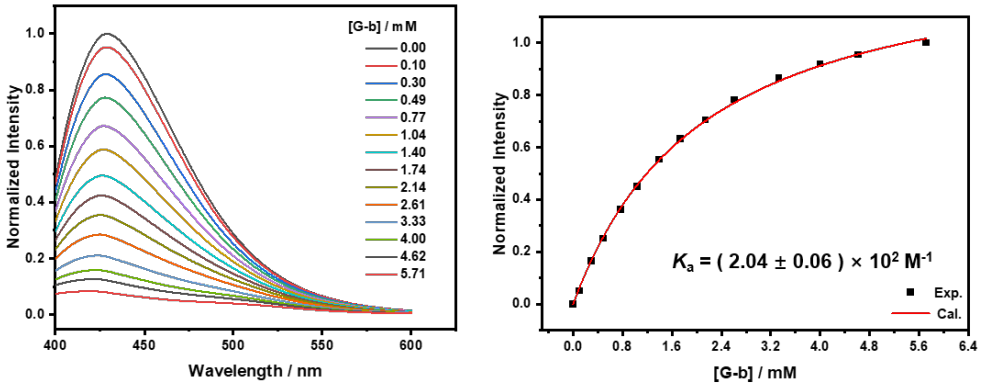


Fig. S14 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-b** in $CHCl_3$, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

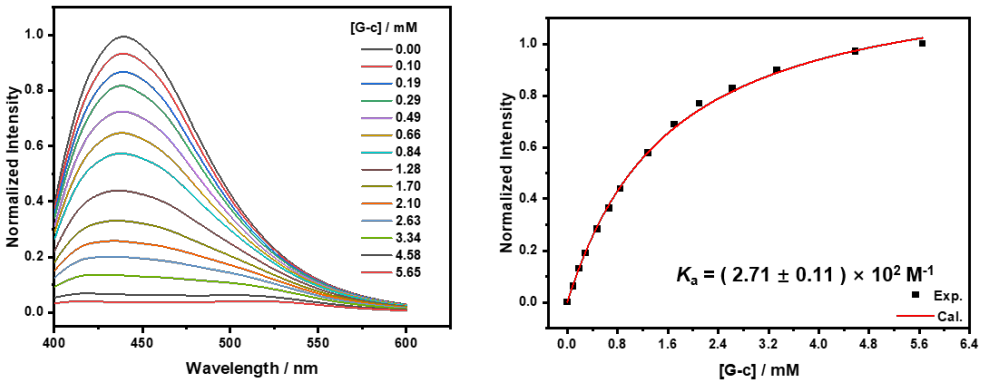


Fig. S15 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-c** in $CHCl_3$, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

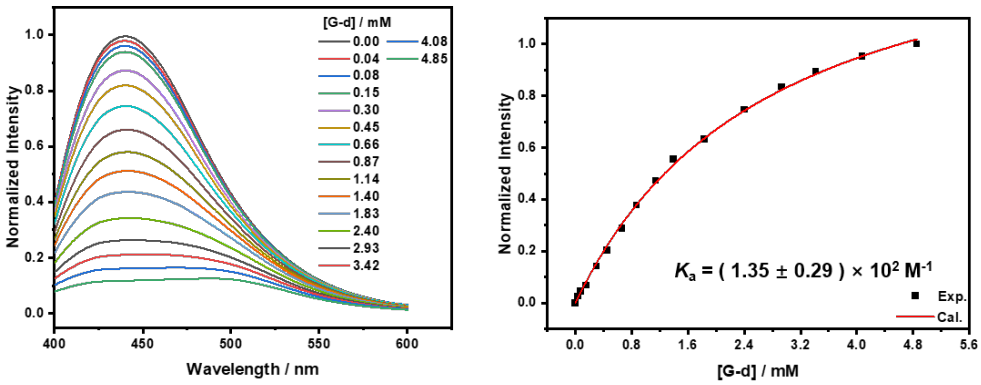


Fig. S16 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-d** in $CHCl_3$, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

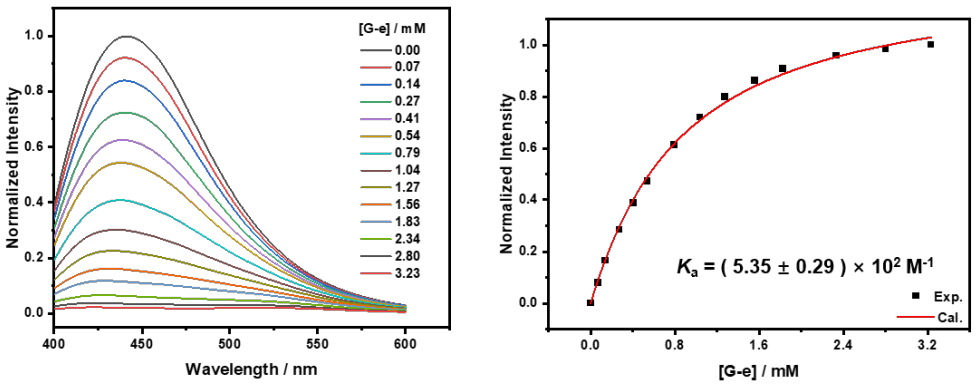


Fig. S17 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-e** in $CHCl_3$, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

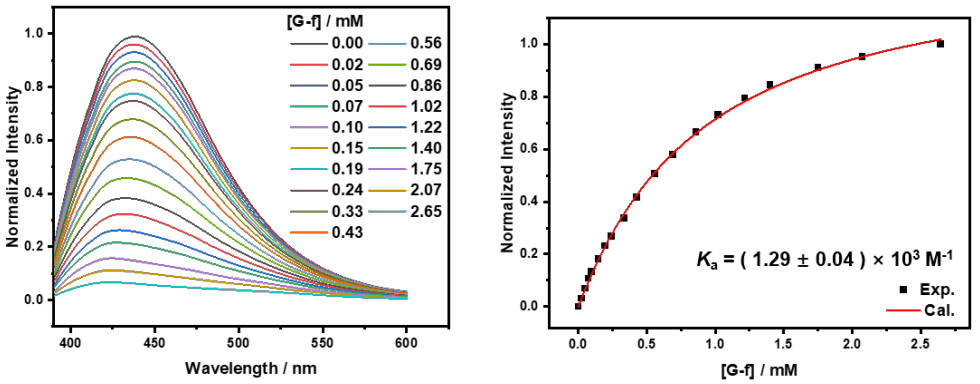


Fig. S18 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-f** in $CHCl_3$, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

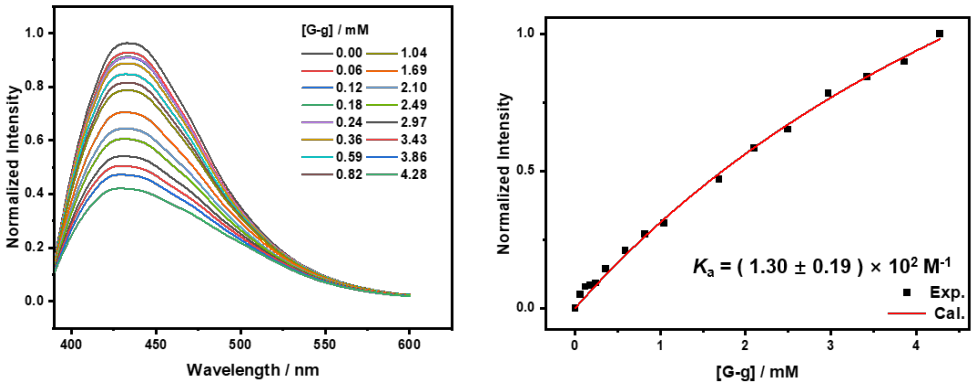


Fig. S19 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-g** in $CHCl_3$, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

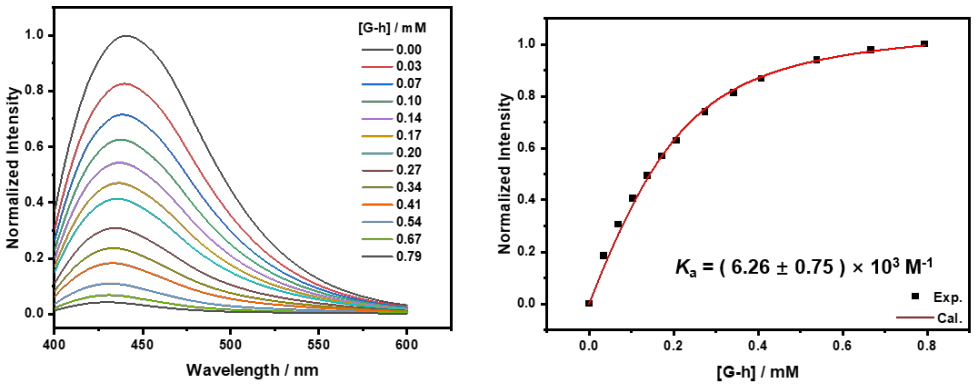


Fig. S20 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-h** in $CHCl_3$, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

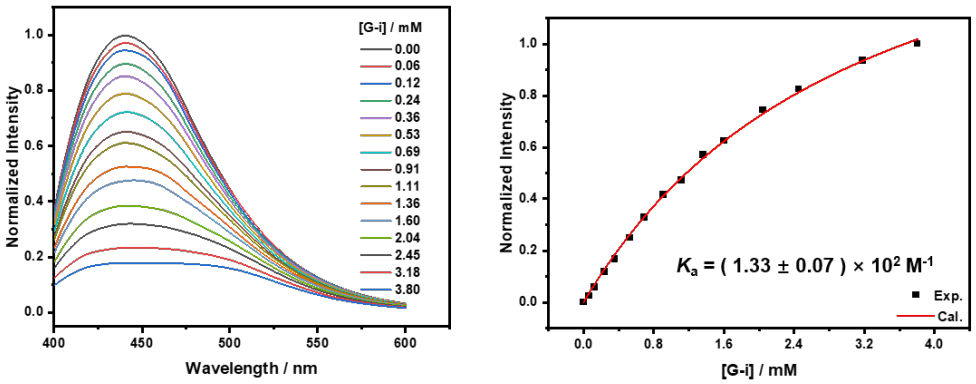


Fig. S21 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-i** in $CHCl_3$, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

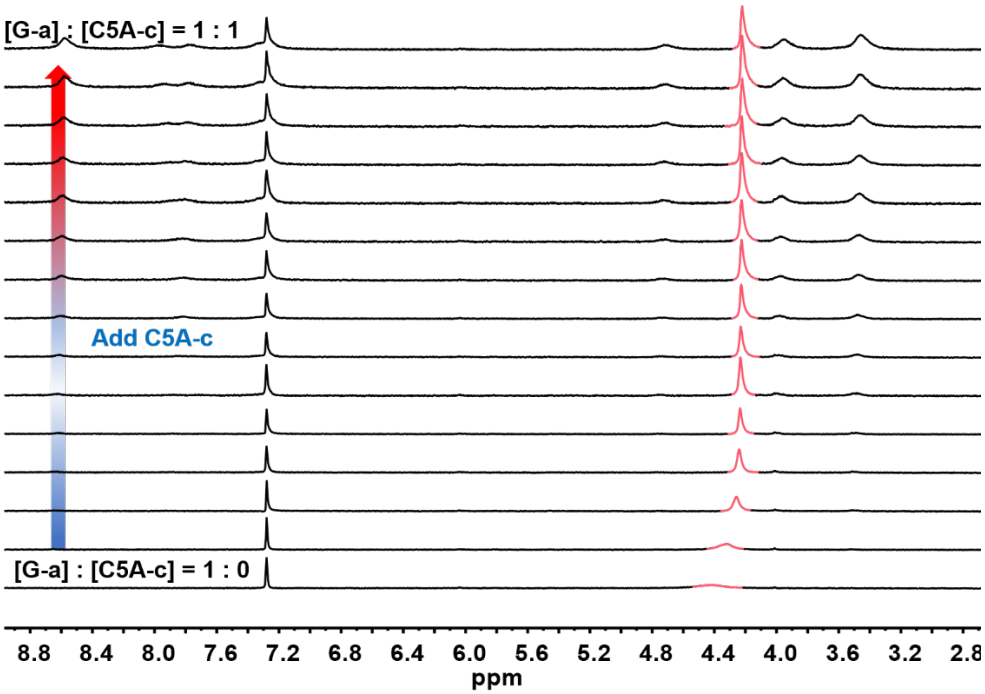


Fig. S22 The ^{1}H NMR titration spectra recorded for the mixture of **G-a** (1.0 mM) and **C5A-c** (0 - 1 equivalent) in PFIH (90v%) and $CDCl_3$. The red peak indicates the resonance of **G-a**.

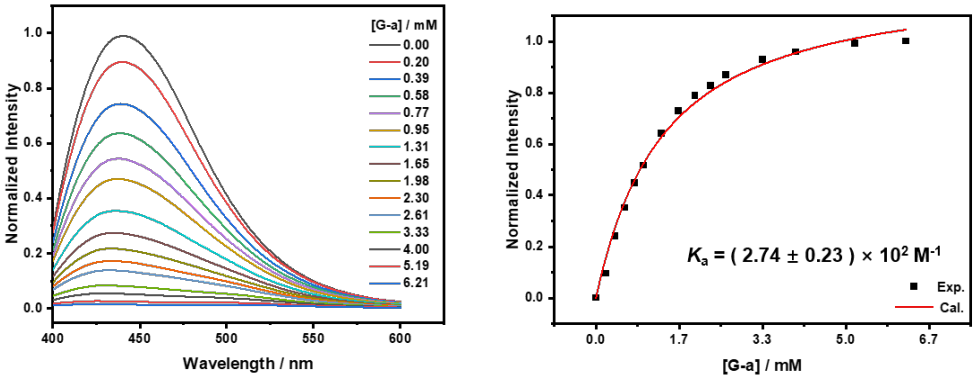


Fig. S23 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-a** in PFIH (40v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

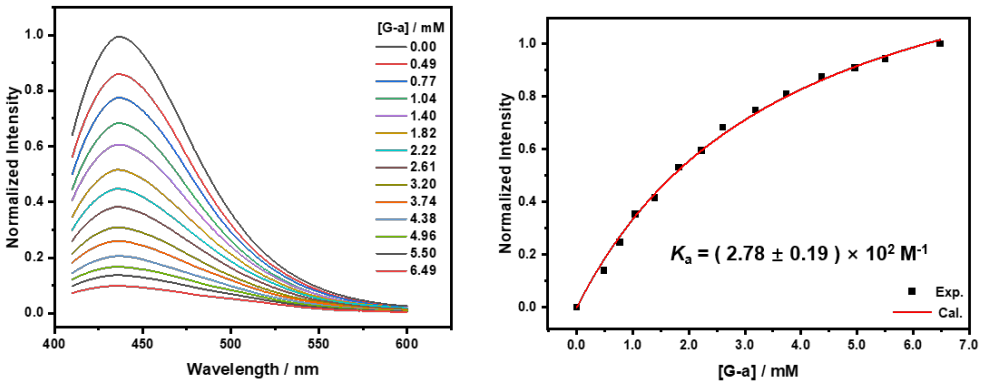


Fig. S24 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-a** in PFIH (60v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

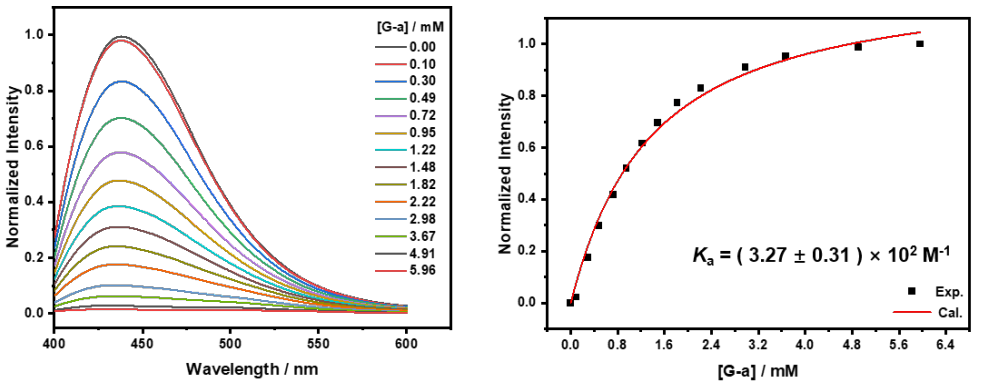


Fig. S25 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-a** in PFIH (70v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

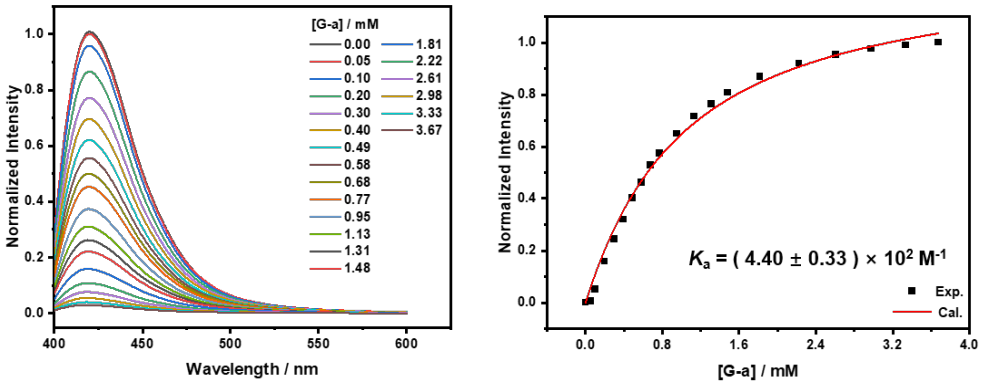


Fig. S26 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-a** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

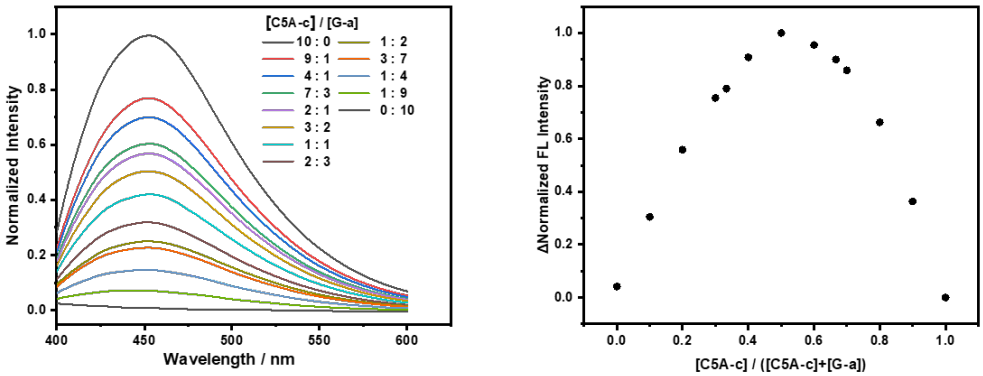


Fig. S27 Job's plot for solutions of **C5A-c** and **G-a** in PFIH (90v%) and chloroform (λ_{ex} = 380 nm, λ_{em} = 430 nm, [**C5A-c**] + [**G-a**] = 0.2 mM, T = 298 K).

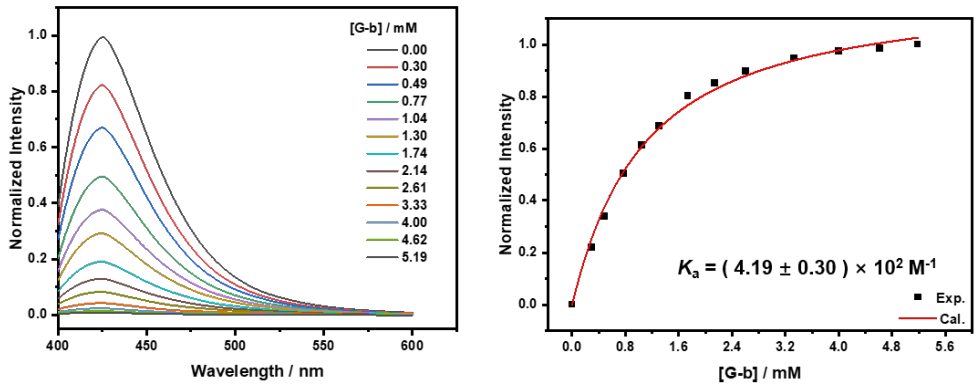


Fig. S28 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-b** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 491 nm was fitted according to a 1:1 binding stoichiometry.

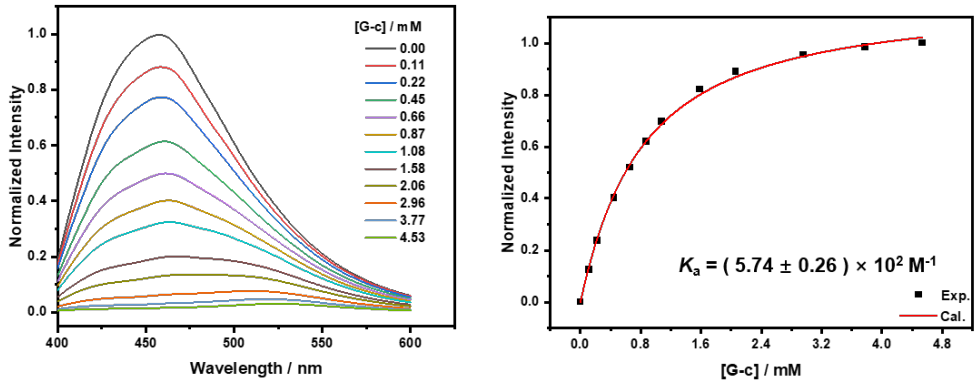


Fig. S29 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-c** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

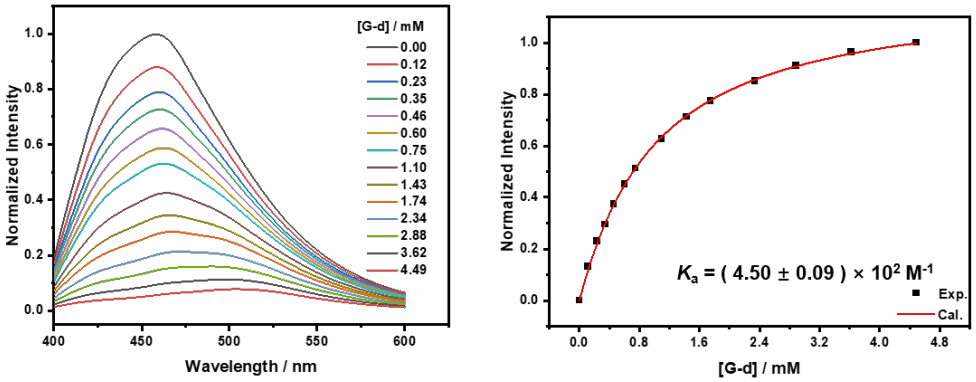


Fig. S30 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-d** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

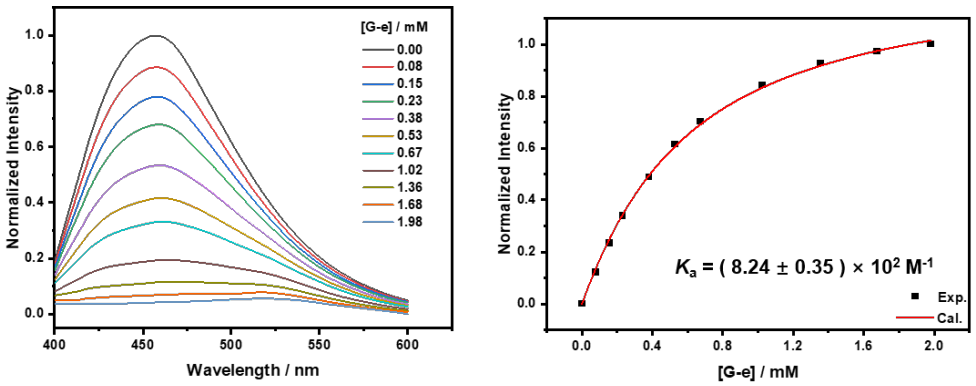


Fig. S31 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-e** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

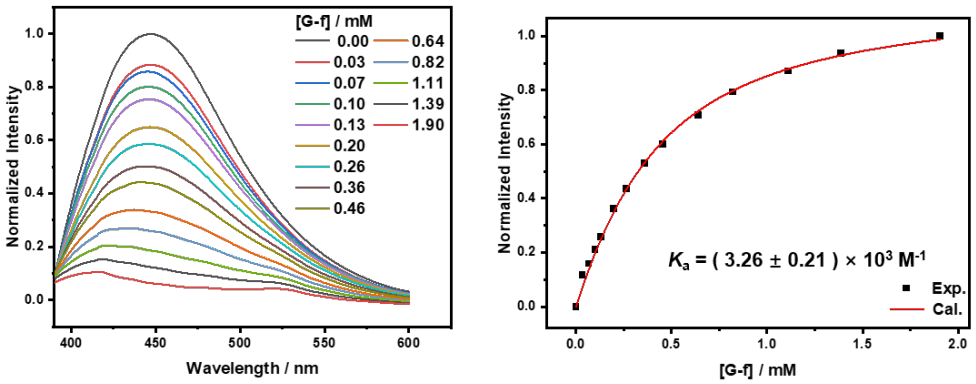


Fig. S32 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-f** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 458 nm was fitted according to a 1:1 binding stoichiometry.

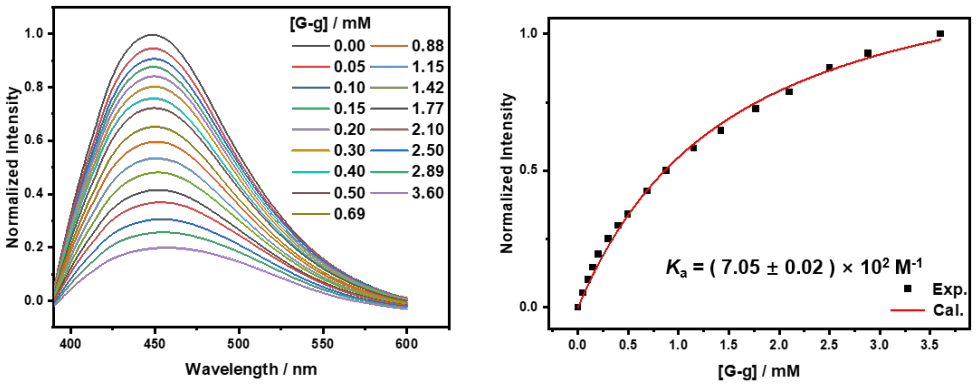


Fig. S33 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-g** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

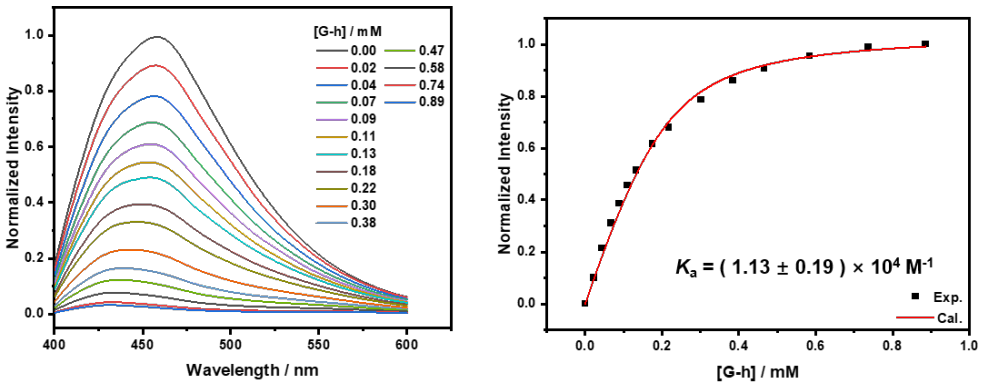


Fig. S34 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-h** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 460 nm was fitted according to a 1:1 binding stoichiometry.

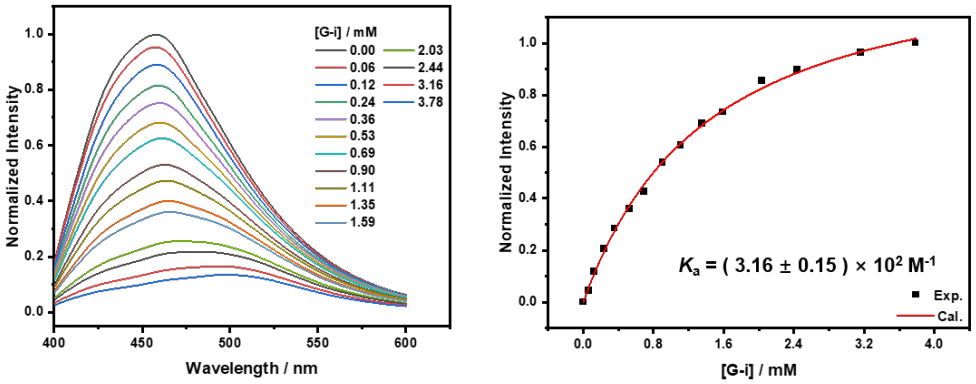


Fig. S35 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-i** in PFIH (80v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

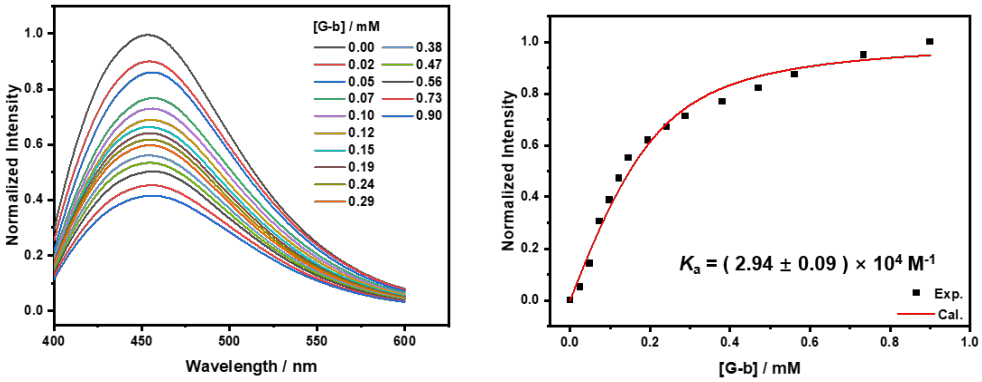


Fig. S36 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-b** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 549 nm was fitted according to a 1:1 binding stoichiometry.

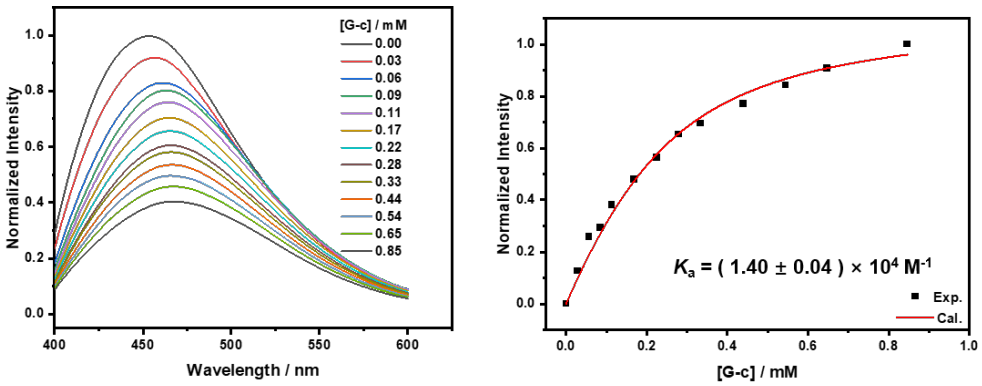


Fig. S37 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-c** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 462 nm was fitted according to a 1:1 binding stoichiometry.

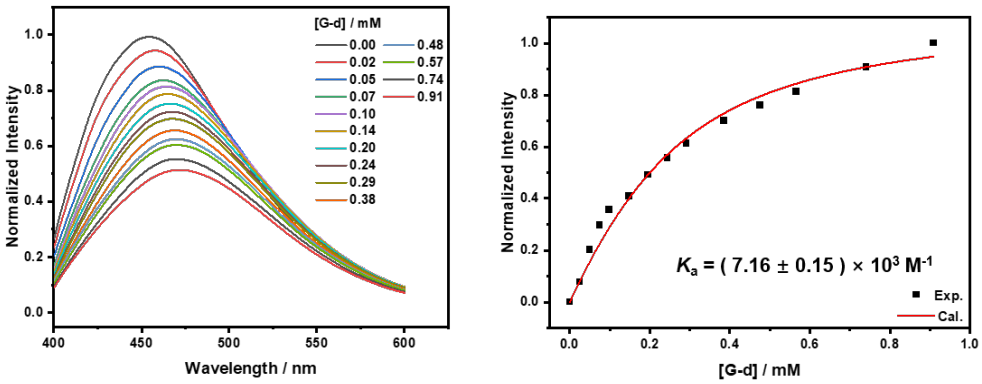


Fig. S38 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-d** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 458 nm was fitted according to a 1:1 binding stoichiometry.

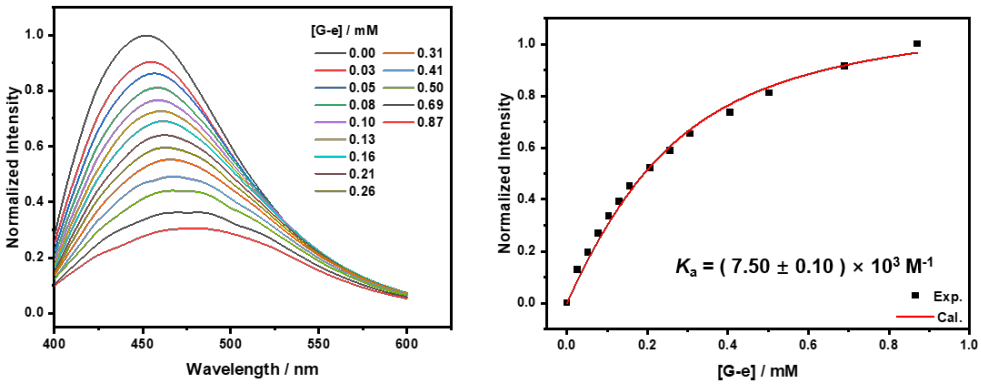


Fig. S39 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-e** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 430 nm was fitted according to a 1:1 binding stoichiometry.

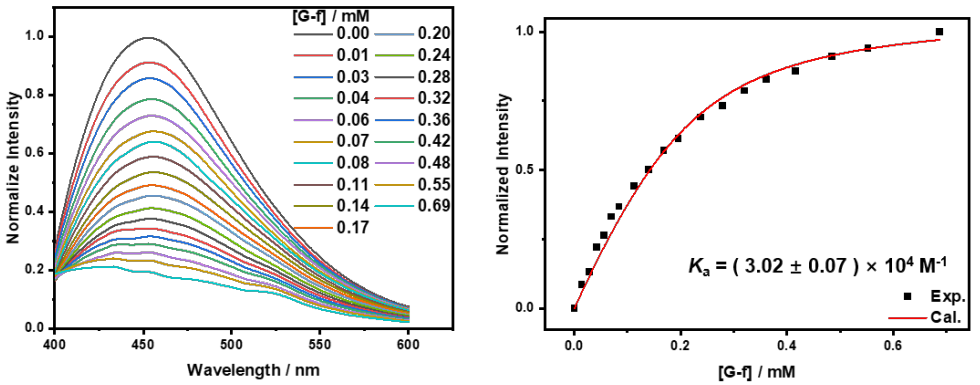


Fig. S40 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-f** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 513 nm was fitted according to a 1:1 binding stoichiometry.

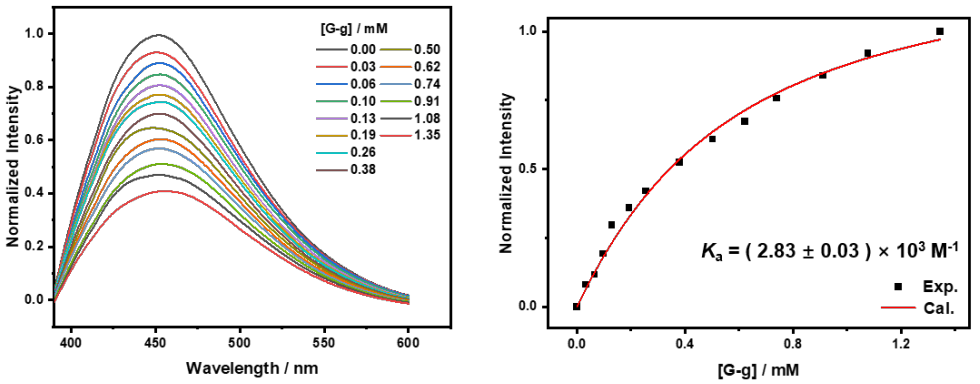


Fig. S41 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-g** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

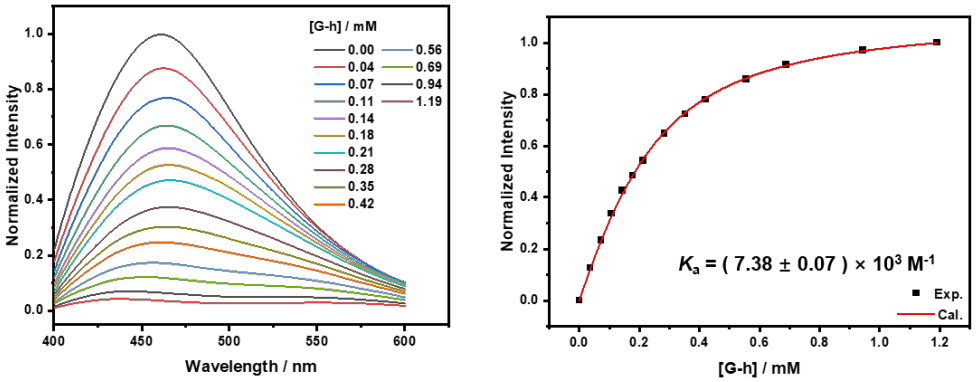


Fig. S42 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-h** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 465 nm was fitted according to a 1:1 binding stoichiometry.

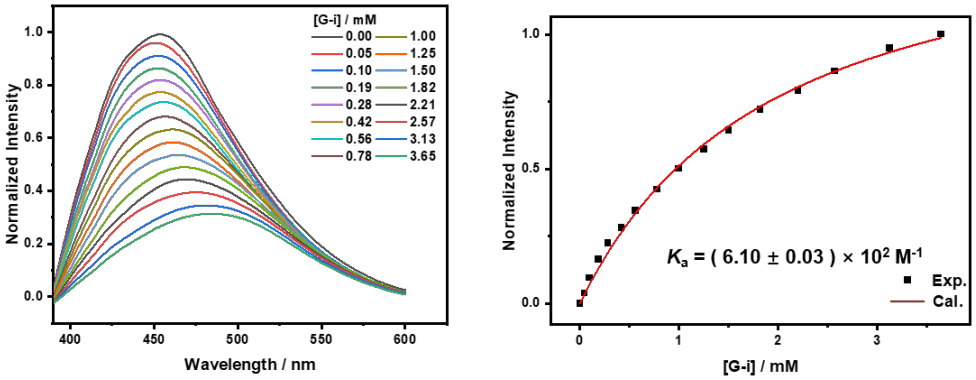


Fig. S43 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-i** in PFIH (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

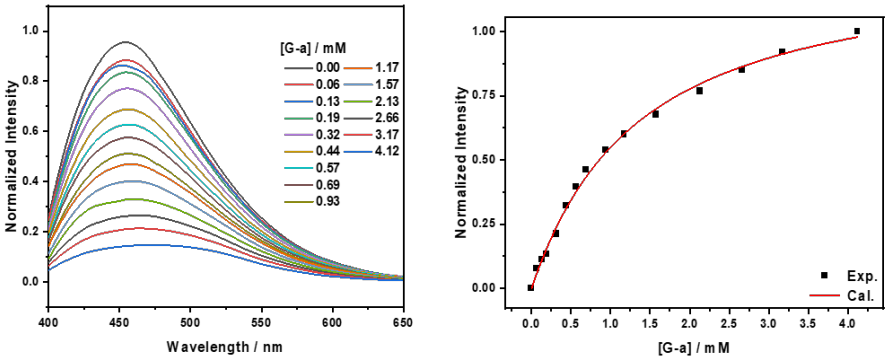


Fig. S44 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-a** in PFIB (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

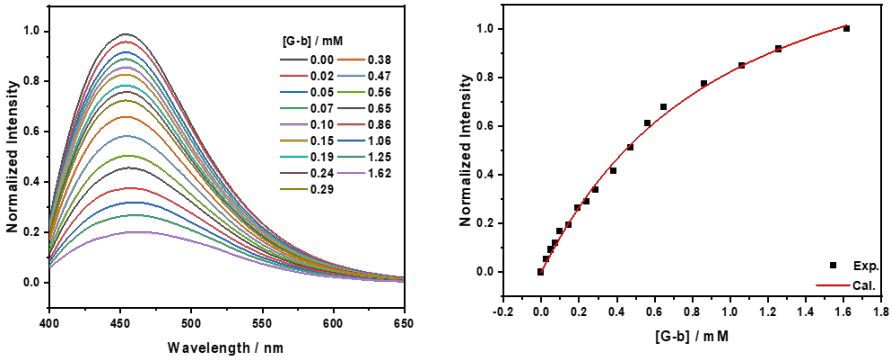


Fig. S45 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-b** in PFIB (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

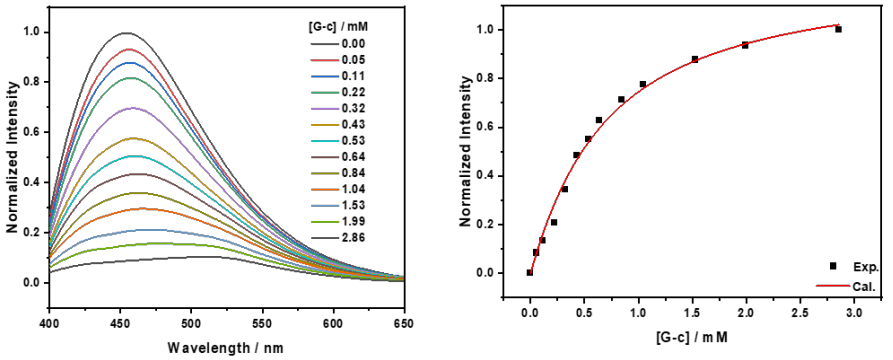


Fig. S46 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-c** in PFIB (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

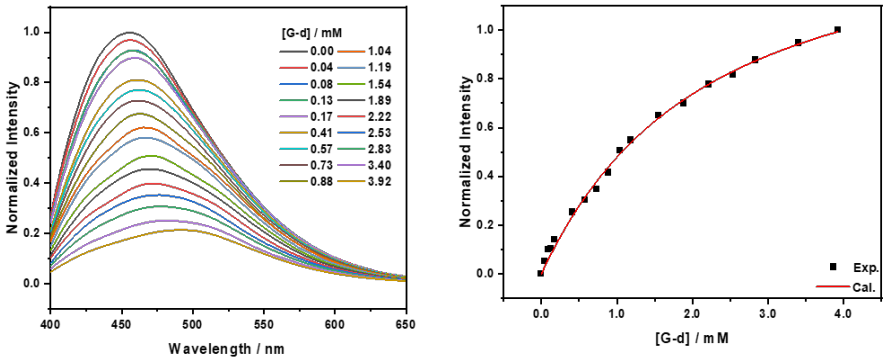


Fig. S47 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.2 mM) with different concentrations of **G-d** in PFIB (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

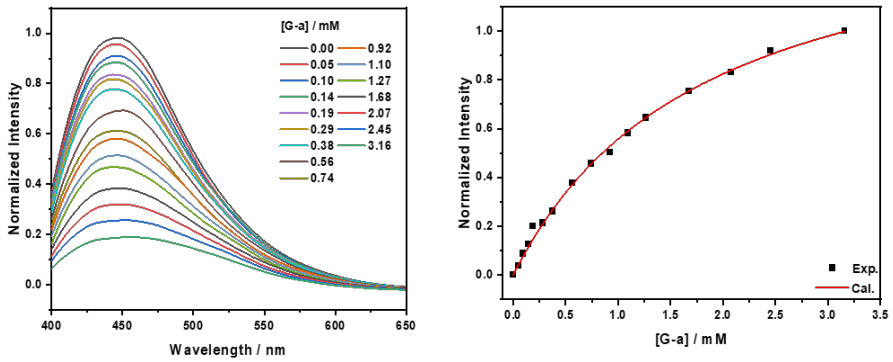


Fig. S48 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.1 mM) with different concentrations of **G-a** in PFIO (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

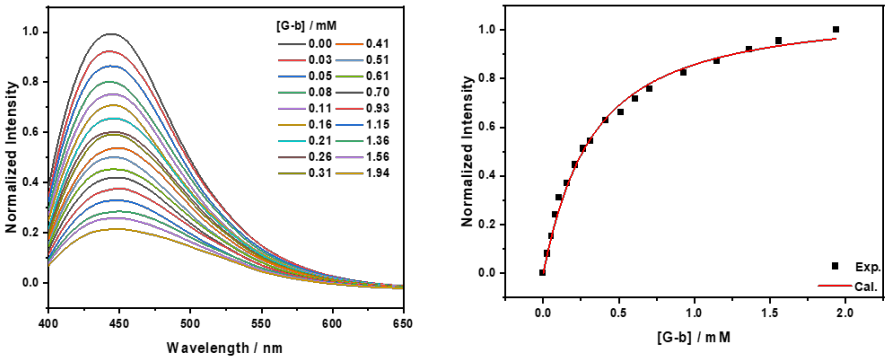


Fig. S49 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.1 mM) with different concentrations of **G-b** in PFIO (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

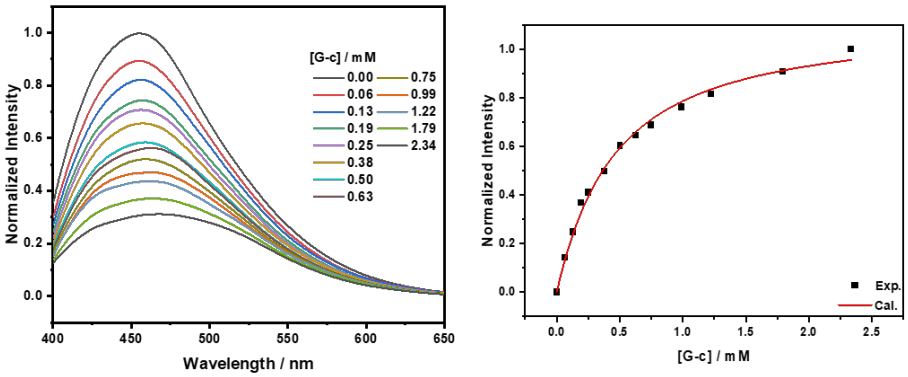


Fig. S50 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.1 mM) with different concentrations of **G-c** in PFIO (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

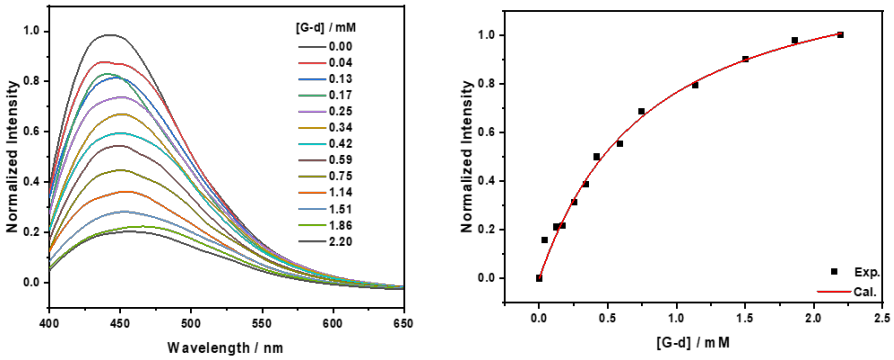


Fig. S51 Fluorescence spectra (λ_{ex} = 380 nm) of **C5A-c** (0.1 mM) with different concentrations of **G-d** in PFIO (90v%) and chloroform, and the associated titration curve at λ_{em} = 450 nm was fitted according to a 1:1 binding stoichiometry.

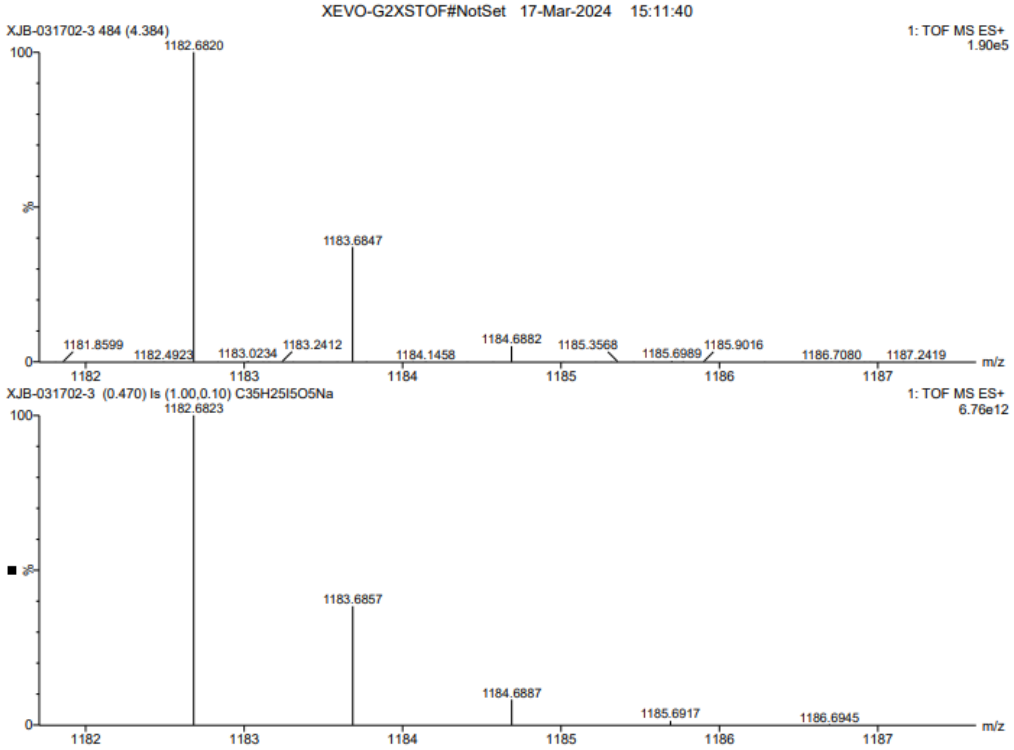


Fig. S52 HR ESI-MS spectrum of compound **2**.

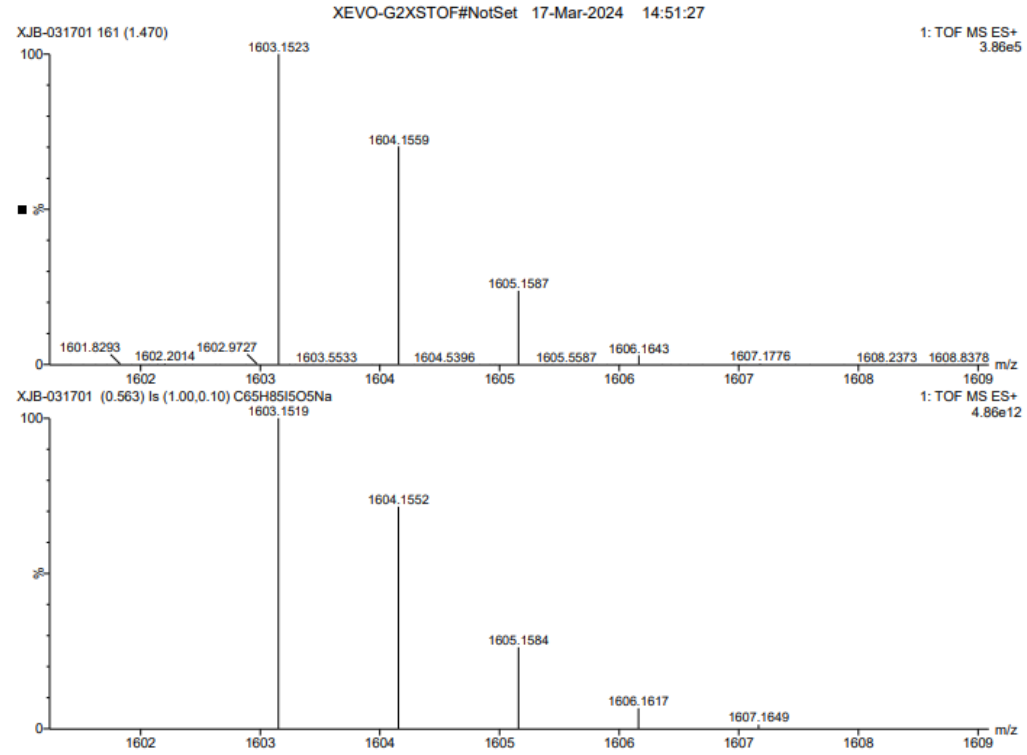


Fig. S53 HR ESI-MS spectrum of compound **4**.

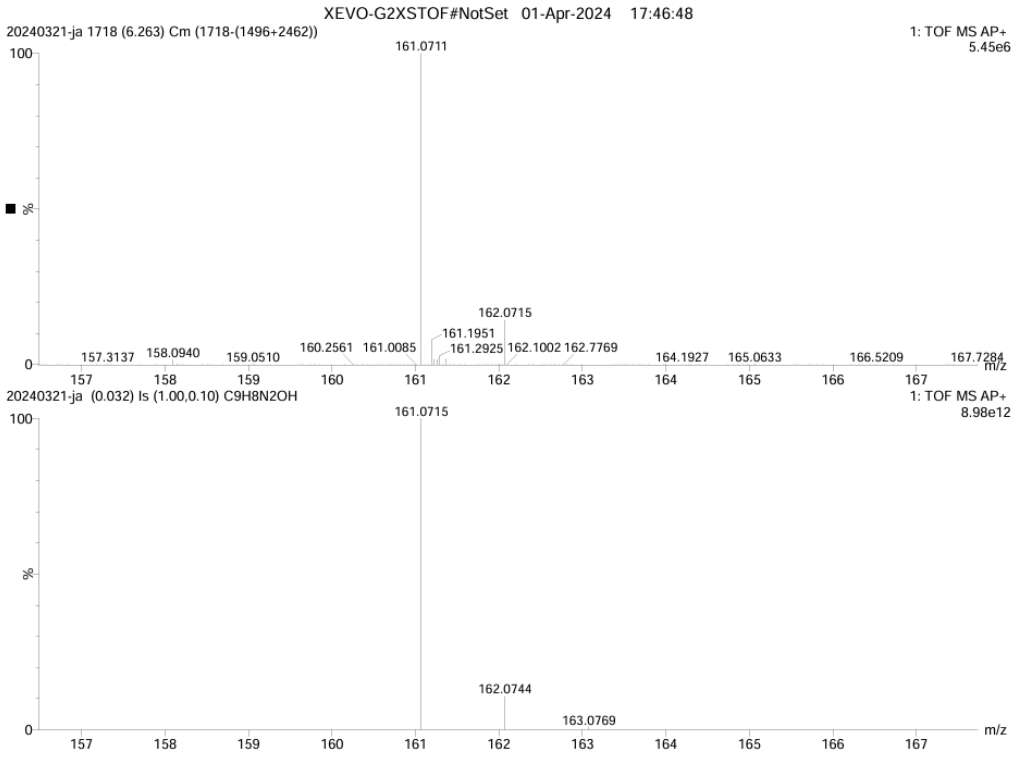


Fig. S54 HR APGC-MS spectrum of compound **5b**.

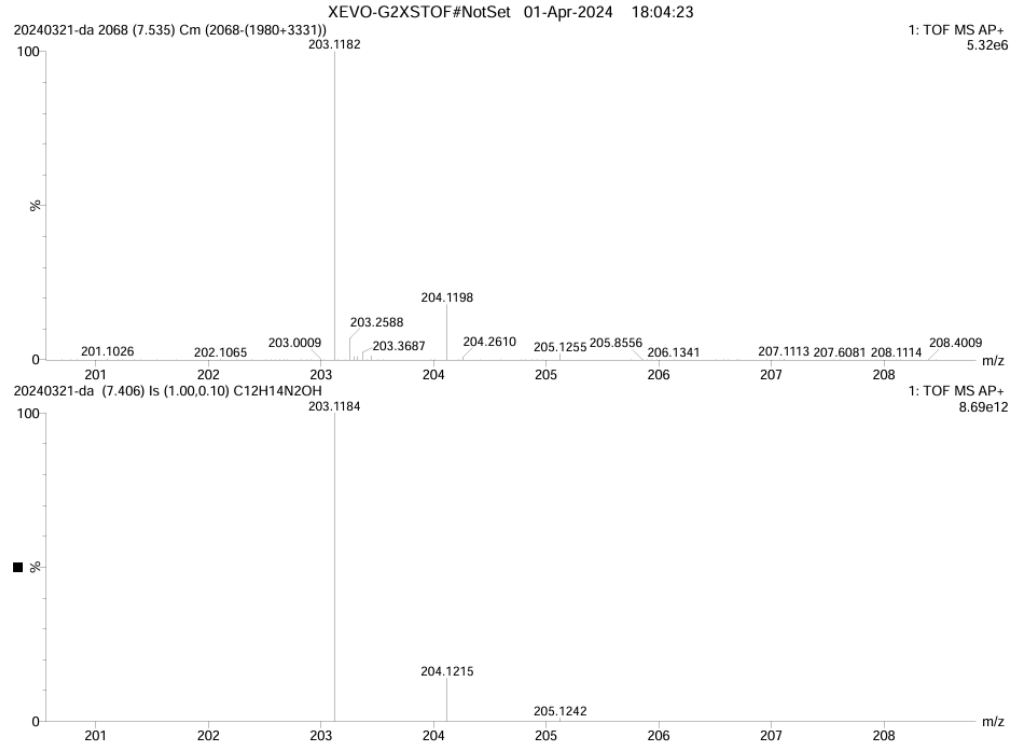


Fig. S55 HR APGC-MS spectrum of compound **5c**.

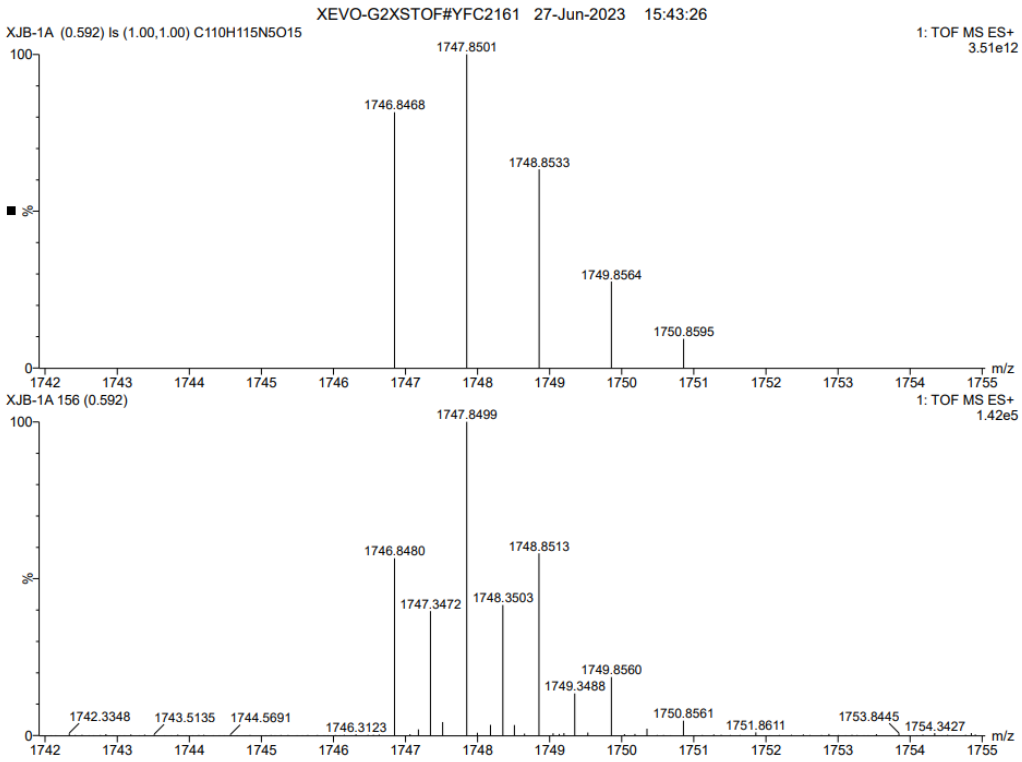


Fig. S56 HR ESI-MS spectrum of compound **C5A-a**.

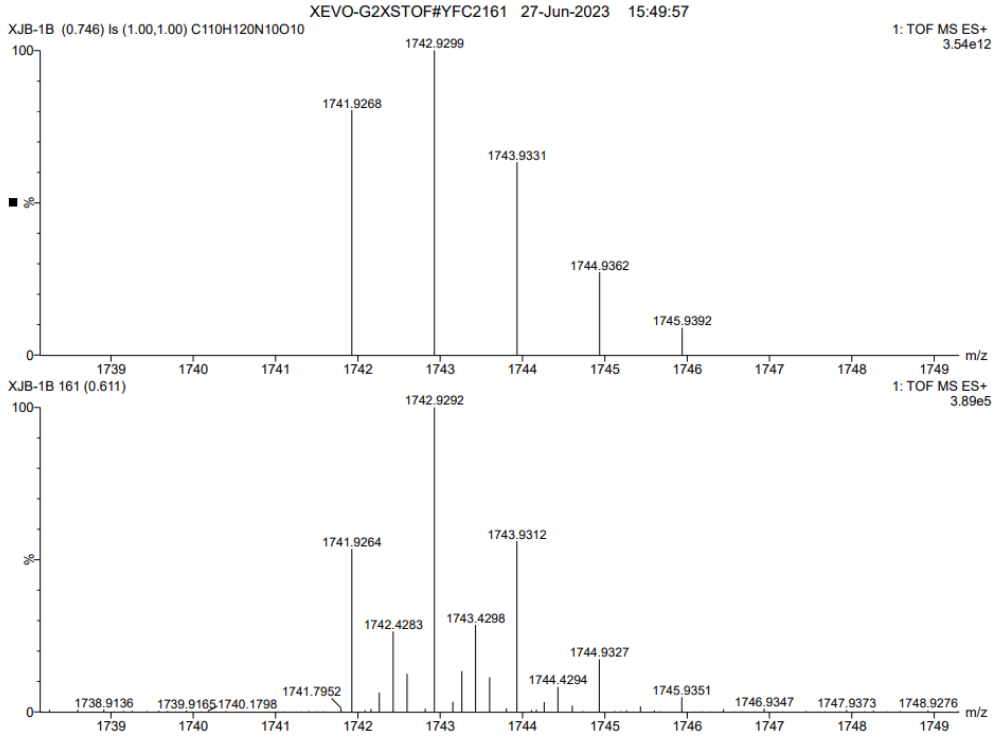


Fig. S57 HR ESI-MS spectrum of compound **C5A-b**.

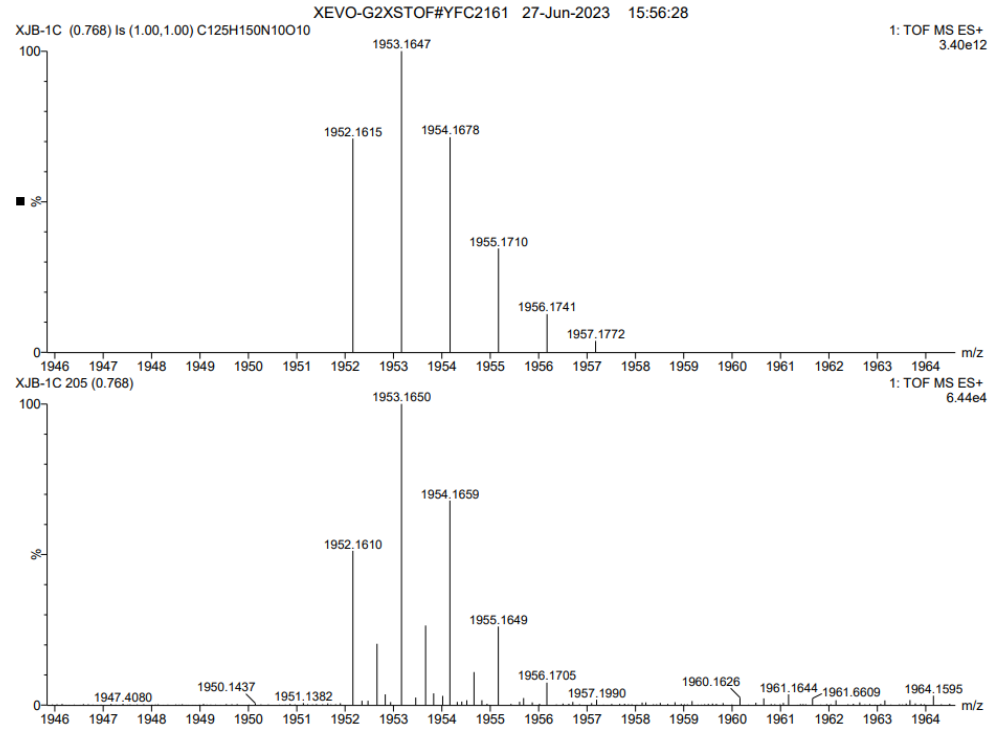


Fig. S58 HR ESI-MS spectrum of compound **C5A-c**.

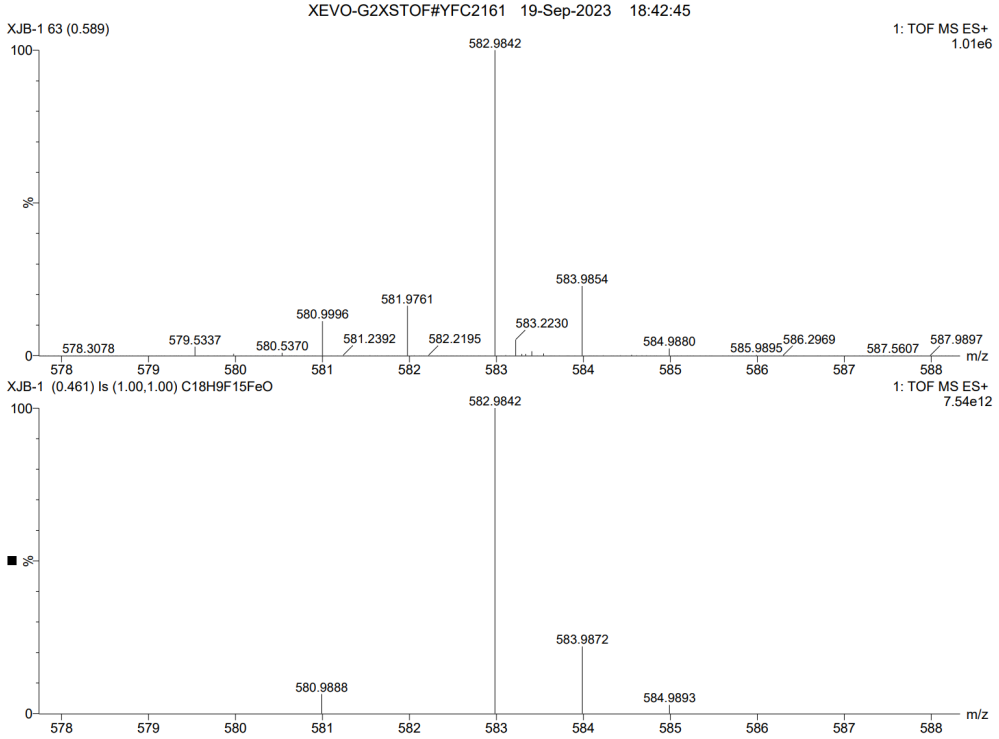


Fig. S59 HR ESI-MS spectrum of compound **G-h**.

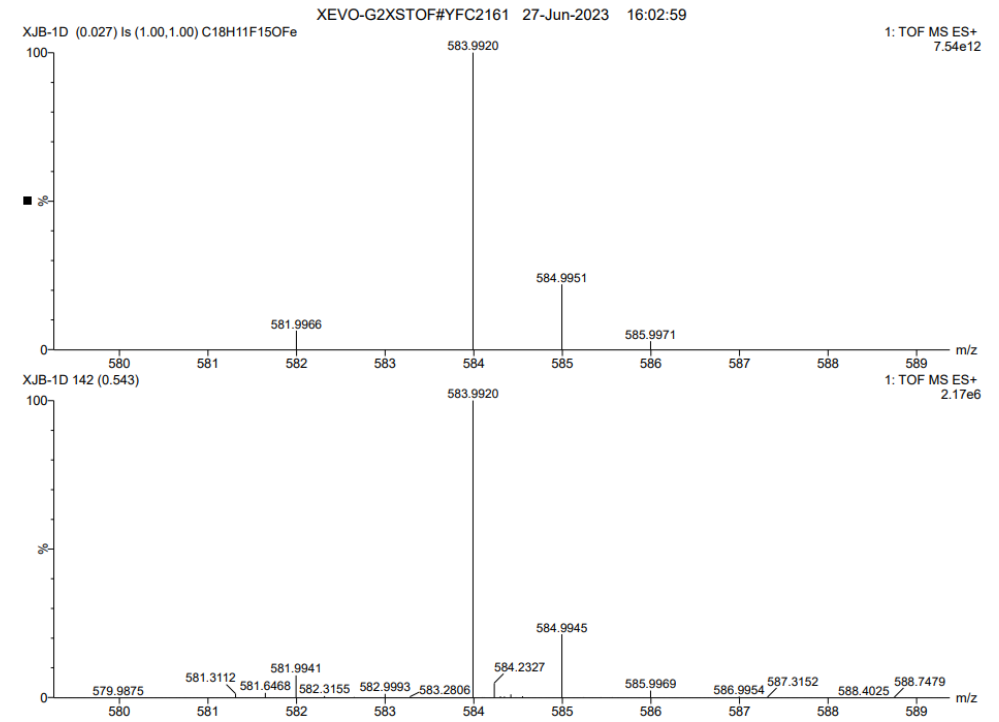


Fig. S60 HR ESI-MS spectrum of compound **G-i**.

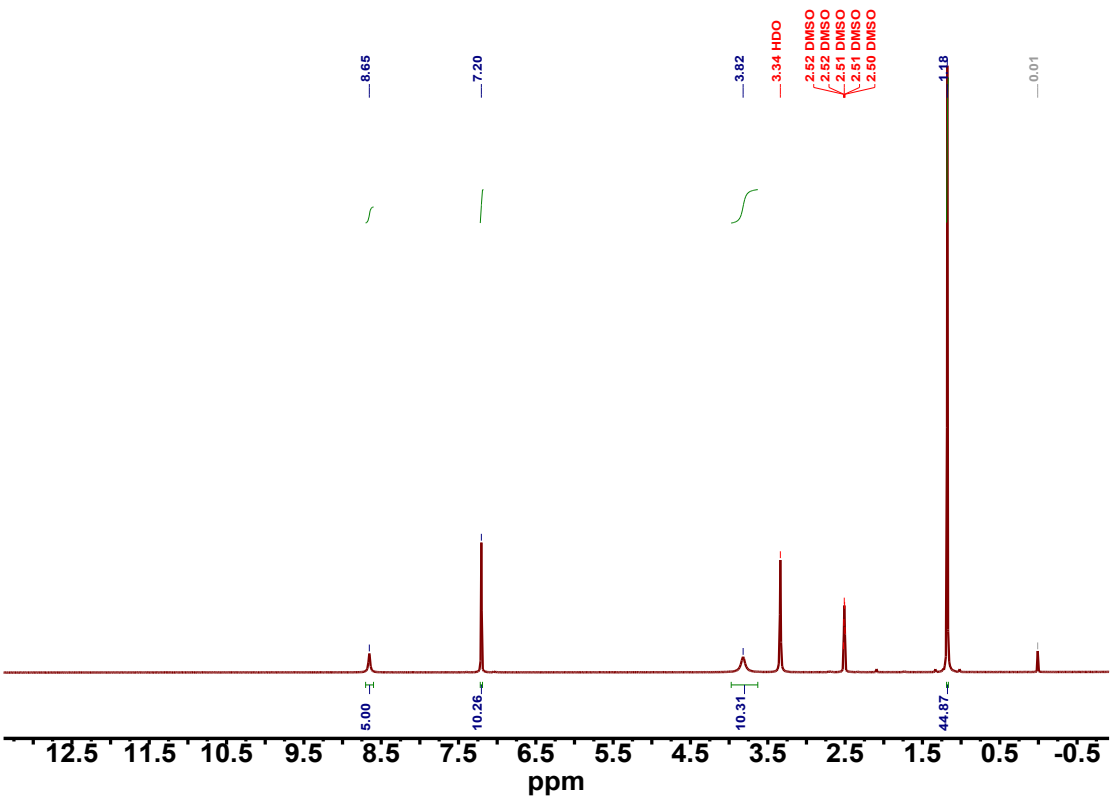


Fig. S61 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of compound **6**.

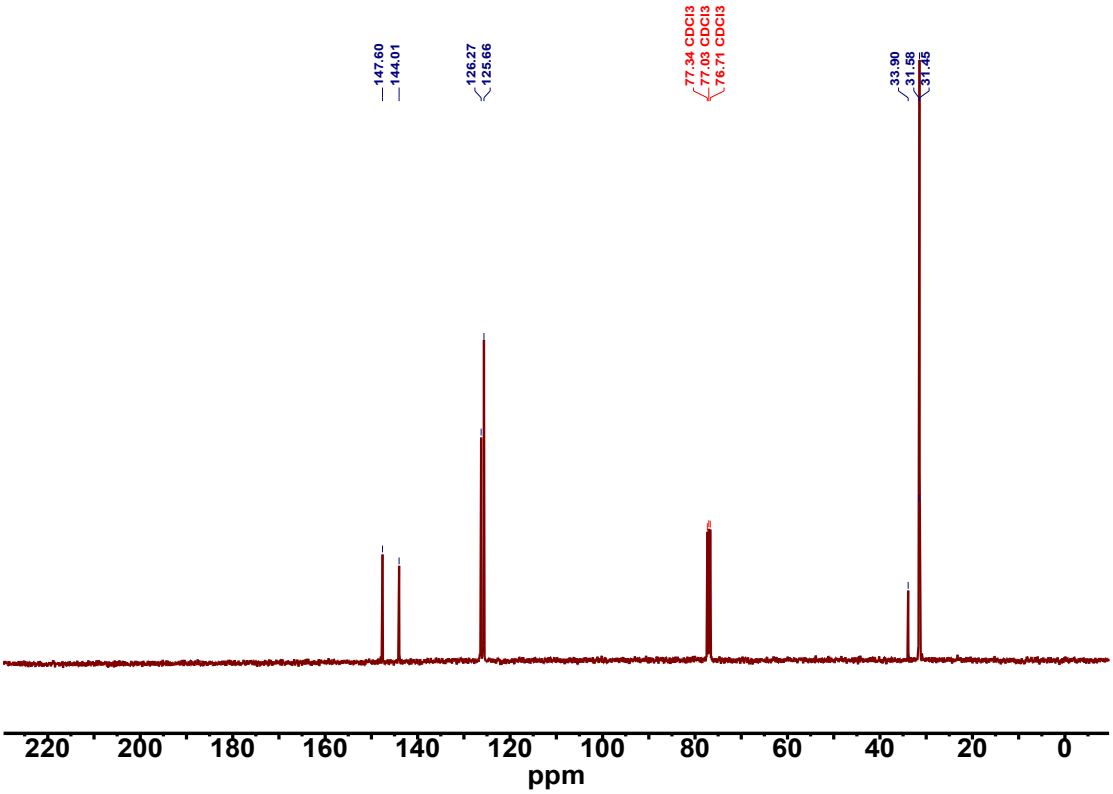


Fig. S62 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **6**.

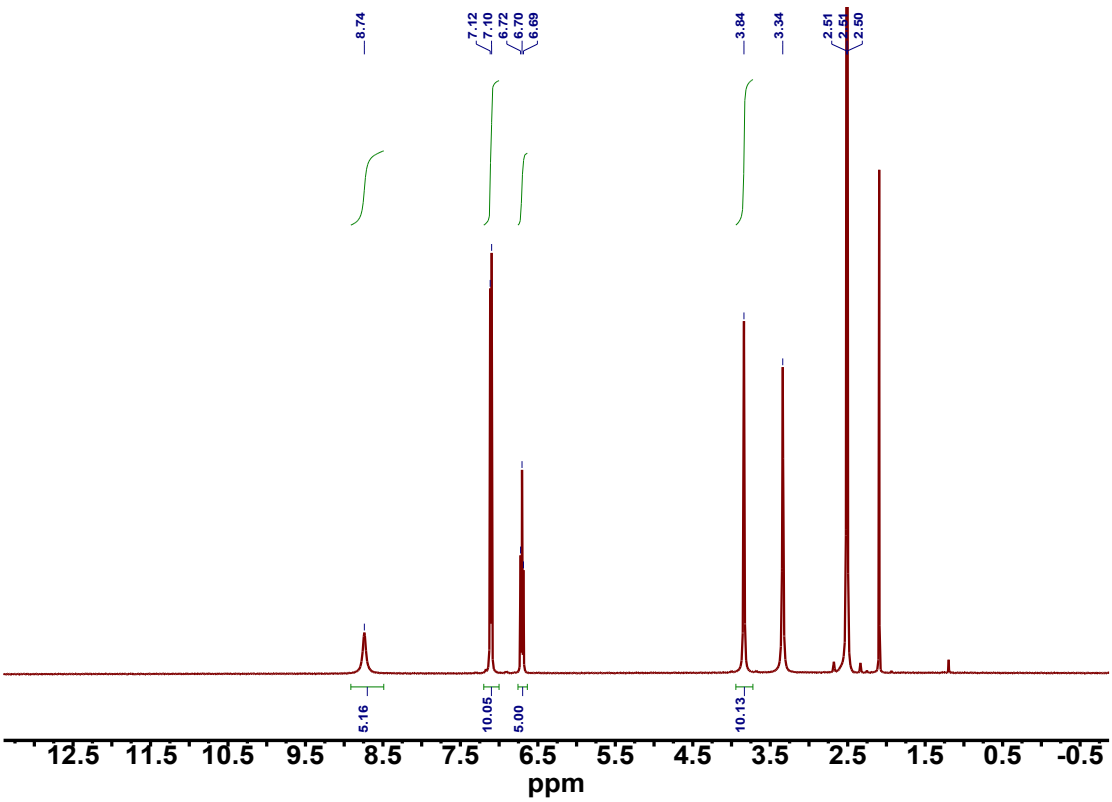


Fig. S63 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of compound **1**.

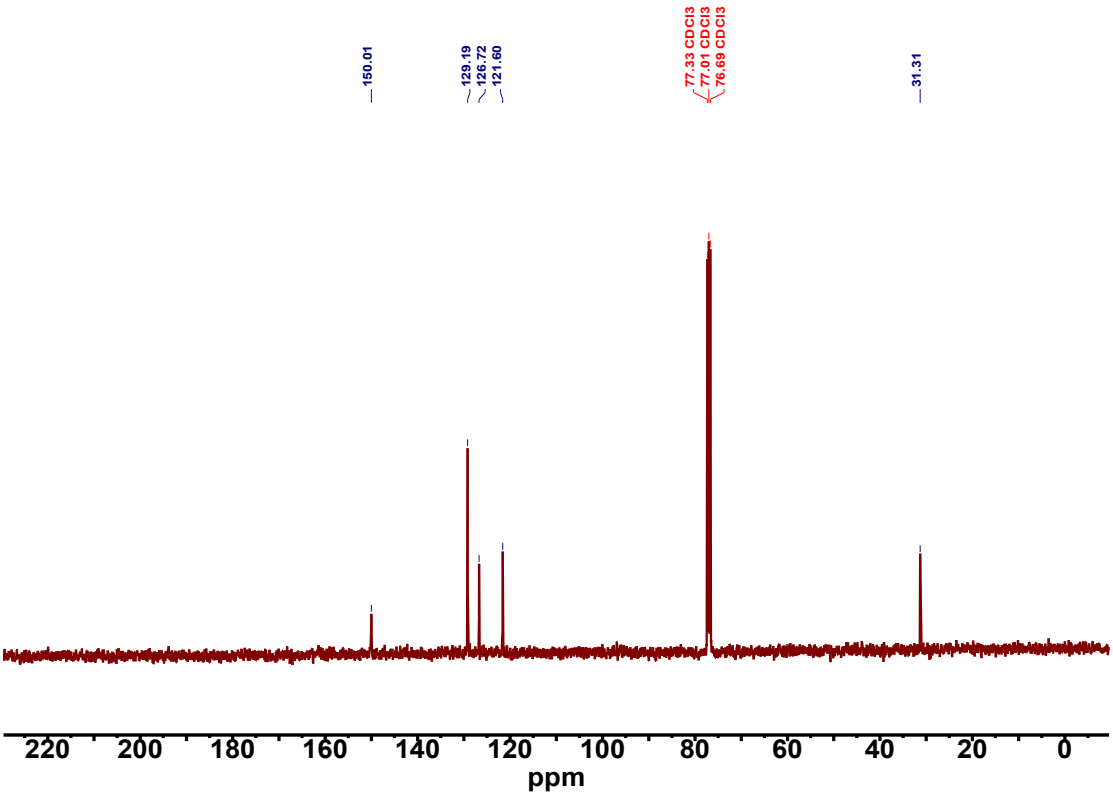


Fig. S64 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **1**.

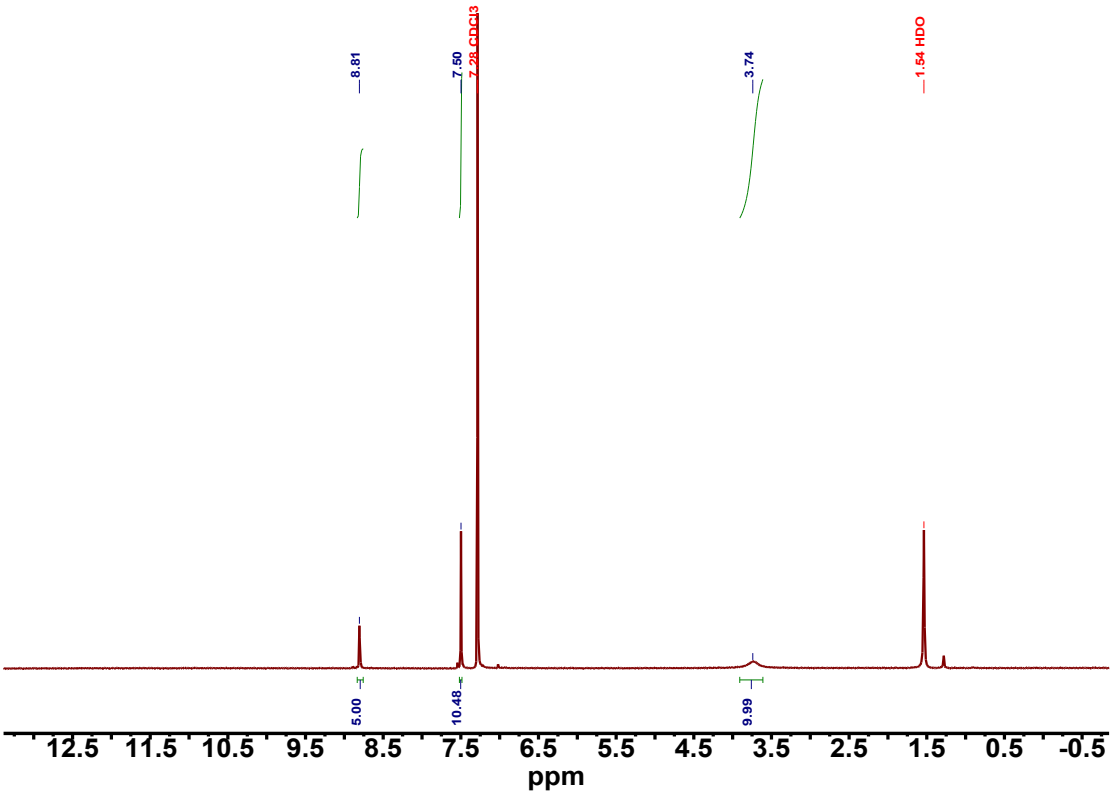


Fig. S65 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of compound **2**.

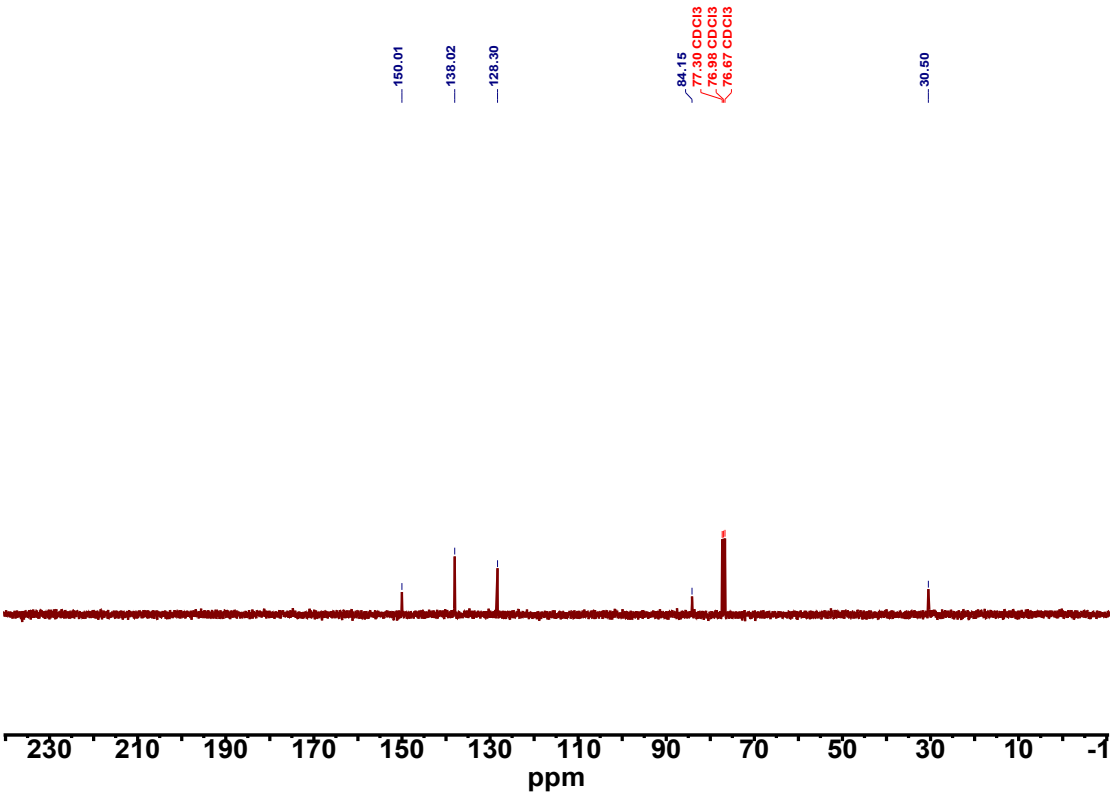


Fig. S66 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **2**.

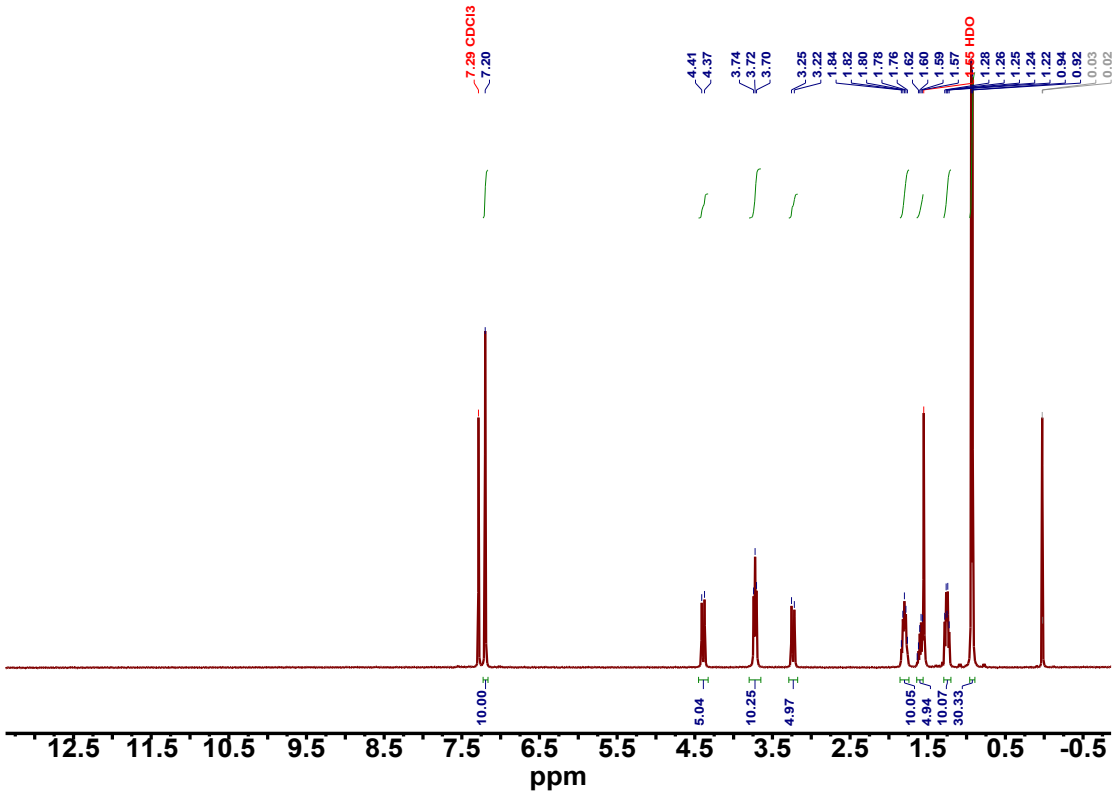


Fig. S67 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of compound **4**.

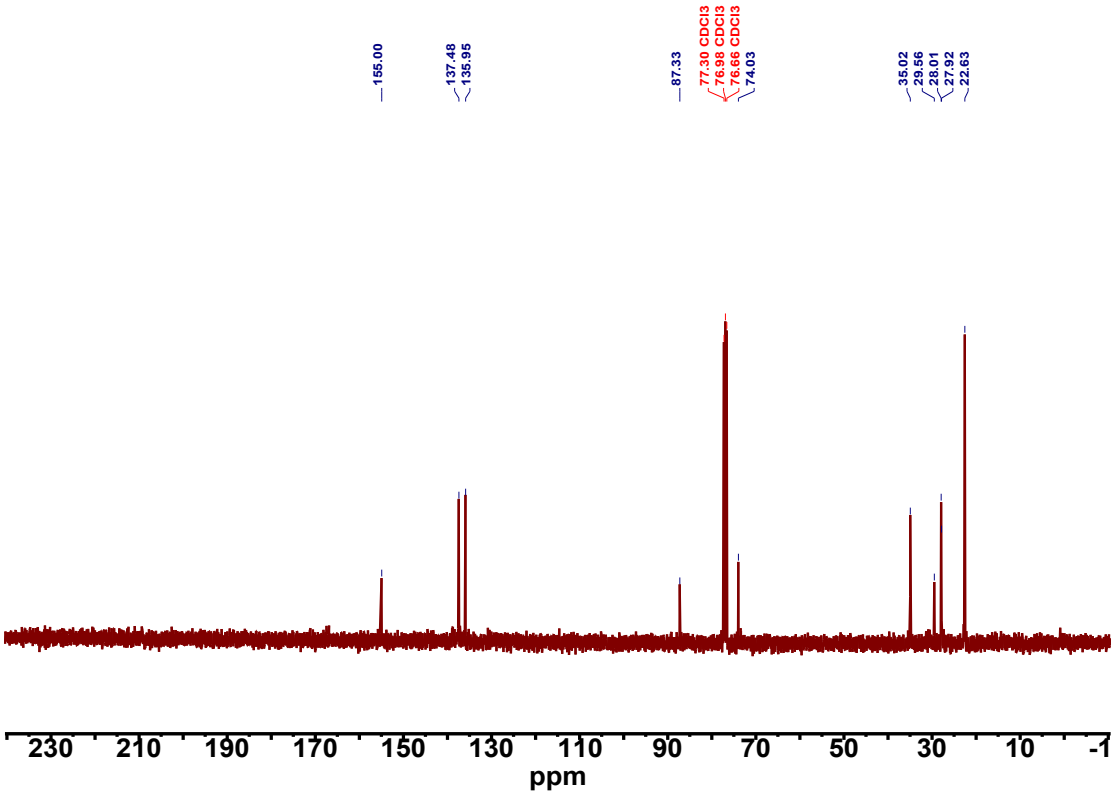


Fig. S68 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **4**.

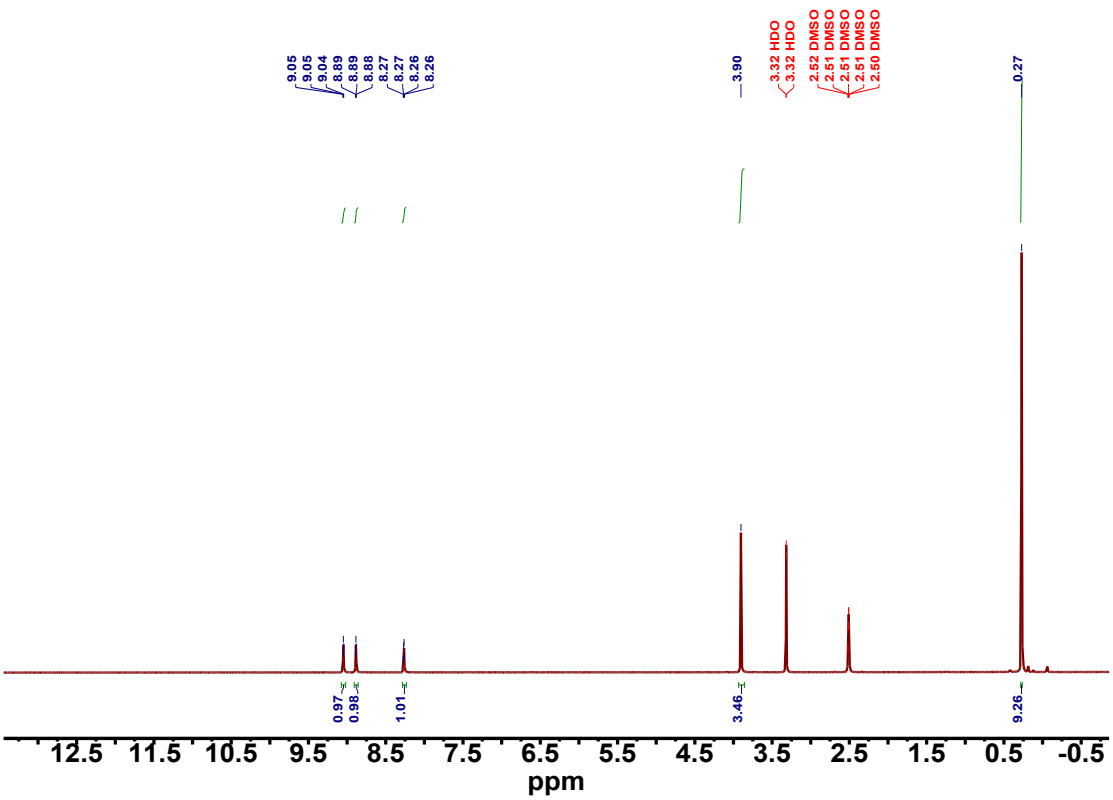


Fig. S69 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of compound **7**.

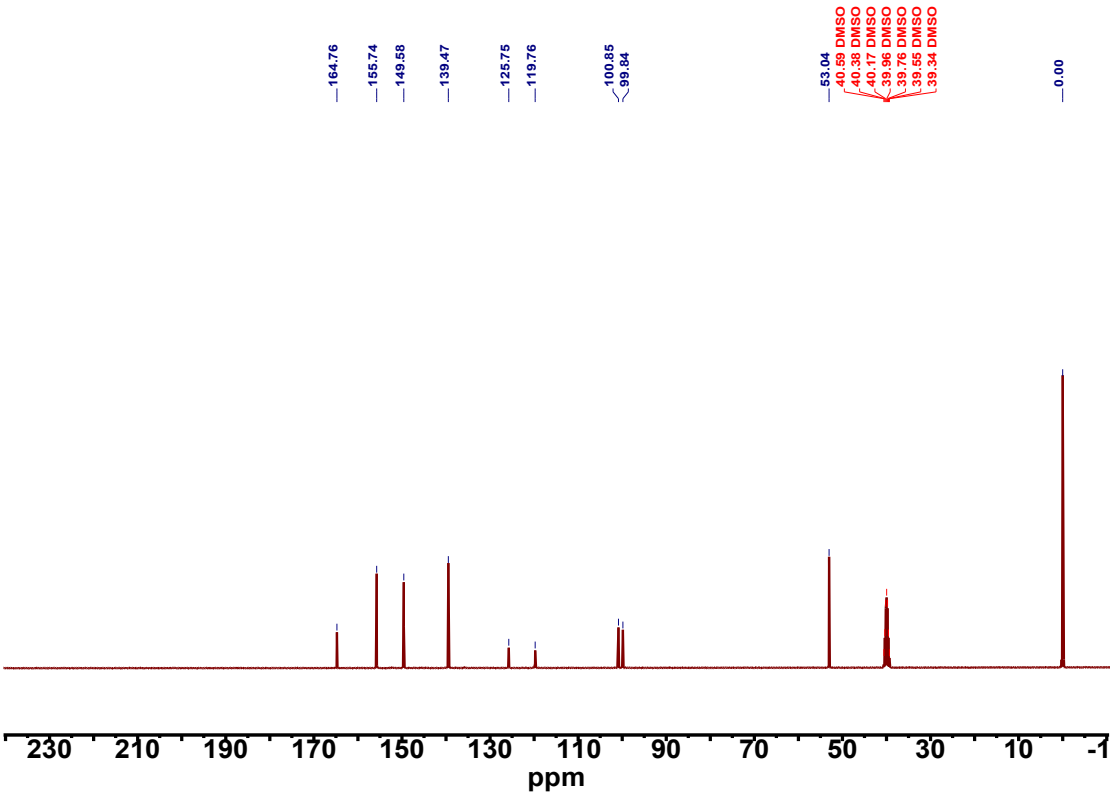


Fig. S70 ^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K) of compound **7.**

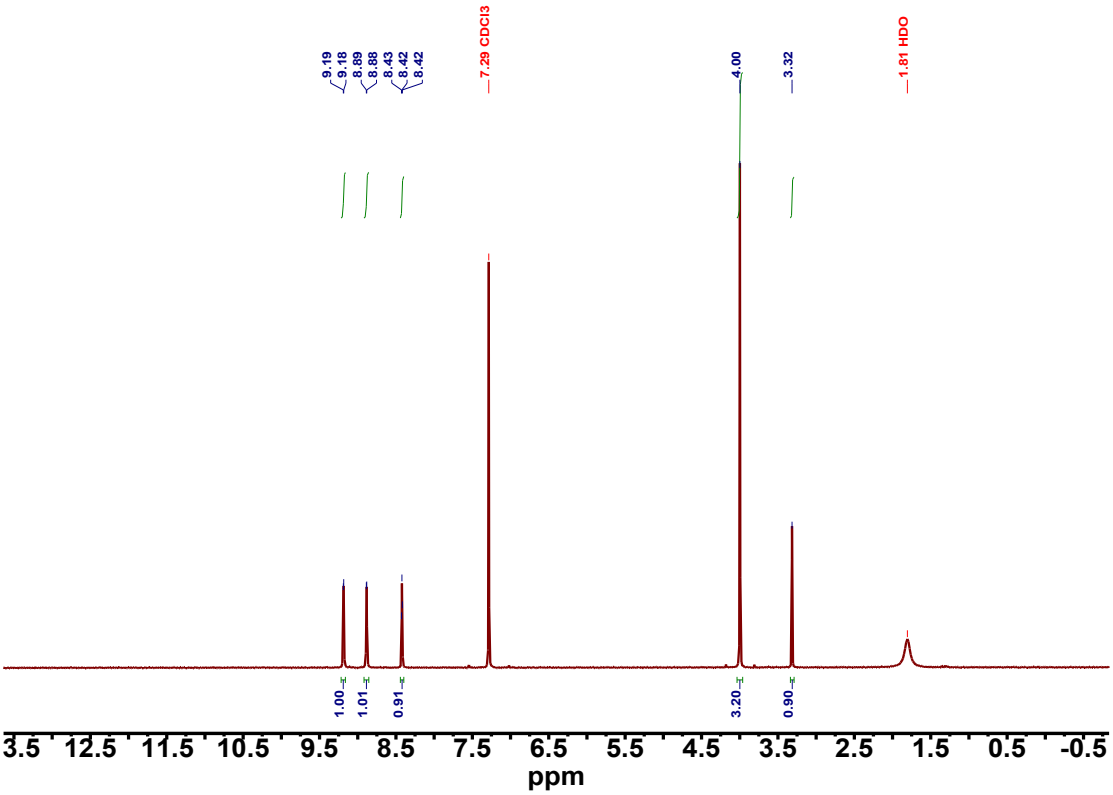


Fig. S71 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of compound **5a**.

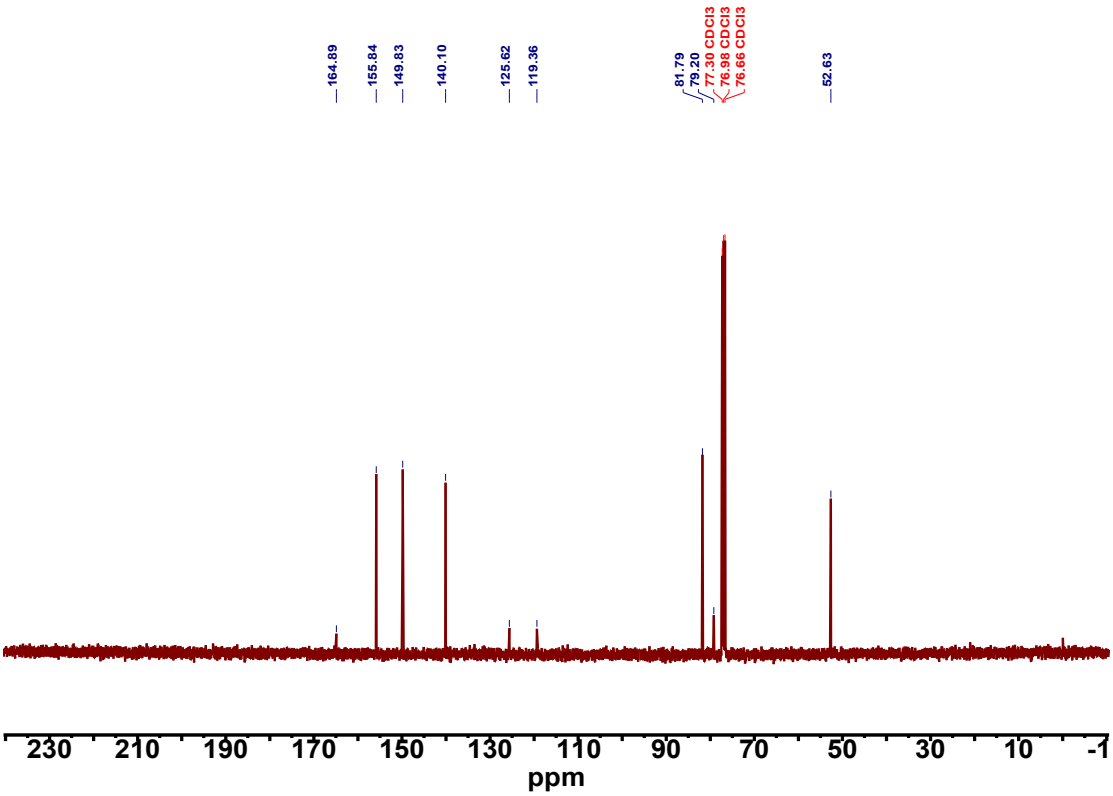


Fig. S72 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **5a**.

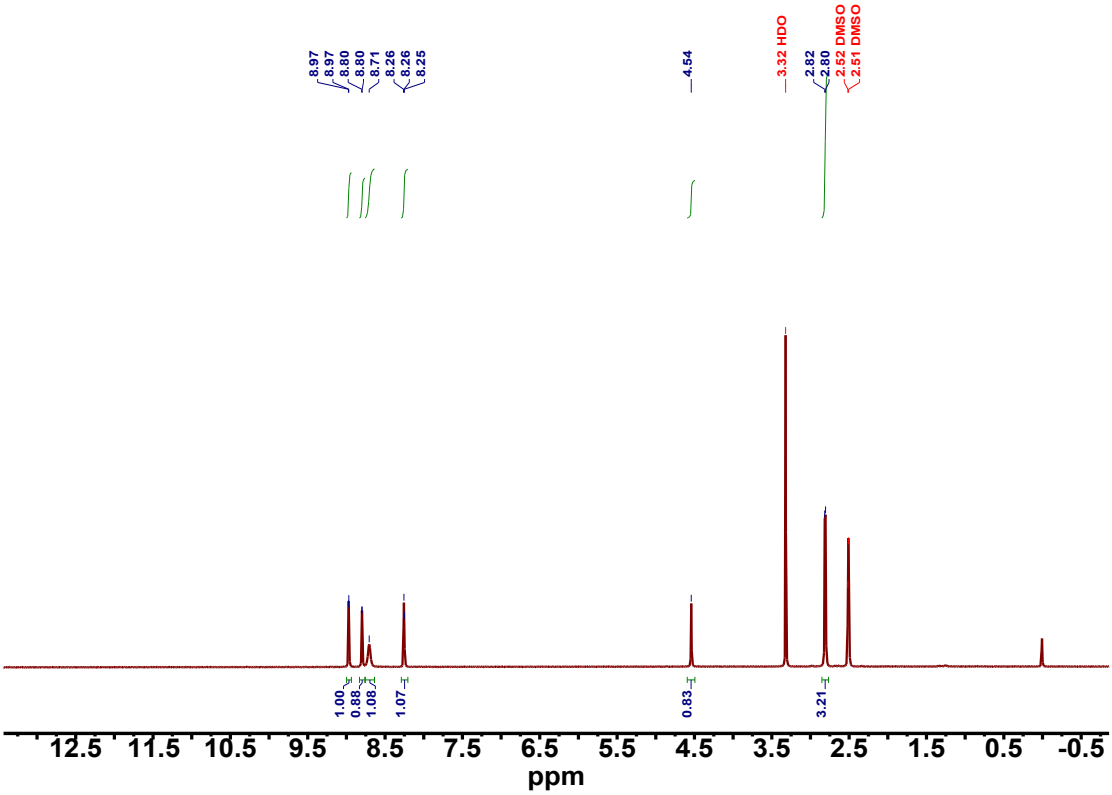


Fig. S73 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of compound **5b**.

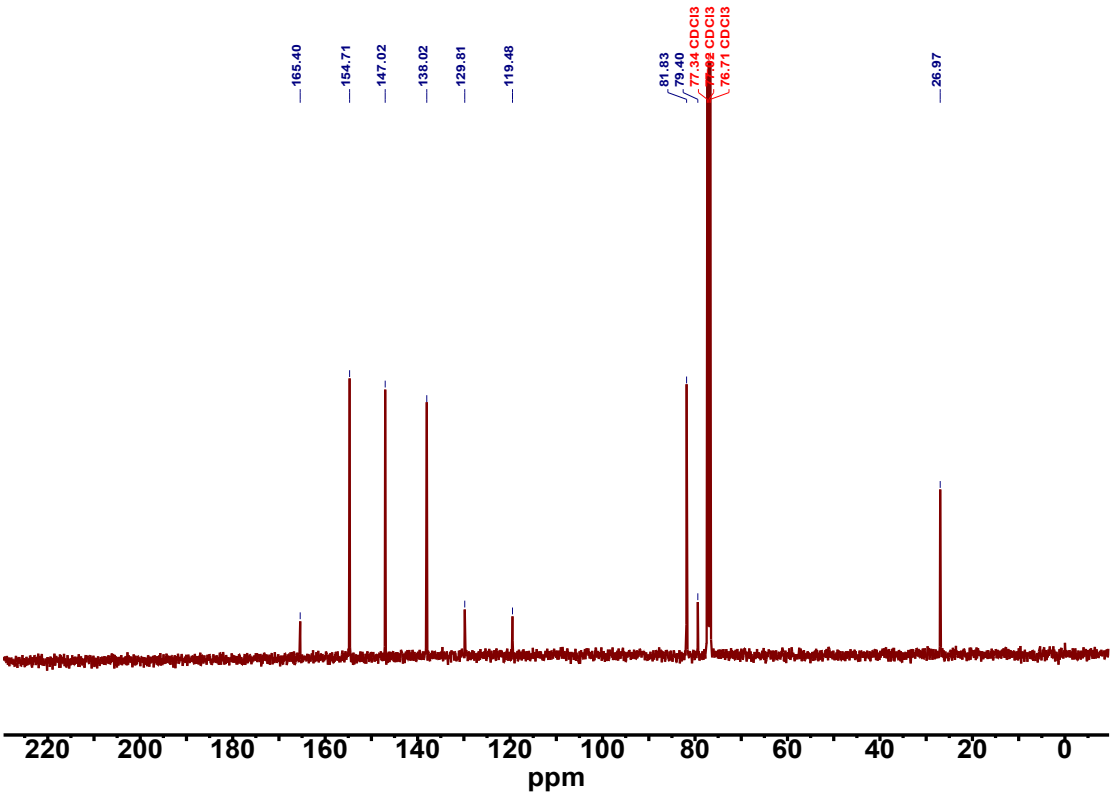


Fig. S74 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **5b**.

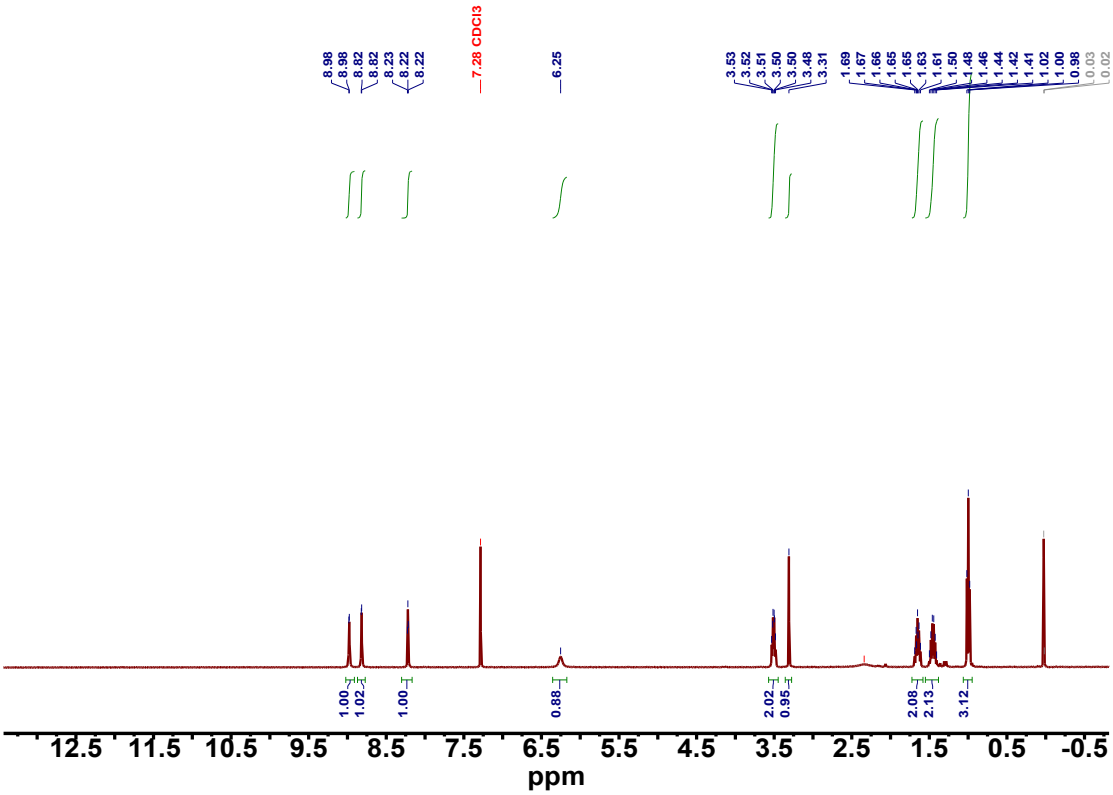


Fig. S75 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of compound **5c**.

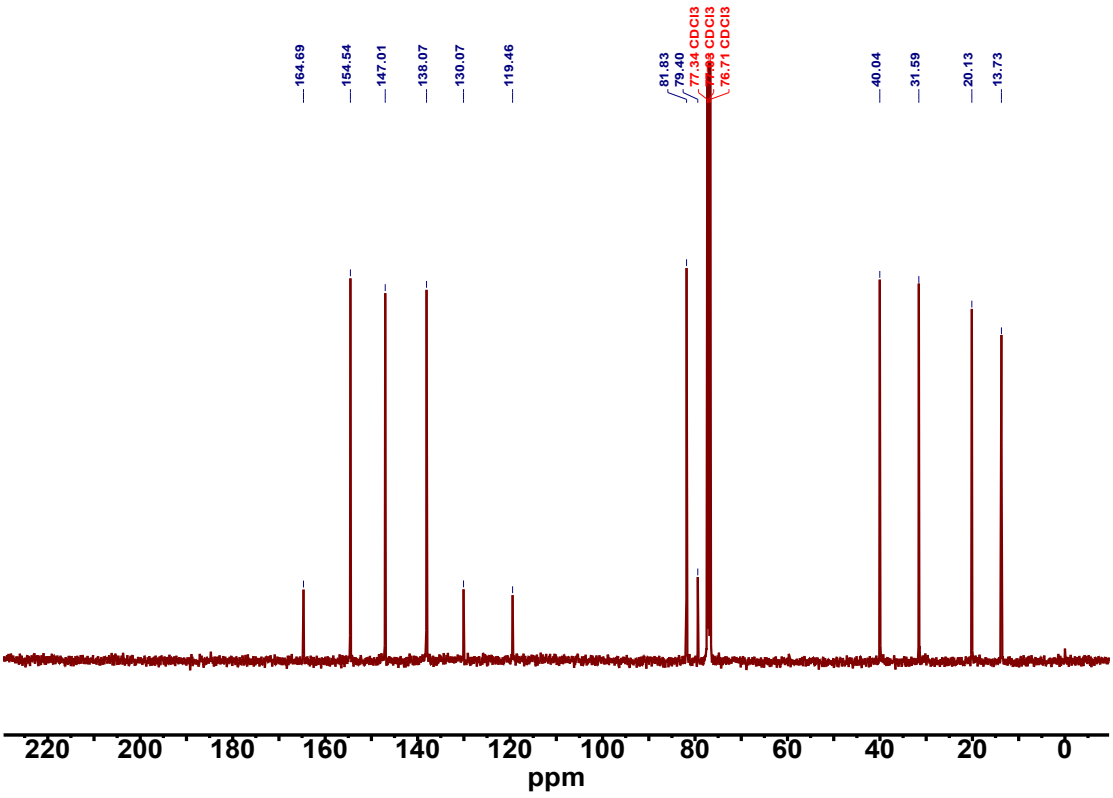


Fig. S76 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **5c**.

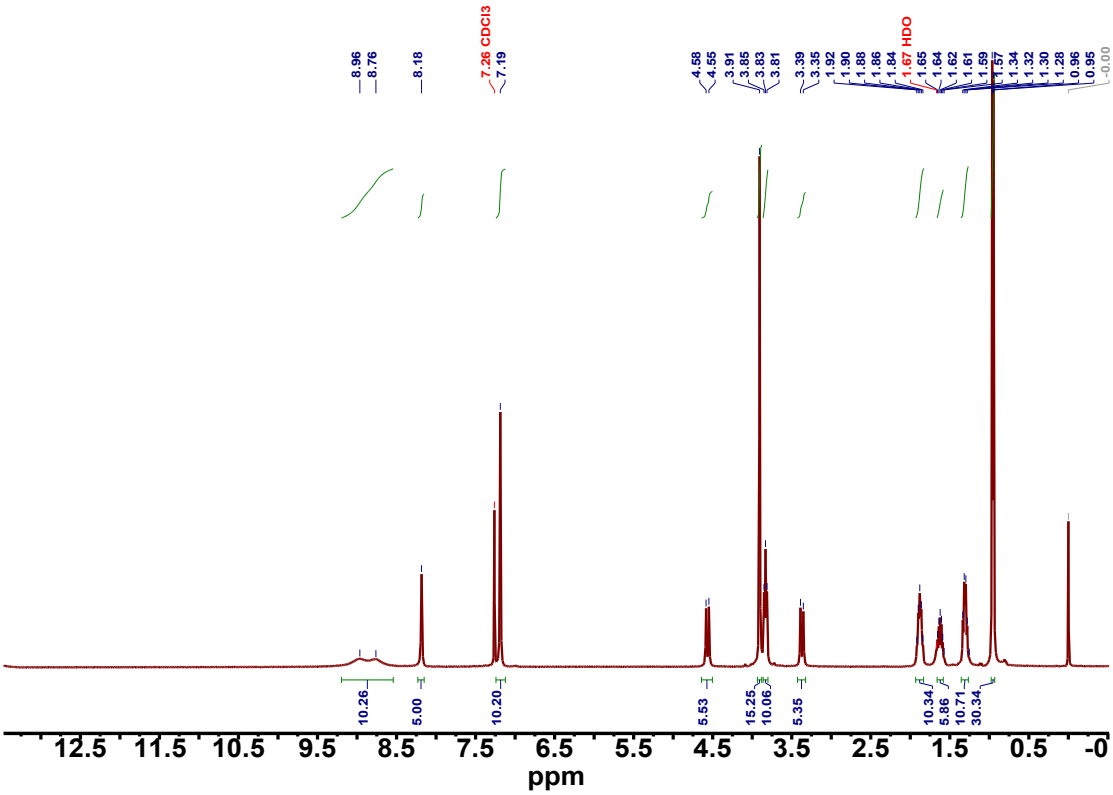


Fig. S77 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **C5A-a**.

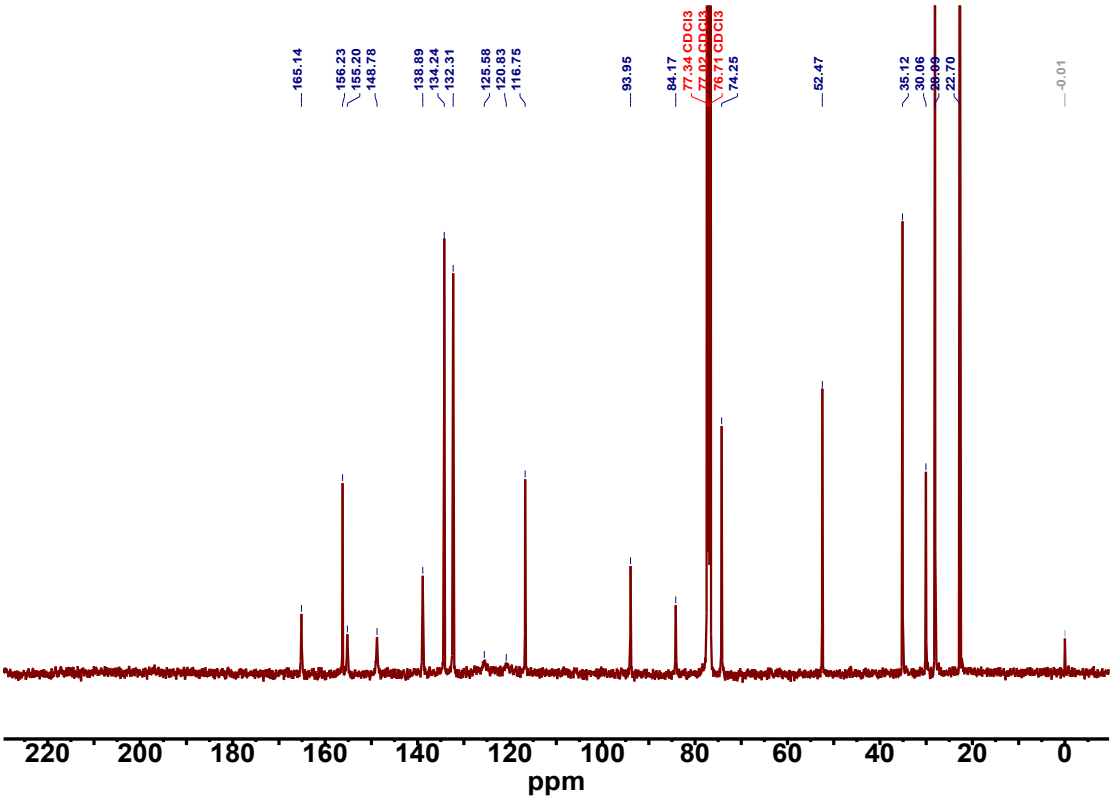


Fig. S78 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **C5A-a**

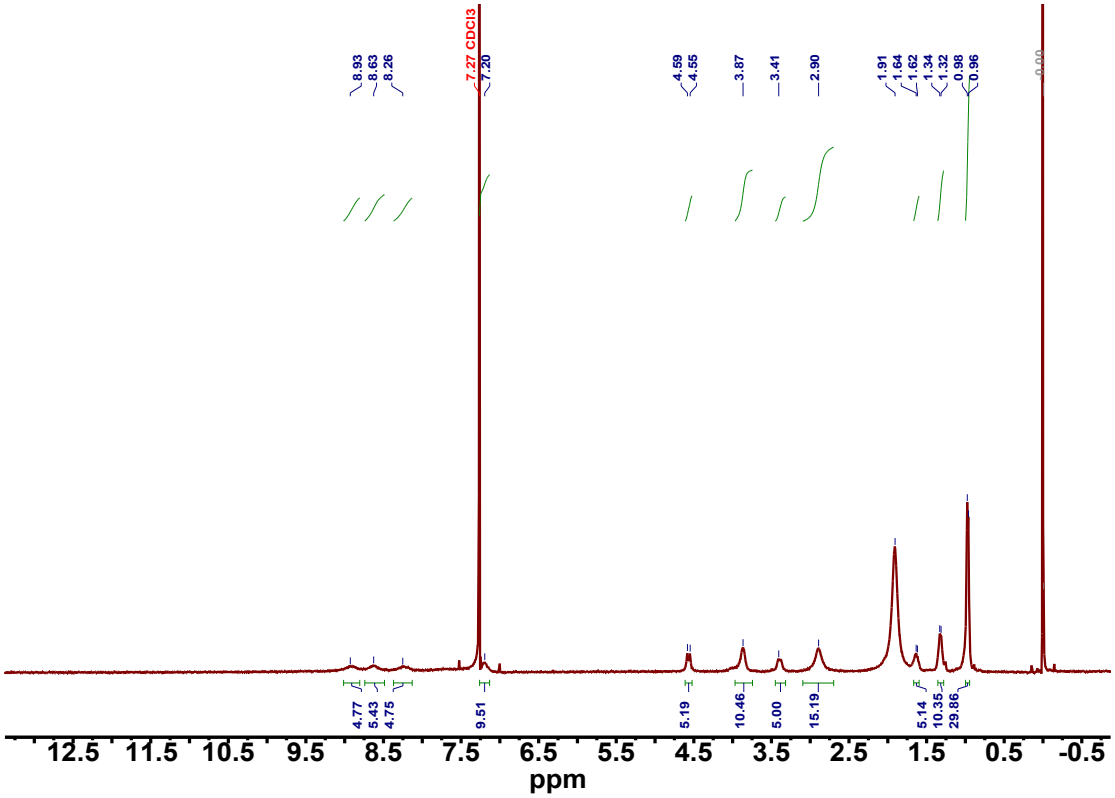


Fig. S79 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **C5A-b**.

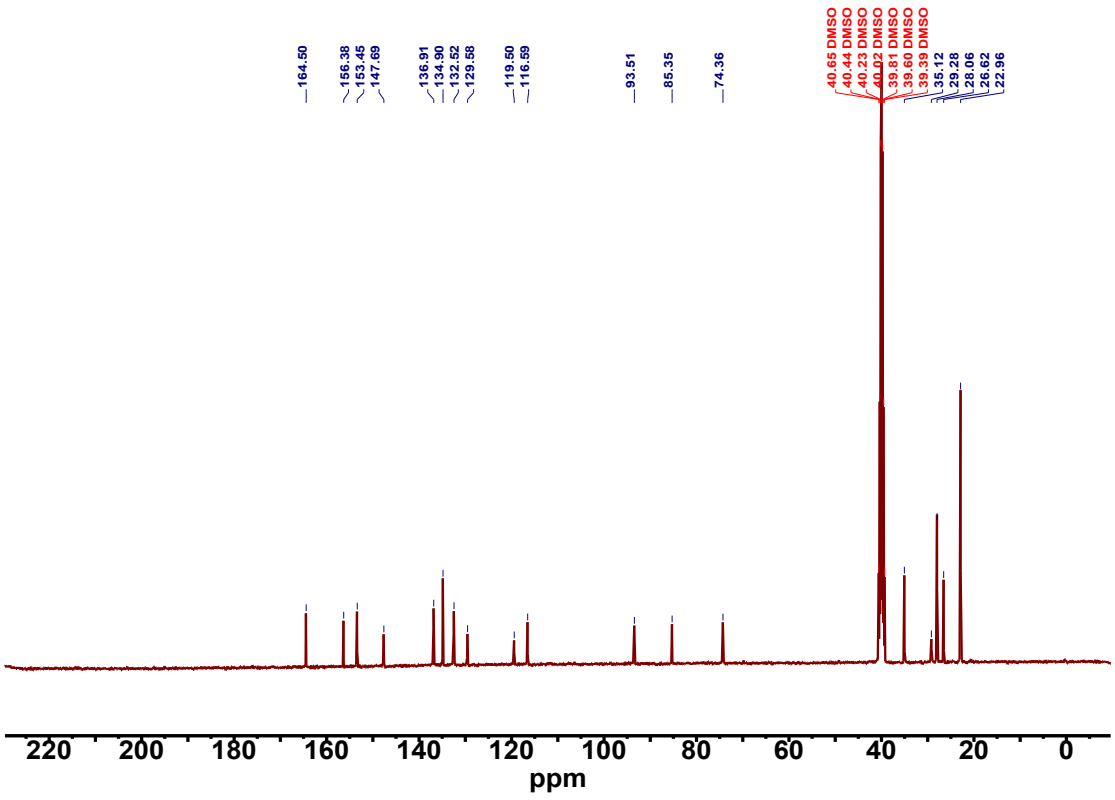


Fig. S80 ^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K) of **C5A-b**.

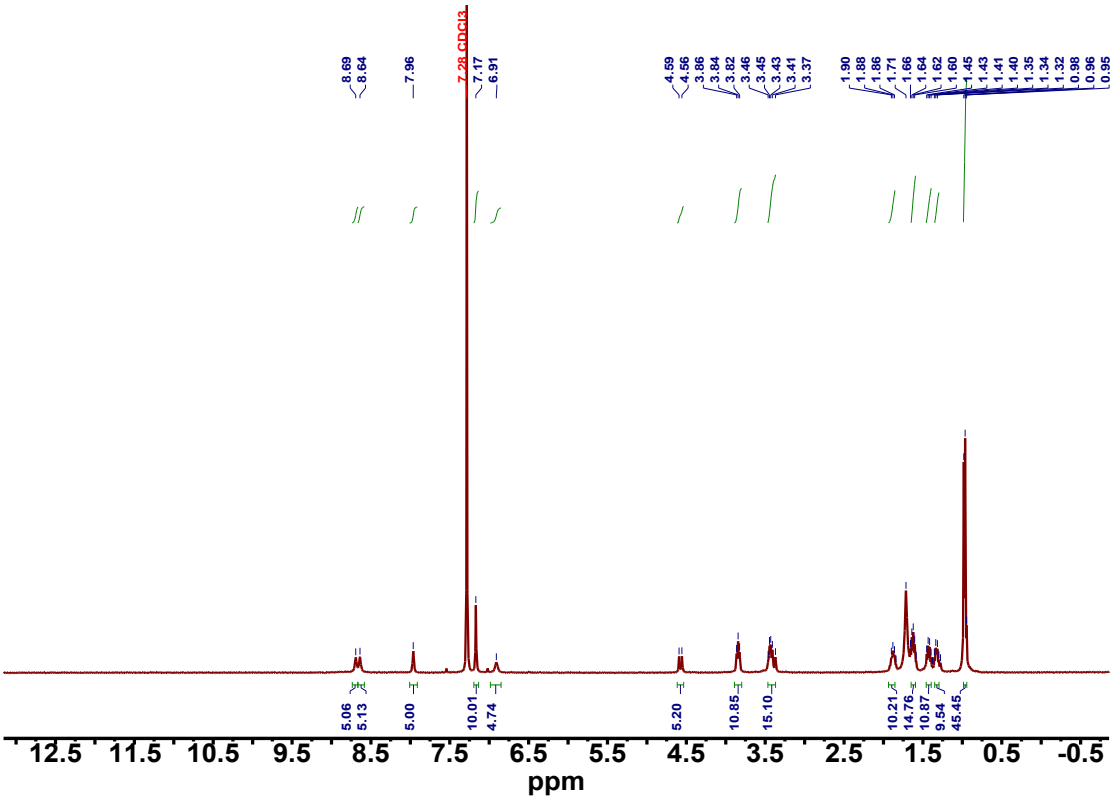


Fig. S81 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **C5A-c**.

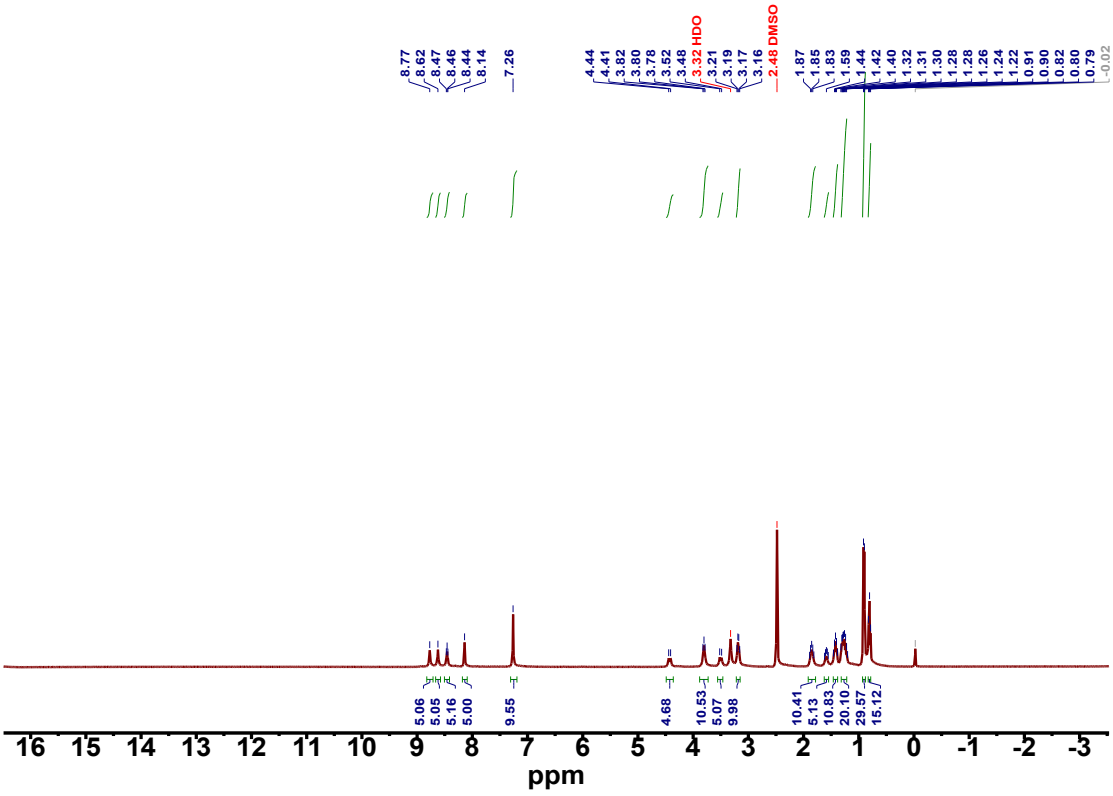


Fig. S82 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **C5A-c**.

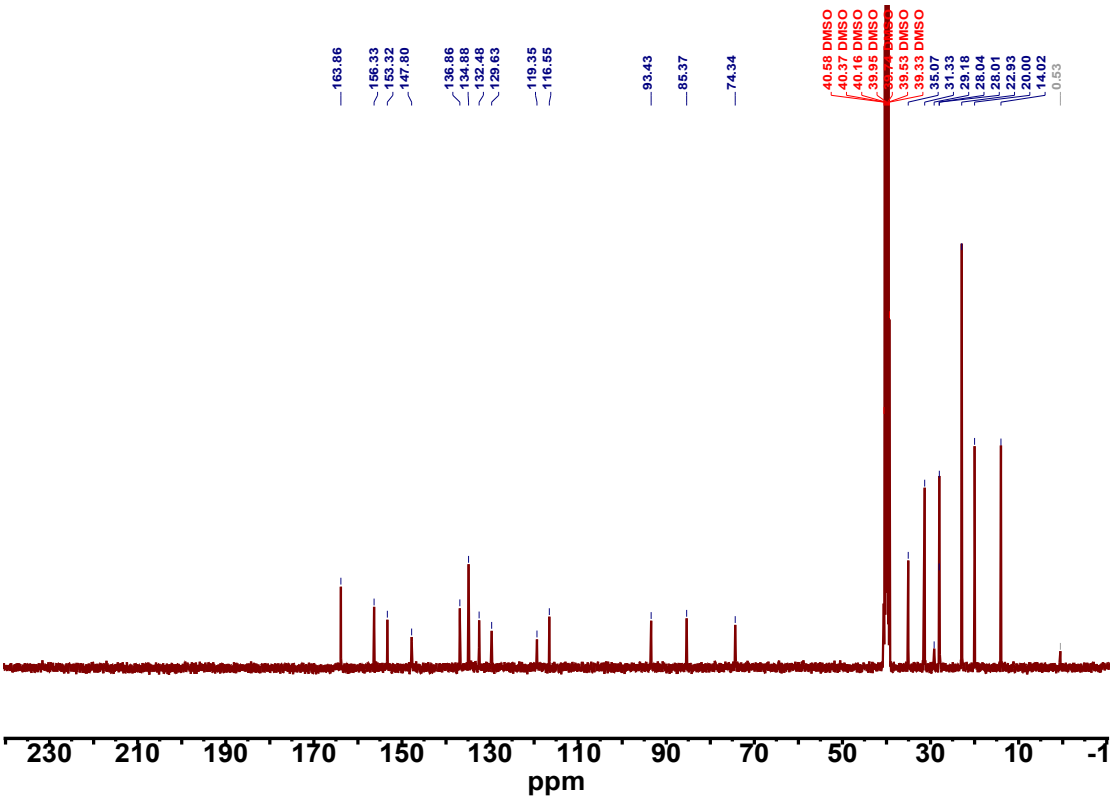


Fig. S83 ^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K) of **C5A-c**.

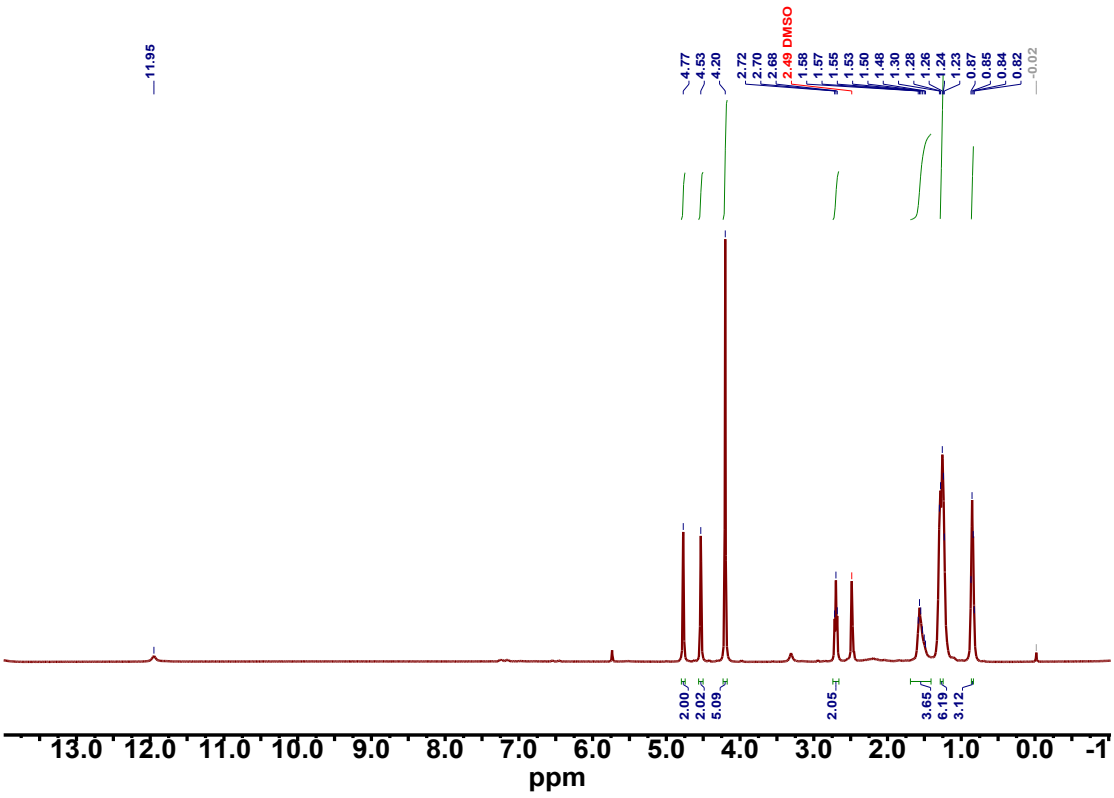


Fig. S84 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **G-f**.

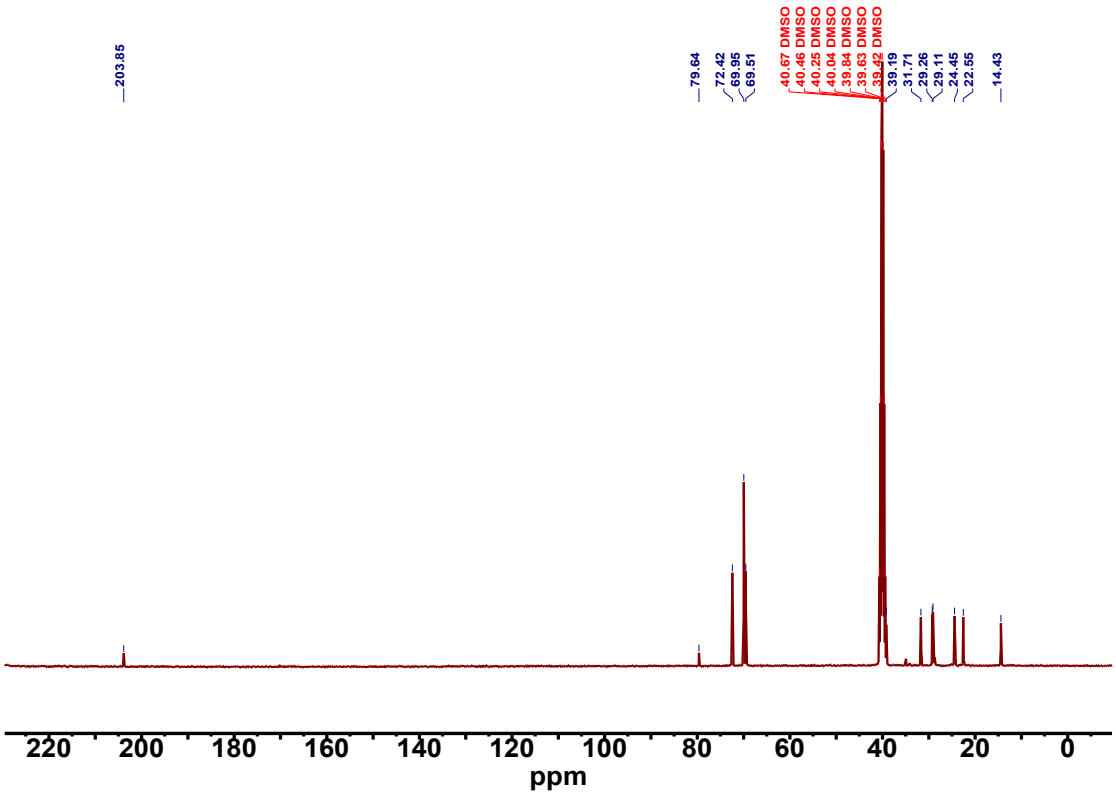


Fig. S85 ^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K) of **G-f**.

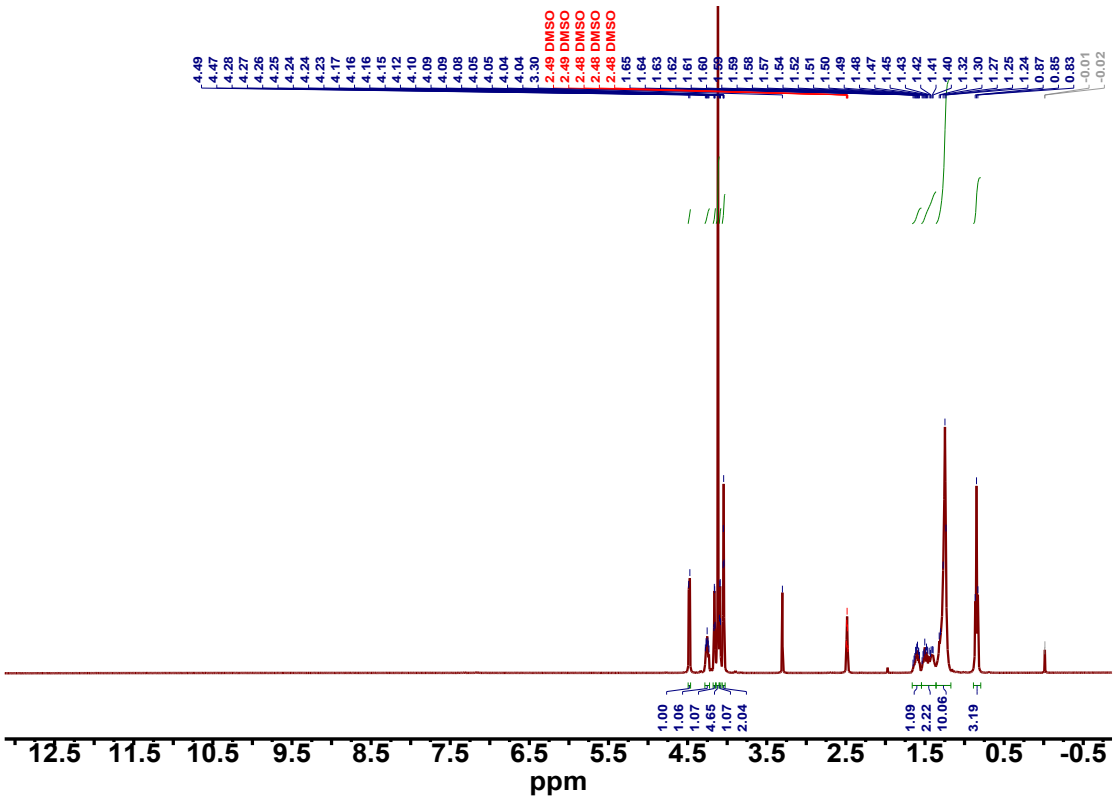


Fig. S86 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **G-g**.

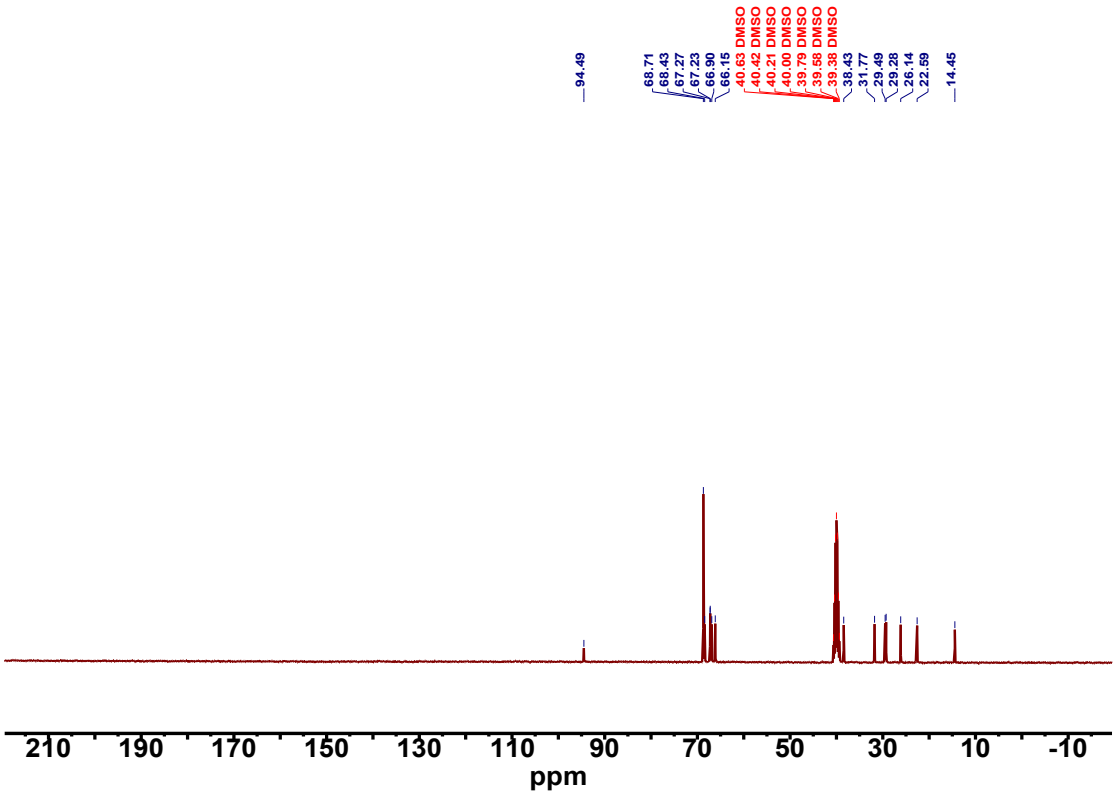


Fig. S87 ^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K) of **G-g**.

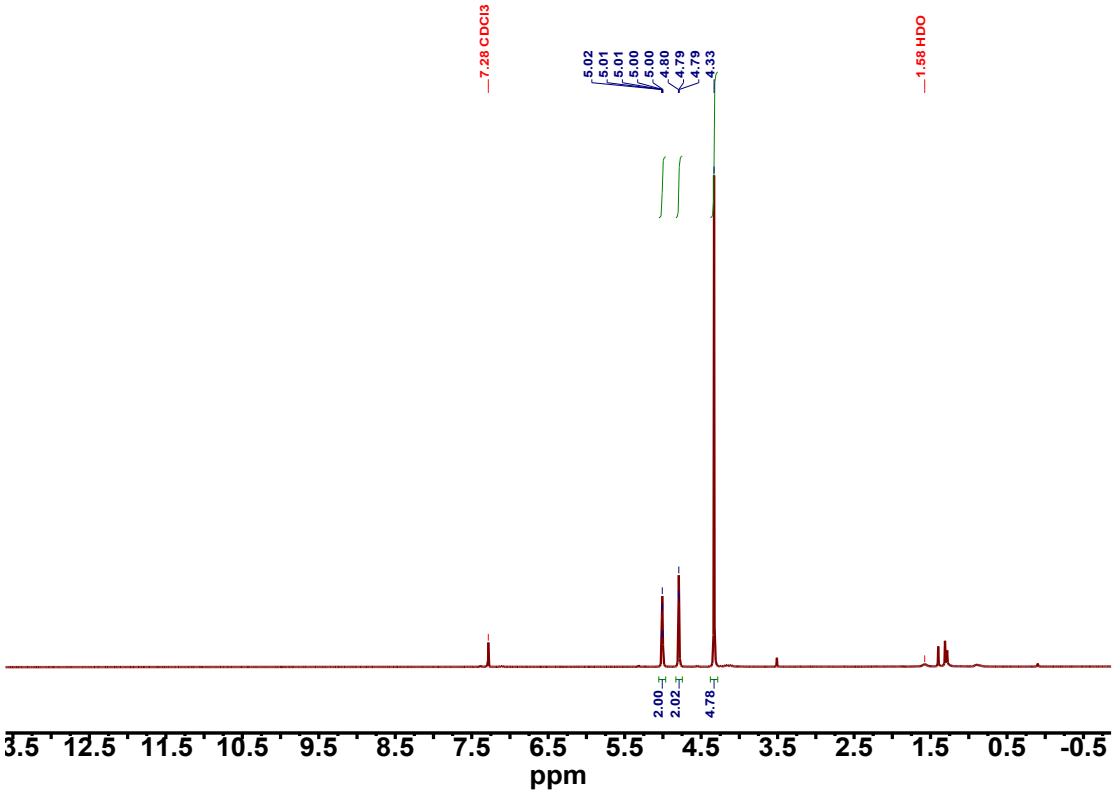


Fig. S88 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **G-h**.

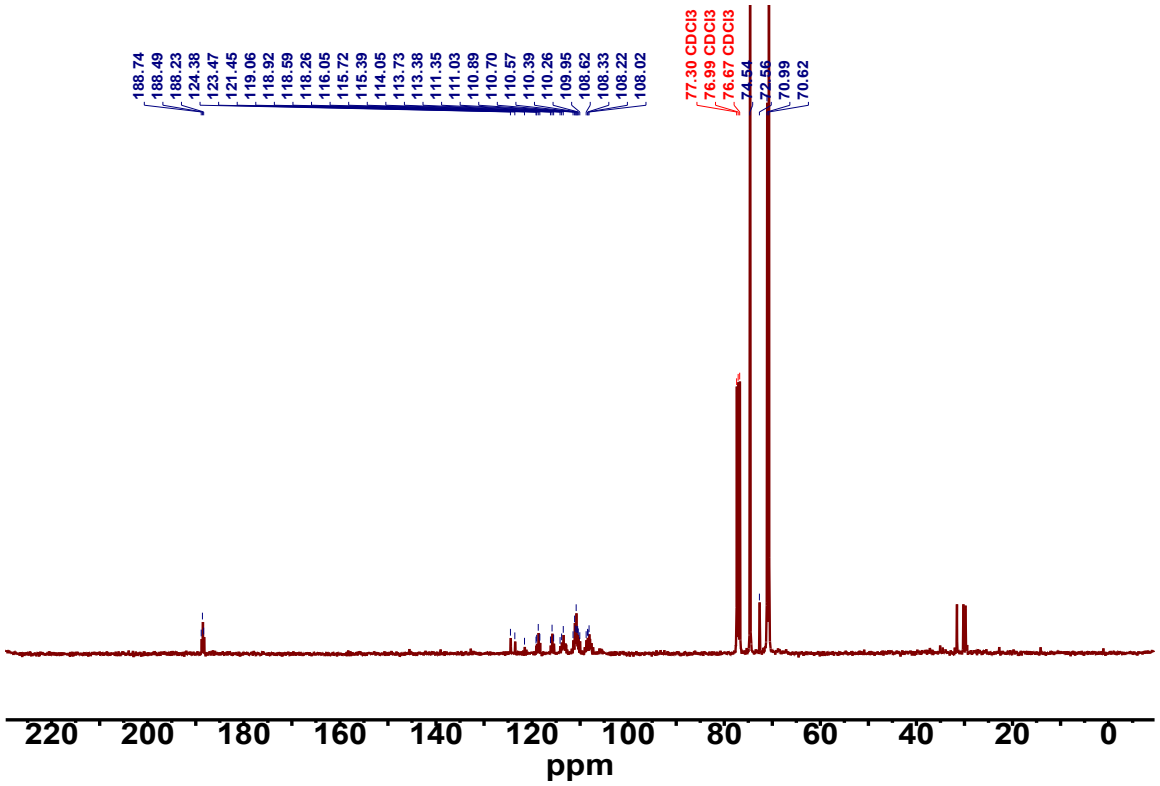


Fig. S89 ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **G-h**.

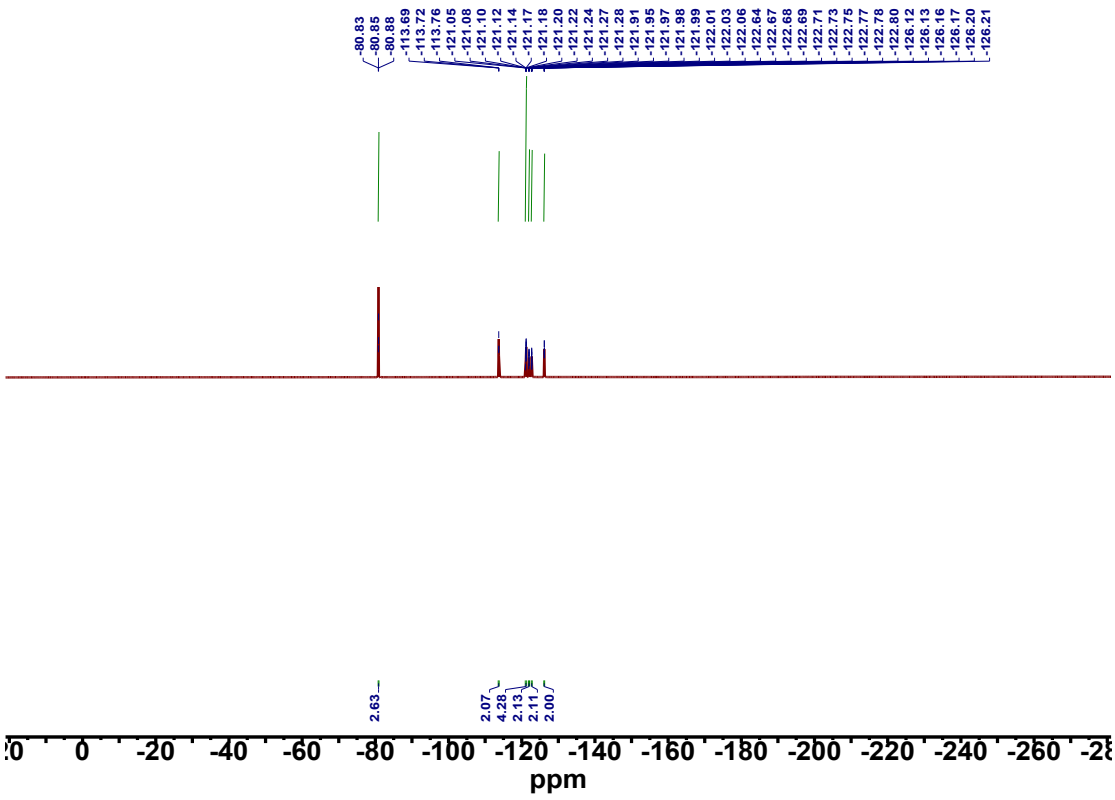


Fig. S90 ^{19}F NMR (376 MHz, $CDCl_3$, 298 K) of **G-h**.

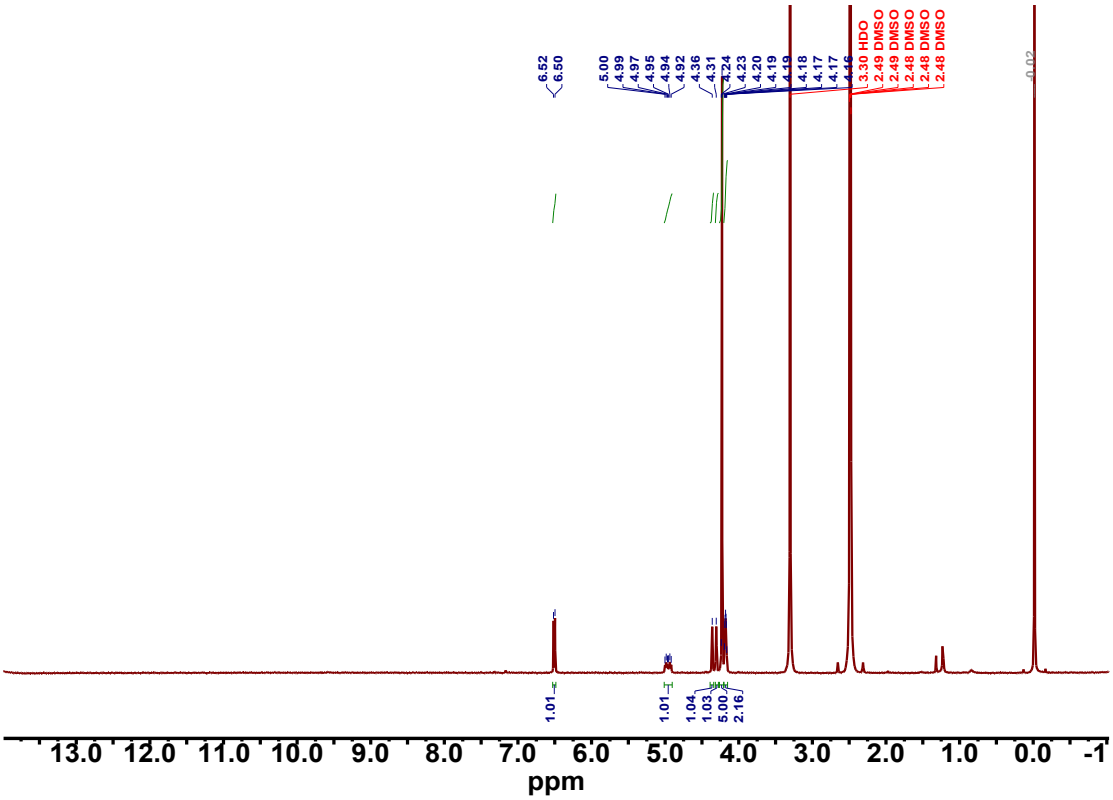


Fig. S91 ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **G-i**.

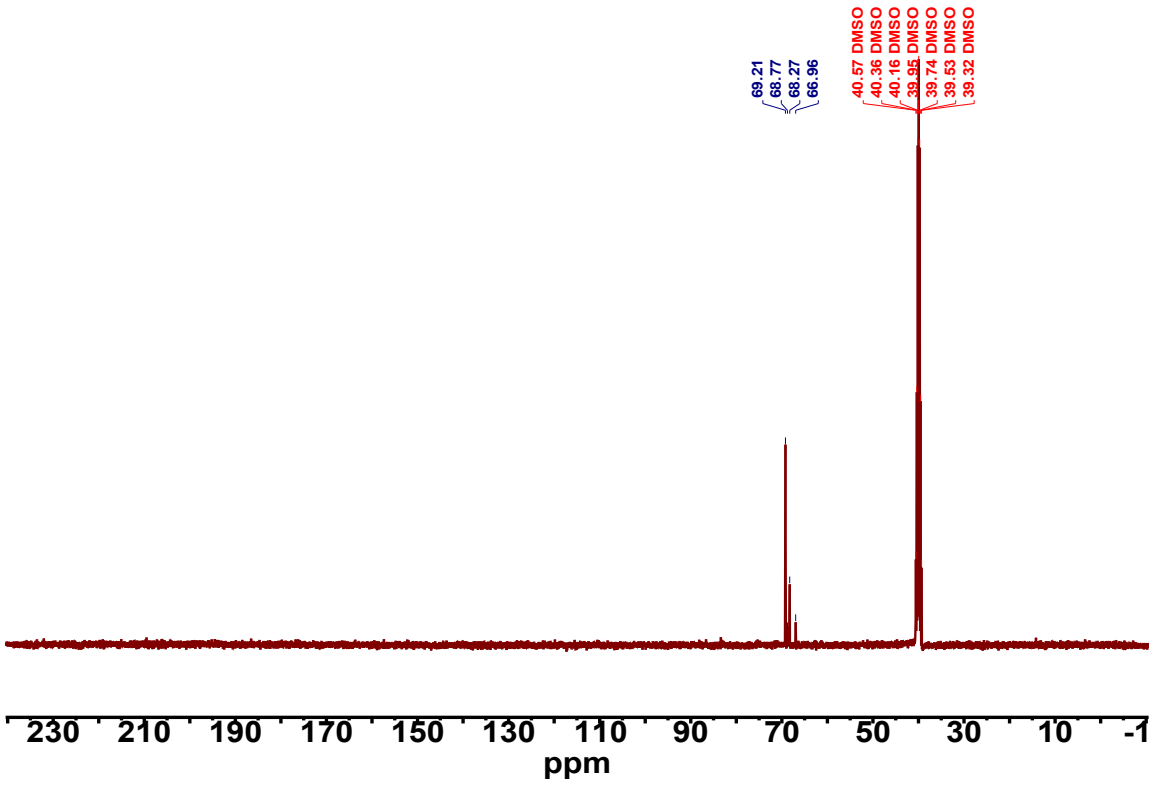


Fig. S92 ^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K) of **G-i**.

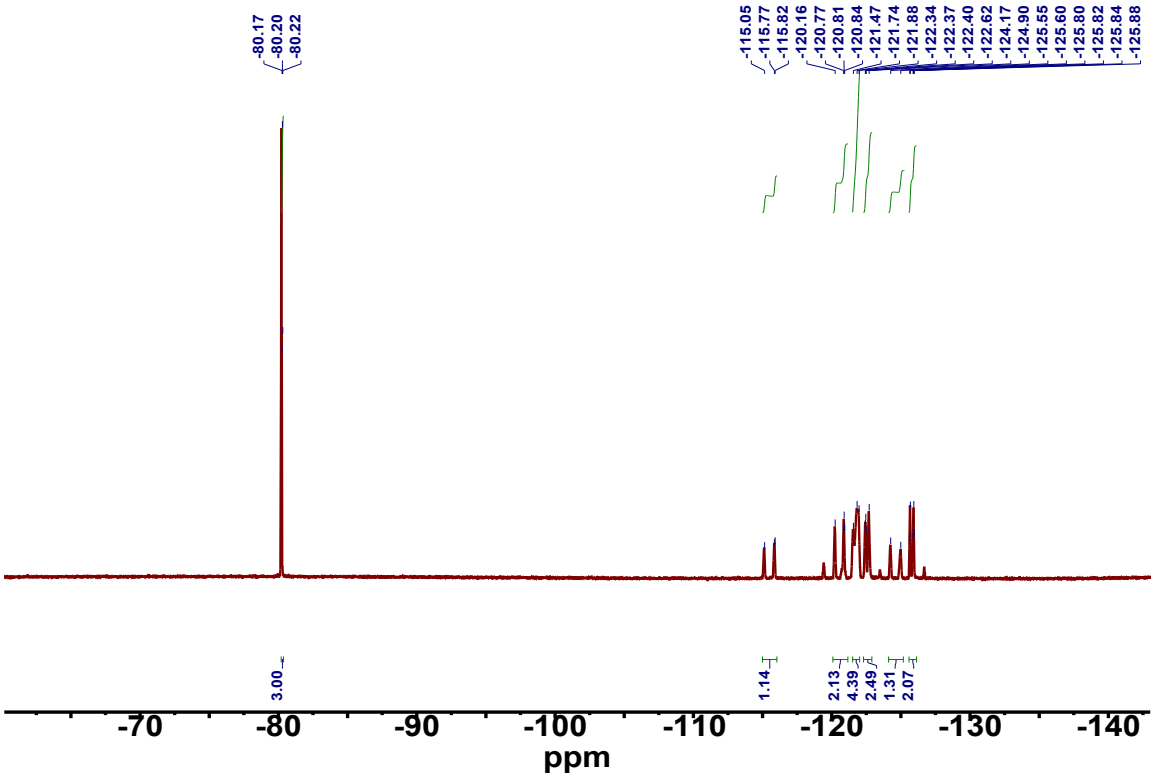


Fig. S93 ^{19}F NMR (376 MHz, DMSO-d_6, 298 K) of **G-i**.

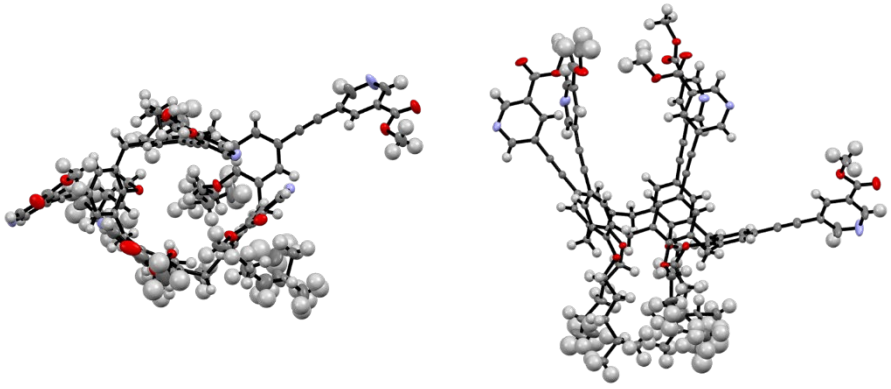


Fig. S94 ORTEP drawing of **C5A-a** (the thermal ellipsoids are displayed at a 30% probability).

CCDC code	2345649
Empirical formula	$C_{110}H_{115}N_5O_{15}$
Formula weight	1747.06
Temperature/K	273.15
Crystal system	triclinic
Space group	P-1
a/Å	14.650(3)
b/Å	17.194(3)
c/Å	20.570(4)

α/°	106.008(10)
β/°	95.714(10)
γ/°	94.420(11)
Volume/Å^3	4925.8(17)
Z	2
ρ_{calc}g/cm^3	1.178
μ/mm^{-1}	0.625
F(000)	1860.0
Crystal size/mm^3	0.2 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.504 to 133.838
Index ranges	-17 ≤ h ≤ 17, -20 ≤ k ≤ 20, -24 ≤ l ≤ 24
Reflections collected	60186
Independent reflections	17034 [R_{int} = 0.1634, R_{sigma} = 0.1686]
Data/restraints/parameters	17034/12/1206
Goodness-of-fit on F^2	1.194
Final R indexes [I>=2σ (I)]	R_1 = 0.1089, wR_2 = 0.2877
Final R indexes [all data]	R_1 = 0.2011, wR_2 = 0.3324
Largest diff. peak/hole / e Å^{-3}	0.85/-0.50

The coordinates of the optimized structure of C5A-c and complex C5A-c•G-a

Table S1. The coordinates of the optimized structure of **C5A-c**

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C	-3.94800000	10.38100000	5.96760000	H	-7.47930000	11.70450000	8.69040000
C	-5.10800000	10.73680000	5.24720000	H	-10.25260000	11.59830000	7.29960000
C	-5.16740000	10.61290000	3.83980000	H	-10.98290000	10.61140000	9.43550000
C	-4.01700000	10.22080000	3.14940000	H	-9.56210000	9.71350000	8.90040000
C	-2.81930000	9.98900000	3.84290000	H	-9.41680000	10.90720000	10.20570000
C	-2.81820000	9.97740000	5.24570000	H	-11.00110000	13.15500000	9.19880000
C	-6.27470000	12.56290000	6.29320000	H	-9.30900000	13.46710000	9.58550000
C	-7.66960000	12.82780000	6.85030000	H	-9.96000000	13.94720000	8.01480000
C	-8.13330000	11.71010000	7.78560000	H	-6.72610000	10.09050000	2.43790000
C	-9.61190000	11.79330000	8.20840000	H	-7.26560000	11.03290000	3.84820000
C	-9.90950000	10.69430000	9.23960000	C	-6.29880000	12.20350000	2.29230000
C	-9.98900000	13.16100000	8.78020000	C	-7.13770000	13.31960000	2.49440000
O	-6.26260000	11.13260000	5.91000000	C	-6.86270000	14.57080000	1.89510000
C	-6.43380000	10.93780000	3.09370000	C	-5.79880000	14.66310000	0.99300000
H	-4.03140000	10.14270000	2.05820000	C	-4.98050000	13.55130000	0.74210000
H	-1.90100000	9.69970000	5.77580000	C	-5.25490000	12.32550000	1.36740000
H	-6.06490000	13.16140000	5.39100000	C	-9.30580000	12.36730000	3.01370000
H	-5.48490000	12.70990000	7.05340000	C	-9.54230000	11.55150000	4.27790000
H	-7.64160000	13.80670000	7.39600000	C	-10.70540000	10.57190000	4.14170000
H	-8.39490000	12.97670000	6.01580000	C	-11.00960000	9.88780000	5.49300000
H	-7.95450000	10.72990000	7.29370000	C	-12.41130000	9.26910000	5.47560000

C	-9.94660000	8.83770000	5.83370000	H	-12.49620000	13.86260000	7.54420000
O	-8.22240000	13.29680000	3.35890000	H	-13.63460000	14.61460000	6.42390000
C	-7.63850000	15.80240000	2.28870000	H	-12.91270000	13.03530000	3.91810000
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H	-4.61250000	11.46510000	1.15260000	H	-11.48020000	13.88680000	3.32530000
H	-9.05260000	11.76180000	2.13230000	H	-5.78410000	19.09140000	6.67650000
H	-10.15730000	13.04270000	2.77730000	H	-6.47830000	17.46760000	6.89610000
H	-8.60130000	11.01400000	4.55960000	C	-4.32460000	17.55260000	7.03760000
H	-9.72550000	12.25540000	5.13150000	C	-4.29200000	16.48860000	7.96600000
H	-11.60890000	11.10330000	3.78310000	C	-3.09890000	16.09460000	8.60770000
H	-10.48380000	9.81130000	3.37010000	C	-1.90010000	16.70590000	8.22450000
H	-10.98540000	10.67730000	6.30180000	C	-1.89590000	17.67550000	7.20950000
H	-12.64170000	8.78030000	6.42870000	C	-3.10910000	18.14610000	6.68020000
H	-13.18260000	10.02770000	5.30370000	C	-6.30950000	16.04560000	9.24330000
H	-12.51420000	8.51150000	4.69140000	C	-7.69070000	16.13070000	8.60160000
H	-10.14980000	8.36360000	6.79970000	C	-8.77160000	16.41850000	9.63950000
H	-9.89880000	8.04320000	5.08250000	C	-10.16350000	16.61020000	9.00440000
H	-8.94860000	9.29020000	5.89840000	C	-11.25750000	16.46630000	10.06790000
H	-8.12480000	16.25800000	1.40010000	C	-10.26910000	17.96120000	8.28840000
H	-8.48220000	15.50680000	2.96160000	O	-5.42300000	15.70660000	8.13230000
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C	-6.66260000	17.00900000	4.34420000	H	-0.95680000	16.39750000	8.68030000
C	-5.67060000	17.83360000	4.93290000	H	-3.09180000	18.95820000	5.94570000
C	-4.72720000	18.44110000	4.10330000	H	-5.99410000	16.97360000	9.73950000
C	-4.74580000	18.21540000	2.71700000	H	-6.21580000	15.18190000	9.94240000
C	-5.76920000	17.44470000	2.14850000	H	-7.67030000	16.90490000	7.79760000
C	-8.91670000	16.67850000	5.18910000	H	-7.89560000	15.17540000	8.05410000
C	-9.62220000	15.33420000	5.06290000	H	-8.80920000	15.57680000	10.37240000
C	-10.99250000	15.32690000	5.73520000	H	-8.50660000	17.31270000	10.23560000
C	-11.74710000	14.00340000	5.49240000	H	-10.32280000	15.79750000	8.23260000
C	-12.87480000	13.83180000	6.51640000	H	-12.25570000	16.57070000	9.62830000
C	-12.29720000	13.92990000	4.06290000	H	-11.22000000	15.48610000	10.55580000
O	-7.48900000	16.35520000	5.24380000	H	-11.16830000	17.22630000	10.85180000
C	-5.61670000	18.02070000	6.42520000	H	-11.28390000	18.14120000	7.91740000
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H	-9.13960000	17.37470000	4.36820000	H	-2.48640000	15.25490000	10.50780000
H	-9.10360000	17.18740000	6.16190000	H	-4.11550000	14.78290000	9.98750000
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H	-10.86200000	15.48110000	6.83520000	C	-2.90620000	11.53910000	7.90650000
H	-11.60200000	16.18180000	5.38970000	C	-1.57000000	11.53390000	7.49110000
H	-11.01940000	13.15450000	5.63130000	C	-0.72680000	12.62000000	7.77370000
H	-13.38080000	12.86810000	6.38830000	C	-1.20240000	13.70440000	8.52870000

C	-4.90040000	12.26850000	10.49360000	C	0.72880000	10.40030000	2.00660000
C	-6.33990000	12.70850000	10.73280000	C	0.84610000	11.54440000	1.17770000
C	-6.84980000	12.25680000	12.10040000	N	2.02140000	11.92390000	0.61960000
C	-8.38810000	12.33440000	12.20720000	C	3.13110000	11.18660000	0.88150000
C	-8.86270000	11.59800000	13.46650000	C	3.09450000	10.03890000	1.69510000
C	-8.88560000	13.78320000	12.21320000	C	1.87930000	9.63240000	2.25530000
O	-4.68760000	12.62630000	9.08470000	C	4.33400000	9.24030000	1.96950000
C	-3.87050000	10.46750000	7.46900000	O	4.41860000	8.04170000	1.71760000
H	-1.17750000	10.69130000	6.91260000	N	5.38450000	9.96980000	2.49170000
H	-0.53790000	14.54530000	8.74020000	C	6.63330000	9.31270000	2.95200000
H	-4.17020000	12.79240000	11.12940000	H	-0.02650000	12.17790000	0.96200000
H	-4.75580000	11.17800000	10.57550000	H	4.06520000	11.53410000	0.41800000
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H	-6.98150000	12.29310000	9.91160000	H	5.24500000	10.94050000	2.80410000
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H	-8.83150000	11.80830000	11.31130000	C	0.57030000	12.68990000	7.20790000
H	-9.95520000	11.61230000	13.54780000	C	1.64280000	12.82170000	6.66260000
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H	-3.57490000	9.48400000	7.89480000	C	3.78120000	13.99550000	6.50270000
H	-4.88700000	10.67420000	7.88970000	C	5.97700000	15.18180000	6.37230000
C	-3.79450000	13.68740000	-0.02080000	O	6.61010000	14.98810000	7.40640000
C	-2.71510000	13.80350000	-0.55610000	H	2.58920000	11.49080000	4.48000000
C	-1.41140000	13.91550000	-1.08330000	H	6.24290000	13.50110000	4.16950000
C	-0.63340000	15.06920000	-0.82000000	H	3.52860000	14.59600000	7.38090000
N	0.66390000	15.17410000	-1.20190000	C	-0.67210000	18.06790000	6.61250000
C	1.23450000	14.12980000	-1.85540000	C	0.34820000	18.28010000	5.99670000
C	0.51350000	12.96460000	-2.18580000	C	1.50890000	18.47230000	5.21780000
C	-0.82600000	12.85920000	-1.80600000	C	2.36940000	17.37750000	4.94920000
C	1.21640000	11.87540000	-2.93720000	N	3.45750000	17.48690000	4.14910000
O	1.77160000	12.06810000	-4.01360000	C	3.73300000	18.69370000	3.58790000
N	1.16790000	10.62460000	-2.34230000	C	2.93880000	19.82900000	3.82600000
C	1.97750000	9.48890000	-2.85370000	C	1.81400000	19.72110000	4.64950000
H	-1.05780000	15.92720000	-0.28020000	C	3.30580000	21.16030000	3.23850000
H	2.29670000	14.23490000	-2.11800000	O	3.77140000	22.07150000	3.91630000
H	-1.41610000	11.97330000	-2.05470000	N	3.12180000	21.25730000	1.87470000
H	0.78720000	10.51150000	-1.40350000	C	3.32630000	22.53570000	1.14830000
H	2.32610000	9.71560000	-3.88850000	H	2.17420000	16.38590000	5.38090000
C	-1.58370000	9.94860000	3.15080000	H	4.61550000	18.73830000	2.93490000
C	-0.51400000	10.10690000	2.60650000	H	1.18190000	20.59010000	4.84960000

H	2.62970000	20.51820000	1.35400000	H	6.77220000	19.55170000	6.60000000
H	3.86930000	23.25730000	1.80220000	C	4.97190000	18.54730000	7.29820000
C	-3.65970000	18.63860000	1.91310000	H	5.38870000	18.21390000	8.26920000
C	-2.67650000	18.87030000	1.24610000	H	4.29160000	17.73530000	6.97280000
C	-1.51860000	19.06720000	0.46560000	C	4.17770000	19.83690000	7.48510000
C	-0.32270000	19.55500000	1.04630000	H	3.32290000	19.68500000	8.15370000
N	0.82060000	19.70450000	0.33310000	H	3.78320000	20.21480000	6.53350000
C	0.82070000	19.37030000	-0.98360000	H	4.79200000	20.63550000	7.91690000
C	-0.32700000	18.87570000	-1.62870000	C	1.98100000	23.12080000	0.69270000
C	-1.51180000	18.73000000	-0.90030000	H	1.43090000	22.38340000	0.07360000
C	-0.32470000	18.51640000	-3.08450000	H	1.33150000	23.30820000	1.57000000
O	-1.06780000	19.05810000	-3.89750000	C	2.18680000	24.41860000	-0.09860000
N	0.59200000	17.54820000	-3.44960000	H	2.85530000	24.23400000	-0.96330000
C	0.59390000	16.96400000	-4.81630000	H	2.71010000	25.16670000	0.52990000
H	-0.27940000	19.82880000	2.10940000	C	0.85990000	24.99300000	-0.58780000
H	1.76900000	19.51000000	-1.52060000	H	0.33170000	24.29410000	-1.24730000
H	-2.42050000	18.35820000	-1.38260000	H	1.01310000	25.91980000	-1.15320000
H	1.14110000	17.05140000	-2.74320000	H	0.18540000	25.22700000	0.24400000
H	-0.08470000	17.55670000	-5.47410000	C	0.16640000	15.49010000	-4.77340000
H	3.98690000	22.33390000	0.27440000	H	0.95230000	14.87870000	-4.28530000
H	1.61920000	17.06680000	-5.23870000	H	-0.73910000	15.36870000	-4.14640000
H	1.31690000	8.59550000	-2.92580000	C	-0.09870000	14.93720000	-6.17950000
N	6.14630000	16.31270000	5.59780000	H	0.78900000	15.09620000	-6.82360000
H	5.52940000	16.49950000	4.80050000	H	-0.92510000	15.49610000	-6.66080000
C	6.95140000	17.46070000	6.09140000	C	-0.43620000	13.44940000	-6.12460000
H	7.44990000	17.17930000	7.04970000	H	0.35910000	12.87570000	-5.62340000
H	7.76470000	17.65180000	5.35320000	H	-0.55940000	13.03030000	-7.12870000
C	6.73610000	9.36480000	4.48380000	H	-1.36330000	13.26130000	-5.57250000
H	6.66100000	10.41170000	4.84040000	C	3.16950000	9.21980000	-1.92360000
H	5.87490000	8.83820000	4.94030000	H	3.80590000	10.12400000	-1.85480000
C	8.05110000	8.74010000	4.96700000	H	2.81590000	9.02370000	-0.89120000
H	8.91200000	9.25800000	4.49920000	C	4.00530000	8.03060000	-2.41320000
H	8.11630000	7.68620000	4.62950000	H	4.36870000	8.21810000	-3.44300000
C	8.17590000	8.80340000	6.48690000	H	3.37200000	7.12360000	-2.47960000
H	8.15310000	9.83600000	6.85520000	C	5.18740000	7.76790000	-1.48440000
H	9.11820000	8.35750000	6.82640000	H	5.88960000	8.60830000	-1.46810000
H	7.36250000	8.26330000	6.98550000	H	5.74680000	6.87810000	-1.79280000
C	6.10390000	18.72620000	6.27810000	H	4.86220000	7.60450000	-0.44510000
H	5.68760000	19.05920000	5.30750000				

Table S2. The coordinates of the optimized structure of **C5A-c•G-a**

C	-3.08250000	3.81840000	0.06560000	C	-1.80450000	3.44040000	2.55500000
C	-3.69470000	3.06950000	1.09290000	C	-1.13080000	4.07640000	1.49920000
C	-3.08690000	2.92060000	2.36070000	C	-1.80190000	4.33560000	0.29470000

C	-4.98210000	1.23040000	0.22500000	H	-7.50740000	0.56140000	2.79120000
C	-6.43330000	0.76270000	0.28030000	H	-8.57900000	0.88240000	5.14180000
C	-7.41690000	1.90750000	0.03130000	H	-7.59450000	2.32960000	5.34160000
C	-8.89420000	1.56640000	0.30200000	H	-9.36890000	1.91650000	2.84000000
C	-9.77650000	2.75580000	-0.10740000	H	-11.15340000	3.23490000	4.03480000
C	-9.35570000	0.30100000	-0.42230000	H	-10.84580000	1.69740000	4.84510000
O	-4.96490000	2.54000000	0.91790000	H	-10.22220000	3.20120000	5.53090000
C	-3.79930000	2.19290000	3.46860000	H	-9.28110000	4.42000000	2.75480000
H	-1.30140000	3.31350000	3.51740000	H	-8.27500000	4.47550000	4.20360000
H	-1.29620000	4.90910000	-0.48790000	H	-7.65530000	3.73430000	2.72460000
H	-4.30010000	0.54860000	0.76220000	H	-3.83040000	-3.61430000	4.12880000
H	-4.63110000	1.39660000	-0.81030000	H	-4.98160000	-2.65680000	3.18440000
H	-6.56350000	-0.03990000	-0.49120000	C	-3.28940000	-3.43060000	2.04350000
H	-6.63660000	0.26590000	1.25920000	C	-3.91700000	-3.38080000	0.78250000
H	-7.12940000	2.77570000	0.66220000	C	-3.26370000	-3.82920000	-0.39400000
H	-7.29470000	2.26140000	-1.02020000	C	-1.96870000	-4.33860000	-0.28870000
H	-9.02400000	1.40730000	1.41210000	C	-1.31340000	-4.36440000	0.95430000
H	-10.80600000	2.62590000	0.24010000	C	-1.99160000	-3.95930000	2.11180000
H	-9.40750000	3.69810000	0.30910000	C	-6.31520000	-3.47380000	1.16120000
H	-9.81500000	2.86870000	-1.20610000	C	-7.02850000	-2.40130000	1.97500000
H	-10.43650000	0.15460000	-0.32360000	C	-8.54230000	-2.59260000	2.00570000
H	-9.13270000	0.34070000	-1.49730000	C	-9.23590000	-1.54460000	2.90070000
H	-8.86940000	-0.59840000	-0.02310000	C	-10.72900000	-1.45390000	2.56550000
H	-3.84200000	2.82350000	4.38180000	C	-9.03240000	-1.86030000	4.38740000
H	-4.87330000	2.04740000	3.15660000	O	-5.15600000	-2.79450000	0.57730000
C	-3.15470000	0.86870000	3.77020000	C	-3.94330000	-3.73220000	-1.73270000
C	-3.84650000	-0.35100000	3.61860000	H	-1.44170000	-4.69440000	-1.17970000
C	-3.18170000	-1.59580000	3.69290000	H	-1.47850000	-4.01470000	3.07660000
C	-1.83060000	-1.61160000	4.05150000	H	-6.01240000	-4.35000000	1.75160000
C	-1.13640000	-0.40900000	4.25940000	H	-6.89320000	-3.81360000	0.27240000
C	-1.80600000	0.81910000	4.14110000	H	-6.59950000	-2.37020000	3.00300000
C	-6.09620000	0.10700000	4.36280000	H	-6.76660000	-1.39610000	1.55600000
C	-7.01560000	1.08920000	3.64890000	H	-8.94430000	-2.51270000	0.96550000
C	-8.07040000	1.68840000	4.57670000	H	-8.79990000	-3.61340000	2.34230000
C	-9.11520000	2.49690000	3.77600000	H	-8.77090000	-0.54050000	2.68980000
C	-10.40110000	2.66610000	4.59210000	H	-11.21770000	-0.66840000	3.15310000
C	-8.55180000	3.85550000	3.34520000	H	-10.89240000	-1.21480000	1.50870000
O	-5.20040000	-0.39900000	3.31360000	H	-11.25280000	-2.39240000	2.77410000
C	-3.88930000	-2.86880000	3.30740000	H	-9.58490000	-1.15920000	5.02260000
H	-1.29750000	-2.56210000	4.14260000	H	-9.37040000	-2.86930000	4.64260000
H	-1.25160000	1.74790000	4.30500000	H	-7.96920000	-1.78570000	4.66620000
H	-5.53200000	0.55150000	5.19490000	H	-4.09890000	-4.75230000	-2.14840000
H	-6.63180000	-0.80250000	4.71280000	H	-4.97900000	-3.31080000	-1.58640000
H	-6.40290000	1.89230000	3.16780000	C	-3.19900000	-2.88710000	-2.73110000

C	-3.74770000	-1.68020000	-3.21810000	H	-1.14920000	4.36350000	-2.10720000
C	-3.09970000	-0.90810000	-4.20570000	H	-1.12600000	1.21480000	-5.05910000
C	-1.83940000	-1.31690000	-4.65170000	H	-5.59550000	2.53320000	-4.86850000
C	-1.23310000	-2.46150000	-4.10760000	H	-5.99280000	3.80180000	-3.64880000
C	-1.93480000	-3.26810000	-3.19650000	H	-7.16960000	0.91400000	-3.71580000
C	-6.16080000	-1.45760000	-3.25080000	H	-7.48040000	2.09580000	-2.44050000
C	-7.02150000	-2.01850000	-2.12400000	H	-8.37000000	3.69320000	-4.37510000
C	-8.43480000	-2.33670000	-2.60310000	H	-8.36070000	2.26620000	-5.40780000
C	-9.29590000	-2.98550000	-1.50070000	H	-9.81790000	2.42650000	-2.67200000
C	-10.78040000	-2.91140000	-1.87390000	H	-11.90500000	2.75660000	-4.02740000
C	-8.86660000	-4.43250000	-1.23500000	H	-10.77000000	4.07700000	-4.30690000
O	-4.88040000	-1.16840000	-2.60790000	H	-10.97380000	2.81440000	-5.52330000
C	-3.70130000	0.37180000	-4.72350000	H	-11.10300000	0.42480000	-3.64860000
H	-1.30500000	-0.72800000	-5.39950000	H	-9.93830000	0.35150000	-4.97150000
H	-1.46770000	-4.18410000	-2.82080000	H	-9.40460000	0.07630000	-3.30190000
H	-6.03860000	-2.14650000	-4.09800000	H	-3.81740000	5.13630000	-1.47540000
H	-6.51850000	-0.46440000	-3.61000000	H	-4.81650000	3.69640000	-1.21040000
H	-6.51680000	-2.91730000	-1.69540000	C	0.27040000	-0.41730000	4.42650000
H	-7.03200000	-1.28420000	-1.27820000	C	1.48050000	-0.39580000	4.43080000
H	-8.92450000	-1.39670000	-2.95270000	C	2.88560000	-0.33740000	4.31820000
H	-8.40280000	-2.99750000	-3.49020000	C	3.55920000	-1.23510000	3.45180000
H	-9.15110000	-2.40210000	-0.54120000	N	4.88560000	-1.13430000	3.19130000
H	-11.41010000	-3.33940000	-1.08600000	C	5.59160000	-0.14240000	3.79430000
H	-11.10720000	-1.87640000	-2.02350000	C	5.00380000	0.74980000	4.71210000
H	-10.99780000	-3.46060000	-2.79640000	C	3.63580000	0.65040000	4.98010000
H	-9.53590000	-4.92570000	-0.52180000	C	5.87360000	1.78140000	5.36390000
H	-8.86270000	-5.03510000	-2.14860000	O	6.90900000	1.49150000	5.95470000
H	-7.85020000	-4.47040000	-0.80830000	N	5.40280000	3.08400000	5.28760000
H	-3.61840000	0.42680000	-5.82950000	C	6.25530000	4.24230000	5.66140000
H	-4.79400000	0.39360000	-4.50150000	H	3.01440000	-2.04510000	2.94530000
C	-3.02360000	1.54880000	-4.07580000	H	6.65620000	-0.06740000	3.53170000
C	-3.70240000	2.35330000	-3.13890000	H	3.14820000	1.32670000	5.68670000
C	-3.03600000	3.33690000	-2.37820000	H	4.60730000	3.30370000	4.68680000
C	-1.68680000	3.58300000	-2.65440000	H	7.09940000	3.89490000	6.30130000
C	-1.00130000	2.81640000	-3.61040000	C	0.26620000	4.29360000	1.58300000
C	-1.67290000	1.81110000	-4.32610000	C	1.47670000	4.30350000	1.58040000
C	-5.96450000	2.71730000	-3.84760000	C	2.88290000	4.19730000	1.55230000
C	-7.27890000	2.01070000	-3.54070000	C	3.49510000	3.06010000	2.13660000
C	-8.43820000	2.58680000	-4.35160000	N	4.83110000	2.84040000	2.08060000
C	-9.81220000	2.18180000	-3.77500000	C	5.61080000	3.75190000	1.44390000
C	-10.92220000	3.00120000	-4.44520000	C	5.07890000	4.91920000	0.86590000
C	-10.07770000	0.68170000	-3.93720000	C	3.70060000	5.14760000	0.91700000
O	-5.04650000	2.12250000	-2.86550000	C	5.98400000	5.93500000	0.23270000
C	-3.75370000	4.04700000	-1.26200000	O	6.20380000	7.02850000	0.74540000

N	6.58570000	5.51910000	-0.93720000	C	4.77230000	-4.92030000	2.29300000
C	7.43410000	6.43120000	-1.74460000	C	3.37410000	-4.92300000	2.30760000
H	2.89110000	2.30010000	2.65420000	C	5.51580000	-5.01570000	3.59220000
H	6.68700000	3.53240000	1.40580000	O	5.42360000	-5.99030000	4.33320000
H	3.26470000	6.04600000	0.47240000	N	6.33760000	-3.94230000	3.87610000
H	6.30150000	4.64350000	-1.39640000	C	7.03720000	-3.82460000	5.18280000
H	7.71710000	7.31960000	-1.13330000	H	2.93210000	-4.72450000	-1.09080000
H	8.37980000	5.89560000	-1.98930000	H	6.54610000	-4.85830000	1.00710000
C	0.39600000	2.97290000	-3.78420000	H	2.82540000	-4.97880000	3.25210000
C	1.60080000	3.02530000	-3.88650000	H	6.31800000	-3.09950000	3.29360000
C	3.00720000	3.03810000	-3.99750000	H	6.83200000	-4.73050000	5.80030000
C	3.81200000	3.55770000	-2.95490000	H	7.56700000	-6.74750000	-2.02170000
N	5.16680000	3.54020000	-3.00590000	H	8.13470000	-3.81230000	4.99200000
C	5.77270000	3.01980000	-4.10460000	H	5.64360000	4.93370000	6.28400000
C	5.03890000	2.50280000	-5.18780000	N	6.17540000	0.70930000	-6.37940000
C	3.64290000	2.50370000	-5.13380000	H	5.94160000	0.09010000	-5.59370000
C	5.73710000	2.01380000	-6.42360000	C	6.79010000	0.06560000	-7.57150000
O	5.92710000	2.74430000	-7.39360000	H	6.67640000	0.73480000	-8.45700000
H	3.36060000	3.99810000	-2.05560000	H	7.88580000	-0.03190000	-7.38810000
H	6.87140000	3.02670000	-4.10720000	C	6.70360000	6.86170000	-3.02540000
H	3.05040000	2.10280000	-5.96030000	H	6.39560000	5.97210000	-3.61050000
C	0.13150000	-2.71820000	-4.38970000	H	5.76120000	7.38370000	-2.76850000
C	1.32680000	-2.83990000	-4.53680000	C	7.59190000	7.77030000	-3.88460000
C	2.73340000	-2.92880000	-4.60350000	H	8.54520000	7.25630000	-4.12040000
C	3.50700000	-1.74920000	-4.75320000	H	7.87460000	8.67600000	-3.31140000
N	4.86010000	-1.75450000	-4.69630000	C	6.89200000	8.17600000	-5.17890000
C	5.49840000	-2.93980000	-4.50990000	H	6.63330000	7.30490000	-5.79270000
C	4.80010000	-4.15380000	-4.38860000	H	7.53100000	8.82540000	-5.78870000
C	3.40280000	-4.15310000	-4.43430000	H	5.96240000	8.72400000	-4.98570000
C	5.54470000	-5.44810000	-4.23220000	C	6.17960000	-1.31330000	-7.84880000
O	5.77990000	-6.19180000	-5.17970000	H	6.31230000	-1.97480000	-6.96930000
N	5.97640000	-5.70730000	-2.94850000	H	6.75650000	-1.79890000	-8.66250000
C	6.63910000	-6.98640000	-2.58990000	C	4.69530000	-1.24610000	-8.23200000
H	3.02520000	-0.77470000	-4.90930000	H	4.57760000	-0.69770000	-9.18720000
H	6.59520000	-2.90240000	-4.45700000	H	4.13550000	-0.65700000	-7.47890000
H	2.83780000	-5.08340000	-4.33270000	C	4.08320000	-2.63950000	-8.34990000
H	5.69890000	-5.10620000	-2.16150000	H	3.02030000	-2.58710000	-8.61140000
H	6.95620000	-7.51770000	-3.51760000	H	4.15980000	-3.19960000	-7.41020000
C	0.06940000	-4.66270000	1.01650000	H	4.57900000	-3.23860000	-9.12280000
C	1.27300000	-4.78560000	1.05080000	C	5.70010000	-7.86900000	-1.75370000
C	2.68110000	-4.85060000	1.08580000	H	5.36060000	-7.32260000	-0.85110000
C	3.43140000	-4.78690000	-0.11380000	H	4.77860000	-8.09200000	-2.32600000
N	4.78730000	-4.79060000	-0.12310000	C	6.39460000	-9.17340000	-1.34250000
C	5.44890000	-4.85580000	1.06160000	H	7.33750000	-8.94840000	-0.80490000

H	6.69340000	-9.74420000	-2.24430000	H	8.57840000	7.85160000	3.71990000
C	5.49320000	-10.03350000	-0.46080000	H	7.30260000	7.10160000	2.75320000
H	5.21450000	-9.51540000	0.46470000	F	1.13990000	-0.39770000	-0.20990000
H	5.99270000	-10.96590000	-0.17240000	C	3.09990000	0.17900000	0.25230000
H	4.56300000	-10.30720000	-0.97190000	C	3.02230000	-1.18580000	-0.19820000
C	6.59560000	-2.54910000	5.91300000	C	2.53940000	-1.18960000	-1.55020000
H	6.91400000	-1.65450000	5.34050000	C	2.25630000	0.15780000	-1.90990000
H	5.48970000	-2.49650000	5.96060000	C	2.60390000	1.00510000	-0.79300000
C	7.18190000	-2.47150000	7.32820000	C	-0.27120000	0.65610000	0.91290000
H	8.28630000	-2.55470000	7.28670000	C	-0.57620000	-0.74490000	0.82170000
H	6.83840000	-3.33330000	7.93320000	C	-0.80430000	-1.07310000	-0.56180000
C	6.78730000	-1.16350000	8.00920000	C	-0.58600000	0.10570000	-1.32360000
H	7.06530000	-0.28800000	7.40100000	C	-0.25180000	1.17540000	-0.41300000
H	7.28010000	-1.05420000	8.98100000	H	3.60100000	0.50820000	1.15730000
H	5.70690000	-1.10110000	8.17840000	H	3.53010000	-2.02050000	0.28340000
C	6.77790000	4.94850000	4.40140000	H	2.50940000	-2.05670000	-2.20030000
H	7.42570000	4.25750000	3.82640000	H	1.96360000	0.50720000	-2.89220000
H	5.93640000	5.20210000	3.72550000	H	2.61510000	2.08750000	-0.80340000
C	7.55360000	6.22560000	4.74610000	H	-0.21800000	1.23130000	1.83130000
H	8.38670000	5.99160000	5.43810000	H	-0.89590000	-1.36920000	1.65750000
H	6.89790000	6.93130000	5.29390000	H	-1.24010000	-1.99960000	-0.92520000
C	8.09740000	6.89530000	3.48700000	H	-0.78950000	0.22090000	-2.38270000
H	8.84110000	6.27030000	2.98060000	H	-0.16460000	2.22080000	-0.6835000

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