Supporting Information

Organic Solid Fluorophores Regulated by Subtle Structure Modification: Color-Tunable and Aggregation-Induced Emission

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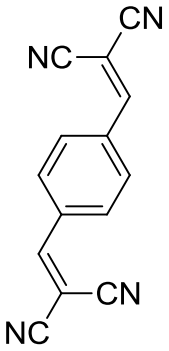
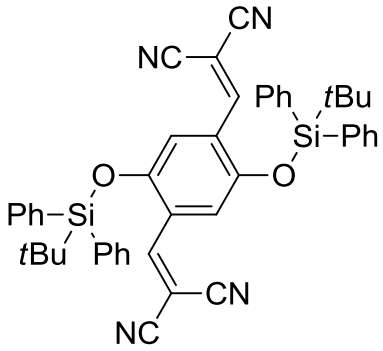
1. General Information

Ethyl ether (Et_2O), tetrahydrofuran (THF), toluene were distilled over sodium and benzophenone. DMF was distilled over CaH_2. Petroleum ether and ethyl acetate for chromatography were distilled before used. All other reagents and solvents were used directly from the corresponding supplier without further purification. All starting materials were purchased from Alfa Aesar, Aladdin, Energy, Accela and use directly. Analytical thin-layer chromatography (TLC) was carried out using commercial silica gel plated (GF254). Nuclear magnetic resonance spectra (^1H, ^{13}C NMR) were recorded on a Bruker AV 300 (^1H at 300 MHz and ^{13}C at 75 MHz), a Bruker Ascend 400 (^1H at 400 MHz, ^{13}C at 101 MHz) or a Bruker Ascend 600 (^1H at 600 MHz, ^{13}C at 151 MHz). The chemical shifts are reported as ppm and solvent residual peaks were shown as following: $CDCl_3$ δ H (7.26 ppm) and δ C (77.16 ppm); d_6-DMSO δ H (2.50 ppm) and δ C (39.52 ppm). UV-visible absorption spectra were measured on Purkinje TU-1950 spectrometer. Fluorescence spectra were recorded on a Hitachi F-7000 spectrometer. Fluorescence quantum yields were measured using Hamamatsu C9920-02G. Fluorescence lifetime was measured using Edinburgh FLS980 spectrometer. Single crystal was collected on Oxford diffraction Eos CCD detector or Bruker CMOS PHOTON 100 detector, respectively. Powder X-Ray diffraction (XRD) was performed on a Hao Yuan DX-2700. The single crystal pictures were taken on Olympus DP80 fluorescent microscopy. Dynamic Light Scattering (DLS) was carried out on Malvern Zetasizer Nano ZS90. High-resolution Mass spectra (HRMS) were obtained on a Bruker Maxis and Microflex and reported as m/z (relative intensity). Accurate masses are presented as molecular ion $[M+Na]^+$ or $[M+H]^+$, respectively.

2. Target Compounds Charts

Compound	Compound
 **1a**	 **1b**
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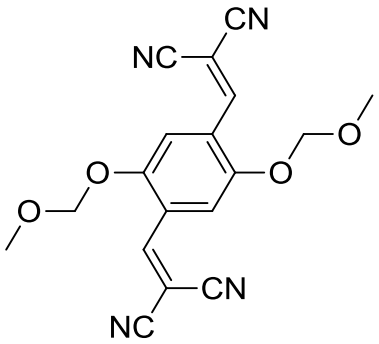
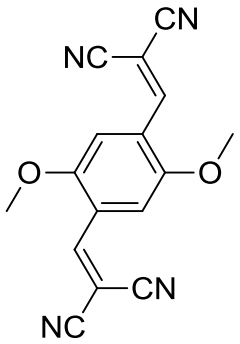
 **1c**	 **1d**
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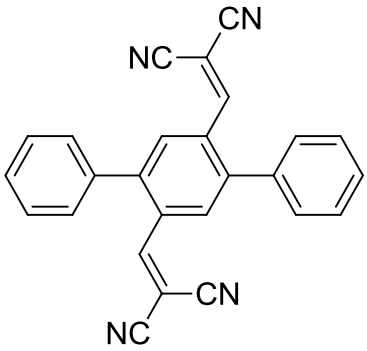
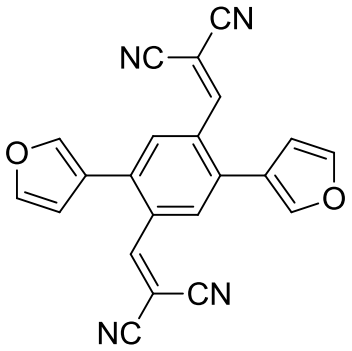
 **2a**	 **2b**
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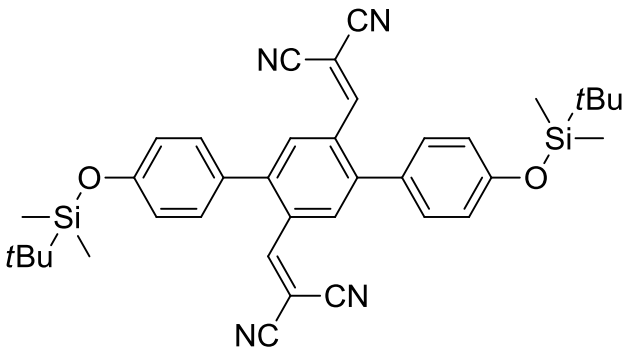
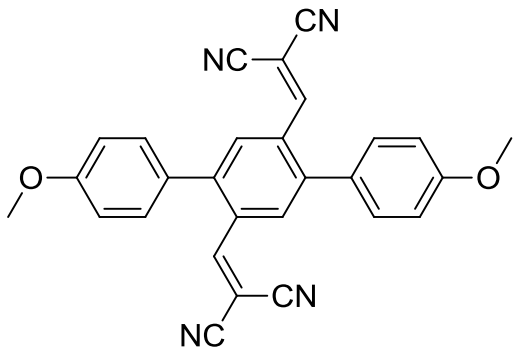
 **2c**	 **2d**
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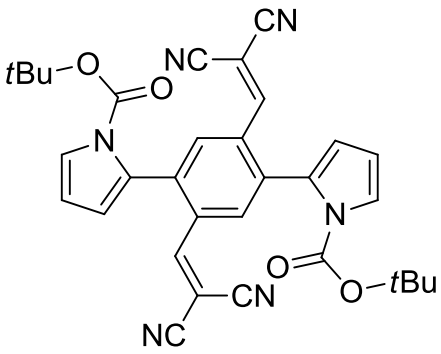
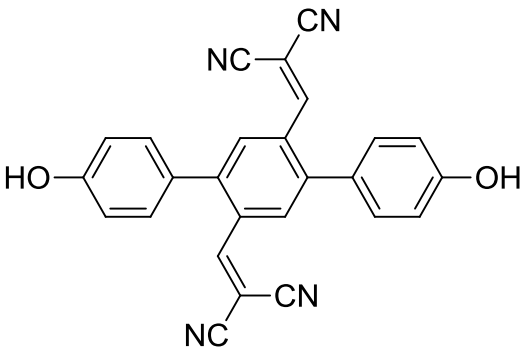
 **2e**	 **2f**
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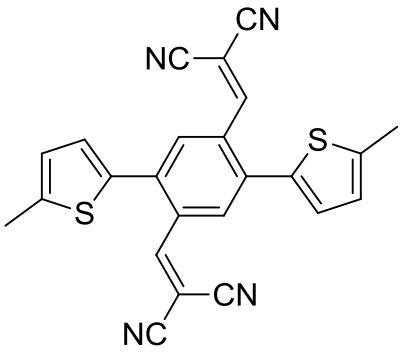
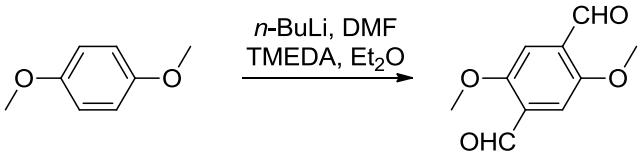
 **2g**	
Data NMR X-ray	

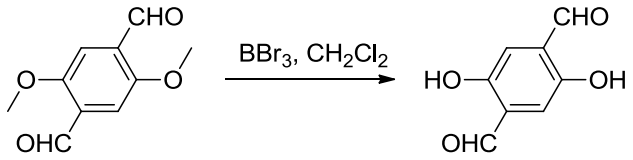
3. Experimental Procedure and Characterization Data

3.1 Reaction procedures



A round-bottom flask was charged with 1,4-dimethoxybenzene (0.692 g, 5.01 mmol), Et_2O (15.0 mL), tetramethylethylenediamine (TMEDA, 3.78 mL, 24.8 mmol) under N_2. Then *n*-BuLi (15.0 mL, 37.5 mmol, 2.5 M solution in hexane) was added dropwise (the resulting mixture turned to yellow). The mixture was allowed to reflux for 23 hrs. After that, the solution was cooled with ice-water bath, and DMF (2.5 mL, 32.3 mmol) was added dropwise. The mixture was stirred for another 15 minutes, and warmed up to room temperature. Aqueous solution of NH_4Cl (25.0 mL, 5% *w*/*v*), water (100.0 mL) were added, and extracted with ethyl acetate (3×50.0 mL). Combined organic phase was washed with water (100.0 mL), brine (100.0 mL), and then dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and residue was recrystalized from ethanol (first crop, 100.0 mL; second crop 15.0mL). Both crops were combined to give yellow crystals in 28 % yield.

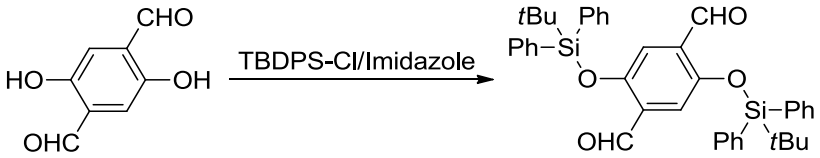
^{1}H-NMR (300 MHz, $CDCl_3$) δ (ppm): 10.50 (s, 2H, CHO), 7.46 (s, 2H, Ar H), 3.94 (s, 6H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 189.40, 155.86, 129.25, 111.02, 56.35.



To a stirred solution of 2,5-dimethoxyterephthaladehyde (0.100 g, 0.52 mmol) in 10.0 mL CH_2Cl_2 at -78^{o}C was added BBr_3 solution (130 μL in 1.0 mL CH_2Cl_2). The mixture was warmed up to room temperature and stirred for 3hrs before the reaction was quenched by water. Then the reaction mixture was adjusted to pH = 10.0 by 2.0 M NaOH and kept the

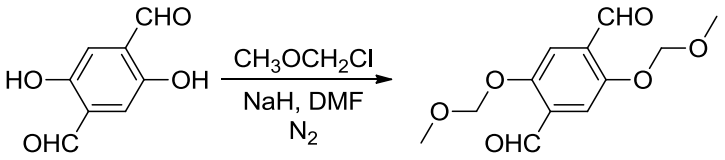
solution at that pH for 10 minutes. After that, the mixture adjusted to pH = 5.0 using 2 M HCl. The resulting solution was extracted with CH_2Cl_2 (3 × 20.0 mL), and combined organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was recrystalized from ethyl acetate to give the desired product in 50% yield.

^{1}H-NMR (600 MHz, d_6-DMSO) δ (ppm): 10.30 (s, 2H), 10.29 (s, 2H), 7.22 (s, 2H, Ar H); ^{13}C-NMR (151 MHz, d_6-DMSO) δ (ppm): 190.21, 152.76, 127.64, 115.13.



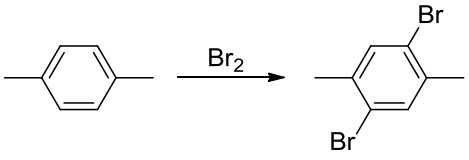
Imidazole (79.7 mg, 1.17 mmol) was added to a stirred solution of 2,5-dihydroxyterephthalaldehyde (50.0 mg, 0.3 mmol) in DMF (5.0 mL) at 50 ℃. Then *tert*-butylchlorodiphenylsilane (0.23 mL, 0.9 mmol) in 3.0 mL DMF was added dropwise to the reaction mixture and kept the reaction stirred overnight at 50^{o}C. After the reaction was complete based on TLC, Et_2O (10.0mL) and saturated $NaHCO_3$ solution (5.0mL) were added. The organic layer was separated, and the aqueous layer was extracted with Et_2O (2 × 5.0mL). Combined organic layer was then successively washed with saturated aqueous NH_4Cl solution, water and brine. Then organic phase was dried over anhydrous Na_2SO_4, concentrated under reduced pressure and purified by column chromatography to give 54% yield.

^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.45 (s, 2H, CHO), 7.67-7.65 (m, 8H, Ar H), 7.47-7.45 (m, 4H, Ar H), 7.40-7.37 (m, 8H, Ar H), 1.09 (s, 18H, CH_3); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 188.94, 152.23, 135.62, 131.48, 131.00, 130.59, 128.23, 119.19, 26.77, 19.82. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{40}H_{42}O_4Si_2Na$, 665.2519, found, 665.2523.



The 2,5-dihydroxyterephthalaldehyde (74 mg, 0.45 mmol) in 6.0 mL anhydrous DMF was added dropwise to a stirred solution of NaH (79 mg, 1.96 mmol) in anhydrous DMF (6.0 mL) at 0^{o}C. After the addition was completed, the mixture was stirred at 0 ℃ for 1 hr. Then reaction was warmed up to room temperature and stirred for another 15 minutes to give a clear solution. Then the reaction was recooled to 0 ℃ and chloromethyl methyl ether (0.107μL, 1.25mmol) was added slowly via syringe. After that, the mixture was warmed up to room temperature again and stirred overnight. Then the reaction was quenched by saturated NH_4Cl (20.0 mL). The aqueous layer was extracted with ethyl acetate (2 × 10.0 mL). Combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The resulting residue was purified by column chromatography to give the desired product in71% yield.

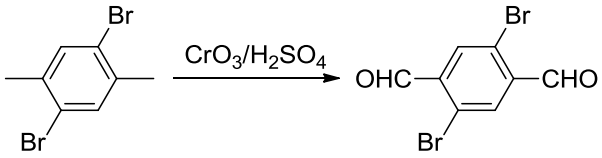
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.50 (s, 2H, CHO), 7.66 (s, 2H, Ar H), 5.29 (s, 4H, CH_2), 3.51 (s, 6H, CH_3); ^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm): 189.02, 154.07, 130.19, 114.66, 95.21, 56.68. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{10}H_{10}O_4Na$, 277.0688, found, 277.0688.



The bromine (5.4 mL, 105 mmol) was added dropwise to a stirred solution of *p*-xylene (6.2 mL, 50 mmol) and iodine (63 mg, 0.25 mmol) at 0^{o}C under dark. After stirred at room temperature for 16 hrs, 20% KOH solution (100.0 mL) was added. Then the aqueous solution was decanted and the resulting residue was recrystallized from EtOH (2 ×30.0mL) to

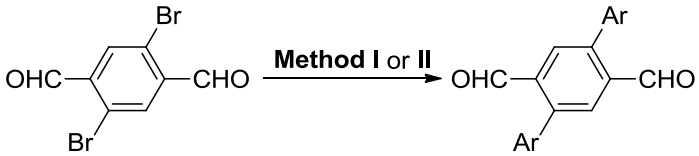
give the desired product in 91% yield.

^{1}H-NMR (600MHz, $CDCl_3$) δ (ppm): 7.39 (s, 2H, Ar H), 2.33 (s, 6H, CH_3); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 137.12, 134.08, 123.49, 22.23.



The sulfuric acid (28.0 mL) was added dropwise to a suspension containing 1,4-dibromo-2,5-dimethylbenzene (8.0 g, 0.03 mol), acetic acid (40.0 mL) and acetic anhydride (80.0 mL) at 0^{o}C. Then CrO_3 (12.0 g, 0.12 mol) was added to the reaction mixture in portions. The resulting solution was stirred vigorously at 0^{o}C for further 5 hrs until the reaction was completed. Then the greenish slurry was poured into ice-water bath and filtered. The white solid was washed with water and cold methanol. After that, the intermediate of diacetate was hydrolyzed under refluxing in a mixture of water (40.0 mL), ethanol (40.0 mL) and sulfuric acid (4.0 mL) for 5 hrs. Then the reaction cooled, the pale yellow product was separated by filtration and the crude product was purified by recrystallization from chloroform in 28%yield.

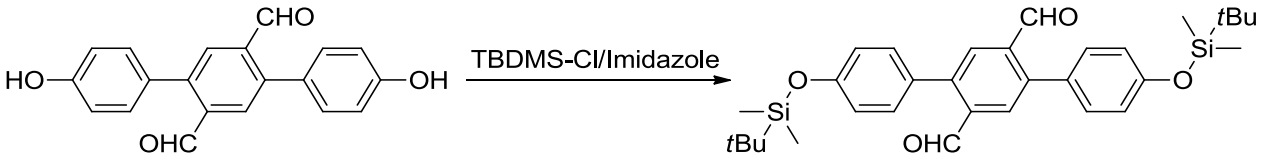
^{1}H-NMR (300MHz, $CDCl_3$) δ (ppm): 10.35 (s, 2H, CHO), 8.16 (s, 2H, Ar H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 189.94, 137.54, 135.16, 125.63.



Method I: 2,5-Dibromobenzene-1,4-dicarbaldehyde (58.4 mg, 0.2 mmol) was dissolved in DMF (0.27 mL). To this solution was added 2M sodium carbonate (0.4 mmol, 2.0 equiv), deionized water (0.13 mL) and corresponding boronic acid (0.5 mmol, 2.5equiv). Then the solution was stirred for 10 minutes. After that, the palladium acetate (4.2 mg, 0.01 mmol,

0.05 equiv) was added under N_2. The resulting solution was kept stirring for at least 12 hrs based on the TLC. Then the organic layer was concentrated under reduced pressure and purified by column chromatography on silica gel to give the corresponding product.

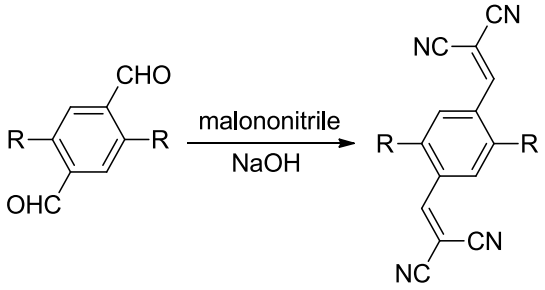
Method II: 2,5-Dibromobenzene-1,4-dicarbaldehyde (200.00 mg, 0.69 mmol), corresponding boronic acid (2.5 eq), $Pd(PPh_3)_4$ (0.05eq), PPh_3 (0.12eq) and 2.0 mL Na_2CO_3 solution (2M) in 10.0 mL toluene was refluxed for 48 hrs under N_2, After the reaction was completed based on the TLC, poured the reaction mixture into water and extracted with EtOAc. The organic layer was washed with brine, water and dried over anhydrous Na_2SO_4. The crude product was purified by flash column chromatography and then recrystallized form EtOH to give desired product.



Imidazole (65.4 mg, 96 mmol) was added to a stirred solution of 4,4''-dihydroxy-[1,1':4',1''-terphenyl]-2',5'-dicarbaldehyde (30.0 mg, 0.094 mmol) in DMF (5.0mL) at 0 ℃. Then *tert*-butyldimethylsilyl chloride (141.7 mg, 0.94mmol) was added dropwise to the reaction mixture and kept the reaction stirred overnight at room temperature. After the reaction was completed based on TLC, Et_2O (6.0mL) and saturated $NaHCO_3$ solution (3.0mL) were added. The organic layer was separated, and the aqueous layer was extracted with Et_2O (2×5.0mL). Combined organic layer was then successively washed with saturated aqueous NH_4Cl solution, water and brine. Then organic phase was dried over anhydrous Na_2SO_4, concentrated under reduced pressure and purified by column chromatography to give 77% yield.

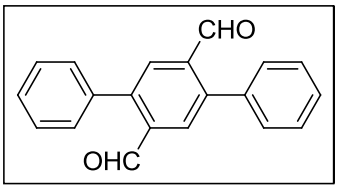
^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.09 (s, 2H, CHO), 8.06 (s, 2H, Ar H), 7.29 (d, 4H,

J= 8.3 Hz , Ar H), 6.97 (d, 4H , *J*= 8.3 Hz, Ar H), 1.02 (s, 18H, CH_3), 0.26 (s, 12H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 192.34, 156.55, 144.08, 136.60, 131.45, 130.20, 129.50, 120.51, 25.81, 18.41. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{32}H_{42}O_4Si_2Na$, 569.2519, found, 569.2521.

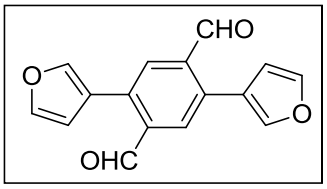


To a stirred solution of corresponding dialdehyde (1.00 equiv) in ethanol were added malononitrile (2.05 equiv) and a drop of 1M NaOH. Then the reaction stirred at room temperature for certain hours. After the reaction was completed based on TLC, the product was purified by either recrystalization or column chromatography.

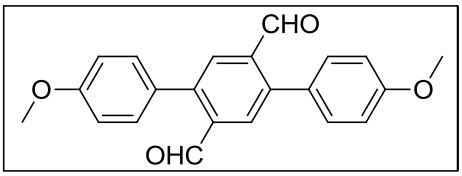
3.2 Compound data



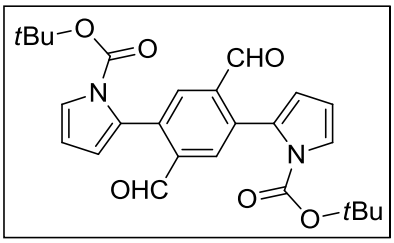
[1,1':4',1''-terphenyl]-2',5'-dicarbaldehyde (Method I): 58% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.09 (s, 2H, CHO), 8.11 (s, 2H, Ar H), 7.55-7.49 (m, 6H, Ar H), 7.48-7.44 (m, 4H, Ar H); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 191.92, 144.72, 136.69, 136.62, 130.33, 130.21, 128.91, 128.85.



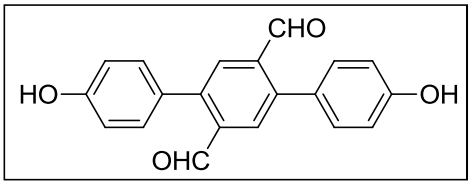
2,5-Di(cyclopenta-1,4-dien-1-yl)terephthalaldehyde (Method II): 88% yield. ^{1}H-NMR (400MHz, $CDCl_3$) δ (ppm): 10.29 (s, 2H, CHO), 8.05 (s, 2H), 7.61-7.59 (m, 4H), 6.64-6.63 (m, 2H); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 191.58, 144.17, 141.81, 137.05, 135.15, 130.23, 121.65, 112.07. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{10}O_4Na$, 289.0477, found, 289.0477.



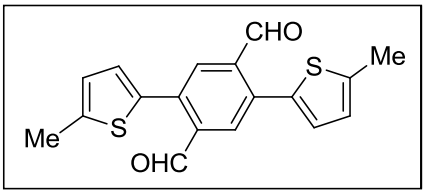
4,4''-Dimethoxy-[1,1':4',1''-terphenyl]-2',5'-dicarbaldehyde (Method II): 58% yield**.** ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.08 (s, 2H, CHO), 8.06 (s, 2H), 7.36 (d, 4H, *J* = 8.3Hz, Ar H), 7.04 (d, 4H, *J* = 8.3 Hz, Ar H), 3.89 (s, 6H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 192.25, 160.24, 143.94, 136.67, 131.45, 130.29, 128.90, 114.39, 55.58.



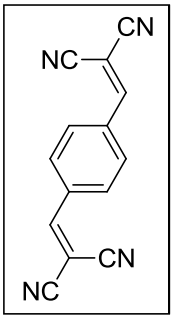
Di-tert-butyl-2,2'-(2,5-diformyl-1,4-phenylene)bis(1H-pyrrole-1-carboxylate) (Method II): 22% yield. ^{1}H-NMR (400MHz, $CDCl_3$) δ (ppm): 9.99 (s, 2H, CHO), 7.95 (s, 2H, Ar H), 7.46 (s, 2H), 6.32-6.31 (m, 4H)，1.35 (s, 18H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 191.23, 148.90, 137.64, 136.80, 130.37, 128.81, 123.46, 117.71, 111.22, 84.88, 27.75. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{26}H_{28}N_2O_6Na$, 487.1845, found, 487.1846.



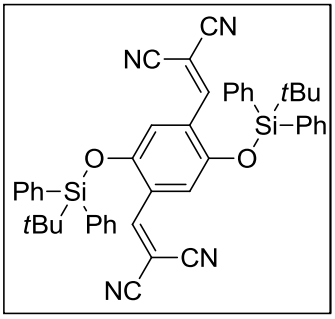
4,4''-Dihydroxy-[1,1':4',1''-terphenyl]-2',5'-dicarbaldehyde (Method II): 62% yield. ^{1}H-NMR (400 MHz, d_6-DMSO) δ (ppm): 9.97 (s, 2H), 9.85 (s, 2H),7.86 (s, 2H, Ar H), 7.32 (d, 4H, *J* = 8.4 Hz, Ar H), 6.93 (d, 4H, *J* = 8.4 Hz, Ar H); ^{13}C-NMR (101 MHz, d_6-DMSO) δ (ppm): 191.77, 158.04, 143.00, 136.01, 131.34, 129.72, 126.73, 115.70. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{20}H_{14}O_4Na$, 341.0790, found, 341.0784.



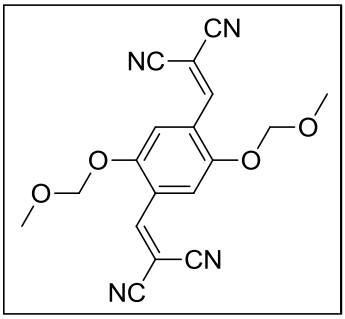
2,5-bis(5-methylthiophen-2-yl)terephthalaldehyde (Method II): 67% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.27 (s, 2H, CHO), 8.08 (s, 2H, Ar H), 6.91 (d, 2H , *J* = 3.4 Hz), 6.83 (d, 2H, *J* = 2.9 Hz), 2.57 (s, 6H, CH_3); ^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm): 191.63, 143.49, 137.03, 136.76, 135.21, 130.72, 130.26, 126.59, 15.57.



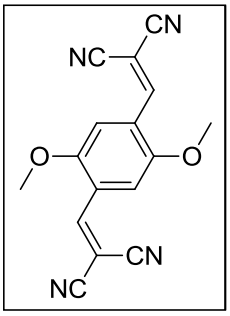
2,2'-(1,4-phenylenebis(methanylylidene))Dimalononitrile: 73% yield. ^{1}H-NMR (300 MHz, d_6-DMSO) δ (ppm): 8.63(s, 2H), 8.09(s, 4H); ^{13}C-NMR (101 MHz, d_6-DMSO) δ (ppm): 159.81, 135.34, 130.87, 113.82, 112.76, 84.71. Compounds chart NMR X-ray



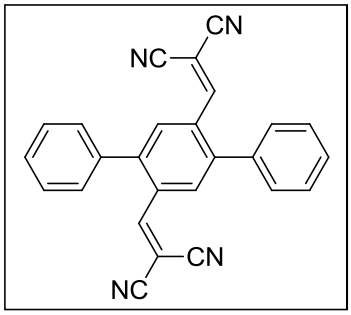
2,2'-((2-((tert-butyldiphenylsilyl)oxy)-5-(2,2-dimethyl-1,1-diphenylpropoxy)-1,4-phenylene)bis(methanylylidene))dimalononitrile: 78% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 7.98 (s, 2H), 7.57 (d, 8H, J = 7.0 Hz, Ar H), 7.47 (d, 4H, J = 7.4 Hz, Ar H), 7.40-7.36 (m, 10H, Ar H), 1.13 (s, 18H, CH_3); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 152.54, 149.79, 135.77, 130.95, 130.48, 128.46, 128.25, 119.13, 113.47, 111.36, 84.64, 26.73, 19.66. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{46}H_{42}N_4O_2Si_2Na$, 761.2744, found, 761.2739. Compounds chart NMR



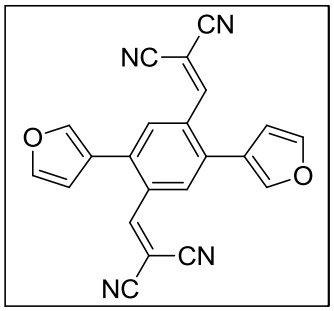
2,2'-((2,5-bis(methoxymethoxy)-1,4-phenylene)Bis(methanylylidene))dimalononitrile: 81% yield**.** ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.25 (s, 2H), 8.08 (s, 2H), 5.28 (s, 4H, CH_2), 3.52 (s, 6H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 152.84, 151.27, 126.51, 114.61, 113.47, 112.18, 95.89, 85.94, 56.91. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{18}H_{14}N_4O_4Na$, 373.0913, found, 373.0908. Compounds chart NMR X-ray



2,2'-((2,5-dimethoxy-1,4-phenylene)bis(methanylylidene))dimalononitrile: 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.29 (s, 2H), 7.84 (s, 2H, Ar H), 3.95 (s, 6H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 152.85, 152.56, 125.89, 113.50, 112.82, 110.86, 84.99, 56.82. Compounds chart NMR X-ray

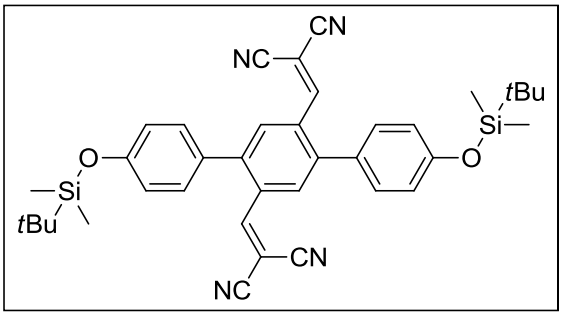


2,2'-([1,1':4',1''-terphenyl]-2',5'-diylbis(methanylylidene))dimalononitrile: 71% yield. ^{1}H-NMR (400 MHz, d_6-DMSO) δ (ppm): 8.35 (s, 2H), 8.21 (s, 4H), 7.62-7.56 (m, 6H, Ar H), 7.50 (d, 4H, *J* = 7.3 Hz, Ar H); ^{13}C-NMR (101 MHz, d_6-DMSO) δ (ppm): 160.26, 141.51, 136.97, 132.99, 130.77, 129.93, 129.05, 113.58, 112.91, 87.55, 79.19. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{26}H_{14}N_4Na$, 405.1116, found, 405.1117. Compounds chart NMR X-ray

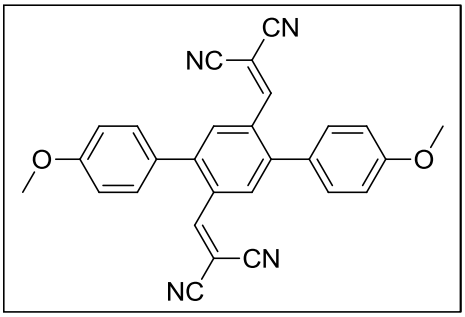


2,2'-((2,5-di(furan-3-yl)-1,4-phenylene)bis(methanylylidene))Dimalononitrile: 63% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.24 (s, 2H), 8.05 (s, 2H), 7.64(t, 2H, *J* = 1.6 Hz), 7.55 (s, 2H), 6.62-6.61 (m, 2H); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 157.36, 145.09, 142.34, 134.28, 132.85, 130.21, 122.40, 112.82, 111.99, 111.35, 87.65. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{22}H_{10}N_4O_2Na$, 385.0701, found, 385.0703.

Compounds chart NMR X-ray

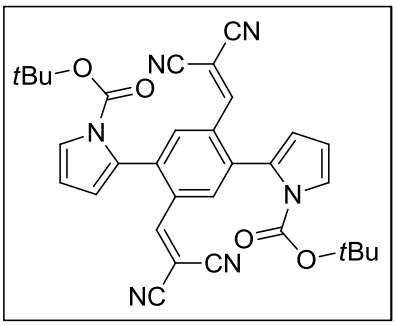


2,2'-((4,4''-bis((tert-butyldimethylsilyl)oxy)-[1,1':4',1''-terphenyl]-2',5'-diyl)Bis(methanylylidene))dimalononitrile: 82% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.21 (s, 2H), 7.85 (s, 2H), 7.21 (d, 4H, *J* = 8.5 Hz, Ar H), 7.00 (d, 4H, *J* = 8.5 Hz, Ar H), 1.02 (s, 18H, CH_3), 0.28 (s, 12H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 158.87, 157.43, 142.93, 132.73, 131.51, 130.77, 129.48, 121.00, 113.07, 112.31, 86.49, 25.77, 18.37, -4.16. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{38}H_{42}N_4O_2Si_2Na$, 665.2744, found, 665.2745. Compounds chart NMR X-ray

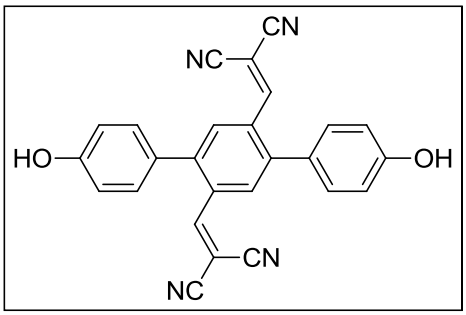


2,2'-((4,4''-dimethoxy-[1,1':4',1''-terphenyl]-2',5'-diyl)Bis(methanylylidene))dimalononitrile: 69% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.22 (s, 2H), 7.84 (s, 2H), 7.27 (d, 4H, *J* = 8.5 Hz, Ar H), 7.07 (d, 4H, *J* = 8.5 Hz, Ar H), 3.91 (s, 6H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 160.97, 158.77, 142.91, 132.79, 131.50, 130.76, 128.94, 115.03, 113.09, 112.29, 86.53, 55.69. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{28}H_{18}N_4O_2Na$, 465.1327, found, 465.1330.

Compounds chart NMR X-ray

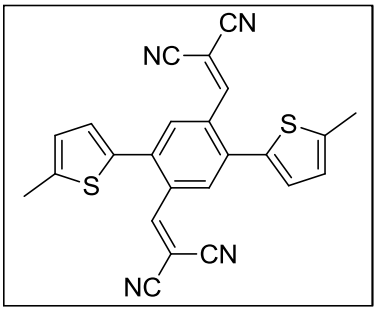


Di-tert-butyl-2,2'-(2,5-bis(2,2-dicyanovinyl)-1,4-phenylene)bis(1H-pyrrole-1-carboxylate): 59%. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.17 (s, 2H), 7.68 (s, 2H), 7.46-7.45 (t, 2H, *J* = 2.6 Hz), 6.35 (d, 4H, *J* = 3.2 Hz), 1.47 (s, 18H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 158.87, 157.44, 142.93, 132.73, 131.51, 130.77, 129.48, 121.01, 113.07, 112.31, 86.48, 25.77, 18.37, -4.16. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{32}H_{28}N_6O_4Na$, 538.2070, found, 538.2074. Compounds chart NMR X-ray



2,2'-((4,4''-dihydroxy-[1,1':4',1''-terphenyl]-2',5'-diyl)Bis(methanylylidene))dimalononitrile: 45% yield. ^{1}H-NMR (400 MHz, d_6-DMSO) δ (ppm): 9.95 (s, 2H, OH), 8.30 (s, 2H), 8.10 (s, 2H), 7.28 (d, 4H, *J* = 8.5 Hz, Ar H), 6.96 (d, 4H, *J* = 8.5 Hz, Ar H); ^{13}C-NMR (101 MHz, d_6-DMSO) δ(ppm): 160.61, 158.44, 140.90, 132.61, 131.35, 130.24, 127.63, 115.84, 113.71, 113.02, 86.61. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{26}H_{14}N_4O_2Na$, 437.1014, found, 437.1017.

Compounds chart NMR



2,2'-((2,5-bis(5-methylthiophen-2-yl)-1,4-phenylene)Bis(methanylylidene))dimalononitrile: 75% yield. ^{1}H-NMR (300 MHz, $CDCl_3$) δ (ppm): 8.22 (s, 2H), 8.08 (s, 2H), 6.89 (s, 4H), 2.59 (s, 6H, CH_3); ^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm): 157.93, 145.48, 135.83, 135.50, 132.32, 130.89, 130.77, 127.40, 113.02, 111.95, 87.32, 15.67. HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd for $C_{24}H_{14}N_4S_2Na$, 445.0558, found, 445.0563. Compounds chart NMR X-ray

4. UV-vis Spectra

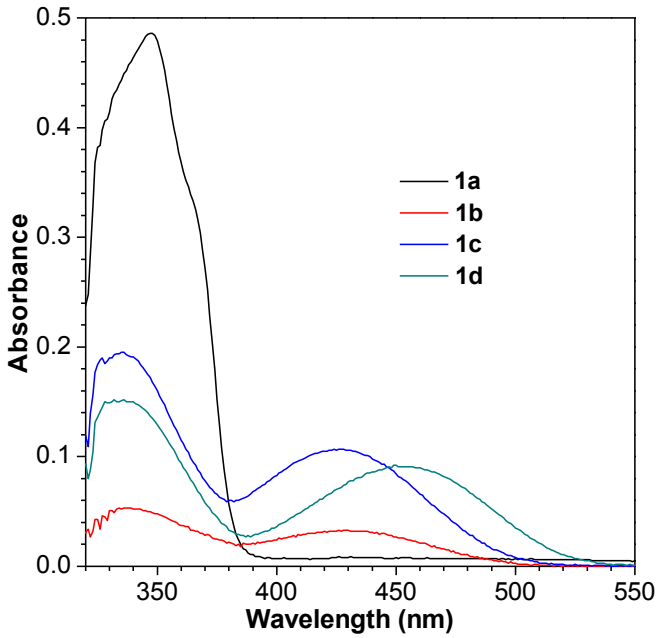


Fig. S1 UV-vis spectra of compounds **1a-1d** (10 μM) in acetone.

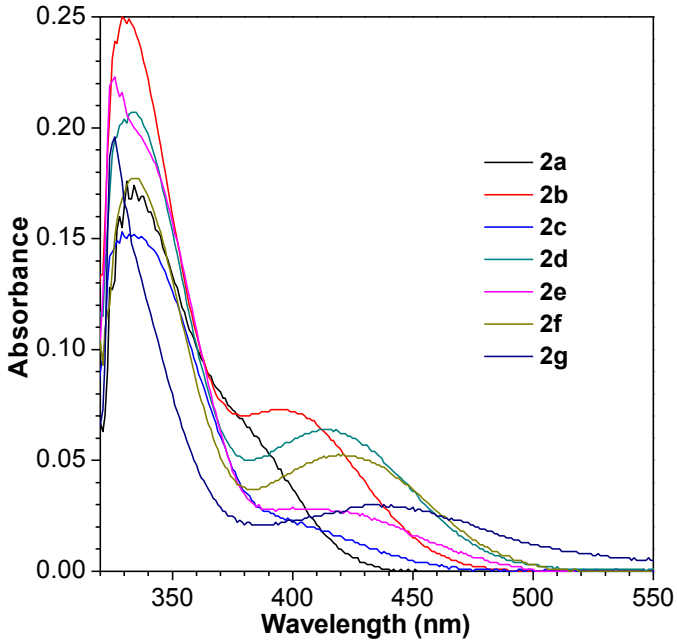
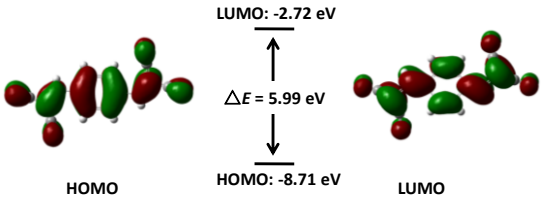
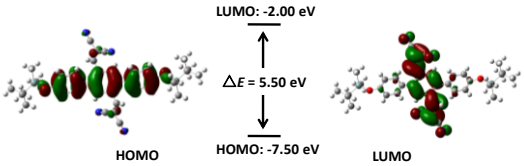
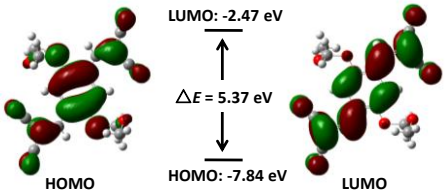
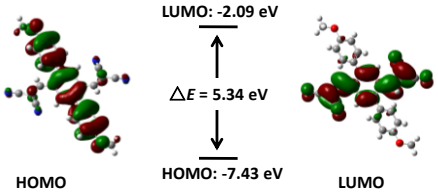
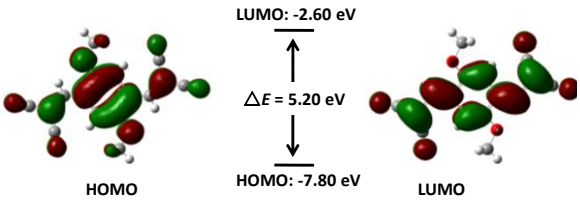
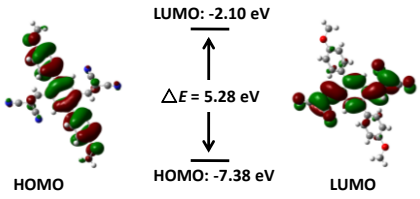
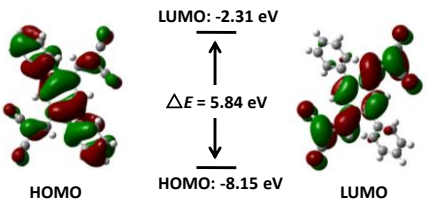
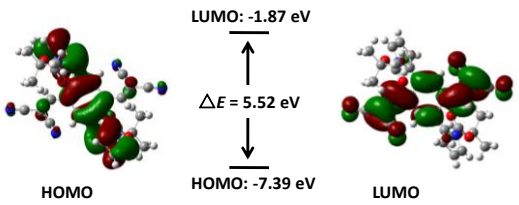
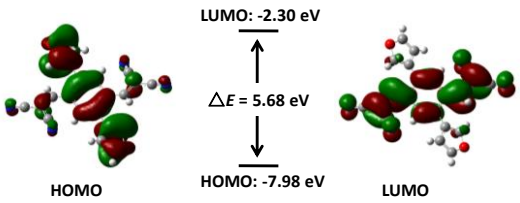
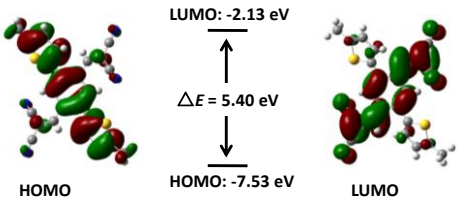


Fig. S2 UV-vis spectra of compounds **2a-2g** (10 μM) in acetone.

5. Theoretical Calculation Based on the Single Crystal

Table S1. Molecular orbital amplitude plots of both HOMO and LUMO

Cmpd[a]		Cmpd[a]	
1a		**2c**	
1c		**2d-g**	
1d		**2d-o**	
2a		**2e**	
2b		**2g**	

[a]The energy gap between HOMO and LUMO of corresponding single crystal were calculated at the CAM-B3LYP/6-31G (d, p) level of theory.

Table S2. Calculated dipole moments for corresponding crystals

Compound	μ_g (D)[a]	μ_e (D)[b]	$\Delta\mu$ (D)[c]
1a	0.0023	0.0050	0.0027
1c	0.0110	0.0103	-0.0007
1d	0.0051	0.0048	-0.0003
2a	0.0036	0.0217	0.0181
2b	0.0022	0.0032	0.0010
2c	0.0145	0.0421	0.0276
2d-g	0.0044	0.0486	0.0442
2d-o	0.0024	0.0108	0.0084
2e	0.0102	0.0216	0.0114
2g	0.001	0.0312	0.0302

[a]μ_g = ground state dipole moment. [b]μ_e = excited state dipole moment. [c]$\Delta\mu = \mu_e - \mu_g$

6. Photoluminescence Properties

6.1 Solid state emission and their CIE diagram

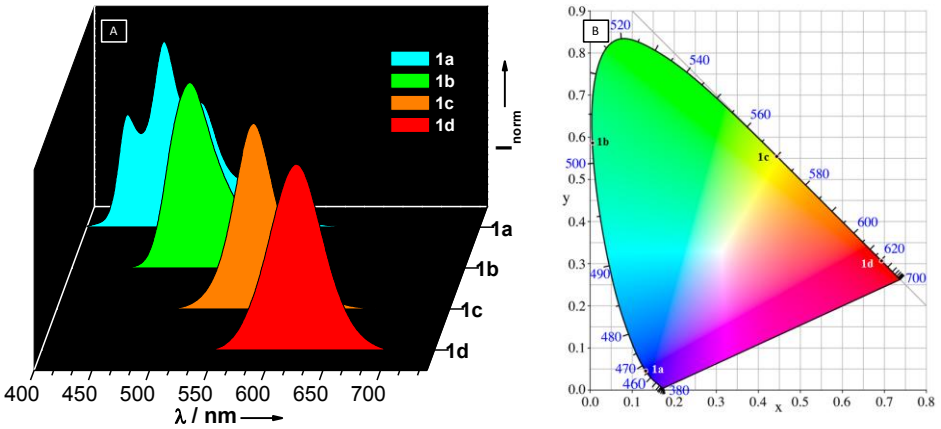


Fig. S3 (A) PL spectra of **1a-1d** in the solid states. (B) PL spectra of compounds **1a-1d** plotted on a CIE 1931 chromaticity diagram.

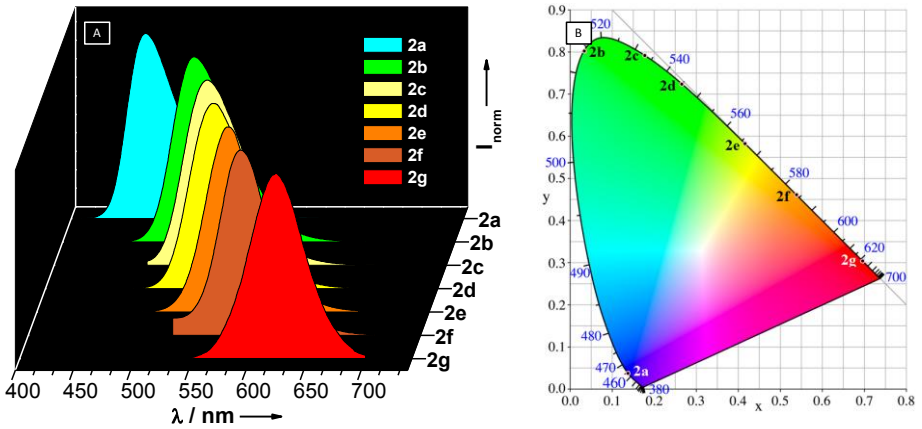


Fig. S4 (A) PL spectra of **2a-2g** in the solid states. (B) PL spectra of compounds **2a-2g** plotted on a CIE chromaticity diagram.

Table S3. Coordinates of compounds **1a-1d** and **2a-2g** on CIE diagram.

Compound	λ_{em} (nm)	Coordinate (X)	Coordinate (Y)
1a	467	0.1314	0.0459
1b	502	0.0049	0.5871
1c	570	0.4441	0.5547
1d	620	0.6915	0.3083
2a	464	0.1374	0.0374
2b	514	0.0328	0.8029
2c	533	0.1778	0.7917
2d	545	0.2658	0.7243
2e	566	0.4158	0.5826
2f	584	0.5385	0.4607
2g	622	0.6954	0.3045

6.2 Single crystal emission

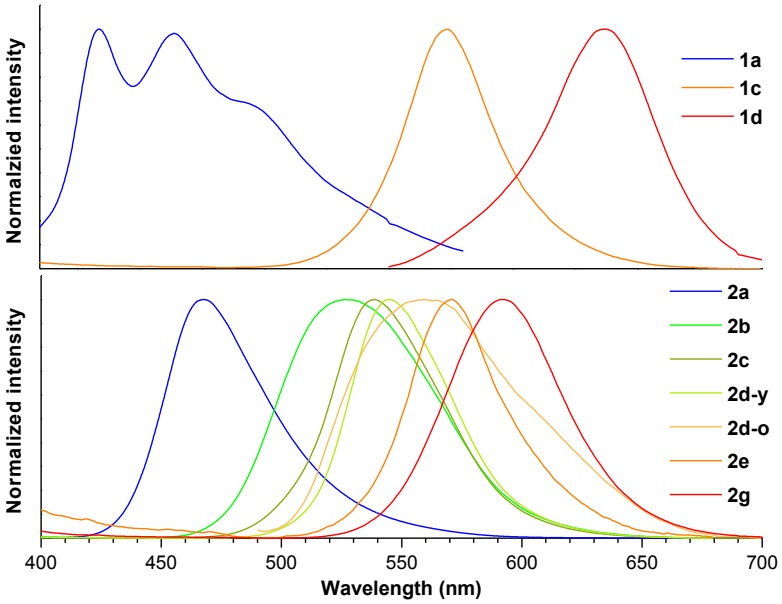


Fig. S5 Normalized PL spectra of corresponding single crystals.

6.3 Summary of the optical properties

Table S4. The fluorescence lifetime of all compounds.

Compd.	Lifetime in solution (ns)	Lifetime in solid sate (ns)	Lifetime in Crystal (ns)
1a	τ_1 = 1.10	τ_1 = 1.11 (65.33%) τ_2 = 3.83 (34.67%)	τ_1 = 1.08 (66.58%) τ_2 = 6.18 (33.42%)
1b	τ_1 = 5.21	τ_1 = 1.57	--
1c	τ_1 = 7.31	τ_1 = 2.46	τ_1 = 1.67 (34.15%) τ_2 = 5.18 (65.85%)
1d	τ_1 = 10.62	τ_1 = 2.53 (33.17%) τ_2 = 9.84 (66.83%)	τ_1 = 1.68 (36.96%) τ_2 = 10.70 (63.04%)
2a	τ_1 = 2.95	τ_1 = 0.47 (79.65%) τ_2 = 2.70 (20.35%)	τ_1 = 2.86
2b	τ_1 = 0.42 (30.58%) τ_2 = 4.40 (69.42%)	τ_1 = 1.73 (66.34%), τ_2 = 4.66 (33.66%)	τ_1 = 0.14 (50.15%) τ_2 = 3.14 (49.85%)
2c	τ_1 = 0.81	τ_1 = 2.84 (13.92%) τ_2 = 9.08 (86.08%)	τ_1 = 4.51 (25.99%) τ_2 = 9.31 (74.01%)
2d	τ_1 = 0.41 (47.59%) τ_2 = 3.09 (52.41%)	τ_1 = 6.27	τ_1 = 6.29 (**2d-g**) τ_1 = 3.89 (**2d-o**)
2e	n. d	τ_1 = 0.21 (29.14%) τ_2 = 7.47 (70.86%)	τ_1 = 5.09 (5.24%) τ_2 = 11.06 (94.76%)
2f	n. d	τ_1 = 4.15	--
2g	τ_1 = 1.75	τ_1 = 2.61	τ_1 = 1.73 (32.07%) τ_2 = 6.40 (67.93%)

Table S5. The rate constants for radiative (k_r) and nonradiative decay (k_{nr}) were calculated from the Φ and τ values according to the formulae $k_r = \Phi_F/\tau$ and $k_{nr} = (1-\Phi_F)/\tau$.

Compd.	Solution		Solid state		Crystal	
	k_r (s^{-1})	k_{nr} (s^{-1})	k_r (s^{-1})	k_{nr} (s^{-1})	k_r (s^{-1})	k_{nr} (s^{-1})
1a	7.272×10^{6}	9.02×10^{8}	6.439×10^{7}	4.234×10^{8}	1.489×10^{7}	4.256×10^{8}
1b	3.013×10^{8}	1.618×10^{8}	7.197×10^{7}	5.650×10^{8}	--	--
1c	7.647×10^{7}	6.03×10^{7}	9.756×10^{6}	3.967×10^{8}	5.528×10^{6}	2.458×10^{8}
1d	7.185×10^{7}	2.232×10^{7}	4.986×10^{6}	1.297×10^{8}	6.532×10^{6}	1.293×10^{8}
2a	4.034×10^{7}	2.986×10^{8}	1.445×10^{8}	9.424×10^{8}	3.240×10^{7}	3.160×10^{8}
2b	4.717×10^{6}	3.097×10^{8}	6.728×10^{7}	3.003×10^{8}	3.963×10^{7}	5.701×10^{8}
2c	4.938×10^{6}	1.229×10^{9}	5.554×10^{7}	6.626×10^{7}	6.675×10^{7}	5.732×10^{7}
2d	4.972×10^{6}	5.475×10^{8}	2.089×10^{7}	1.386×10^{8}	7.790×10^{7} (**2d-y**) 2.031×10^{7} (**2d-o**)	8.108×10^{7} (**2d-y**) 2.368×10^{8} (**2d-o**)
2e	--	--	4.856×10^{7}	8.786×10^{7}	4.009×10^{7}	5.293×10^{7}
2f	--	--	4.182×10^{7}	1.776×10^{9}	--	--
2g	2.229×10^{7}	5.49×10^{8}	2.813×10^{7}	2.122×10^{8}	4.306×10^{7}	1.608×10^{8}

6.4 Solvent effect of Target Compounds

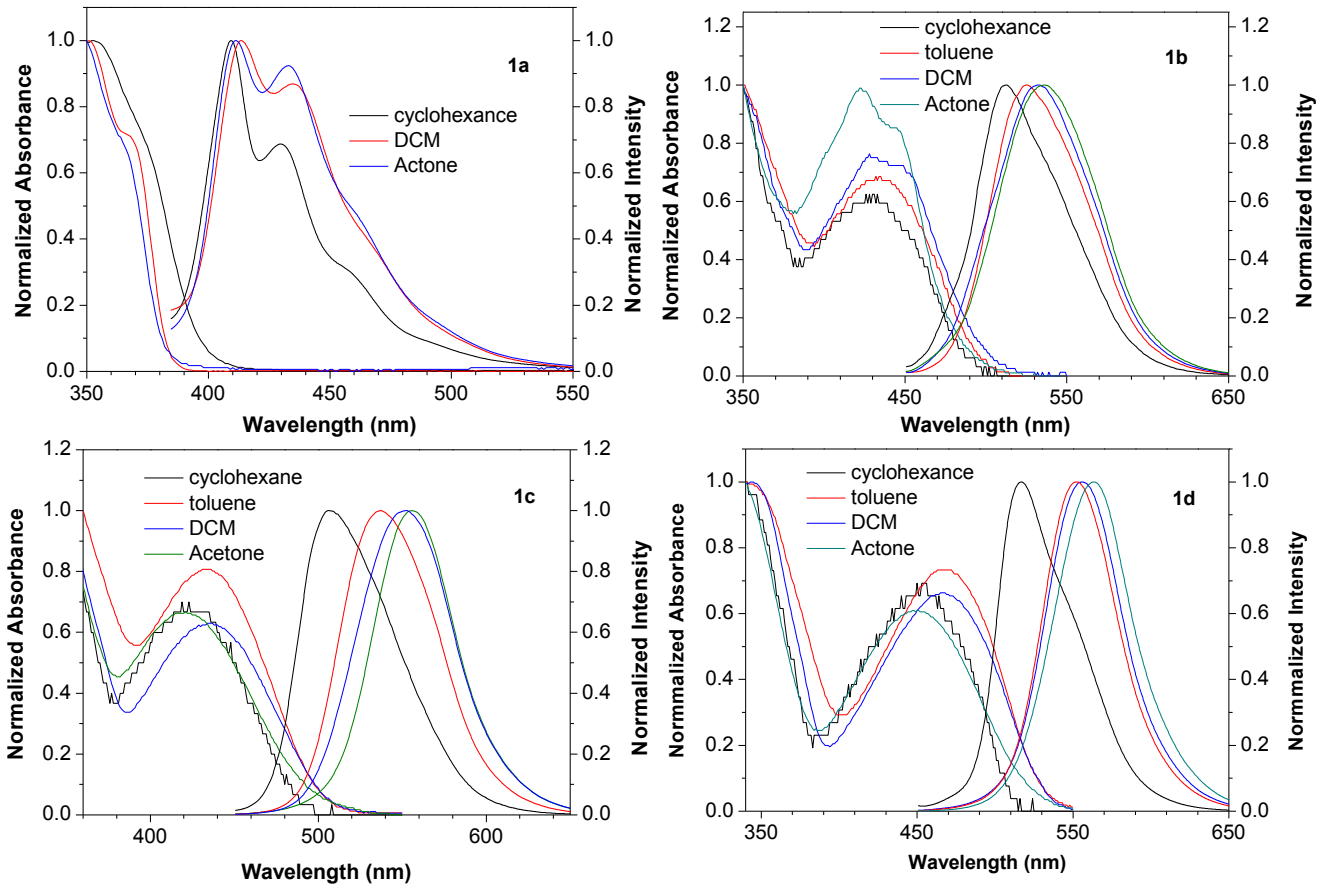


Fig. S6 UV-vis and PL spectra of compounds **1b-1d** in different solution.

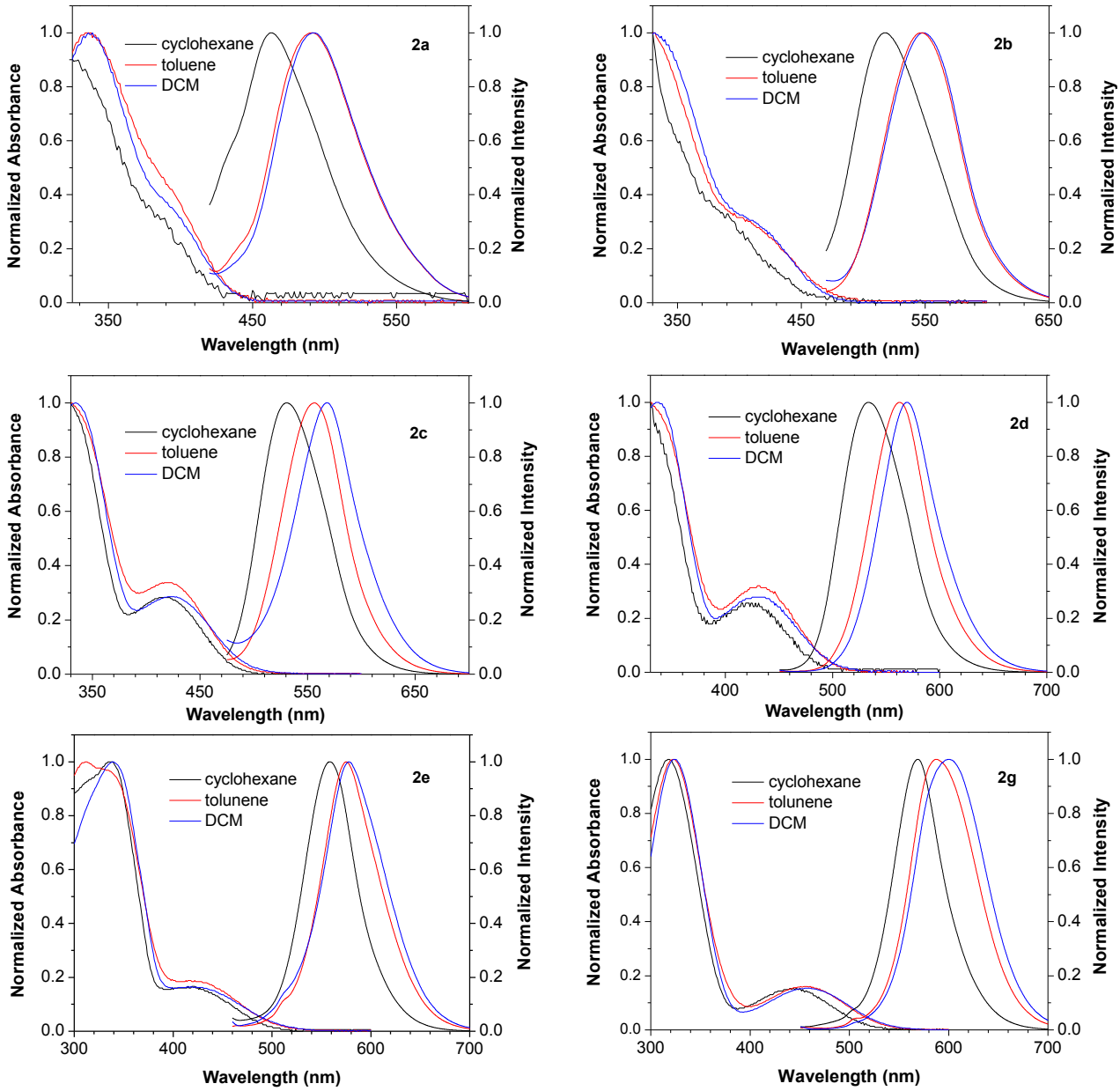


Fig. S7 UV-vis and PL spectra of compounds **2a**-**2g** in different solution.

6.5 Aggregation-induced emission properties of target compounds

Nanoaggregates preparation: 1 mM stock solutions of target compounds in acetone were firstly prepared. Then aliquots of above stock solution were transferred into 5 mL volumetric flasks. And appropriate amounts of water were added to obtain 10 μM solution with different water fractions (0 vol%, 30 vol%, 50 vol%, 70 vol%, 90 vol%, 99 vol%). After that, the PL measurements of the resulting solutions were performed immediately.

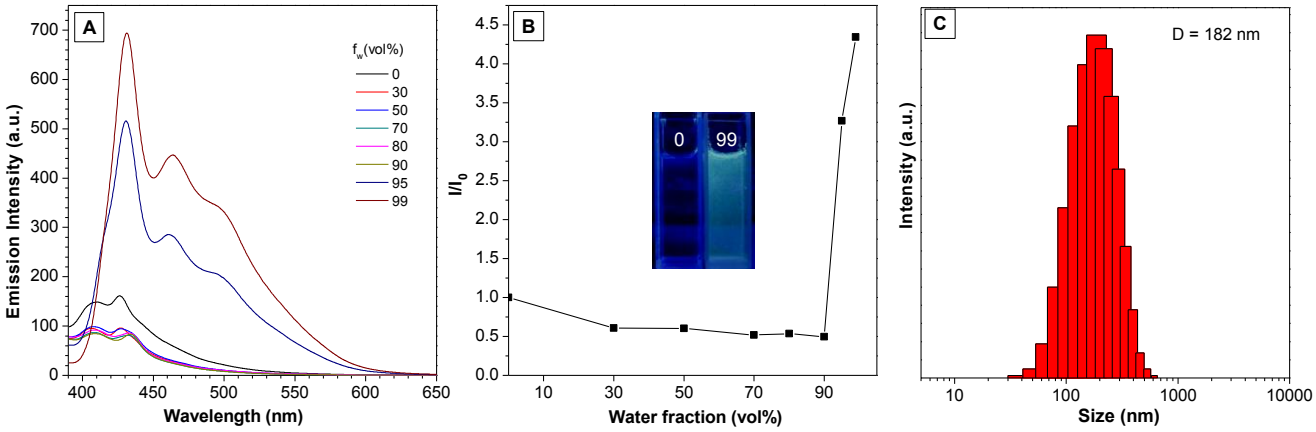


Fig. S8 (A) PL spectra of **1a** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **1a**. Inset: photograph of **1a** in acetone/water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **1a** (10 μM) in acetone/water (1:99, v/v).

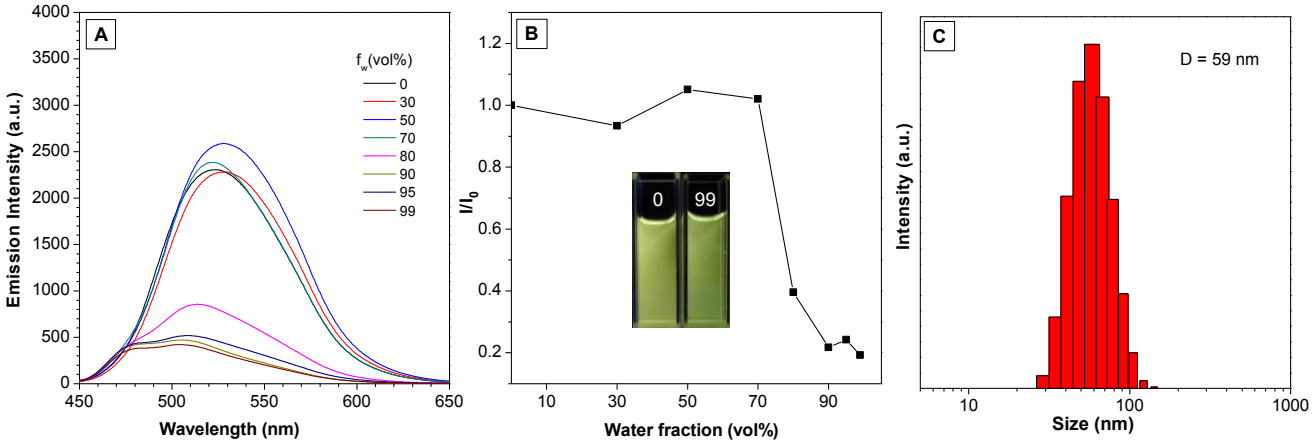


Fig. S9 (A) PL spectra of **1b** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **1b**. Inset: photograph of **1b** in acetone/water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **1b** (10 μM) in acetone/water (1:99, v/v).

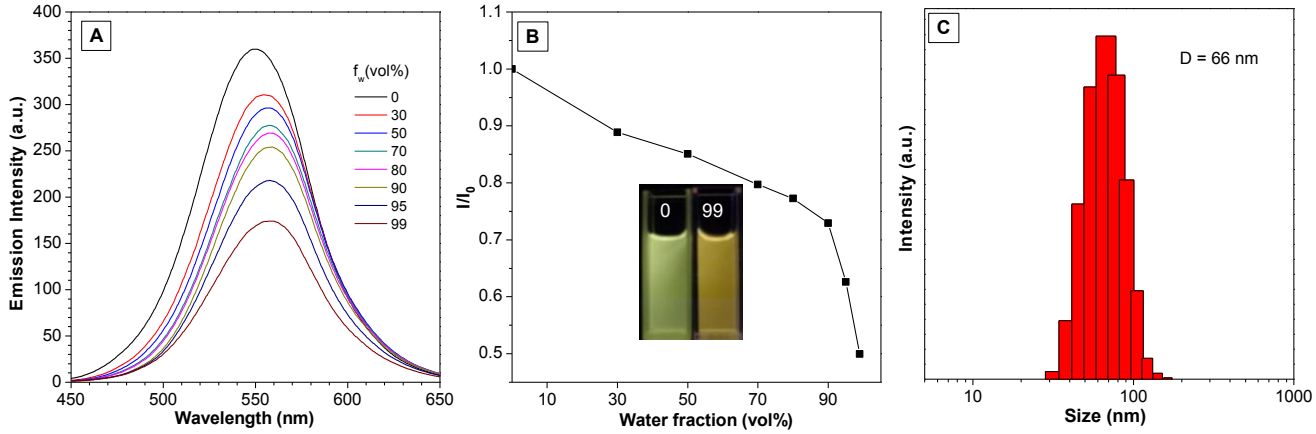


Fig. S10 (A) PL spectra of **1c** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **1c**. Inset: photograph of **1c** in acetone/water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **1c** (10 μM) in acetone/water (1:99, v/v).

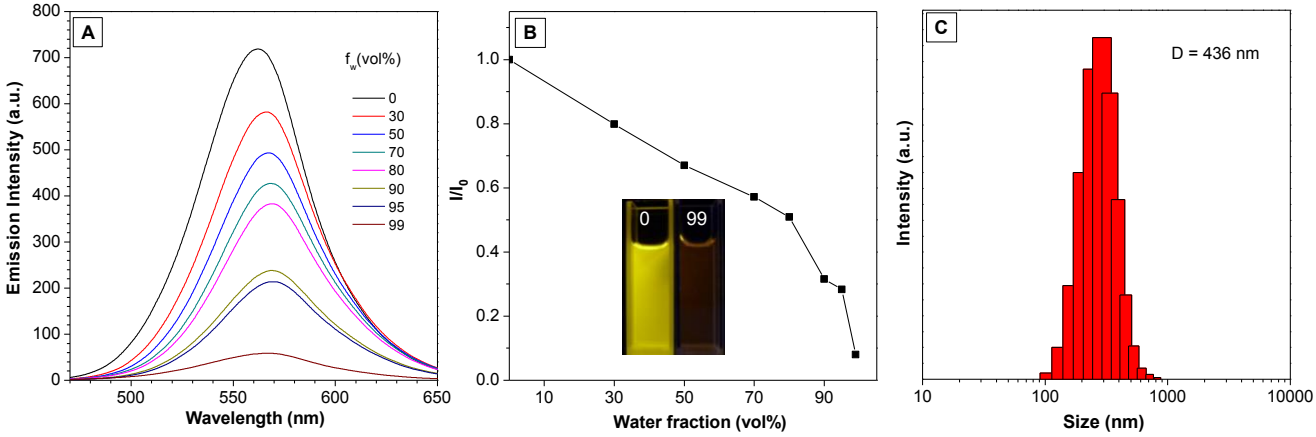


Fig. S11 (A) PL spectra of **1d** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **1d**. Inset: photograph of **1d** in acetone/water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **1d** (10 μM) in acetone/water (1:99, v/v).

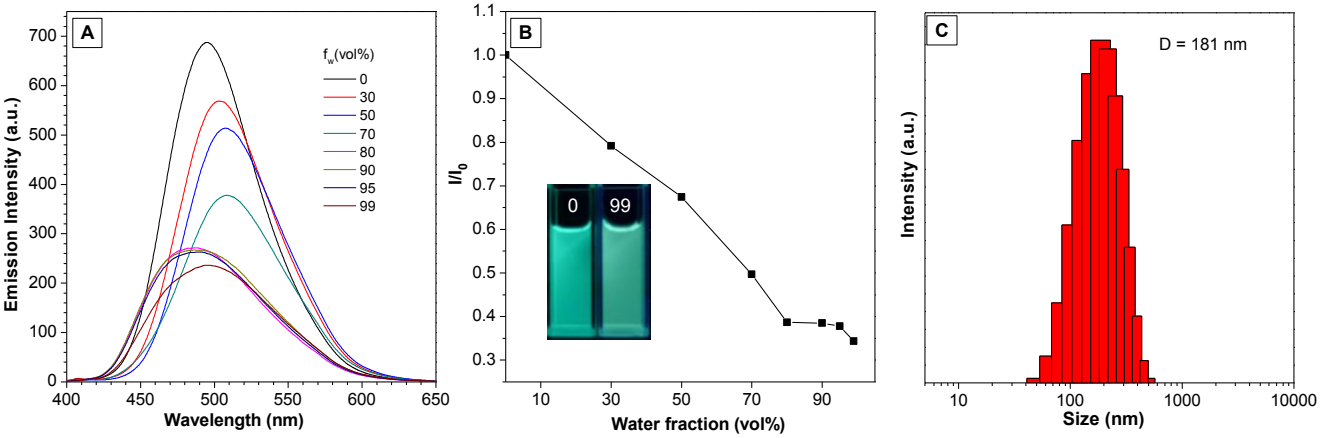


Fig. S12 (A)PL spectra of **2a** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **2a**. Inset: photograph of **2a** in acetone/water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **2a** (10 μM) in acetone/water (1:99, v/v).

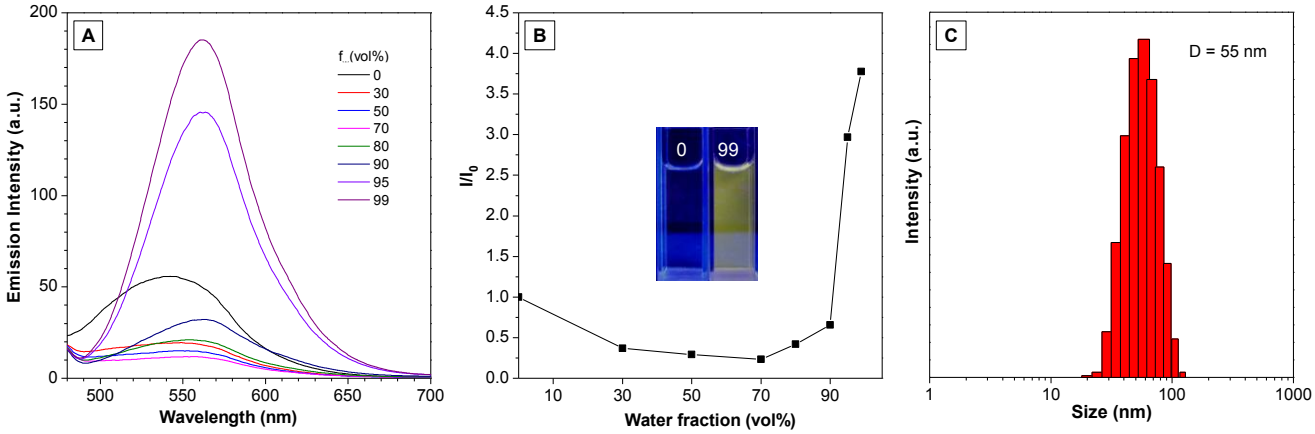


Fig. S13 (A) PL spectra of **2b** (10 μM) in acetone and acetone/watermixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **2b**. Inset: photograph of **2b** in acetone/ water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **2b** (10 μM) in acetone/water (1:99, v/v).

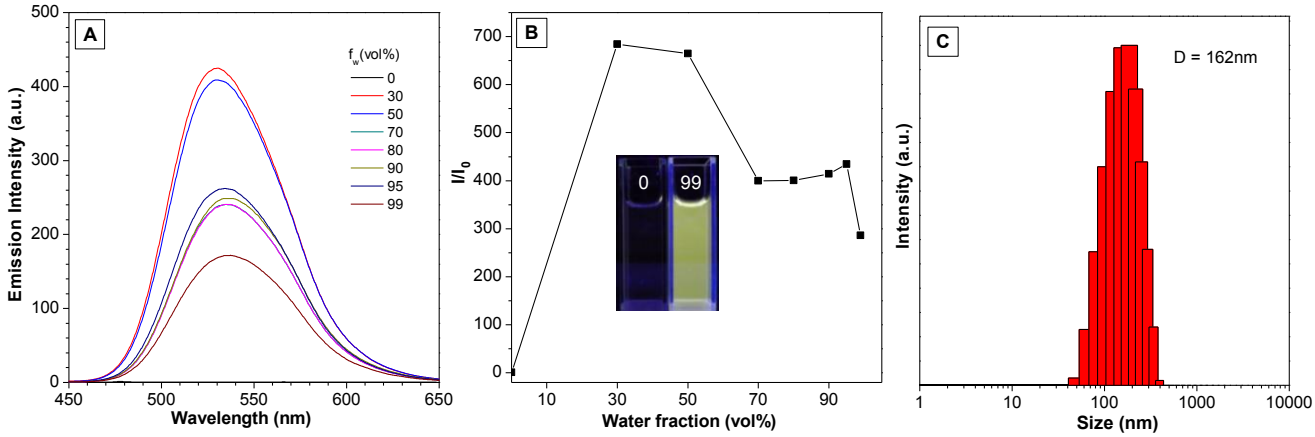


Fig. S14 (A) PL spectra of **2c** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **2c**. Inset: photograph of **2c** in acetone/ water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **2c** (10 μM) in acetone/water (1:99, v/v).

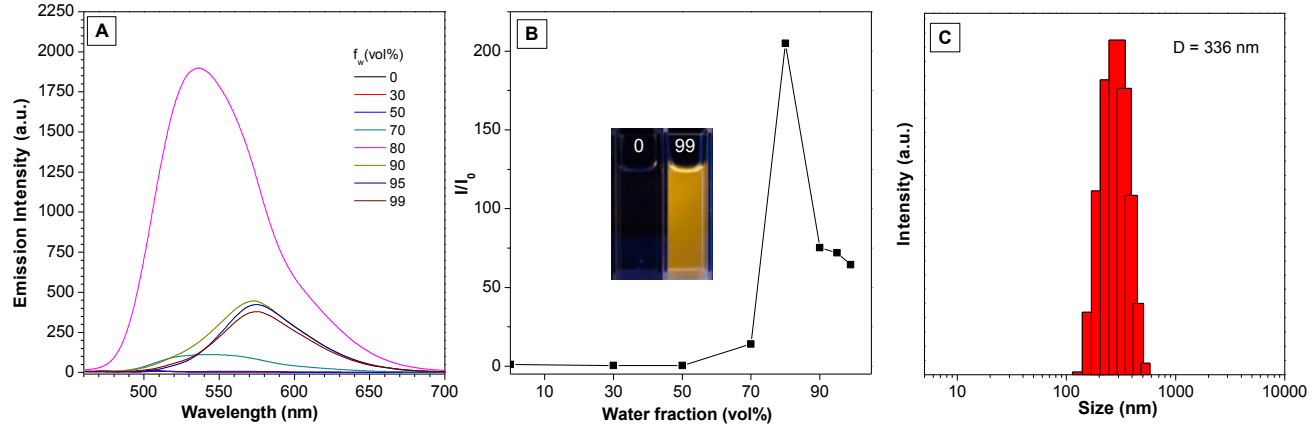


Fig. S15 (A) PL spectra of **2d** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **2d**. Inset: photograph of **2d** in acetone/ water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **2d** (10 μM) in acetone/water (1:99, v/v).

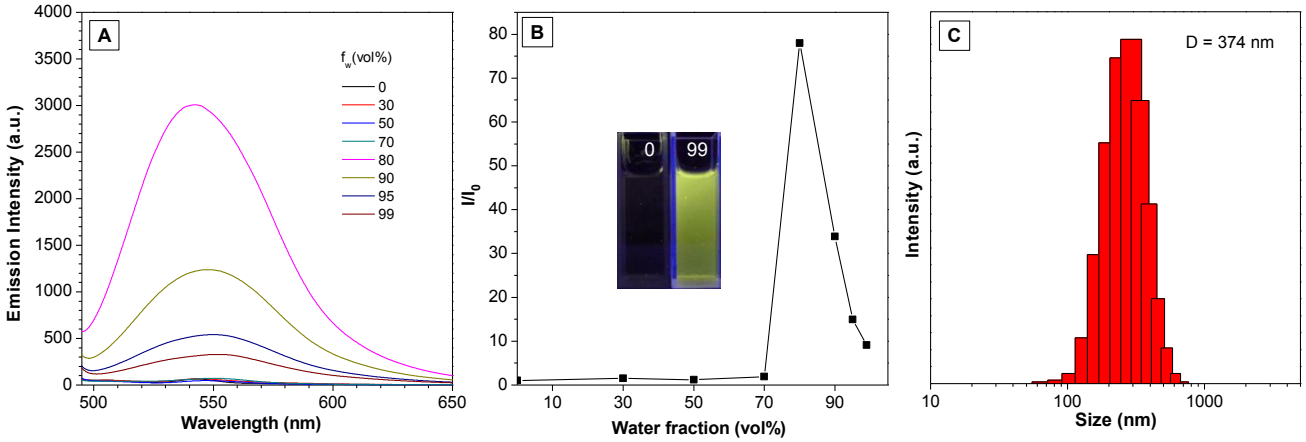


Fig. S16 (A) PL spectra of **2f** (10μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **2f**. Inset: photograph of **2f** in acetone/ water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **2f** (10 μM) in acetone/water (1:99, v/v).

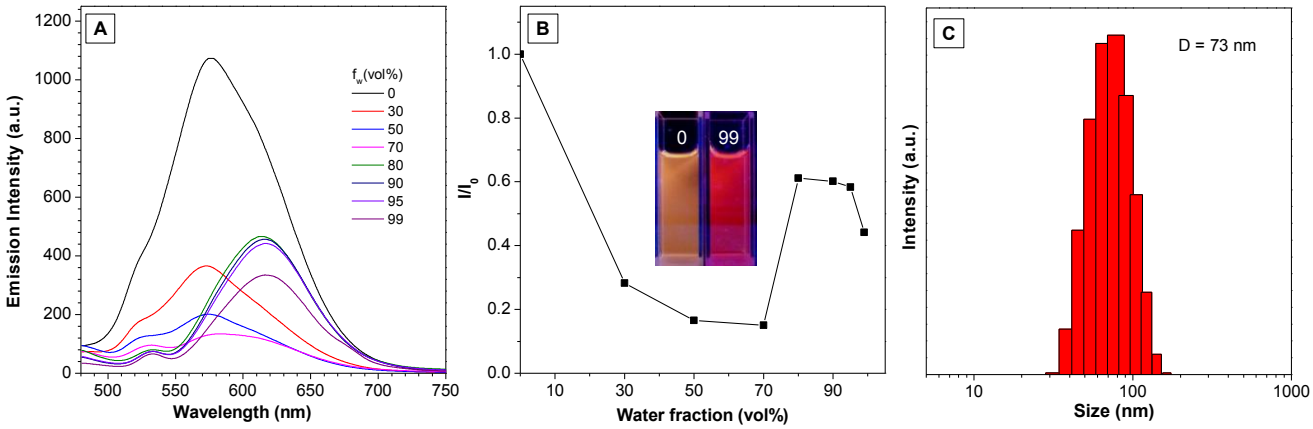


Fig. S17 (A) PL spectra of **2g** (10 μM) in acetone and acetone/water mixtures with different water fractions (f_w). (B) Plots of emission intensity versus the composition of the water mixtures of **2g**. Inset: photograph of **2g** in acetone/ water mixtures with f_w values of 0, and 99% under irradiation of 365 nm UV light. (C) Particle size distribution of **2g** (10 μM) in acetone/water (1:99, v/v).

7. Mechanochromic Luminescence Properties

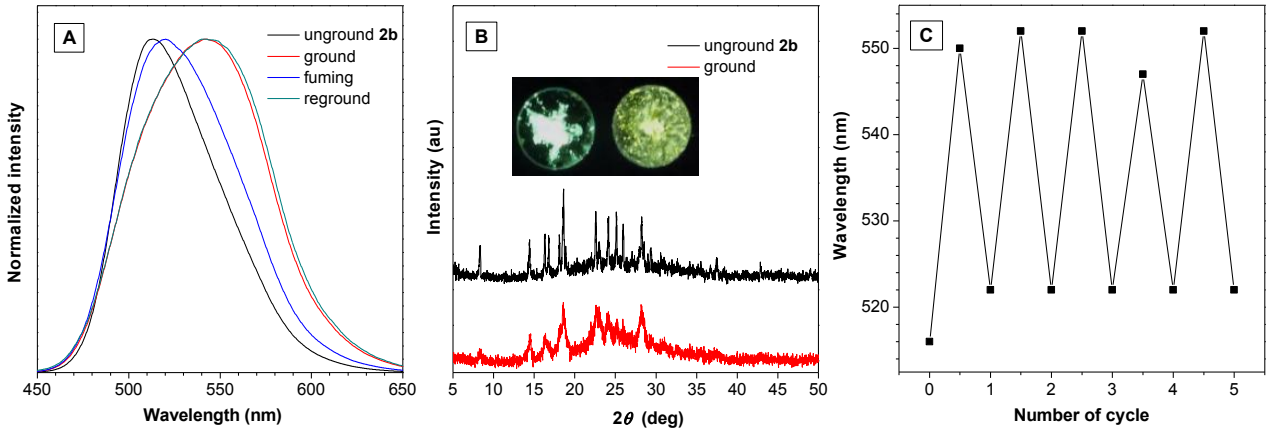


Fig. S18 (A) Normalized PL spectra of **2b** under different condition. (B) Powder XRD diffractions of **2b**. Inset: photograph of **2b** taken under illumination with UV light (365 nm) at different conditions. (C) Reversible switching of emission by repeated grinding/fuming cycles.

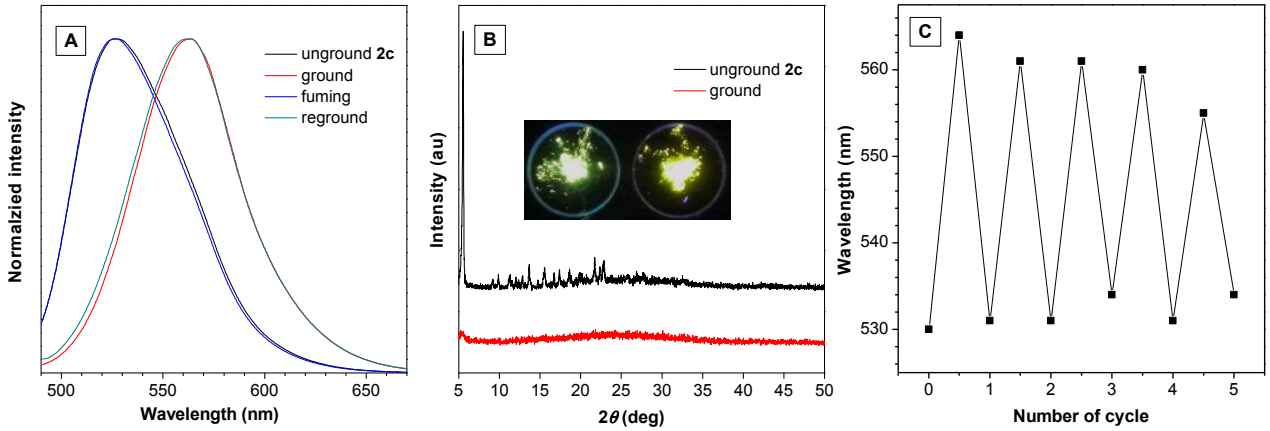


Fig. S19 (A) Normalized PL spectra of **2c** under different condition. (B) Powder XRD diffractions of **2c**. Inset: photograph of **2c** taken under illumination with UV light (365 nm) at different conditions. (C) Reversible switching of emission by repeated grinding/fuming cycles.

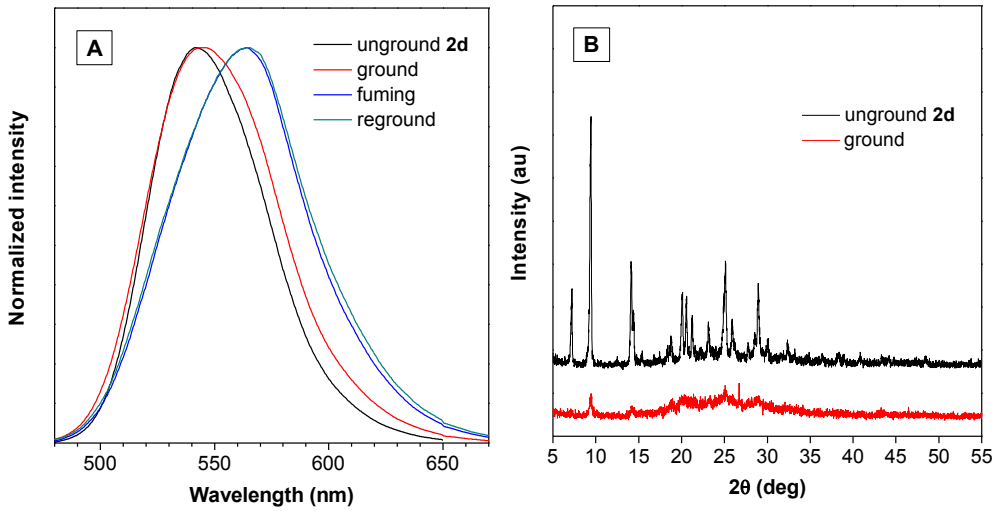
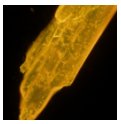
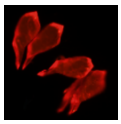


Fig. S20 (A) Normalized PL spectra of **2d** under different condition. (B) Powder XRD diffractions of **2d**.

8. X-ray Single Crystals Data and Their Packing Mode

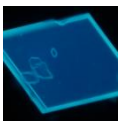
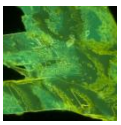
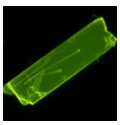
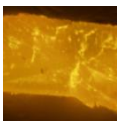
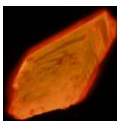
8.1 single crystal data summary

Table S6. Crystallographic data of series **1**.

Crystal	**1a**	**1c**	**1d**
formula	$C_{14}H_6N_4$	$C_{18}H_{14}N_4O_4$	$C_{16}H_{10}N_4O_2$
crystal system	monoclinic	monoclinic	monoclinic
space group	P 1 21/n 1	P 1 21/c 1	P 1 21/c 1
a [Å]	6.9562(4)	10.1736(3)	3.9933(4)
b[Å]	8.6030(4)	4.9312(2)	16.4932(9)
c[Å]	10.0638(8)	17.7827(8)	10.7618(6)
β [deg]	104.584(7)	96.441(4)	93.630(6)
V [Å^3]	582.86(6)	886.49(7)	707.37(9)
Z	2	2	2
μ [mm^{-1}]	0.671	0.797	0.776
T [K]	293	293	293
θ_{min}-θ_{max}[deg]	7.0050-71.6570	4.8090-71.9580	5.3750-71.2330
R	0.0457	0.0396	0.0433
wR_2	0.1345	0.1161	0.1314
GOOF	1.050	1.028	1.044
crystal pictures[a]			
CCDC number	1056239	1056280	1403124
	Compounds chart	Compounds chart	Compounds chart
	Data	Data	Data
	NMR	NMR	NMR

[a]The fluorescent pictures of corresponding single crystals were taken by Olympus DP-80 fluorescence microscopy under UV irradiation.

Table S7. Crystallographic data of series **2**.

Crystal	**2a**	**2b**	**2c**	**2e**	**2g**
formula	$C_{26}H_{14}N_4$	$C_{22}H_{10}N_4O_2$	$C_{38}H_{42}N_4O_2Si_2$	$C_{32}H_{28}N_6O_4$	$C_{24}H_{14}N_4S_2$
crystal system	monoclinic	monoclinic	triclinic	monoclinic	monoclinic
space group	P 1 21/n 1	C 2/c	P -1	C 1 2/c 1	P 1 21/c 1
a [Å]	12.4262 (9)	10.8800 (4)	9.7516 (5)	20.3875 (9)	9.0866 (3)
b[Å]	7.2914 (5)	7.8430 (3)	12.8129 (6)	6.9526 (2)	10.3527 (4)
c[Å]	12.8993 (8)	21.0513 (10)	16.8155 (9)	21.3637 (7)	11.6224 (4)
β [deg]	118.312 (3)	91.528 (4)	99.248 (5)	95.544 (3)	104.969 (4)
V [Å^3]	1028.92 (12)	1795.71 (13)	1981.19 (18)	3014.04 (19)	1056.23 (7)
Z	2	4	2	4	2
μ [mm^{-1}]	0.075	0.732	1.079	0.683	2.423
T [K]	293	291	293	293	293
θ_{min}-θ_{max}[deg]	3.1390-26.4140	4.1730-69.5230	4.6380-68.5880	5.7680-66.1850	3.9370-71.5460
R	0.0770	0.0405	0.0770	0.0430	0.0389
wR_2	0.2330	0.1209	0.2412	0.1208	0.1118
GOOF	1.094	1.074	1.036	1.037	1.036
crystal pictures[a]					
CCDC number	1439334	1439332	1443616	1442948	1442404
	Compounds chart	Compounds chart	Compounds chart	Compounds chart	Compounds chart
	Data	Data	Data	Data	Data
	NMR	NMR	NMR	NMR	NMR

[a] The fluorescent pictures of corresponding single crystals were taken by Olympus DP-80 fluorescence microscopy under UV irradiation.

Table S8. Crystallographic data of **2d-g** and **2d-o**.

Crystal	**2d-g**	**2d-o**
formula	$C_{28}H_{18}N_4O_2$	$C_{28}H_{18}N_4O_2$
crystal system	monoclinic	triclinic
space group	P 1 21/c 1	P -1
a [Å]	6.7023 (2)	6.5174 (4)
b[Å]	14.1338 (4)	9.8469 (5)
c[Å]	12.7266 (4)	10.3476 (5)
β [deg]	100.447 (3)	95.997 (5)
V [Å^3]	1185.58 (7)	575.82 (7)
Z	2	11
μ [mm^{-1}]	0.646	0.665
T [K]	293	293
θ_{min}-θ_{max}[deg]	8.7080-71.9270	8.4320-72.4360
R	0.0505	0.0418
wR_2	0.1373	0.1177
GOOF	1.048	1.0717
CCDC number	1472574	1499316
	Compounds chart	
	Data	
	NMR	

8.2 X-ray single crystallographic packing of the corresponding compounds

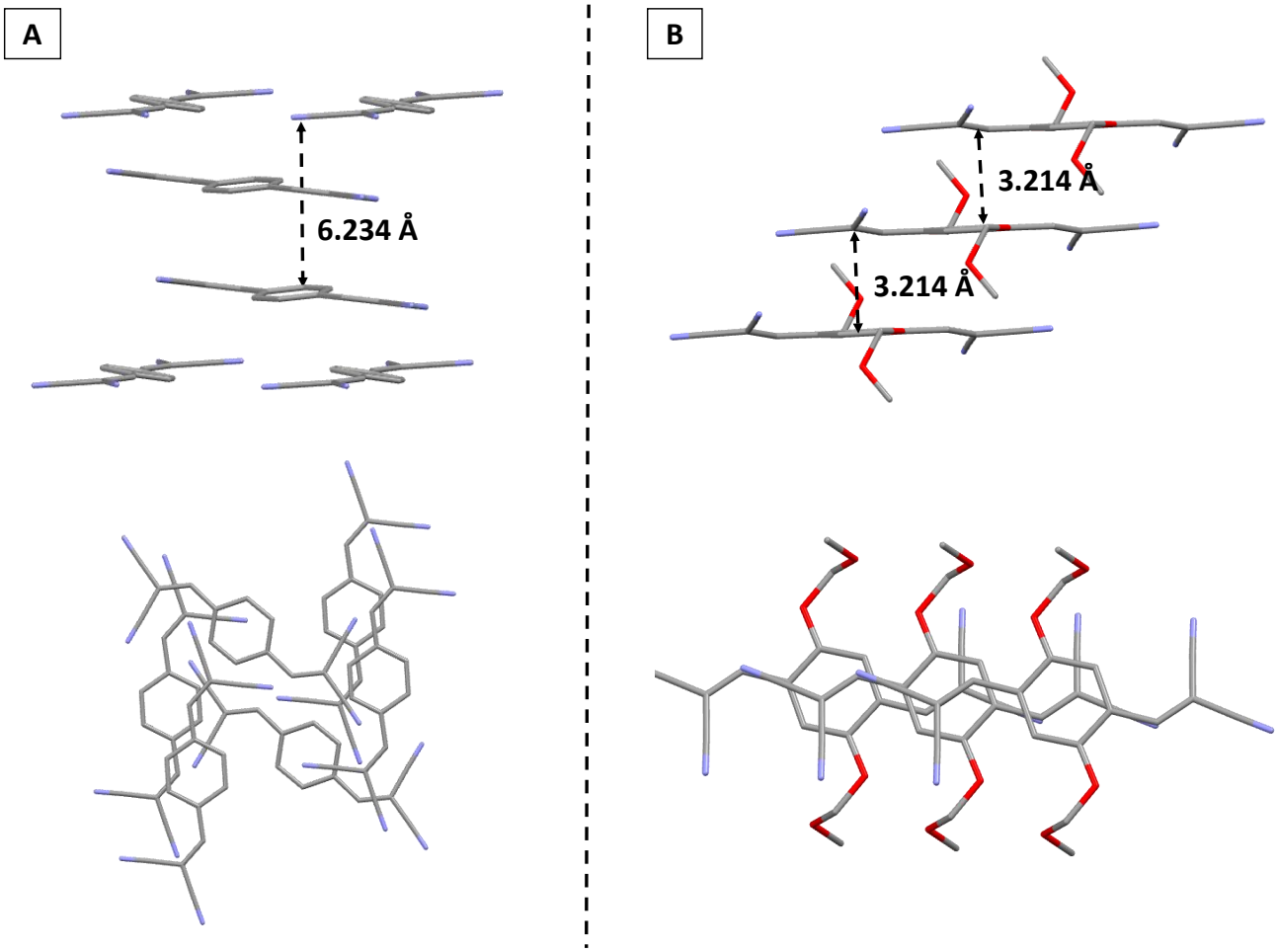


Fig. S21 Side and top view of crystal packing mode of 1**a** (A) and **1c** (B). Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

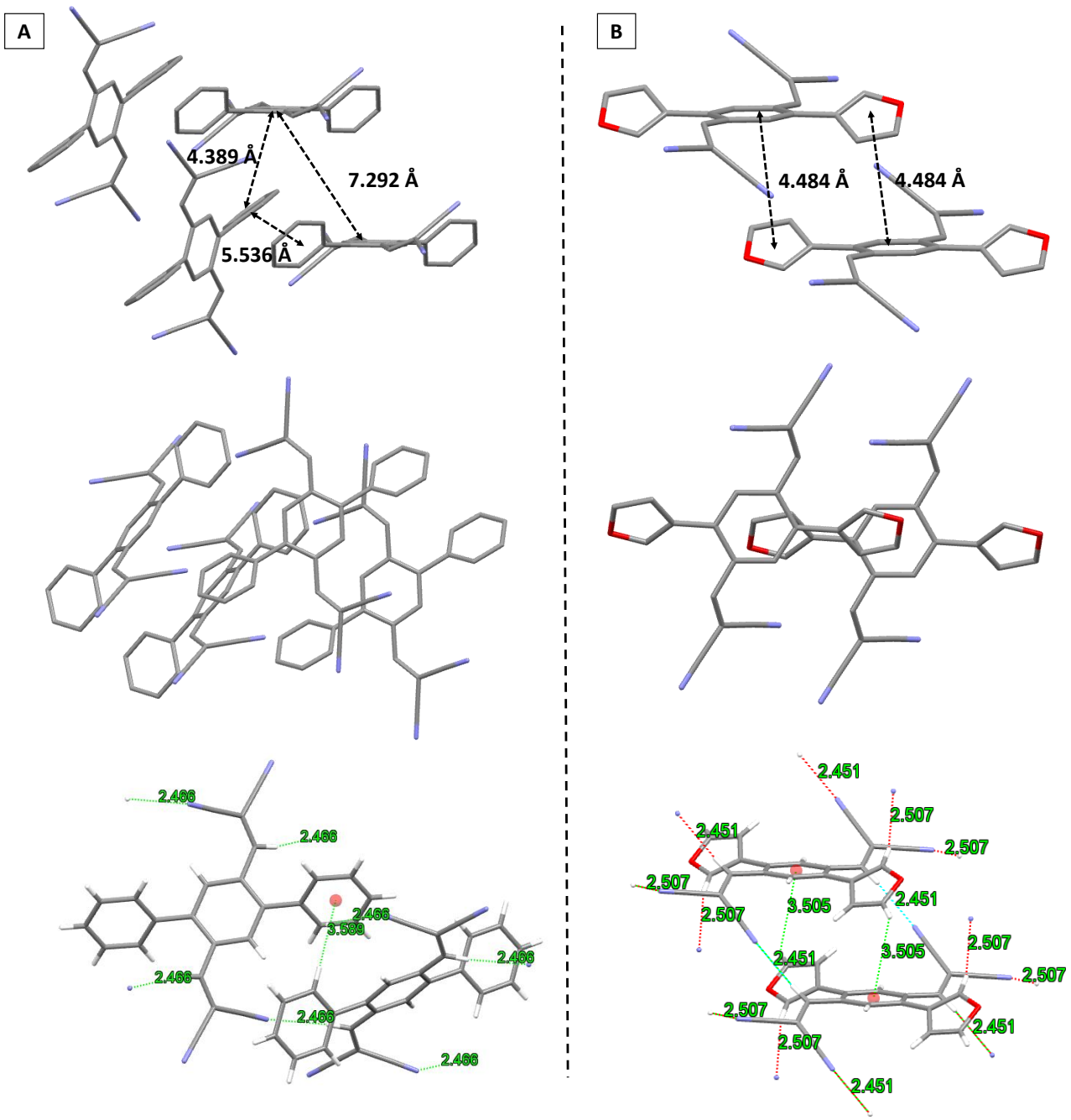


Fig. S22 Side and top view of crystal packing mode as well as short contacts of **2a** (A) and **2b** (B). Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

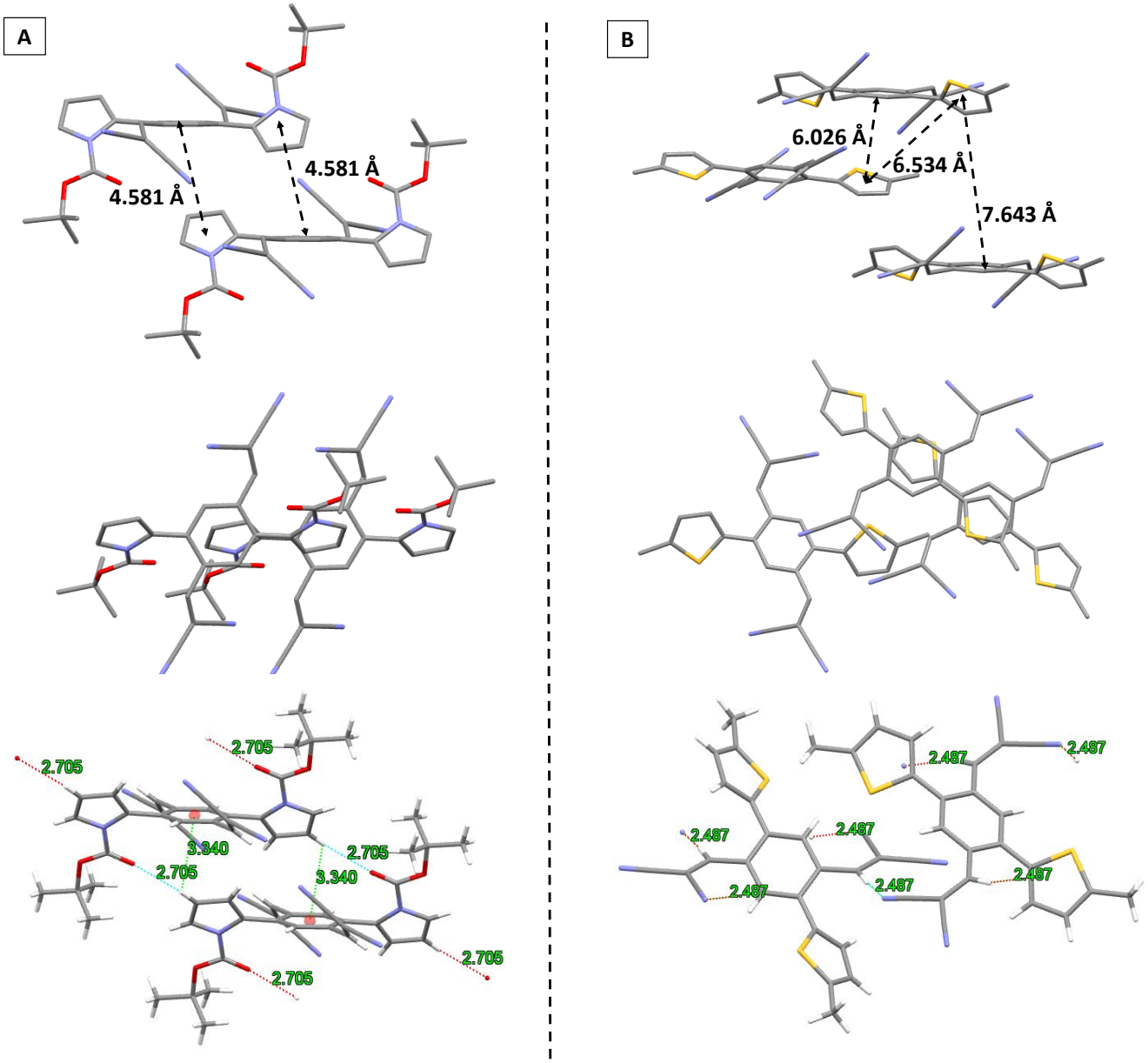


Fig. S23 Side and top view of crystal packing mode as well as short contacts of **2c** (A) and **2g** (B). Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

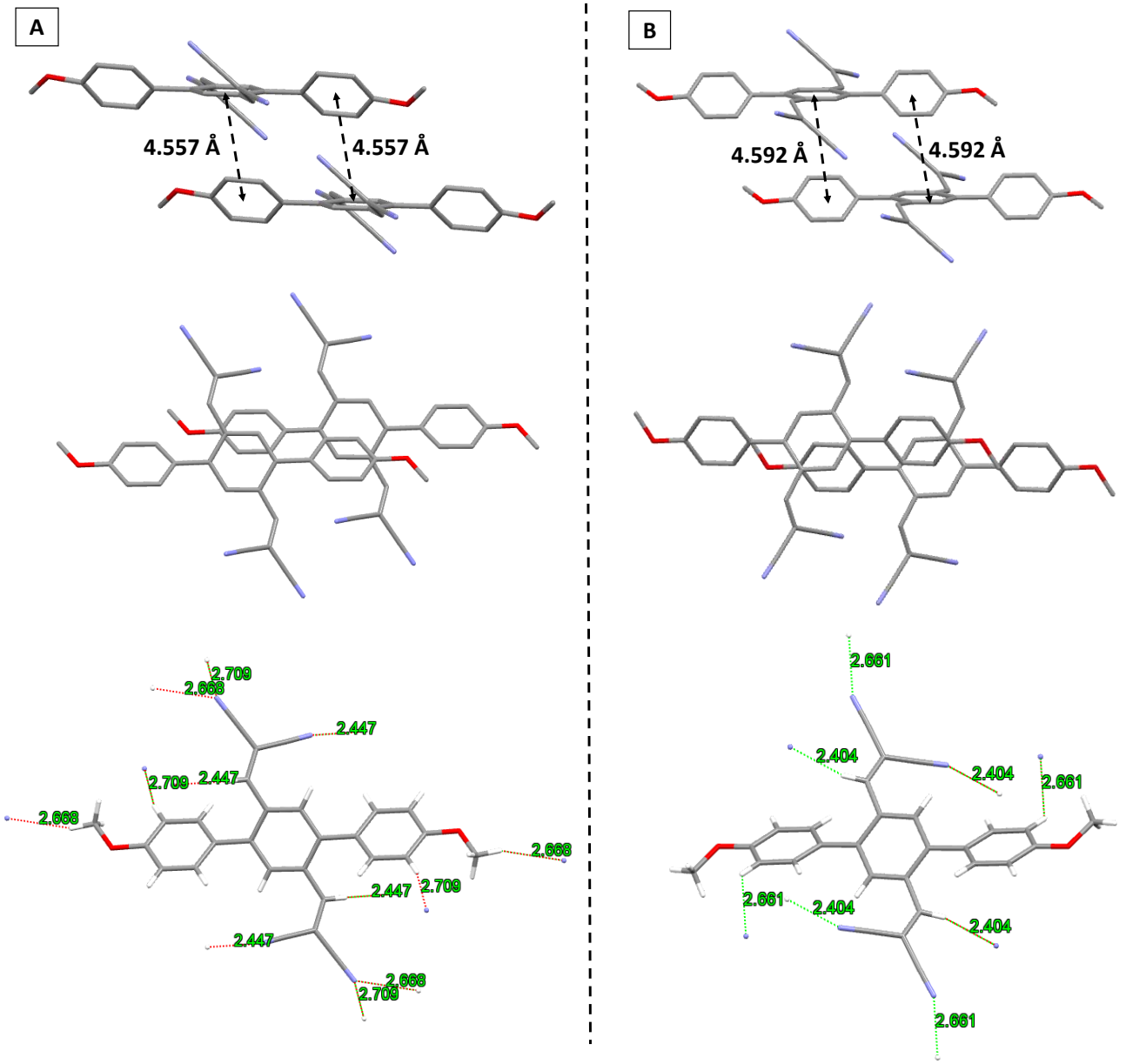


Fig.S24 Side and top view of crystal packing mode as well as short contacts of **2d-y** (A) and **2d-o** (B). Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

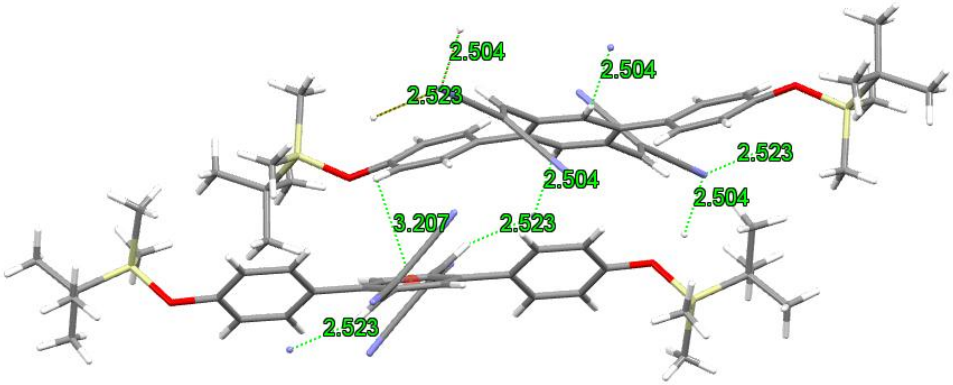
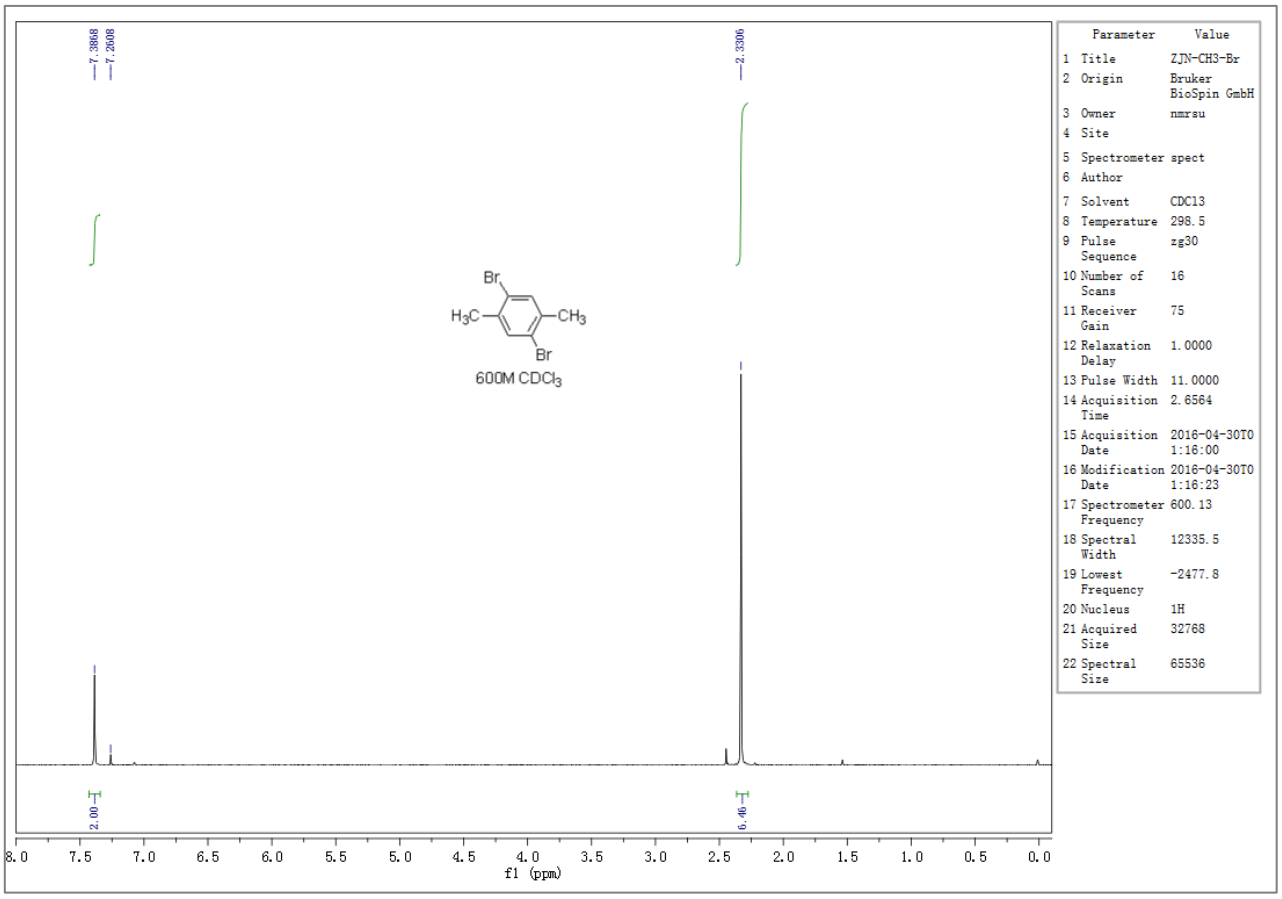


Fig.S25 Illustration of short contacts of **2c**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

9. NMR Spectra



	Parameter	Value
1	Title	ZJN-CH3-Br
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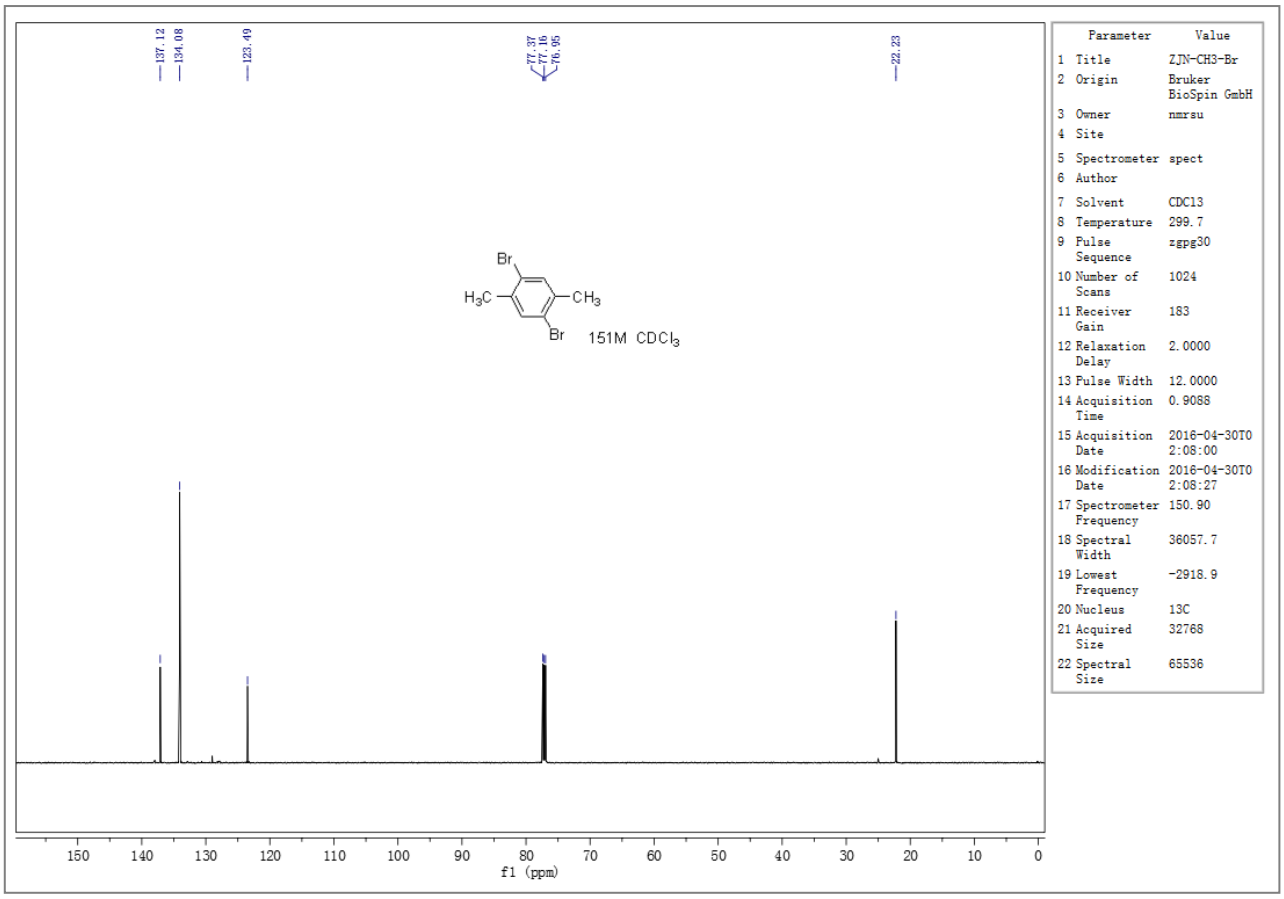
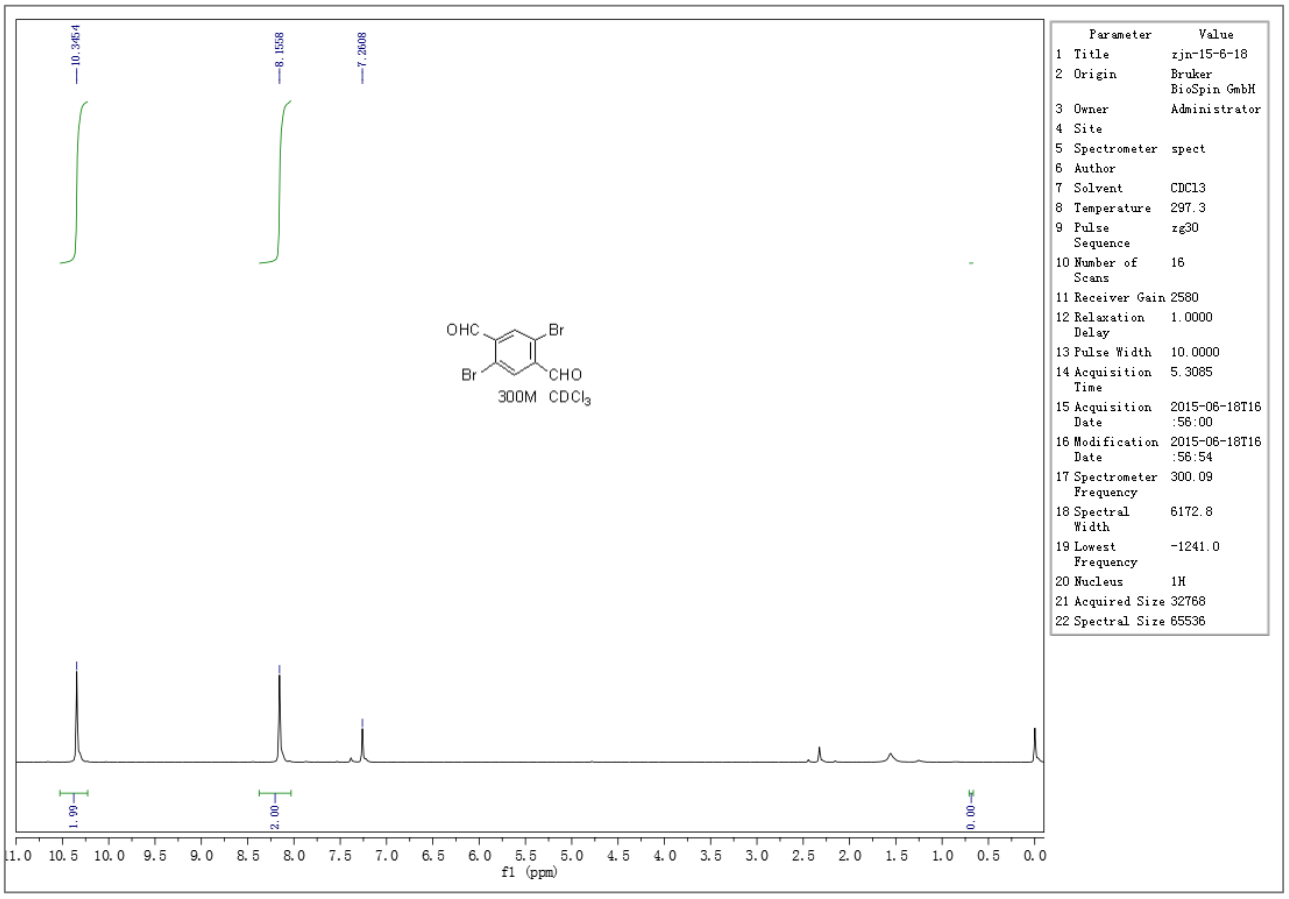
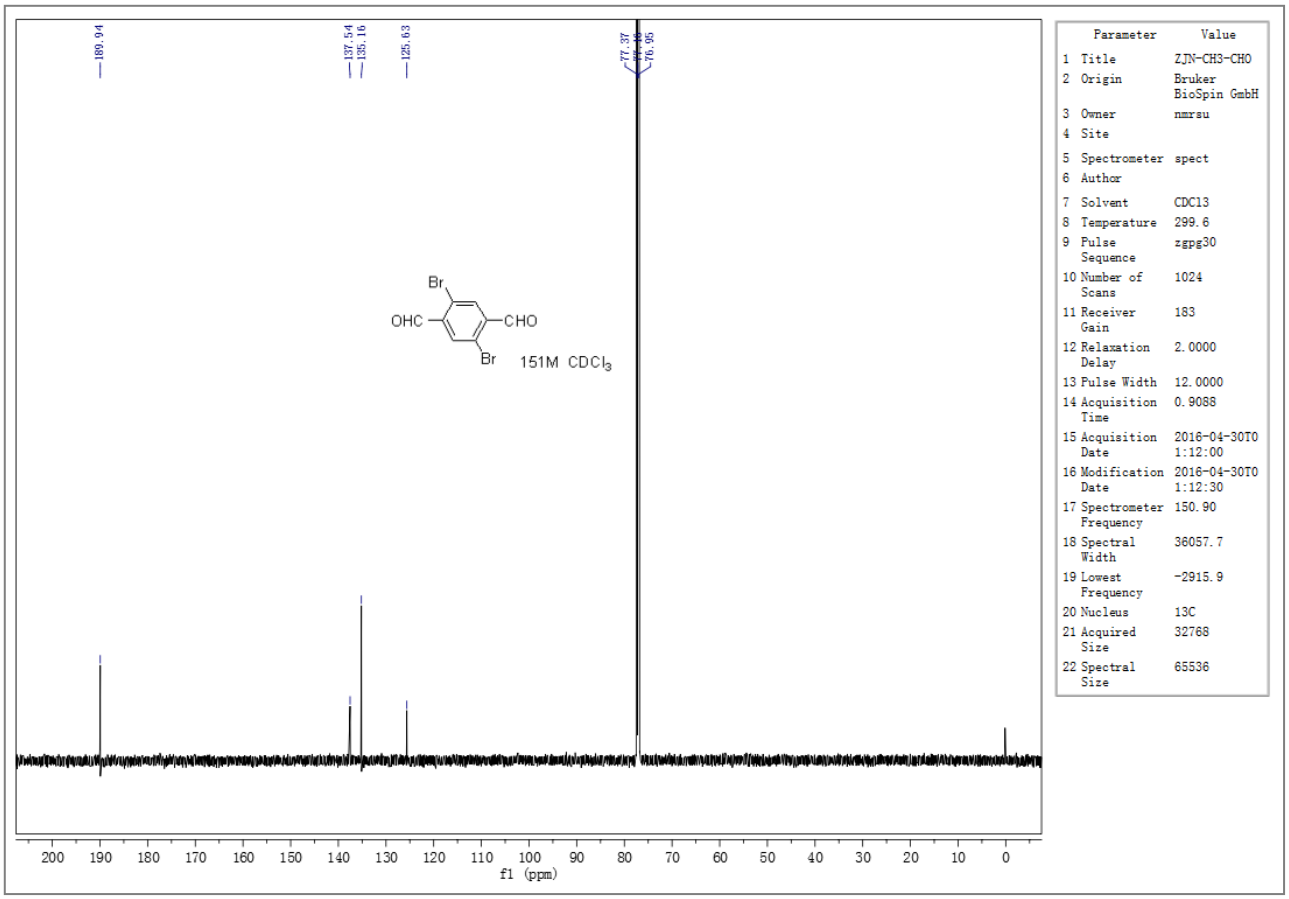
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.5
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	75
12	Relaxation Delay	1.0000
13	Pulse Width	11.0000
14	Acquisition Time	2.6564
15	Acquisition Date	2016-04-30T01:16:00
16	Modification Date	2016-04-30T01:16:23
17	Spectrometer Frequency	600.13
18	Spectral Width	12335.5
19	Lowest Frequency	-2477.8
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



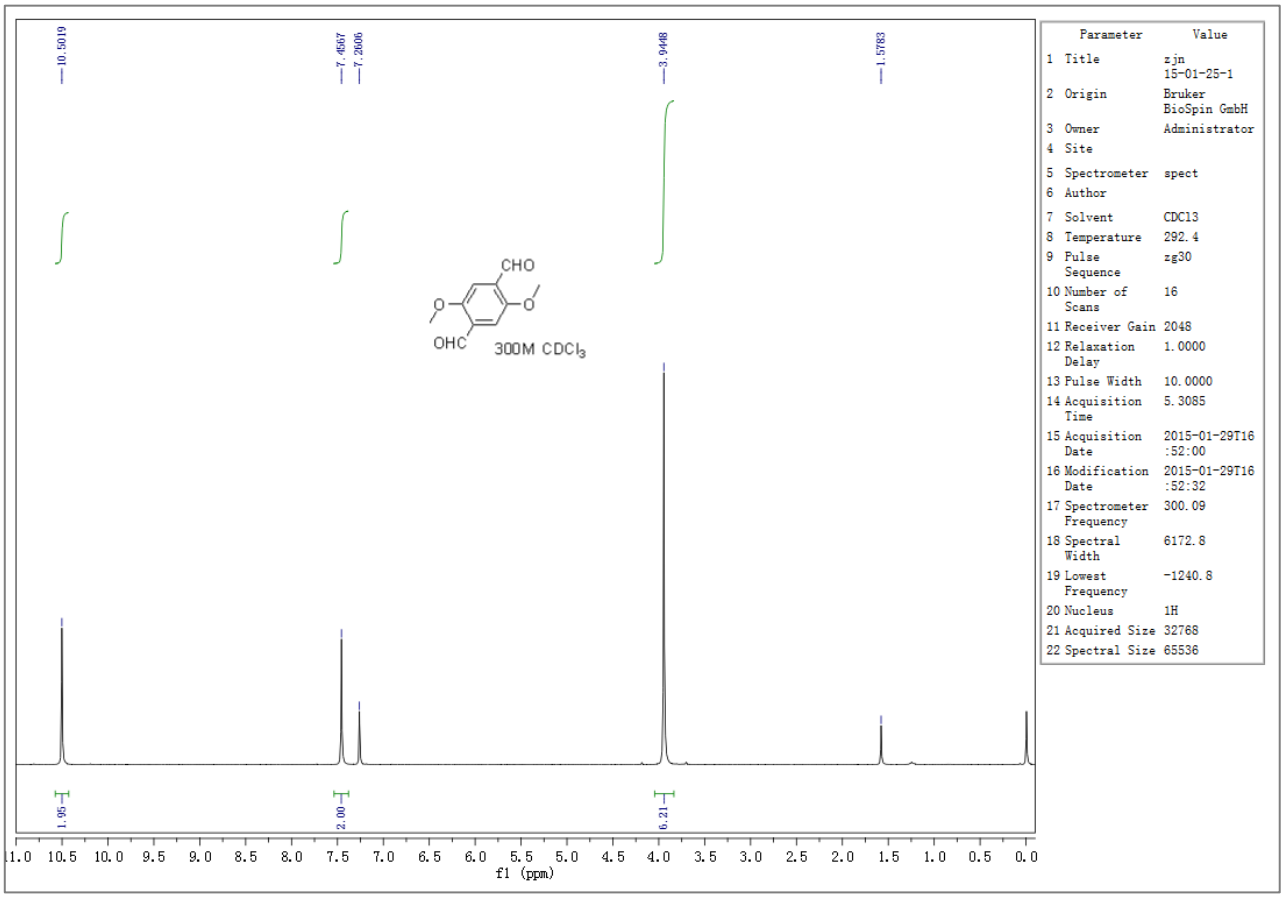
	Parameter	Value
1	Title	ZJN-CH3-Br
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	299.7
9	Pulse Sequence	zgpg30
10	Number of Scans	1024
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2016-04-30T02:08:00
16	Modification Date	2016-04-30T02:08:27
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2918.9
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



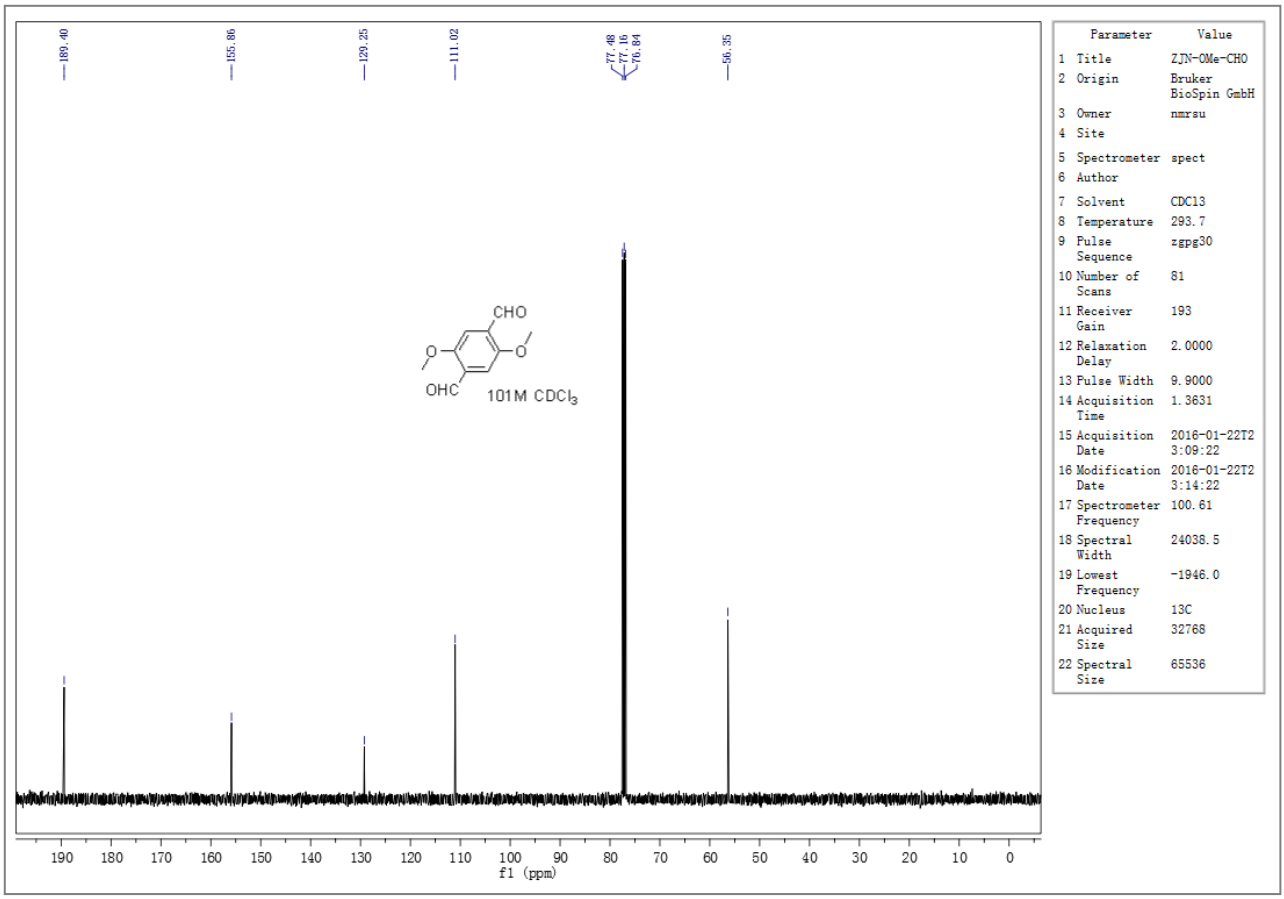
	Parameter	Value
1	Title	zjn-15-6-18
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.3
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	2580
12	Relaxation Delay	1.0000
13	Pulse Width	10.0000
14	Acquisition Time	5.3085
15	Acquisition Date	2015-06-18T16:56:00
16	Modification Date	2015-06-18T16:56:54
17	Spectrometer Frequency	300.09
18	Spectral Width	6172.8
19	Lowest Frequency	-1241.0
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



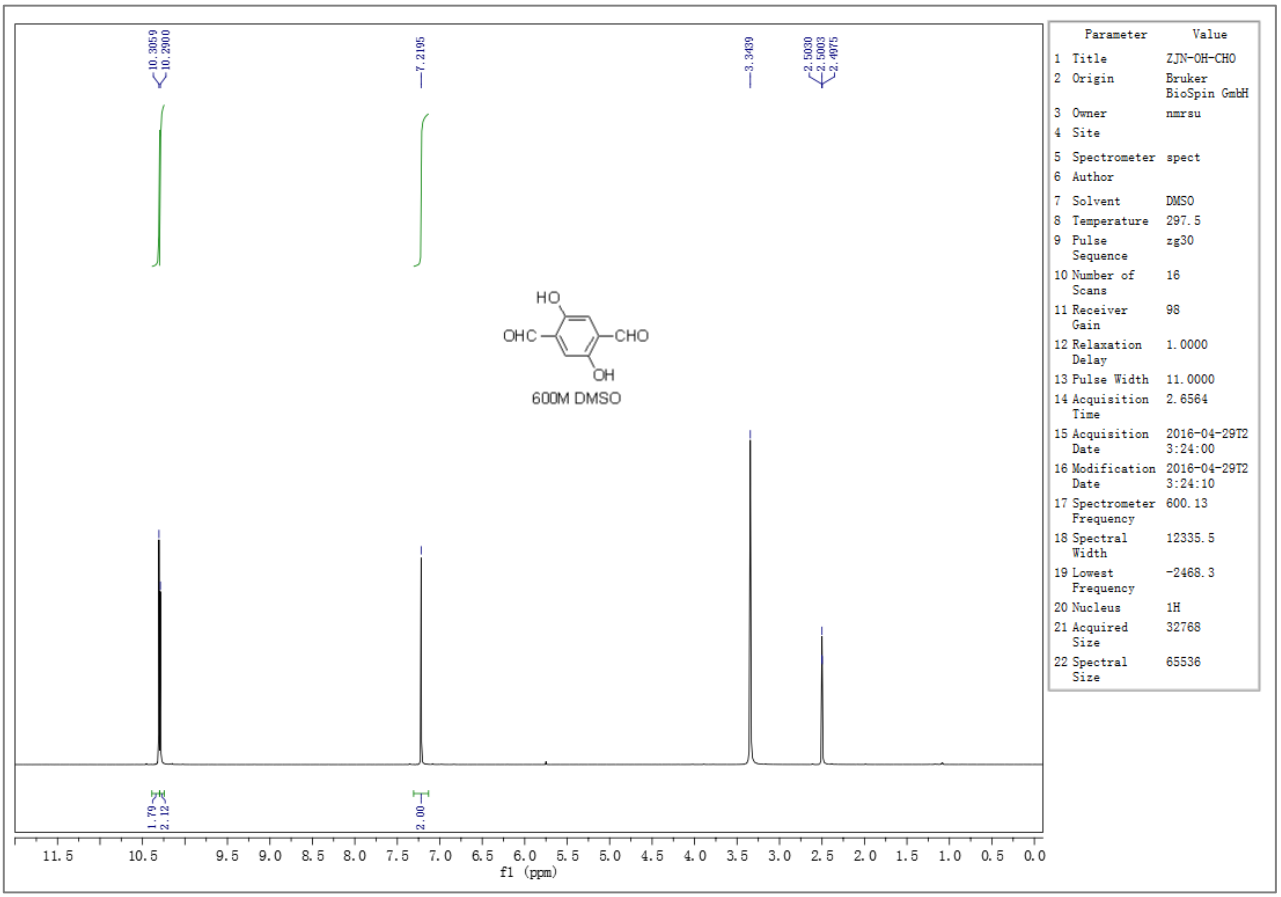
	Parameter	Value
1	Title	ZJN-CH3-CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	299.6
9	Pulse Sequence	zgpg30
10	Number of Scans	1024
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2016-04-30T01:12:00
16	Modification Date	2016-04-30T01:12:30
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2915.9
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



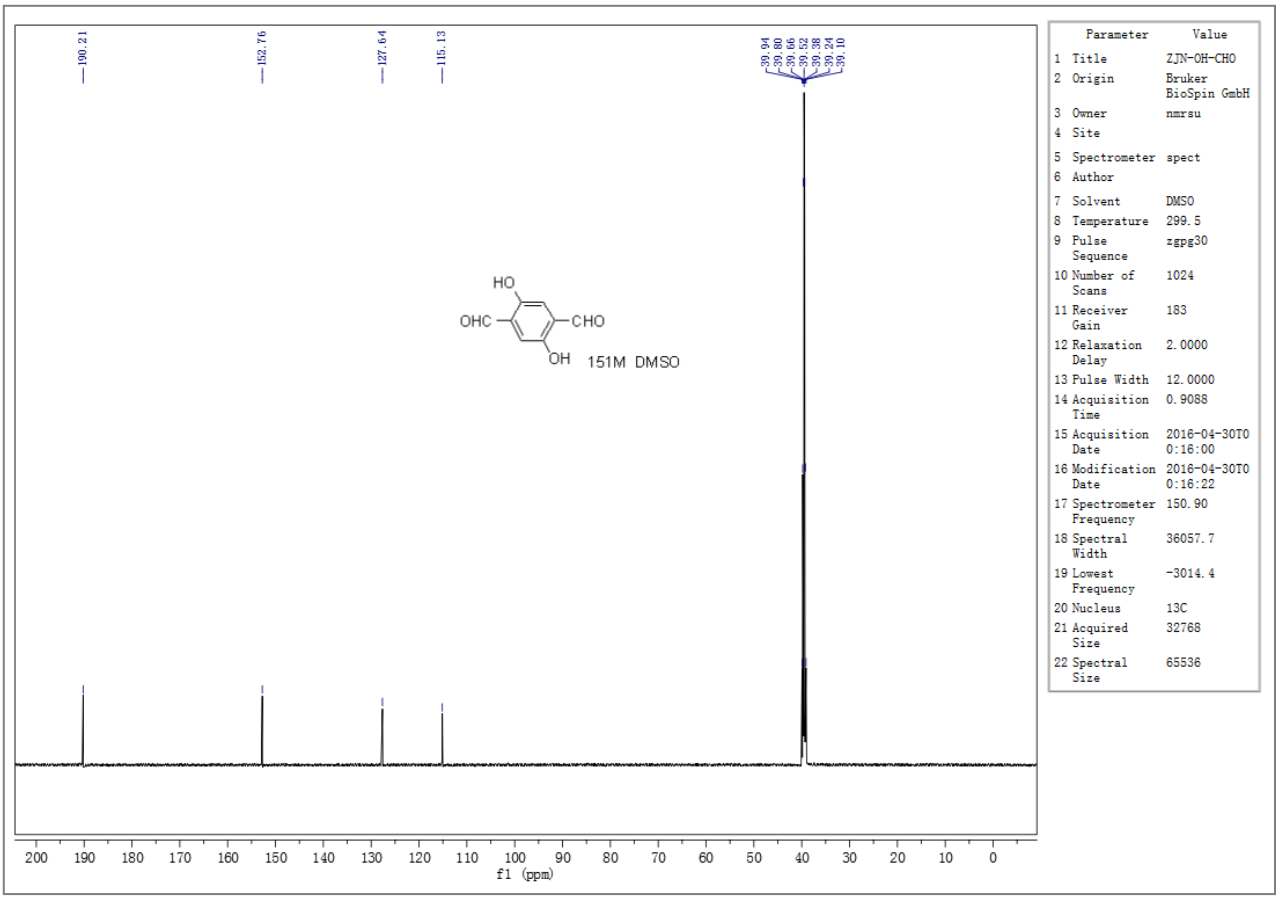
	Parameter	Value
1	Title	zjn 15-01-25-1
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	292.4
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	2048
12	Relaxation Delay	1.0000
13	Pulse Width	10.0000
14	Acquisition Time	5.3085
15	Acquisition Date	2015-01-29T16:52:00
16	Modification Date	2015-01-29T16:52:32
17	Spectrometer Frequency	300.09
18	Spectral Width	6172.8
19	Lowest Frequency	-1240.8
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



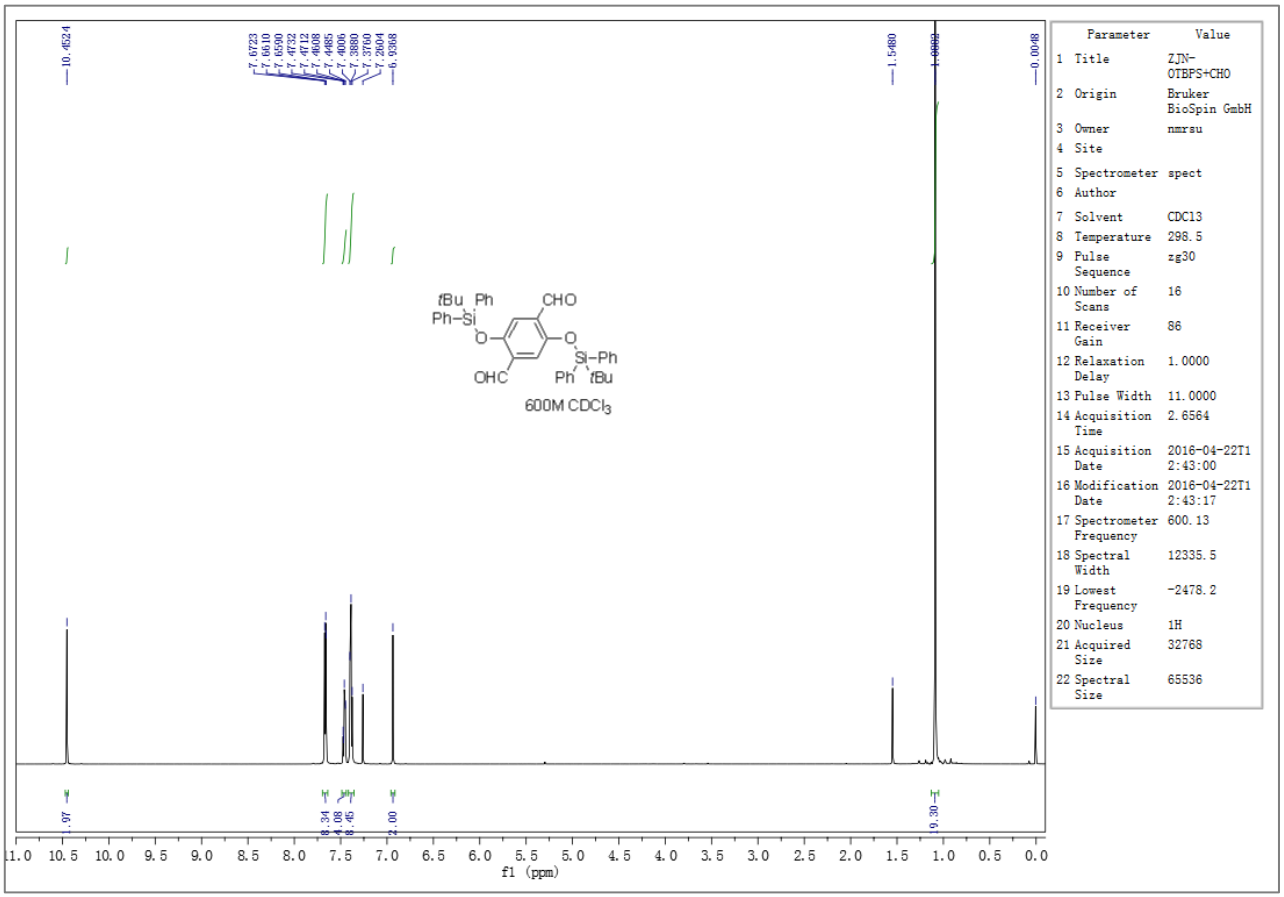
	Parameter	Value
1	Title	ZJN-OMe-CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	293.7
9	Pulse Sequence	zgpg30
10	Number of Scans	81
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2016-01-22T23:09:22
16	Modification Date	2016-01-22T23:14:22
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1946.0
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



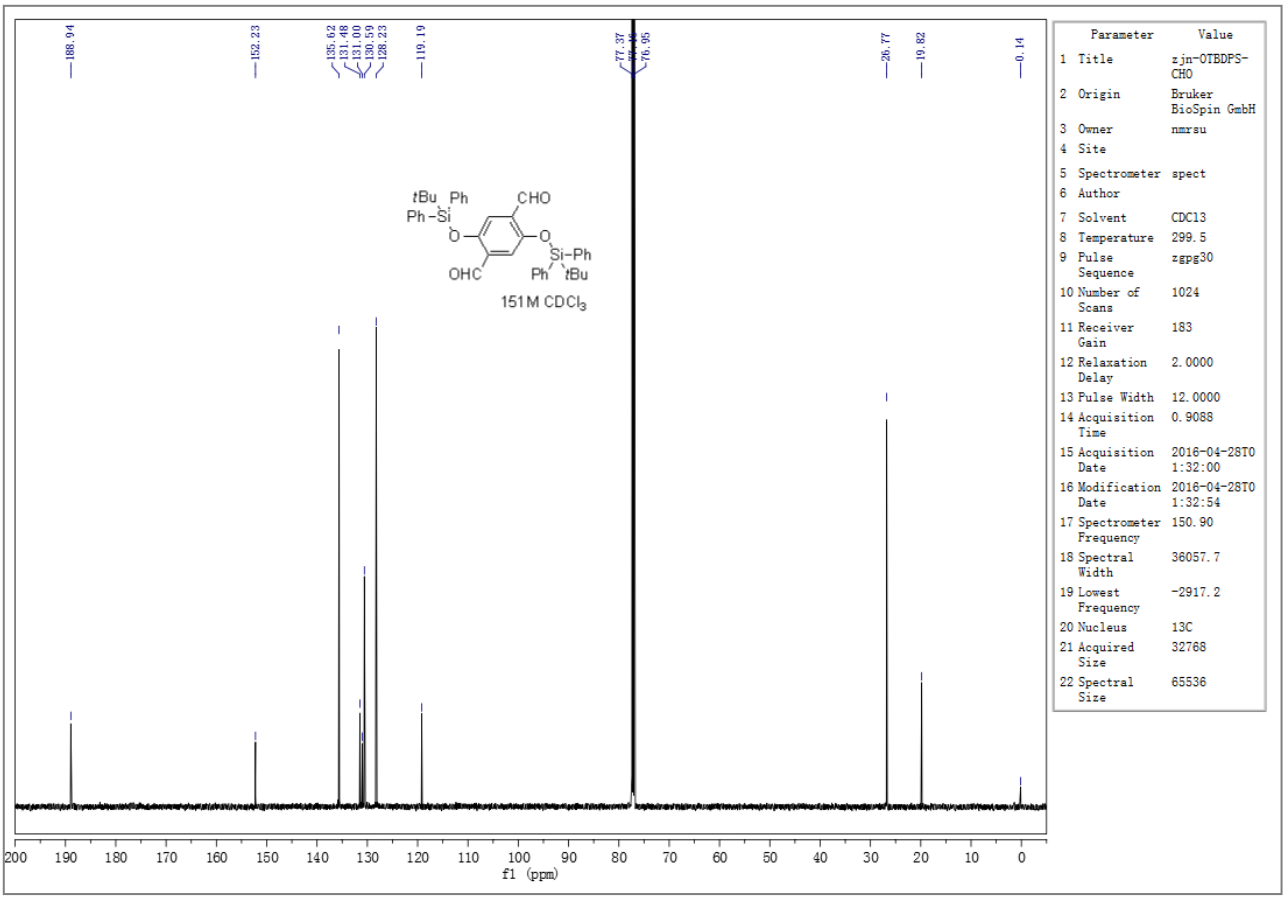
	Parameter	Value
1	Title	ZJN-OH-CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	297.5
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	98
12	Relaxation Delay	1.0000
13	Pulse Width	11.0000
14	Acquisition Time	2.6564
15	Acquisition Date	2016-04-29T2 3:24:00
16	Modification Date	2016-04-29T2 3:24:10
17	Spectrometer Frequency	600.13
18	Spectral Width	12335.5
19	Lowest Frequency	-2468.3
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



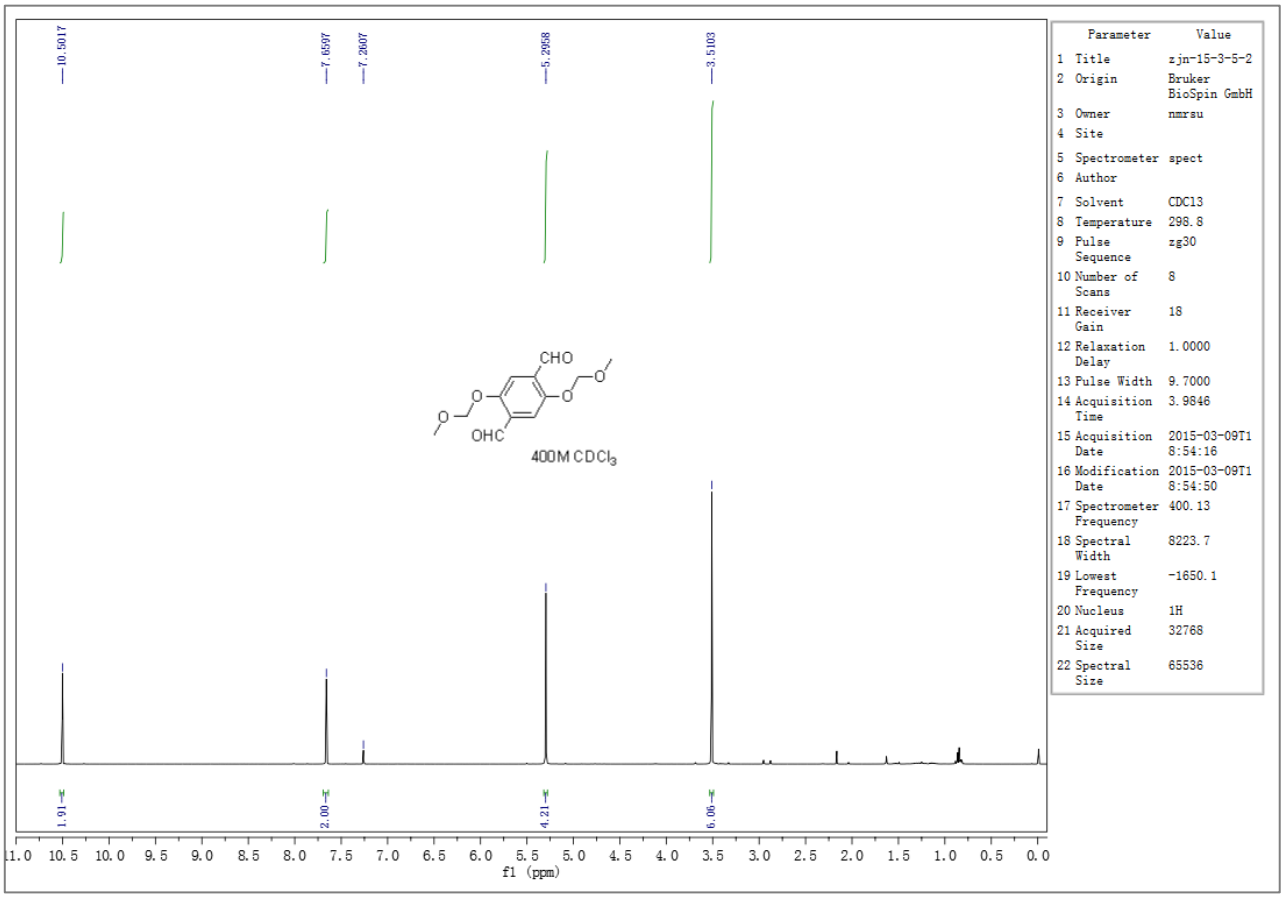
	Parameter	Value
1	Title	ZJN-OH-CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	299.5
9	Pulse Sequence	zgpg30
10	Number of Scans	1024
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2016-04-30T0 0:16:00
16	Modification Date	2016-04-30T0 0:16:22
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-3014.4
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



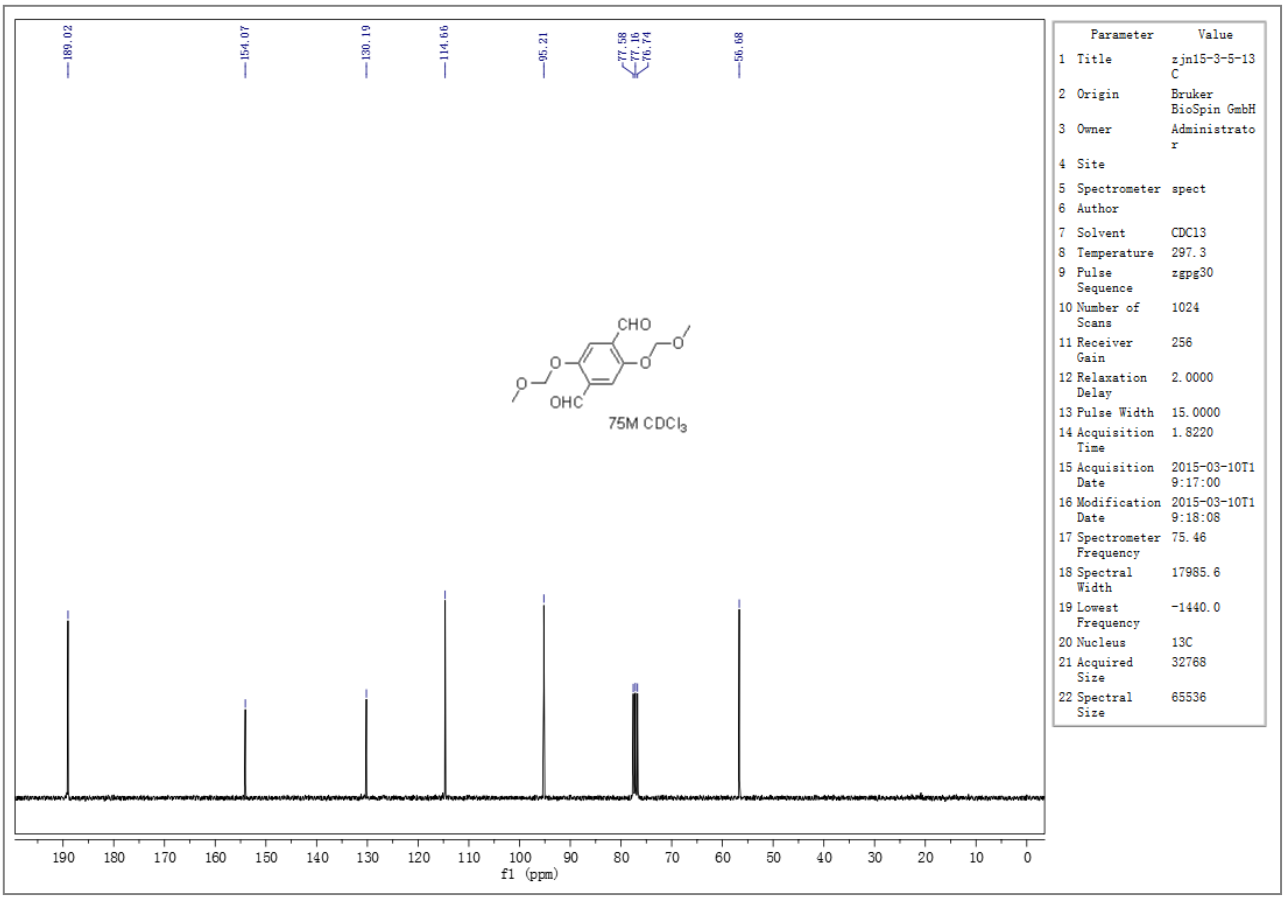
	Parameter	Value
1	Title	ZJN-OTBPS+CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.5
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	86
12	Relaxation Delay	1.0000
13	Pulse Width	11.0000
14	Acquisition Time	2.6564
15	Acquisition Date	2016-04-22T12:43:00
16	Modification Date	2016-04-22T12:43:17
17	Spectrometer Frequency	600.13
18	Spectral Width	12335.5
19	Lowest Frequency	-2478.2
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



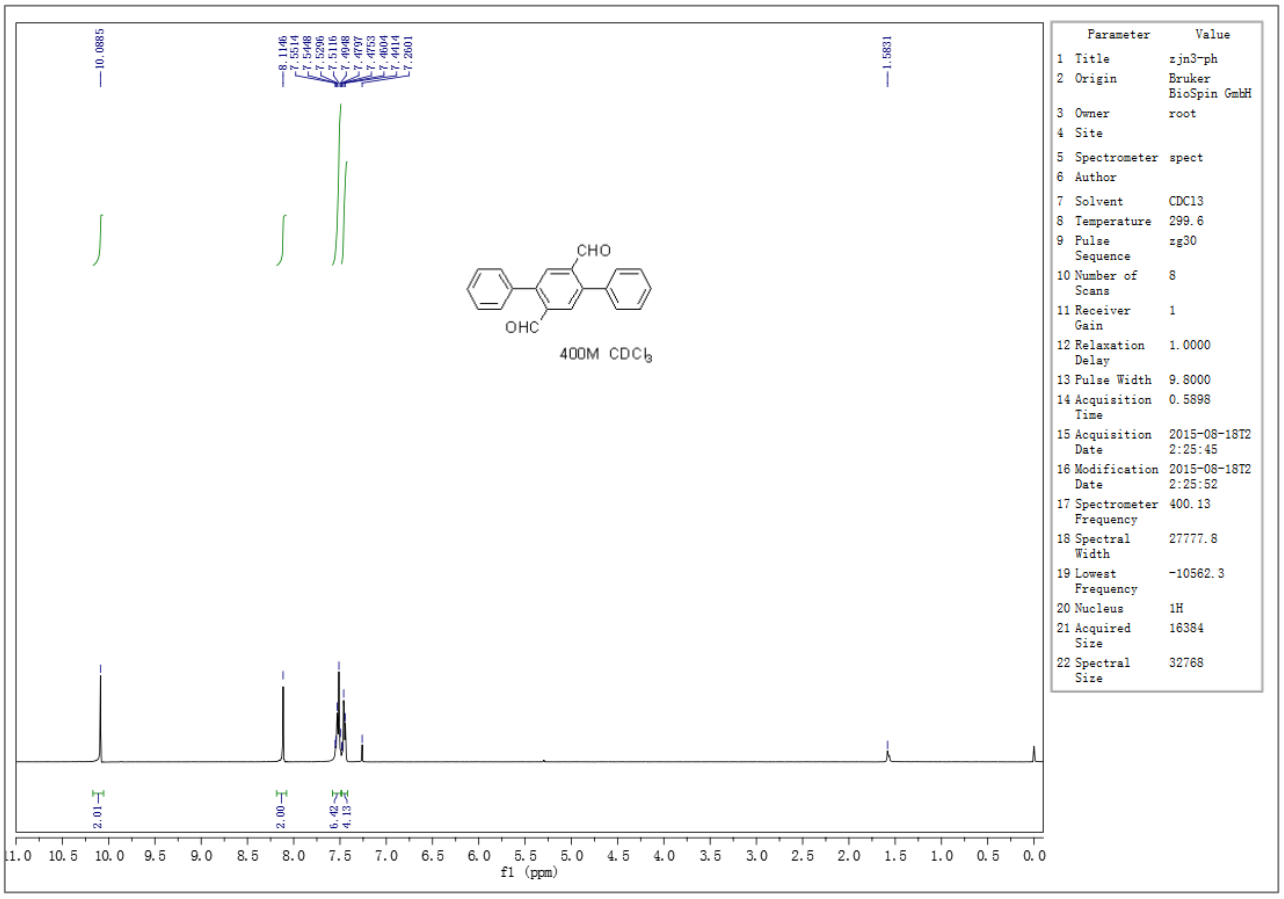
	Parameter	Value
1	Title	zjn-OTBDPS-CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	299.5
9	Pulse Sequence	zgpg30
10	Number of Scans	1024
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2016-04-28T01:32:00
16	Modification Date	2016-04-28T01:32:54
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2917.2
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



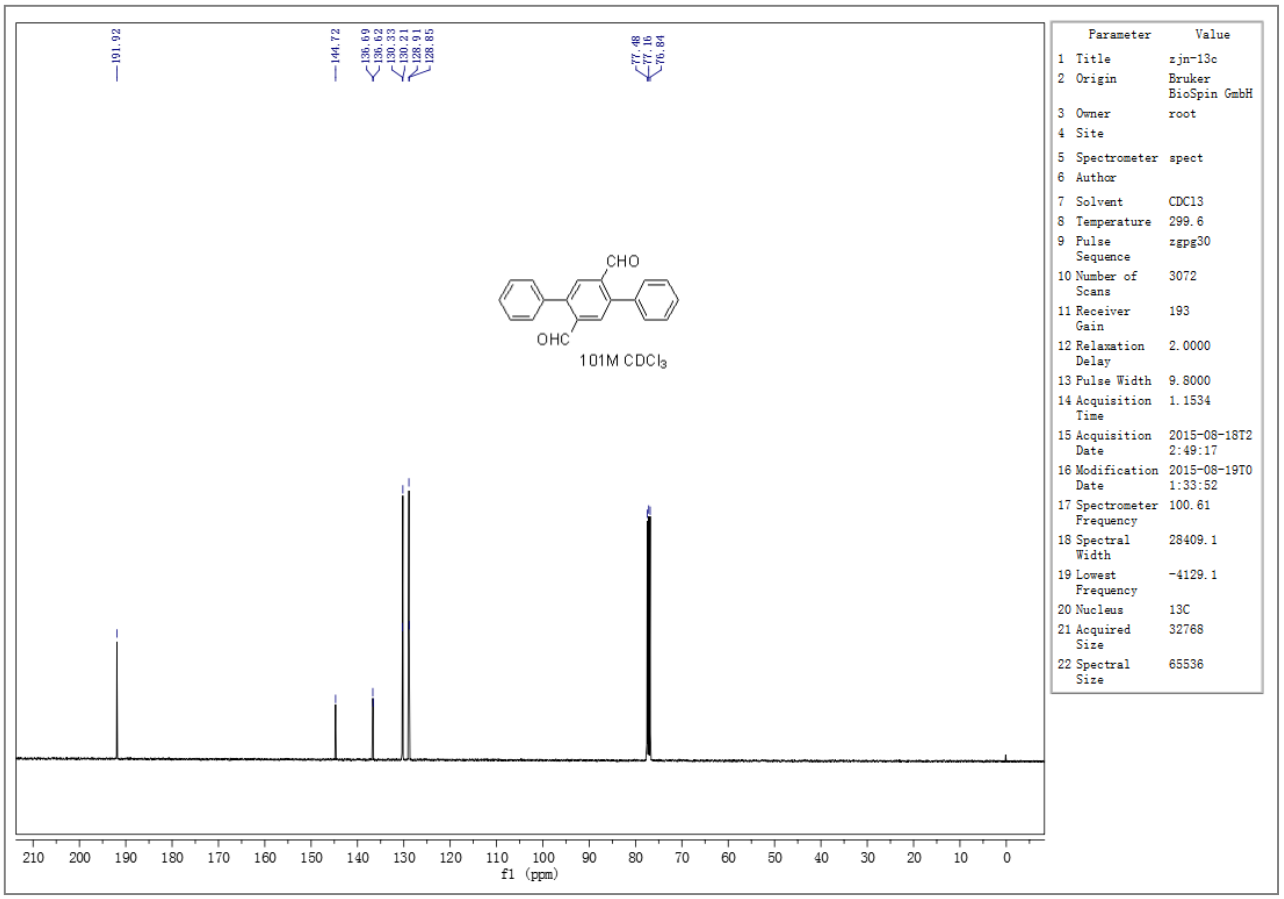
	Parameter	Value
1	Title	zjn-15-3-5-2
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.8
9	Pulse Sequence	zg30
10	Number of Scans	8
11	Receiver Gain	18
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-03-09T18:54:16
16	Modification Date	2015-03-09T18:54:50
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.1
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



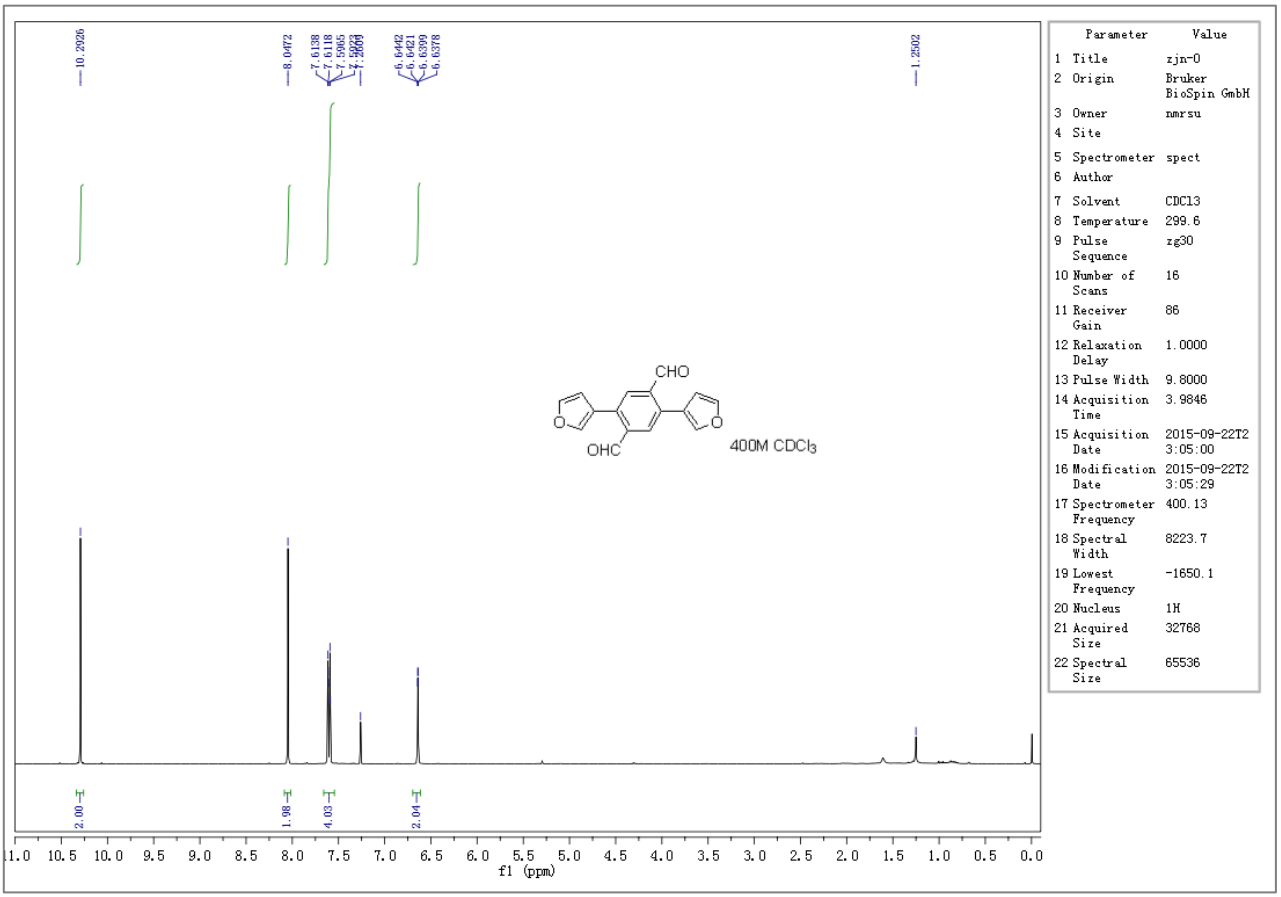
	Parameter	Value
1	Title	zjn15-3-5-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.3
9	Pulse Sequence	zgpg30
10	Number of Scans	1024
11	Receiver Gain	256
12	Relaxation Delay	2.0000
13	Pulse Width	15.0000
14	Acquisition Time	1.8220
15	Acquisition Date	2015-03-10T19:17:00
16	Modification Date	2015-03-10T19:18:08
17	Spectrometer Frequency	75.46
18	Spectral Width	17985.6
19	Lowest Frequency	-1440.0
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



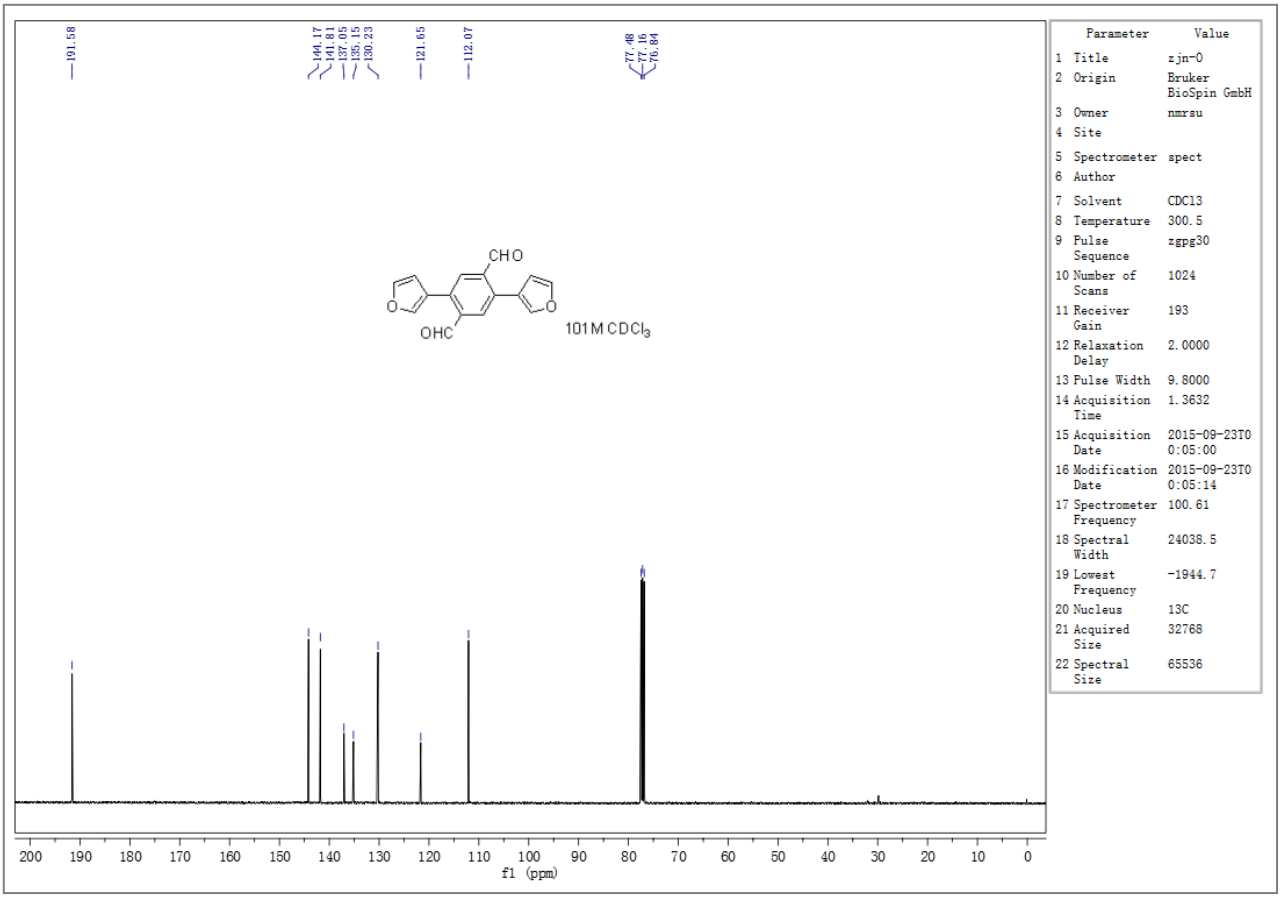
	Parameter	Value
1	Title	zjn3-ph
2	Origin	Bruker BioSpin GmbH
3	Owner	root
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDC13
8	Temperature	299.6
9	Pulse Sequence	zg30
10	Number of Scans	8
11	Receiver Gain	1
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.5898
15	Acquisition Date	2015-08-18T2 2:25:45
16	Modification Date	2015-08-18T2 2:25:52
17	Spectrometer Frequency	400.13
18	Spectral Width	27777.8
19	Lowest Frequency	-10562.3
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768



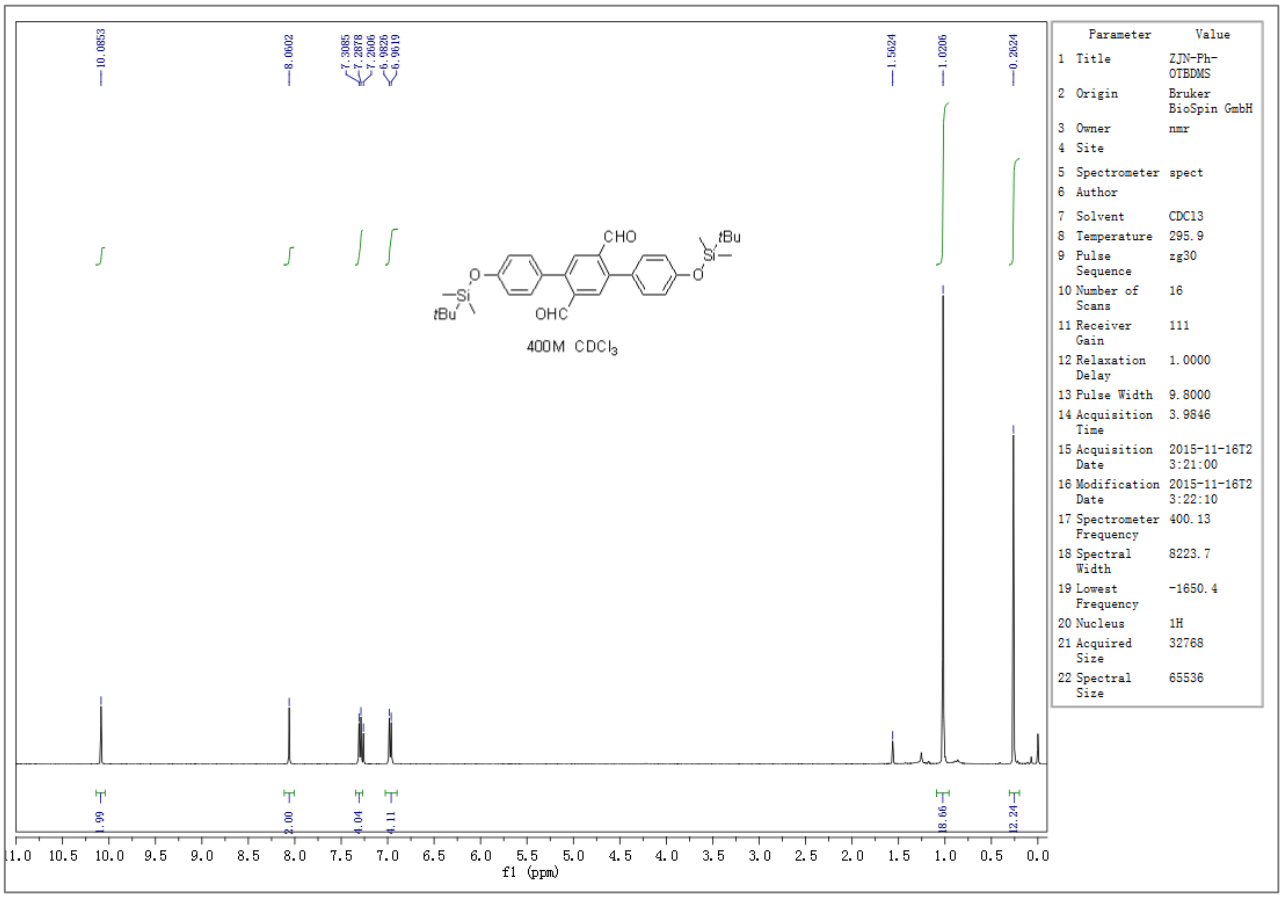
	Parameter	Value
1	Title	zjn-13c
2	Origin	Bruker BioSpin GmbH
3	Owner	root
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDC13
8	Temperature	299.6
9	Pulse Sequence	zgpg30
10	Number of Scans	3072
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	1.1534
15	Acquisition Date	2015-08-18T2 2:49:17
16	Modification Date	2015-08-19T0 1:33:52
17	Spectrometer Frequency	100.61
18	Spectral Width	28409.1
19	Lowest Frequency	-4129.1
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



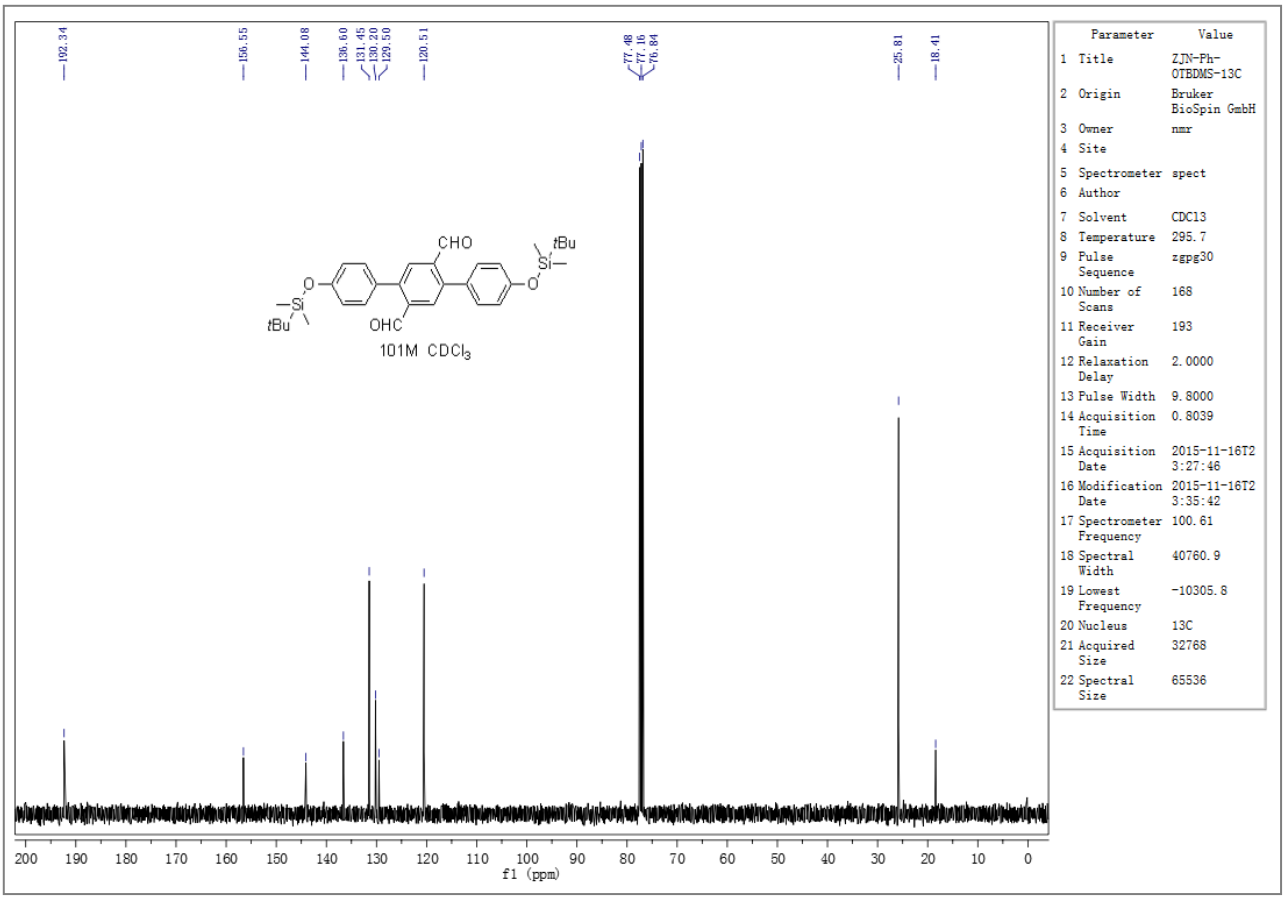
	Parameter	Value
1	Title	zjn-0
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	299.6
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	86
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-09-22T2 3:05:00
16	Modification Date	2015-09-22T2 3:05:29
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.1
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



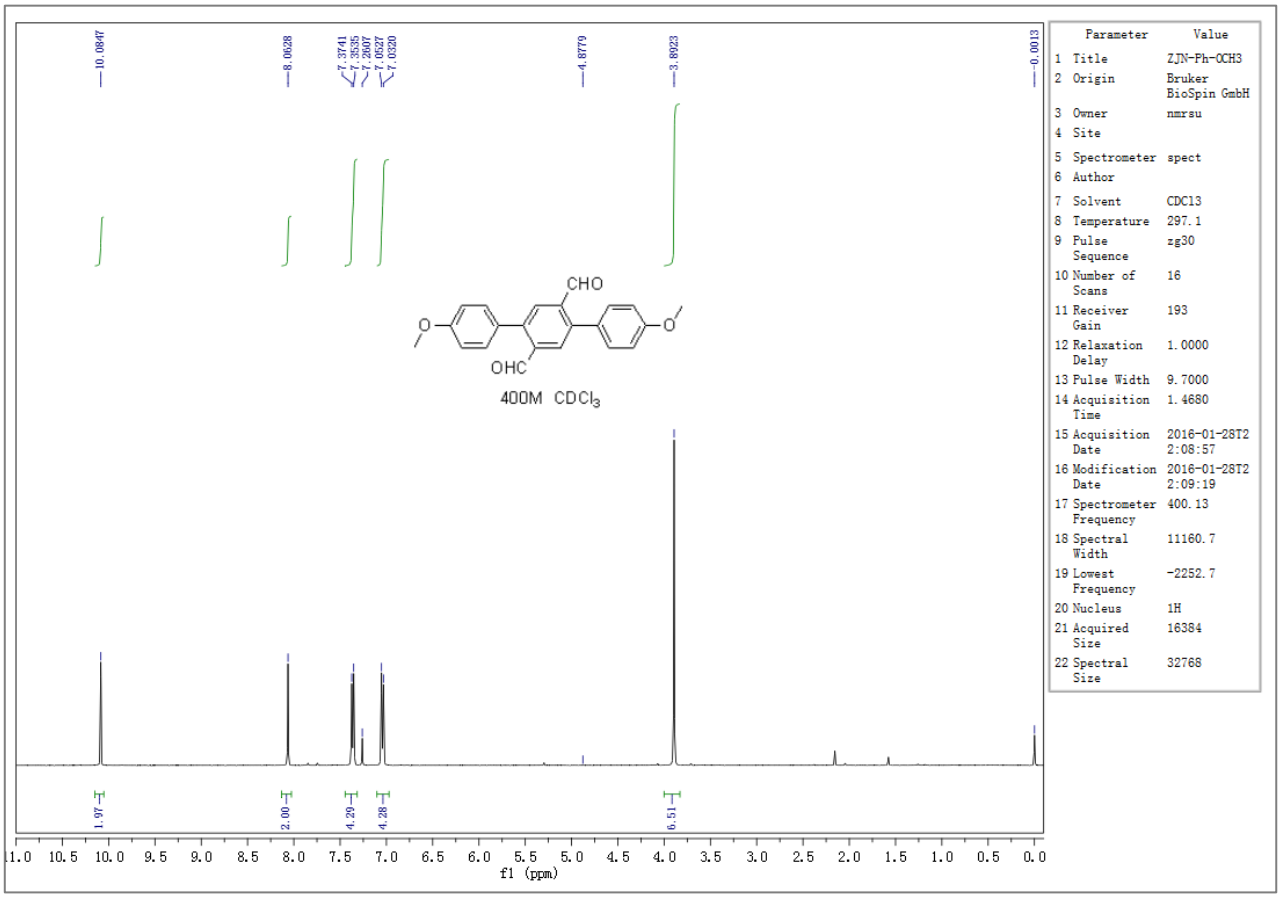
	Parameter	Value
1	Title	zjn-0
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	300.5
9	Pulse Sequence	zgpg30
10	Number of Scans	1024
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	1.3632
15	Acquisition Date	2015-09-23T0 0:05:00
16	Modification Date	2015-09-23T0 0:05:14
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1944.7
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



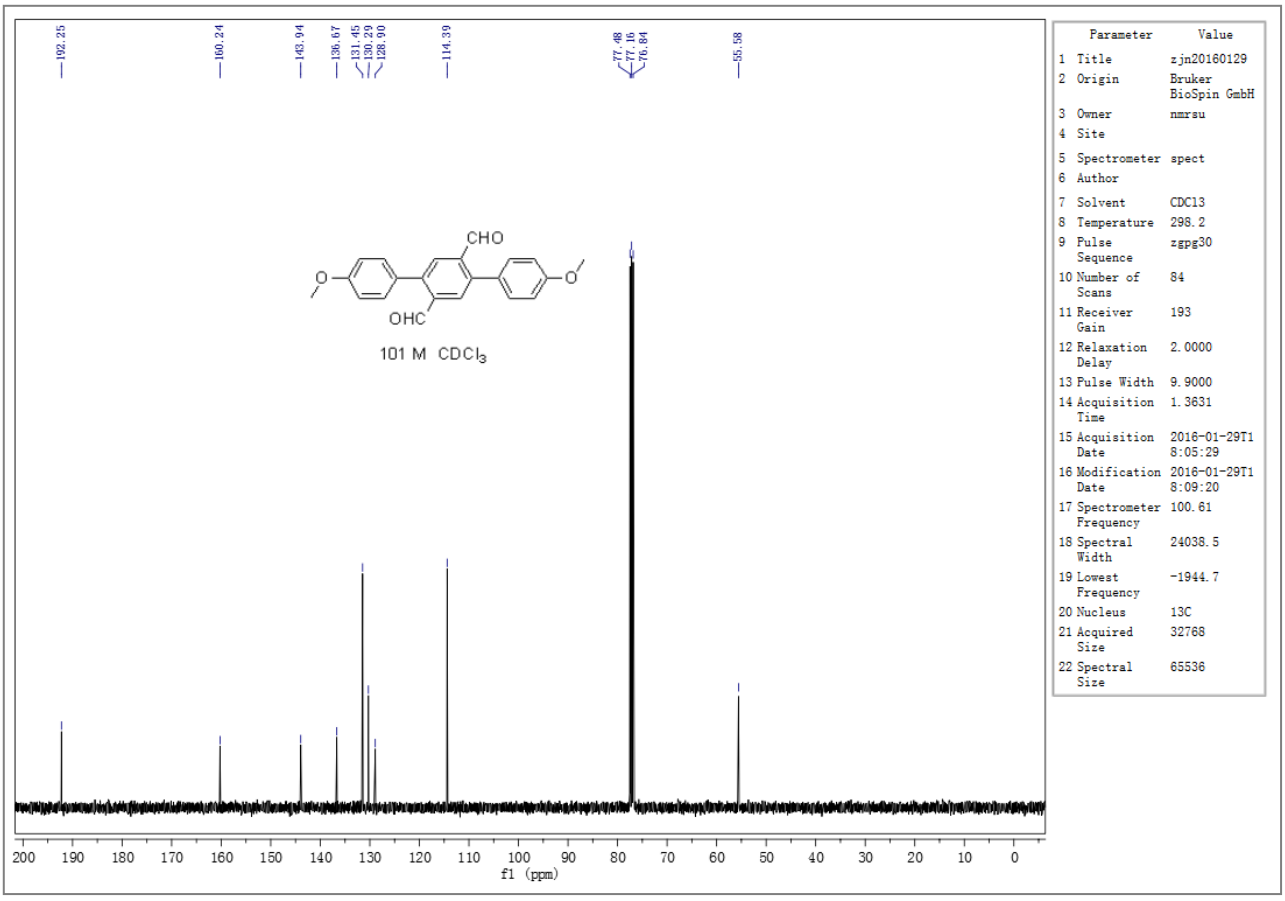
	Parameter	Value
1	Title	ZJN-Ph-OTBDMS
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	295.9
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	111
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-11-16T23:21:00
16	Modification Date	2015-11-16T23:22:10
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.4
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



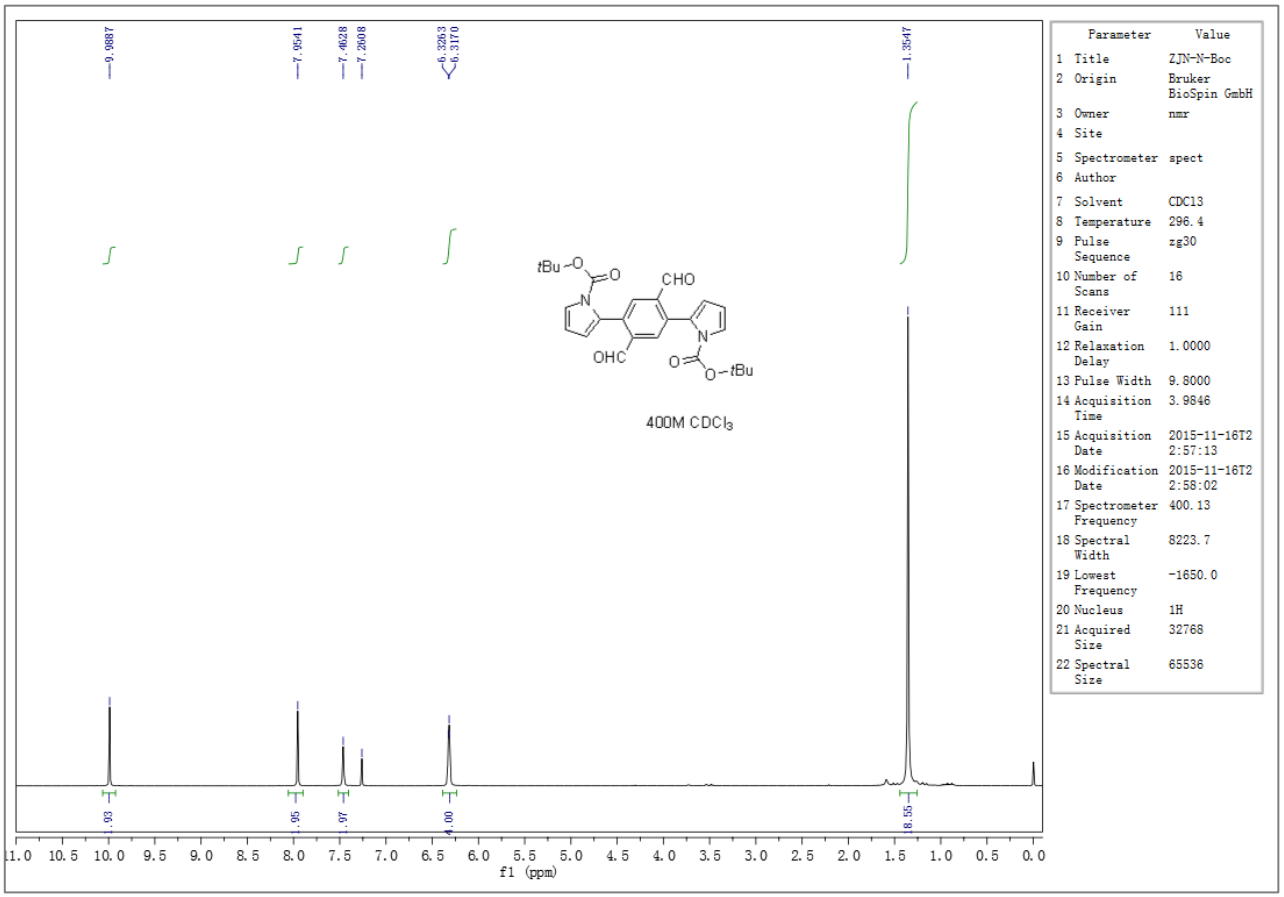
	Parameter	Value
1	Title	ZJN-Ph-OTBDMS-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	295.7
9	Pulse Sequence	zgpg30
10	Number of Scans	168
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.8039
15	Acquisition Date	2015-11-16T23:27:46
16	Modification Date	2015-11-16T23:35:42
17	Spectrometer Frequency	100.61
18	Spectral Width	40760.9
19	Lowest Frequency	-10305.8
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



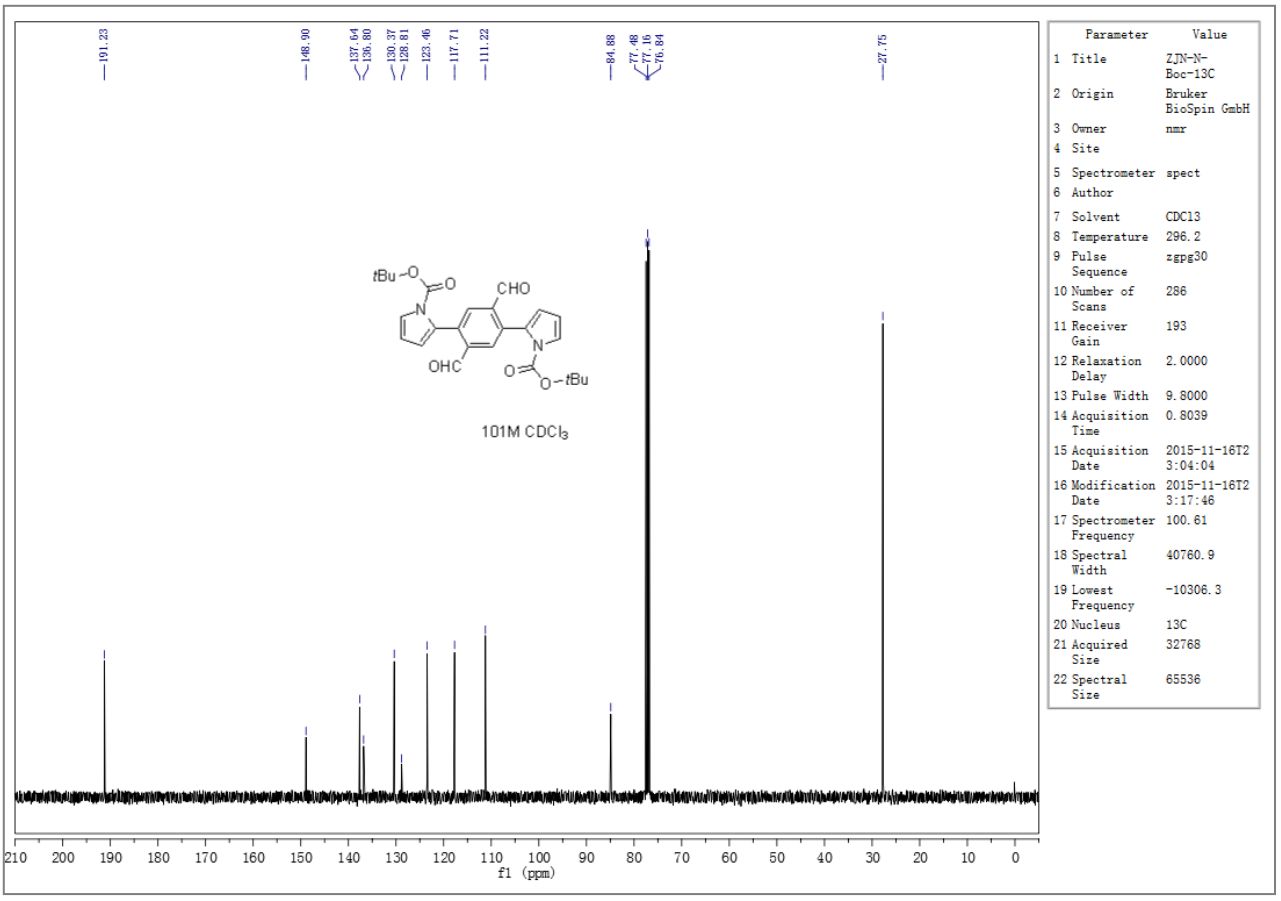
	Parameter	Value
1	Title	ZJN-Ph-OCH3
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.1
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	193
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	1.4680
15	Acquisition Date	2016-01-28T2 2:08:57
16	Modification Date	2016-01-28T2 2:09:19
17	Spectrometer Frequency	400.13
18	Spectral Width	11160.7
19	Lowest Frequency	-2252.7
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768



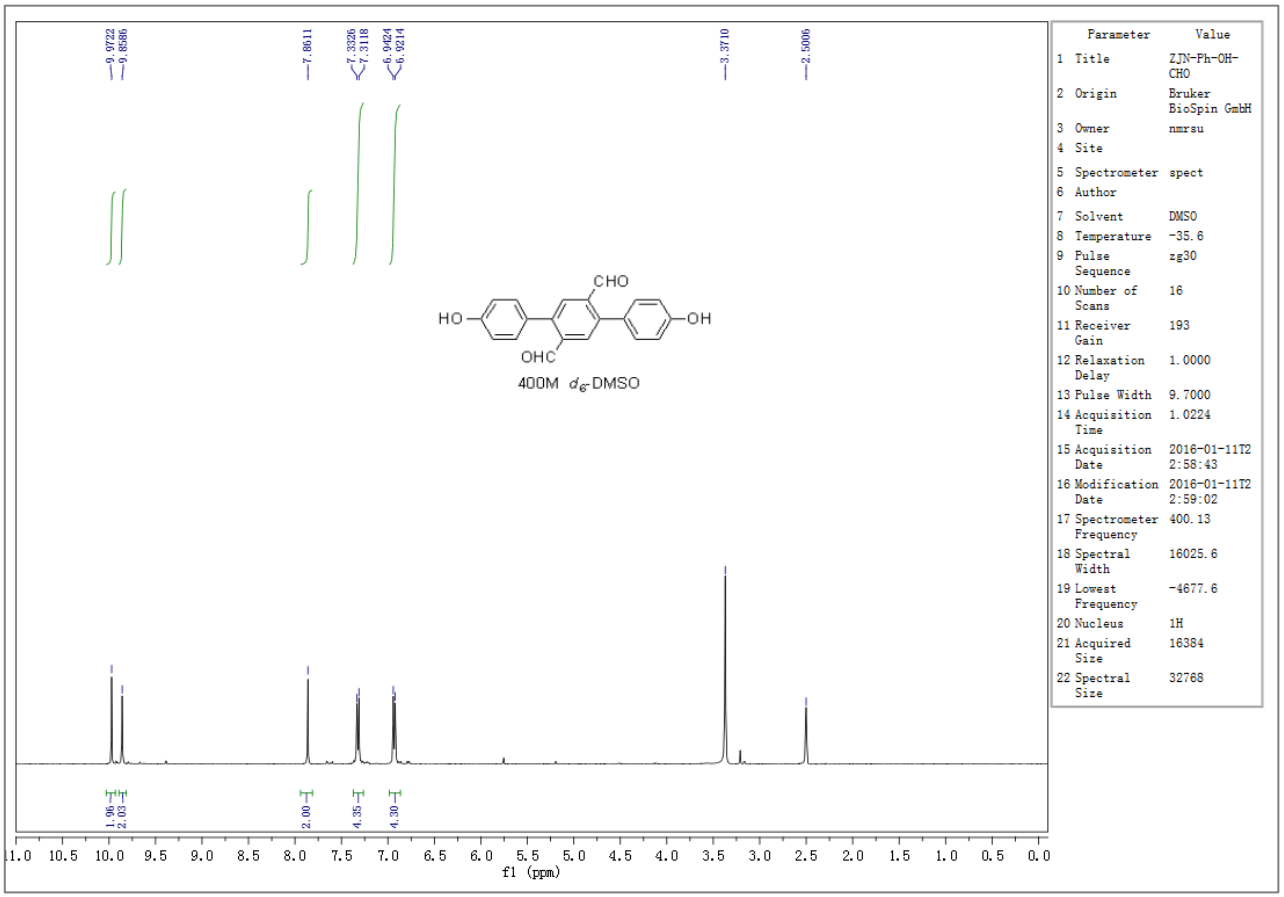
	Parameter	Value
1	Title	zjn20160129
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.2
9	Pulse Sequence	zgpg30
10	Number of Scans	84
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2016-01-29T1 8:05:29
16	Modification Date	2016-01-29T1 8:09:20
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1944.7
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



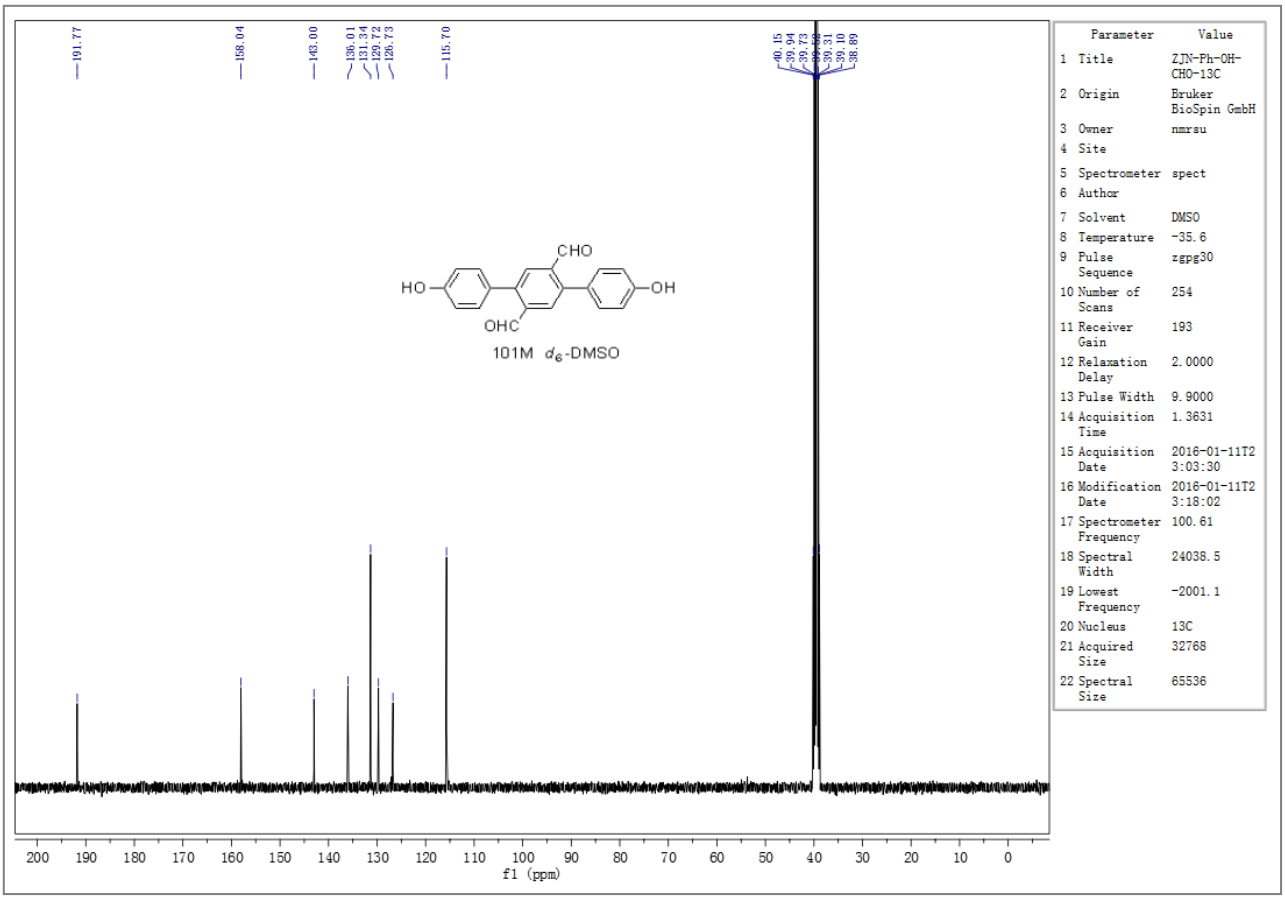
	Parameter	Value
1	Title	ZJN-N-Boc
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	296.4
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	111
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-11-16T12:57:13
16	Modification Date	2015-11-16T12:58:02
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.0
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



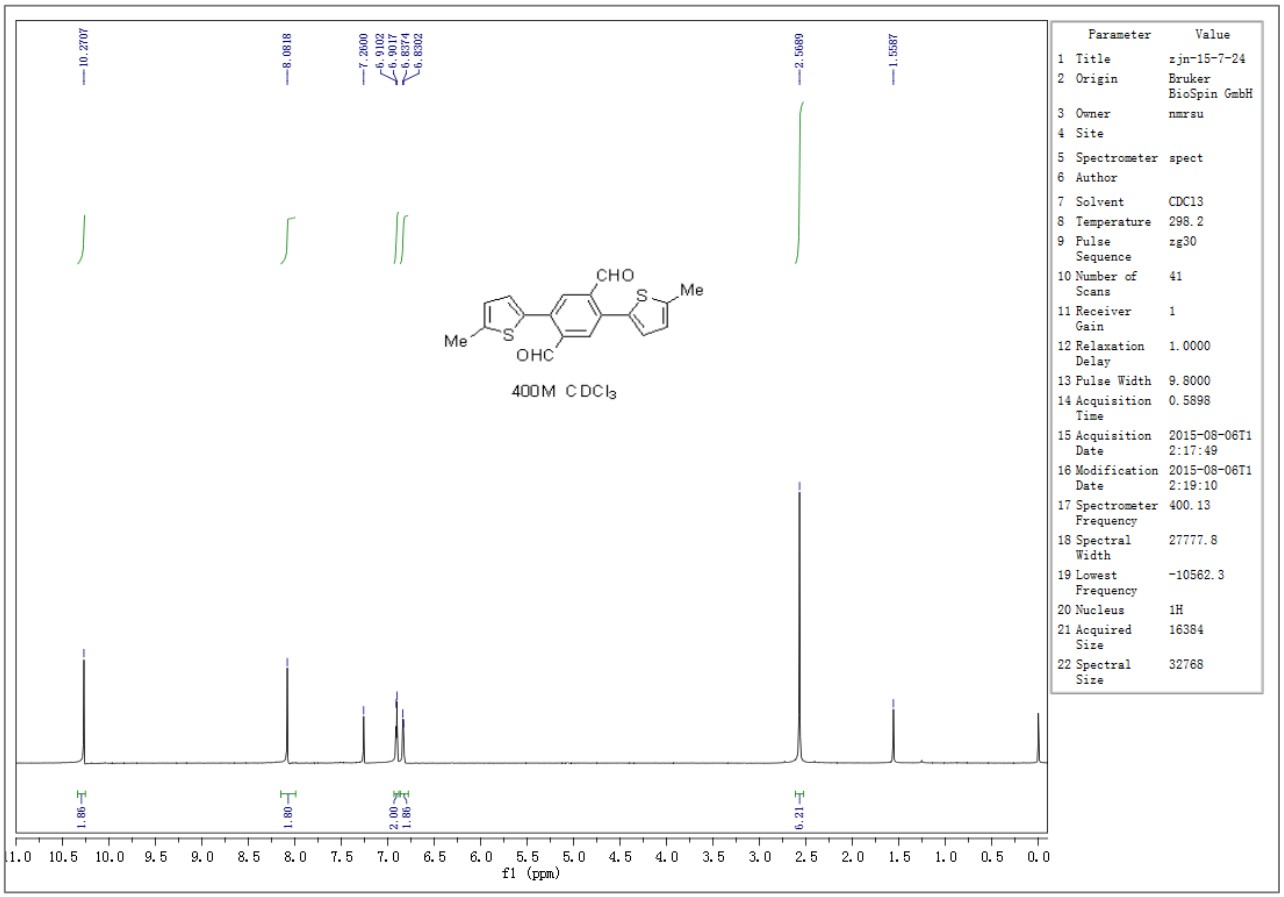
	Parameter	Value
1	Title	ZJN-N-Boc-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	296.2
9	Pulse Sequence	zgpg30
10	Number of Scans	286
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.8039
15	Acquisition Date	2015-11-16T13:04:04
16	Modification Date	2015-11-16T13:17:46
17	Spectrometer Frequency	100.61
18	Spectral Width	40760.9
19	Lowest Frequency	-10306.3
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



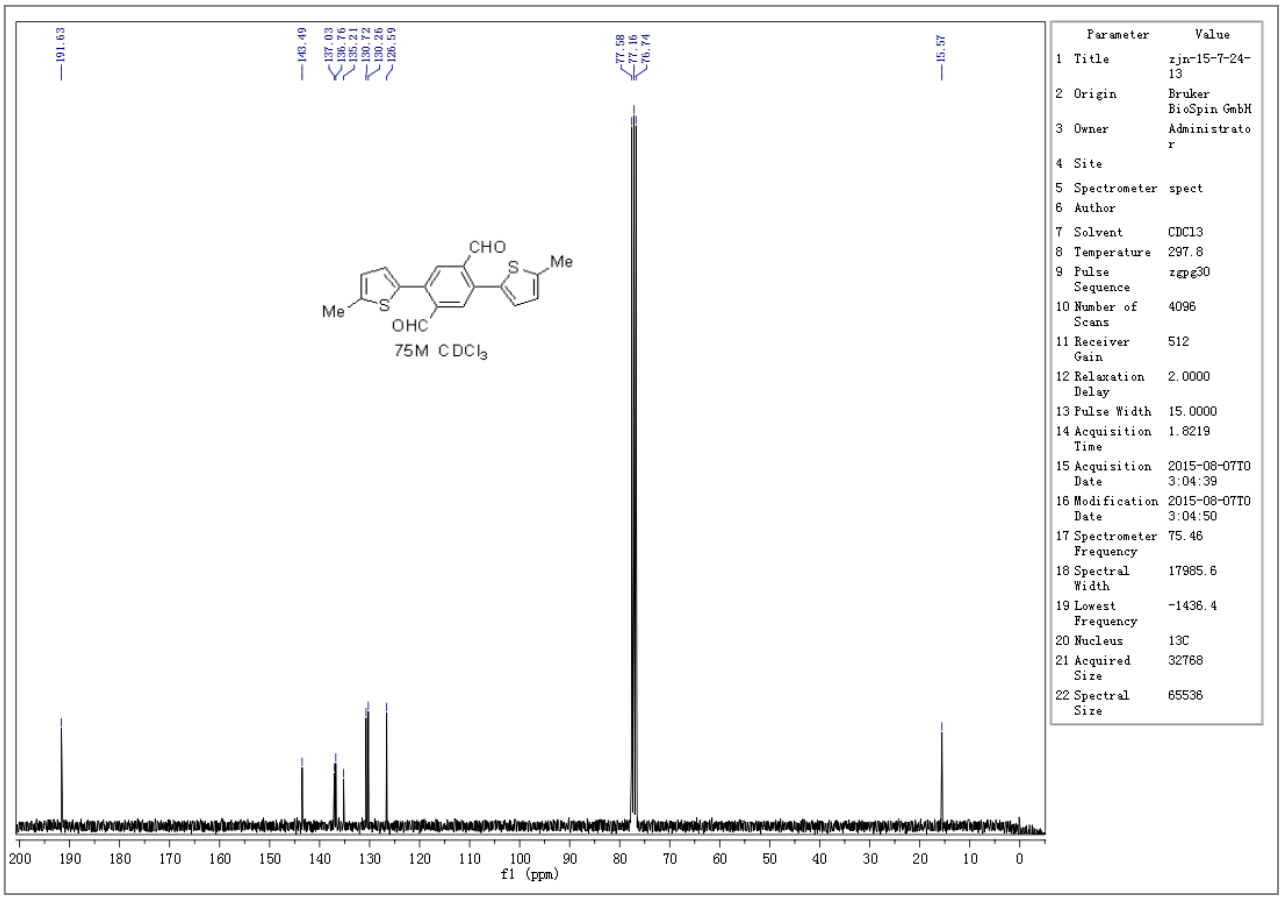
	Parameter	Value
1	Title	ZJN-Ph-OH-CHO
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	-35.6
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	193
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	1.0224
15	Acquisition Date	2016-01-11T2 2:58:43
16	Modification Date	2016-01-11T2 2:59:02
17	Spectrometer Frequency	400.13
18	Spectral Width	16025.6
19	Lowest Frequency	-4677.6
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768



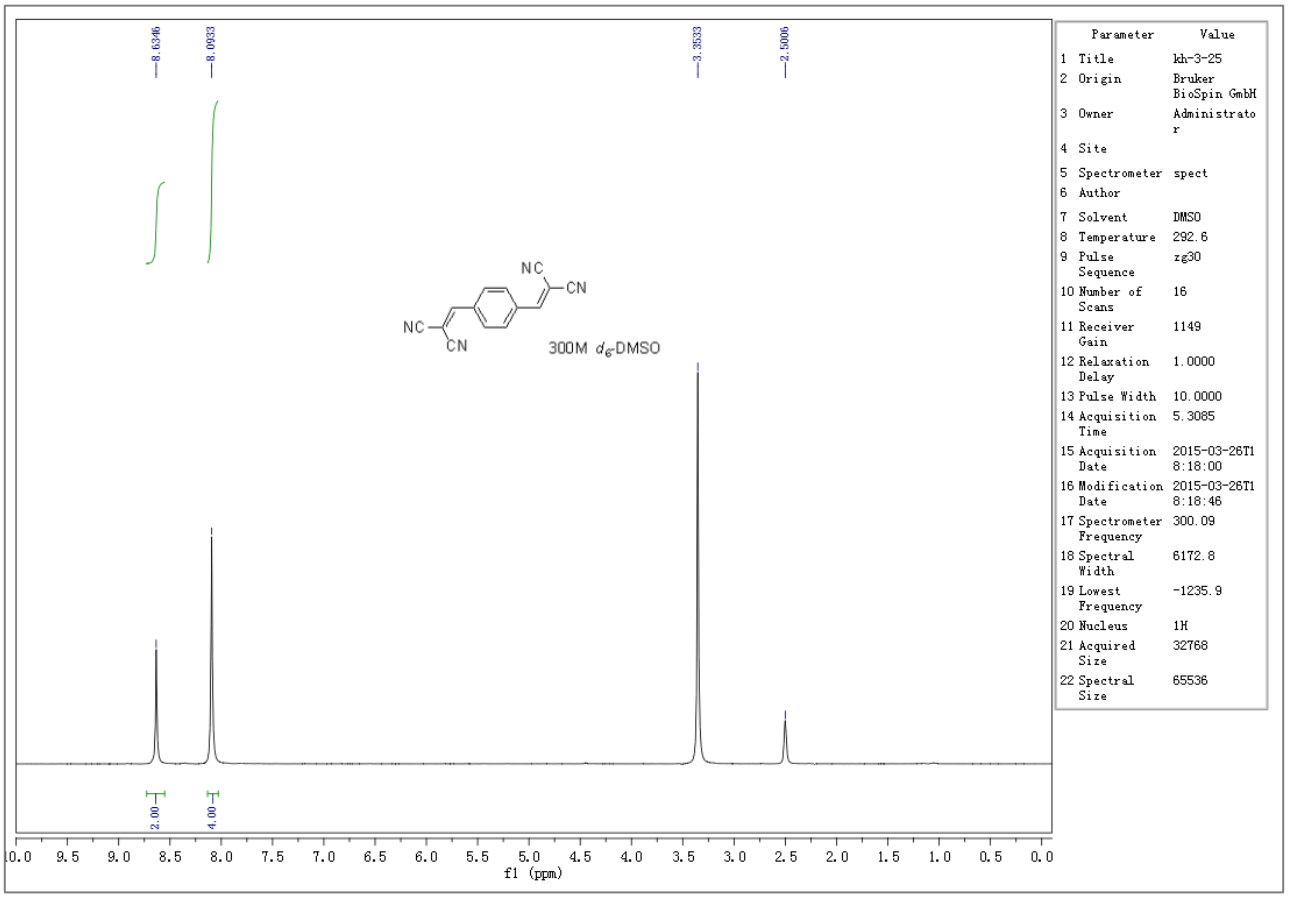
	Parameter	Value
1	Title	ZJN-Ph-OH-CHO-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	-35.6
9	Pulse Sequence	zgpg30
10	Number of Scans	254
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2016-01-11T2 3:03:30
16	Modification Date	2016-01-11T2 3:18:02
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-2001.1
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



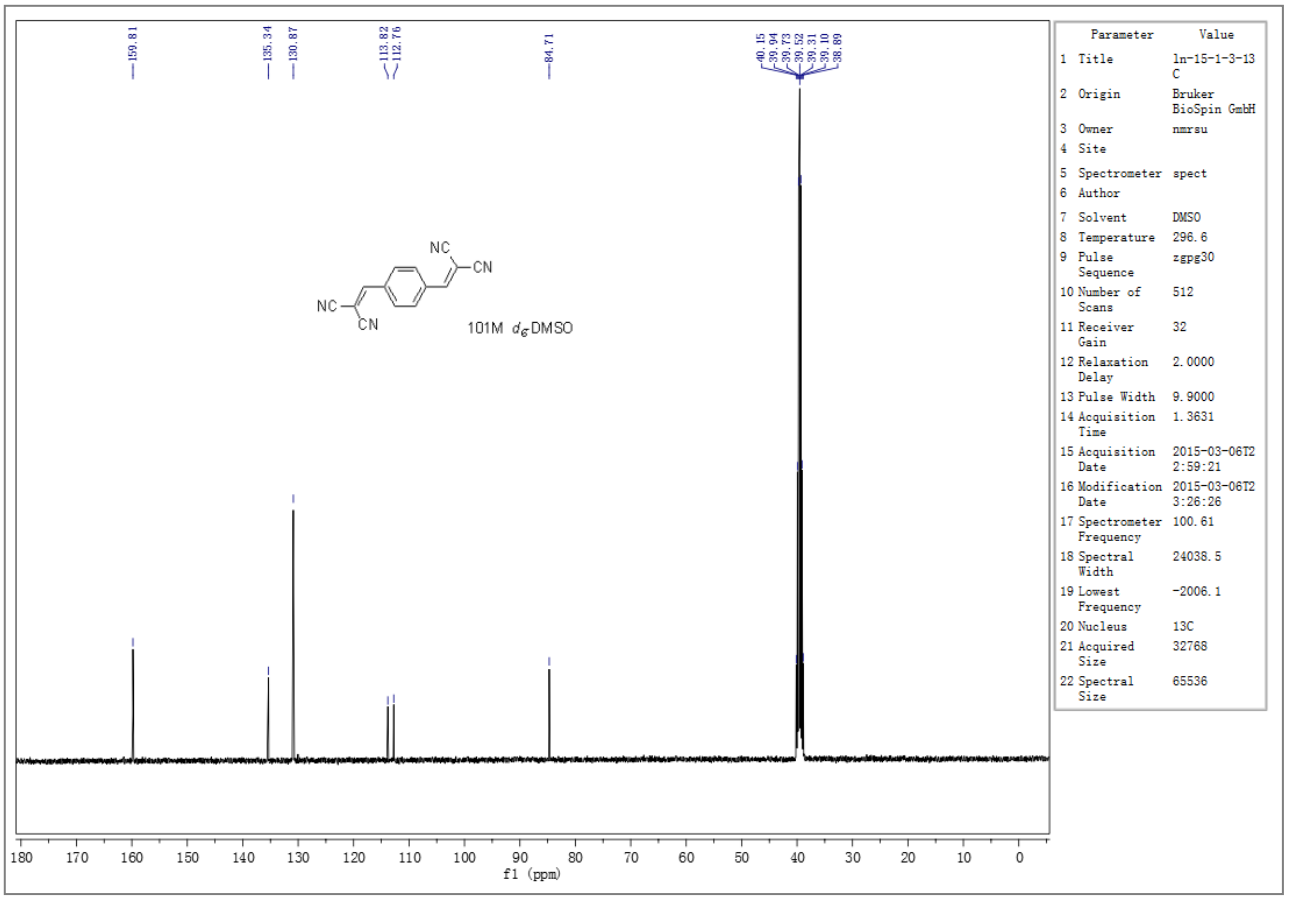
	Parameter	Value
1	Title	zjn-15-7-24
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.2
9	Pulse Sequence	zg30
10	Number of Scans	41
11	Receiver Gain	1
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.5898
15	Acquisition Date	2015-08-06T12:17:49
16	Modification Date	2015-08-06T12:19:10
17	Spectrometer Frequency	400.13
18	Spectral Width	27777.8
19	Lowest Frequency	-10562.3
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768



	Parameter	Value
1	Title	zjn-15-7-24-13
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.8
9	Pulse Sequence	zgpg30
10	Number of Scans	4096
11	Receiver Gain	512
12	Relaxation Delay	2.0000
13	Pulse Width	15.0000
14	Acquisition Time	1.8219
15	Acquisition Date	2015-08-07T03:04:39
16	Modification Date	2015-08-07T03:04:50
17	Spectrometer Frequency	75.46
18	Spectral Width	17985.6
19	Lowest Frequency	-1436.4
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

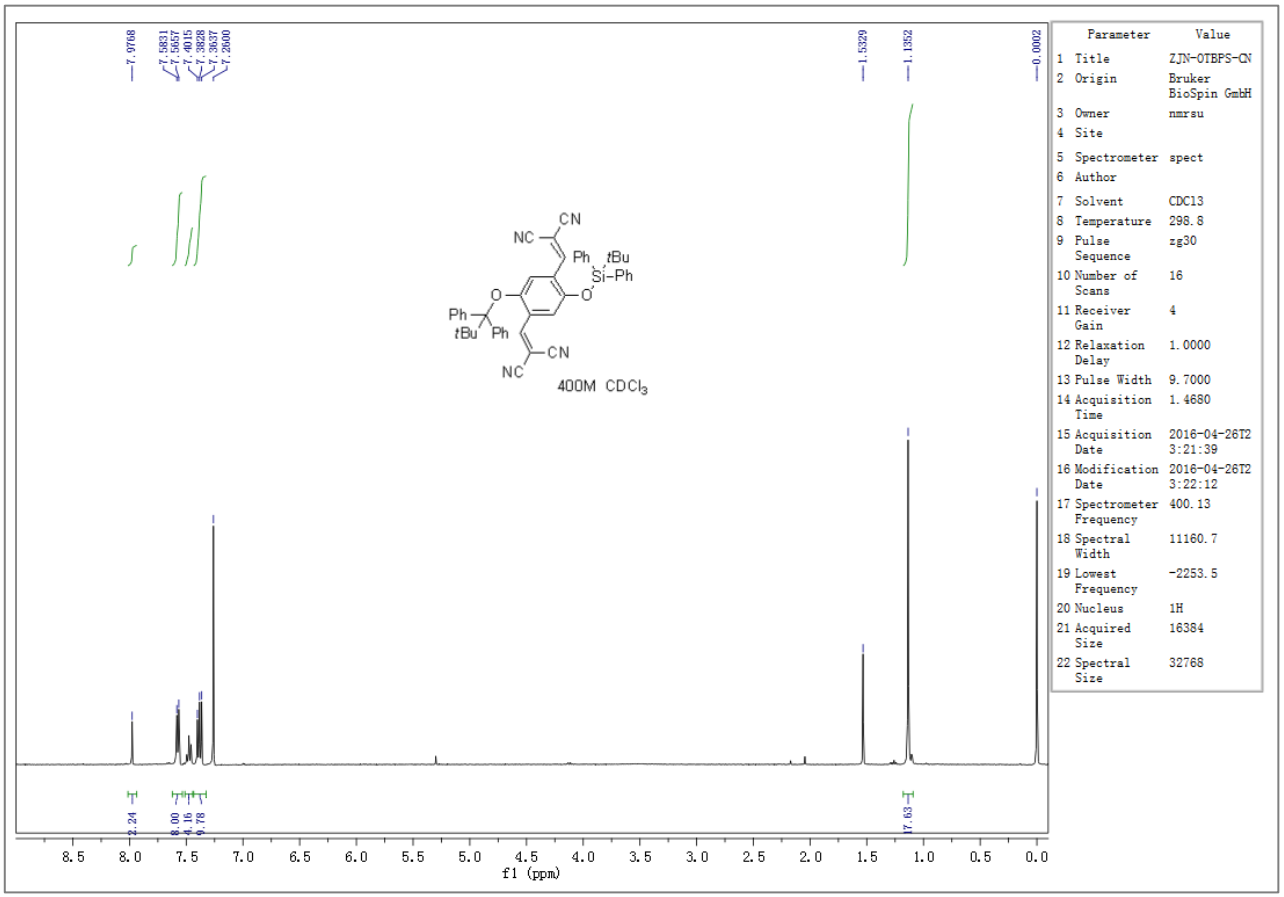


	Parameter	Value
1	Title	kh-3-25
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	292.6
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	1149
12	Relaxation Delay	1.0000
13	Pulse Width	10.0000
14	Acquisition Time	5.3085
15	Acquisition Date	2015-03-26T18:18:00
16	Modification Date	2015-03-26T18:18:46
17	Spectrometer Frequency	300.09
18	Spectral Width	6172.8
19	Lowest Frequency	-1235.9
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

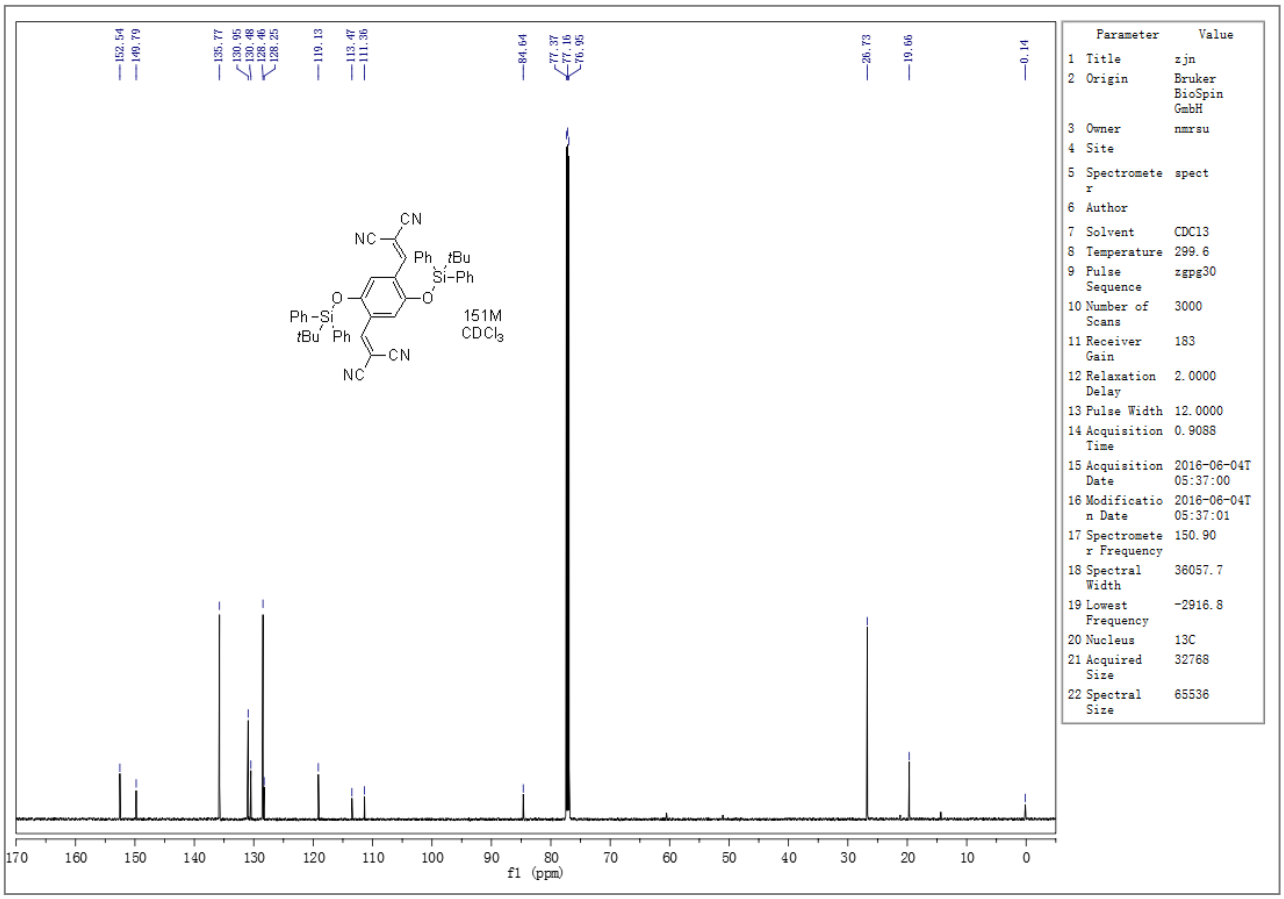


	Parameter	Value
1	Title	ln-15-1-3-13 C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	296.6
9	Pulse Sequence	zgpg30
10	Number of Scans	512
11	Receiver Gain	32
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2015-03-06T12:59:21
16	Modification Date	2015-03-06T13:26:26
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-2006.1
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

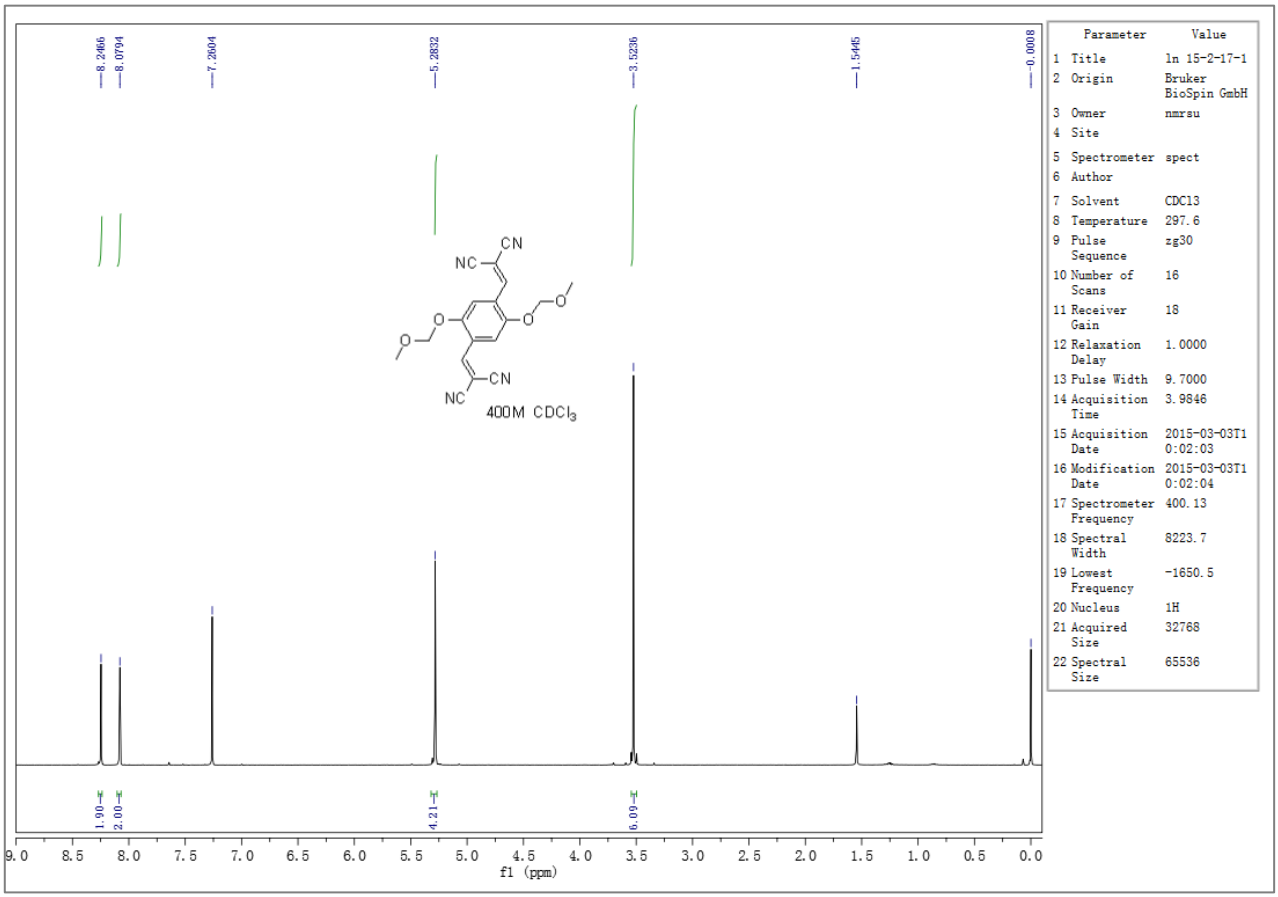


	Parameter	Value
1	Title	ZJN-0TBPS-CN
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.8
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	4
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	1.4680
15	Acquisition Date	2016-04-26T23:21:39
16	Modification Date	2016-04-26T23:22:12
17	Spectrometer Frequency	400.13
18	Spectral Width	11160.7
19	Lowest Frequency	-2253.5
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768

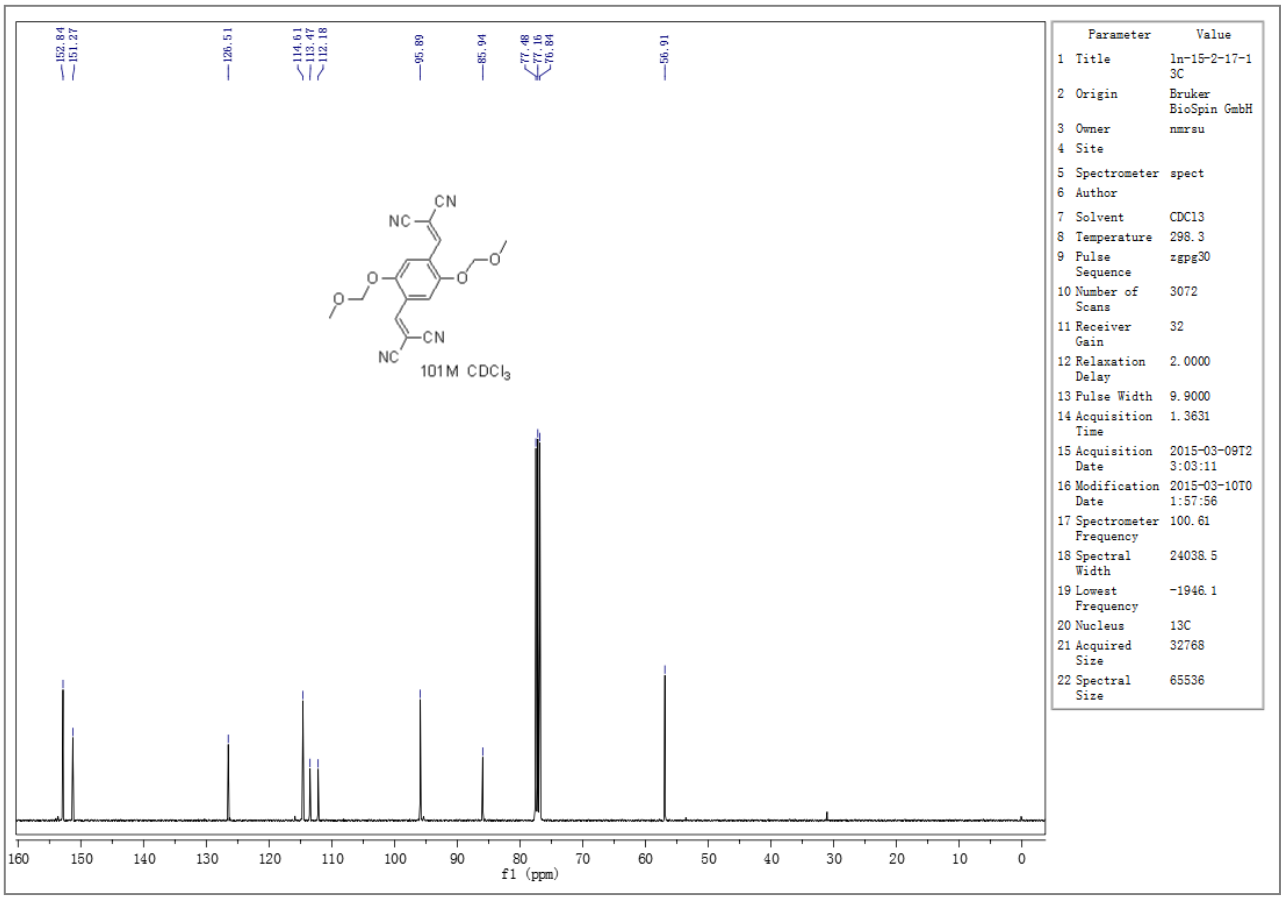


	Parameter	Value
1	Title	zjn
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	299.6
9	Pulse Sequence	zgpg30
10	Number of Scans	3000
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2016-06-04T05:37:00
16	Modification Date	2016-06-04T05:37:01
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2916.8
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data

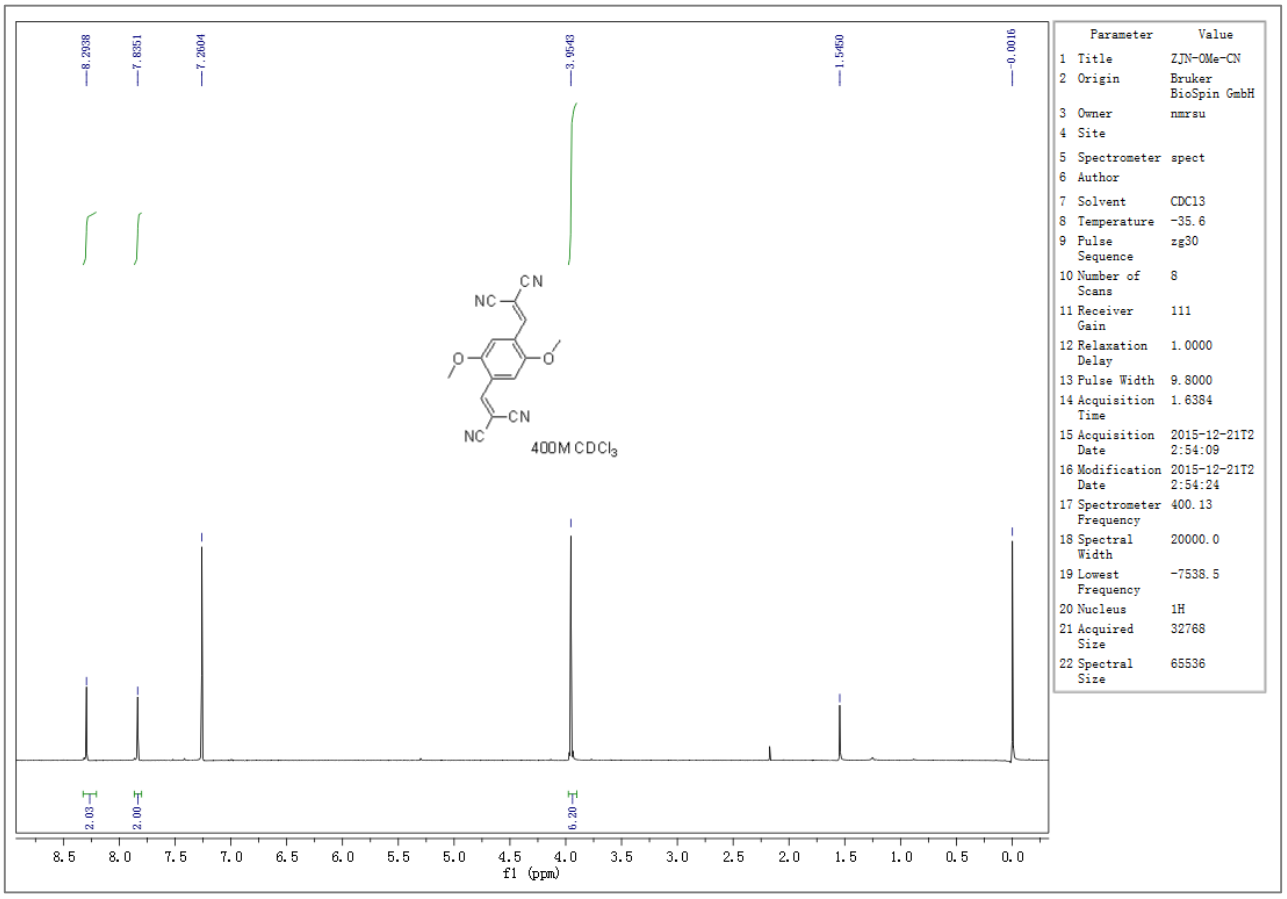


	Parameter	Value
1	Title	ln 15-2-17-1
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.6
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	18
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-03-03T10:02:03
16	Modification Date	2015-03-03T10:02:04
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.5
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

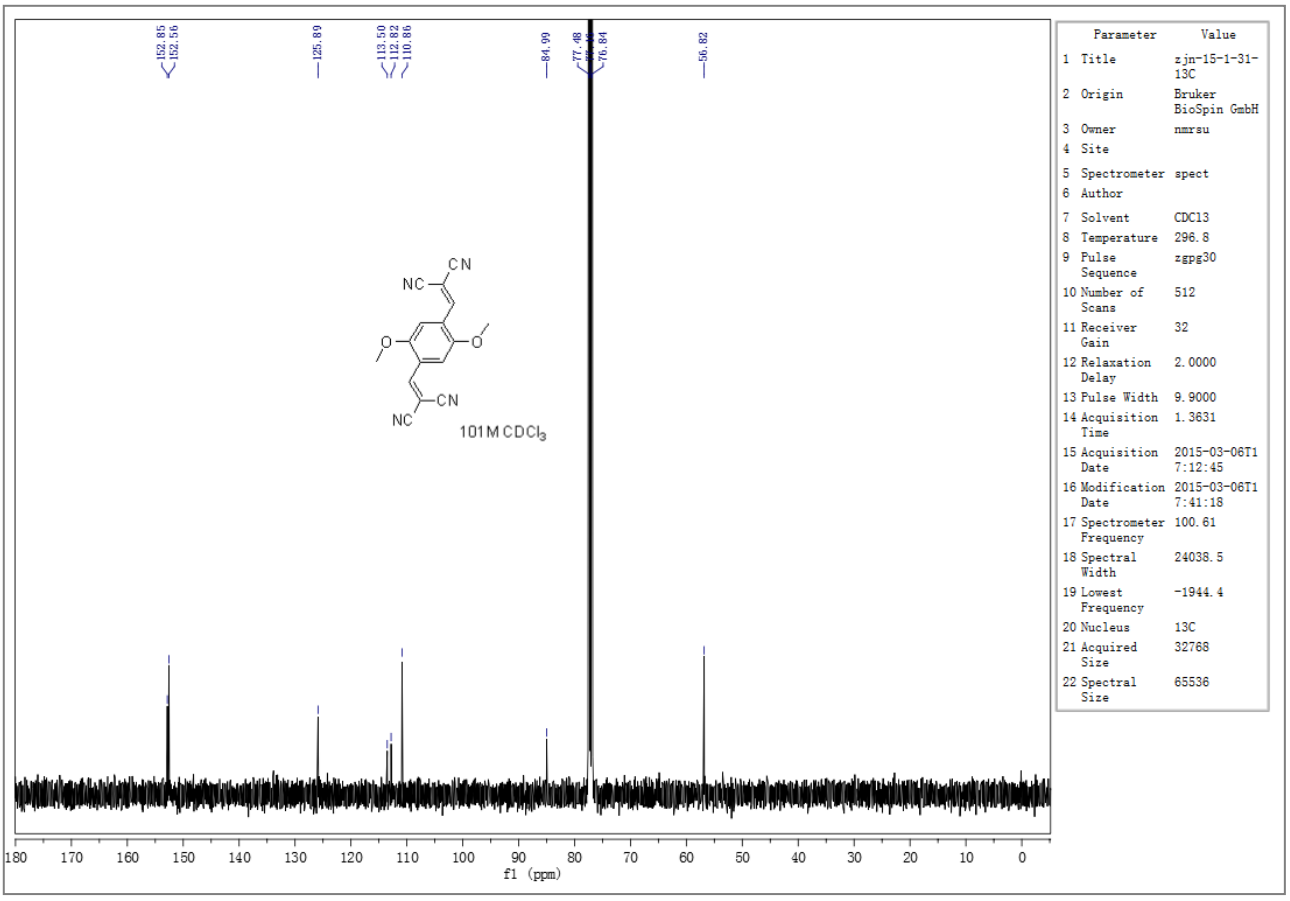


	Parameter	Value
1	Title	ln-15-2-17-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.3
9	Pulse Sequence	zgpg30
10	Number of Scans	3072
11	Receiver Gain	32
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2015-03-09T23:03:11
16	Modification Date	2015-03-10T01:57:56
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1946.1
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

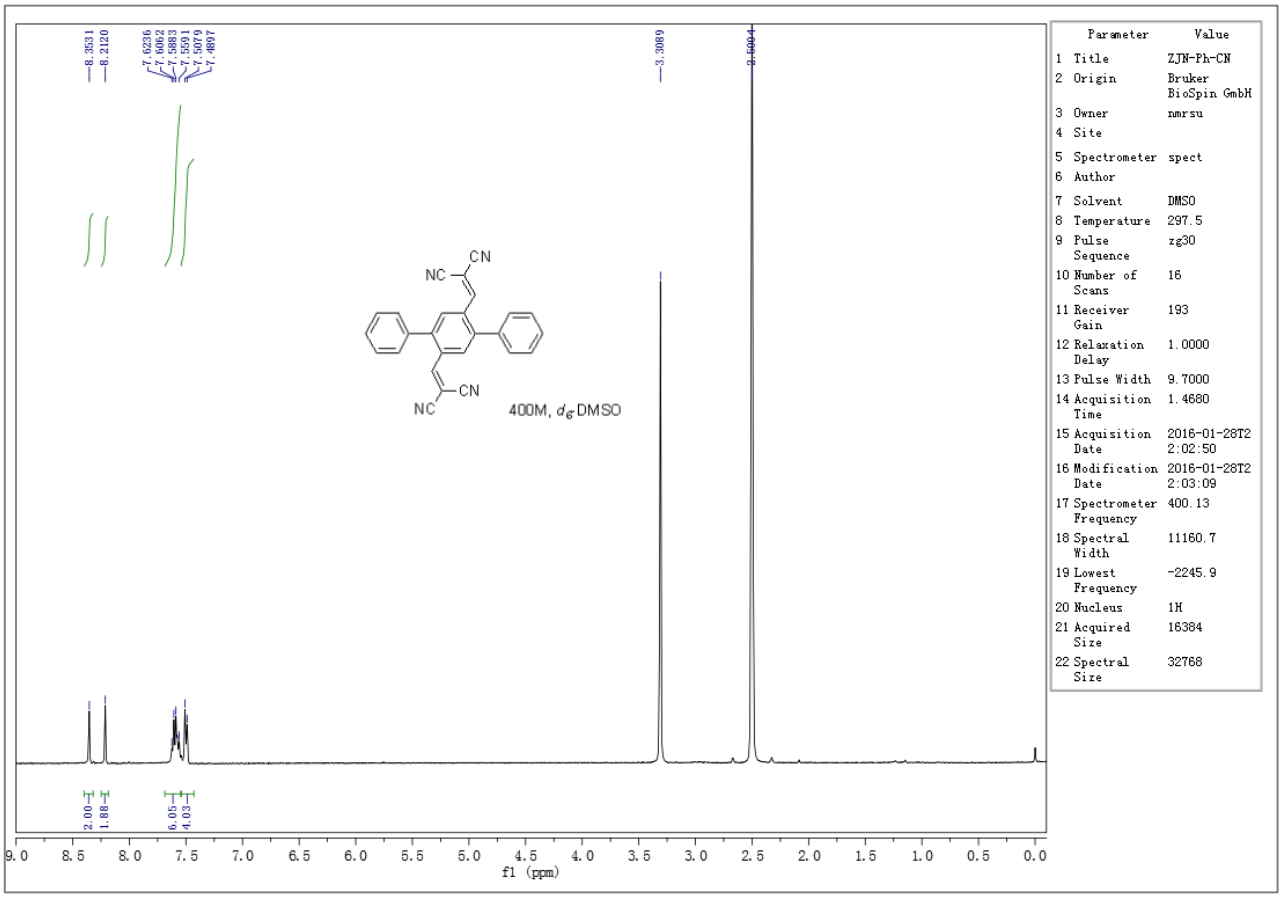


	Parameter	Value
1	Title	ZJN-OMe-CN
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	-35.6
9	Pulse Sequence	zg30
10	Number of Scans	8
11	Receiver Gain	111
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	1.6384
15	Acquisition Date	2015-12-21T2 2:54:09
16	Modification Date	2015-12-21T2 2:54:24
17	Spectrometer Frequency	400.13
18	Spectral Width	20000.0
19	Lowest Frequency	-7538.5
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

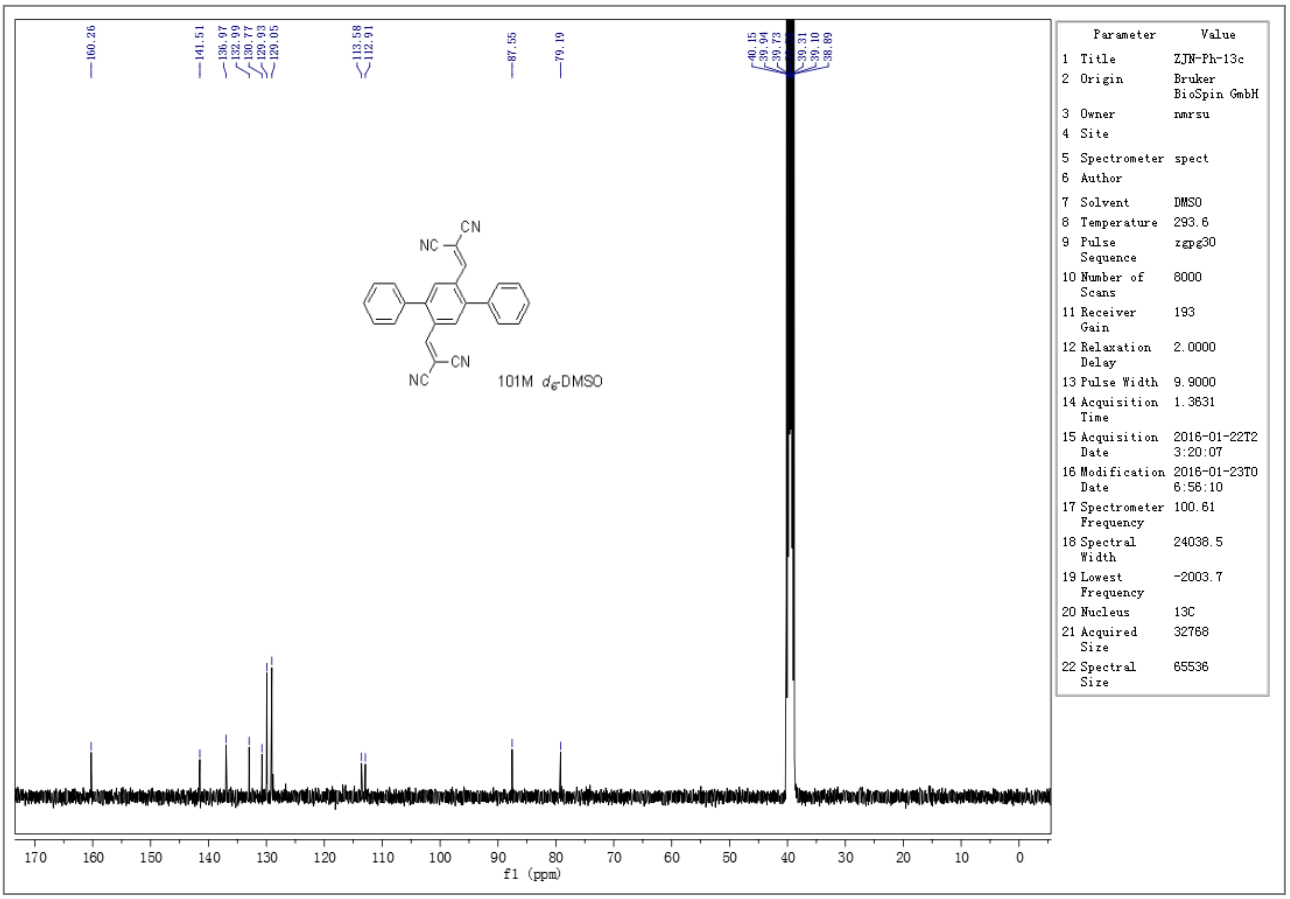


	Parameter	Value
1	Title	zjn-15-1-31-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	296.8
9	Pulse Sequence	zgpg30
10	Number of Scans	512
11	Receiver Gain	32
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2015-03-06T1 7:12:45
16	Modification Date	2015-03-06T1 7:41:18
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1944.4
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

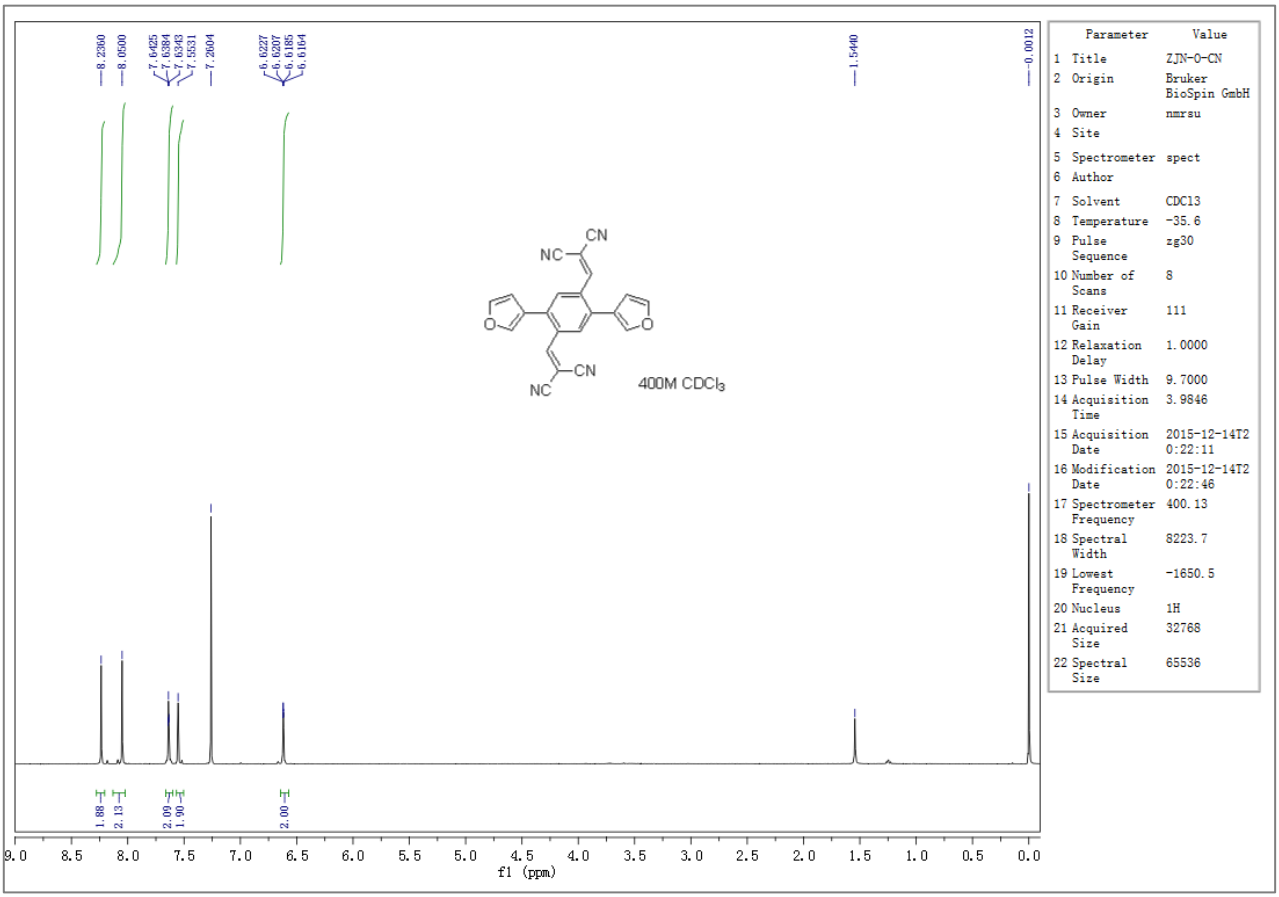


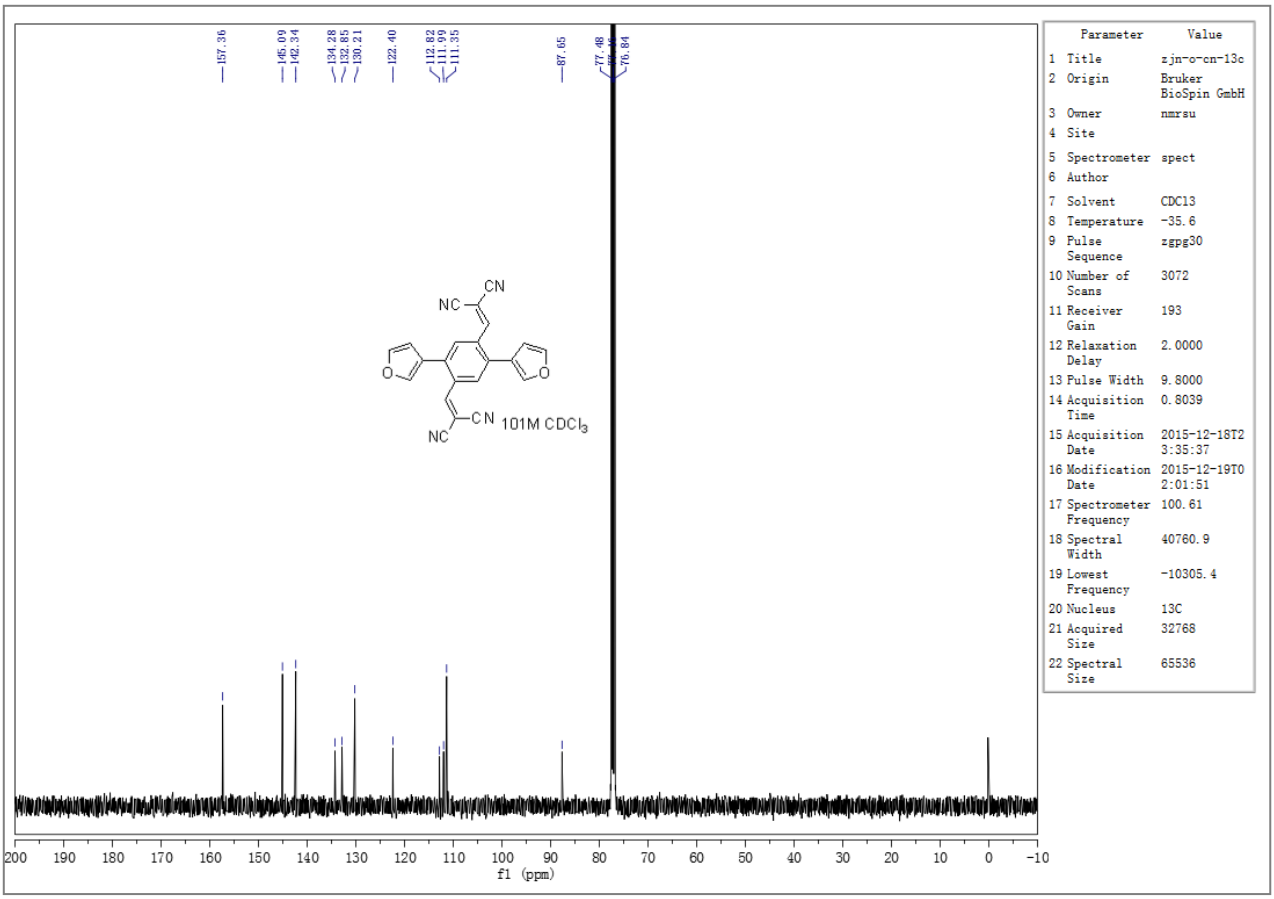
	Parameter	Value
1	Title	ZJN-Ph-CN
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	297.5
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	193
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	1.4680
15	Acquisition Date	2016-01-28T2 2:02:50
16	Modification Date	2016-01-28T2 2:03:09
17	Spectrometer Frequency	400.13
18	Spectral Width	11160.7
19	Lowest Frequency	-2245.9
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768



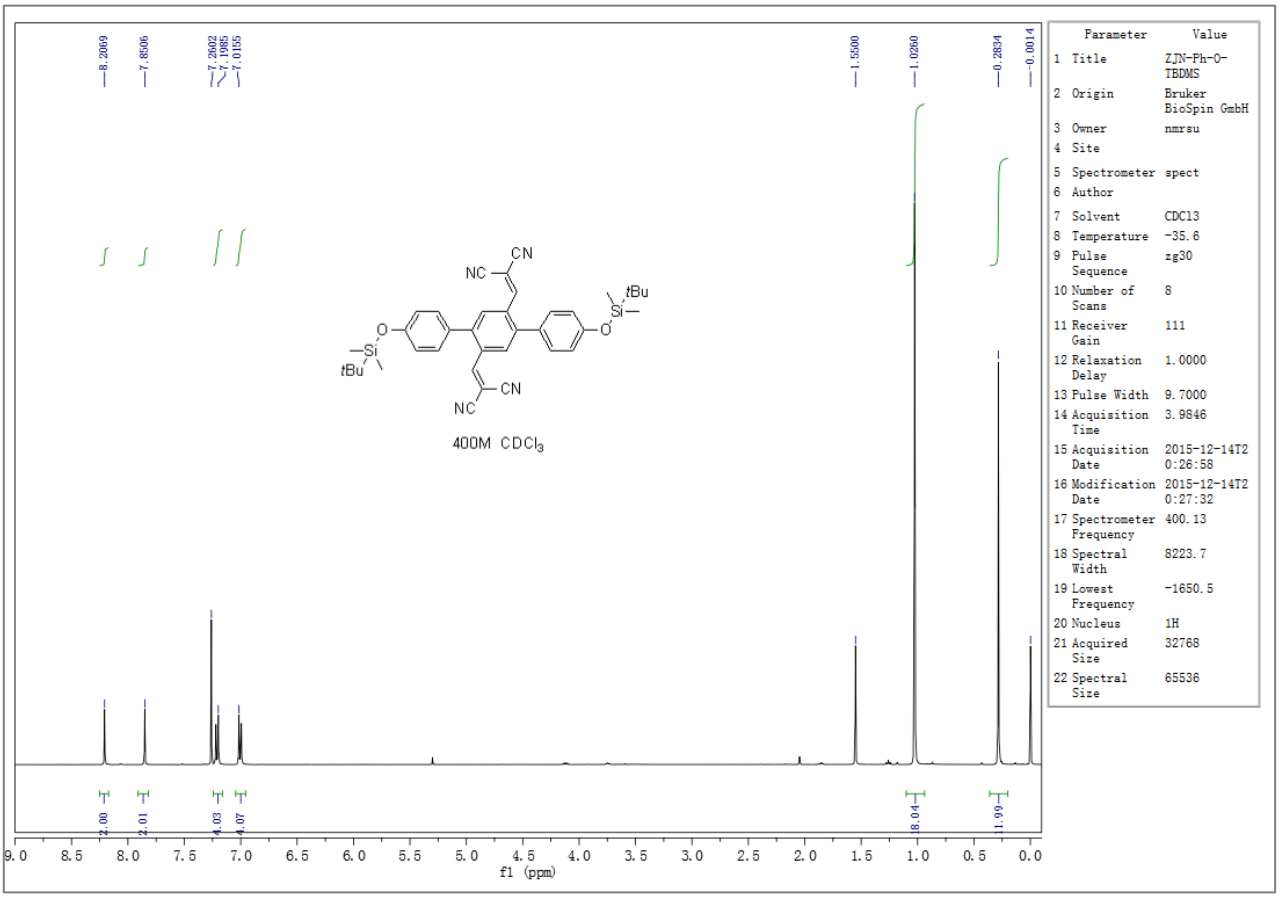
	Parameter	Value
1	Title	ZJN-Ph-13c
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	DMSO
8	Temperature	293.6
9	Pulse Sequence	zgpg30
10	Number of Scans	8000
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.9000
14	Acquisition Time	1.3631
15	Acquisition Date	2016-01-22T2 3:20:07
16	Modification Date	2016-01-23T0 6:56:10
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-2003.7
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

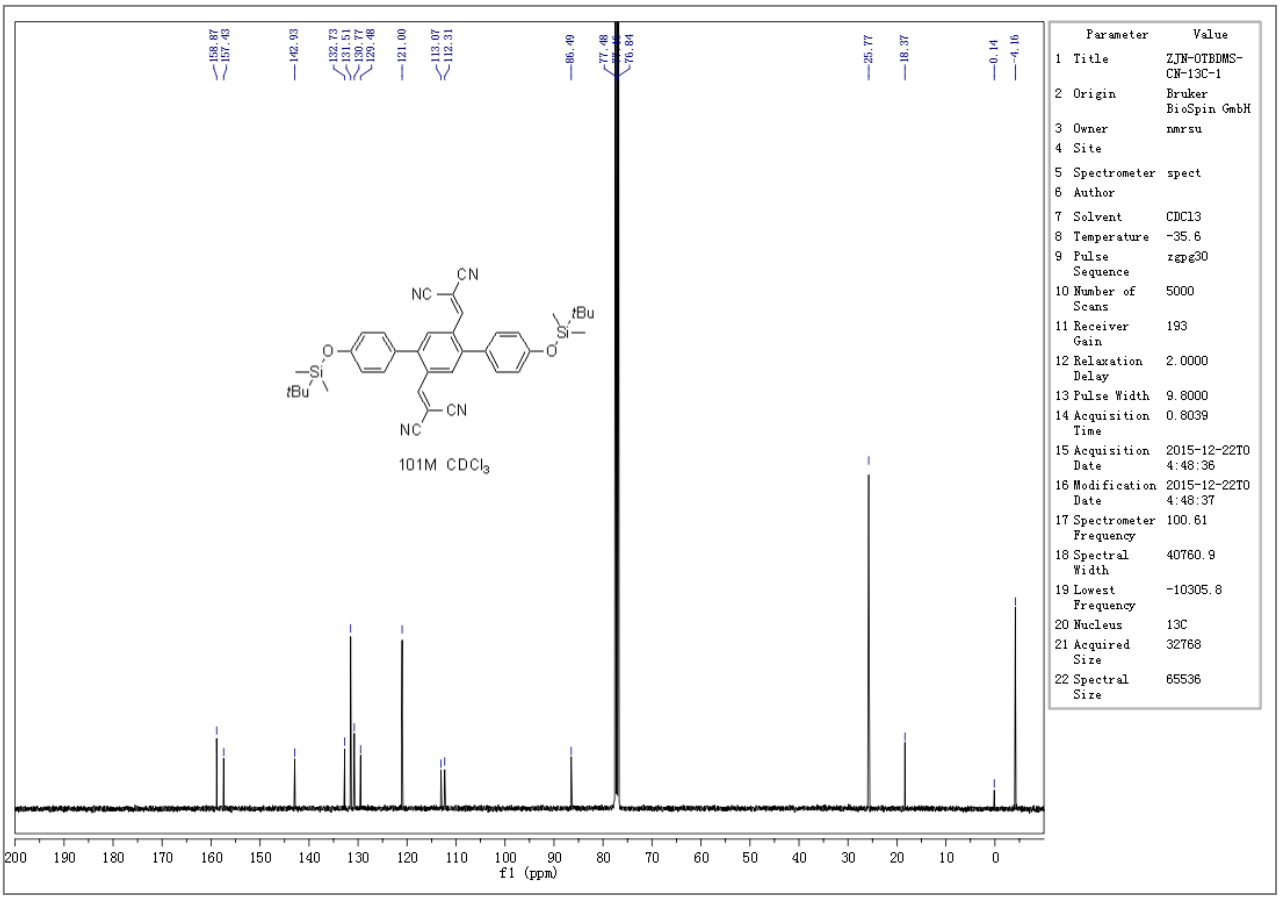




Compounds chart Data X-ray

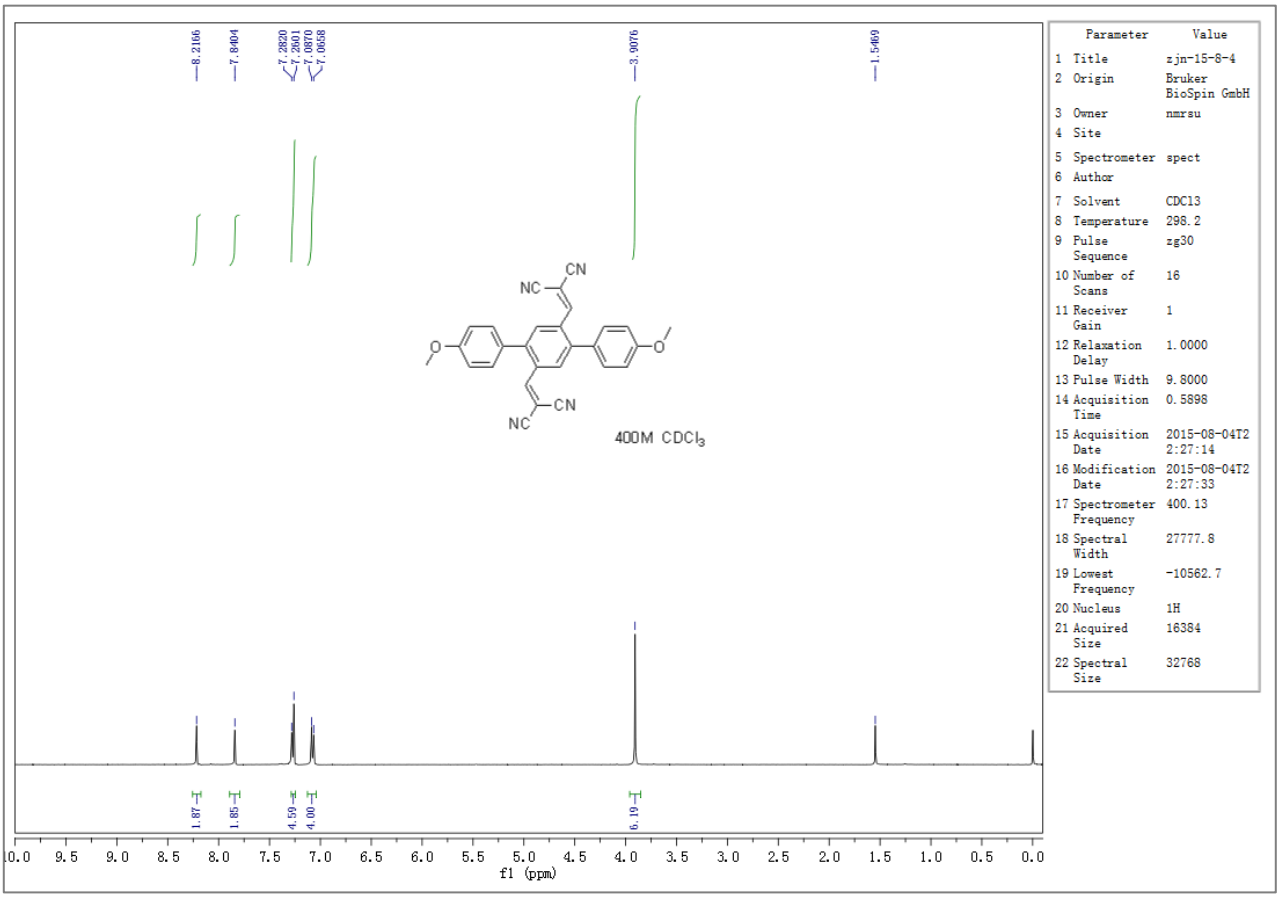


	Parameter	Value
1	Title	ZJN-Ph-O-TBDMS
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	-35.6
9	Pulse Sequence	zg30
10	Number of Scans	8
11	Receiver Gain	111
12	Relaxation Delay	1.0000
13	Pulse Width	9.7000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-12-14T2 0:26:58
16	Modification Date	2015-12-14T2 0:27:32
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.5
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

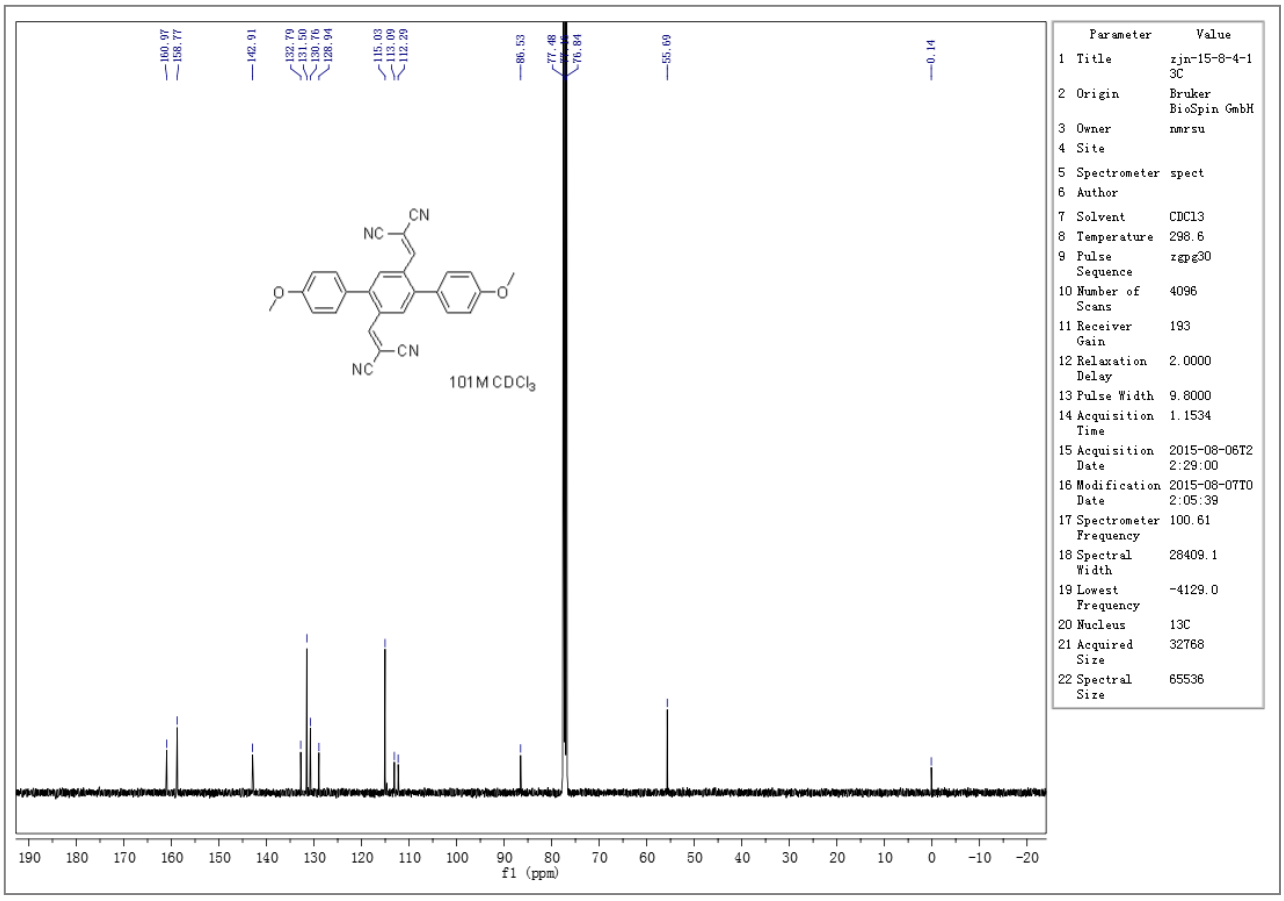


	Parameter	Value
1	Title	ZJN-OTBDMS-CN-13C-1
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	-35.6
9	Pulse Sequence	zgpg30
10	Number of Scans	5000
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.8039
15	Acquisition Date	2015-12-22T0 4:48:36
16	Modification Date	2015-12-22T0 4:48:37
17	Spectrometer Frequency	100.61
18	Spectral Width	40760.9
19	Lowest Frequency	-10305.8
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

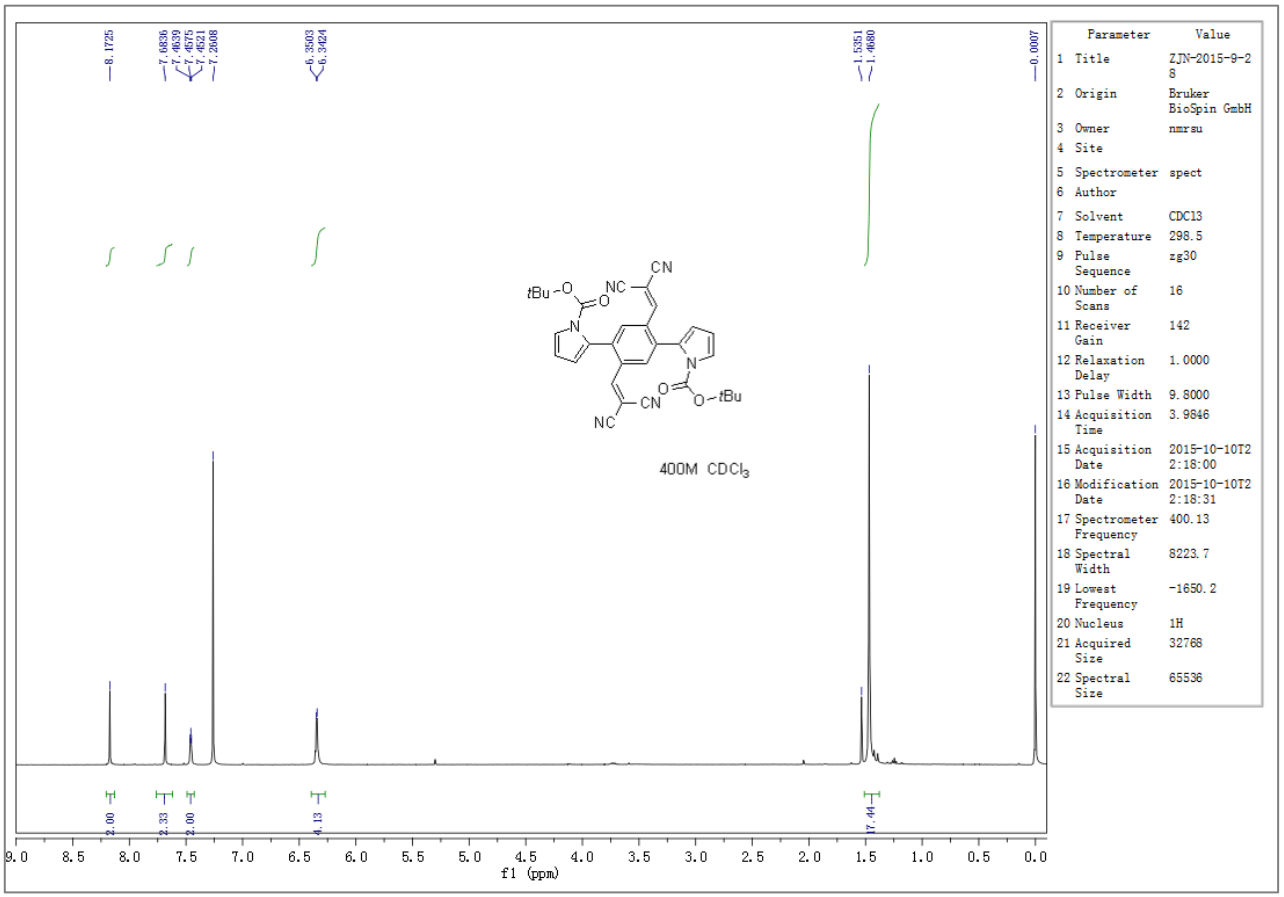


	Parameter	Value
1	Title	zjn-15-8-4
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.2
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	1
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.5898
15	Acquisition Date	2015-08-04T2 2:27:14
16	Modification Date	2015-08-04T2 2:27:33
17	Spectrometer Frequency	400.13
18	Spectral Width	27777.8
19	Lowest Frequency	-10562.7
20	Nucleus	1H
21	Acquired Size	16384
22	Spectral Size	32768

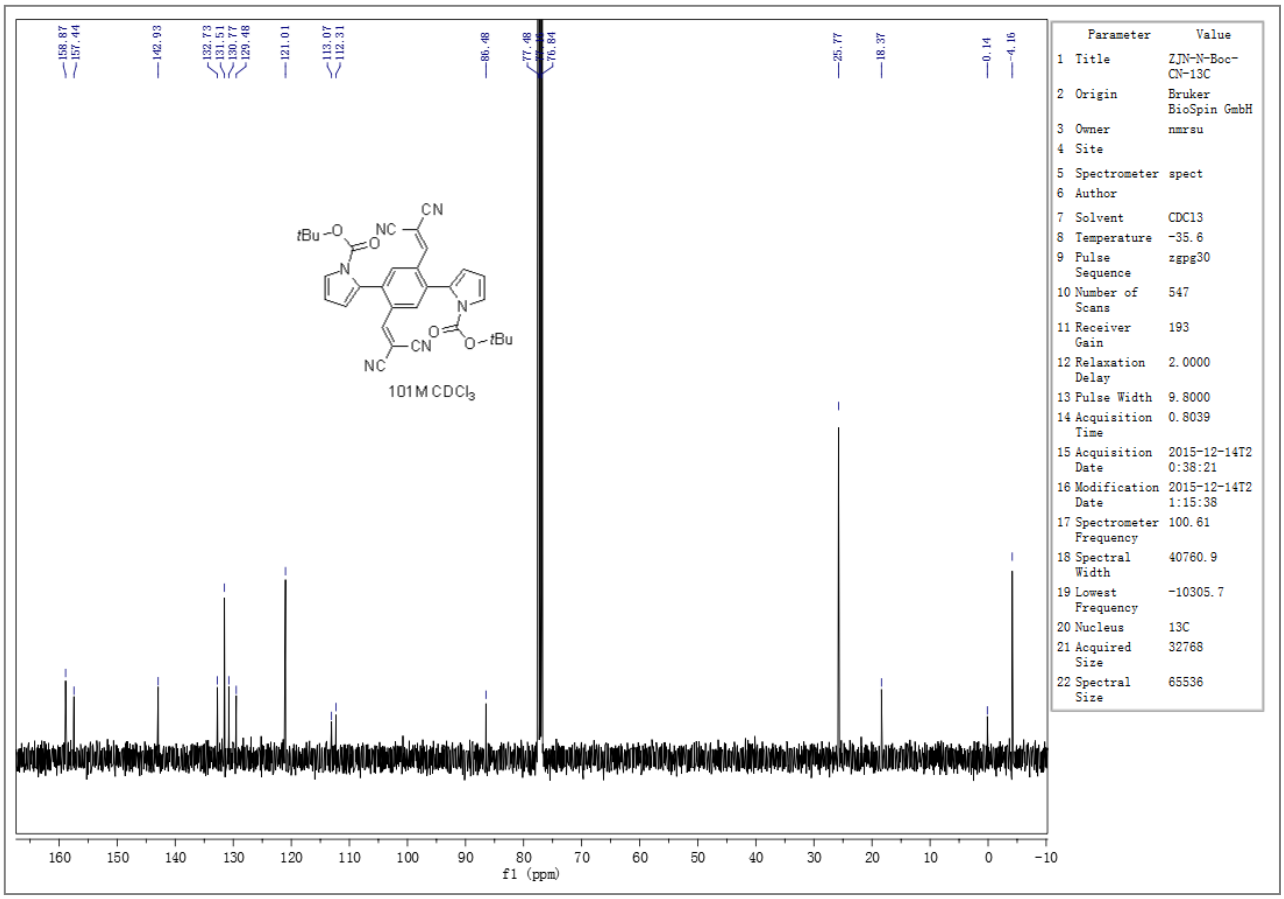


	Parameter	Value
1	Title	zjn-15-8-4-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.6
9	Pulse Sequence	zgpg30
10	Number of Scans	4096
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	1.1534
15	Acquisition Date	2015-08-06T2 2:29:00
16	Modification Date	2015-08-07T0 2:05:39
17	Spectrometer Frequency	100.61
18	Spectral Width	28409.1
19	Lowest Frequency	-4129.0
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

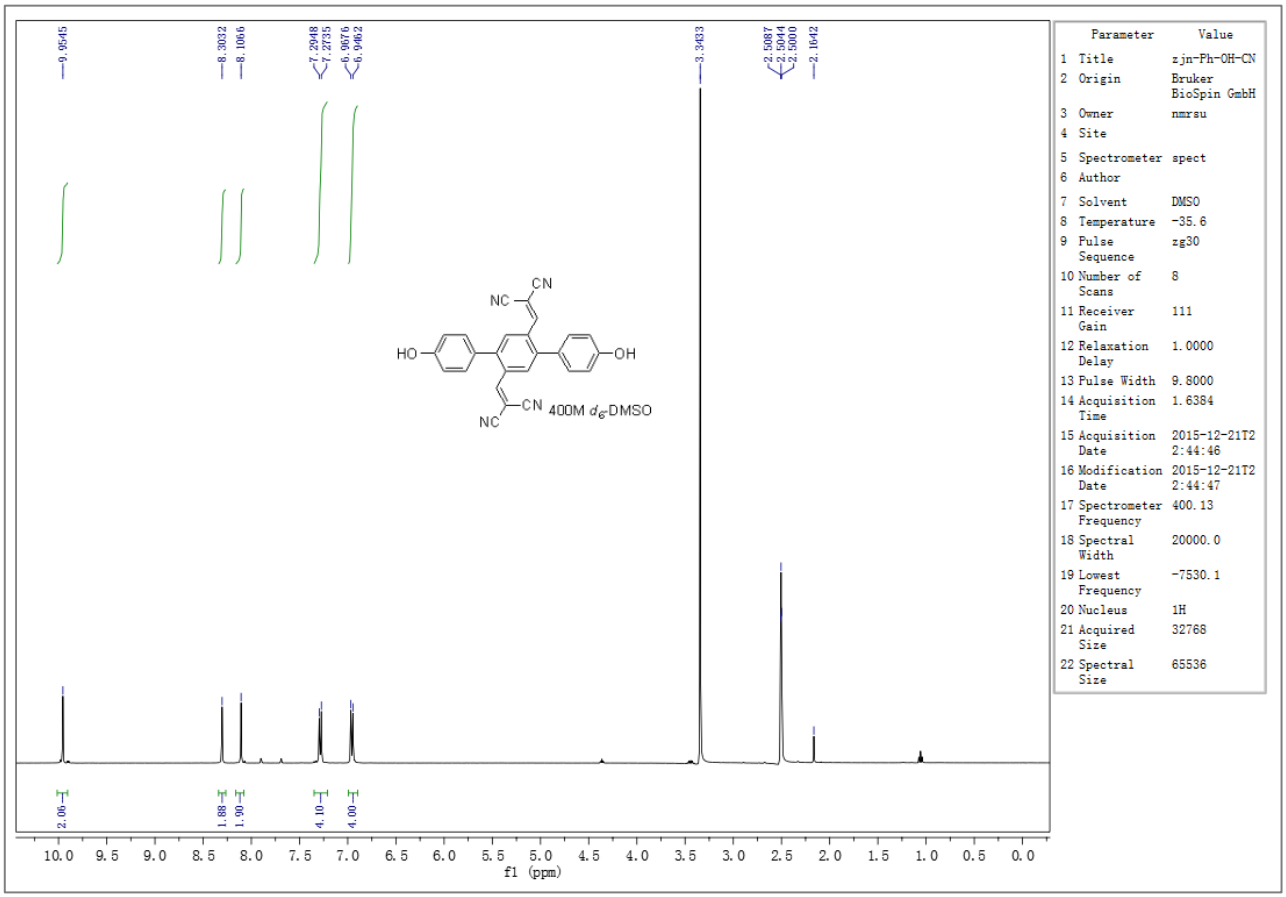


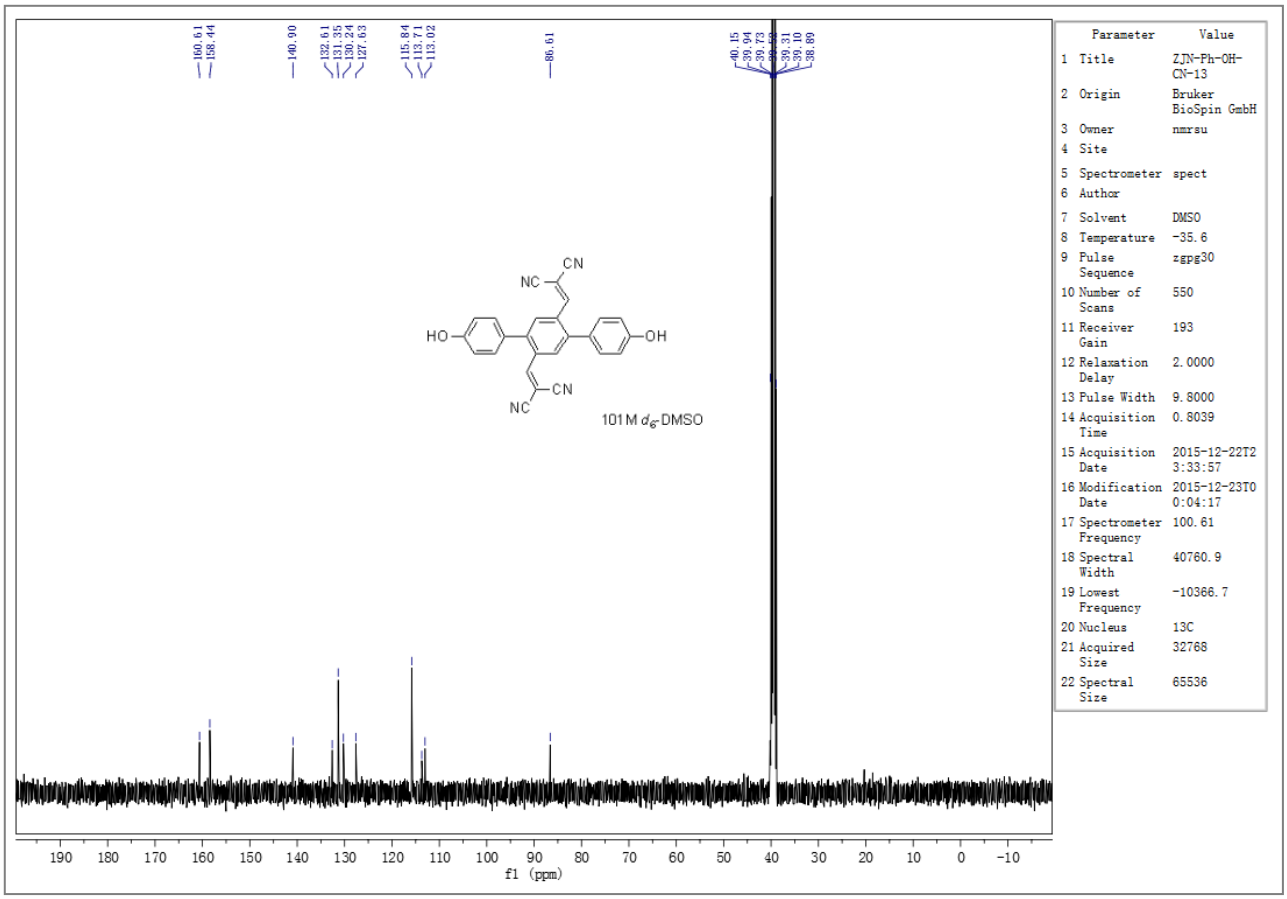
	Parameter	Value
1	Title	ZJN-2015-9-28
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	298.5
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	142
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	3.9846
15	Acquisition Date	2015-10-10T22:18:00
16	Modification Date	2015-10-10T22:18:31
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.2
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



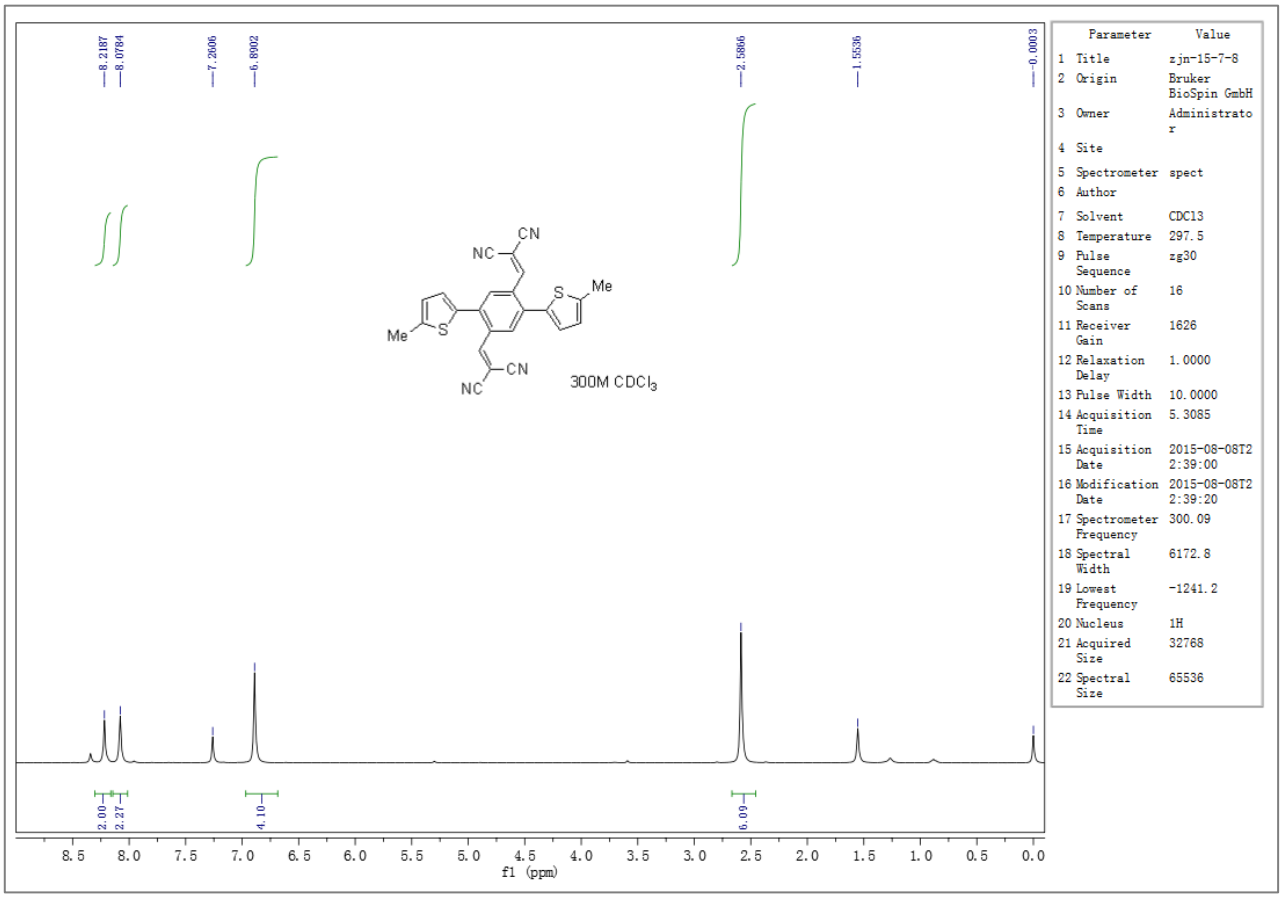
	Parameter	Value
1	Title	ZJN-N-Boc-CN-13C
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	-35.6
9	Pulse Sequence	zgpg30
10	Number of Scans	547
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	0.8039
15	Acquisition Date	2015-12-14T20:38:21
16	Modification Date	2015-12-14T21:15:38
17	Spectrometer Frequency	100.61
18	Spectral Width	40760.9
19	Lowest Frequency	-10305.7
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

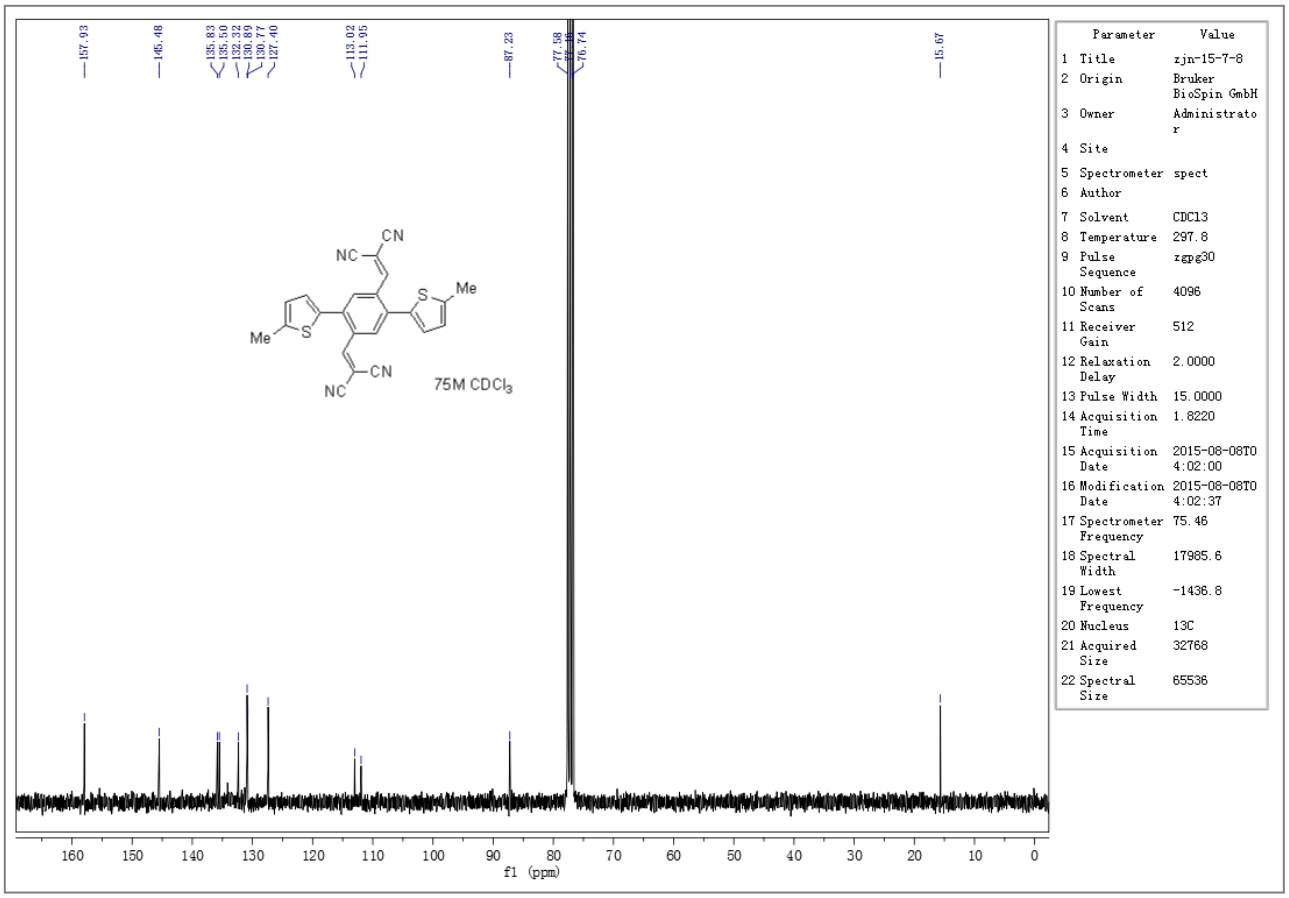




Compounds chart Data



	Parameter	Value
1	Title	zjn-15-7-8
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.5
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	1626
12	Relaxation Delay	1.0000
13	Pulse Width	10.0000
14	Acquisition Time	5.3085
15	Acquisition Date	2015-08-08T2 2:39:00
16	Modification Date	2015-08-08T2 2:39:20
17	Spectrometer Frequency	300.09
18	Spectral Width	6172.8
19	Lowest Frequency	-1241.2
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



	Parameter	Value
1	Title	zjn-15-7-8
2	Origin	Bruker BioSpin GmbH
3	Owner	Administrator
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.8
9	Pulse Sequence	zgpg30
10	Number of Scans	4096
11	Receiver Gain	512
12	Relaxation Delay	2.0000
13	Pulse Width	15.0000
14	Acquisition Time	1.8220
15	Acquisition Date	2015-08-08T0 4:02:00
16	Modification Date	2015-08-08T0 4:02:37
17	Spectrometer Frequency	75.46
18	Spectral Width	17985.6
19	Lowest Frequency	-1436.8
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray