Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Regulation of circular dichroism behavior and construction of tunable solid-state circularly polarized luminescence based on BINOL derivatives

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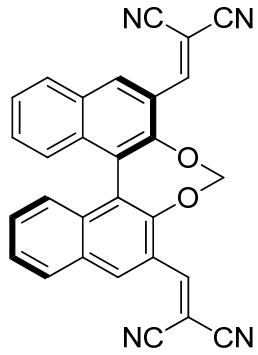
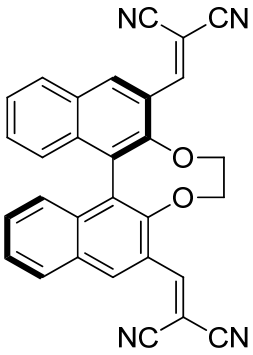
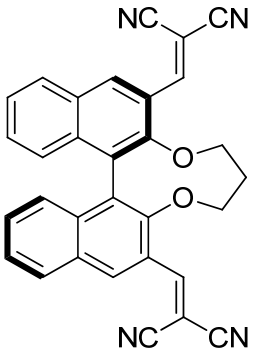
1. General Information

Tetrahydrofuran (THF) was 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 (^{1}H, ^{13}C NMR) were recorded on a Bruker AV 300 (^{1}H at 300 MHz, ^{13}C at 75 MHz), a Bruker Ascend 400 (^{1}H at 400 MHz, ^{13}C at 101 MHz) or a Bruker Ascend 600 (^{1}H 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. Circular dichroisms (CD) were recorded on a Chirascan spectrometer. Circularly polarized luminescences (CPL) were recorded on a JASCO CPL-300 spectrometer. Fluorescence quantum yields were measured using Hamamatsu C9920-02G. Single crystal was collected on Oxford diffraction Eos CCD detector or Bruker CMOS PHOTON 100 detector, respectively. 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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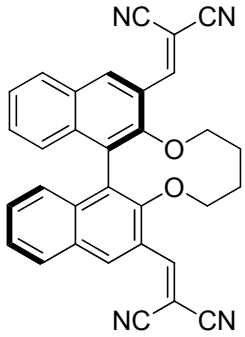	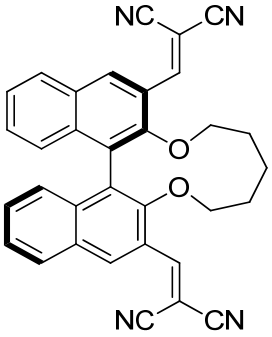	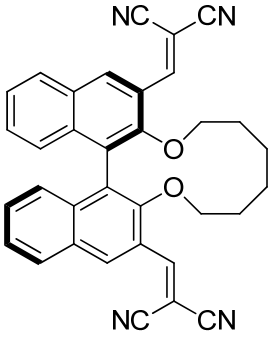
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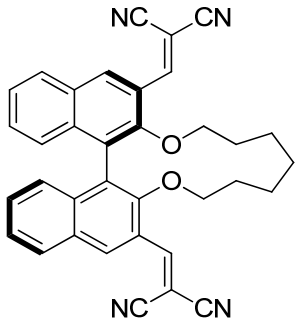	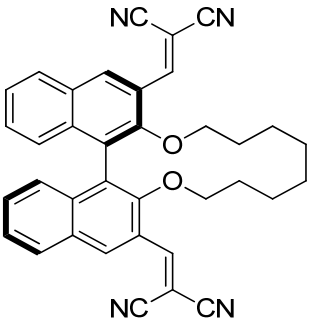	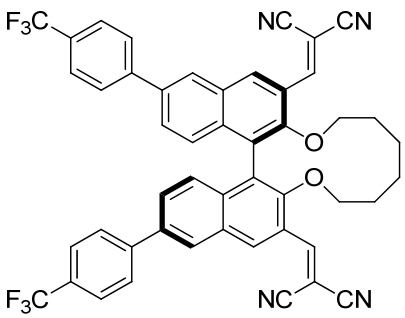
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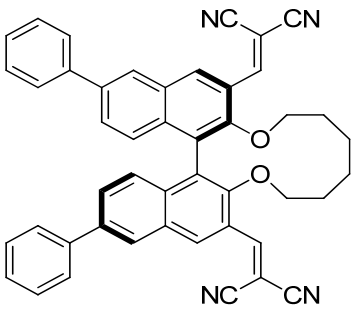	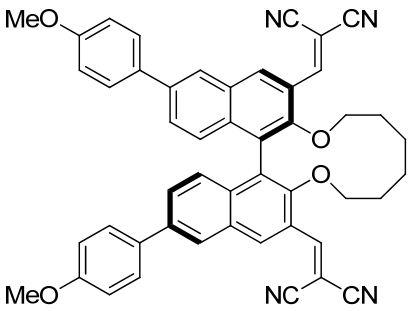	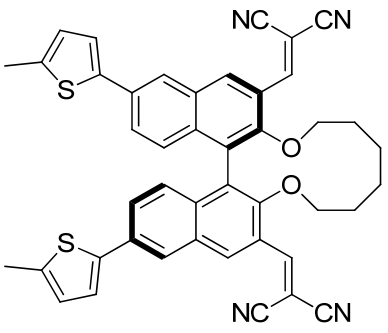
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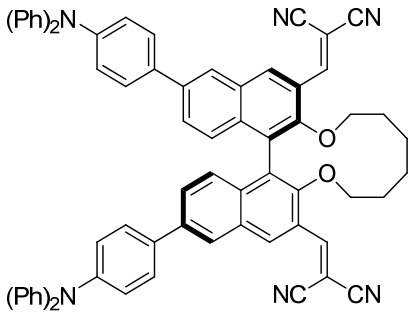	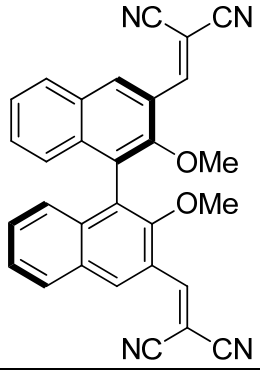	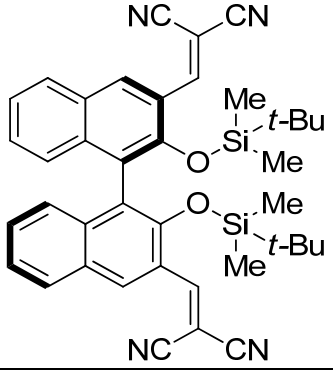
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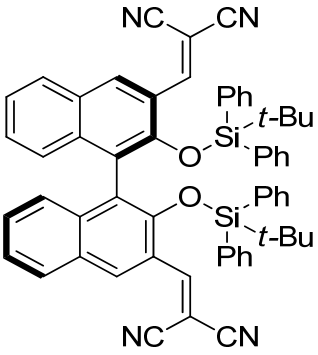
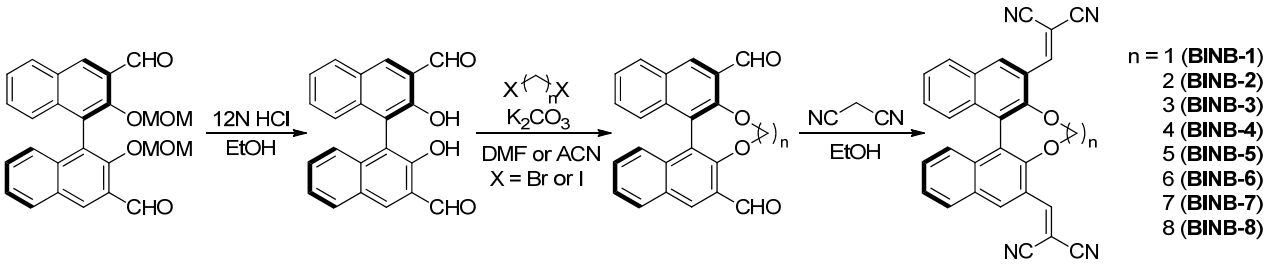
		
BINUB-3 Data NMR		

3. Experimental Procedure and Characterization Data

3.1 Reaction procedures

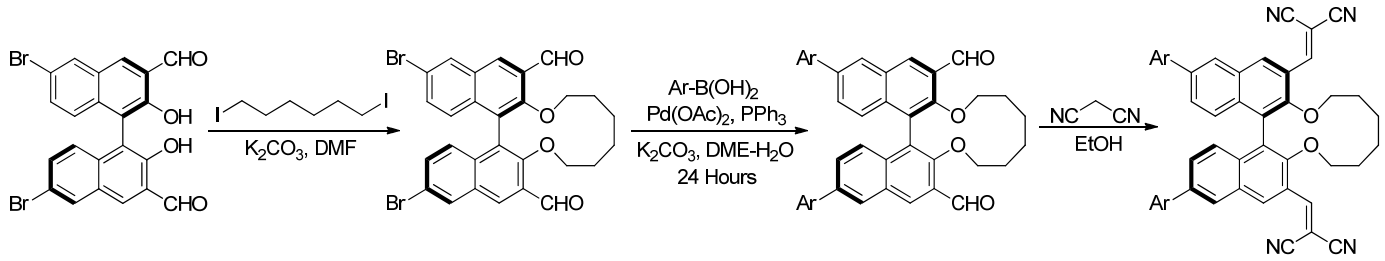


Scheme S1. Synthetic route of **BINB** derivatives.

Remove –MOM group: (*R*)-2,2'-bis(methoxymethoxy)-[1,1'-binaphthalene]-3,3'-dicarbaldehyde (860 mg, 2.0 mmol) was dissolved in THF (12.00 mL). The temperature of the reaction mixture was reduced to 0 °C, and then 12 N HCl (6.00 mL) was added over 5 min with stirring. Then the reaction mixture was allowed to stir at room temperature for approximately 3 hours. After completion of the reaction, filter afforded desired product in 84% yield.

Introduction of alkyl chain group: To a stirred solution containing corresponding dialdehyde (1.00 equiv) and K_2CO_3 (6.00 equiv for diiodomethane, 10.00 equiv for other di-bromo or di-iodo alkanes) in DMF were added corresponding di-bromo alkanes or di-iodo alkanes (1.00 to 3.00 equiv) slowly. Then the reaction was stirred at room temperature for 12 hours (for diiodomethane, the reaction need reflux for 12 hours). After the reaction was completed based on TLC, the solvent was removed under reduced pressure and purified by column chromatography on silica gel (Petroleum ether / EtOAc) to give desired product.

Introduction of malononitrile: To a stirred solution of corresponding di-aldehyde (1.00 equiv) in ethanol were added malononitrile (3.00 equiv) and NaOH (0.05 equiv, 0.1 M in ethanol). Then the reaction kept stirring at room temperature for certain hours. After the reaction was completed based on TLC, the product was purified by column chromatography on silica gel to give desired product.

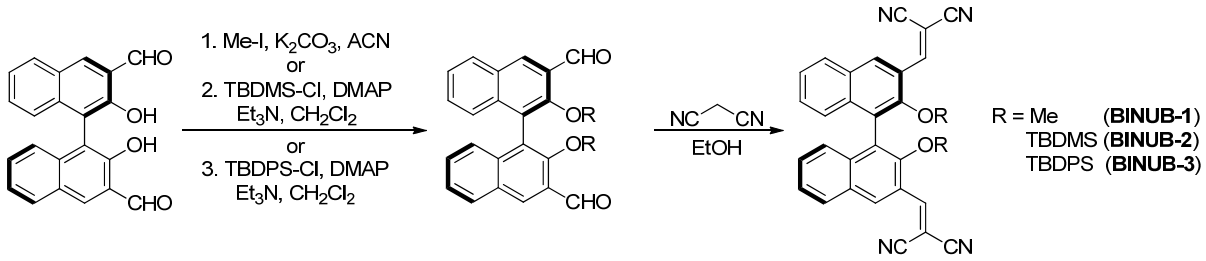


Scheme S2. Synthetic route of **BINB-6** derivatives.

Introduction of alkyl chain group: To a stirred solution containing corresponding di-aldehyde (100.00 mg, 0.20 mmol) and K_2CO_3 (138.00 mg, 1.00 mmol) in DMF (10.00 mL) were added 1,6-diiodo hexane (33.00 μL, 0.20 mmol) slowly. Then the reaction was stirred at 80 ^oC for 24 hours. After the reaction was completed based on TLC, the mixture was diluted with water, followed by extraction with EtOAc. The organic phase were combined and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel (Petroleum ether / EtOAc) to give desired product.

Introduction of varied electron donating group: Di-aldehyde (0.10 mmol), corresponding boronic acid (0.30 mmol), K_2CO_3 (83.00 mg, 0.60 mmol), $Pd(OAc)_2$ (5.00 mg, 0.02 mmol) and PPh_3 (6.00 mg, 0.02 mmol) were dissolved in 1.00 mL DME-H_2O (v / v = 1:1). The mixture was stirred at room temperature under N_2 for 24 hours. Then the reaction was diluted with water, followed by extraction with CH_2Cl_2. The organic phase were combined and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel (Petroleum ether / EtOAc) to give desired product.

Introduction of malononitrile: To a stirred solution of corresponding di-aldehyde (1.00 equiv) in ethanol were added malononitrile (3.00 equiv) and NaOH (0.20 equiv, 0.1 M in ethanol). Then the reaction kept stirring at room temperature for certain hours. After the reaction was completed based on TLC, the product was purified by column chromatography on silica gel to give desired product.



Scheme S3. Synthetic route of **BINUB** derivatives.

Introduction of -Me group: Potassium carbonate (110.40 mg, 0.8 mmol) was added to a stirred solution of corresponding dialdehyde (68.40 mg, 0.2 mmol) in acetonitrile (5.00 mL) at room temperature. Then, methyl iodide (74 μL, 1.2 mmol) was added to the reaction mixture and kept the reaction stirred at room temperature overnight. After the reaction was completed based on TLC, the solvent was removed under reduced pressure and purified by column chromatography on silica gel (Petroleum ether/EtOAc) to give desired product in 82% yield.

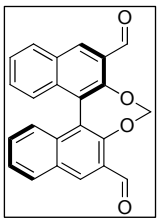
Introduction of -TBDMS group: Corresponding dialdehyde (0.35 mmol) was added to a stirred solution of *tert*-butylchlorodimethylsilane (150.72 mg, 3.5 mmol), DMAP (17.25 mg, 0.14 mmol) and NEt_3 (489.00 μL, 3.5 mmol) in DMF (2.00 mL) at room temperature under N_2. Then the reaction stirred at room temperature for 4 hours. After the reaction was completed based on TLC, the solvent was removed under reduced pressure and purified by column chromatography on silica gel (Petroleum ether/EtOAc) to give desired product in 74% yield.

Introduction of -TBDPS group: Corresponding dialdehyde (0.2 mmol) was added to a stirred solution of *tert*-butylchlorodiphenylsilane (275.00 mg, 1.0 mmol), DMAP (13.00 mg, 0.1 mmol) and NEt_3 (95.00 μL, 0.7 mmol) in CH_2Cl_2 (1.00 mL) at room temperature under N_2. Then the reaction stirred at room temperature for 15 hours. After the reaction was completed based on TLC, the solvent was removed under reduced pressure and purified by column chromatography on silica gel (Petroleum ether/EtOAc) to give desired product in 81%

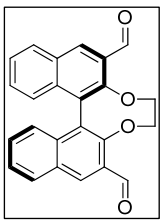
yield.

Introduction of malononitrile: To a stirred solution of corresponding di-aldehyde (1.00 equiv) in ethanol were added malononitrile and base (NaOH or piperidine). The reaction kept stirring at room temperature for certain hours. After the reaction was completed based on TLC, the product was purified by column chromatography on silica gel to give desired product.

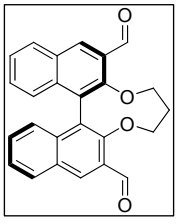
3.2 Compound data



(*R*)-dinaphtho[2,1-*d*:1',2'-*f*][1,3]dioxepine-2,6-dicarbaldehyde. 68% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.60 (s, 2H, CHO), 8.61 (s, 2H, Ar H), 8.09 (d, 2H, *J* = 8.3 Hz, Ar H), 7.55-7.51 (m, 2H, Ar H), 7.42 (t, 4H, *J* = 3.7 Hz, Ar H), 5.90 (s, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 189.49, 151.15, 134.94, 132.29, 130.89, 130.80, 129.28, 127.44, 126.85, 126.73, 126.48, 104.12.

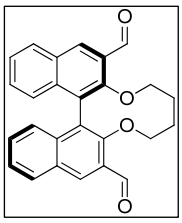


(*R*)-4,5-dihydrodinaphtho[2,1-*e*:1',2'-*g*][1,4]dioxocine-2,7-dicarbaldehyde. 38% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.54 (s, 2H, CHO), 8.60 (s, 2H, Ar H), 8.06 (d, 2H, *J* = 8.2 Hz, Ar H), 7.47 (t, 2H, *J* = 7.3 Hz, Ar H), 7.34 (t, 2H, *J* = 8.0 Hz, Ar H), 7.13 (d, 2H, *J* = 8.6 Hz, Ar H), 4.61-4.56 (m, 2H, CH_2), 4.23-4.18 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 190.17, 156.19, 135.97, 134.07, 130.44, 130.25, 129.58, 127.92, 126.89, 126.20, 125.23, 74.04.

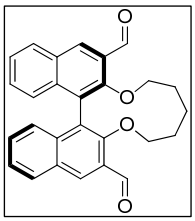


(*R*)-5,6-dihydro-4*H*-dinaphtho[2,1-*f*:1',2'-*h*][1,5]dioxonine-2,8-dicarbaldehyde. 49% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.44 (s, 2H, CHO), 8.57 (s, 2H, Ar H), 8.06 (d, 2H, *J* = 8.2 Hz, Ar H), 7.47 (t, 2H, *J* = 7.4 Hz, Ar H), 7.36 (t, 2H, *J* = 8.0 Hz, Ar H), 7.05 (d, 2H, *J* = 8.5 Hz, Ar H), 4.49-4.45 (m, 2H, CH_2), 4.31-4.27 (m, 2H, CH_2), 1.92-1.88 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 190.06, 153.71, 136.60, 134.66, 130.29, 130.04, 129.87, 128.46, 126.60, 126.09, 125.91,

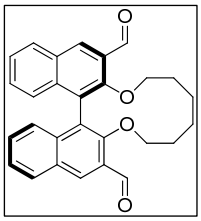
76.34, 31.28.



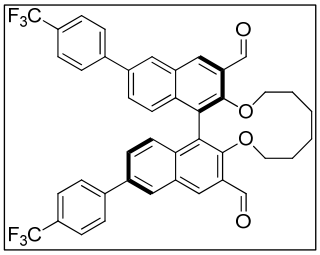
(*R*)-4,5,6,7-tetrahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxecine-2,9-dicarbaldehyde. 51% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.52 (s, 2H, CHO), 8.60 (s, 2H, Ar H), 8.04 (d, 2H, *J* = 8.2 Hz, Ar H), 7.46 (t, 2H, *J* = 7.3 Hz, Ar H), 7.37 (t, 2H, *J* = 7.6 Hz, Ar H), 7.04 (d, 2H, *J* = 8.5 Hz, Ar H), 4.20-4.14 (m, 4H, CH_2), 1.76-1.70 (m, 2H, CH_2), 1.53-1.49 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 190.05, 153.32, 136.88, 133.92, 130.26, 129.97, 129.92, 128.22, 126.70, 126.15, 125.32, 76.14, 25.62.



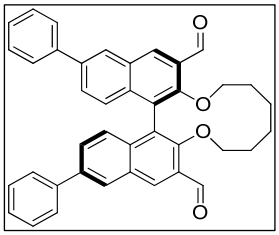
(*R*)-9,10,11,12-tetrahydro-8*H*-dinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclounde cine-6,14-dicarbaldehyde. 32% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.55 (s, 2H, CHO), 8.58 (s, 2H, Ar H), 8.03 (d, 2H, *J* = 8.1 Hz, Ar H), 7.48-7.45 (m, 2H, Ar H), 7.43-7.40 (m, 2H, Ar H), 7.20 (t, 2H, *J* = 8.5 Hz, Ar H), 4.43-4.40 (m, 2H, CH_2), 4.05-4.01 (m, 2H, CH_2), 1.61-1.56 (m, 2H, CH_2), 1.49-1.42 (m, 2H, CH_2), 1.20-1.16 (s, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 190.44, 155.13, 136.75, 133.94, 130.20, 129.92, 129.63, 128.36, 125.93, 125.51, 125.13, 74.95, 28.12, 21.19.



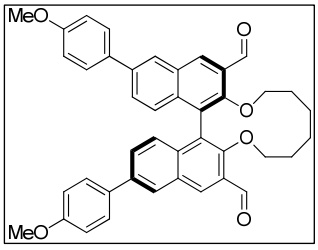
(*R*)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-dicarbaldehyde. 17% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.56 (s, 2H, CHO), 8.61 (s, 2H, Ar H), 8.05 (d, 2H, *J* = 8.2 Hz, Ar H), 7.46 (t, 2H, *J* = 7.3 Hz, Ar H), 7.36 (t, 2H, *J* = 7.7 Hz, Ar H), 7.12 (d, 2H, *J* = 8.5 Hz, Ar H), 3.84-3.80 (m, 2H, CH_2), 3.53-3.49 (m, 2H, CH_2), 1.24-1.22 (m, 2H, CH_2), 1.04-0.99 (m, 2H, CH_2), 0.86-0.83 (s, 4H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 190.65, 156.02, 137.20, 132.11, 130.51, 129.94, 129.54, 129.12, 126.00, 125.79, 125.62, 76.08, 29.45, 25.73.



(*R*)-12,17-bis(4-(trifluoromethyl)phenyl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-dicarbaldehyde. 47% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.66 (s, 2H, CHO), 8.68 (s, 2H, Ar H), 8.25 (s, 2H, Ar H), 7.79-7.73 (m, 8H, Ar H), 7.71-7.69 (m, 2H, Ar H), 7.47 (d, 2H, *J* = 8.9 Hz, Ar H), 4.33-4.29 (m, 2H, CH_2), 3.89-3.84 (m, 2H, CH_2), 1.75-1.73 (m, 2H, CH_2), 1.54 (s, 2H, CH_2), 1.27-1.25 (m, 2H, CH_2), 1.12-1.09 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 190.58, 154.94, 143.68, 137.22, 135.59, 133.30, 130.06, 129.85, 129.82, 129.48, 129.13, 128.46, 127.62, 126.65, 126.12, 126.09, 125.25, 123.44, 123.29, 72.94, 28.44, 22.75.

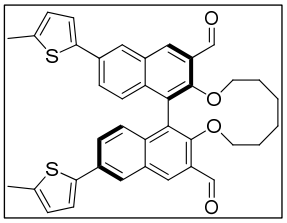


(*R*)-12,17-diphenyl-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-dicarbaldehyde. 86% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.67 (s, 2H, CHO), 8.65 (s, 2H, Ar H), 8.23 (d, 2H, *J* = 1.6 Hz, Ar H), 7.73-7.71 (m, 2H, Ar H), 7.70-7.68 (m, 4H, Ar H), 7.50-7.43 (m, 6H, Ar H), 7.41-7.37 (m, 2H, Ar H), 4.31-4.24 (m, 2H, CH_2), 3.86-3.79 (m, 2H, CH_2), 1.78-1.72 (m, 2H, CH_2), 1.31-1.27 (m, 4H, CH_2), 1.14-1.07 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 190.88, 154.47, 153.56, 140.22, 138.76, 135.26, 132.90, 129.99, 129.56, 129.33, 129.16, 127.91, 127.89, 127.37, 126.37, 123.35, 72.50, 28.47, 22.80.

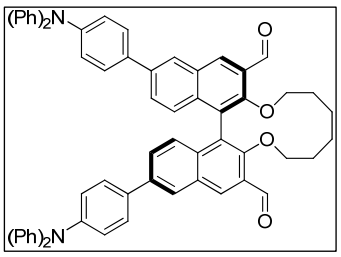


(*R*)-12,17-bis(4-methoxyphenyl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-dicarbaldehyde. 65% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.66 (s, 2H, CHO), 8.62 (s, 2H, Ar H), 8.16 (d, 2H, *J* = 1.3 Hz, Ar H), 7.69-7.67 (m, 2H, Ar H), 7.62 (d, 4H, *J* = 8.7 Hz, Ar H), 7.42 (d, 2H, *J* = 8.9 Hz, Ar H), 7.02 (d, 4H, *J* = 8.7 Hz, Ar H), 4.27-4.23 (m, 2H, CH_2), 3.87 (s, 6H, CH_3), 3.83-3.79 (m, 2H, CH_2), 1.75-1.72 (m, 2H, CH_2), 1.54-1.48 (m, 2H, CH_2), 1.30-1.25 (m, 2H, CH_2), 1.11-1.07 (m, 2H, CH_2); ^{13}C-NMR (151

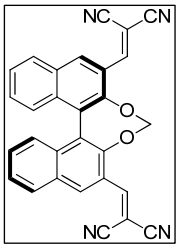
MHz, $CDCl_3$) δ (ppm): 190.95, 159.70, 154.21, 138.36, 134.93, 132.68, 132.64, 130.08, 129.38, 129.30, 128.40, 127.08, 126.31, 123.39, 114.64, 72.38, 55.54, 28.46, 22.81.



(*R*)-12,17-bis(5-methylthiophen-2-yl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-dicarbaldehyde. 68% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 10.62 (s, 2H, CHO), 8.56 (s, 2H, Ar H), 8.12 (d, 2H, *J* = 1.2 Hz, Ar H), 7.65-7.63 (m, 2H, Ar H), 7.33 (d, 2H, *J* = 8.9 Hz, Ar H), 7.19 (d, 2H, *J* = 3.5 Hz, Ar H), 6.75 (d, 2H, *J* = 2.5 Hz, Ar H), 4.24-4.20 (m, 2H, CH_2), 3.81-3.76 (m, 2H, CH_2), 2.52 (s, 6H, CH_3), 1.72-1.69 (m, 2H, CH_2), 1.51-1.50 (m, 2H, CH_2), 1.07-1.05 (m, 2H, CH_2), 0.90-0.84 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 190.72, 154.24, 140.96, 140.49, 134.94, 132.48, 132.36, 129.92, 129.36, 127.99, 126.61, 126.27, 125.40, 123.83, 123.38, 72.48, 28.39, 22.73, 15.63.

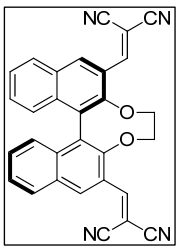


(*R*)-12,17-bis(4-(diphenylamino)phenyl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-dicarbaldehyde. 52% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 10.67 (s, 2H, CHO), 8.63 (s, 2H, Ar H), 8.18 (d, 2H, *J* = 1.4 Hz, Ar H), 7.71-7.69 (m, 2H, Ar H), 7.56 (d, 4H, *J* = 8.7 Hz, Ar H), 7.43 (d, 2H, *J* = 8.9 Hz, Ar H), 7.30-7.26 (m, 8H, Ar H), 7.19-7.14 (m, 12H, Ar H), 7.07-7.04 (m, 4H, Ar H), 4.29-4.23 (m, 2H, CH_2), 3.84-3.78 (m, 2H, CH_2), 1.76-1.72 (m, 2H, CH_2), 1.59-1.54 (m, 2H, CH_2), 1.31-1.25 (m, 2H, CH_2), 1.11-1.07 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 190.91, 154.19, 147.79, 147.66, 138.19, 134.93, 133.67, 132.65, 130.05, 129.48, 129.27, 129.22, 127.94, 127.00, 126.31, 124.81, 123.70, 123.33, 72.32, 28.44, 22.79.

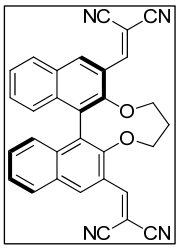


(*R*)-2,2'-(dinaphtho[2,1-*d*:1',2'-*f*][1,3]dioxepine-2,6-diylbis(methanylylidene))dimalononitrile (BINB-1). 72% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm):

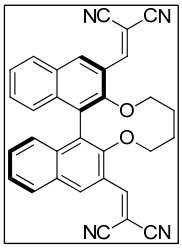
9.06 (s, 2H), 8.40 (s, 2H, Ar H), 8.11 (d, 2H, *J* = 8.2 Hz, Ar H), 7.60 (t, 2H, *J* = 7.4 Hz, Ar H), 7.48 (t, 2H, *J* = 7.9 Hz, Ar H), 7.37 (d, 2H, *J* = 8.6 Hz, Ar H), 5.75 (s, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 153.36, 148.58, 134.67, 131.97, 130.93, 130.69, 130.31, 127.25, 126.62, 126.40, 123.12, 113.83, 112.75, 103.68, 84.74. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{29}H_{14}N_4O_2Na^+$, 473.1009, found, 473.1002. Compounds chart NMR X-ray#



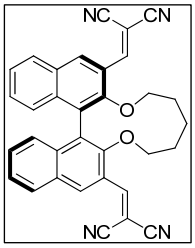
(*R*)-2,2'-((4,5-dihydrodinaphtho[2,1-*e*:1',2'-*g*][1,4]dioxocine-2,7-diyl)bis(methanylylidene))dimalononitrile (BINB-2). 62% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.99 (s, 2H), 8.34 (s, 2H, Ar H), 8.07 (d, 2H, *J* = 8.2 Hz, Ar H), 7.56-7.52 (m, 2H, Ar H), 7.41-7.37 (m, 2H, Ar H), 7.04 (d, 2H, *J* = 8.5 Hz, Ar H), 4.57-4.50 (m, 2H, CH_2), 4.05-3.98 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 154.49, 153.62, 135.76, 132.58, 130.49, 130.35, 130.22, 126.95, 126.69, 124.72, 124.03, 113.90, 112.72, 84.55, 73.19. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{30}H_{16}N_4O_2Na^+$, 487.1165, found, 487.1172. Compounds chart NMR X-ray



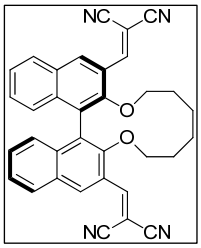
(*R*)-2,2'-((5,6-dihydro-4*H*-dinaphtho[2,1-*f*:1',2'-*h*][1,5]dioxonine-2,8-diyl)bis(methanylylidene))dimalononitrile (BINB-3). 56% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.90 (s, 2H), 8.21 (s, 2H, Ar H), 8.06 (d, 2H, *J* = 8.2 Hz, Ar H), 7.53 (t, 2H, *J* = 7.4 Hz, Ar H), 7.40 (t, 2H, *J* = 7.8 Hz, Ar H), 6.95 (d, 2H, *J* = 8.5 Hz, Ar H), 4.43-4.39 (m, 2H, CH_2), 4.07-4.04 (m, 2H, CH_2), 1.93-1.89 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 155.29, 152.15, 136.17, 132.23, 30.60, 130.24, 130.09, 126.85, 126.13, 125.65, 123.99, 113.79, 112.63, 84.03, 75.69, 30.82. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{31}H_{18}N_4O_2Na^+$, 501.1322, found, 501.1320. Compounds chart NMR#



(*R*)-2,2'-((4,5,6,7-tetrahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxecine-2,9-diyl) bis(methanylylidene))dimalononitrile (BINB-4). 47% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.91 (s, 2H), 8.31 (s, 2H, Ar H), 8.04 (d, 2H, *J* = 8.2 Hz, Ar H), 7.52 (t, 2H, *J* = 7.4 Hz, Ar H), 7.42 (t, 2H, *J* = 8.2 Hz, Ar H), 6.99 (d, 2H, *J* = 8.5 Hz, Ar H), 4.12 (t, 2H, *J* = 11.6 Hz, CH_2), 3.93-3.89 (m, 2H, CH_2), 1.75-1.66 (m, 2H, CH_2), 1.50-1.41 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 155.68, 151.59, 136.36, 132.63, 130.72, 130.16, 129.97, 126.92, 126.30, 125.21, 123.76, 113.83, 112.71, 83.82, 75.30, 28.19. HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{32}H_{21}N_4O_2^+$, 493.1659, found, 493.1608. Compounds chart NMR X-ray#

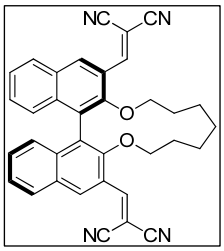


(*R*)-2,2'-((9,10,11,12-tetrahydro-8*H*-dinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacycl oundecine-6,14-diyl)bis(methanylylidene))dimalononitrile (BINB-5). 33% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.83 (s, 2H), 8.38 (s, 2H, Ar H), 8.02 (d, 2H, *J* = 8.2 Hz, Ar H), 7.51 (t, 2H, *J* = 7.2 Hz, Ar H), 7.44 (t, 2H, *J* = 7.7 Hz, Ar H), 7.12 (d, 2H, *J* = 8.5 Hz, Ar H), 4.24-4.20 (m, 2H, CH_2), 3.93-3.89 (m, 2H, CH_2), 1.59-1.56 (m, 2H, CH_2), 1.50-1.45 (m, 2H, CH_2), 1.18-1.14 (s, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 156.65, 152.91, 136.14, 132.48, 130.57, 130.09, 129.76, 126.70, 125.41, 124.64, 124.06, 113.79, 112.65, 83.85, 74.10, 28.19, 20.74. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{33}H_{22}N_4O_2Na^+$, 529.1635, found, 529.1636. Compounds chart NMR X-ray

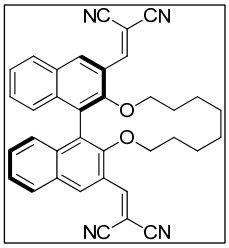


(*R*)-2,2'-((2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclodod ecine-9,20-diyl)bis(methanylylidene))dimalononitrile (BINB-6). 54% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.93 (s, 2H), 8.37 (s, 2H, Ar H), 8.07 (d, 2H, *J* = 8.2 Hz, Ar H), 7.52 (t, 2H, *J* = 7.2 Hz, Ar H), 7.41 (t, 2H, *J* = 7.8 Hz, Ar H), 7.06 (d, 2H, *J* = 8.5 Hz, Ar H), 3.69-3.66 (m, 2H, CH_2), 3.47-3.43 (m, 2H, CH_2),

1.30-1.26 (m, 2H, CH_2), 1.17-1.15 (m, 2H, CH_2), 0.91 (s, 4H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 155.83, 153.37, 136.76, 132.06, 130.54, 130.35, 129.96, 126.84, 125.61, 125.00, 124.88, 113.94, 112.73, 84.17, 75.89, 29.80, 26.21. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{34}H_{24}N_4O_2Na^+$, 543.1791, found, 1063.3710 ($2M+Na^+$). Compounds chart NMR

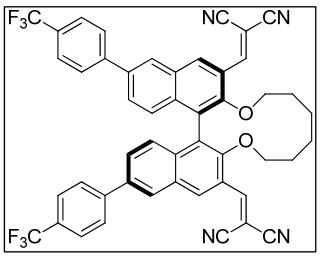


(*R*)-2,2'-((3,4,5,6,7,8-hexahydro-2H-dinaphtho[2,1-b:1',2'-d][1,6]dioxacyclotridecine-10,21-diyl)bis(methanylylidene))dimalononitrile (BINB-7). 35% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.92 (s, 2H), 8.44 (s, 2H, Ar H), 8.03 (d, 2H, J = 8.2 Hz, Ar H), 7.51 (t, 2H, J = 7.3 Hz, Ar H), 7.41 (t, 2H, J = 7.6 Hz, Ar H), 7.02 (d, 2H, J = 8.6 Hz, Ar H), 4.04-4.00 (m, 2H, CH_2), 3.82-3.78 (m, 2H, CH_2), 1.57-1.54 (m, 2H, CH_2), 1.44-1.41 (m, 2H, CH_2), 1.33-1.21 (m, 4H, CH_2), 1.14-1.10 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 156.30, 153.01, 136.70, 132.16, 130.55, 130.20, 129.77, 126.74, 125.57, 125.17, 124.57, 113.95, 112.85, 83.76, 74.48, 27.76, 24.96, 23.04. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{35}H_{26}N_4O_2Na^+$, 557.1948, found, 557.1947. Compounds chart NMR X-ray

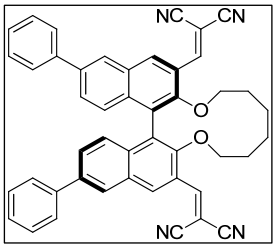


(*R*)-2,2'-((2,3,4,5,6,7,8,9-octahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclotetradecine-11,22-diyl)bis(methanylylidene))dimalononitrile (BINB-8). 30% yield (two steps). ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.95 (s, 2H), 8.42 (s, 2H, Ar H), 8.04 (d, 2H, J = 8.2 Hz, Ar H), 7.52 (t, 2H, J = 7.4 Hz, Ar H), 7.41 (t, 2H, J = 8.0 Hz, Ar H), 7.00 (d, 2H, J = 8.5 Hz, Ar H), 3.91-3.87 (m, 2H, CH_2), 3.73-3.69 (m, 2H, CH_2), 1.69-1.64 (m, 2H, CH_2), 1.51 (s, 2H, CH_2), 1.35-1.34 (m, 2H, CH_2), 1.20-1.18 (m, 6H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 156.05, 153.02, 136.74, 132.03, 130.52, 130.25, 129.88, 126.83, 125.53, 125.28, 124.86, 113.97, 112.88, 83.78, 74.55, 26.80, 24.17, 23.28. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{36}H_{28}N_4O_2Na^+$,

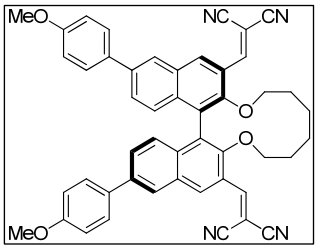
571.2104, found, 571.2089. Compounds chart NMR X-ray



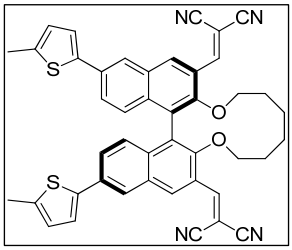
(*R*)-2,2'-((12,17-bis(4-(trifluoromethyl)phenyl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-diyl)bis(methanylylidene))dimalononitrile (BINB-6A). 70% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 9.00 (s, 2H), 8.53 (s, 2H, Ar H), 8.24 (d, 2H, *J* = 1.6 Hz, Ar H), 7.80-7.73 (m, 10H, Ar H), 7.41 (d, 2H, *J* = 8.9 Hz, Ar H), 4.06-4.01 (m, 2H, CH_2), 3.75-3.71 (m, 2H, CH_2), 1.78-1.73 (m, 2H, CH_2), 1.51-1.47 (m, 2H, CH_2), 1.39-1.35 (m, 2H, CH_2), 1.13-1.07 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 155.96, 151.67, 143.13, 138.15, 134.71, 132.48, 130.39, 130.23, 130.18, 129.97, 129.89, 128.19, 127.67, 126.47, 126.21, 126.19, 125.83, 125.17, 123.36, 122.45, 113.80, 112.78, 108.82, 84.54, 71.01, 28.72, 22.66. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{48}H_{30}F_6N_4O_2Na^+$, 831.2165, found, 831.2173. Compounds chart NMR X-ray



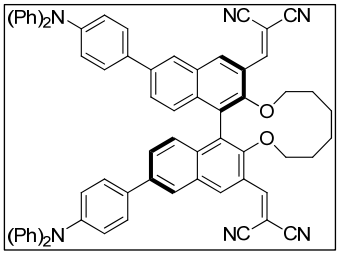
(*R*)-2,2'-((12,17-diphenyl-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-diyl)bis(methanylylidene))dimalononitrile (BINB-6B). 45% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 9.00 (s, 2H), 8.54 (s, 2H, Ar H), 8.22 (s, 2H, Ar H), 7.76 (d, 2H, *J* = 8.9 Hz, Ar H), 7.69 (d, 4H, *J* = 7.7 Hz, Ar H), 7.50 (t, 4H, *J* = 7.6 Hz, Ar H), 7.43-7.38 (m, 4H, Ar H), 4.06-4.01 (m, 2H, CH_2), 3.74-3.69 (m, 2H, CH_2), 1.77-1.74 (m, 2H, CH_2), 1.52-1.47 (m, 2H, CH_2), 1.39-1.34 (m, 2H, CH_2), 1.11-1.08 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 156.12, 151.21, 139.67, 139.64, 134.42, 132.33, 130.33, 130.11, 129.25, 128.23, 127.64, 127.36, 126.19, 125.57, 122.54, 113.97, 112.90, 84.01, 70.83, 28.72, 22.70. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{46}H_{32}N_4O_2Na^+$, 695.2417, found, 695.2404. Compounds chart NMR#



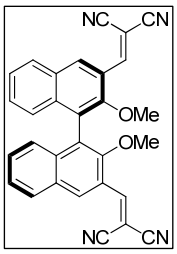
(*R*)-2,2'-((12,17-bis(4-methoxyphenyl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-diyl)bis(methanylylidene))dimalononitrile (BINB-6C). 67% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.98 (s, 2H), 8.53 (s, 2H, Ar H), 8.16 (s, 2H, Ar H), 7.73-7.71 (m, 2H, Ar H), 7.63 (d, 4H, *J* = 8.6 Hz, Ar H), 7.35 (d, 2H, *J* = 8.9 Hz, Ar H), 7.03 (d, 4H, *J* = 8.7 Hz, Ar H), 4.04-3.99 (m, 2H, CH_2), 3.87 (s, 6H, CH_3), 3.72-3.67 (m, 2H, CH_2), 1.78-1.72 (m, 2H, CH_2), 1.49-1.46 (m, 2H, CH_2), 1.39-1.36 (m, 2H, CH_2), 1.10-1.07 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 159.94, 156.18, 150.93, 139.24, 134.10, 132.14, 132.03, 130.20, 130.14, 128.42, 126.76, 126.12, 125.50, 122.58, 114.72, 114.02, 112.95, 83.80, 70.77, 55.55, 28.69, 22.71. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{48}H_{36}N_4O_4Na^+$, 755.2629, found, 755.2624. Compounds chart NMR



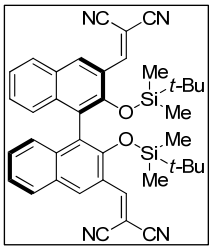
(*R*)-2,2'-((12,17-bis(5-methylthiophen-2-yl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-diyl)bis(methanylylidene))dimalononitrile (BINB-6D). 49% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.88 (s, 2H), 8.49 (s, 2H, Ar H), 8.10 (s, 2H, Ar H), 7.68 (d, 2H, *J* = 13.4 Hz, Ar H), 7.27-7.23 (m, 4H, Ar H), 6.78 (d, 2H, *J* = 4.7 Hz, Ar H), 4.00-3.94 (m, 2H, CH_2), 3.71-3.64 (m, 2H, CH_2), 2.54 (s, 6H, CH_3), 1.77-1.68 (m, 2H, CH_2), 1.47-1.42 (m, 2H, CH_2), 1.37-1.31 (m, 2H, CH_2), 1.08-1.04 (m, 2H, CH_2); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 155.90, 150.91, 141.21, 140.37, 133.89, 133.08, 131.85, 130.02, 128.37, 126.90, 126.14, 125.57, 124.86, 124.28, 122.55, 113.92, 112.79, 83.88, 70.94, 28.56, 22.65, 15.72. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{44}H_{32}N_4O_2Na^+$, 735.1859, found, 735.1864. Compounds chart NMR



(*R*)-2,2'-((12,17-bis(4-(diphenylamino)phenyl)-2,3,4,5,6,7-hexahydrodinaphtho[2,1-*b*:1',2'-*d*][1,6]dioxacyclododecine-9,20-diyl)bis(methanylylidene))dimalononitrile (BINB-6E). 82% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.97 (s, 2H), 8.53 (s, 2H, Ar H), 8.16 (s, 2H, Ar H), 7.74-7.72 (m, 2H, Ar H), 7.35 (d, 4H, *J* = 8.9 Hz, Ar H), 7.74-7.72 (m, 2H, Ar H), 7.31-7.27 (m, 8H, Ar H), 7.17-7.14 (m, 12H, Ar H), 7.08-7.04 (m, 4H, Ar H), 4.04-3.98 (m, 2H, CH_2), 3.72-3.66 (m, 2H, CH_2), 1.77-1.72 (m, 2H, CH_2), 1.54-1.43 (m, 2H, CH_2), 1.39-1.36 (m, 2H, CH_2), 1.13-1.04 (m, 2H, CH_2); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 156.17, 150.93, 148.12, 147.57, 139.14, 134.12, 132.98, 132.14, 130.20, 130.01, 129.51, 127.98, 126.72, 126.13, 125.51, 124.89, 124.86, 123.65, 123.59, 123.48, 123.40, 122.57, 114.01, 112.93, 83.82, 70.74, 28.69, 22.71. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{70}H_{50}N_6O_2Na^+$, 1029.3893, found, 1029.3850. Compounds chart NMR

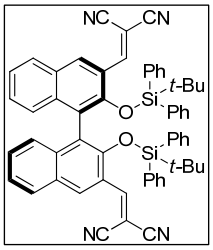


(*R*)-2,2'-((2,2'-dimethoxy-[1,1'-binaphthalene]-3,3'-diyl)bis(methanylylidene))dimalononitrile (BINUB-1). 54% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.98 (s, 2H), 8.36 (s, 2H, Ar H), 8.07 (d, 2H, *J* = 8.2 Hz, Ar H), 7.55 (t, 2H, *J* = 7.8 Hz, Ar H), 7.46 (t, 2H, *J* = 7.8 Hz, Ar H), 7.14 (d, 2H, *J* = 8.4 Hz, Ar H), 3.36 (s, 6H, CH_3); ^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 155.09, 154.30, 136.73, 132.22, 130.71, 130.44, 129.98, 126.92, 125.55, 124.55, 124.48, 113.89, 112.86, 84.18, 62.93. Compounds chart NMR



(*R*)-2,2'-((2,2'-bis((tert-butyldimethylsilyl)oxy)-[1,1'-binaphthalene]-3,3'-diyl)bis(methanylylidene))dimalononitrile (BINUB-2). 52% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm): 8.83 (s, 2H), 8.25 (s, 2H, Ar H), 7.99 (d, 2H, *J* = 8.0 Hz, Ar H), 7.48-7.44 (m, 2H, Ar H), 7.42-7.38 (m, 2H, Ar H), 7.14 (d, 2H, *J* = 8.4 Hz, Ar H), 0.81 (s, 18H, *t*-Bu), -0.09 (s, 6H, CH_3), -1.15 (s, 6H, CH_3);

^{13}C-NMR (101 MHz, $CDCl_3$) δ (ppm): 156.84, 149.86, 137.64, 131.62, 130.25, 128.86, 126.57, 125.84, 124.46, 122.57, 113.75, 112.72, 83.21, 25.47, 18.34, -3.68, -4.43. Compounds chart NMR



(*R*)-2,2'-((2,2'-bis((tert-butyldiphenylsilyl)oxy)-[1,1'-binaphthalene]-3,3'-diyl)bis(methanylylidene))dimalononitrile (BINUB-3). 36% yield. ^{1}H-NMR (600 MHz, $CDCl_3$) δ (ppm): 8.36 (s, 2H), 7.91 (d, 2H, *J* = 7.9 Hz, Ar H), 7.88 (s, 2H, Ar H), 7.81 (d, 4H, *J* = 7.1 Hz, Ar H), 7.52 (t, 2H, *J* = 7.5 Hz, Ar H), 7.43-7.35 (m, 14H, Ar H), 7.23 (t, 4H, *J* = 7.6 Hz, Ar H), 7.18 (d, 2H, *J* = 7.9 Hz, Ar H), 0.43 (s, 18H, CH_3); ^{13}C-NMR (151 MHz, $CDCl_3$) δ (ppm): 158.23, 149.93, 137.18, 135.40, 135.04, 132.39, 131.48, 130.99, 129.94, 128.94, 128.73, 128.36, 125.82, 124.05, 123.12, 113.00, 112.12, 83.46, 25.47, 19.49. Compounds chart NMR

4. UV-vis Spectra

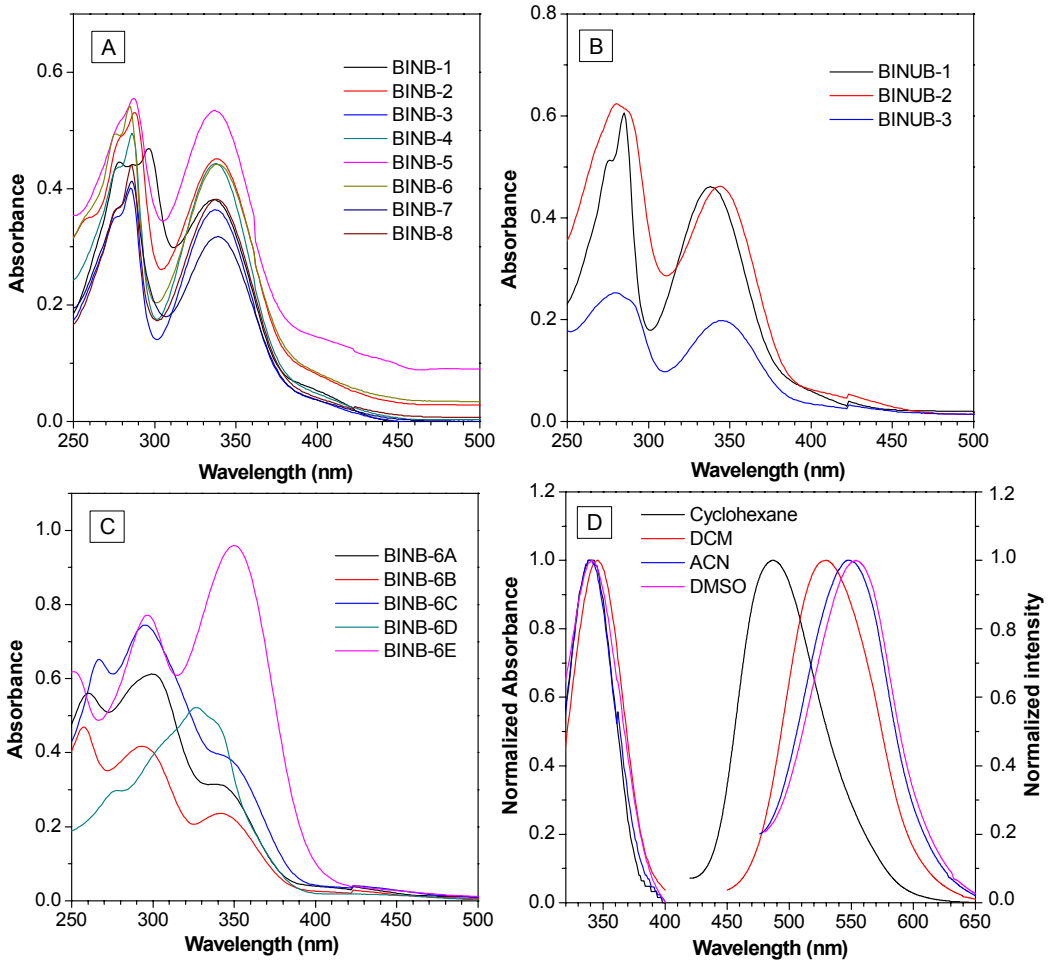


Fig. S1 UV-vis spectra of compounds (A) **BINB-1** to **BINB-8** (10 μM) (B) **BINUB-1** to **BINUB-3** (10 μM) (C) **BINB-6A** to **BINB-6E** (10 μM) (D) UV-vis and emission spectra of **BINB-6** in different solvents (10 μM).

5. Photoluminescence Properties

5.1 Optical properties of BINUB-1 to BINUB-3

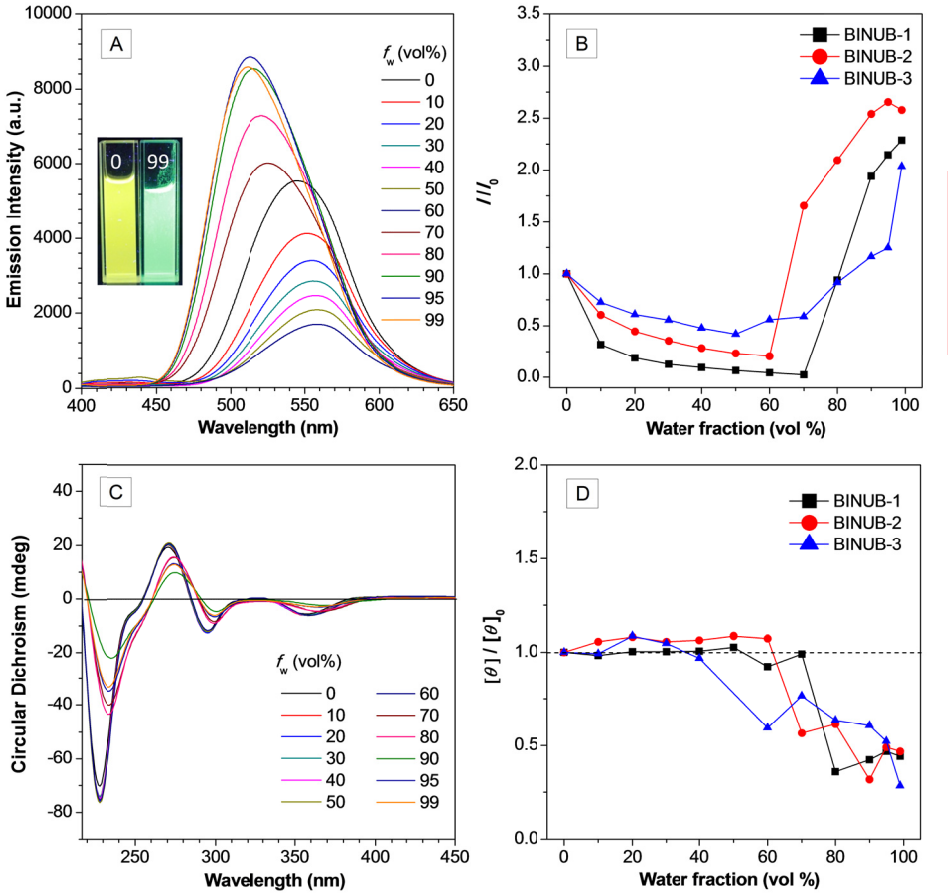


Fig. S2 (A) Emission spectra and (C) CD spectra of **BINUB-2** in acetonitrile/water mixtures with different water fraction (f_w). (B) Plot of emission intensity at 520 nm and (D) CD intensity at 230 nm *versus* the composition of f_w for **BINUB-1** to **BINUB-3**. Inset in A: photograph of **BINUB-2** in acetonitrile/water mixtures with f_w values of 0 and 99% under 365 nm UV irradiation.

5.2 Solid state emission and their CIE diagram

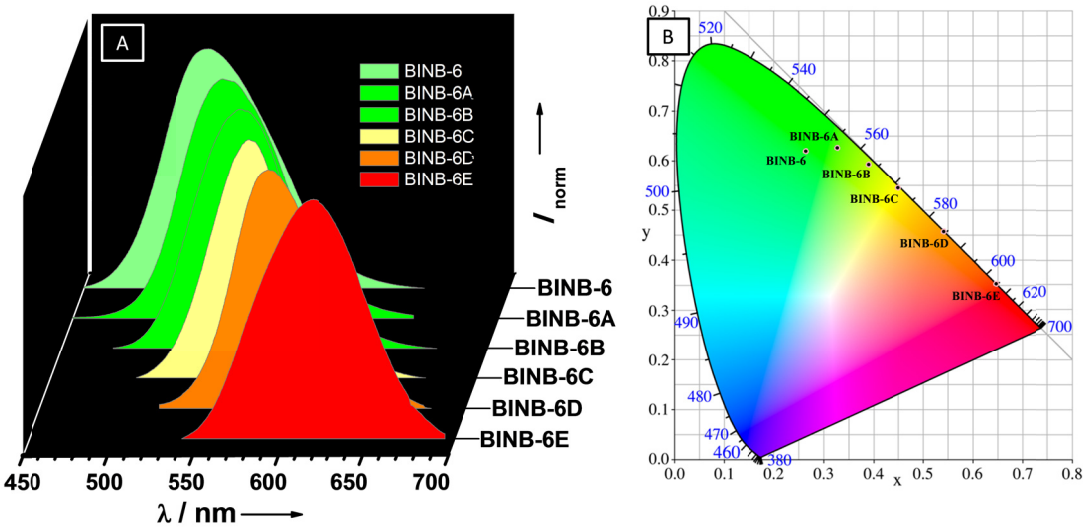


Fig. S3 (A) Emission spectra of **BINB-6** to **BINB-6E** in the solid states. (B) Emission spectra of compounds **BINB-6** to **BINB-6E** plotted on a CIE 1931 chromaticity diagram.

Table S1. Coordinates of compounds **BINB-6** to **BINB-6E** on CIE diagram.

Compd	λ_{em} (nm)	Coordinate (X)	Coordinate (Y)
BINB-6	518	0.2634	0.6195
BINB-6A	538	0.327	0.6271
BINB-6B	555	0.3888	0.5937
BINB-6C	566	0.4491	0.5447
BINB-6D	584	0.5408	0.4572
BINB-6E	617	0.646	0.3536

5.3 Emission of BINB6 to BINB-6D after self-assembly.

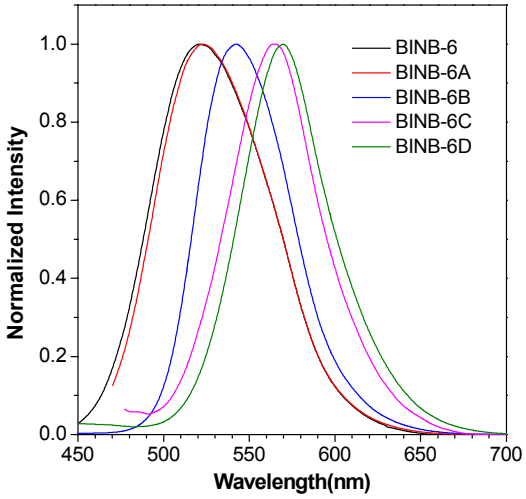


Fig. S4 Emission spectra of **BINB-6** to **BINB-6D** after self-assembly.

5.4 Summary of the optical properties

Table S2. Optical properties of **BINB-1** to **BINB-5**, and **BINB-7** to **BINB-8**.

Compds	Solution state[a]					Solid state		
	λ_{abs} [nm][a]	ε [$M^{-1}cm^{-1}$]	λ_{em} [nm]	Φ_F [%][b]	τ_{avg} [ns][c]	λ_{em} [nm]	Φ_F [%][b]	τ_{avg} [ns][c]
BINB-1	337	38100	552	8.3	4.76	525	17.2	6.13
BINB-2	338	45100	514	6.1	2.88	512	13.7	4.16
BINB-3	337	36400	540	9.9	4.79	515	11.9	3.44
BINB-4	338	44300	544	7.6	3.59	514	12.5	4.41
BINB-5	337	53500	544	9.9	5.00	524	12.7	3.63
BINB-7	339	31800	553	10.6	5.37	522	13.1	3.98
BINB-8	338	38200	551	10.1	5.08	523	14.3	4.19

[a]Acetonitrile solution (10 μM); [b]Absolute fluorescence quantum yield measured using the calibrated integrating sphere system. Longest wavelength absorption maximum in acetonitrile. [c]Mean fluorescence lifetime (τ_{avg}) calculated by using the equation $\tau_{avg} = A_1\tau_1 + A_2\tau_2$.

Table S3. Optical properties of **BINUB-1** to **BINUB-3**.

Compds	Solution state[a]					Solid state		
	λ_{abs} [nm][a]	ε [$M^{-1}cm^{-1}$]	λ_{em} [nm]	Φ_F [%][b]	τ_{avg} [ns][c]	λ_{em} [nm]	Φ_F [%][b]	τ_{avg} [ns][c]
BINUB-1	338	46100	546	7.7	4.77	519	18.0	7.06
BINUB-2	344	46200	545	12.3	6.53	510	14.4	5.54
BINUB-3	346	19800	531	8.9	5.32	486	11.5	4.09

[a]Acetonitrile solution (10 μM); [b]Absolute fluorescence quantum yield measured using the calibrated integrating sphere system. Longest wavelength absorption maximum in acetonitrile. [c]Mean fluorescence lifetime (τ_{avg}) calculated by using the equation $\tau_{avg} = A_1\tau_1 + A_2\tau_2$.

Table S4. The fluorescence lifetime of all compounds.

Compds	Lifetime in solution (ns)	Lifetime in solid (ns)	Compds	Lifetime in solution (ns)	Lifetime in solid (ns)
BINB-1	τ_1 = 3.55 (5%) τ_2 = 4.83 (95%)	τ_1 = 2.58 (55%) τ_2 = 10.48 (45%)	**BINB-6A**	τ_1 = 2.92 (11%) τ_2 = 5.29 (89%)	τ_1 = 4.85
BINB-2	τ_1 = 3.00 (76%) τ_2 = 2.48 (24%)	τ_1 = 2.3 (64%) τ_2 = 7.36 (36%)	**BINB-6B**	τ_1 = 2.05 (13%) τ_2 = 4.69 (87%)	τ_1 = 6.34
BINB-3	τ_1 = 1.67 (17%) τ_2 = 5.44 (83%)	τ_1 = 2.22 (70%) τ_2 = 6.28 (30%)	**BINB-6C**	τ_1 = 0.89 (98%) τ_2 = 5.15 (2%)	τ_1 = 7.54
BINB-4	τ_1 = 1.45 (29%) τ_2 = 4.46 (71%)	τ_1 = 2.49 (42%) τ_2 = 5.80 (58%)	**BINB-6D**	τ_1 = 0.95 (37%) τ_2 = 5.16 (63%)	τ_1 = 6.15
BINB-5	τ_1 = 5.00	τ_1 = 1.88 (56%) τ_2 = 5.85 (44%)	**BINB-6E**	τ_1 = 1.36 (11%) τ_2 = 4.72 (89%)	τ_1 = 9.06
BINB-6	τ_1 = 1.59 (5%) τ_2 = 5.17 (95%)	τ_1=5.38	**BINUB-1**	τ_1 = 4.77	τ_1 = 7.06
BINB-7	τ_1 = 5.37	τ_1 = 3.98	**BINUB-2**	τ_1 = 6.53	τ_1 = 5.54
BINB-8	τ_1 = 5.08	τ_1 = 2.32 (47%) τ_2 = 5.85 (53%)	**BINUB-3**	τ_1 = 5.32	τ_1 = 4.09

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 $k_{nr} = (1-\Phi_F)/\tau$.

Compds	Solution state		Film state		Compds	Solution state		Film state	
	k_r (s^{-1})	k_{nr} (s^{-1})	k_r (s^{-1})	k_{nr} (s^{-1})		k_r (s^{-1})	k_{nr} (s^{-1})	k_r (s^{-1})	k_{nr} (s^{-1})
BINB-1	1.744×10^7	1.926×10^8	2.806×10^7	1.351×10^8	**BINB-6A**	1.829×10^7	1.805×10^8	2.722×10^7	1.790×10^8
BINB-2	2.118×10^7	3.260×10^8	3.293×10^7	2.075×10^8	**BINB-6B**	1.517×10^7	2.147×10^8	1.877×10^7	1.390×10^8
BINB-3	2.067×10^7	1.881×10^8	3.459×10^7	2.561×10^8	**BINB-6C**	5.051×10^6	1.005×10^9	1.459×10^7	1.180×10^8
BINB-4	2.117×10^7	2.574×10^8	2.834×10^7	1.984×10^8	**BINB-6D**	1.950×10^6	2.766×10^8	7.805×10^6	1.548×10^8
BINB-5	1.980×10^7	1.802×10^8	3.499×10^7	2.405×10^8	**BINB-6E**	6.897×10^5	2.292×10^8	1.876×10^6	1.085×10^8
BINB-6	1.727×10^7	1.835×10^8	2.993×10^7	1.559×10^8	**BINUB-1**	1.614×10^7	1.935×10^8	2.549×10^7	1.161×10^8
BINB-7	1.974×10^7	1.665×10^8	3.291×10^7	2.183×10^8	**BINUB-2**	1.884×10^7	1.343×10^8	2.599×10^7	1.545×10^8
BINB-8	1.988×10^7	1.770×10^8	3.413×10^7	2.045×10^8	**BINUB-3**	1.673×10^7	1.712×10^8	2.812×10^7	2.164×10^8

5.5 Aggregation-induced emission properties of target compounds

Nanoaggregates preparation: 1 mM stock solutions of target compounds in acetonitrile 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%, 10 vol%, 20 vol%, 30 vol%, 40 vol%, 50 vol%, 60 vol%, 70 vol%, 80 vol%, 90 vol%, 95 vol%, 99 vol%). After that, the PL measurements of the resulting solutions were performed immediately.

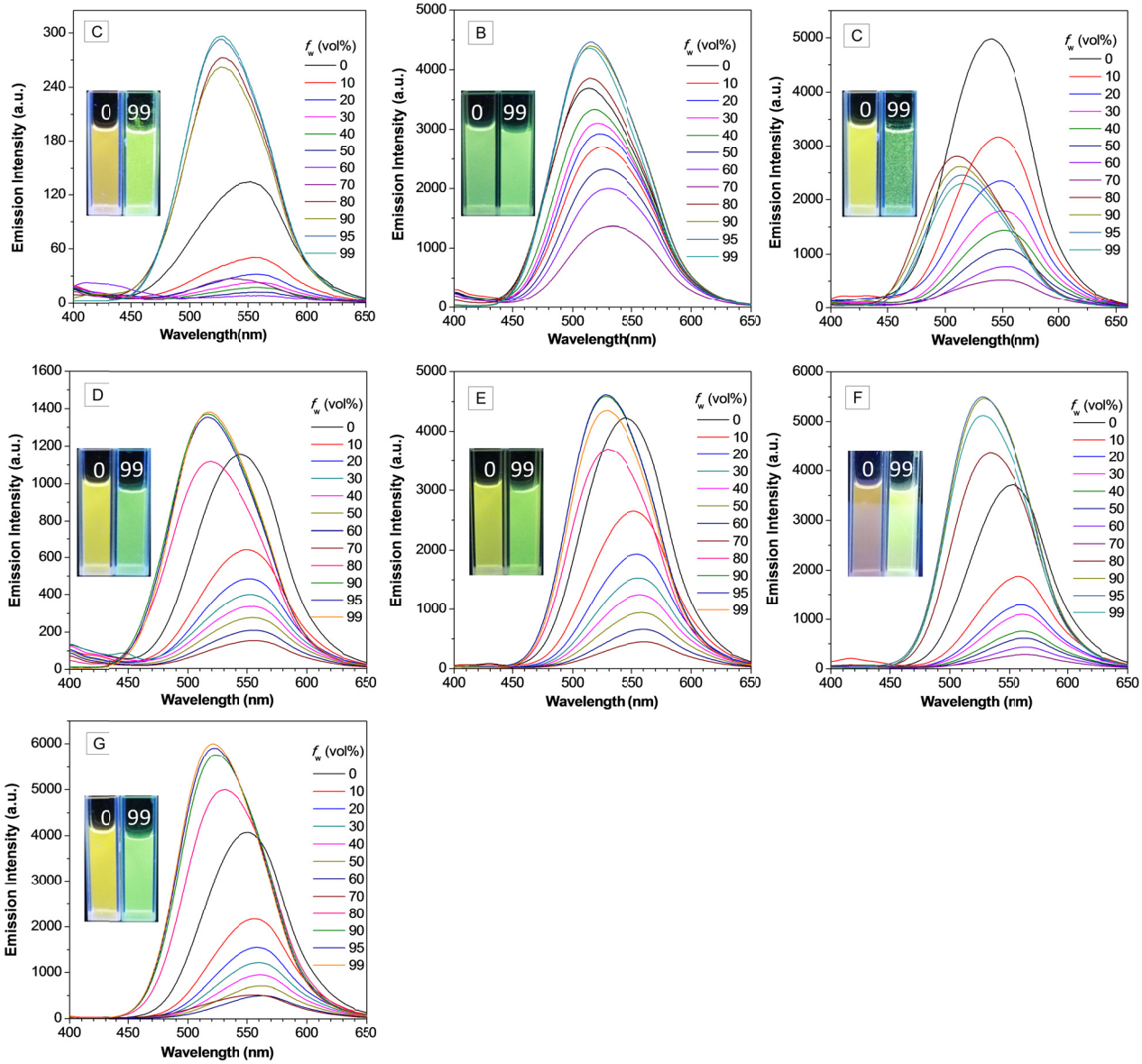


Fig. S5 Emission spectra of (A) **BINB-1**, (B) **BINB-2**, (C) **BINB-3**, (D) **BINB-4**, (E) **BINB-5**, (F) **BINB-7**, (G) **BINB-8** (10 μM) in acetonitrile and acetonitrile/water mixtures with different f_w. Inset: photograph of corresponding fluorogens in acetonitrile/water mixtures with f_w values of 0 and 99% under 365 nm UV irradiation.

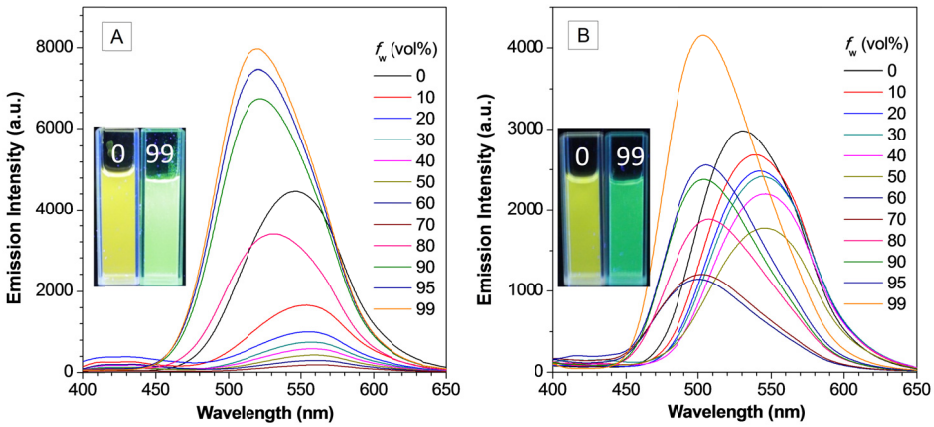


Fig. S6 Emission spectra of (A) **BINUB-1**, (B) **BINUB-2** (10 μM) in acetonitrile and acetonitrile/water mixtures with different f_w. Inset: photograph of corresponding fluorogens in acetonitrile/water mixtures with f_w values of 0 and 99% under 365 nm UV irradiation.

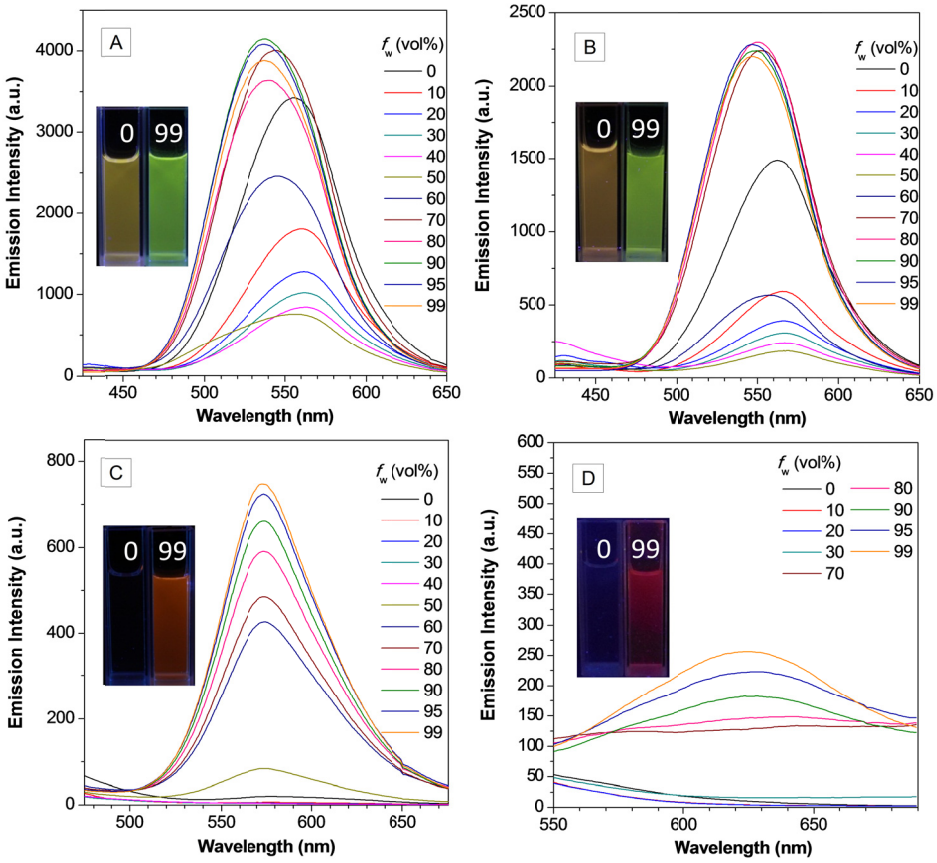


Fig. S7 Emission spectra of (A) **BINB-6A**, (B) **BINB-6B**, (C) **BINB-6D**, (**D**) **BINB-6E** (10 μM) in acetonitrile and acetonitrile/water mixtures with different f_w. Inset: photograph of corresponding fluorogens in acetonitrile/water mixtures with f_w values of 0 and 99% under 365 nm UV irradiation.

5.6 Dynamic light scattering (DLS) of target compounds

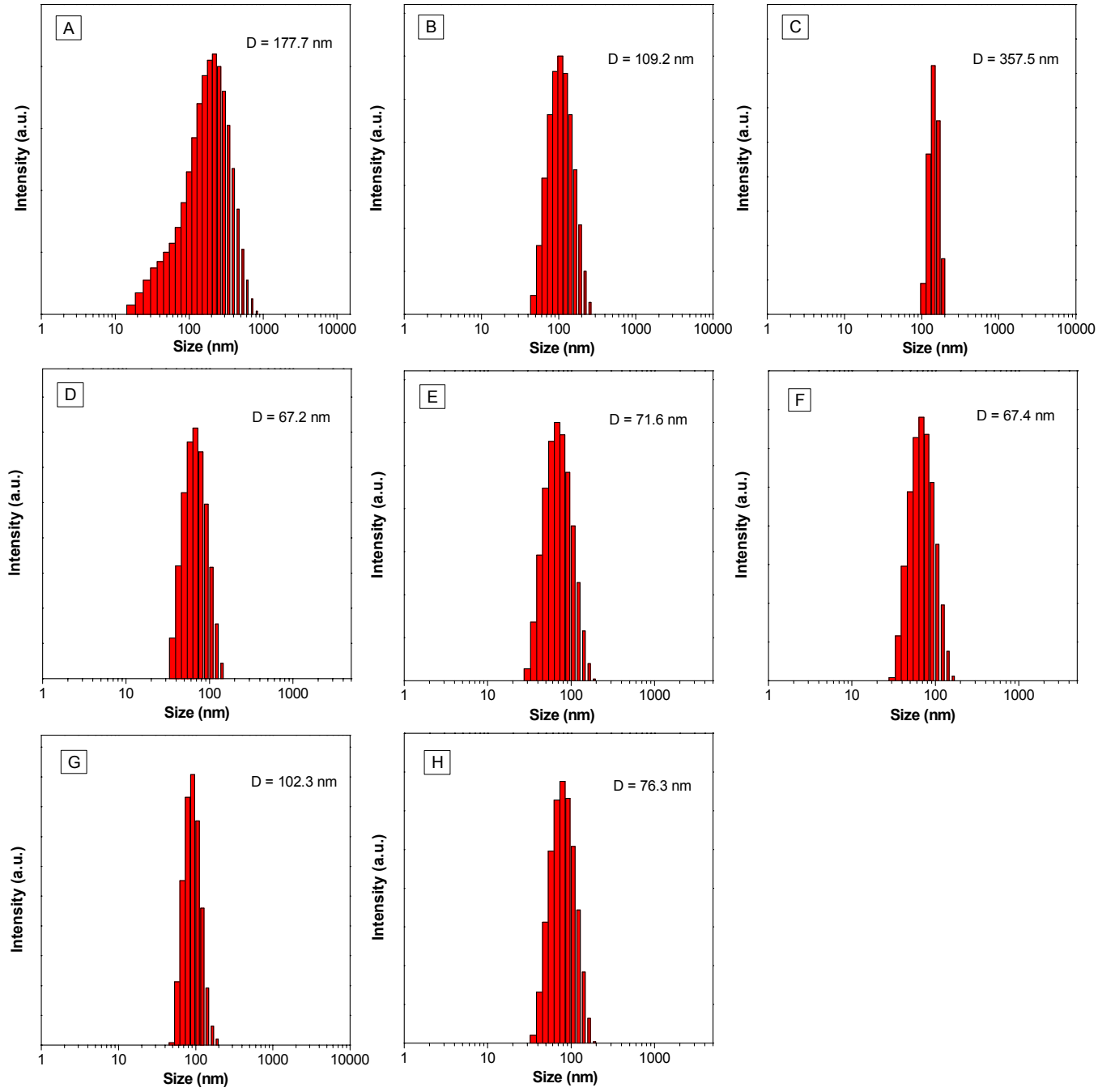


Fig. S8 Particle size distribution of (A) **BINB-1**, (B) **BINB-2**, (C) **BINB-3**, (D) **BINB-4**, (E) **BINB-5**, (F) **BINB-6**, (G) **BINB-7**, (H) **BINB-8** (10 μM) in acetonitrile/water (1:99, v/v).

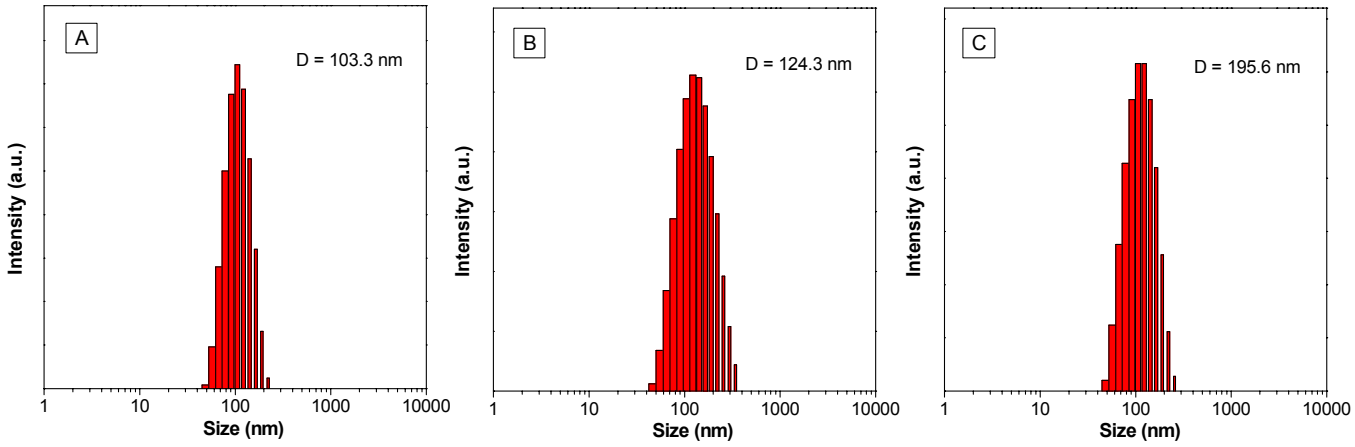


Fig. S9 Particle size distribution of (A) **BINUB-1**, (B) **BINUB-2**, (C) **BINUB-3** (10 μM) in acetonitrile/water (1:99, v/v).

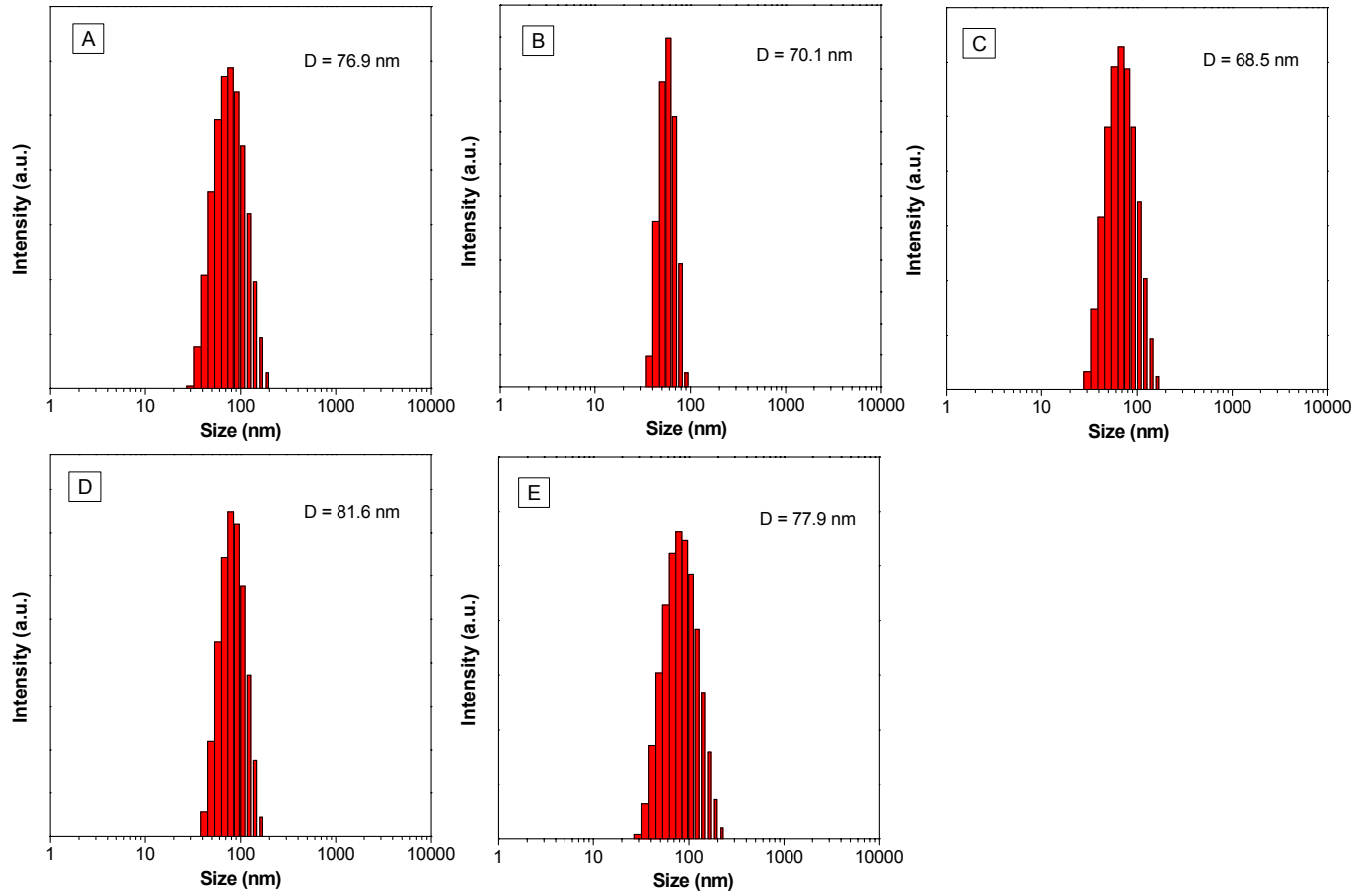


Fig. S10 Particle size distribution of (A) **BINB-6A**, (B) **BINB-6B**, (C) **BINB-6C**, (D) **BINB-6D**, (E) **BINB-6E** (10 μM) in acetonitrile/water (1:99, v/v).

5.7 Circular dichroism (CD) spectra of target compounds

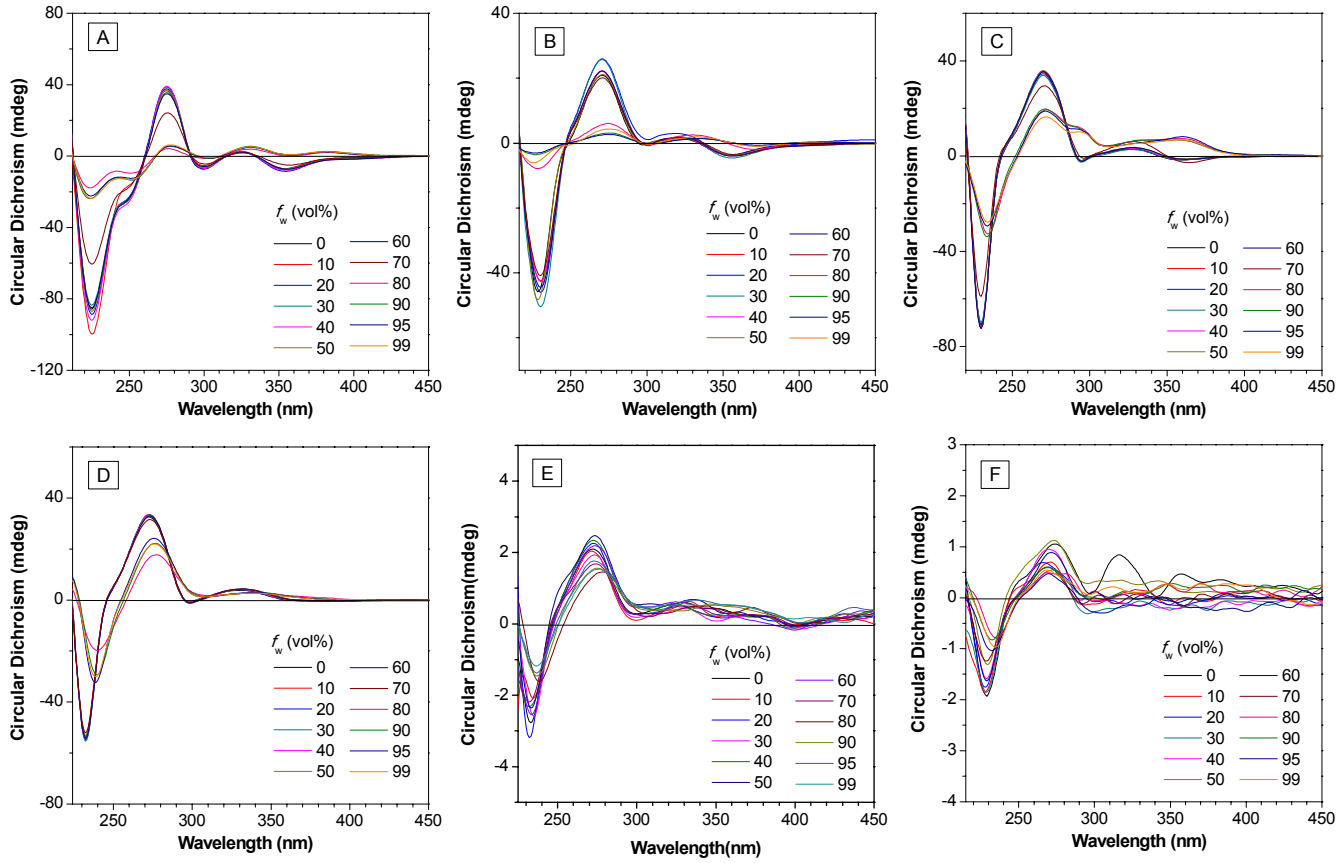


Fig. S11 CD spectra of (A) **BINB-1**, (B) **BINB-3**, (C) **BINB-4**, (D) **BINB-5**, (E) **BINB-7**, (F) **BINB-8** (10 μM) in acetonitrile/water mixtures with different f_w.

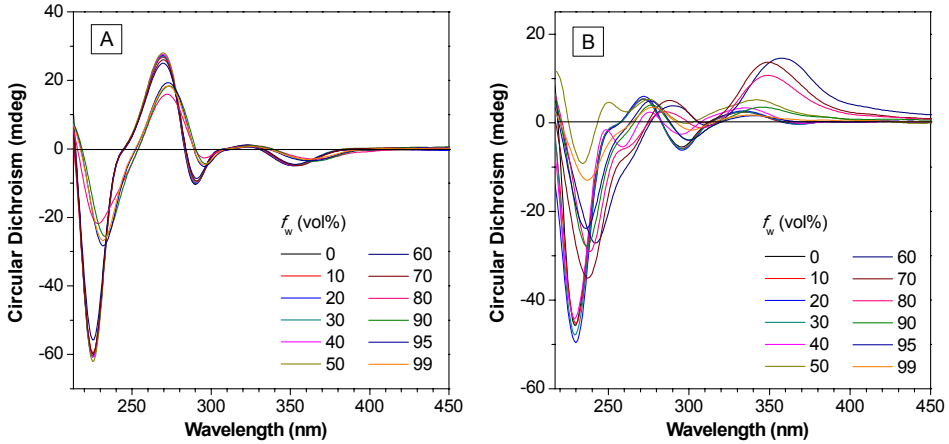


Fig. S12 CD spectra of (A) **BINUB-1**, (B) **BINUB-3** (10 μM) in acetonitrile/water mixtures with different f_w.

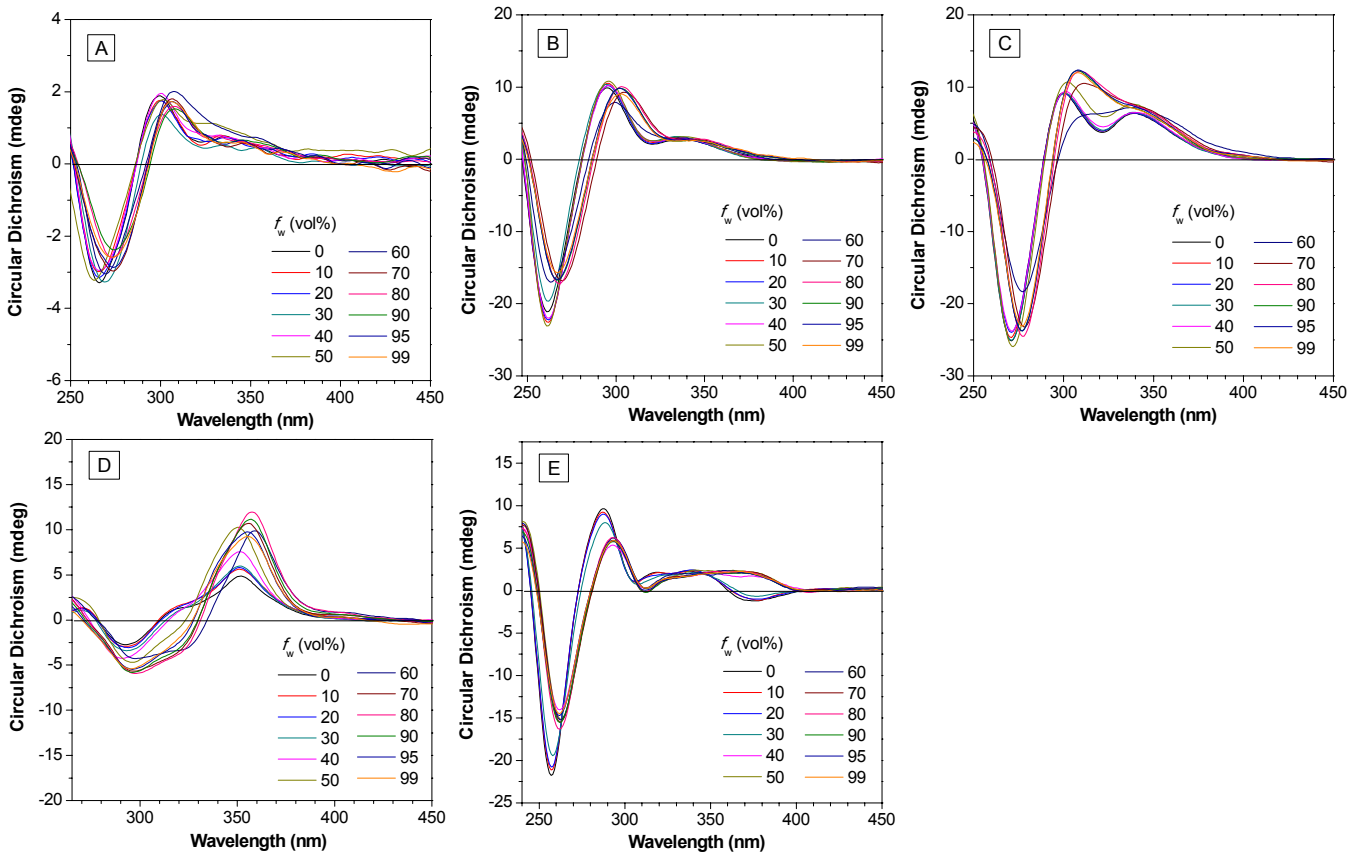
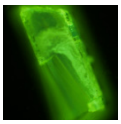
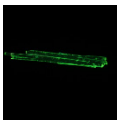


Fig. S13 CD spectra of (A) **BINB-6A**, (B) **BINB-6B**, (C) **BINB-6C**, (D) **BINB-6D**, (E) **BINB-6E** (10 μM) in acetonitrile/water mixtures with different f_w.

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

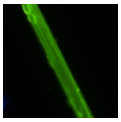
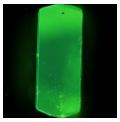
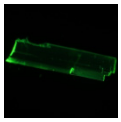
6.1 single crystal data summary

Table S6. Crystallographic data.

Crystal	BINB-1	BINB-2	BINB-4	BINB-5
formula	$C_{29}H_{14}N_4O_2$	$C_{30}H_{16}N_4O_2$	$C_{32}H_{20}N_4O_2$	$C_{33}H_{22}N_4O_2$
crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
space group	P 2 (1)	C 2	P 2 (1)	C 222 (1)
a [Å]	5.0052 (2)	25.4902 (8)	7.9714 (4)	12.0721 (6)
b[Å]	15.6076 (4)	8.4676 (3)	22.5703 (8)	17.9566 (12)
c[Å]	14.6006 (4)	16.9657 (5)	9.1047 (4)	12.2305 (6)
β [deg]	91.275 (3)	104.889 (2)	115.426 (7)	90.00
V [Å^3]	1140.30 (6)	3538.9 (2)	1479.42 (11)	2651.3 (3)
Z	2	6	2	4
μ [mm^{-1}]	0.687	0.679	2.266	0.646
T [K]	293	293	293	293
θ_{min}-θ_{max} [deg]	5.6610-71.6150	3.5770-71.7750	5.3690-71.5160	4.3920-71.5610
R	0.0332	0.0315	0.0561	0.0396
wR_2	0.0919	0.0887	0.1700	0.1069
GOOF	1.030	1.038	1.061	1.054
crystal pictures[a]				
CCDC number	1823469	1823470	1823471	1823472
	Compounds chart	Compounds chart	Compounds chart	Compounds chart
	Data	Data	Data	Data
	NMR	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.

Crystal	BINB-6A	BINB-7	BINB-8
formula	$C_{48}H_{30}F_6N_4O_2$	$C_{35}H_{26}N_4O_2$	$C_{36}H_{28}N_4O_2$
crystal system	orthorhombic	monoclinic	triclinic
space group	C222 (1)	P 21/c	P 1
a [Å]	18.4373 (19)	8.5584 (3)	8.8302 (3)
b[Å]	25.7446 (19)	18.7684 (5)	18.7601 (8)
c[Å]	11.6266 (7)	17.4034 (4)	19.0270 (7)
β [deg]	90.00	94.951 (3)	94.387 (3)
V [Å^3]	5518.7 (8)	2785.04 (13)	2926.02 (19)
Z	4	12	4
μ [mm^{-1}]	0.625	0.641	0.623
T [K]	153	293	293
θ_{min}-θ_{max} [deg]	2.95-62.11	0.809-0.825	4.1350-69.2690
R	0.0854	0.0467	0.0585
wR_2	0.2375	0.1369	0.1822
GOOF	1.103	1.033	1.070
crystal pictures[a]			
CCDC number	1823473	1856064	1823474
	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.

6.2 X-ray single crystallographic packing of the corresponding compounds

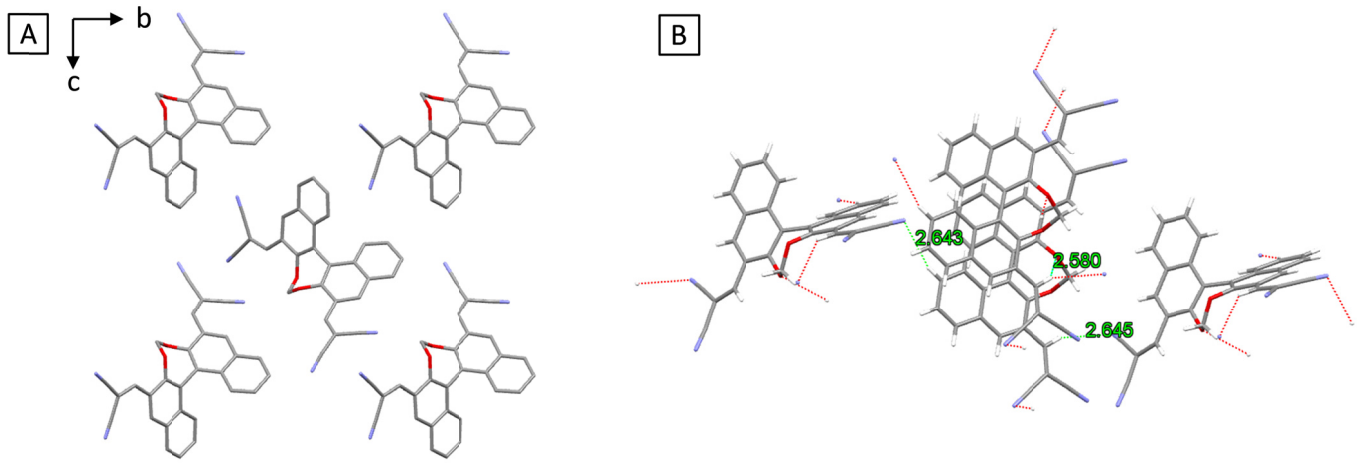


Fig. S14 Crystal packing mode (A) as well as short contacts (B) of **BINB-1**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

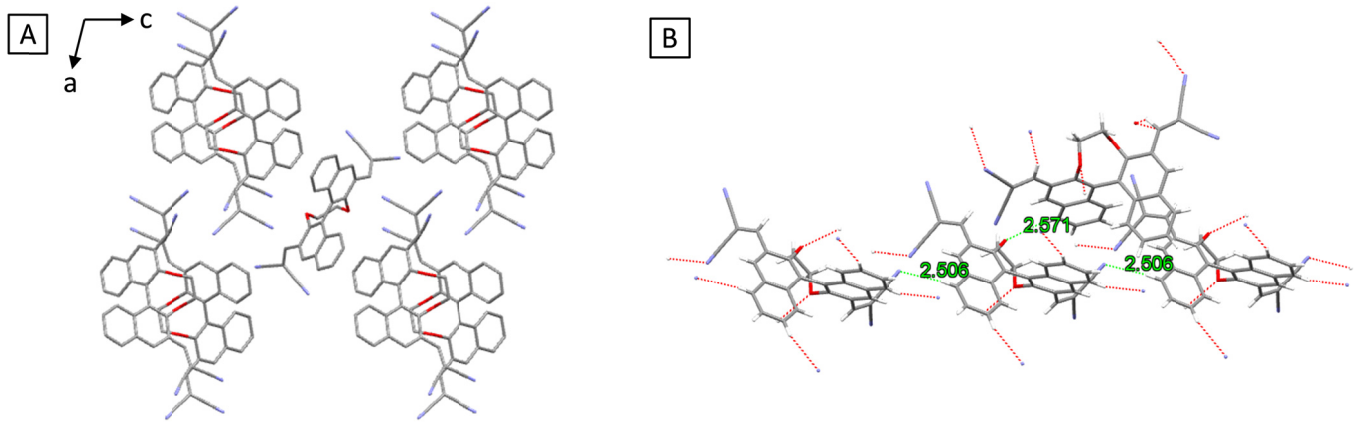


Fig. S15 Crystal packing mode (A) as well as short contacts (B) of **BINB-2**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

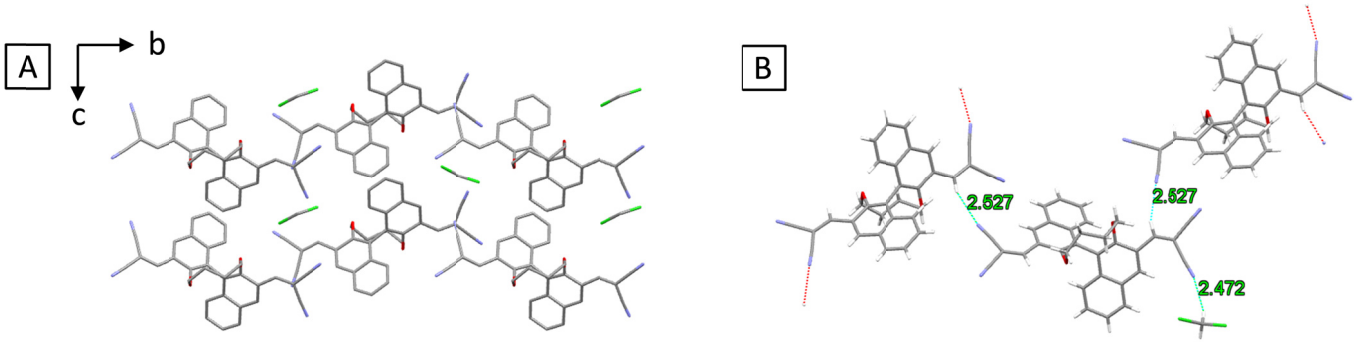


Fig. S16 Crystal packing mode (A) as well as short contacts (B) of **BINB-4**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

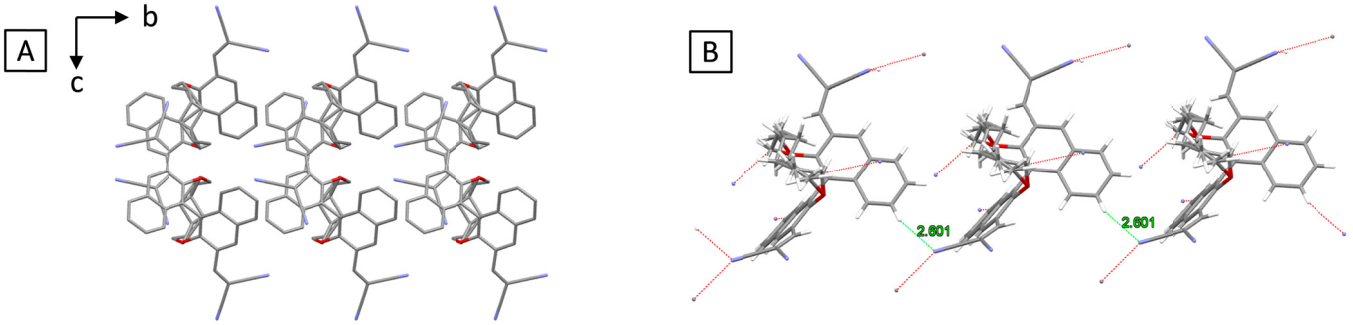


Fig. S17 Crystal packing mode (A) as well as short contacts (B) of **BINB-5**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

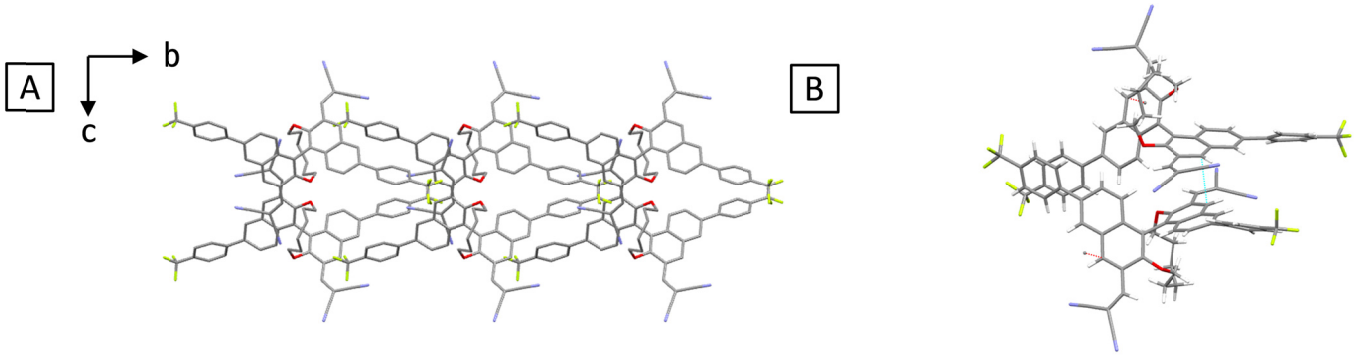


Fig. S18 Crystal packing mode (A) as well as short contacts (B) of **BINB-6A**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

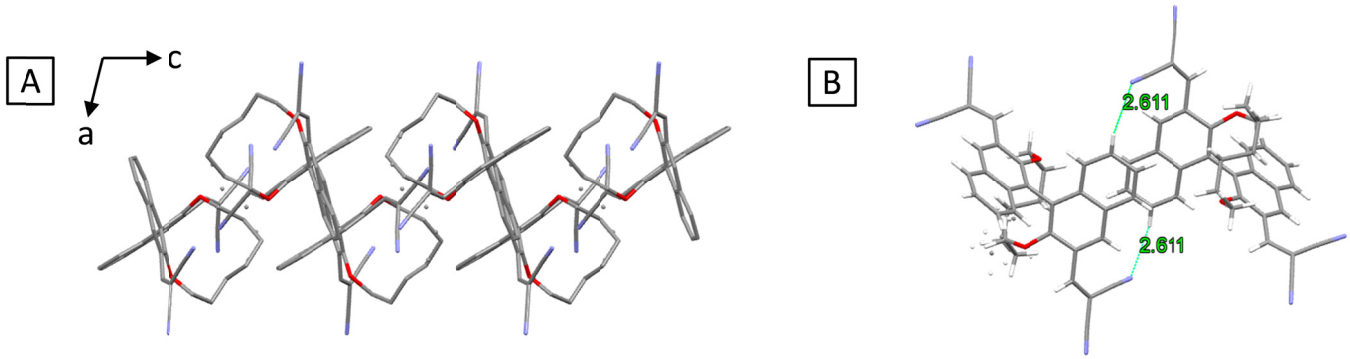


Fig. S19 Crystal packing mode (A) as well as short contacts (B) of **BINB-7**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

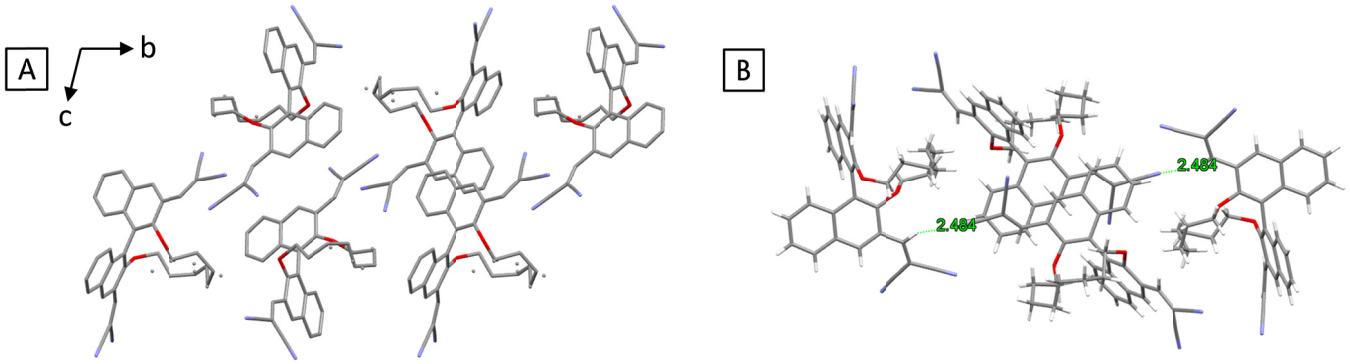


Fig. S20 Crystal packing mode (A) as well as short contacts (B) of **BINB-8**. Carbon, hydrogen, and nitrogen atoms are shown in gray, white, and blue, respectively.

7. Molecular dynamics simulations.

To obtain the torsion angles distribution, we performed molecular dynamics (MD) simulations for **BINB-2** and **BINB-6** by using GROMACS software package (version 5.1).[1] We first performed the geometry optimization and then carried out the electrostatic potential for each molecule by ωb97xd/6-31G** method using Gaussian 09 package.[2] The partial charges of the atoms reproducing the electrostatic potential were obtained by using restrained electrostatic potential (RESP) fit method.[3,4] The atom types and parameters of the two molecules were built from the general amber force field (GAFF).[5] We set up model by placing each molecule into the center of a cubic box and then solvated by the pre-equilibrated TIP3P water molecules.[6] For **BINB-2** and **BINB-6**, the length of box was both 4 nm, containing 2145 and 2204 water molecules respectively.

For each molecule, we first performed the energy minimization by using steepest descent algorithm. And then we performed the 500 ps MD simulations under the NVT (P = 1 bar, T = 300 K) ensemble. The temperature was controlled by the velocity rescaling thermostat.[7] Then we performed the 50 ns MD simulations under the NPT (P = 1 bar, T = 300 K) ensemble coupled by Parrinello-Rahman barostat.[8] The Newton's classical equations of motion were integrated at a time step of 2 fs using the classical leapfrog algorithm. For each molecule, we ran two independent 50 ns MD trajectories and we chose conformations in the last 40 ns for torsion angles analysis. The torsion angles of **BINB-2** and **BINB-6** were distributed around 71 degree and 111 degree respectively.

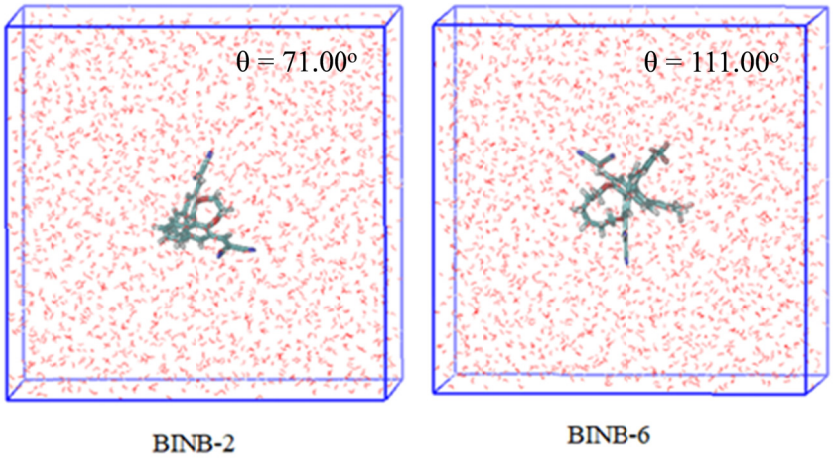


Fig. S21 The snapshots of the final equilibrated BINB-2 and BINB-6 in aqueous solution and their torsion angles distribution.

References

(1) M. J. Abraham, D. van der Spoel, E. Lindahl, B. Hess and the GROMACS development team, GROMACS User Manual version 5.1, 2015.

(2) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, et al. Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford, CT, 2009.

(3) C. I. Bayly, P. Cieplak, W. Cornell and P. A. Kollman, *J. Phys. Chem*., 1993, **97**, 10269–10280.

(4) W. D. Cornell, P. Cieplak, C. I. Bayly and P. A. Kollman, *J. Am. Chem. Soc*., 1993, **115**, 9620–9631.

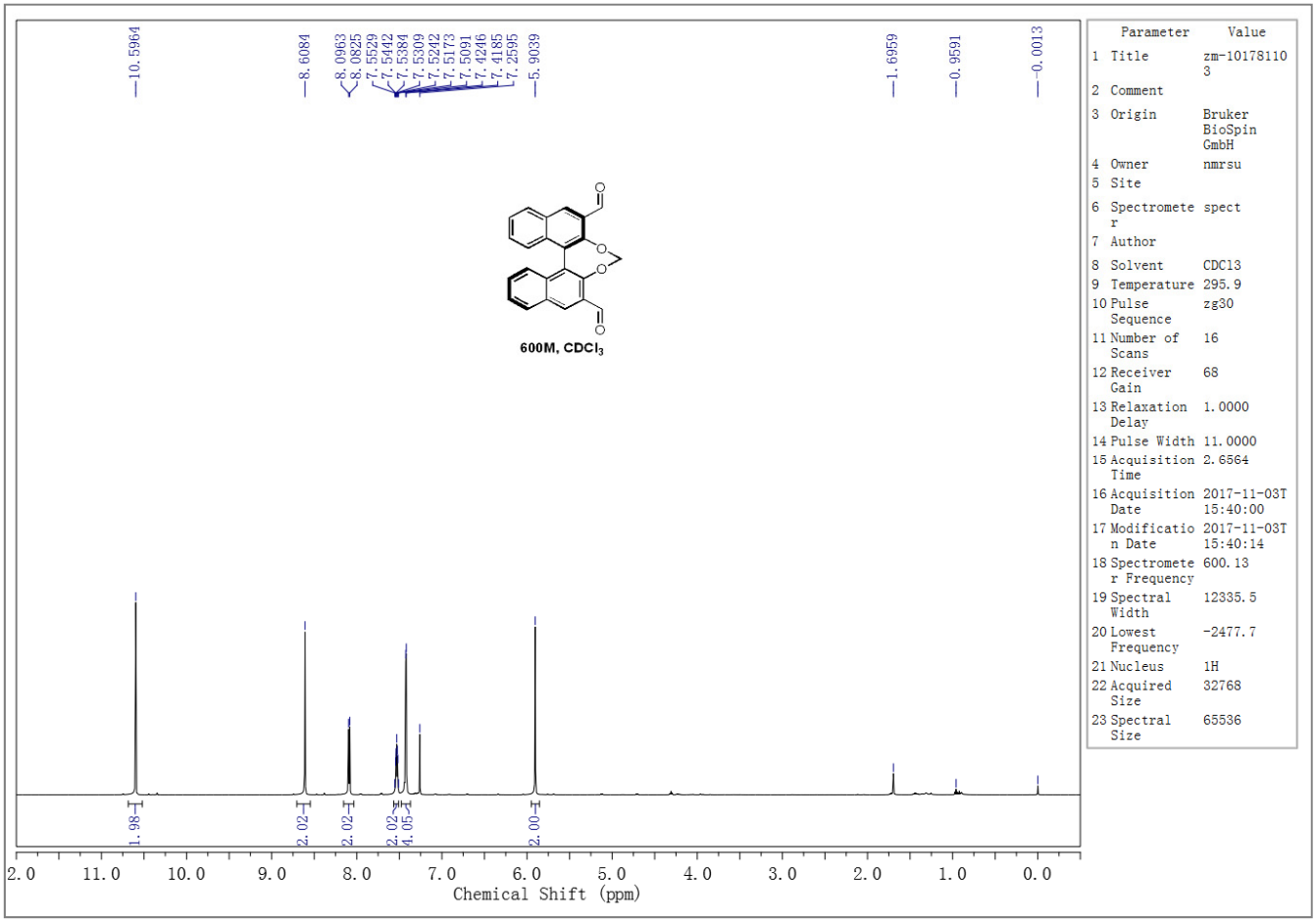
(5) J. Wang, R. M. Wolf, J. W. Caldwell, P. A. Kollman and D. A. J. Case, *Comput. Chem*., 2004, **25**, 1157–1174.

(6) W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey and M. L. J. Klein, *Chem. Phys*., 1983, **79**, 926–935.

(7) G. Bussi, D. Donadio and M. Parrinello, *J. Chem. Phys*., 2007, **126**, 014101.

(8) M. Parrinello and A. Rahman, *J. Appl. Phys*., 1981, **52**, 7182–7190.

8. NMR Spectra



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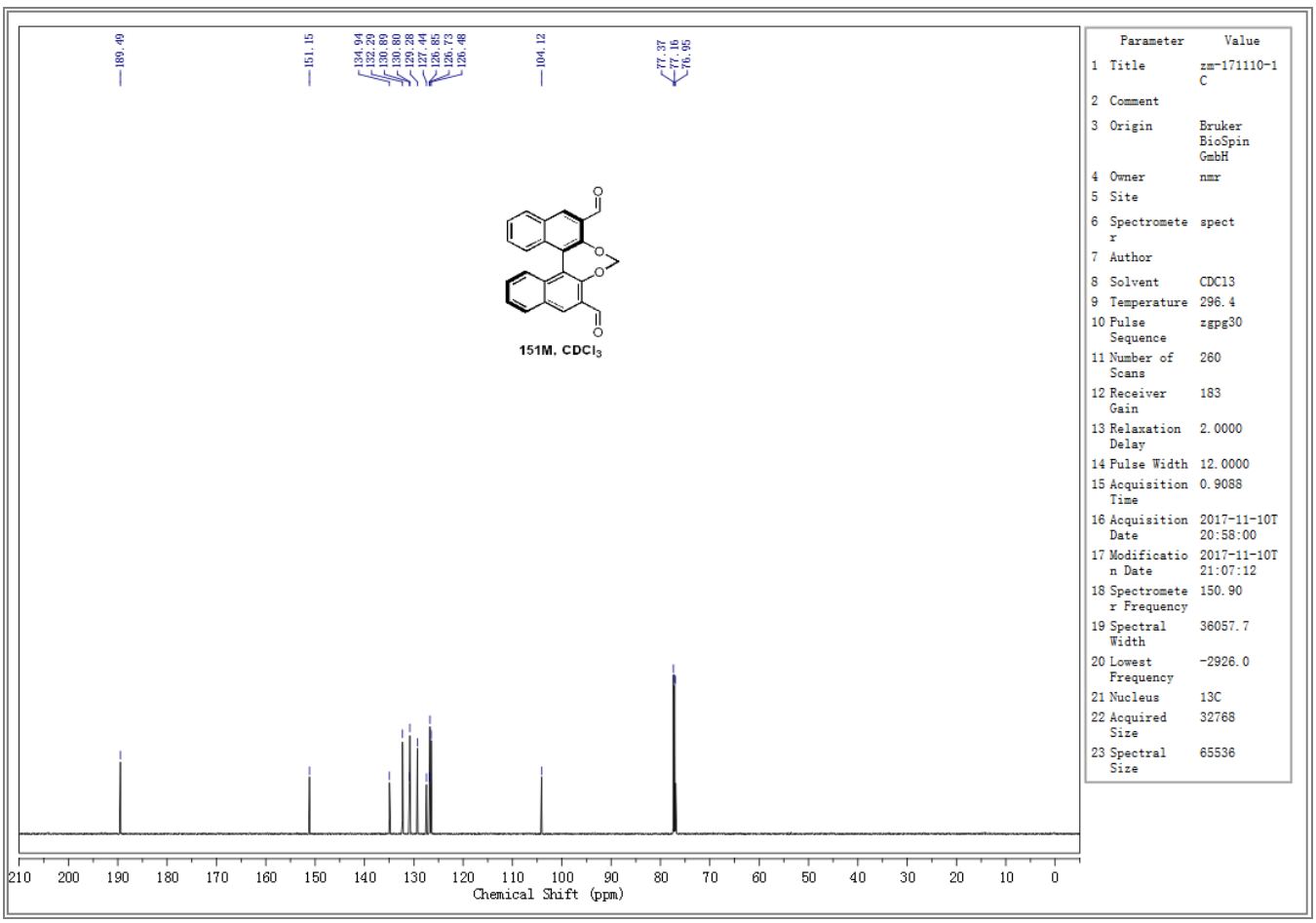
20	Lowest Frequency	-2477.7
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536



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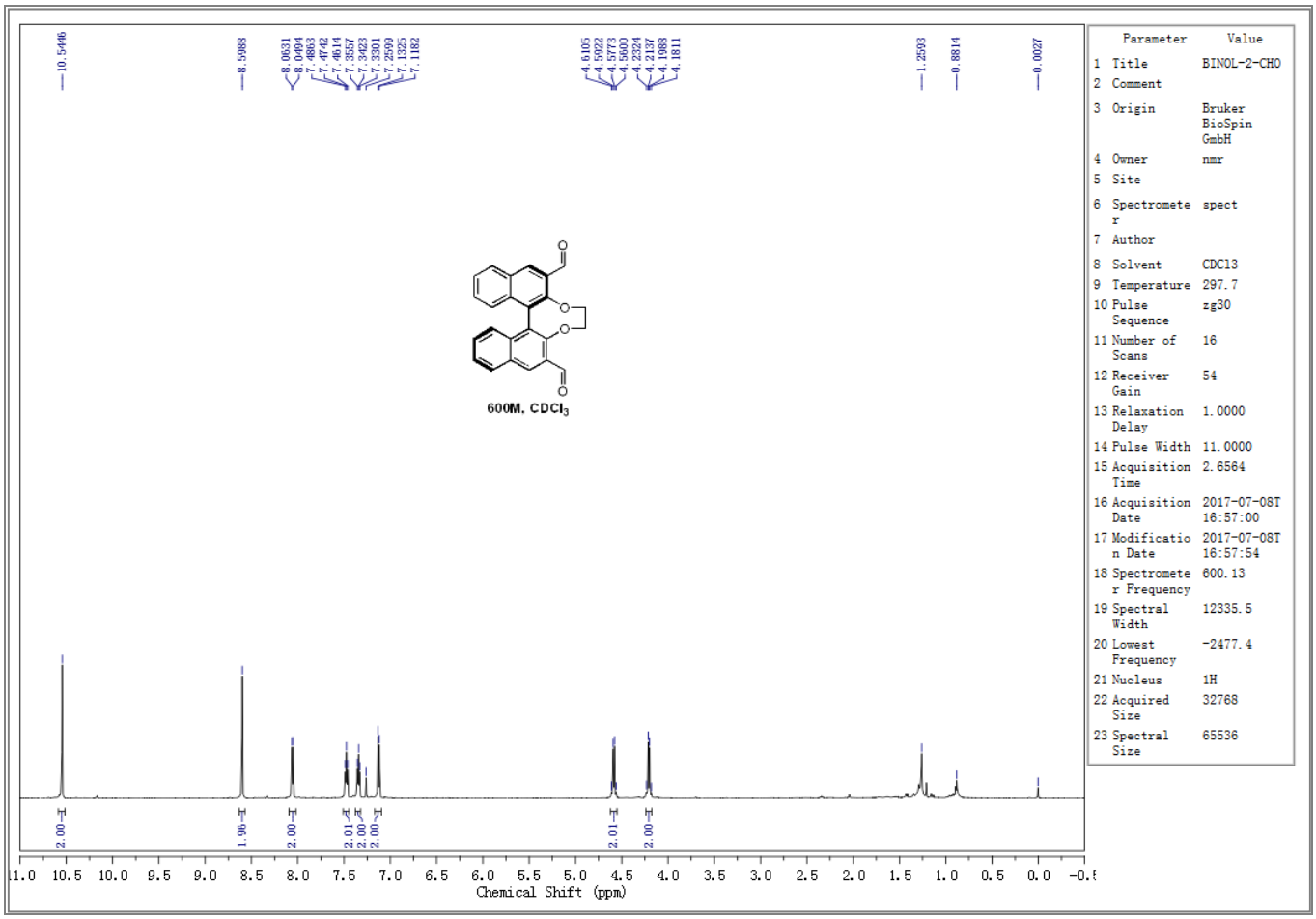

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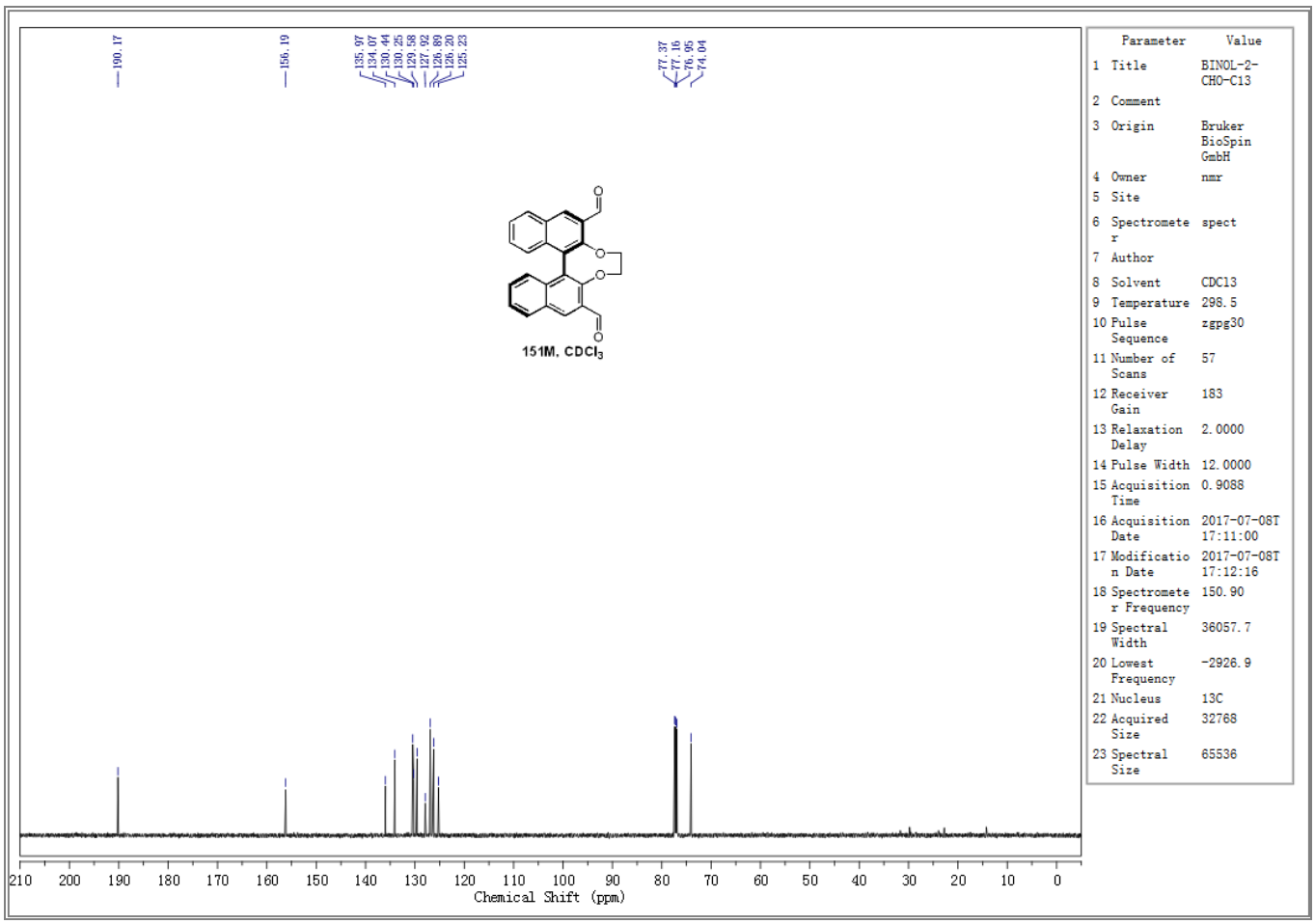

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22	Acquired Size	32768
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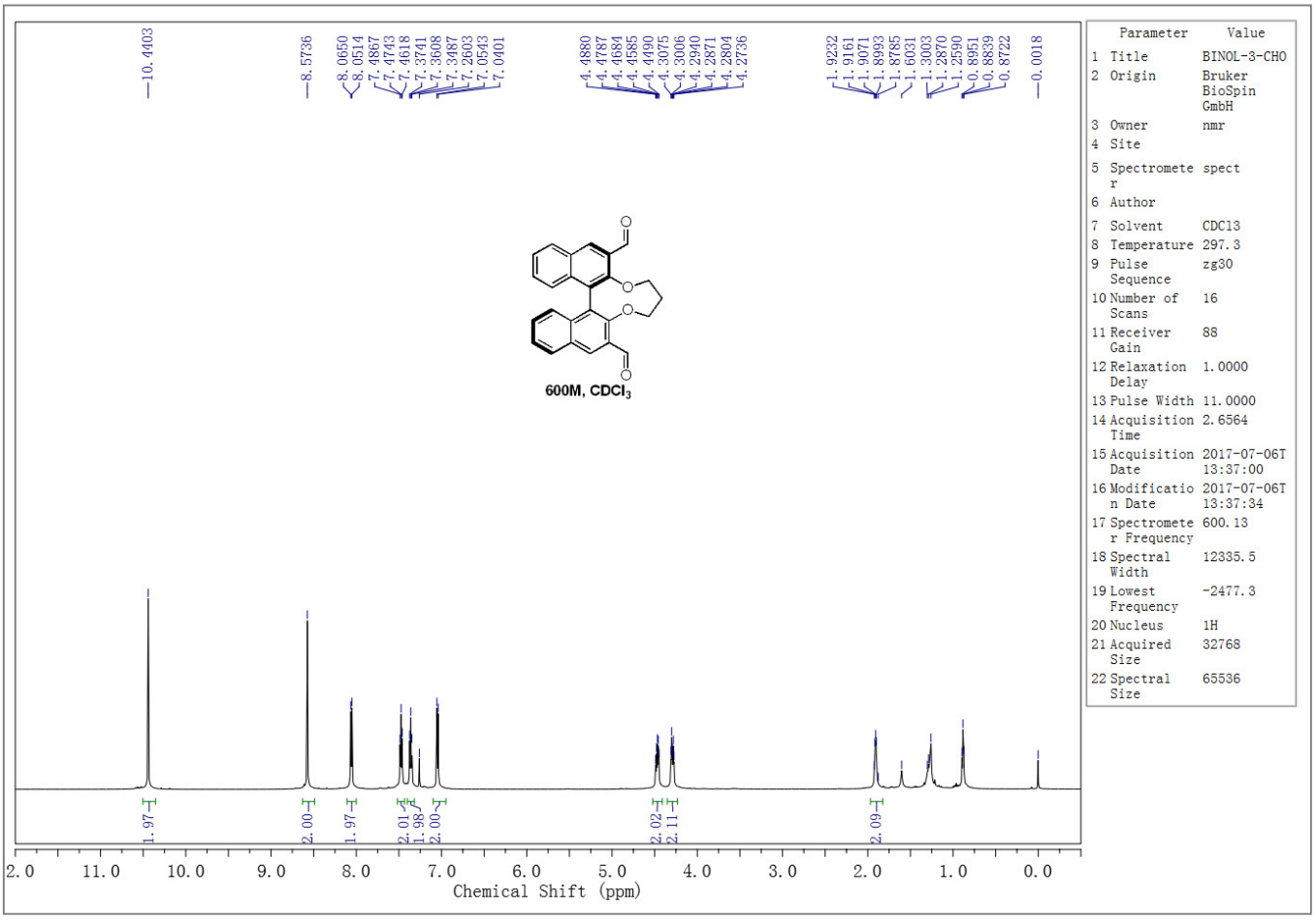

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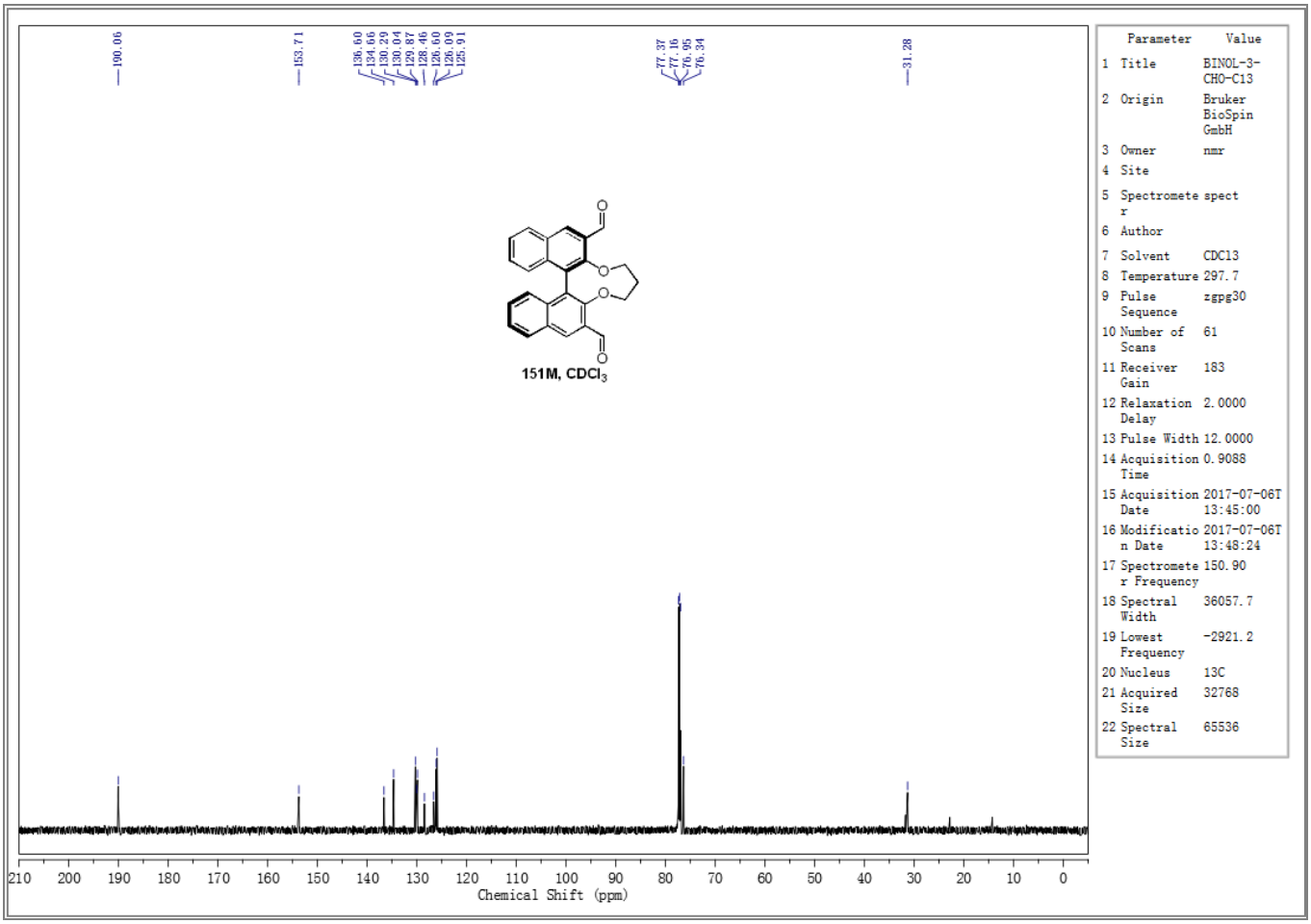
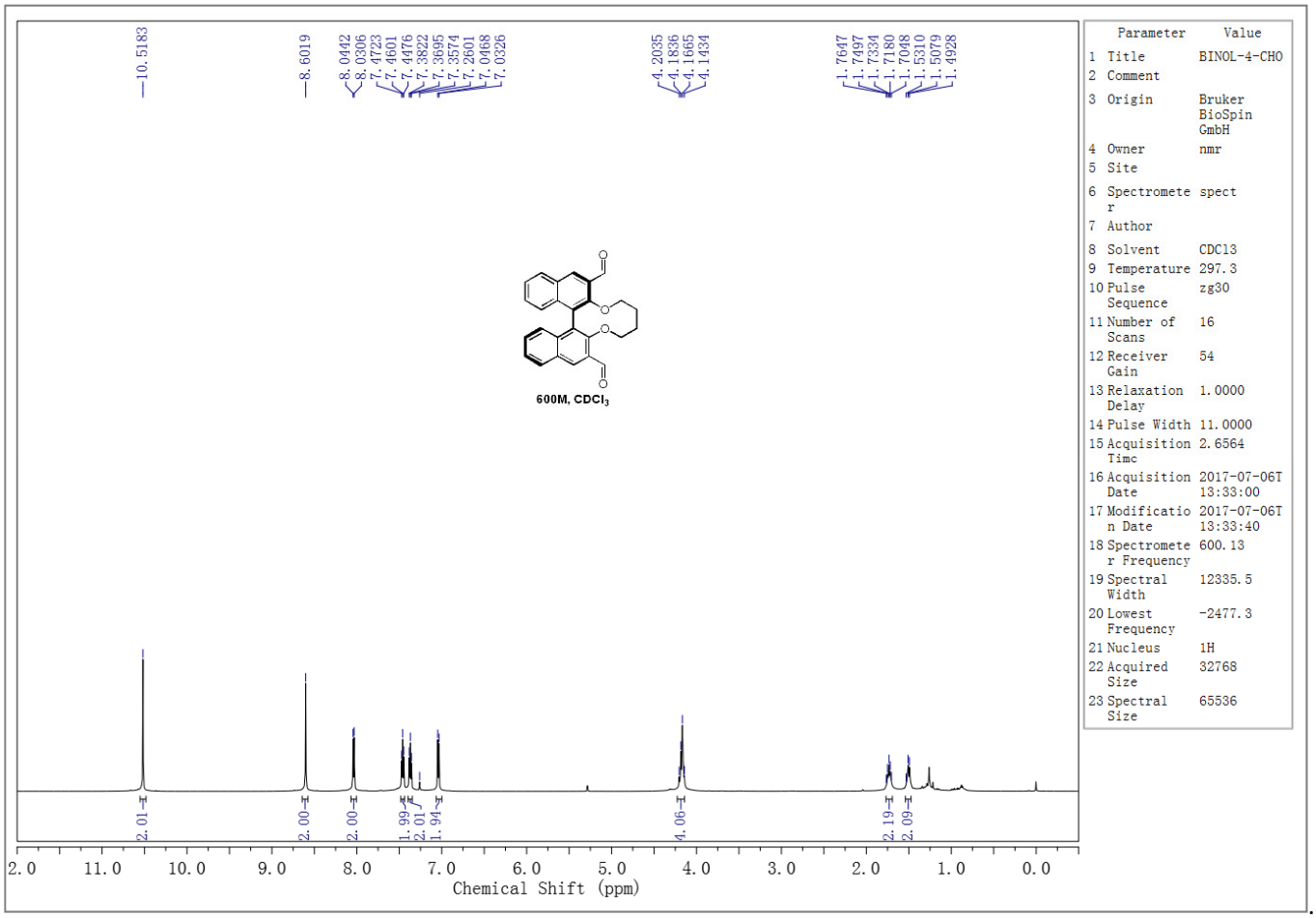
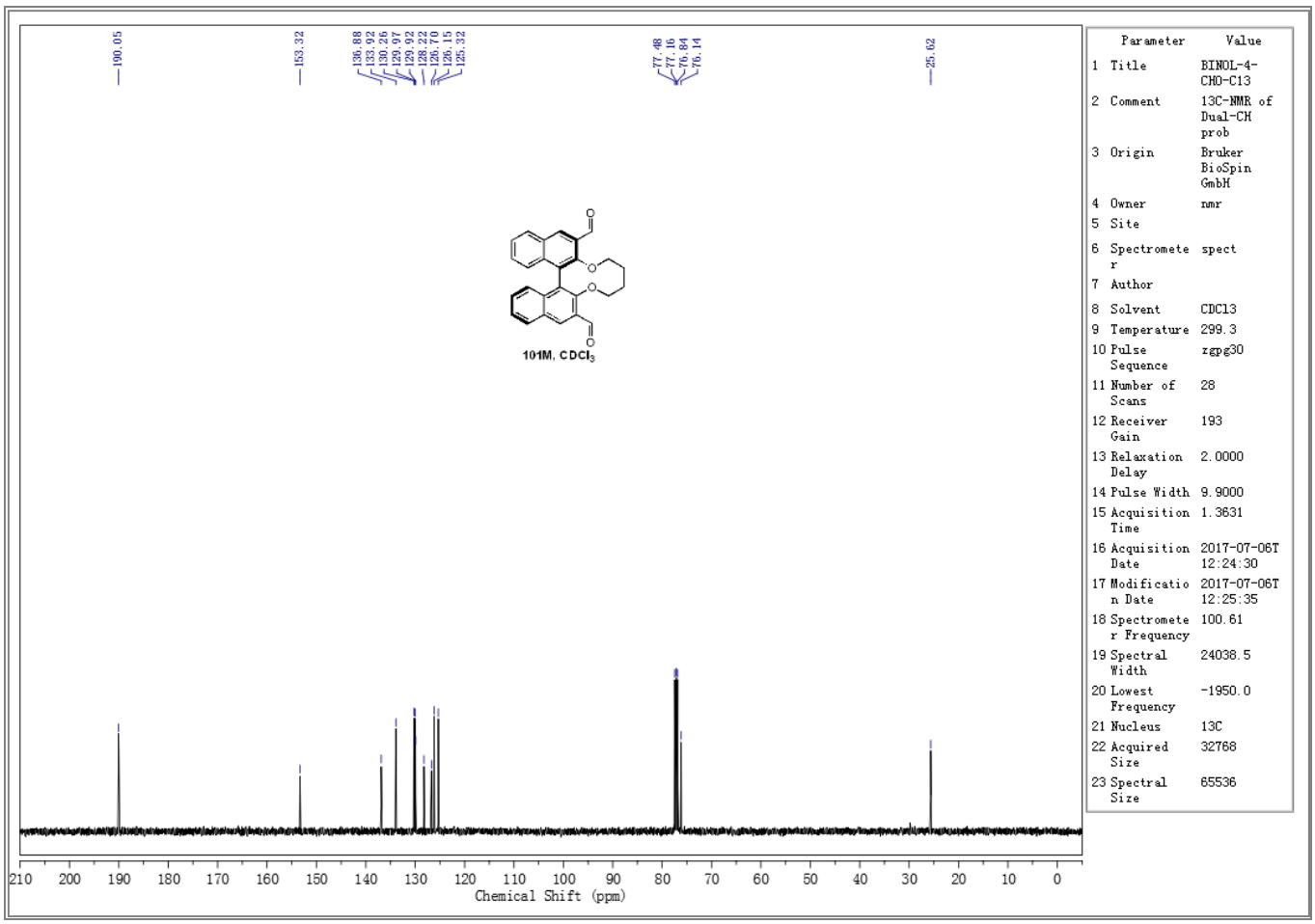
6	Author	
7	Solvent	CDCl3
8	Temperature	297.3
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	88
12	Relaxation Delay	1.0000
13	Pulse Width	11.0000
14	Acquisition Time	2.6564
15	Acquisition Date	2017-07-06T 13:37:00
16	Modification Date	2017-07-06T 13:37:34
17	Spectrometer Frequency	600.13
18	Spectral Width	12335.5
19	Lowest Frequency	-2477.3
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



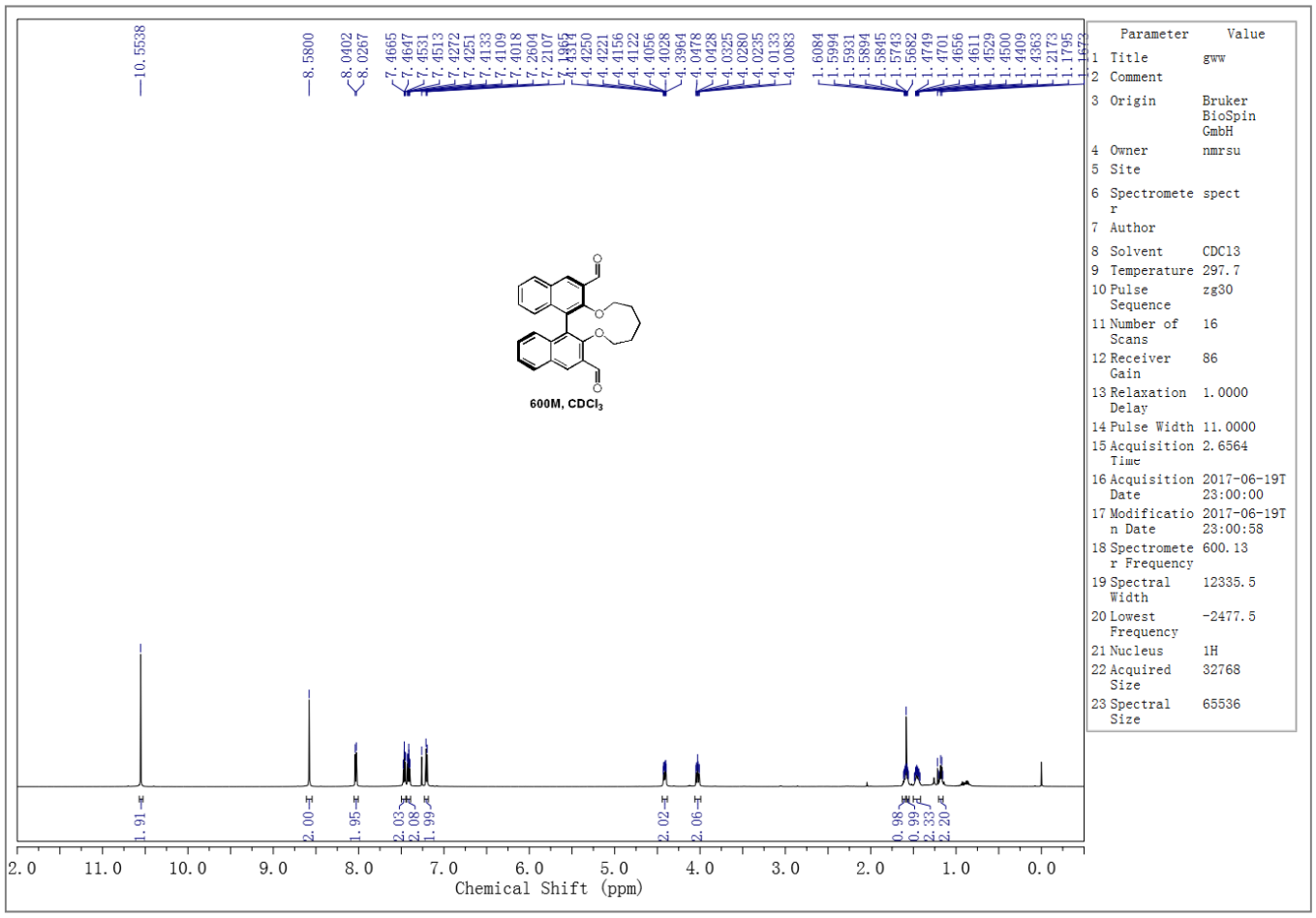
	Parameter	Value
1	Title	BINOL-3-CHO-C13
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect r
6	Author	
7	Solvent	CDCl3
8	Temperature	297.7
9	Pulse Sequence	zgpg30
10	Number of Scans	61
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2017-07-06T 13:45:00
16	Modification Date	2017-07-06T 13:48:24
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2921.2
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

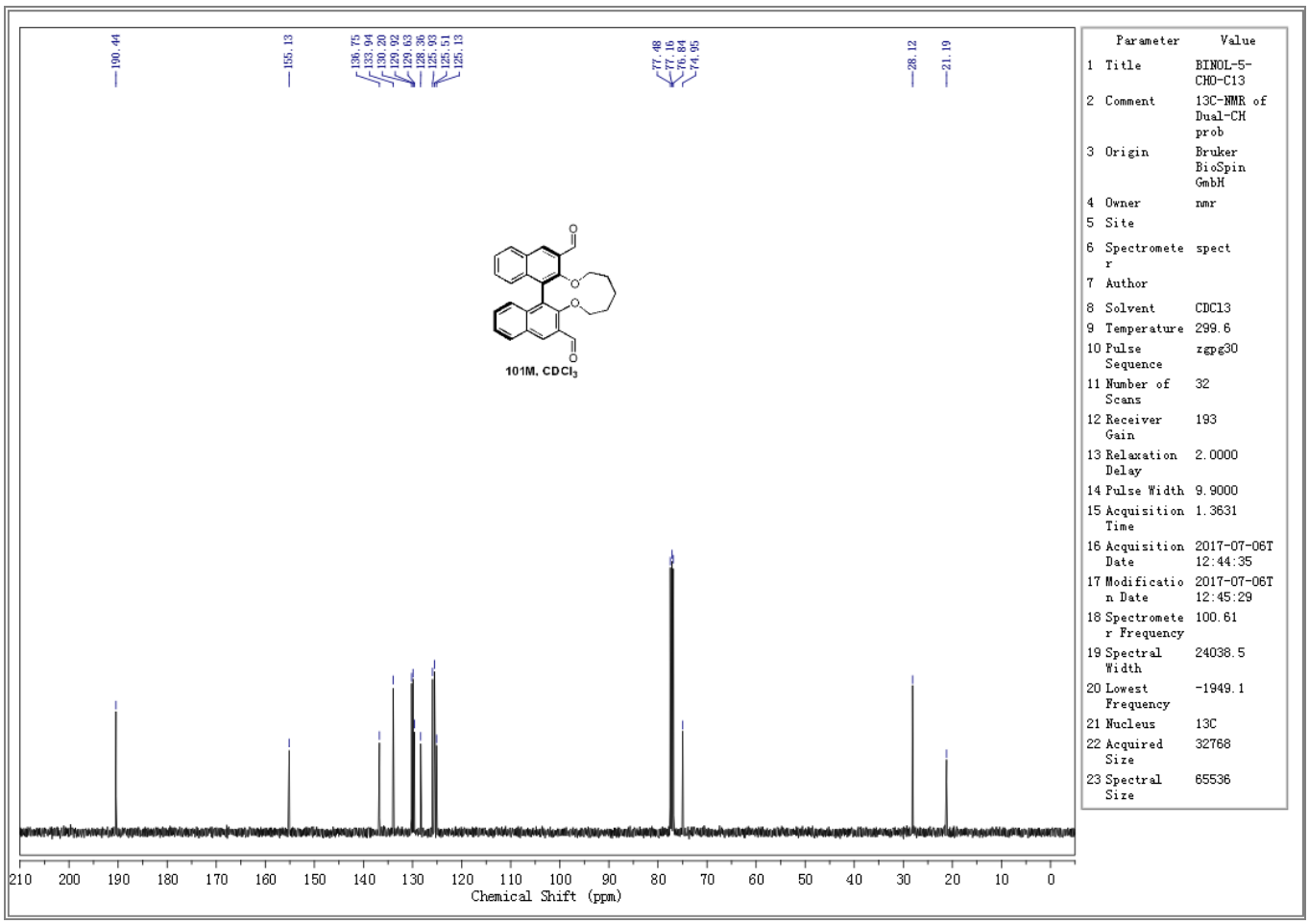


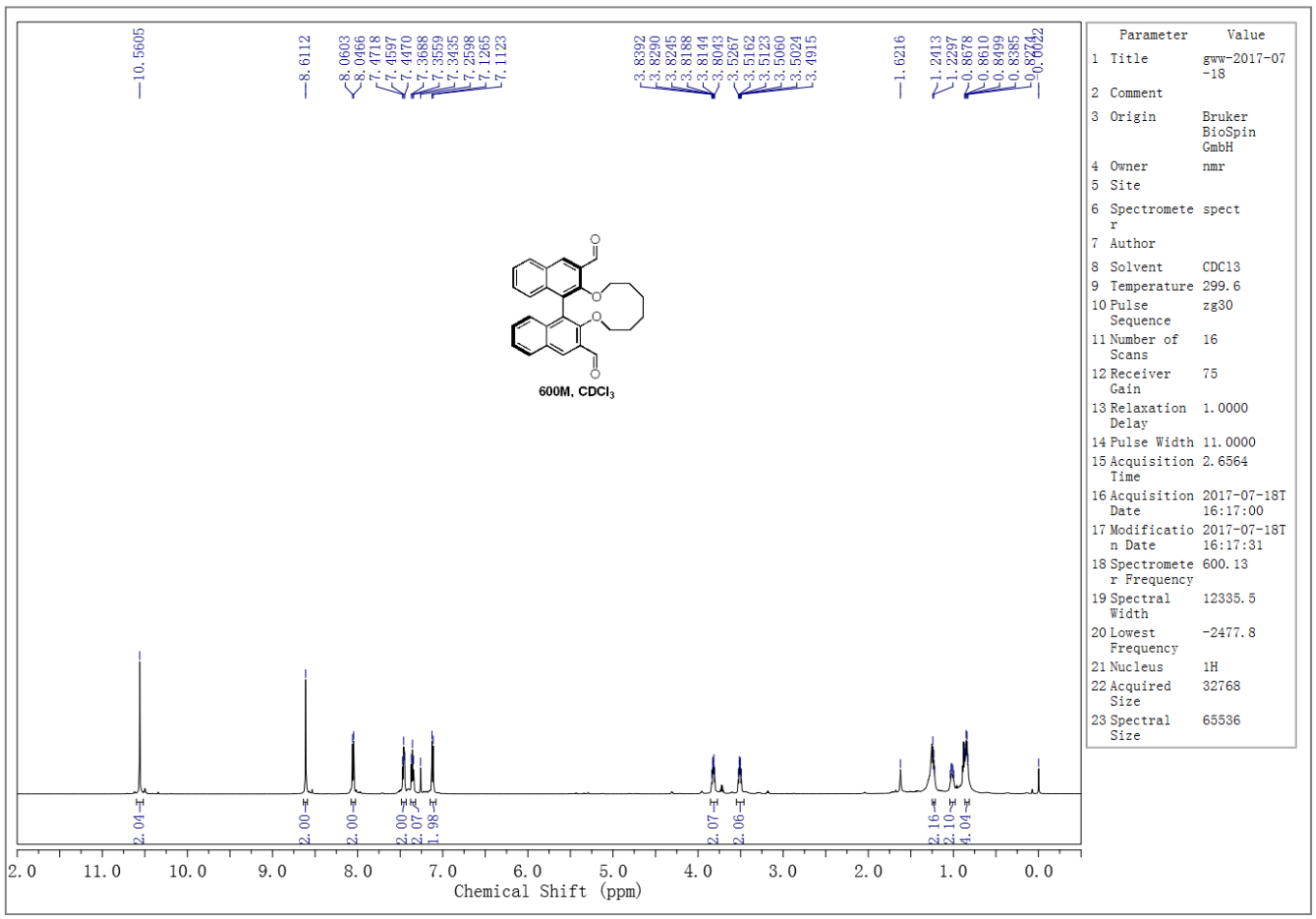
	Parameter	Value
1	Title	BINOL-4-CHO
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	297.3
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	54
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-06T 13:33:00
17	Modification Date	2017-07-06T 13:33:40
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.3
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536



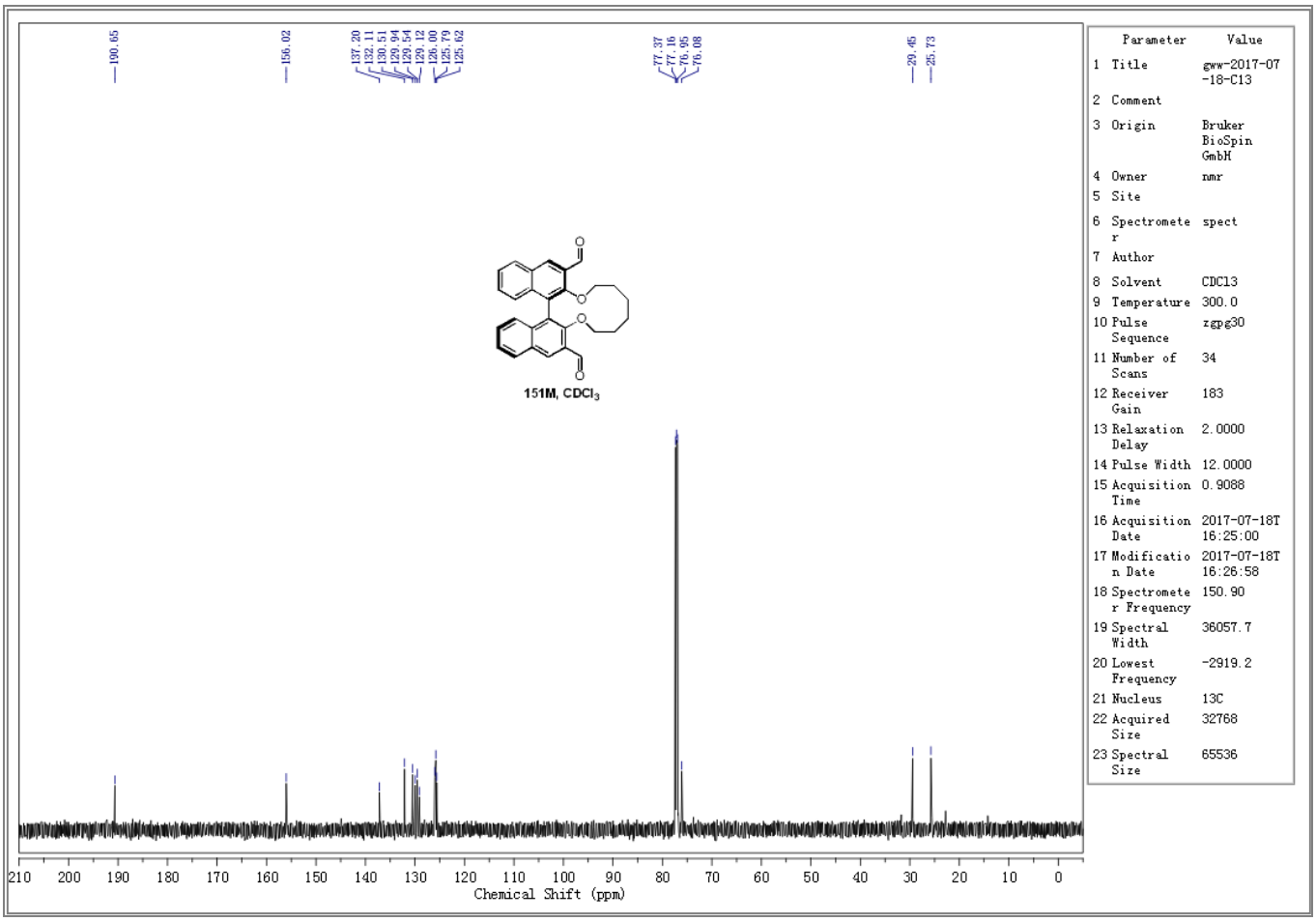
	Parameter	Value
1	Title	BINOL-4-CHO-C13
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.3
10	Pulse Sequence	zgpg30
11	Number of Scans	28
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-07-06T 12:24:30
17	Modification Date	2017-07-06T 12:25:35
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1950.0
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536


10.5538
8.5800
8.0402
8.0267
7.4665
7.4647
7.4531
7.4513
7.4272
7.4251
7.4133
7.4109
7.4018
7.2604
7.2107
4.4250
4.4221
4.4156
4.4122
4.4056
4.4028
4.3964
4.0478
4.0428
4.0325
4.0280
4.0235
4.0133
4.0083
1.6084
1.5994
1.5931
1.5894
1.5845
1.5743
1.5682
1.4749
1.4701
1.4656
1.4611
1.4529
1.4500
1.4409
1.4363
1.2173
1.1795
600M, CDCl3
1.91
2.00
1.95
2.03
2.08
1.99
2.02
2.06
0.98
0.99
2.33
2.20
Chemical Shift (ppm)
Parameter Value
1 Title gww
2 Comment
3 Origin Bruker BioSpin GmbH
4 Owner nmrsu
5 Site
6 Spectrometer spect
7 Author
8 Solvent CDCl3
9 Temperature 297.7
10 Pulse Sequence zg30
11 Number of Scans 16
12 Receiver Gain 86
13 Relaxation Delay 1.0000
14 Pulse Width 11.0000
15 Acquisition Time 2.6564
16 Acquisition Date 2017-06-19T 23:00:00
17 Modification Date 2017-06-19T 23:00:58
18 Spectrometer Frequency 600.13
19 Spectral Width 12335.5
20 Lowest Frequency -2477.5
21 Nucleus 1H
22 Acquired Size 32768
23 Spectral Size 65536

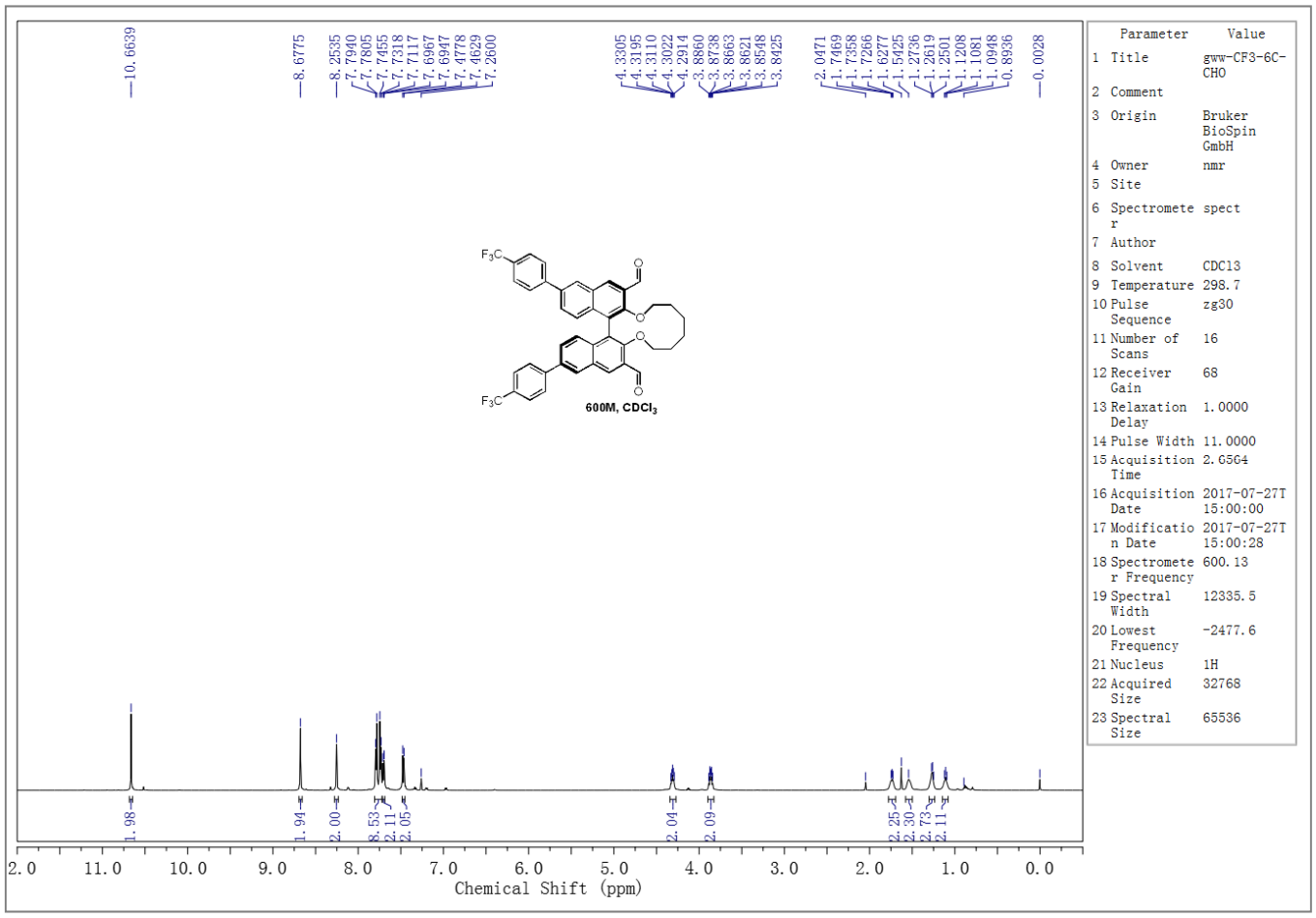

190.44
155.13
136.75
133.94
130.20
129.92
129.63
128.36
125.93
125.51
125.13
77.48
77.16
76.84
74.95
28.12
21.19
101M, CDCl3
Chemical Shift (ppm)
Parameter Value
1 Title BINOL-5-CHO-C13
2 Comment 13C-NMR of Dual-CH prob
3 Origin Bruker BioSpin GmbH
4 Owner nmr
5 Site
6 Spectrometer spect
7 Author
8 Solvent CDCl3
9 Temperature 299.6
10 Pulse Sequence zgpg30
11 Number of Scans 32
12 Receiver Gain 193
13 Relaxation Delay 2.0000
14 Pulse Width 9.9000
15 Acquisition Time 1.3631
16 Acquisition Date 2017-07-06T 12:44:35
17 Modification Date 2017-07-06T 12:45:29
18 Spectrometer Frequency 100.61
19 Spectral Width 24038.5
20 Lowest Frequency -1949.1
21 Nucleus 13C
22 Acquired Size 32768
23 Spectral Size 65536



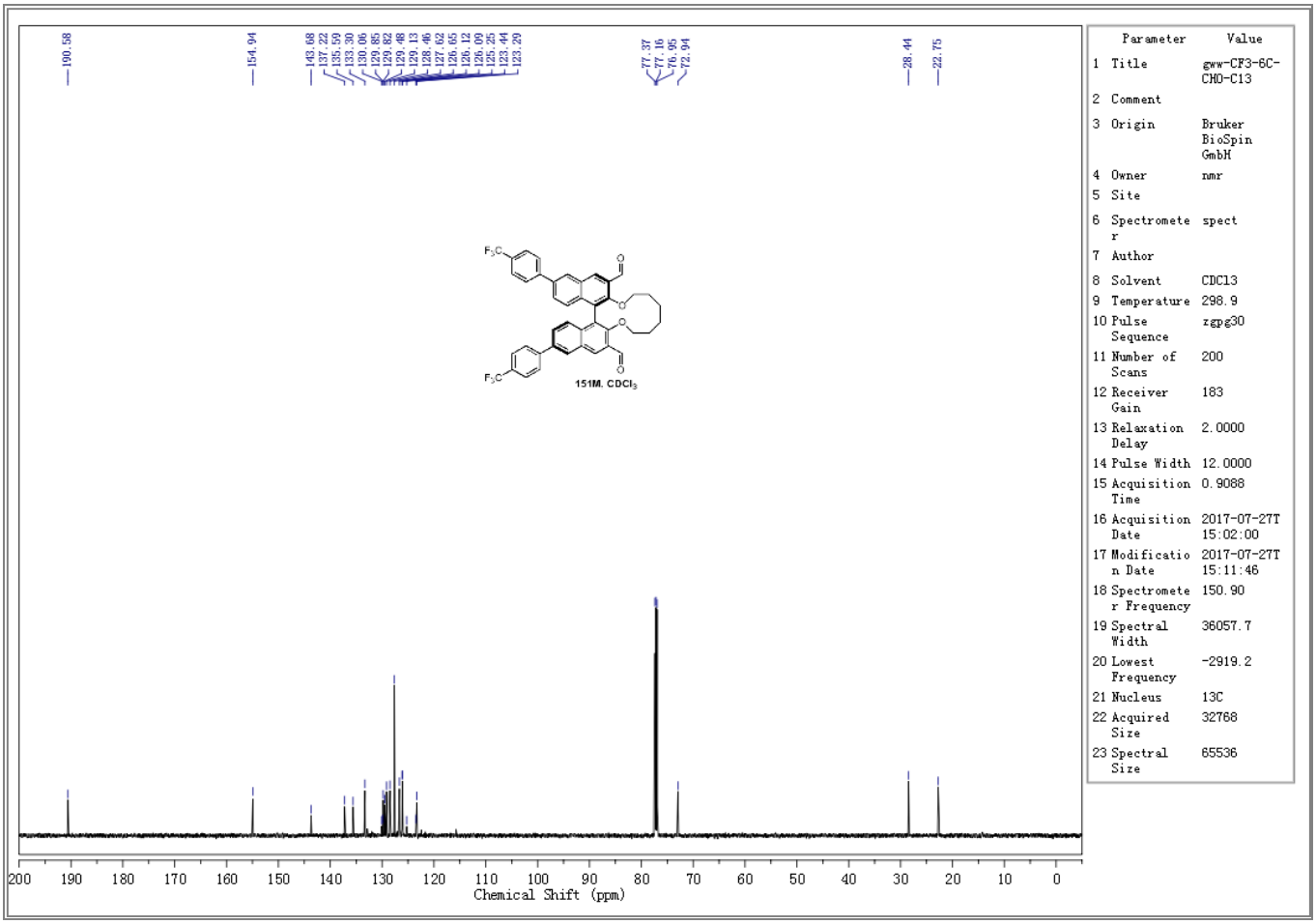
	Parameter	Value
1	Title	gww-2017-07-18
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.6
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	75
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-18T16:17:00
17	Modification Date	2017-07-18T16:17:31
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.8
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536



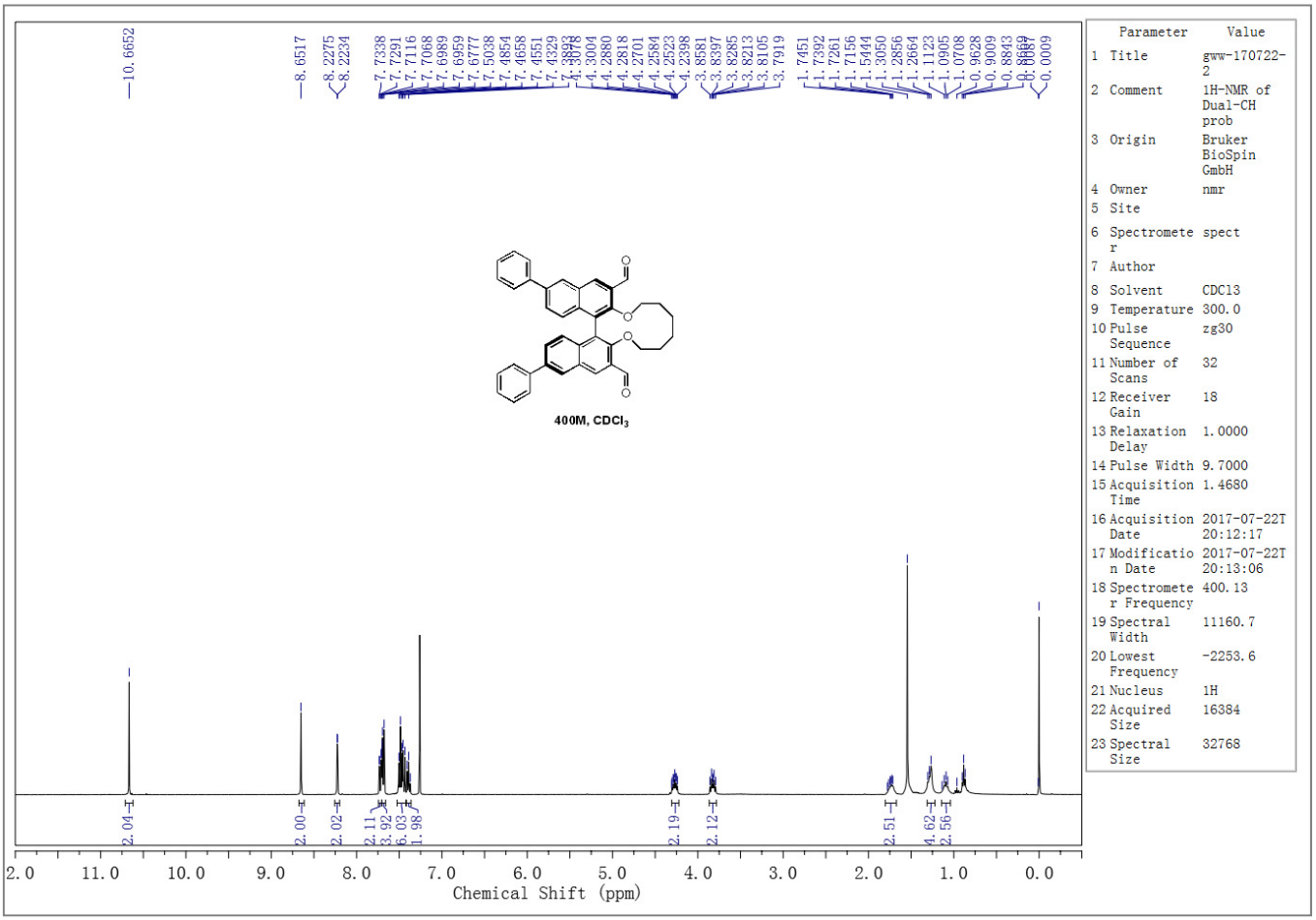
	Parameter	Value
1	Title	gww-2017-07-18-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	300.0
10	Pulse Sequence	zgpg30
11	Number of Scans	34
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-18T16:25:00
17	Modification Date	2017-07-18T16:26:58
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2919.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



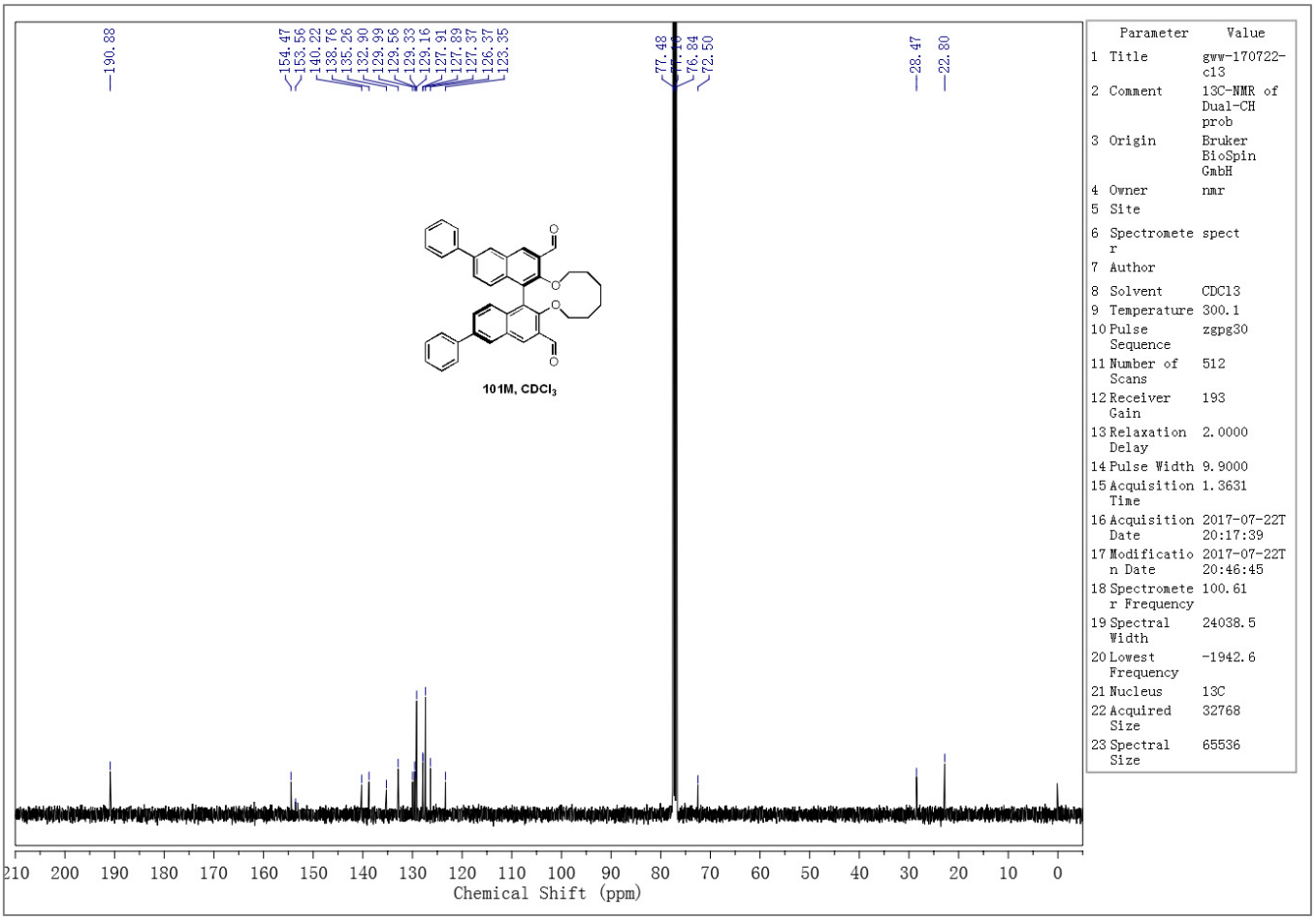
Parameter	Value
1 Title	gww-CF3-6C-CHO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	CDCl3
9 Temperature	298.7
10 Pulse Sequence	zg30
11 Number of Scans	16
12 Receiver Gain	68
13 Relaxation Delay	1.0000
14 Pulse Width	11.0000
15 Acquisition Time	2.6564
16 Acquisition Date	2017-07-27T 15:00:00
17 Modification Date	2017-07-27T 15:00:28
18 Spectrometer Frequency	600.13
19 Spectral Width	12335.5
20 Lowest Frequency	-2477.6
21 Nucleus	1H
22 Acquired Size	32768
23 Spectral Size	65536



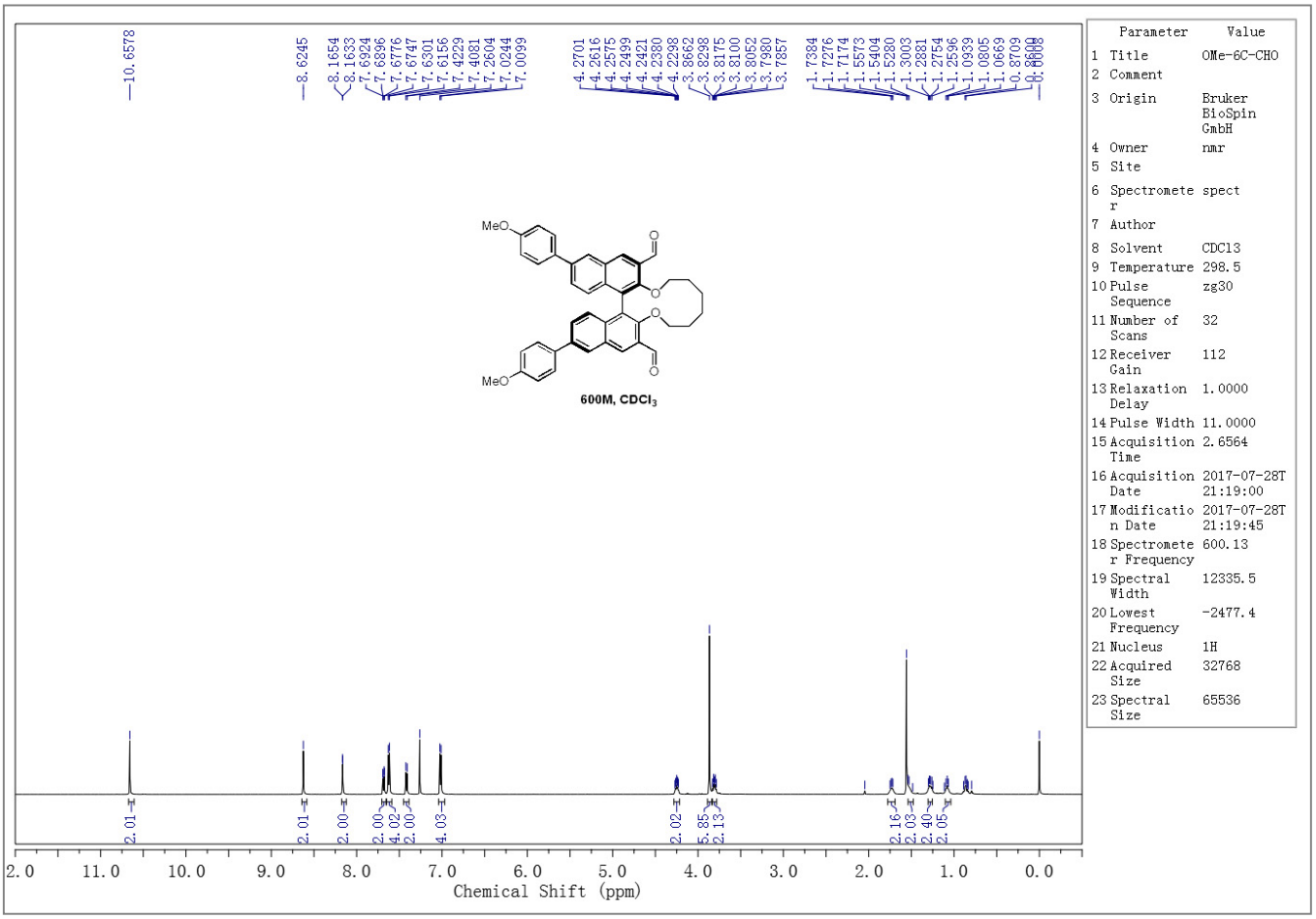
Parameter	Value
1 Title	gww-CF3-6C-CHO-C13
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	CDCl3
9 Temperature	298.9
10 Pulse Sequence	zgpg30
11 Number of Scans	200
12 Receiver Gain	183
13 Relaxation Delay	2.0000
14 Pulse Width	12.0000
15 Acquisition Time	0.9088
16 Acquisition Date	2017-07-27T 15:02:00
17 Modification Date	2017-07-27T 15:11:46
18 Spectrometer Frequency	150.90
19 Spectral Width	36057.7
20 Lowest Frequency	-2919.2
21 Nucleus	13C
22 Acquired Size	32768
23 Spectral Size	65536



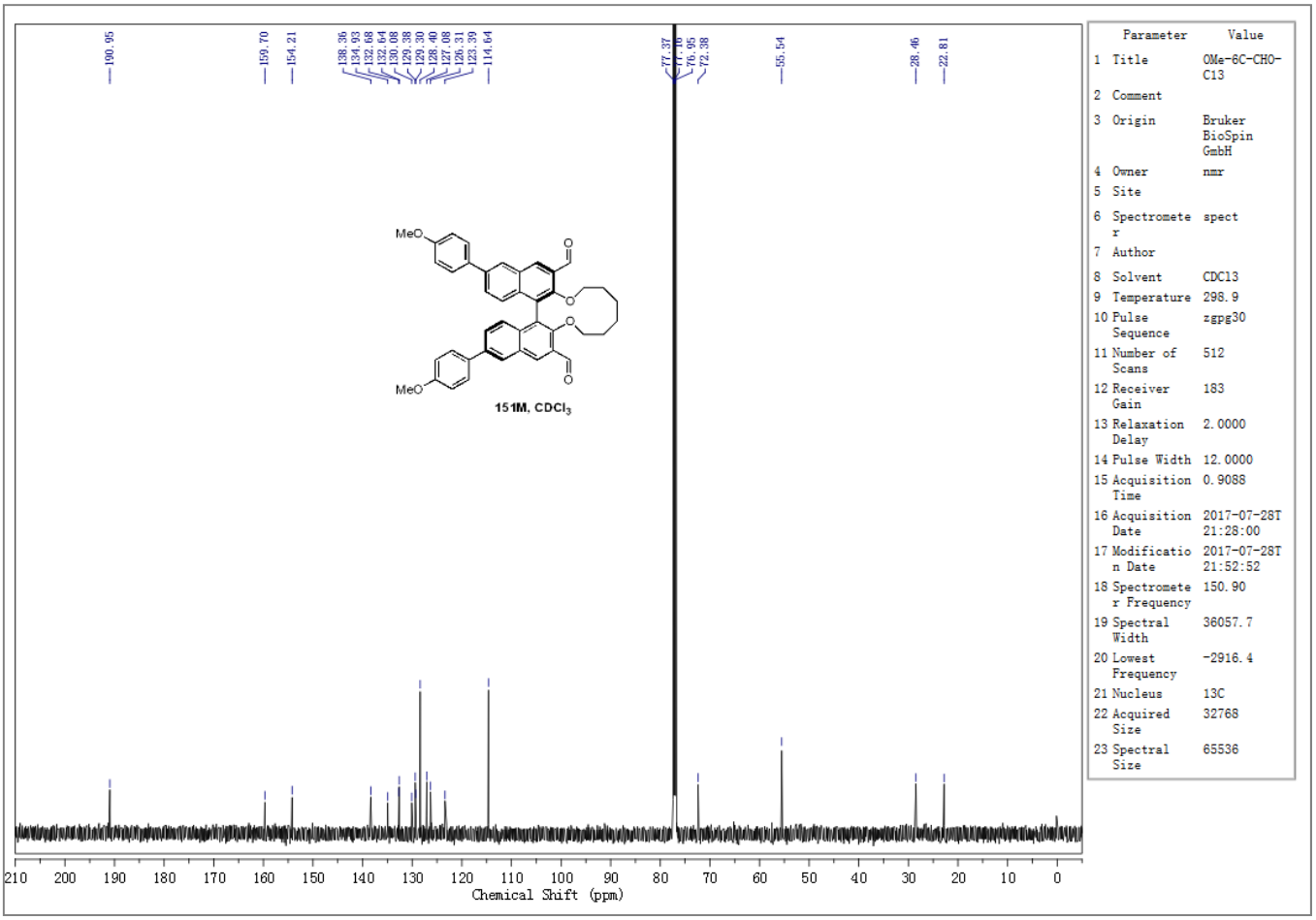
	Parameter	Value
1	Title	gww-170722-2
2	Comment	1H-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	300.0
10	Pulse Sequence	zg30
11	Number of Scans	32
12	Receiver Gain	18
13	Relaxation Delay	1.0000
14	Pulse Width	9.7000
15	Acquisition Time	1.4680
16	Acquisition Date	2017-07-22T 20:12:17
17	Modification Date	2017-07-22T 20:13:06
18	Spectrometer Frequency	400.13
19	Spectral Width	11160.7
20	Lowest Frequency	-2253.6
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	32768



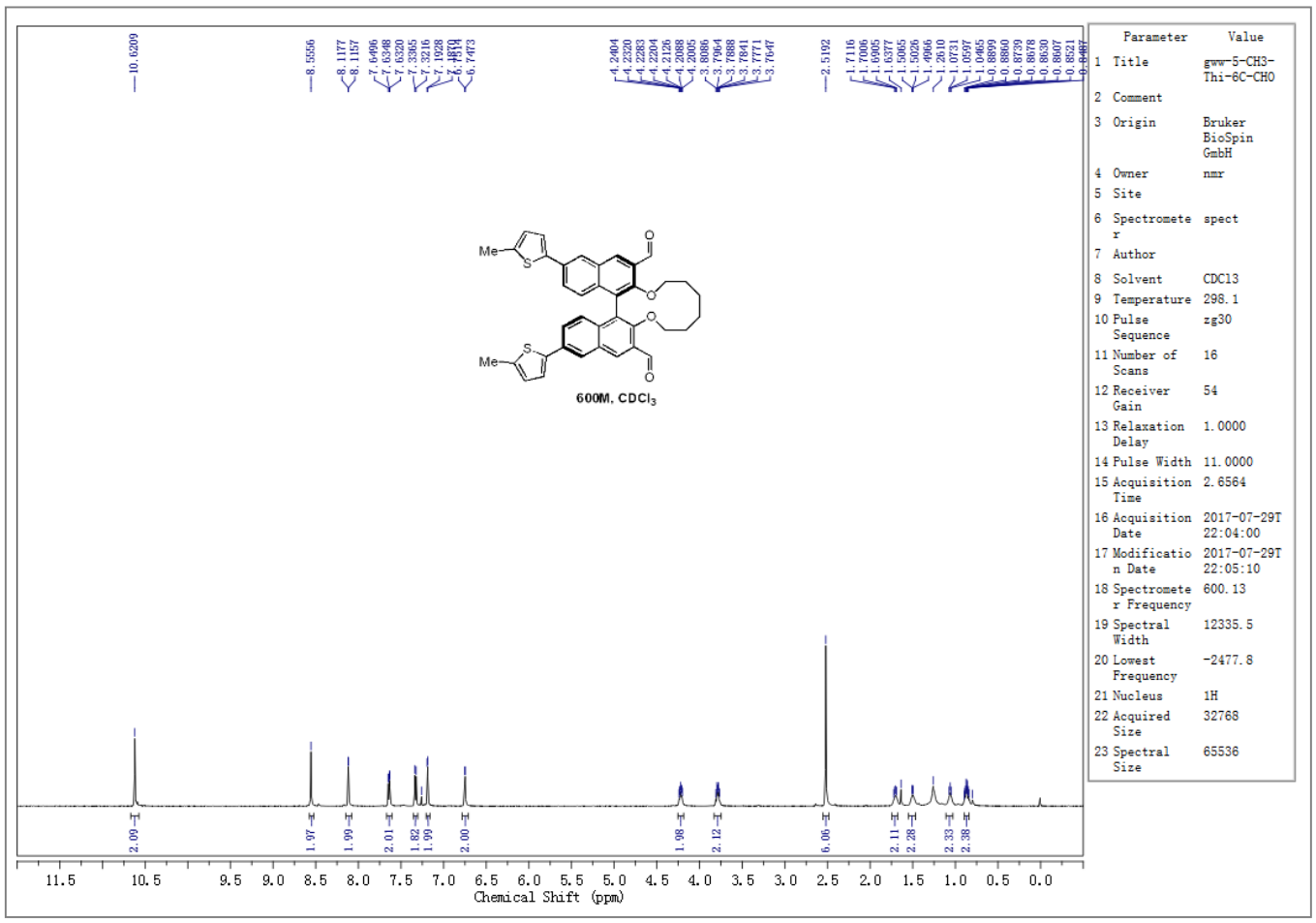
	Parameter	Value
1	Title	gww-170722-c13
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	300.1
10	Pulse Sequence	zgpg30
11	Number of Scans	512
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-07-22T 20:17:39
17	Modification Date	2017-07-22T 20:46:45
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1942.6
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



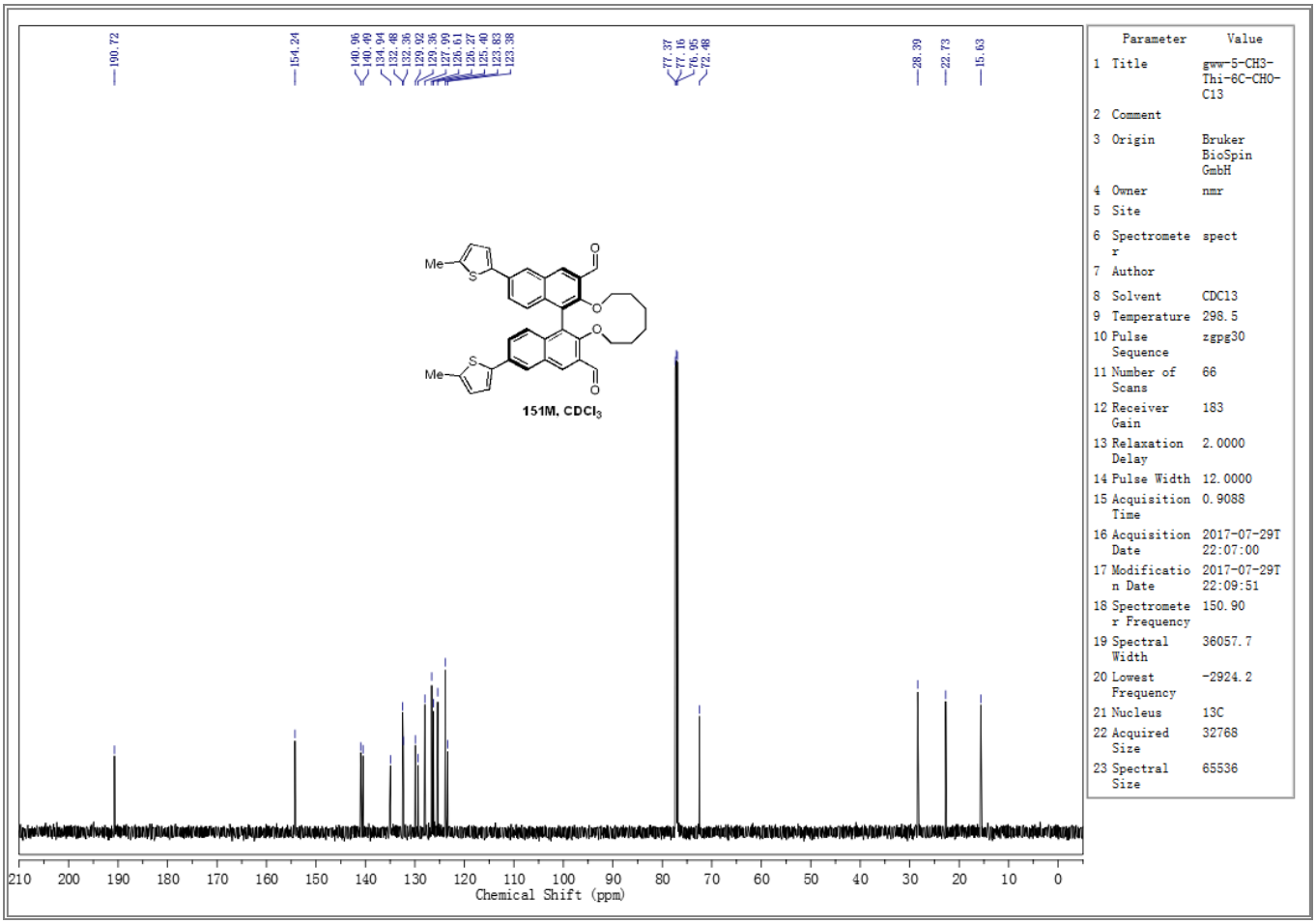
	Parameter	Value
1	Title	OMe-6C-CHO
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.5
10	Pulse Sequence	zg30
11	Number of Scans	32
12	Receiver Gain	112
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-28T 21:19:00
17	Modification Date	2017-07-28T 21:19:45
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.4
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536



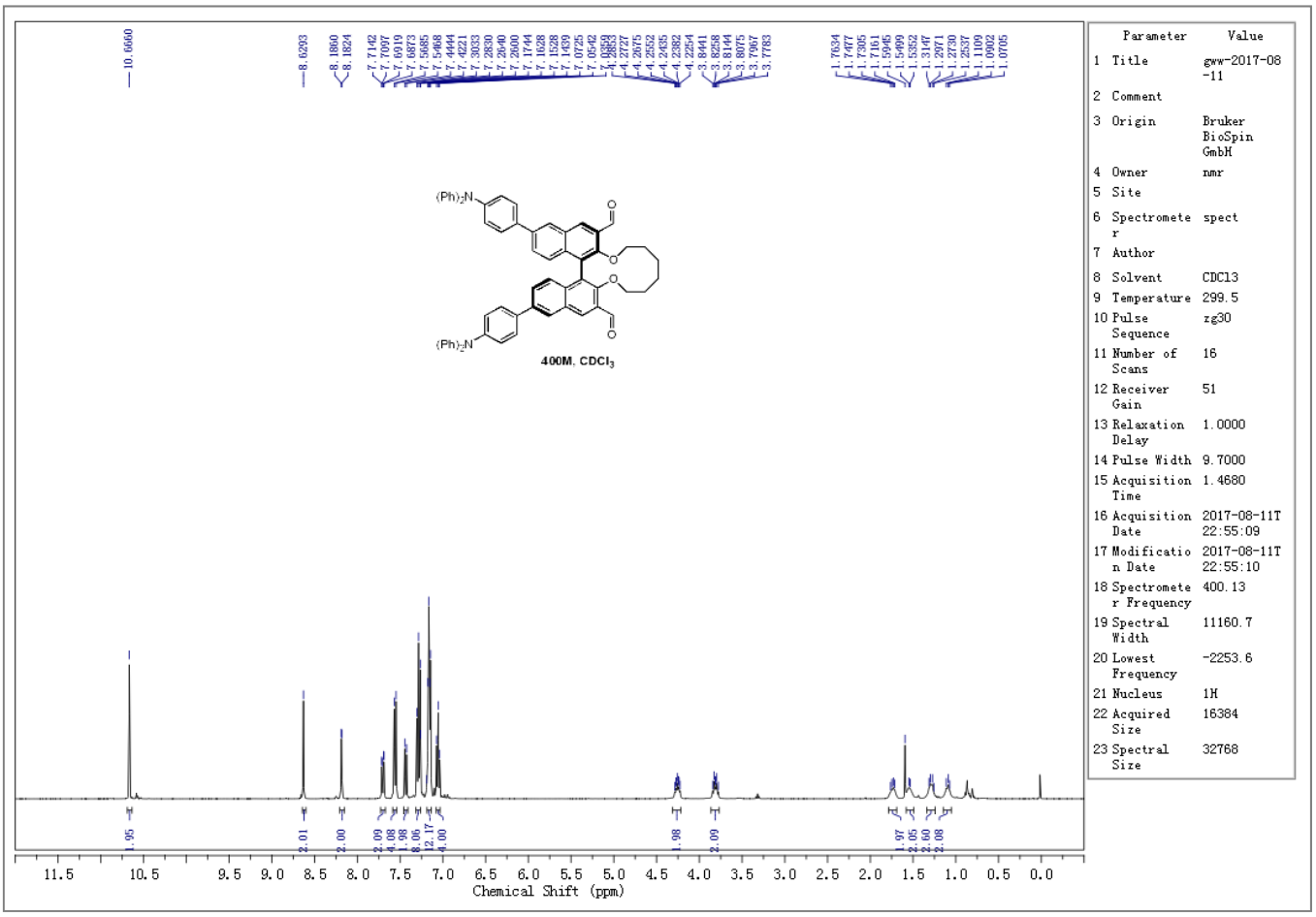
	Parameter	Value
1	Title	OMe-6C-CHO-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.9
10	Pulse Sequence	zgpg30
11	Number of Scans	512
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-28T 21:28:00
17	Modification Date	2017-07-28T 21:52:52
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2916.4
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



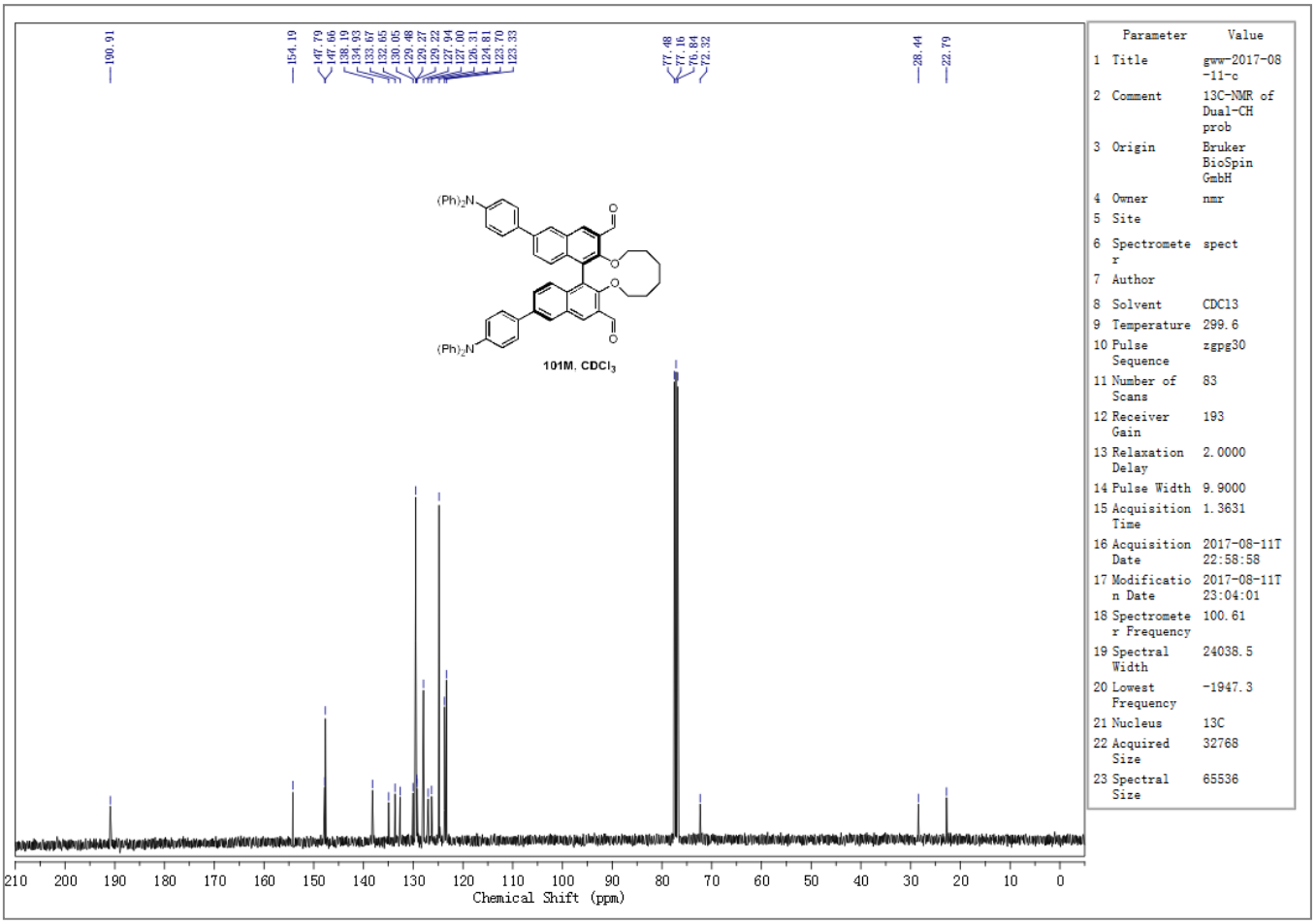
	Parameter	Value
1	Title	gww-5-CH3-Thi-6C-CHO
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.1
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	54
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-29T 22:04:00
17	Modification Date	2017-07-29T 22:05:10
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.8
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536



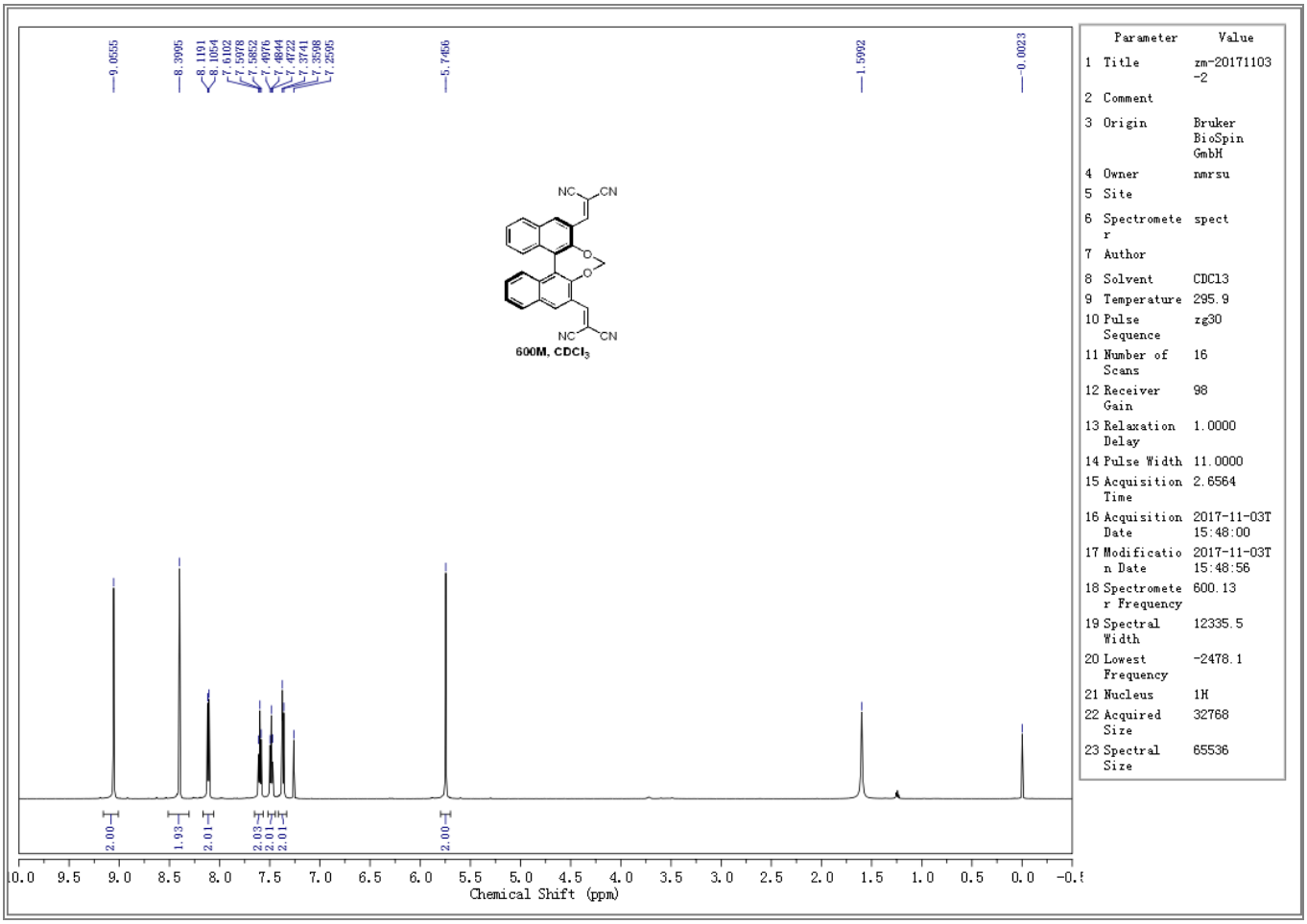
	Parameter	Value
1	Title	gww-5-CH3-Thi-6C-CHO-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.5
10	Pulse Sequence	zgpg30
11	Number of Scans	66
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-29T 22:07:00
17	Modification Date	2017-07-29T 22:09:51
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2924.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536



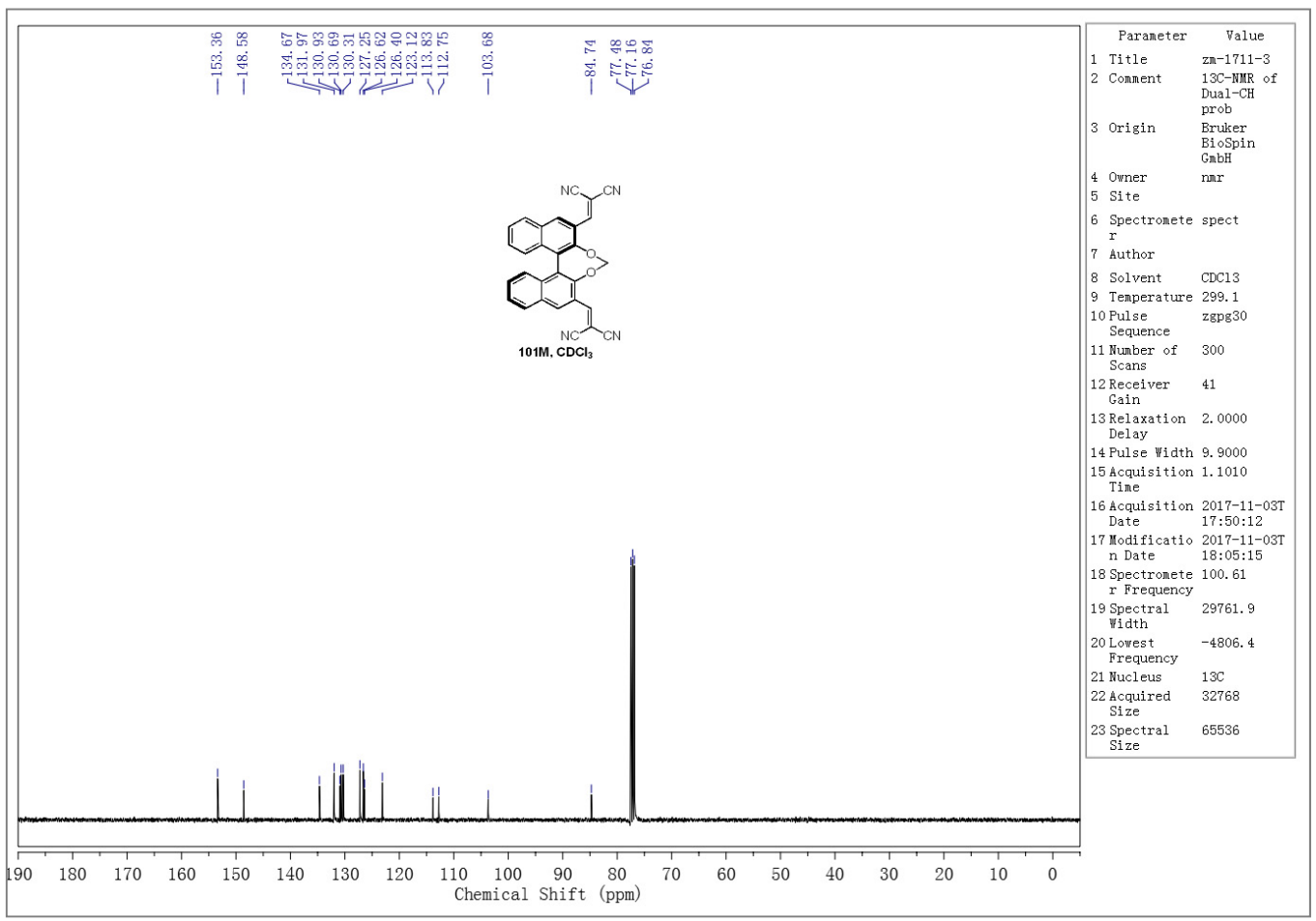
	Parameter	Value
1	Title	gww-2017-08-11
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.5
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	51
13	Relaxation Delay	1.0000
14	Pulse Width	9.7000
15	Acquisition Time	1.4680
16	Acquisition Date	2017-08-11T 22:55:09
17	Modification Date	2017-08-11T 22:55:10
18	Spectrometer Frequency	400.13
19	Spectral Width	11160.7
20	Lowest Frequency	-2253.6
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	32768



	Parameter	Value
1	Title	gww-2017-08-11-c
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.6
10	Pulse Sequence	zgpg30
11	Number of Scans	83
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-08-11T 22:58:58
17	Modification Date	2017-08-11T 23:04:01
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1947.3
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

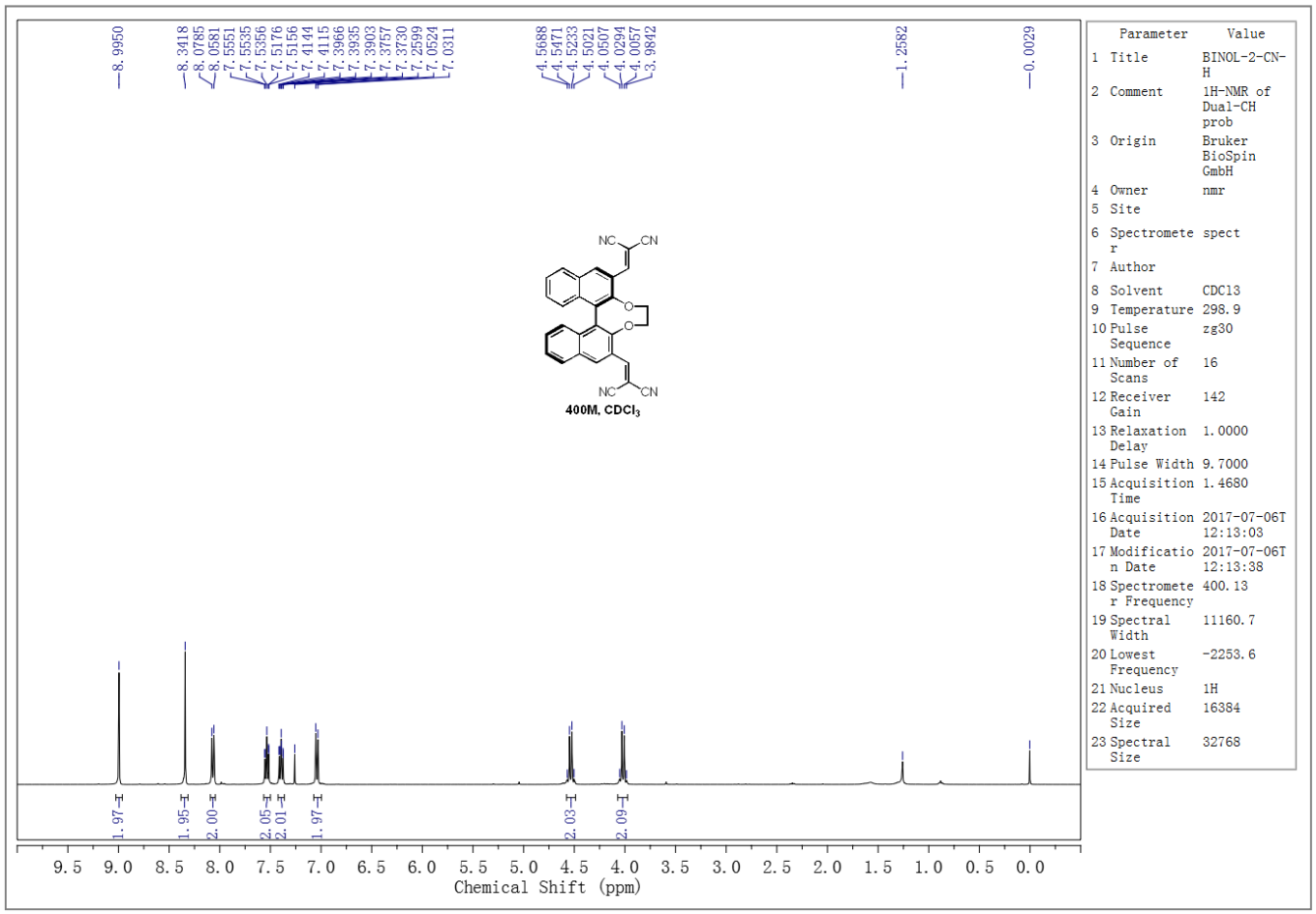


	Parameter	Value
1	Title	zm-20171103-2
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	295.9
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	98
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-11-03T 15:48:00
17	Modification Date	2017-11-03T 15:48:56
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2478.1
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

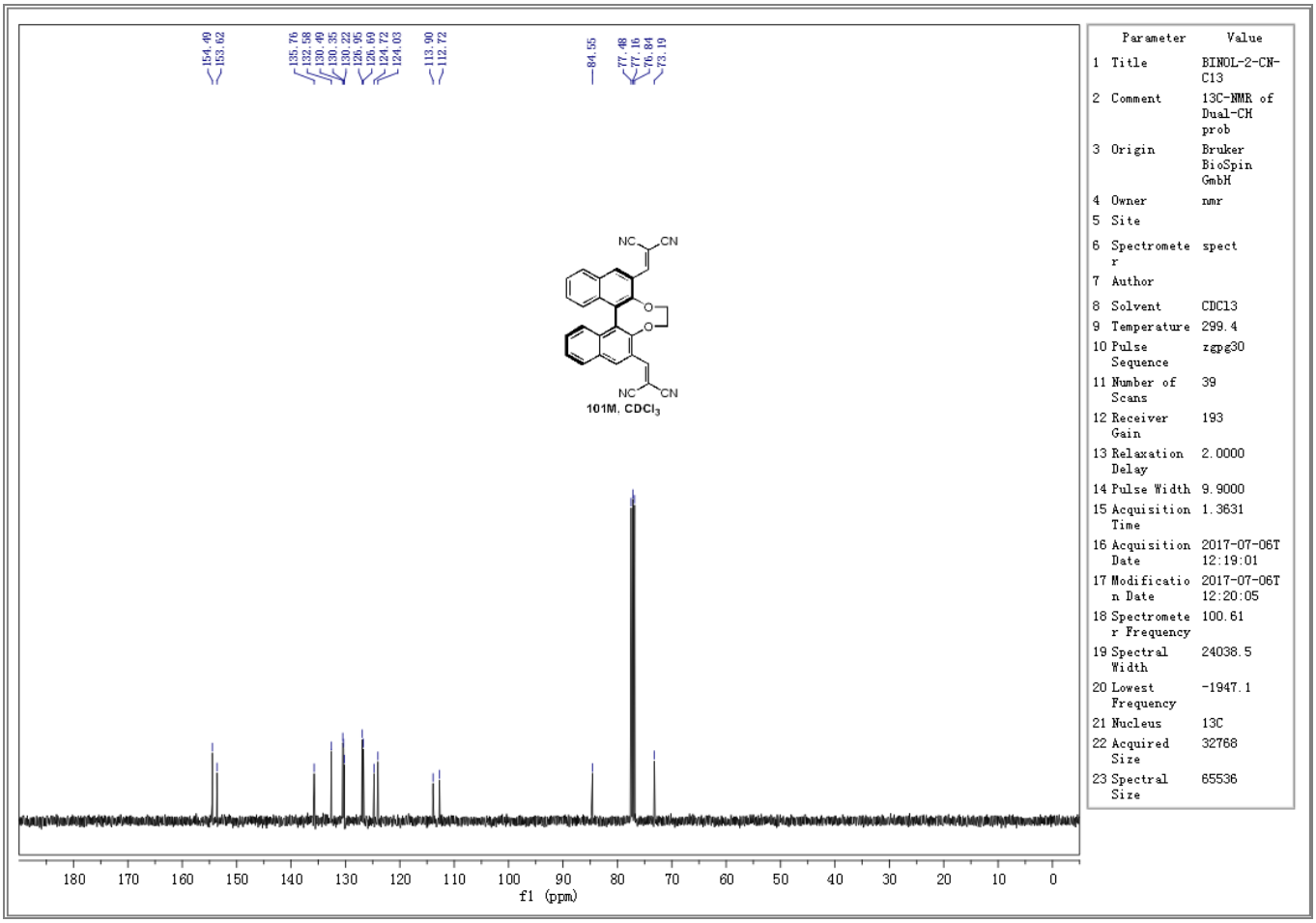


	Parameter	Value
1	Title	zm-1711-3
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.1
10	Pulse Sequence	zgpg30
11	Number of Scans	300
12	Receiver Gain	41
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.1010
16	Acquisition Date	2017-11-03T 17:50:12
17	Modification Date	2017-11-03T 18:05:15
18	Spectrometer Frequency	100.61
19	Spectral Width	29761.9
20	Lowest Frequency	-4806.4
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data X-ray

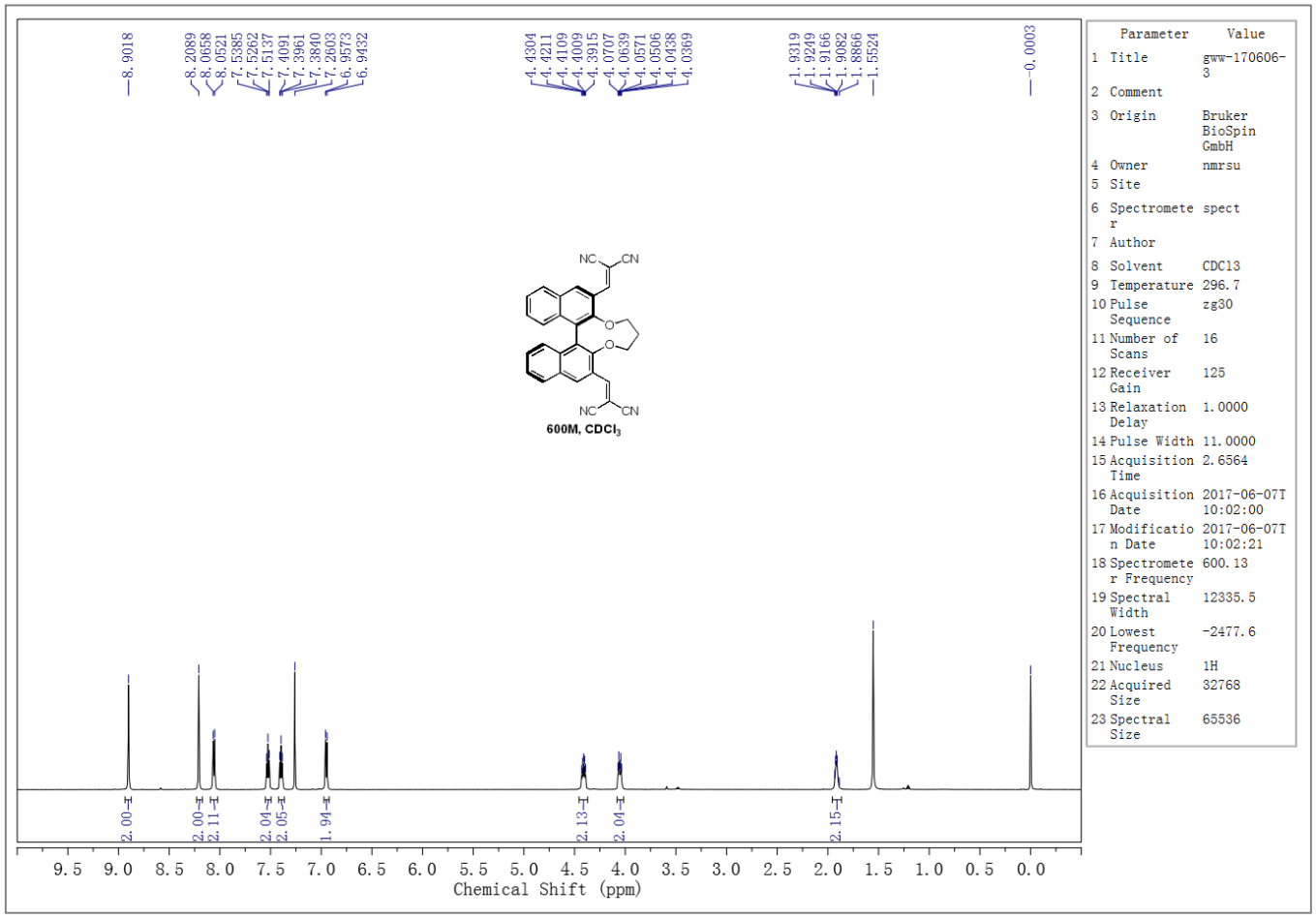


	Parameter	Value
1	Title	BINOL-2-CN-H
2	Comment	1H-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.9
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	142
13	Relaxation Delay	1.0000
14	Pulse Width	9.7000
15	Acquisition Time	1.4680
16	Acquisition Date	2017-07-06T 12:13:03
17	Modification Date	2017-07-06T 12:13:38
18	Spectrometer Frequency	400.13
19	Spectral Width	11160.7
20	Lowest Frequency	-2253.6
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	32768

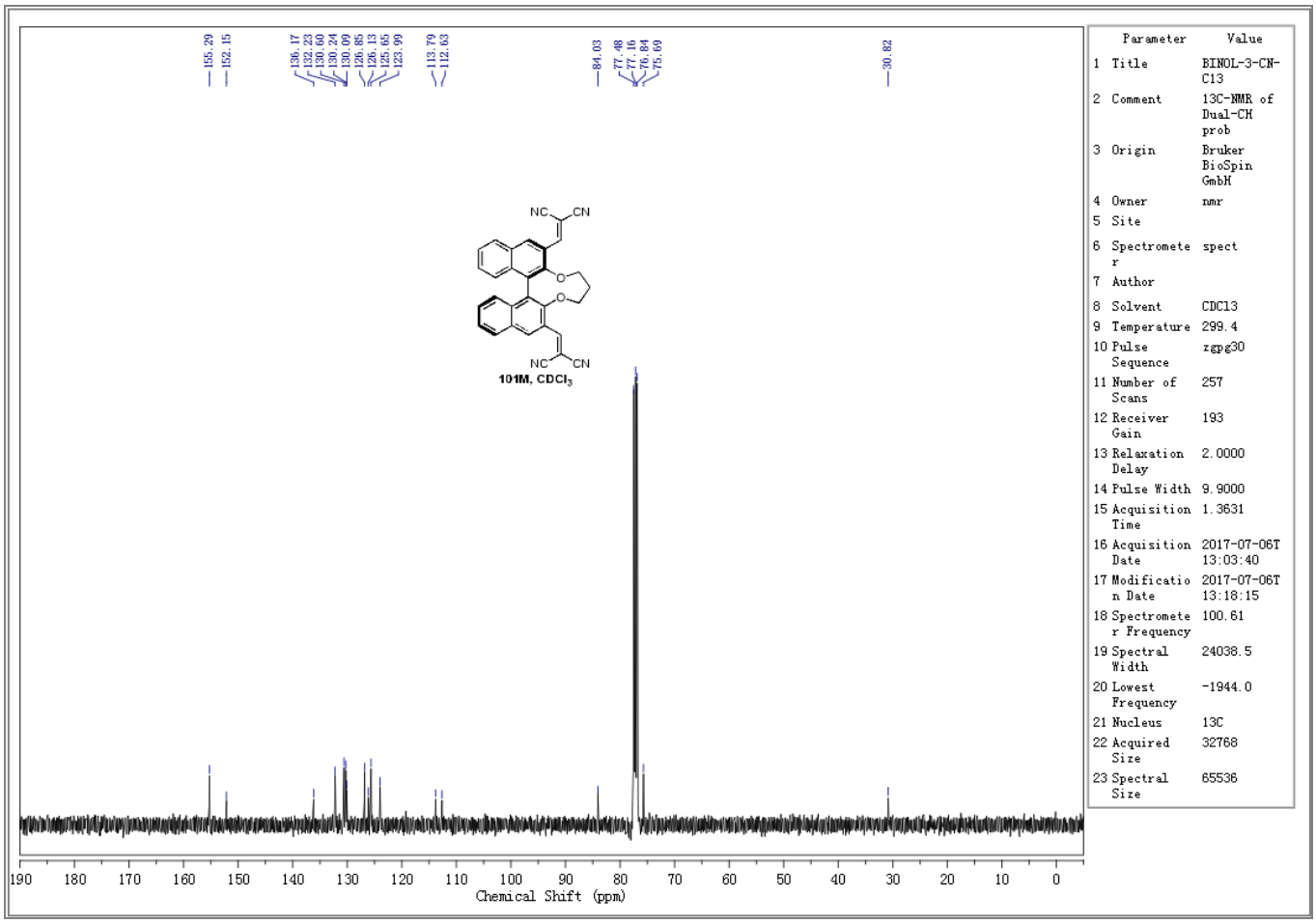


	Parameter	Value
1	Title	BINOL-2-CN-C13
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.4
10	Pulse Sequence	zgpg30
11	Number of Scans	39
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-07-06T 12:19:01
17	Modification Date	2017-07-06T 12:20:05
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1947.1
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data X-ray

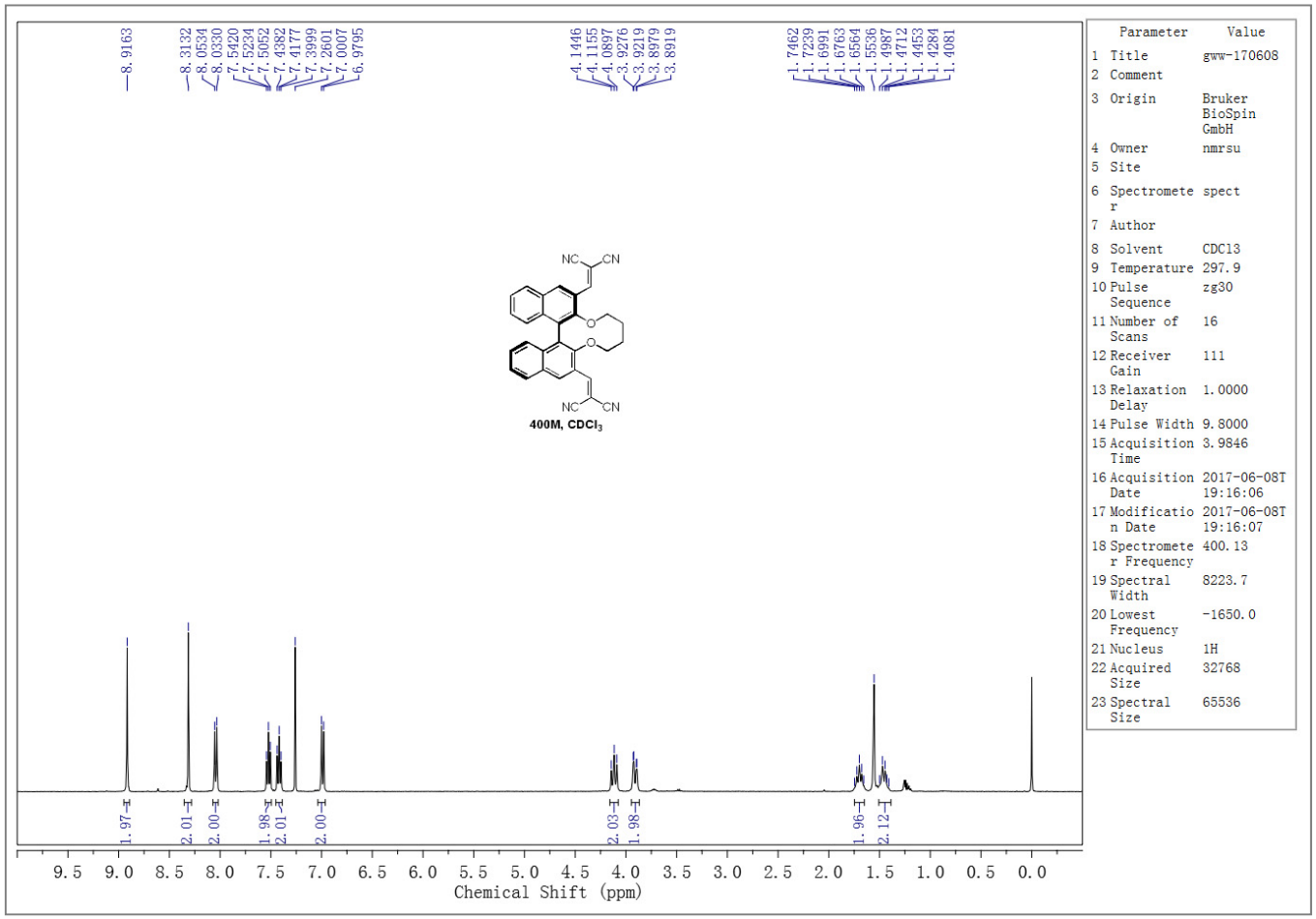


	Parameter	Value
1	Title	gww-170606-3
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	296.7
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	125
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-06-07T 10:02:00
17	Modification Date	2017-06-07T 10:02:21
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.6
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

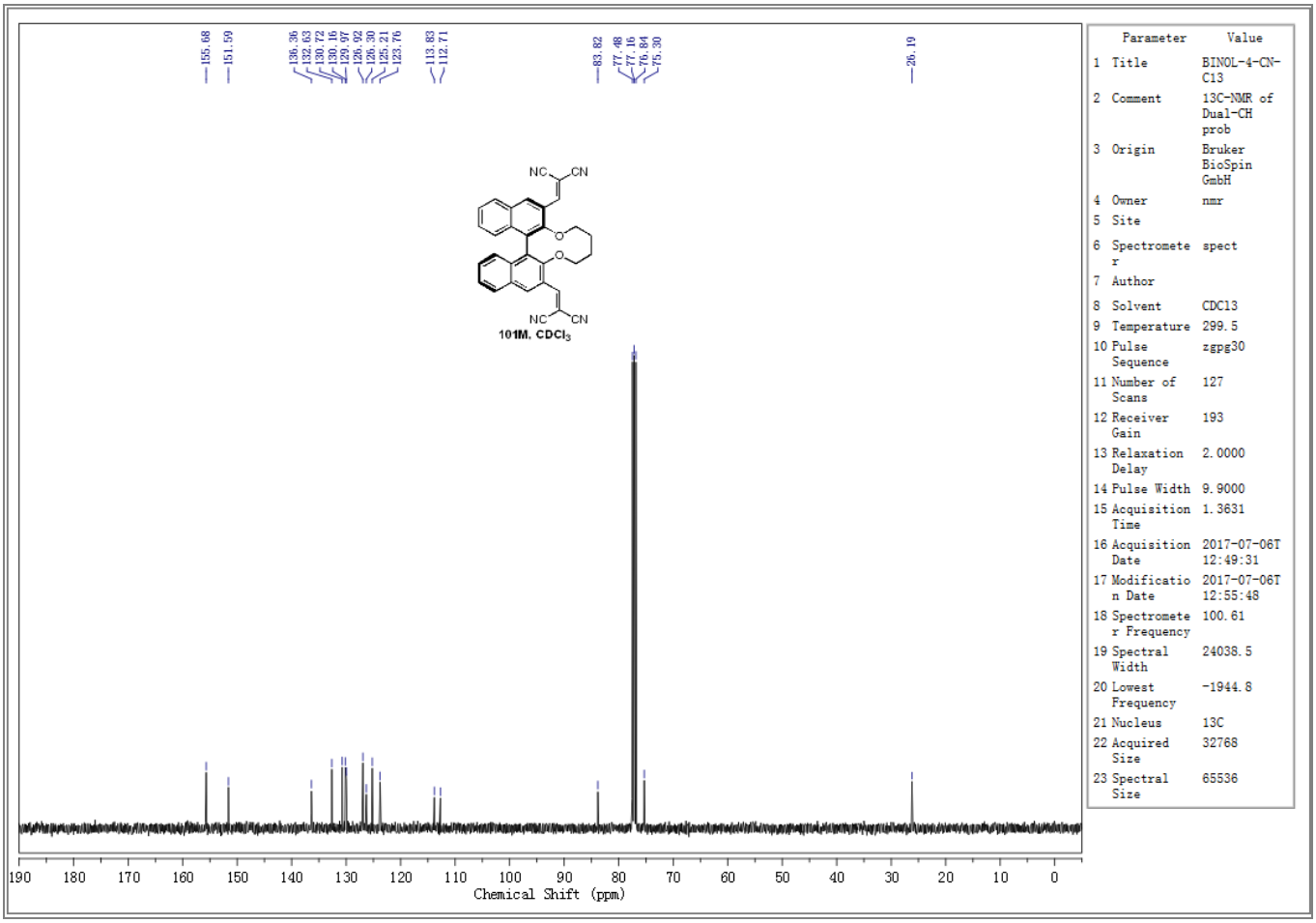


	Parameter	Value
1	Title	BINOL-3-CN-C13
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.4
10	Pulse Sequence	zgpg30
11	Number of Scans	257
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-07-06T 13:03:40
17	Modification Date	2017-07-06T 13:18:15
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1944.0
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data

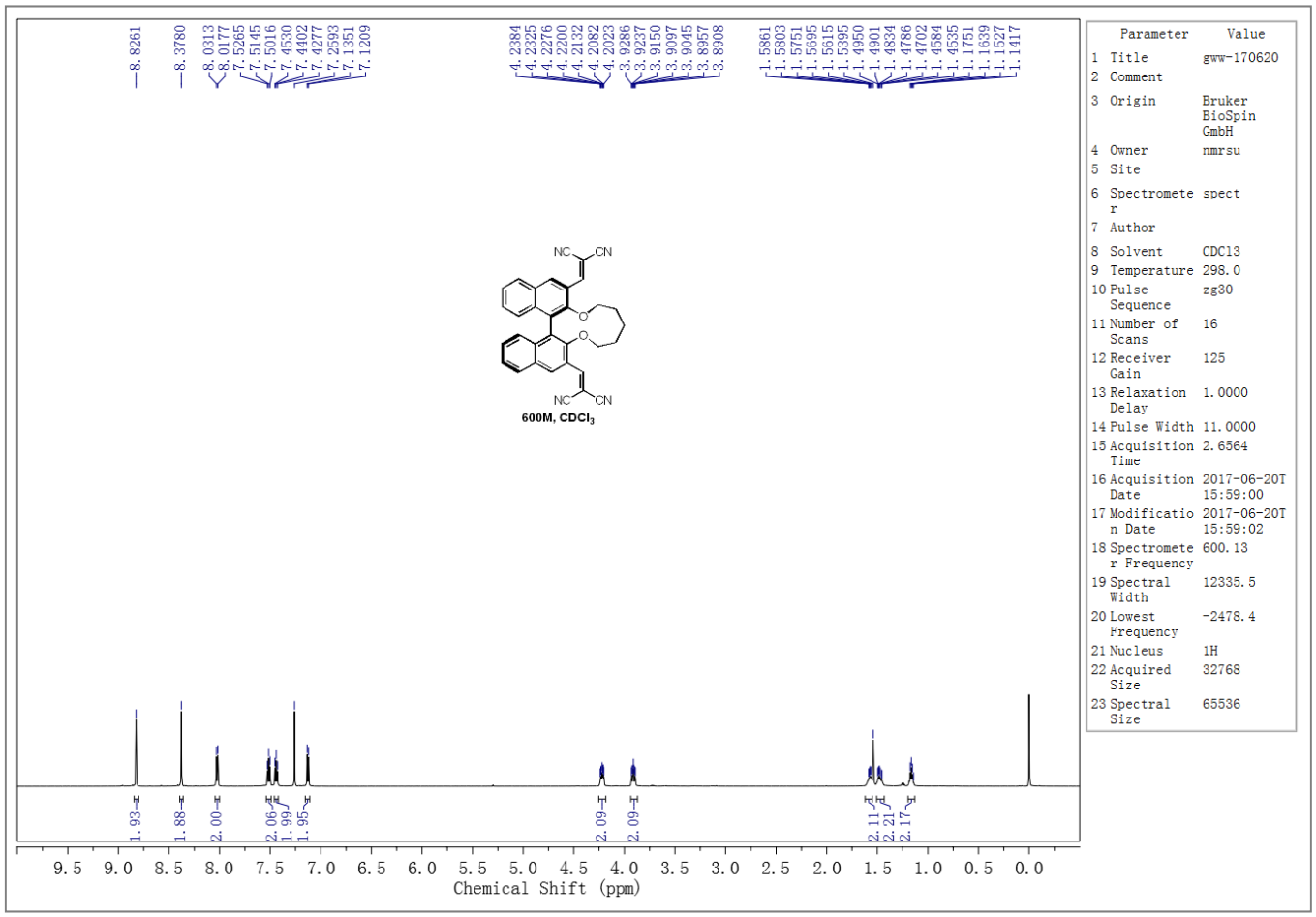


	Parameter	Value
1	Title	gww-170608
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	297.9
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	111
13	Relaxation Delay	1.0000
14	Pulse Width	9.8000
15	Acquisition Time	3.9846
16	Acquisition Date	2017-06-08T 19:16:06
17	Modification Date	2017-06-08T 19:16:07
18	Spectrometer Frequency	400.13
19	Spectral Width	8223.7
20	Lowest Frequency	-1650.0
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

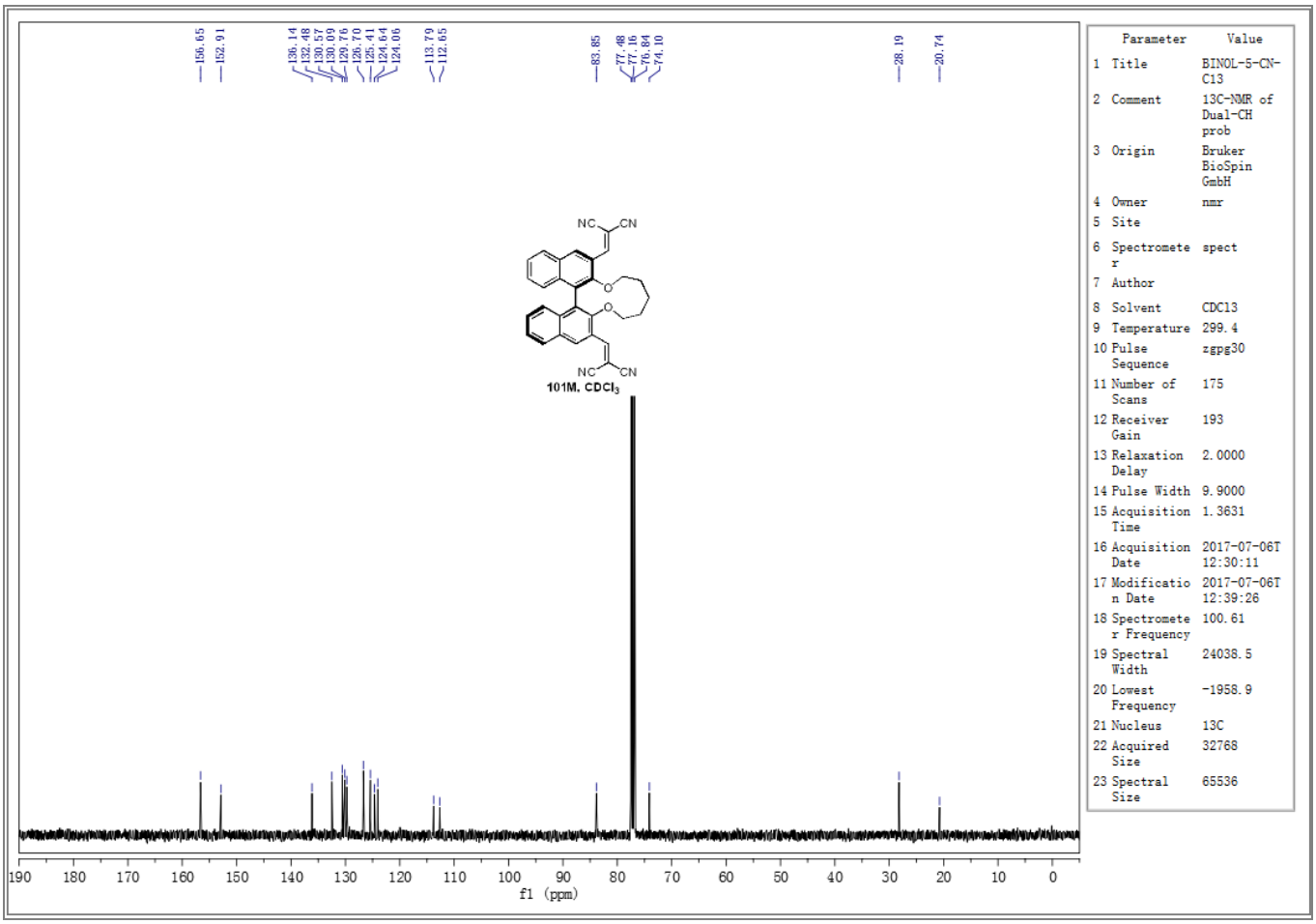


	Parameter	Value
1	Title	BINOL-4-CN-C13
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.5
10	Pulse Sequence	zgpg30
11	Number of Scans	127
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-07-06T 12:49:31
17	Modification Date	2017-07-06T 12:55:48
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1944.8
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data X-ray

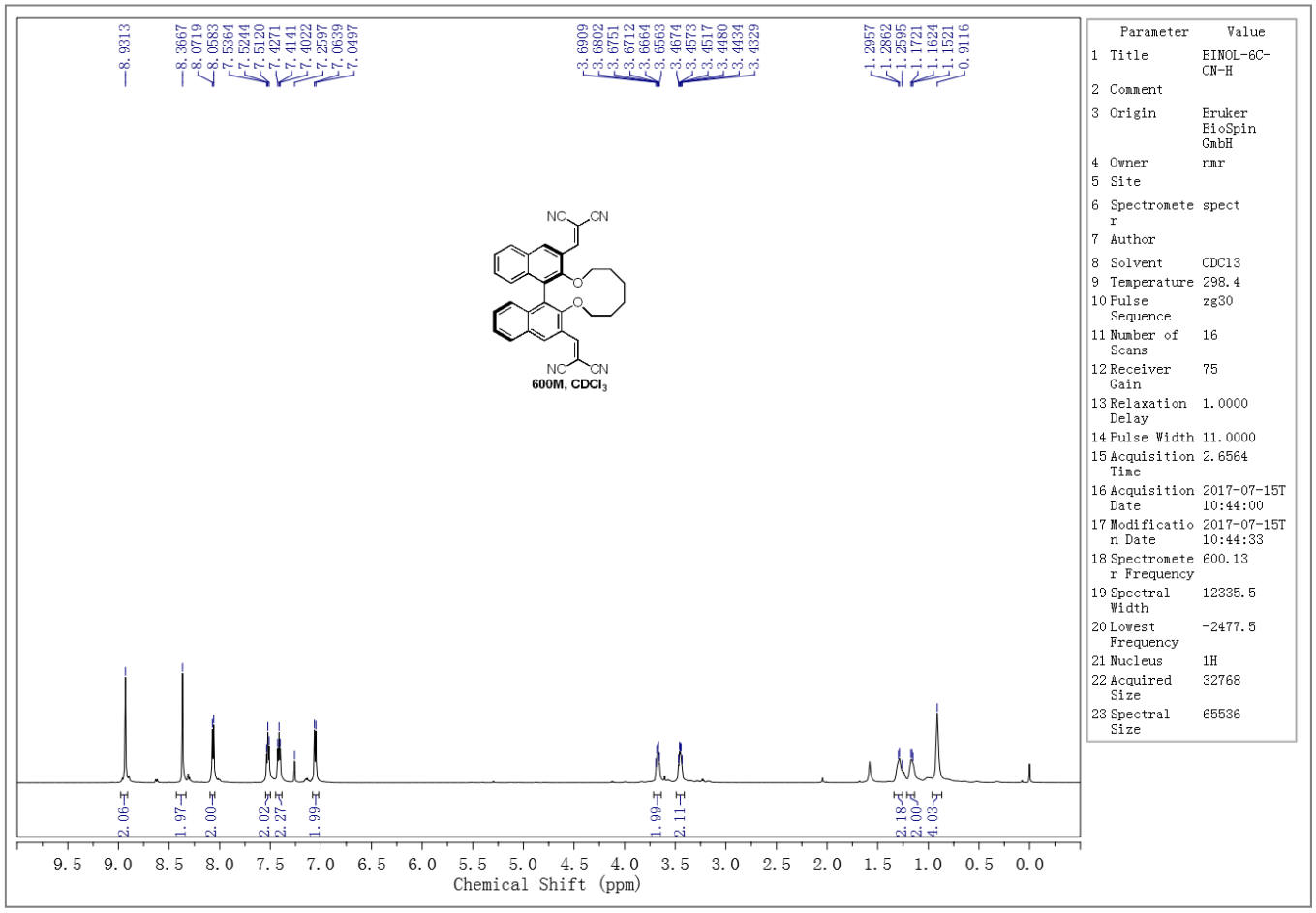


	Parameter	Value
1	Title	gww-170620
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.0
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	125
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-06-20T 15:59:00
17	Modification Date	2017-06-20T 15:59:02
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2478.4
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

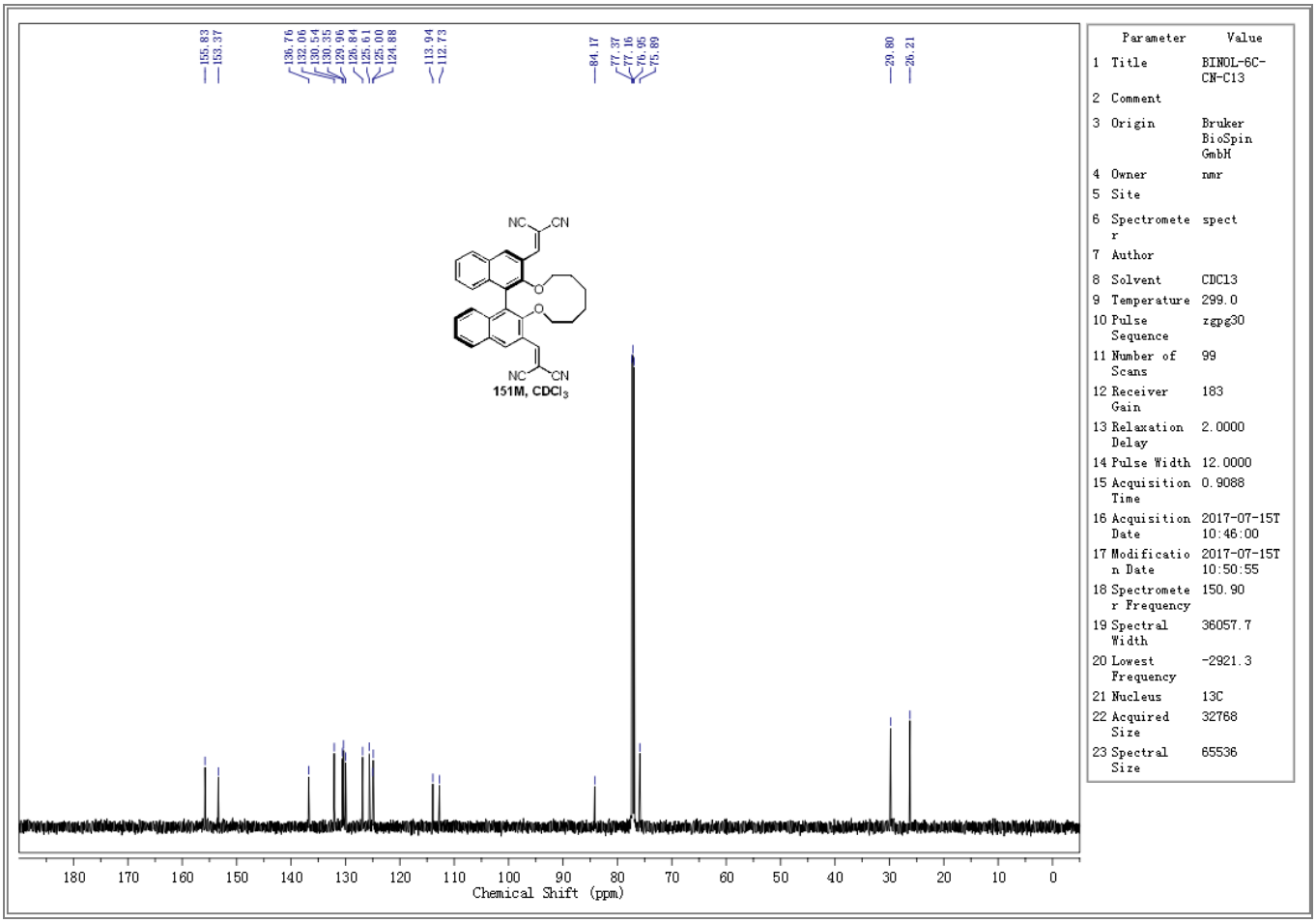


	Parameter	Value
1	Title	BINOL-5-CN-C13
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.4
10	Pulse Sequence	zgpg30
11	Number of Scans	175
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-07-06T 12:30:11
17	Modification Date	2017-07-06T 12:39:26
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1958.9
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data X-ray

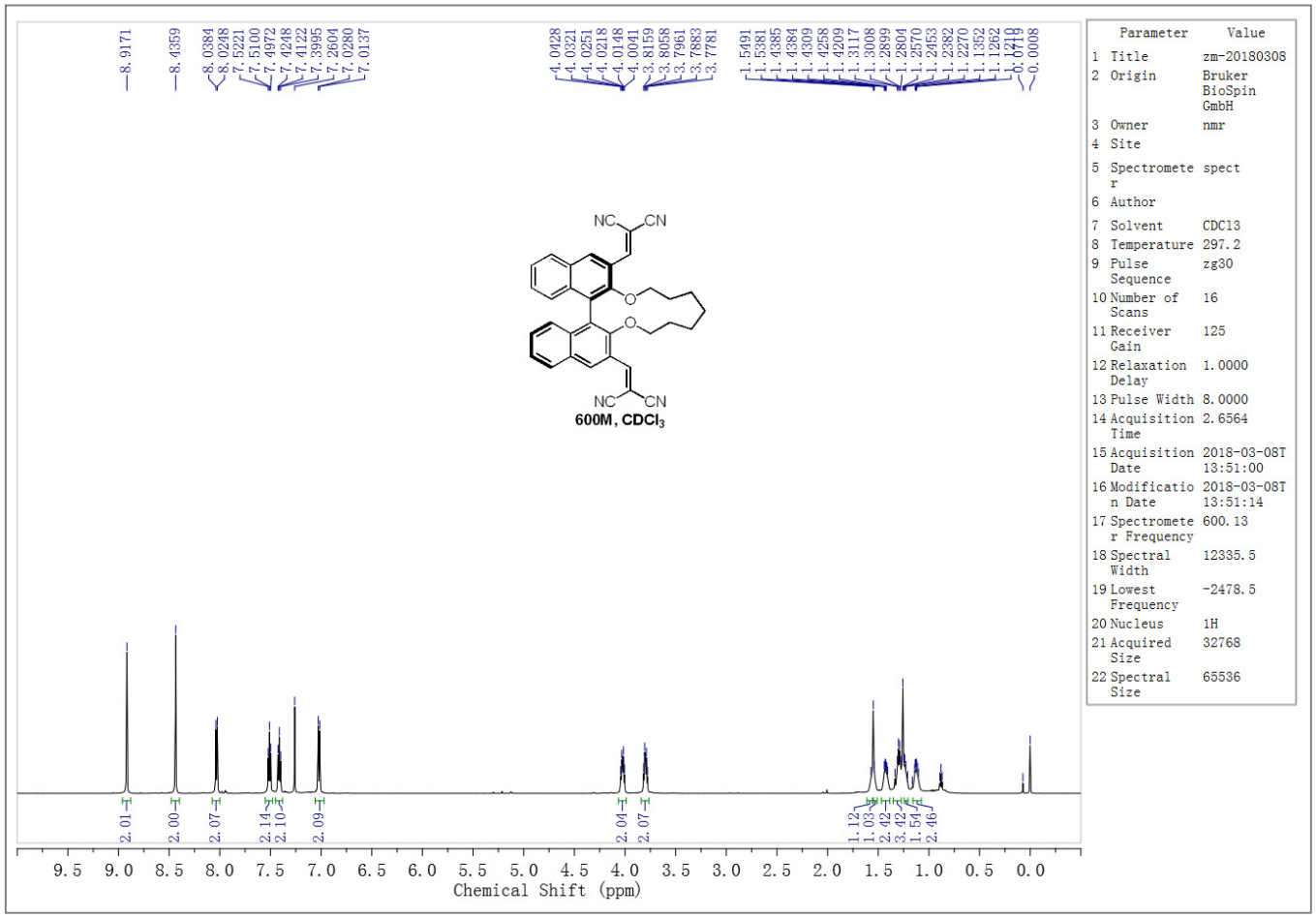


	Parameter	Value
1	Title	BINOL-6C-CN-H
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.4
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	75
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-15T 10:44:00
17	Modification Date	2017-07-15T 10:44:33
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.5
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

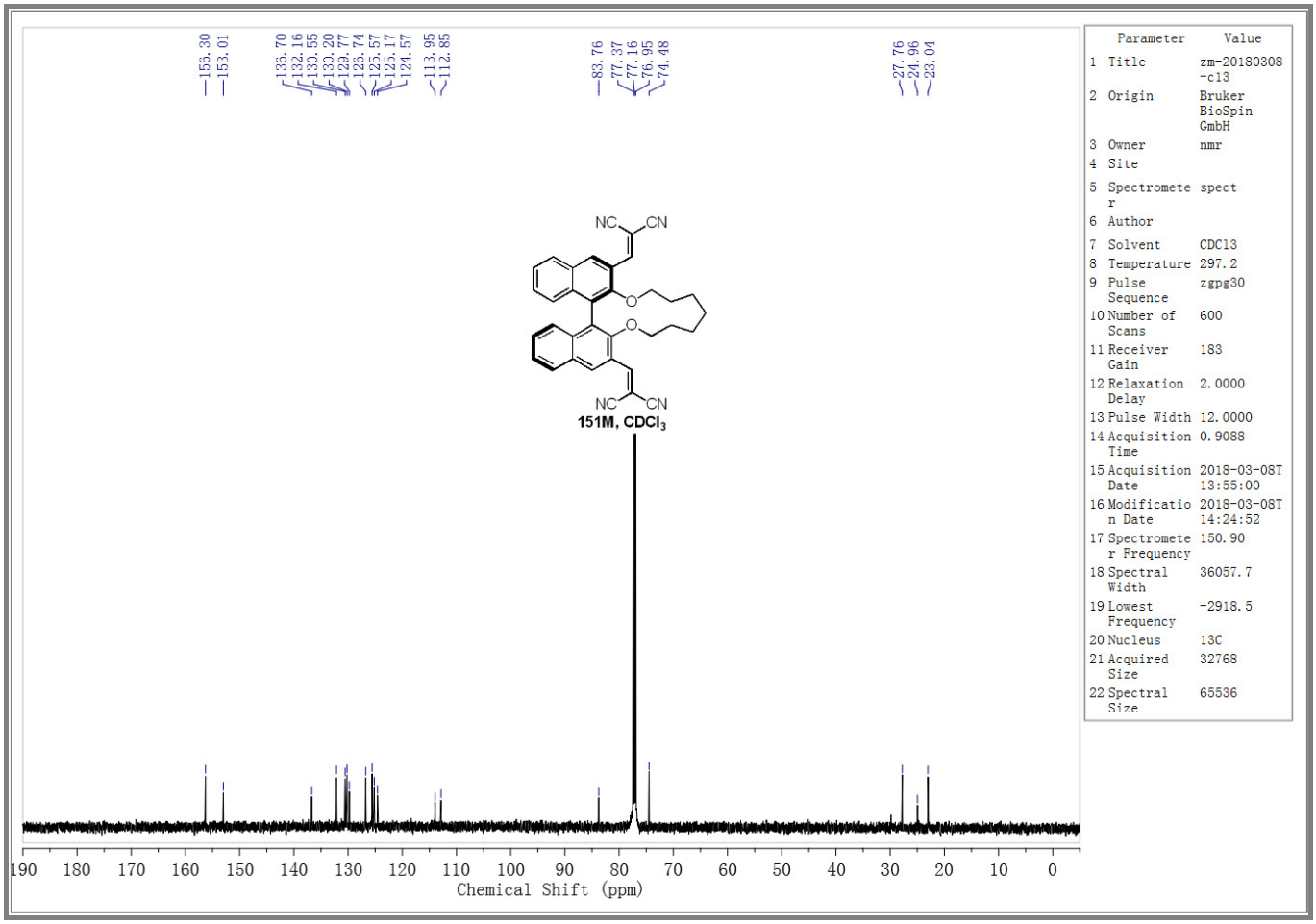


	Parameter	Value
1	Title	BINOL-6C-CN-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.0
10	Pulse Sequence	zgpg30
11	Number of Scans	99
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-15T 10:46:00
17	Modification Date	2017-07-15T 10:50:55
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2921.3
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data

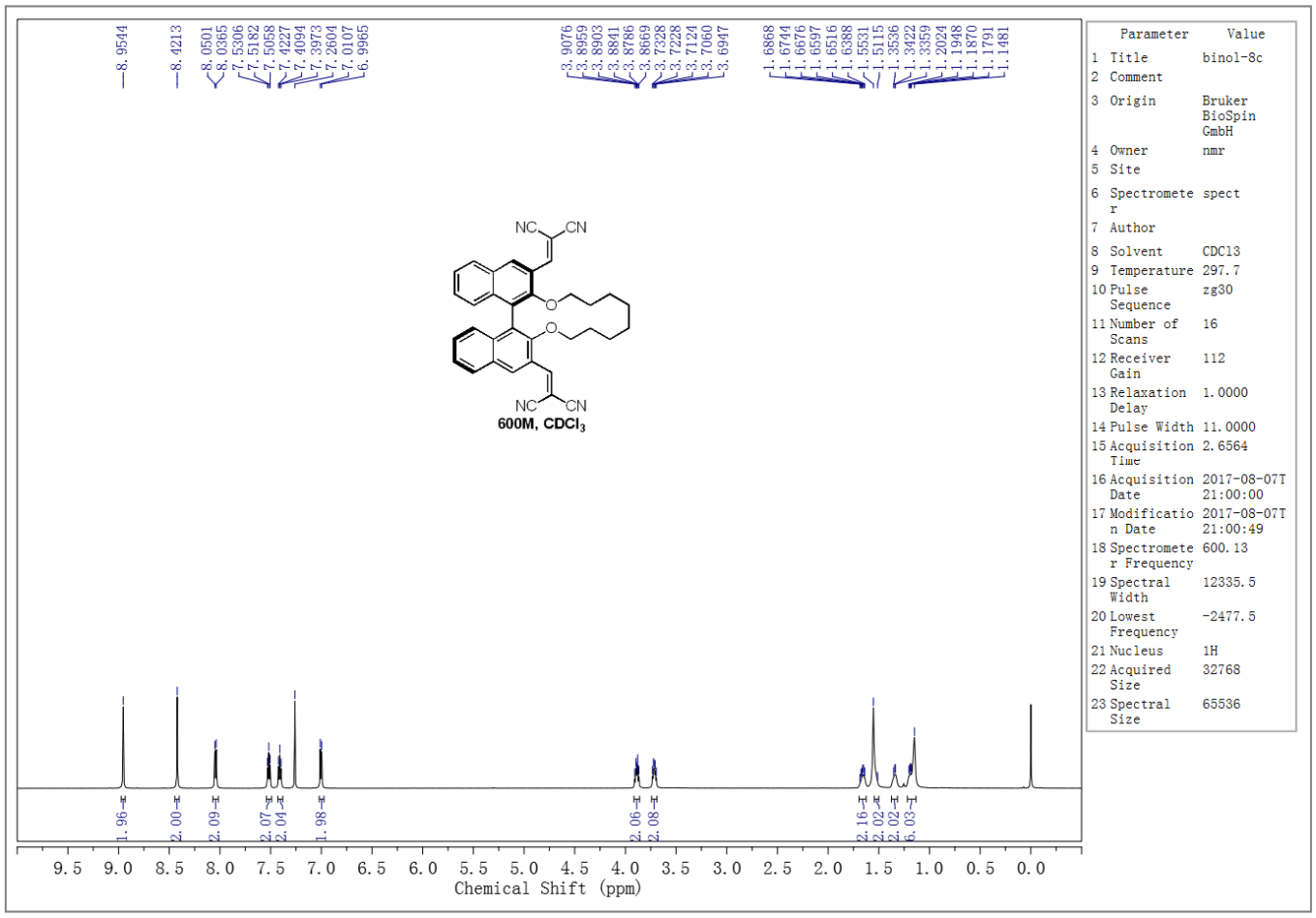


	Parameter	Value
1	Title	zm-20180308
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.2
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	125
12	Relaxation Delay	1.0000
13	Pulse Width	8.0000
14	Acquisition Time	2.6564
15	Acquisition Date	2018-03-08T 13:51:00
16	Modification Date	2018-03-08T 13:51:14
17	Spectrometer Frequency	600.13
18	Spectral Width	12335.5
19	Lowest Frequency	-2478.5
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

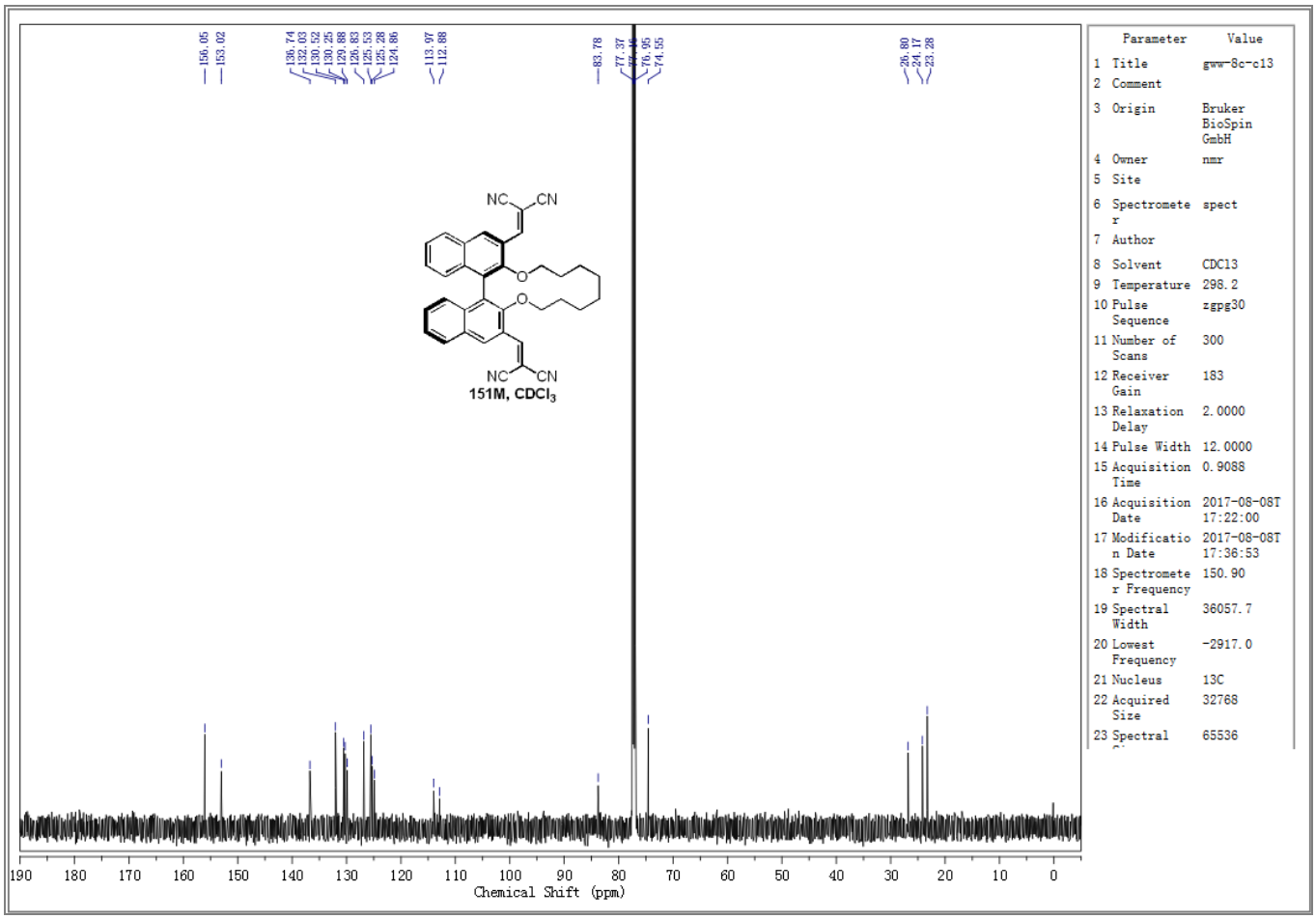


	Parameter	Value
1	Title	zm-20180308 -c13
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	297.2
9	Pulse Sequence	zgpg30
10	Number of Scans	600
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2018-03-08T 13:55:00
16	Modification Date	2018-03-08T 14:24:52
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2918.5
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data X-ray

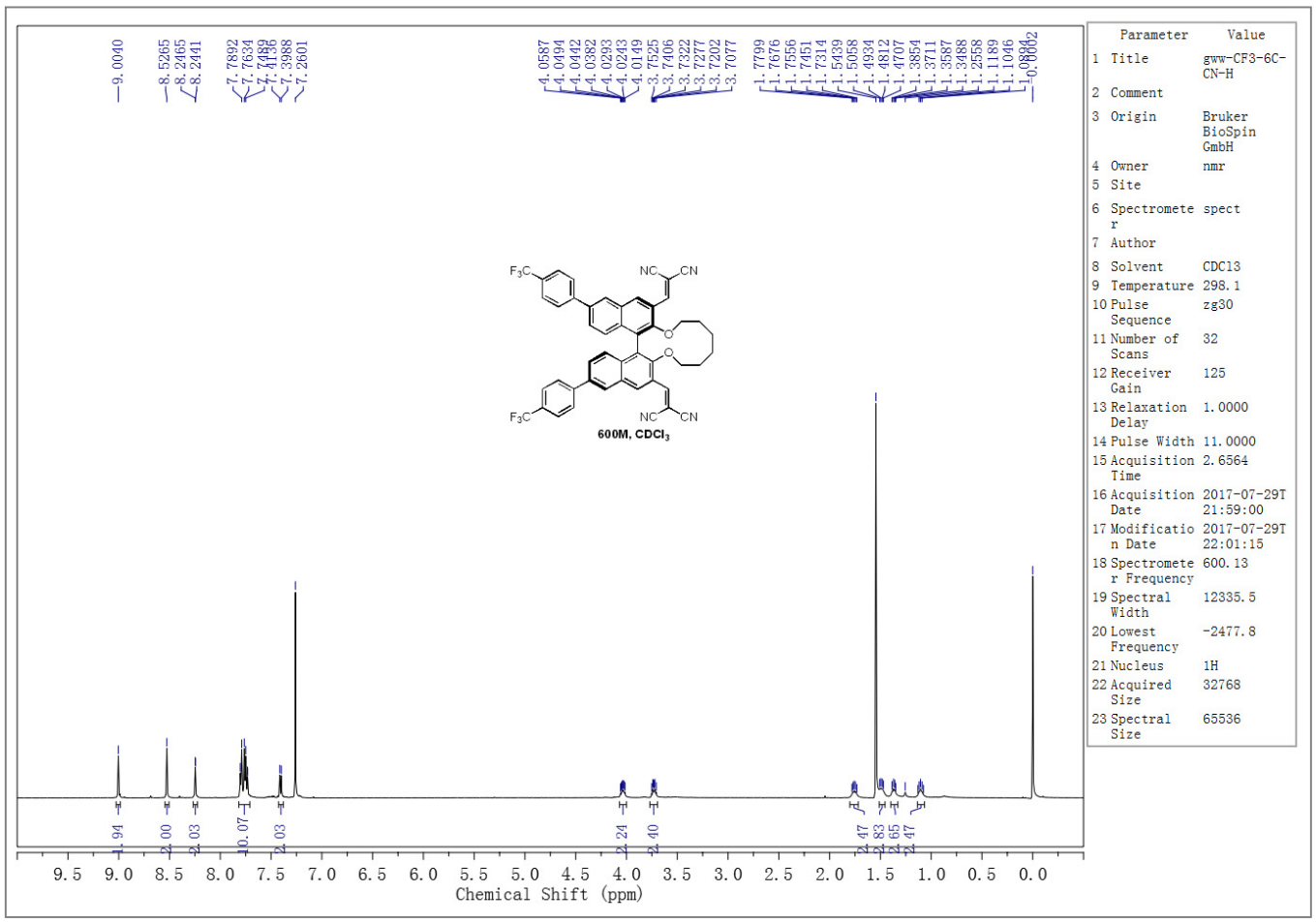


	Parameter	Value
1	Title	binol-8c
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	297.7
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	112
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-08-07T 21:00:00
17	Modification Date	2017-08-07T 21:00:49
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.5
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

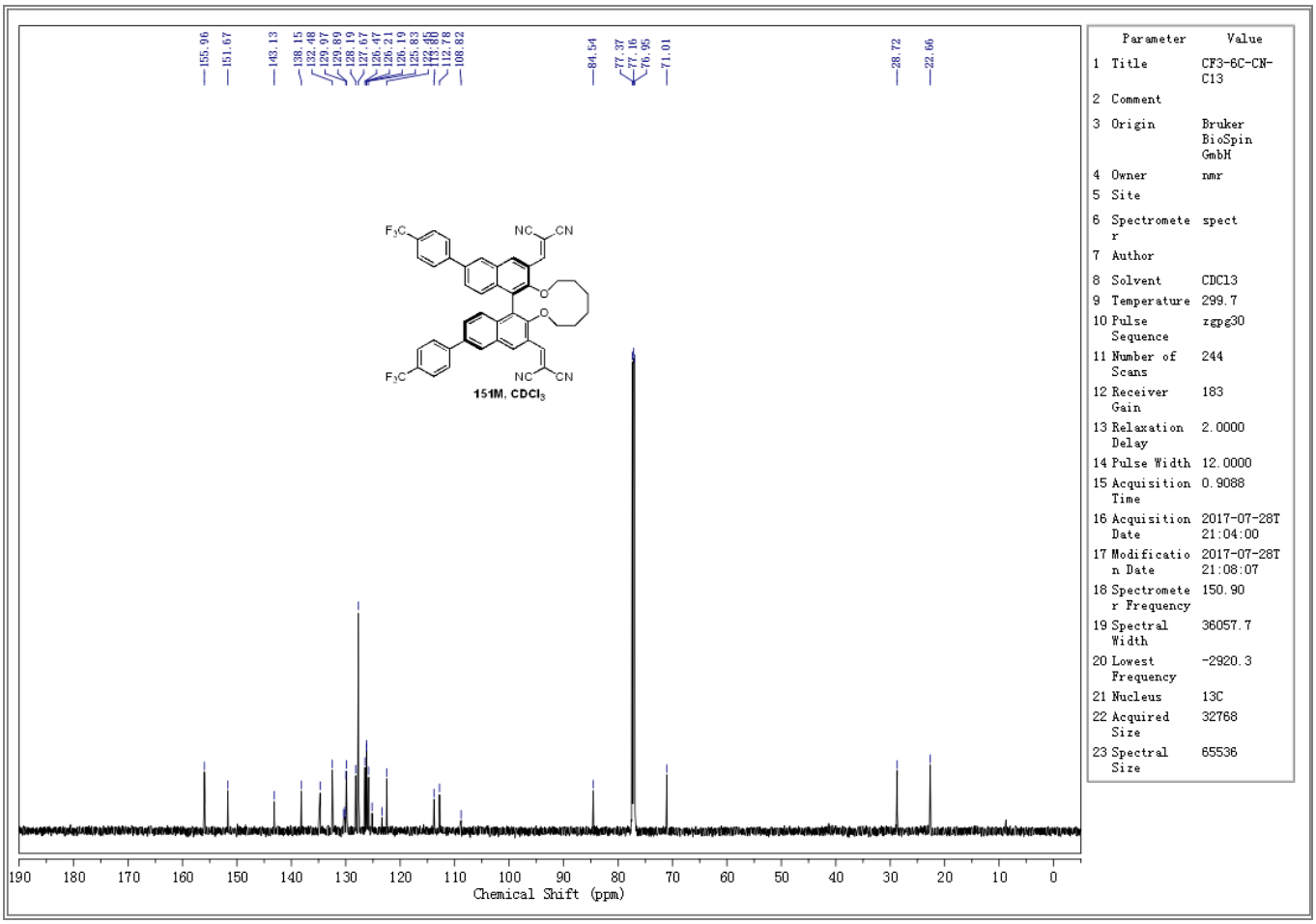


	Parameter	Value
1	Title	gww-8c-c13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.2
10	Pulse Sequence	zgpg30
11	Number of Scans	300
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-08-08T 17:22:00
17	Modification Date	2017-08-08T 17:36:53
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2917.0
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral	65536

Compounds chart Data X-ray

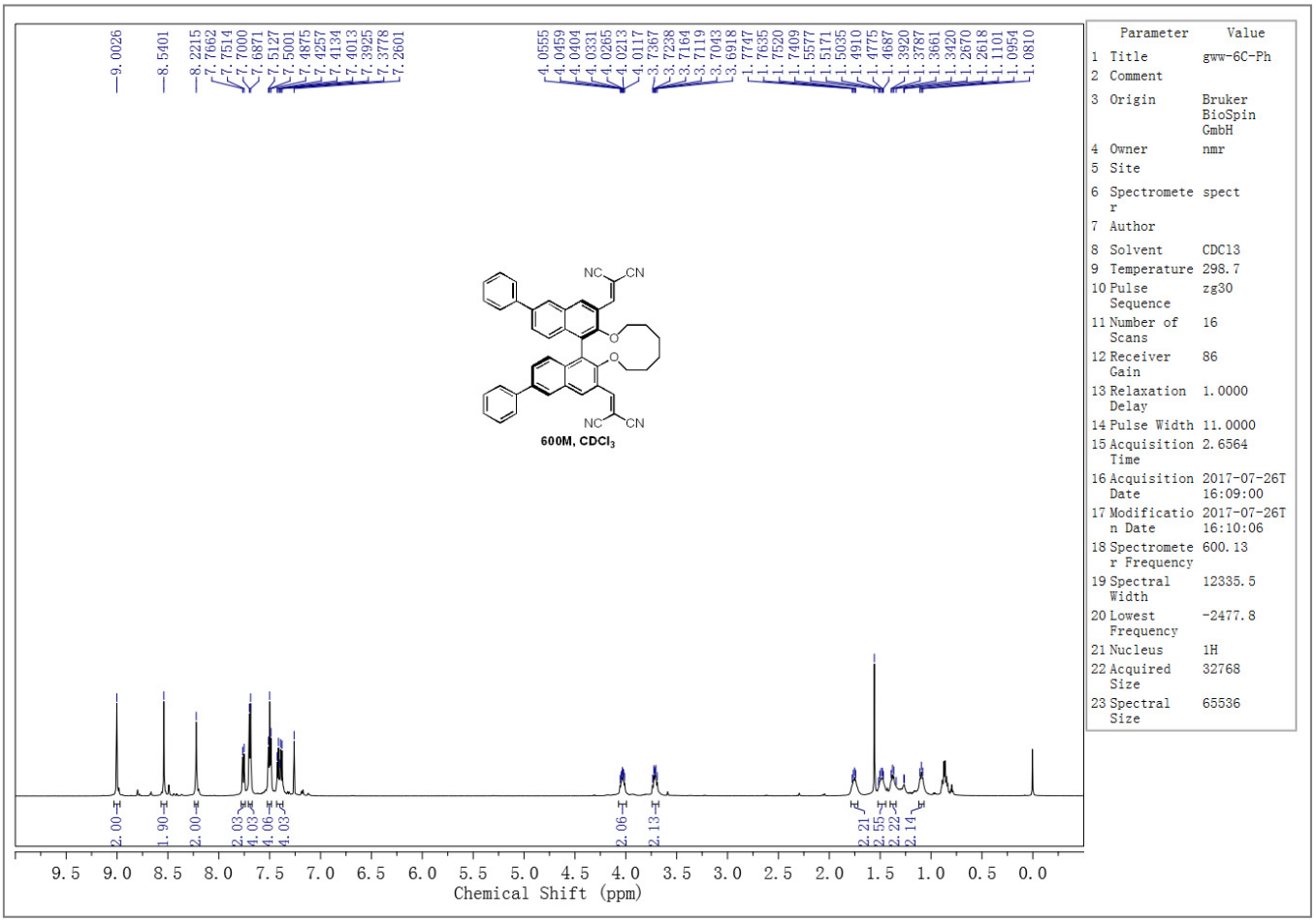


	Parameter	Value
1	Title	gww-CF3-6C-CN-H
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.1
10	Pulse Sequence	zg30
11	Number of Scans	32
12	Receiver Gain	125
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-29T 21:59:00
17	Modification Date	2017-07-29T 22:01:15
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.8
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

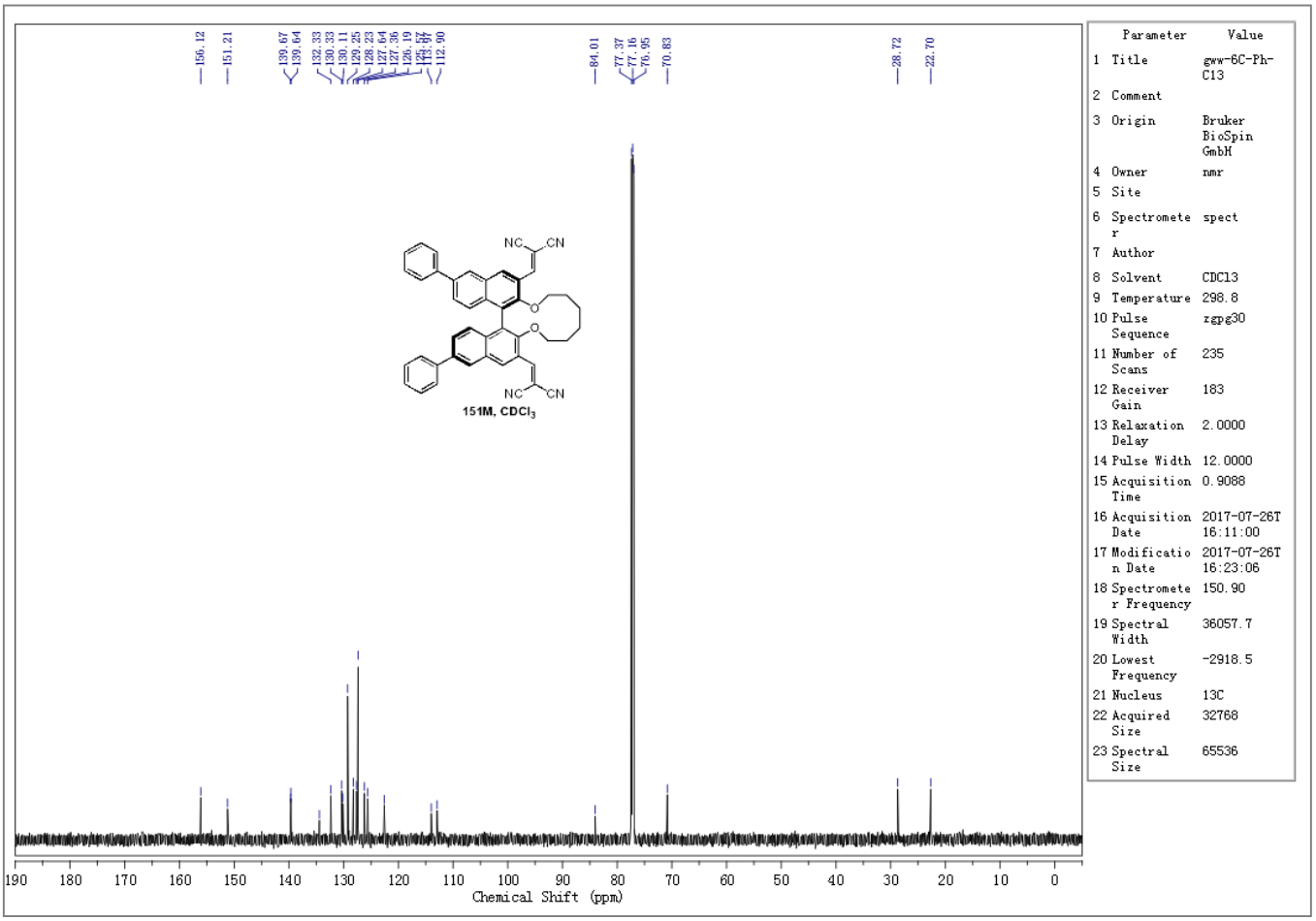


	Parameter	Value
1	Title	CF3-6C-CN-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.7
10	Pulse Sequence	zgpg30
11	Number of Scans	244
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-28T 21:04:00
17	Modification Date	2017-07-28T 21:08:07
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2920.3
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data X-ray

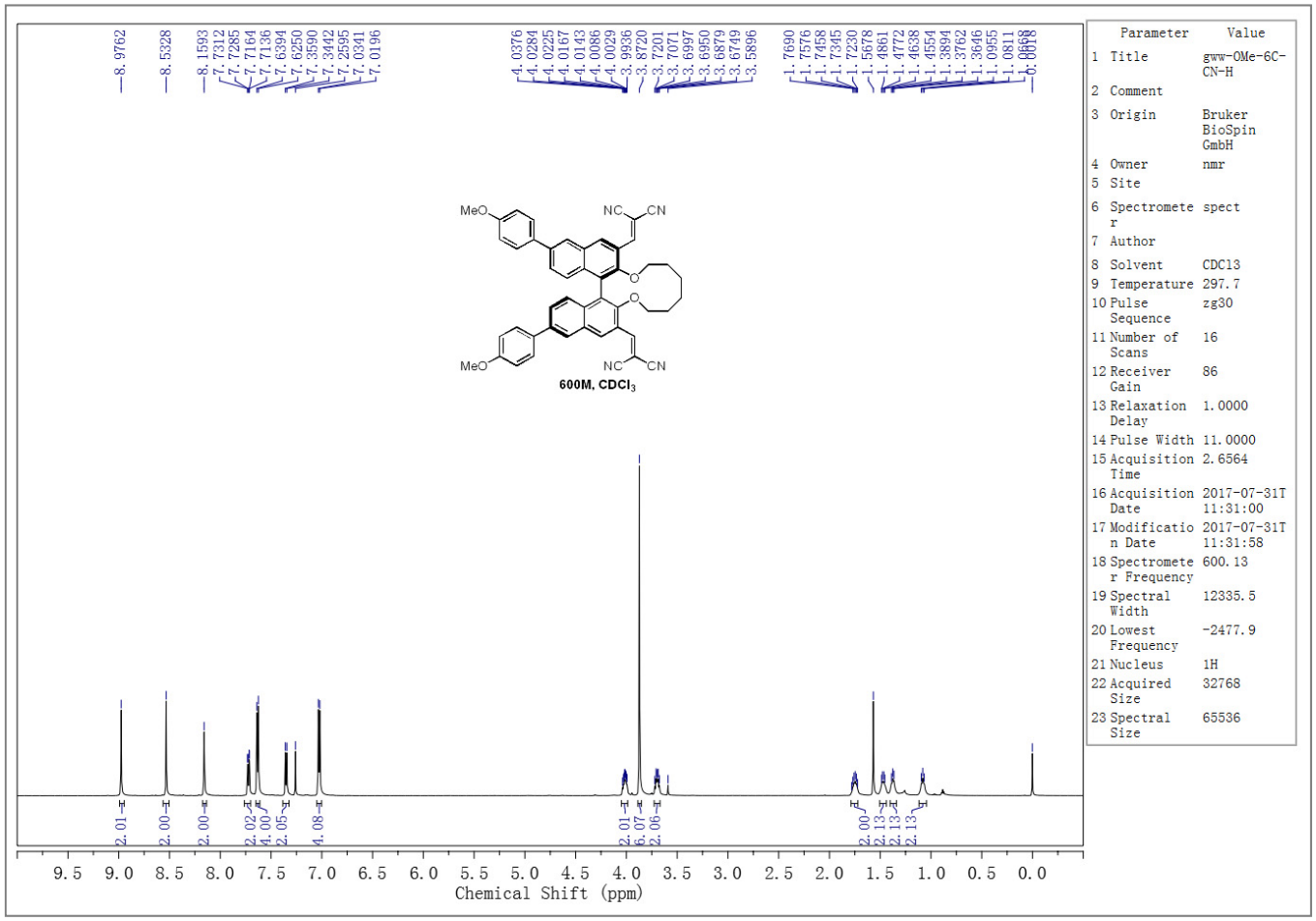


	Parameter	Value
1	Title	gww-6C-Ph
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.7
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	86
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-26T 16:09:00
17	Modification Date	2017-07-26T 16:10:06
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.8
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

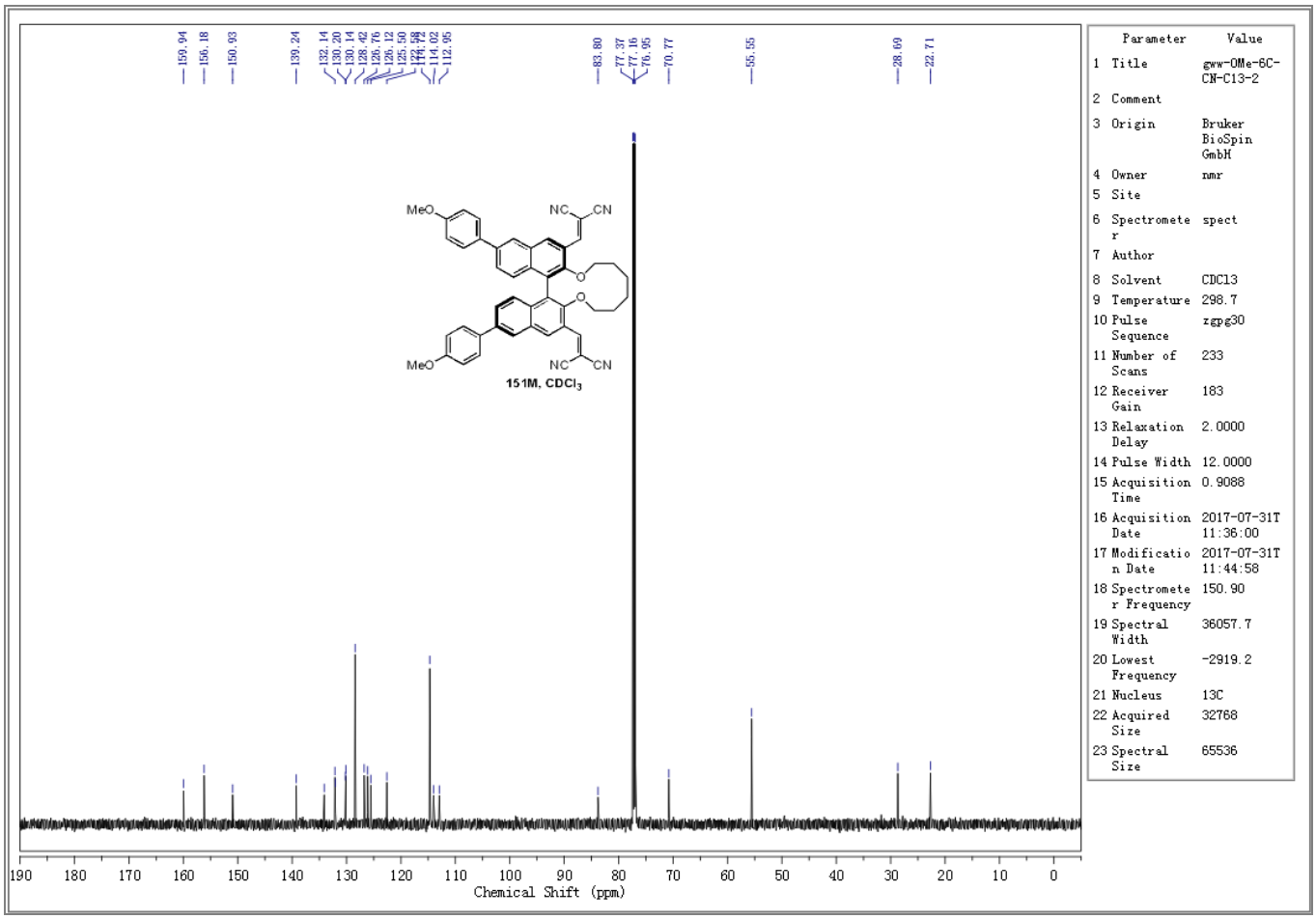


	Parameter	Value
1	Title	gww-6C-Ph-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.8
10	Pulse Sequence	zgpg30
11	Number of Scans	235
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-26T 16:11:00
17	Modification Date	2017-07-26T 16:23:06
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2918.5
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data

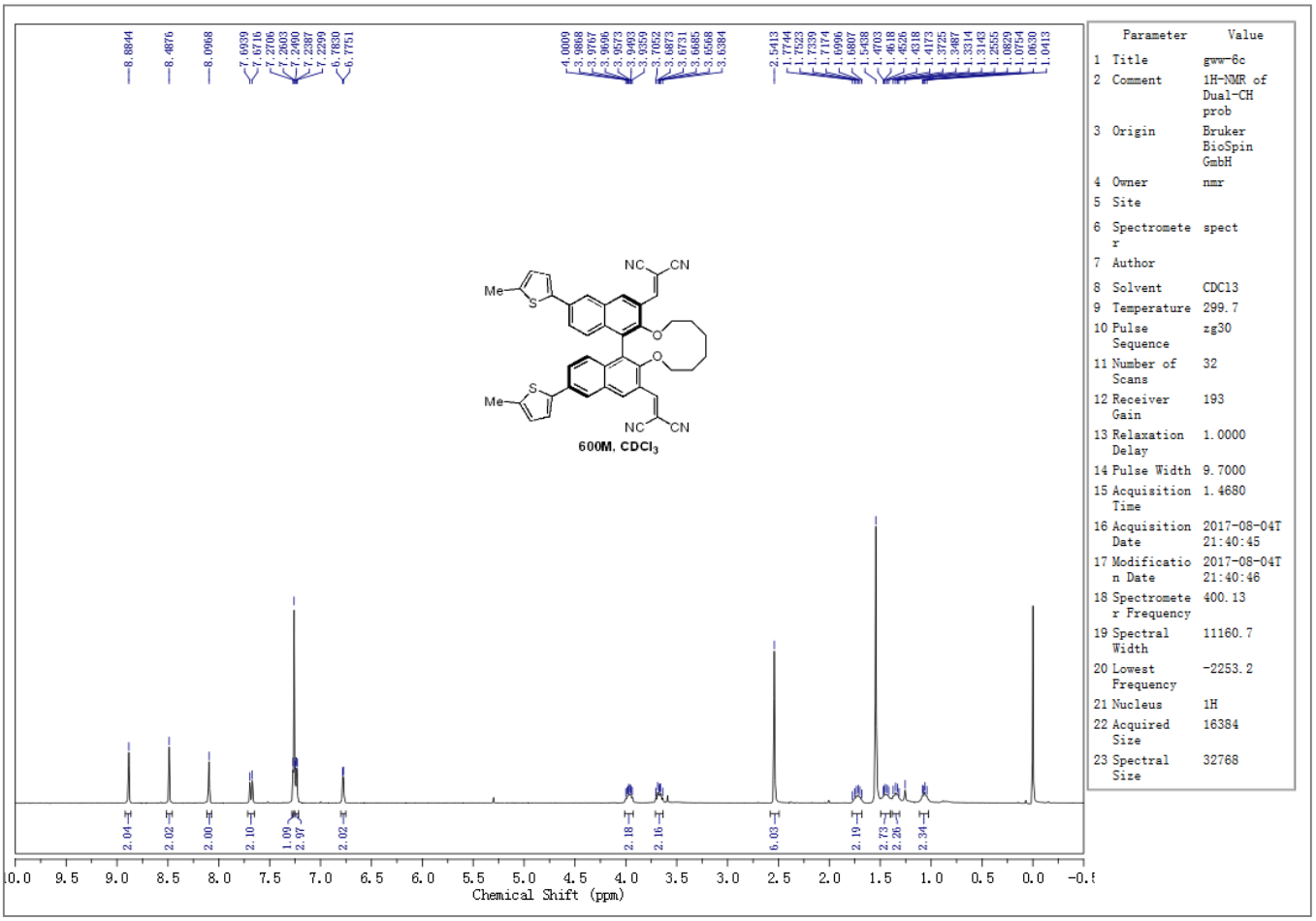


	Parameter	Value
1	Title	gww-OMe-6C-CN-H
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	297.7
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	86
13	Relaxation Delay	1.0000
14	Pulse Width	11.0000
15	Acquisition Time	2.6564
16	Acquisition Date	2017-07-31T 11:31:00
17	Modification Date	2017-07-31T 11:31:58
18	Spectrometer Frequency	600.13
19	Spectral Width	12335.5
20	Lowest Frequency	-2477.9
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

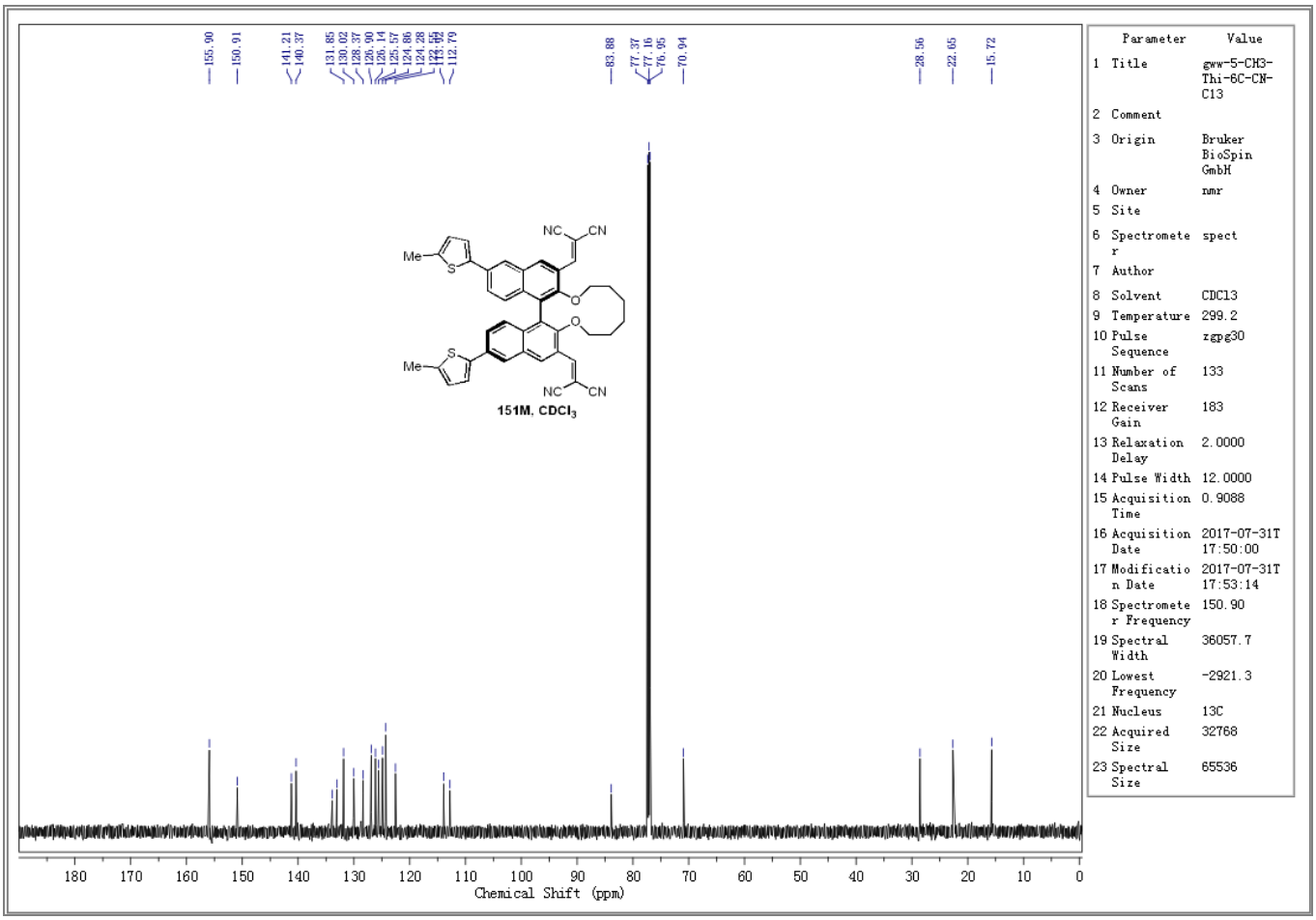


	Parameter	Value
1	Title	gww-OMe-6C-CN-C13-2
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	298.7
10	Pulse Sequence	zgpg30
11	Number of Scans	233
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-31T 11:36:00
17	Modification Date	2017-07-31T 11:44:58
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2919.2
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data

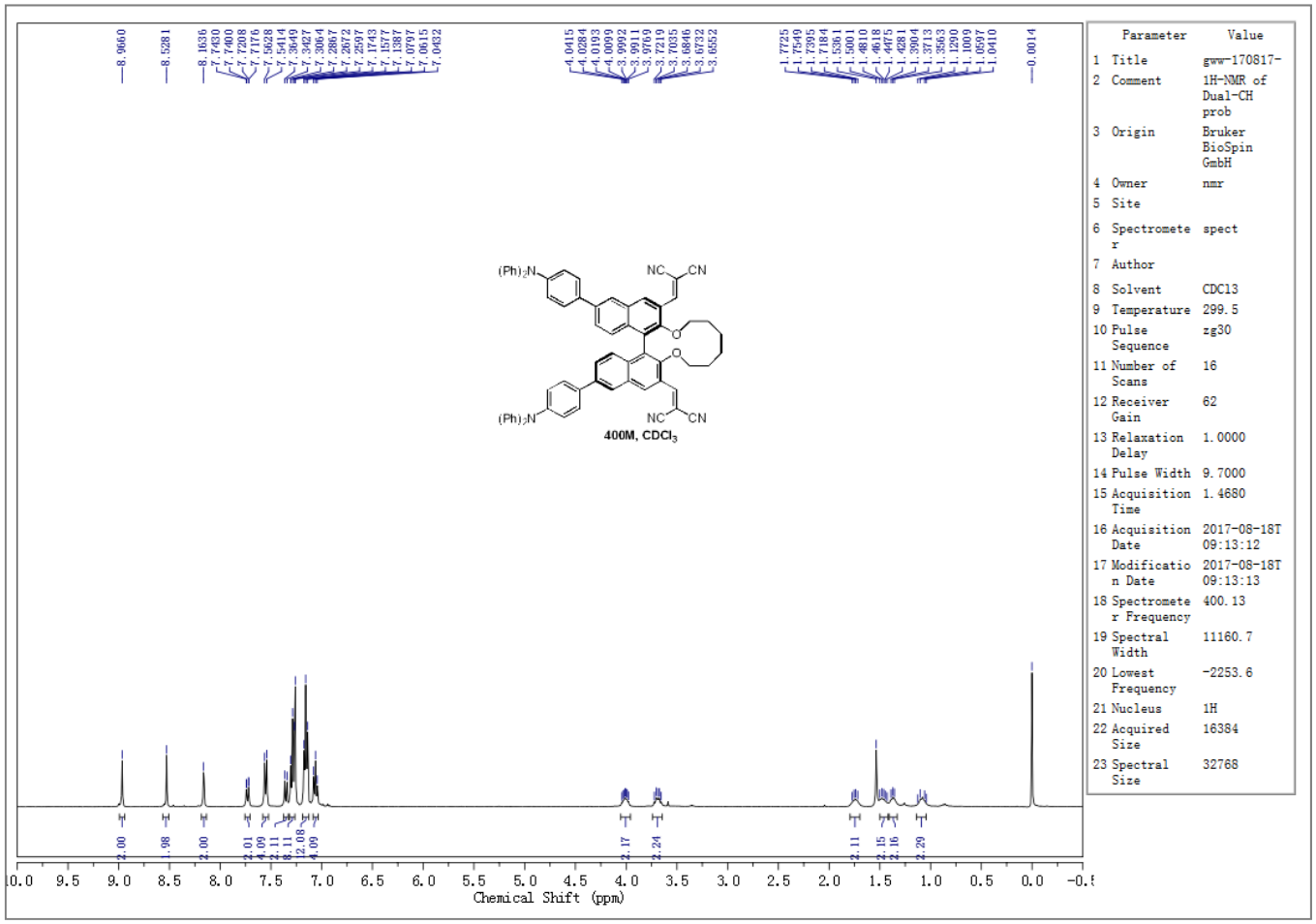


	Parameter	Value
1	Title	gww-6c
2	Comment	1H-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.7
10	Pulse Sequence	zg30
11	Number of Scans	32
12	Receiver Gain	193
13	Relaxation Delay	1.0000
14	Pulse Width	9.7000
15	Acquisition Time	1.4680
16	Acquisition Date	2017-08-04T 21:40:45
17	Modification Date	2017-08-04T 21:40:46
18	Spectrometer Frequency	400.13
19	Spectral Width	11160.7
20	Lowest Frequency	-2253.2
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	32768

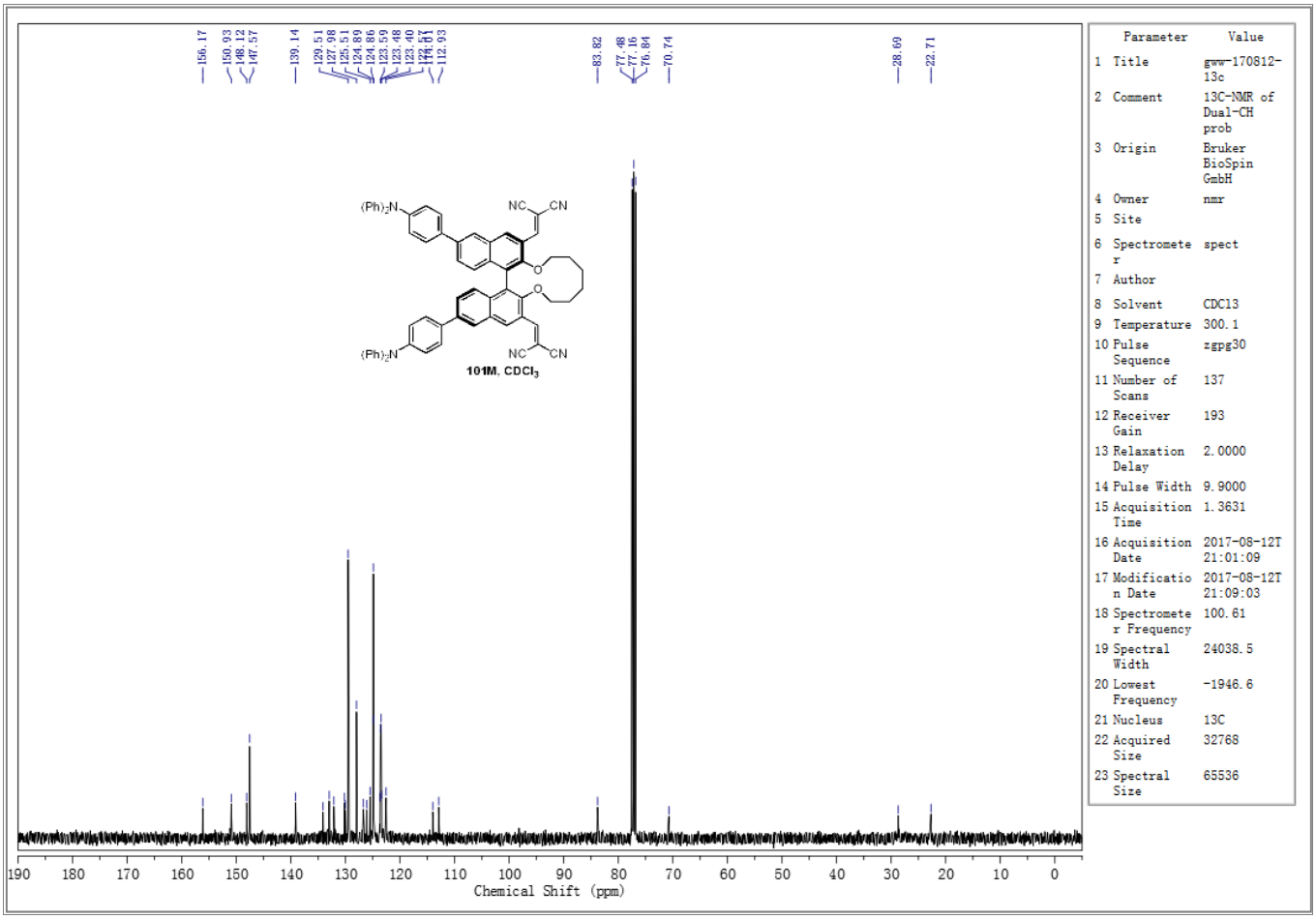


	Parameter	Value
1	Title	gww-5-CH3-Thi-6C-CN-C13
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.2
10	Pulse Sequence	zgpg30
11	Number of Scans	133
12	Receiver Gain	183
13	Relaxation Delay	2.0000
14	Pulse Width	12.0000
15	Acquisition Time	0.9088
16	Acquisition Date	2017-07-31T 17:50:00
17	Modification Date	2017-07-31T 17:53:14
18	Spectrometer Frequency	150.90
19	Spectral Width	36057.7
20	Lowest Frequency	-2921.3
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data

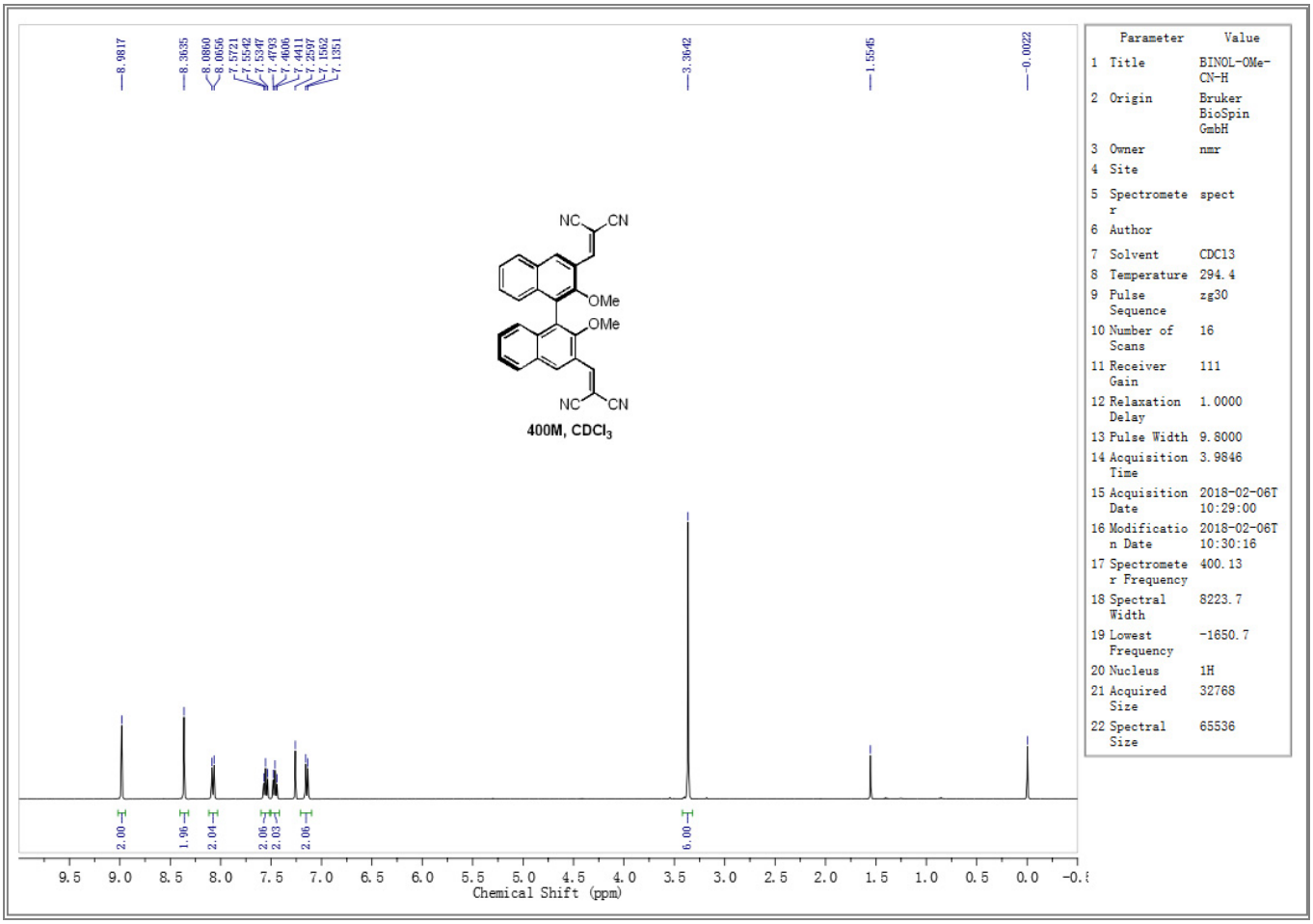


	Parameter	Value
1	Title	gww-170817-
2	Comment	1H-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	299.5
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	62
13	Relaxation Delay	1.0000
14	Pulse Width	9.7000
15	Acquisition Time	1.4680
16	Acquisition Date	2017-08-18T 09:13:12
17	Modification Date	2017-08-18T 09:13:13
18	Spectrometer Frequency	400.13
19	Spectral Width	11160.7
20	Lowest Frequency	-2253.6
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	32768

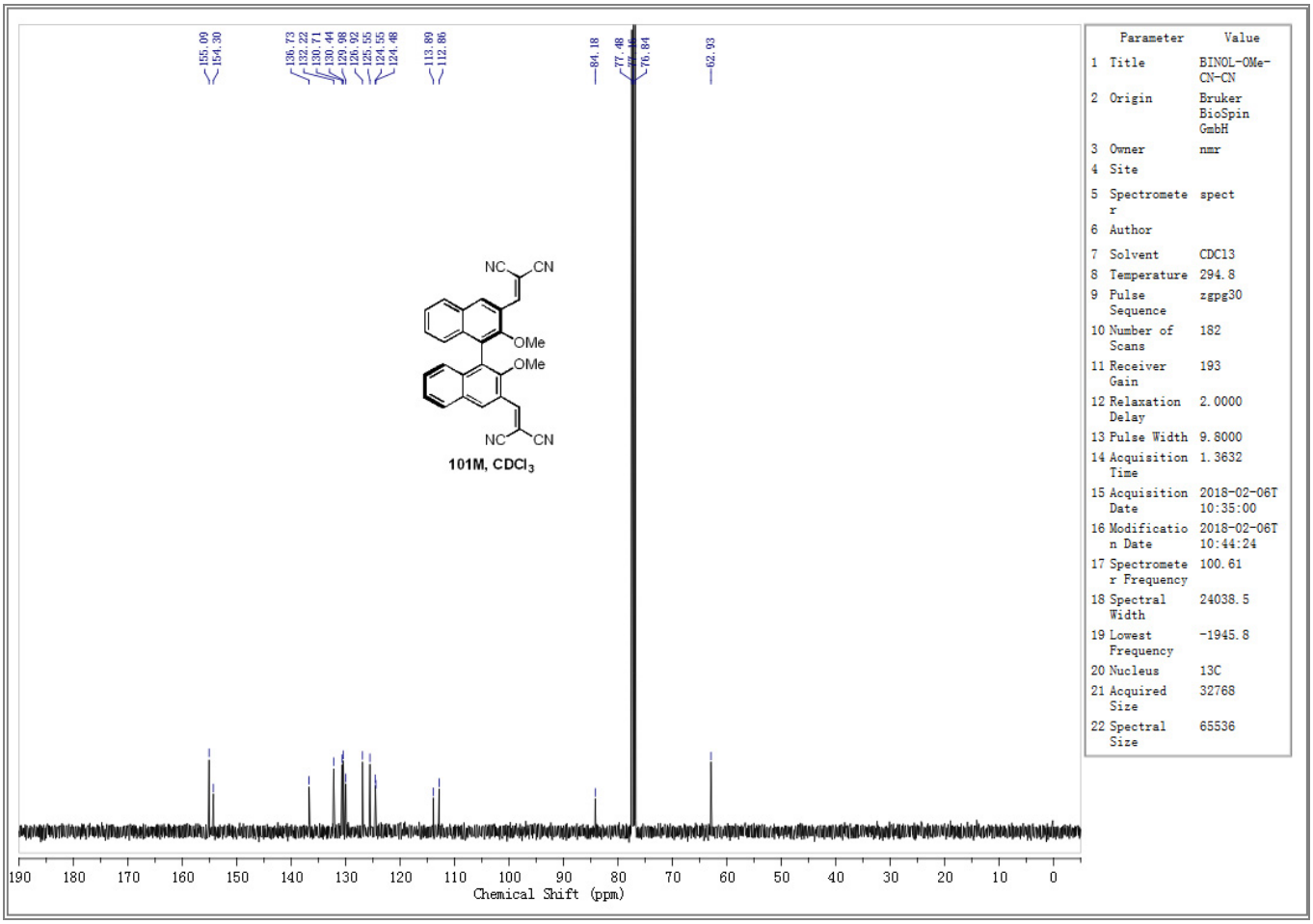


	Parameter	Value
1	Title	gww-170812-13c
2	Comment	13C-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	300.1
10	Pulse Sequence	zgpg30
11	Number of Scans	137
12	Receiver Gain	193
13	Relaxation Delay	2.0000
14	Pulse Width	9.9000
15	Acquisition Time	1.3631
16	Acquisition Date	2017-08-12T 21:01:09
17	Modification Date	2017-08-12T 21:09:03
18	Spectrometer Frequency	100.61
19	Spectral Width	24038.5
20	Lowest Frequency	-1946.6
21	Nucleus	13C
22	Acquired Size	32768
23	Spectral Size	65536

Compounds chart Data

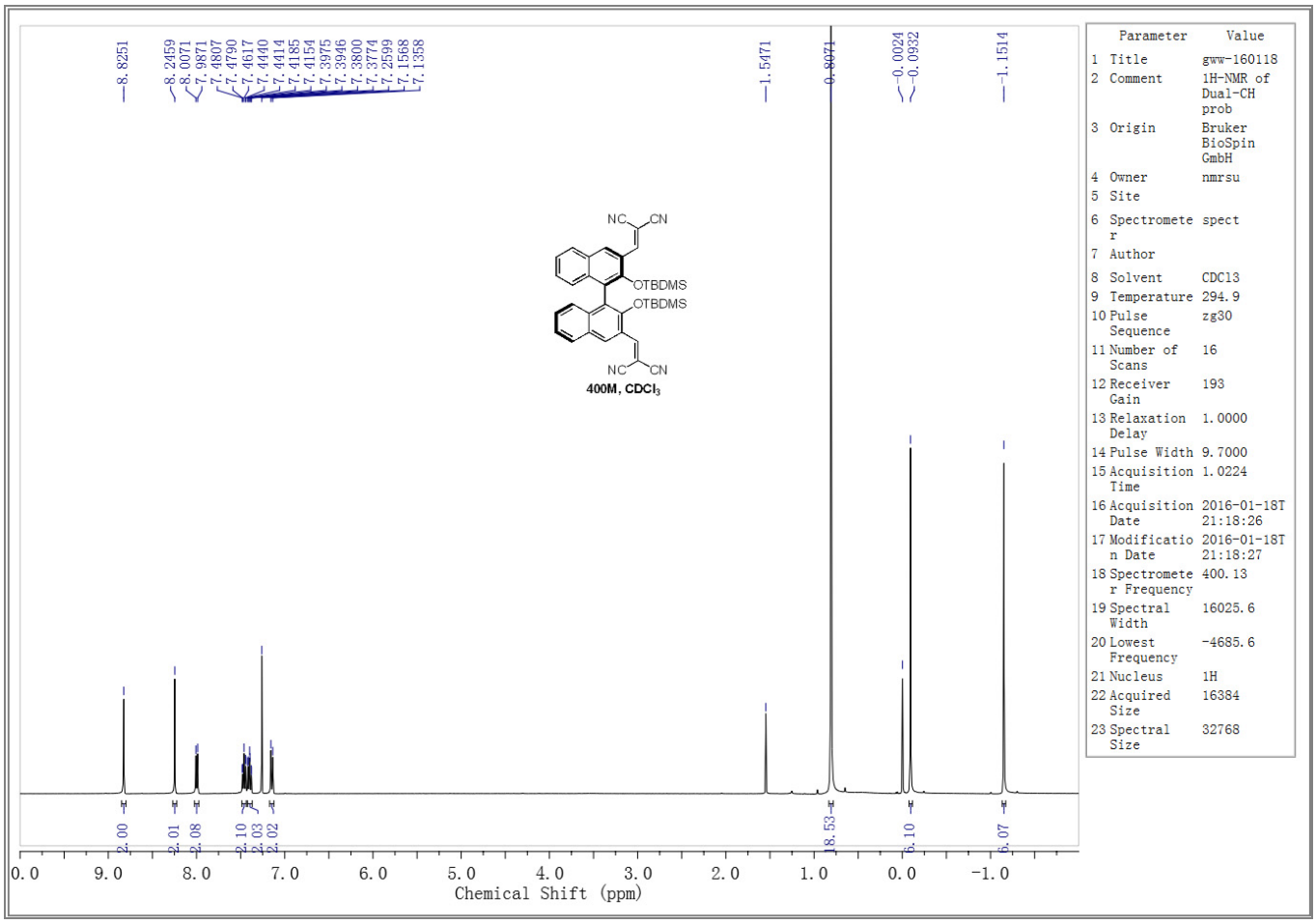


	Parameter	Value
1	Title	BINOL-OMe-CN-H
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	294.4
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	111
12	Relaxation Delay	1.0000
13	Pulse Width	9.8000
14	Acquisition Time	3.9846
15	Acquisition Date	2018-02-06T 10:29:00
16	Modification Date	2018-02-06T 10:30:16
17	Spectrometer Frequency	400.13
18	Spectral Width	8223.7
19	Lowest Frequency	-1650.7
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

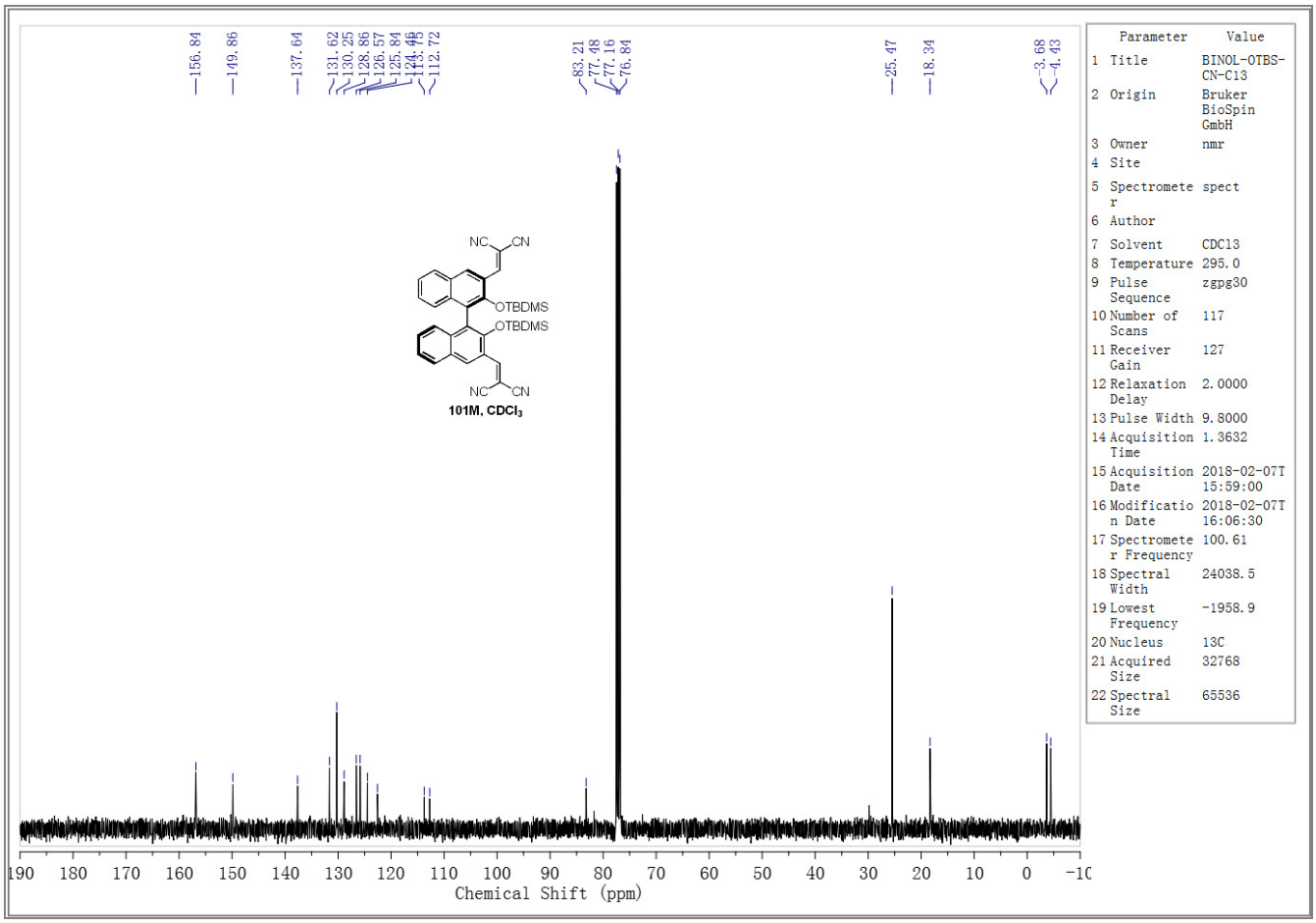


	Parameter	Value
1	Title	BINOL-OMe-CN-CN
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	294.8
9	Pulse Sequence	zgpg30
10	Number of Scans	182
11	Receiver Gain	193
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	1.3632
15	Acquisition Date	2018-02-06T 10:35:00
16	Modification Date	2018-02-06T 10:44:24
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1945.8
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data

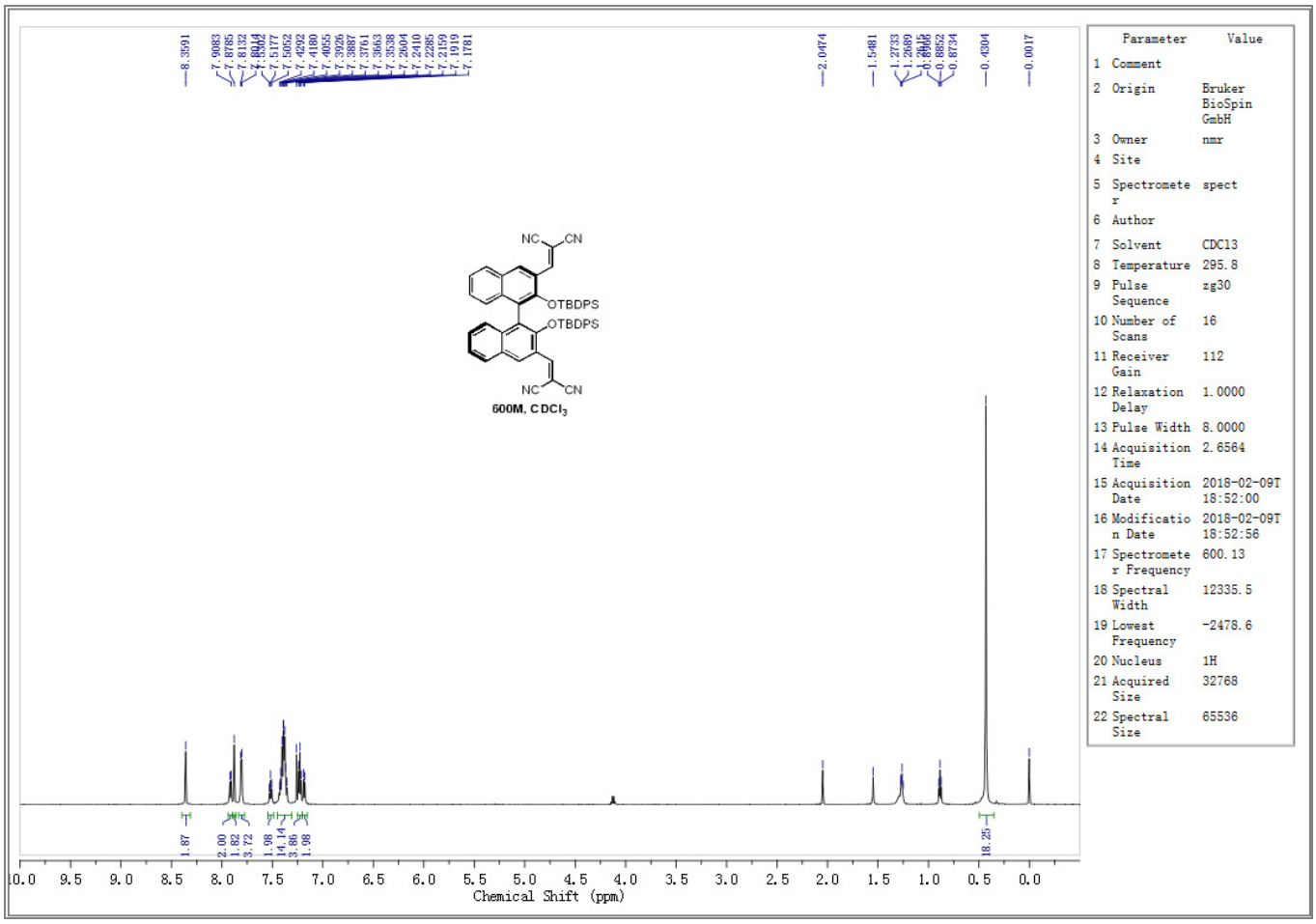


	Parameter	Value
1	Title	gww-160118
2	Comment	1H-NMR of Dual-CH prob
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	294.9
10	Pulse Sequence	zg30
11	Number of Scans	16
12	Receiver Gain	193
13	Relaxation Delay	1.0000
14	Pulse Width	9.7000
15	Acquisition Time	1.0224
16	Acquisition Date	2016-01-18T 21:18:26
17	Modification Date	2016-01-18T 21:18:27
18	Spectrometer Frequency	400.13
19	Spectral Width	16025.6
20	Lowest Frequency	-4685.6
21	Nucleus	1H
22	Acquired Size	16384
23	Spectral Size	32768

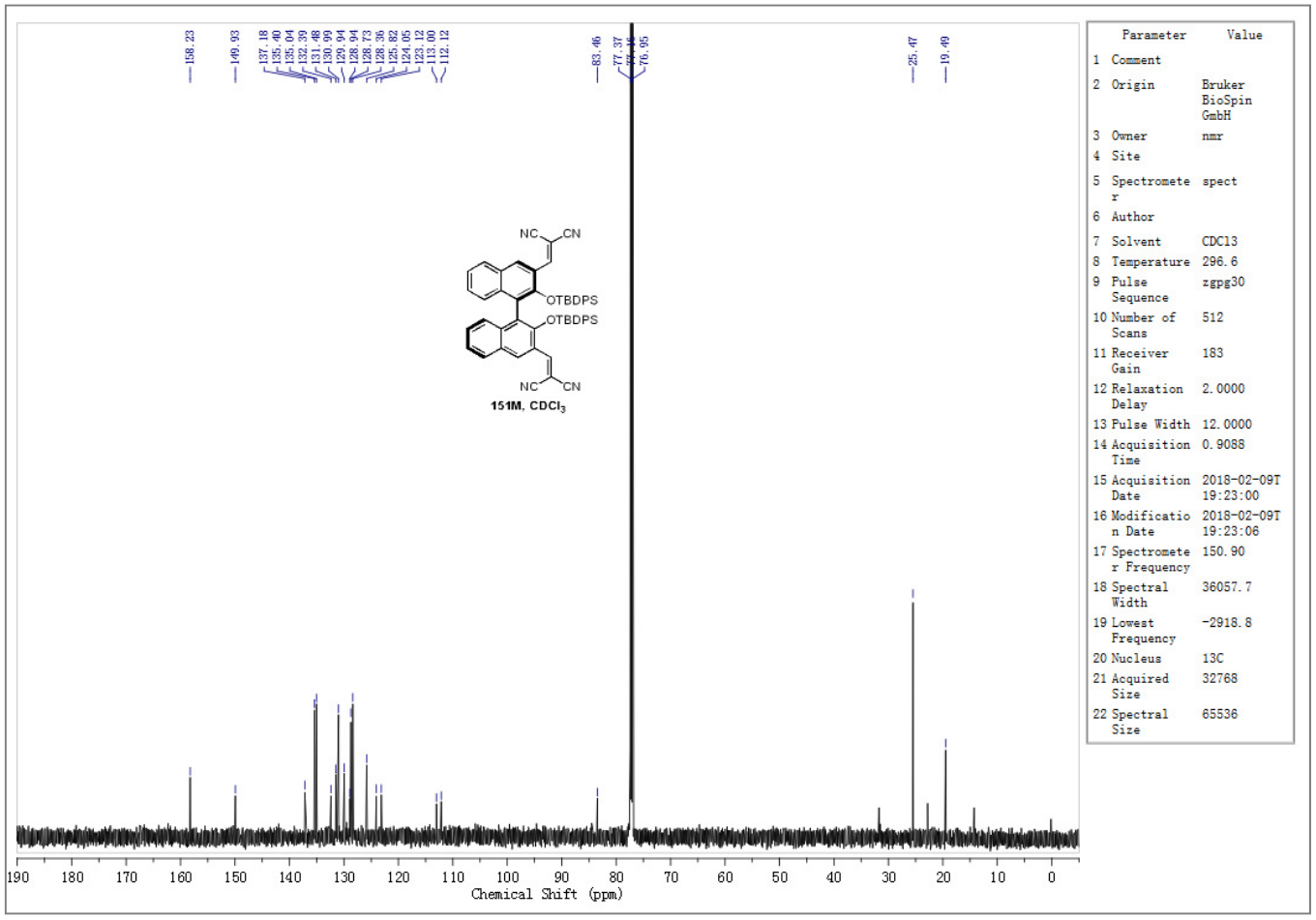


	Parameter	Value
1	Title	BINOL-OTBS-CN-C13
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	295.0
9	Pulse Sequence	zgpg30
10	Number of Scans	117
11	Receiver Gain	127
12	Relaxation Delay	2.0000
13	Pulse Width	9.8000
14	Acquisition Time	1.3632
15	Acquisition Date	2018-02-07T 15:59:00
16	Modification Date	2018-02-07T 16:06:30
17	Spectrometer Frequency	100.61
18	Spectral Width	24038.5
19	Lowest Frequency	-1958.9
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data



	Parameter	Value
1	Comment	
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	295.8
9	Pulse Sequence	zg30
10	Number of Scans	16
11	Receiver Gain	112
12	Relaxation Delay	1.0000
13	Pulse Width	8.0000
14	Acquisition Time	2.6564
15	Acquisition Date	2018-02-09T 18:52:00
16	Modification Date	2018-02-09T 18:52:56
17	Spectrometer Frequency	600.13
18	Spectral Width	12335.5
19	Lowest Frequency	-2478.6
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



	Parameter	Value
1	Comment	
2	Origin	Bruker BioSpin GmbH
3	Owner	nmr
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl3
8	Temperature	296.6
9	Pulse Sequence	zgpg30
10	Number of Scans	512
11	Receiver Gain	183
12	Relaxation Delay	2.0000
13	Pulse Width	12.0000
14	Acquisition Time	0.9088
15	Acquisition Date	2018-02-09T 19:23:00
16	Modification Date	2018-02-09T 19:23:06
17	Spectrometer Frequency	150.90
18	Spectral Width	36057.7
19	Lowest Frequency	-2918.8
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536

Compounds chart Data