

Blue Fluorescent Dihydro-indenoindene Derivatives with Unusual Low Oxidation Potentials for Multifunctional OLEDs Materials

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SUPPLEMENTARY INFORMATION

(23 pages)

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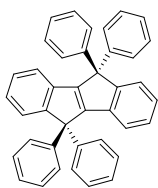
General information

All reactions regarding air or moisture sensitive compounds were performed in dry reaction vessels under nitrogen or argon atmosphere. Analytical thin-layer chromatography (TLC) was performed on Merck 60 F₂₅₄ silica gel plates, indicated by UVP UVGC-25 Compact UV Lamp. Visualization was accomplished with UV light. Fractional flash column chromatography was carried out using 32-63 μm silica gel.

Materials All reagents were purchased from Acros Organic, Sigma-Aldrich, TCI, or Alfa-Aesar, used directly without further purification. Solvents used for experiments were reagent grade unless mentioned elsewhere. Diethyl ether and toluene were advanced dried over Na with benzophenone-ketyl intermediate as an indicator.

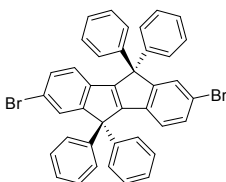
Instruments ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE III HD (600 MHz ^1H , 150 MHz ^{13}C) spectrometer in CD_2Cl_2 with tetramethylsilane or CH_2Cl_2 as an internal reference. Chemical shifts (δ) and coupling constants (J) are reported in ppm and Hz, respectively. Splitting patterns are described as following: doublet, d; triplet, t; quartet, q; multiplet, m. Data are reported as δ (splitting pattern, J). Mass and High-resolution mass spectra were recorded on LCQ Advantage GC/LC/MS and Finnigan MAT 95S spectrometers. Data are reported in m/z . Combustion analyses were performed on a PerkinElmer 2400-CHN analyzer by the Northern Instrument Center of Taiwan. Absorption spectra were measured on a Thermo Scientific Evolution 60S spectrophotometer using spectrophotometric CH_2Cl_2 . Upon excitation, emission spectra were measured on a JASCO FP-6500 fluorescence spectrometer in the same solutions. Fluorescence quantum yields were measured using Coumarin 1 (99% in EtOAc)¹ as a standard. Cyclic voltammetry (CV) experiments were performed in dichloromethane solutions containing 0.1 M tetrabutylammonium perchlorate as a supporting electrolyte on a CHI 611D Electrochemical analyzer. Platinum, carbon, and Ag/AgCl electrodes were used as counter, working, and reference electrodes respectively. Differential scanning calorimetry (DSC) analyses were performed on a METTLER TOLEDO DSC 1 differential scanning calorimeter. Sample was heated (10 $^\circ\text{C}/\text{min}$) to melt and then cooled rapidly by liquid nitrogen. Melting point was obtained during the heating progress. T_g was recorded during the second round of heating (10 $^\circ\text{C}/\text{min}$). Thermogravimetric analyses (TGA) were performed on a PerkinElmer Pyris 1 TGA thermogravimetric analyzer.

5,5,10,10-Tetraphenyl-5,10-dihydroindeno[2,1-a]indene (1)



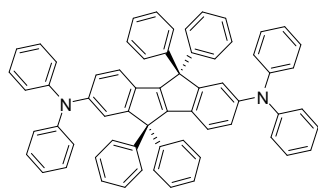
To a 250 mL, three-necked, round-bottomed flask was placed a solution of (Z)-2,2'-dibromostilbene² (6761 mg, 20 mmol) in diethyl ether (100 mL). The reaction flask was cooled to 0 °C, and *n*-BuLi (1.6 M in hexanes, 27.5 mL, 44 mmol) was added dropwise. It was stirred at this temperature for 30 minutes followed by adding a solution of benzophenone (8018 mg, 44 mmol) in diethyl ether (20 mL). The resulting mixture was gradually warmed to ambient temperature and then quenched with saturated NaHCO₃ (aq) (50 mL). After filtration, the precipitants were washed by distilled water (100 mL) and hexanes (100 mL), and then dried under reduce pressure. The crude residue dissolved in acetic acid (50 mL) was placed in another 100 mL, two-necked, round-bottomed flask. HCl (12 N, 36 μL, 1 mmol) was then added and the reaction mixture was refluxed for 2 hours. After cooling to ambient temperature, saturated NaHCO₃ (aq) (50 mL) was added again and stirred vigorously for 20 minutes. The precipitation was filtered and the yellow solids were washed by distilled water (100 mL), methanol (100 mL), and hexanes (100 mL) in turn, and then dried under reduce pressure to give **1**, which was further re-crystallized from CH₂Cl₂ to afford 2441 mg of pure **1** (24 %): *T*_m 376 °C (DSC); M.W.: 508.65; ¹H NMR (600 MHz, CDCl₃) δ 7.42 (dd, *J* = 6.8, 1.8, 2H), 7.30-7.23 (m, 20H), 7.18-7.11 (m, 6H); ¹³C NMR (150 MHz, CD₂Cl₂) δ 157.7, 155.7, 143.0, 138.6, 128.7, 128.6, 127.4, 127.3, 126.2, 125.3, 121.1, 63.4; EI-MS (negative) calcd for C₄₀H₂₈ [M⁻]: 508.2, found: 508.3; TLC R_f 0.75 (CH₂Cl₂/hexanes, 1/3).

2,7-Dibromo-5,5,10,10-tetraphenyl-5,10-dihydroindeno[2,1-a]indene (2)³



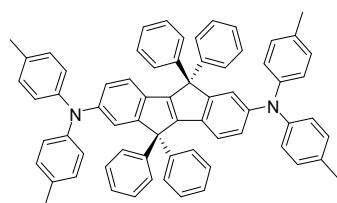
To a 250 mL, three-necked, round-bottomed flask was placed a suspension of **1** (1017 mg, 2 mmol), CuBr₂ (3350 mg, 15 mmol), and Al₂O₃ (10050 mg) in CCl₄ (20 mL). The reaction mixture was heated to reflux for 16 hours. After cooling to ambient temperature, the excess amount of CuBr₂ and Al₂O₃ were filtered thru Celite. The filtrate was evaporated under reduce pressure and re-crystallized from toluene to afford 1093 mg of pure **2** (82 %): *T*_m 393 °C (DSC); M.W.: 666.44; ¹H NMR (600 MHz, CD₂Cl₂) δ 7.54 (d, *J* = 1.7, 2H), 7.31-7.24 (m, 22H), 7.03 (d, *J* = 8.2, 2H); ¹³C NMR (150 MHz, CD₂Cl₂) δ 159.6, 155.2, 141.8, 137.3, 130.7, 129.0, 128.7, 128.5, 127.7, 122.3, 120.4, 63.6; TLC R_f 0.70 (CH₂Cl₂/hexanes, 1/3); Anal. Calcd for C₄₀H₂₆Br₂: C, 72.09, H, 3.93. Found: C, 72.30, H, 3.94.

2,7-Bis(*N,N*,-diphenylamino)-5,5,10,10-octaphenyl-5,10-dihydroindeno[2,1-*a*]indene (**3a**)⁴



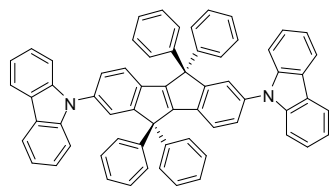
To a 25 mL, two-necked, round-bottomed flask was placed **2** (666 mg, 1 mmol), Pd₂(dba)₃ (18 mg, 0.02 mmol), NaO(*t*-Bu) (288 mg, 3 mmol), P(*t*-Bu)₃ (0.03 M in toluene, 2 mL, 0.06 mmol), and diphenylamine (372 mg, 2.2 mmol) in toluene (20 mL). The reaction mixture was refluxed for 4 hours. After cooling to ambient temperature, it was filtered and the precipitant was washed by toluene (100 mL). The crude residue was sublimated at 383 °C under 5 x 10⁻⁶ Torr to afford 573 mg of pure **3a** (68 %): *T*_m 363 °C (DSC); *T*_d 492 °C (TGA); *T*_g 163 °C (DSC); M.W.: 843.06; ¹H NMR (600 MHz, CD₂Cl₂) δ 7.23 (s, 20H), 7.20 (d, *J* = 2.0, 2H), 7.16 (t, *J* = 15.8, 8H), 6.99-6.94 (m, 24H), 6.74 (dd, *J* = 8.2, 2.0, 2H); ¹³C NMR (150 MHz, CD₂Cl₂) δ 158.7, 154.1, 147.9, 146.1, 143.3, 133.4, 129.4, 128.7, 128.6, 127.1, 124.4, 123.1, 122.5, 121.4, 120.9, 63.3; TLC *R*_f 0.75 (CH₂Cl₂/hexanes, 1/3); HR-ESI-MS (positive) calcd for C₆₄H₄₆N₂ [*M*⁺]: 842.3661, found: 842.3693; Anal. Calcd for C₆₄H₄₆N₂: C, 91.18, H, 5.50, N, 3.32. Found: C, 90.99, H, 5.42, N, 3.59.

2,7-Bis(*N,N*,-di(*p*-tolyl)-amino)-5,5,10,10-octaphenyl-5,10-dihydroindeno[2,1-*a*]indene (**3b**)



To a 25 mL, two-necked, round-bottomed flask was placed **2** (666 mg, 1 mmol), Pd₂(dba)₃ (18 mg, 0.02 mmol), NaO(*t*-Bu) (288 mg, 3 mmol), P(*t*-Bu)₃ (0.03 M in toluene, 2 mL, 0.06 mmol), and di-*p*-tolylamine (434 mg, 2.2 mmol) in toluene (20 mL). The reaction mixture was refluxed for 4 hours. After cooling to ambient temperature, it was filtered and the precipitant was washed by toluene (100 mL). The crude residue was sublimated at 393 °C under 5 x 10⁻⁶ Torr to afford 557 mg of pure **3b** (62 %): *T*_m 433 °C (DSC); *T*_d 514 °C (TGA); *T*_g 165 °C (DSC); M.W.: 899.17; ¹H NMR (600 MHz, CD₂Cl₂) δ 7.23 (s, 20H), 7.15 (d, *J* = 2.0, 2H), 6.98 (d, *J* = 8.3, 8H), 6.91 (d, *J* = 8.3, 2H), 6.86 (d, *J* = 8.3, 8H), 6.65 (dd, *J* = 8.3, 2.0, 2H), 2.25 (s, 12H); ¹³C NMR (150 MHz, CD₂Cl₂) δ 158.6, 153.8, 146.5, 145.6, 143.6, 132.9, 130.0, 128.8, 128.6, 127.1, 124.7, 121.4, 120.7, 120.4, 63.3, 20.8; TLC *R*_f 0.75 (CH₂Cl₂/hexanes, 1/3); HR-ESI-MS (positive) calcd for C₆₈H₅₄N₂ [*M*⁺]: 898.4287, found: 898.4313; Anal. Calcd for C₆₈H₅₄N₂: C, 90.83, H, 6.05, N, 3.12. Found: C, 90.72, H, 5.98, N, 3.30.

Bis(9-carbazolyl)-5,5,10,10-octaphenyl-5,10-dihydroindeno[2,1-*a*]indene (**3c**)



To a 25 mL, two-necked, round-bottomed flask was placed **2** (666 mg, 1 mmol), Pd₂(dba)₃ (18 mg, 0.02 mmol), NaO(*t*-Bu) (288 mg, 3 mmol), P(*t*-Bu)₃ (0.03 M in toluene, 2 mL, 0.06 mmol), and carbazole (368 mg, 2.2 mmol) in toluene (20 mL). The reaction mixture was refluxed for 4 hours. After cooling to ambient temperature, it was filtered and the precipitant was washed by toluene (100 mL). The crude residue was sublimated at 393 °C under 5 x 10⁻⁶ Torr to afford 537 mg of pure **3c** (64 %): *T*_m 435 °C (DSC); *T*_d 546 °C (TGA); *T*_g 204 °C (DSC); M.W.: 839.03; ¹H NMR (600 MHz, CD₂Cl₂) δ 8.10 (d, *J* = 7.8, 4H), 7.71 (s, 2H), 7.46-7.44 (m, 12H), 7.36-7.30 (m, 20H), 7.23-7.23 (m, 4H); ¹³C NMR (150 MHz, CD₂Cl₂) δ 159.5, 142.6, 141.0, 137.5, 136.0, 129.1, 128.7, 128.7, 127.7, 126.2, 126.0, 124.2, 123.7, 122.1, 120.5,

120.3, 110.1, 63.8; TLC R_f 0.75 (CH_2Cl_2 /hexanes, 1/3); HR-ESI-MS (positive) calcd for $\text{C}_{64}\text{H}_{42}\text{N}_2\text{Na}$ [$\text{M}^{2+} + \text{Na}$]: 442.1572, found: 442.2563; Anal. Calcd for $\text{C}_{64}\text{H}_{42}\text{N}_2$: C, 91.62, H, 5.05, N, 3.34. Found: C, 91.46, H, 4.98, N, 3.56.

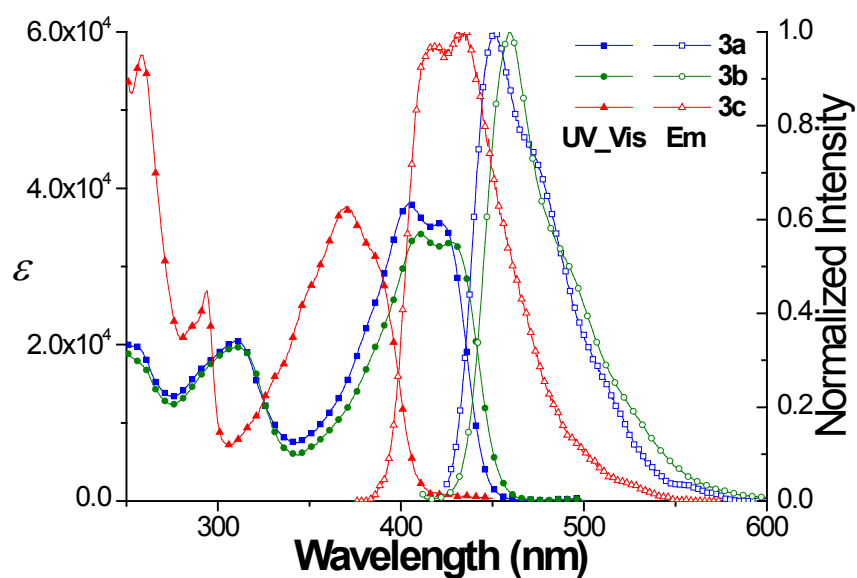


Figure S1. Stacked Plots of the Absorption and Emission Spectra for **3a–c**.

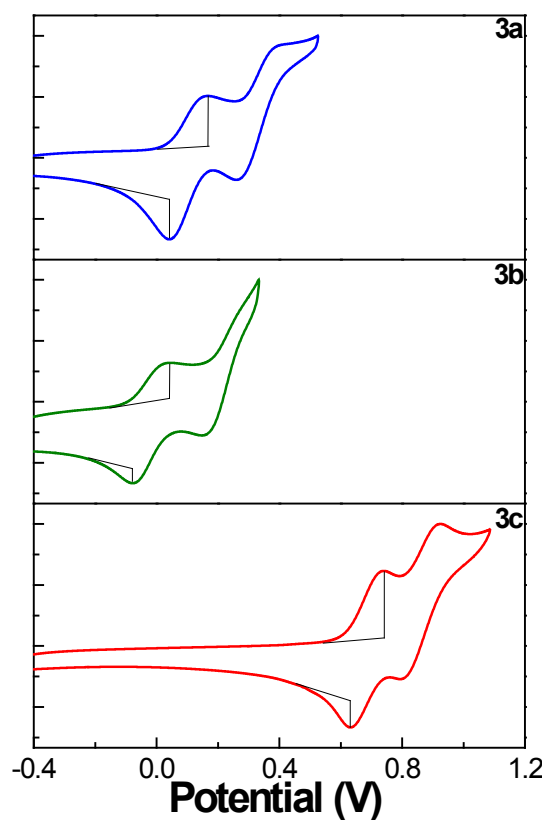


Figure S2. Plots of the Cyclic Voltammograms for **3a–c**.

Device fabrication and measurements

All the materials were commercially available or synthesized as described, and subjected to gradient sublimation twice prior to use. The cathode was an indium tin oxide (ITO) coated glass with the sheer resistance of $\sim 30 \Omega/\square$. Pre-patterned ITO substrate was cleaned sequentially by sonication in detergent solution, doubly distilled water, and EtOH for 5 min in turn before blow-drying with a stream of nitrogen. Advanced surface cleaning was accomplished by oxygen plasma treatment for 3 min. hole injection layer (HIL) was then spin-coated at a rate of 3000 rpm on the substrate before it was loaded into the vacuum chamber. Furthermore, a layer by layer deposition was carried out thermally at a rate of 0.1-0.3 nm/s under a pressure of 5×10^{-6} Torr. Electroluminescence efficiencies and spectra were recorded on a Keithley 2400 source meter and Photo Research PR-655 SpectraScan spectroradiometer, respectively. All the measurements were made at atmospheric conditions. Device configurations are described as following: Hole-only device, ITO/NPB (40 nm)/**3a** (50 nm)/NPB (40 nm)/Anode; electron-only device, ITO/BCP (40 nm)/**3a** (50 nm)/TPBI (40 nm)/LiF (1 nm)/Anode; A, ITO/electron transporting layer (ETL)/EL/ETL/electron injection layer (EIL)/Anode; A, ITO/emitting layer (EL)/electron transporting layer (ETL)/electron injection layer (EIL)/Anode; B, ITO/HTL/EL/ETL/EIL/Anode; C and E, ITO/HTL/EL/EIL/Anode; D, ITO/HIL/EL/ETL/EIL/Anode, where HIL, HTL, EM, ETL, EIL, and Anode correspond to 30 nm of PEDOT:PSS, 20 nm of **3a** or 40 nm of NPB, 40 nm of **3a-c** or **Alq₃**, 40 nm of TPBI, 1 nm of LiF, and 150 nm of Al, respectively.

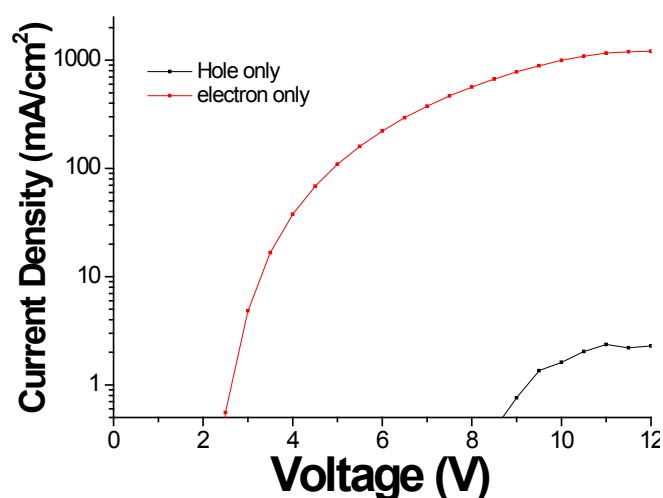


Figure S3. Stacked Plots of the I - V Curves in Hole and Electron Only Devices for **3a**.

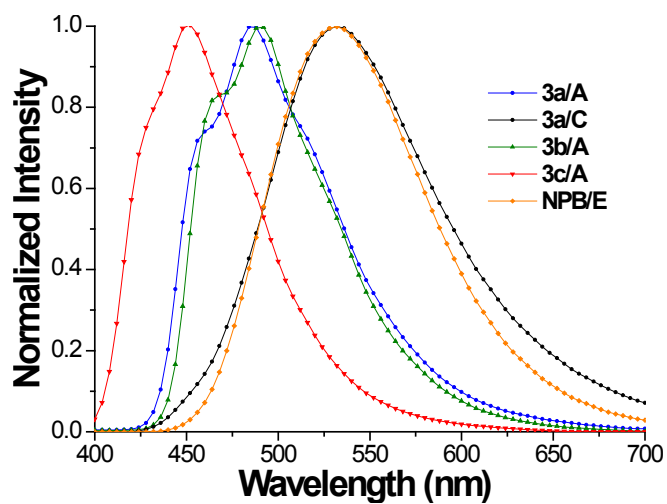


Figure S4. Stacked Plots of the EL Spectra for 3a-c and NPB.

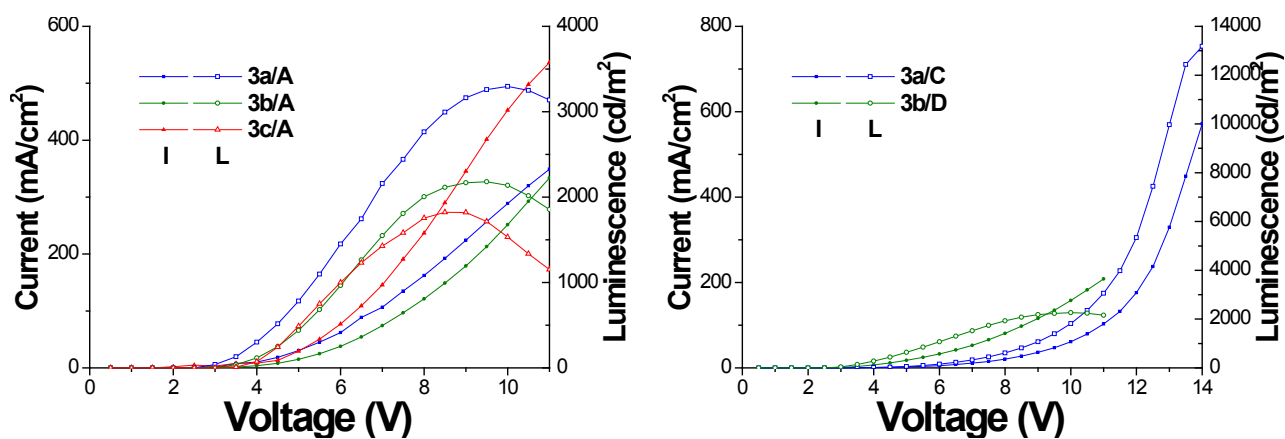


Figure S5. Stacked Plots of the I - V - L Curves for 3a-c.

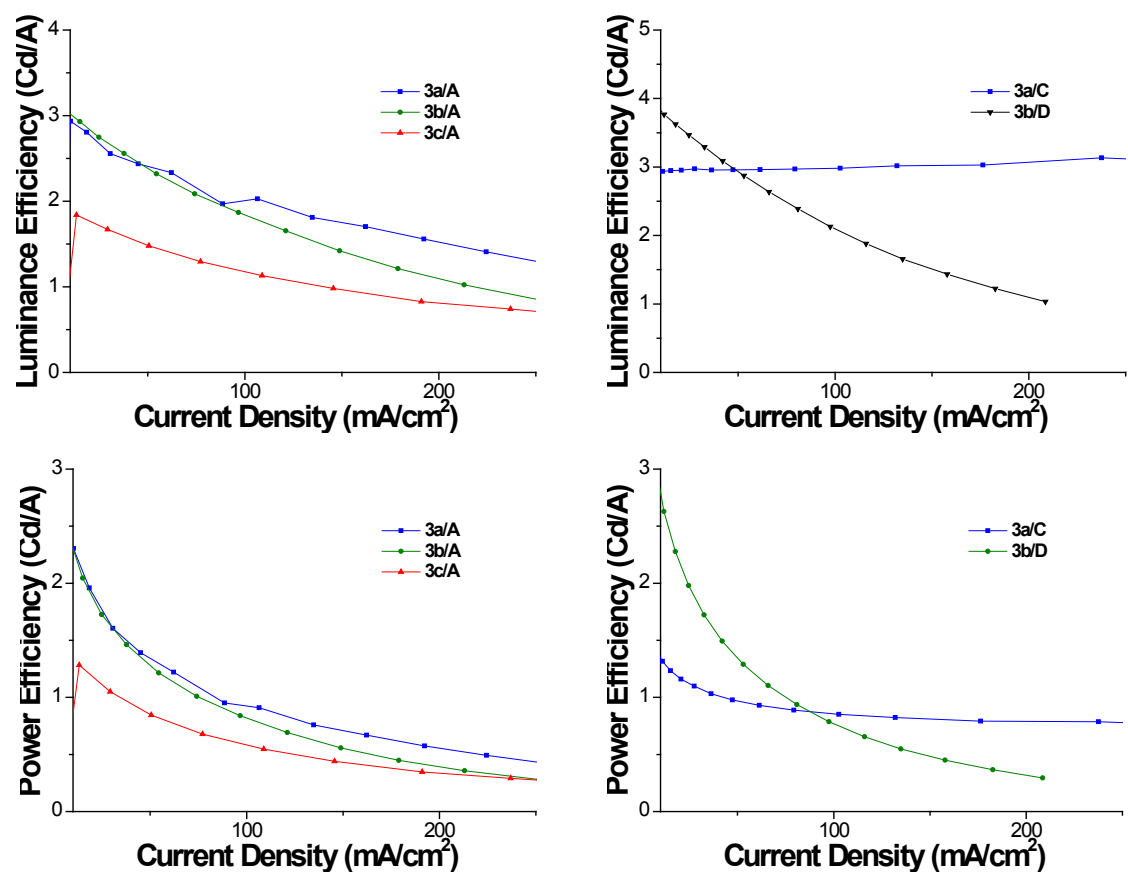
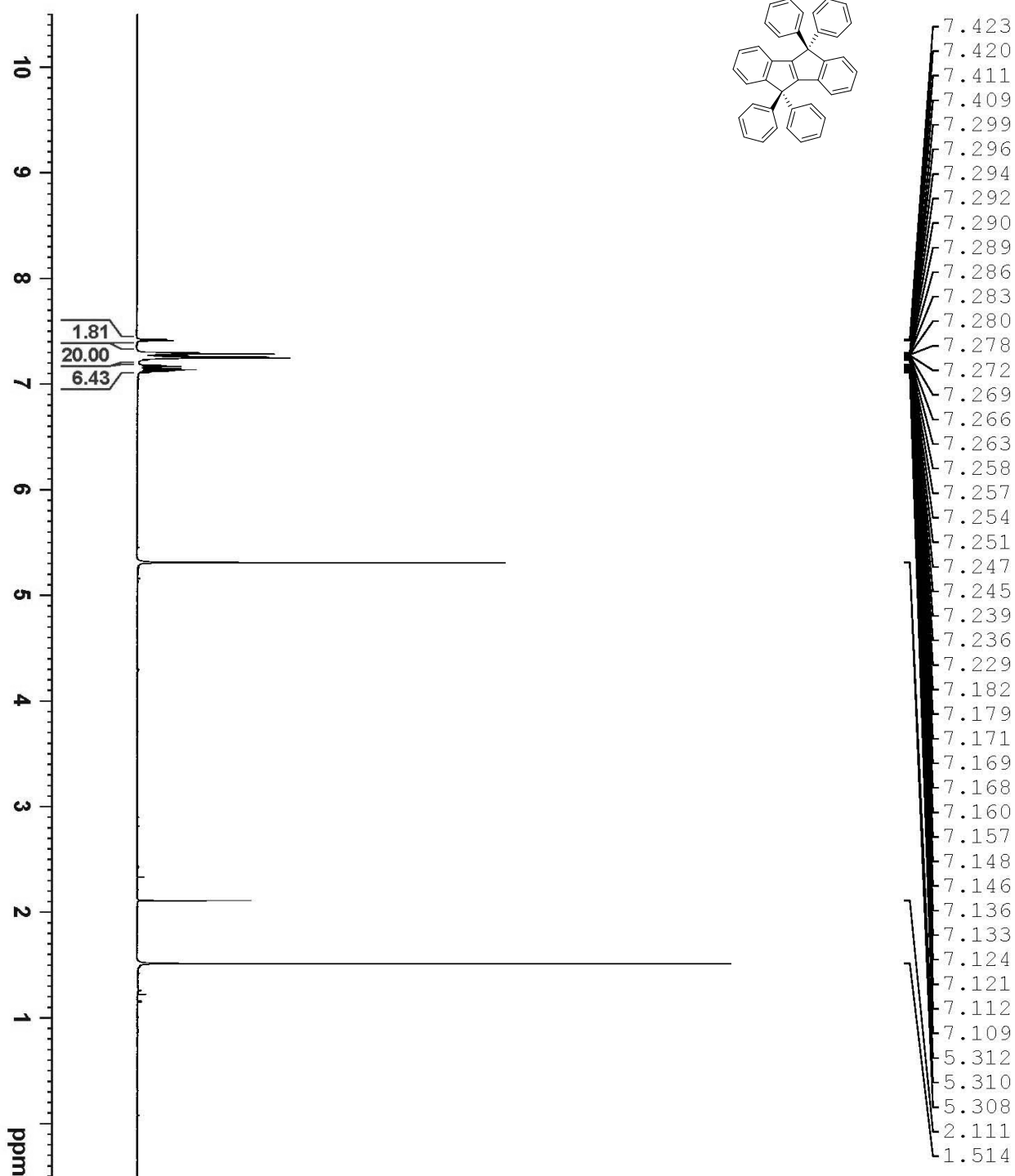


Figure S6. Stacked Plots of the $I-\eta_c$ and $I-\eta_p$ Curves for 3a–c.



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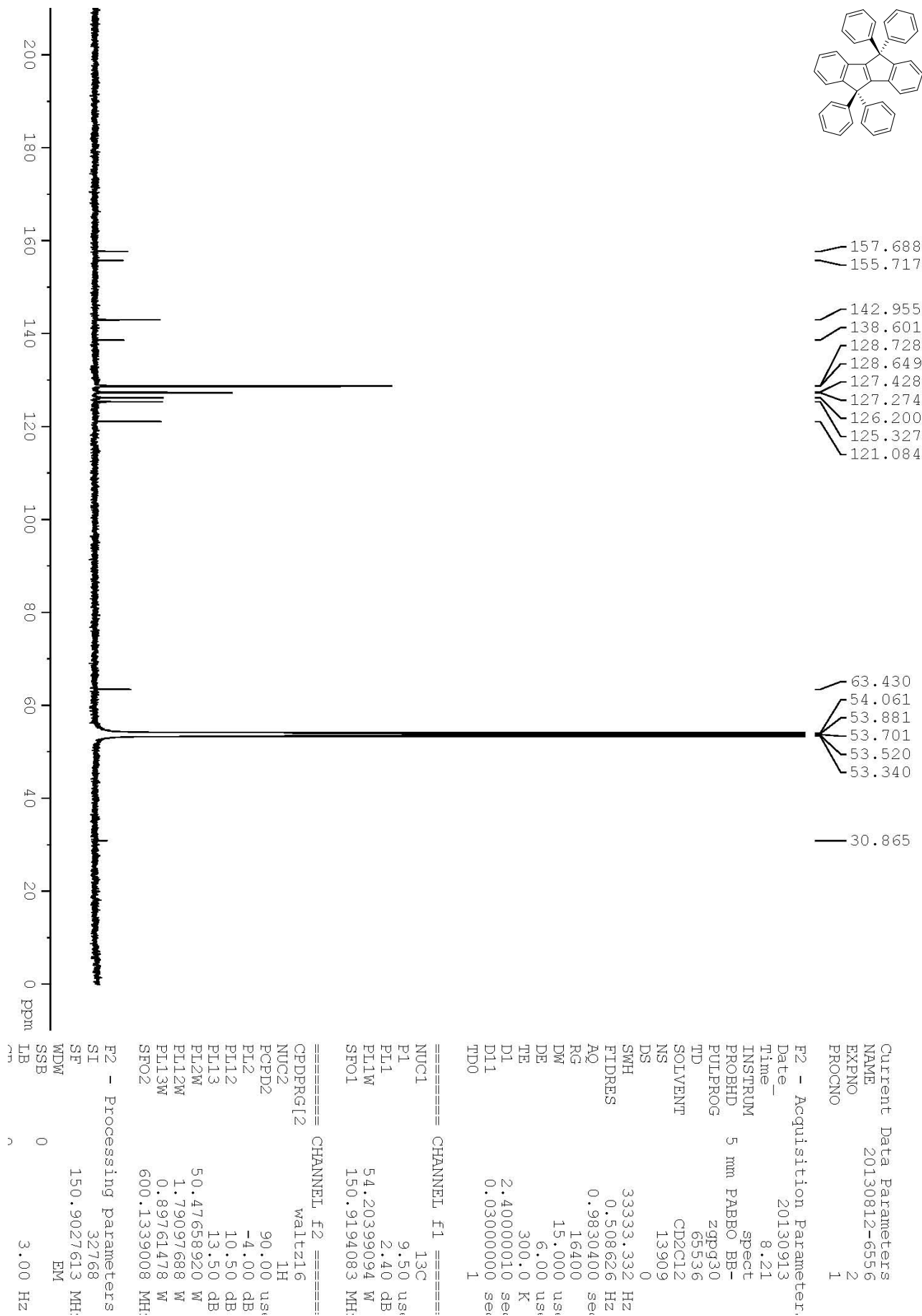
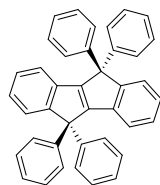
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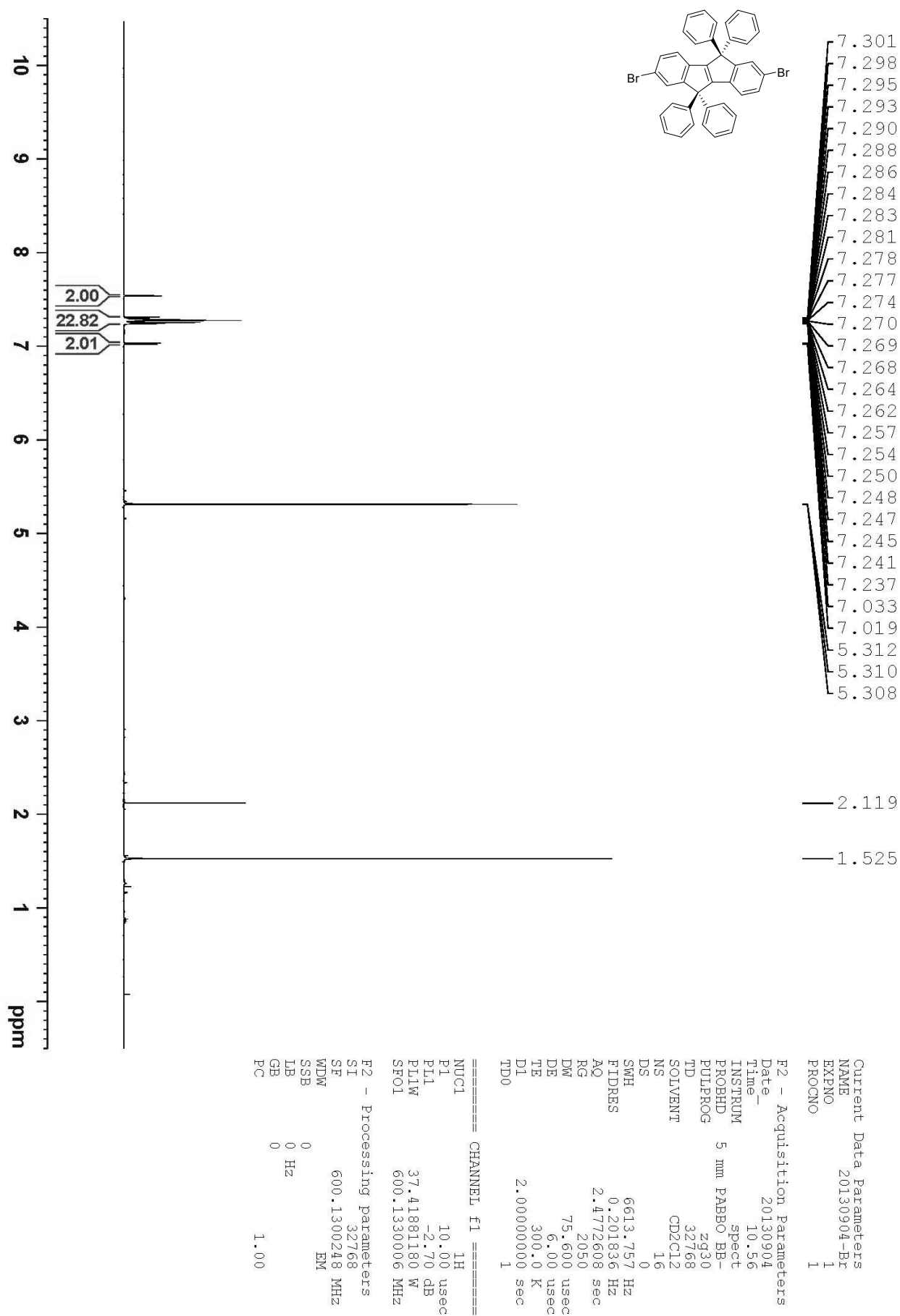
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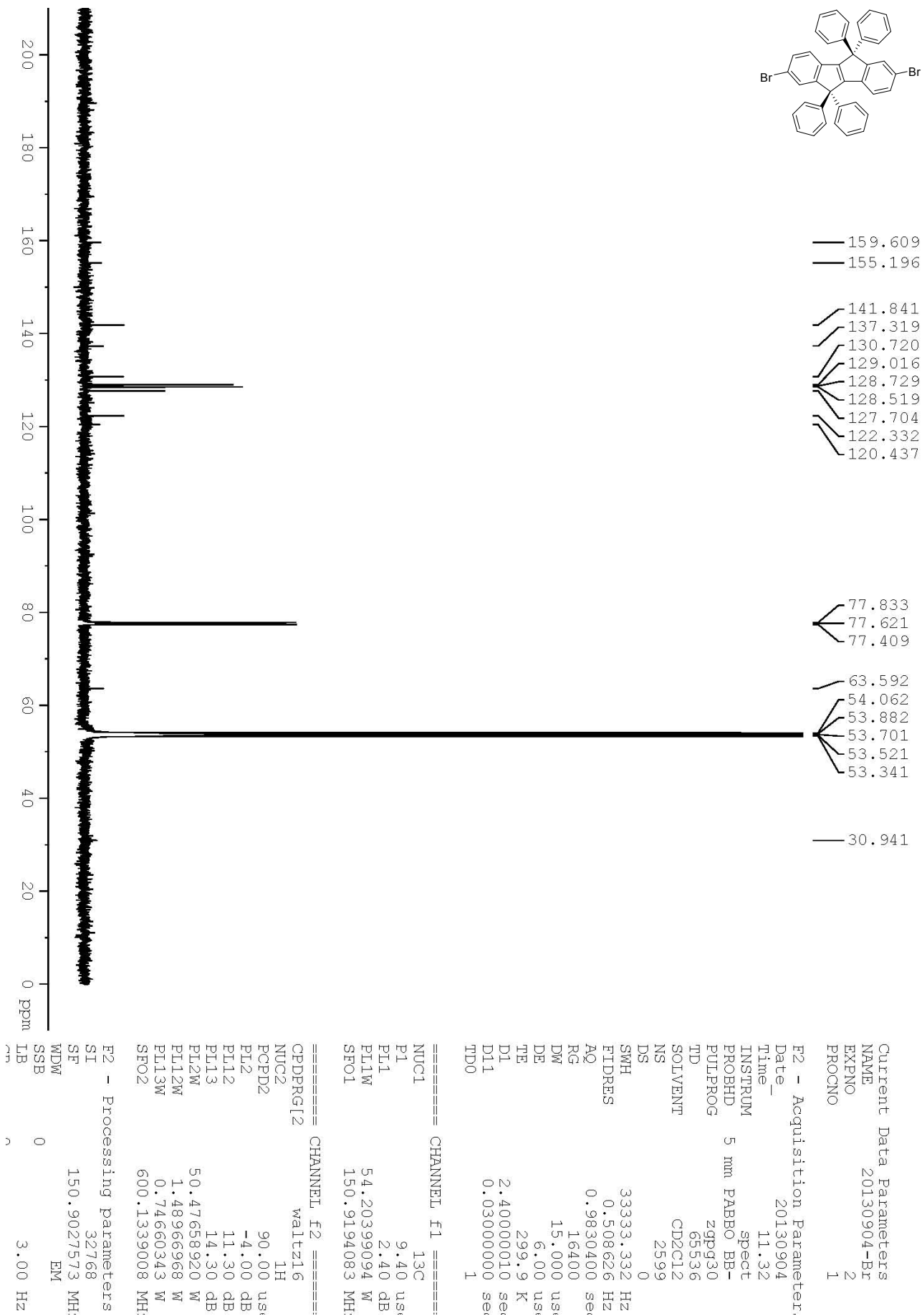
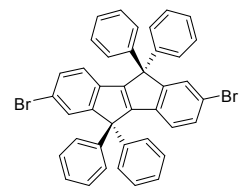
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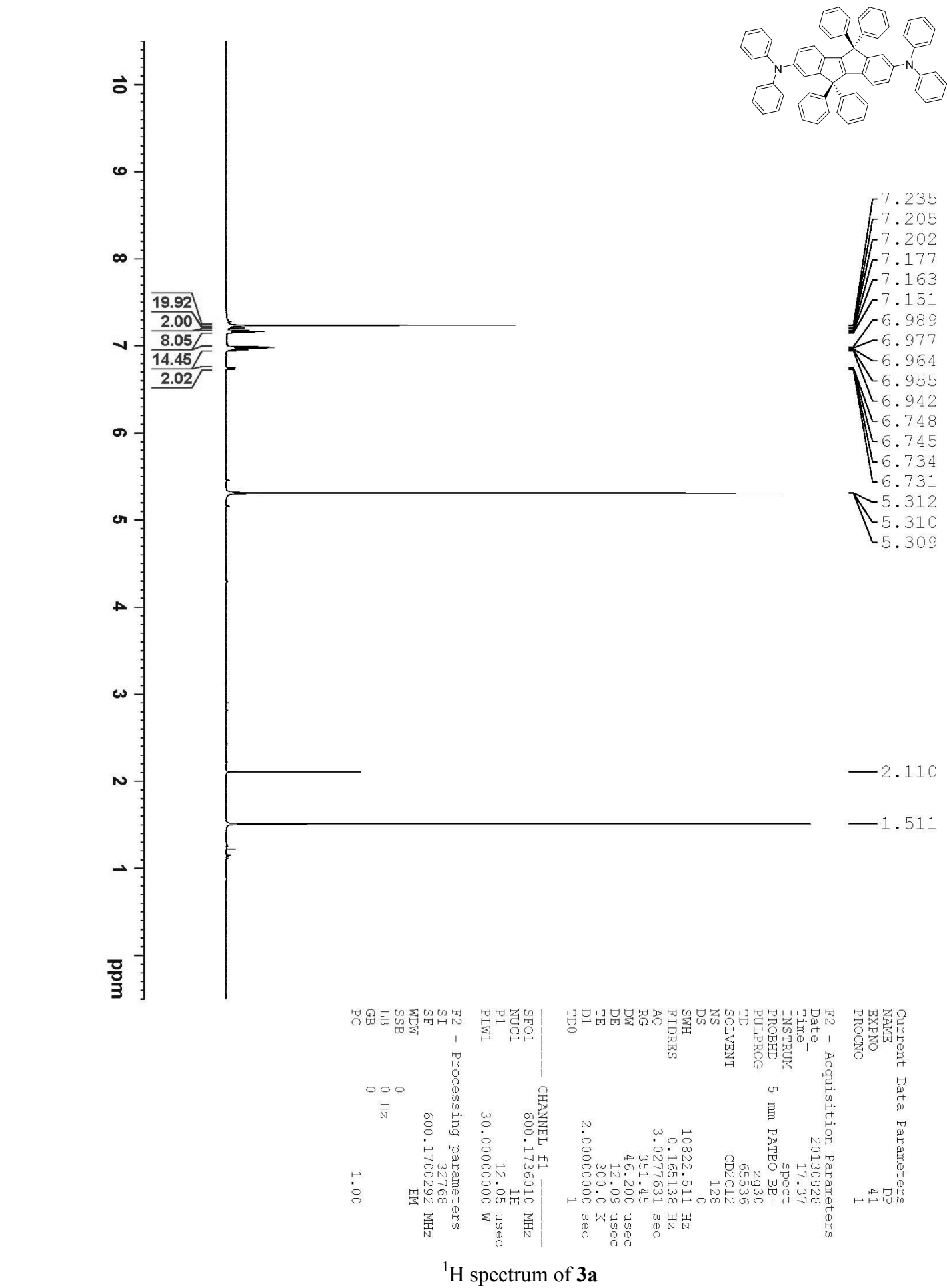
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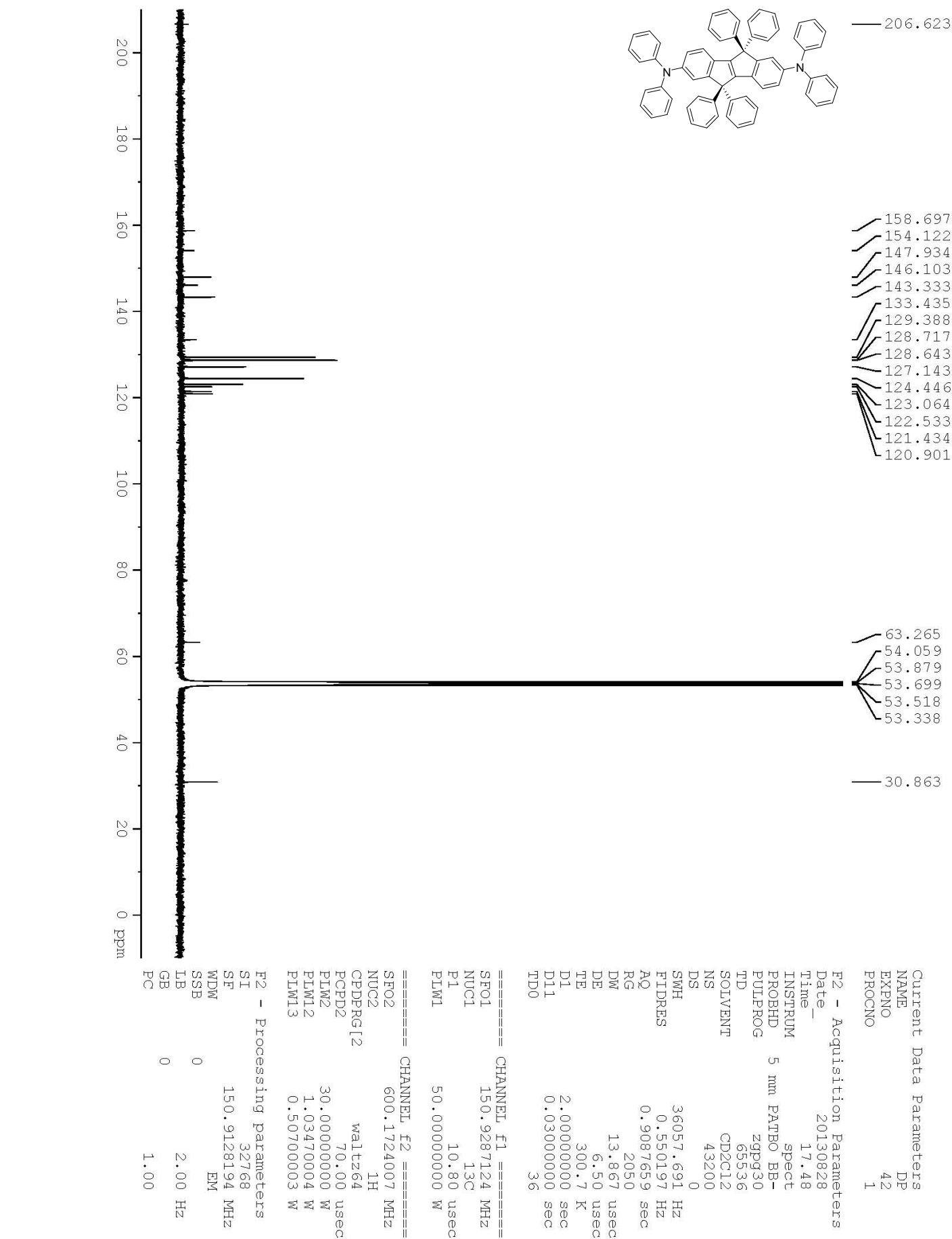


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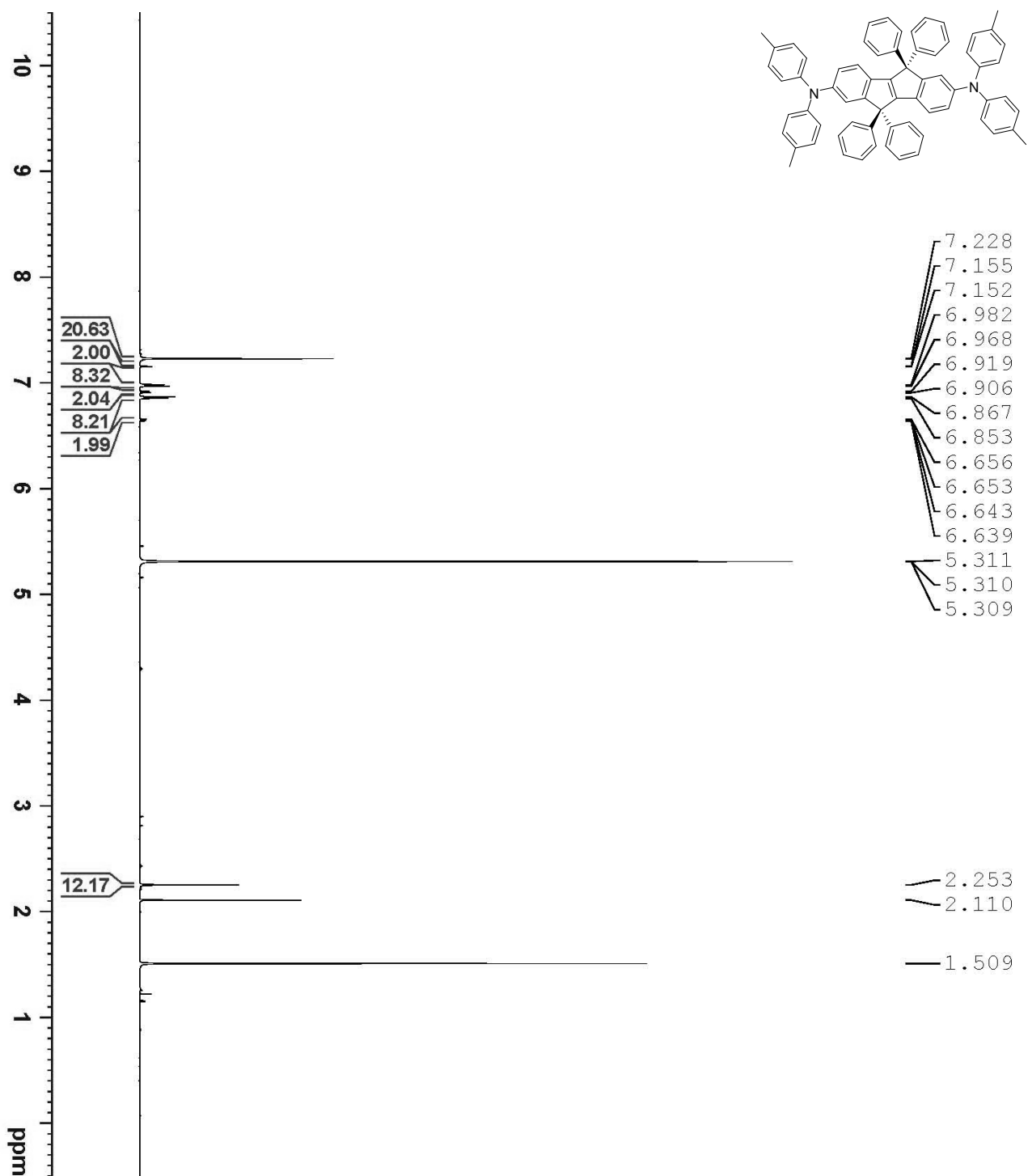


¹³C NMR spectrum of **2**





¹³C NMR spectrum of **3a**



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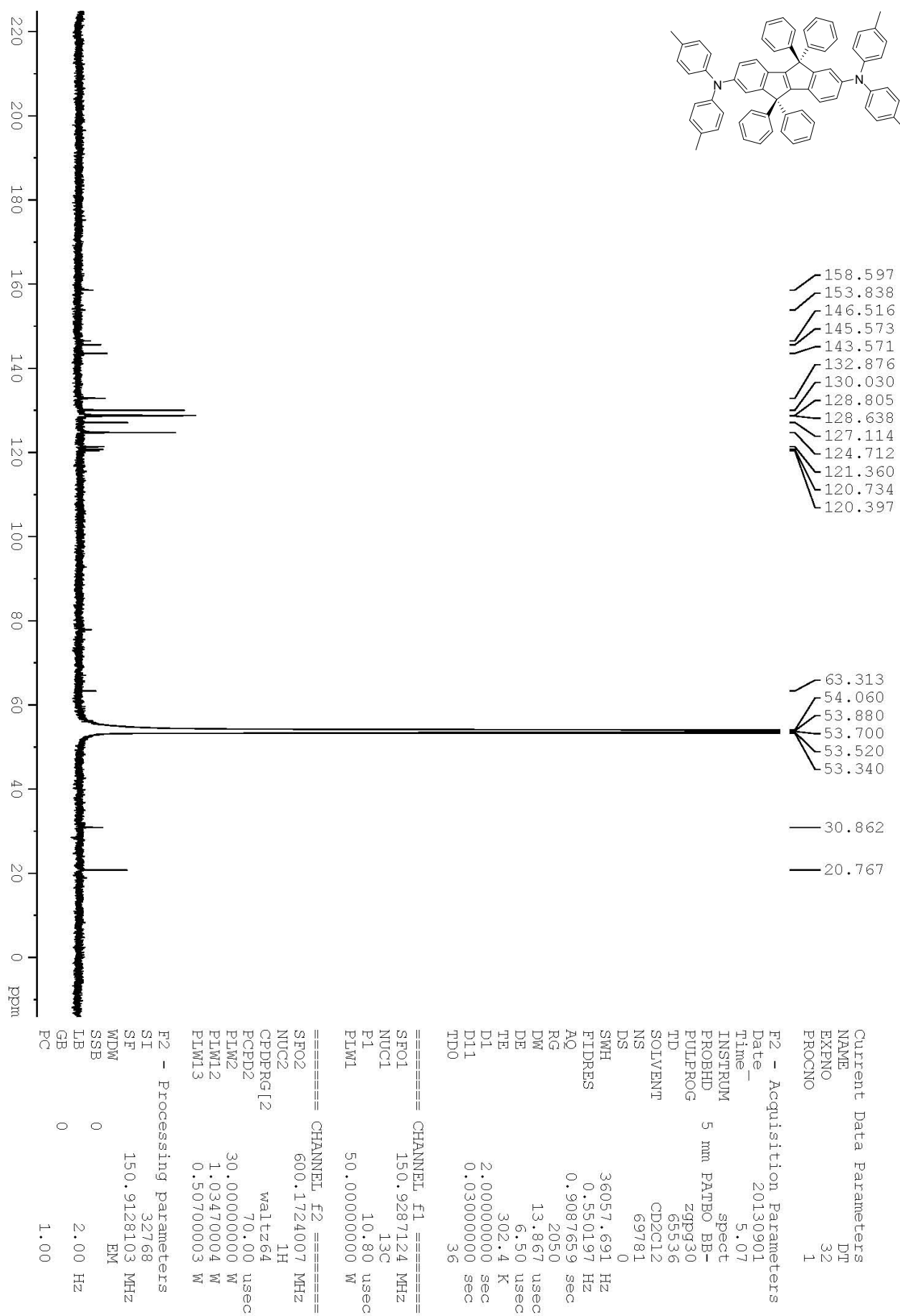
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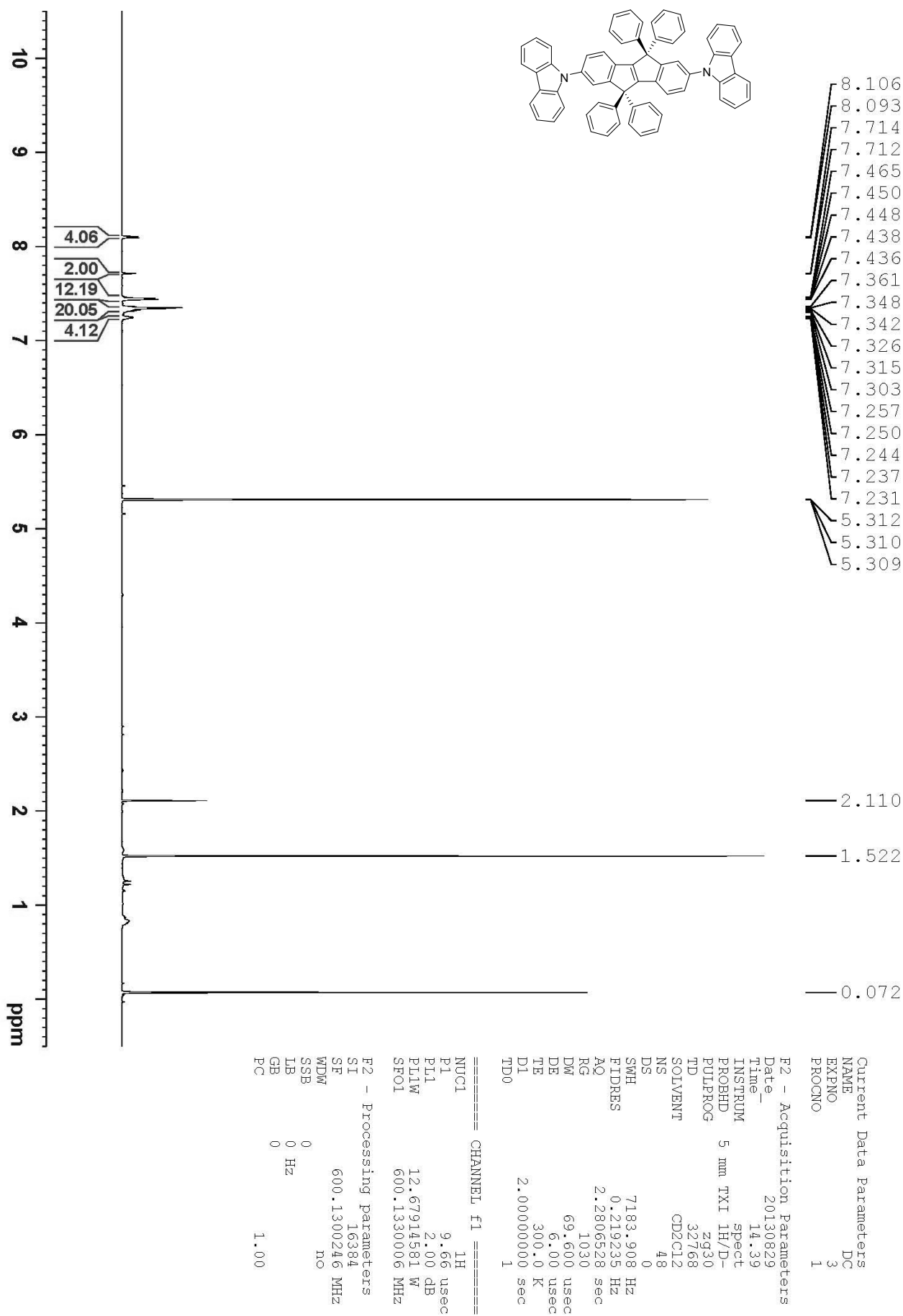
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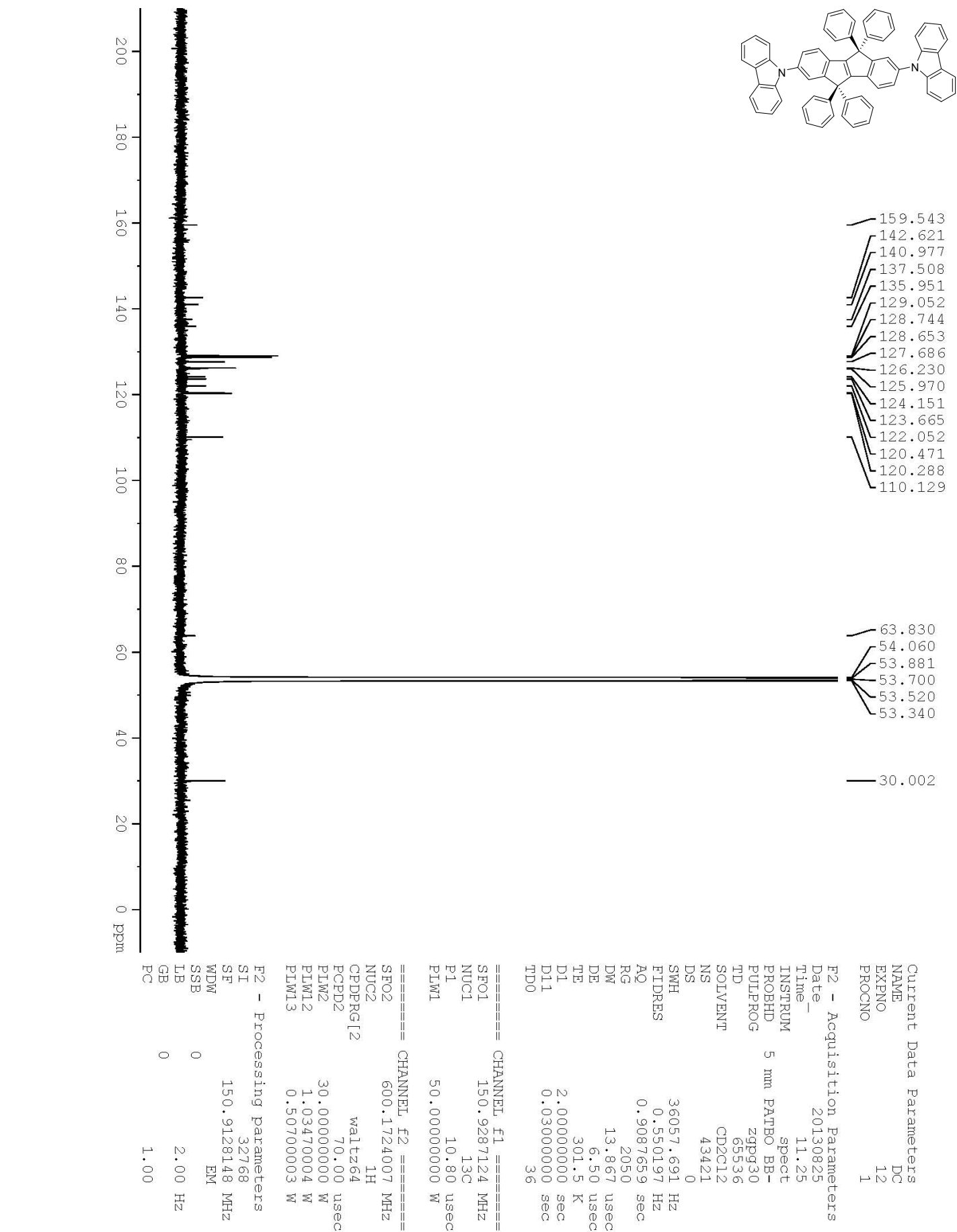
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¹H spectrum of 3b

 ^{13}C NMR spectrum of **3b**





¹³C NMR spectrum of **3c**

DFT Calculation data⁵

3a

Excited State	1:	Singlet-A	2.8255 eV	438.80 nm	f=0.9099	<S**2>=0.000
	222 -> 223	0.70160				
Excited State	2:	Singlet-A	3.3597 eV	369.04 nm	f=0.0002	<S**2>=0.000
	221 -> 223	0.70138				
Excited State	3:	Singlet-A	3.5182 eV	352.41 nm	f=0.0039	<S**2>=0.000
	221 -> 225	-0.13505				
	222 -> 224	0.68181				
Excited State	4:	Singlet-A	3.5692 eV	347.37 nm	f=0.0445	<S**2>=0.000
	221 -> 224	-0.15328				
	222 -> 225	0.67033				
Excited State	5:	Singlet-A	3.8174 eV	324.79 nm	f=0.1069	<S**2>=0.000
	221 -> 227	-0.14040				
	222 -> 226	0.63792				
	222 -> 227	0.10227				
	222 -> 228	-0.15403				
	222 -> 229	0.14966				
Excited State	6:	Singlet-A	3.8200 eV	324.56 nm	f=0.0573	<S**2>=0.000
	222 -> 226	0.16705				
	222 -> 228	0.66509				
Excited State	7:	Singlet-A	3.8335 eV	323.42 nm	f=0.0790	<S**2>=0.000
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	222 -> 227	0.65561				
	222 -> 228	0.11412				
Excited State	8:	Singlet-A	3.8820 eV	319.38 nm	f=0.0400	<S**2>=0.000
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	222 -> 226	-0.13329				
	222 -> 227	-0.10951				
	222 -> 229	0.65285				

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	222 -> 230	0.16519				
	222 -> 231	0.62074				
	222 -> 232	0.20662				
3b						
Excited State	1:	Singlet-A	2.7772 eV	446.44 nm	f=0.9585	<S**2>=0.000
	238 -> 239	0.70167				
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	238 -> 241	0.67022				
Excited State	5:	Singlet-A	3.7462 eV	330.96 nm	f=0.0528	<S**2>=0.000
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	238 -> 243	0.65232				
	238 -> 244	0.12893				
Excited State	6:	Singlet-A	3.7711 eV	328.77 nm	f=0.0844	<S**2>=0.000
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Excited State	7:	Singlet-A	3.8006 eV	326.22 nm	f=0.0885	<S**2>=0.000
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	238 -> 244	0.57583				
	238 -> 245	-0.19791				

Excited State	8:	Singlet-A	3.8268 eV	323.99 nm	f=0.1215	<S**2>=0.000
	237 -> 244	-0.14475				
	238 -> 242	0.15918				
	238 -> 244	0.28174				
	238 -> 245	0.58470				
Excited State	9:	Singlet-A	3.8876 eV	318.92 nm	f=0.0068	<S**2>=0.000
	238 -> 246	0.65547				
	238 -> 247	-0.22636				
Excited State	10:	Singlet-A	3.8990 eV	317.99 nm	f=0.0262	<S**2>=0.000
	238 -> 246	0.23060				
	238 -> 247	0.61620				
	238 -> 248	0.17562				
3c						
Excited State	1:	Singlet-A	3.0249 eV	409.88 nm	f=0.6741	<S**2>=0.000
	220 -> 221	0.70200				
Excited State	2:	Singlet-A	3.3077 eV	374.84 nm	f=0.0000	<S**2>=0.000
	219 -> 221	0.70276				
Excited State	3:	Singlet-A	3.6837 eV	336.58 nm	f=0.0001	<S**2>=0.000
	217 -> 221	0.15110				
	218 -> 221	0.68751				
Excited State	4:	Singlet-A	3.6838 eV	336.56 nm	f=0.0000	<S**2>=0.000
	217 -> 221	0.68767				
	218 -> 221	-0.15118				
Excited State	5:	Singlet-A	3.7766 eV	328.30 nm	f=0.0903	<S**2>=0.000
	216 -> 221	0.68980				
Excited State	6:	Singlet-A	3.8805 eV	319.51 nm	f=0.0000	<S**2>=0.000
	219 -> 225	-0.14402				
	220 -> 224	0.66232				
Excited State	7:	Singlet-A	3.9191 eV	316.36 nm	f=0.0627	<S**2>=0.000
	219 -> 222	0.29998				
	220 -> 223	0.59870				
	220 -> 225	0.13859				

Excited State	8:	Singlet-A	3.9203 eV	316.26 nm	f=0.0000	<S**2>=0.000
	219 -> 223	0.30809				
	220 -> 222	0.61561				
Excited State	9:	Singlet-A	3.9447 eV	314.30 nm	f=0.0168	<S**2>=0.000
	214 -> 221	0.13274				
	219 -> 224	-0.19669				
	220 -> 223	-0.12619				
	220 -> 225	0.60710				
	220 -> 226	0.11053				
Excited State	10:	Singlet-A	4.2099 eV	294.51 nm	f=0.0551	<S**2>=0.000
	219 -> 224	-0.13153				
	220 -> 225	-0.19102				
	220 -> 226	0.64666				

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