Electronic Supplementary Material (ESI) for Chemical Communications
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Supporting Information

Novel bis(fluorenyl)benzothiadiazole-cored carbazole dendrimers as highly efficient solution-processed non-doped green emitters for organic light-emitting diodes

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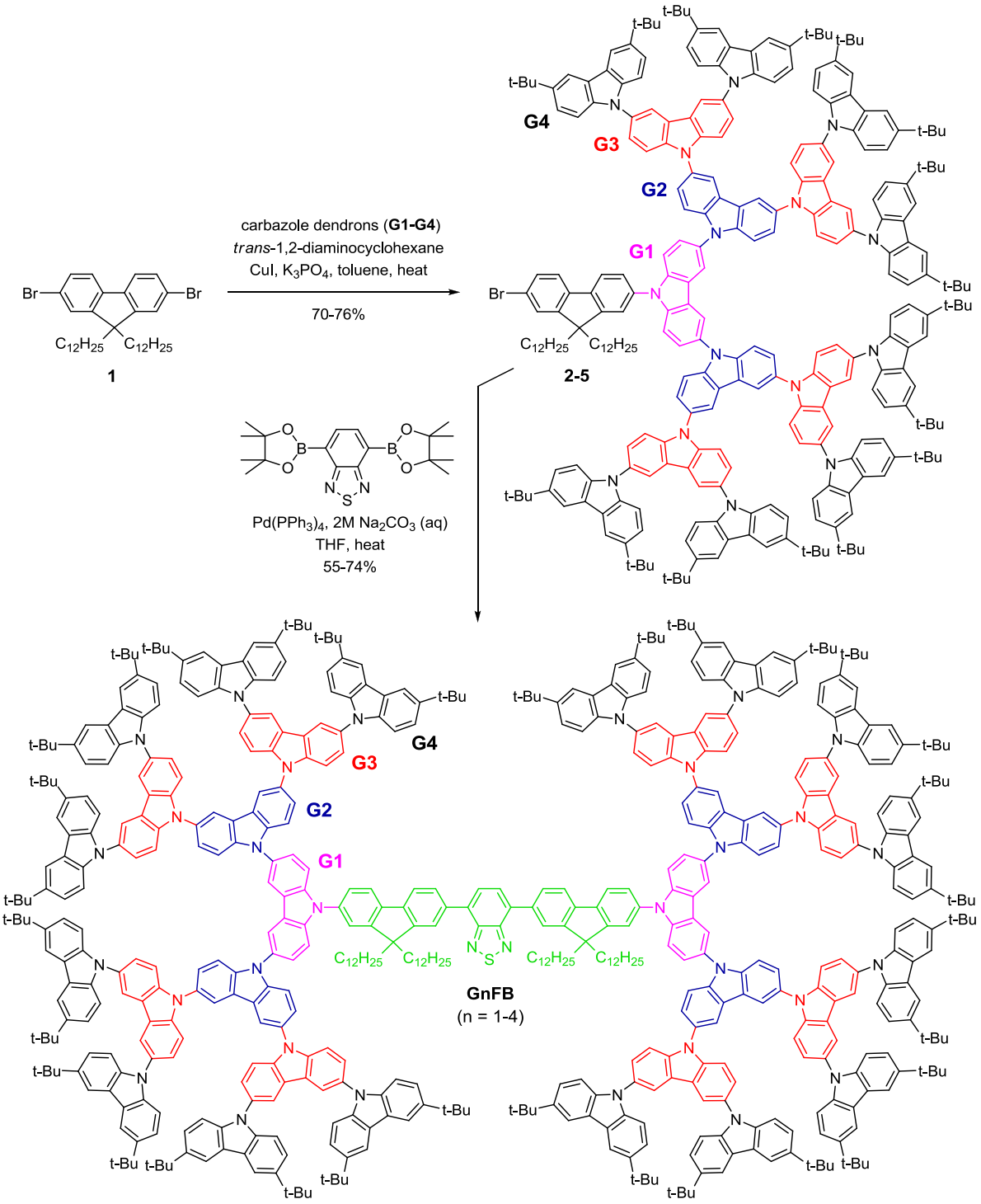
1. General Procedures

All reagents were purchased from Aldrich, Acros or Fluka and used without further purification. All solvents were supplied by Thai companies and used without further distillation. Tetrahydrofuran (THF) was refluxed with sodium and benzophenone, and distilled. CH_2Cl_2 for cyclic voltammetry (CV) measurements was washed with conc. H_2SO_4 and distilled twice from calcium hydride. Chromatographic separations were carried out on silica gel Merck Silica gel 60 (0.0630-0.200 mm).

^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on a Brüker AVANCE 300 MHz spectrometer with tetramethylsilane as the internal reference using $CDCl_3$ as solvent in all cases. Infrared (IR) spectra were measured on a Perkin-Elmer FTIR spectroscopy spectrum RXI spectrometer as KBr disc. Ultraviolet-visible (UV-Vis) spectra were recorded as a diluted solution in spectroscopic grade CH_2Cl_2 on a Perkin-Elmer UV Lambda 25 spectrometer. Photoluminescence spectra and the fluorescence quantum yields (Φ_F) were recorded with a Perkin-Elmer LS 50B Luminescence Spectrometer as a dilute solution in spectroscopic grade dichloromethane and thin film obtained by spin casting. The fluorescence quantum yields (Φ_F) were determined by comparison with a fluorescence standard of quinine sulfate in 0.1% H_2SO_4 (Φ_F = 0.58).[1] Differential scanning calorimetry (DSC) analysis and thermal gravimetric analysis (TGA) were performed on a METTLER DSC823e thermal analyzer and a Rigaku TG-DTA 8120 thermal analyzer, respectively, with heating rate of 10 ^oC/min under nitrogen atmosphere. Cyclic voltammetry (CV) measurements were carried out on an Autolab potentiostat PGSTAT 12 with a three electrode system (platinum counter electrode, glassy carbon working electrode and Ag/Ag^+ reference electrode) at scan rate of 50 mV/s in CH_2Cl_2 under argon atmosphere. The concentration of analytical materials and tetrabutyl ammonium hexafluorophosphate (*n*-Bu_4NPF_6) were 10^{-3} M and 0.1 M, respectively. Melting points were measured using an Electrothermal IA 9100 series of digital melting point instrument and are uncorrected. High resolution mass spectrometry (HRMS) analysis was performed by Mass Spectrometry Unit, Mahidol University, Thailand. The atomic force microscopy (AFM) analysis was performed on Park System model XE 100 using standard non contact mode with resonance of 316.17 KHz at Ubon Ratchathani University.

2. Synthesis and Characterization

The synthesis of **GnFB** is outlined in Scheme S1.



Scheme S1. Synthetic route to **G1FB**

Synthesis of 1

To a mixture of 2,7-dibromofluorene (19.34 g, 59.70 mmol) and tetrabutyl ammonium bromide (1.5 g, 4.5 mmol) in DMSO (100 ml) was added an aqueous NaOH solution (50% wt/V, 20 ml) follow by 1-bromododecane (32.40 g, 30.12 mmol). After being stirred at room temperature for 3 h, the reaction mixture was extracted with EtOAc (100 ml x 3). The combined organic phase was washed with water (100 ml), HCl solution (1 M, 50 ml), brine solution (100 ml), dried over Na_2SO_4 anhydrous, filtered and the organic phase was removed in vacuum. Purification by column chromatography using silica gel eluent with hexane gave yellow oil (32.52 g, 82%); ^{1}H-NMR (300 MHz, CDCl3) δ 7.50-7.37 (6H, m), 1.95-2.01 (4H, m), 1.40-1.0 (40H, m) and 0.95 (6H, m) ppm.

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Synthesis of 2-5

A mixture of 2,7-dibromo-9,9-didodecylfluorene (**1**) (27.29 mmol), carbazole dendrons **G1-4**[3] (7.15 mmol), copper iodide (3.64 mmol), potassium phosphate (18.21 mmol) and *trans*-diaminocyclohexane in toluene (70 ml) was refluxed for 24 h under N_2 atmosphere. After cooling, the reaction mixture was extracted with CH_2Cl_2 (50 ml x 3). The combined organic phase was washed with water (100 ml), brine solution (100 ml), dried over Na_2SO_4 anhydrous, filtered and the solvent was remove in vacuum. The crude product was purified by column chromatography over silica gel eluting with a mixture of CH_2Cl_2:hexane (1:9).

2 (G1): light yellow viscous (73%); ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.25 (2H, s), 7.85 (1H, d, *J* = 7.98 Hz), 7.63 (1H, d, *J* = 8.48 Hz), 7.56 (6H, m), 7.45 (2H, d, *J* = 8.48 Hz), 1.98 (4H, m), 1.53 (18H, m), 1.25 (40H, m) and 0.95 (6H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 153.27, 152.50, 152.17, 151.02, 142.93, 142.78, 140.50, 140.01, 139.47, 139.35, 138.86, 137.39, 136.90, 130.25, 127.29, 127.01, 126.32, 125.54, 125.35, 123.64, 123.49, 123.42, 122.98, 121.48, 121.35, 121.18, 120.90, 119.83, 55.40, 40.40, 34.80, 32.11, 31.97, 30.10, 29.78, 29.39, 24.00 and 22.73 ppm; FT-IR (KBr) ν 3046, 2954, 2927, 2852, 1609, 1579, 1489, 1469, 1364, 1324, 1294, 1265, 1235, 1033, 877, 809, 739 and 614 cm^{-1}; MALDI-TOF (*m/z*) (M^+) calcd for $C_{45}H_{56}BrN$: 689.359; found 689.221.

3 (G2): yellow solid (76%); m.p. 129-130 ^{o}C; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.30 (2H, s), 8.20 (4H, s), 7.99(1H, d, *J* = 8.40 Hz), 7.75-7.56 (8H, m), 7.50 (4H, d, *J* = 8.40 Hz), 7.45-7.37 (5H, m), 2.10 (4H, m), 1.44 (36H), 1.25 (40H, m) and 0.95 (6H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 153.29, 152.66, 142.58, 140.64, 140.52, 140.22, 139.99, 139.19, 136.11, 131.01, 130.89, 130.41, 126.44, 126.03, 124.06, 123.59, 123.21, 121.79, 121.41, 121.28, 119.43, 116.25, 111.15, 111.08, 109.12, 55.90, 55.57, 40.36, 40.25, 34.76, 32.08, 31.87, 30.07, 30.00, 29.73, 29.37, 29.29, 24.03, 22.65 and 14.09 ppm; FT-IR (KBr) ν 3441, 3050, 2953, 2927, 2852, 1629, 1609, 1579, 1362, 1322, 1294, 1261, 1232, 1031, 875, 809, 739, 654 and 610 cm^{-1}.; MALDI-TOF (*m/z*) (MH^+) calcd for $C_{61}H_{66}N$: 812.511; found 812.435.

4 (G3): yellow solid (70%); m.p. 235-237 ^{o}C; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.60 (2H, s), 8.31 (4H, s), 8.20 (8H, s), 8.08 (1H, d, *J* = 8.0 Hz), 7.90-7.77 (7H, m), 7.72-7.63 (8H, m), 7.51-7.48 (10H, m), 7.40-7.37 (8H, d, *J* = 8.5 Hz), 2.15-2.13 (4H, m), 1.56-1.43 (72H, m),1.29-1.04 (34H, m) and 0.91-0.80 (12H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 153.21, 151.21, 151.04, 143.04, 142.55, 141.79, 141.58, 141.45, 141.39, 140.25, 140.04, 137.66, 135.43, 134.90, 130.78, 129.97, 129.91, 127.89, 127.51, 127.25, 126.44, 126.05, 125.91, 124.12, 123.82, 123.58, 123.14, 121.86, 121.28, 120.85, 120.10, 119.89, 119.45, 116.23, 111.78, 111.11, 109.14, 55.65, 55.46, 40.39, 36.08, 34.75, 34.53, 34.00, 32.28, 32.07, 31.85, 31.62, 30.08, 29.59, 29.40, 29.28, 26.95, 25.31, 24.08, 22.64, 22.38, 20.73 and 14.08 ppm; FT-IR (KBr) ν 3432, 3046, 2958, 2923, 2857, 1629, 1609, 1579, 1489, 1362, 1322, 1294, 1278, 1261, 1232, 1029, 875, 809, 737, 652 and 610 cm^{-1}; MALDI-TOF (*m/z*) (M^+) calcd for $C_{49}H_{59}NS$: 693.436; found 693.361.

5 (G4): yellow solid (75%); m.p. 246-248 ^{o}C; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.74 (2H, s), 8.62 (4H, s), 8.30 (8H, s), 8.18 (16H, s), 7.95-7.86 (14H, m), 7.71-7.62 (18H, m), 7.46 (17H, d, *J* = 8.1 Hz), 7.36 (17H, d, *J* = 8.4 Hz), 2.15-2.13 (4H, m), 1.48 (144H, s) and 1.30-0.81 (46H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 155.54, 153.33, 153.12, 152.11, 148.19, 142.56, 142.41, 142.17, 141.96, 141.82, 141.66, 141.55, 141.43, 140.90, 140.51, 140.24, 140.05, 139.41, 137.05, 135.63, 131.91, 130.81, 130.37, 130.01, 129.87, 129.78, 128.92, 127.73, 127.05, 126.48, 126.32, 126.06, 125.23, 124.11, 124.02, 123.83, 123.57, 123.35, 123.15, 122.31, 122.05, 121.81, 121.48, 120.81, 119.93, 119.47, 118.72, 116.23, 114.47, 111.85, 111.50, 111.07, 110.43, 109.12, 65.66, 55.97, 47.96, 39.89, 35.10, 34.75, 34.59, 33.85, 32.07, 31.85, 30.55, 30.11, 29.90, 29.74, 29.63, 29.60, 29.42, 29.28, 29.14, 28.34, 26.96, 26.15, 24.60, 22.93, 22.80, 22.64, 22.45, 21.67, 19.56, and 14.11 ppm; FT-IR (KBr) ν 3432, 3050, 2953, 2927, 2861, 1629, 1612, 1579, 1487, 1362, 1322, 1276, 1261, 1232, 1031, 875, 807, 737, 654 and 612 cm^{-1}; MALDI-TOF (*m/z*) (M^+) calcd for $C_{49}H_{59}NS$: 693.436; found 693.361.

Synthesis of GnFB

A mixture of **2-5** (0.13 mmol) and 2,1,3-benzothiadiazole-4,7-bis(boronic acid pinacol ester) (0.043 mmol), $Pd(PPh_3)_4$ (0.0087 mmol) and 2 M Na_2CO_3 (10 ml) in THF (20 ml) was degassed with N_2 for 5 min. The reaction mixture was stirred at reflux under N_2 for 24 h. After being cooled to room temperature, water (50 ml) was added. The reaction mixture was extracted with CH_2Cl_2 (50 ml x 3), washed with water (50 ml), and

brine solution (50 ml), dried over Na_2SO_4 anhydrous, filtered and the solvents were remove to dryness. The crude product was purified by column chromatography over silica gel eluting with a mixture of CH_2Cl_2:hexane (1:9).

G1FB: yellow solid (74%); m.p. 68-70 ^oC; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.64 (1H, d, *J* = 9.3 Hz), 8.25-8.18 (9H, m), 8.09-8.04 (1H, m), 7.91 (1H, d, *J* = 8.4 Hz), 7.79 (1H, d, *J* = 7.8 Hz), 7.70 (1H, d, *J* = 7.8 Hz), 7.72-7.65 (2H, m), 7.57-7.50 (4H, m), 7.42 (4H, d, *J* = 9.3 Hz), 7.34 (2H, d, *J* = 10.8 Hz), 2.09-2.07 (4H, m), 1.51 (18H, m),1.15 (12H, m) and 0.84-0.80 (10H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 154.43, 153.11, 151.45, 142.87, 140.73, 139.51, 139.43, 137.21, 136.45, 133.60, 128.45, 127.98, 125.49, 124.04, 123.62, 123.47, 121.55, 121.02, 119.90, 116.35, 109.32, 55.62, 40.34, 34.79, 32.09, 31.92, 30.13, 29.68, 29.41, 29.34, 24.15, 22.68 and 14.11 ppm; FT-IR (KBr) ν 3441, 3041, 2953, 2923, 2852, 1612, 1581, 1487, 1467, 1364, 1322, 1294, 1261, 1232, 875, 809, 741, 665 and 614 cm^{-1}; MALDI-TOF (*m/z*) (M^+) calcd for $C_{69}H_{69}NS_2$: 975.487; found 975.489.

G2FB: yellow solid (64%); m.p. 158-160 ^oC; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.28 (4H, s), 8.25-8.18 (9H, m), 8.17 (8H, s), 8.14-7.98 (10H, m), 7.77-7.66 (12H, m), 7.47 (8H, d, *J* = 8.4 Hz), 7.36 (8H, d, *J* = 8.4 Hz), 2.18 (8H, m), 1.68-1.48 (48H, m), 1.34-0.88 (32H, m) and 0.85-0.78 (12H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 154.39, 153.56, 151.51, 142.56, 140.56, 140.39, 140.19, 136.79, 136.11, 133.58, 130.90, 128.55, 128.05, 126.00, 125.91, 124.13, 124.00, 123.56, 123.15, 121.86, 121.39, 120.14, 119.39, 116.23, 111.16, 109.10, 55.77, 40.30, 34.74, 32.05, 31.83, 30.11, 29.70, 29.60, 29.55, 29.39, 29.26, 24.20, 22.62 and 14.06 ppm; FT-IR (KBr) ν 3046, 2958, 2923, 2852, 1631, 1609, 1579, 1484, 1467, 1452, 1362, 1324, 1294, 1259, 1232, 1103, 1033, 877, 807, 739, 654 and 612 cm^{-1}; MALDI-TOF (*m/z*) (M^+) calcd for $C_{184}H_{222}N_8S$: 2576.737; found 2576.948.

G3FB: yellow solids (55%); m.p. 218-220 ^oC; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.58 (4H, s), 8.28 (8H, s), 8.16-8.03 (26H, m), 7.87-7.84 (12H, m), 7.69-7.60 (16H, m), 7.46 (16H, dd, *J* = 1.5 Hz, *J* = 8.7 Hz), 7.35 (16H,d, *J* = 8.7 Hz), 2.24 (8H, m), 1.46 (144H, m) and 1.39-0.85 (92H, m) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.54, 141.42, 140.23, 130.78, 123.81, 123.55, 123.12, 116.21, 109.11, 34.73, 32.04, 31.81, 29.61, 29.25, 22.60, 14.05 ppm; FT-IR (KBr) ν 3437, 2953, 2923, 2852, 1658, 1640, 1629, 1609, 1491, 1482, 1467, 1449, 1362, 1322, 1296, 1278, 1261, 1232, 1020, 875, 807 cm^{-1}; MALDI-TOF (*m/z*) (MH^+) calcd for $C_{312}H_{343}N_{16}S$: 4345.705; found 4345.720.

G4FB: yellow solid (57%); m.p. >250 ^oC; ^{1}H-NMR (300 MHz, $CDCl_3$) δ 8.72 (4H, s), 8.59 (8H, s), 8.26 (16H, m), 8.14 (32H, m), 8.07-7.86 (34H, m), 7.73-7.52 (36H, m), 7.43 (32H, d, *J* = 8.1 Hz), 7.32 (32H, *J* = 8.7 Hz), 2.27 (8H, m), 1.41 (288H, s) and 1.39-0.75 (92H, m) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$) δ 154.41, 153.90, 151.48, 142.53, 142.13, 141.65, 141.39, 140.20, 137.09, 135.61, 133.61, 130.79, 129.99, 129.77, 128.71, 128.11, 126.45, 126.04, 124.21, 124.00, 123.80, 123.54, 123.11, 121.74, 120.15, 119.45, 116.21, 112.14, 111.67, 111.03, 109.08, 84.05, 59.79, 55.92, 53.23, 40.39, 38.69, 36.35, 34.71, 32.03, 31.80, 30.15, 29.71, 29.62, 29.57, 29.43, 29.24, 27.10, 24.28, 22.59, 19.74 and 14.06 ppm; FT-IR (KBr) ν 3046, 2958, 2923, 2861, 1629, 1607, 1581, 1464, 1452, 1322, 1294, 1278, 1259, 1232, 1033, 1022, 875, 807, 739, 667, 654 and 610 cm^{-1}; MALDI-TOF (*m/z*) (MH^+) calcd for $C_{568}H_{583}N_{32}S$: 7888.641; found 7888.408.

2. Computer quantum calculation results

The ground state geometries of **GnFB** were fully optimized using PM6 level, as implemented in Gaussian 09.[4]

3. Device fabrication and testing

Double layer green OLED devices using **GnFB** as a non-doped green emissive layer (EML) with the device configuration of ITO/PEDOT:PSS/**GnFB**(spin-coating)/BCP(40 nm)/LiF(0.5 nm)/Al(150 nm) were fabricated and characterized as followed. The patterned indium tin oxide (ITO) glass substrate with a sheet resistance 14 Ω/□ (purchased from Kintec Company) was thoroughly cleaned by successive ultrasonic treatment in detergent, deionised water, isopropanol, and acetone, and then dried at 60 ^oC in a vacuum oven. A 50 nm thick PEDOT:PSS hole injection layer was spin-coated on top of ITO from a 0.75 wt.% dispersion in water at a spin speed of 3000 rpm for 20 s and dried at 200 ^oC for 15 min under vacuum. Thin film of **GnFB** was deposited by spin-coating $CHCl_3$:toluene solution (1:1) of **GnFB** (1% w/v) on top of

PEDOT:PSS layer at a spin speed of 3000 rpm for 30 second to get a 40 nm thick of EML. The film thickness was measured by using a Tencor α-Step 500 surface profiler. Then BCP was deposited onto the surface of the **GnFB** film as electron-transporting layer (ETL) with a thickness of 40 nm by evaporation from resistively heated alumina crucibles at evaporation rate of 0.5-1.0 nm/s in vacuum evaporator deposition (ES280, ANS Technology) under a base pressure of ~10^{-5} mbar. The film thickness was monitored and recorded by quartz oscillator thickness meter (TM-350, MAXTEK). The chamber was vented with dry air to load the cathode materials and pumped back; a 0.5 nm thick LiF and a 150 nm thick aluminum (Al) layers were the subsequently deposited through a shadow mask on the top of BCP film without braking vacuum to from an active diode areas of 4 mm^2. The measurement of device efficiency was performed according to M.E. Thomson's protocol and the device external quantum efficiencies were calculated using procedure reported previously.[5] Current density-voltage-luminescence (*J-V-L*) characteristics were measured simultaneous by the use of a Keithley 2400 source meter and a Newport 1835C power meter equipped with a Newport 818-UV/CM calibrated silicon photodiode. The EL spectra were acquired by an Ocean Optics USB4000 multichannel spectrometer. All the measurements were performed under ambient atmosphere at room temperature soon after breaking the chamber.

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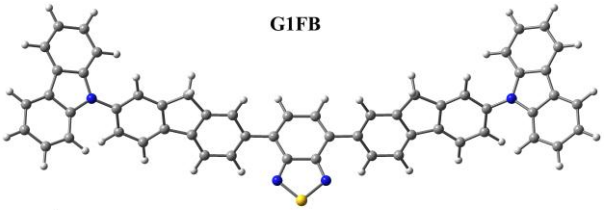

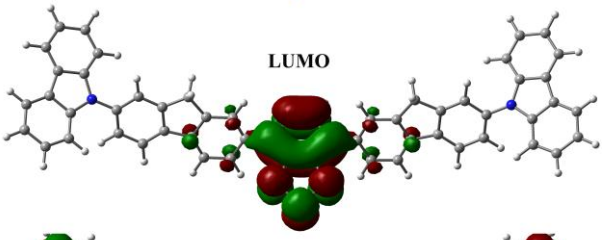

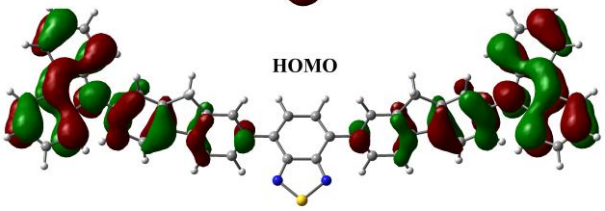

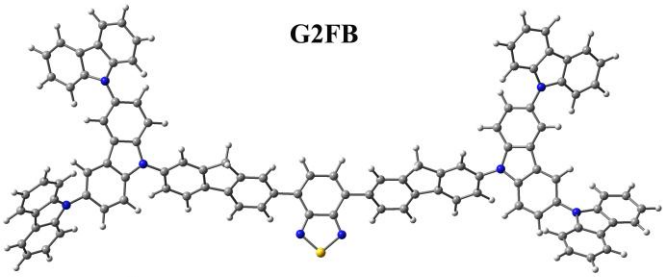

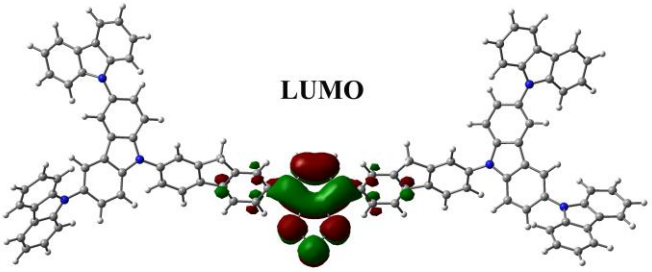

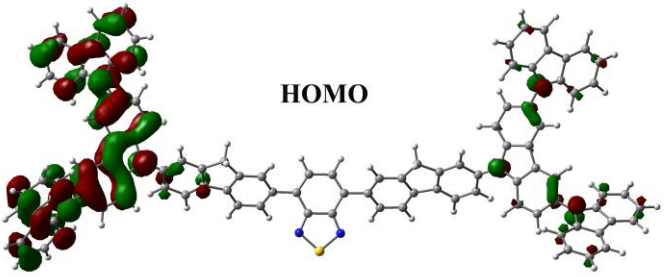

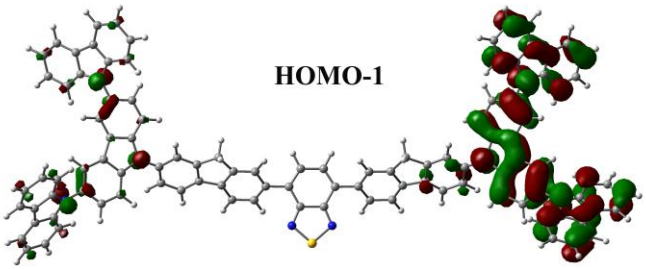

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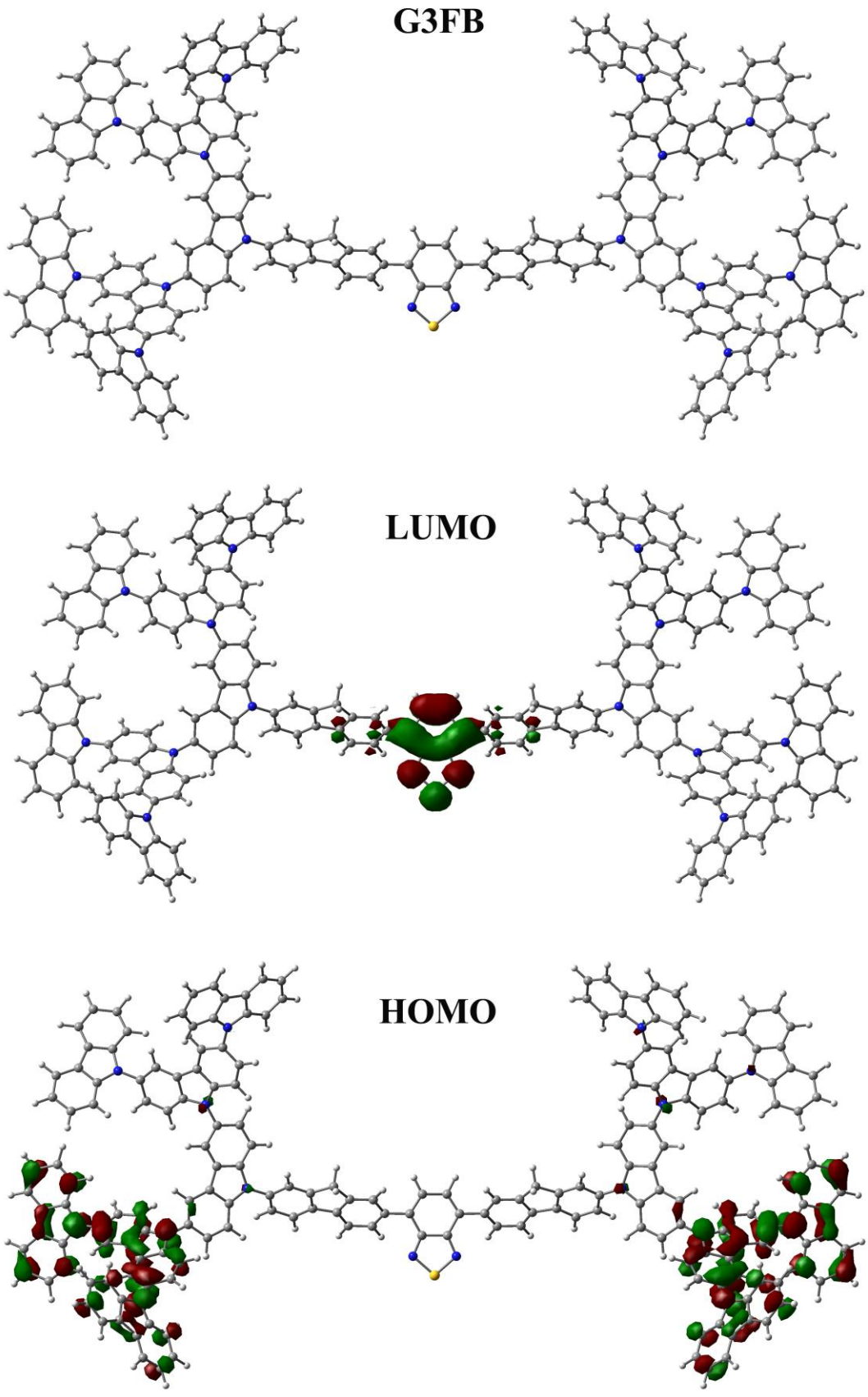

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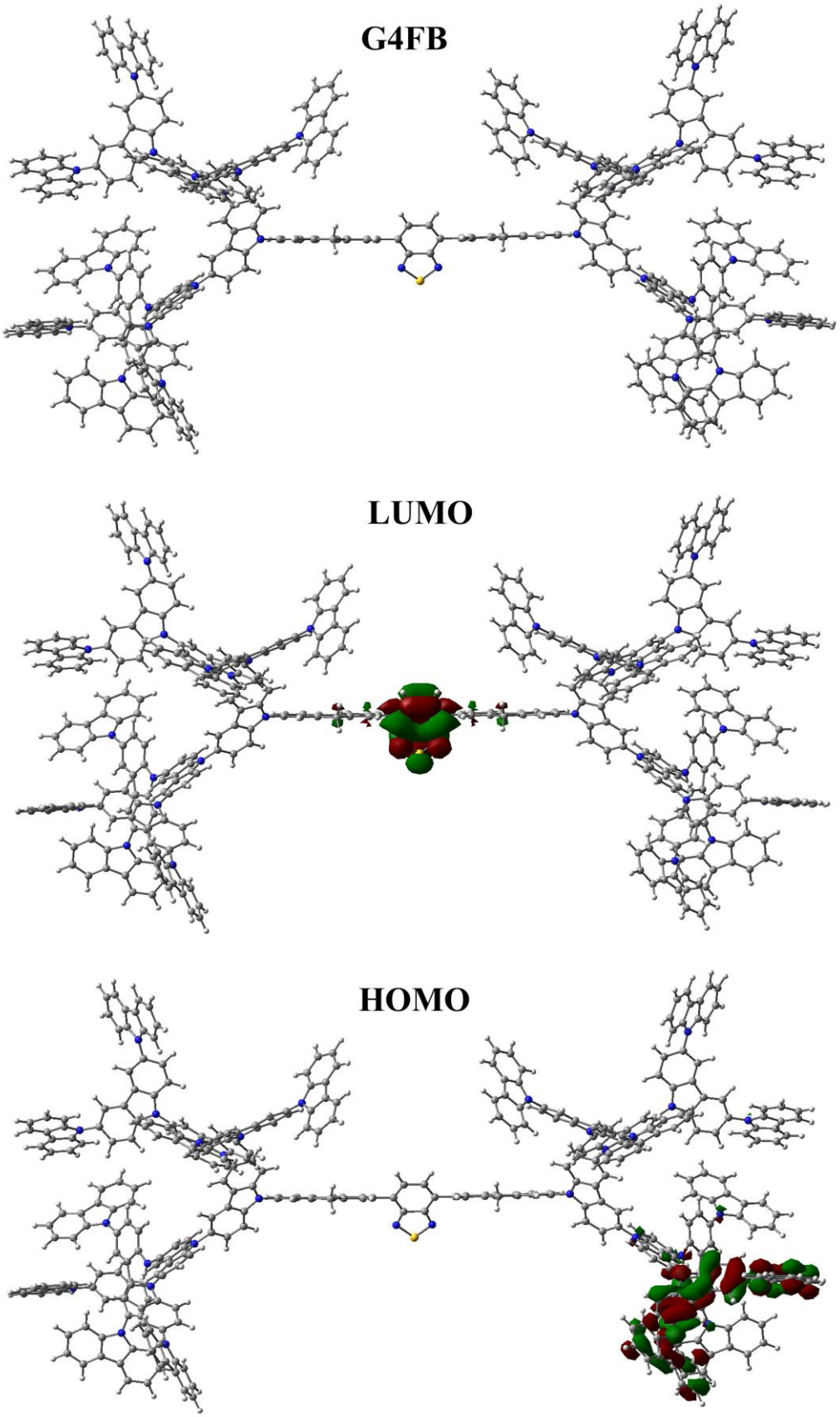
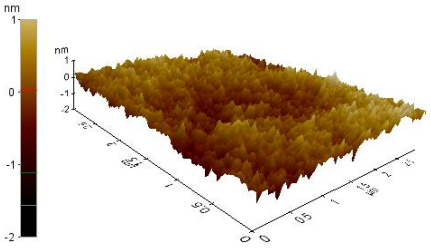


Figure S1 The optimized geometry (Uppermost), and FMO of **GnFB** calculated by PM6 level of theory.



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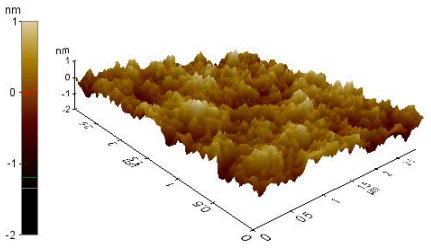
G1FB



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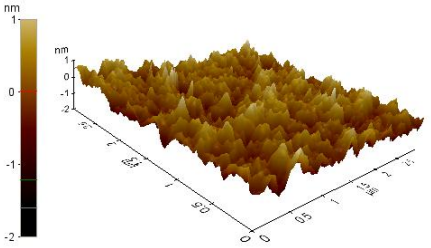
Drive	19.04 (%)

G2FB



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Source	Topography
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Data Height	153 (pxl)
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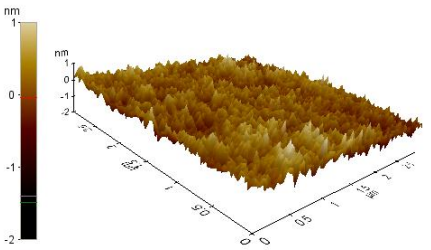
Y Scan Size	2.99 (µm)
Scan Rate	0.3 (Hz)
Z Servo Gain	3.35
Set Point	6.39 (nm)
Amplitude	19.86 (nm)
Sel. Frequency	302.99E3 (Hz)
Drive	23.35 (%)

G3FB



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Scan Rate	0.3 (Hz)
Z Servo Gain	3.35
Set Point	6.39 (nm)
Amplitude	19.86 (nm)
Sel. Frequency	302.99E3 (Hz)
Drive	23.35 (%)

G4FB

Figure S2 Tapping mode AFM image of spin-coated films of **GnFB**.

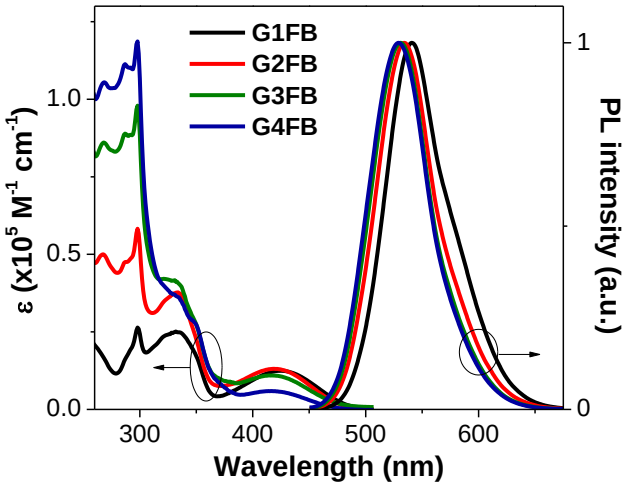


Figure S3 UV-Vis absorption and PL spectra of **GnFB** measured CH_2Cl_2 solution.

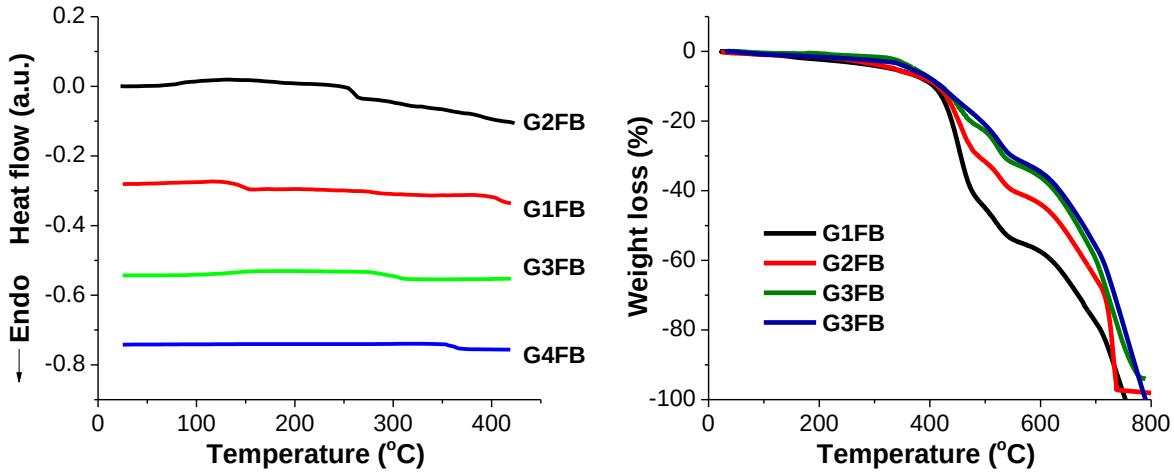
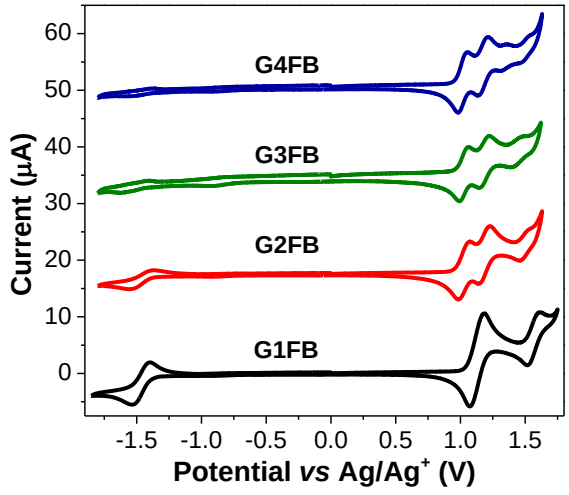


Figure S4 DSC (1st heating scan) and TGA curves of **GnFB** measured at 10 °C/min under N_2.



Compd	$E_{1/2}$ *vs* Ag/Ag^+ (V)
G1FB	-1.47, 1.12, 1.56
G2FB	-1.46, 1.03, 1.18, 1.50
G3FB	-1.47, 1.02, 1.18, 1.45
G4FB	-1.45, 1.02, 1.17, 1.34, 1.50

Figure S5 (a) CV curves of **GnFB** measured in CH_2Cl_2 at a scan rate of 50 mV/s.

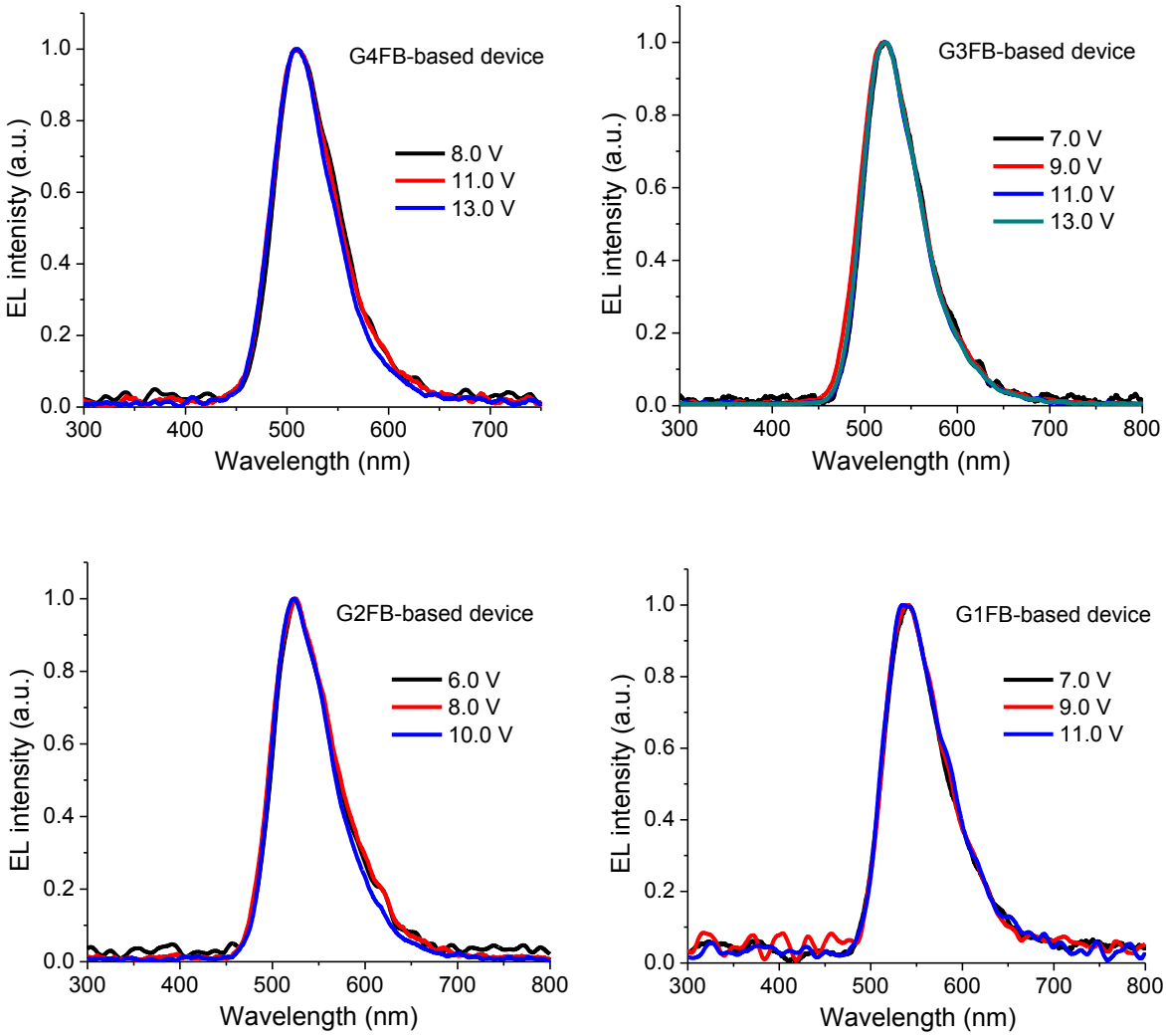


Figure S6 (a) Normalized EL spectra at different applied voltages of **the double layer OLED**.

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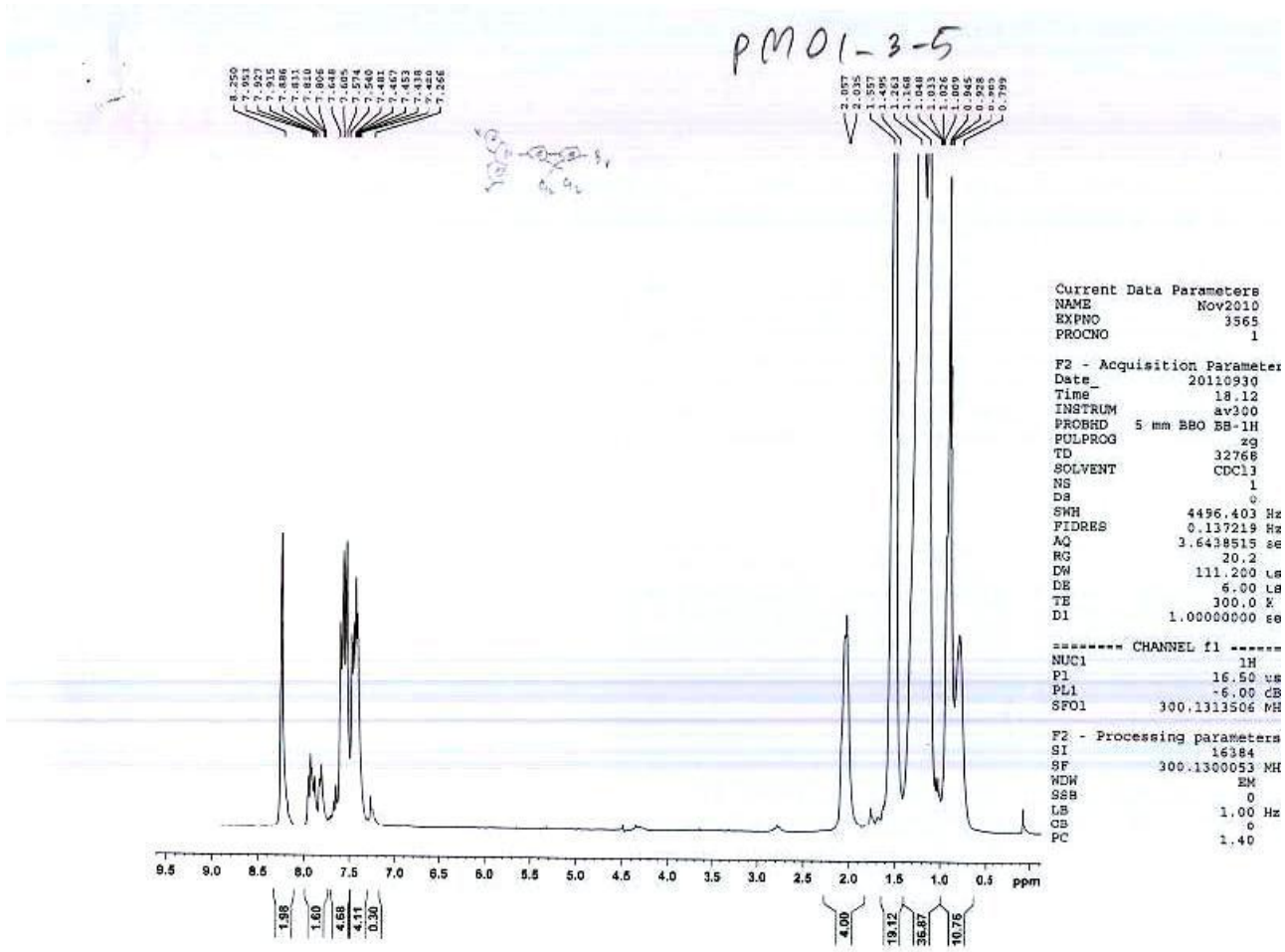
Compound 2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FIDRES 0.137219 Hz
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DE 6.00 us
TE 300.0 K
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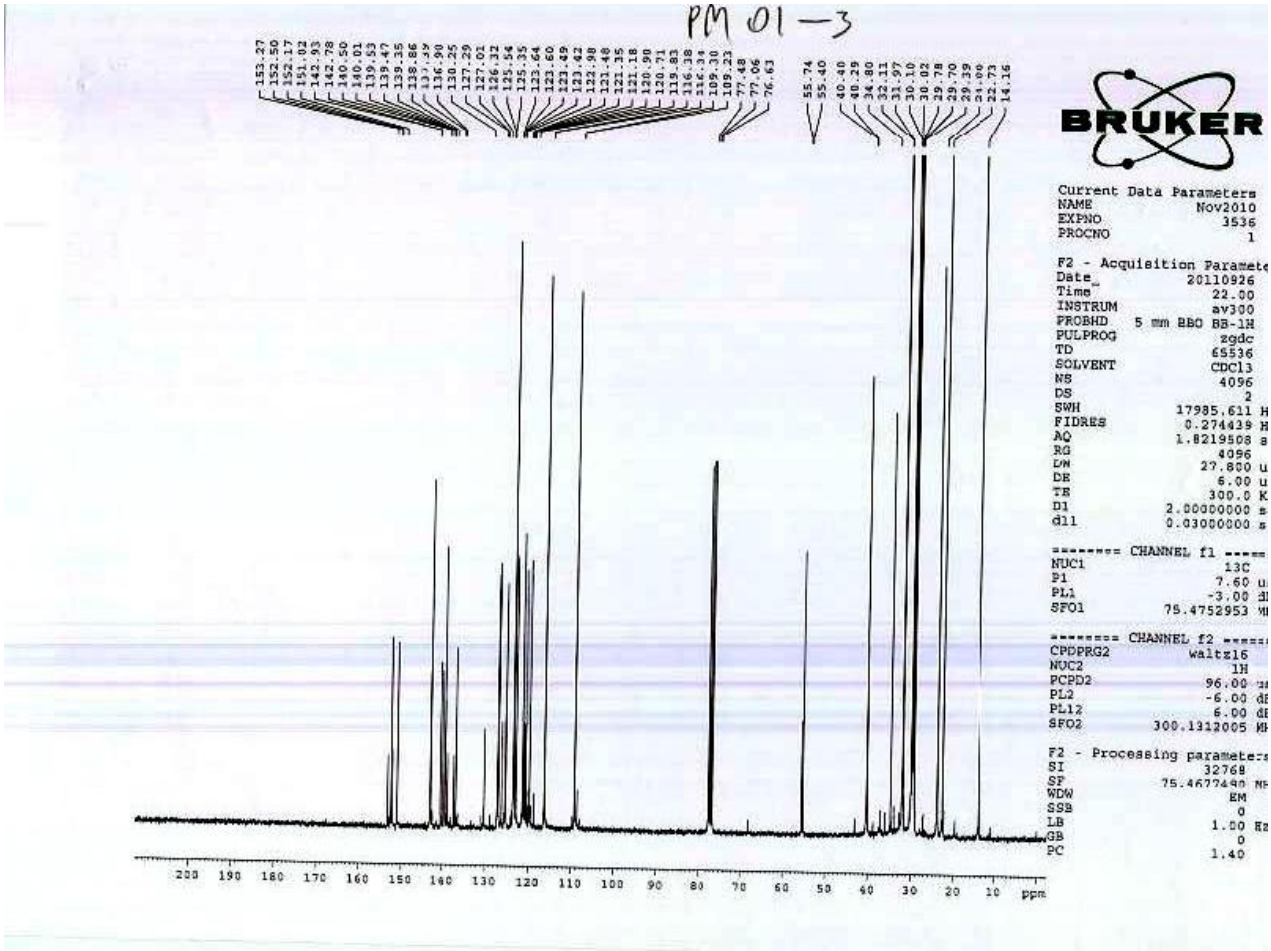
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DE 6.00 u
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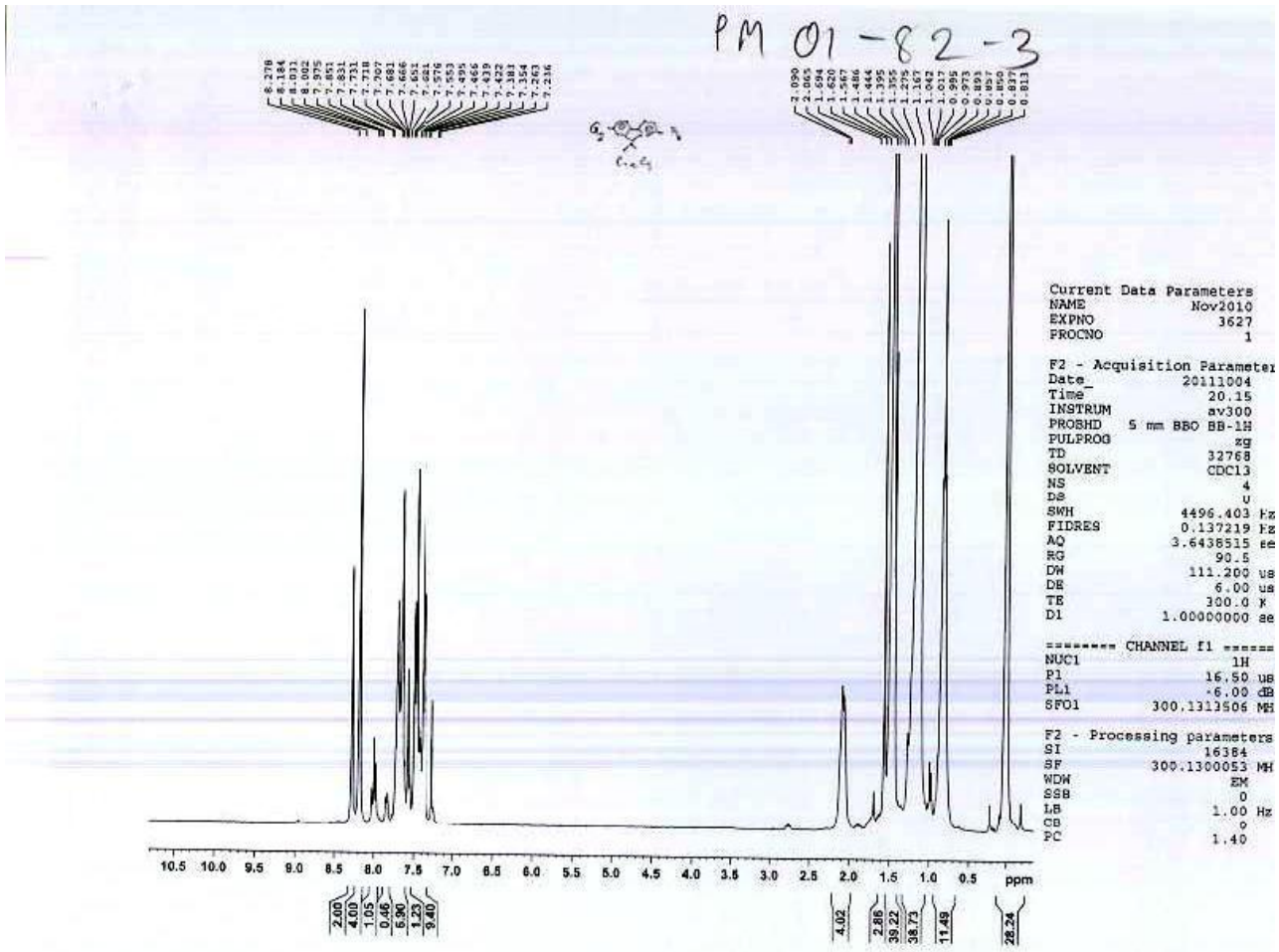
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SOLVENT CDCl3
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FIDRES 0.137219 Hz
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RG 90.5
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DE 6.00 us
TE 300.0 K
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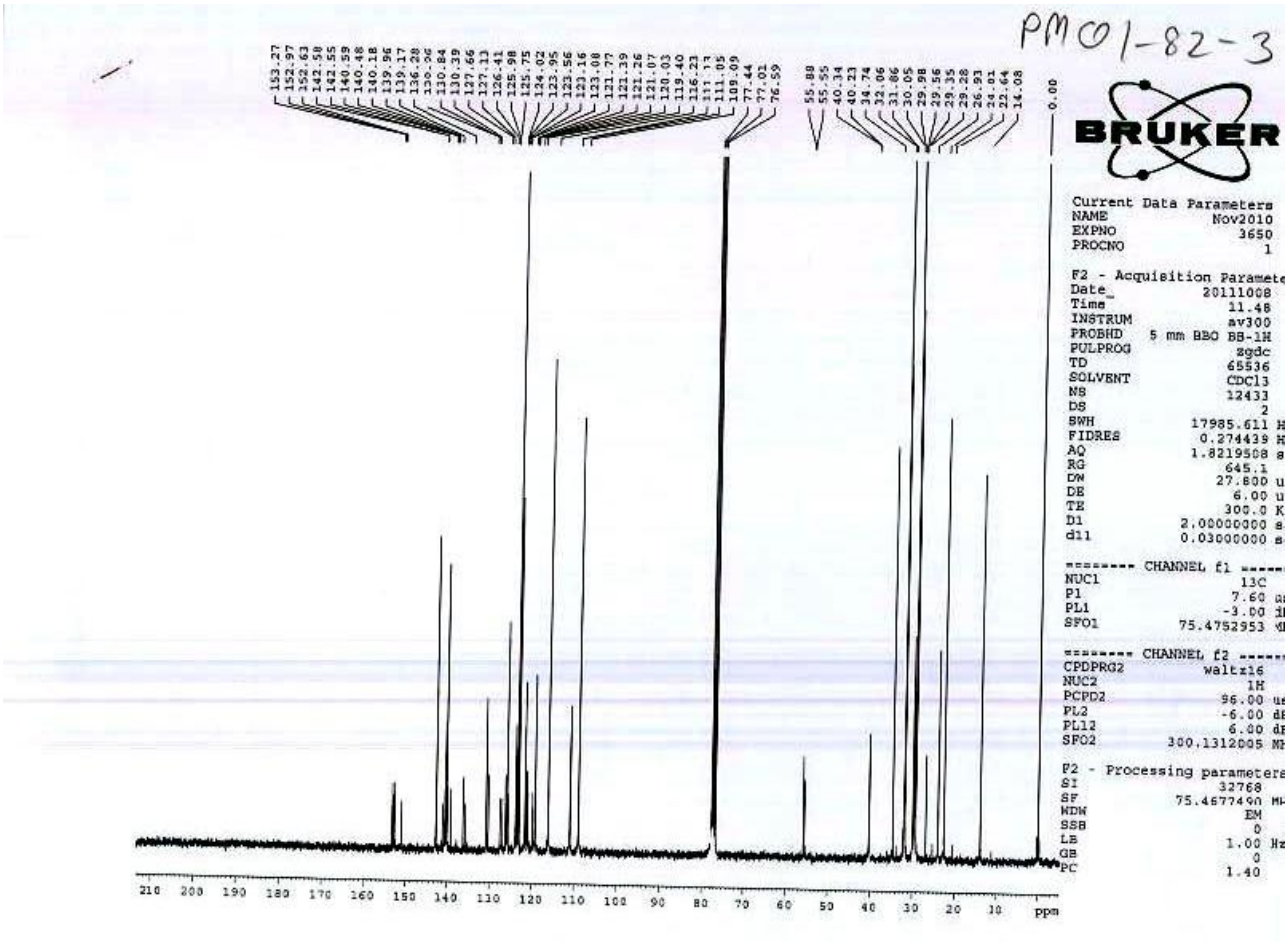
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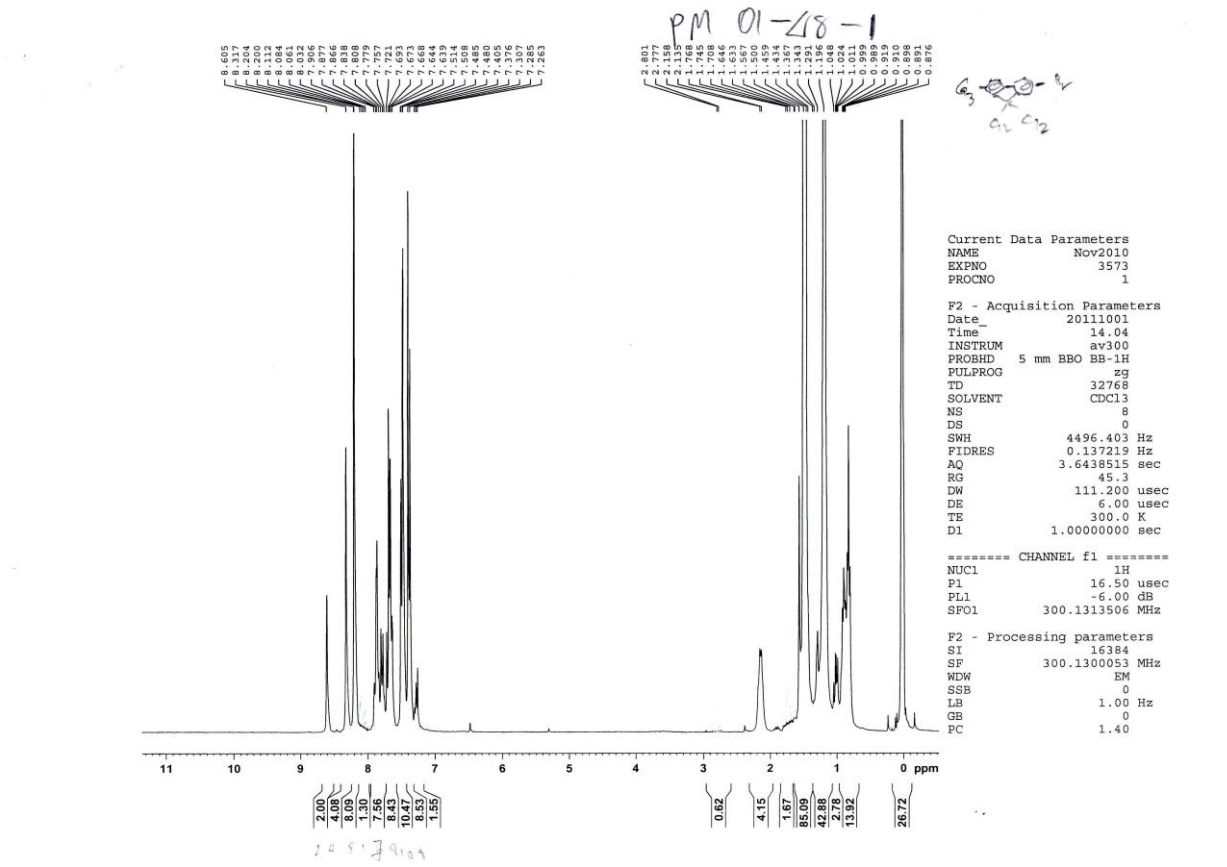
Compound 4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DE 6.00 usec
TE 300.0 K
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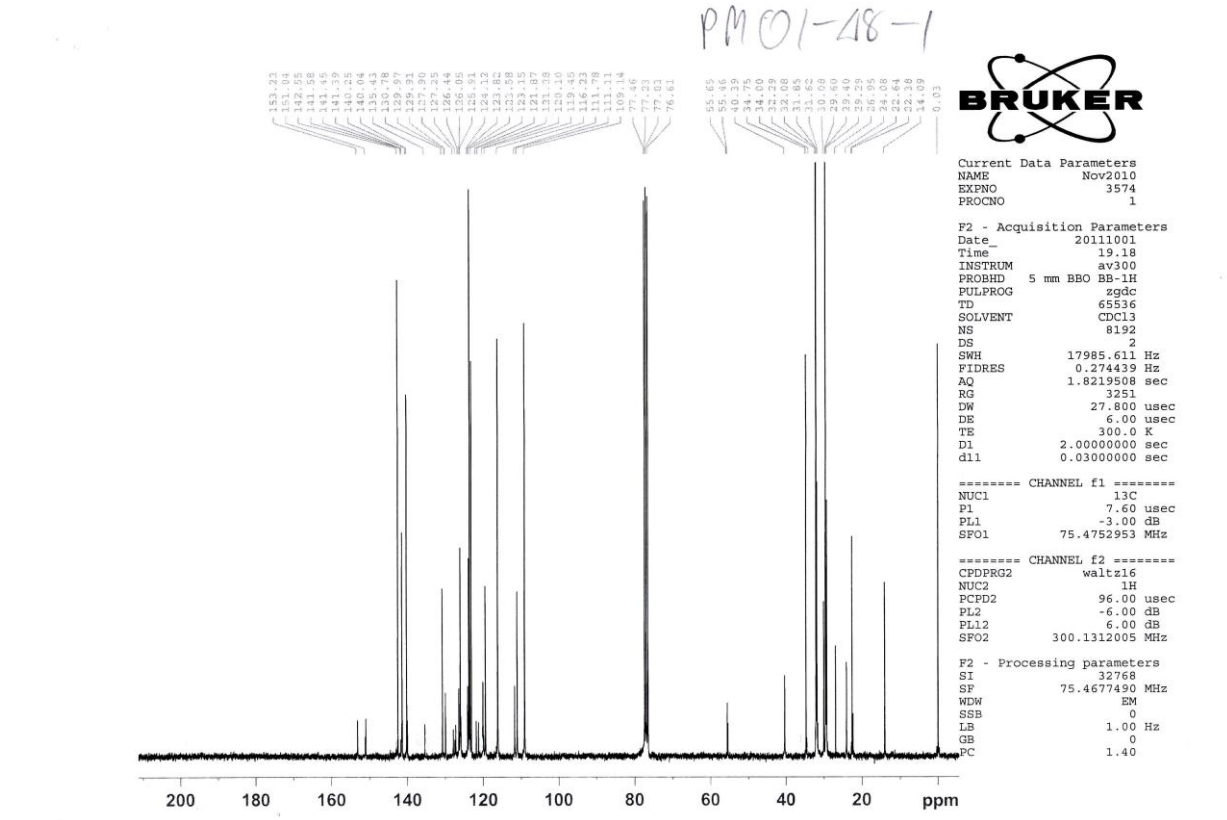
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FIDRES 0.274439 Hz
AQ 1.8219508 sec
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DE 6.00 usec
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d11 0.03000000 sec
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P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
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NUC2 1H
PCPD2 96.00 usec
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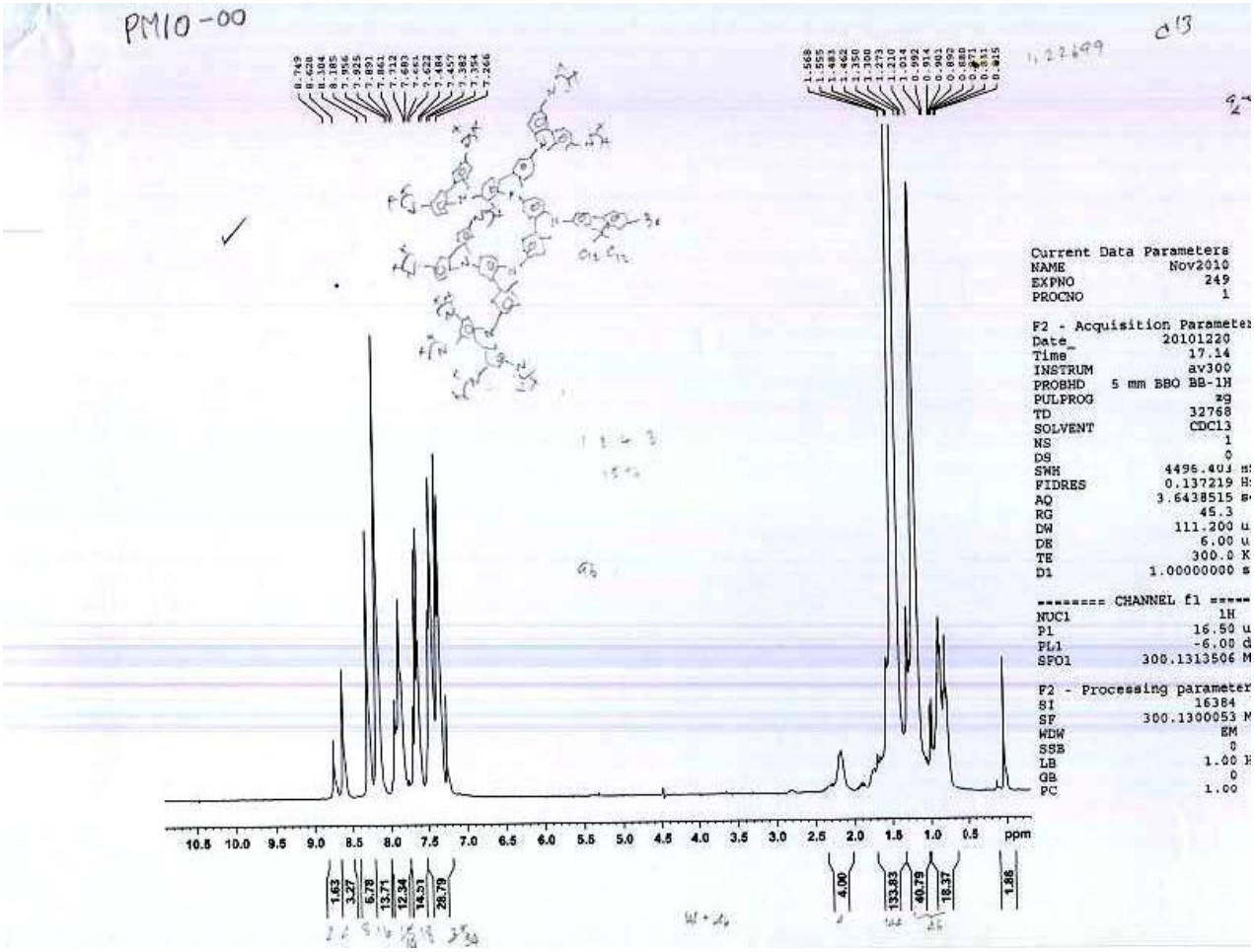
Compound 5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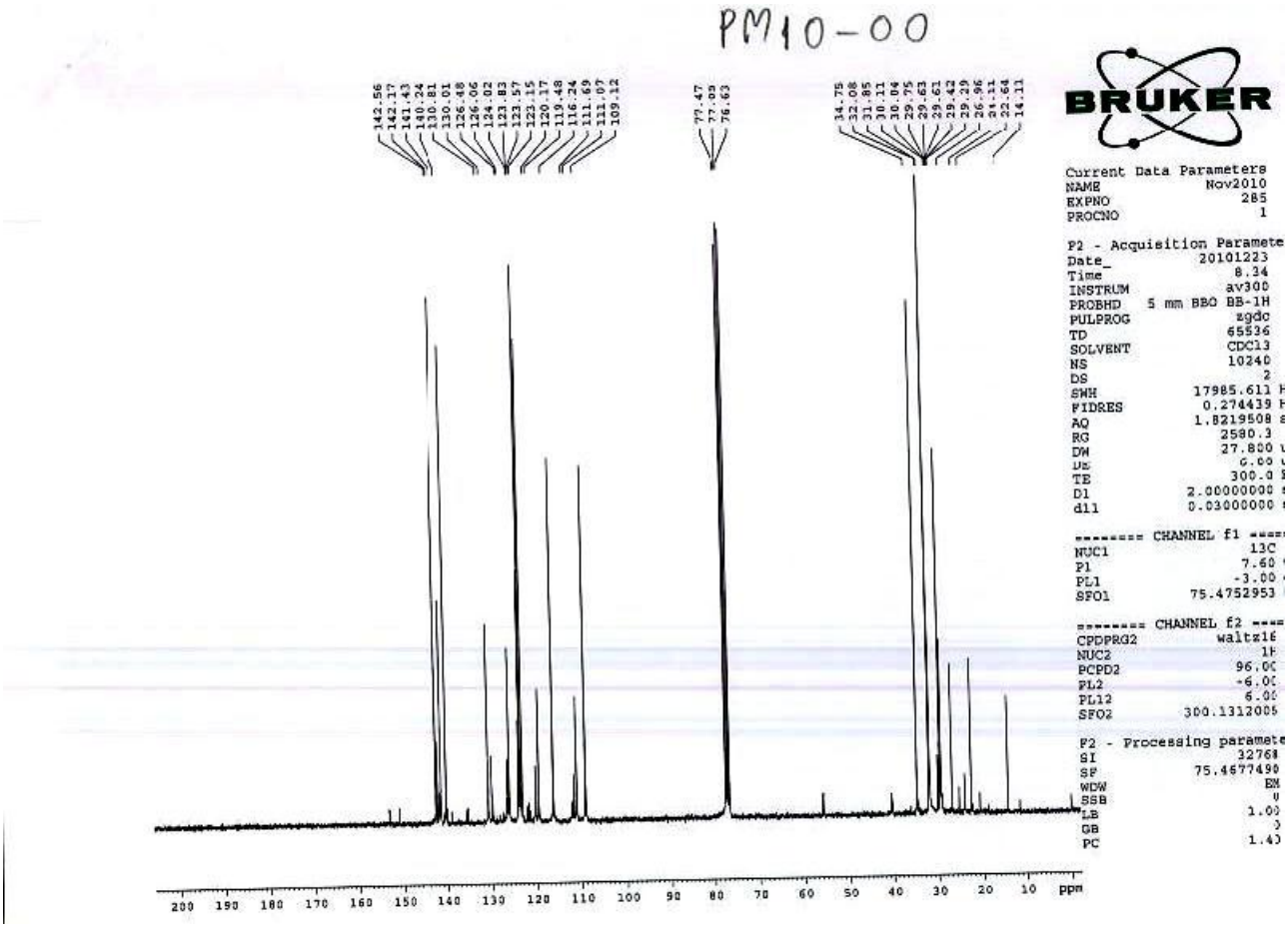
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NUC1 13C
P1 7.60
PL1 -3.00
SFO1 75.4752953
CHANNEL f2
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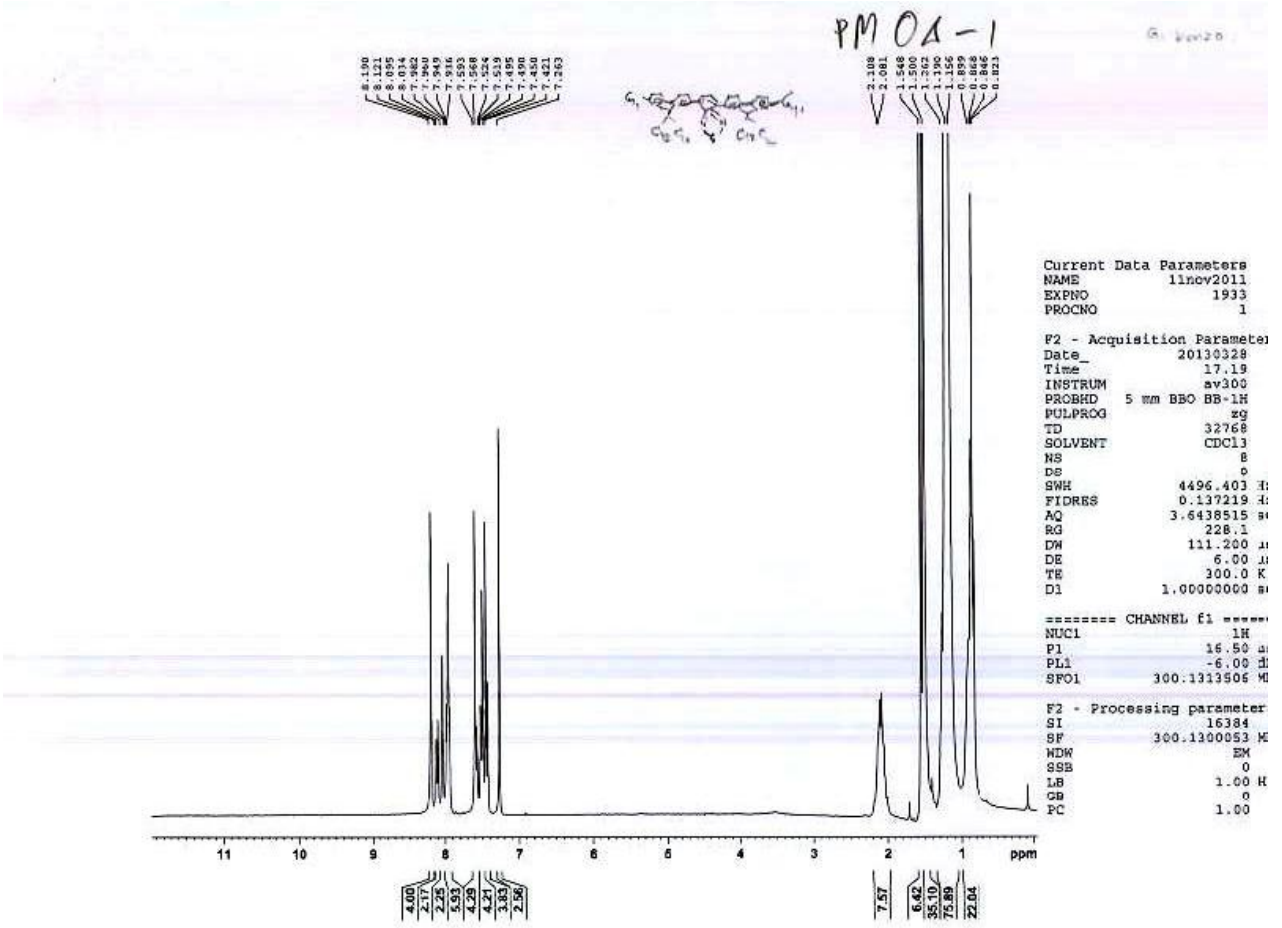

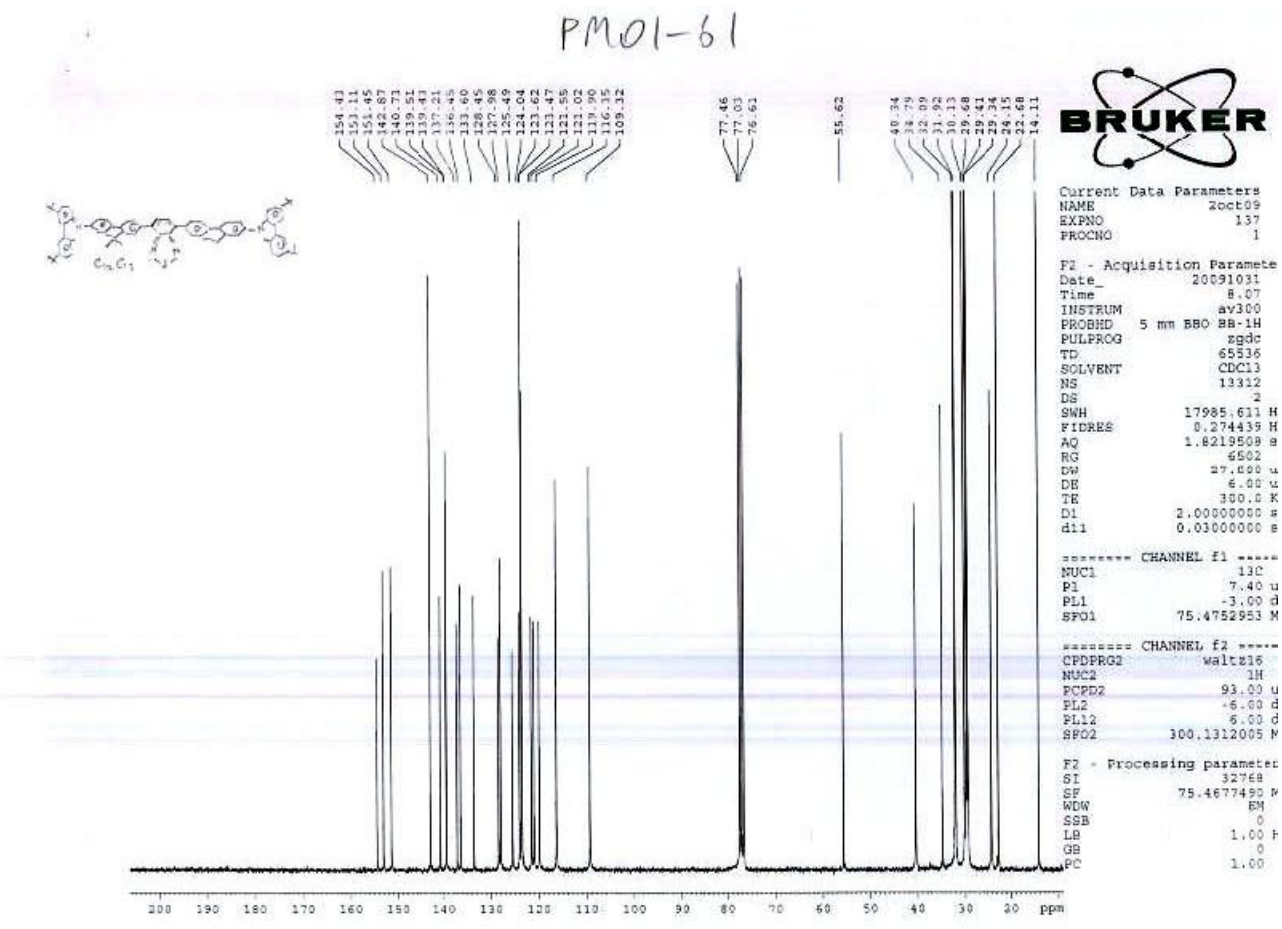

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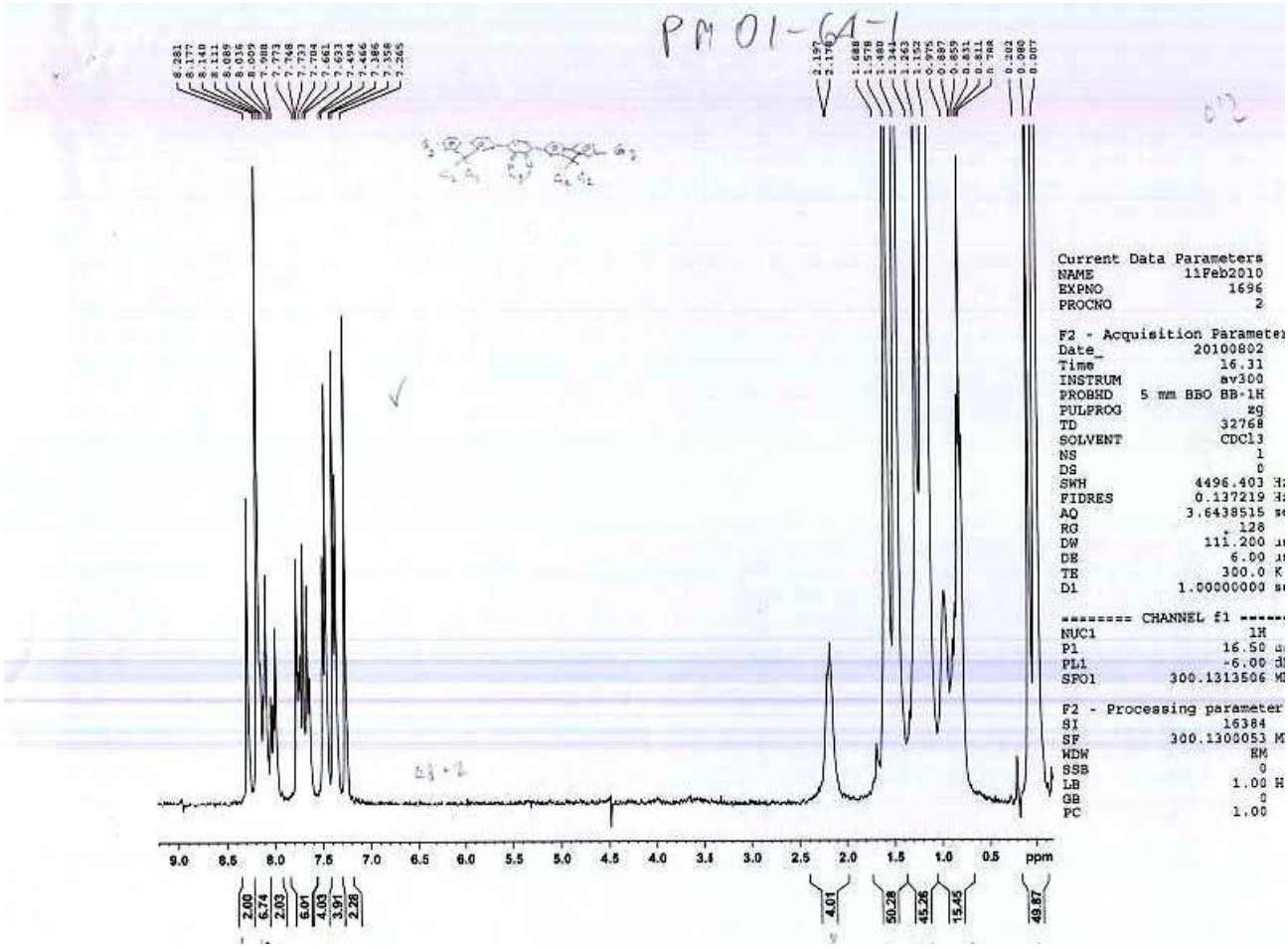

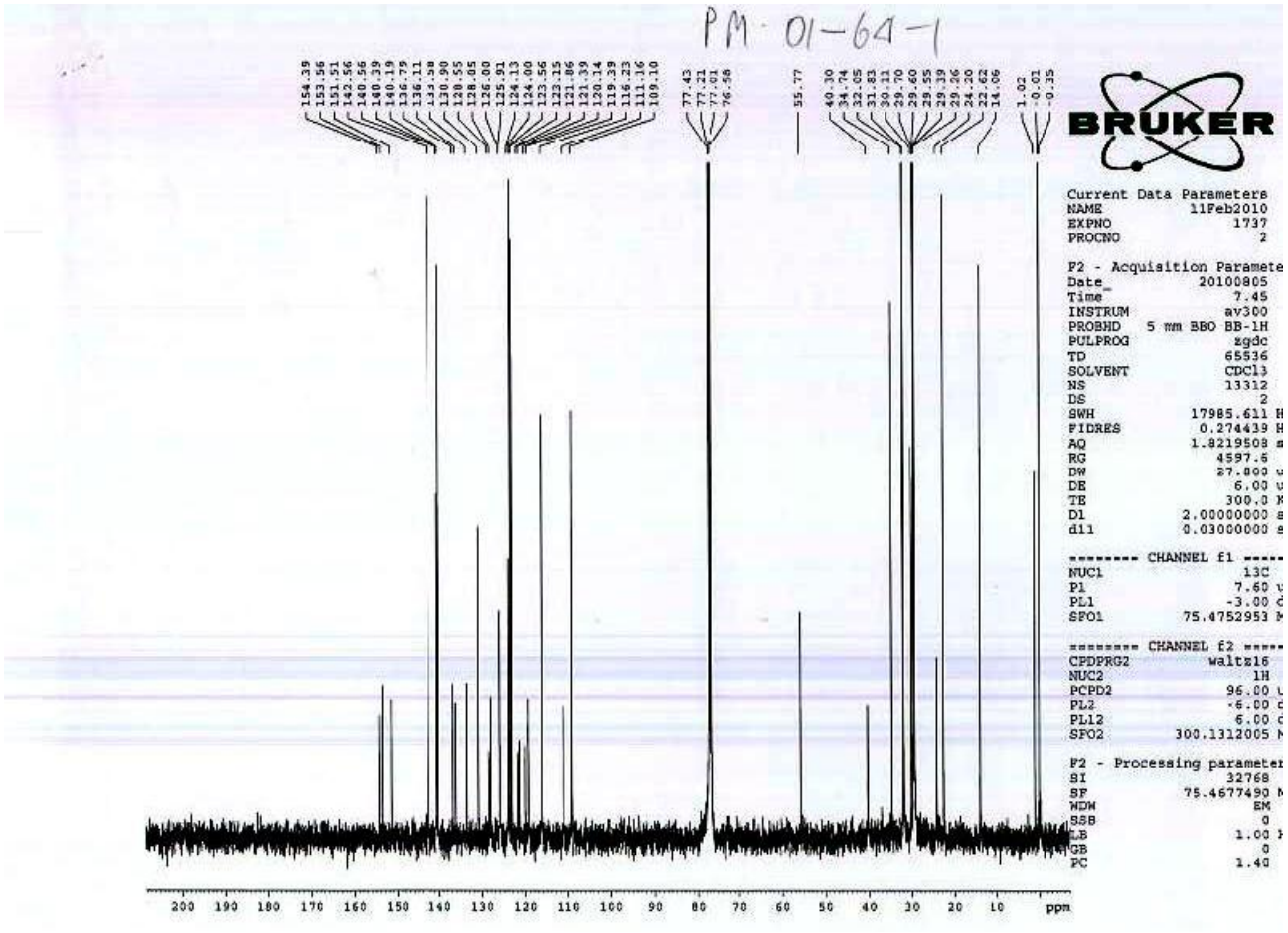

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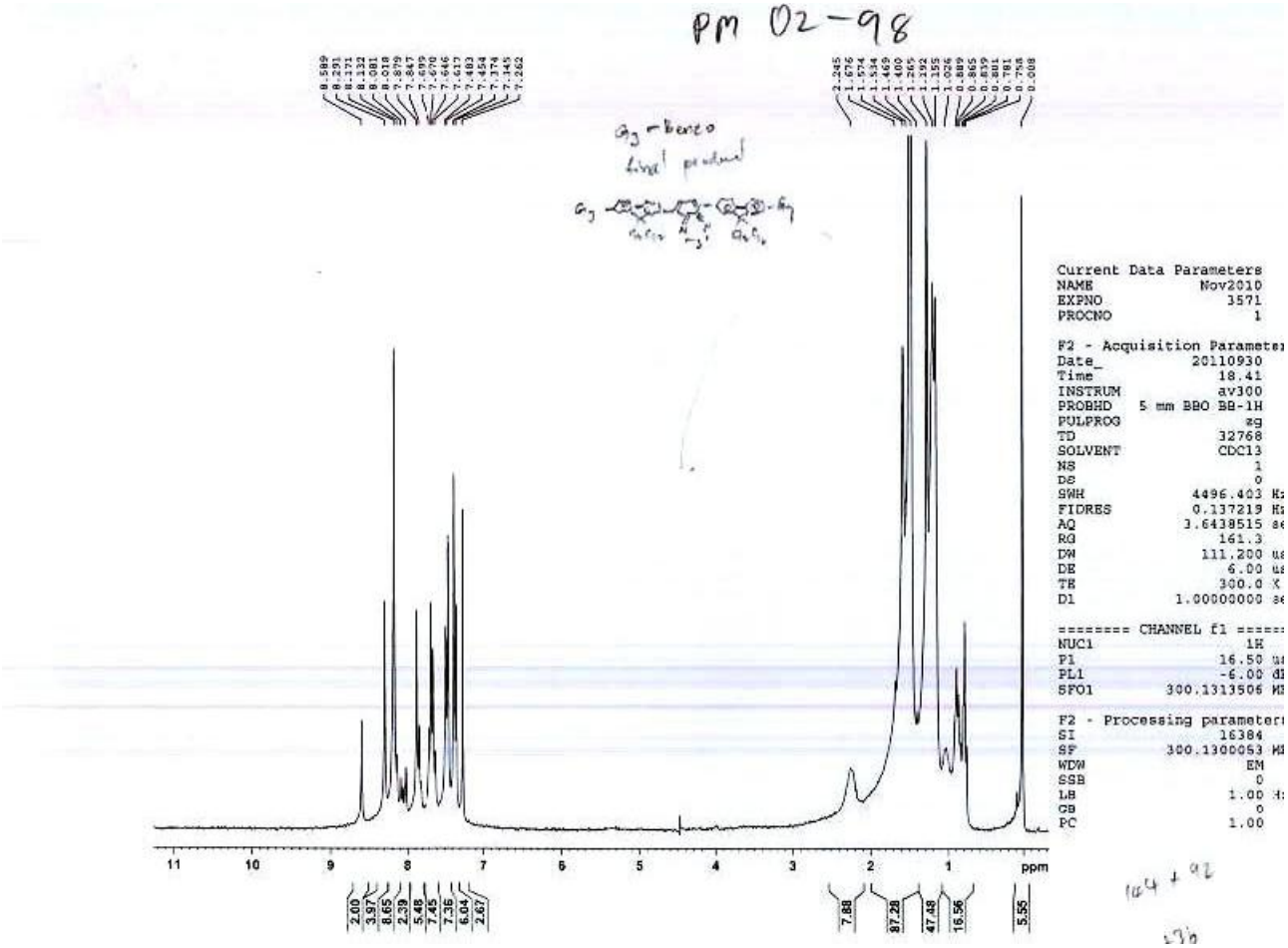

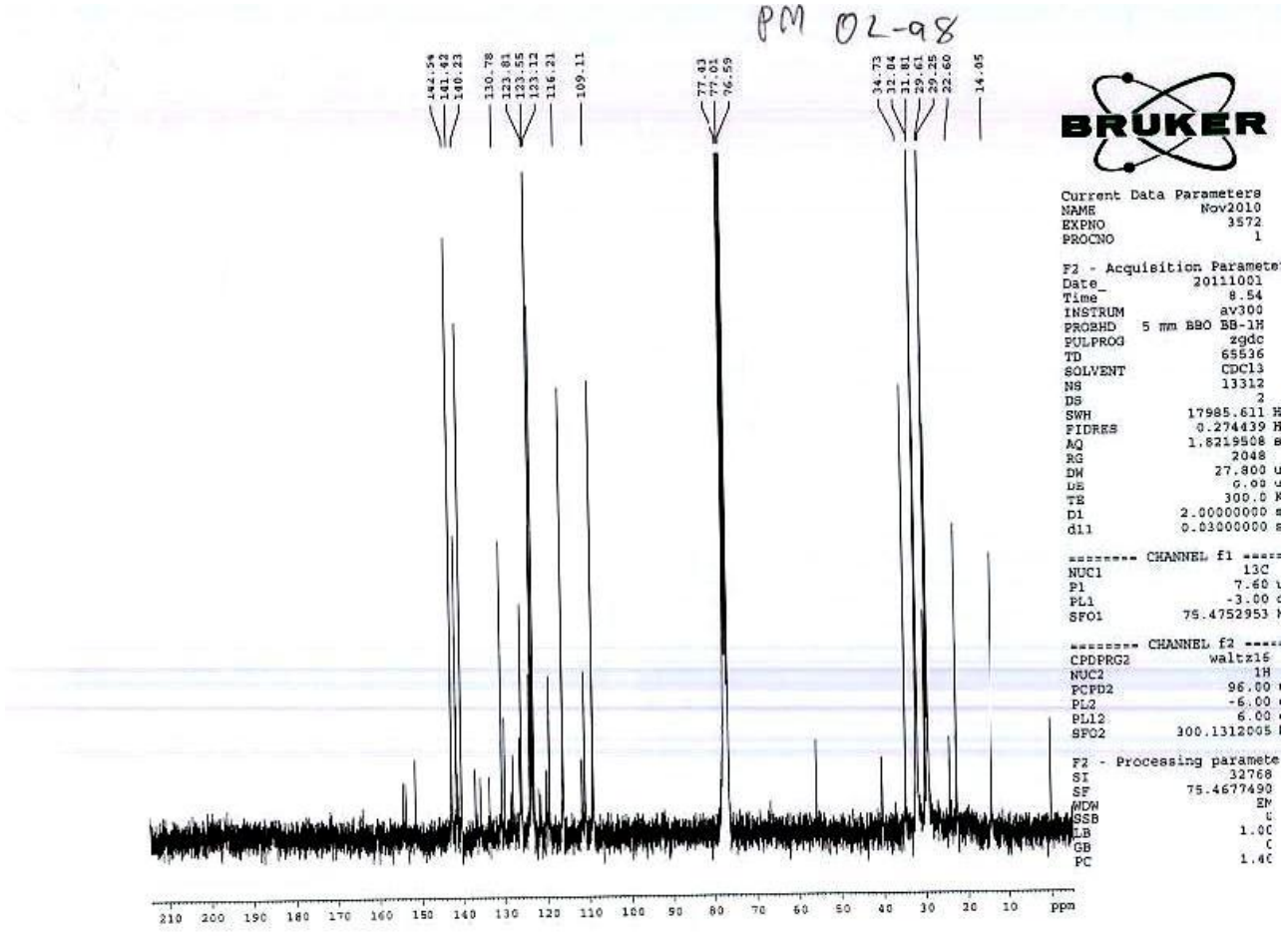

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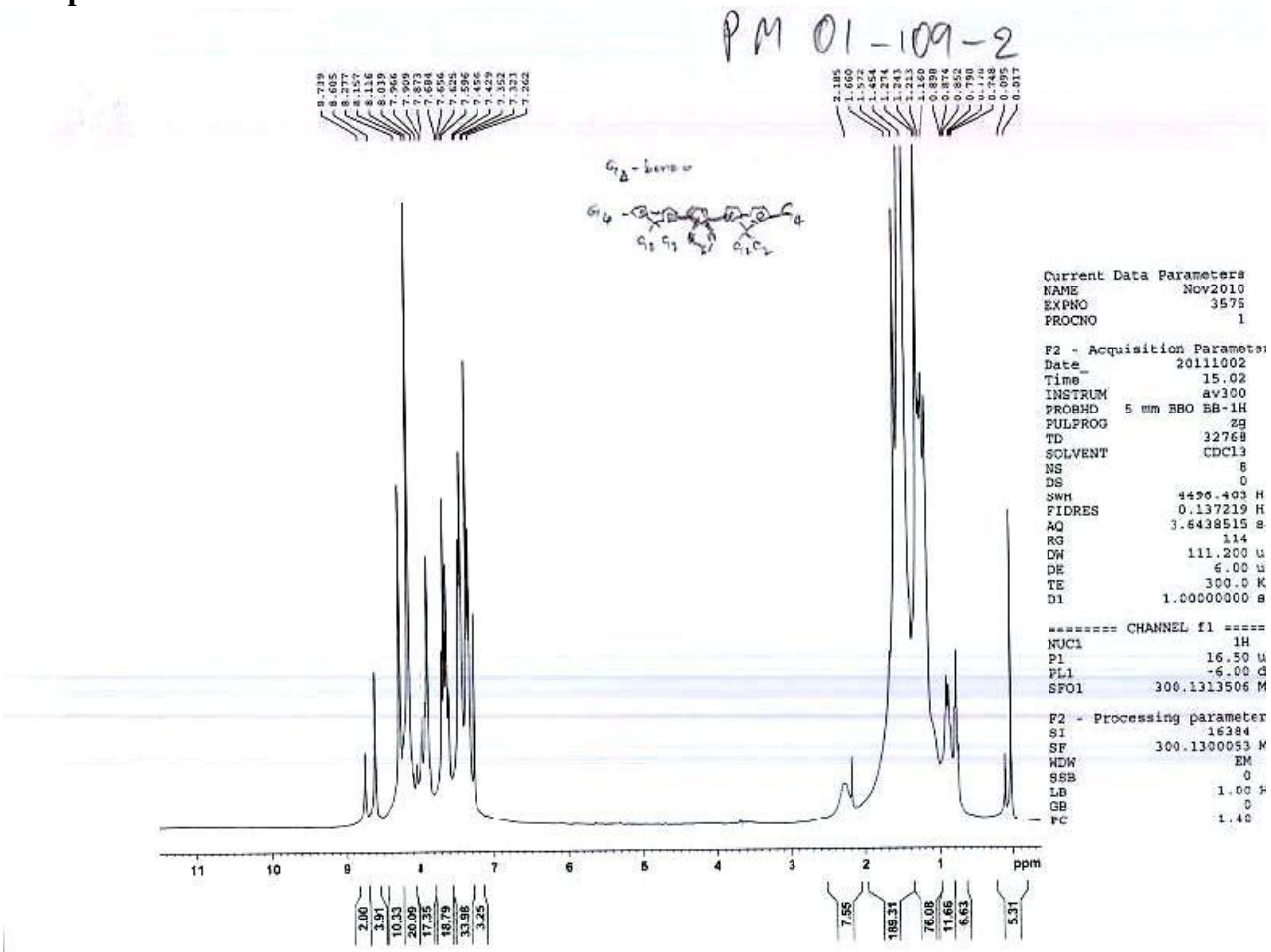

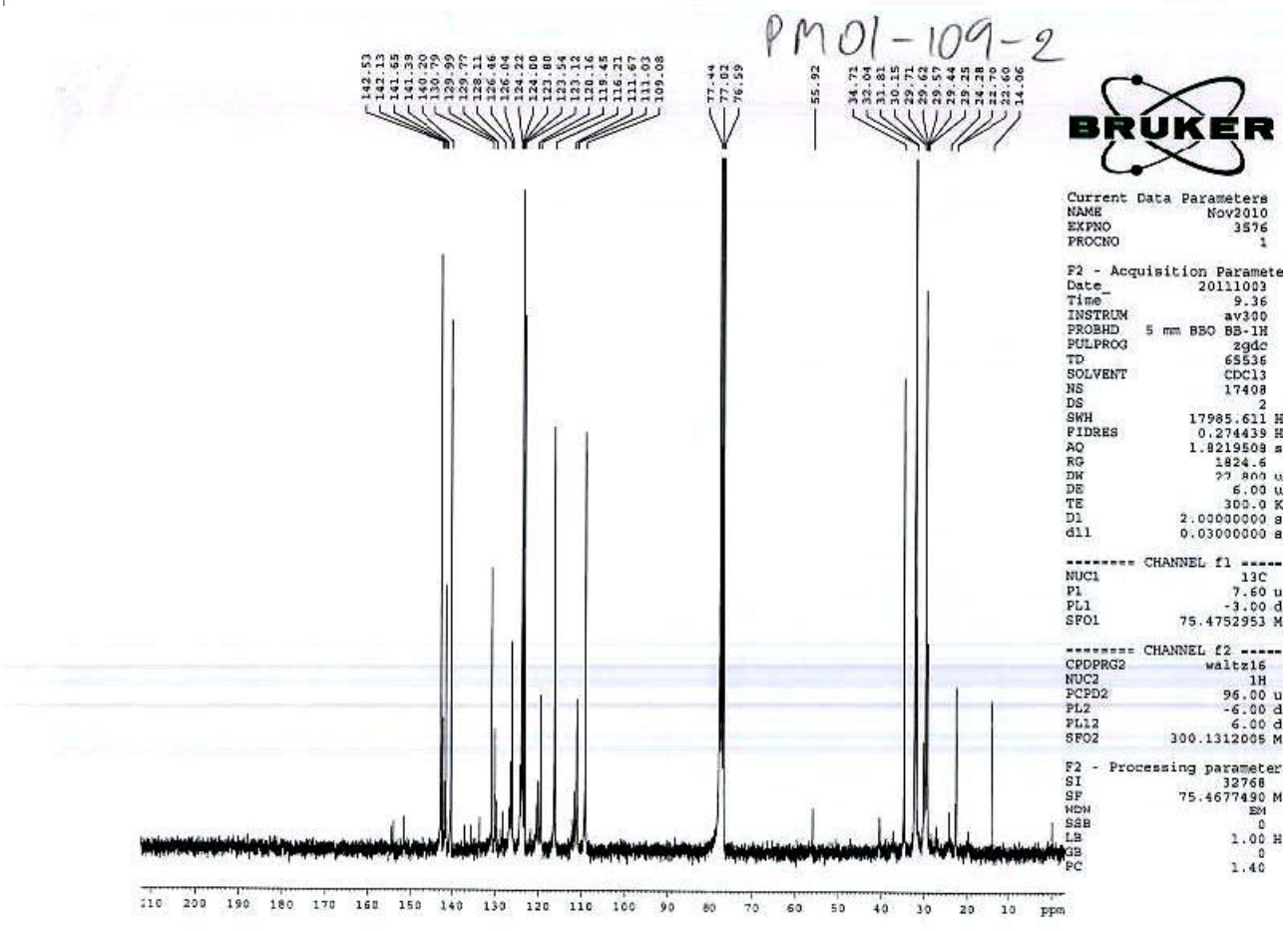

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