Supporting Information

Disodium Benzodipyrrole Sulfonate as Neutral Hole-Transporting Materials for Perovskite Solar Cells

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1. Synthesis of BDPSO Compounds

General

All reactions were carried out in a dry reaction vessel under nitrogen atmosphere. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230–400 mesh silica gel containing a fluorescent indicator (purchased from Merck). Flash silica gel column chromatography was performed on a silica gel 60N (Kanto, spherical and neutral, 140–325 mesh) as described by Still *et al.* (*J. Org. Chem.* **1978**, *43*, 2923–2924).

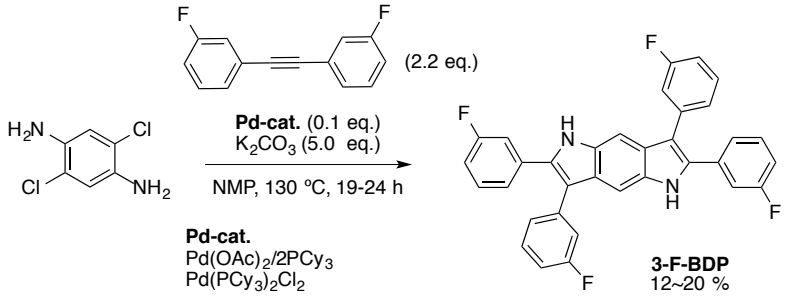
Proton nuclear magnetic resonance (^{1}H-NMR), carbon nuclear magnetic resonance (^{13}C-NMR) and fluorine nuclear magnetic resonance (^{19}F-NMR) were recorded using JEOL ECZ-500 (500 MHz) NMR spectrometer. Chemical data of protons, carbons and fluorines are reported in parts per million (ppm, δ scale) downfield from an internal standard, tetramethylsilane (δ 0.0), DMSO-d_6 (δ 39.5) or THF-d_8 (δ 66.5), $C_6H_5CF_3$ (δ –63.8), respectively. Mass spectra were obtained using JEOL JMS-T100LC equipped with an atmospheric pressure chemical ionization (APCI) or electrospray ionization (ESI) unit and a time-of-flight mass analyzer.

Materials

Commercial reagents were purchased from Tokyo Kasei Co., Aldrich., and other commercial suppliers and used as purchased. Anhydrous solvents were purchased from Kanto and purified by a solvent purification system (GlassCoutour) equipped with columns of activated alumina and copper catalyst prior to use. Other solvents were used as received. Bis(2-fluorophenyl)acetylene, bis(3-fluorophenyl)acetylene, bis(4-fluorophenyl)acetylene were synthesized by a method reported by Lee *et al.*[1] 2,3,6,7-Tetraphenylbenzo[1,2-*b*:4,5-*b*']dipyrrole (**BDP**) were synthesized by a method reported by Kinsley *et al.*[2]

Synthetic Procedures

General Procedure for the Synthesis of BDP Cores: 3-F-BDP



A procedure reported by Senanayake *et al.* was modified for BDP core synthesis.[3] A mixture of 2,5-dichloro-1,4-phenylenediamine (1.77 g, 10 mmol), bis(3-fluorophenyl)acetylene (4.71 g, 22 mmol), $Pd(PCy_3)_2Cl_2$ (0.10 mmol) or $Pd(OAc)_2/2PCy_3$ (0.10 mmol), and potassium carbonate (6.98 g, 5.0 mmol) in

NMP (40 mL or 100 mL) was stirred at 130 ºC for 19 h. NMP was removed by vacuum distillation and the residue was passed over a short column of silica gel (eluent: ethyl acetate). Silica gel column chromatography (eluent: hexane/dichloromethane = 1/1) followed by washing by methanol and acetone afforded the title compound as a yellow solid (1050 mg, 20%).

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 11.31 (s, 2H, N*H*), 7.51–7.49 (m, 2H, Ar*H*), 7.42 (q, *J* = 7.3 Hz, 6H, Ar*H*), 7.28–7.14 (m, *12*H, Ar*H*).

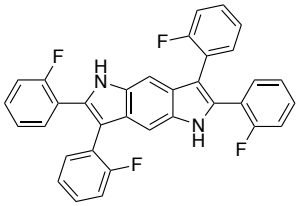
^{13}C-NMR (125 MHz, DMSO-d_6) δ: 162.49 (d, *J* = 242 Hz), 162.10 (d, *J* = 242 Hz), 138.04 (d, *J* = 7.2 Hz), 134,65 (d, *J* = 8.4 Hz), 133.96 (d, *J* = 2.4 Hz), 133.73 (s), 130.74 (d, *J* = 9.6 Hz), 130.66 (d, *J* = 9.6 Hz), 126.78 (s), 125.96 (s), 124.21 (s), 116.14 (d, *J* = 22.6 Hz), 114.51 (d, *J* = 21.6 Hz), 114.37 (d, *J* = 20.8 Hz), 113.02 (d, *J* = 20.4 Hz), 111.71 (s), 98.40 (s).

^{19}F-NMR (470 MHz, DMSO-d_6) δ: –115.32, –115.69.

HRMS (APCI$^+$) *m/z* Calcd. for $C_{42}H_{21}F_4N_2$ ([M+H]$^+$): 533.1641; Found: 533.1619.

m.p. 308–309 ºC.

2-F-BDP



Using $Pd(OAc)_2$ (10 mol%) and PCy_3 (20 mol%) as catalyst. Pale yellow solid (25%).

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 11.25 (s, 2H, N*H*), 7.41–7.33 (m, 10H, Ar*H*), 7.27–7.19 (m, 8H, Ar*H*).

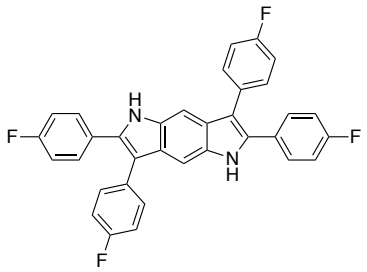
^{13}C-NMR (125 MHz, THF-d_8) δ: 160.53 (d, *J* = 245 Hz), 159.93 (d, *J* = 247 Hz), 134.22 (s), 132.51 (d, *J* = 3.6 Hz), 131.30 (d, *J* = 3.6 Hz), 130.87 (s), 129.13 (d, *J* = 8.4 Hz), 127.71 (d, *J* = 8.4 Hz), 126.94 (s), 124.17 (d, *J* = 15.6 Hz), 123.88 (d, *J* = 2.4 Hz), 123.80 (d, *J* = 3.6 Hz), 121.73 (d, *J* = 13.2 Hz), 115.81 (d, *J* = 18.2 Hz), 115.61 (d, *J* = 22.8 Hz), 108.46 (s), 98.77 (d, *J* = 2.4 Hz).

^{19}F-NMR (470 MHz, DMSO-d_6) δ: –116.10, –116.44.

HRMS (APCI$^+$) *m/z* Calcd. for $C_{42}H_{21}F_4N_2$ ([M+H]$^+$): 533.1641; Found: 533.1664.

m.p. 311–312 ºC.

4-F-BDP



Using $Pd(OAc)_2$ (10 mol%) and PCy_3 (20 mol%) as catalyst. Yellow solid (42%).

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 11.12 (s, 2H, N*H*), 7.46 (dd, *J* = 8.6, 5.7 Hz, 4H, Ar*H*), 7.42–7.39 (m, 6H, Ar*H*), 7.28 (t, *J* = 8.6 Hz, 4H, Ar*H*), 7.23 (t, *J* = 8.9 Hz, 4H, Ar*H*)

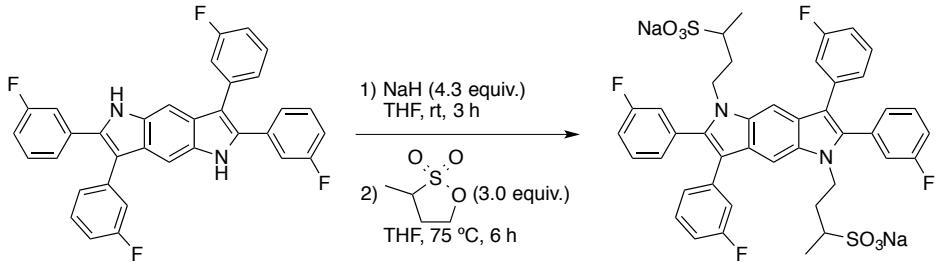
^{13}C-NMR (125 MHz, THF-d_8) δ: 162.18 (d, *J* = 245 Hz), 161.43 (d, *J* = 242 Hz), 134.34 (s), 134.27 (s), 132.65 (d, *J* = 2.4 Hz), 131.63 (d, *J* = 8.4 Hz), 130.06 (d, *J* = 7.2 Hz), 129.89 (s), 127.54 (s) 115.21 (d, *J* = 20.4 Hz), 111.98 (s), 98.18 (s) (some of the peaks were overlapped).

^{19}F-NMR (470 MHz, DMSO-d_6) δ: –116.94, –119.15.

HRMS (APCI$^+$) *m/z* Calcd. for $C_{42}H_{21}F_4N_2$ ([M+H]$^+$): 533.1641; Found: 533.1618.

m.p. 305–308 ºC.

General Procedure for the Synthesis of BDPSO Derivatives: 3-F-br-4C



A mixture of 3-F-BDP (534 mg, 1.0 mmol), sodium hydride (60% dispersion in oil, 173 mg, 4.3 mmol) in THF (20 mL) was stirred at room temperature for 3 h. 2,4-Butanesultone (410 mg, 3.0 mmol) was then added to the reaction mixture and stirred at 75 ºC for 6 h. After cooling to room temperature, minimum amount of methanol was added to quench the remaining sodium hydride. The solid materials were collected by filtration, which was washed with small amount of THF. The obtained solid was sonicated with methanol, collected by filtration, and followed by recrystallization using acetone/water mixture (minimal amount of water in boiling acetone) to give the title compound as a pale yellow solid (600 mg, 71%).

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 7.81 (s, 2H, Ar*H*), 7.52 (q, *J* = 7.4 Hz, 2H, Ar*H*), 7.37 (q, *J* = 7.4 Hz, 2H, Ar*H*), 7.32–7.23 (m, 8H, Ar*H*), 7.01–6.97 (m, 4H, Ar*H*), 4.26–4.20 (m, 4H, NCH_2), 2.24–2.22 (m, 2H, CH_2CH), 2.10–2.08 (m, 2H, CH_2CH), 1.50–1.47 (m, 2H, C*H*), 0.90 (d, *J* = 6.9 Hz, 6H, CH_3).

^{13}C-NMR (125 MHz, DMSO-d_6) δ: 162.14 (d, *J* = 241 Hz), 161.93 (d, *J* = 242 Hz), 137.44 (d, *J* = 8.4 Hz), 137.25 (s), 133.98 (d, *J* = 8.4 Hz), 133.90 (s), 133.90 (d, *J* = 8.4 Hz), 130.33 (d, *J* = 9.6 Hz), 127.26 (s),

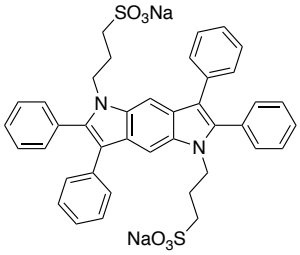
125.52 (s), 124.50 (s), 117.63 (d, J = 21.6 Hz), 115.47 (d, J = 21.6 Hz), 115.44 (d, J = 20.4 Hz), 112.52 (s), 112.14 (d, J = 20.4 Hz), 98.30 (s), 51.55 (s), 41.65 (s), 32.15 (s), 15.47 (d, J = 2.3 Hz).

^{19}F-NMR (470 MHz, DMSO-d_6) δ: –115.07, –115.94.

HRMS (ESI$^-$) *m/z* Calcd. for $C_{42}H_{34}F_4N_2NaO_6S_2$ ([M-Na]$^-$): 825.1692; Found: 825.1681.

m.p. 405 ºC (dec.)

3C



Following the general procedure, this reaction was performed on 1.0 mmol scale. Obtained in 81% yield (606 mg) as pale white solid.

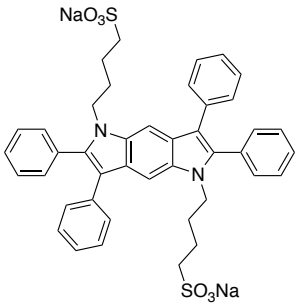
^{1}H-NMR (500 MHz, DMSO-d_6) δ: 7.76 (s, 2H, Ar*H*), 7.46–7.41 (m, 6H, Ar*H*), 7.37–7.36 (m, 4H, Ar*H*), 7.34–7.32 (m, 4H, Ar*H*), 7.28 (t, J = 7.4 Hz, 4H, Ar*H*), 7.14 (t, J = 7.2 Hz, 2H, Ar*H*), 4.18 (t, J = 7.2 Hz, 4H, NCH_2), 2.15 (t, J = 7.7 Hz, 4H, CH_2S), 1.88–1.82 (m, 4H, $CH_2CH_2CH_2$).

^{13}C NMR (125 MHz, DMSO-d_6) δ: 138.15, 135.32, 133.89, 132.12, 130.94, 129.40, 128.48, 128.34, 128.13, 125.14, 124.69, 113.32, 98.14, 48.88, 42.66, 25.62.

HRMS (ESI$^-$) *m/z* Calcd. for $C_{40}H_{34}N_2NaO_6S_2$ ([M-Na]$^-$): 725.1756; Found: 725.1767.

m.p. 412 ºC (dec.)

4C



Following the general procedure, this reaction was performed on 1.0 mmol scale. Obtained in 72% yield (559 mg) as pale yellow solid.

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 7.67 (s, 2H, Ar*H*), 7.46–7.38 (m, 10H, Ar*H*), 7.33–7.29 (m, 8H, Ar*H*), 7.15–7.13 (m, 2H, Ar*H*), 4.05 (t, J = 7.4 Hz, 4H, NCH_2), 2.23 (t, J = 7.7 Hz, 4H, CH_2S), 1.65–1.59 (m, 4H, CH_2), 1.44–1.38 (m, 4H, CH_2).

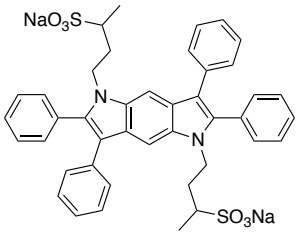
^{13}C-NMR (125 MHz, DMSO-d_6) δ: 138.20, 135.20, 133.78, 132.15, 130.37, 129.37, 128.50, 128.42, 128.23,

125.21, 124.69, 113.21, 97.90, 50.85, 43.20, 28.52, 22.61.

HRMS (ESI$^-$) *m/z* Calcd. for $C_{42}H_{38}N_2NaO_6S_2$ ([M-Na]$^-$): 753.2069; Found: 753.2090.

m.p. 396 ºC (dec.)

br-4C



Following the general procedure, this reaction was performed on 3.0 mmol scale. Obtained in 78% yield (1.82 g) as pale white solid.

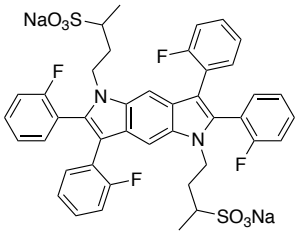
^{1}H NMR (500 MHz, DMSO-d_6) δ: 7.74 (s, 2H, Ar*H*), 7.46–7.42 (m, 6H, Ar*H*), 7.39–7.37 (m, 4H, Ar*H*), 7.34–7.32 (m, 4H, Ar*H*), 7.28 (t, *J* = 7.7 Hz, 4H, Ar*H*), 7.14 (t, *J* = 7.4 Hz, 2H, Ar*H*), 4.21–4.11 (m, 4H, NC*H*2), 2.23–2.12 (m, 4H, CH_2CH), 1.52–1.46 (m, 2H, CH$_2$C*H*), 0.86 (d, *J* = 6.9 Hz, 6H, CH_3).

^{13}C NMR (125 MHz, DMSO-d_6) δ: 138.03, 135.38, 133.78, 132.13, 130.94, 129.35, 128.48, 128.31, 128.15, 125.12, 124.72, 113.17, 98.02, 51.73, 41.62, 32.11, 15.42.

HRMS (ESI$^-$) *m/z* Calcd. for $C_{42}H_{38}N_2NaO_6S_2$ ([M-Na]$^-$): 753.2069; Found: 753.2103.

m.p. 405 ºC (dec.)

2-F-br-4C



Following the general procedure, this reaction was performed on 1.0 mmol scale (without recrystallization in acetone/water, using ethanol instead of methanol for washing since this compound can be dissolved in methanol). Obtained in 87% yield (738 mg) as pale yellow solid.

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 7.50–7.42 (m, 4H, Ar*H*), 7.40–7.22 (m, 10H, Ar*H*), 7.16 (t, *J* = 8.3 Hz, 4H, Ar*H*), 4.21–4.01 (m, 4H, NCH_2), 2.17–2.07 (m, 4H, CH_2CH), 1.48–1.38 (m, 2H, CH$_2$C*H*), 0.79 (d, *J* = 6.3 Hz, 6H, CH_3)

^{13}C-NMR (125 MHz, DMSO-d_6) δ: 159.91 (d, *J* = 245 Hz), 159.59 (d, *J* = 244 Hz), 133.47 (d, *J* = 16.8 Hz), 133.08 (d, *J* = 10.8 Hz), 133.13–132.99 (m), 132.14 (s), 131.15 (d, *J* = 8.4 Hz), 128.24 (d, *J* = 7.2 Hz), 125.07 (d, *J* = 4.8 Hz), 124.50 (m), 124.32 (s), 122.31 (d, *J* = 15.6 Hz), 119.59 (d, *J* = 15.6 Hz), 115.73 (d, *J*

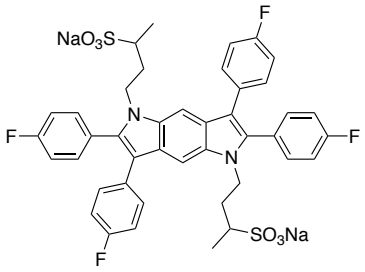
= 21.6 Hz), 108.69–108.457 (m), 98.17 (s), 51.64 (s), 41.98 (s), 21.90 (d, *J* = 20.4 Hz), 15.15 (d, *J* = 12.0 Hz) (some of the peaks were overlapped).

^{19}F-NMR (470 MHz, DMSO-d_6) δ: –115.29, –115.47, –115.57.

HRMS (ESI$^-$) *m/z* Calcd. for $C_{42}H_{34}F_4N_2NaO_6S_2$ ([M-Na]$^-$): 825.1692; Found: 825.1692.

m.p. 367 ºC (dec.)

4-F-br-4C



Following the general procedure, this reaction was performed on 1.0 mmol scale. Obtained in 67% yield (568 mg) as pale yellow solid.

^{1}H-NMR (500 MHz, DMSO-d_6) δ: 7.78 (s, 2H, Ar*H*), 7.43 (dd, *J* = 8.3, 5.4 Hz, 4H, Ar*H*), 7.35 (dd, *J* = 8.6, 5.7 Hz, 4H, Ar*H*), 7.29 (t, *J* = 8.6 Hz, 4H, Ar*H*), 7.12 (t, *J* = 8.9 Hz, 4H, Ar*H*), 4.24–4.17 (m, 4H, NCH_2), 2.27–2.22 (m, 2H, CH_2CH), 2.10–2.07 (m, 2H, CH_2CH), 1.50–1.47 (m, 2H, CH$_2$C*H*), 0.89 (d, *J* = 6.9 Hz, 6H, CH_3)

^{13}C-NMR (125 MHz, DMSO-d_6) δ: 162.01 (d, *J* = 222 Hz), 160.07 (d, *J* = 218 Hz), 136.92 (s), 133.76 (s), 133.07 (d, *J* = 8.4 Hz), 131.46 (s), 131.07 (d, *J* = 8.4 Hz), 128.32 (s), 124.62 (s), 115.61 (d, *J* = 21.6 Hz), 115.23 (d, *J* = 21.6 Hz), 112.41 (s), 98.10 (s), 51.57 (s), 41.55 (s), 32.20 (s), 15.71 (s).

^{19}F-NMR (470 MHz, DMSO-d_6) δ: –115.94, –120.18.

HRMS (ESI$^-$) *m/z* Calcd. for $C_{42}H_{34}F_4N_2NaO_6S_2$ ([M-Na]$^-$): 825.1692; Found: 825.1674.

m.p. 411 ºC (dec.)

2. Device Fabrication and Characterization

Materials

The following chemicals were obtained from commercial suppliers and used as received: lead(II) iodide (99.99%, TCI), methylammonium iodide (>98%, TCI), $PC_{61}BM$ (99.5%, Lumtec Co., Taiwan), C_{60} (99.5%, Lumtec Co., Taiwan), bathocuproine (>99.0%, TCI). Superdehydrated dimethylformamide and chlorobenzene were purchased from Wako, Japan.

Device Fabrication

The patterned ITO glass was ultrasonically cleaned using a surfactant, rinsed with deionized water, and then given 10 min UV−ozone treatment. An acetone/deionized water (volume ratio, 1:1. For **3F-br-4C**, 1:4 ratio was used after further optimization, and for **br-4C**, 1:2 ratio was used after further optimization) mixed solution of BDPSO (100 μL, 4 mg mL^{-1}) was sealed, mixed overnight and filtered through a 0.45μm PVDF syringe filter before use. The solution was spin-coated onto an ITO substrate at 500 rpm for 3 s and then 3000 rpm for 30 s under air, and was annealed at 130 °C for 10 min under air and 10 min under N_2. Next, a $MAPbI_3$ precursor solution (100 μL) consisting of lead(II) iodide (507.1 mg, 1.10 mmol) and methylammonium iodide (174.9 mg, 1.10 mmol) dissolved in 1.0 mL of dimethylformamide was dropped onto the BDPSO film, and the film was spin-coated at 500 rpm for 3 s and then at 3800 rpm for 20 s. Chlorobenzene (100 μL) was dropped onto the perovskite-coated BDPSO film 8 s after the rotation speed was increased to 3800 rpm, and the film was heated at 100 °C for 10 min. Then 30 nm of C_{60} and 15 nm of bathocuproine were evaporated successively onto the perovskite film. Device fabrication was completed by thermal evaporation of a 100 nm-thick film of Ag as the cathode.

Device Characterization

Current–voltage characteristics were measured by means of AM 1.5G illumination at 100 mW cm^{-2} with a solar simulator (Sumitomo Heavy Industries Advanced Machinery) under ambient conditions with a delay time of 30 ms. *J–V* curves for all devices were measured by masking the devices with a metal mask with an area of 9 mm^2. The light intensity of the solar simulator was calibrated with a standard silicon solar cell (PV Measurements). For the external quantum efficiency (EQE) measurement, a constant power mode was employed using monochromatized photons from halogen or xenon lamps. All the measurements were carried out under an ambient atmosphere. Transient photocurrent (TPC) and photovoltage (TPV) were measured by Paios measurement system (Fluxim). TPC and TPV decay curves were measured under white bias light with intensity equivalent to 1.0-Sun (100 mW cm^2) and 0.9-Sun (90 mW cm^2) respectively generated by LED. Light-soaking stability of encapsulated devices (filled with nitrogen) examined at a maximum-power-point by using a fixed resistance under continuous full-sun illumination at 35°C with UV cutting filter (SIGMAKOKI CO.,LTD, SCF-50S-42L).

Comparison of Performance Parameters Obtained using Device of Different Sizes

A. Performance Parameters of 9.0 mm^2 Devices using Different HTMs[a]

HTM	V_{oc}/V	J_{sc}/mA cm^{-2}	FF	PCE/%	R_s/Ω cm^2	R_{sh}/kΩ cm^2
3C	$0.91_{\pm 0.04}$	$17.49_{\pm 0.63}$	$0.79_{\pm 0.02}$	$12.88_{\pm 0.62}$	$2.6_{\pm 0.5}$	$3.2_{\pm 0.9}$
4C	$0.90_{\pm 0.03}$	$17.51_{\pm 0.56}$	$0.77_{\pm 0.02}$	$12.09_{\pm 0.23}$	$2.7_{\pm 0.3}$	$2.5_{\pm 0.7}$
br-4C	$1.00_{\pm 0.01}$	$19.48_{\pm 0.35}$	$0.79_{\pm 0.01}$	$15.58_{\pm 0.28}$	$3.7_{\pm 0.4}$	$3.1_{\pm 1.0}$
2F-br-4C	$0.94_{\pm 0.02}$	$19.92_{\pm 0.40}$	$0.79_{\pm 0.01}$	$14.40_{\pm 0.57}$	$3.6_{\pm 0.5}$	$3.5_{\pm 1.5}$
3F-br-4C	$1.04_{\pm 0.02}$	$19.78_{\pm 0.41}$	$0.80_{\pm 0.01}$	$16.95_{\pm 0.31}$	$3.3_{\pm 0.3}$	$4.2_{\pm 1.7}$
4F-br-4C	$0.98_{\pm 0.03}$	$18.14_{\pm 0.36}$	$0.80_{\pm 0.01}$	$14.41_{\pm 0.39}$	$3.2_{\pm 0.2}$	$3.9_{\pm 1.4}$
PEDOT:PSS	$0.83_{\pm 0.03}$	$18.85_{\pm 0.72}$	$0.79_{\pm 0.02}$	$12.52_{\pm 0.69}$	$2.9_{\pm 0.8}$	$5.5_{\pm 1.5}$

[a]Data obtained by averaging 5 optimal devices, root mean square error (RMSE) are shown as subscript

B. Performance Parameters of 1.0 mm^2 Devices using Different HTMs[a]

HTM	V_{oc}/V	J_{sc}/mA cm^{-2}	FF	PCE/%	R_s/Ω cm^2	R_{sh}/kΩ cm^2
3C	$0.89_{\pm 0.03}$	$17.46_{\pm 0.63}$	$0.80_{\pm 0.01}$	$12.98_{\pm 0.54}$	$2.5_{\pm 0.3}$	$3.3_{\pm 0.8}$
4C	$0.87_{\pm 0.06}$	$17.21_{\pm 0.78}$	$0.76_{\pm 0.02}$	$12.27_{\pm 0.31}$	$2.4_{\pm 0.4}$	$2.0_{\pm 0.6}$
br-4C	$0.99_{\pm 0.02}$	$19.66_{\pm 0.67}$	$0.77_{\pm 0.03}$	$15.42_{\pm 0.63}$	$3.5_{\pm 0.6}$	$1.9_{\pm 0.9}$
2F-br-4C	$0.91_{\pm 0.02}$	$18.36_{\pm 0.49}$	$0.81_{\pm 0.02}$	$13.90_{\pm 0.75}$	$2.2_{\pm 0.5}$	$4.6_{\pm 1.7}$
3F-br-4C	$1.04_{\pm 0.01}$	$19.83_{\pm 0.63}$	$0.81_{\pm 0.01}$	$16.68_{\pm 0.57}$	$2.6_{\pm 0.4}$	$3.9_{\pm 0.9}$
4F-br-4C	$0.94_{\pm 0.01}$	$18.36_{\pm 0.45}$	$0.80_{\pm 0.02}$	$13.76_{\pm 0.71}$	$2.4_{\pm 0.3}$	$4.2_{\pm 1.3}$
PEDOT:PSS	$0.80_{\pm 0.01}$	$18.46_{\pm 0.78}$	$0.81_{\pm 0.02}$	$12.65_{\pm 0.46}$	$1.9_{\pm 0.5}$	$4.4_{\pm 1.1}$

[a]Data obtained by averaging 8 optimal devices, root mean square error (RMSE) are shown as subscript

As shown in the Tables above, the data obtained using 1.0 mm^2 devices (1.0 mm^2 mask on a 4.0 mm^2 cell), and 9.0 mm^2 devices gave very similar results and same tendency.

3. Instruments

Absorption spectra were measured with JASCO V-670 spectrometer. Emission spectra were measured with HITACHI F-4500 spectrometer. Differential pulse voltammetry (DPV) were conducted with HOKUTO DENKO HZ-7000 voltammetric analyzer. Measurements were carried out in a one-compartment cell under Ar gas, equipped with a platinum counter electrode, a glassy-carbon working electrode, and an Ag/Ag^+ reference electrode. The supporting electrolyte was a 0.5 M N-methyl pyrrolidone (NMP) solution of tetrabutylammonium hexafluorophosphate. All potentials were corrected against Fc/Fc^+. Photoelectron yield spectroscopy (PYS) measurement were performed with PYS-201 (Sumitomo Heavy Industries, Ltd). Atomic force microscopy (AFM) measurement was performed on Bruker Multimode 8 with a silicon nitride cantilever (SCANASYST-AIR or SANASYST-AIR-HR). Thermogravimetric (TG) analysis and differential thermal analysis (DTA) was conducted with Rigaku ThermoPlus 2 thermal analyzer TG-8120. Sample was placed in an aluminum pan and heated to 500 ºC at the rate of 10 K/min, under N_2 purge at a flow rate of 100 mL/min. Al_2O_3 was used as a reference material. Scanning electron microscopic (SEM) images were obtained with an FEI Magellan 400L field emission scanning electron microscope. X-ray diffraction (XRD) patterns were collected on a Rigaku Smartlab diffractometer equipped with a Cu Kα radiation source.

4. Absorption and Emission in Solution

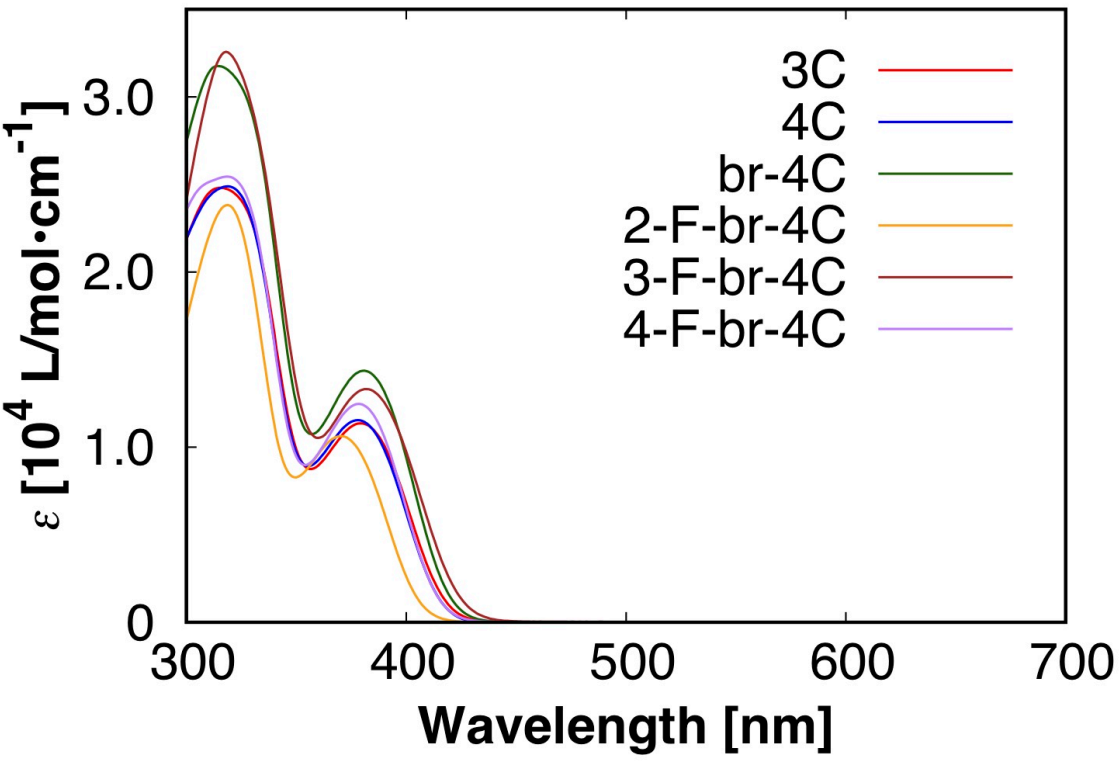


Figure S1. Absorption spectra of BDPSOs in NMP (ca. 3×10^{-5} M).

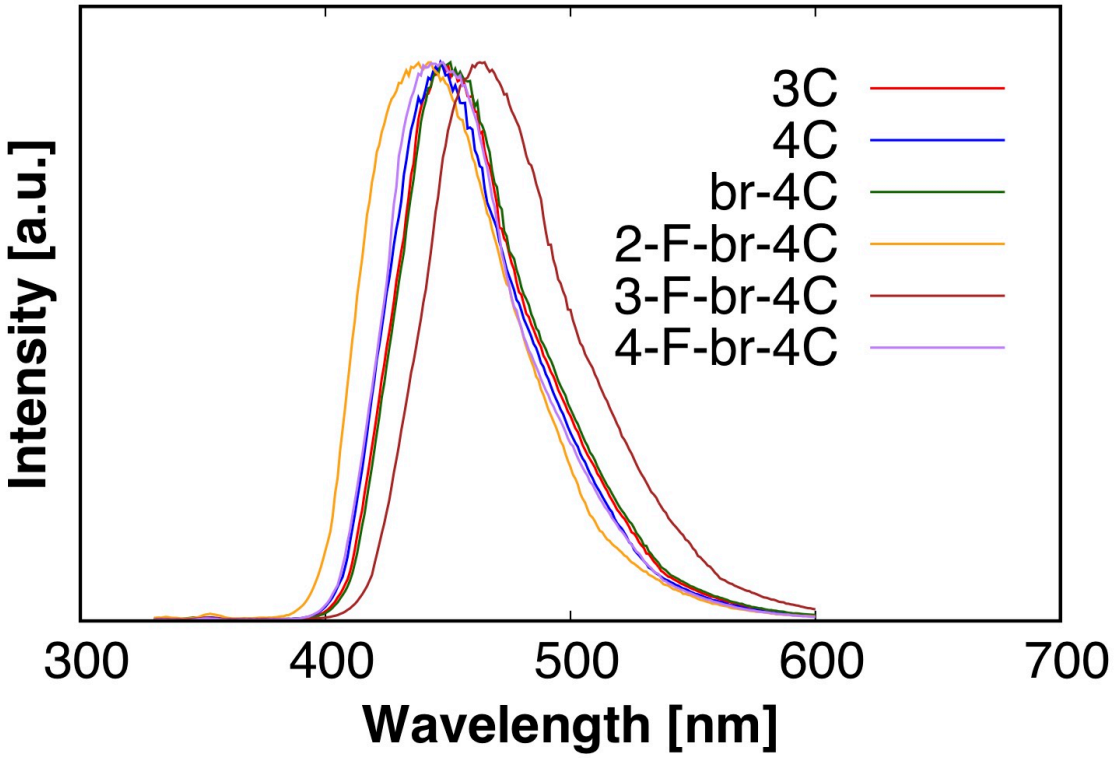


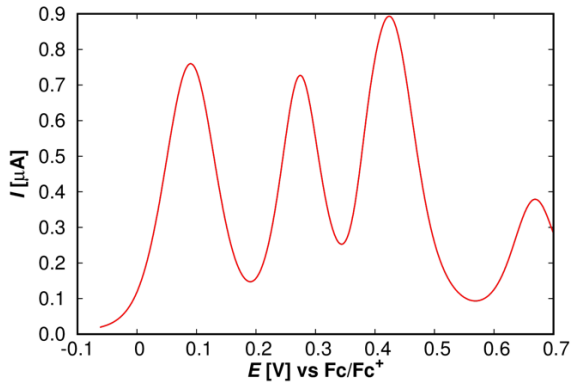
Figure S2. Emission spectra of BDPSOs in NMP (ca. 3.0×10^{-6} M).

Table S1. Absorption and emission properties of BDPSOs in NMP.

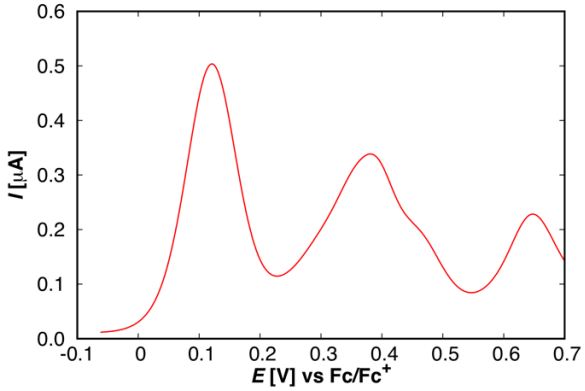
	λ_{abs} [nm]	$\varepsilon \times 10^{-5}$ [L/mol·cm^{-1}]	Absorption onset [nm]	Optical bandgap [eV]	λ_{em} [nm]
3C	315, 379	2.5, 1.1	419	2.96	450
4C	319, 378	2.5, 1.2	417	2.97	446
br-4C	314, 381	3.2, 1.4	420	2.95	450
2-F-br-4C	319, 371	2.4, 1.1	407	3.05	440
3-F-br-4C	318, 382	3.3, 1.3	425	2.92	463
4-F-br-4C	318, 378	2.5, 1.2	415	2.99	447

5. DPV measurement of BDPSO solution

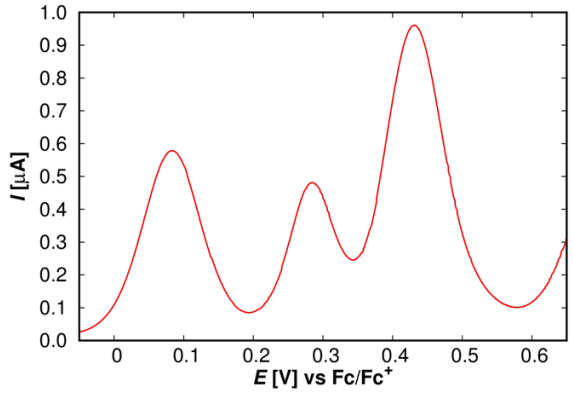
3C



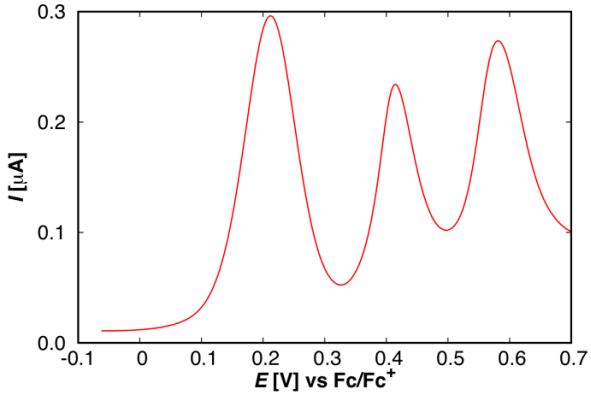
4C



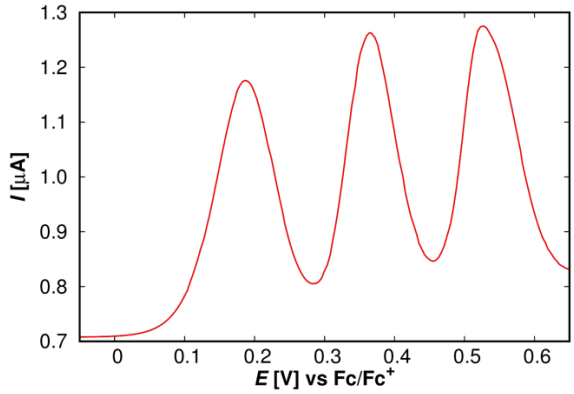
br-4C



2-F-br-4C



3-F-br-4C



4-F-br-4C

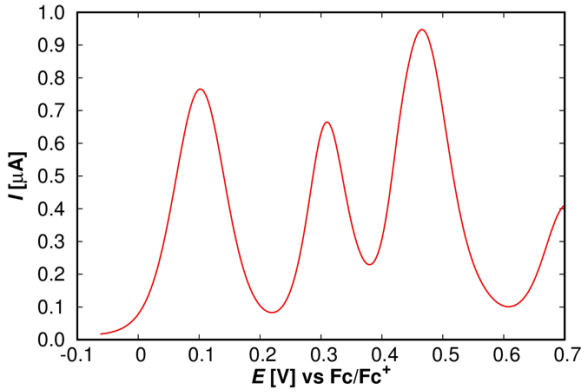


Figure S3. Differential pulse voltammograms of BDPSO derivatives in NMP solution.

Table S2. Energy levels of BDPSO derivatives in NMP solution.

	E_{ox} [V] vs Fc/Fc^+	HOMO [eV]	Optical bandgap [eV]	LUMO [eV]
3C	0.09, 0.27, 0.42	4.89	2.96	1.93
4C	0.12, 0.38	4.92	2.97	1.95
br-4C	0.08, 0.28, 0.53	4.88	2.95	1.93
2-F-br-4C	0.21, 0.41, 0.58	5.01	3.05	1.96
3-F-br-4C	0.19, 0.36, 0.63	4.99	2.92	2.07
4-F-br-4C	0.10, 0.31, 0.47	4.90	2.99	1.91

6. Thin-Film Transmittance and Absorptance

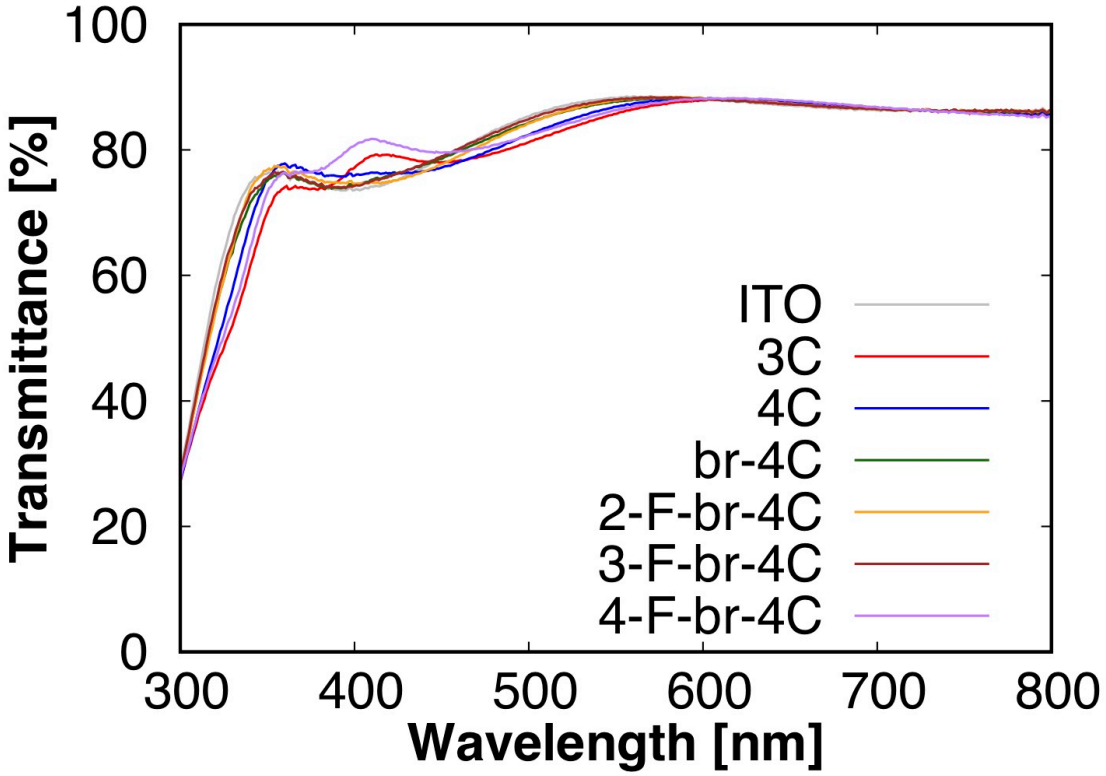


Figure S4. Transmittance spectra of BDPSO thin films on ITO.

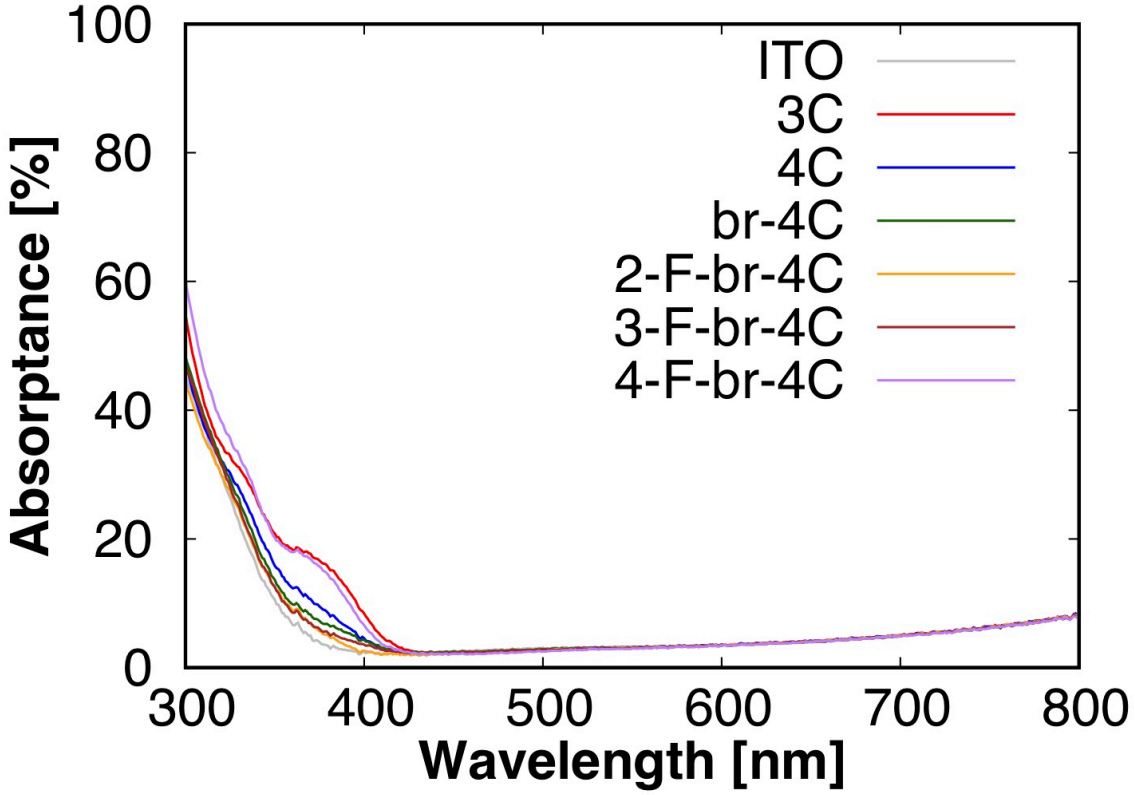


Figure S5. Absorptance spectra of BDPSO thin films on ITO calculated from transmittance and reflectance.

7. PYS Measurement on BDPSO Thin Films

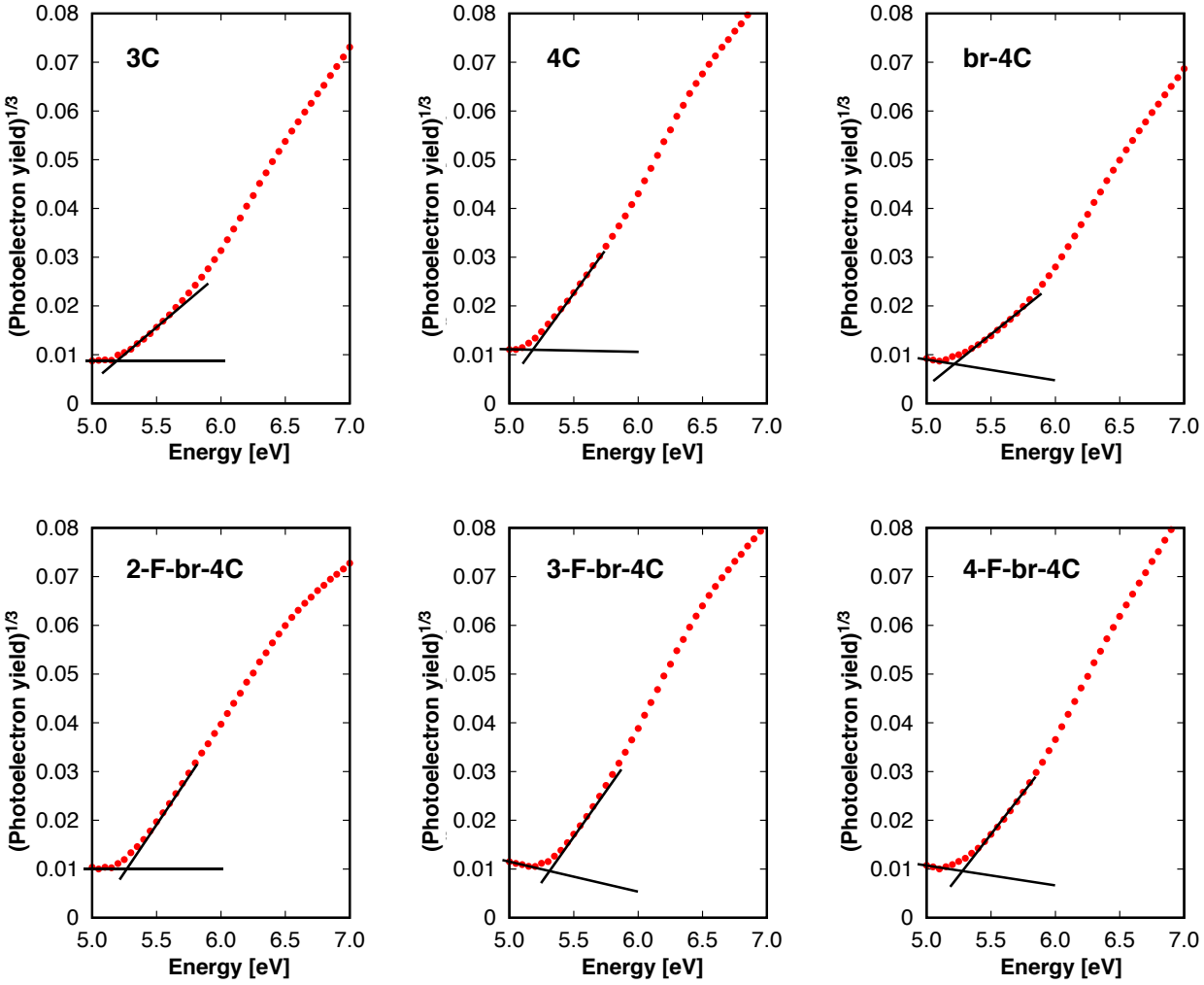


Figure S6. PYS data of BDPSO thin films on ITO.

Table S3. IPs and EAs of BDPSO thin films on ITO. Electron affinity (EA) of the thin films were calculated considering the onset of the absorptance spectra as the optical band gap.

	IP	Absorption onset	Optical bandgap	EA
	[eV]	[nm]	[eV]	[eV]
3C	5.21	417	2.97	2.24
4C	5.21	413	3.00	2.21
br-4C	5.22	418	2.97	2.25
2-F-br-4C	5.27	391	3.17	2.10
3-F-br-4C	5.32	415	2.93	2.38
4-F-br-4C	5.32	414	2.99	2.33

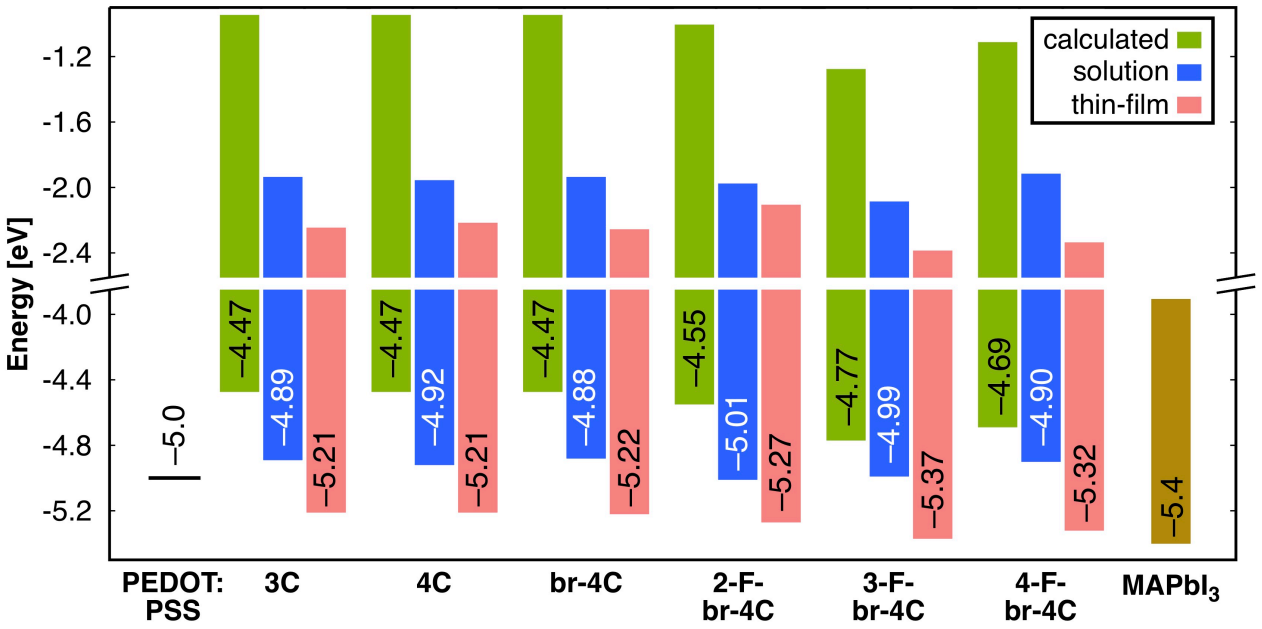
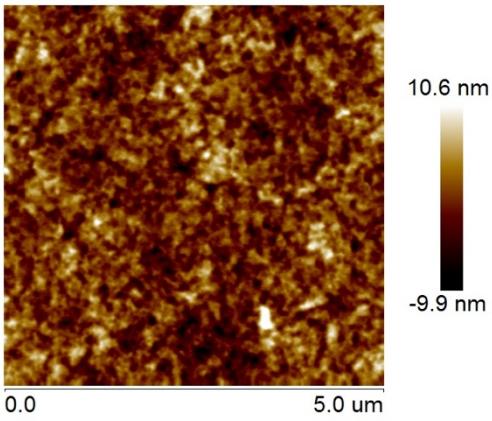


Figure S7. Comparison of energy levels of BDPSO derivatives obtained by DFT calculation (calculated at B3LYP/6-31G(d) level, green boxes), DPV measurement in NMP solution (blue boxes), and PYS measurement on the thin-films (pink boxes).

8. AFM Images of BDPSO Thin Films

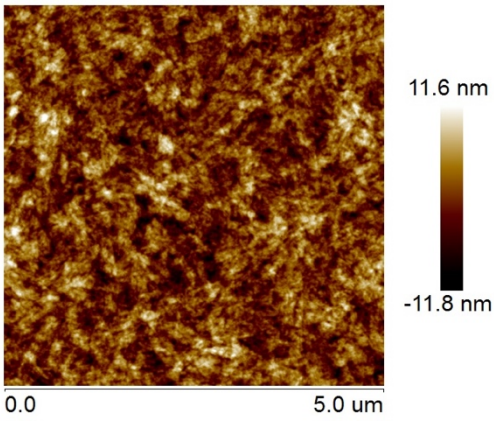
3C

d = 7 nm, R_q = 2.9 nm



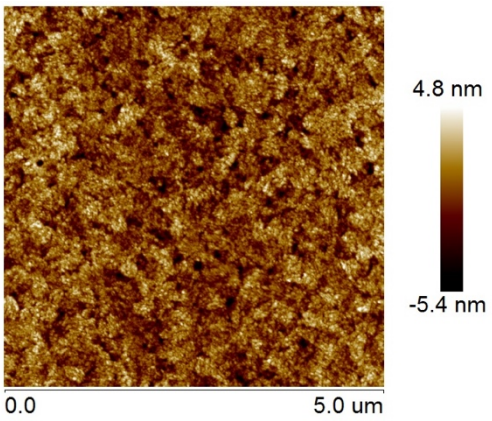
4C

d = 10 nm, R_q = 2.2 nm



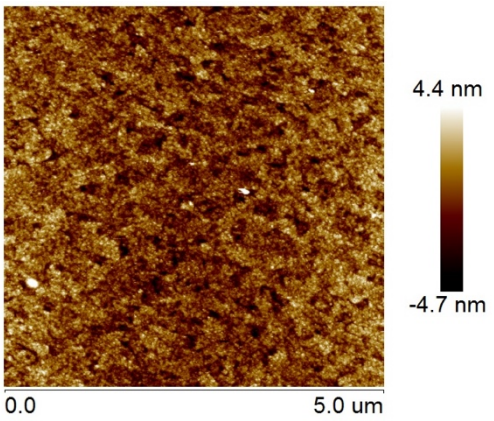
br-4C

d = 4 nm, R_q = 1.5 nm



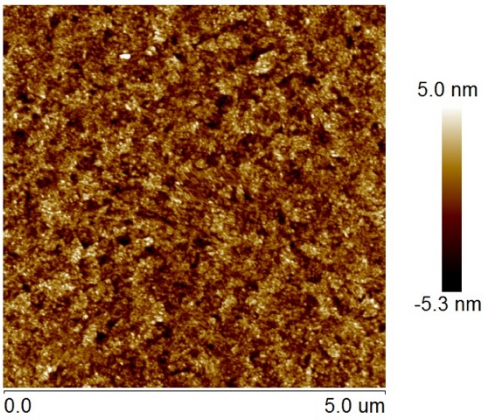
2-F-br-4C

d = 3 nm, R_q = 1.3 nm



3-F-br-4C

d = 8 nm, R_q = 1.5 nm



4-F-br-4C

d = 14 nm, R_q = 3.0 nm

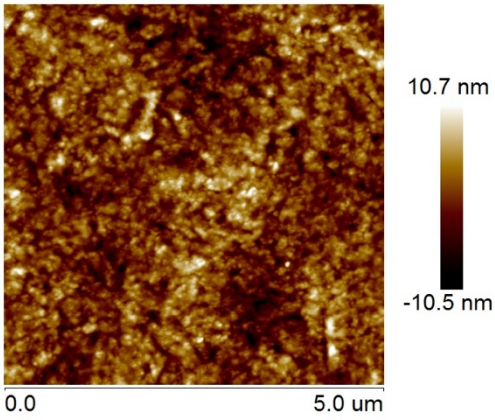
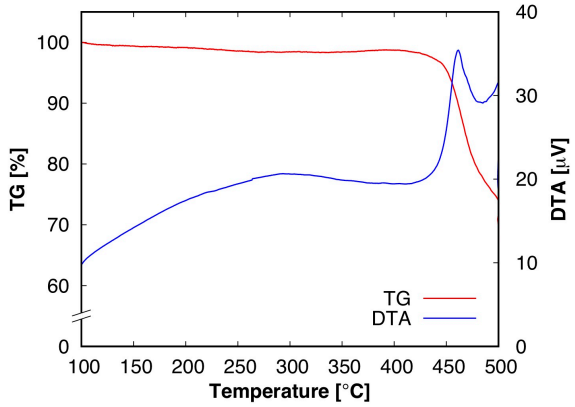


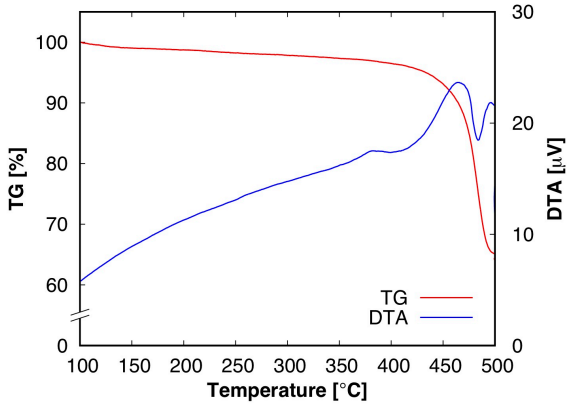
Figure S8. AFM images of BDPSO thin films on ITO. d: thickness, R_q: root mean square roughness.

9. Thermal Analyses of BDPSOs

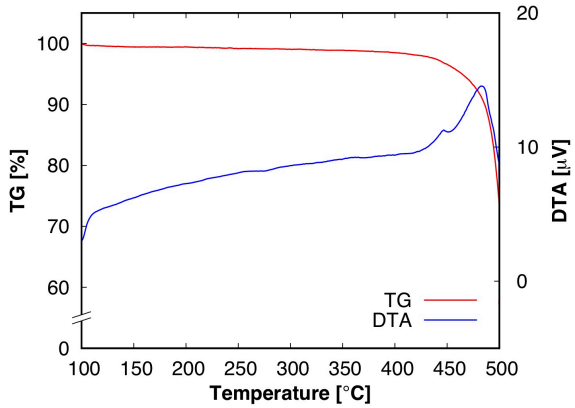
3C



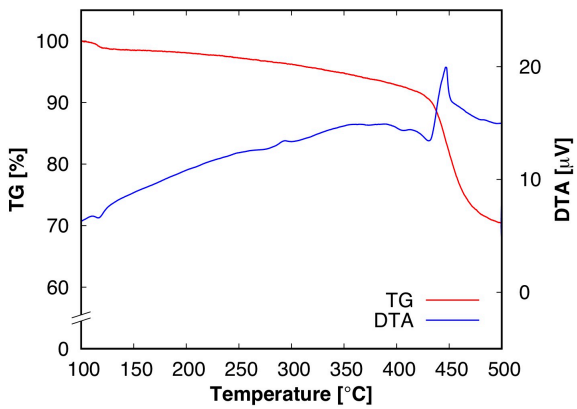
4C



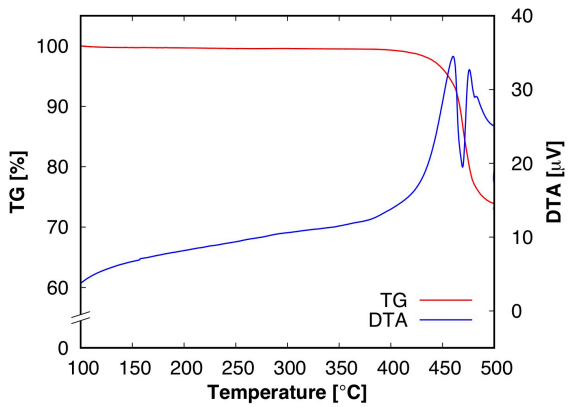
br-4C



2-F-br-4C



3-F-br-4C



4-F-br-4C

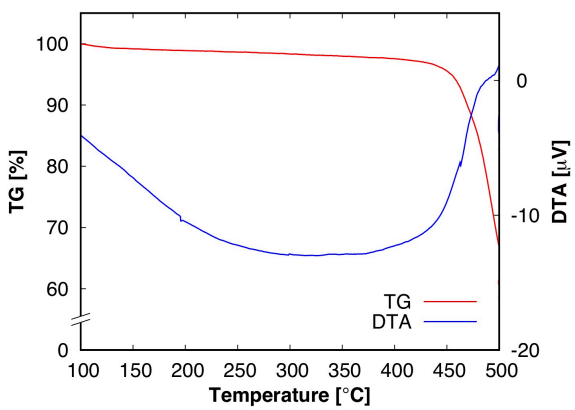


Figure S9. TG and DTA curves of BDPSO derivatives.

10. Computational Studies

Computational studies were performed on Gaussian 09, Revision B.01.[4] The geometries of molecules were optimized with density functional theory (DFT) using B3LYP hybrid functional with a basis set limited to 6-31G(d). Alkyl chains on nitrogen atom were replaced with methyl groups.

Cartesian Coordinates from Calculation of 1,5-dimethyl-2,3,6,7-tetraphenylbenzo[1,2-*b*:4,5-*b'*]dipyrrole

Total energy: *E* (B3LYP/6-31G(d)) = –1498.23380588 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.981573	-0.954266	0.040078
2	6	0	0.335361	-1.406865	0.044235
3	6	0	1.338051	-0.429399	-0.010840
4	6	0	0.981580	0.954255	-0.040670
5	6	0	-0.335364	1.406854	-0.044653
6	6	0	-1.338042	0.429387	0.010438
7	1	0	0.581044	-2.463031	0.077952
8	1	0	-0.581048	2.463028	-0.078095
9	6	0	2.781173	-0.491578	-0.022158
10	6	0	3.241283	0.817564	-0.056875
11	7	0	2.154127	1.694651	-0.061273
12	6	0	-2.781178	0.491551	0.022042
13	6	0	-3.241262	-0.817591	0.056666
14	7	0	-2.154115	-1.694708	0.060571
15	6	0	-4.633165	-1.307137	0.089319
16	6	0	-5.536476	-0.811775	1.045482
17	6	0	-6.414900	-2.710657	-0.799282
18	6	0	-6.856721	-1.256972	1.075750
19	1	0	-5.192233	-0.076286	1.765628
20	6	0	-7.300840	-2.210024	0.156429
21	1	0	-6.753053	-3.445556	-1.525207
22	1	0	-7.539159	-0.862315	1.823840
23	6	0	4.633169	1.307129	-0.089541
24	6	0	5.536680	0.811242	-1.045254
25	6	0	6.414718	2.711199	0.798583
26	6	0	6.856918	1.256451	-1.075532
27	1	0	5.192592	0.075347	-1.765057
28	6	0	7.300850	2.210035	-0.156670
29	1	0	6.752713	3.446528	1.524145
30	1	0	7.539500	0.861388	-1.823277
31	6	0	-2.170843	-3.121893	0.321089
32	1	0	-1.564590	-3.351763	1.205617
33	1	0	-3.193327	-3.451813	0.501535
34	1	0	-1.765808	-3.682759	-0.530584
35	6	0	2.171075	3.122082	-0.320378
36	1	0	3.193003	3.451083	-0.505665
37	1	0	1.560749	3.353134	-1.201745
38	1	0	1.770786	3.682831	0.533648
39	6	0	5.094607	2.262520	0.834276
40	1	0	4.417526	2.637902	1.597021
41	6	0	-5.094786	-2.261978	-0.834972

42	1	0	-4.417840	-2.636895	-1.598068
43	6	0	-3.585234	1.726748	-0.058202
44	6	0	-3.284733	2.826328	0.767027
45	6	0	-4.651007	1.857584	-0.966764
46	6	0	-4.020367	4.008763	0.687477
47	1	0	-2.477253	2.740622	1.488904
48	6	0	-5.391064	3.036367	-1.040279
49	1	0	-4.890138	1.027755	-1.624729
50	6	0	-5.078705	4.119648	-0.215870
51	1	0	-3.770328	4.842285	1.339395
52	1	0	-6.209386	3.112288	-1.752076
53	6	0	3.585188	-1.726788	0.058319
54	6	0	3.284883	-2.826423	-0.766857
55	6	0	4.650758	-1.857543	0.967176
56	6	0	4.020501	-4.008881	-0.687015
57	1	0	2.477573	-2.740820	-1.488937
58	6	0	5.390774	-3.036302	1.040977
59	1	0	4.889703	-1.027628	1.625098
60	6	0	5.078602	-4.119681	0.216580
61	1	0	3.770579	-4.842444	-1.338925
62	1	0	6.208929	-3.112204	1.752969
63	1	0	5.653189	-5.040095	0.278998
64	1	0	8.329839	2.558333	-0.183579
65	1	0	-5.653281	5.040088	-0.278021
66	1	0	-8.329831	-2.558317	0.183330

Cartesian Coordinates from Calculation of 1,5-dimethyl-2,3,6,7-tetrakis(2-fluorophenyl)benzo[1,2-*b*:4,5-*b'*]dipyrrole

Total energy: *E* (B3LYP/6-31G(d)) = –1895.16842189 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.998971	0.930988	0.129937
2	6	0	-0.307000	1.411973	0.084132
3	6	0	-1.325126	0.459569	-0.052436
4	6	0	-0.999040	-0.931037	-0.129836
5	6	0	0.306930	-1.412023	-0.084030
6	6	0	1.325053	-0.459620	0.052543
7	1	0	-0.533989	2.471226	0.144683
8	1	0	0.533924	-2.471277	-0.144560
9	6	0	-2.763506	0.554839	-0.120757
10	6	0	-3.248051	-0.739439	-0.234012
11	7	0	-2.186198	-1.637023	-0.248201
12	6	0	2.763428	-0.554887	0.120931
13	6	0	3.247979	0.739388	0.234076
14	7	0	2.186130	1.636977	0.248264
15	6	0	4.648364	1.174632	0.378522
16	6	0	5.471653	0.648434	1.388183
17	6	0	6.561782	2.490737	-0.403258
18	6	0	6.808006	1.028203	1.505678
19	1	0	5.042147	-0.064415	2.084951
20	6	0	7.353460	1.951742	0.611639

21	1	0	6.953726	3.202536	-1.122452
22	1	0	7.420353	0.607413	2.297748
23	6	0	-4.648406	-1.174704	-0.378717
24	6	0	-5.471489	-0.648568	-1.388577
25	6	0	-6.561969	-2.490809	0.402711
26	6	0	-6.807811	-1.028363	-1.506339
27	1	0	-5.041844	0.064249	-2.085292
28	6	0	-7.353442	-1.951868	-0.612375
29	1	0	-6.954056	-3.202576	1.121859
30	1	0	-7.419994	-0.607621	-2.298561
31	6	0	2.257898	3.073720	0.424280
32	1	0	1.466972	3.396608	1.108589
33	1	0	3.220850	3.340823	0.862008
34	1	0	2.145964	3.604039	-0.528426
35	6	0	-2.257976	-3.073767	-0.424205
36	1	0	-3.220818	-3.340836	-0.862202
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44	6	0	3.921396	-4.113787	0.767788
45	1	0	2.398919	-2.813441	1.559462
46	6	0	5.333923	-3.158008	-0.939460
47	6	0	4.986127	-4.237362	-0.126670
48	1	0	3.644924	-4.947276	1.407459
49	1	0	6.148353	-3.216891	-1.654470
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51	6	0	-3.215711	2.913707	-0.850309
52	6	0	-4.608768	1.977481	0.845066
53	6	0	-3.921485	4.113684	-0.767862
54	1	0	-2.399291	2.813128	-1.559720
55	6	0	-5.333587	3.158285	0.939942
56	6	0	-4.985966	4.237474	0.126860
57	1	0	-3.645137	4.947050	-1.407748
58	1	0	-6.147779	3.217358	1.655207
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60	1	0	-8.392788	-2.254954	-0.701285
61	1	0	5.544943	-5.166439	-0.195053
62	1	0	8.392829	2.254809	0.700344
63	9	0	-4.484575	-2.606132	1.501343
64	9	0	-4.952629	0.959533	1.665831
65	9	0	4.484138	2.606171	-1.501415
66	9	0	4.953135	-0.959071	-1.664929

Cartesian Coordinates from Calculation of 1,5-dimethyl-2,3,6,7-tetrakis(3-fluorophenyl)benzo[1,2-*b*:4,5-*b'*]dipyrrole

Total energy: *E* (B3LYP/6-31G(d)) = –1895.16824062 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.003228	-0.917507	0.164529
2	6	0	0.301898	-1.401229	0.202661
3	6	0	1.326025	-0.462547	0.020220
4	6	0	1.003210	0.917521	-0.164574
5	6	0	-0.301918	1.401243	-0.202697
6	6	0	-1.326042	0.462562	-0.020252
7	1	0	0.521622	-2.452501	0.355600
8	1	0	-0.521644	2.452516	-0.355627
9	6	0	2.766407	-0.561861	-0.004009
10	6	0	3.256690	0.722347	-0.196860
11	7	0	2.192514	1.620492	-0.286934
12	6	0	-2.766426	0.561876	0.003976
13	6	0	-3.256706	-0.722324	0.196891
14	7	0	-2.192535	-1.620485	0.286869
15	6	0	-4.660182	-1.163954	0.308737
16	6	0	-5.532451	-0.533067	1.212940
17	6	0	-6.483342	-2.592215	-0.366362
18	6	0	-6.863334	-0.935685	1.312394
19	1	0	-5.157058	0.270840	1.836708
20	6	0	-7.355829	-1.976657	0.523020
21	1	0	-7.524697	-0.439601	2.016996
22	6	0	4.660174	1.163967	-0.308666
23	6	0	5.532441	0.533101	-1.212886
24	6	0	6.483366	2.592137	0.366541
25	6	0	6.863335	0.935692	-1.312303
26	1	0	5.157036	-0.270767	-1.836697
27	6	0	7.355846	1.976609	-0.522867
28	1	0	7.524695	0.439627	-2.016921
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32	1	0	-1.847591	-3.669901	-0.073495
33	6	0	2.238069	3.008836	-0.709616
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35	1	0	1.633652	3.148514	-1.613734
36	1	0	1.847883	3.669907	0.073811
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38	1	0	4.526353	2.705233	1.224280
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40	1	0	-4.526331	-2.705312	-1.224112
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46	6	0	-5.325207	3.034287	-1.318793
47	1	0	-4.881042	0.960844	-1.679627
48	6	0	-4.983461	4.199661	-0.629347
49	1	0	-6.148836	3.054632	-2.027305

50	6	0	3.542844	-1.797634	0.210221
51	6	0	3.199775	-2.970900	-0.485438
52	6	0	4.615294	-1.851423	1.119766
53	6	0	3.918906	-4.137209	-0.261136
54	1	0	2.394074	-2.975608	-1.211766
55	6	0	5.325228	-3.034288	1.318643
56	1	0	4.881055	-0.960857	1.679536
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58	1	0	6.148872	-3.054643	2.027137
59	1	0	5.516411	-5.133805	0.771578
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61	1	0	-5.516383	5.133819	-0.771785
62	1	0	-8.386177	-2.310490	0.585347
63	9	0	-6.942811	-3.594937	-1.145598
64	9	0	-3.572180	5.251928	0.944706
65	9	0	6.942853	3.594799	1.145844
66	9	0	3.572178	-5.251884	-0.944882

Cartesian Coordinates from Calculation of 1,5-dimethyl-2,3,6,7-tetrakis(4-fluorophenyl)benzo[1,2-*b*:4,5-*b'*]dipyrrole

Total energy: *E* (B3LYP/6-31G(d)) = –1895.16725192 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.955321	-0.981722	-0.024982
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4	6	0	-0.955311	0.981722	0.024994
5	6	0	0.373564	1.397893	0.021546
6	6	0	1.348773	0.392299	-0.016753
7	1	0	-0.647914	-2.447523	-0.038535
8	1	0	0.647926	2.447522	0.038534
9	6	0	-2.792626	-0.415023	0.028509
10	6	0	-3.217441	0.905860	0.043490
11	7	0	-2.107402	1.753619	0.034624
12	6	0	2.792635	0.415024	-0.028527
13	6	0	3.217451	-0.905858	-0.043512
14	7	0	2.107413	-1.753622	-0.034597
15	6	0	4.596246	-1.430648	-0.067495
16	6	0	5.512580	-0.974545	-1.031875
17	6	0	6.343937	-2.863262	0.854323
18	6	0	6.823500	-1.444074	-1.059462
19	1	0	5.188424	-0.245461	-1.767146
20	6	0	7.217832	-2.385690	-0.115325
21	1	0	6.692239	-3.590605	1.580324
22	1	0	7.535266	-1.097990	-1.801726
23	6	0	-4.596239	1.430648	0.067481
24	6	0	-5.512544	0.974585	1.031909
25	6	0	-6.343968	2.863198	-0.854364
26	6	0	-6.823467	1.444105	1.059508
27	1	0	-5.188361	0.245539	1.767206
28	6	0	-7.217832	2.385669	0.115334

29	1	0	-6.692296	3.590500	-1.580393
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33	1	0	3.098473	-3.543608	-0.455160
34	1	0	1.683235	-3.720750	0.604321
35	6	0	-2.087040	3.186130	0.264460
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42	1	0	4.354129	-2.725627	1.644429
43	6	0	3.630835	1.628723	0.030316
44	6	0	3.372789	2.715419	-0.825771
45	6	0	4.690041	1.753022	0.947872
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48	6	0	5.469315	2.906714	1.005624
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53	6	0	-3.630833	-1.628718	-0.030314
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57	1	0	-2.571135	-2.637801	1.554417
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60	6	0	-5.177854	-3.956735	-0.142689
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62	1	0	-6.285715	-3.005533	-1.713867
63	9	0	-8.484486	2.848961	0.140177
64	9	0	-5.925451	-5.081565	-0.198461
65	9	0	5.925427	5.081583	0.198526
66	9	0	8.484482	-2.848993	-0.140160

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12. References

1) Park, K.; Bae, G.; Moon, J.; Choe, J.; Song, K. H.; Lee, S. *J. Org. Chem.* **2010**, *75*, 6244.
2) Kinsley, D. A.; Plant, S. G. P. *J. Chem. Soc.* **1958**, 1.
3) Shen, M.; Li, G.; Lu, B. Z.; Hossain, A.; Roschangar, F.; Farina, V.; Senanayake, C. H. *Org. Lett.* **2004**, *6*, 4129.
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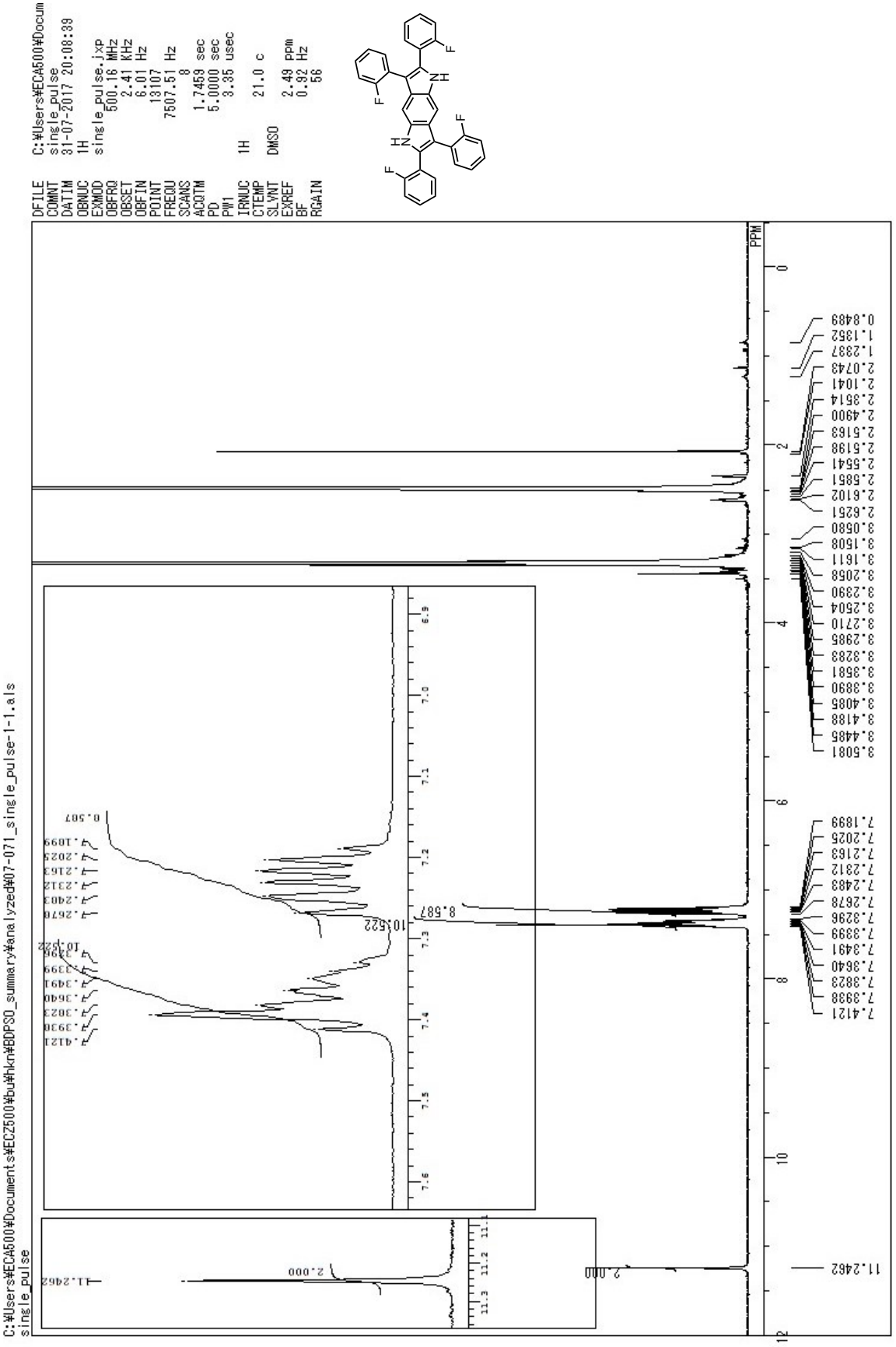
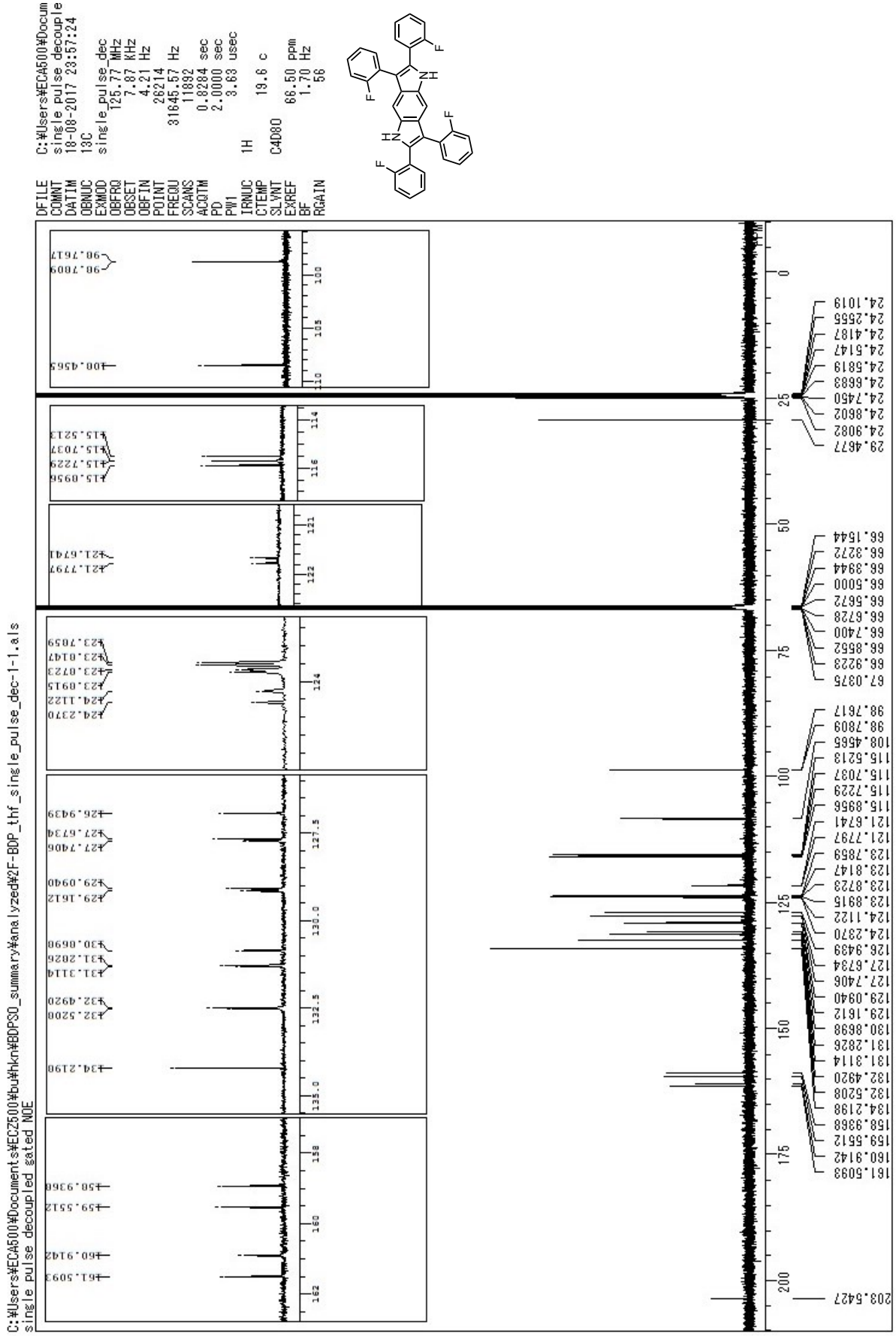
13. ^{1}H-, ^{13}C- and ^{19}F-NMR Spectra

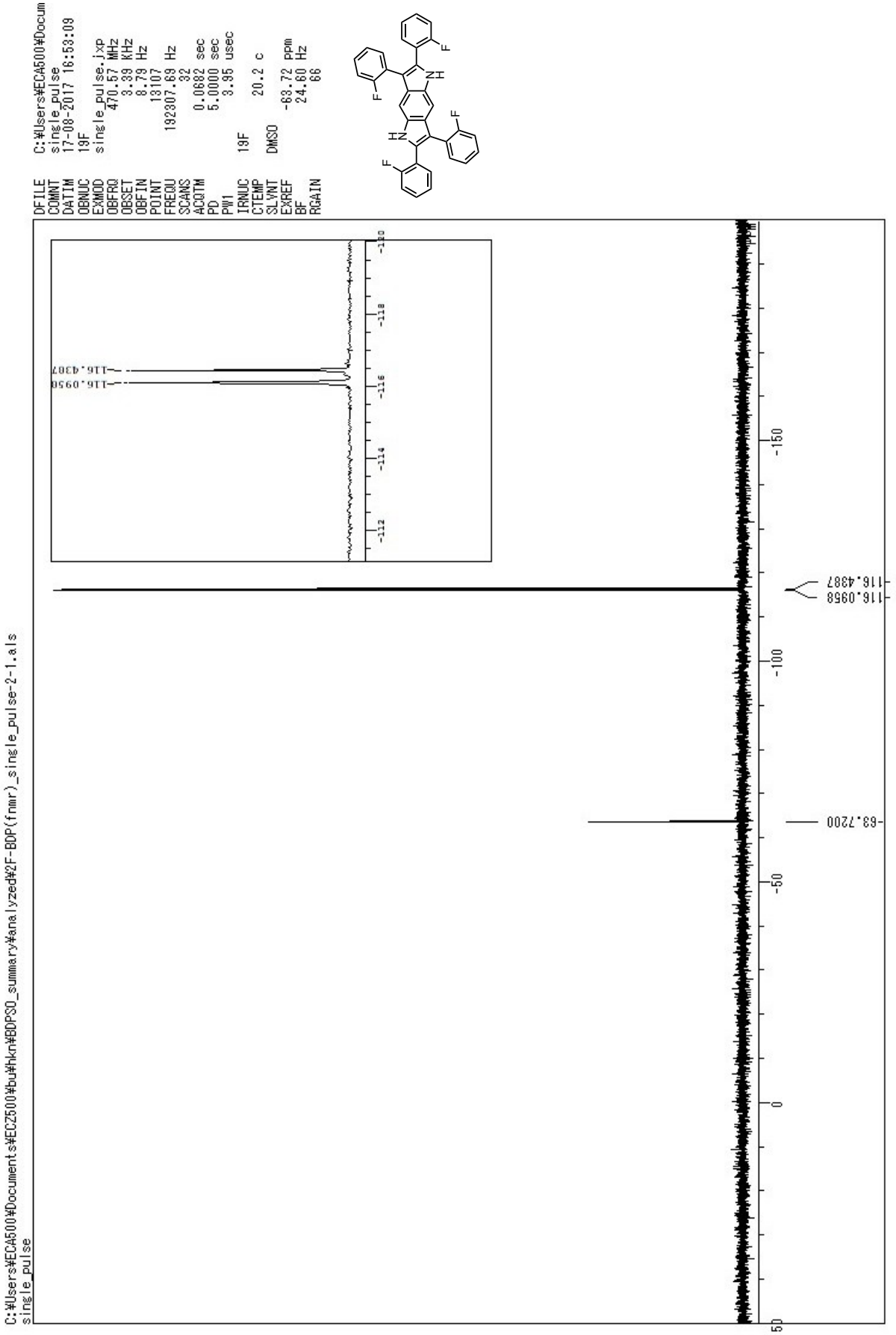
^{1}H-NMR spectrum of **2-F-BDP**



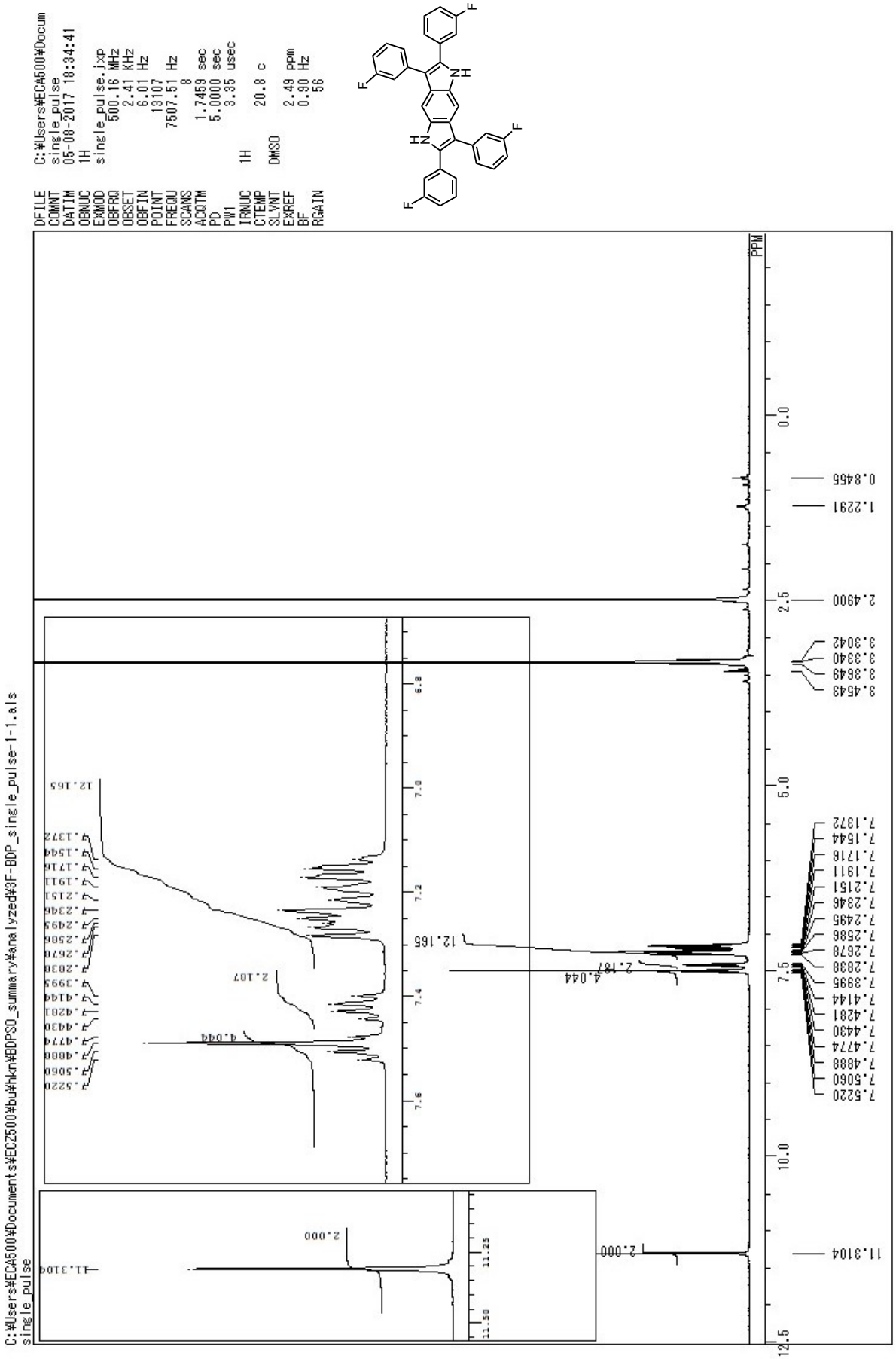
^{13}C-NMR spectrum of **2-F-BDP**



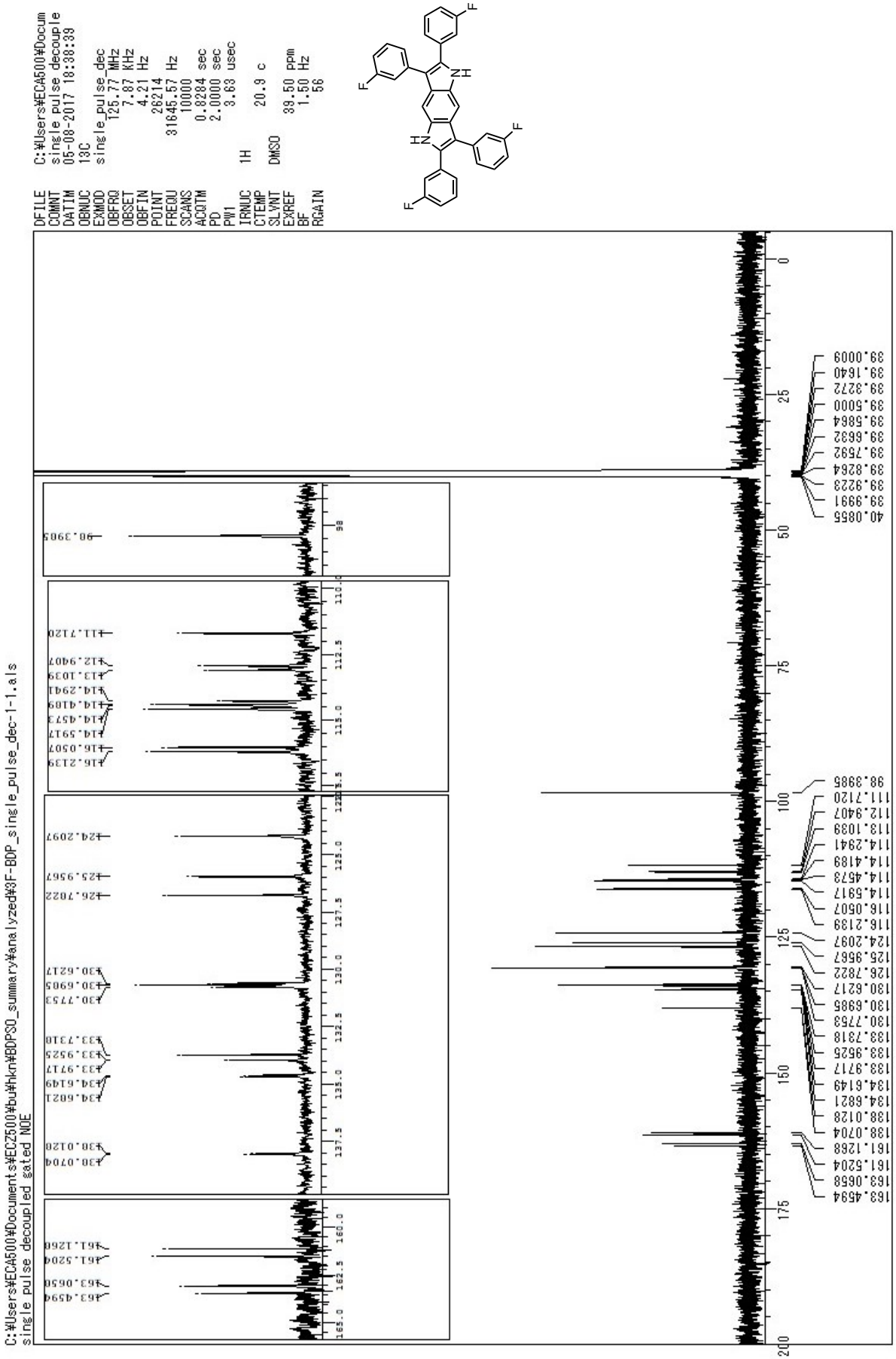
^{19}F-NMR spectrum of **2-F-BDP**



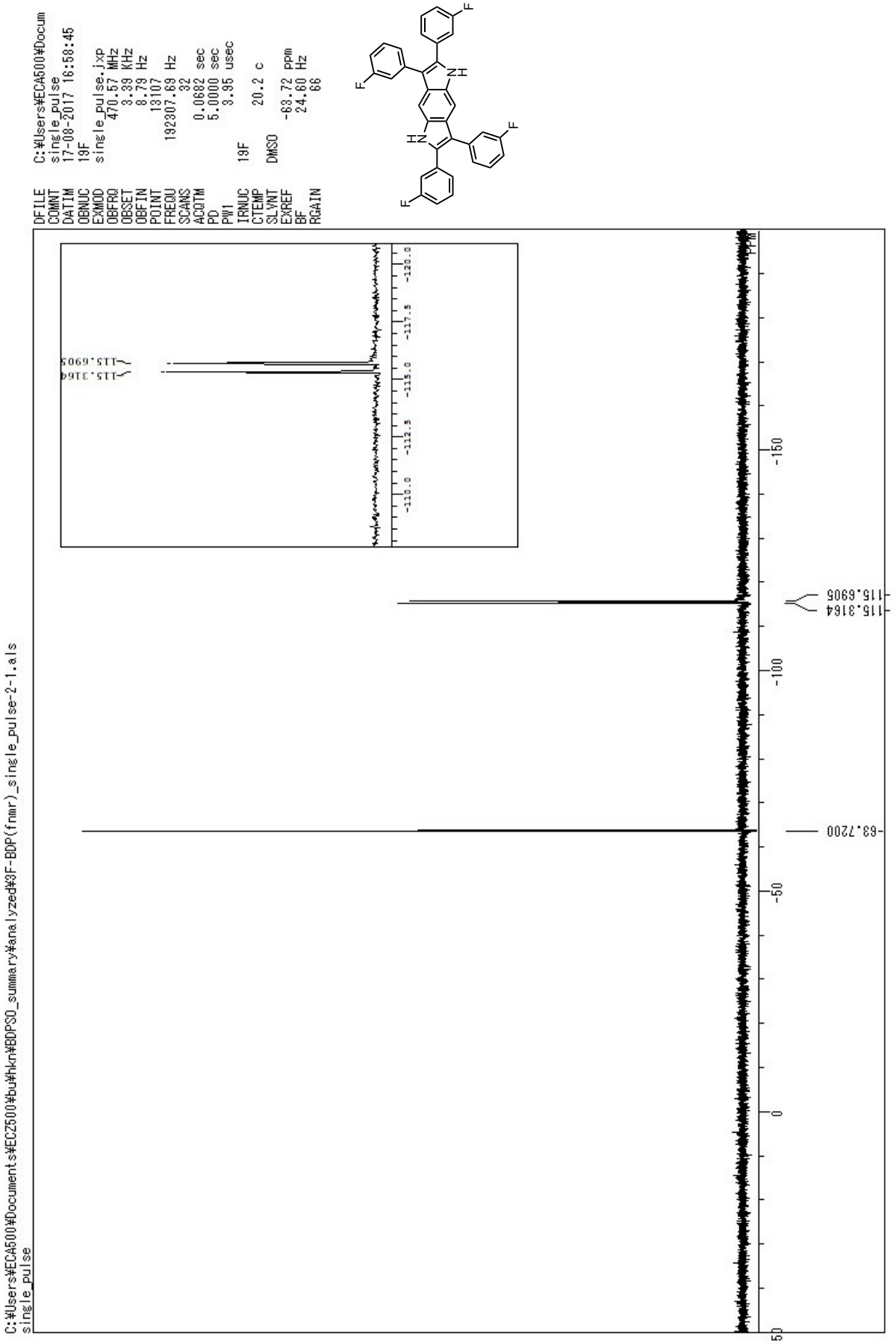
^{1}H-NMR spectrum of **3-F-BDP**



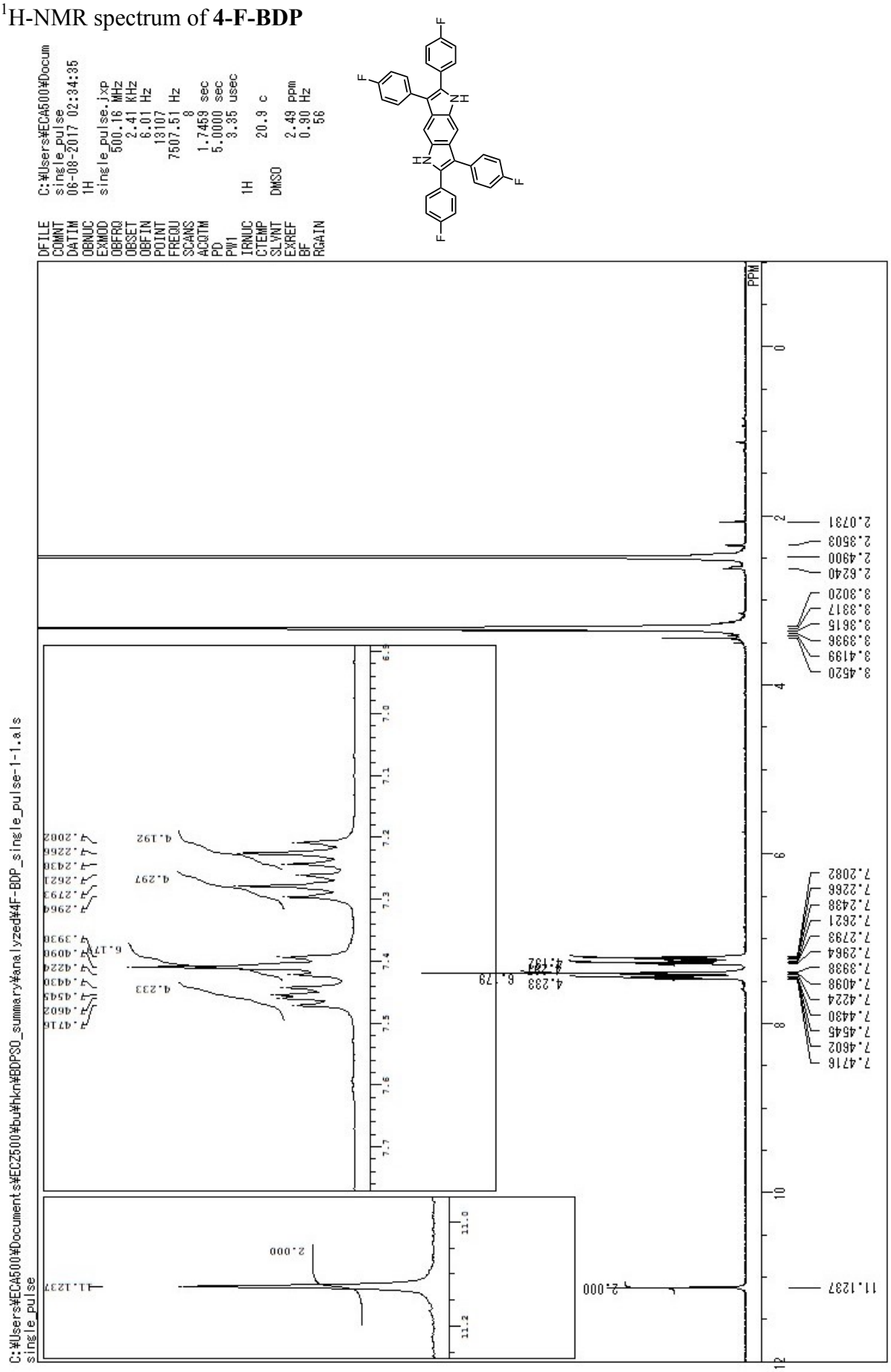
^{13}C-NMR spectrum of **3-F-BDP**



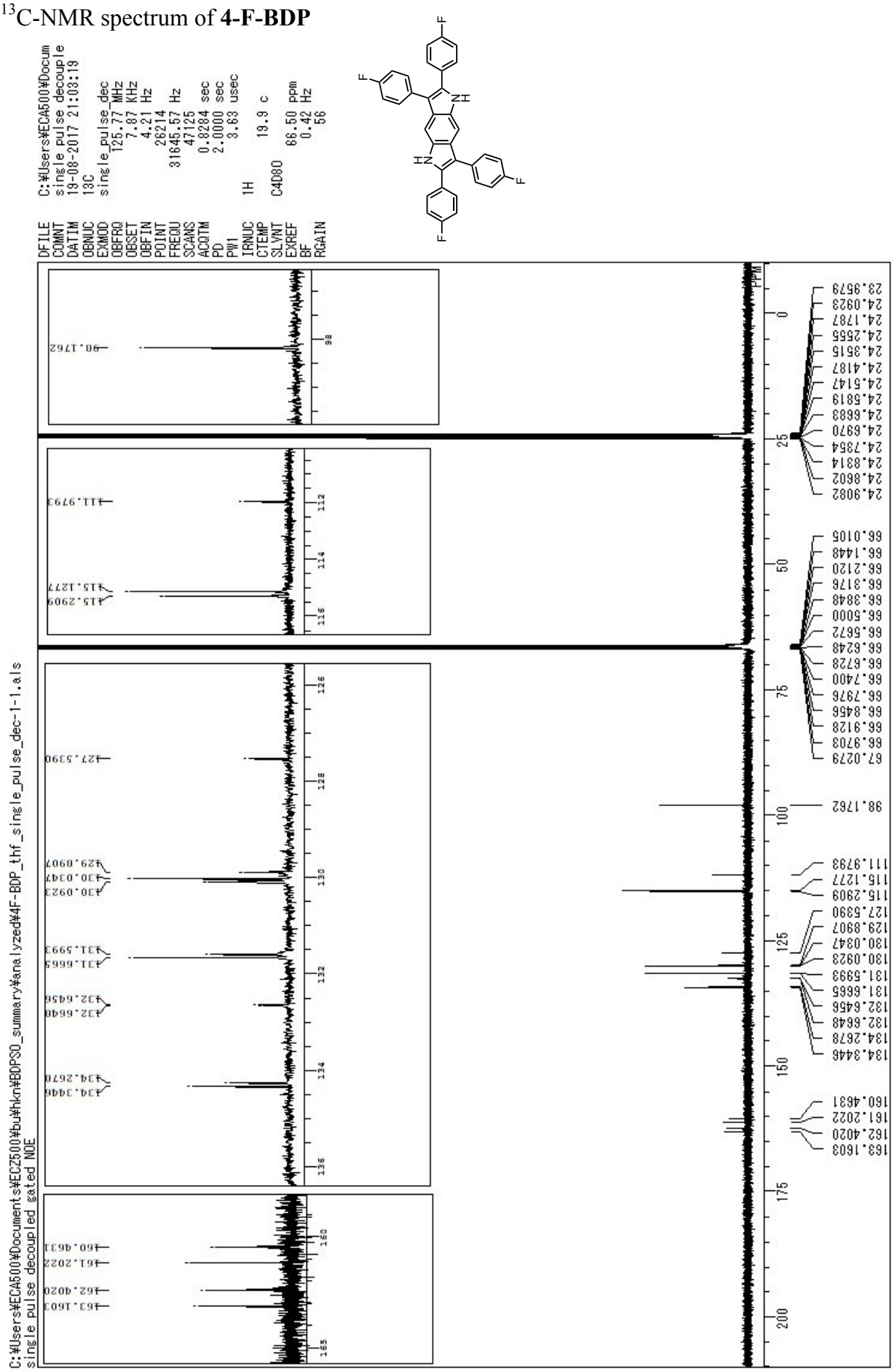
^{19}F-NMR spectrum of **3-F-BDP**



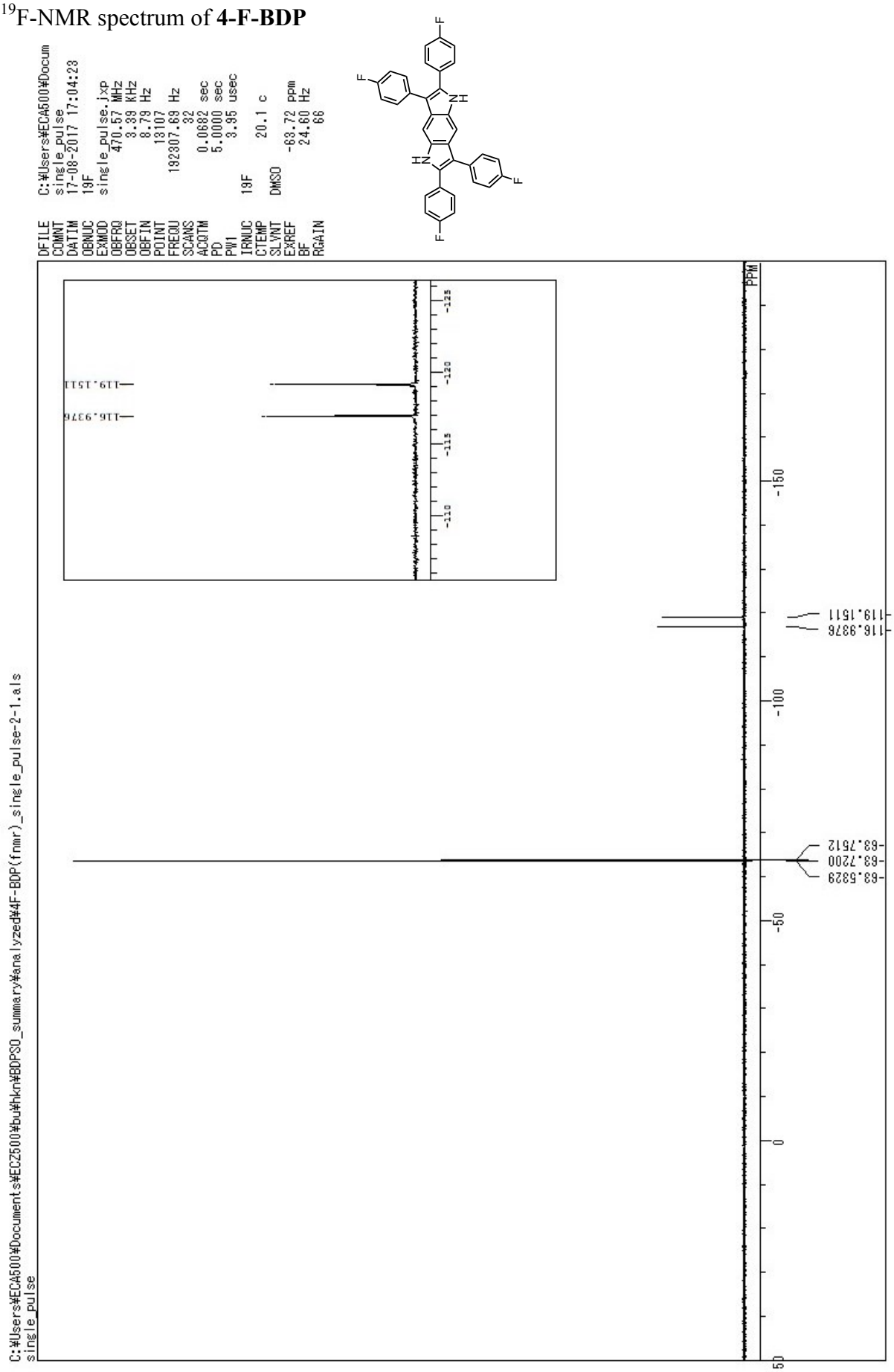
^{1}H-NMR spectrum of **4-F-BDP**



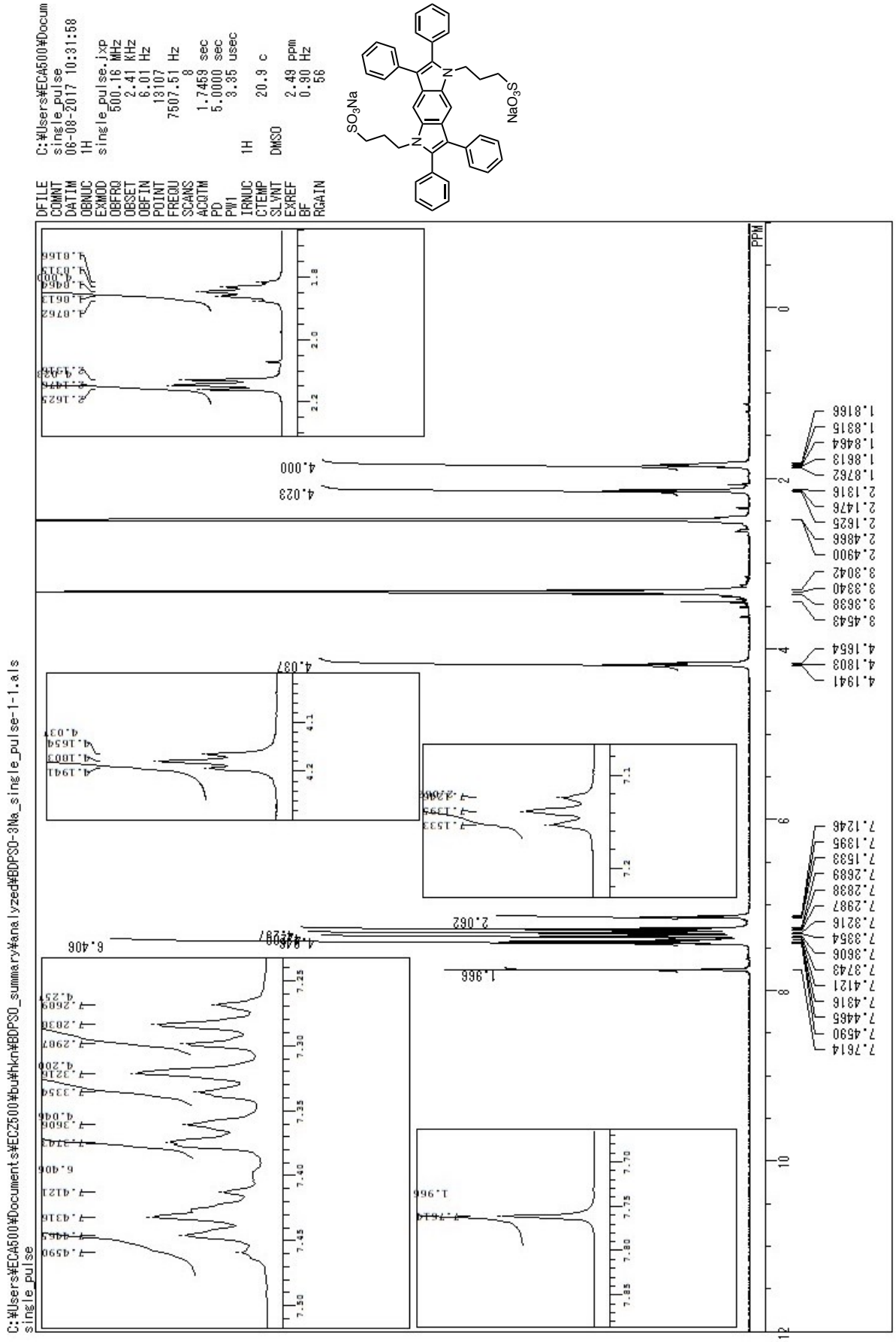
^{13}C-NMR spectrum of **4-F-BDP**



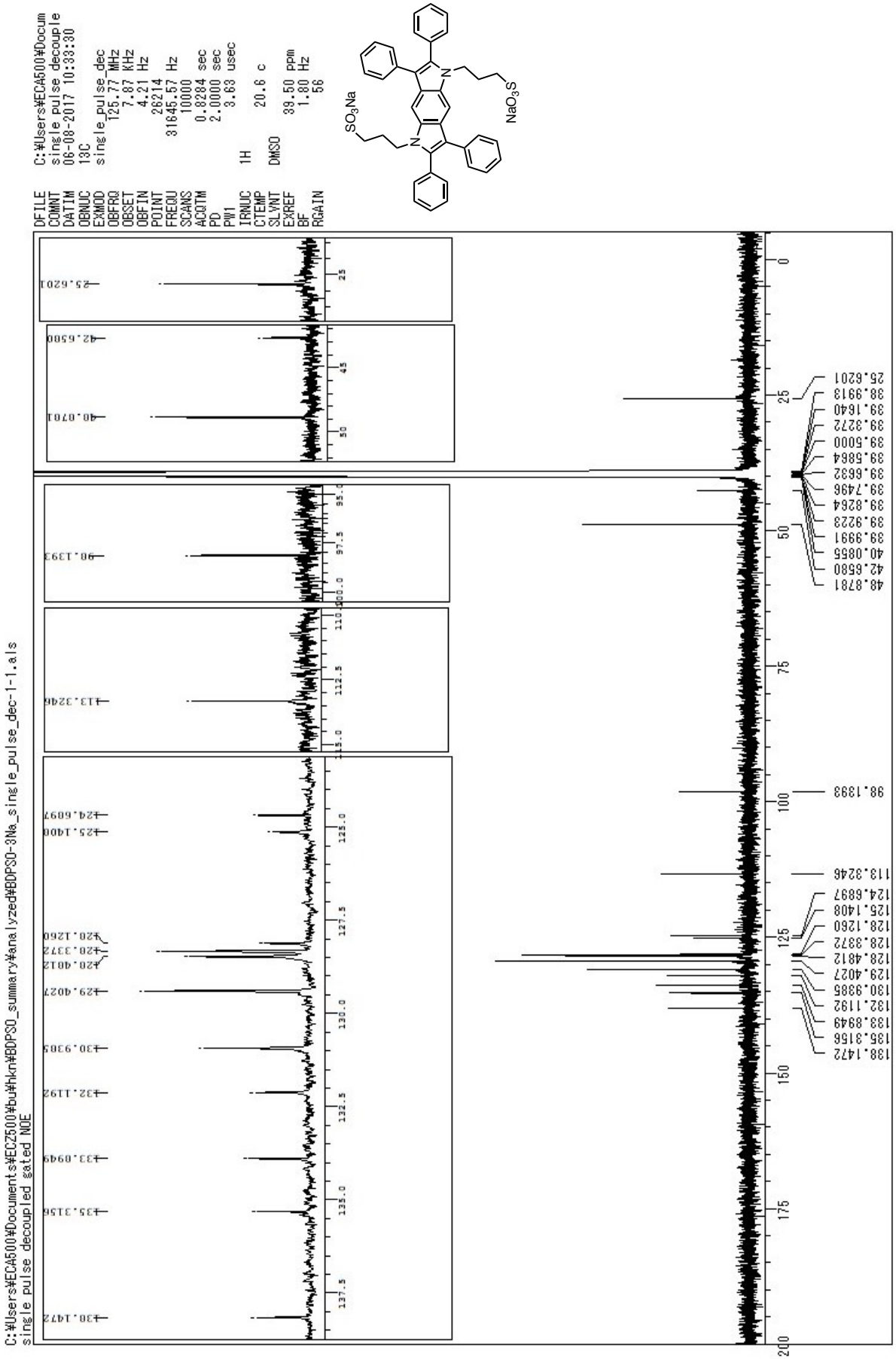
^{19}F-NMR spectrum of **4-F-BDP**



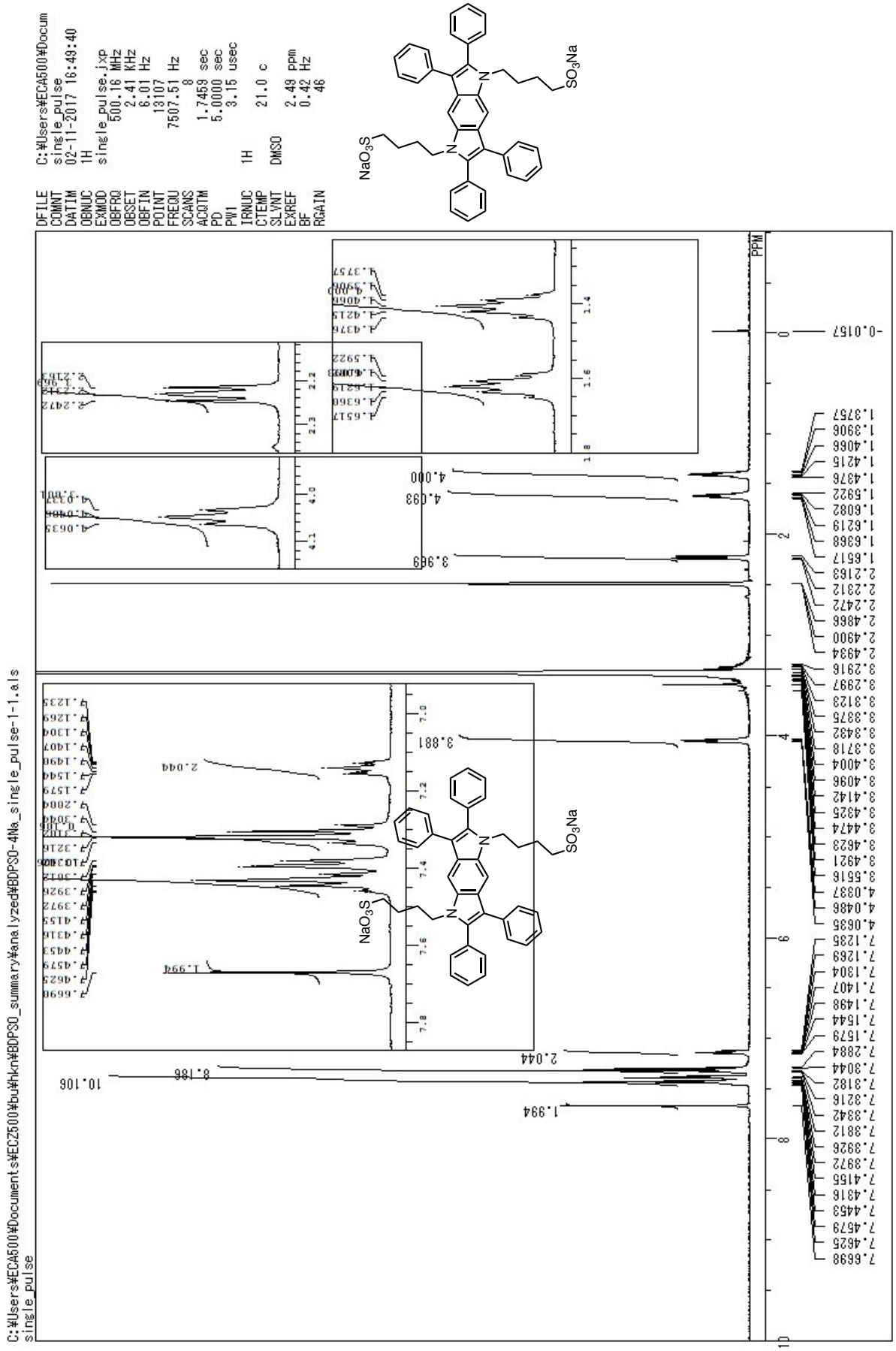
^{1}H-NMR spectrum of **3C**



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



^{1}H-NMR spectrum of **4C**



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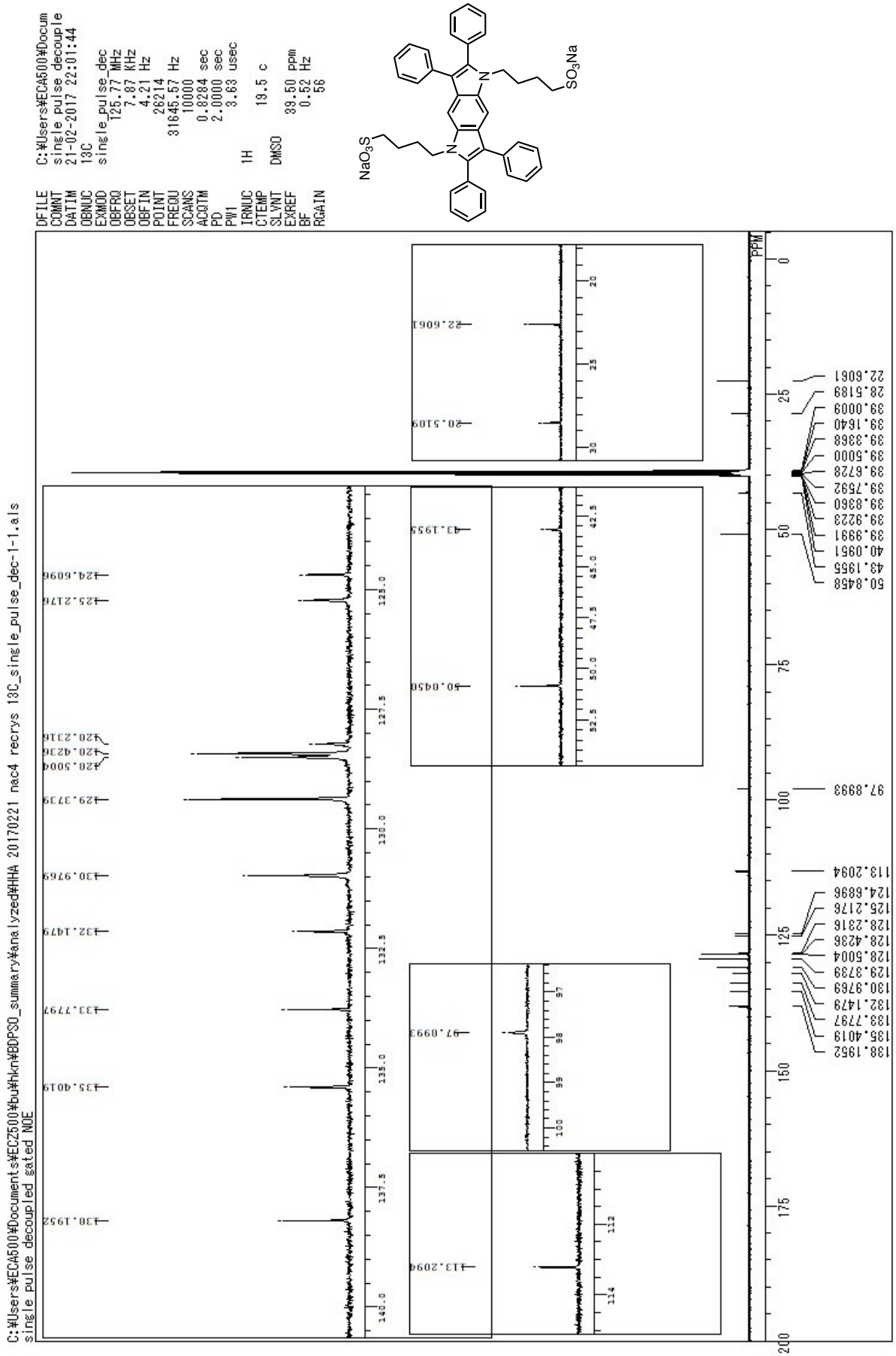
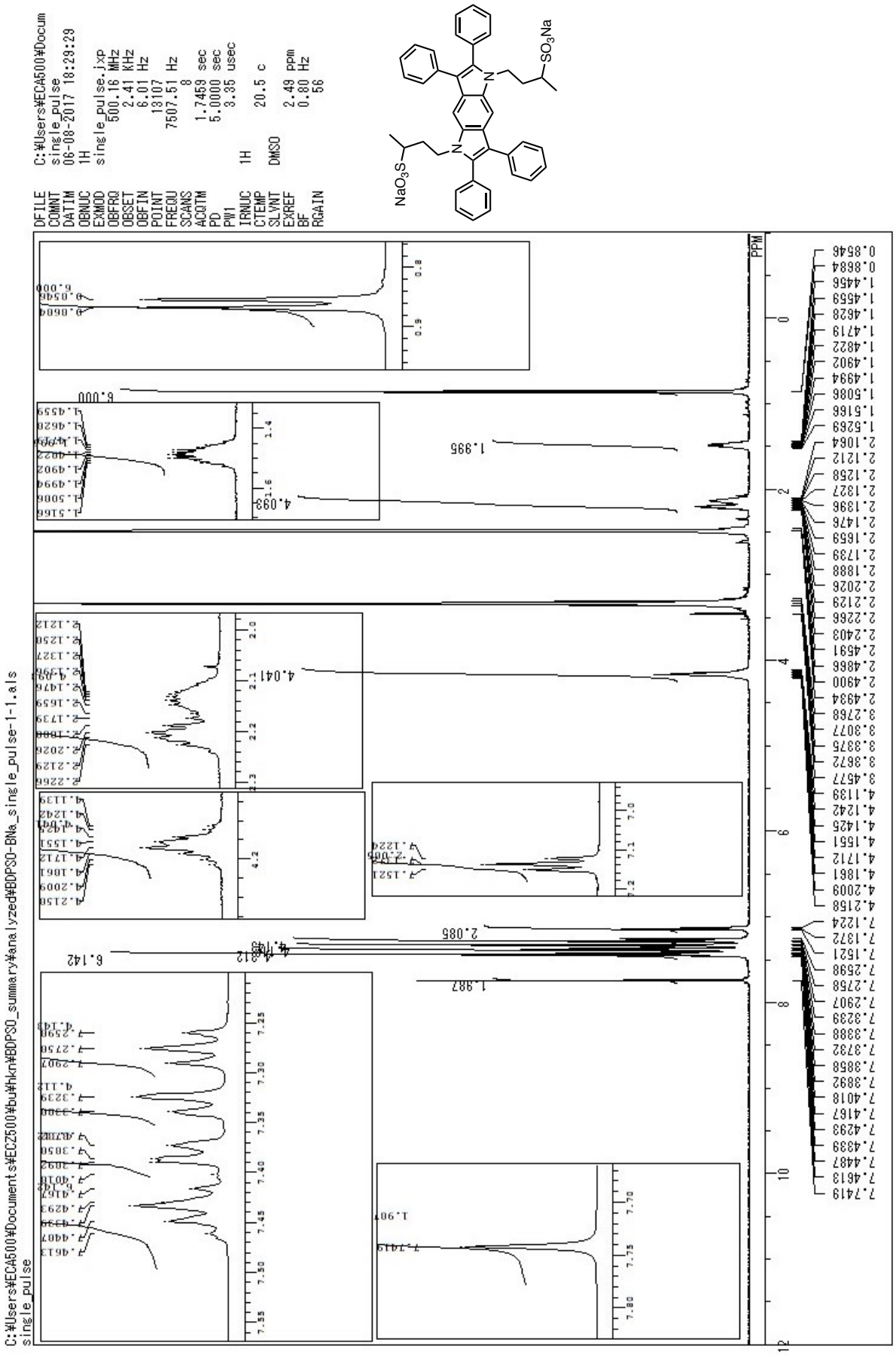
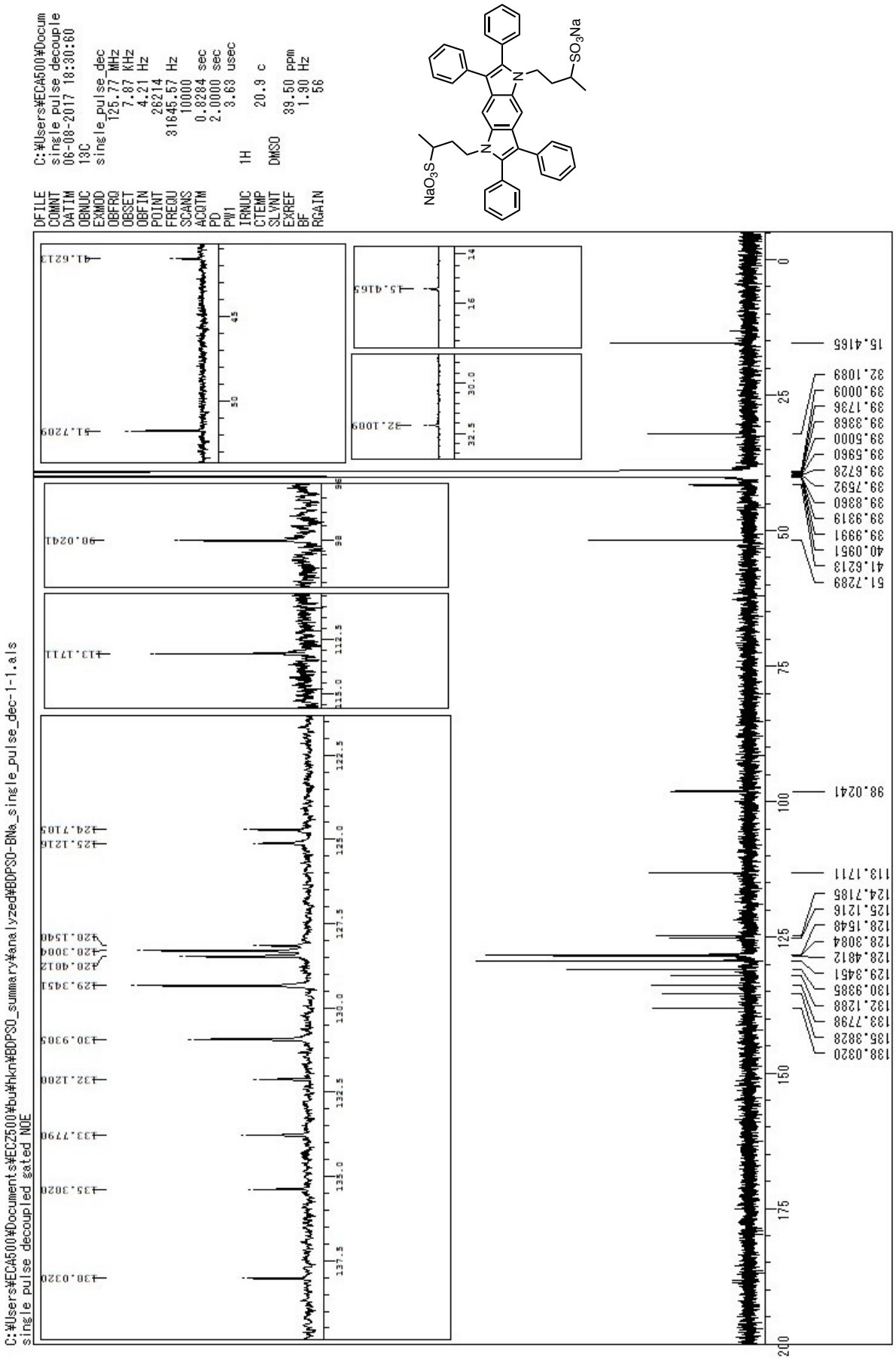


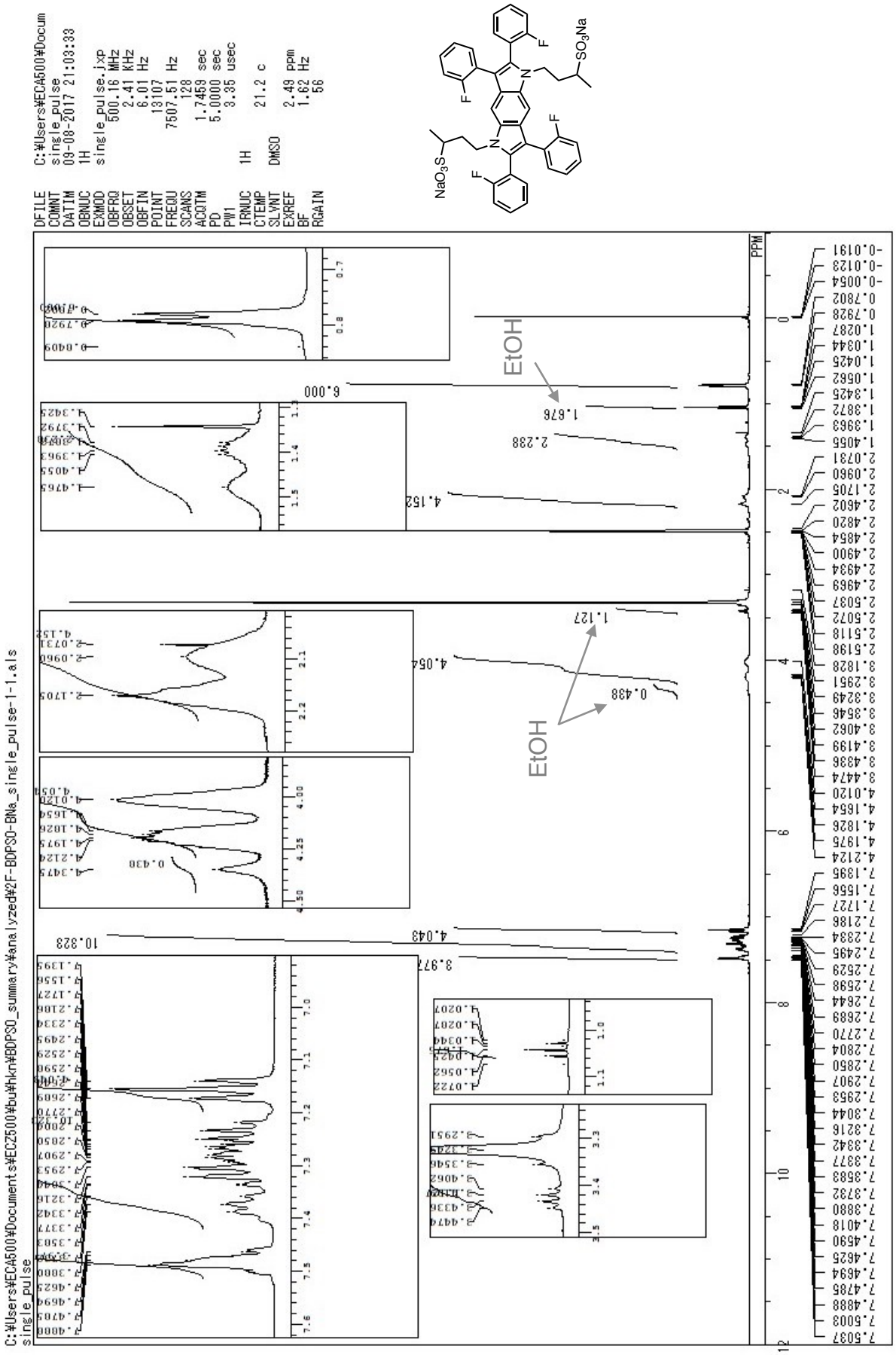
^{1}H-NMR spectrum of **br-4C**



^{13}C-NMR spectrum of **br-4C**



^{1}H-NMR spectrum of **2-F-br-4C**



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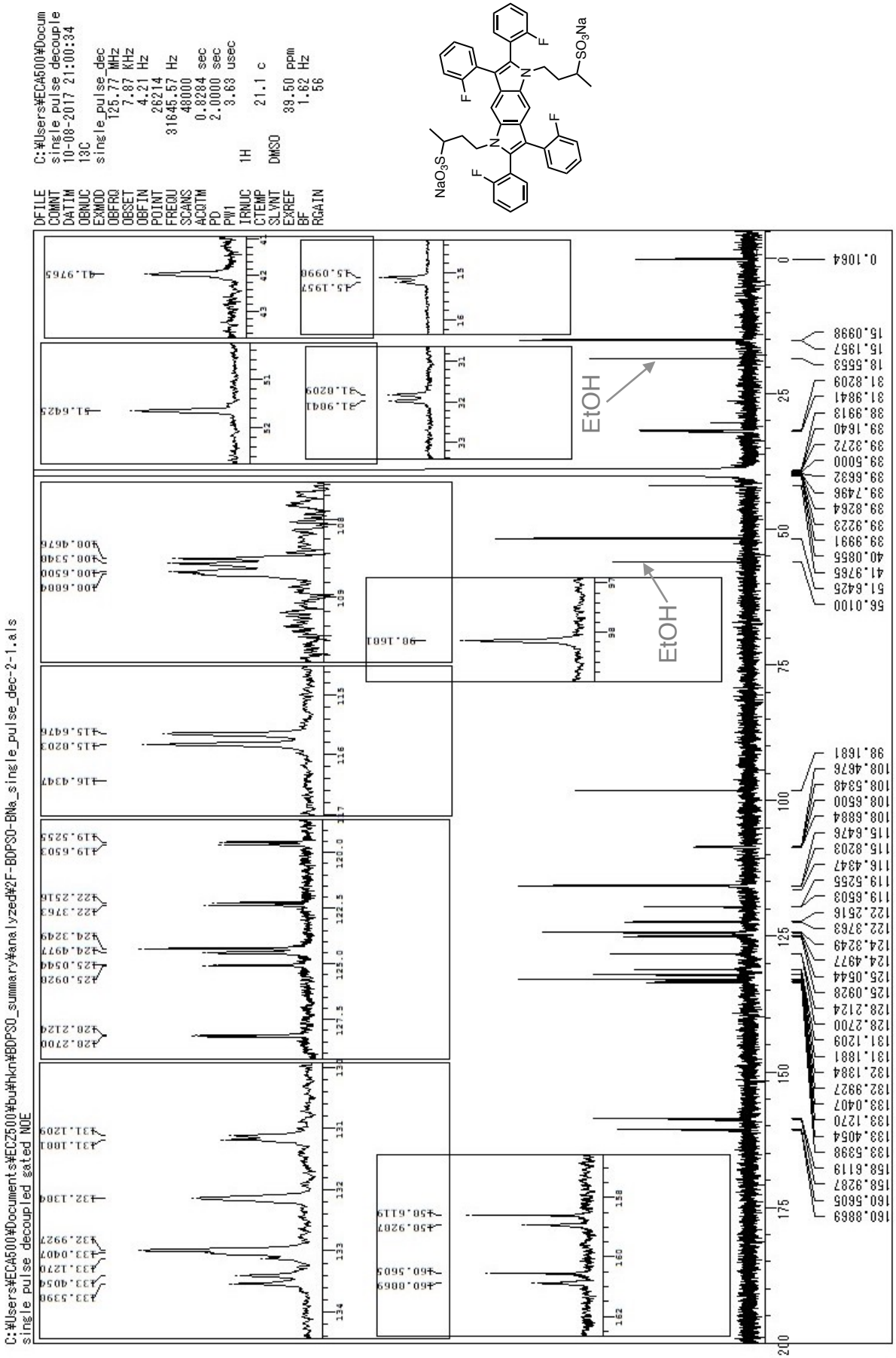
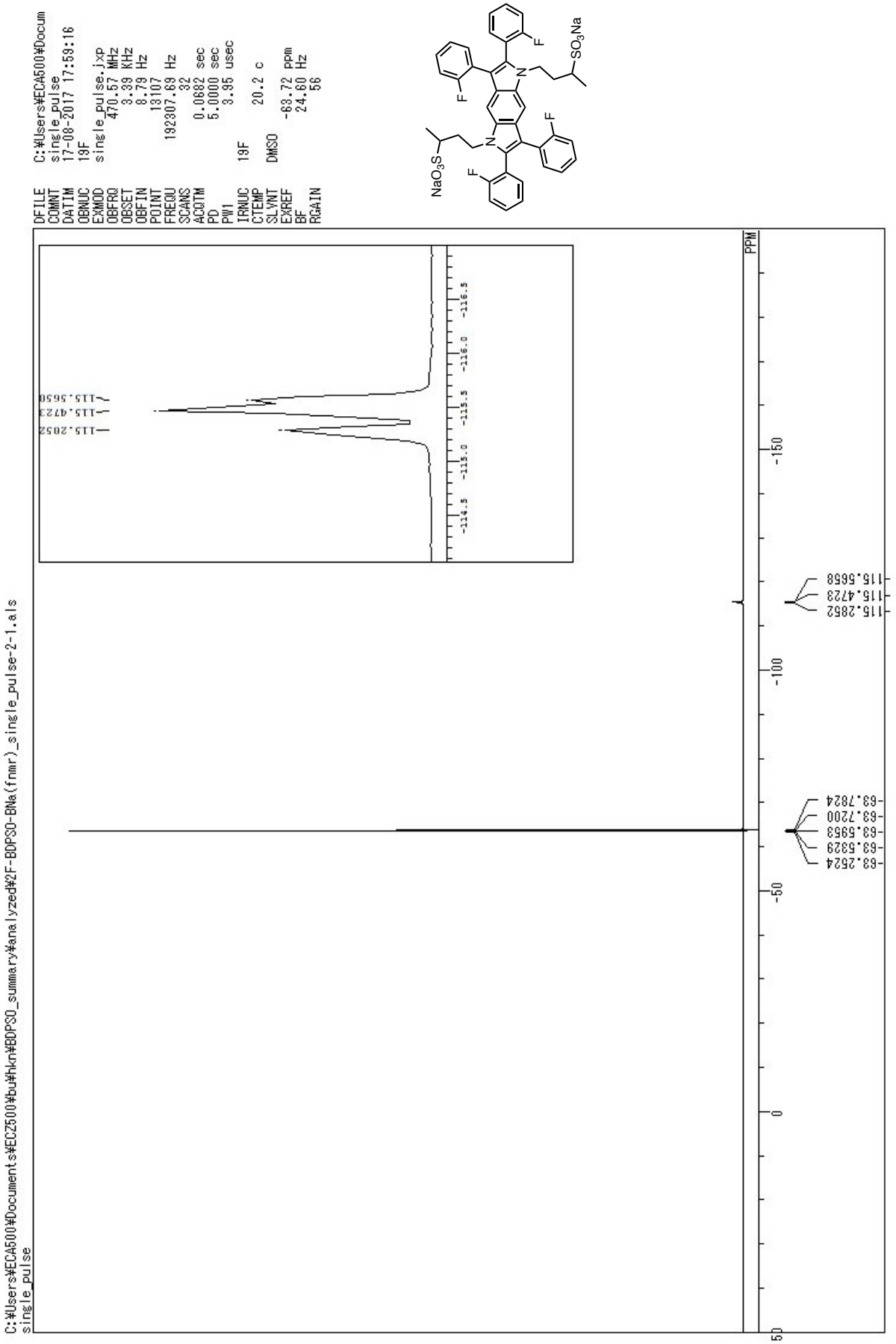


^{19}F-NMR spectrum of **2-F-br-4C**



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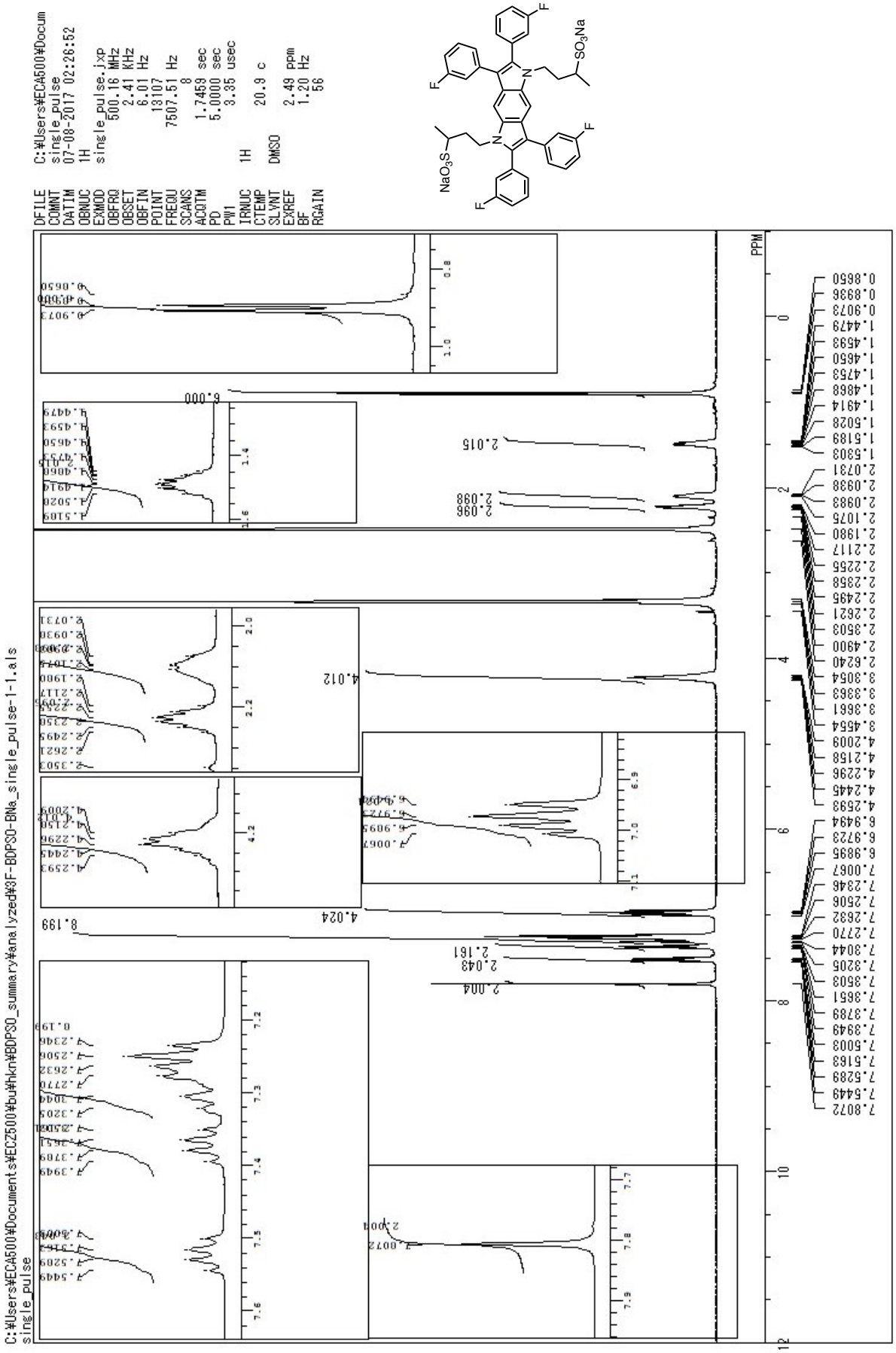

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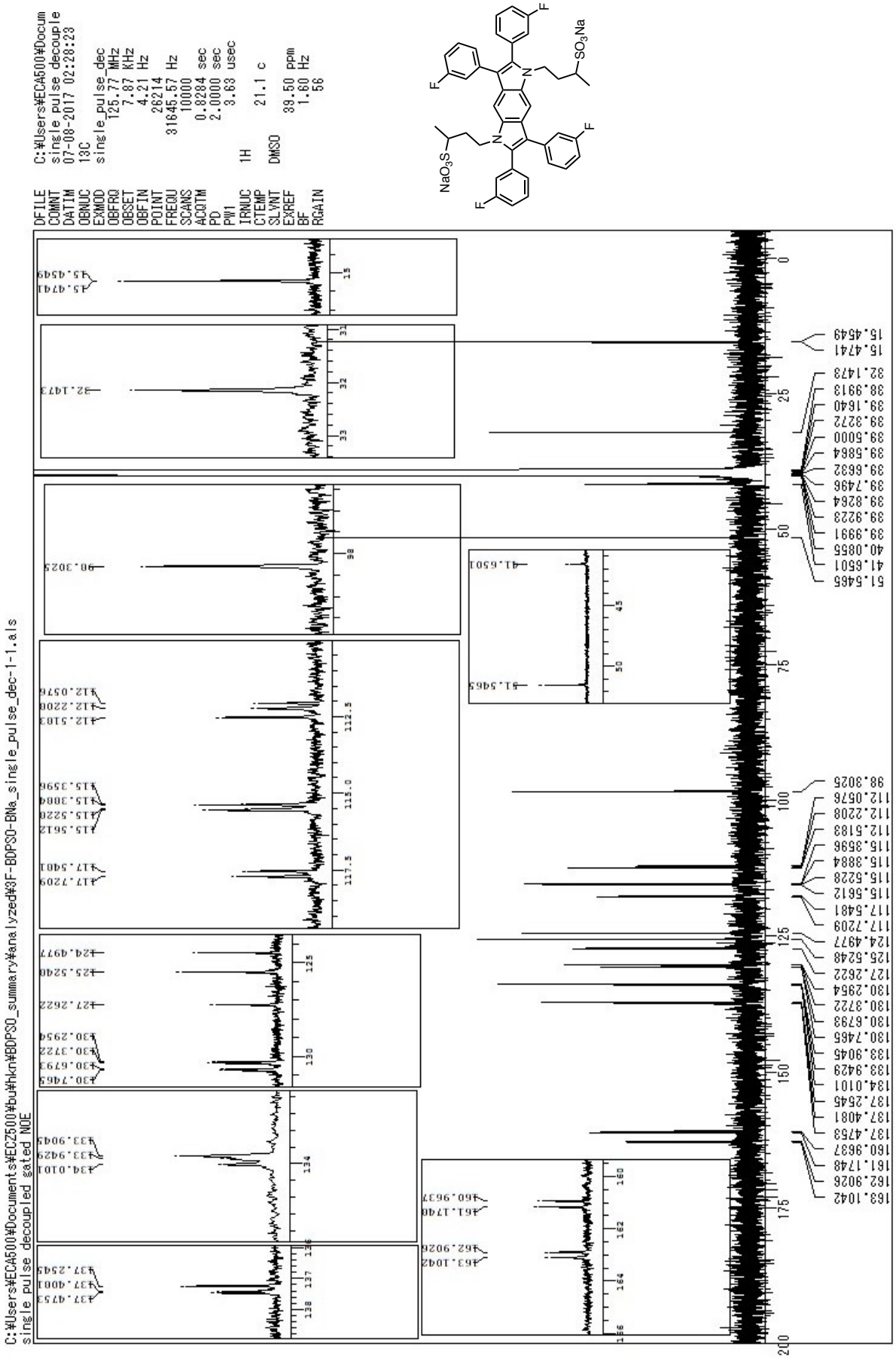
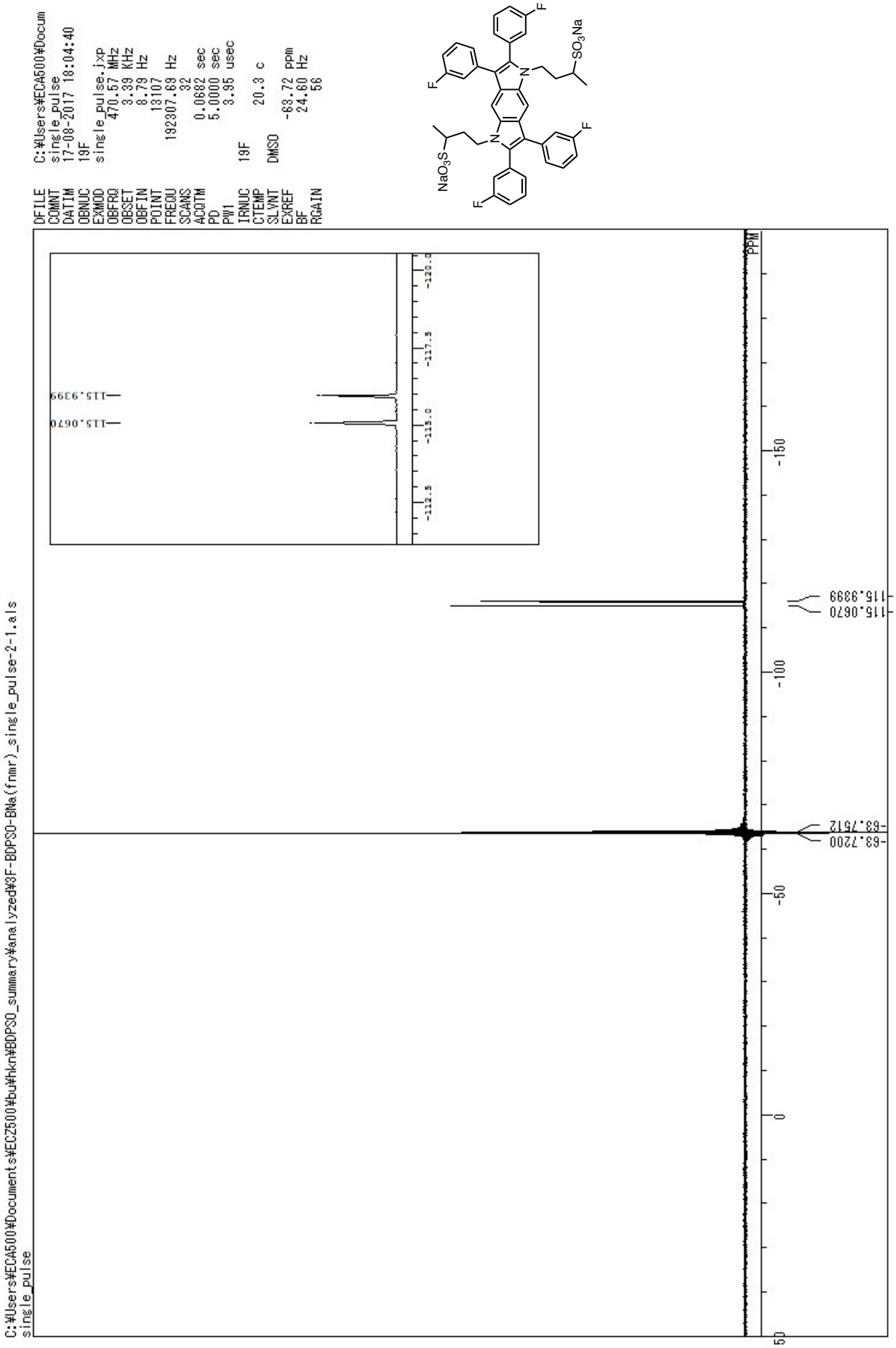
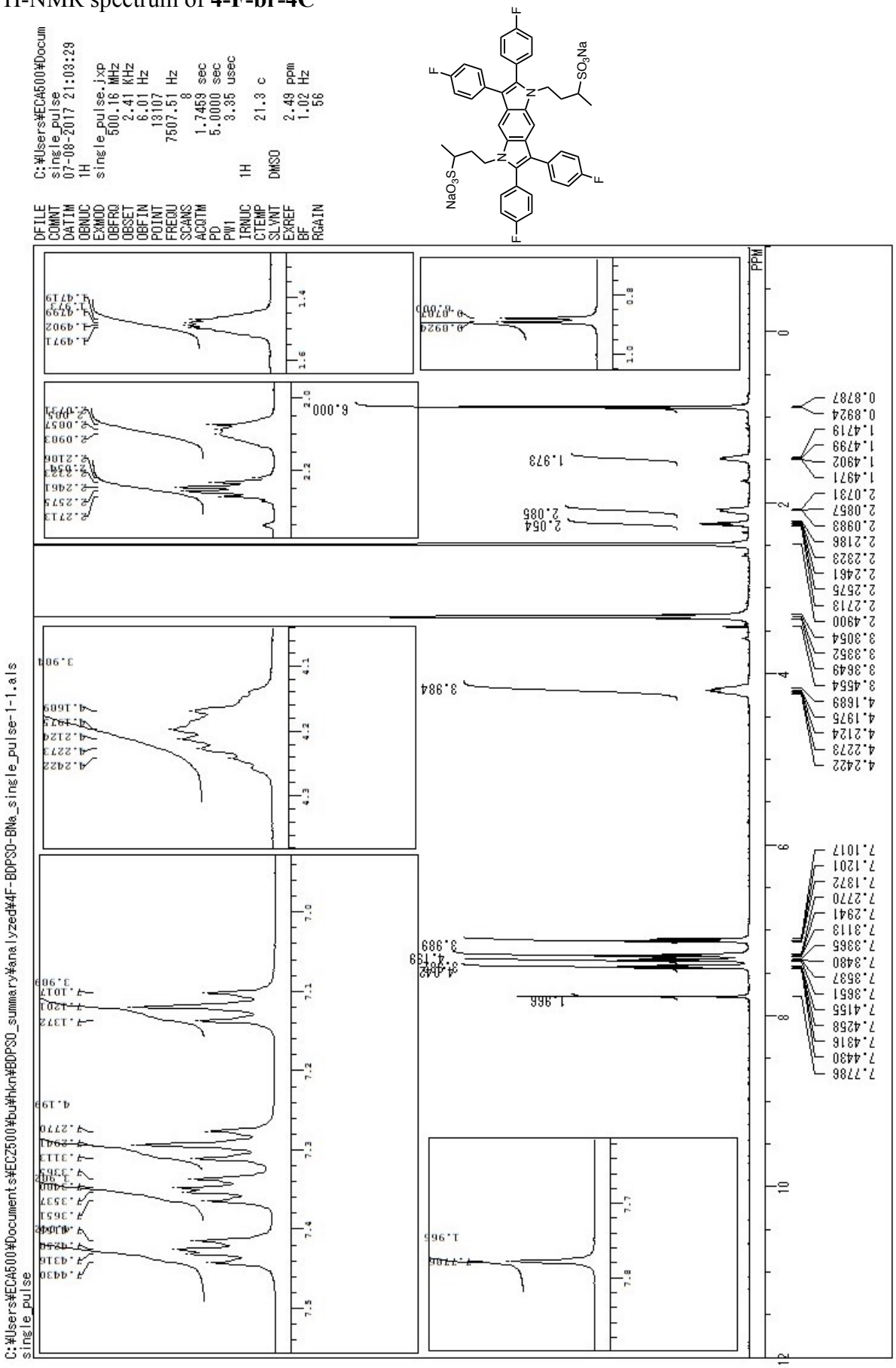


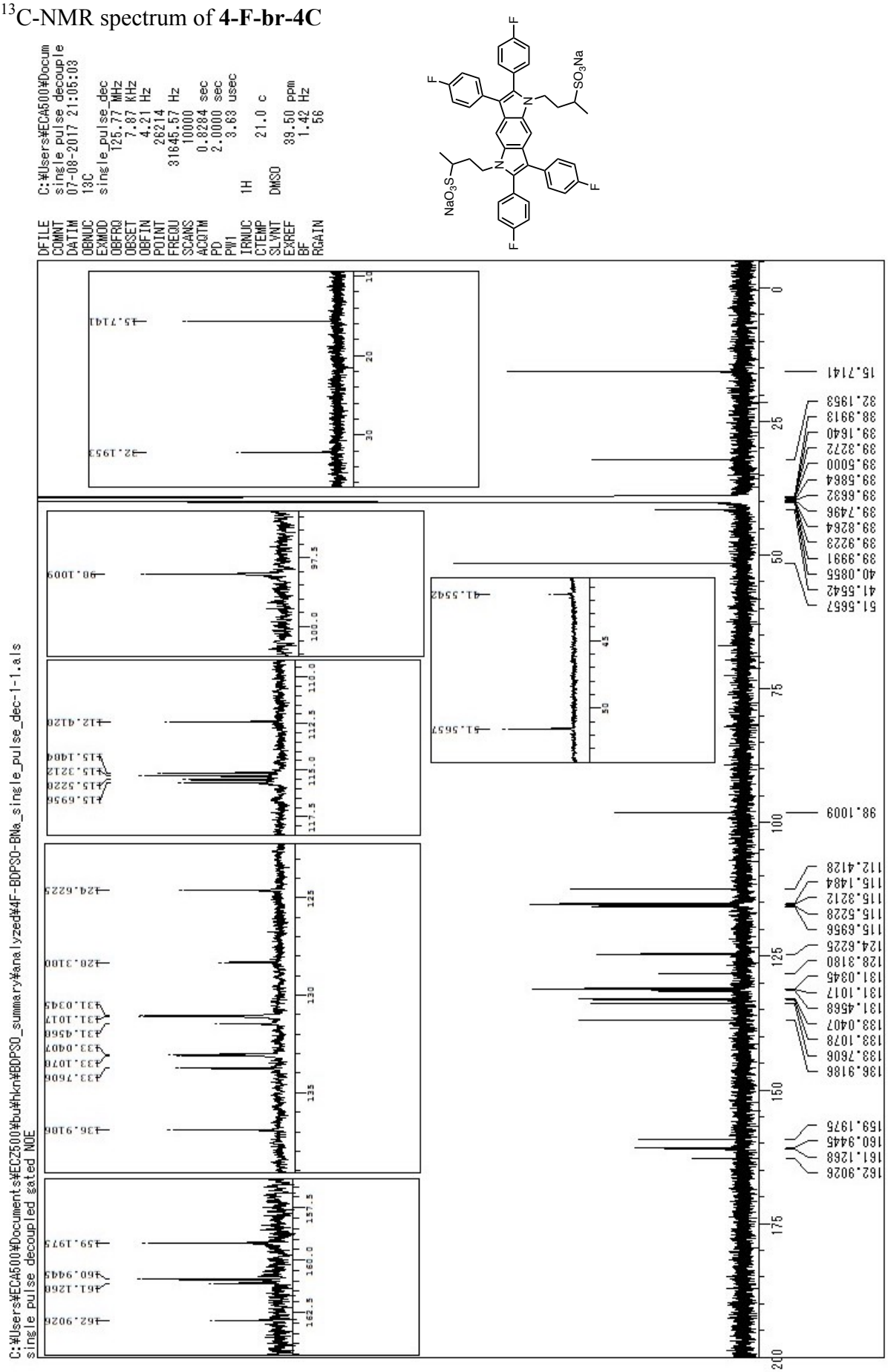
^{19}F-NMR spectrum of **3-F-br-4C**



^{1}H-NMR spectrum of **4-F-br-4C**



^{13}C-NMR spectrum of **4-F-br-4C**



^{19}F-NMR spectrum of **4-F-br-4C**