Electronic Supplementary Information

Pyrazino[2,3-g]Quinoxaline Dyes for Solar Cell Applications

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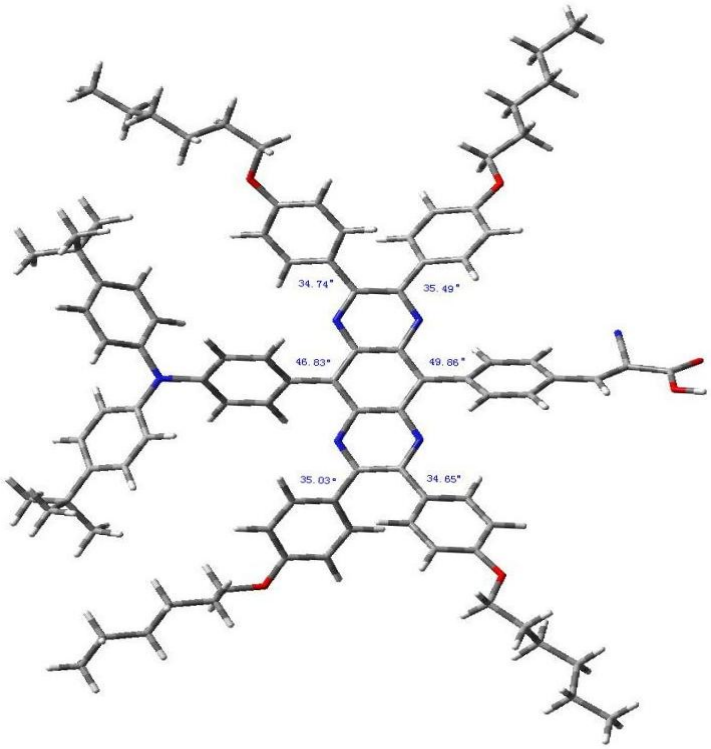
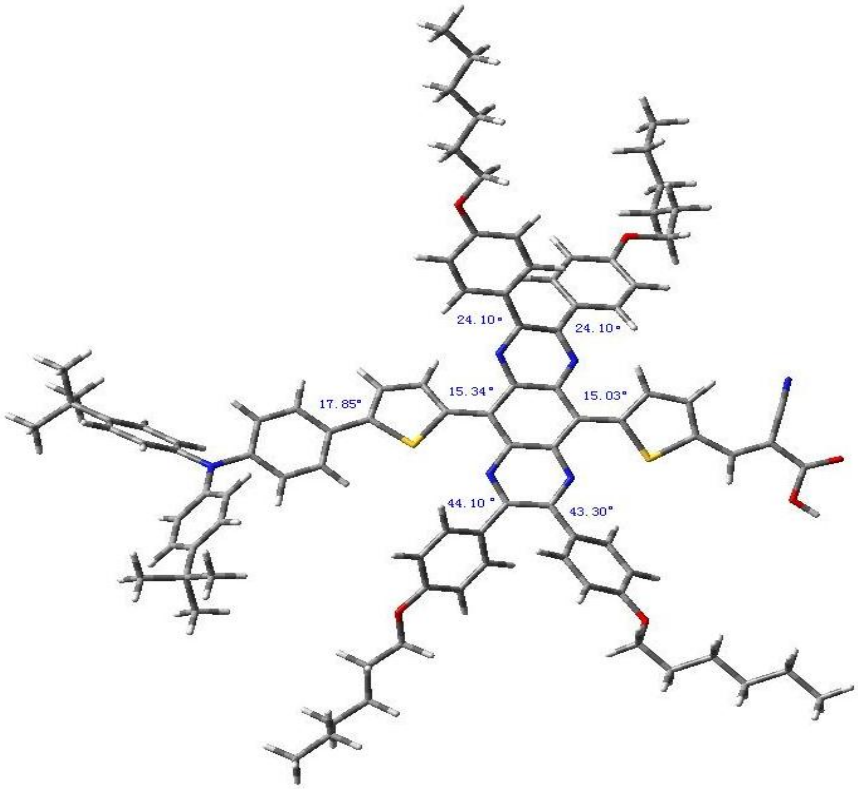
The optimized ground state molecular structures and the corresponding dihedral angles of PQ-1 and PQ-2



PQ-1



PQ-2

The fluorescence spectra of PQ-1and PQ-2

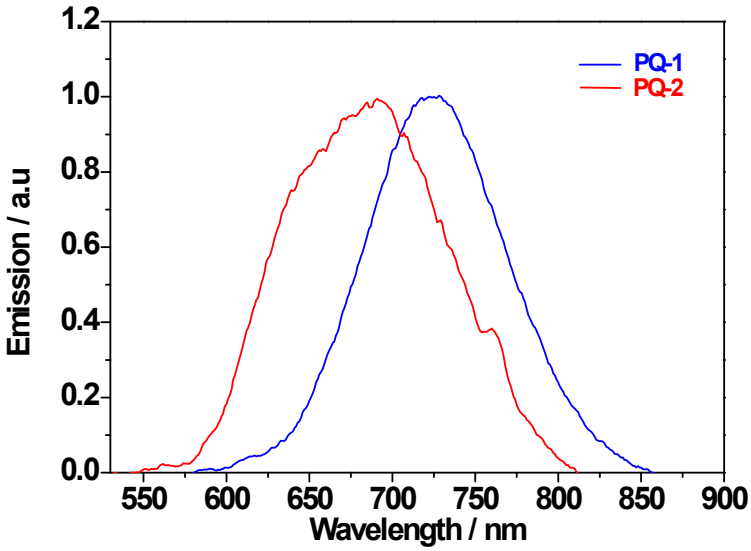
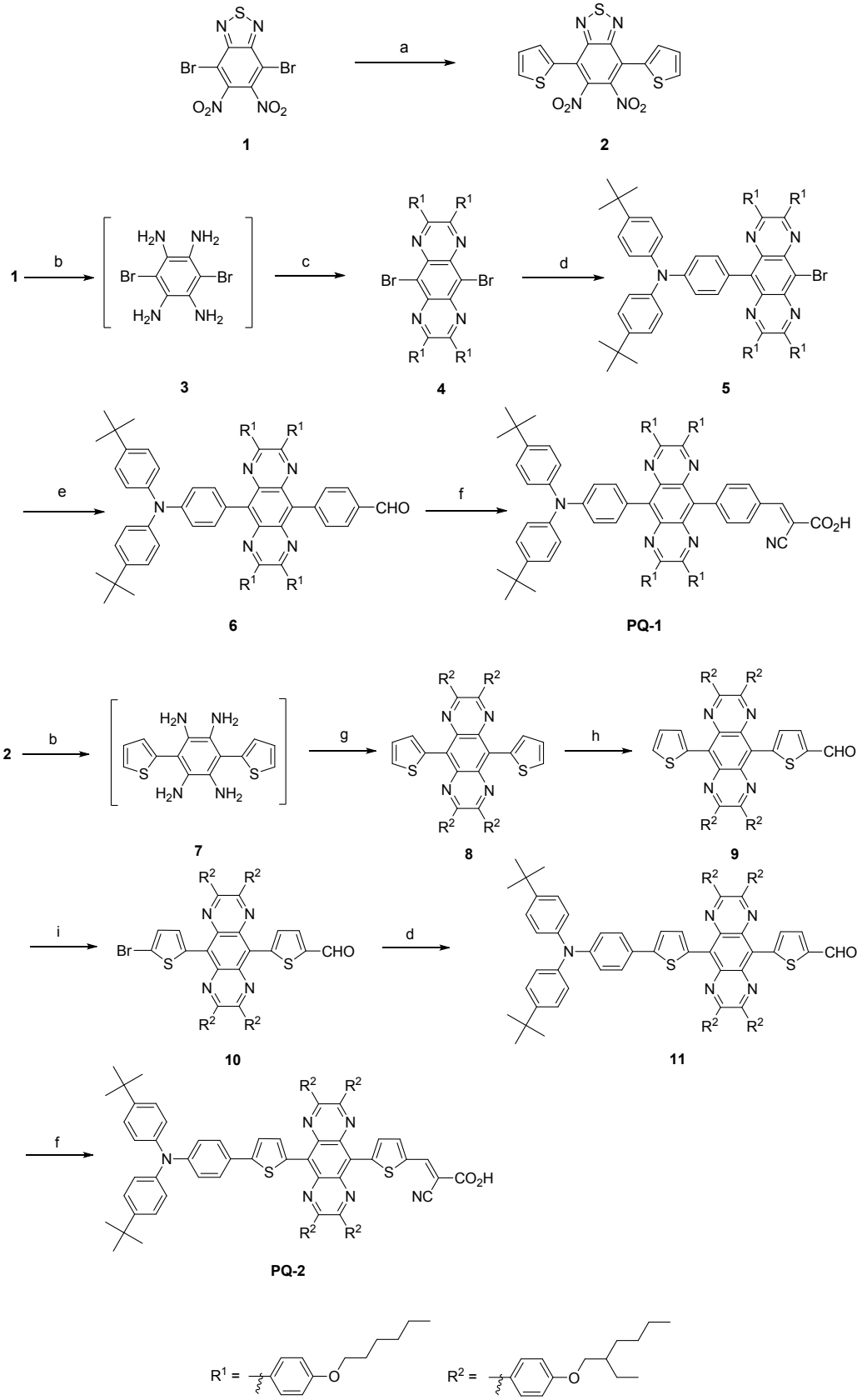


Fig.S1. Emission spectra of **PQ-1**(excited at 560 nm) and **PQ-2** (excited at 512 nm) in diluted CH_2Cl_2 .

Synthetic procedures and characterization data

Scheme S1. Synthetic routes to **PQ-1** and **PQ-2** dyes



Reagents and conditions: (a) 2-tributylstannylthiophene, $Pd(PPh_3)_4$, THF, reflux; (b) Zn, HOAc; (c) 4,4'-(hexyloxy)benzil, HOAc; (d) 4-(bis(4-*tert*-butylphenyl)amino)phenylboronic acid, $Pd(PPh_3)_4$, K_2CO_3, PhMe, reflux; (e) 4-formyl-phenylboronic acid, $Pd(PPh_3)_4$, K_2CO_3, PhMe, reflux; (f) cyanoacetic acid, peperidine, THF, reflux; (g) 4,4'-[(2-ethylhexyl)oxy]benzyl, HOAc; (h) $POCl_3$, DMF, 1,2-dichloroethane; (i) NBS, THF.

5,6-Dinitro-4,7-di(thiophen-2-yl)benzo[c][1,2,5]thiadiazole (**2**). A mixture of 4,7-dibromo-5,6-dinitrobenzo[c][1,2,5]thiadiazole (**1**) (1.92 g, 5.0 mmol), 2-tributylstannylthiophene (4.48 g, 12.0 mmol), $Pd(PPh_3)_4$ (0.17 g, 0.15 mmol) and dry THF (50 mL) was refluxed for 15 h under a nitrogen atmosphere. The mixture was concentrated under a reduced pressure and purified by silica gel column chromatography (eluting with dichloromethane/petroleum ether, 50/50, v/v) to afford compound **2** (1.60 g, 82%) as a grown solid. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 7.32 (dd, J = 4.8, 3.8 Hz, 2H), 7.51 (dd, J = 4.0, 1.2 Hz, 2H), 8.06 (dd, J = 5.2, 1.2 Hz, 2H); HR-MS (EI): m/z $[M]^+$ cacld for $C_{14}H_6N_4O_4S_3$, 389.9551; found, 389.9556.

2,3,7,8-Tetra(*p*-hexyloxyphenyl)-5,10-dibromopyrazino[2,3-g]quinoxaline (**4**). The compound **1** (0.60 g, 1.6 mmol) was dissolved in glacial acetic acid (30 mL), followed by adding activated zinc powder (2.4 g) in one portion. After stirring at 70 ^{0}C for 1 h, the mixture solution including the intermediate 3,6-dibromo-1,2,4,5-benzenetetramine **3** which was extremely sensitive to air was filtered to remove the unreactive zinc powder. To the filtrate was added 4,4'-(hexyloxy)benzil (1.3 g, 3.2 mmol) and the mixture was stirred at 100 ^{0}C for another 20 h. After removal of the solvent, the residue was dissolved in dichloromethane (100 mL), washed with saturated $NaHCO_3$ solution (100 mL), water (100 mL), and brine (100 mL), respectively. The organic phase was dried over anhydrous $MgSO_4$, concentrated in vacuum and purified by silica gel column chromatography (eluting with dichloromethane/petroleum ether, 20/50, v/v) to afford the quinoxaline product **4** (0.33 g, 20%) as an orange solid. M.p.175-177 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.92 (t, J = 13.2 Hz, 12H), 1.26–1.54 (m, 24H), 1.78-1.84 (m, 8H), 4.00 (t, J = 12.9 Hz, 8H), 6.91 (d, J = 8.7 Hz, 8H), 7.77 (d, J = 8.7 Hz, 8H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.86, 154.37, 138.17, 131.91, 130.44, 114.41, 68.16, 31.59, 29.17, 25.71, 22.61, 14.05. HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{58}H_{68}Br_2N_4O_4$, 1042.3607; found, 1042.3602.

2,3,7,8-Tetra(*p*-hexyloxyphenyl)-5-[*p*-(bis(*p*-*tert*-butylphenyl)amino)phenyl]-10-bromopyrazino[2,3-g]quinoxaline (**5**). A mixture of the compound **4** (150 mg, 0.14 mmol), 4-(bis(4-*tert*-butylphenyl)amino)phenylboronic acid (70 mg, 0.17 mmol), $Pd(PPh_3)_4$ (25 mg, 15 mol% relative to the compound **4**), K_2CO_3 (83 mg, 0.6 mmol) in toluene (20 mL) and H_2O (3 mL) was refluxed for 15 h under a nitrogen atmosphere. After removal of the solvents, the residue was dissolved in dichloromethane (50 mL), washed with brine (50 mL), and dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was purified by silica gel column chromatography (eluting with dichloromethane/petroleum ether 20/50, v/v) to afford a mixture of compound **5** and the double cross-coupling compound. The mixed products were difficult to separate and thus the crude compound **5** was directly used in the next reaction.

2,3,7,8-Tetra(*p*-hexyloxyphenyl)-5-[*p*-(bis(*p*-*tert*-butylphenyl)amino)phenyl]-10-(4''-formylphenyl) pyrazino[2,3-g]quinoxaline (**6**). A mixture of the crude compound **5** (150 mg), 4-formylphenylboronic acid (25 mg, 0.17 mmol), $Pd(PPh_3)_4$ (20 mg, 15%mol), K_2CO_3 (69 mg, 0.5 mmol) in toluene (20 mL) and H_2O (3 mL) was refluxed for 15 h under a nitrogen atmosphere. After removal of the solvents, the residue was dissolved in dichloromethane (50 mL), washed with brine (50 mL) and dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was purified by silica gel column chromatography (eluting with dichloromethane/petroleum ether 20/50, v/v) to afford the crude compound **6** (95 mg, 62%) as a brown solid which was unpurified and directly used in the next reaction.

3-{*p*-[2,3,7,8-Tetra(*p*-hexyloxyphenyl)-5-[*p*-(bis(*p*-*tert*-butylphenyl)amino)phenyl]pyrazino[2,3-*g*](quinoxalin-10-yl)]phenyl}-2-cyanoacrylic acid (**PQ-1**). To a solution of the crude compound **6** (95 mg), cyanoacetic acid (10 mg, 0.12 mmol) and tetrahydrofuran (15 mL) was added a few drops of piperdine and then the reaction mixture was refluxed for 8 h under a nitrogen atmosphere. After the completion of the reaction, acetic acid (2 mL) was added into the mixture, and the solvents were removed under a reduced pressure. The residue was dissolved in dichloromethane (50 mL), washed with water (30 mL) and brine (30 mL), respectively. The organic phase was dried over anhydrous $MgSO_4$. After removal of the solvents, the residue was purified by silica gel column chromatography (eluting with methanol–dichloromethane 10/100, v/v) to afford the dye **PQ-1** (56 mg, 56%) as a deep brown solid. M.p.>220 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.87–0.93 (m, 12H), 1.25–1.45 (m, 44H), 1.76-1.80 (m, 8 H), 3.94-3.97 (t, J = 11.6 Hz, 8 H), 6.74 (d, J = 7.2 Hz, 4H), 6.81 (d, J = 8.0 Hz, 4H), 7.24–7.34 (m, 10H), 7.57–7.59 (m, 8H), 7.95 (br. s, 2H), 8.17 (br. s, 2H), 8.50 (br. s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.35, 160.22, 151.41, 150.90, 147.59, 145.73, 145.10, 136.76, 136.31, 135.54, 135.29, 132.24, 132.16, 131.65, 131.50, 131.08, 130.80, 130.39, 129.90, 129.73, 128.65, 128.56, 127.21, 125.98, 124.65, 120.15, 114.36, 114.21, 68.08, 34.36, 33.71, 31.92, 31.62, 31.59, 31.55, 29.78, 29.69, 29.65, 29.60, 29.46, 29.33, 29.26, 29.21, 29.10, 27.22, 25.74, 25.72, 24.77, 22.68, 14.10**;** IR(KBr) ν 3026, 2969, 2854, 2230, 1716, 1683, 1651, 1558, 1540, 1507 cm^{-1};HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{94}H_{104}N_6O_6$, 1412.8017; found, 1412.8012.

2,3,7,8-Tetra[*p*-(2-ethylhexyloxy)phenyl]-5,10-dithienylpyrazino[2,3-g]quinoxaline (**8**). The compound **2** (0.50g, 1.3 mmol) was dissolved in glacial acetic acid (30 mL) followed by addition of activated zinc powder (2.0 g) in one portion. After being stirred at 70 ^{0}C for 1 h, the solution mixture including the intermediate 3,6-dithienyl-1,2,4,5-benzenetetramine **7**, which was extremely sensitive to air, was filtered to remove the unreactive zinc powder. To the filtrate was added 4,4'-[(2-ethylhexyl)oxy]benzil (1.21 g, 2.6 mmol) and then the mixture was stirred at 100 ^{0}C for 20 h. After removal of the solvent, the residue was dissolved in dichloromethane (100 mL), washed with saturated $NaHCO_3$ solution (100 mL), water (100 mL) and brine (100 mL), respectively. The organic phase was dried over anhydrous $MgSO_4$, concentrated in vacuum and purified by silica gel column chromatography (eluting

with dichloromethane/petroleum ether 20/50, v/v) to afford the quinoxaline **8** (0.64 g, 42%) as a deep grown solid. M.p.124-126 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.90–0.96 (m, 24H), 1.33–1.40 (m, 18H), 1.40–1.49 (m, 14H), 1.72–1.78 (m, 4H), 3.89 (d, *J* = 5.6 Hz, 8H), 6.91 (d, *J* = 8.8 Hz, 8H), 7.36 (t, *J* = 4.1 Hz , 2H), 7.71 (d, *J* = 4.4 Hz, 2H), 7.81 (d, *J* = 8.8 Hz, 8H), 8.45 (d, *J* = 4.4 Hz, 2H); HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{74}H_{90}N_4O_4S_2$, 1162.6404; found, 1162.6400.

2,3,7,8-Tetra[*p*-(2-ethylhexyloxy)phenyl]-5-(5-formylthienyl)-10-thienylpyrazino[2,3-g]quinoxaline (9). To a mixture of the quinoxaline **8** (0.70g, 0.6 mmol), anhydrous DMF (88 mg, 1.2 mmol) and 1,2-dichloroethane (40 mL) was added $POCl_3$ (110 mg, 0.72 mmol) dropwise through a syringe at 0 ^{0}C under a nitrogen atmosphere. Then the mixture was stirred at 70 ^{0}C for 5 h before being poured into water. The organic phase was separated and washed with saturated $NaHCO_3$ solution (30 mL), water (30 mL) and brine (30 mL) respectively. The organic phase was dried over anhydrous $MgSO_4$, concentrated in vacuum and purified by silica gel column chromatography (eluting with dichloromethane) to afford the compound **9** (0.58 g, 81%) as a deep red solid. M.p.128-130 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.90–0.97 (m, 24H), 1.25–1.35 (m, 18H), 1.35–1.55 (m, 14H), 1.71–1.77 (m, 4H), 3.90 (d, *J* = 5.4 Hz, 8H), 6.92 (dd, *J* =9.0, 2.7 Hz, 8H), 7.36 (t, *J* = 5.8 Hz , 1H), 7.74–7.81 (m, 9H), 7.97 (d, *J* = 4.4 Hz, 1H), 8.49 (d, *J* = 4.4 Hz, 2H), 10.08 (s, 1H); HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{74}H_{90}N_4O_4S_2$, 1190.6353; found, 1190.6347.

2,3,7,8-Tetra[*p*-(2-ethylhexyloxy)phenyl]-5-(5-formylthienyl)-10-(5-bromothienyl)pyrazino[2,3-g]quinoxaline (**10**). To a solution of the compound **9** (0.50 g, 0.42 mmol) in tetrahydrofuran (40 mL) was added dropwise a solution of *N*-bromosuccinimide (90 mg, 0.50 mmol) in tetrahydrofuran (5 mL) in dark at 0 ^{0}C. Then the mixture was stirred at room temperature for additional 8 h before being poured into water. Dichloromethane (100 mL) was added into the resulting mixture, and the organic phase was separated, washed with brine (50 mL) and dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was purified by flash silica gel column chromatography (eluting with dichloromethane/petroleum ether 20/50, v/v) to afford the brominated compound **10** (0.43 g, 83%) as a deep red solid. M.p.126-128 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.90–0.97 (m, 24H), 1.30–1.40 (m, 18H), 1.40–1.59 (m, 14H), 1.75–1.77 (m, 4H), 3.89 (d, *J* =4.0 Hz, 8H), 6.92 (dd, *J* =8.4, 6.4 Hz, 8H), 7.27 (d, *J* =4.0 Hz, 1H), 7.74 (dd, *J* =8.8, 3.2 Hz, 8H), 7.92 (d, *J* = 4.0 Hz, 1H), 8.47 (t, *J* = 3.8 Hz, 2H), 10.06 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 183.62, 160.87, 160.78, 152.50, 152.12, 145.25, 144.87, 136.65, 136.42, 135.64, 135.09, 134.90, 134.51, 131.90, 130.64, 130.53, 130.45, 129.15, 128.14, 125.47, 119.32, 114.48, 70.70, 39.40, 30.55, 29.13, 23.88, 23.07, 14.12, 11.16; HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{75}H_{89}BrN_4O_5S_2$, 1268.5458; found, 1268.5452.

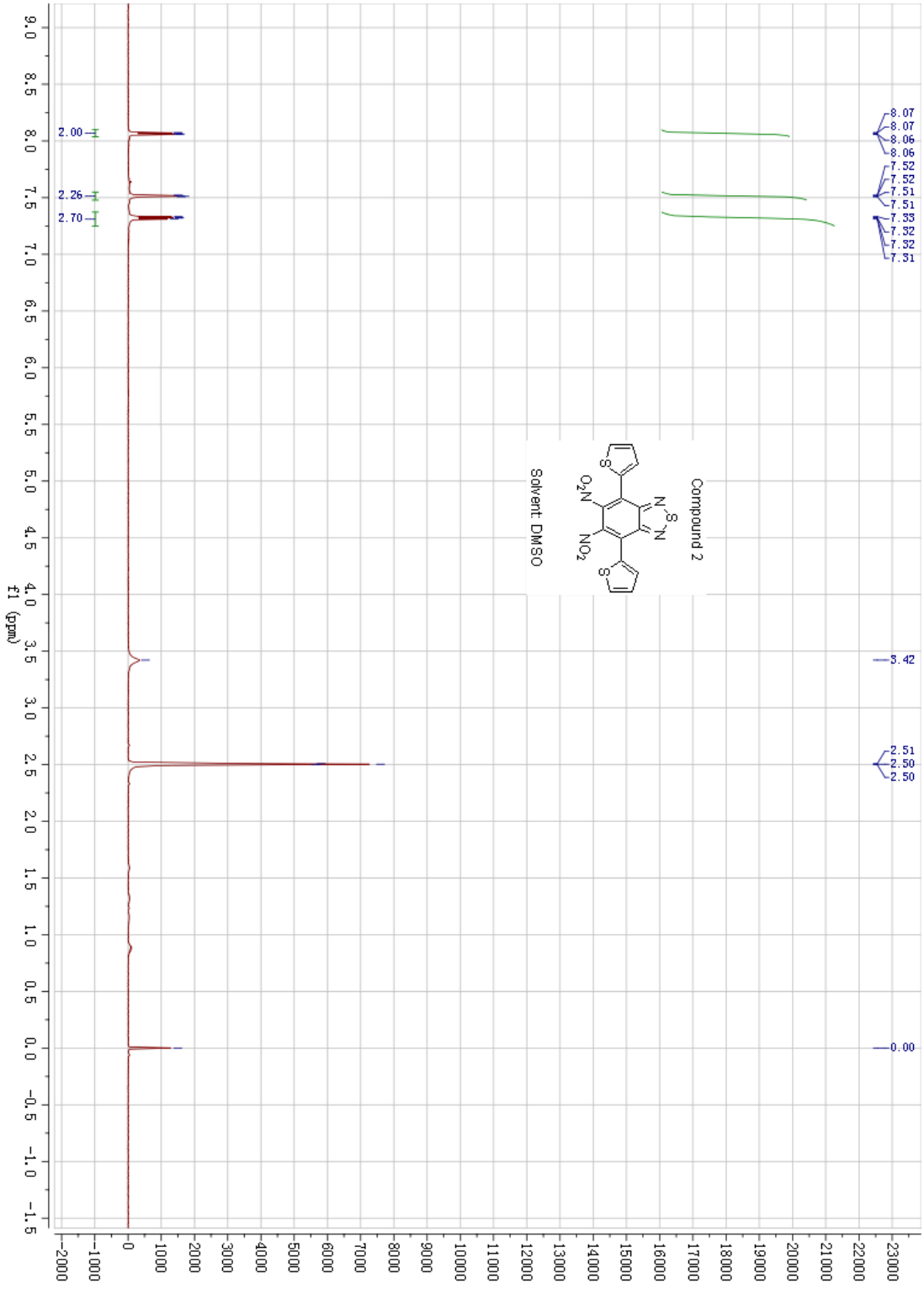
2,3,7,8-Tetra[*p*-(2-ethylhexyloxy)phenyl]-5-(5-formylthienyl)-10-[5-[*p*-(bis(*p*-*tert*-butylphenyl)amino)phenyl]thien-2-yl]pyrazino[2,3-g]quinoxaline (**11**). A mixture of the compound **10** (380 mg, 0.30 mmol), 4-[bis(4-*tert*-butylphenyl)amino]phenylboronic acid (144 mg, 0.36 mmol), $Pd(PPh_3)_4$ (25 mg, 5

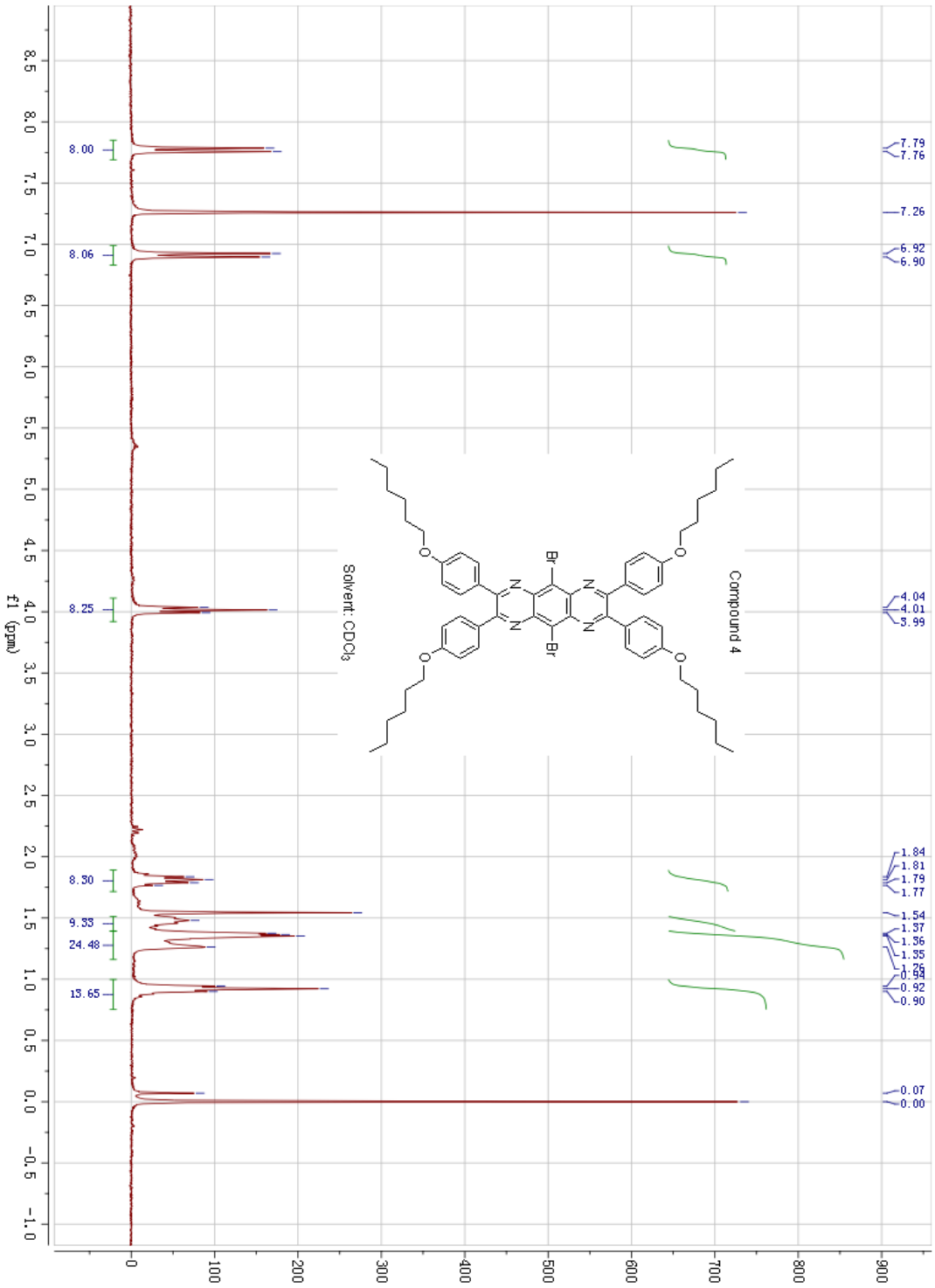
mol% relative to the compound **6**), K_2CO_3 (165 mg, 1.2 mmol) in toluene (20 mL) and H_2O (3 mL) was refluxed for 15 h under a nitrogen atmosphere. After removal of the solvents, the residue was dissolved in dichloromethane (50 mL), washed with brine (50 mL) and dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was purified by silica gel column chromatography (eluting with dichloromethane/petroleum ether 20/50, v/v) to afford the compound **11** (0.34 g, 75%). M.p.178-180 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.93–0.97 (m, 26H), 1.34 (s, 18H), 1.40–1.55 (m, 32H), 1.73–1.77 (m, 4H), 3.88–3.91 (m, 8H), 6.93 (dd, *J* = 8.4, 3.2 Hz, 8H), 7.10–7.14 (m, 5H), 7.31 (d, *J* = 8.4 Hz, 4H), 7.48 (d, *J* = 4.0 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.79 (d, *J* = 8.8 Hz, 4H), 7.83 (d, *J* = 8.8 Hz, 4H), 7.90 (d, *J* = 4.0 Hz, 1H), 8.51 (d, *J* =4.0 Hz, 1H), 8.57 (d, *J* = 4.0 Hz, 1H), 10.08 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 183.58, 160.80, 160.64, 152.29, 152.59, 149.59, 147.84, 146.06, 145.26, 145.00, 144.79, 136.78, 135.82, 134.93, 134.25, 133.38, 131.91, 131.86, 130.79, 130.64, 129.56, 128.13, 126.58, 126.15, 124.29, 122.74, 114.50, 114.42, 70.70, 39.39, 34.35, 31.46, 30.54, 29.10, 23.87, 23.06, 14.10, 11.14; HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{101}H_{119}N_5O_5S_2$, 1545.8653; found, 1545.8649.

3-{*p*-[2,3,7,8-Tetra(*p*-(2-ethylhexyloxy)phenyl]-5-[(*p*-(bis(*p*-*tert*-butylphenyl)amino)phenyl)thien-2-yl]pyrazino[2,3-*g*](quinoxalin-10-yl)]thien-2-yl}-2-cyano acrylic acid (**PQ-2**). To a solution of the compound **7** (200 mg, 0.13mmol), cyanoacetic acid (20 mg, 0.24 mmol) in tetrahydrofuran (30 mL) was added a few drops of piperdine, followed by refluxing for 8 h under a nitrogen atmosphere. Then, acetic acid (2 mL) was added into the mixture and the solvent removed under a reduced pressure. The residue was dissolved in dichloromethane (50 mL), washed with water (30 mL) and brine (30 mL), respectively. The organic phase was dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was purified by silica gel column chromatography (eluting with methanol–dichloromethane 10/100, v/v) to afford the dye **PQ-2** (136 mg, 65%) as a dark red solid. M.p.>230 ^{0}C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.93-0.97 (m, 26H), 1.34 (s, 18H), 1.35–1.55 (m, 32H), 1.73-1.77 (m, 4H), 3.88-3.91 (m, 8H), 6.93 (d, *J* = 8.4 Hz, 4H), 6.98 (d, *J* = 8.4 Hz, 4H), 7.10-7.14 (m, 5H), 7.31 (d, *J* = 8.4 Hz, 4H), 7.48 (d, *J* = 4.0 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.78–7.84 (m, 8H), 7.84 (dd, *J* = 8.7, 2.1 Hz, 8H), 8.51 (s, 1H), 8.68 (d, *J* = 4.0 Hz, 1H), 8.78 (d, *J* = 4.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.84, 160.64, 152.55, 152.02, 151.59, 149.91, 147.87, 147.31, 146.08, 144.79, 138.23, 137.31, 136.76, 135.72, 135.10, 133.41, 131.97, 130.70, 130.52, 129.82, 128.09, 126.59, 126.17, 124.32, 123.69, 122.71, 122.07, 116.47, 114.69, 114.39, 96.28, 70.69, 39.44, 39.38, 34.36, 31.95, 31.49, 30.55, 29.72, 29.48, 29.38, 29.28, 29.15, 29.12, 24.73, 23.89, 23.08, 14.10; IR(KBr) *v* 3032, 2943, 2895, 2850, 2218，1698, 1684, 1603, 1572, 1519, 1457 cm^{-1}; HR-MS (MALDI): m/z $[M]^+$ cacld for $C_{104}H_{120}N_6O_6S_2$, 1612.8711; found, 1612.8705.

^{1}H and ^{13}C NMR spectra of the compounds

^{1}H NMR spectra of the compounds

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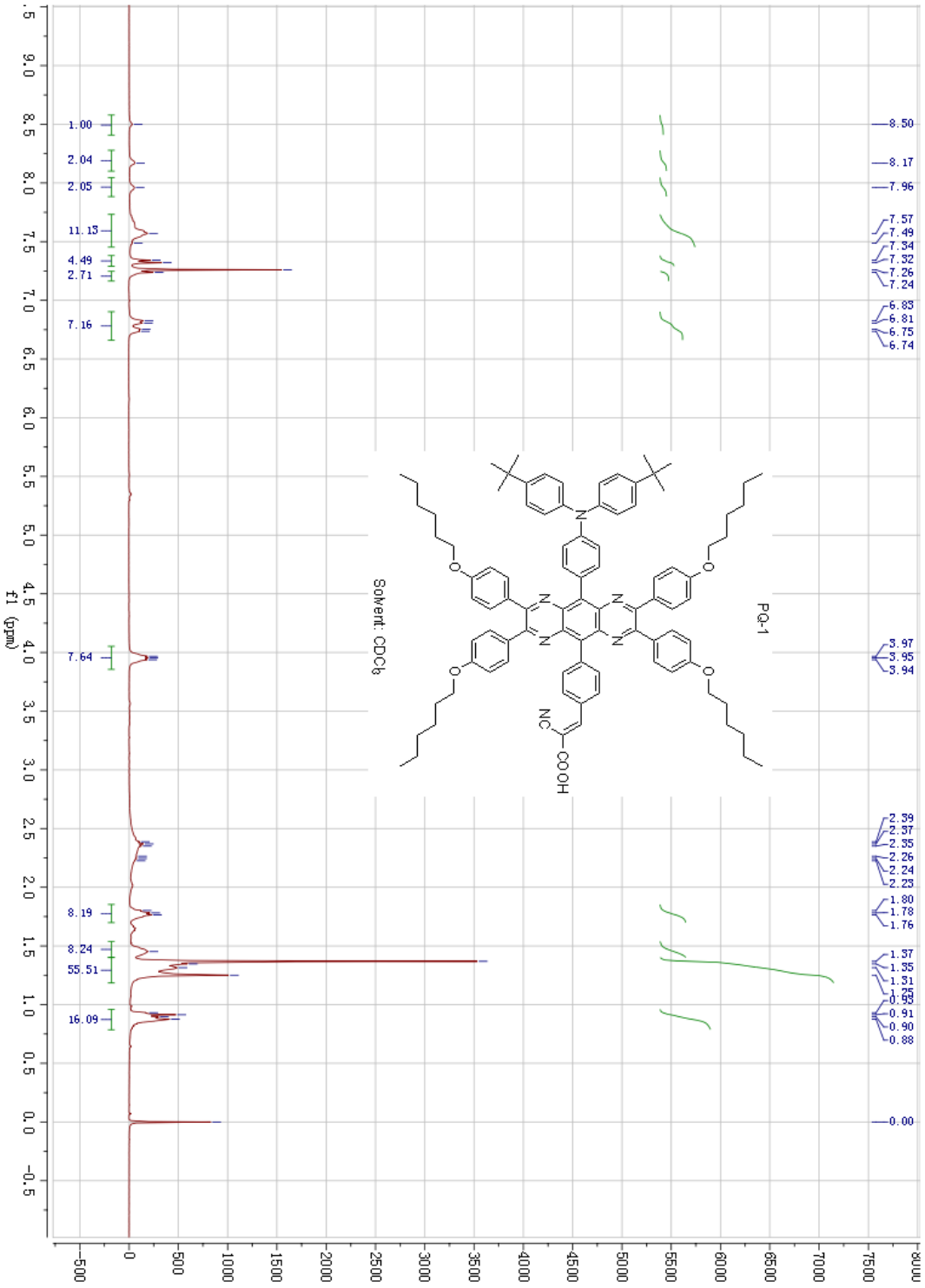
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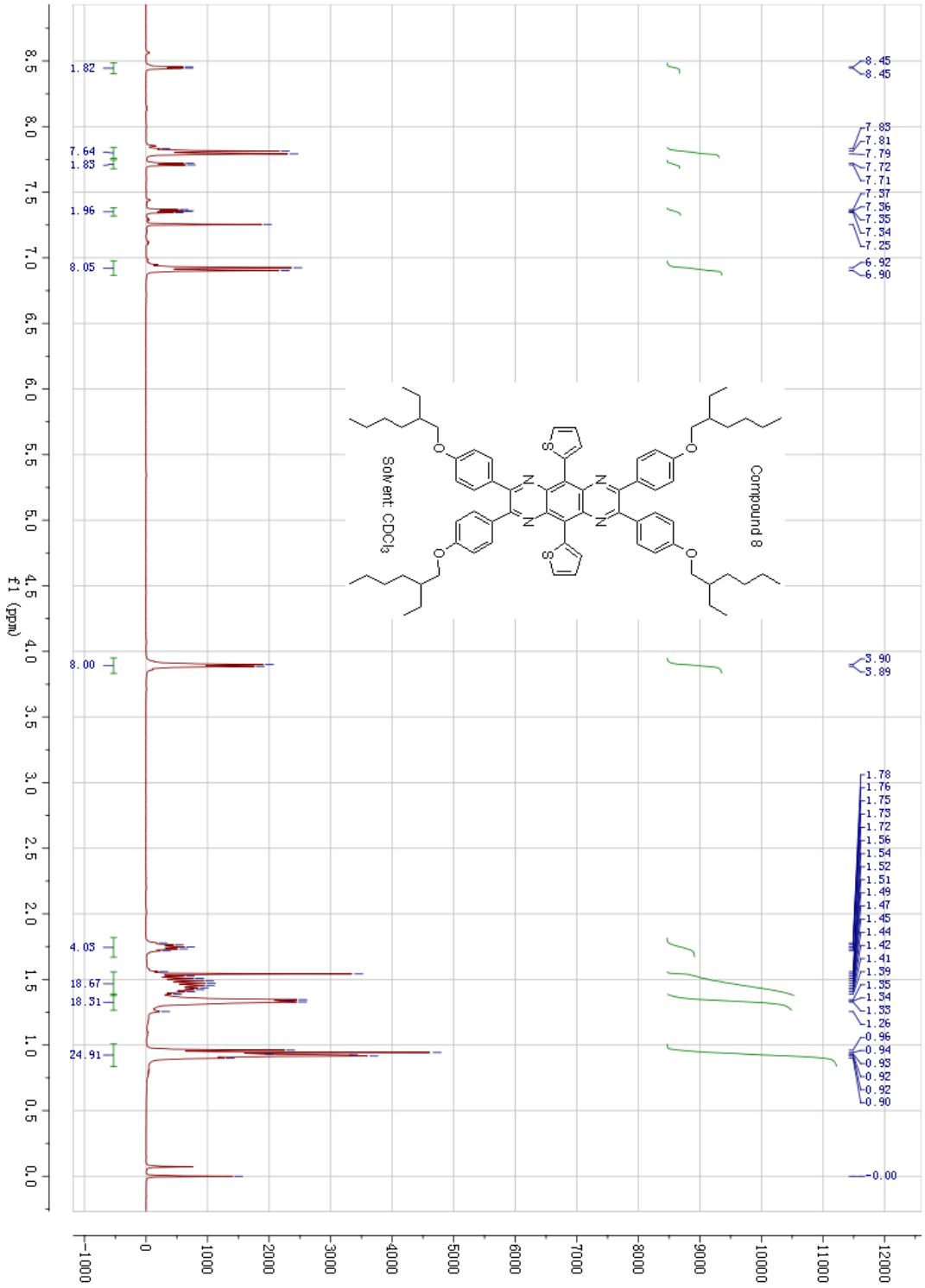
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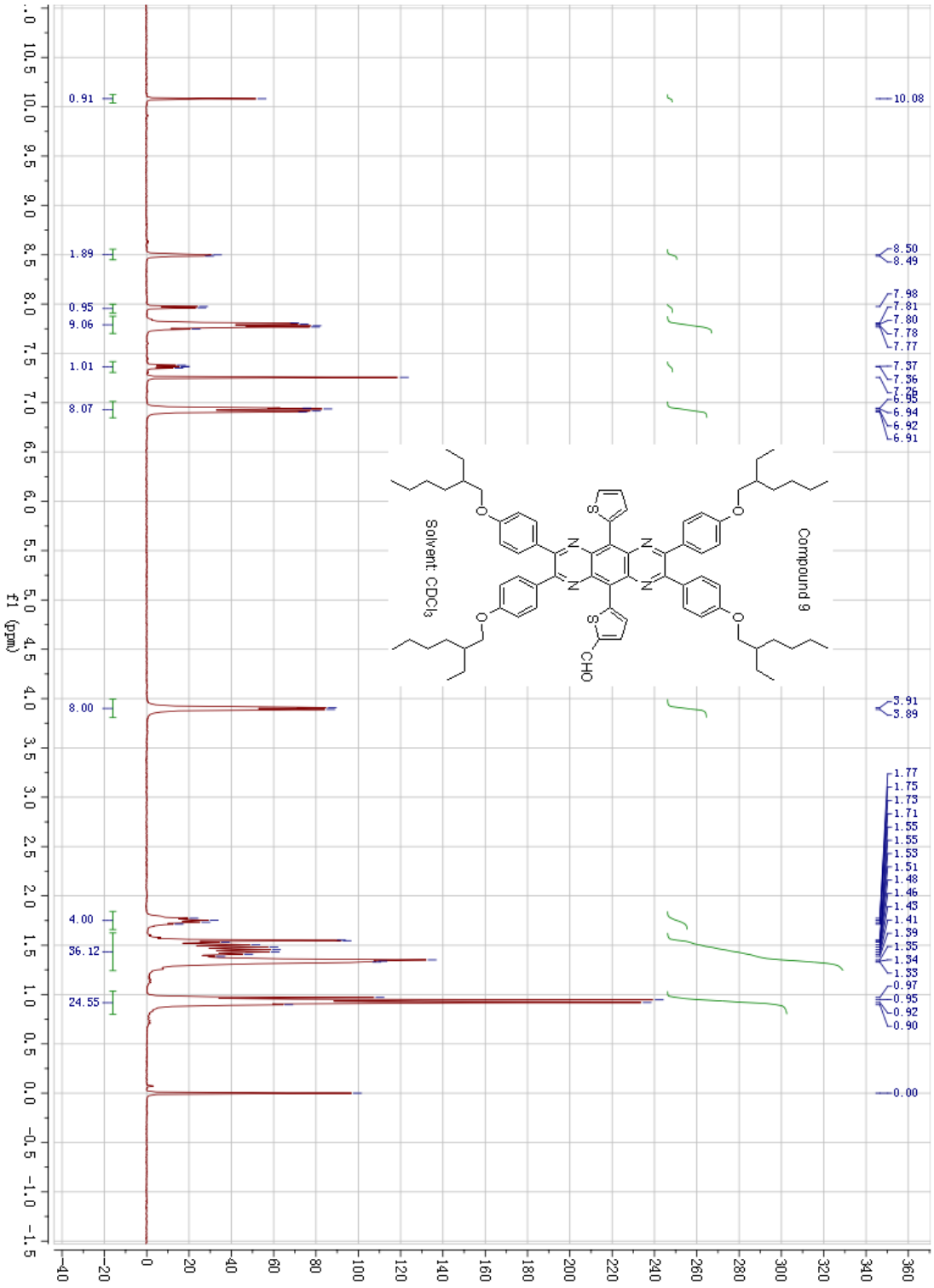
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7.80
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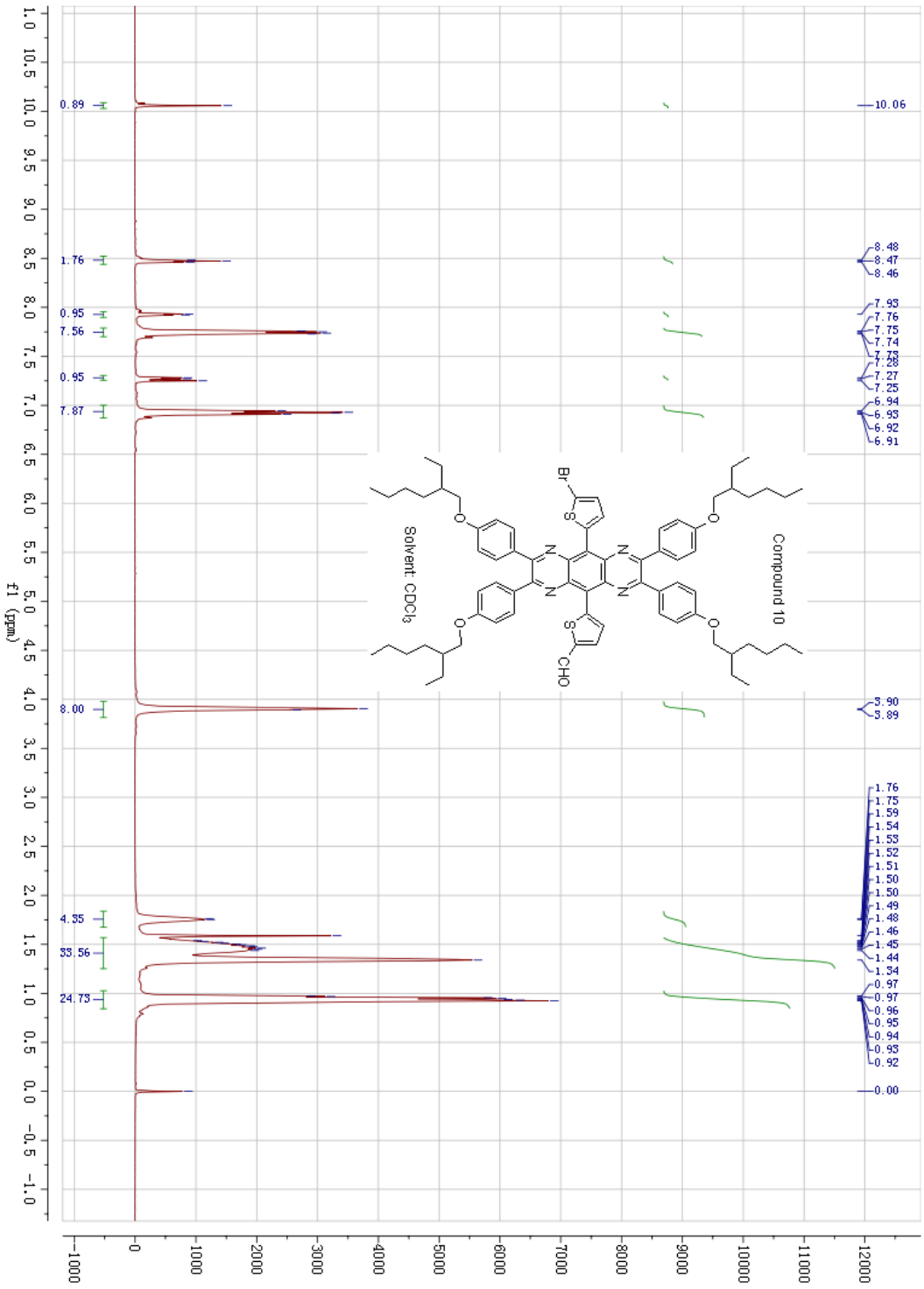
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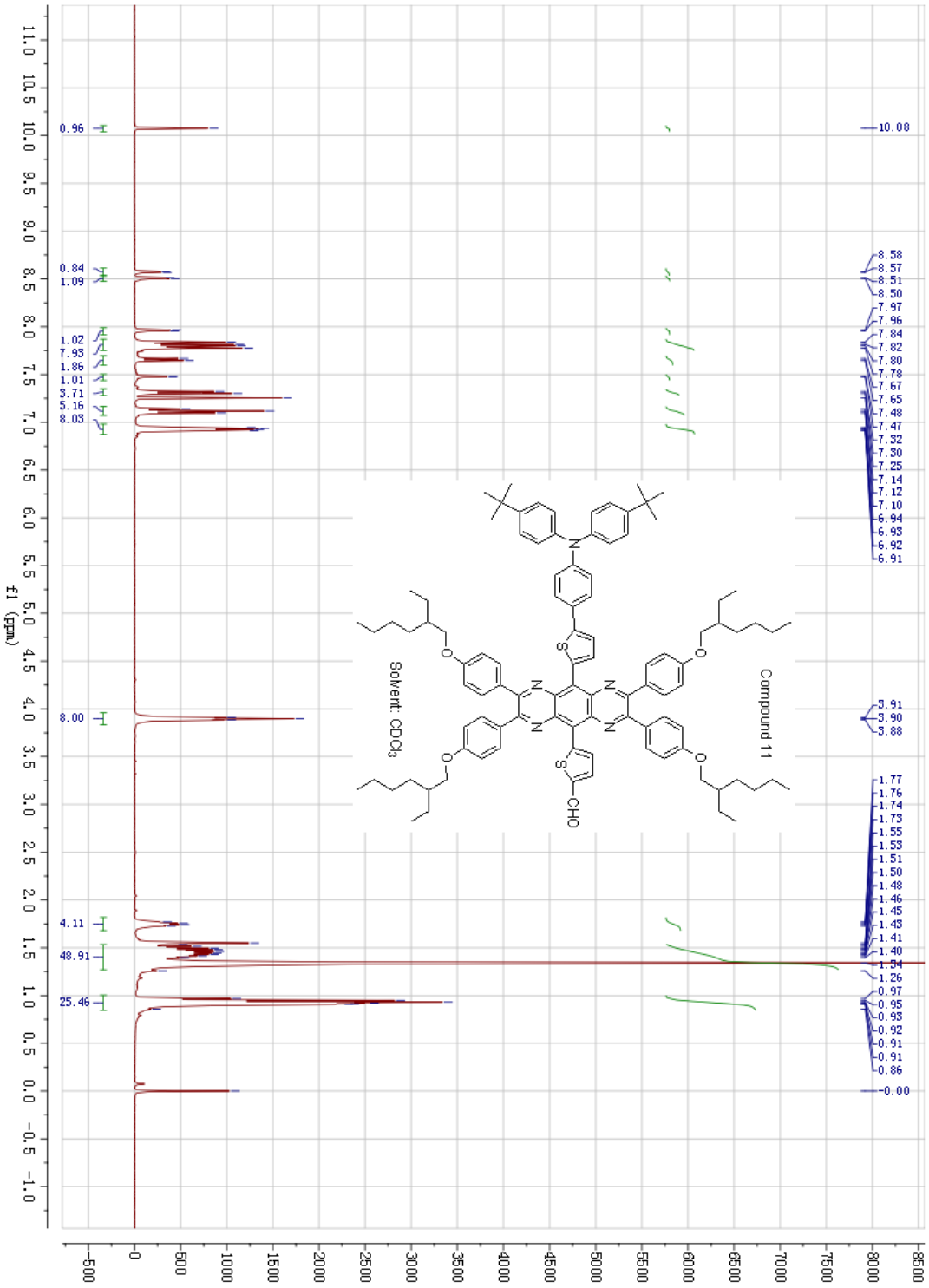
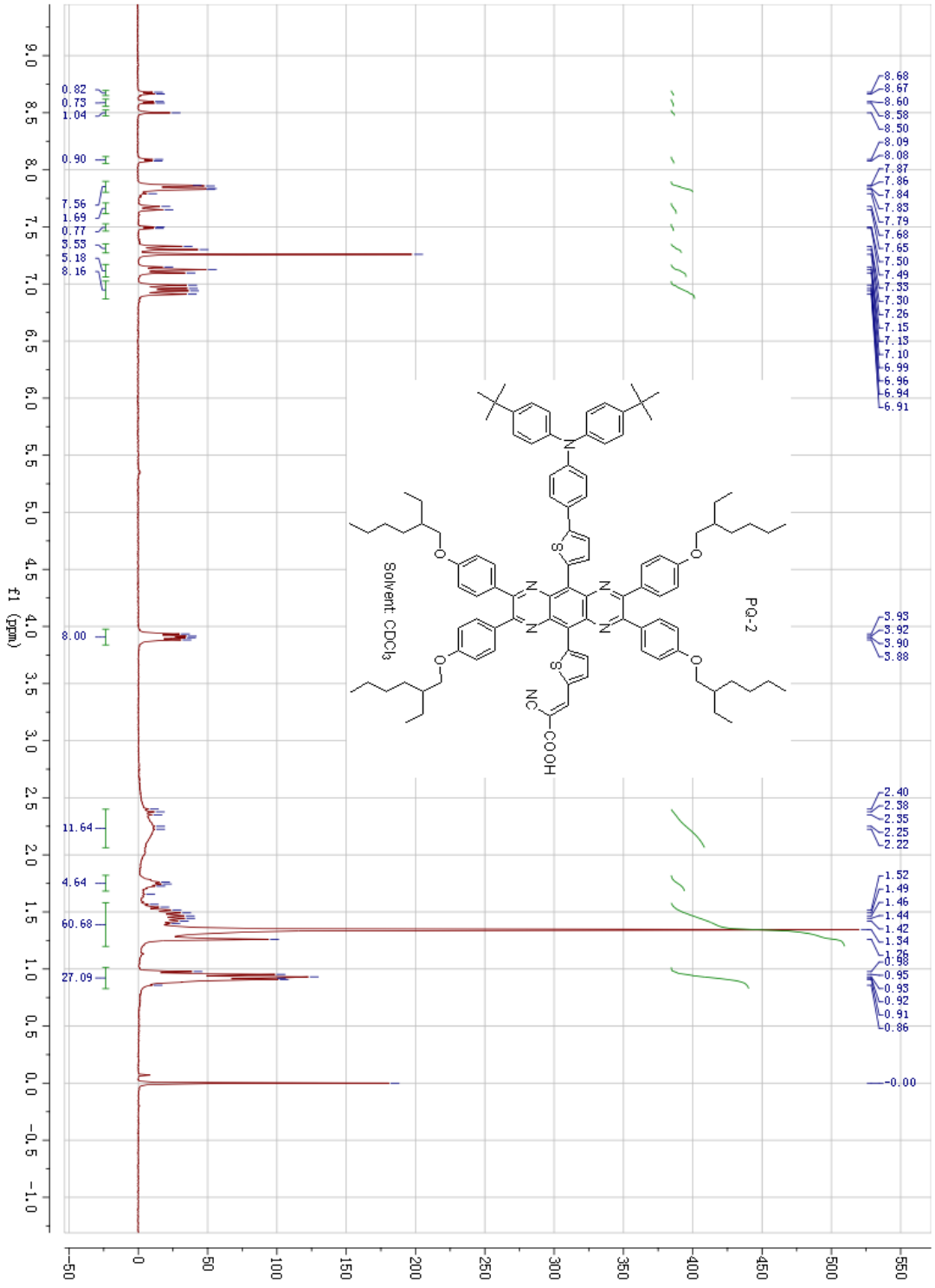
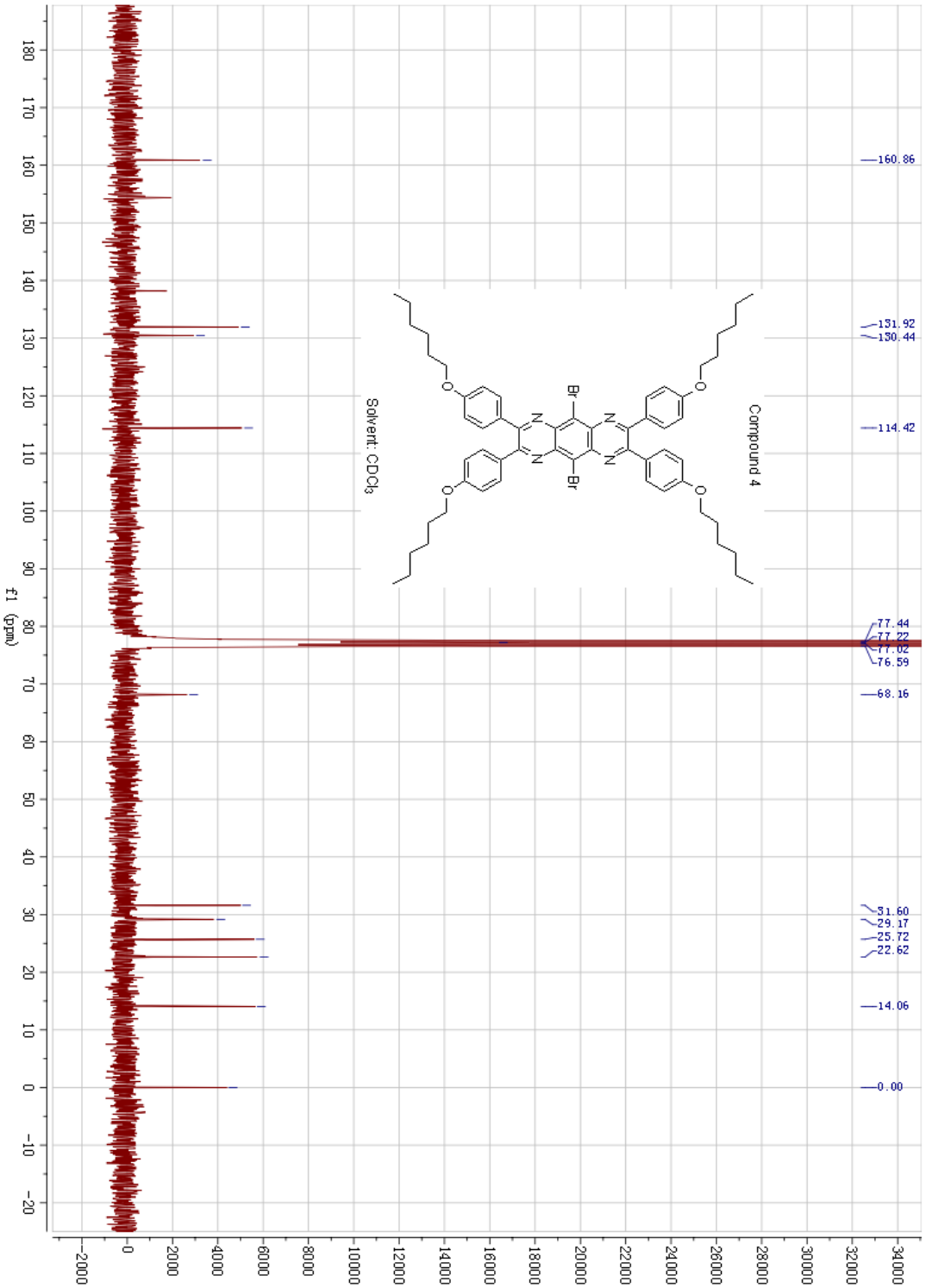
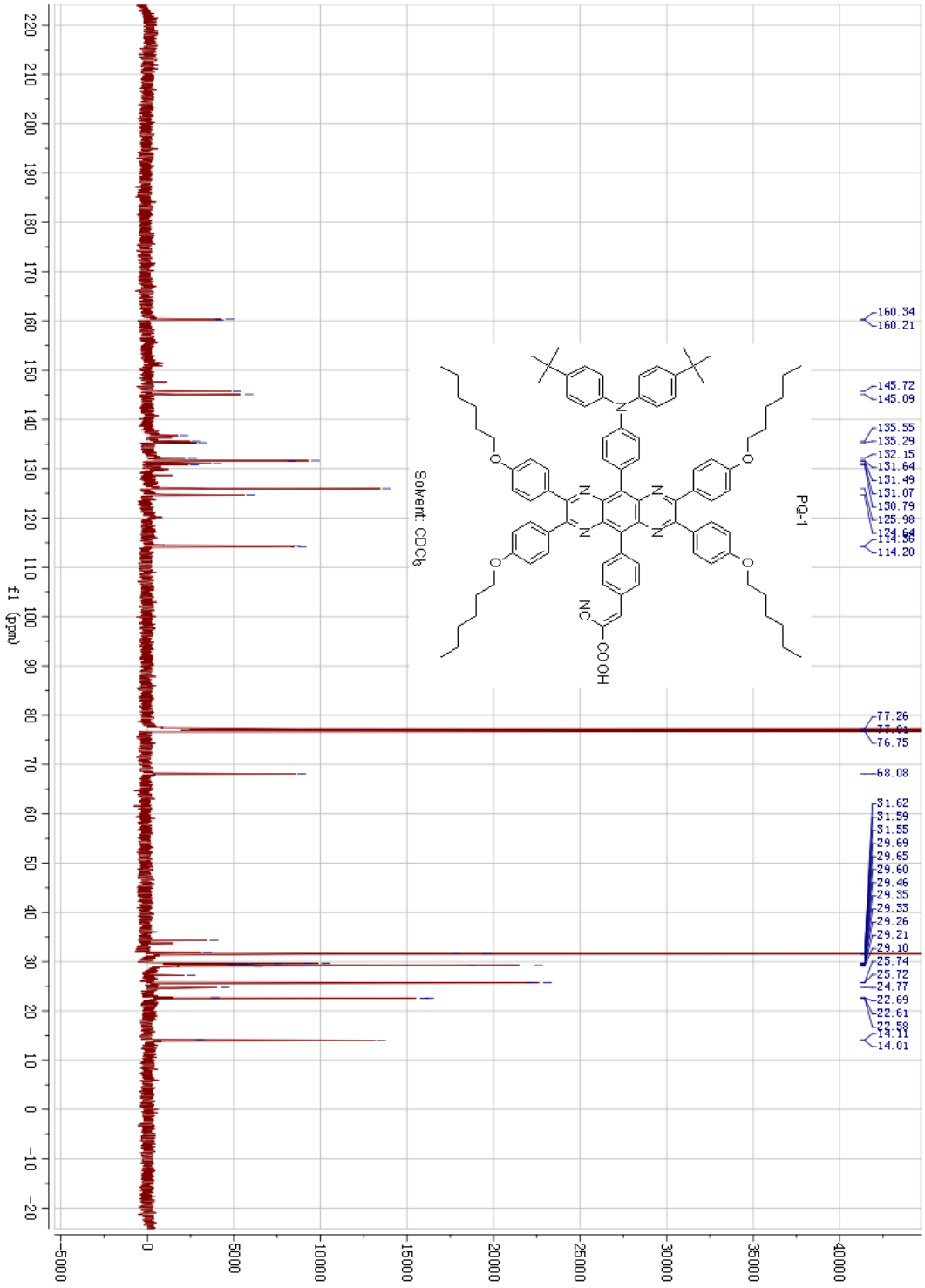
1.76
0.95
7.56
0.95
7.87
8.00
4.35
33.56
24.73
10.06
8.48
8.47
8.46
7.93
7.76
7.75
7.74
7.73
7.28
7.27
7.25
6.94
6.93
6.92
6.91
3.90
3.89
1.76
1.75
1.59
1.54
1.53
1.52
1.51
1.50
1.50
1.49
1.48
1.46
1.45
1.44
1.34
0.97
0.97
0.96
0.95
0.94
0.93
0.92
0.00

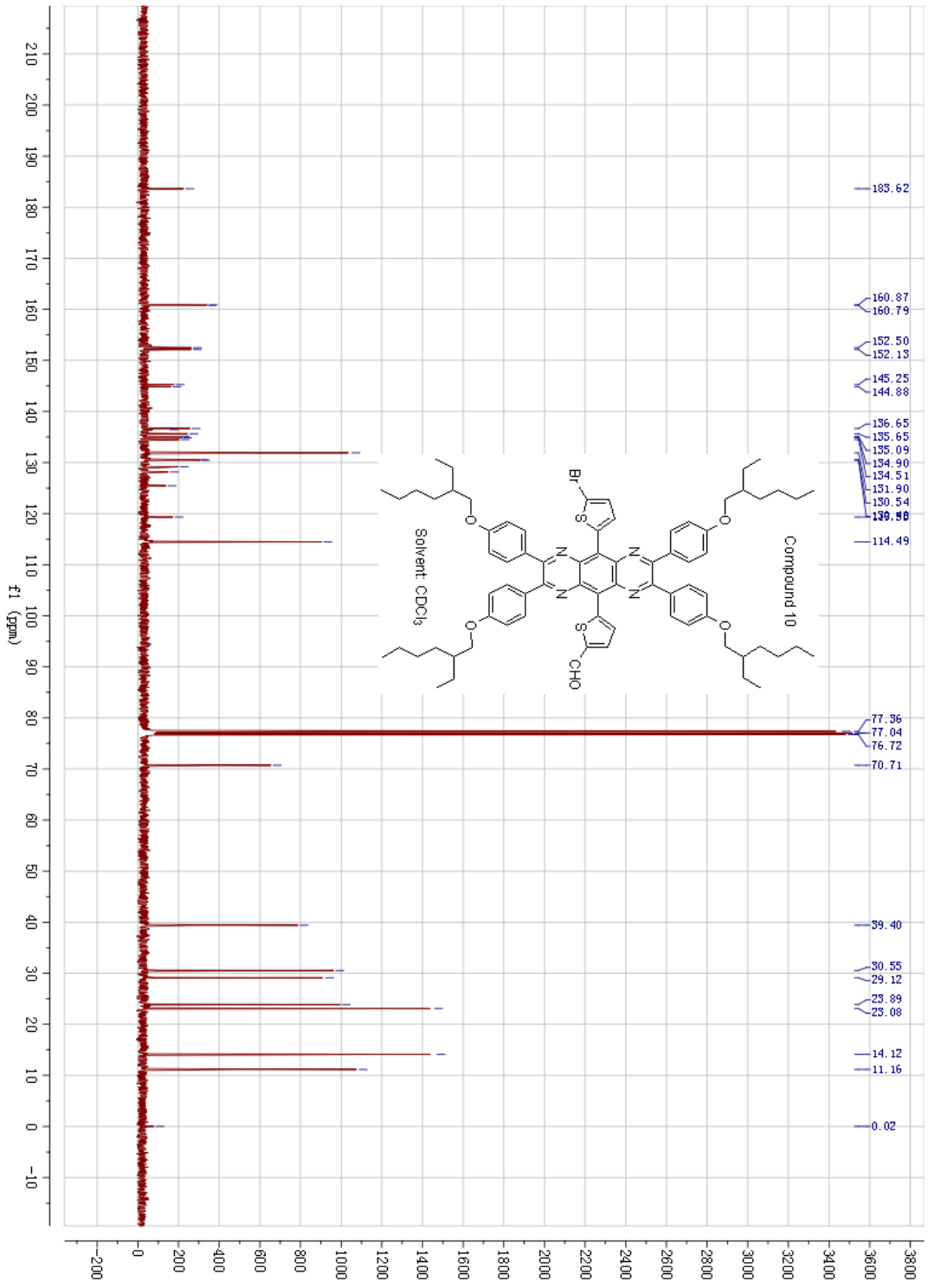

Solvent: CDCl3
Compound 11
f1 (ppm)

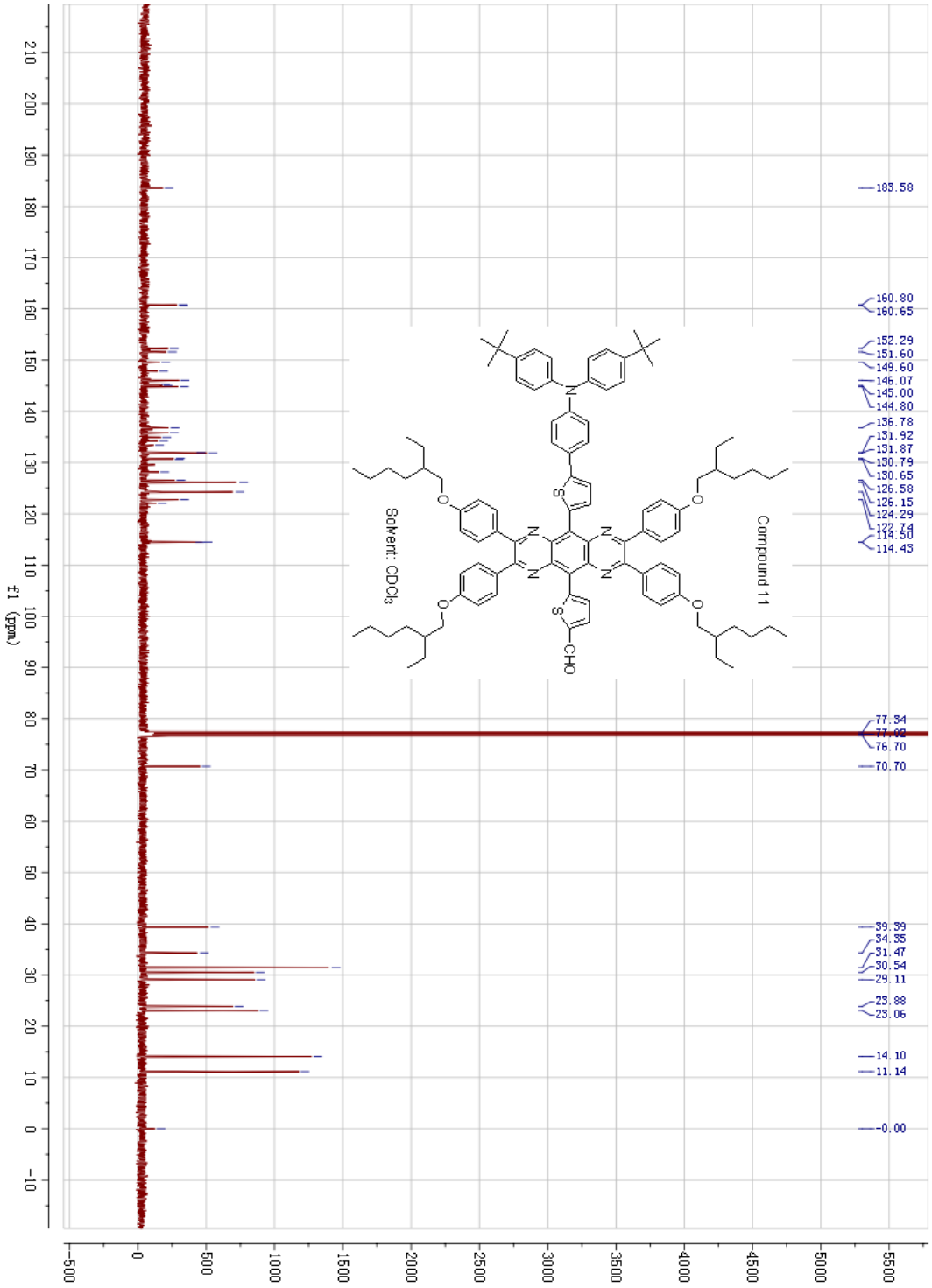

f1 (ppm)
Solvent: CDCl3
PQ-2
NC
COOH

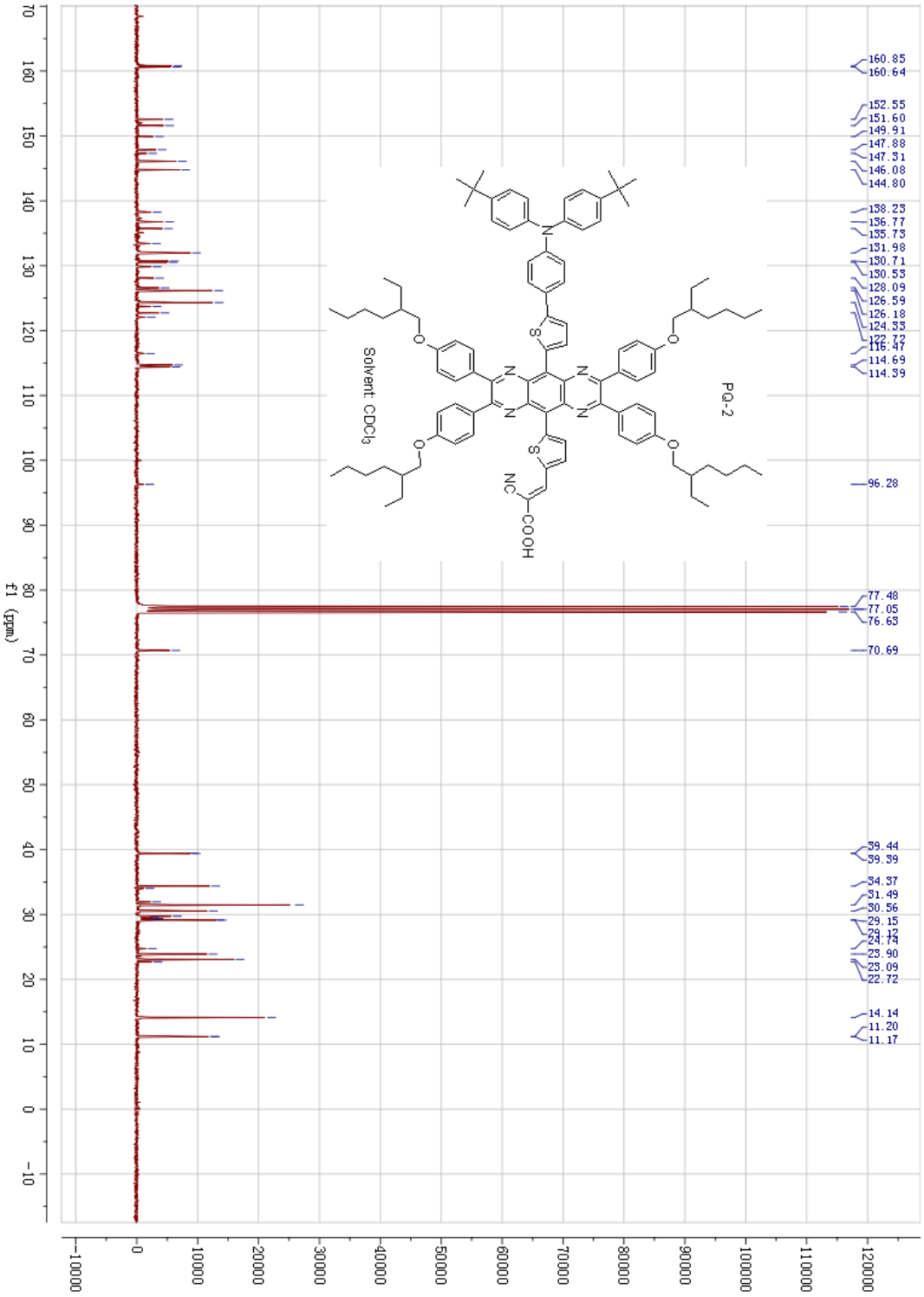
^{13}C NMR spectra of the compounds




f1 (ppm)
Solvent: CDCl3
PQ-1
160.34
160.21
145.72
145.09
135.55
135.29
132.15
131.64
131.49
131.07
130.79
125.98
114.20
77.26
76.75
68.08
31.62
31.59
31.55
29.69
29.65
29.60
29.46
29.35
29.33
29.26
29.21
29.10
25.74
25.72
24.77
22.69
22.61
22.58
14.11
14.01


f1 (ppm)
183.62
160.87
160.79
152.50
152.13
145.25
144.88
136.65
135.65
135.09
134.90
134.51
131.90
130.54
114.49
77.36
77.04
76.72
70.71
39.40
30.55
29.12
25.89
25.08
14.12
11.16
0.02
Solvent: CDCl3
Compound 10
Br
S
N
O
CHO


183.58
160.80
160.65
152.29
151.60
149.60
146.07
145.00
144.80
136.78
131.92
131.87
130.79
130.65
126.58
126.15
124.29
122.74
114.43
77.34
77.02
76.70
70.70
39.39
34.35
31.47
30.54
29.11
23.88
23.06
14.10
11.14
0.00
Solvent: CDCl3
Compound 11
CHO
f1 (ppm)


160.85
160.64
152.55
151.60
149.91
147.88
147.31
146.08
144.80
138.23
136.77
135.73
131.98
130.71
130.53
128.09
126.59
126.18
124.33
122.72
116.47
114.69
114.39
96.28
77.48
77.05
76.63
70.69
39.44
39.39
34.37
31.49
30.56
29.15
24.74
23.90
23.09
22.72
14.14
11.20
11.17
Solvent: CDCl3
PQ-2
NC
COOH
f1 (ppm)