

Fluorine-free Blue-green Emitters for Light-Emitting Electrochemical Cells.

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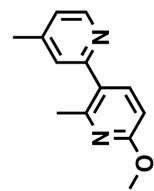
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SUPPORTING INFORMATION

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TXR059



NAME 08-22-Baranoff-18
EXPNO 10
PROCNO 1
Date 20130822
Time 14.21
INSTRUM spect
PROBID 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6008.615 Hz
FIDRES 0.183399 Hz
AQ 2.726447 sec
RG 203
DW 83.200 usc
DE 12.89 usc
TE 280.9 K
D1 1.000000 sec
TDO 1
===== CHANNEL f1 ======
NUC1 1H
P1 12.80 usec
PL 1.00 dB
P1W 9.5725906 W
SF01 300.1318534 MHz
SF 32783
SF 300.130259 MHz
WDW EM
SSB 0
LB 0.30 Hz
QSB 0
PC 1.00

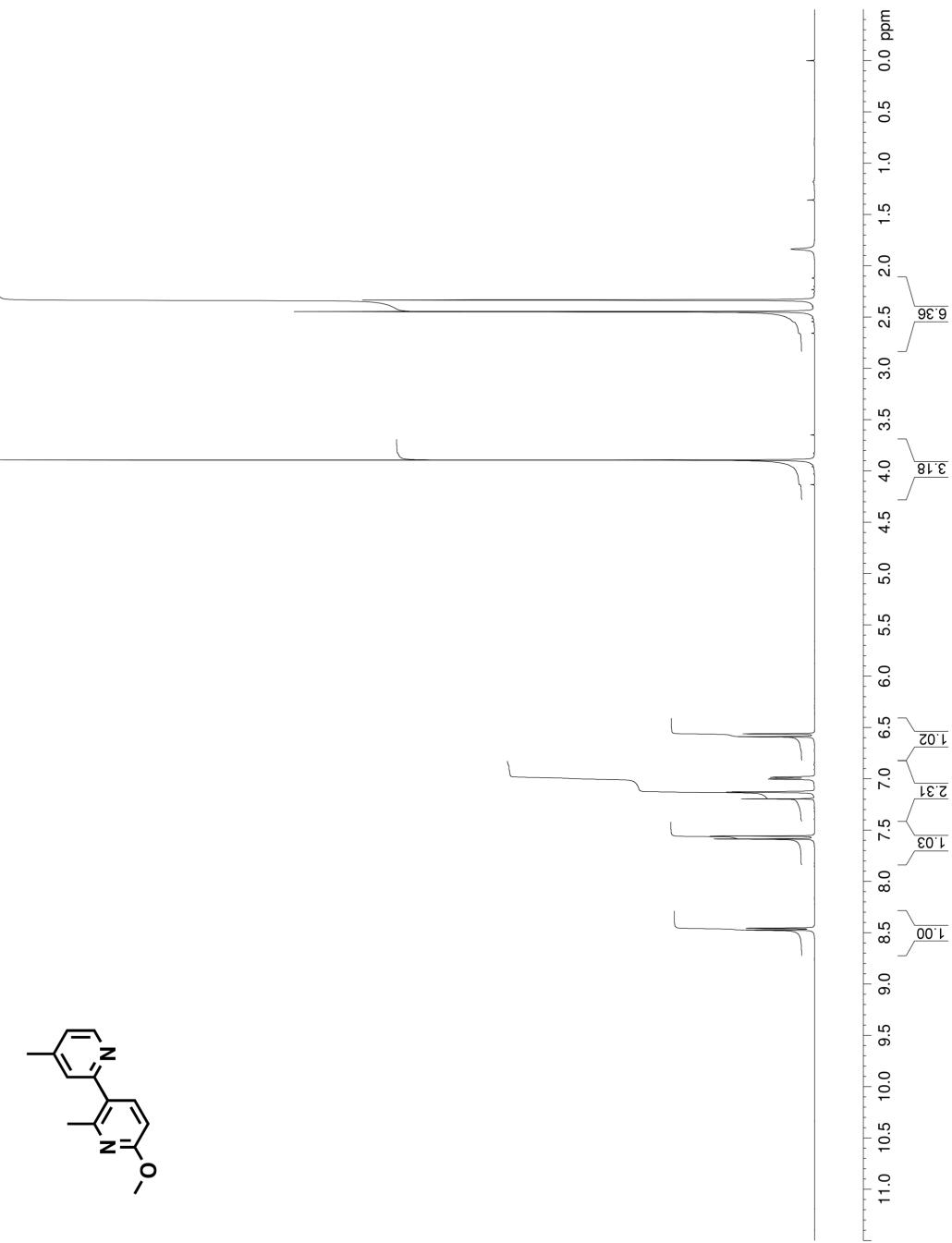


Figure S1. ^1H NMR of **L1** in CDCl_3 .

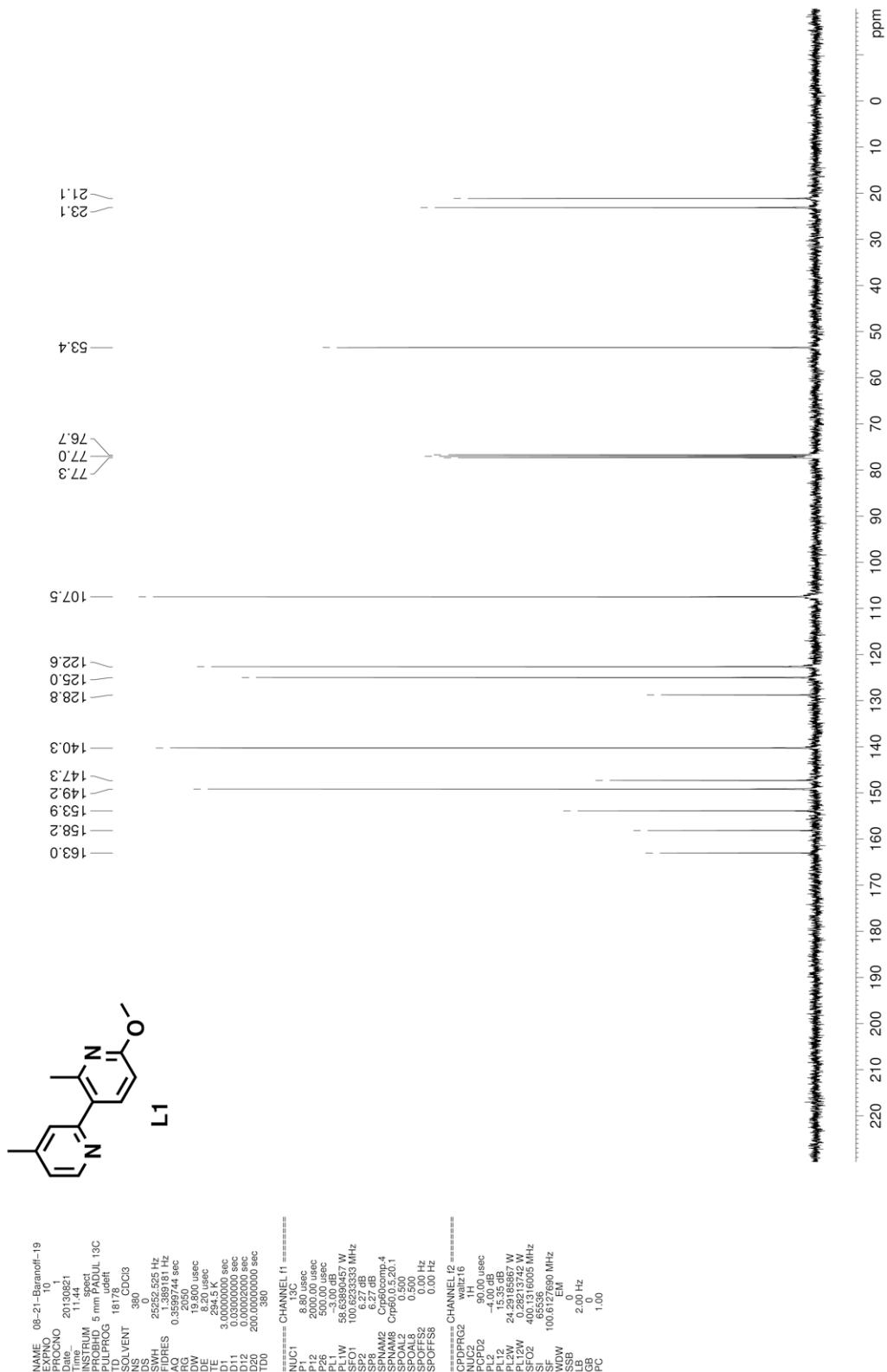
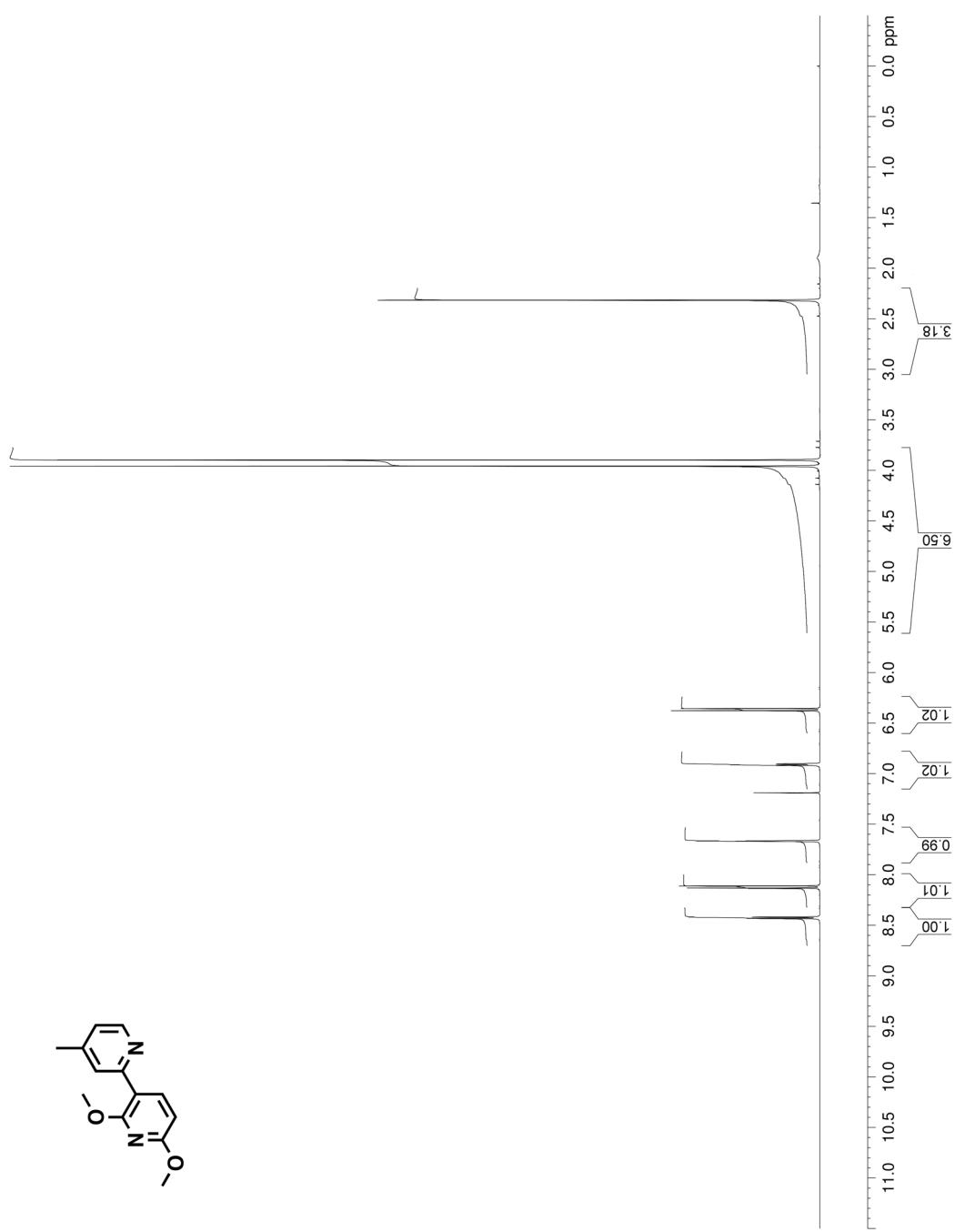


Figure S2. ¹³C NMR of **L1** in CDCl₃.

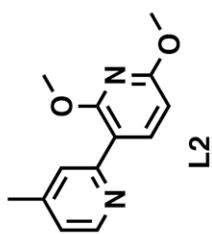


```

NAME 06-12-Baranoff-11
EXPNO 10
PROCNO 1
Date 20130612
Time 21:11
INSTRUM spect
PROBID 5 mm PADUL-13C
PULPROG
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250987 Hz
AQ 1.9923444 sec
RG 256
DW 60.800 usec
DE 16.98 usec
TE 294.1 K
D1 1.5000000 sec
TDO 1
===== CHANNEL_11 =====
NUC1      1H
P1        9.50 usec
PL1       -4.00 dB
PL1W      24.2515867 W
SF01      400.1324710 MHz
SF        32768
SF      400.1300380 MHz
WDW
SSB      0
EM
LB      0.30 Hz
GB      1.00
PC

```

Figure S3. ¹H NMR of L2 in CDCl₃.



```

NAME: 06-12-Baranoff-3
EXPNO: 10
PROCNO: 1
Date: 20130612
INSTRUM: 13C
PROBHD: 5 mm P/DUL_13C
PULPROG: udelt
TD: 18178
SOLVENT: CDCl3
DS: 0
SWH: 2552.525 Hz
FIDRES: 1.389181 Hz
AQ: 0.399744 sec
RG: 20.00
DW: 10.00 usec
DE: 8.20 usec
TE: 294.6 K
D1: 3.000000 sec
D1: 0.0300000 sec
D1: 0.0100000 sec
D2: 200.000000 sec
TD0: 380
=====
===== CHANNEL 11 =====
NUC1: 13C
P1: 8.80 usec
P12: 200.00 usec
P26: 500.00 usec
PL1: -3.00 dB
PL1W: 58.6398457 W
SP1: 100.000003 MHz
SP2: 6.277 GB
SP8: 6.277 GB
SPNAM2: Crp80comp4
SPNAM3: Crp60.520.1
SPDQ1: 0.500
SPDQ2: 0.500
SPOFF1: 0.00 Hz
SPOFF2: 0.00 Hz
SPOFF8: 0.00 Hz
=====
===== CHANNEL 12 =====
NUC1: 1H
PCPD2: 90.00 usec
PL2: -4.00 dB
PL12: 15.55 dB
PL1W: 24.5848957 W
PL1W: 400.01516005 MHz
SFQ2: 65536
SF: 100.0127690 MHz
WOW: 0
SB: 200.0 Hz
GB: 0
PC: 1.00

```

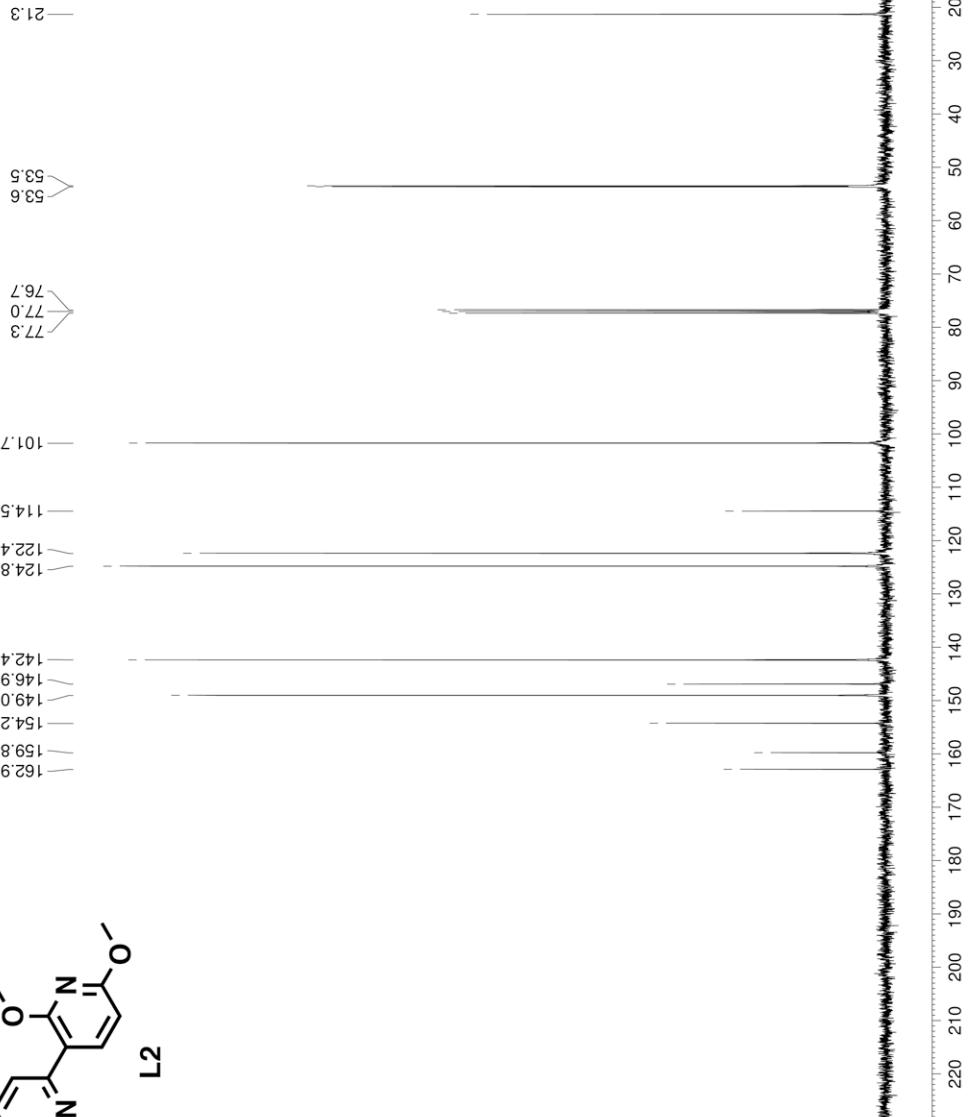


Figure S4. ^{13}C NMR of L2 in CDCl_3 .

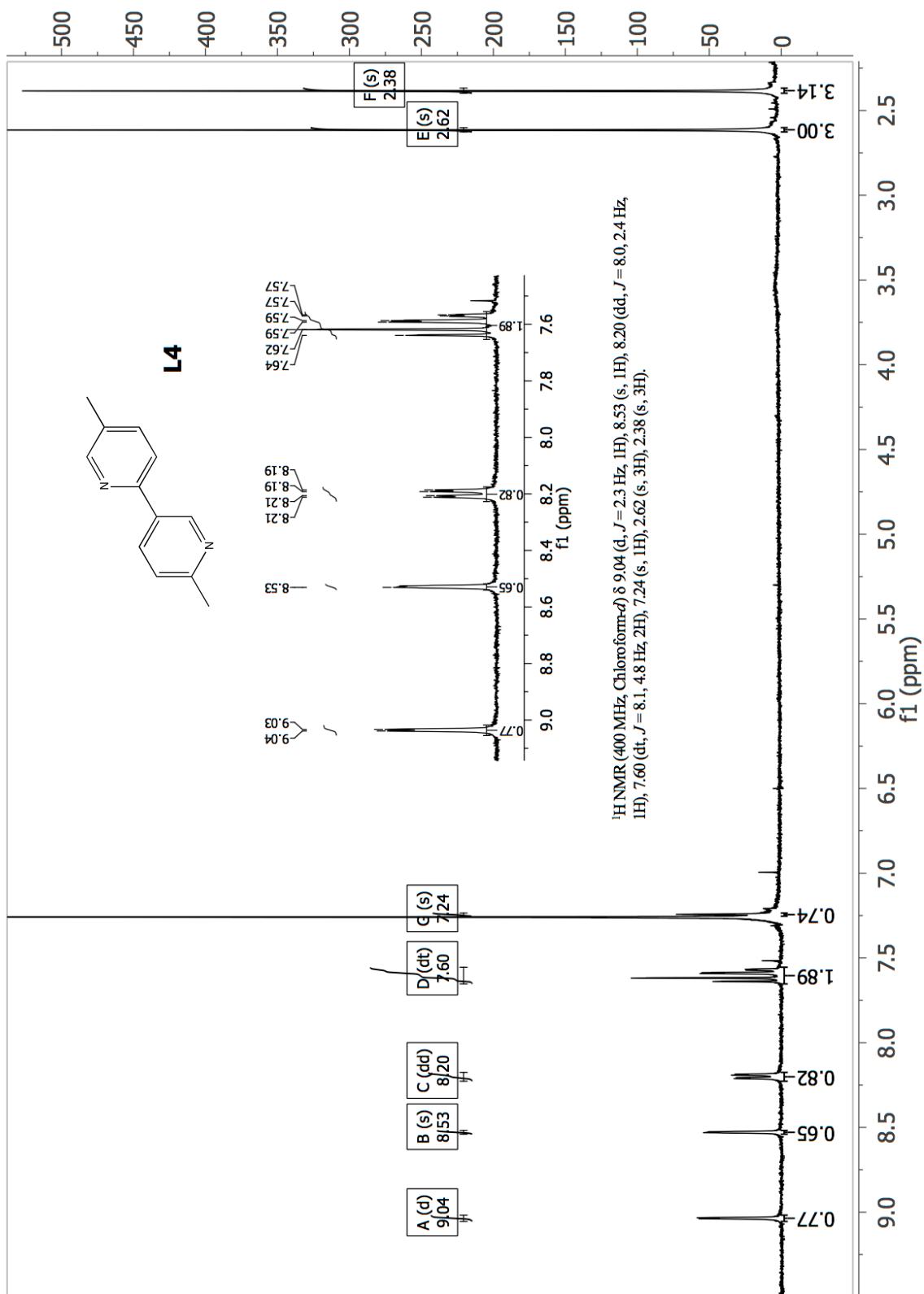


Figure S5. ¹H NMR of L4 in CDCl₃.

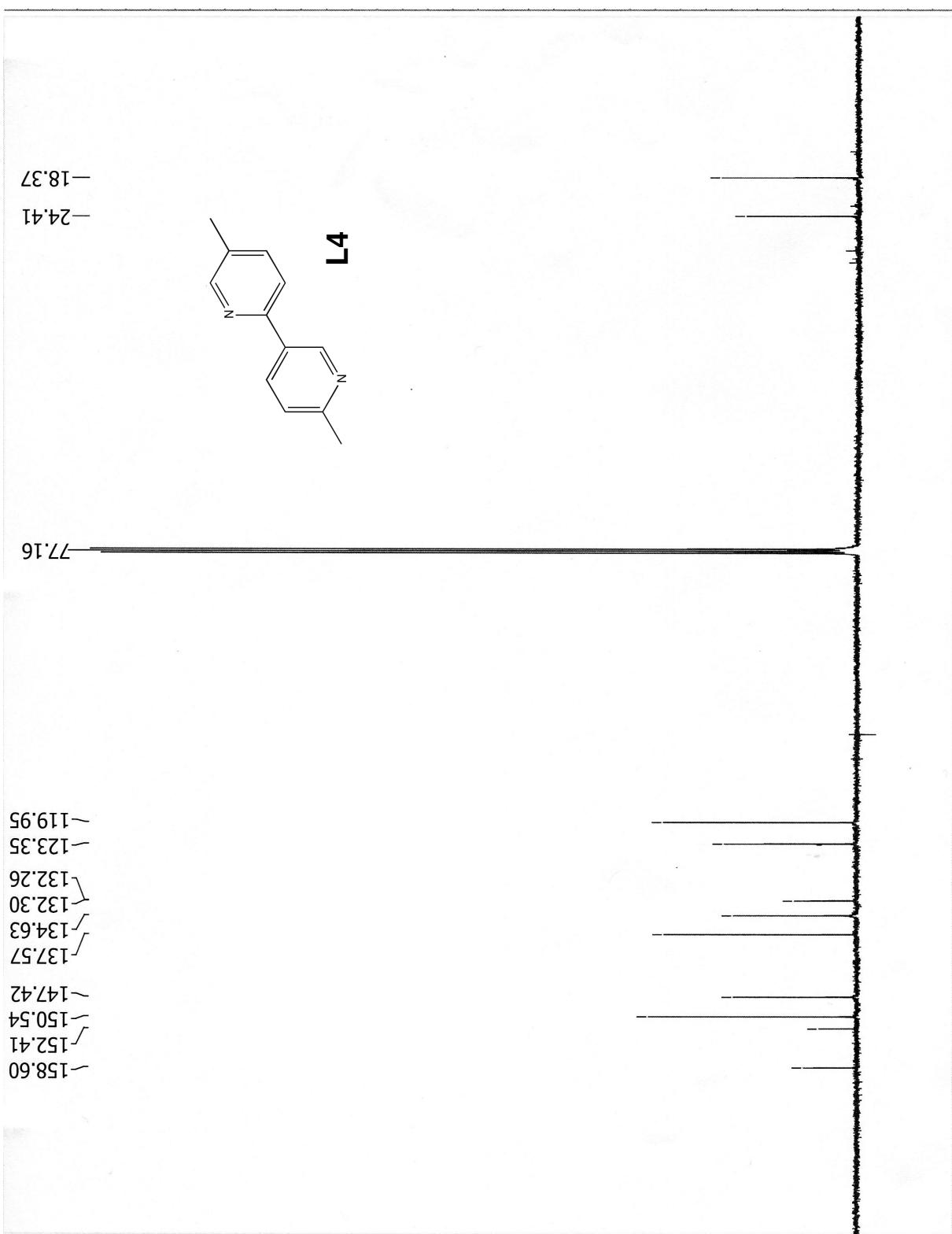


Figure S6. ^{13}C NMR of **L4** in CDCl_3 .

EB323

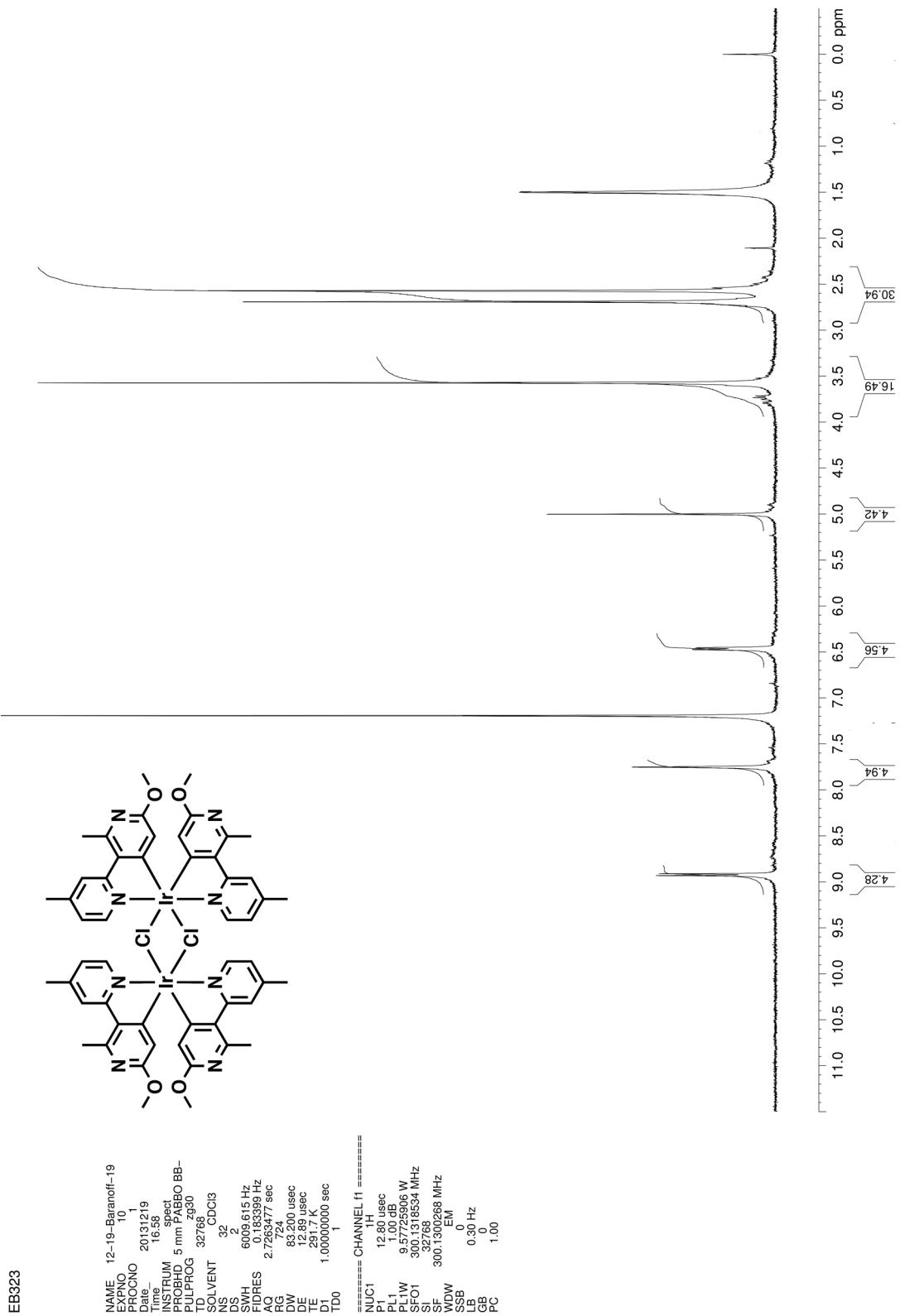


Figure S7. ¹H NMR of **D1** in CDCl₃.

```

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EXPNO 1
PROCNO 1
Date 20131219
Time 17:04
INSTRUM spect
PROBID 5 mm PABBO BB-
PULPROG
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.083399 Hz
AQ 2.763477 sec
RG 322
DW 83.200 usec
DE 12.89 usec
TE 291.6 K
D1 1.0000000 sec
TDO 1

```

```

===== CHANNEL f1 =====
NUC1 1H
P1 12.80 usec
PL1 1.00 dB
PL1W 9.5/259.06 W
SF01 300.1318834 MHz
SF 327.68 MHz
WDW
SSB 0
EM
LB 0.30 Hz
GB 0
PC 1.00

```

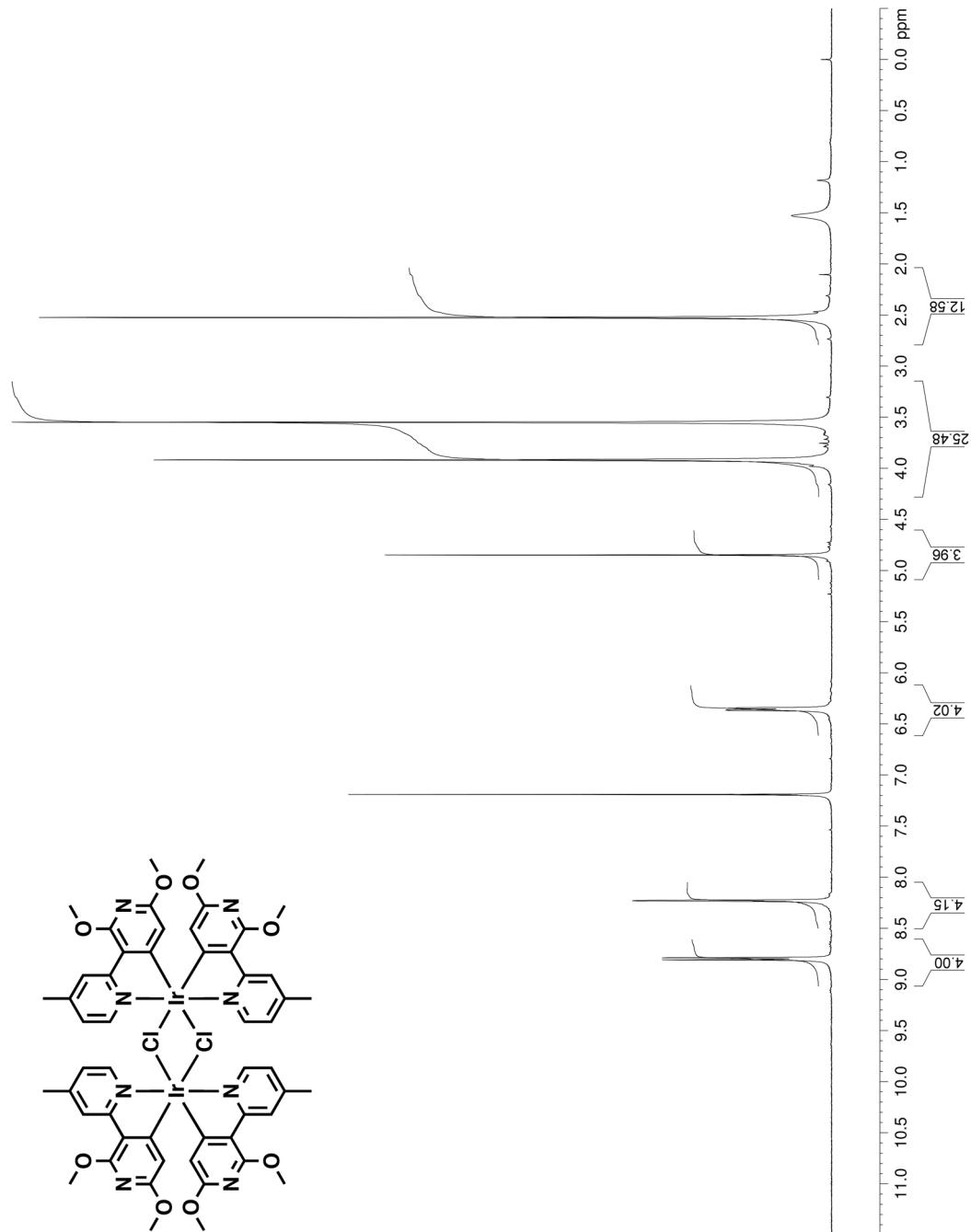
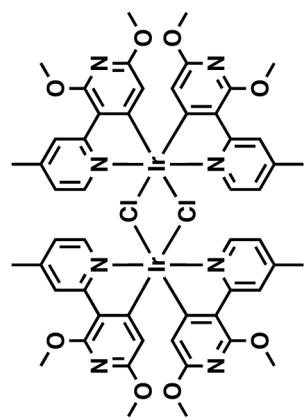


Figure S8. ^1H NMR of **D2** in CDCl_3 .

Complex 1

^1H NMR (700 MHz , Acetonitrile- d_3) δ 8.47 (d, $J = 1.8 \text{ Hz}$, 1H), 7.97 (s, 1H), 7.85 (d, $J = 5.8 \text{ Hz}$, 1H), 7.49 (dd, $J = 5.9, 1.9 \text{ Hz}$, 1H), 7.43 (d, $J = 6.0 \text{ Hz}$, 1H), 6.86 (dd, $J = 5.9, 0.9 \text{ Hz}$, 1H), 5.34 (s, 1H), 3.76 (s, 3H), 2.81 (s, 3H), 2.51 (s, 3H), 1.40 (s, 9H).

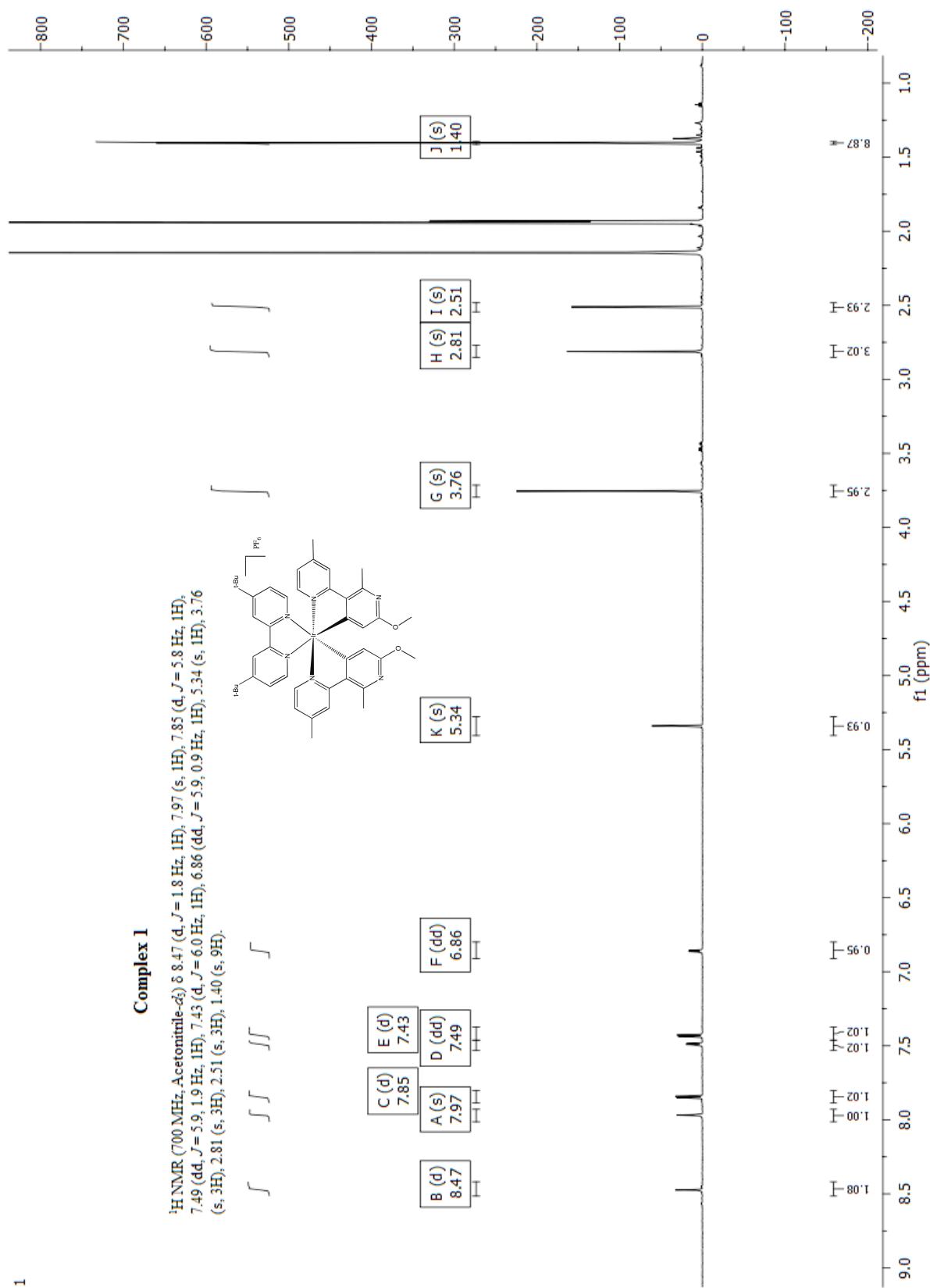


Figure S9. ^1H NMR of **Complex 1** in CD_3CN .

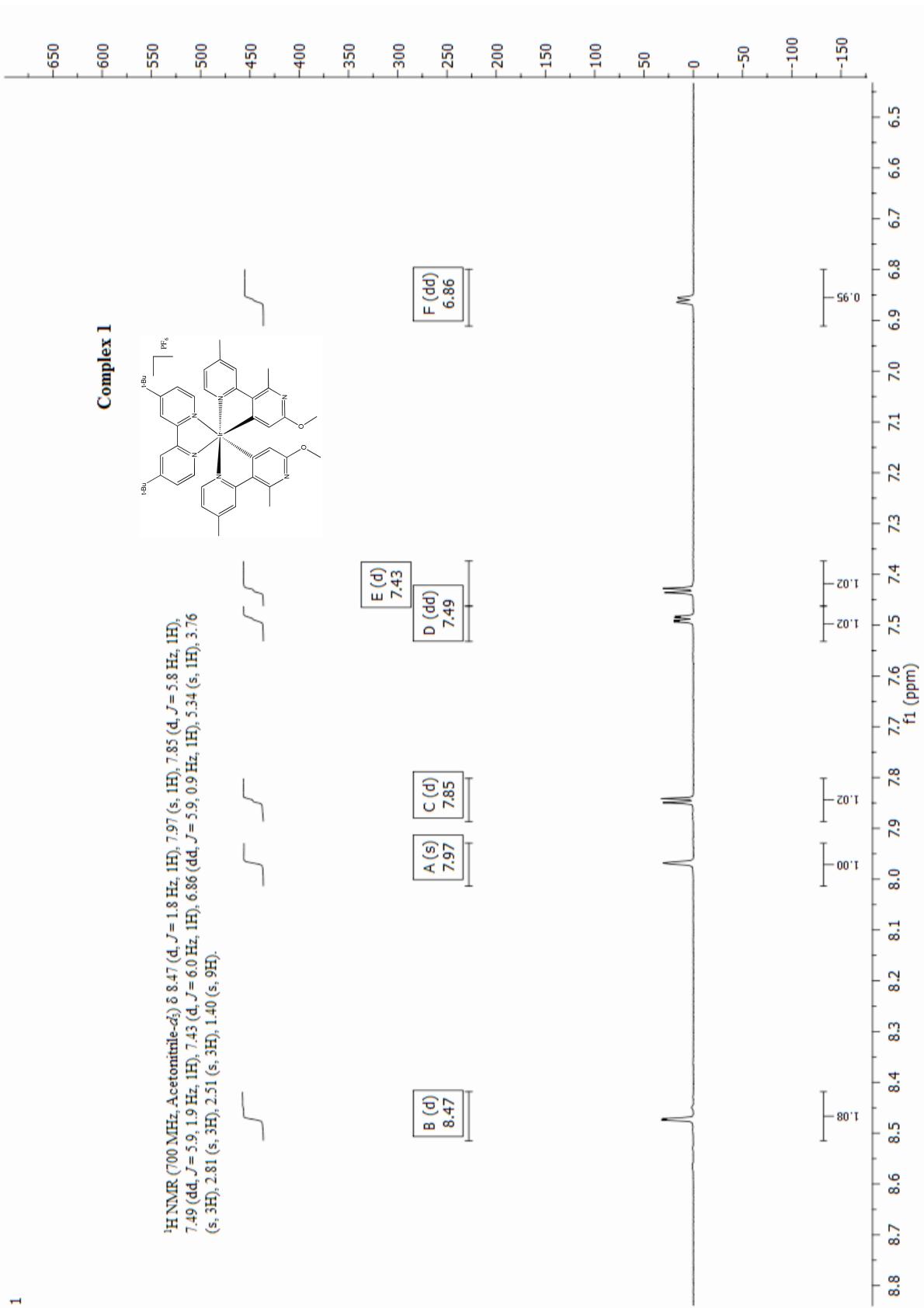


Figure S10. ¹H NMR of **Complex 1** (aromatic part) in CD_3CN .

1

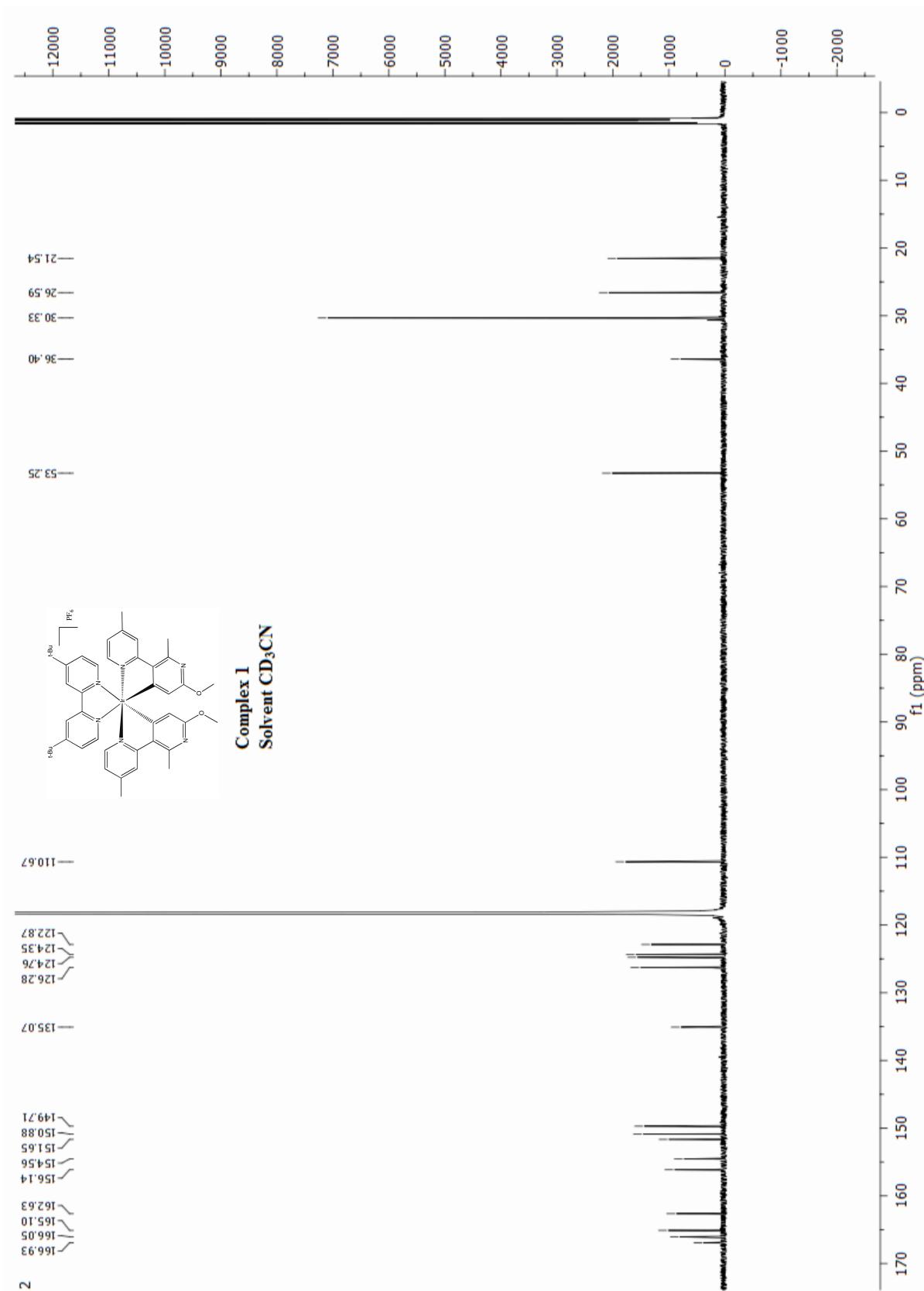


Figure S11. ^{13}C NMR of **Complex 1** in CD_3CN .

Complex 2

^1H NMR (700 MHz, Acetonitrile-d₃) δ 8.49 (d, J = 1.8 Hz, 1H), 8.40 (m, 1H), 7.95 (d, J = 5.9 Hz, 1H), 7.52 (dd, J = 5.9, 2.0 Hz, 1H), 7.34 (d, J = 6.0 Hz, 1H), 6.79 (dd, J = 6.1, 1.8 Hz, 1H), 5.16 (s, 1H), 4.10 (s, 3H), 3.81 (s, 3H), 2.49 (s, 3H), 1.43 (s, 9H).

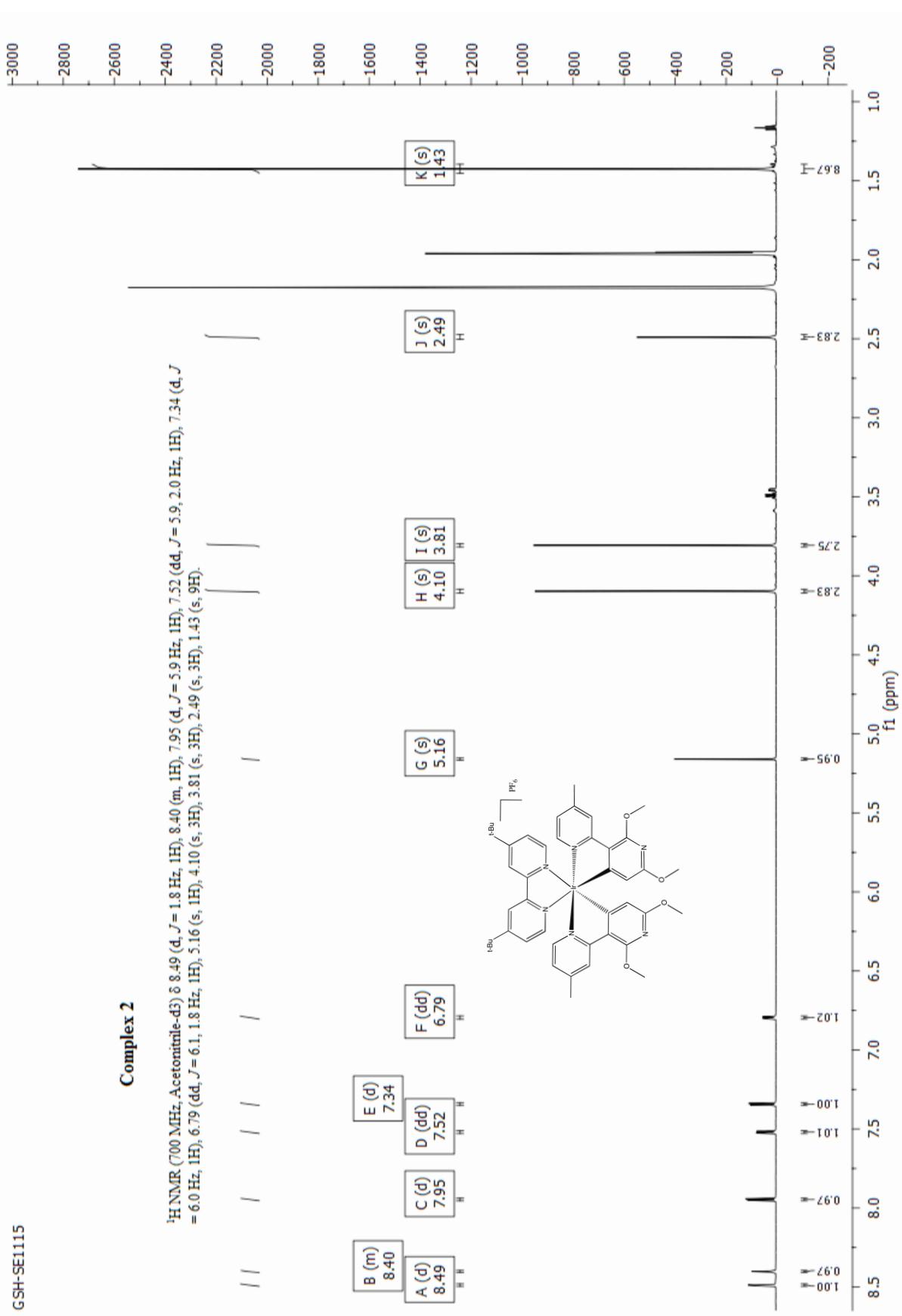


Figure S12. ^1H NMR of Complex 2 in CD_3CN .

Complex 2

¹H NMR (γ 00 MHz, Acetonitrile-d3) δ 8.49 (d, J = 1.8 Hz, 1H), 8.40 (m, 1H), 7.95 (d, J = 5.9 Hz, 1H), 7.52 (dd, J = 5.9, 2.0 Hz, 1H), 7.34 (d, J = 6.0 Hz, 1H), 6.79 (dd, J = 6.1, 1.8 Hz, 1H), 5.16 (s, 1H), 4.10 (s, 3H), 3.81 (s, 3H), 2.49 (s, 3H), 1.43 (s, 9H).

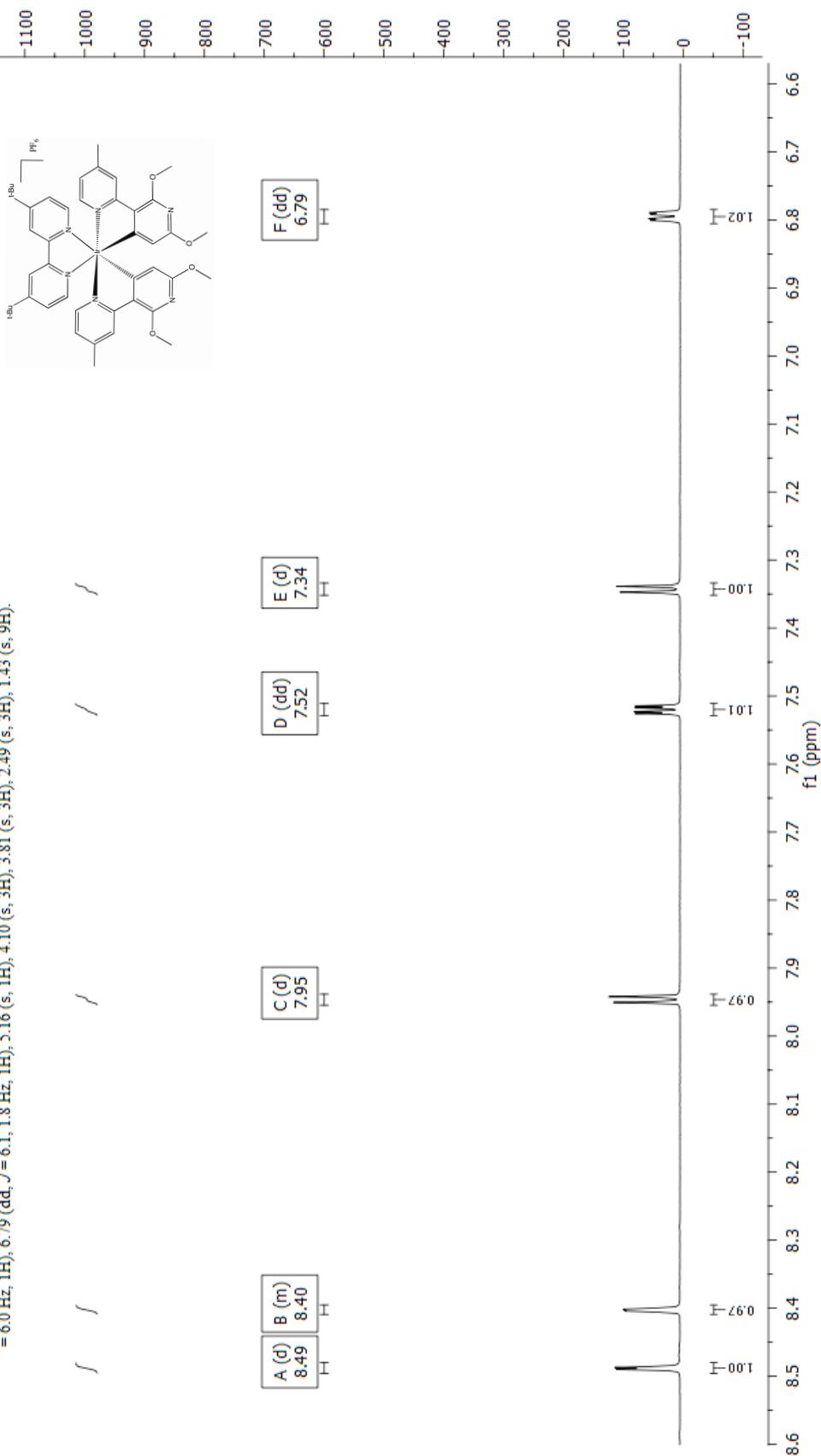
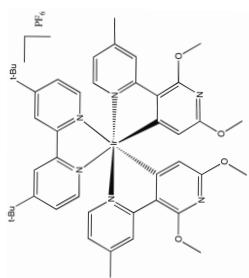


Figure S13. ¹H NMR of **Complex 2** (aromatic part) in CD₃CN.

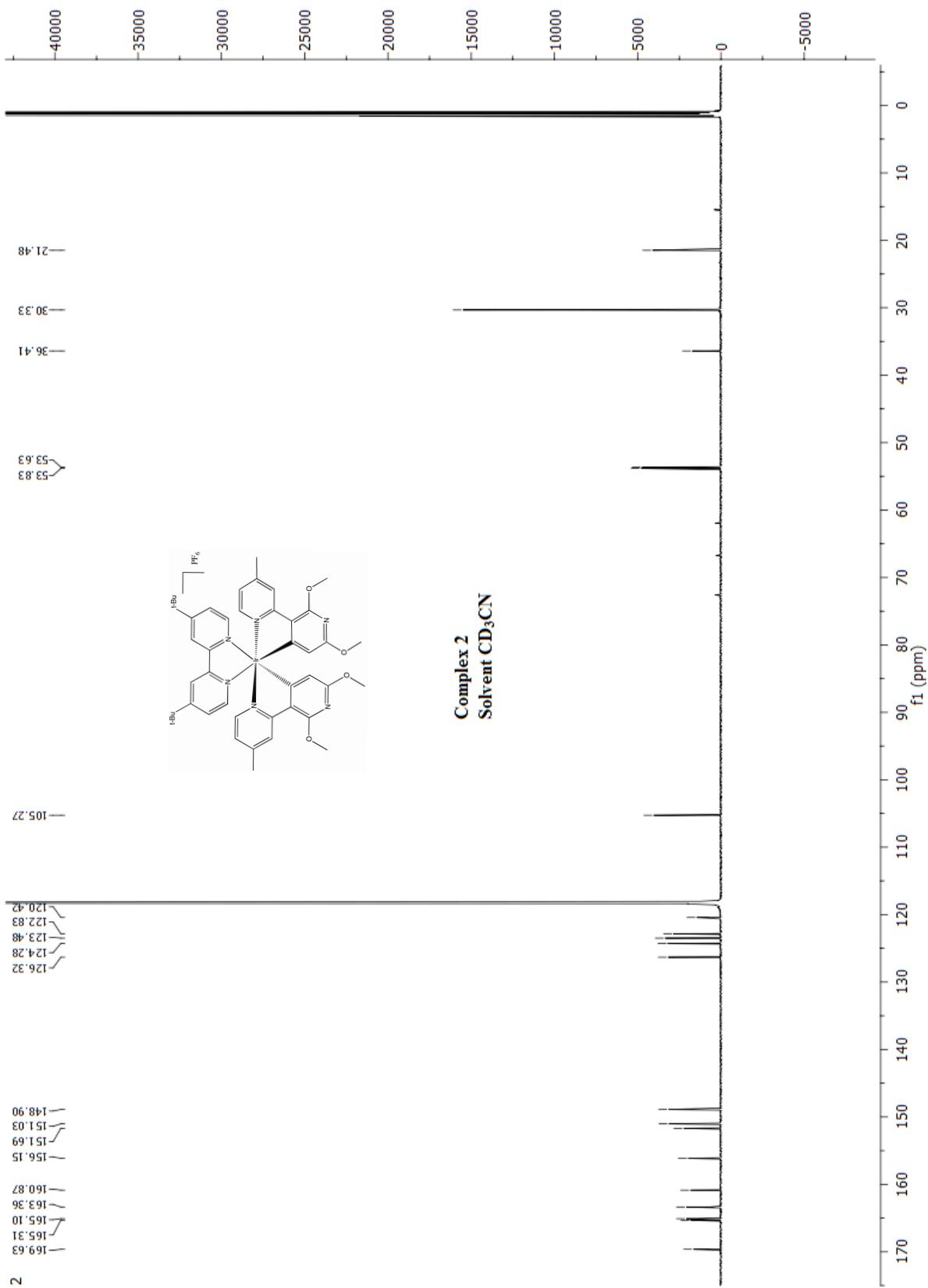


Figure S14. ^{13}C NMR of **Complex 2** in CD_3CN .

Complex 3

^1H NMR (700 MHz, Acetonitrile- d_3) δ 8.54 (d, J = 8.4 Hz, 1H), 8.48 (d, J = 1.6 Hz, 1H), 7.94 (d, J = 5.9 Hz, 1H), 7.80 (m, 1H), 7.51 (m, 2H), 6.92 (m, 1H), 5.12 (s, 1H), 4.07 (s, 3H), 3.79 (s, 3H), 1.41 (s, 9H).

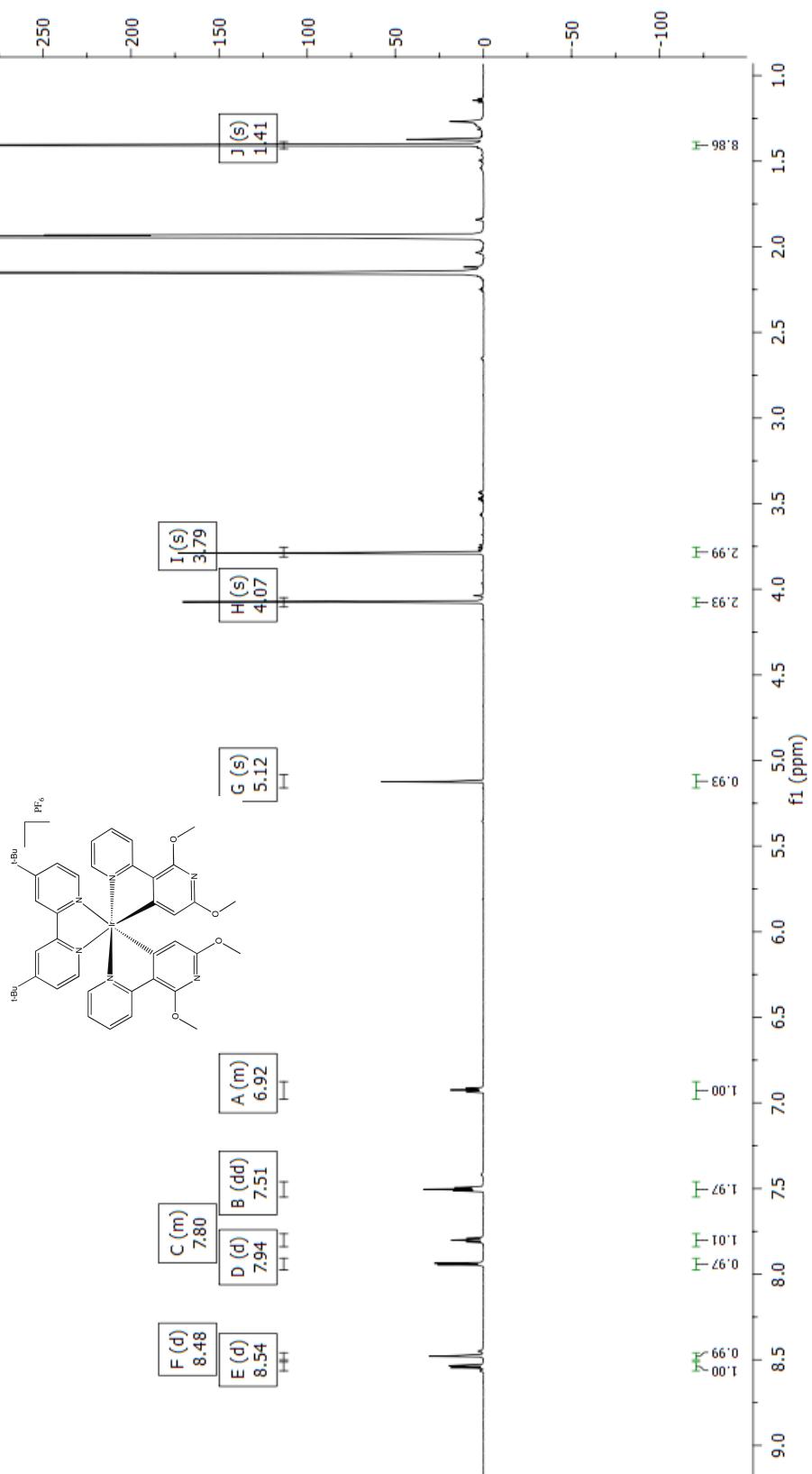


Figure S15. ^1H NMR of Complex 3 in CD_3CN .

Complex 3

^1H NMR (700 MHz, Acetonitrile- d_3) δ 8.54 (d, $J = 8.4$ Hz, 1H), 8.48 (d, $J = 1.6$ Hz, 1H), 7.94 (d, $J = 5.9$ Hz, 1H), 7.80 (m, 1H), 7.51 (m, 2H), 6.92 (m, 1H), 5.12 (s, 1H), 4.07 (s, 3H), 3.79 (s, 3H), 1.41 (s, 9H).

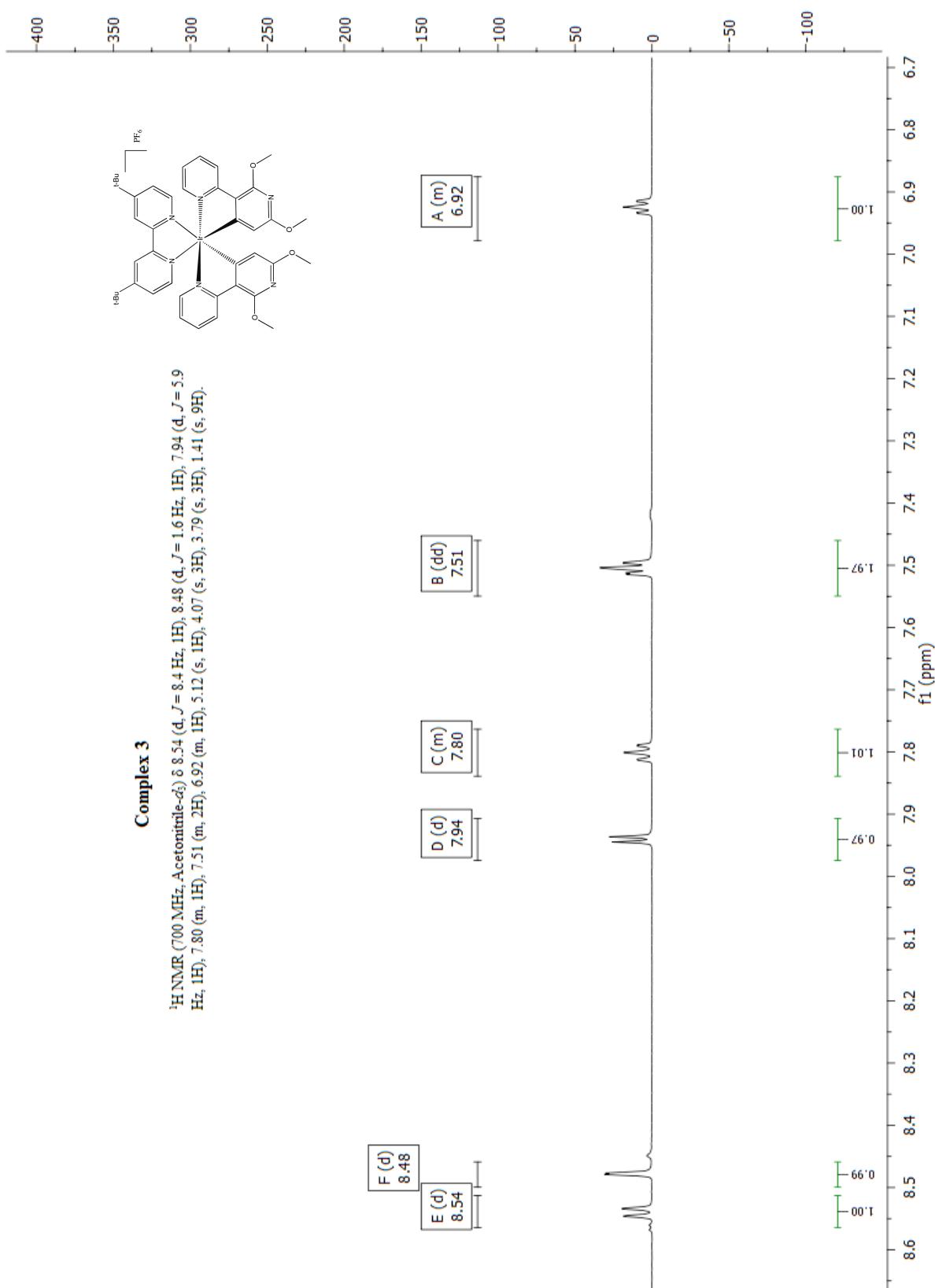
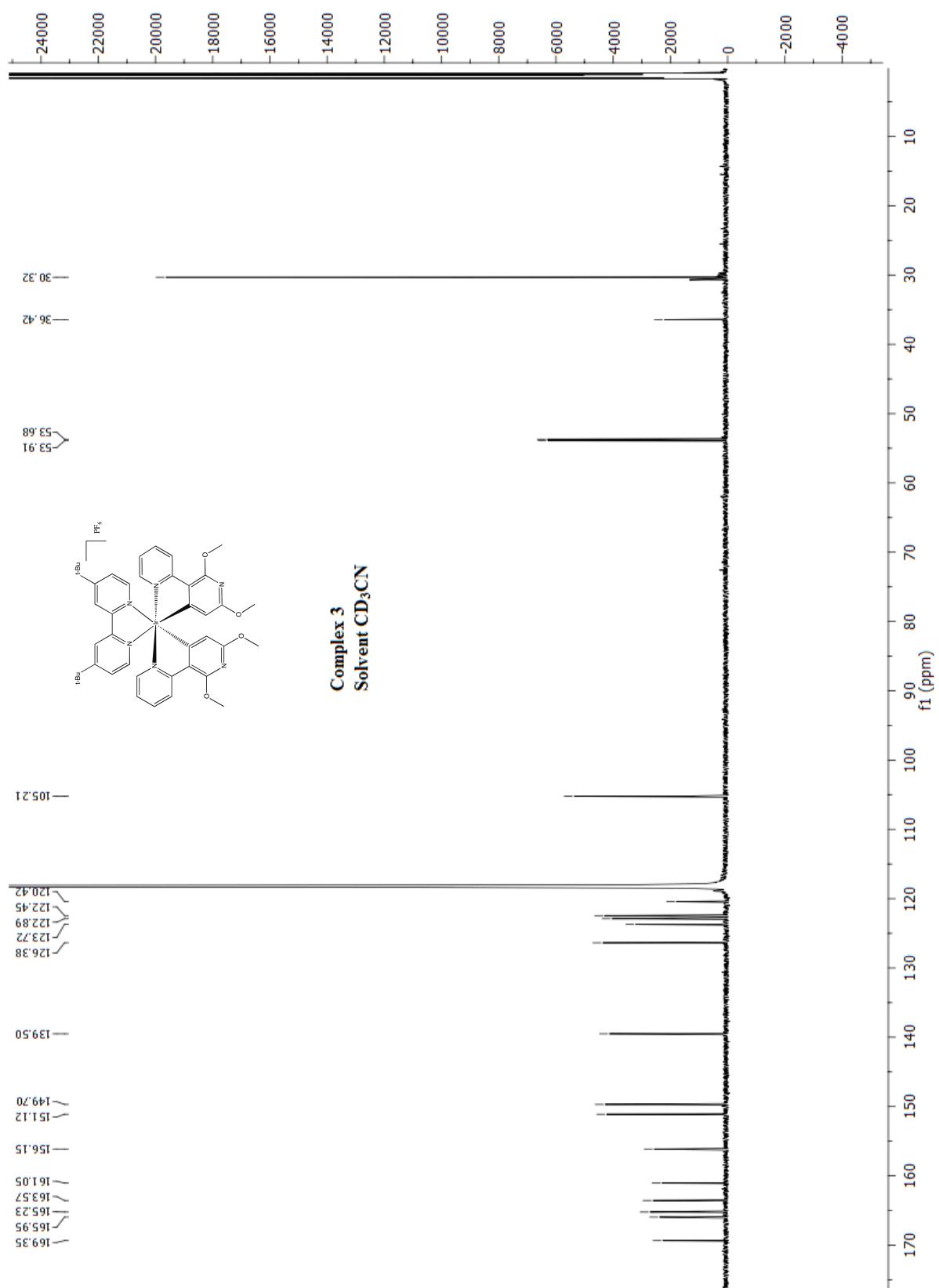


Figure S16. ^1H NMR of Complex 3 (aromatic part) in CD_3CN .



Complex 4

^1H NMR (700 MHz, Acetonitrile- d_3) δ 8.68 (s, 1H), 8.49 (d, $J = 0.9$ Hz, 1H), 8.01 (d, $J = 8.3$ Hz, 1H), 7.84 (d, $J = 5.8$ Hz, 1H), 7.73 (d, $J = 8.1$ Hz, 1H), 7.50 (dd, $J = 5.9, 1.0$ Hz, 2H), 7.30 (s, 1H), 6.14 (s, 1H), 2.25 (s, 3H), 2.12 (s, 3H), 1.41 (s, 9H).

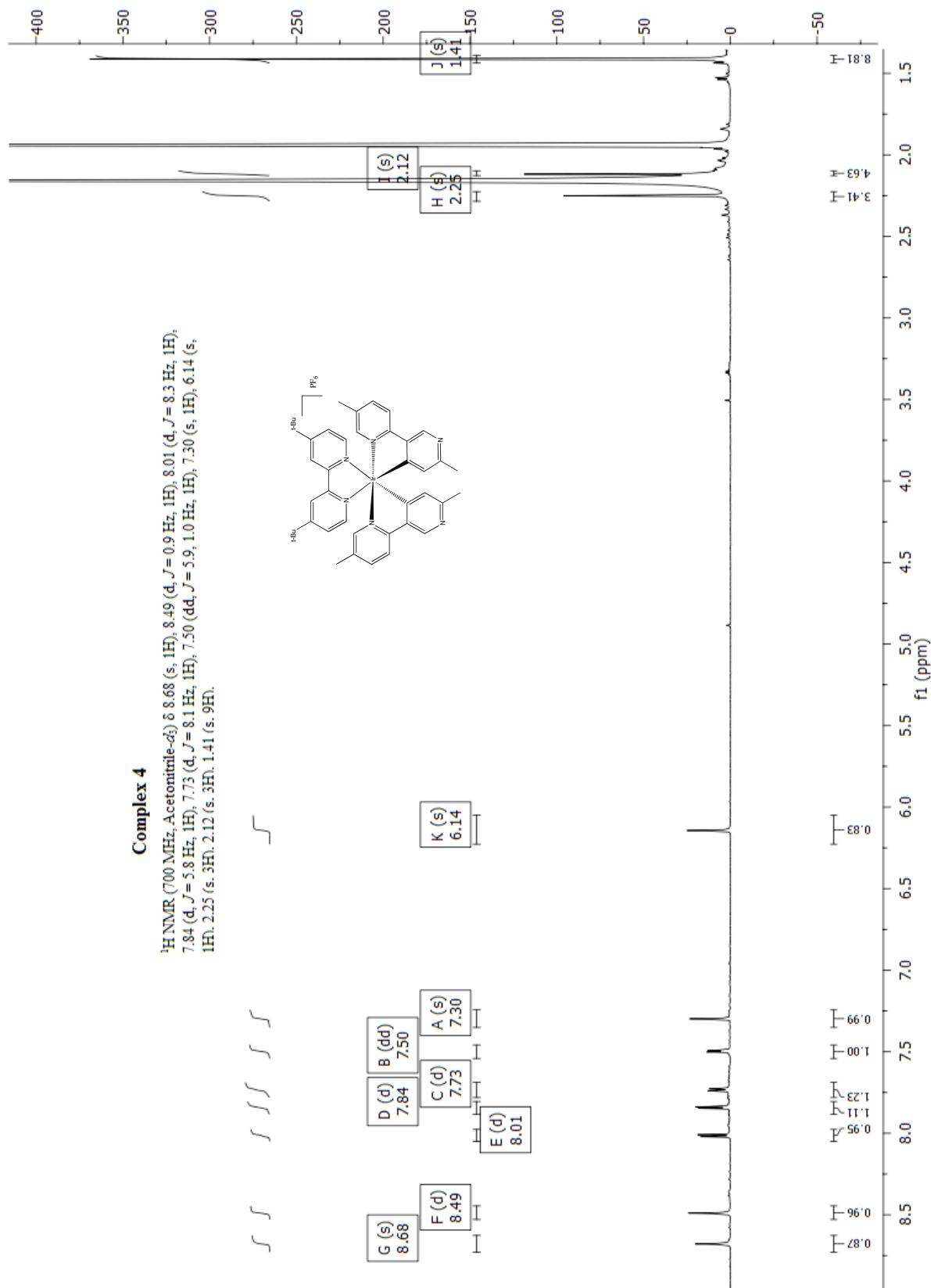


Figure S18. ^1H NMR of Complex 4 in CD_3CN .

Complex 4

^1H NMR (700 MHz, Acetonitrile- d_6) δ 8.68 (s, 1H), 8.49 (d, $J = 8.3$ Hz, 1H), 8.01 (d, $J = 8.3$ Hz, 1H), 7.84 (d, $J = 5.8$ Hz, 1H), 7.73 (d, $J = 8.1$ Hz, 1H), 7.50 (dd, $J = 5.9, 1.0$ Hz, 1H), 7.30 (s, 1H), 6.14 (s, 1H), 2.25 (s, 3H), 2.12 (s, 3H), 1.41 (s, 9H).

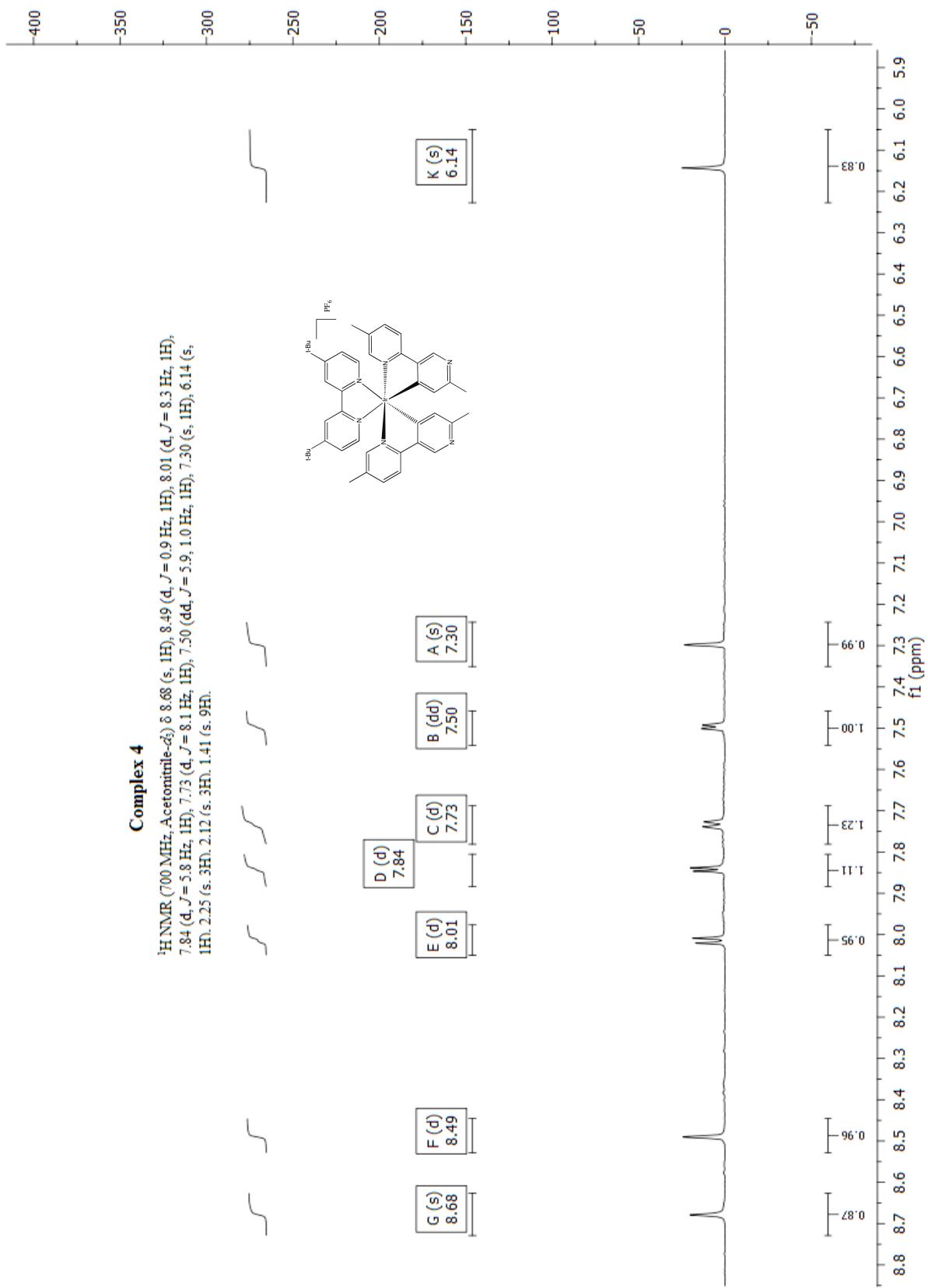


Figure S19. ^1H NMR of Complex 4 (aromatic part) in CD_3CN .

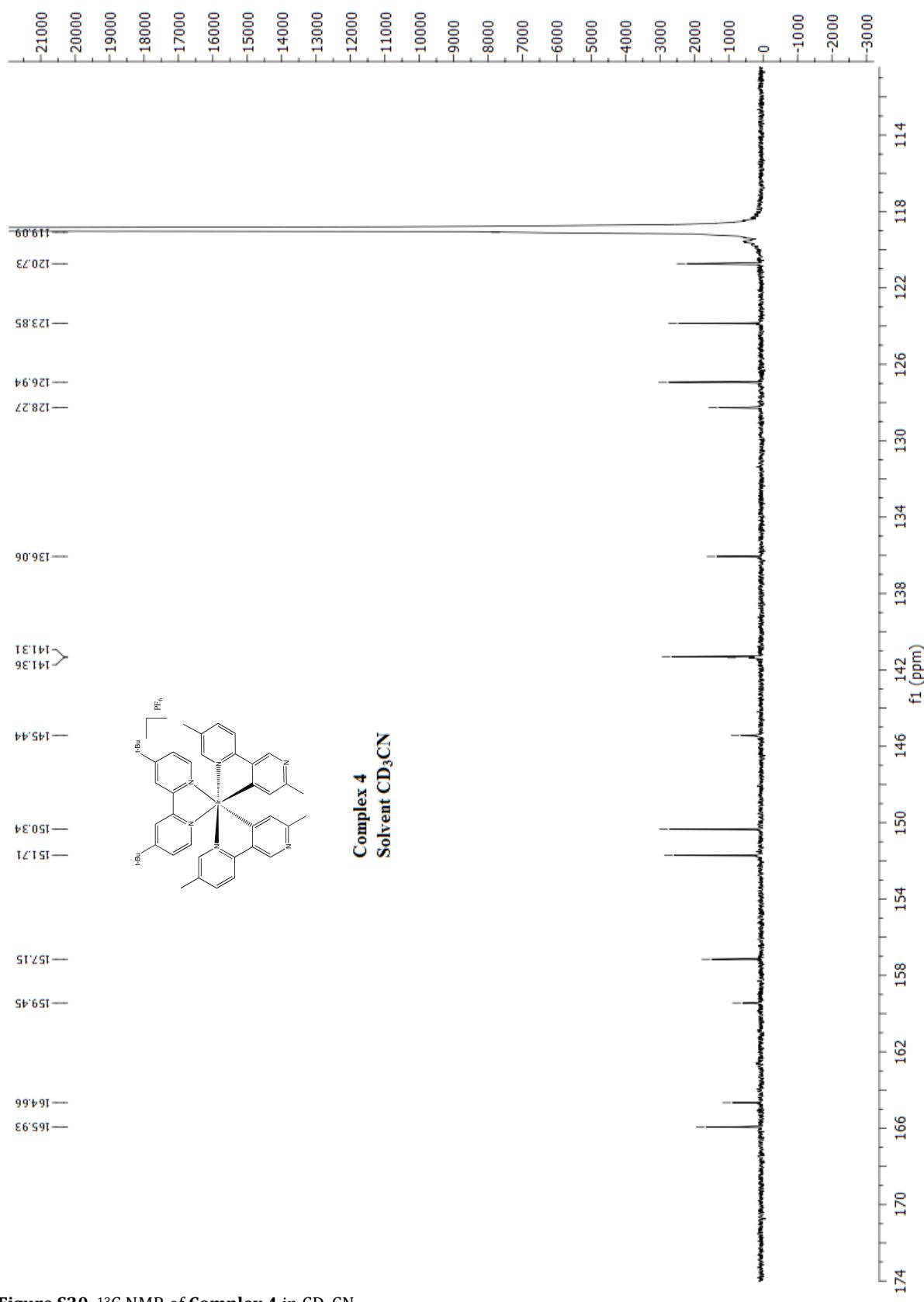


Figure S20. ¹³C NMR of Complex 4 in CD₃CN.

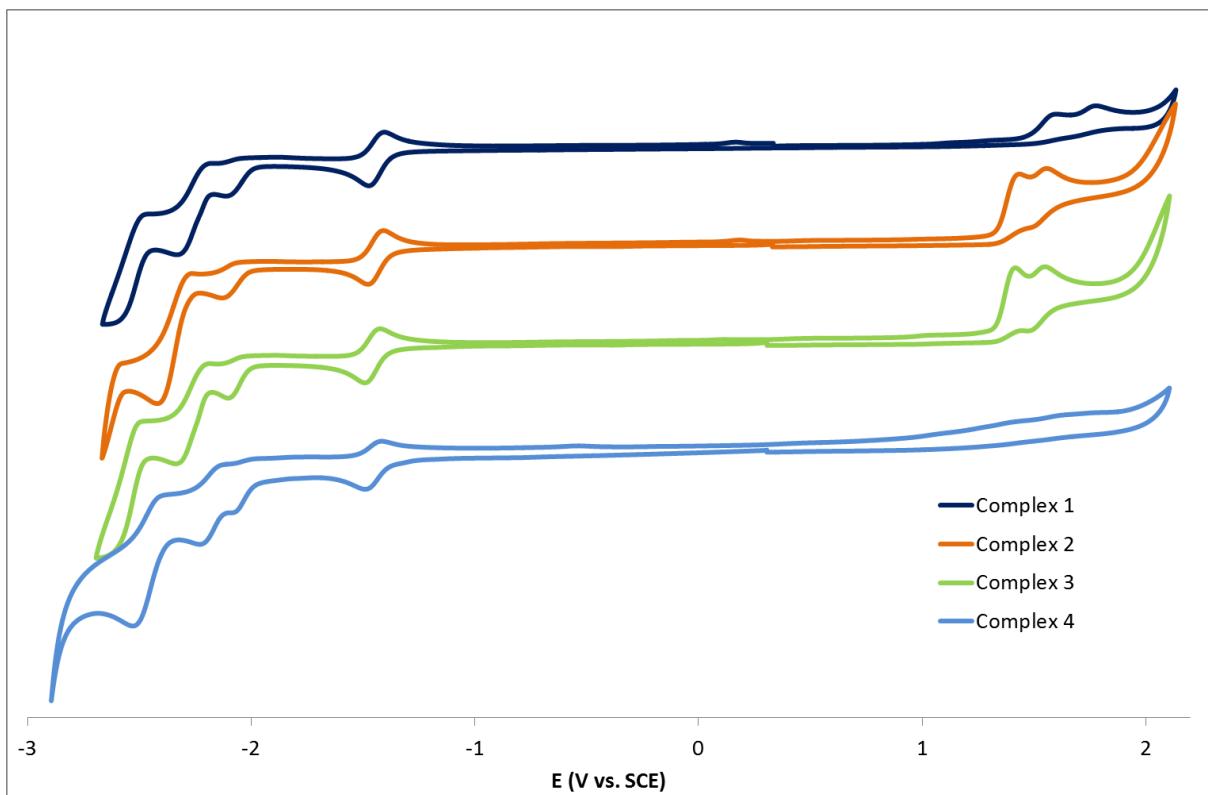


Figure S21. Complete cyclic voltammetries for **1-4** recorded in deaerated CH_3CN ; supporting electrolyte TBAPF_6 0.1 M. Working electrode: glassy carbon; counter electrode: Pt wire; reference electrode: SCE. The Fc^+/Fc couple was used as an internal standard and the potential was then referred to SCE ($E(\text{SCE}) = E(\text{Fc}^+/\text{Fc}) + 0.38 \text{ V}$).