Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and characterisation of homoleptic 2,9-diaryl-1,10-phenanthroline copper(I) complexes: influencing selectivity in photoredox-catalysed atom-transfer radical addition reactions

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Supplementary Information

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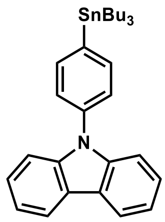
I. Preparation of Materials

Experimental procedures for the preparation of previously unreported compounds are described below. These procedures were not optimised.

9-(4-(Tributylstannyl)phenyl)-9*H*-carbazole



n-BuLi (1.46 mL, 1.6 M in hexane, 2.33 mmol) was added drop wise to a magnetically stirred solution of 9-(4-bromophenyl)-9H-carbazole[1] (500 mg, 1.55 mmol) in THF (5 mL) maintained at –78 ˚C under N_2. After 1 h, Bu_3SnCl (505 mg, 1.55 mmol) was added dropwise. The ensuing mixture was slowly warmed to room temperature over 4 h and then concentrated under reduced pressure. The resulting pale-yellow residue was redissolved in CH_2Cl_2 (10 mL) and filtered through a Celite® plug then concentrated under reduced pressure. The ensuing residue was subjected to flash column chromatography (hexanes; silica gel) to provide the 9-(4-(tributylstannyl)phenyl)-9*H*-carbazole (610 mg, 74% yield) as a colourless oil.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 7.8 Hz, 2H), 7.77–7.65 (m, 2H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.50 (complex m, 4H), 7.31 (t, *J* = 7.2 Hz, 2H), 1.70–1.60 (m, 6H), 1.21–1.14 (m, 6H), 0.97–0.94 (m, 9H) ppm.
^{13}C NMR (100 MHz, $CDCl_3$): δ 141.8, 141.0, 137.9, 137.6, 126.5, 126.0, 123.5, 120.4, 120.0, 110.0, 29.3, 27.6, 13.8, 9.9 ppm.
IR (NaCl): 1694, 1653, 1586, 1559, 1501, 1452, 1231, 748, 725 cm^{-1}.

1. G. K.-M. So, G. Cheng, J. Wang, X. Chang, C.-C. Kwok, H. Zhang, C.-M. and W. Sun, *Chem. – Asian J.* 2013, *12*, **2017**, 1490.

II. Cyclic Voltammetry

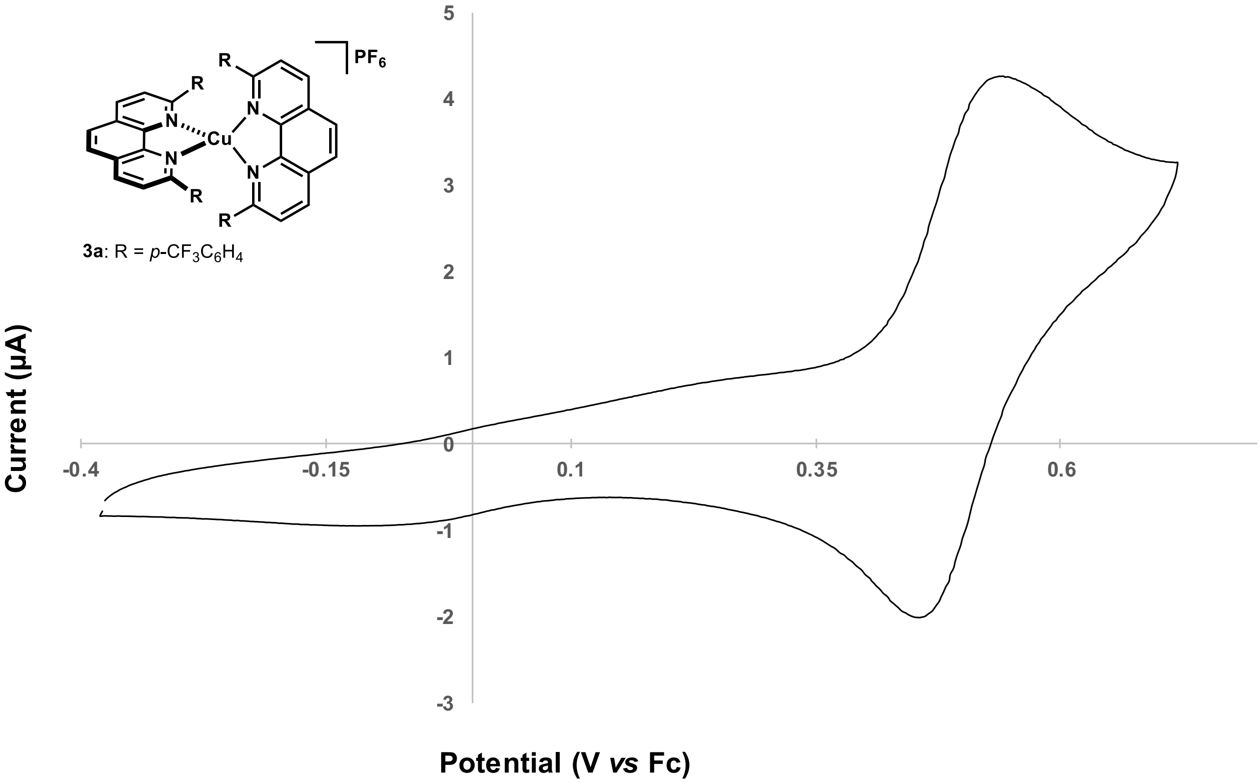


Figure S1a: Cyclic voltammogram of complex **3a** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

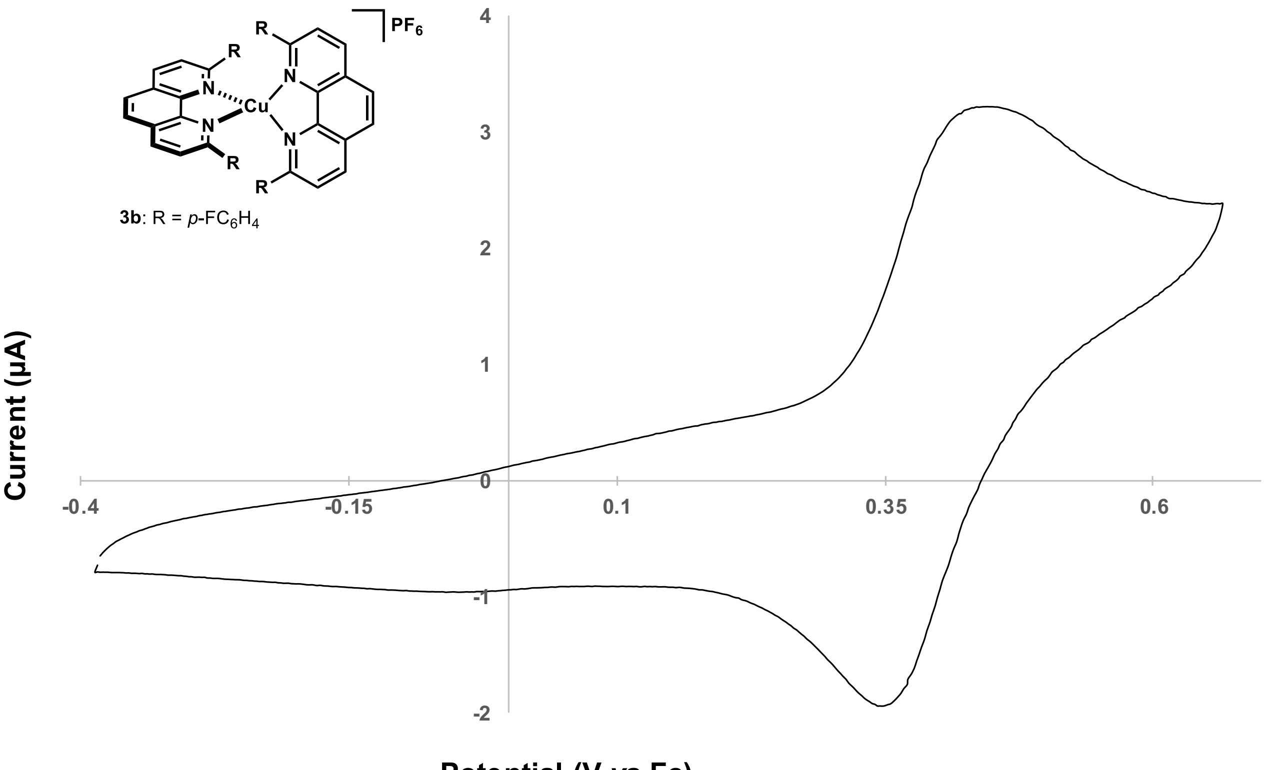


Figure S1b: Cyclic voltammogram of complex **3b** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

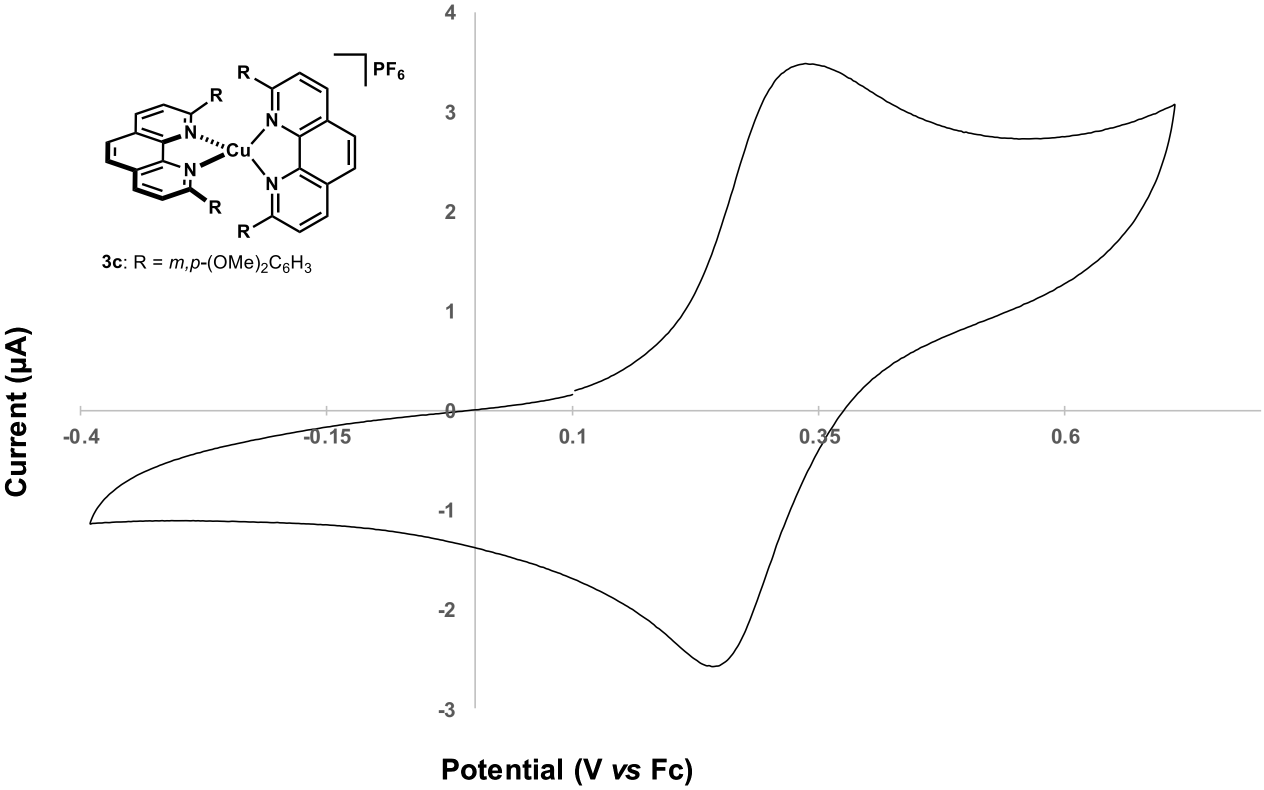


Figure S1c: Cyclic voltammogram of complex **3c** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

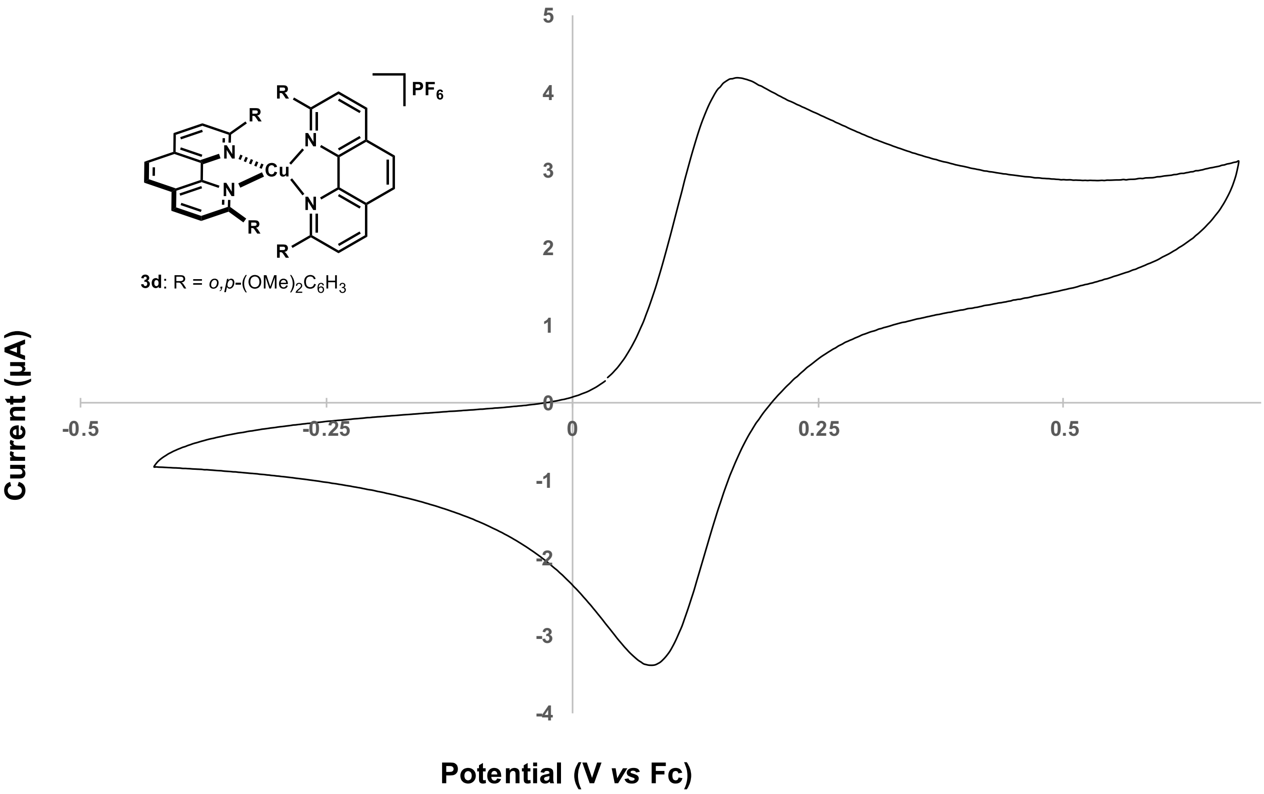


Figure S1d: Cyclic voltammogram of complex **3d** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

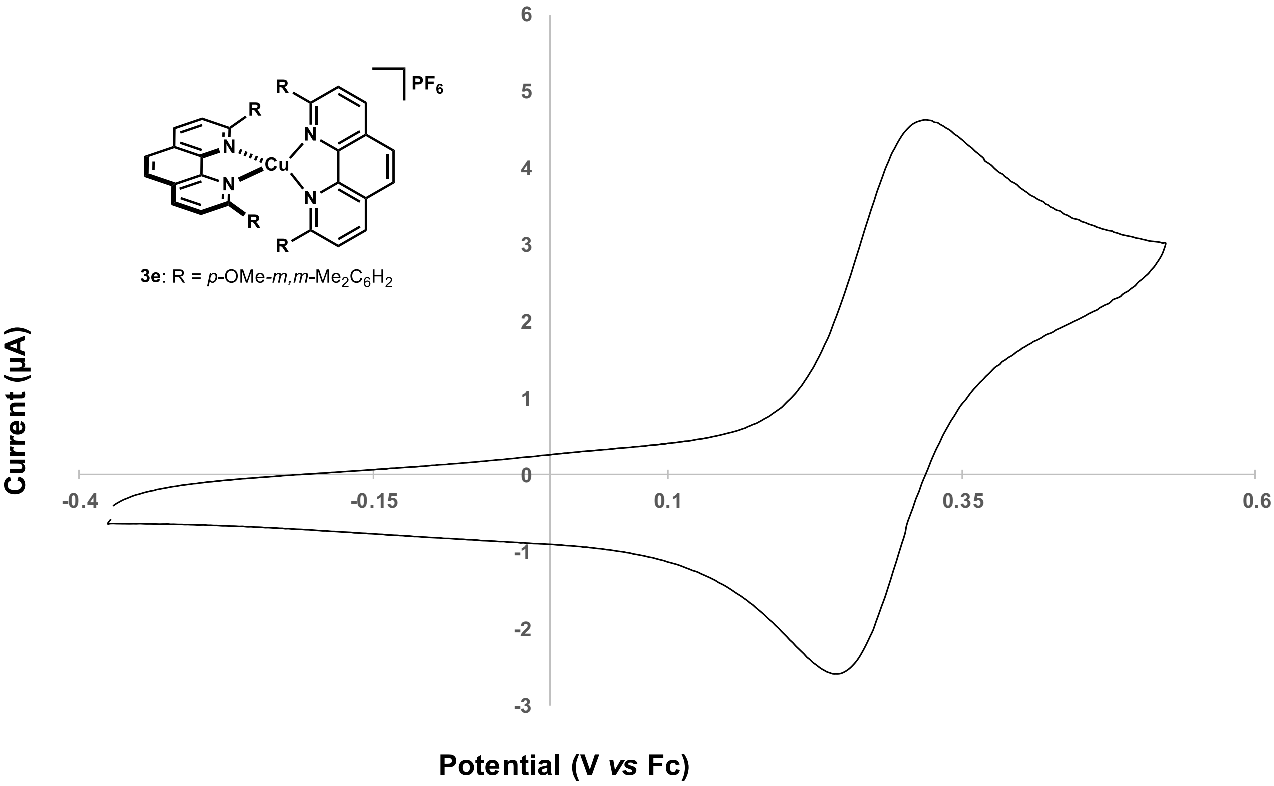


Figure S1e: Cyclic voltammogram of complex **3e** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

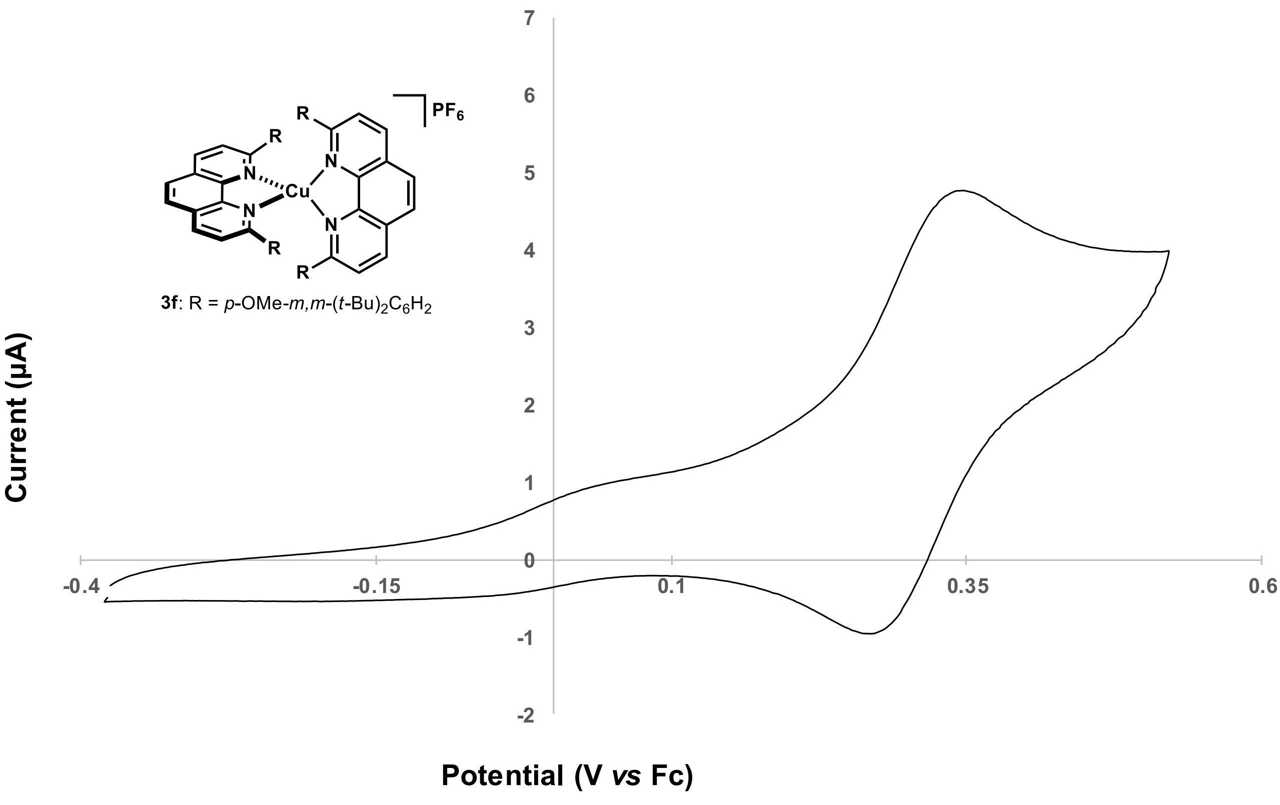


Figure S1f: Cyclic voltammogram of complex **3f** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

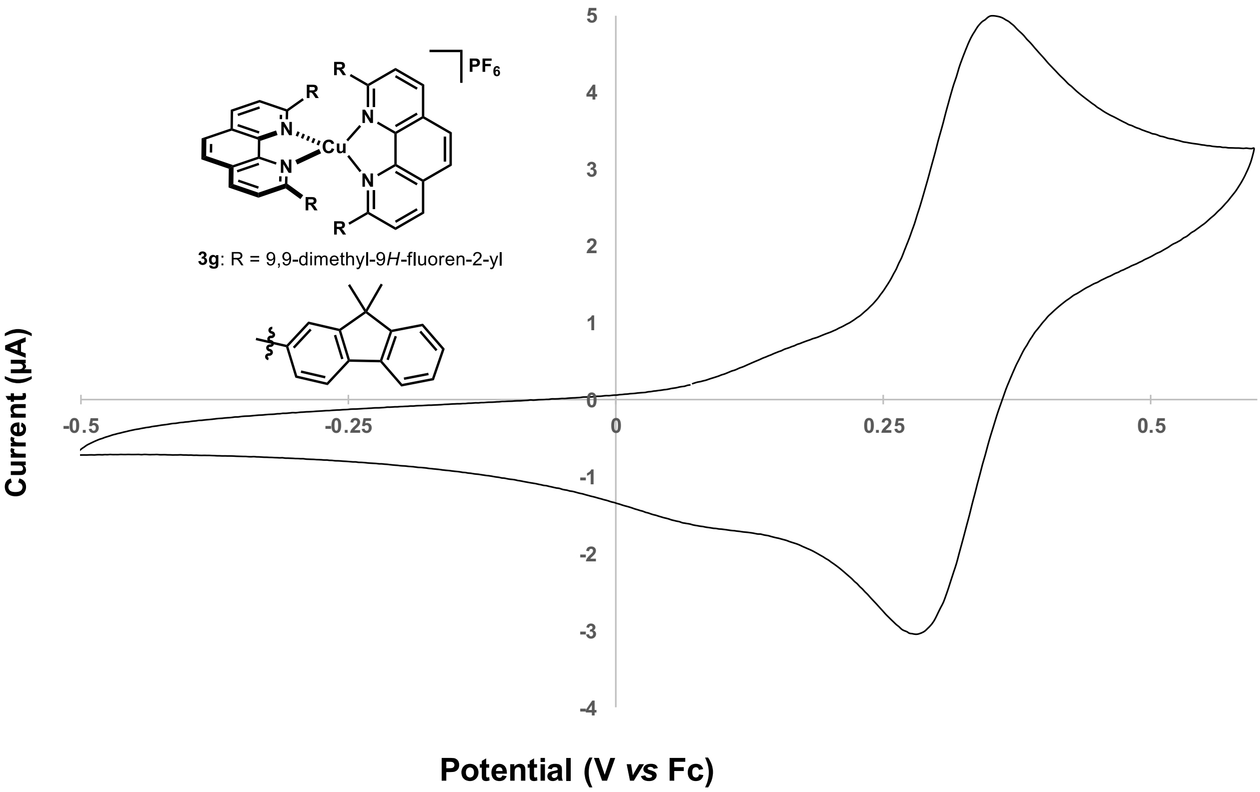


Figure S1g: Cyclic voltammogram of complex **3g** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

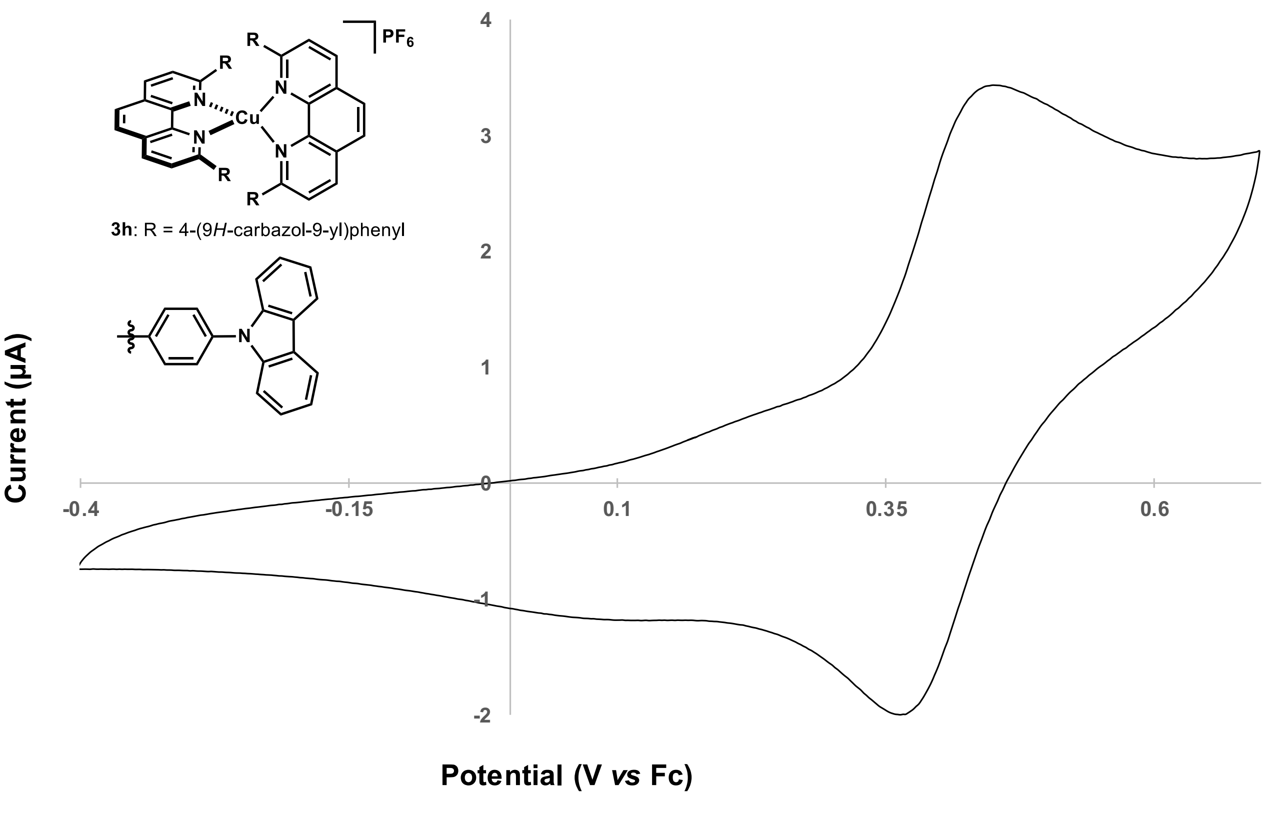


Figure S1h: Cyclic voltammogram of complex **3h** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

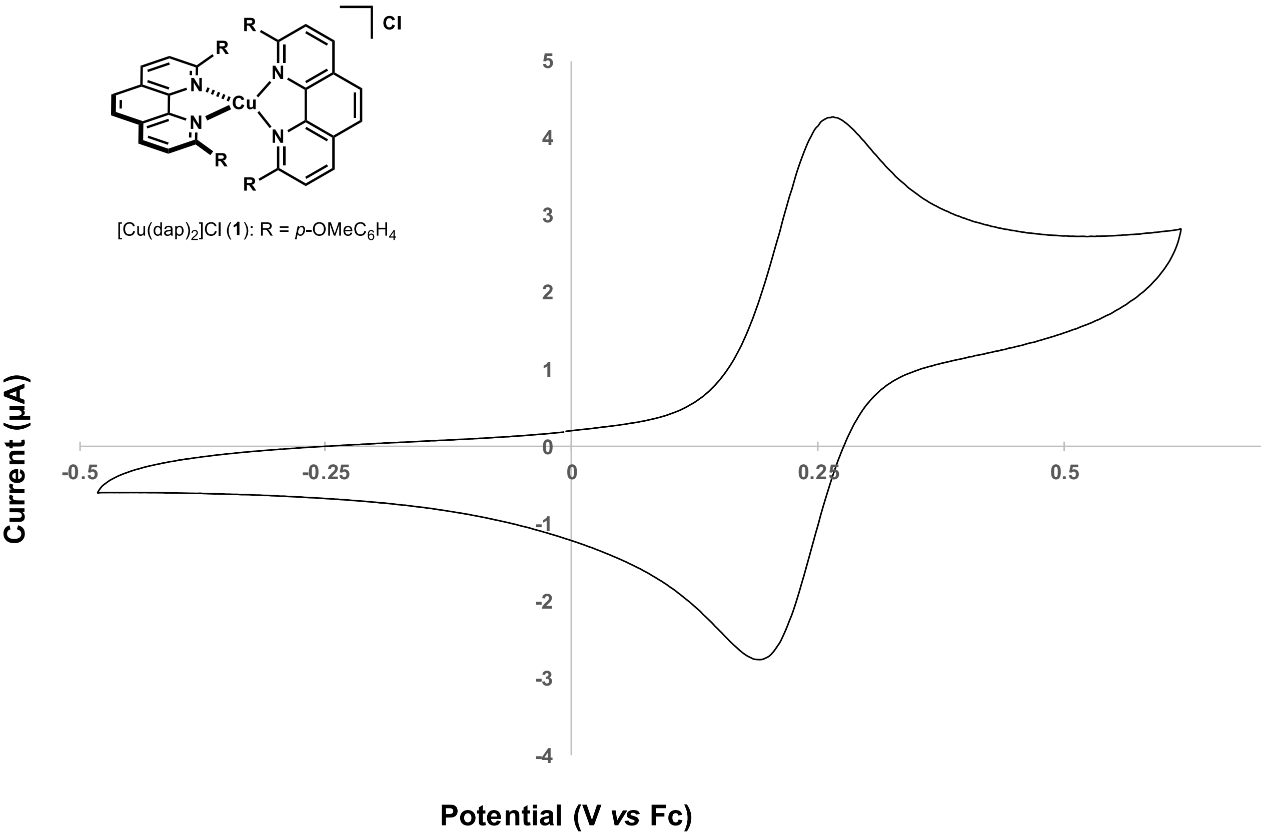


Figure S1i: Cyclic voltammogram of complex **1** in MeCN (0.25 mM) using NBu_4PF_6 (0.1 M) as supporting electrolyte at scan rate of 100 mV s^{-1}.

III. Absorption Spectra

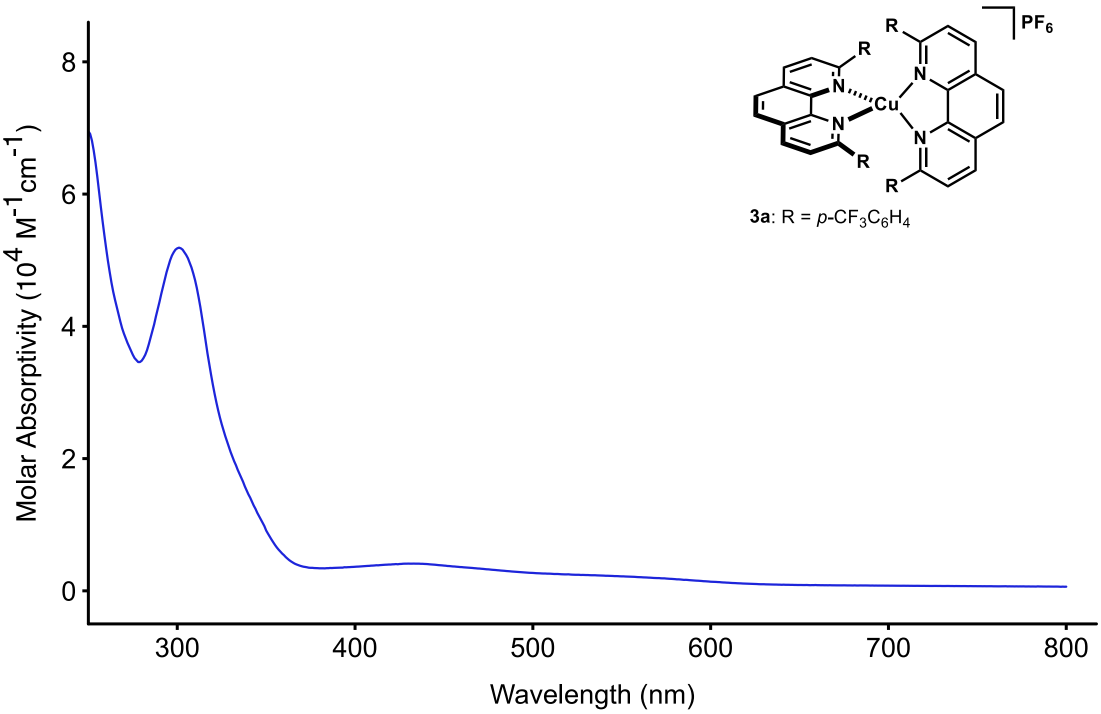


Figure S2a: Absorption spectrum of complex **3a** in CH_2Cl_2 (10^{-5} M).

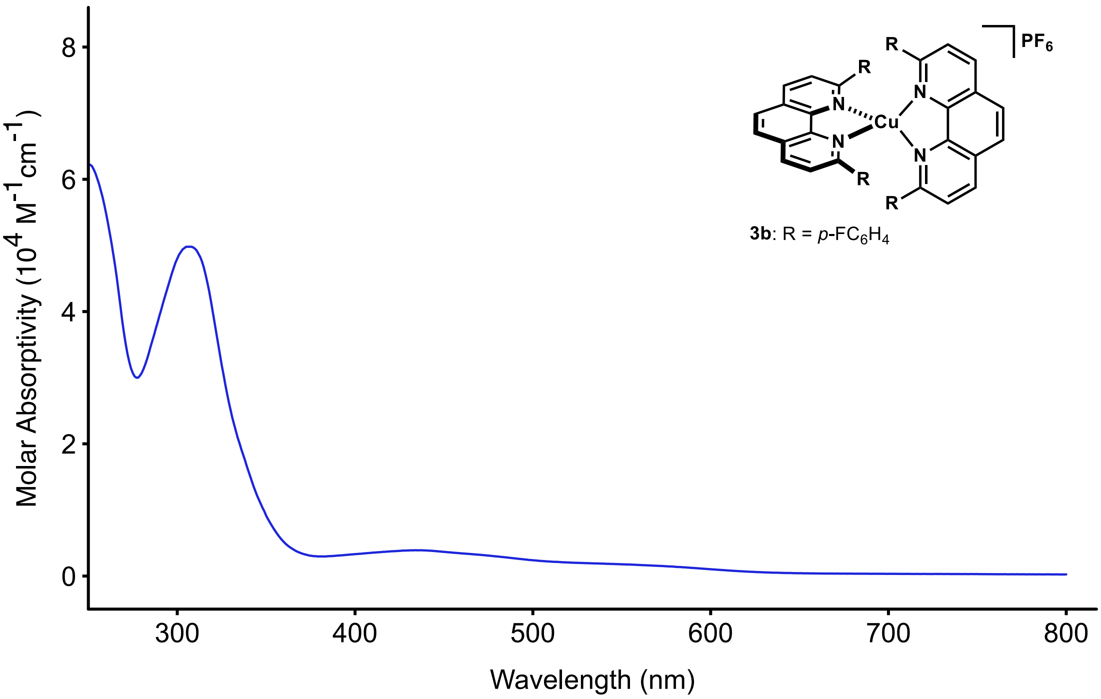


Figure S2b: Absorption spectrum of complex **3b** in CH_2Cl_2 (10^{-5} M).

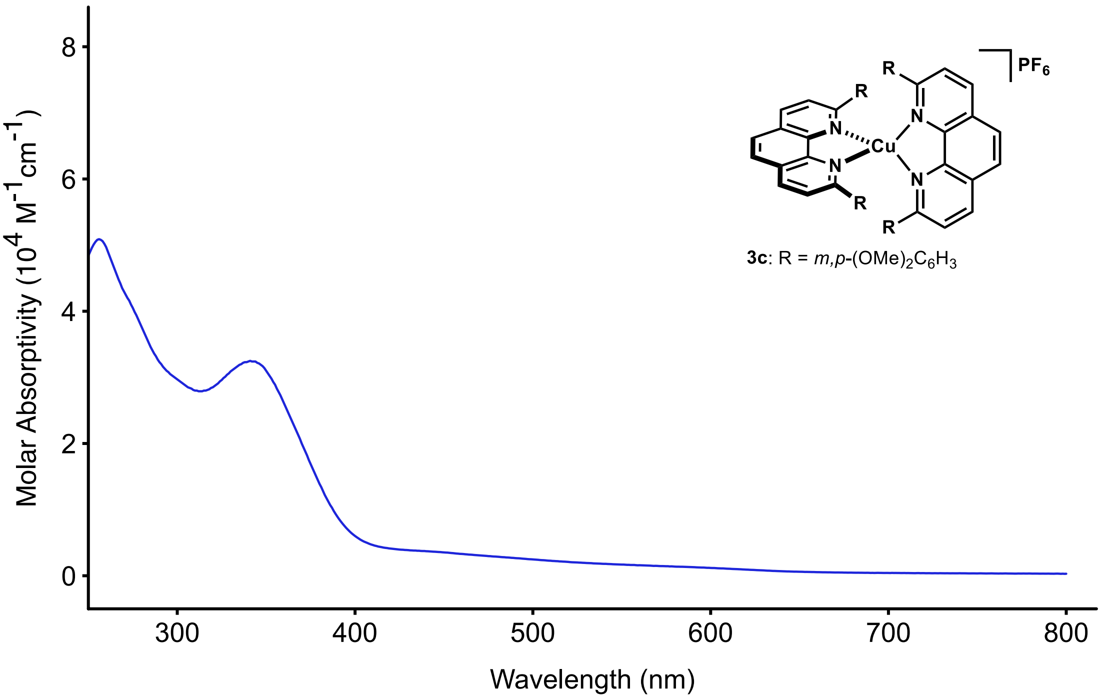


Figure S2c: Absorption spectrum of complex **3c** in CH_2Cl_2 (10^{-5} M).

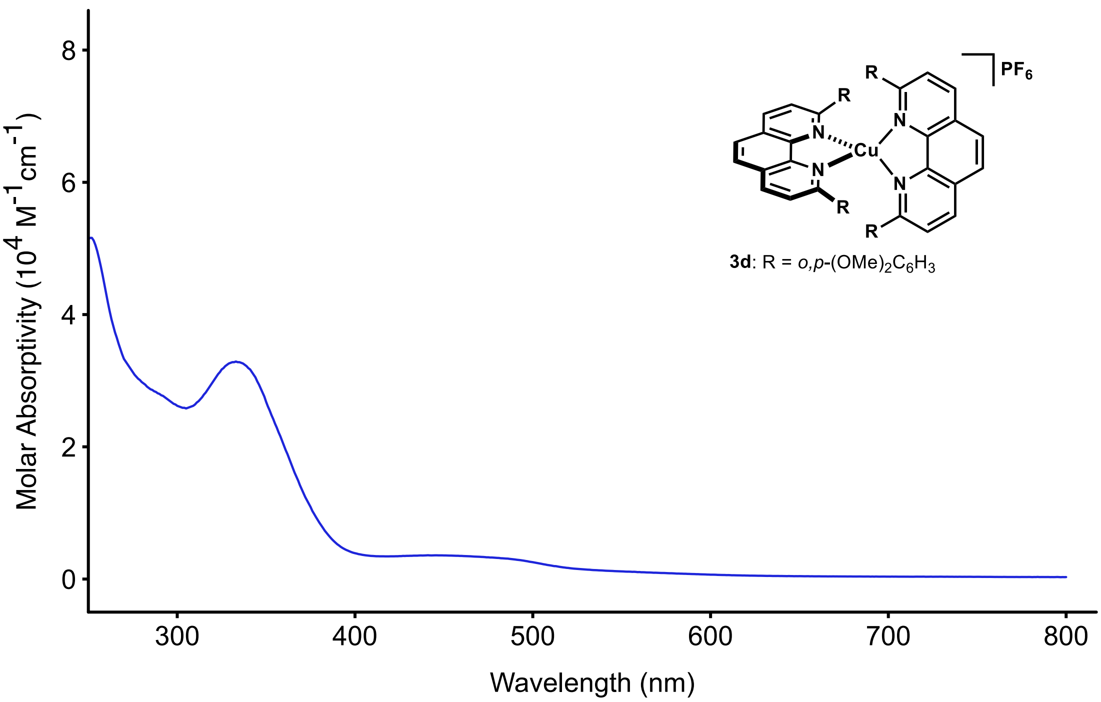


Figure S2d: Absorption spectrum of complex **3d** in CH_2Cl_2 (10^{-5} M).

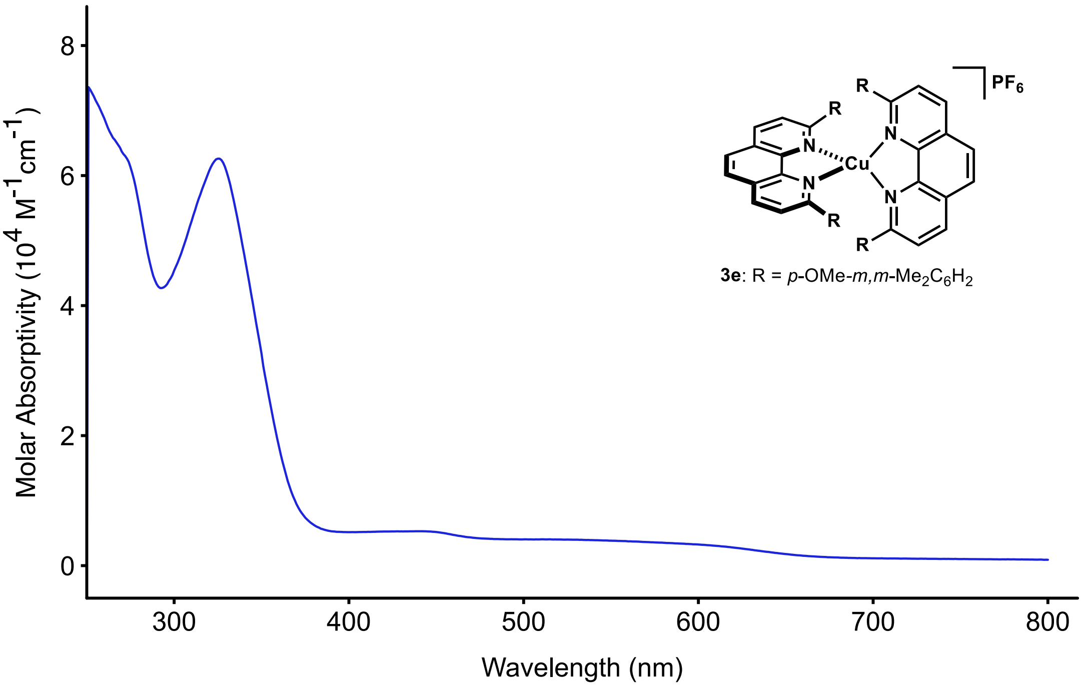


Figure S2e: Absorption spectrum of complex **3e** in CH_2Cl_2 (10^{-5} M).

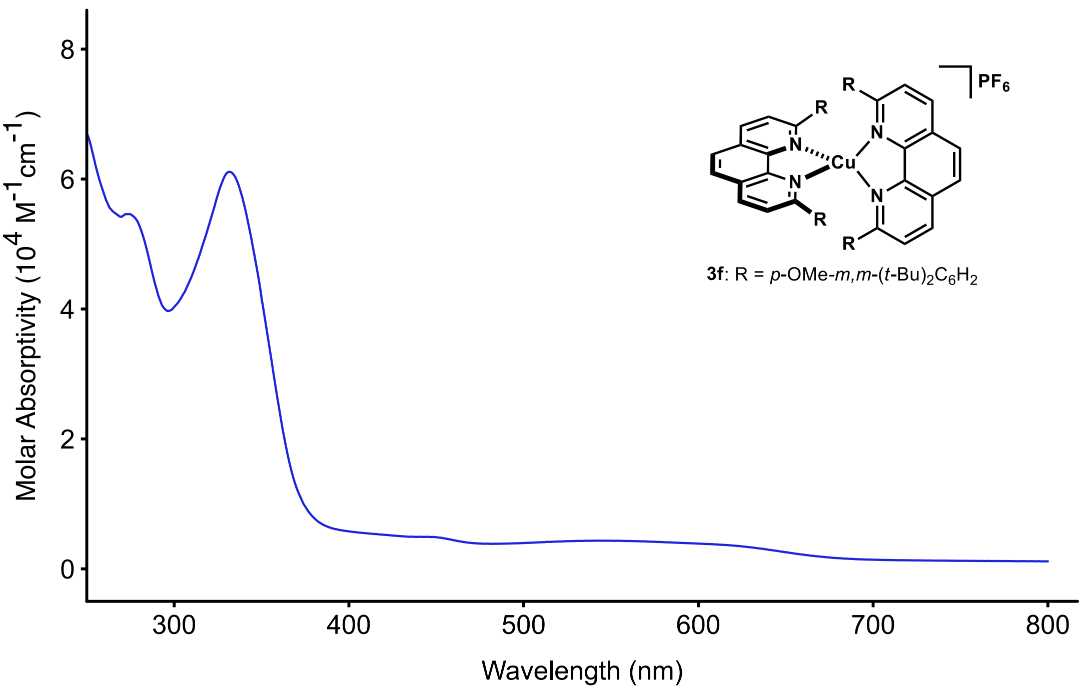


Figure S2f: Absorption spectrum of complex **3f** in CH_2Cl_2 (10^{-5} M).

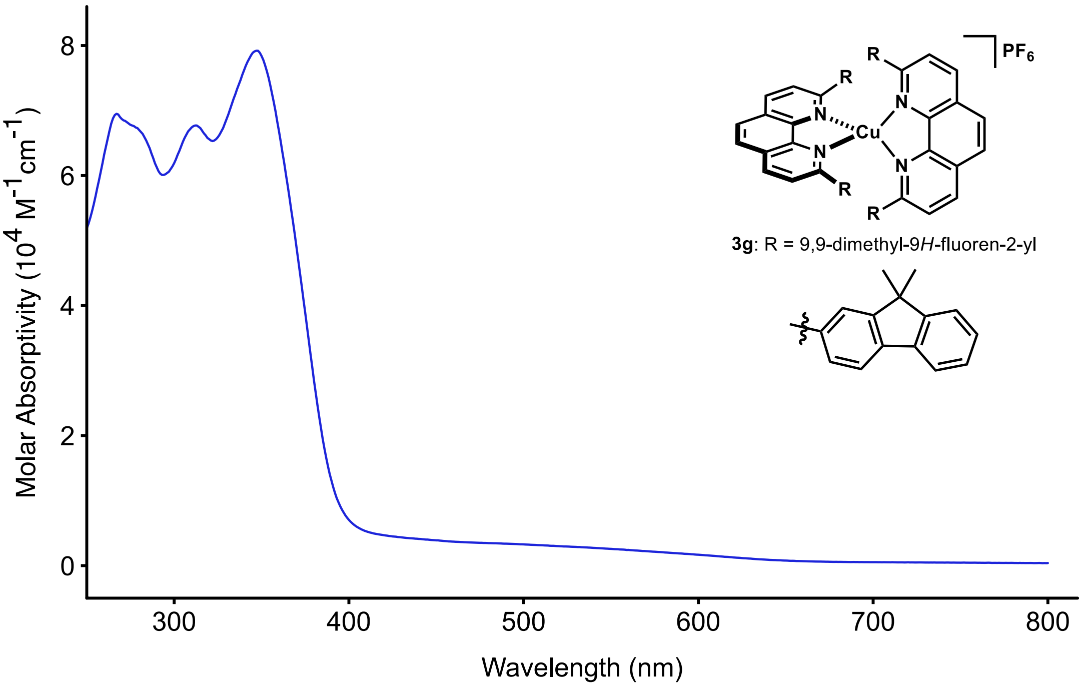


Figure S2g: Absorption spectrum of complex **3g** in CH_2Cl_2 (10^{-5} M).

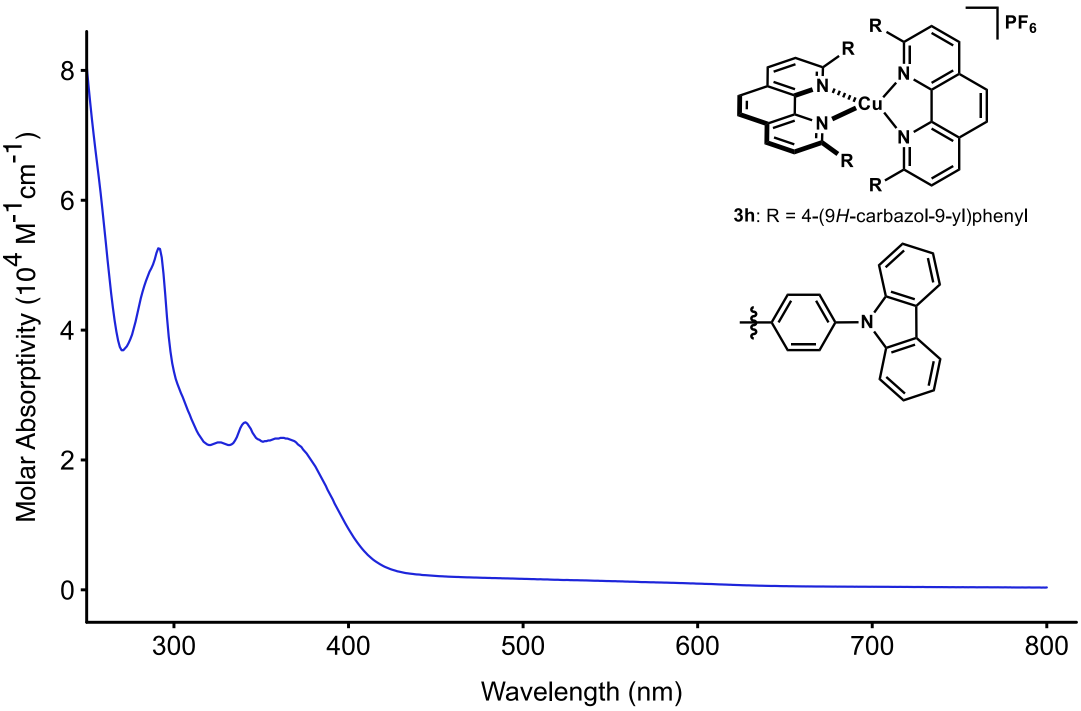


Figure S2h: Absorption spectrum of complex **3h** in CH_2Cl_2 (10^{-5} M).

IV. Excitation Spectra

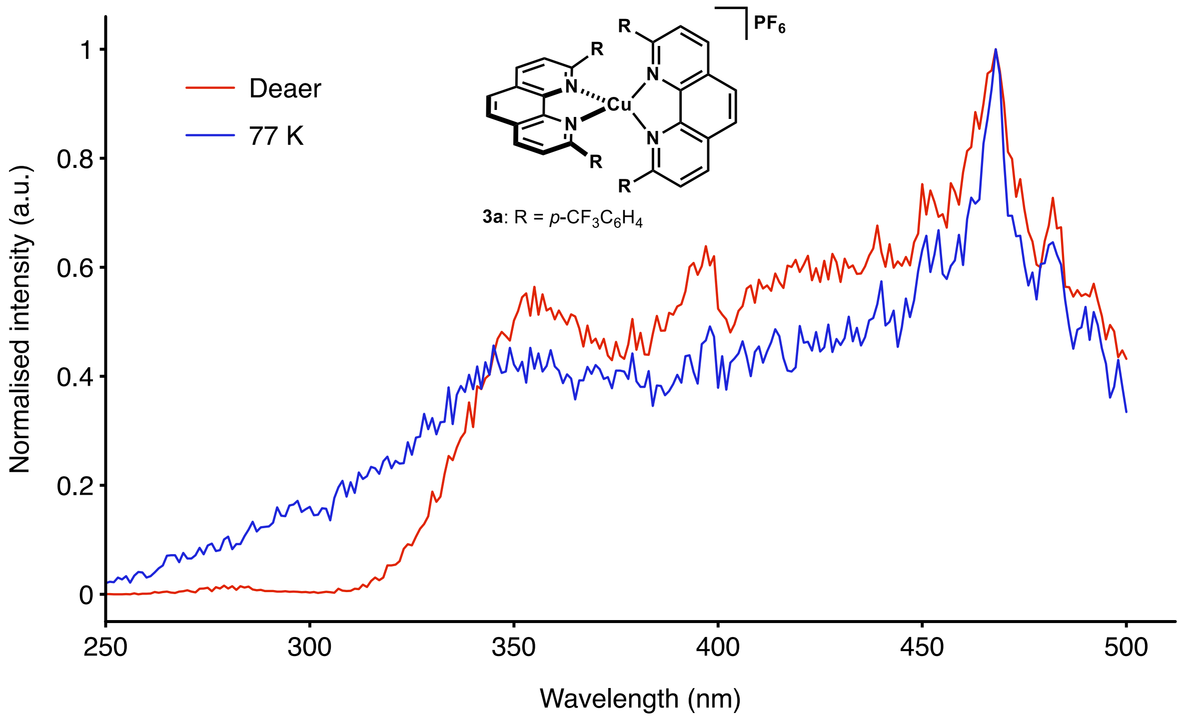


Figure S3a: Excitation spectrum of complex **3a** in CH_2Cl_2 (10^{-5} M).

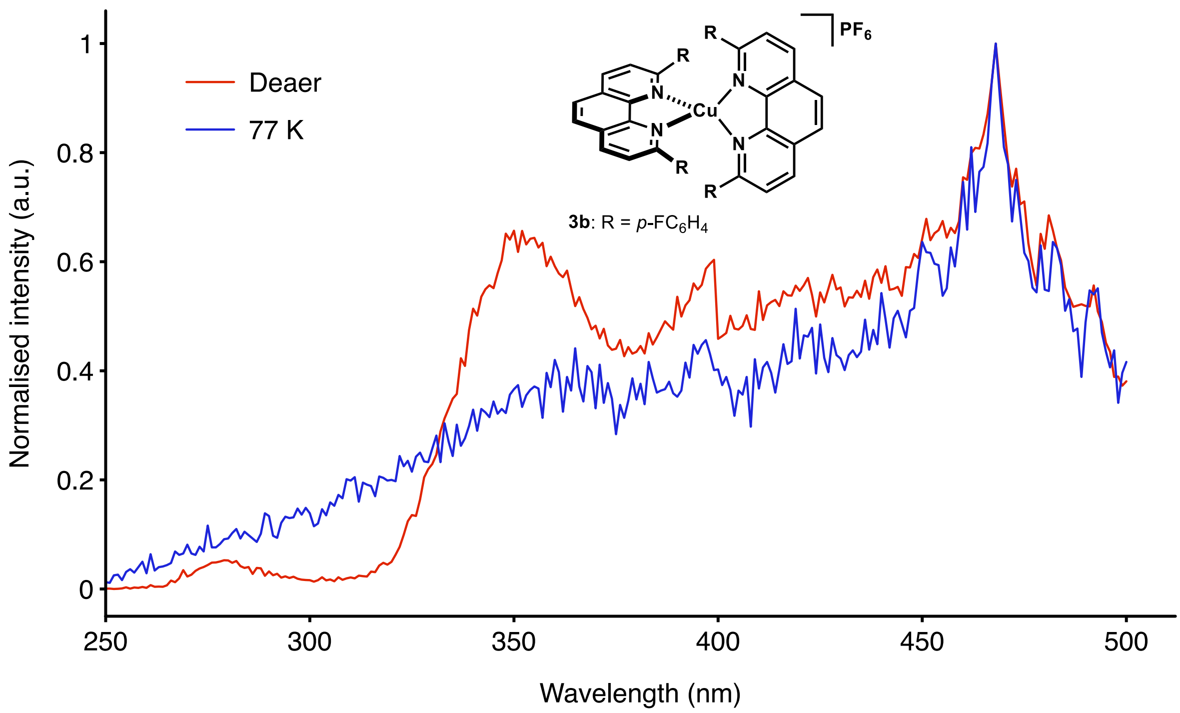


Figure S3b: Excitation spectrum of complex **3b** in CH_2Cl_2 (10^{-5} M).

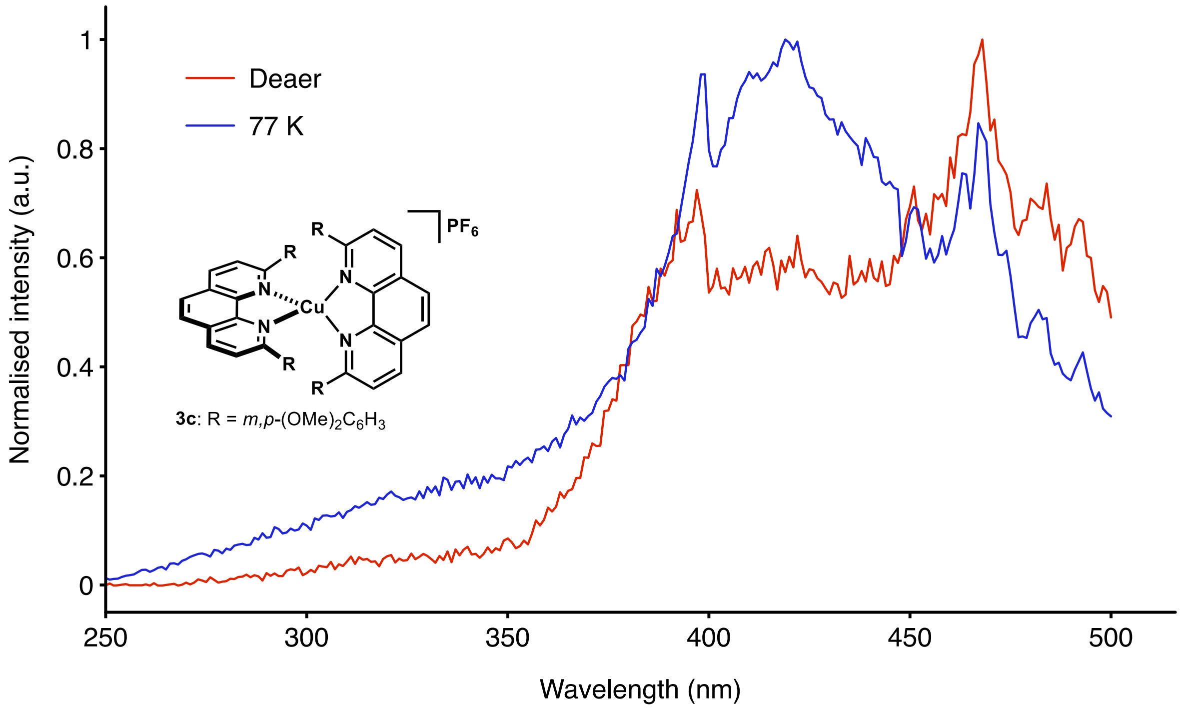


Figure S3c: Excitation spectrum of complex **3c** in CH_2Cl_2 (10^{-5} M).

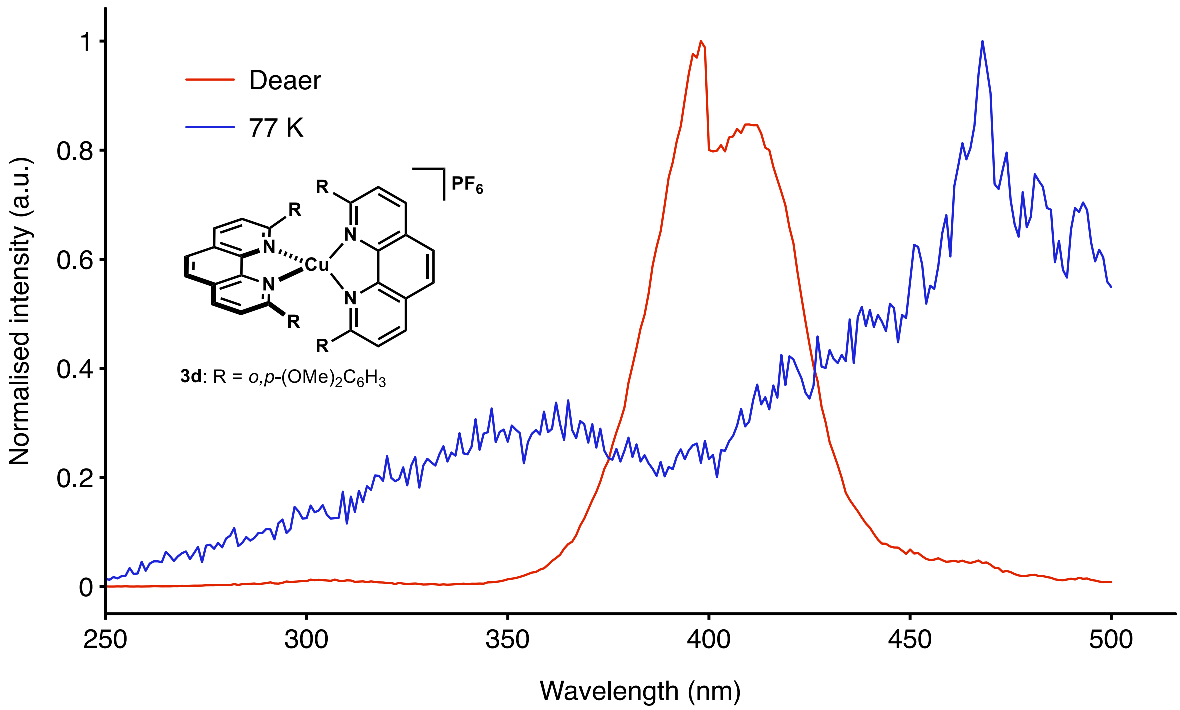


Figure S3d: Excitation spectrum of complex **3d** in CH_2Cl_2 (10^{-5} M).

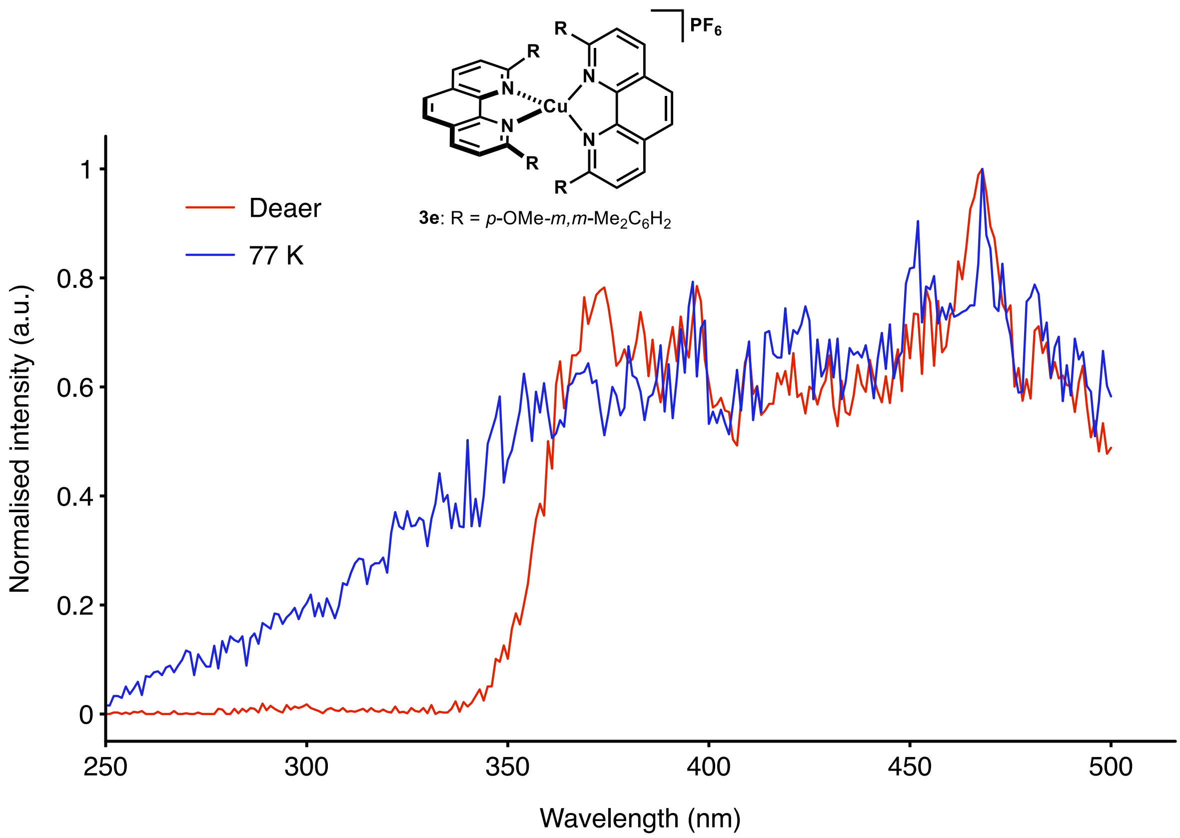


Figure S3e: Excitation spectrum of complex **3e** in CH_2Cl_2 (10^{-5} M).

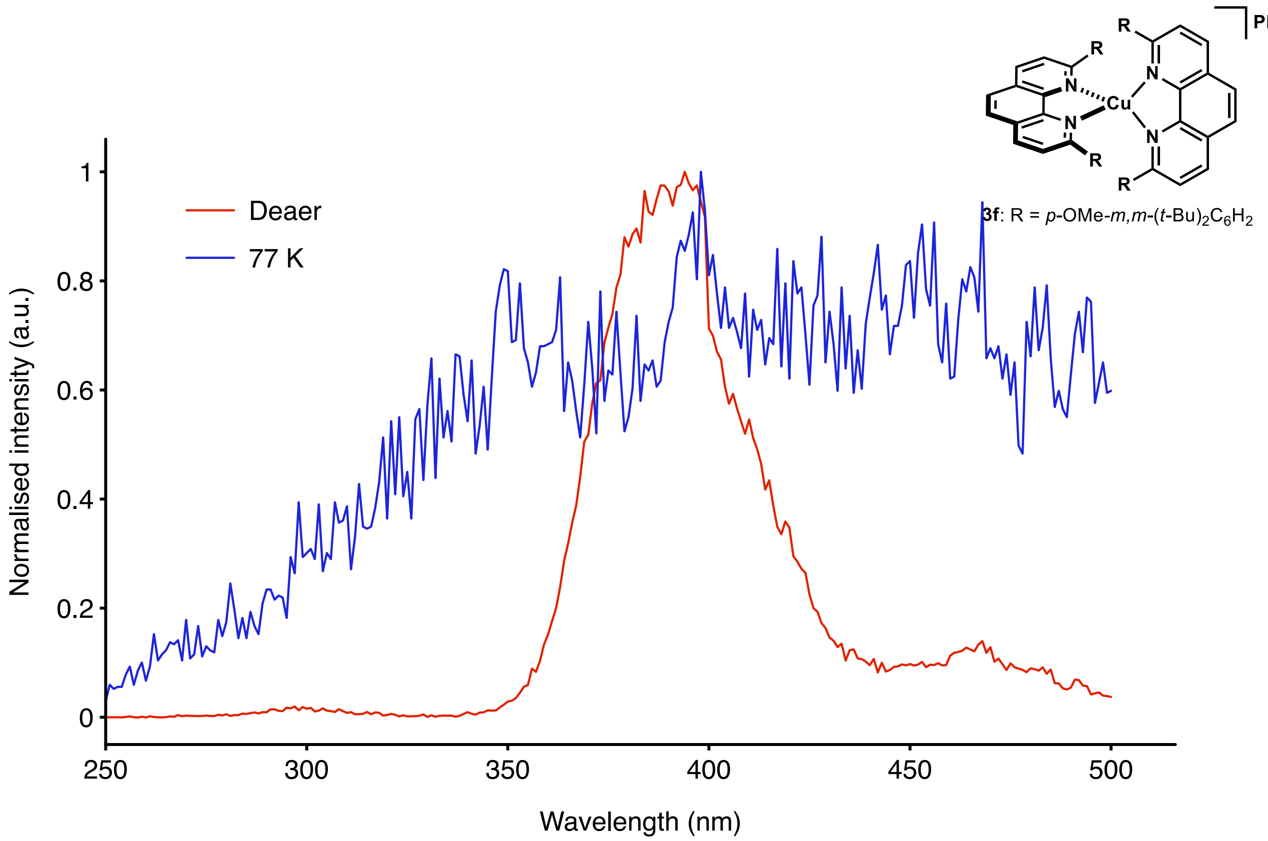


Figure S3f: Excitation spectrum of complex **3f** in CH_2Cl_2 (10^{-5} M).

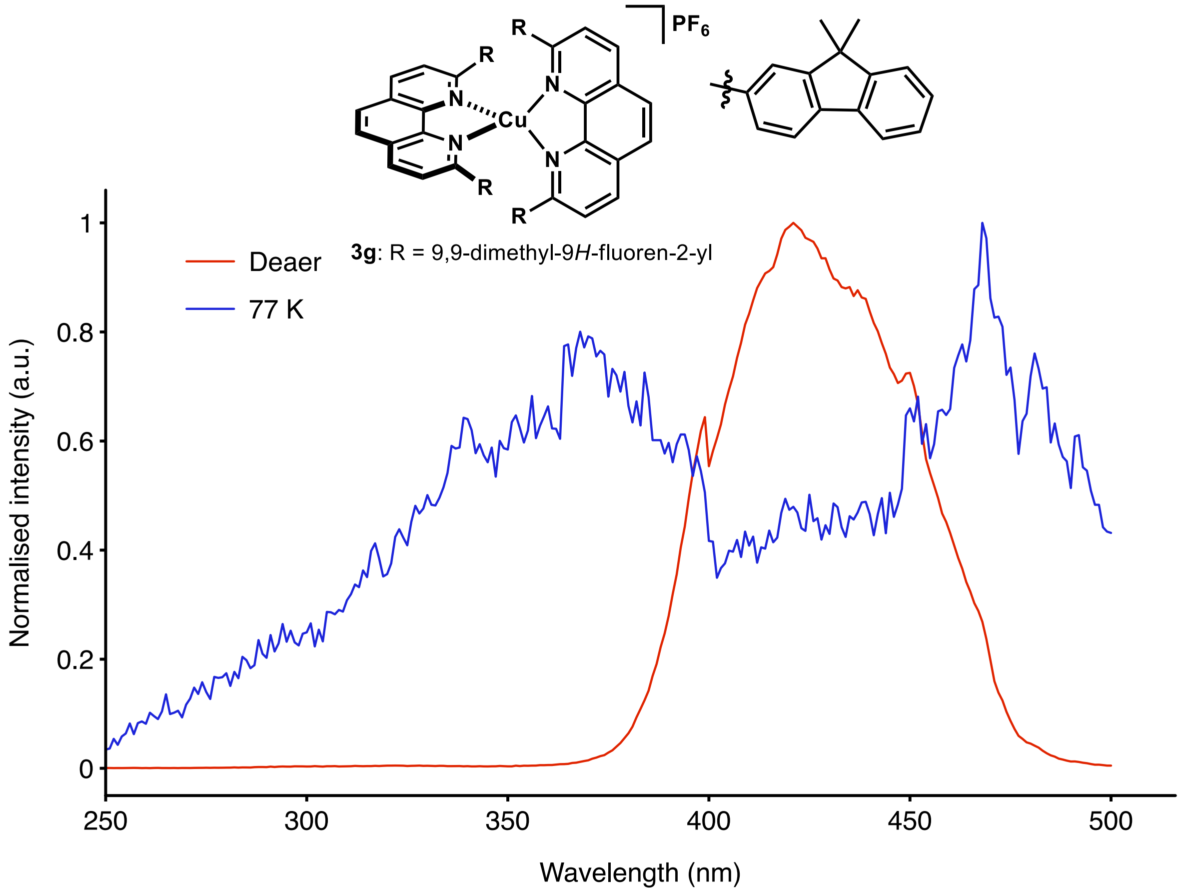


Figure S3g: Excitation spectrum of complex **3g** in CH_2Cl_2 (10^{-5} M).

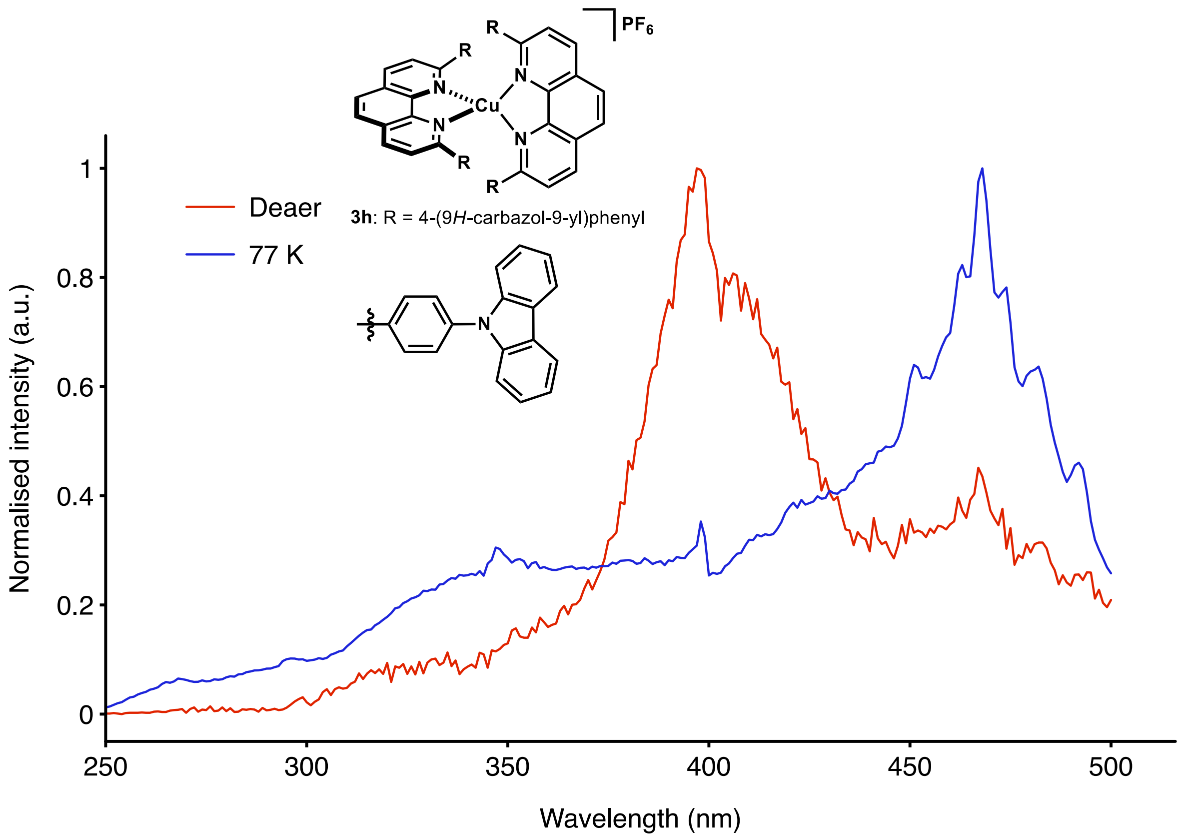


Figure S3h: Excitation spectrum of complex **3h** in CH_2Cl_2 (10^{-5} M).

V. Emission Spectra

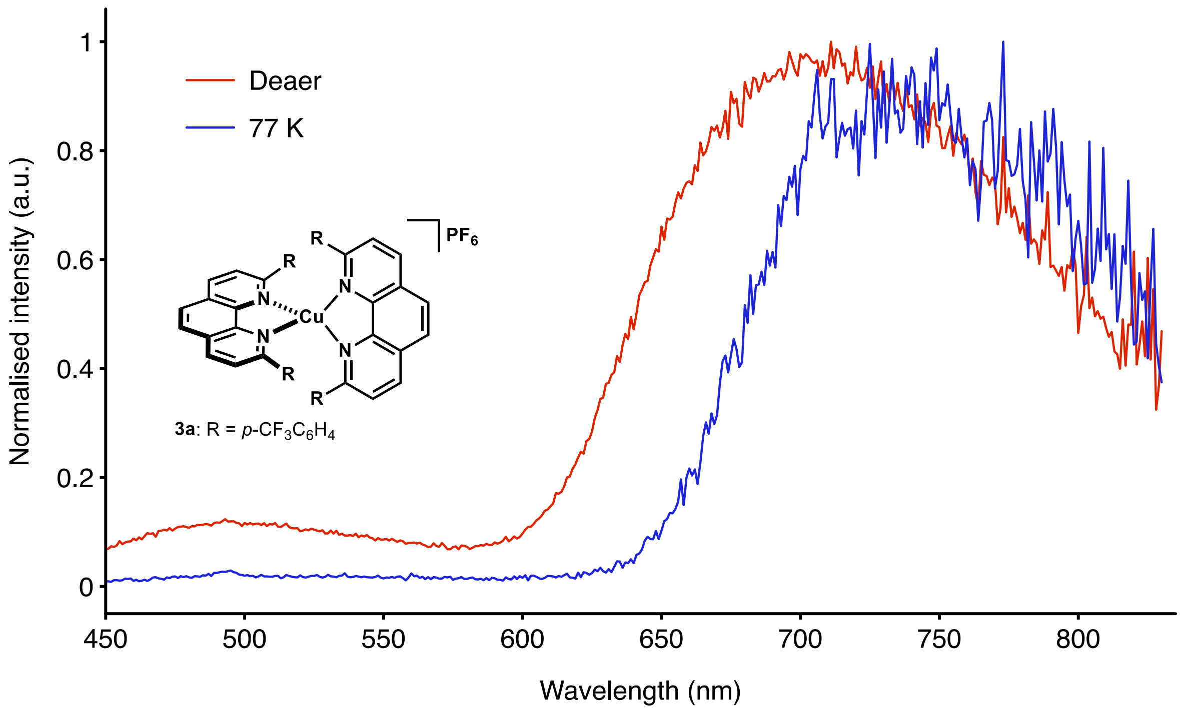


Figure S4a: Emission spectrum of complex **3a** in CH_2Cl_2 (10^{-5} M).

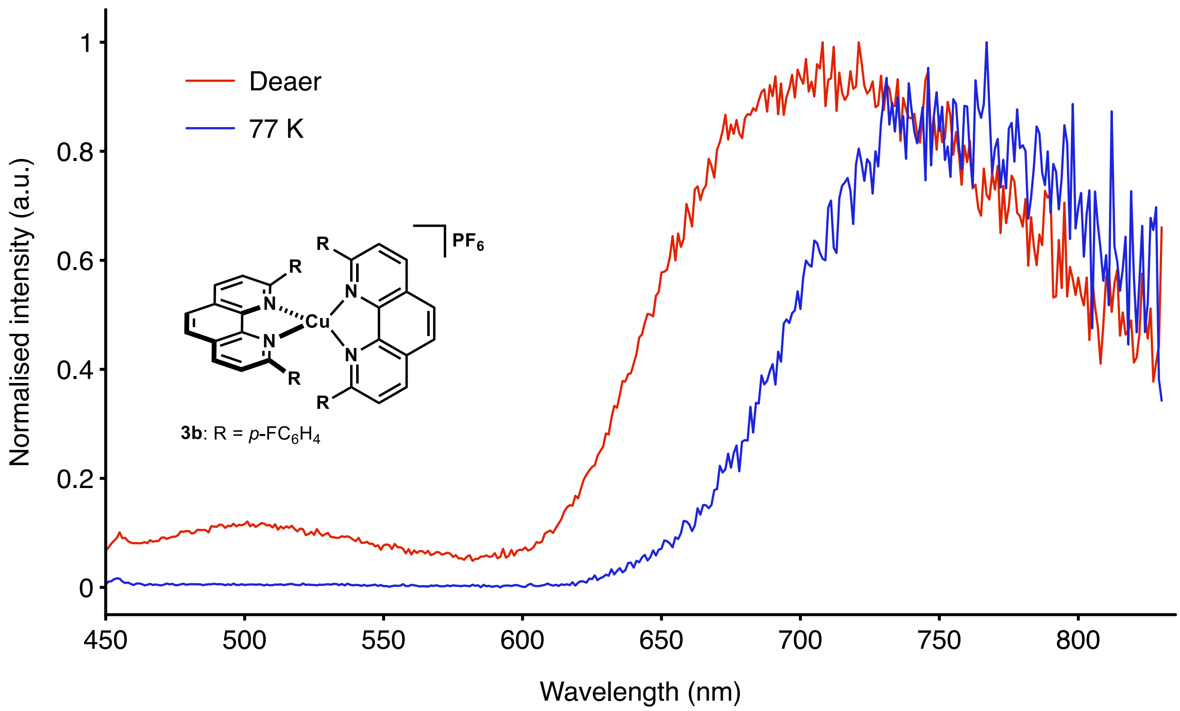


Figure S4b: Emission spectrum of complex **3b** in CH_2Cl_2 (10^{-5} M).

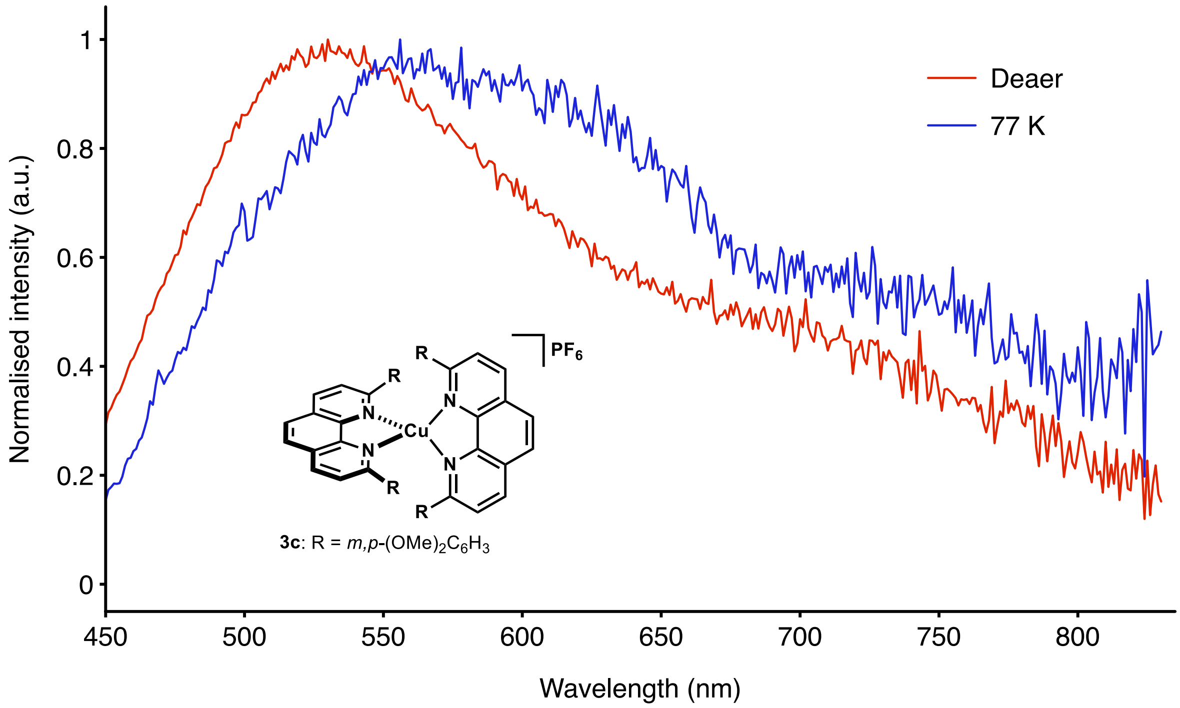


Figure S4c: Emission spectrum of complex **3c** in CH_2Cl_2 (10^{-5} M).

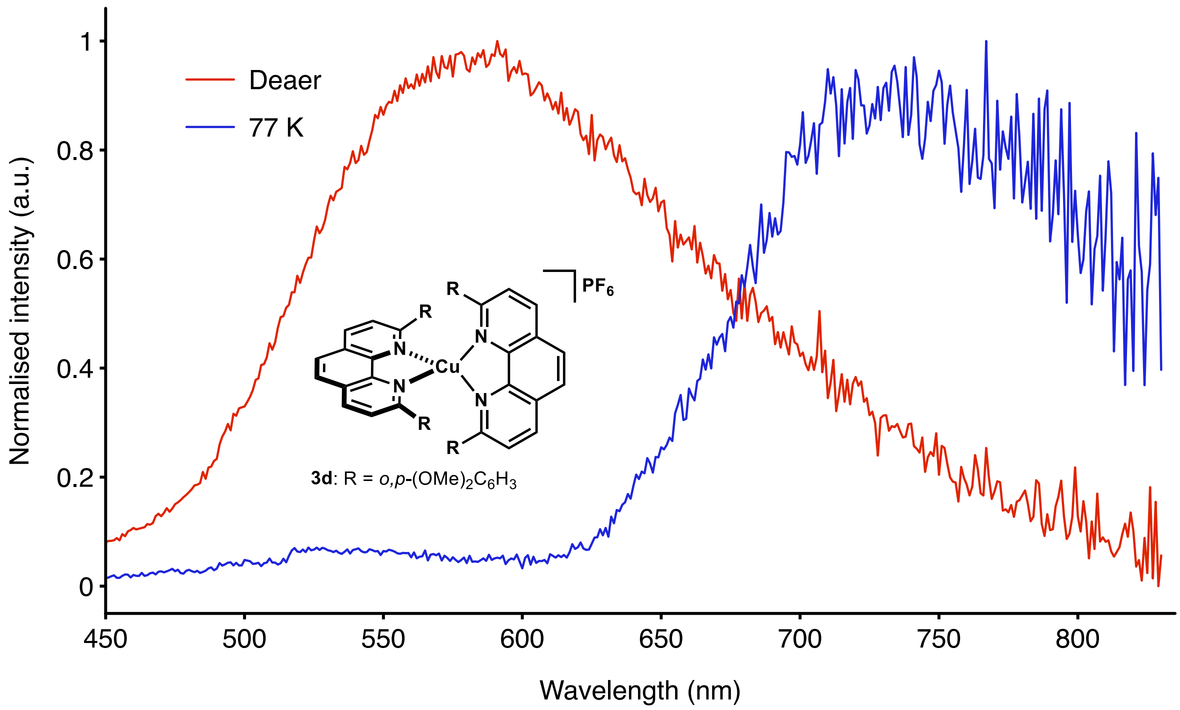


Figure S4d: Emission spectrum of complex **3d** in CH_2Cl_2 (10^{-5} M).

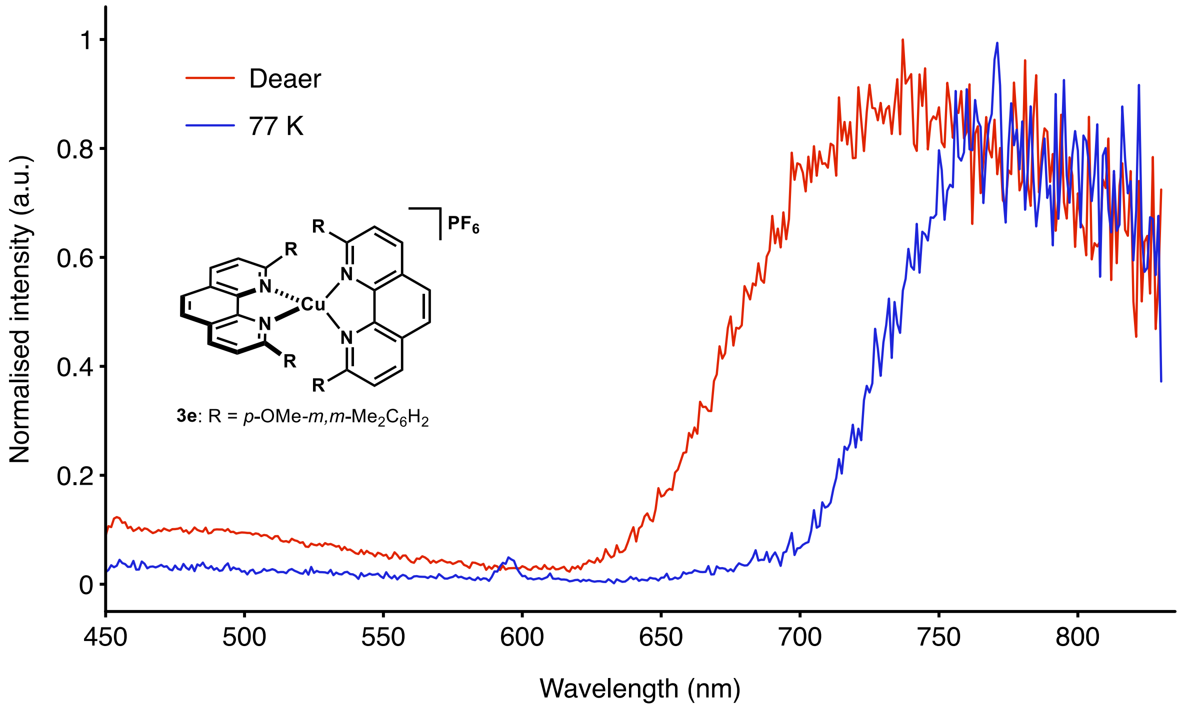


Figure S4e: Emission spectrum of complex **3e** in CH_2Cl_2 (10^{-5} M).

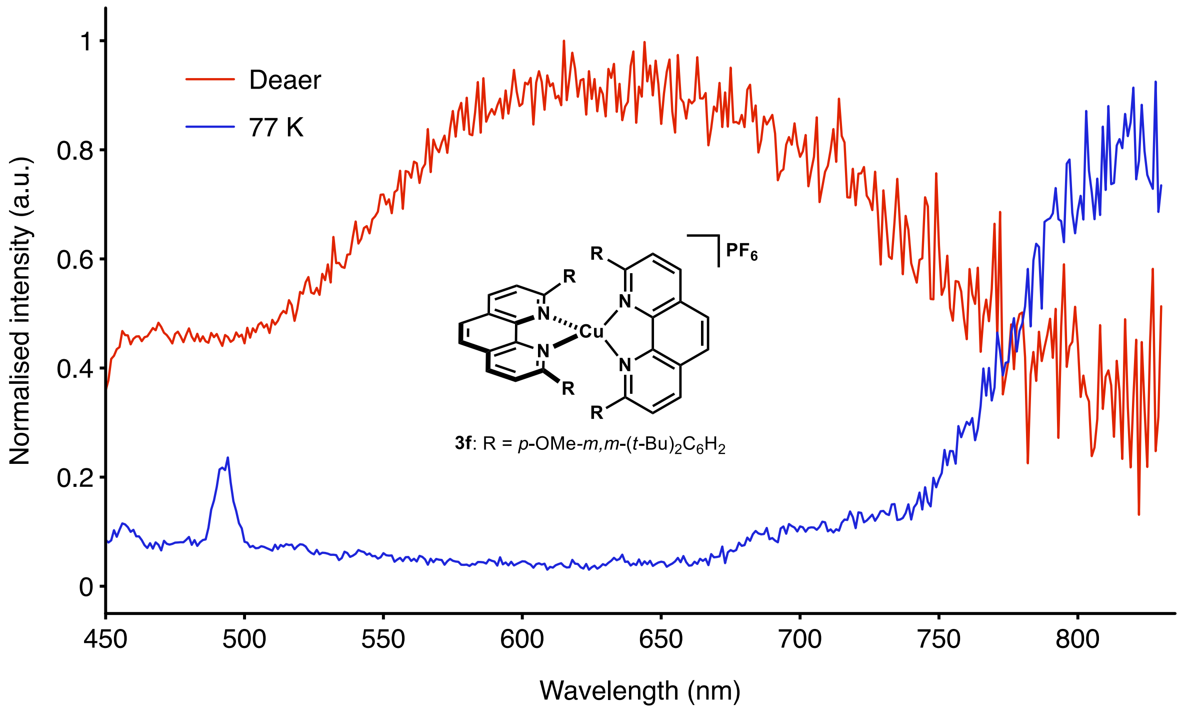


Figure S4f: Emission spectrum of complex **3f** in CH_2Cl_2 (10^{-5} M).

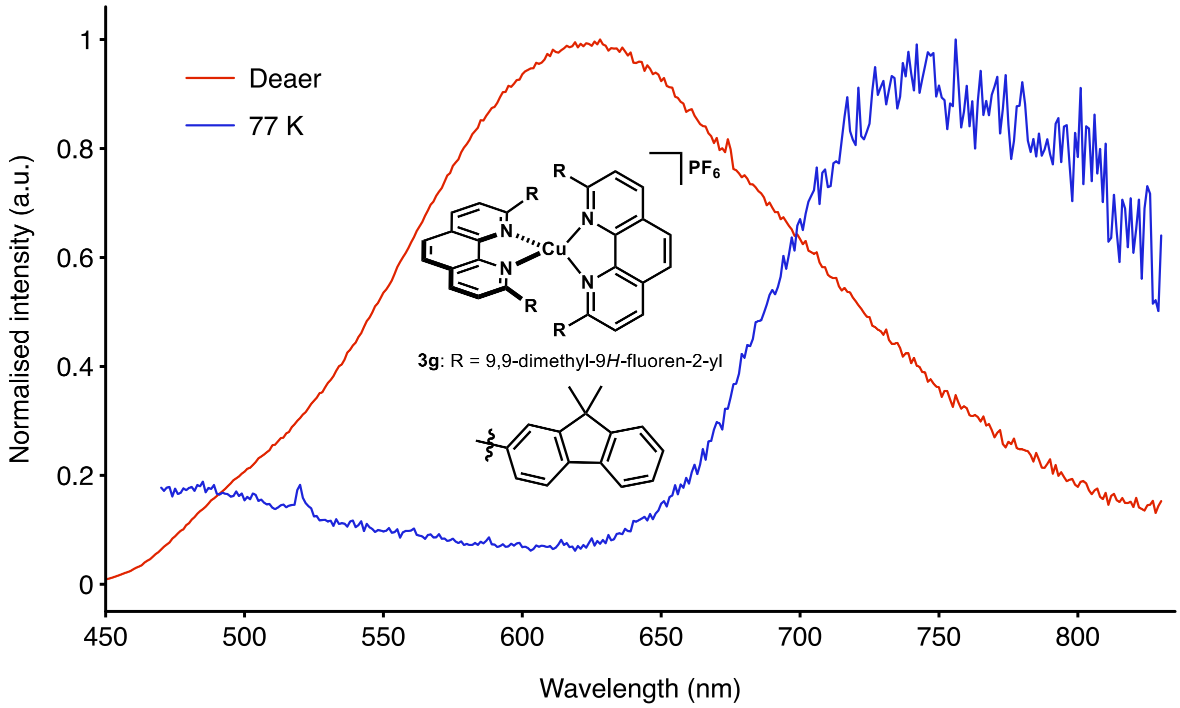


Figure S4g: Emission spectrum of complex **3g** in CH_2Cl_2 (10^{-5} M).

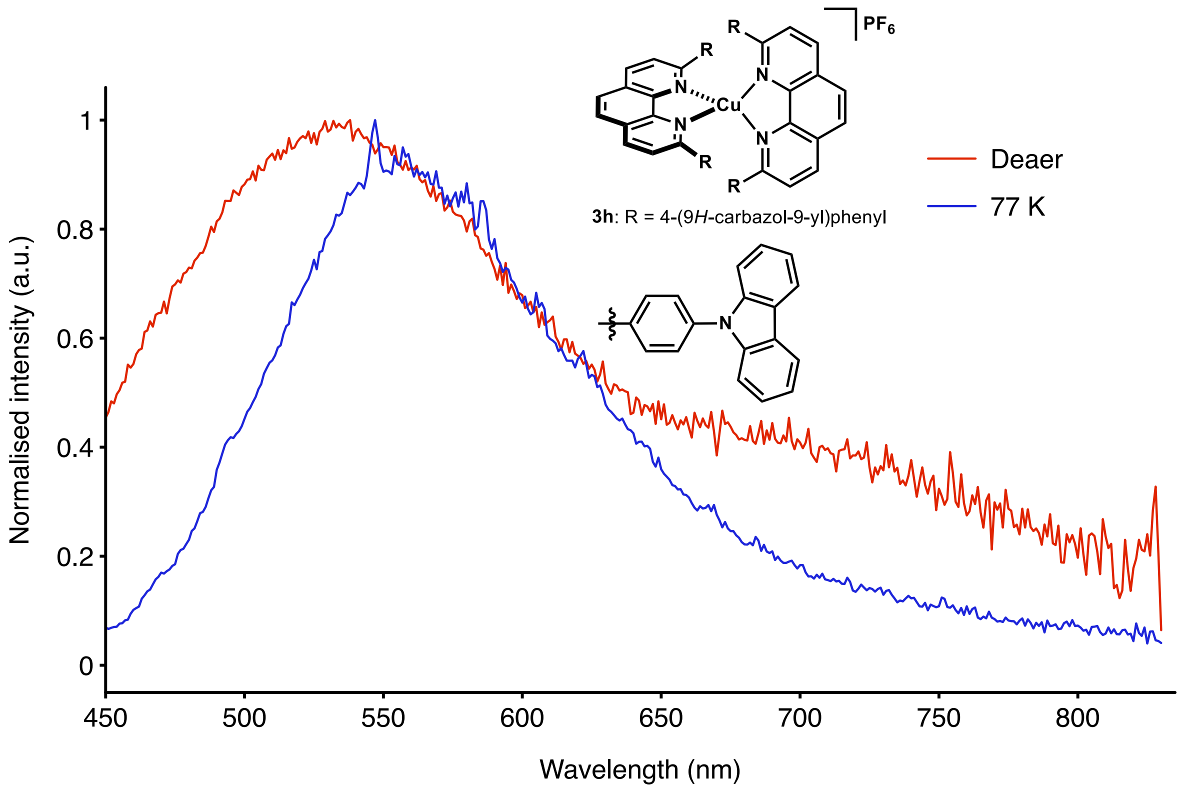


Figure S4h: Emission spectrum of complex **3h** in CH_2Cl_2 (10^{-5} M).

VI. X-Ray Crystallographic Data

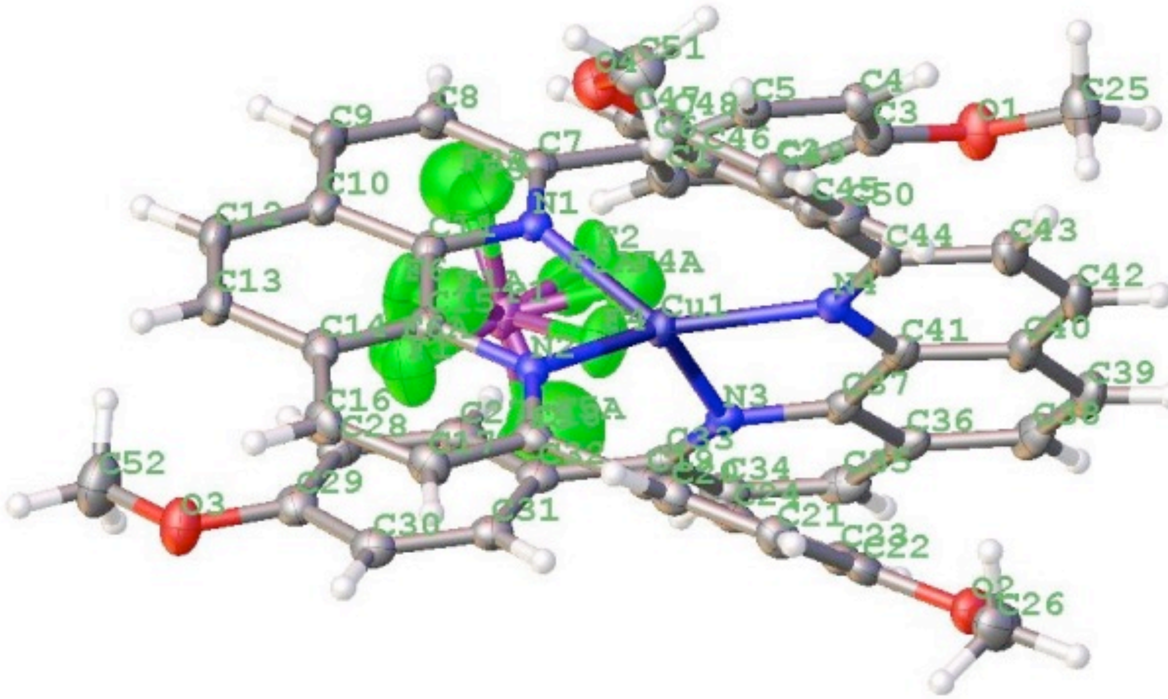


Figure S5a: ORTEP representation of copper(I) complex **1.PF$_6$**. Thermal ellipsoids are drawn at the 50% probability level.

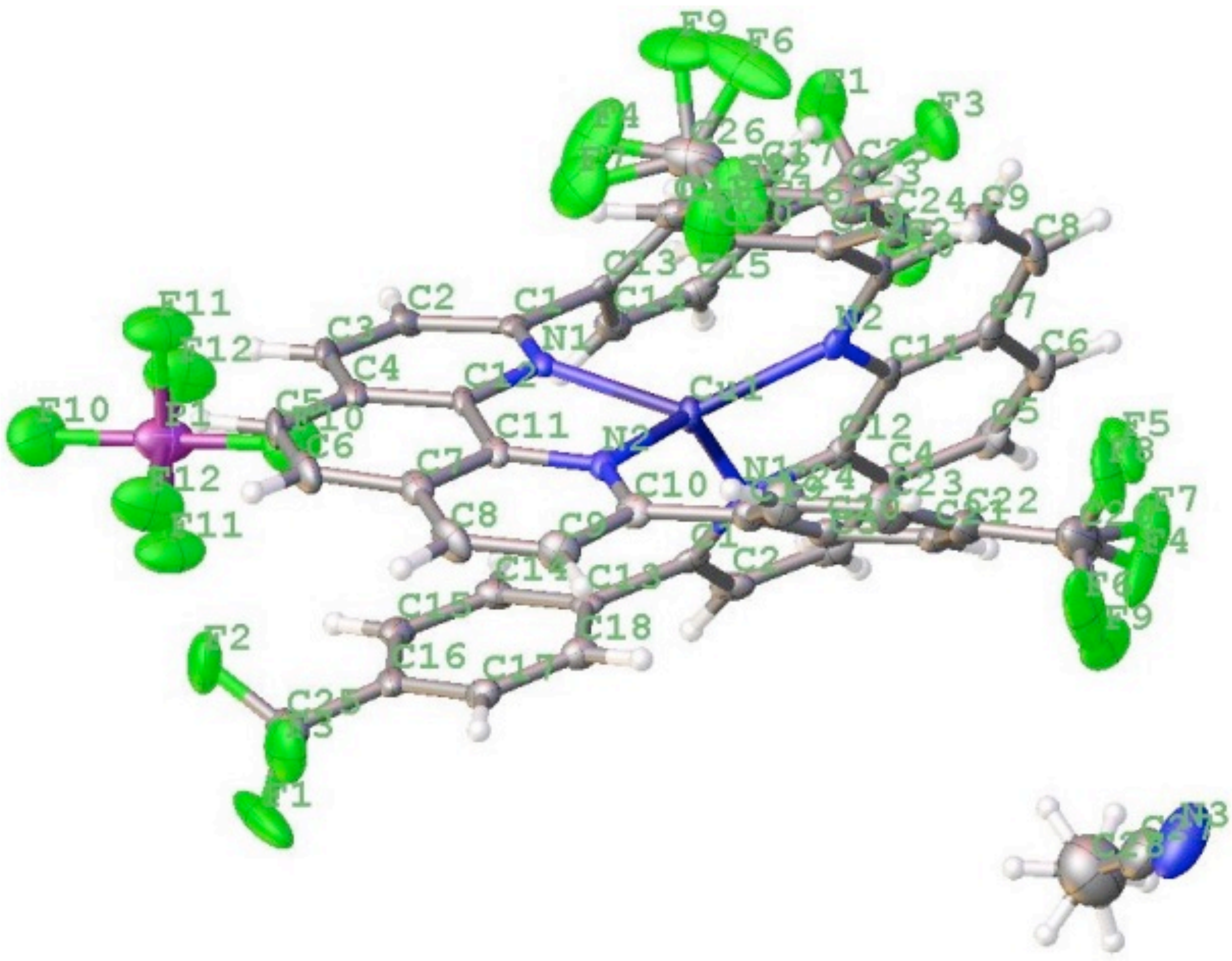


Figure S5b: ORTEP representation of copper(I) complex **3a** Thermal ellipsoids are drawn at the 50% probability level.

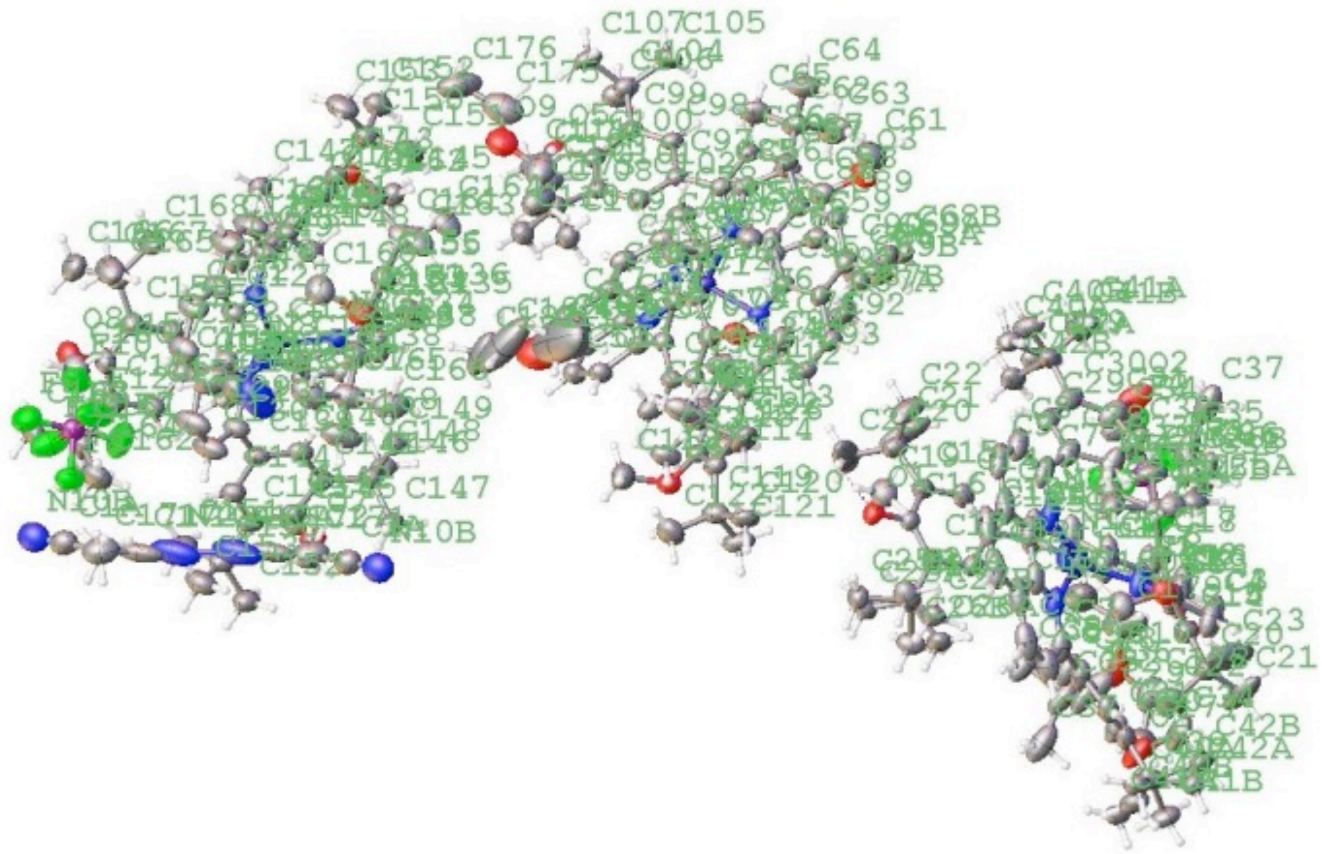


Figure S5c: ORTEP representation of copper(I) complex **3f** Thermal ellipsoids are drawn at the 50% probability level.

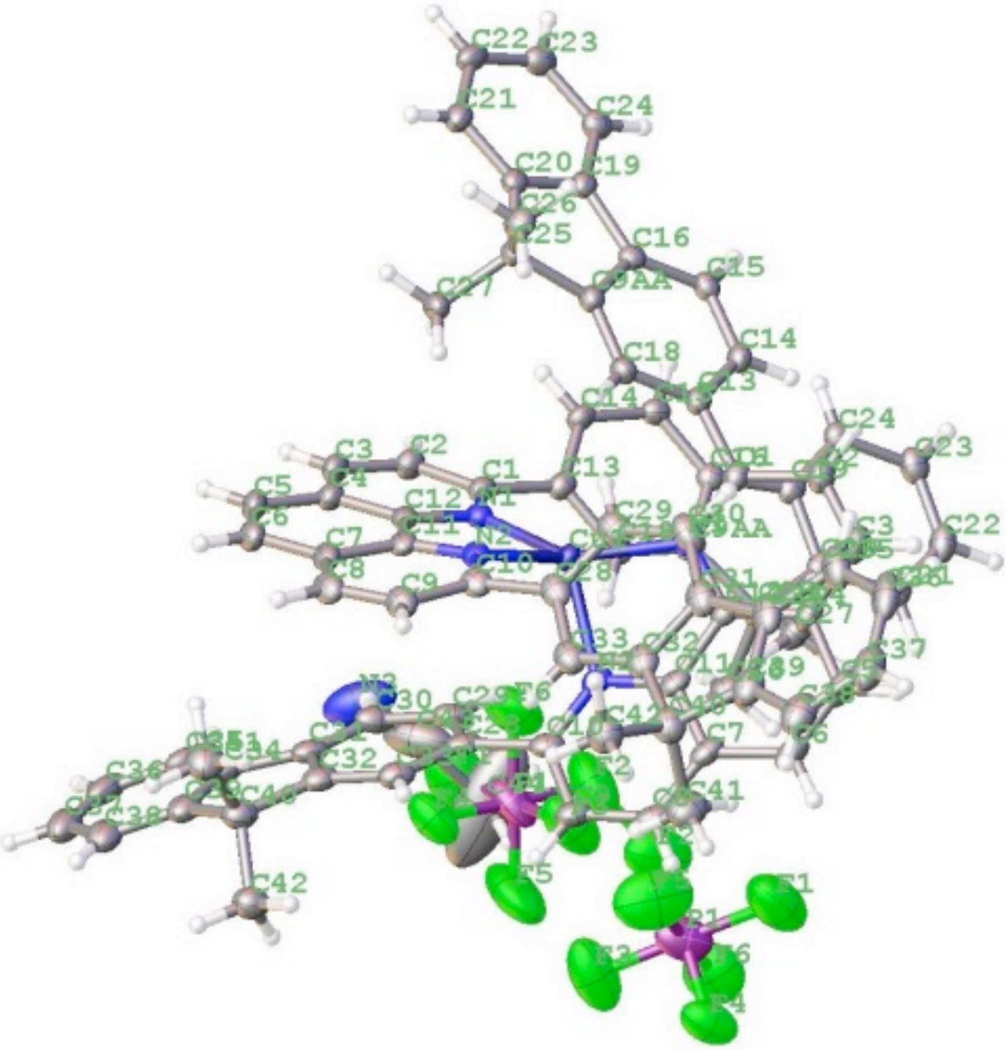


Figure S5d: ORTEP representation of copper(I) complex **3g** Thermal ellipsoids are drawn at the 50% probability level.

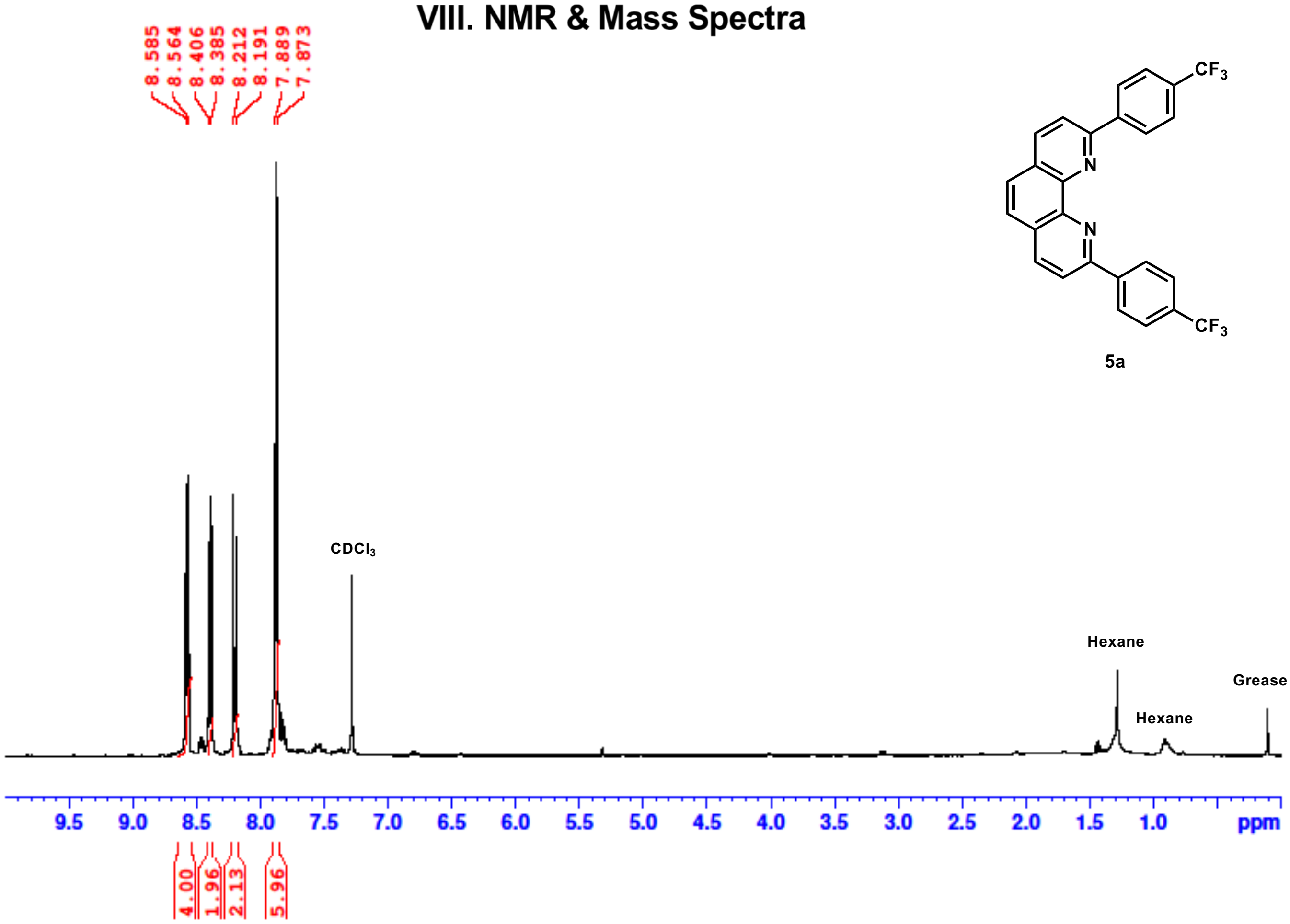
VII. Reported Electrochemical Data

Table S1. Reported electrochemical data for $[Cu(dmp)_2]PF_6$ and complexes **8a**–**d** in degassed CH_3CN (unless otherwise noted) (V vs. SCE).[2–6] [a]Measurements were performed in CH_2Cl_2.

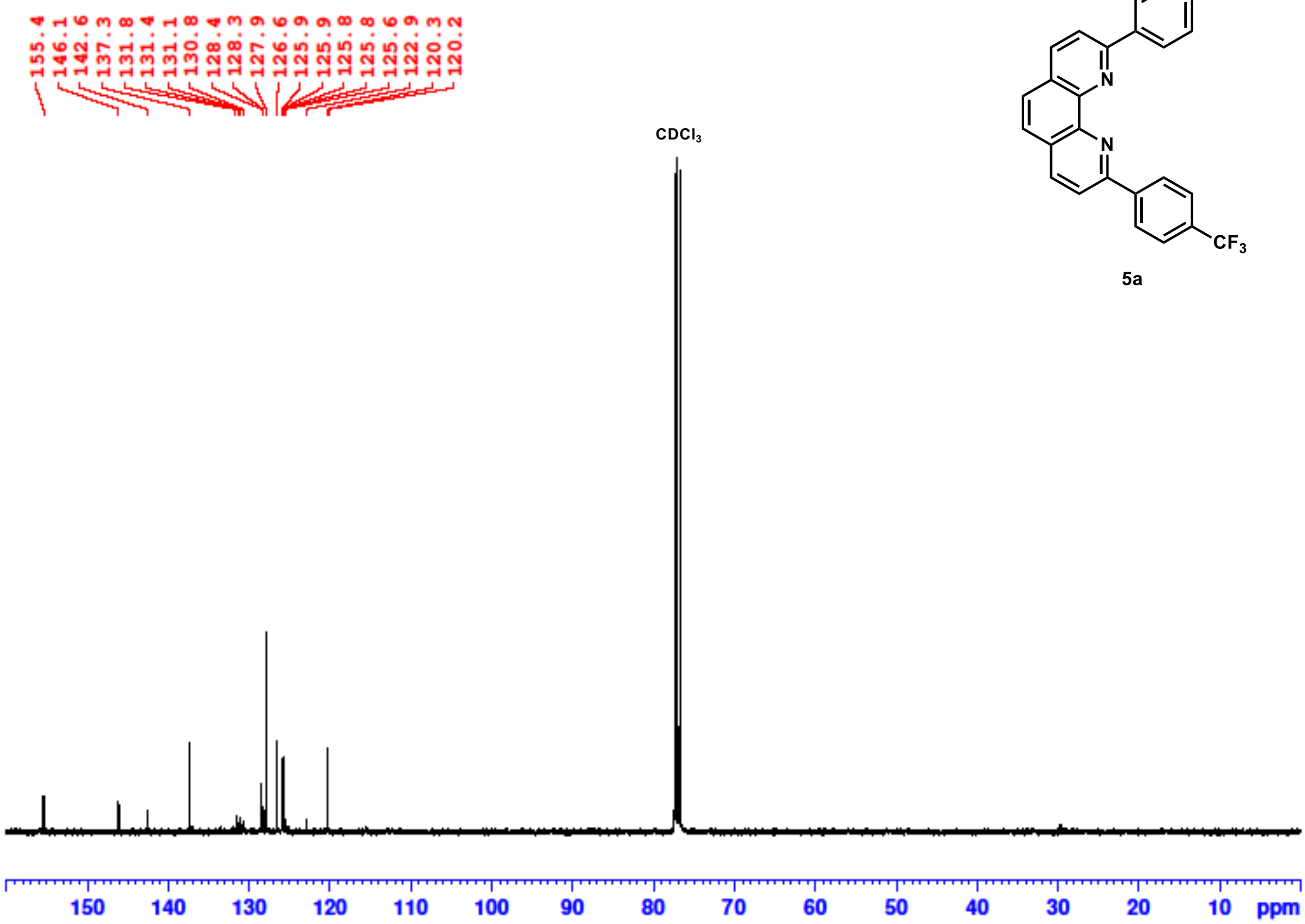
[M]	$E_{1/2}$ (M^+/M^*)	$E_{1/2}$ (M^*/M^-)	$E_{1/2}$ (M^+/M)	$E_{1/2}$ (M/M^-)	ref.
$[Cu(dmp)_2]PF_6$	–1.54	–	+0.63	–	2
8a	–1.44	+1.00	+1.20	–1.73	3
8b	–1.34	+1.04	+1.34	–1.64	4
8c	–1.35	+1.01	+1.26[a]	–1.60[a]	5
8d	–1.02	+0.63	+1.25	–1.64	6

2. D. R. McMillin, M. T. Buckner and B. T. Ahn, *Inorg. Chem.,* 1977, **16**, 943.
3. Y. Zhang, M. Heberle, M. Wätchler, M. Karnahl and B. Dietzek, *RSC adv.*, 2016, **6**, 105801.
4. E. Mejía, S.-P. Luo, M. Karnahl, A. Friedrich, S. Tschierlei, A.-E. Surkus, H. Junge, S. Gladiali, S. Lochbrunner and M. Beller, *Chem. Eur. J.*, 2013, **19**, 15972.
5. (*a*) S. Kuang, D. G. Cuttell, D. R. McMillin, P. E. Fanwick, R. A. Walton and W. Lafayette, *Inorg. Chem.*, 2002, **41**, 3313; (*b*) D. G. Cuttell, S.-M kuang, P. E. Fanwick, D. R. McMillan and R. A. Walton, *J. Am. Chem. Soc.*, 2002, **124**, 6.
6. A. Call, C. Casadevall, F. Acuña-Parés, A. Casitas and J. Lloret-Fillol, *Chem. Sci.*, 2017, **8**, 4739.

VIII. NMR & Mass Spectra



5a



5a

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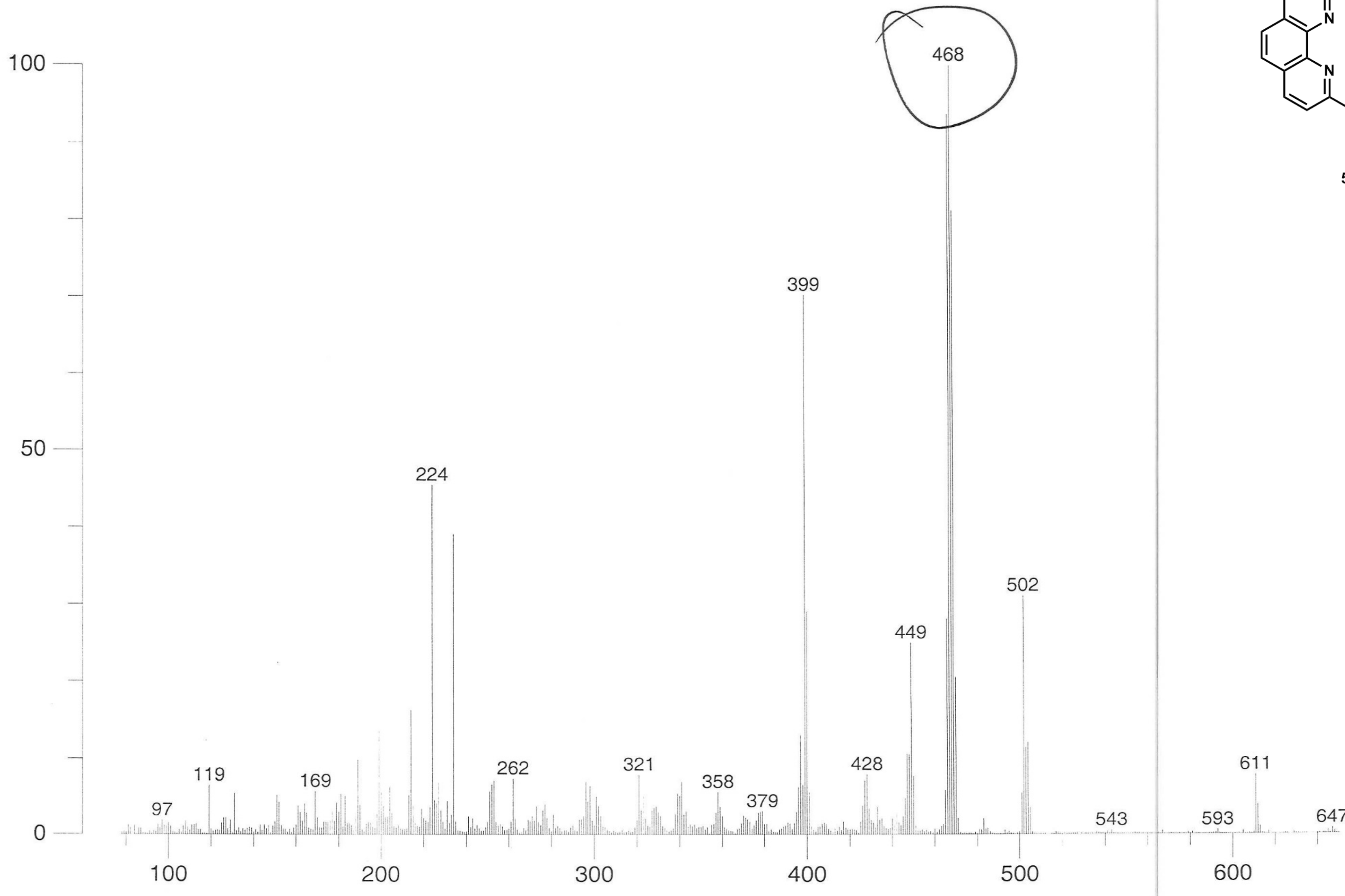

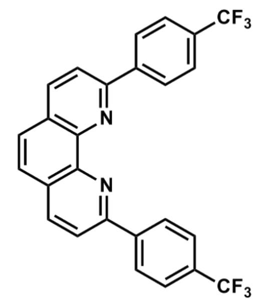

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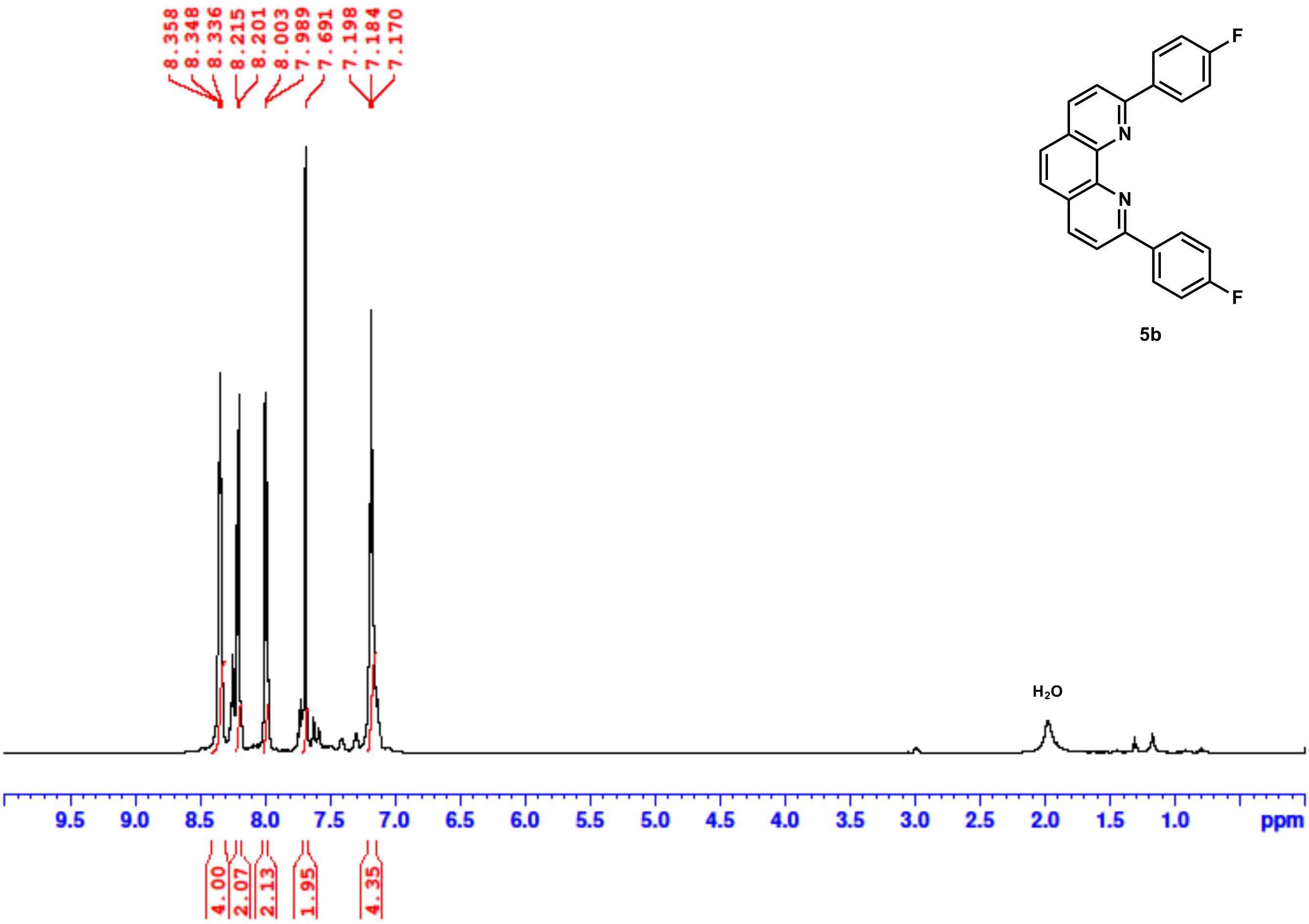
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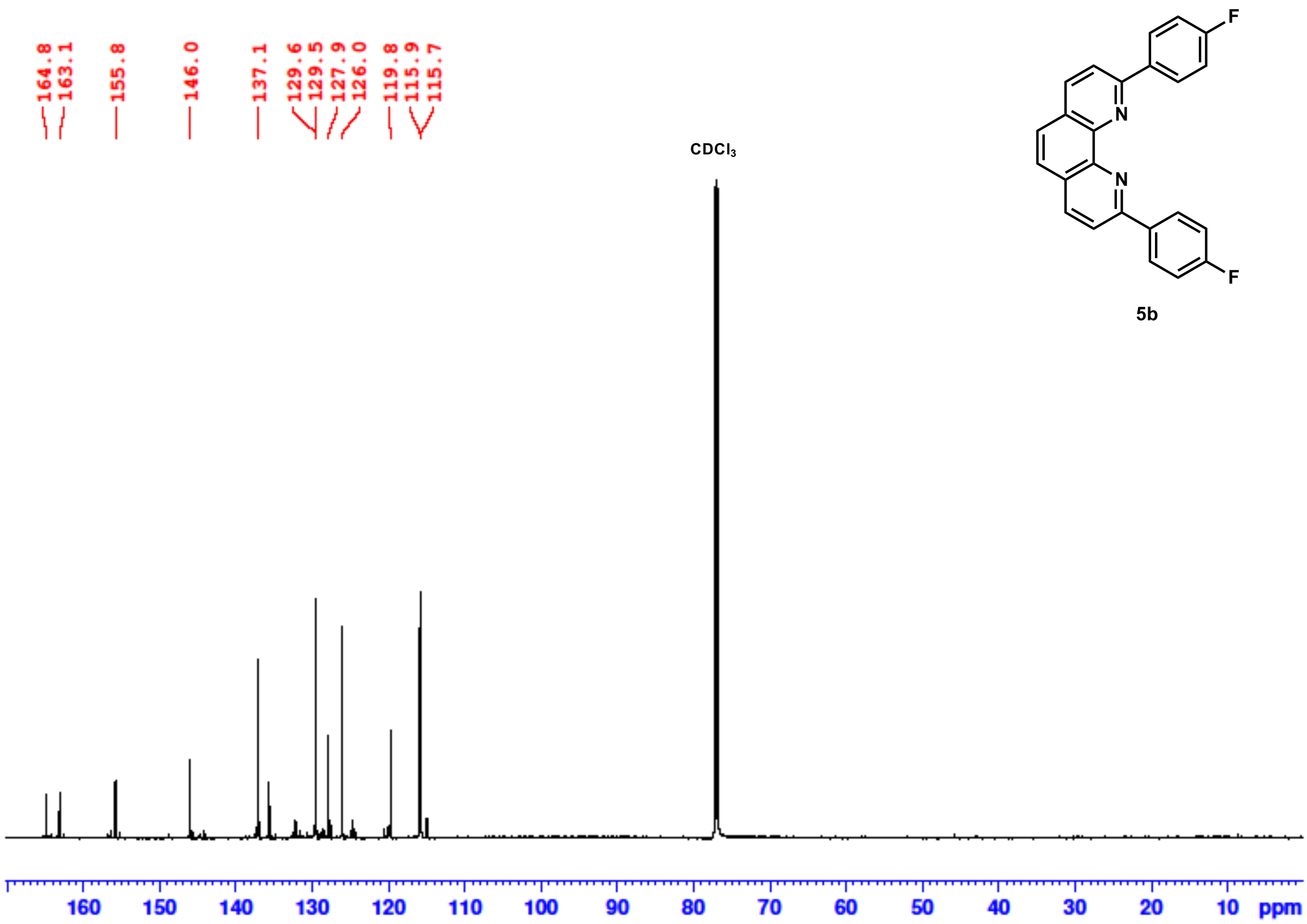
N
F
5b
H$_2$O
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00
2.07
2.13
1.95
4.35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155.8
146.0
137.1
129.6
129.5
127.9
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119.8
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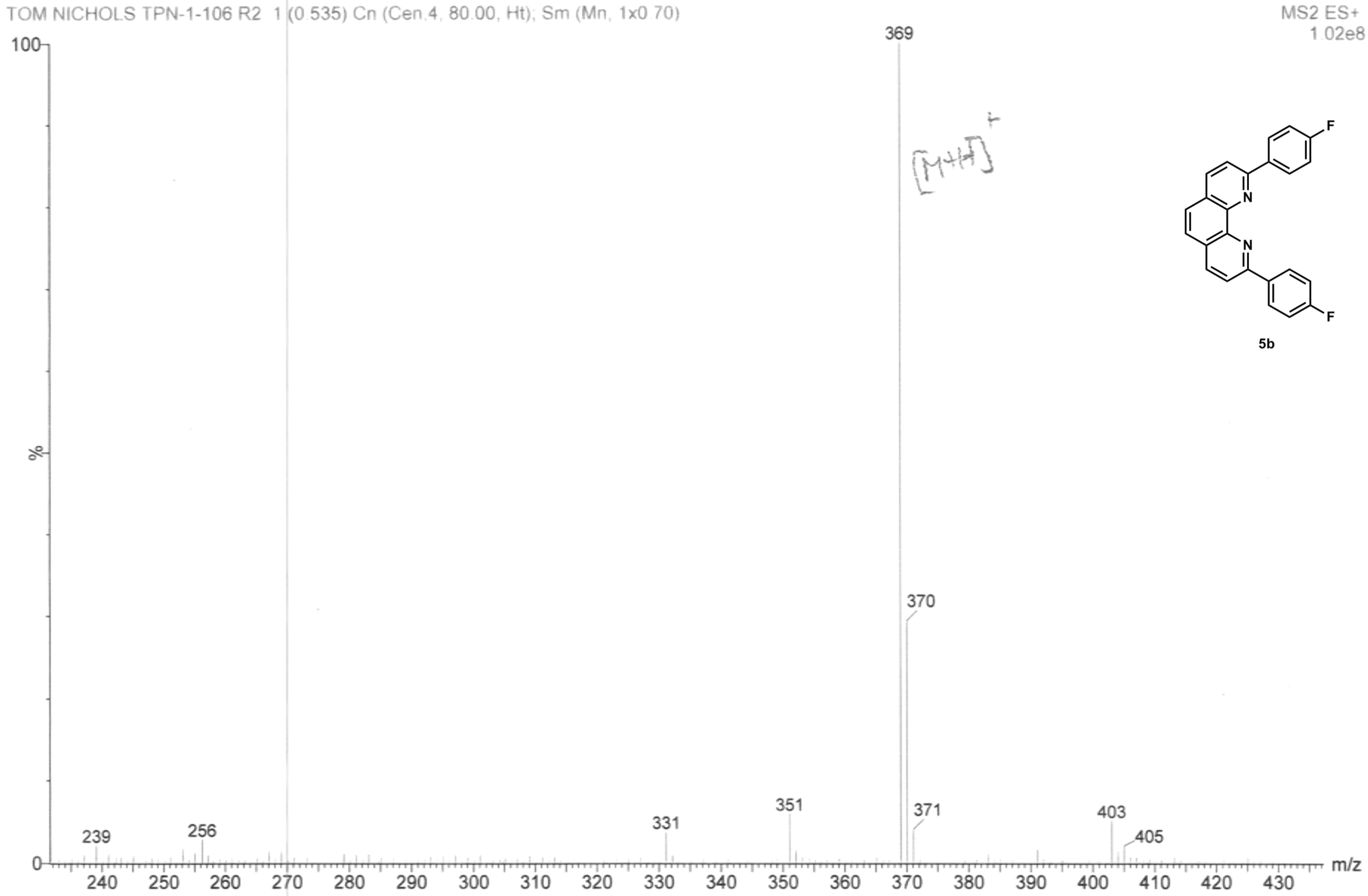
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100
%
0
369
[M+H]+
370
371
351
331
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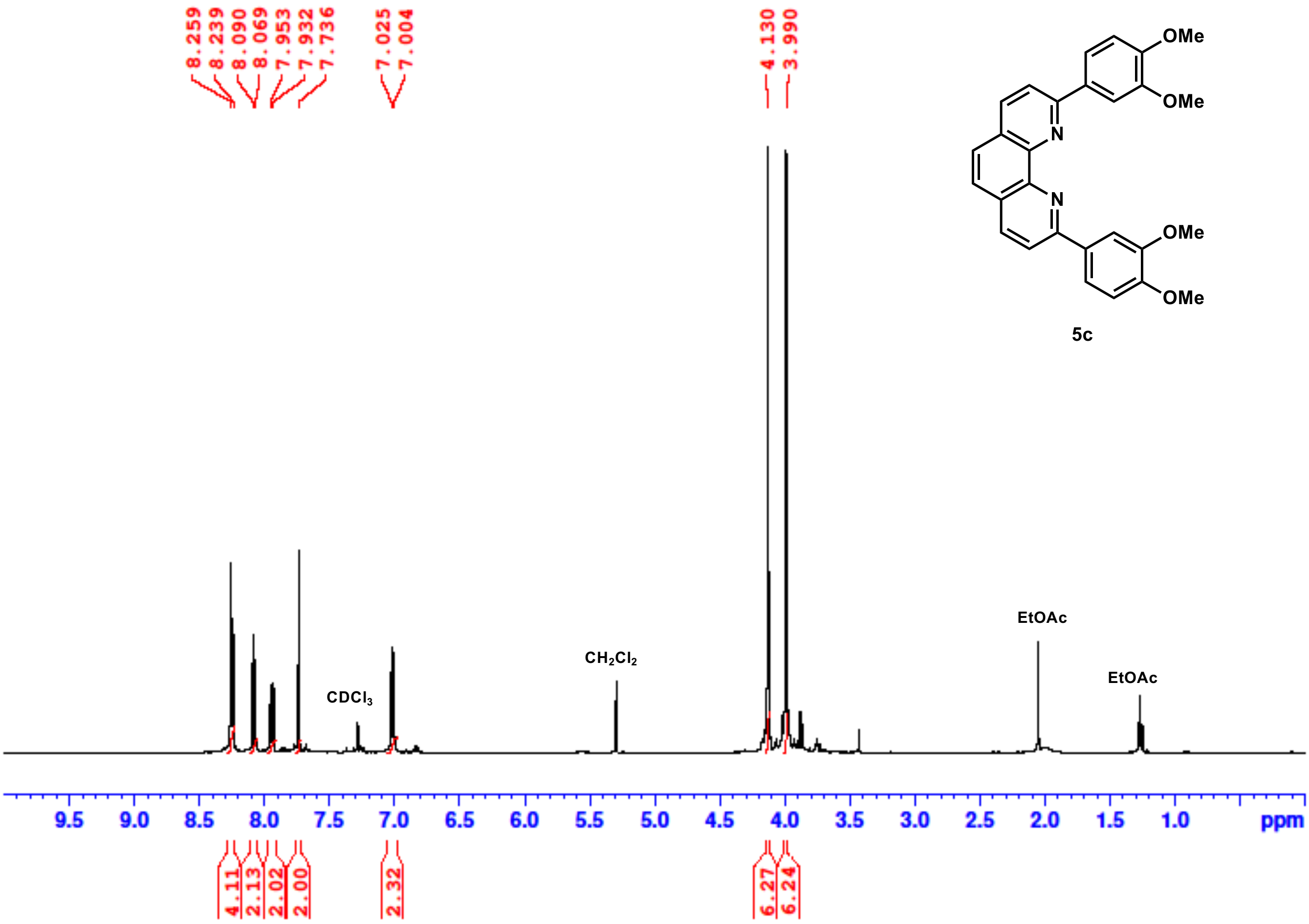
F
5b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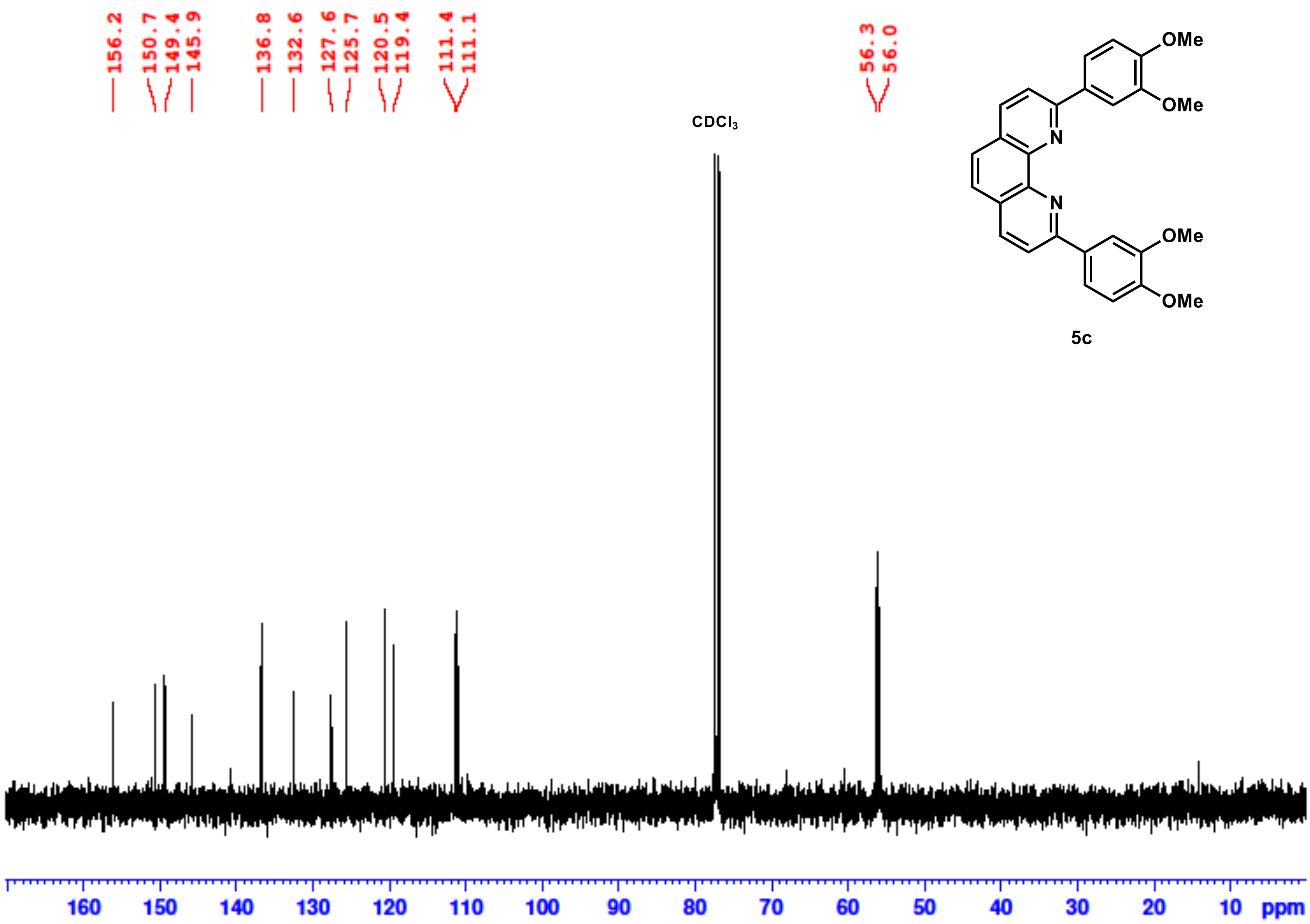
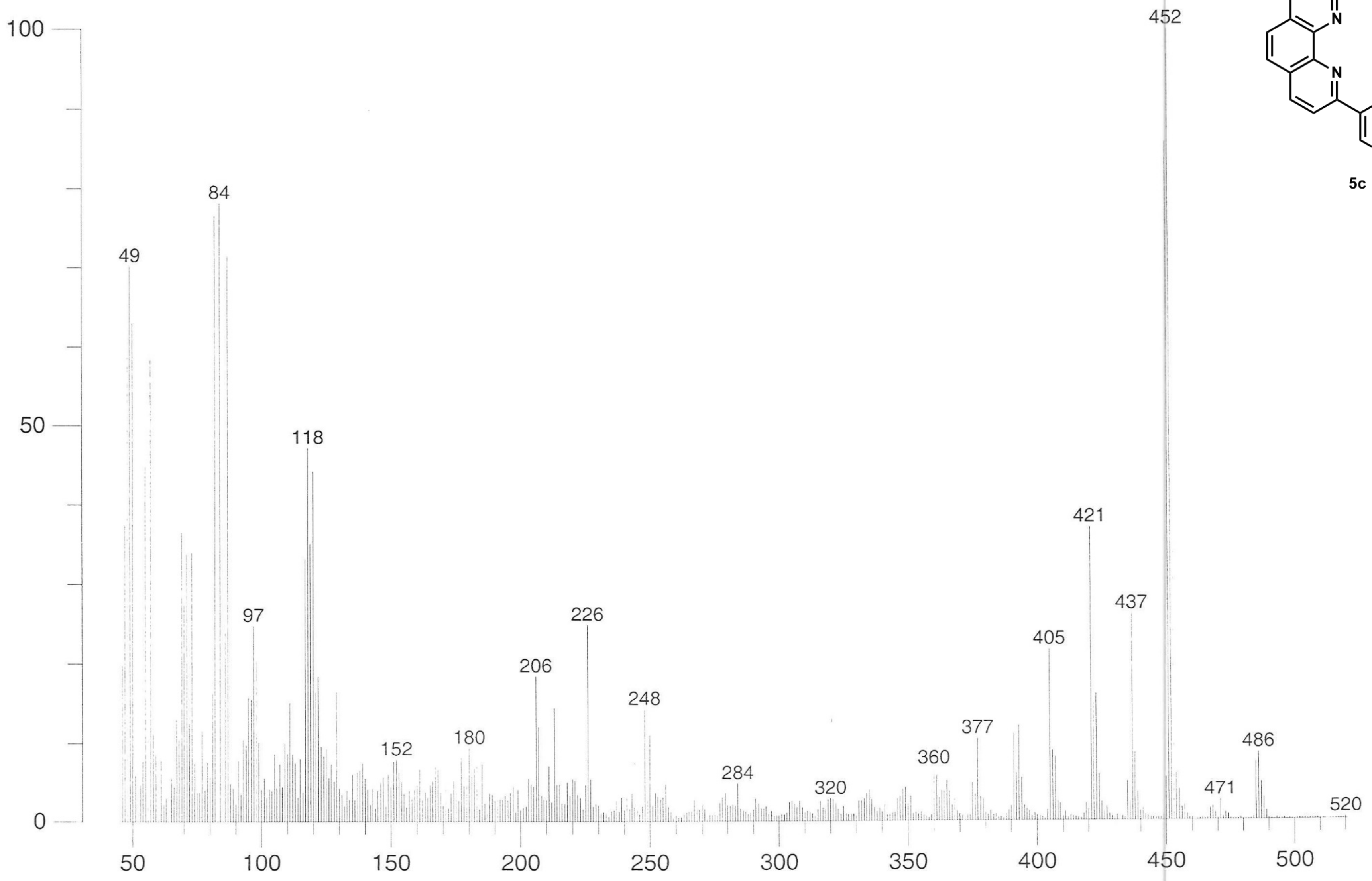
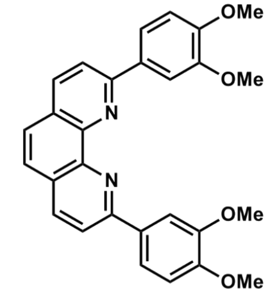
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.11
2.13
2.02
2.00
2.32
6.27
6.24

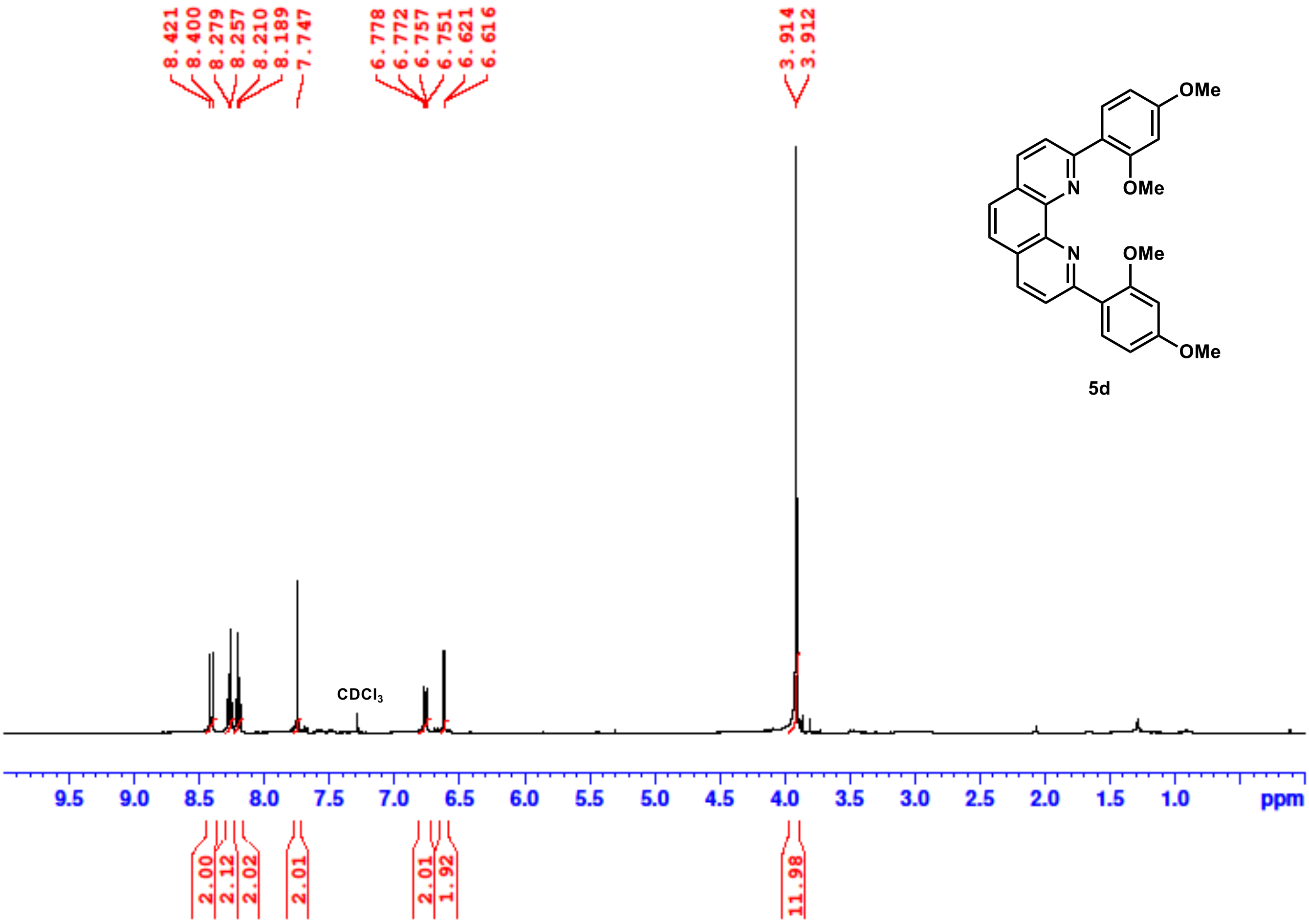

156.2
150.7
149.4
145.9
136.8
132.6
127.6
125.7
120.5
119.4
111.4
111.1
56.3
56.0
CDCl3
OMe
OMe
N
N
OMe
OMe
5c
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

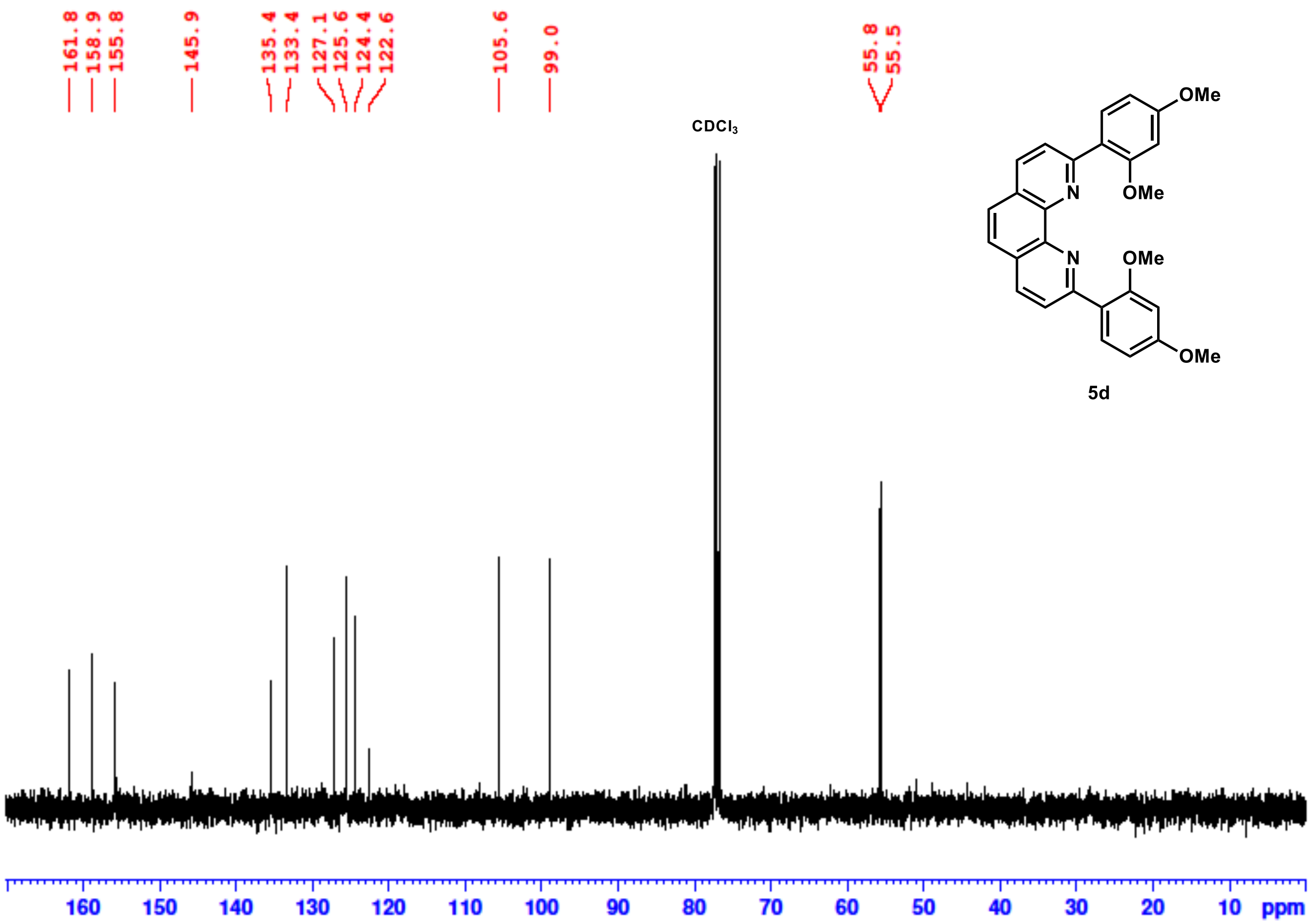
tnicho0010 Scan 1 (Av 115, 115 Acq) 100%=146478 mv 4 Nov 115 16:06
LRP +EI tom nicholls TPN-1-83 nommass

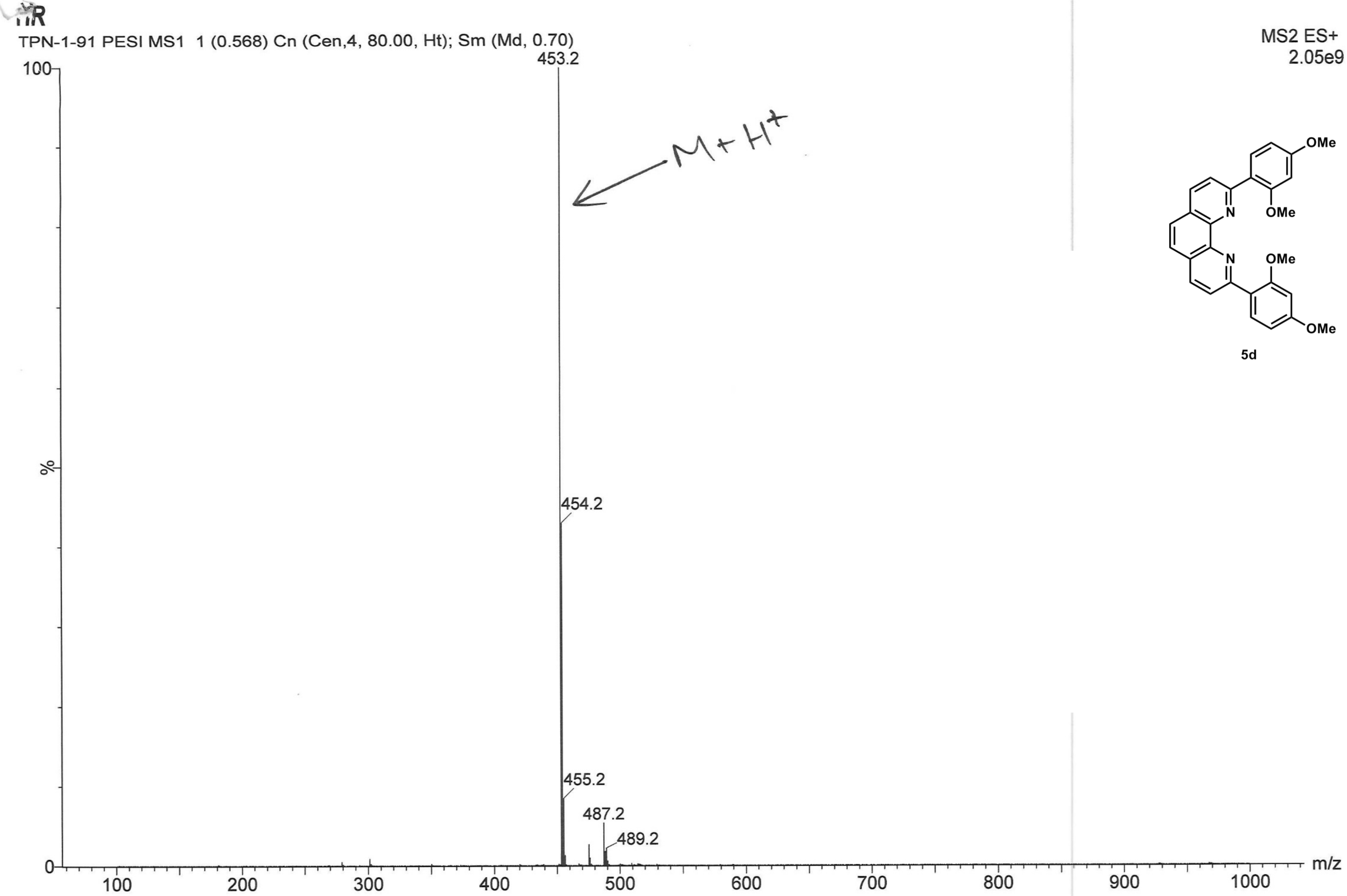




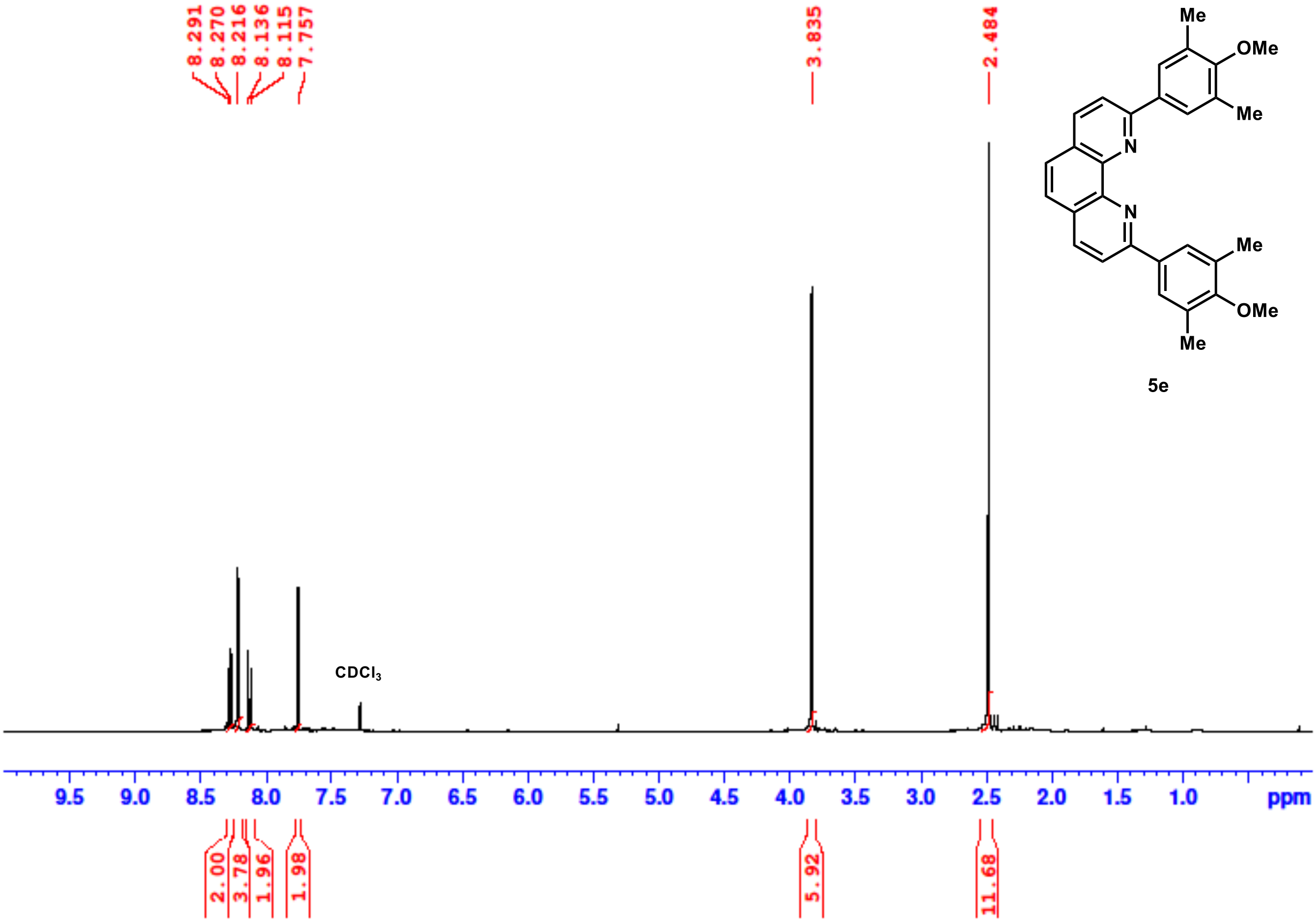
5c

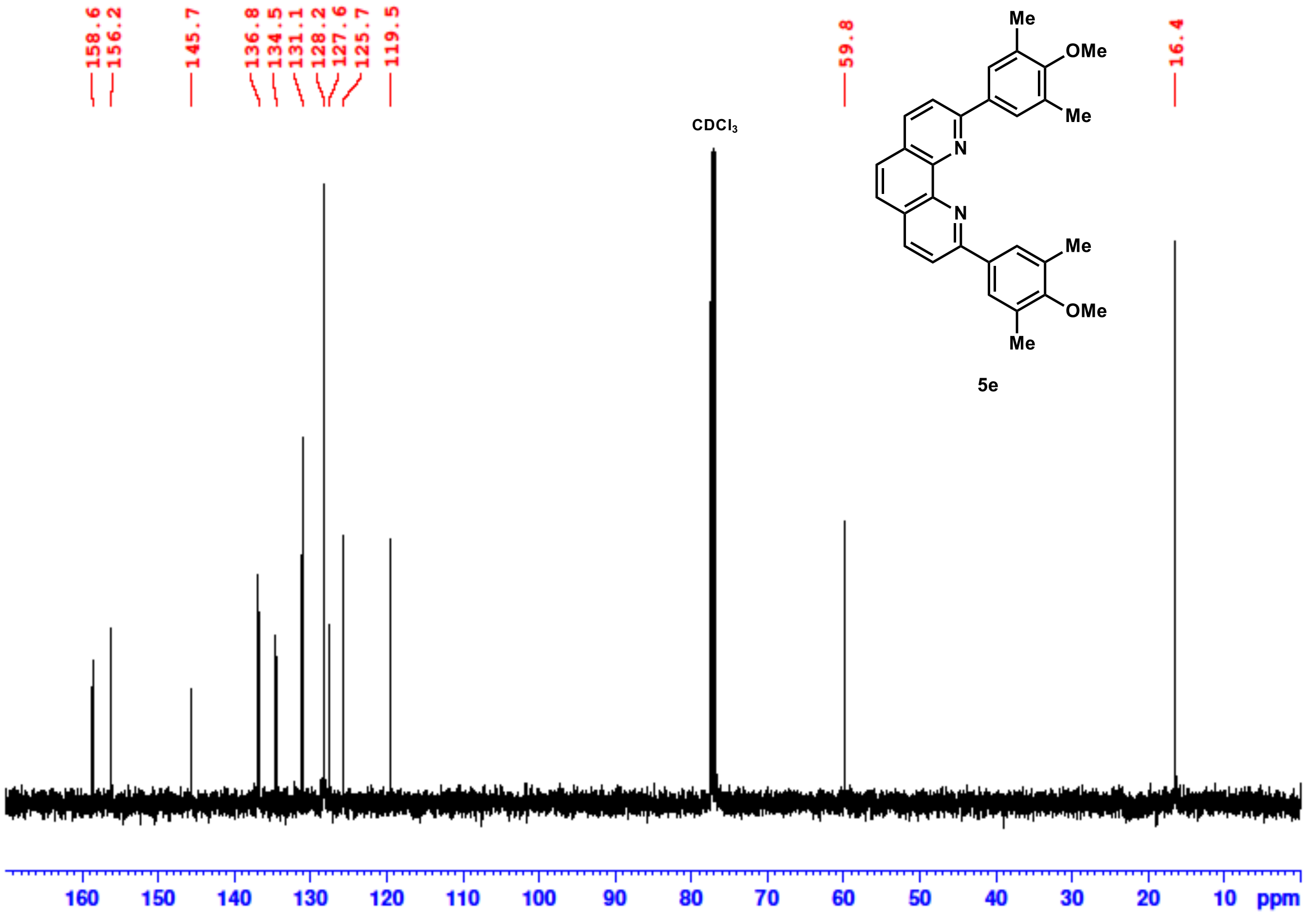

8.421
8.400
8.279
8.257
8.210
8.189
7.747
6.778
6.772
6.757
6.751
6.621
6.616
3.914
3.912
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
2.12
2.02
2.01
2.01
1.92
11.98
OMe
OMe
OMe
OMe
N
N
5d


161.8
158.9
155.8
145.9
135.4
133.4
127.1
125.6
124.4
122.6
105.6
99.0
55.8
55.5
CDCl3
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
OMe
OMe
OMe
OMe
N
N
5d

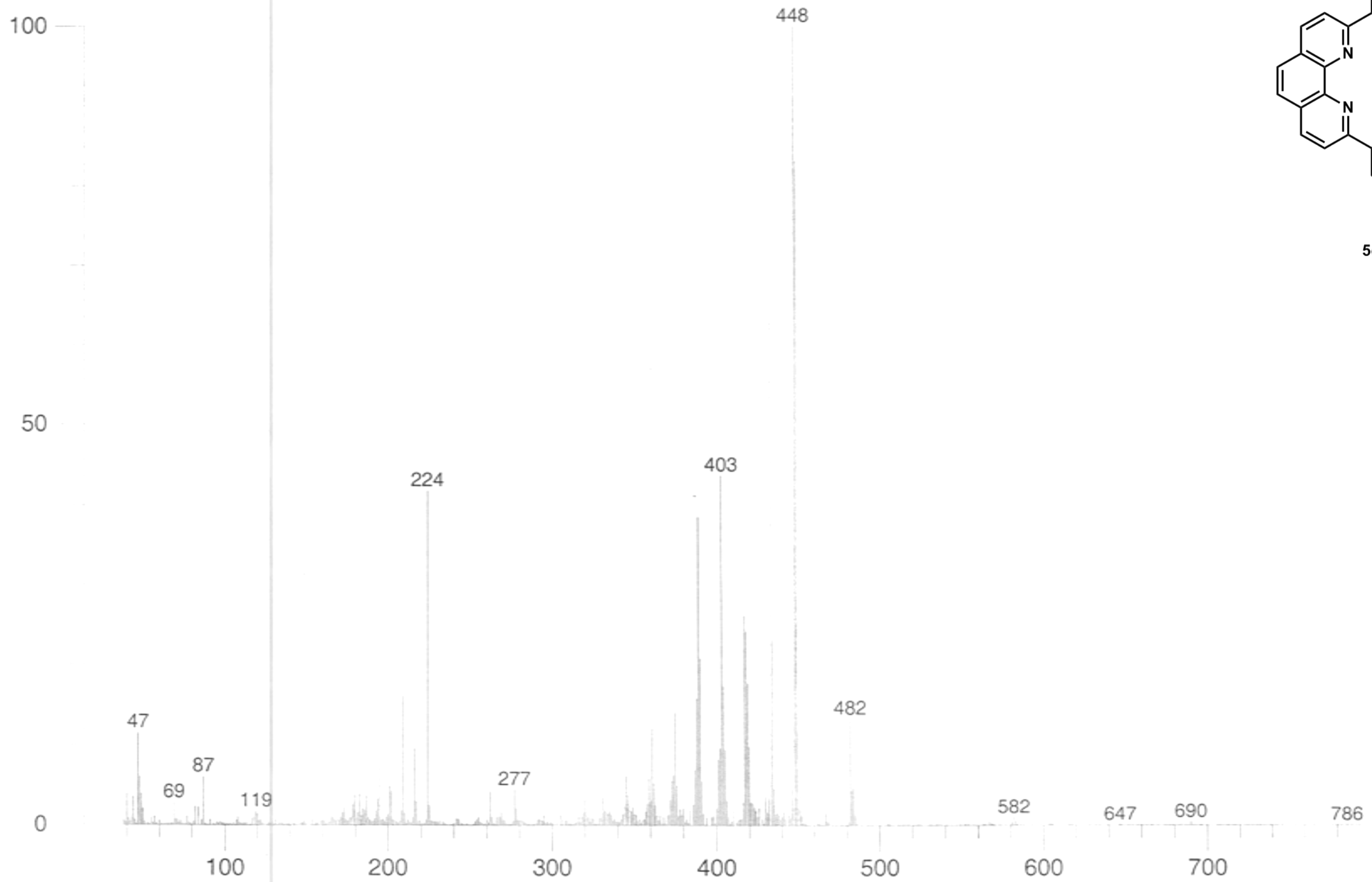


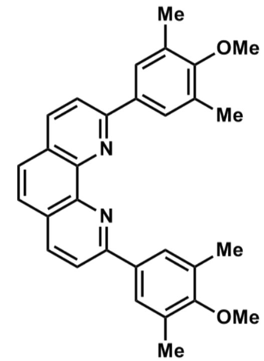
HR
TPN-1-91 PESI MS1 1 (0.568) Cn (Cen,4, 80.00, Ht); Sm (Md, 0.70)
MS2 ES+
2.05e9
453.2
M+H+
454.2
455.2
487.2
489.2
100
%
0
100
200
300
400
500
600
700
800
900
1000
m/z
OMe
OMe
OMe
OMe
N
N
5d


8.291
8.270
8.216
8.136
8.115
7.757
3.835
2.484
Me
OMe
Me
N
N
Me
OMe
Me
5e
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
3.78
1.96
1.98
5.92
11.68

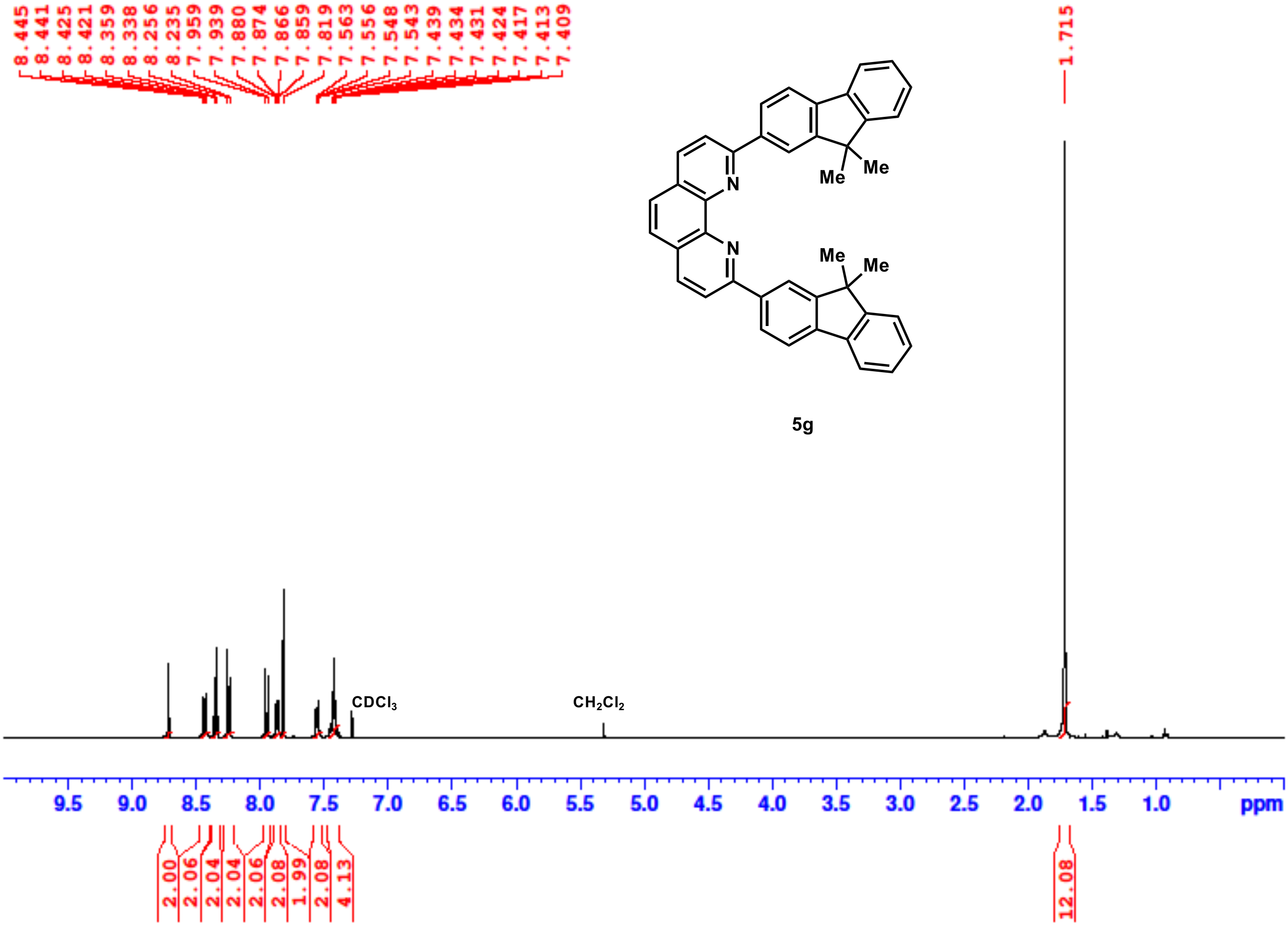

158.6
156.2
145.7
136.8
134.5
131.1
128.2
127.6
125.7
119.5
59.8
16.4
CDCl3
Me
OMe
Me
N
N
Me
OMe
Me
5e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

tnicho0014 Scan 2 (Av 41-42 Acq) 100%=145516 mv 12 Jan 116 14:40
LRP +EI tom nicholls TPN-1-98 nom mass2



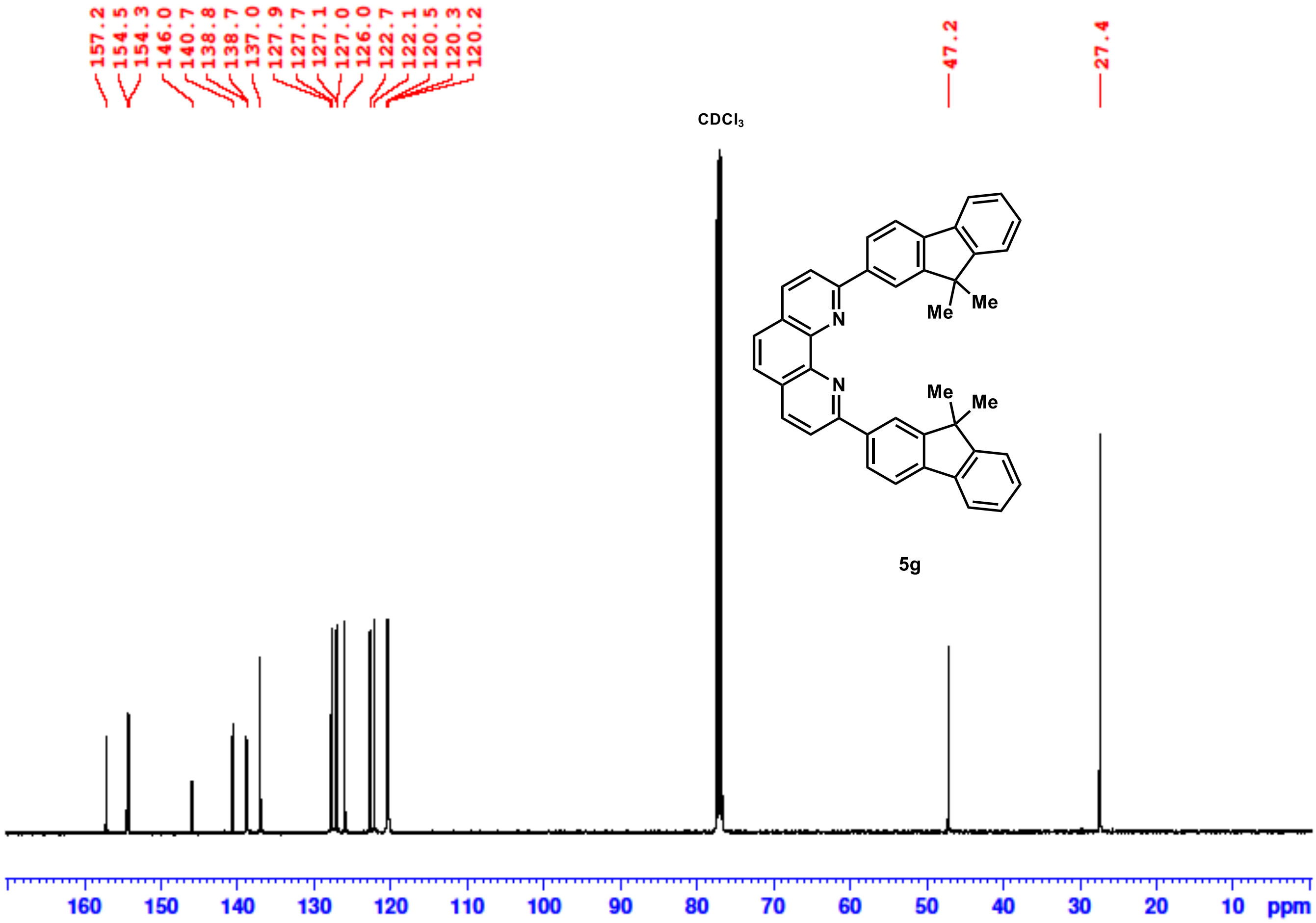


5e



8.445
8.441
8.425
8.421
8.359
8.338
8.256
8.235
7.959
7.939
7.880
7.874
7.866
7.859
7.819
7.563
7.556
7.548
7.543
7.439
7.434
7.431
7.424
7.417
7.413
7.409
1.715
Me
Me
Me
Me
N
N
CDCl3
CH2Cl2
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
2.06
2.04
2.04
2.06
2.08
1.99
2.08
4.13
12.08

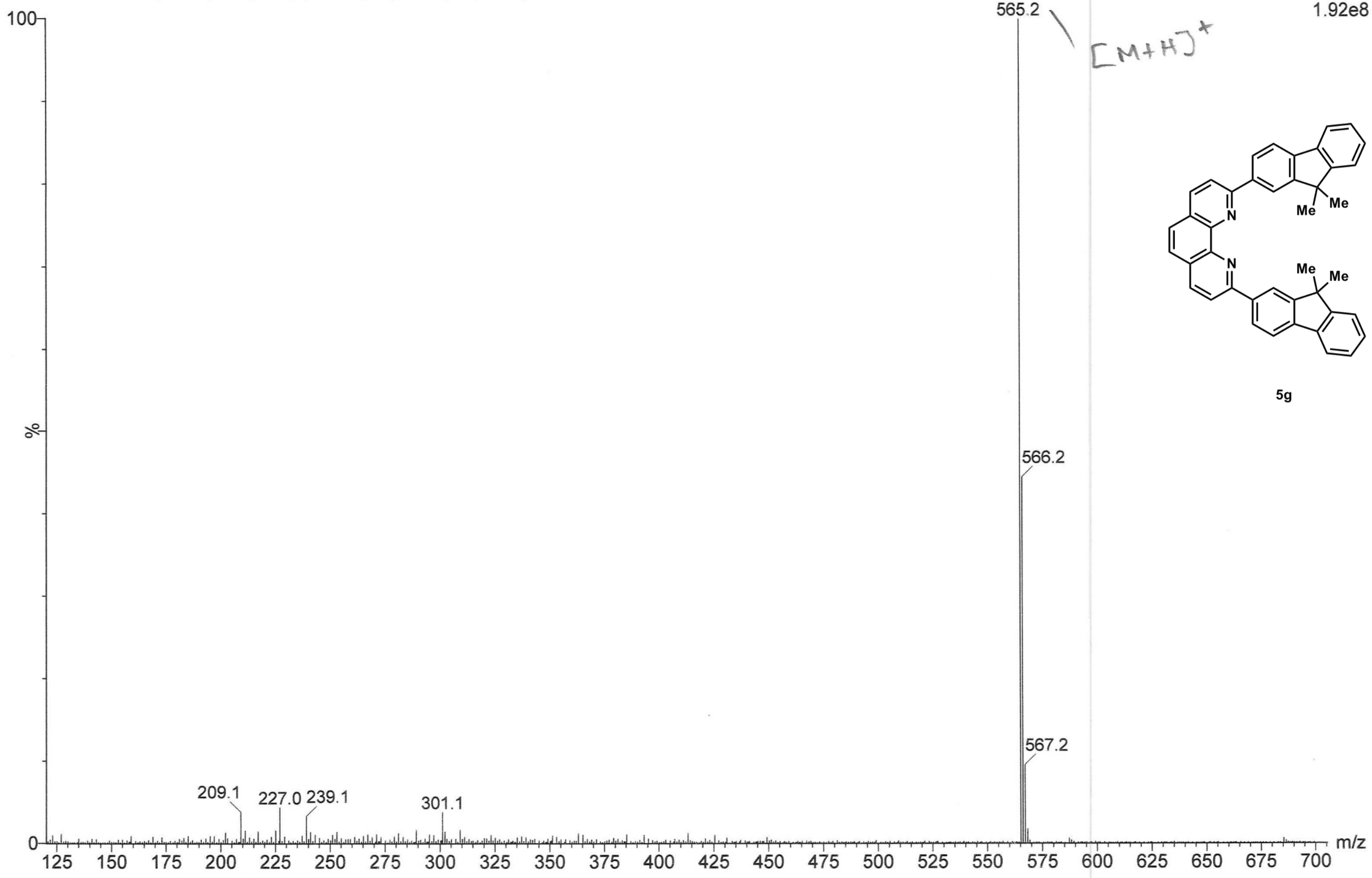
5g

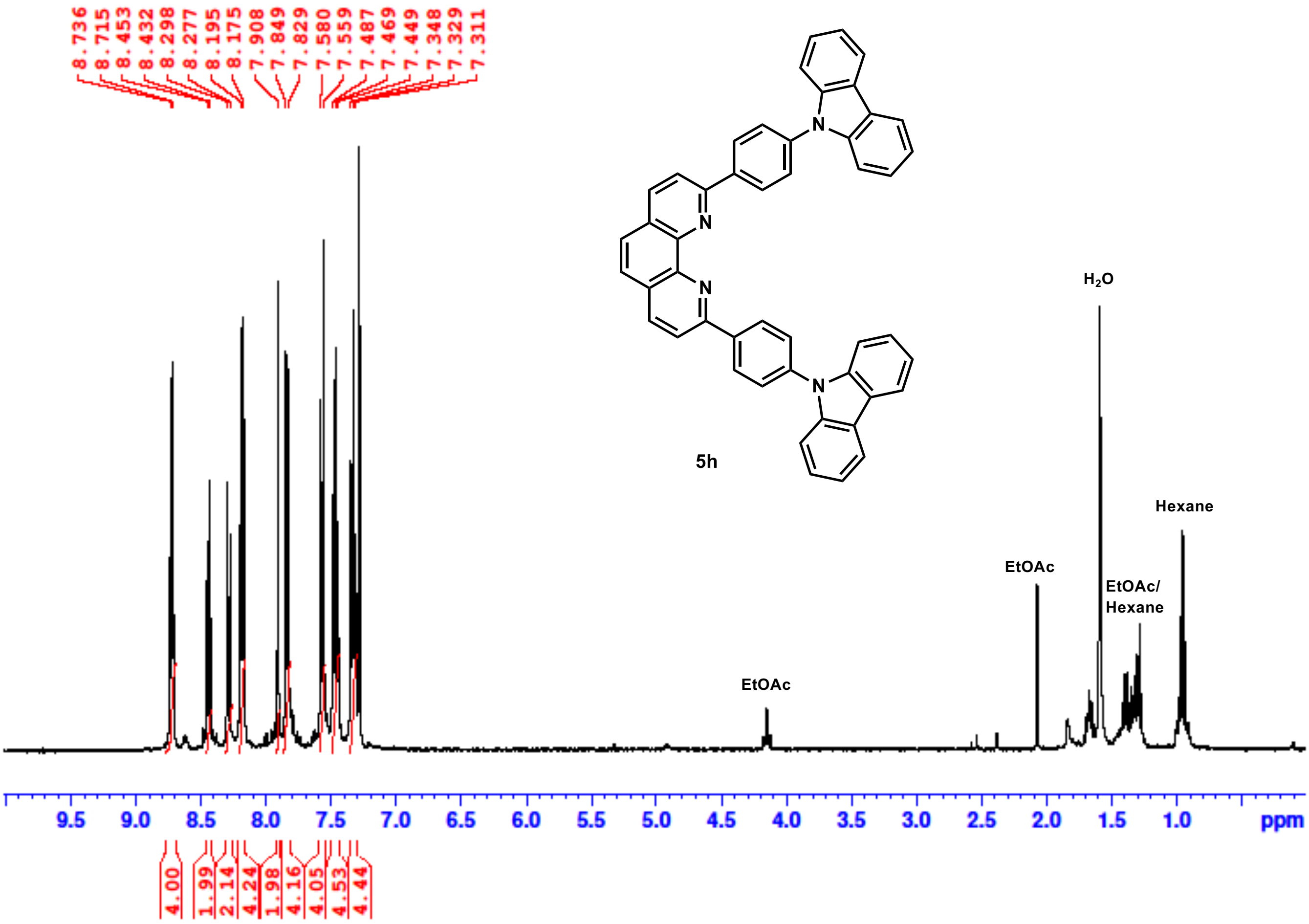


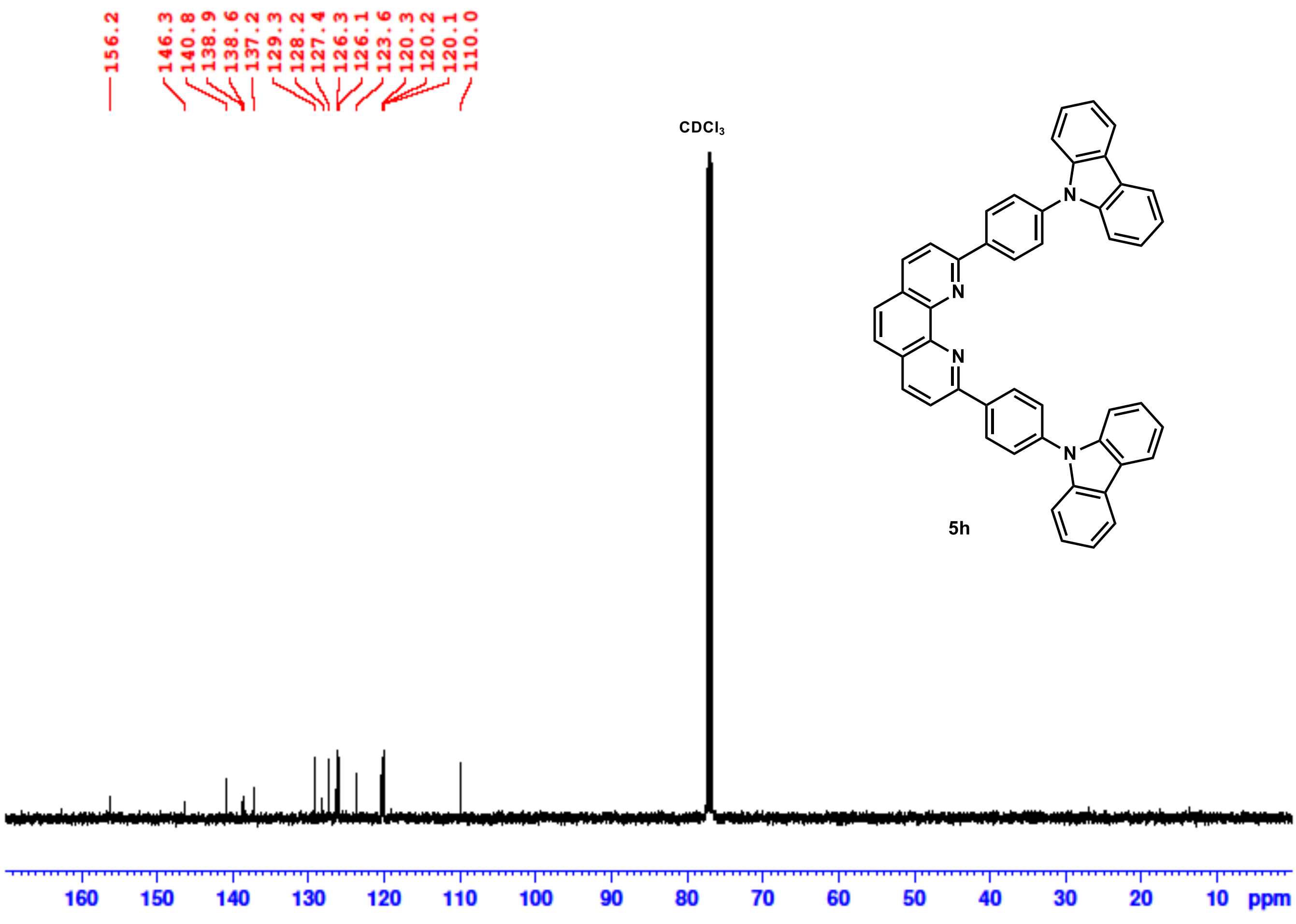
157.2
154.5
154.3
146.0
140.7
138.8
138.7
137.0
127.9
127.7
127.1
127.0
126.0
122.7
122.1
120.5
120.3
120.2
47.2
27.4
CDCl3
Me
Me
Me
Me
N
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

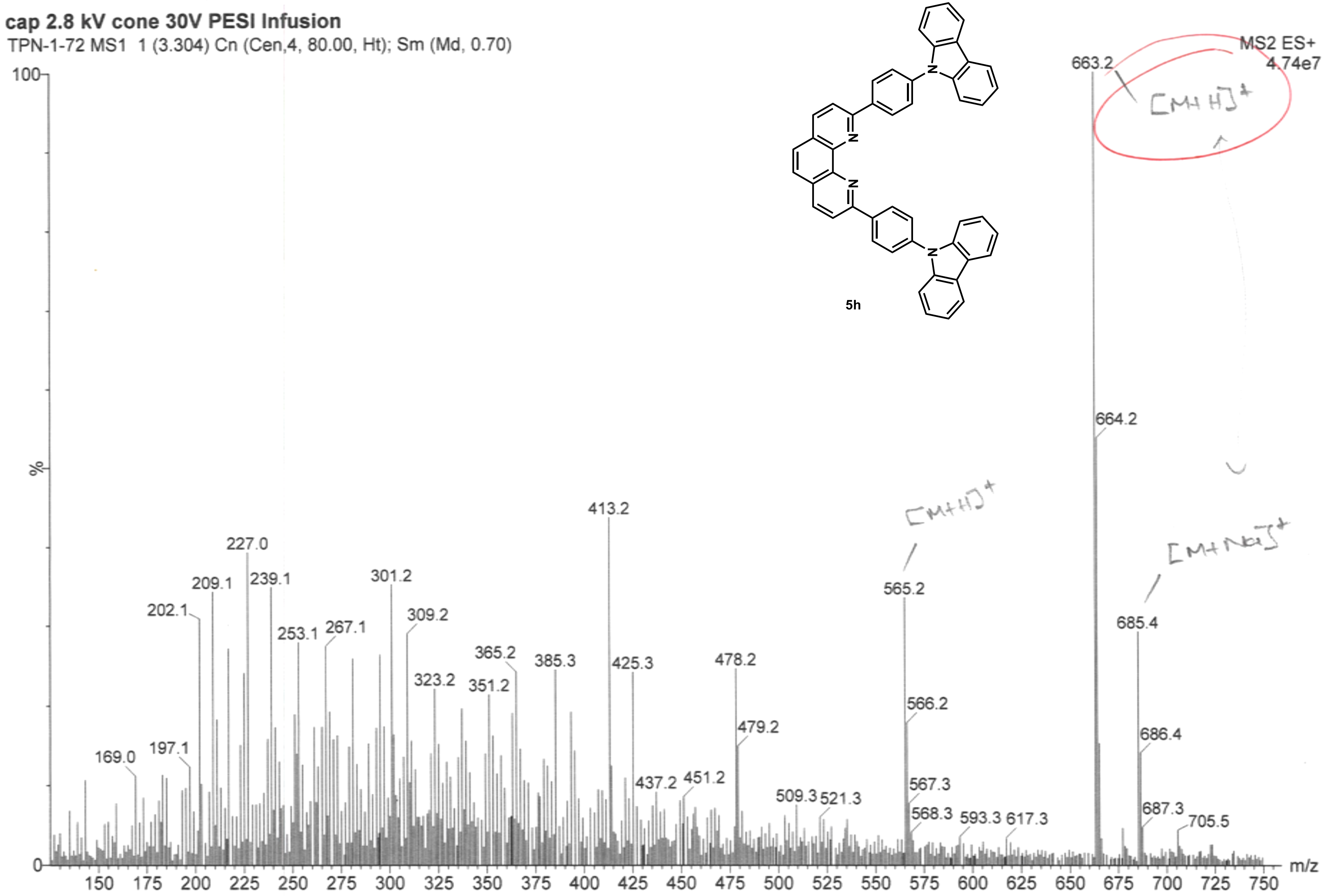
5g

cap 2.8 kV cone 30V PESI Infusion
TPN-1-65 MS1 1 (1.101) Cn (Cen,4, 80.00, Ht); Sm (Md, 0.70)

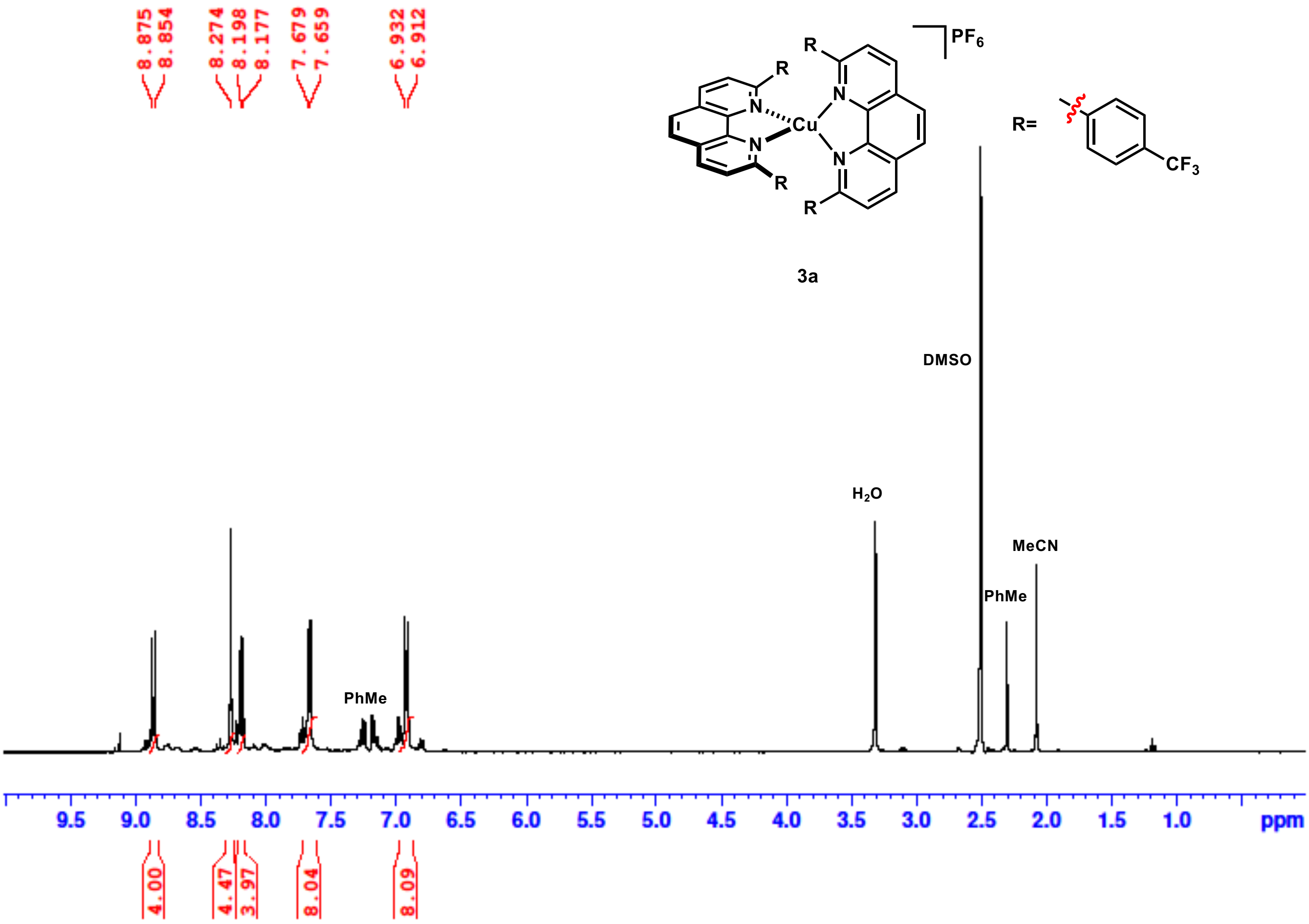


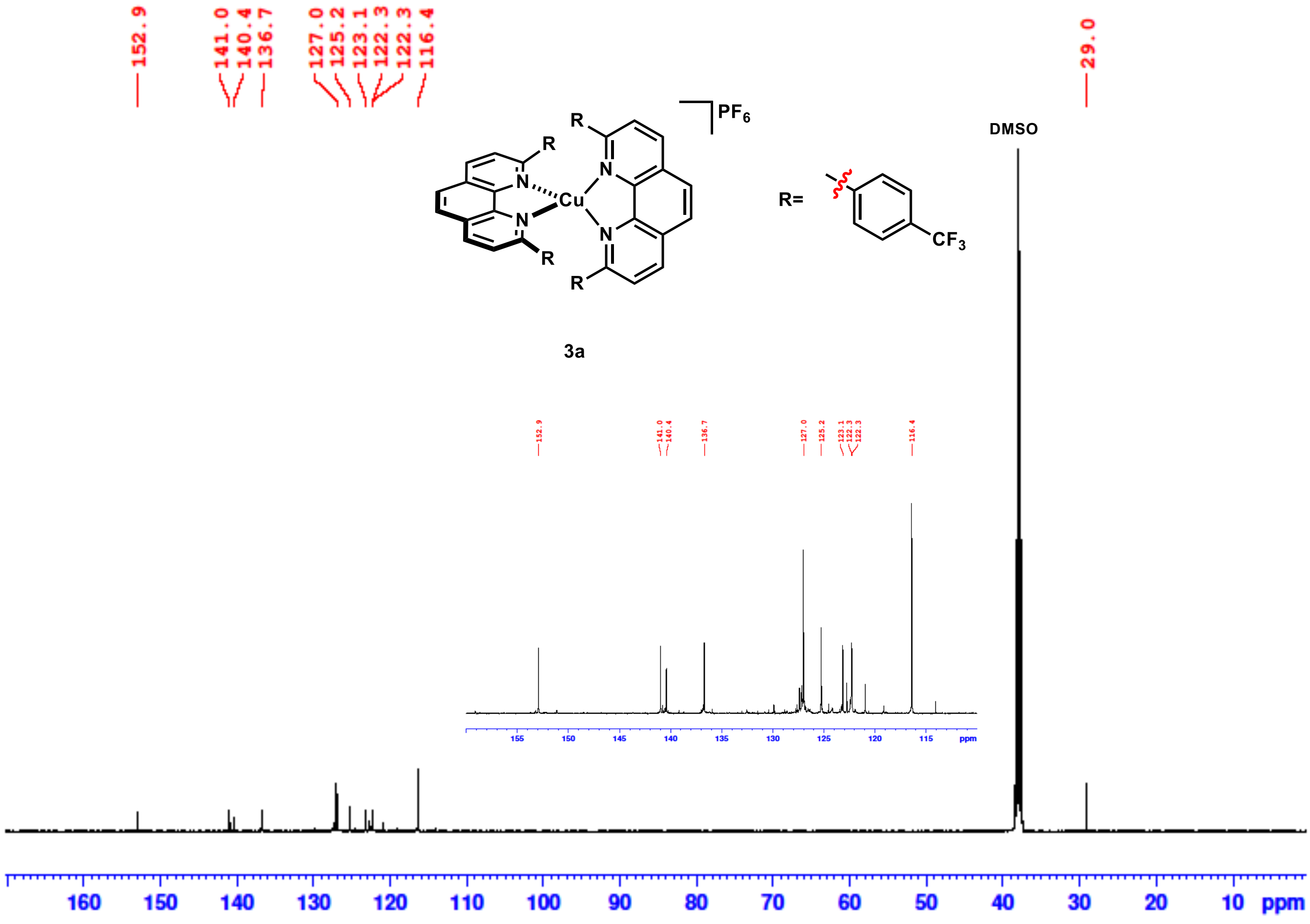

8.736 8.715 8.453 8.432 8.298 8.277 8.195 8.175 7.908 7.849 7.829 7.580 7.559 7.487 7.469 7.449 7.348 7.329 7.311
N
N
5h
H_2O
Hexane
EtOAc
EtOAc/
Hexane
EtOAc
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00 1.99 2.14 4.24 1.98 4.16 4.05 4.53 4.44

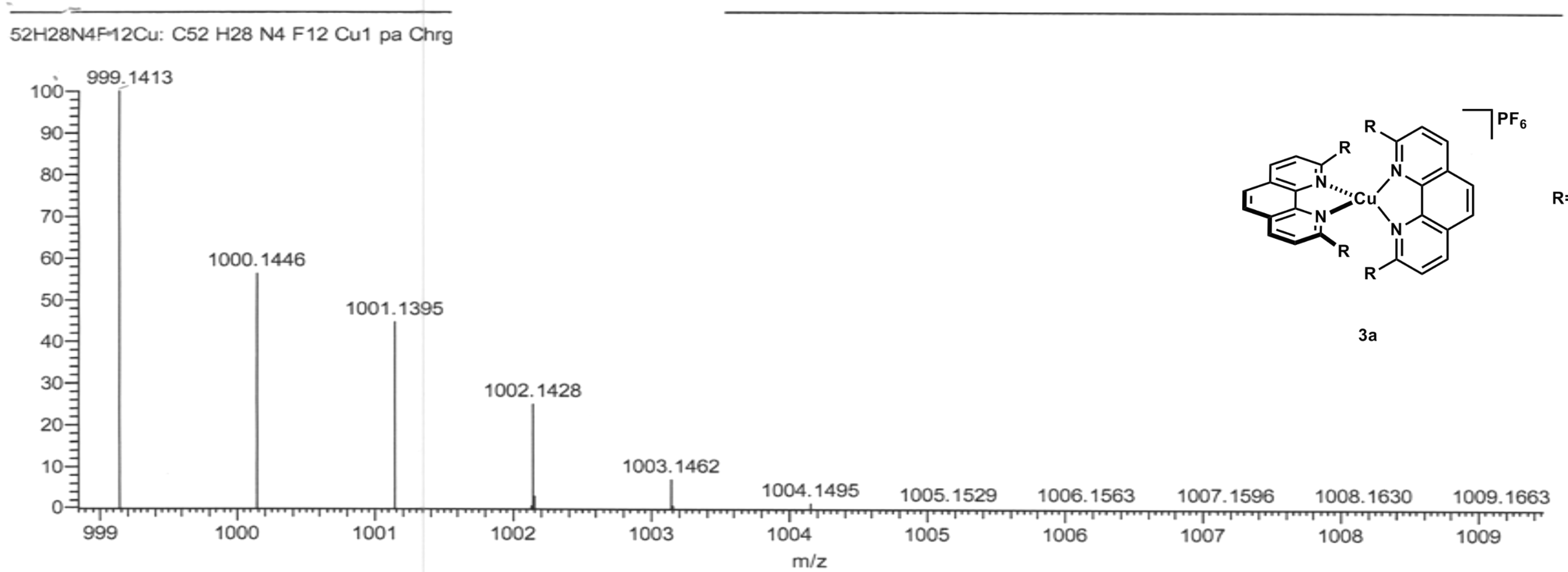

156.2
146.3 140.8 138.9 138.6 137.2 129.3 128.2 127.4 126.3 126.1 123.6 120.3 120.2 120.1 110.0
$CDCl_3$
N
N
5h
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


cap 2.8 kV cone 30V PESI Infusion
TPN-1-72 MS1 1 (3.304) Cn (Cen,4, 80.00, Ht); Sm (Md, 0.70)
MS2 ES+
4.74e7
100
%
0
663.2
[M+H]+
664.2
685.4
[M+Na]+
686.4
687.3
705.5
565.2
[M+H]+
566.2
567.3
568.3
593.3
617.3
509.3
521.3
478.2
479.2
437.2
451.2
413.2
425.3
385.3
365.2
351.2
323.2
309.2
301.2
267.1
253.1
239.1
227.0
209.1
202.1
197.1
169.0
150
175
200
225
250
275
300
325
350
375
400
425
450
475
500
525
550
575
600
625
650
675
700
725
750
m/z

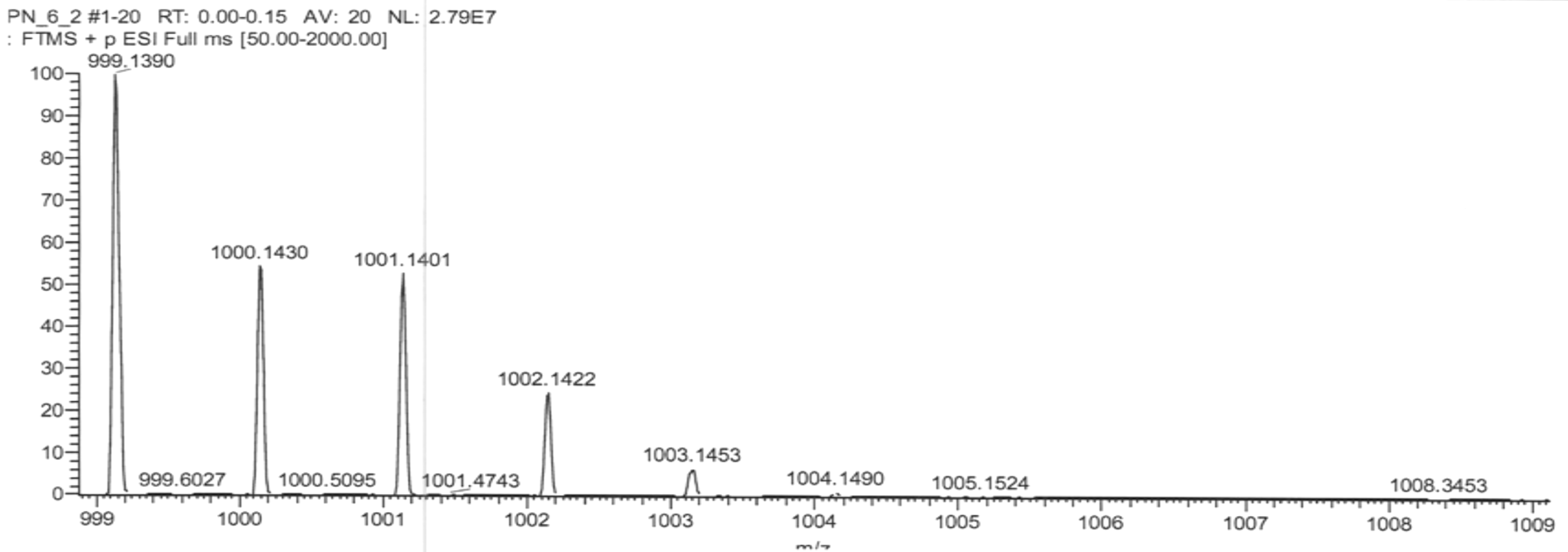
5h

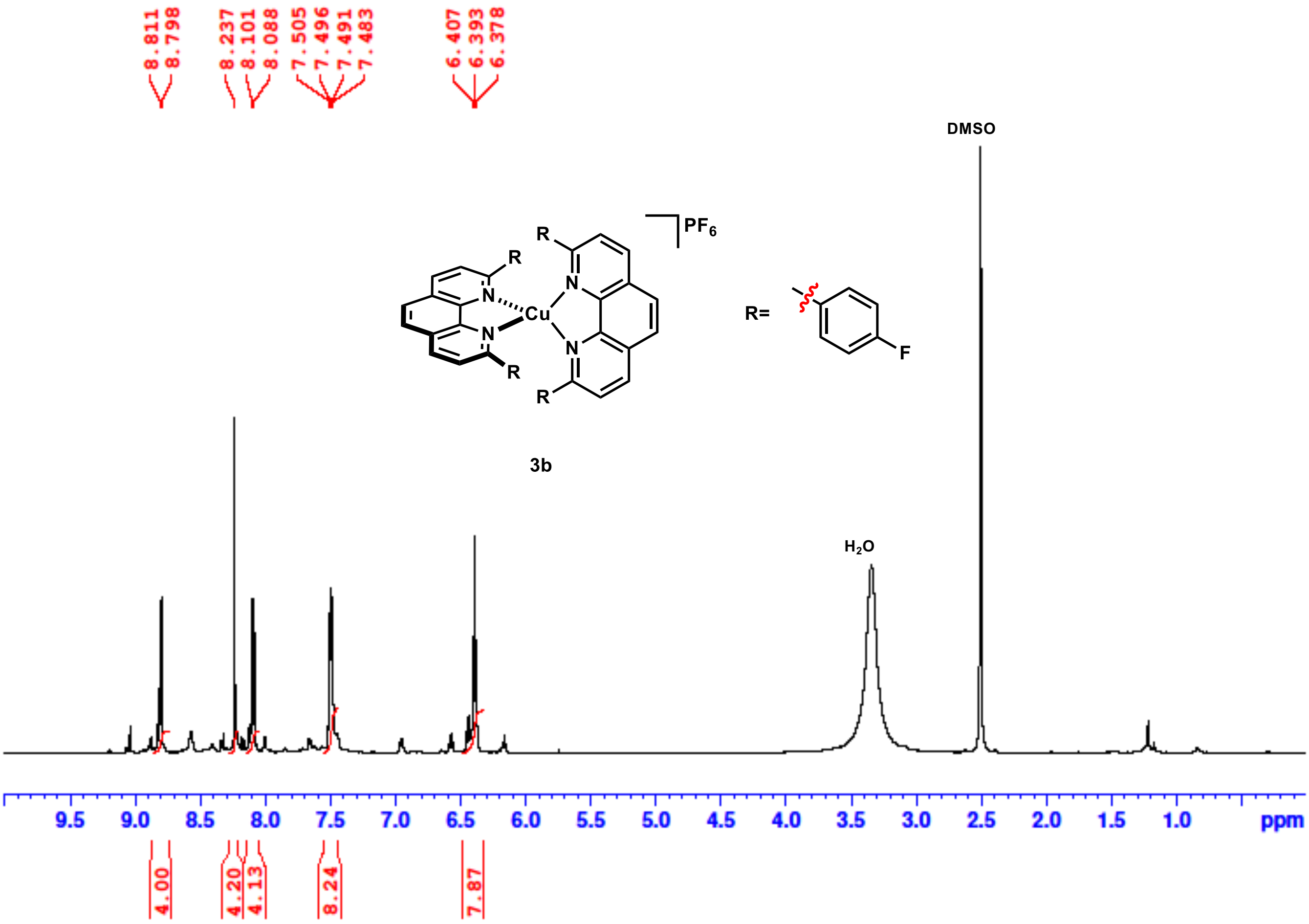

8.875
8.854
8.274
8.198
8.177
7.679
7.659
6.932
6.912
PF6
R=
CF3
3a
DMSO
H2O
MeCN
PhMe
PhMe
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00
4.47
3.97
8.04
8.09

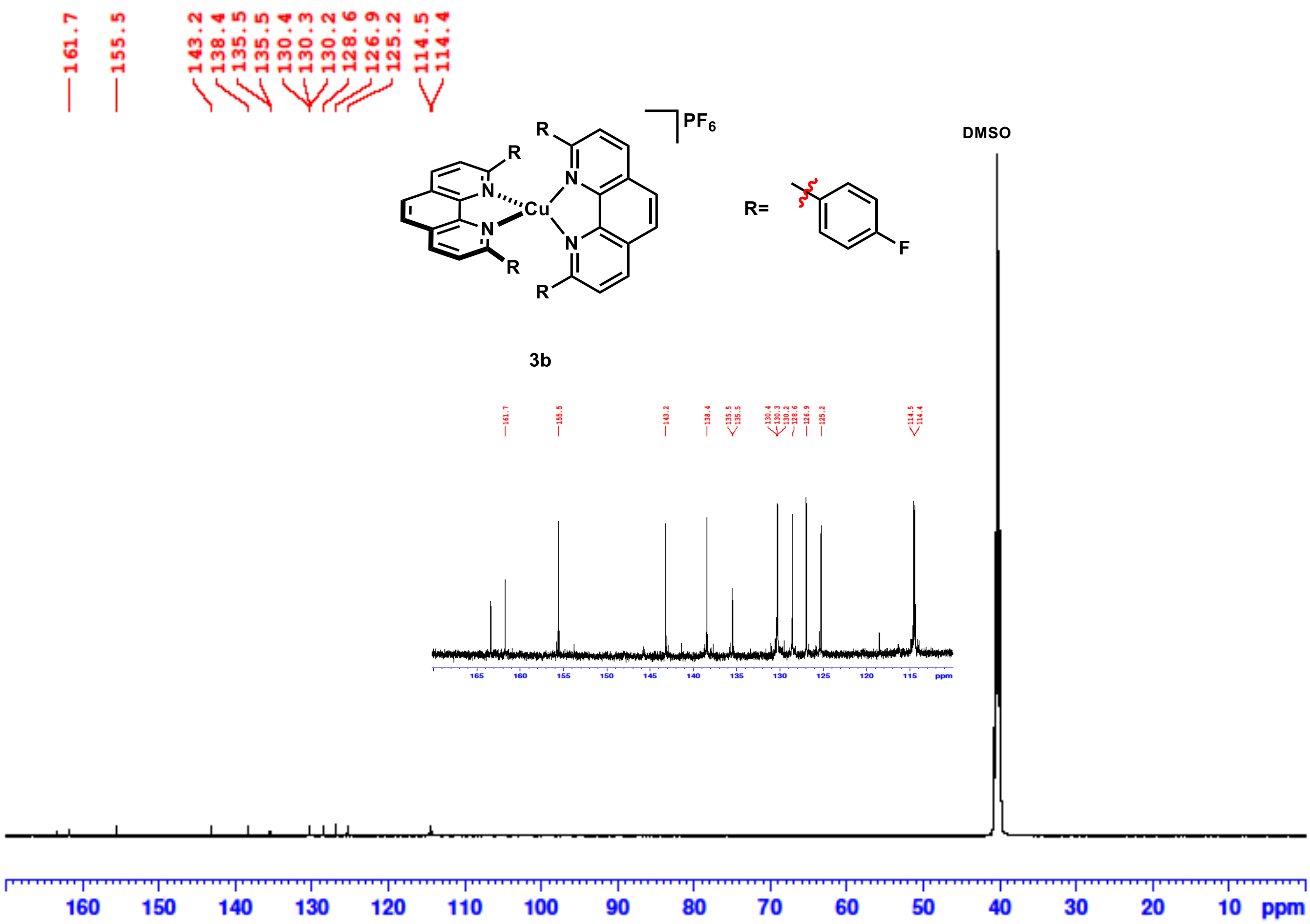

152.9
141.0
140.4
136.7
127.0
125.2
123.1
122.3
122.3
116.4
29.0
PF6
R=
CF3
3a
DMSO
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


52H28N4F12Cu: C52 H28 N4 F12 Cu1 pa Chrg
999.1413
1000.1446
1001.1395
1002.1428
1003.1462
1004.1495
1005.1529
1006.1563
1007.1596
1008.1630
1009.1663
m/z
PF6
R
N
Cu
R=
CF3

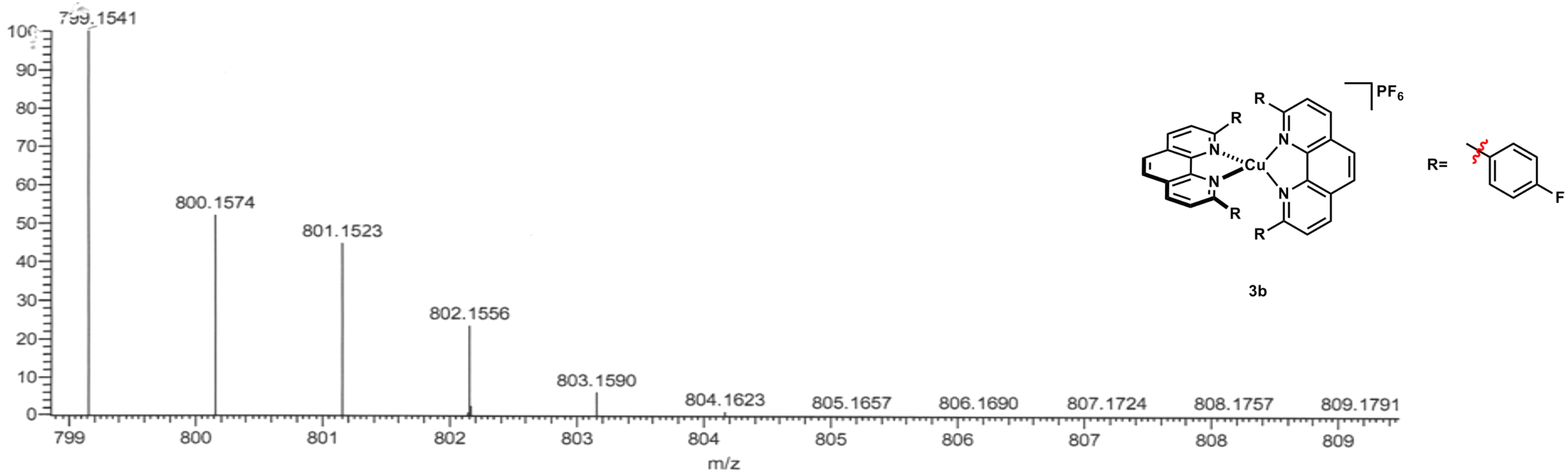
3a


PN_6_2 #1-20 RT: 0.00-0.15 AV: 20 NL: 2.79E7
: FTMS + p ESI Full ms [50.00-2000.00]
999.1390
999.6027
1000.1430
1000.5095
1001.1401
1001.4743
1002.1422
1003.1453
1004.1490
1005.1524
1008.3453


8.811
8.798
8.237
8.101
8.088
7.505
7.496
7.491
7.483
6.407
6.393
6.378
DMSO
PF6
R=
F
3b
H2O
ppm
4.00
4.20
4.13
8.24
7.87

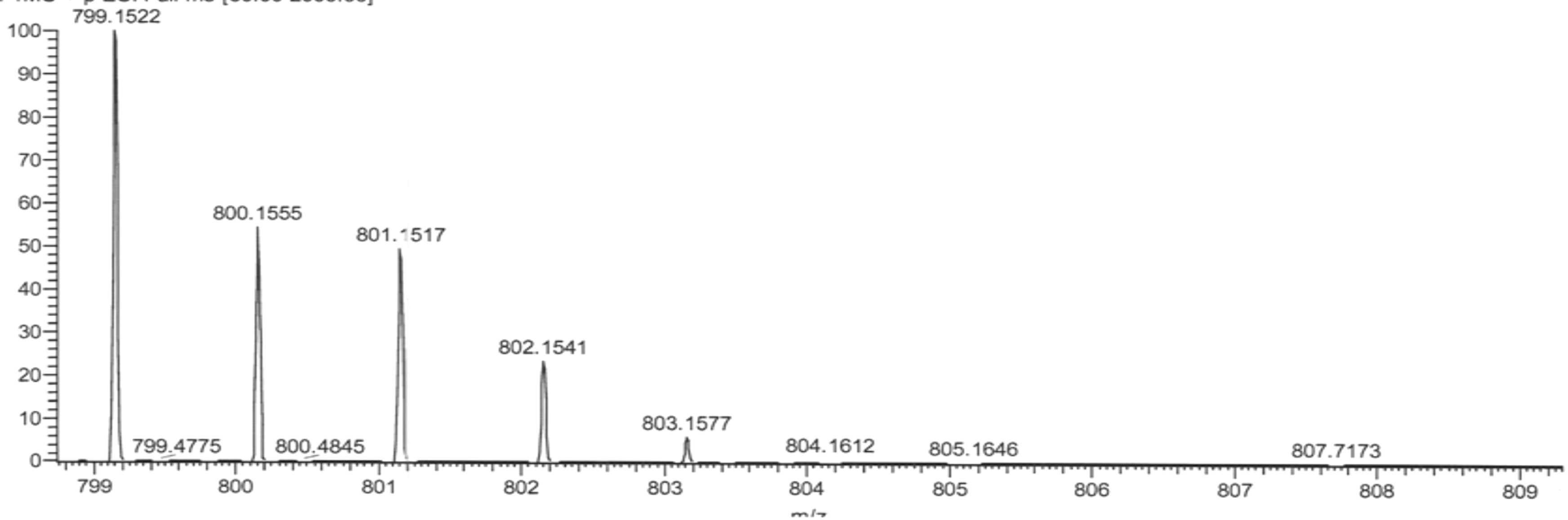

161.7
155.5
143.2
138.4
135.5
135.5
130.4
130.3
130.2
128.6
126.9
125.2
114.5
114.4
DMSO
PF6
R=
F
3b
ppm

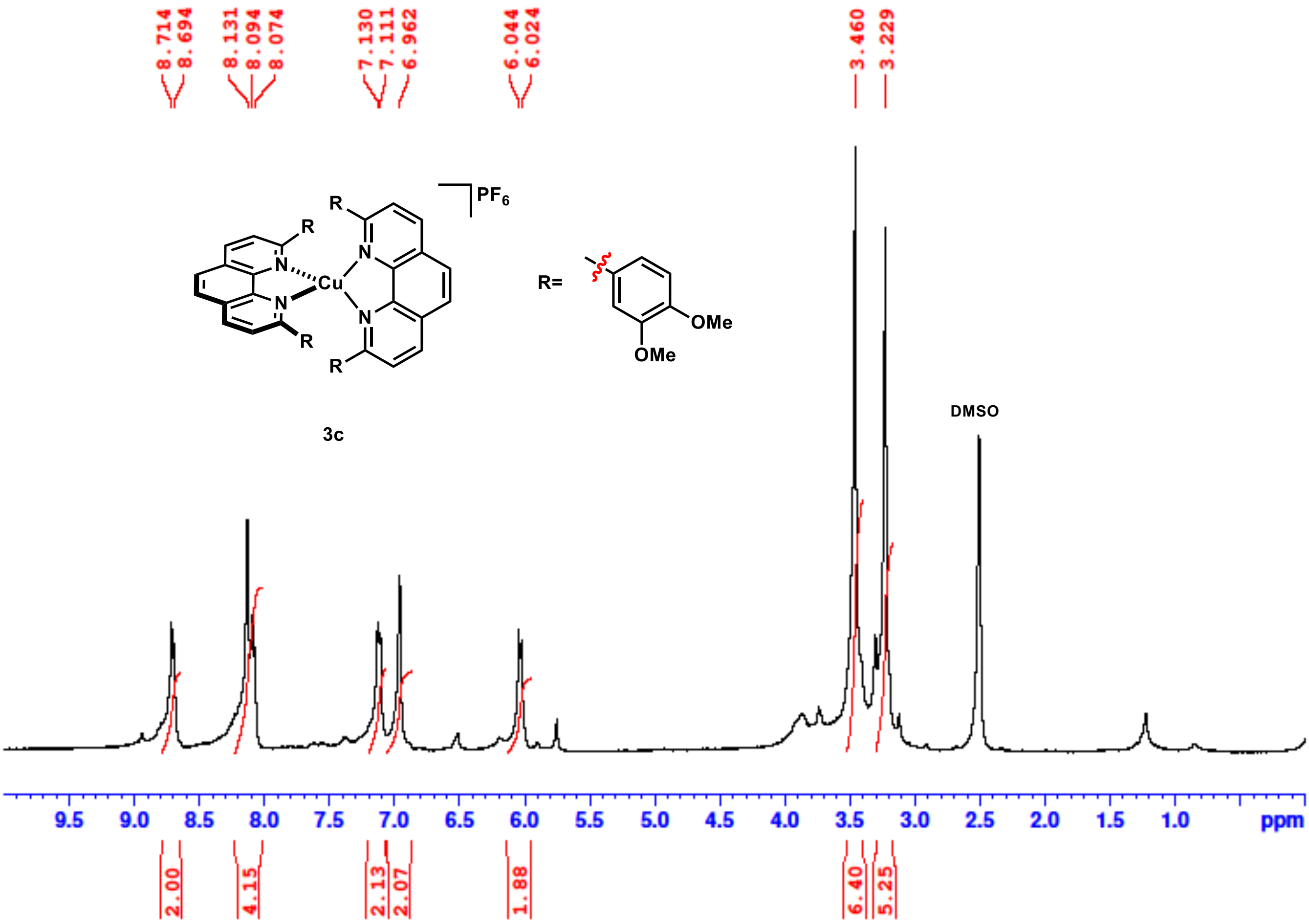
48H28N4F4Cu: C48 H28 N4 F4 Cu1 pa Chrg 1

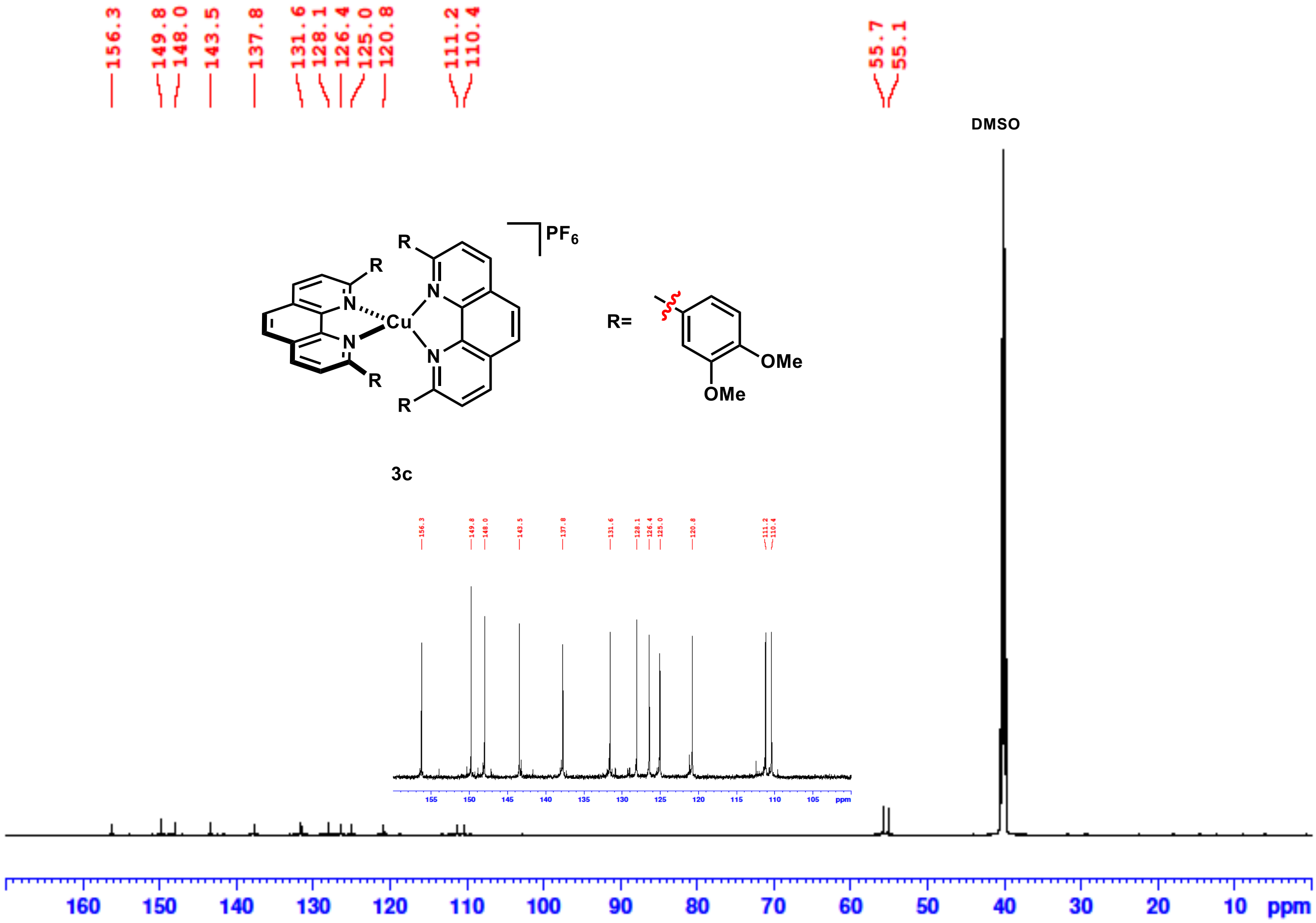


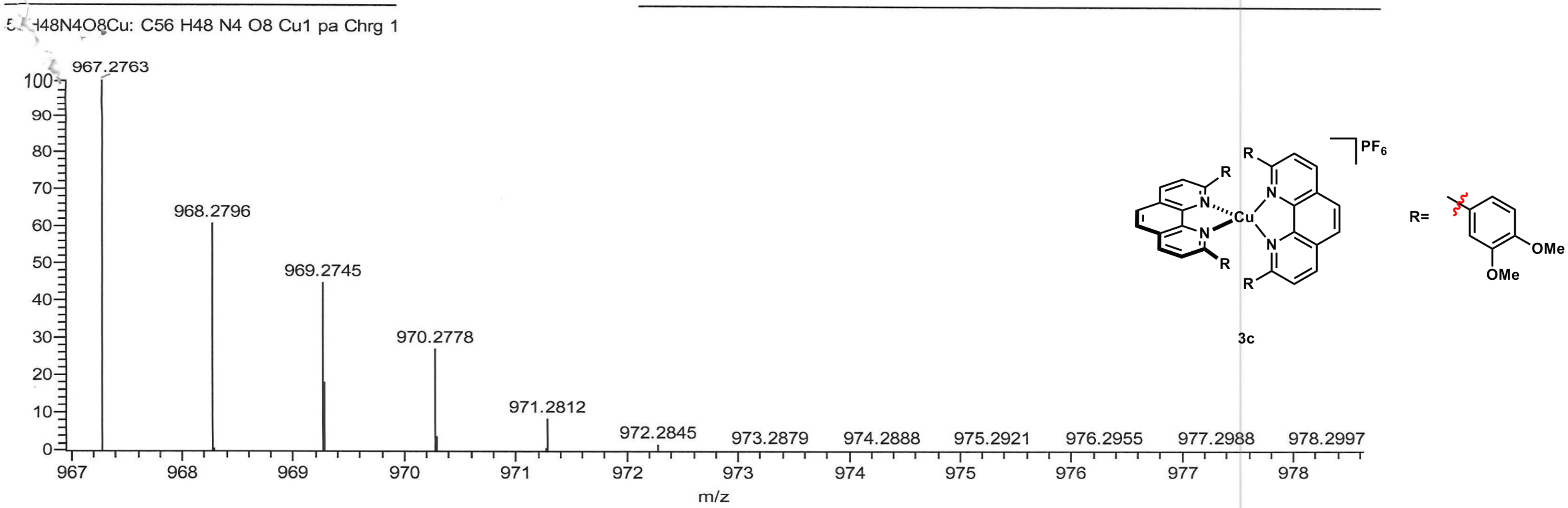
3b

PN_10_2 #2-19 RT: 0.01-0.14 AV: 18 NL: 7.16E7
: FTMS + p ESI Full ms [50.00-2000.00]

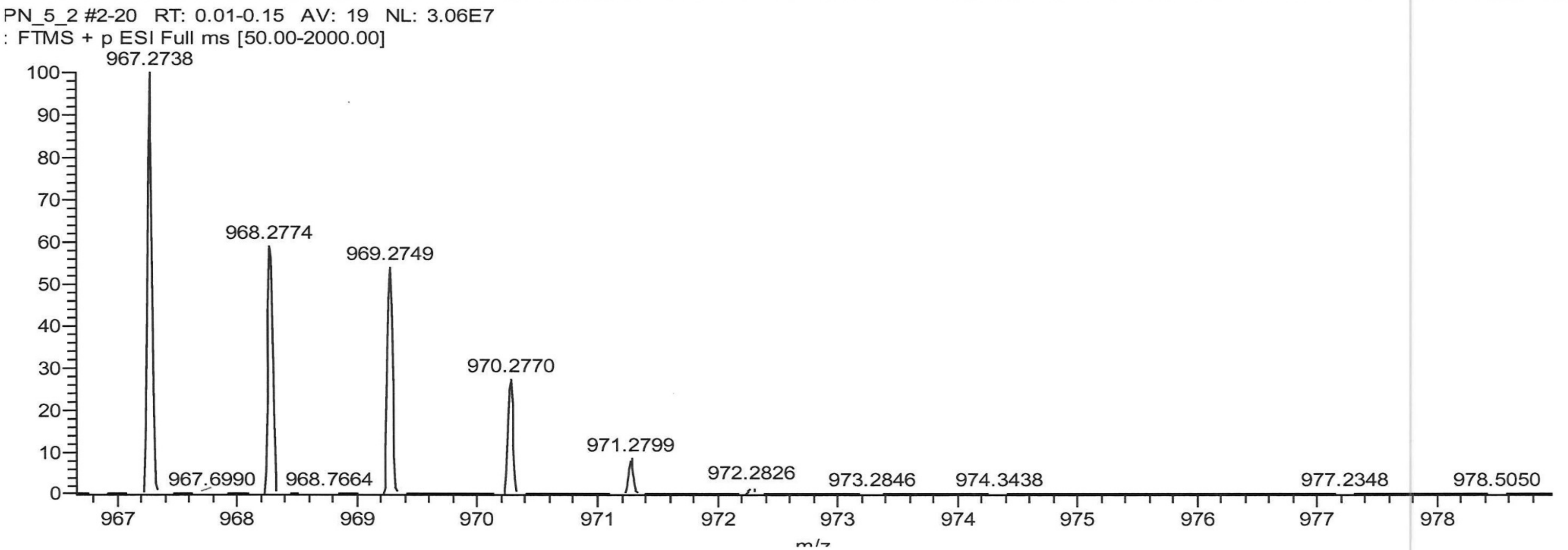


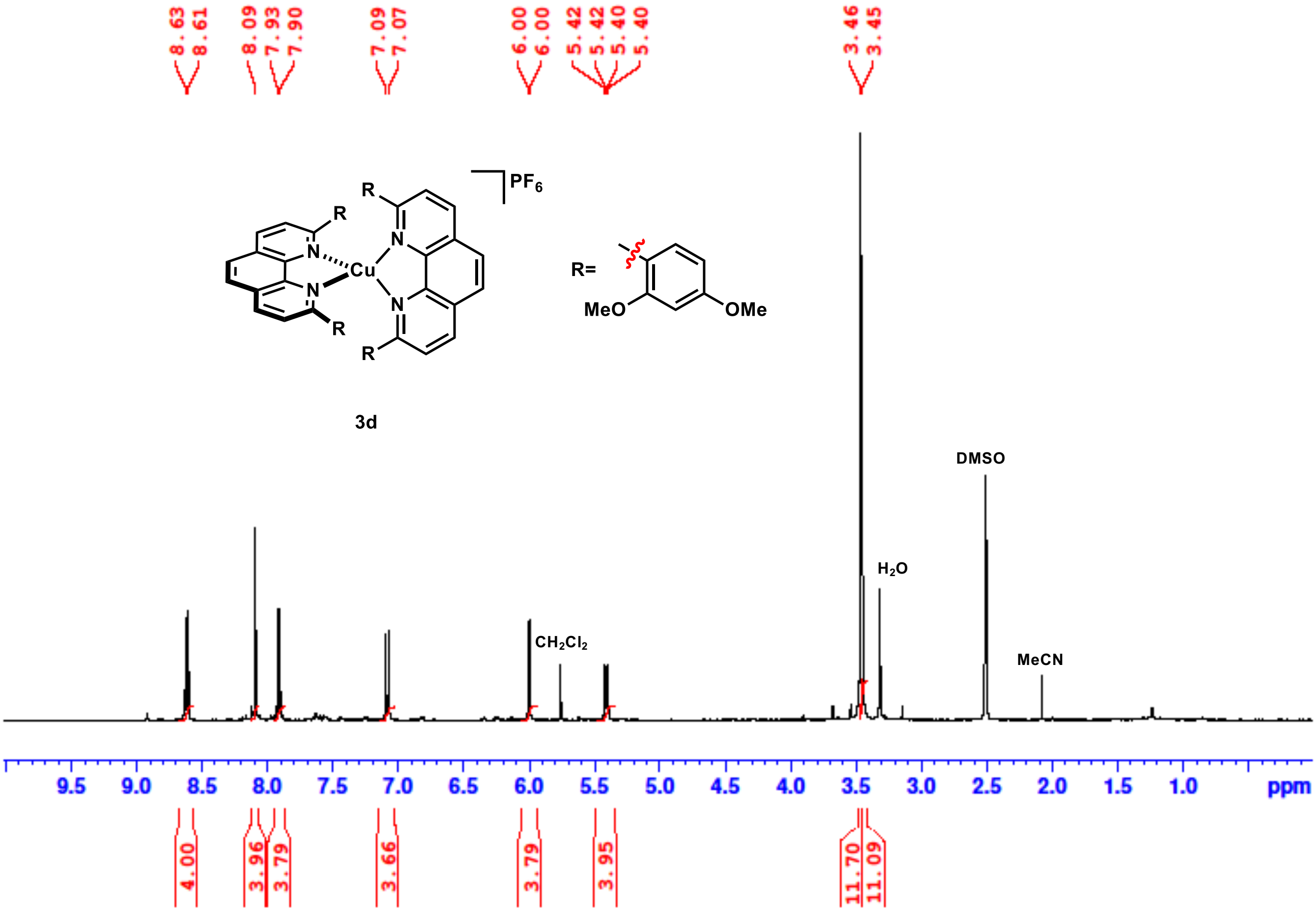

8.714
8.694
8.131
8.094
8.074
7.130
7.111
6.962
6.044
6.024
3.460
3.229
PF6
R
N
Cu
R=
OMe
OMe
3c
DMSO
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
4.15
2.13
2.07
1.88
6.40
5.25


156.3
149.8
148.0
143.5
137.8
131.6
128.1
126.4
125.0
120.8
111.2
110.4
55.7
55.1
DMSO
PF6
R
N
Cu
R=
OMe
OMe
3c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

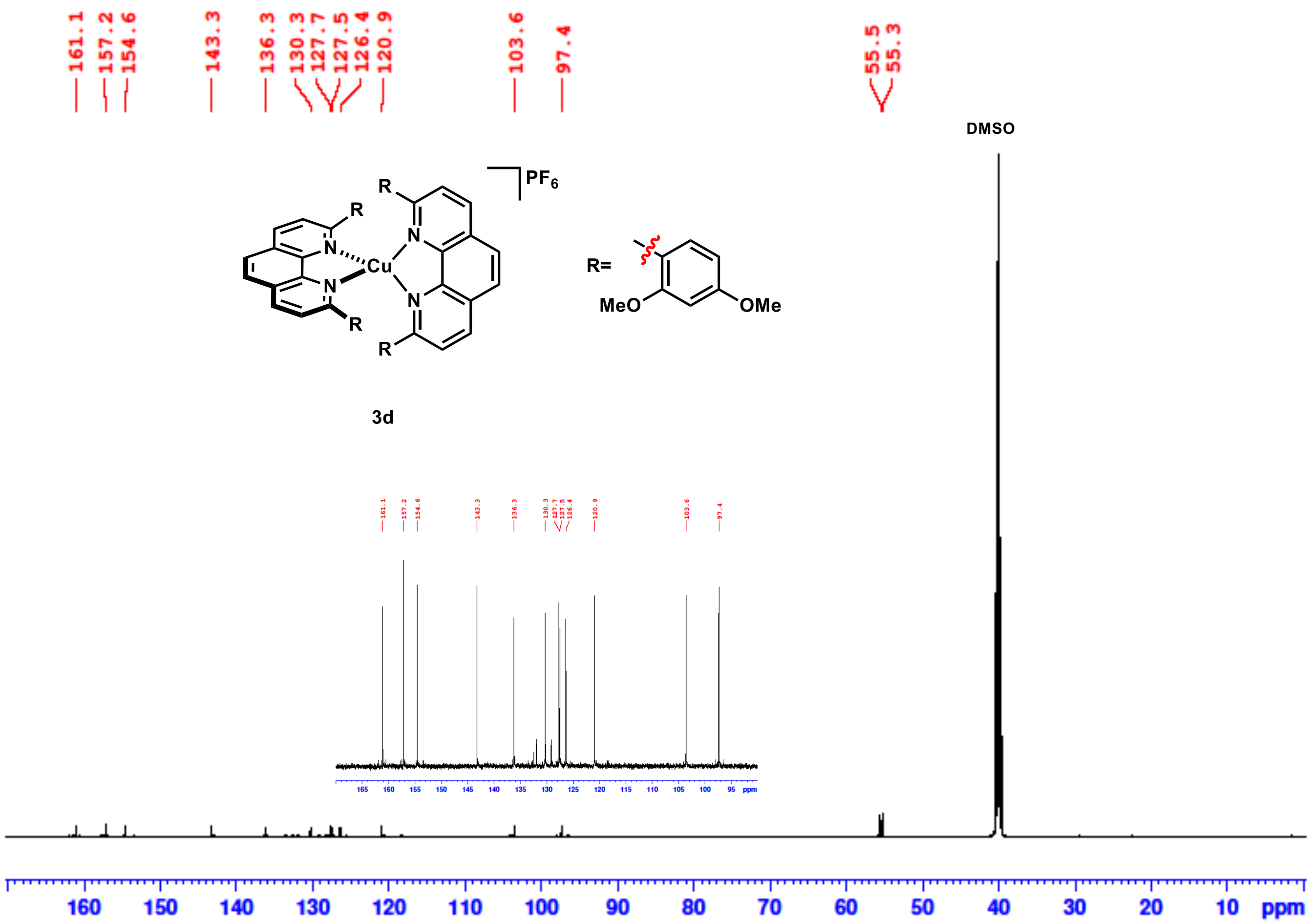

5.H48N4O8Cu: C56 H48 N4 O8 Cu1 pa Chrg 1
967.2763
968.2796
969.2745
970.2778
971.2812
972.2845
973.2879
974.2888
975.2921
976.2955
977.2988
978.2997
m/z
R
N
Cu
PF6
R=
OMe

3c


PN_5_2 #2-20 RT: 0.01-0.15 AV: 19 NL: 3.06E7
: FTMS + p ESI Full ms [50.00-2000.00]
967.2738
967.6990
968.2774
968.7664
969.2749
970.2770
971.2799
972.2826
973.2846
974.3438
977.2348
978.5050

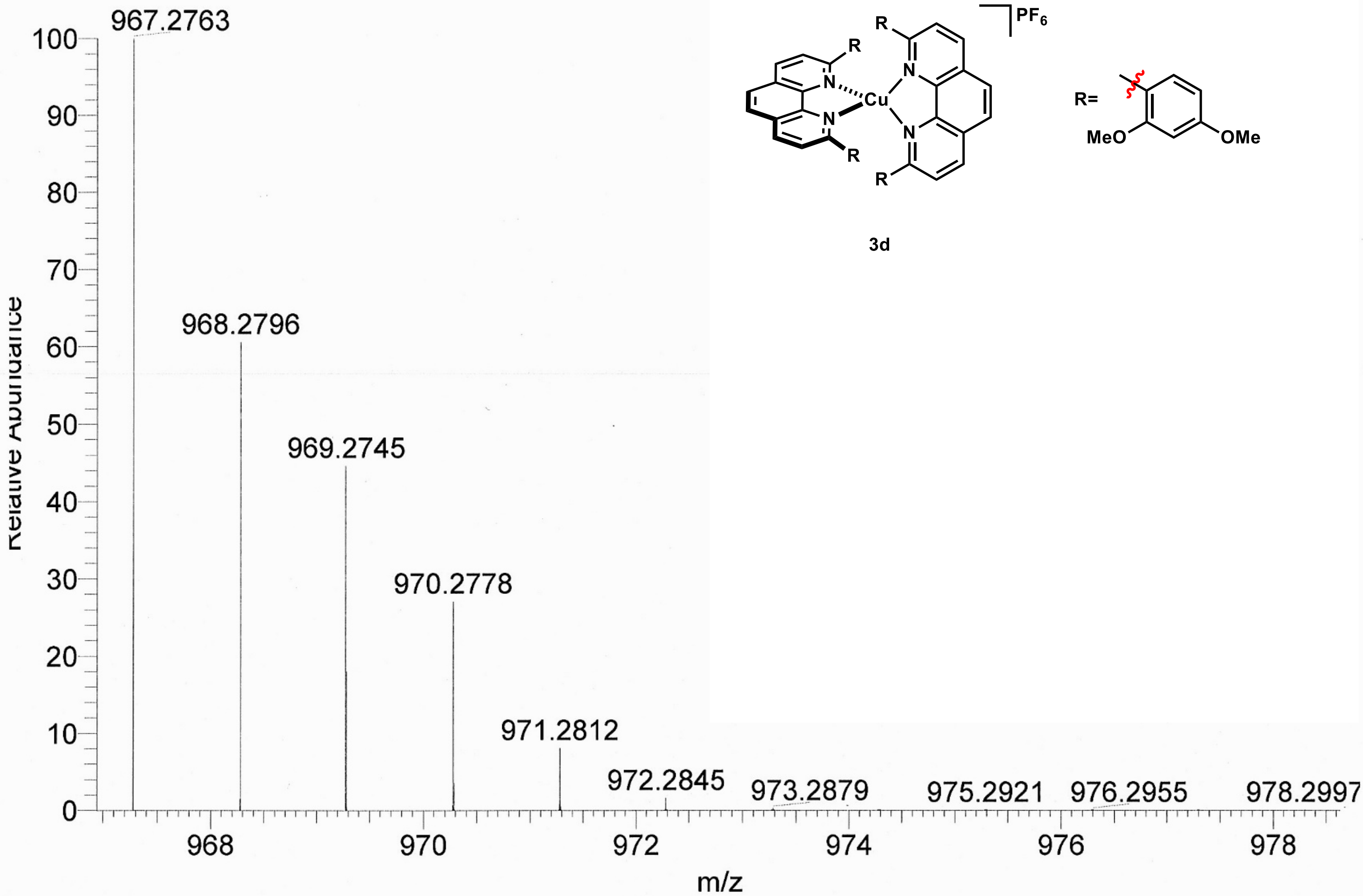


8.63
8.61
8.09
7.93
7.90
7.09
7.07
6.00
6.00
5.42
5.42
5.40
5.40
3.46
3.45
PF6
R=
MeO
OMe
3d
DMSO
H2O
CH2Cl2
MeCN
ppm
4.00
3.96
3.79
3.66
3.79
3.95
11.70
11.09



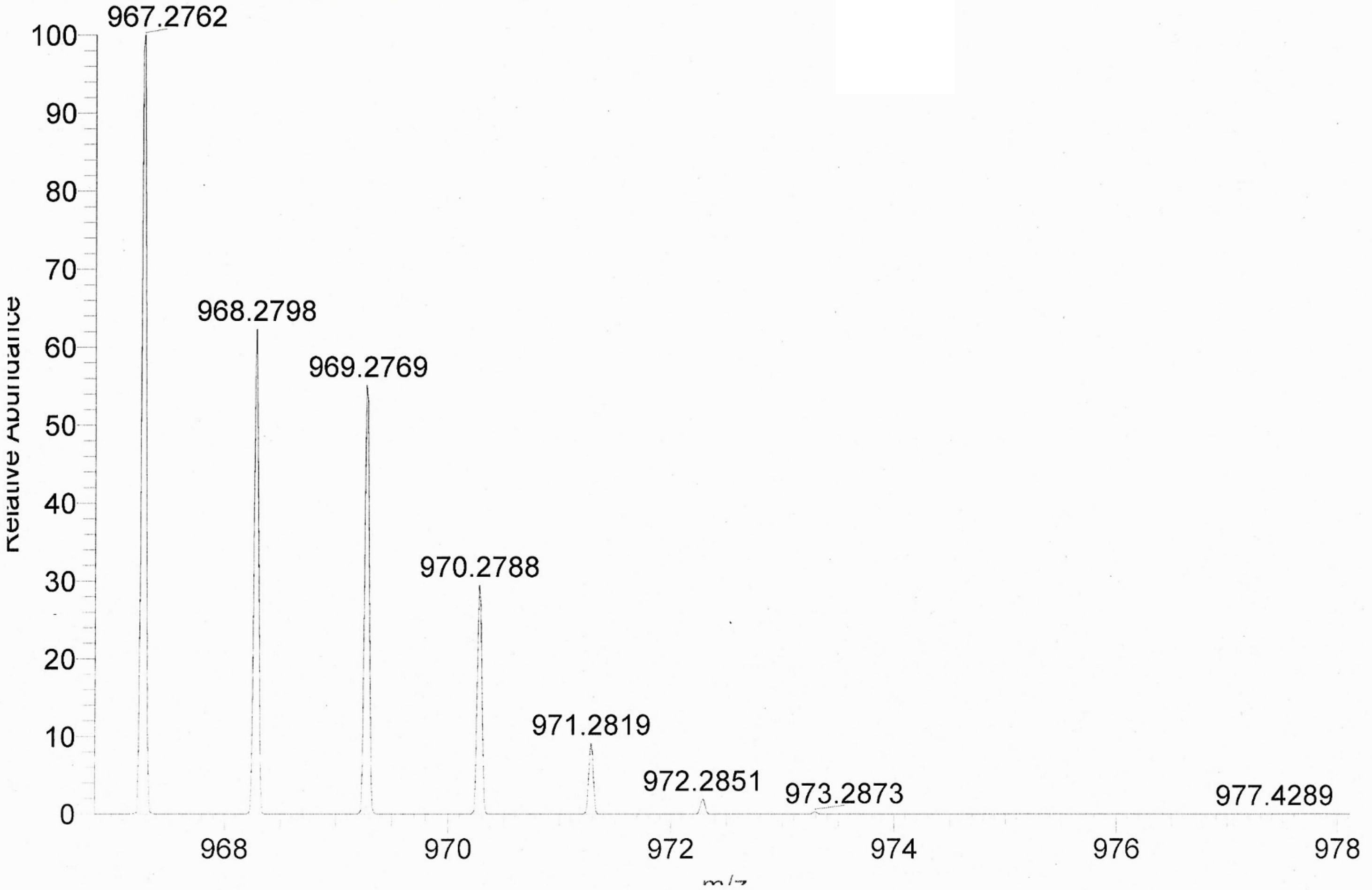
161.1
157.2
154.6
143.3
136.3
130.3
127.7
127.5
126.4
120.9
103.6
97.4
55.5
55.3
DMSO
PF6
R=
MeO
OMe
3d
ppm

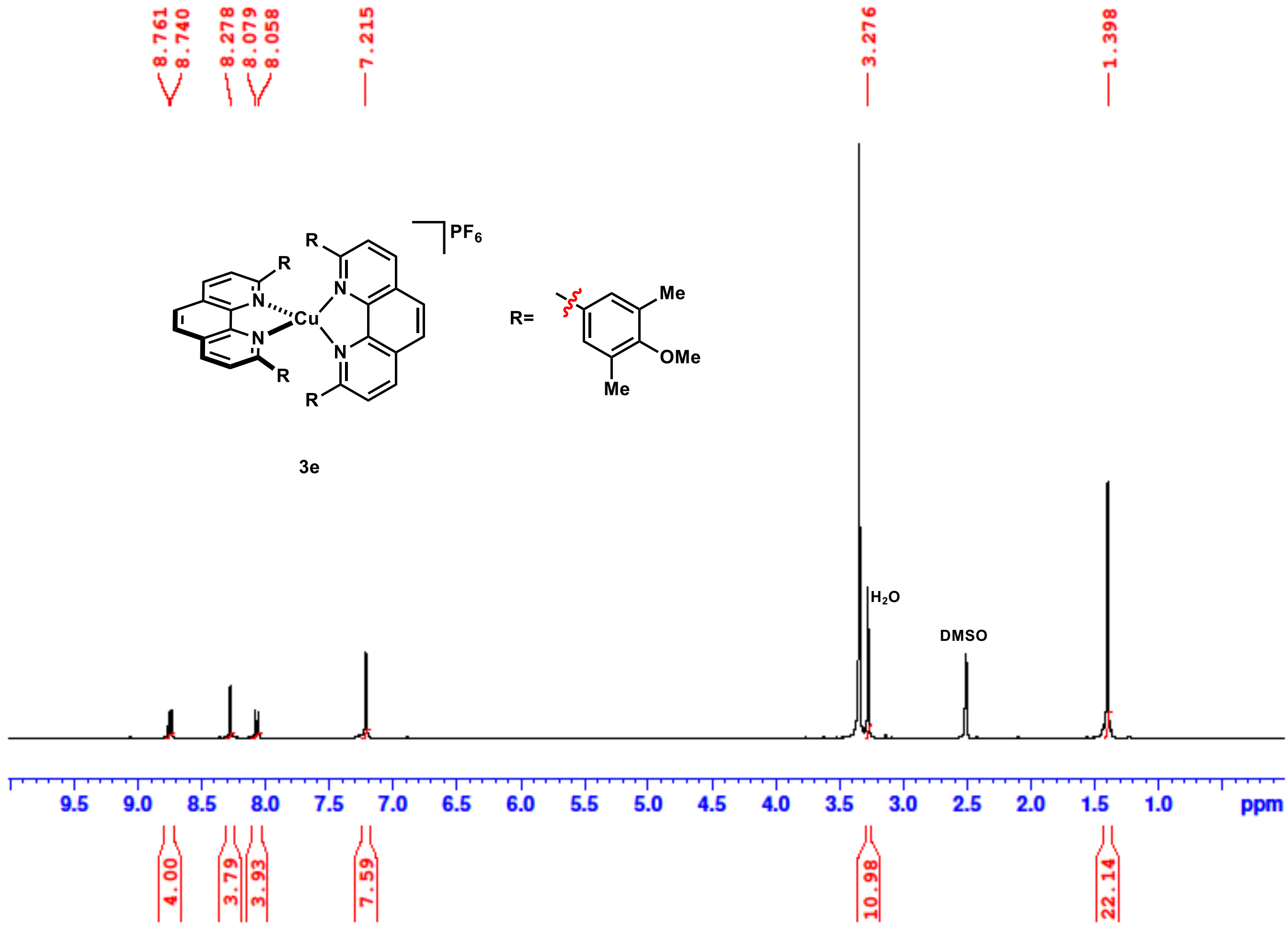
uC56H47N4O8 +H: Cu1 C56 H48 N4 O8 pa Chrg 1

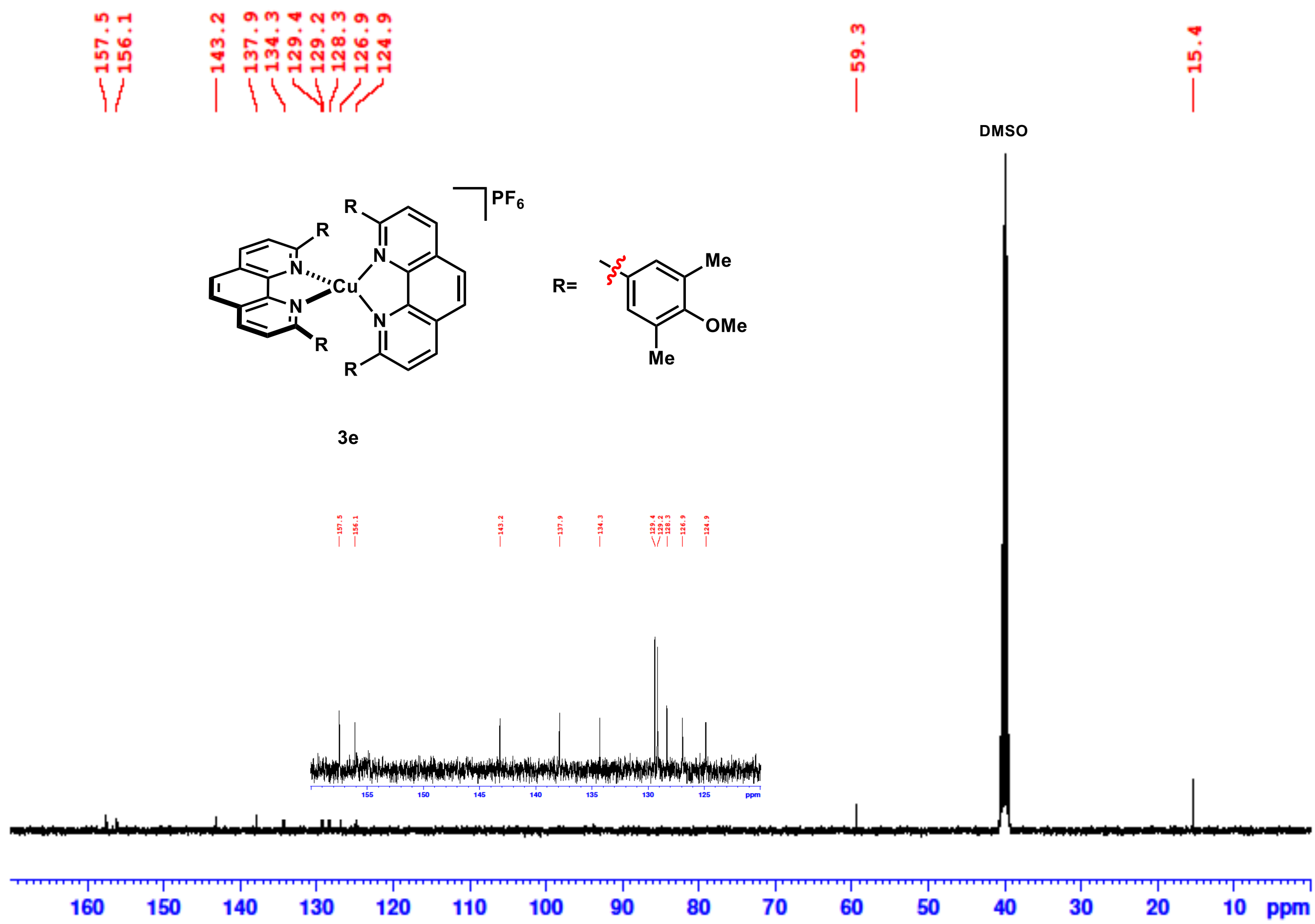


3d

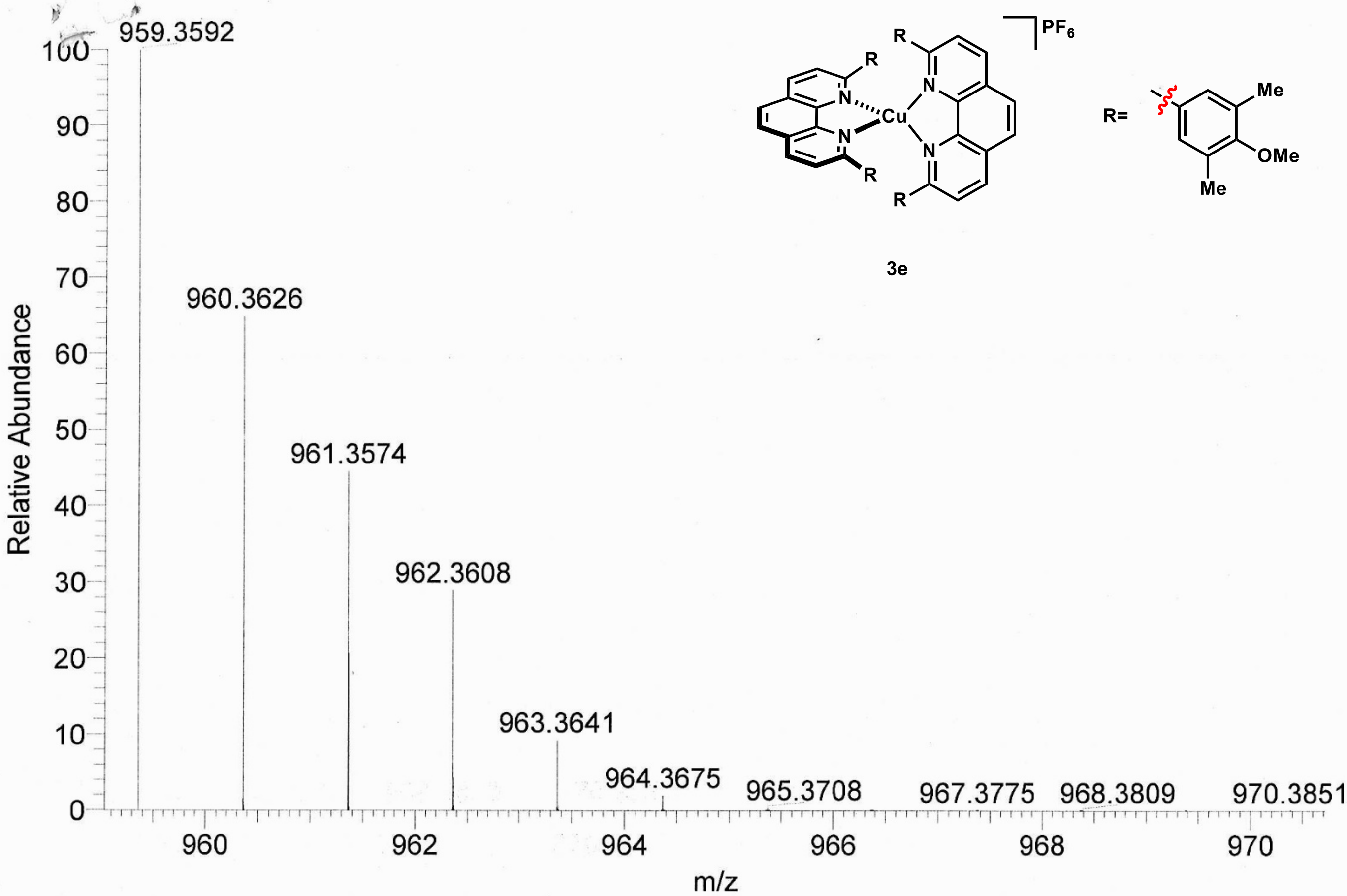
N-1-93 #3-27 RT: 0.05-0.62 AV: 25 NL: 1.14E7
FTMS + p ESI Full ms [150.00-2000.00]




8.761
8.740
8.278
8.079
8.058
7.215
3.276
1.398
PF6
R
N
Cu
R=
Me
OMe
3e
H2O
DMSO
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00
3.79
3.93
7.59
10.98
22.14

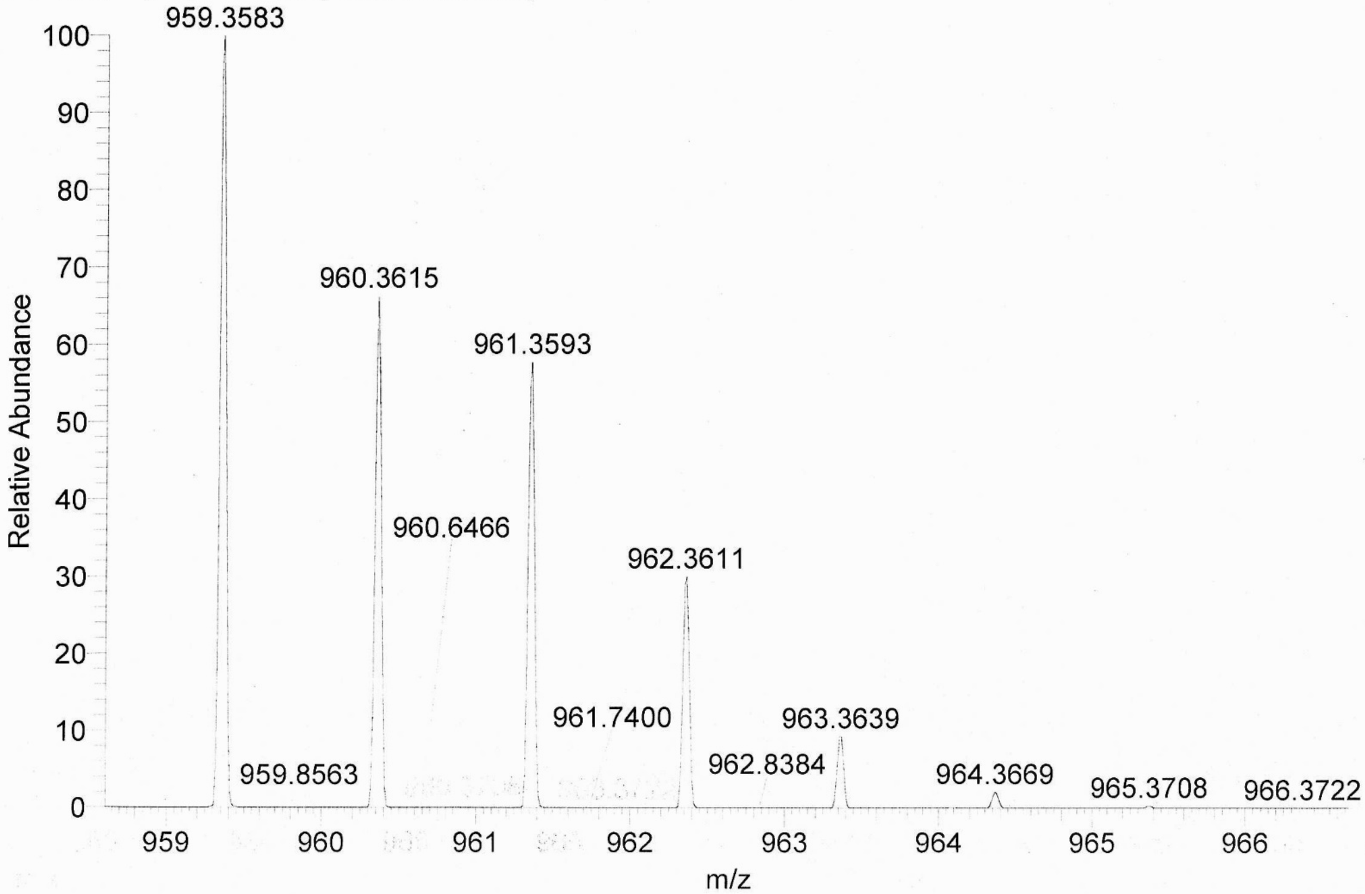

157.5
156.1
143.2
137.9
134.3
129.4
129.2
128.3
126.9
124.9
59.3
15.4
DMSO
PF6
R
N
Cu
R=
Me
OMe
3e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

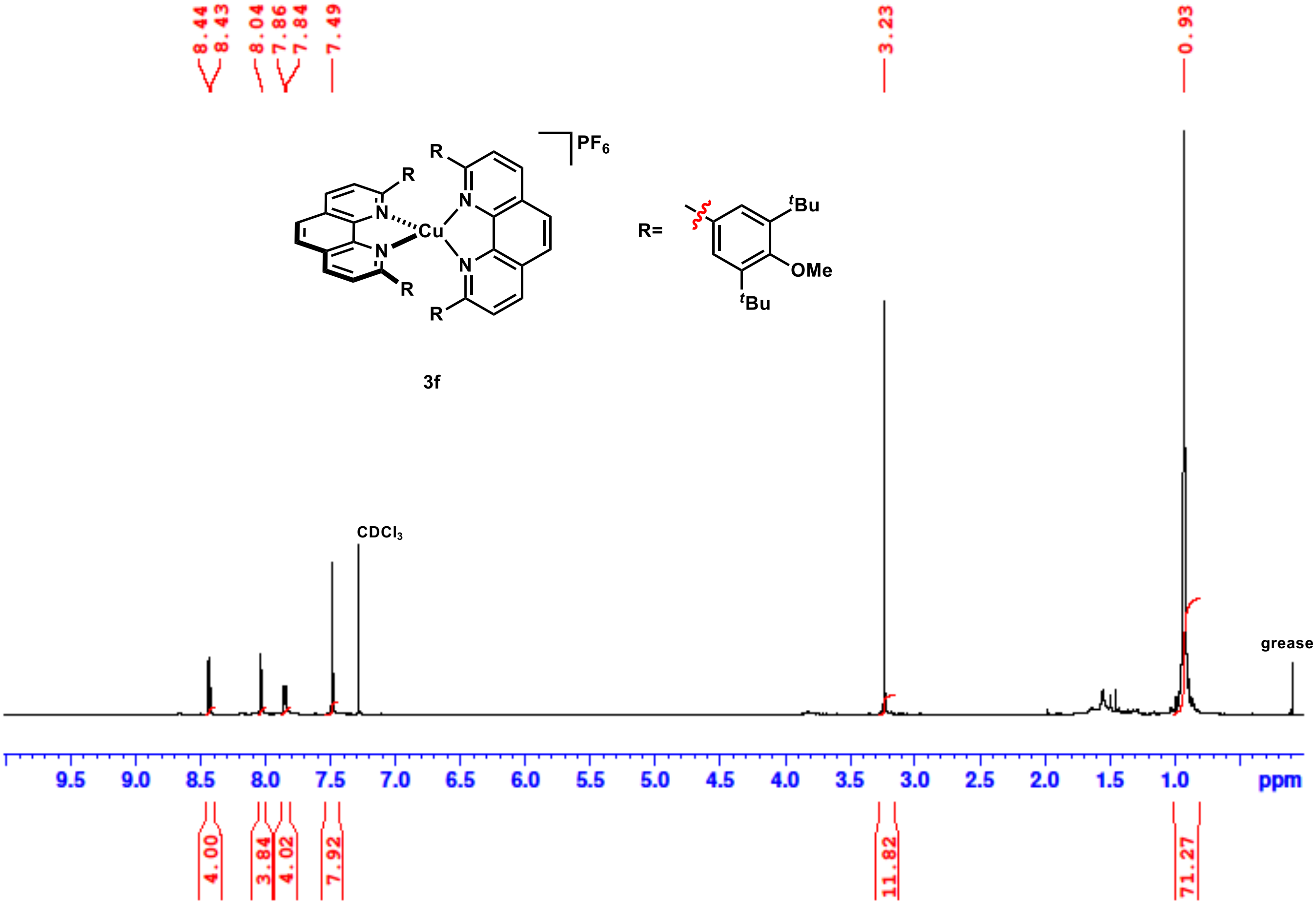
CuC60H56N4O4: Cu1 C60 H56 N4 O4 pa Chrg 1

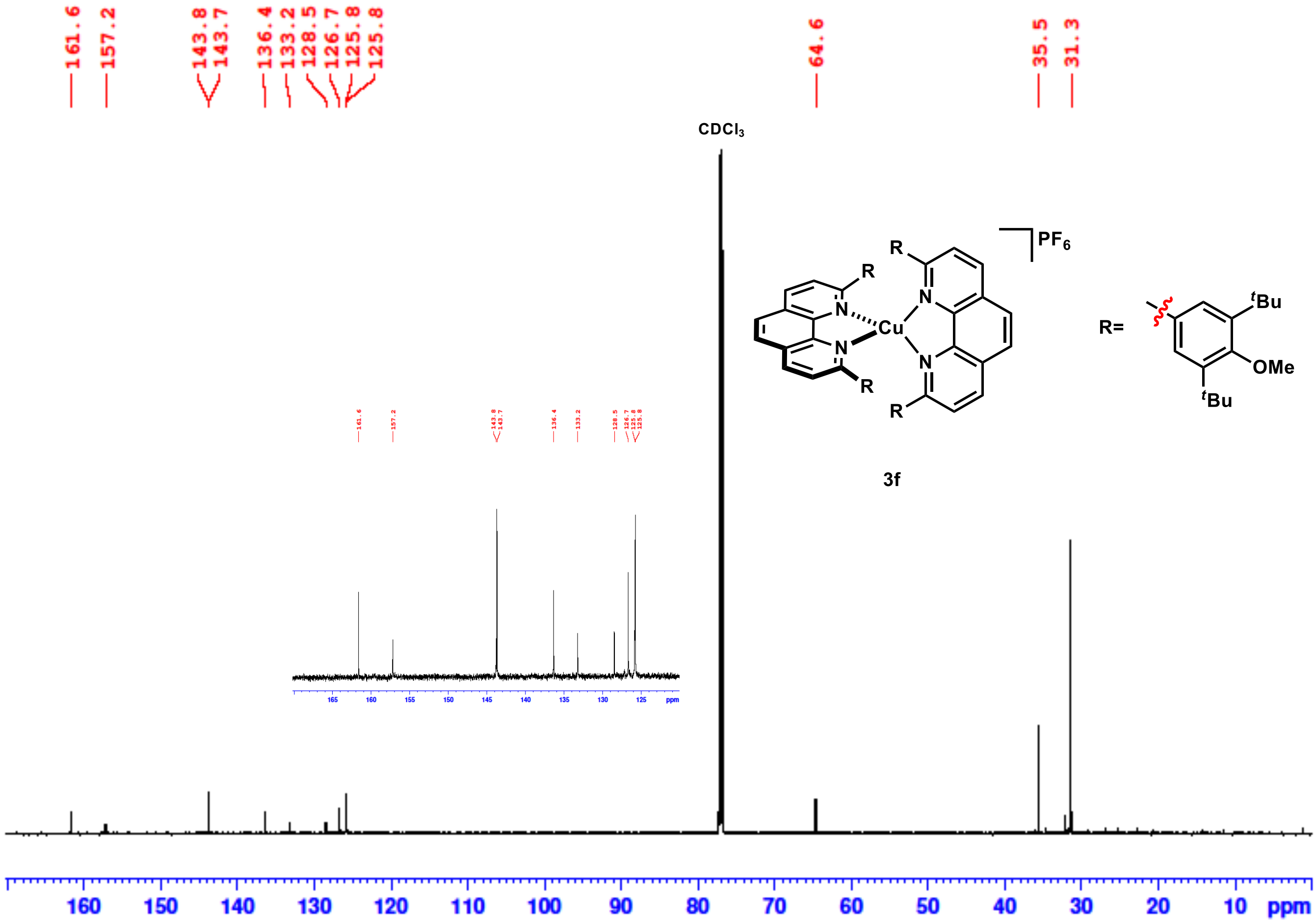


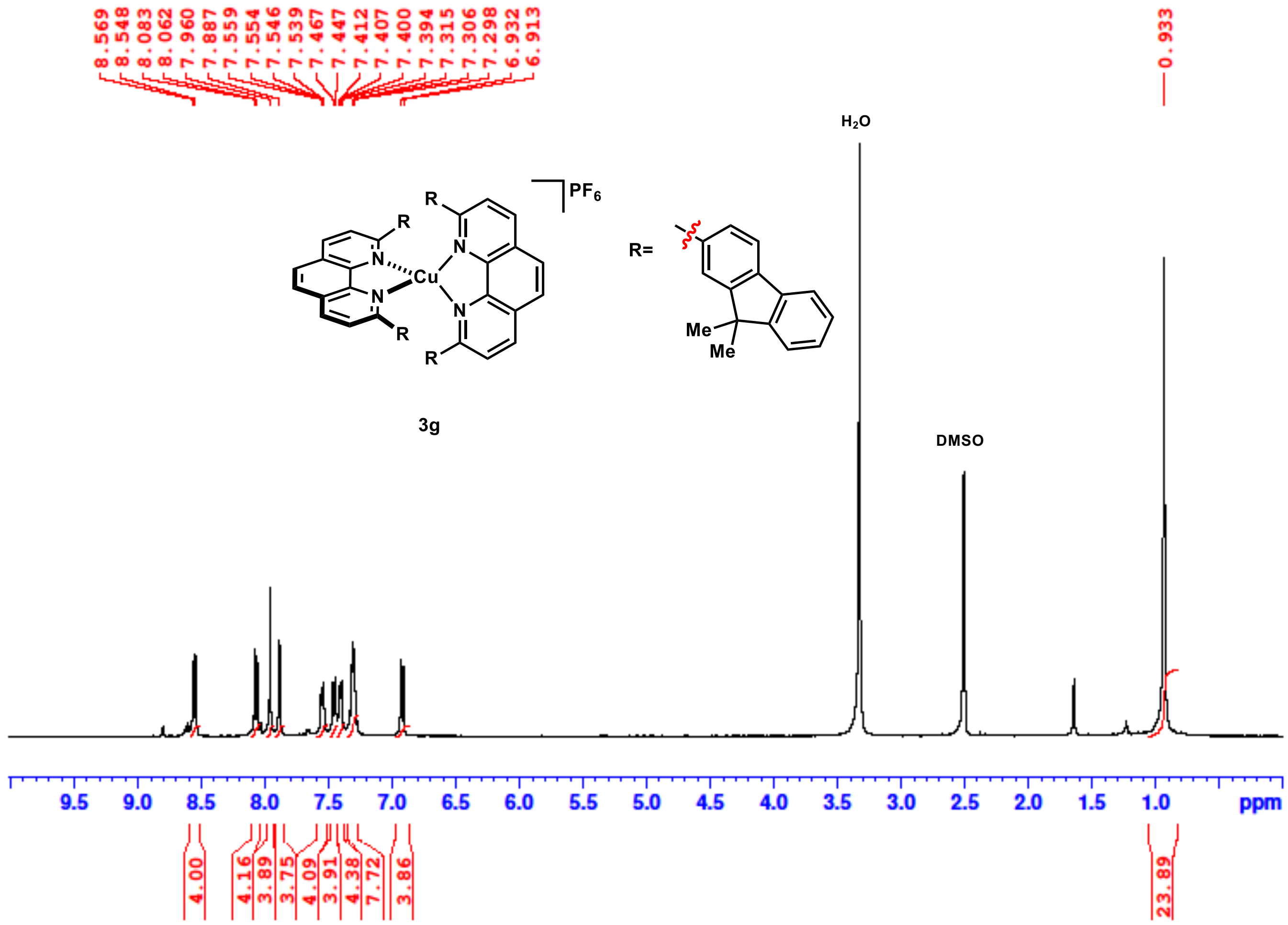
3e

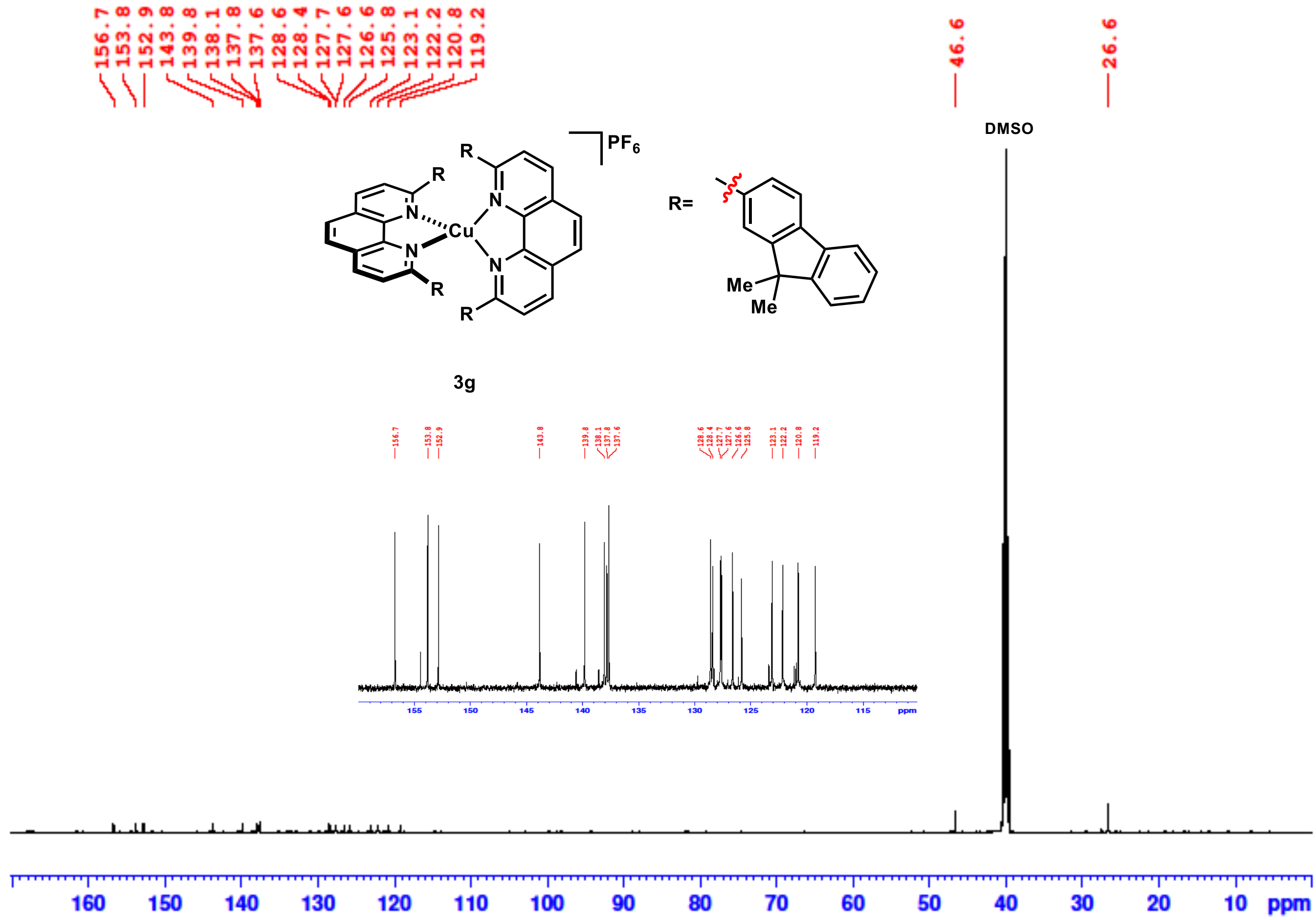
tpn-99 #1-37 RT: 0.01-0.29 AV: 37 NL: 2.48E7
T: FTMS + p ESI Full ms [150.00-2000.00]

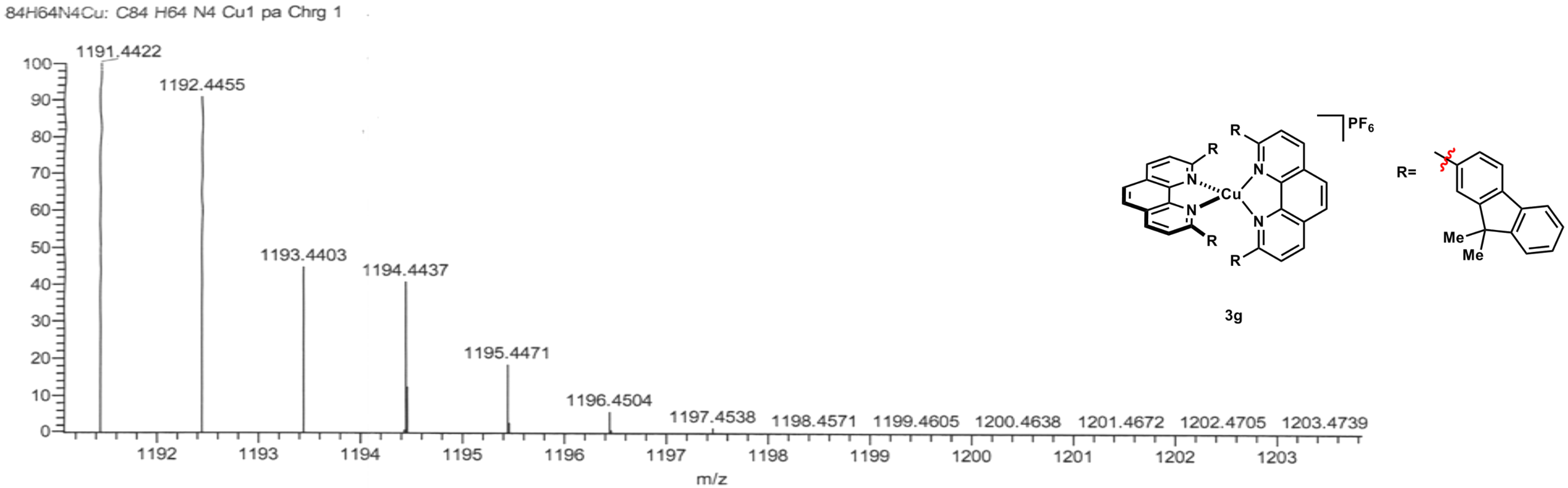


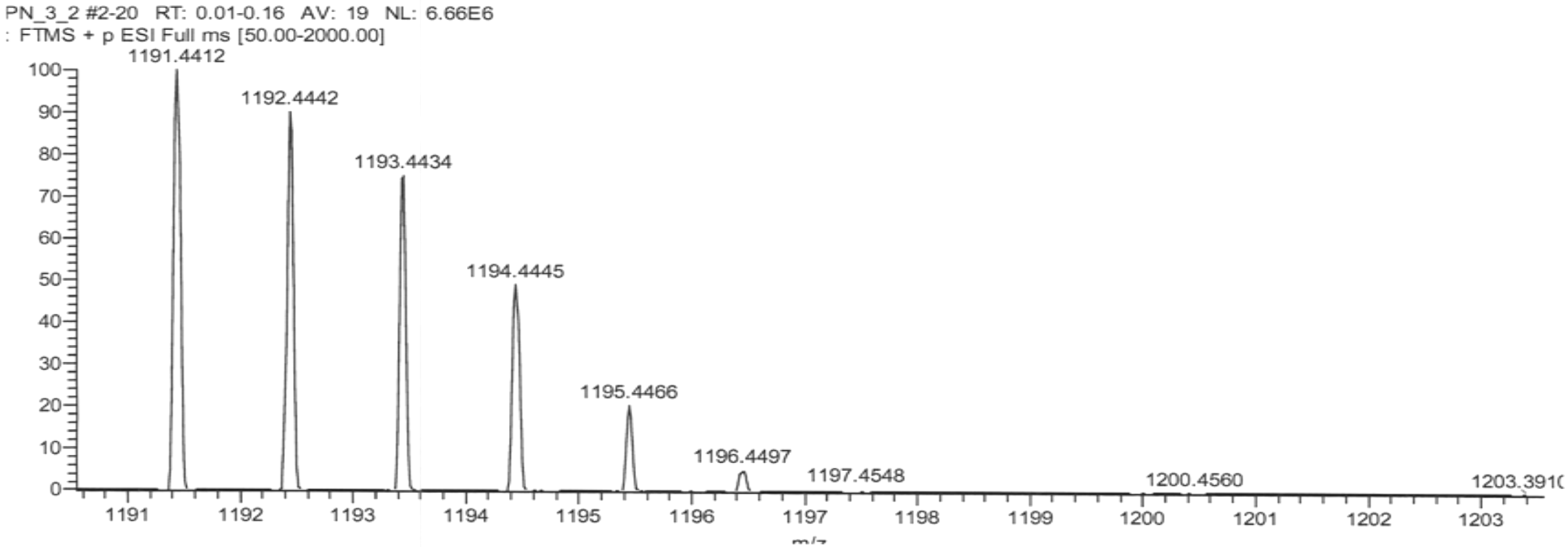

8.44
8.43
8.04
7.86
7.84
7.49
3.23
0.93
PF6
R
N
Cu
R=
tBu
OMe
3f
CDCl3
grease
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
4.00
3.84
4.02
7.92
11.82
71.27

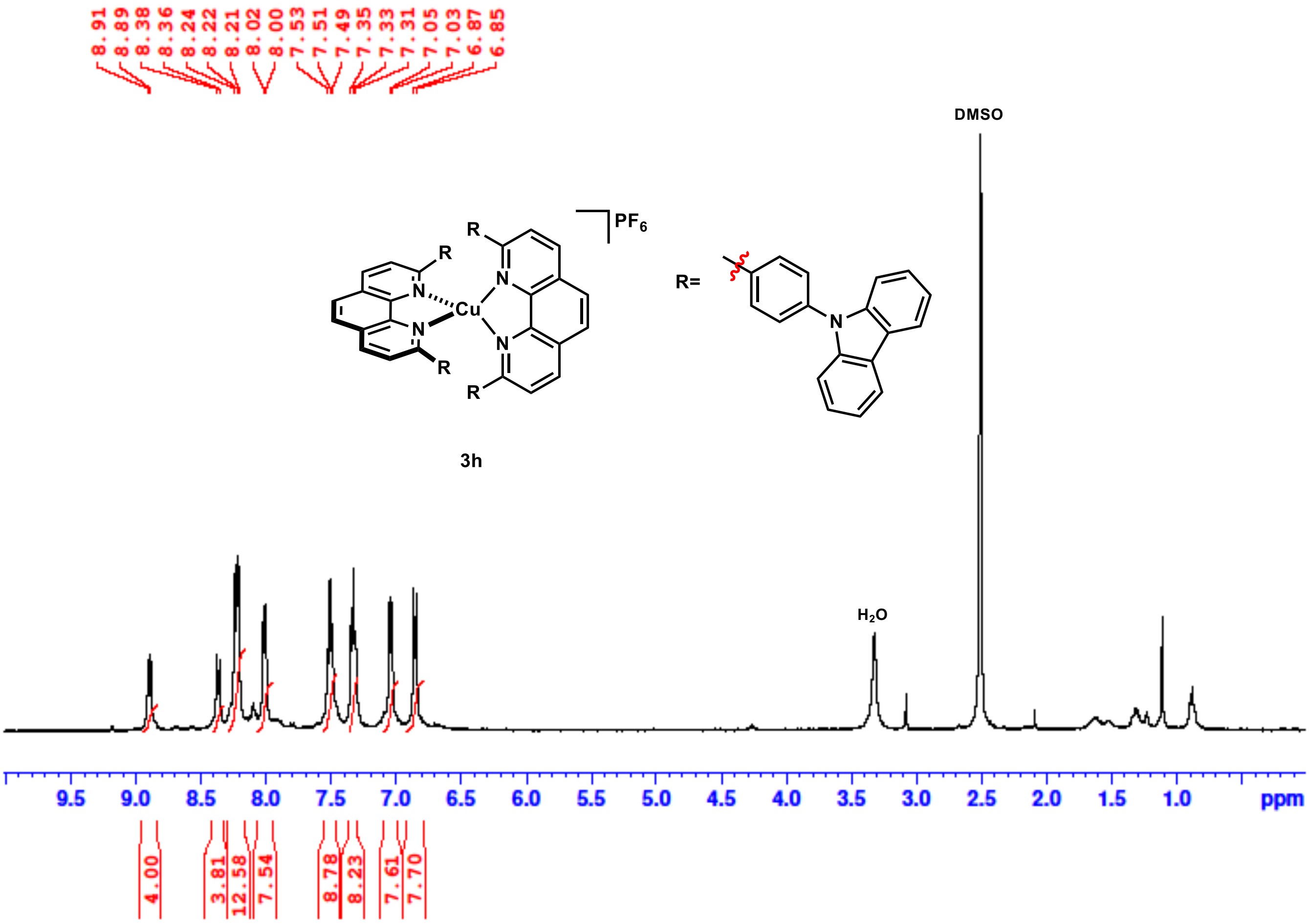

161.6
157.2
143.8
143.7
136.4
133.2
128.5
126.7
125.8
125.8
64.6
35.5
31.3
CDCl3
PF6
R
N
Cu
R=
tBu
OMe
3f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

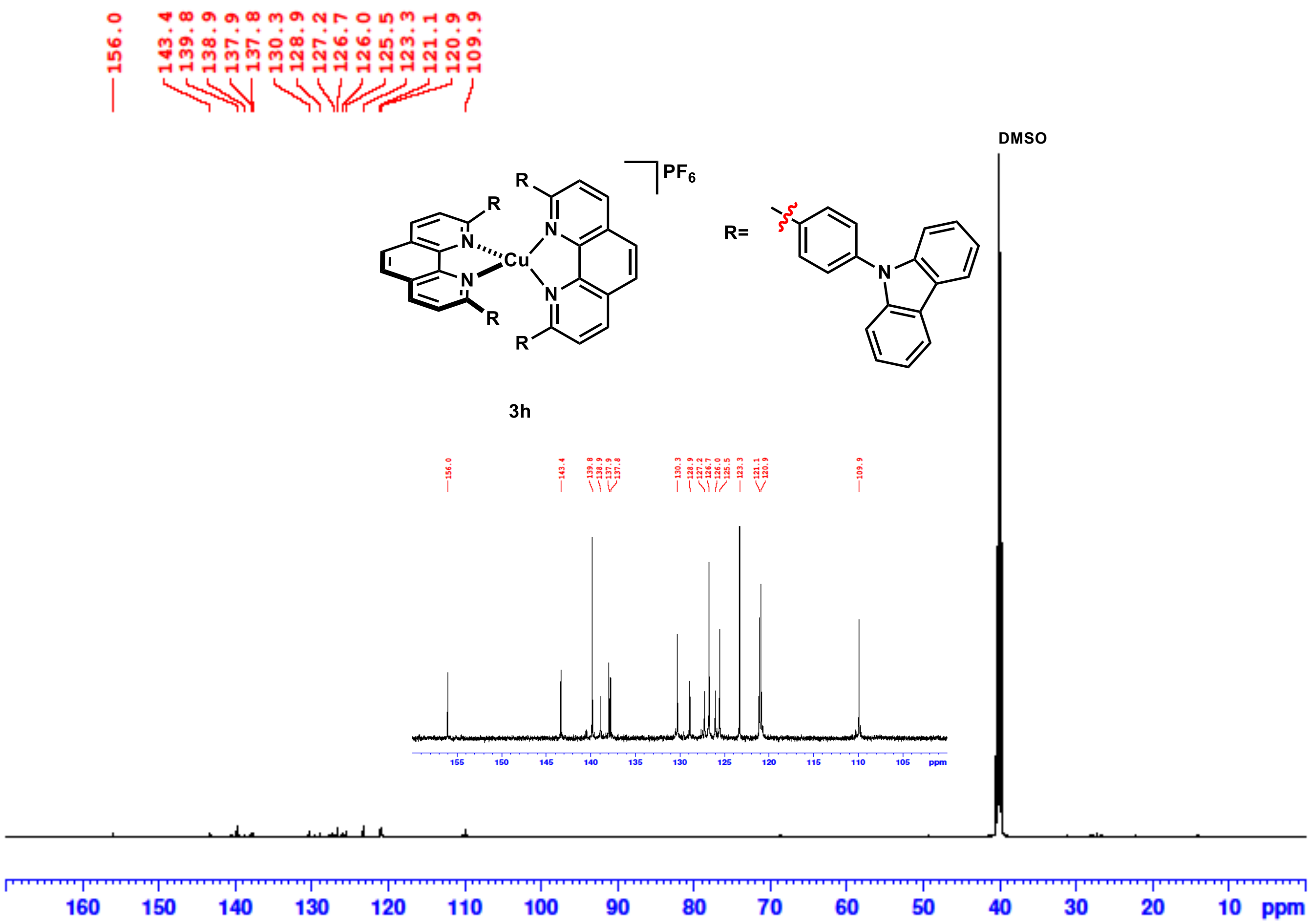

8.569
8.548
8.083
8.062
7.960
7.887
7.559
7.554
7.546
7.539
7.467
7.447
7.412
7.407
7.400
7.394
7.315
7.306
7.298
6.932
6.913
0.933
H2O
DMSO
PF6
R=
Me
Me
3g
ppm
4.00
4.16
3.89
3.75
4.09
3.91
4.38
7.72
3.86
23.89


156.7
153.8
152.9
143.8
139.8
138.1
137.8
137.6
128.6
128.4
127.7
127.6
126.6
125.8
123.1
122.2
120.8
119.2
46.6
26.6
DMSO
PF6
R=
Me
Me
3g
ppm


84H64N4Cu: C84 H64 N4 Cu1 pa Chrg 1
1191.4422
1192.4455
1193.4403
1194.4437
1195.4471
1196.4504
1197.4538
1198.4571
1199.4605
1200.4638
1201.4672
1202.4705
1203.4739
m/z
PF6
R
N
Cu
R=
Me
Me
3g

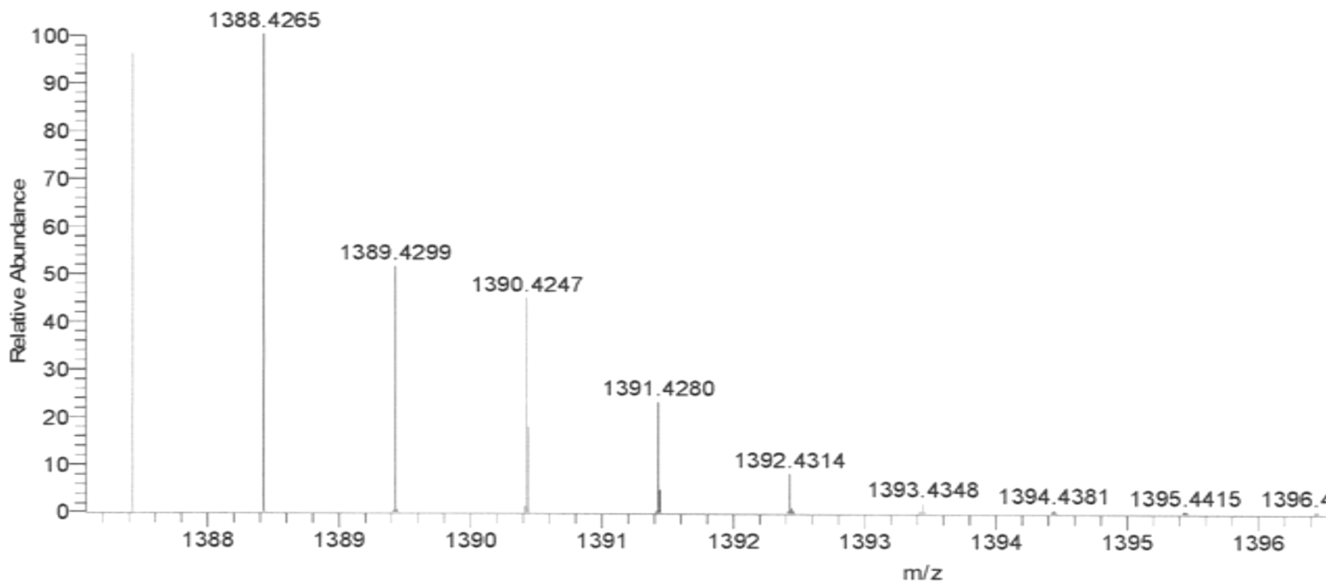

PN_3_2 #2-20 RT: 0.01-0.16 AV: 19 NL: 6.66E6
: FTMS + p ESI Full ms [50.00-2000.00]
1191.4412
1192.4442
1193.4434
1194.4445
1195.4466
1196.4497
1197.4548
1200.4560

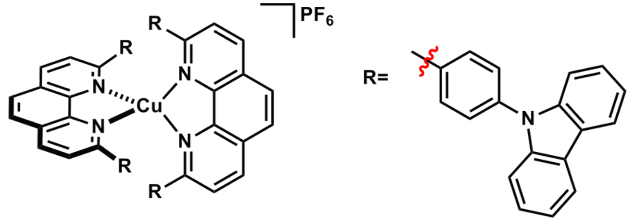

8.91
8.89
8.38
8.36
8.24
8.22
8.21
8.02
8.00
7.53
7.51
7.49
7.35
7.33
7.31
7.05
7.03
6.87
6.85
DMSO
PF6
R=
N
Cu
R
3h
H2O
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
4.00
3.81
12.58
7.54
8.78
8.23
7.61
7.70


156.0
143.4
139.8
138.9
137.9
137.8
130.3
128.9
127.2
126.7
126.0
125.5
123.3
121.1
120.9
109.9
DMSO
PF6
R=
N
Cu
R
3h
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

C:\Xcalibur\data\2017\03_March\TN_04 21/04/2017 11:49:16 AM

C96H60N8Cu: C96 H60 N8 Cu1 pa Chrg 1





3h

TN_04 #2-28 RT: 0.02-0.40 AV: 27 NL: 9.06E4
T: FTMS + p ESI Full ms [150.00-2000.00]