Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Influence of the oxazole ring connection on the fluorescence of oxazoyl-triphenylamine biphotonic DNA probes

Blaise Dumat,[a] Elodie Faurel-Paul,[a] Pauline Fornarelli,[a] Nicolas Saettel,[a] Germain Metgé,[b] Céline Fiorini-Debuisschert,[b] Fabrice Charra,[b] Florence Mahuteau-Betzer*[a] and Marie-Paule Teulade-Fichou*[a]

Electronic Supplementary information

1- Additional figures

2- Analyses: NMR spectra and HPLC chromatograms

1- Additional figures

	λ_{abs} (nm)	λ_{em} (nm)	ε (L mol^{-1} cm^{-1})	Φ_F
TP-3(Ox5Py)	447	634	58530	0.058
TP-3(Ox2Py)	477	690	48650	0.022
TP-3(Ox5Bzim)	410	540	60300	0.53
TP-3Py	492	666	66000	0.13
TP-3Bzim	440	604	57200	0.42

Table 1. Linear optical properties of the TP-Oxazole dyes and of the parent compounds TP-Py and TP-Bzim in glycerol

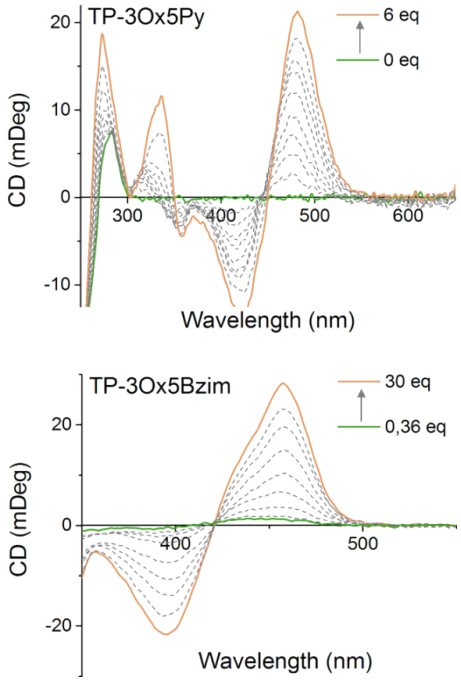
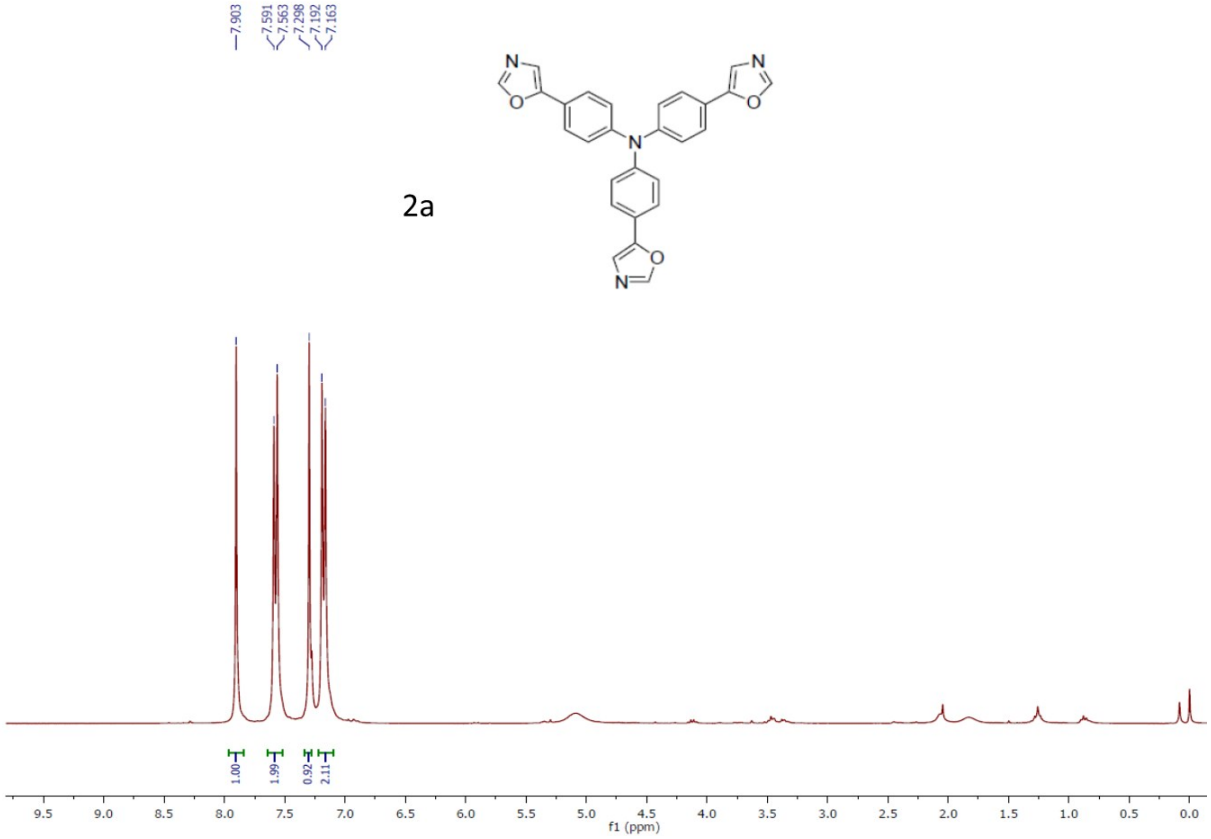
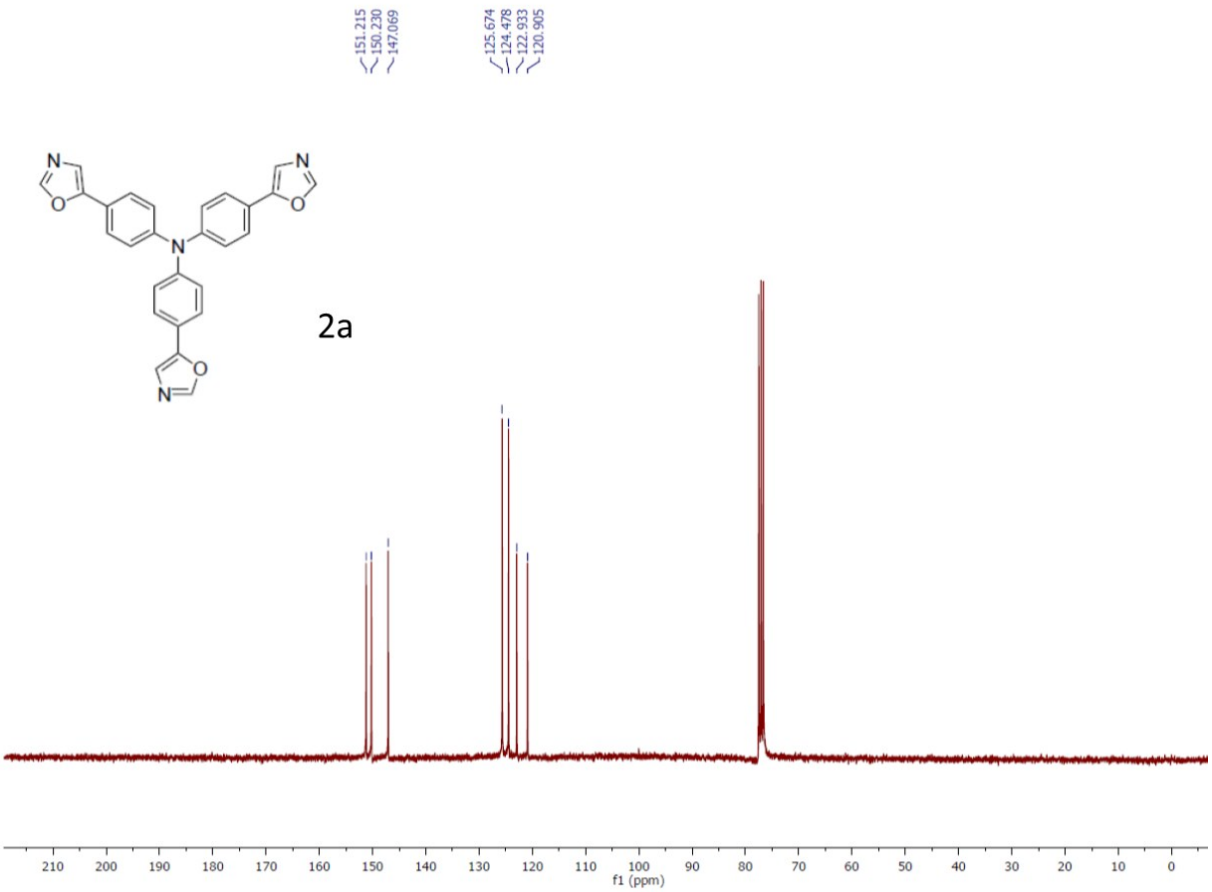
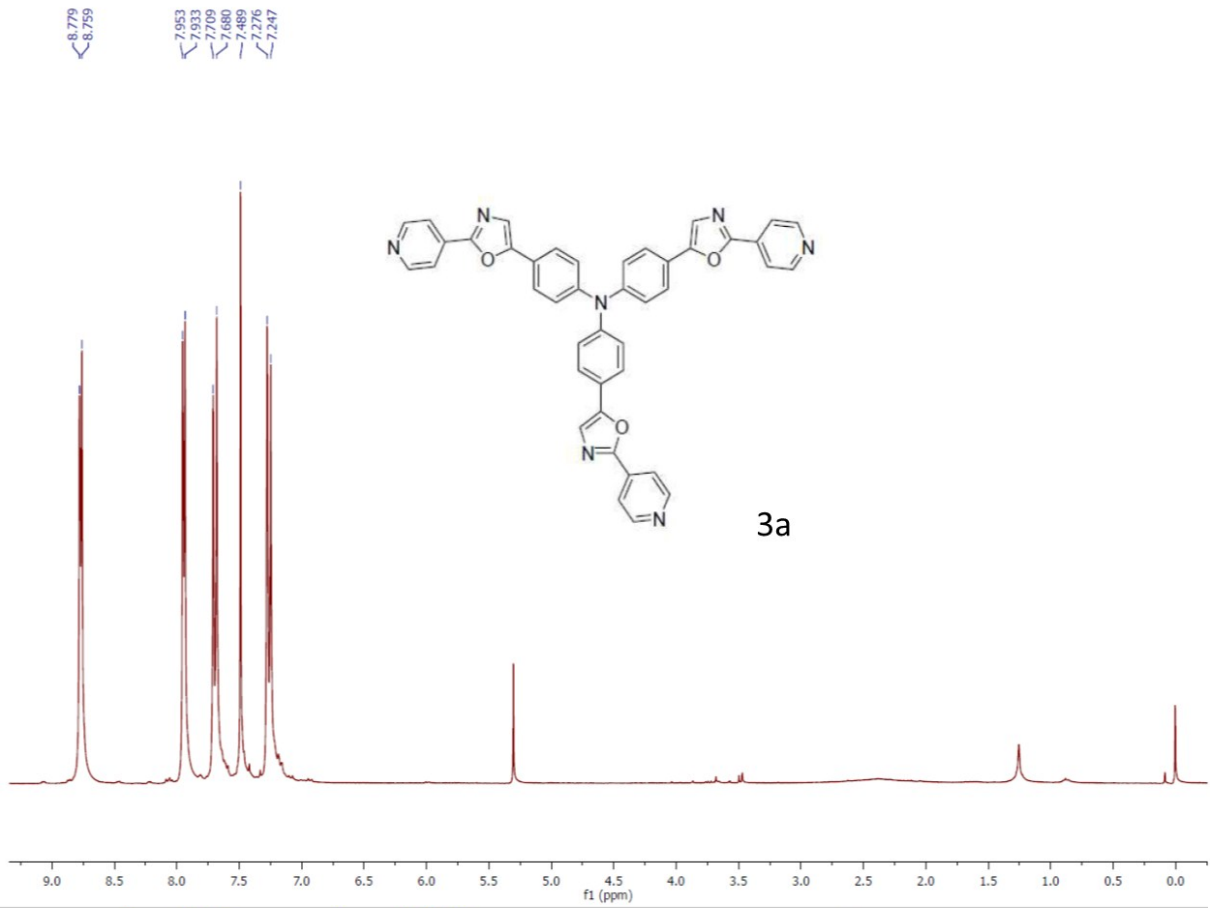


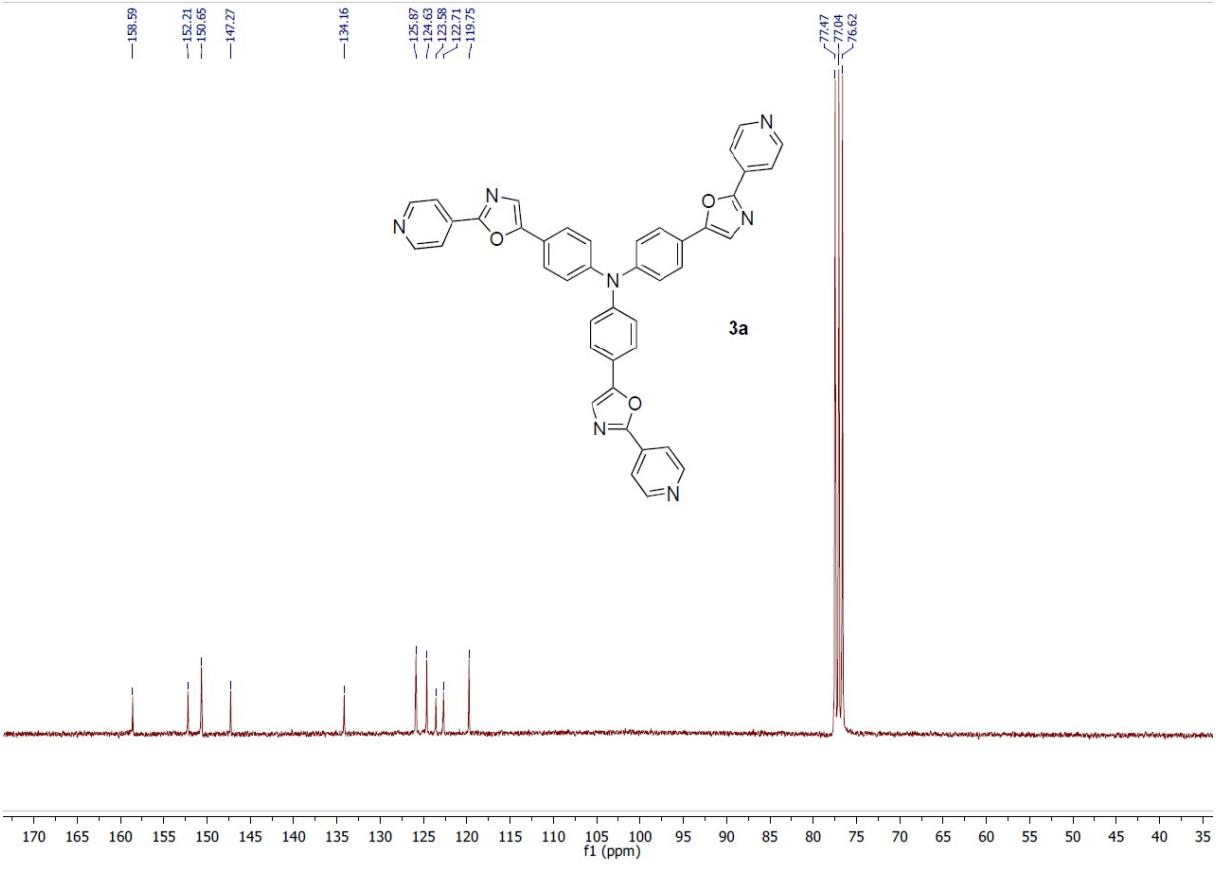
Figure 1. Circular dichroism spectra of drewAT upon addition of TP-3Ox5Py. Increasing amounts of TP-3Ox5Py (molar equivalents indicated on the graphs) are added to a 2 µM solution of drewAT in 10 mM sodium cacodylate pH 7.2 buffer with 100 mM NaCl. Circular dichroism spectra of drew AT at steady TP-3Ox5Bzim concentration according to Chaires's protocol (N. C. Garbett, P. A. Ragazzon, J. B. Chaires Nature Protocols, 2007, 2, 3166-3172)

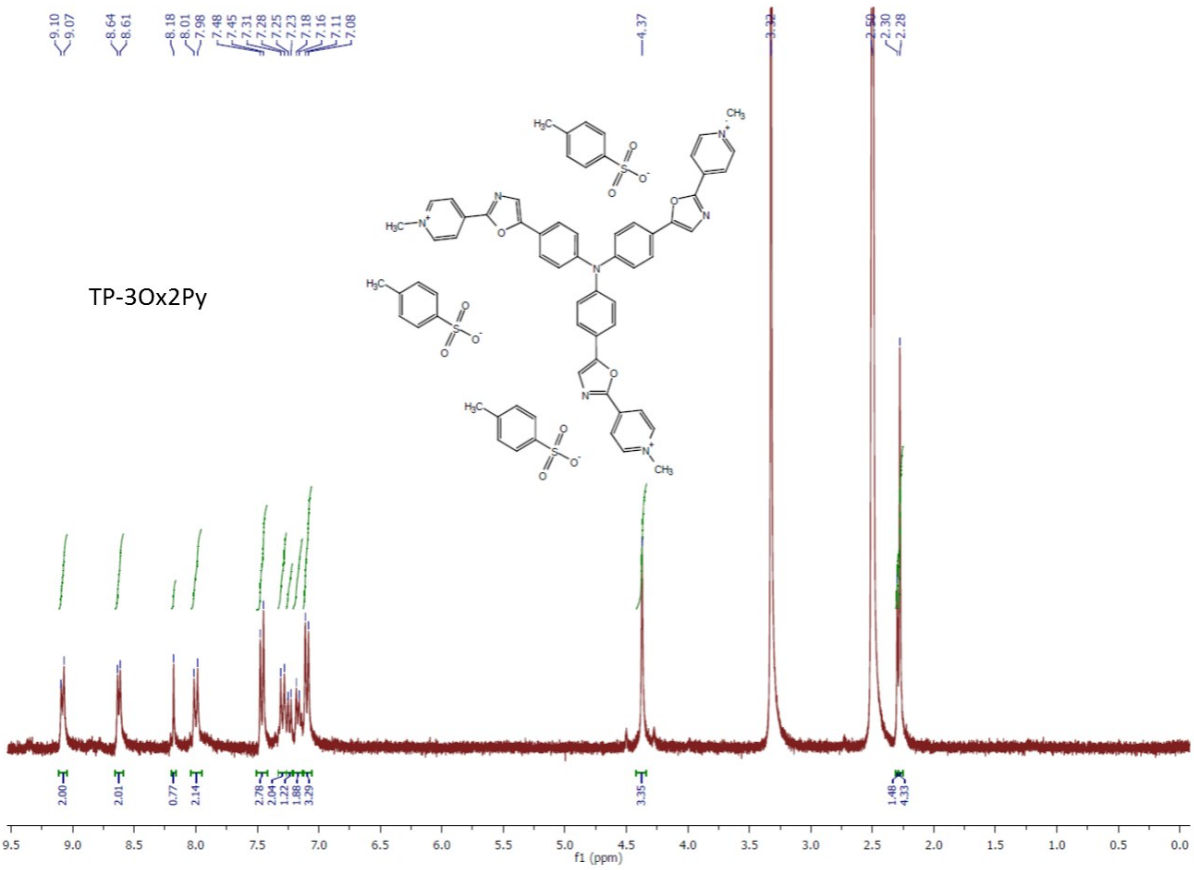
2- Analyses: NMR spectra and HPLC chromatograms

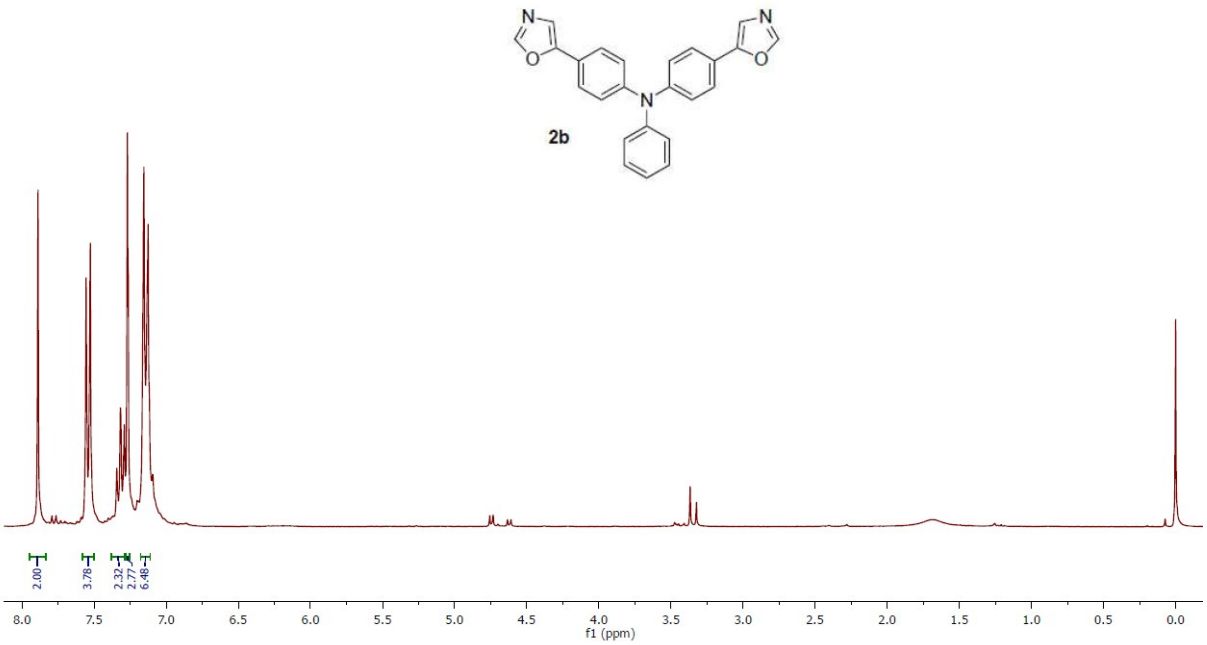


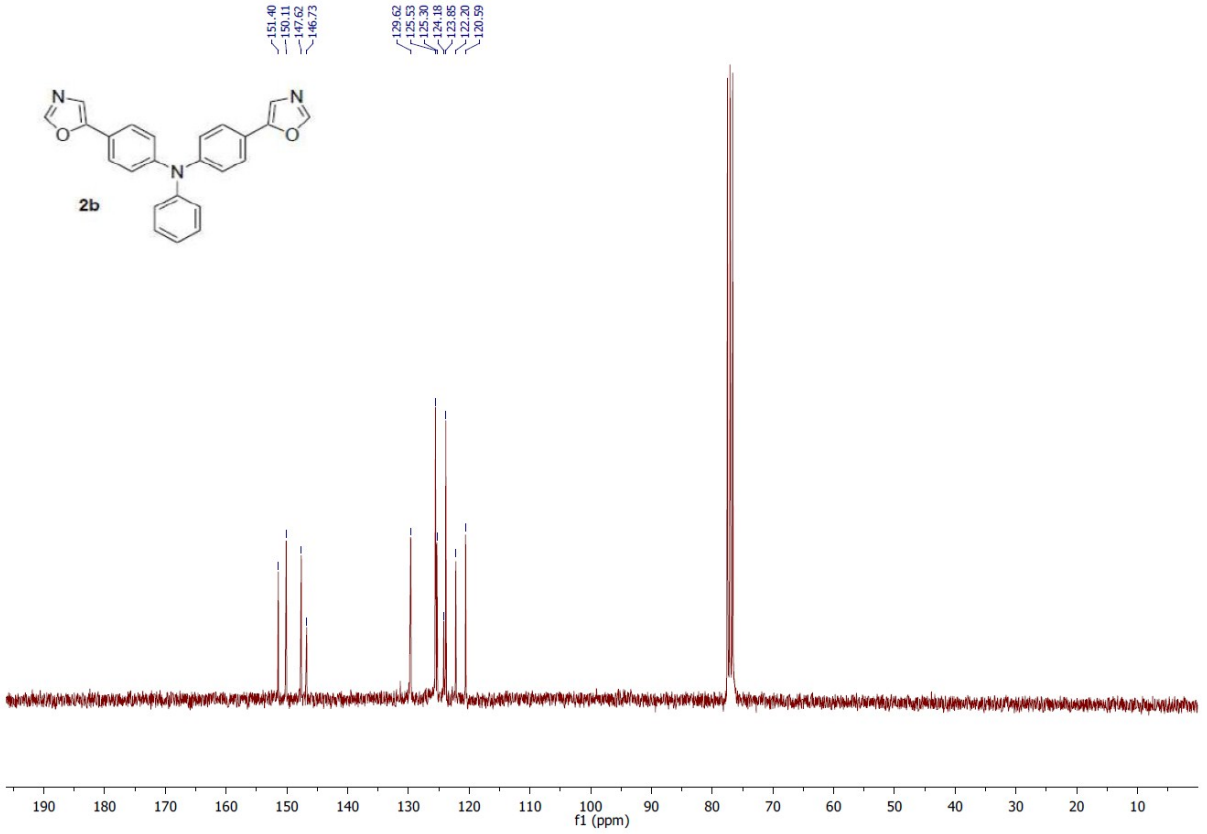


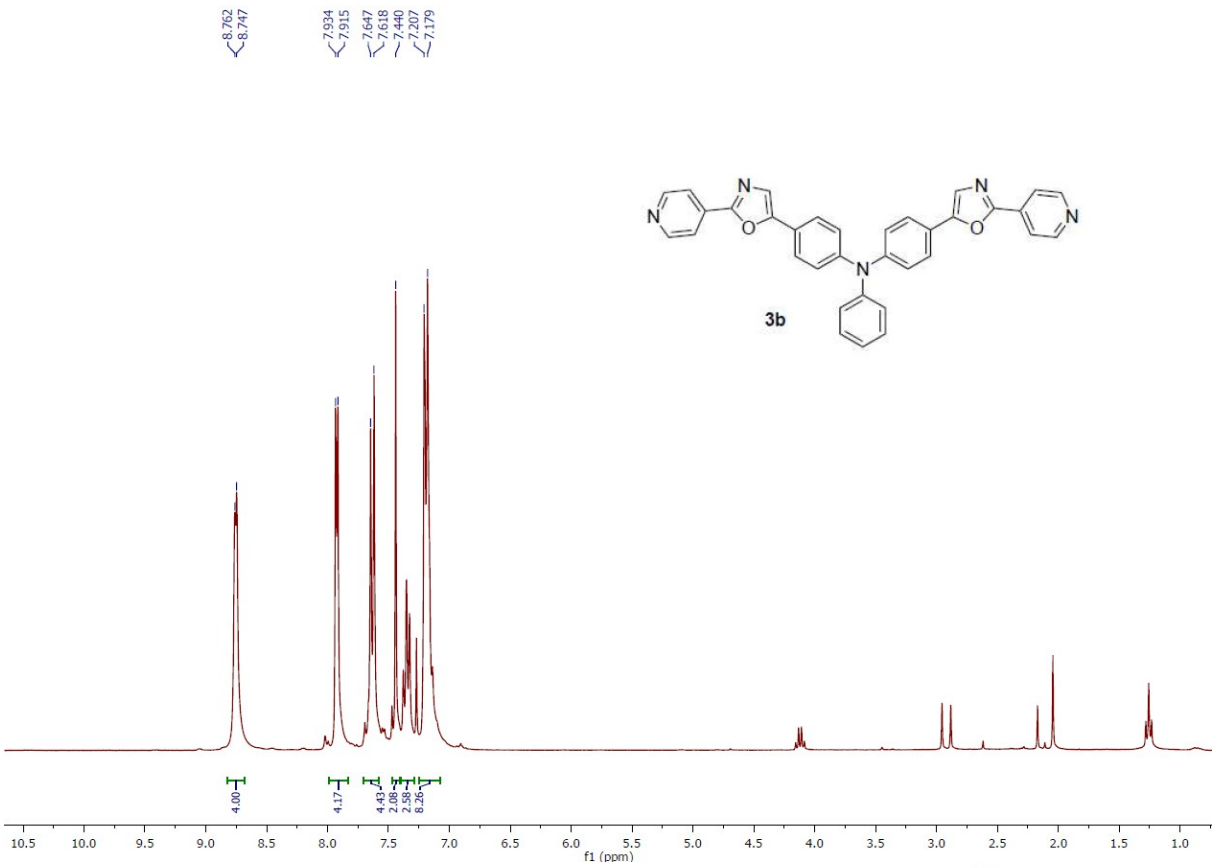

8.779
8.759
7.953
7.933
7.709
7.680
7.489
7.276
7.247
3a
f1 (ppm)

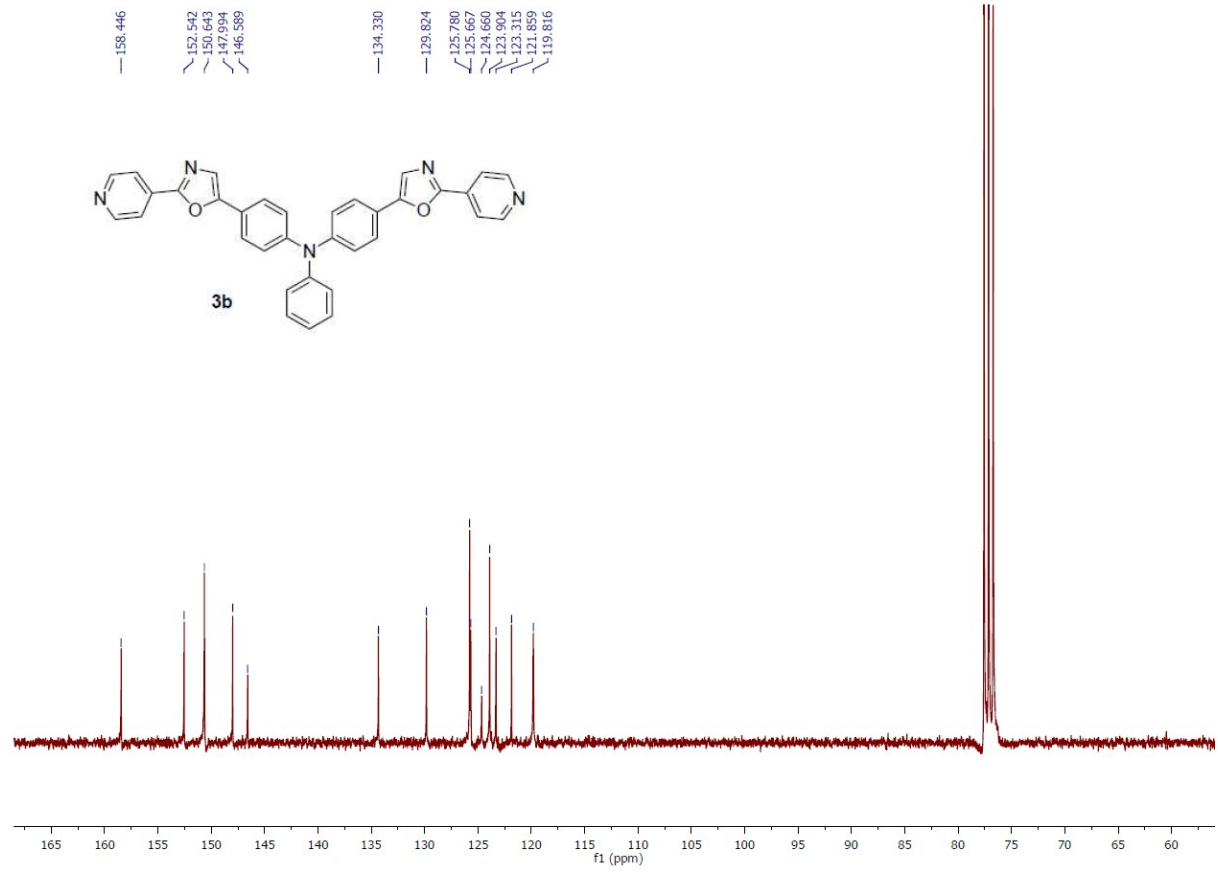

158.59
152.21
150.65
147.27
134.16
125.87
124.63
123.58
122.71
119.75
77.47
77.04
76.62
3a
f1 (ppm)

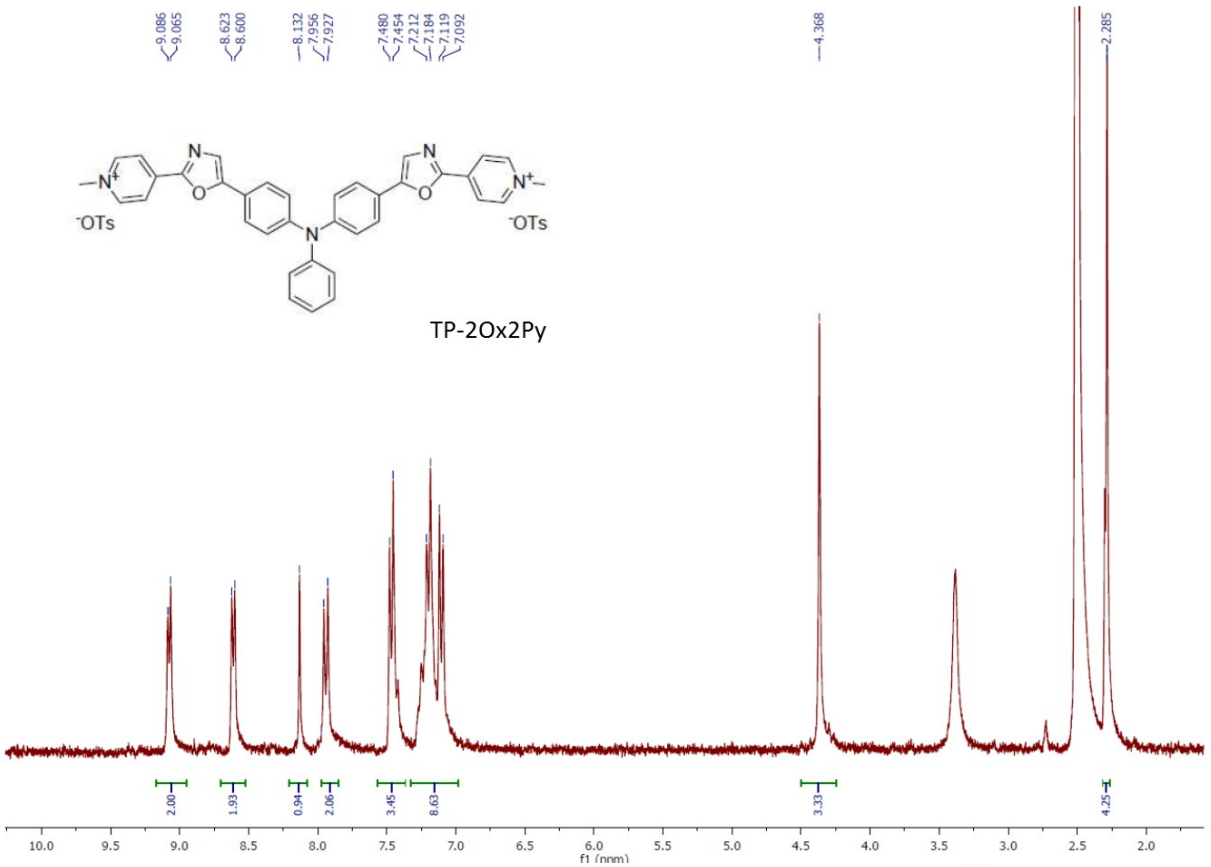

TP-3Ox2Py
9.10
9.07
8.64
8.61
8.18
8.01
7.98
7.48
7.45
7.31
7.28
7.25
7.23
7.18
7.16
7.11
7.08
4.37
3.32
2.50
2.30
2.28
2.00
2.01
0.77
2.14
2.78
2.04
1.22
1.88
3.29
3.35
1.48
4.33
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

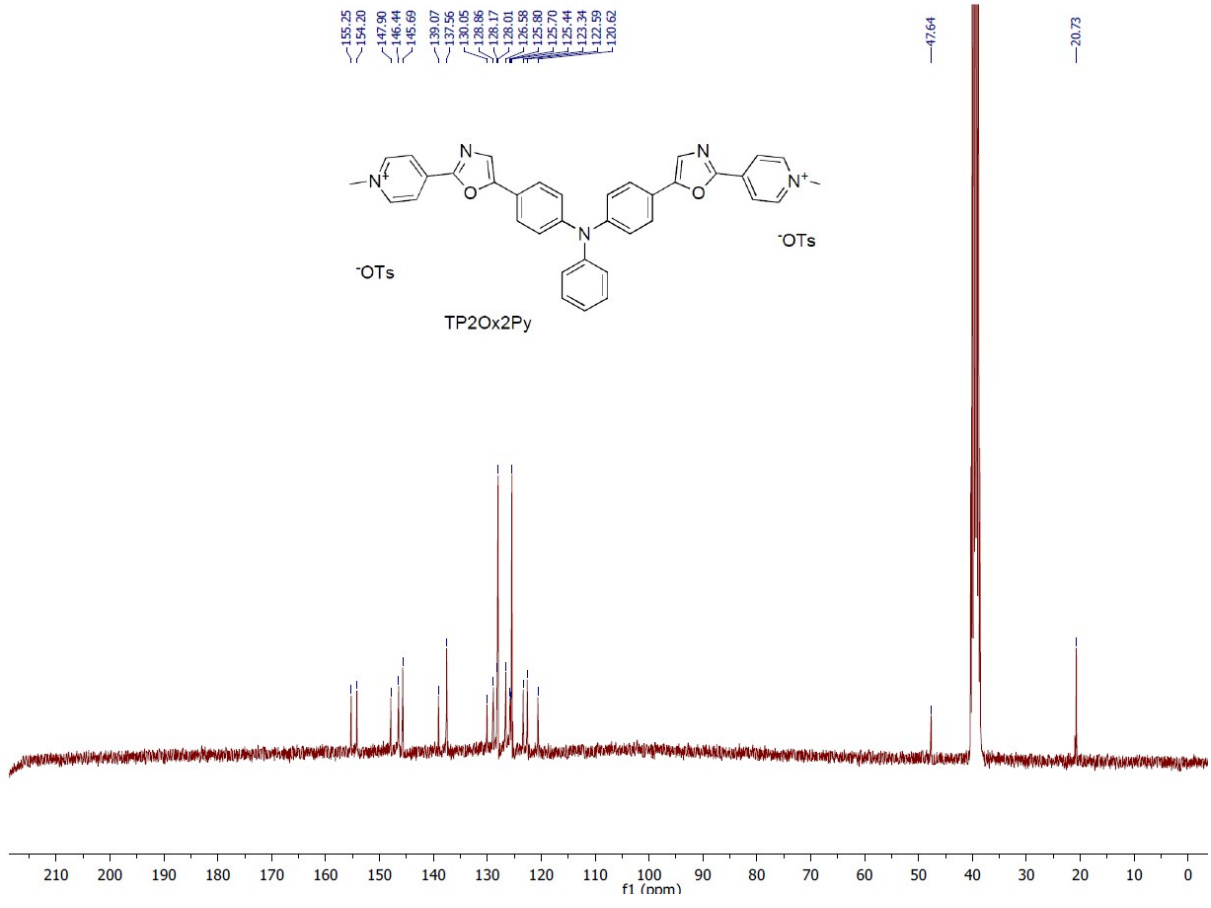

2b
2.00
3.78
2.32
2.77
6.48
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

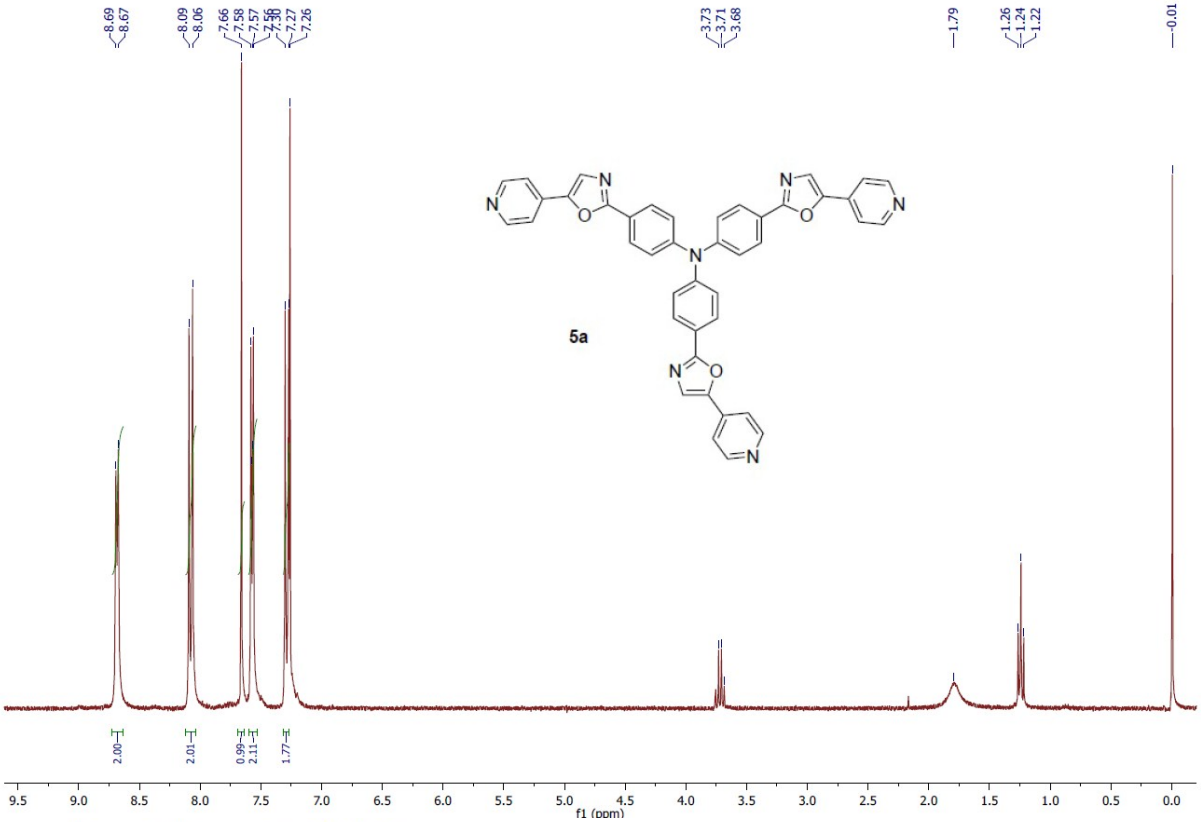

151.40
150.11
147.62
146.73
129.62
125.53
125.30
124.18
123.85
122.20
120.59
2b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

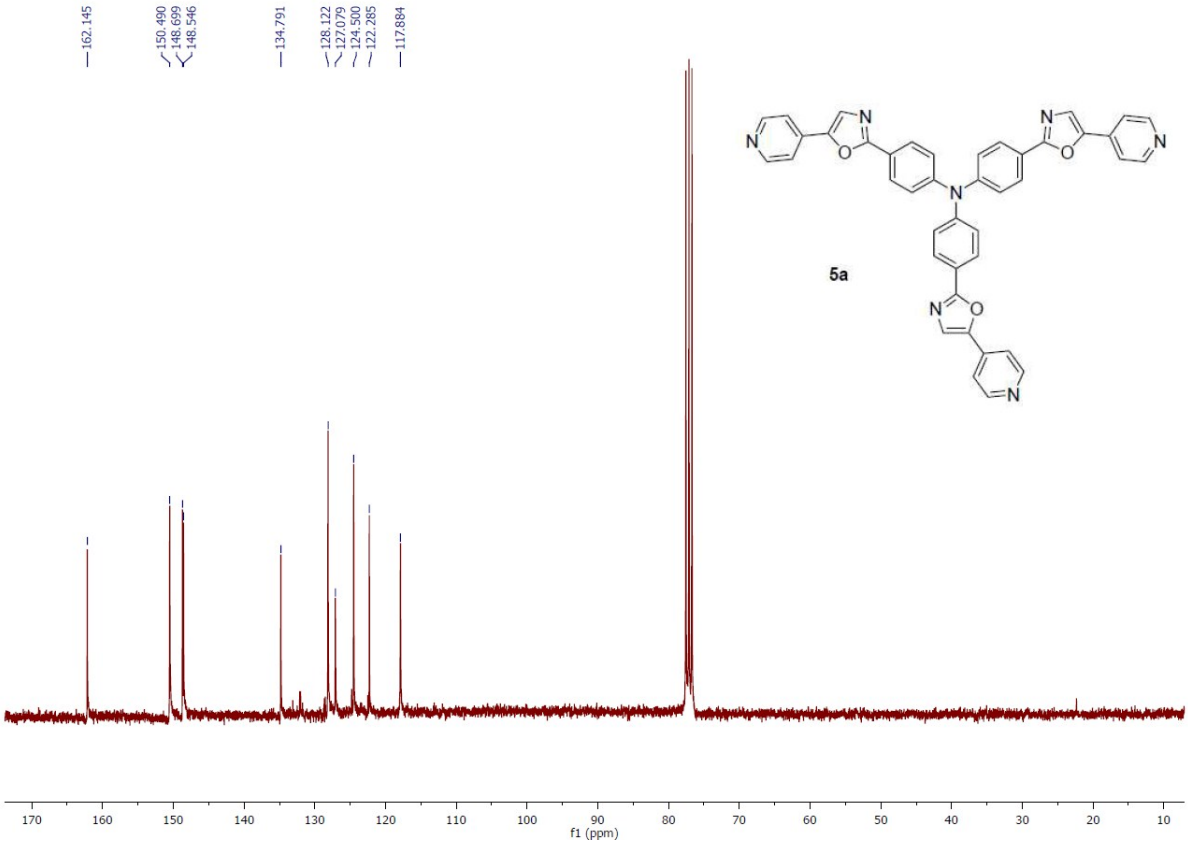

8.762
8.747
7.934
7.915
7.647
7.618
7.440
7.207
7.179
3b
4.00
4.17
4.43
2.08
2.58
8.26
f1 (ppm)

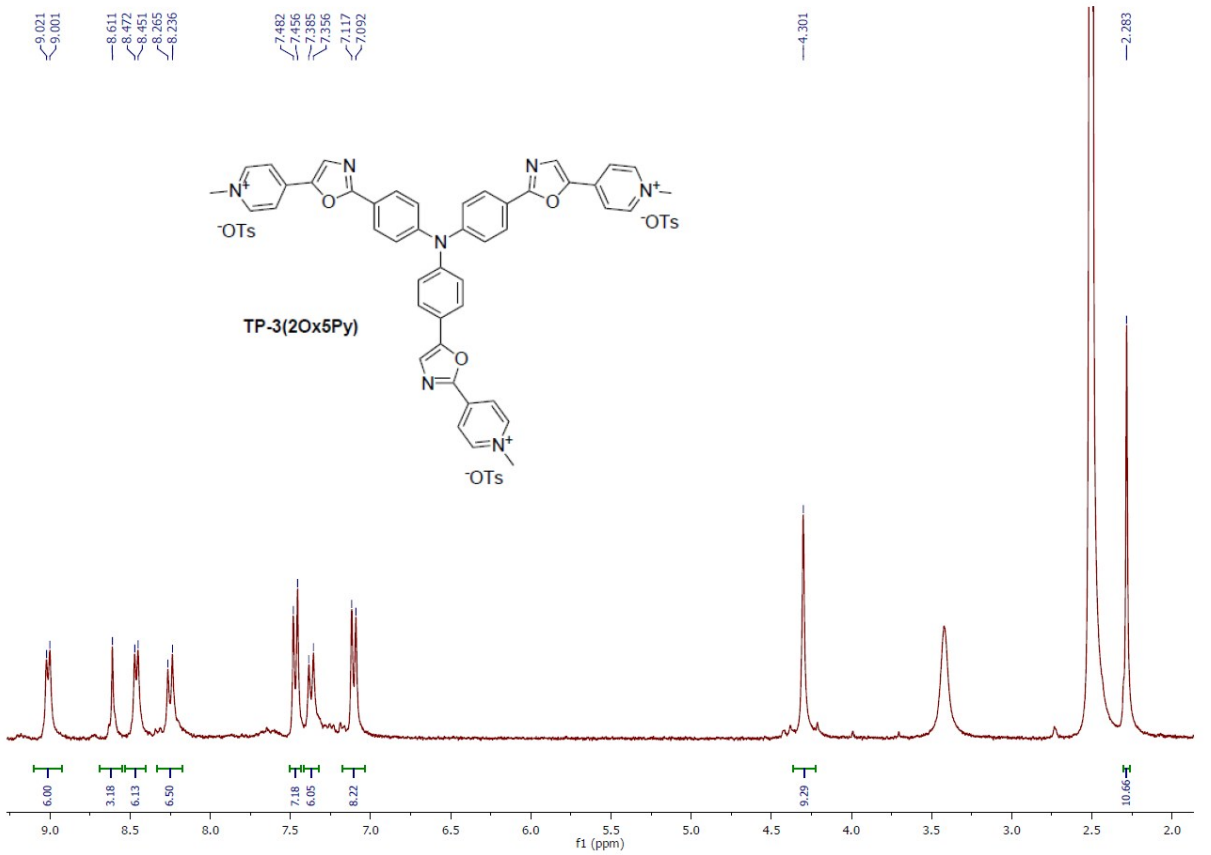

158.446
152.542
150.643
147.994
146.589
134.330
129.824
125.780
125.667
124.660
123.904
123.315
121.859
119.816
3b
f1 (ppm)

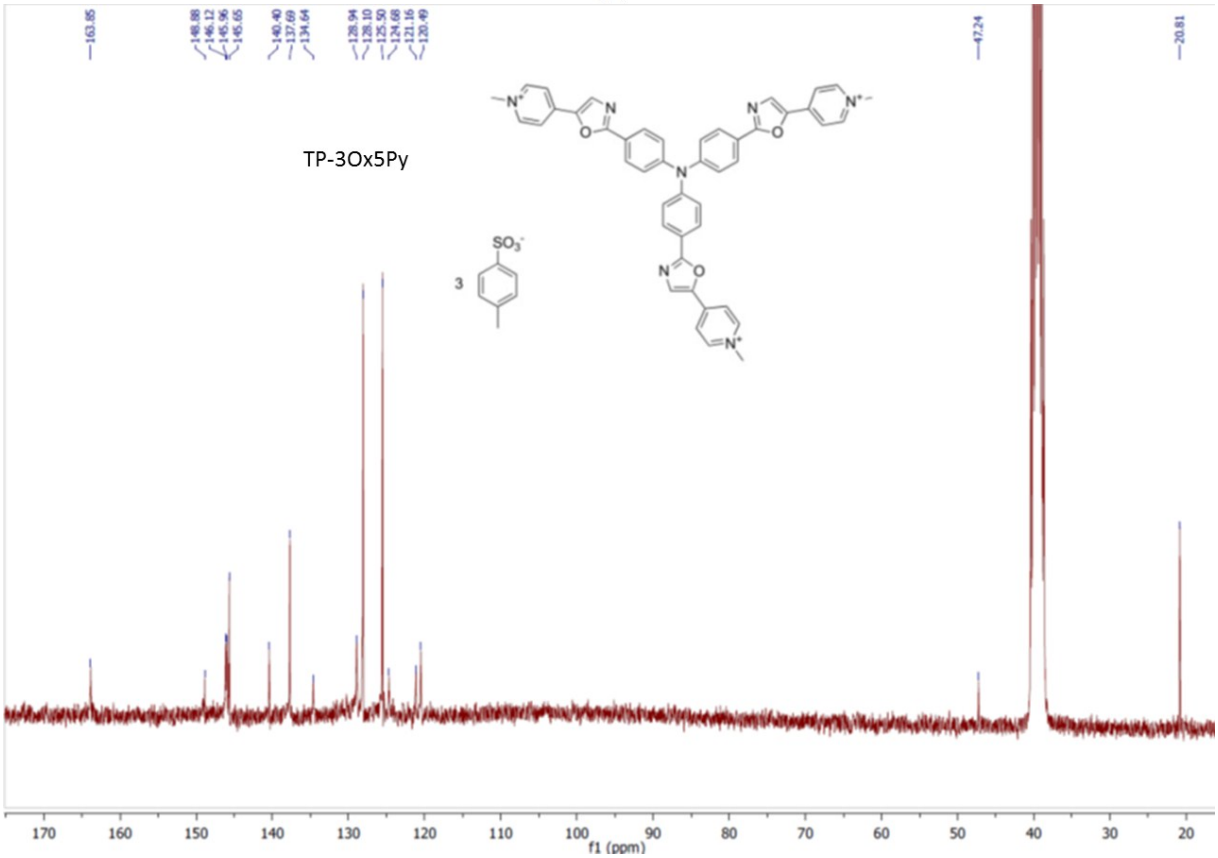

9.086
9.065
8.623
8.600
8.132
7.956
7.927
7.480
7.454
7.212
7.184
7.119
7.092
4.368
2.285
N
N
N+
N+
-OTs
-OTs
TP-2Ox2Py
2.00
1.93
0.94
2.06
3.45
8.63
3.33
4.25
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)

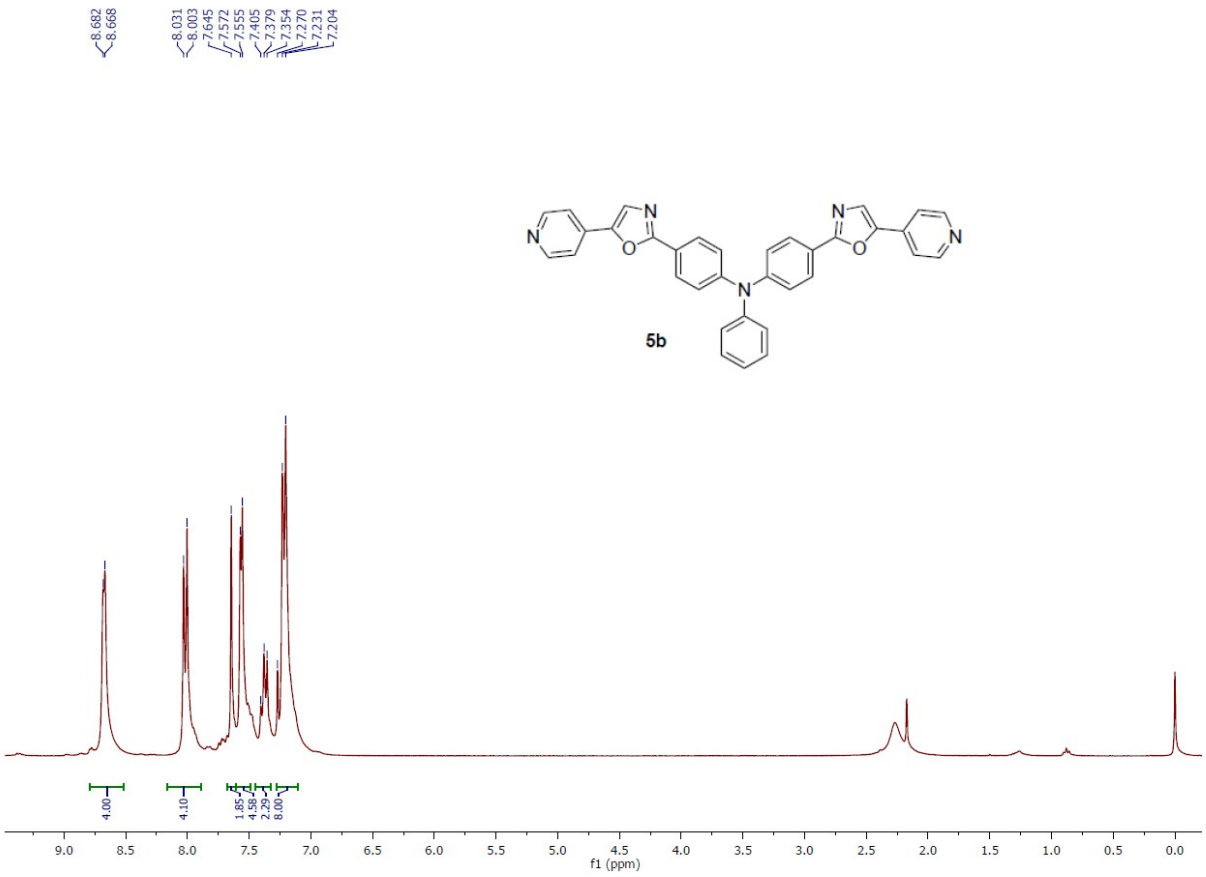

155.25
154.20
147.90
146.44
145.69
139.07
137.56
130.05
126.86
126.17
126.01
125.80
125.70
125.44
123.34
122.59
120.62
47.64
20.73
N
N
N+
N+
-OTs
-OTs
TP2Ox2Py
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

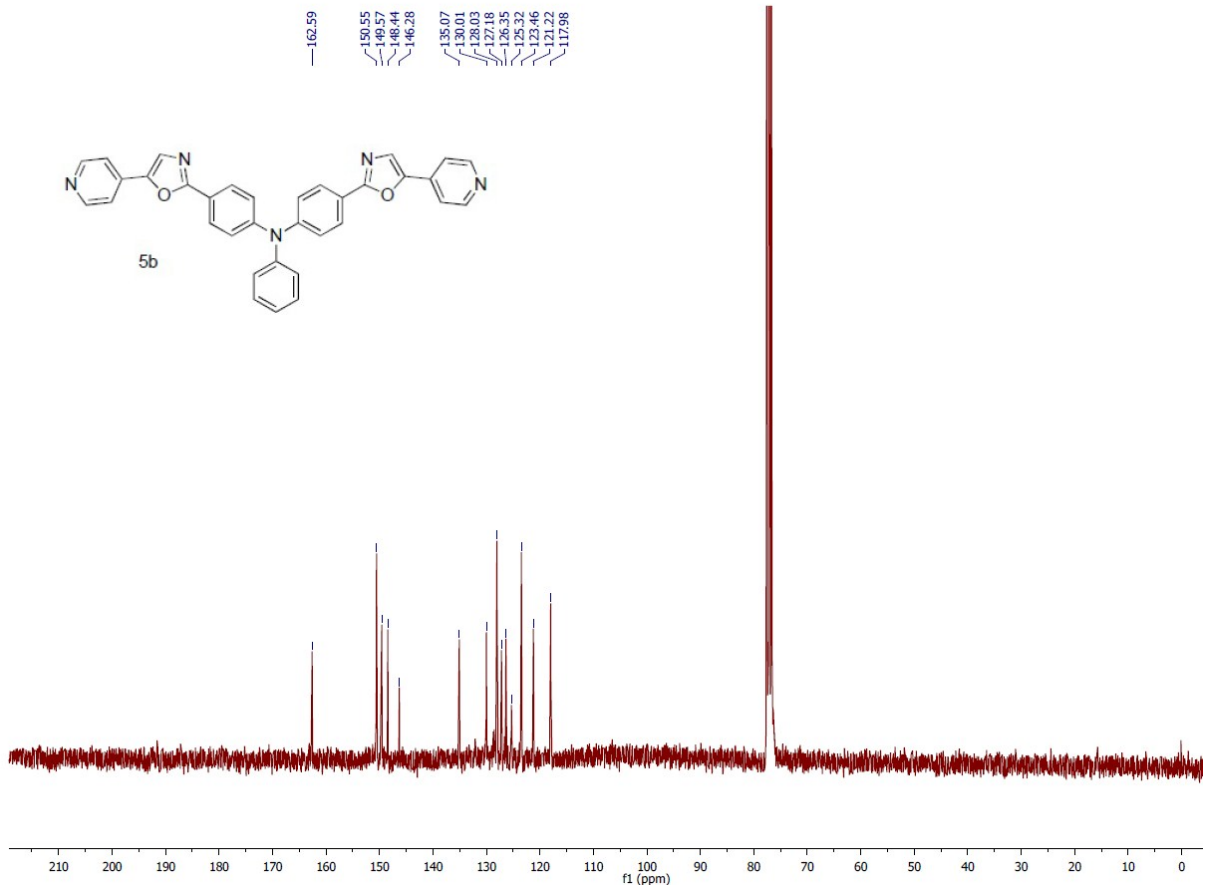

8.69
8.67
8.09
8.06
7.66
7.58
7.57
7.36
7.27
7.26
3.73
3.71
3.68
1.79
1.26
1.24
1.22
0.01
2.00
2.01
0.99
2.11
1.77
5a
f1 (ppm)

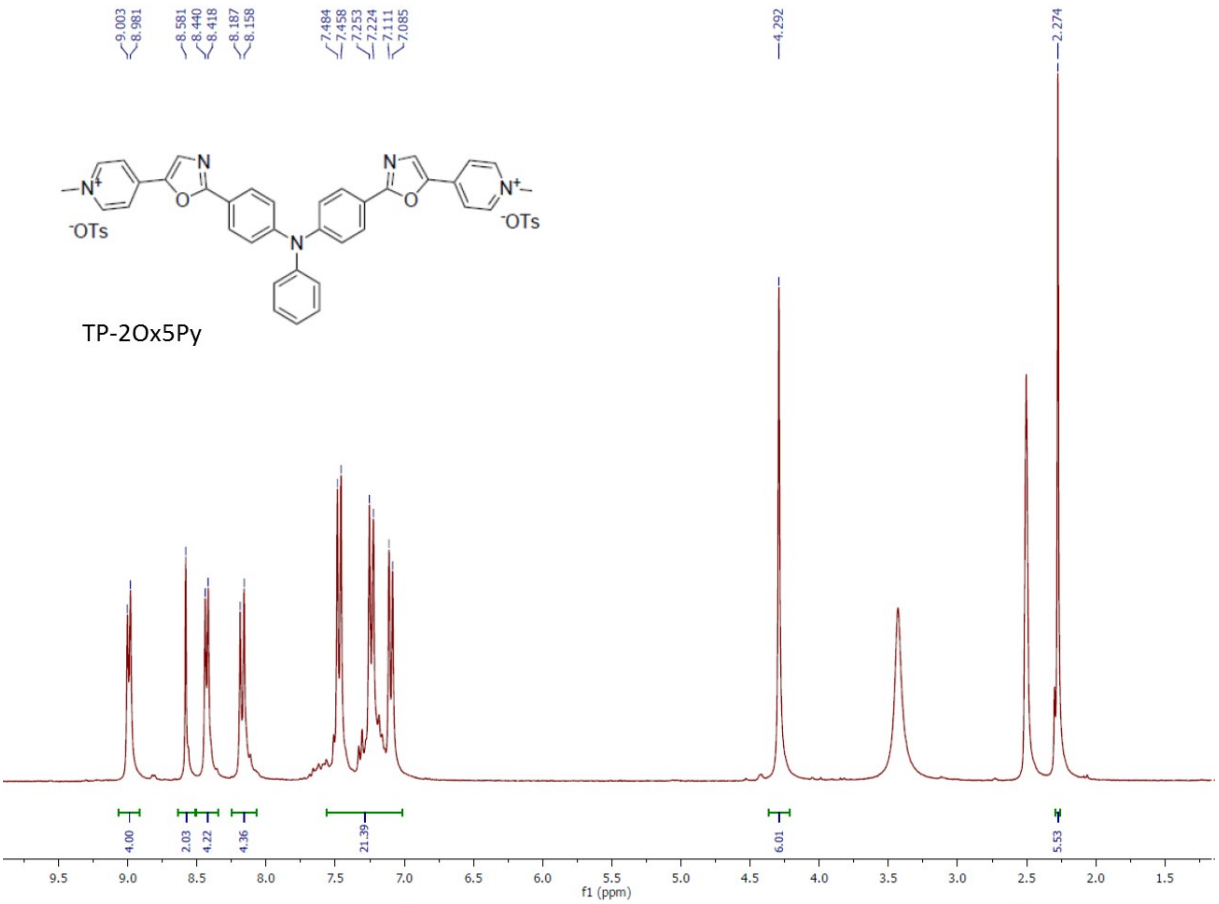

162.145
150.490
148.699
148.546
134.791
128.122
127.079
124.500
122.285
117.884
5a
f1 (ppm)


9.021
9.001
8.611
8.472
8.451
8.265
8.236
7.482
7.456
7.385
7.356
7.117
7.092
4.301
2.283
TP-3(2Ox5Py)
⁻OTs
⁻OTs
⁻OTs
6.00
3.18
6.13
6.50
7.18
6.05
8.22
9.29
10.66
f1 (ppm)

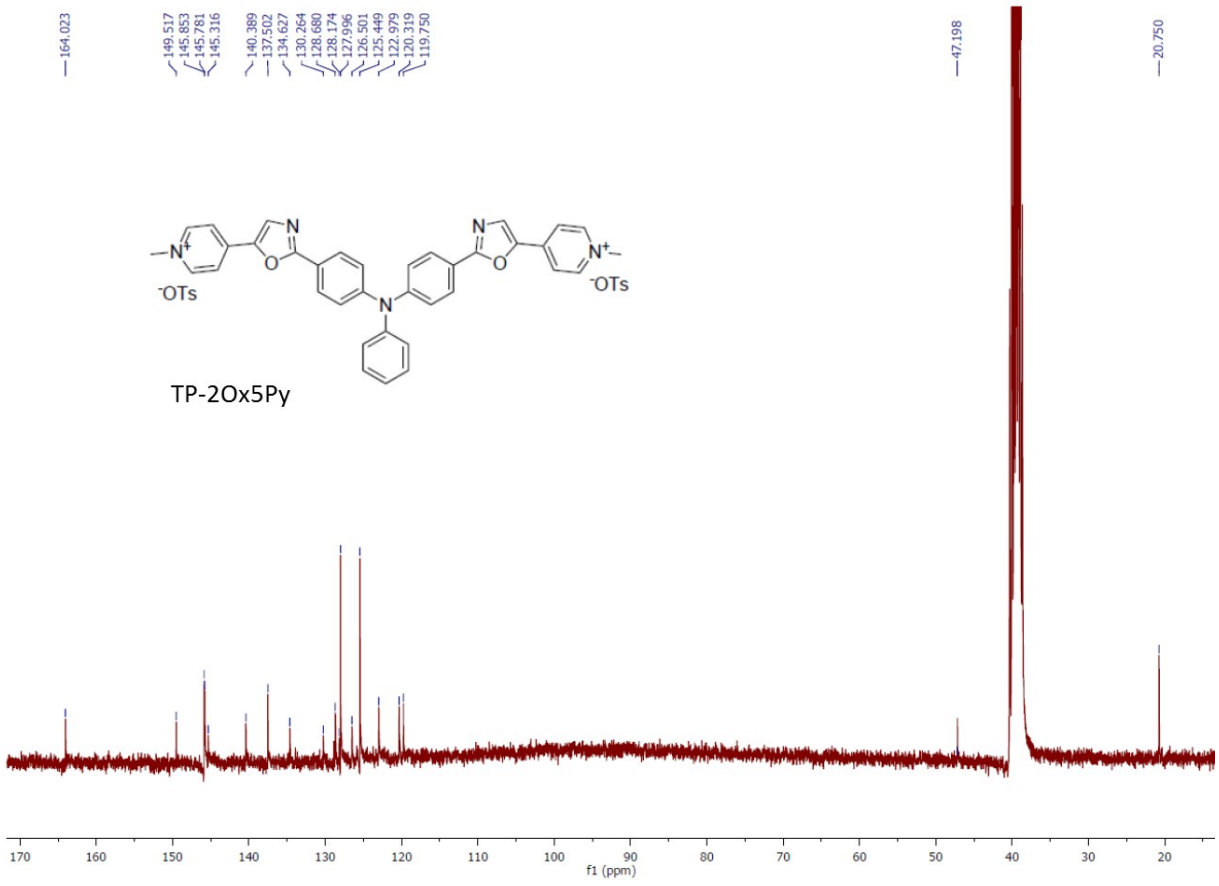

163.85
148.88
146.12
145.96
145.65
140.40
137.69
134.64
128.94
128.10
125.50
124.68
121.16
120.49
47.24
20.81
TP-3Ox5Py
SO3⁻
3
f1 (ppm)


8.682
8.668
8.031
8.003
7.645
7.572
7.555
7.405
7.379
7.354
7.270
7.231
7.204
5b
4.00
4.10
1.85
4.87
2.29
8.00
f1 (ppm)

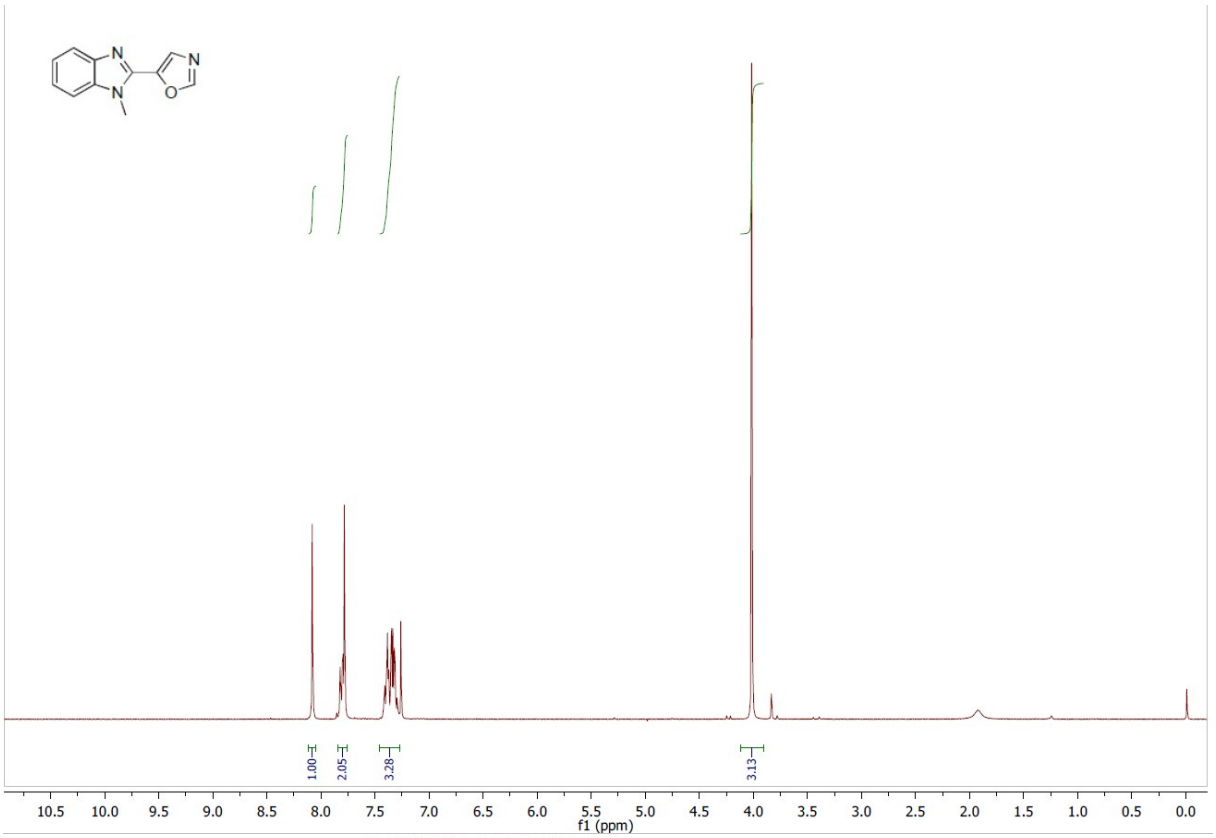

162.59
150.55
149.57
148.44
146.28
135.07
130.01
128.03
127.18
126.35
125.32
123.46
121.22
117.98
5b
f1 (ppm)

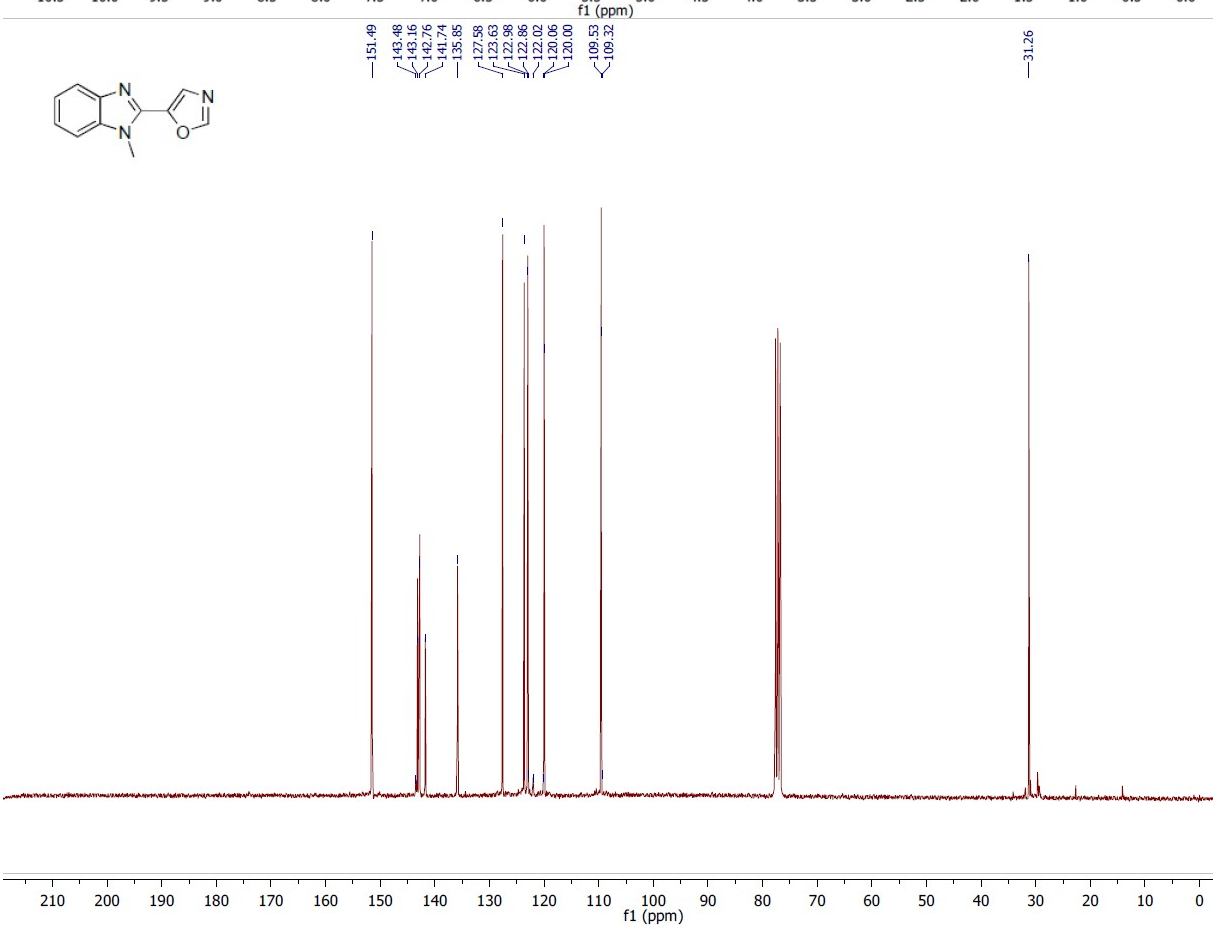


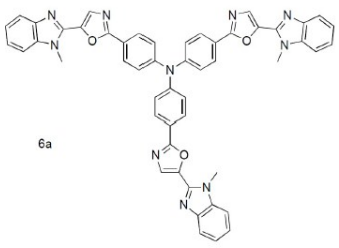
TP-2Ox5Py



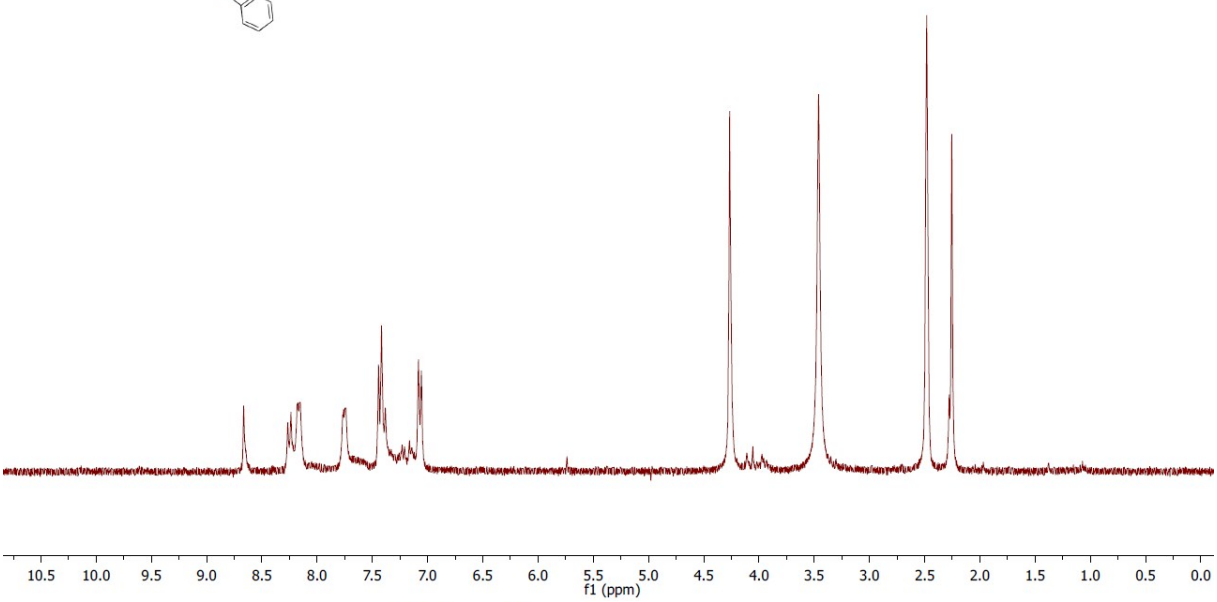
TP-2Ox5Py


1.00
2.05
3.28
3.13
10.5 10.0 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 0.5 0.0
f1 (ppm)

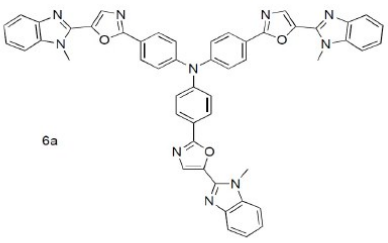

151.49
143.48
143.16
142.76
141.74
135.85
127.58
123.63
122.98
122.86
122.02
120.06
120.00
109.53
109.32
31.26
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



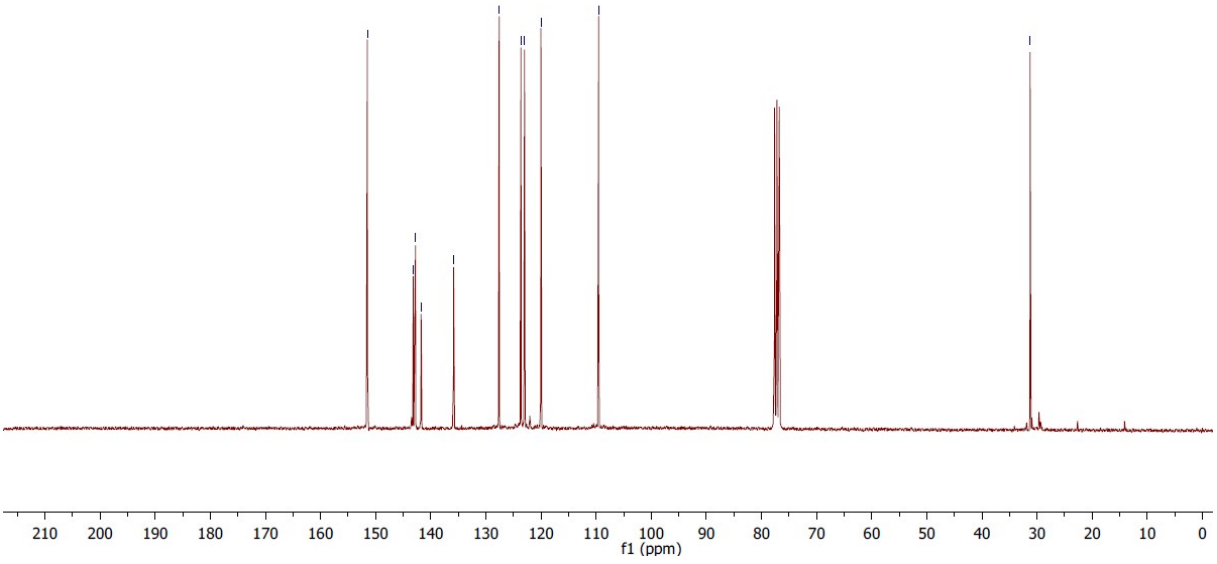
6a

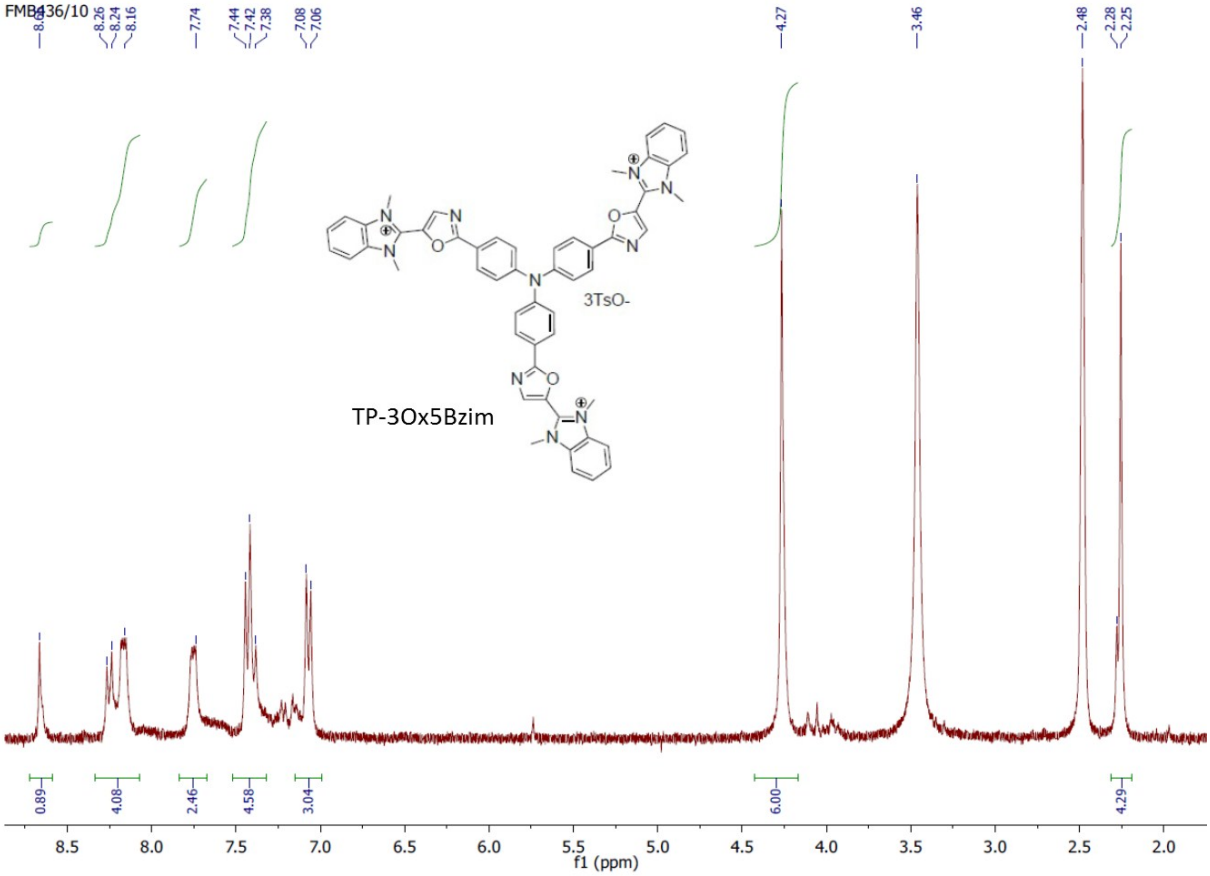


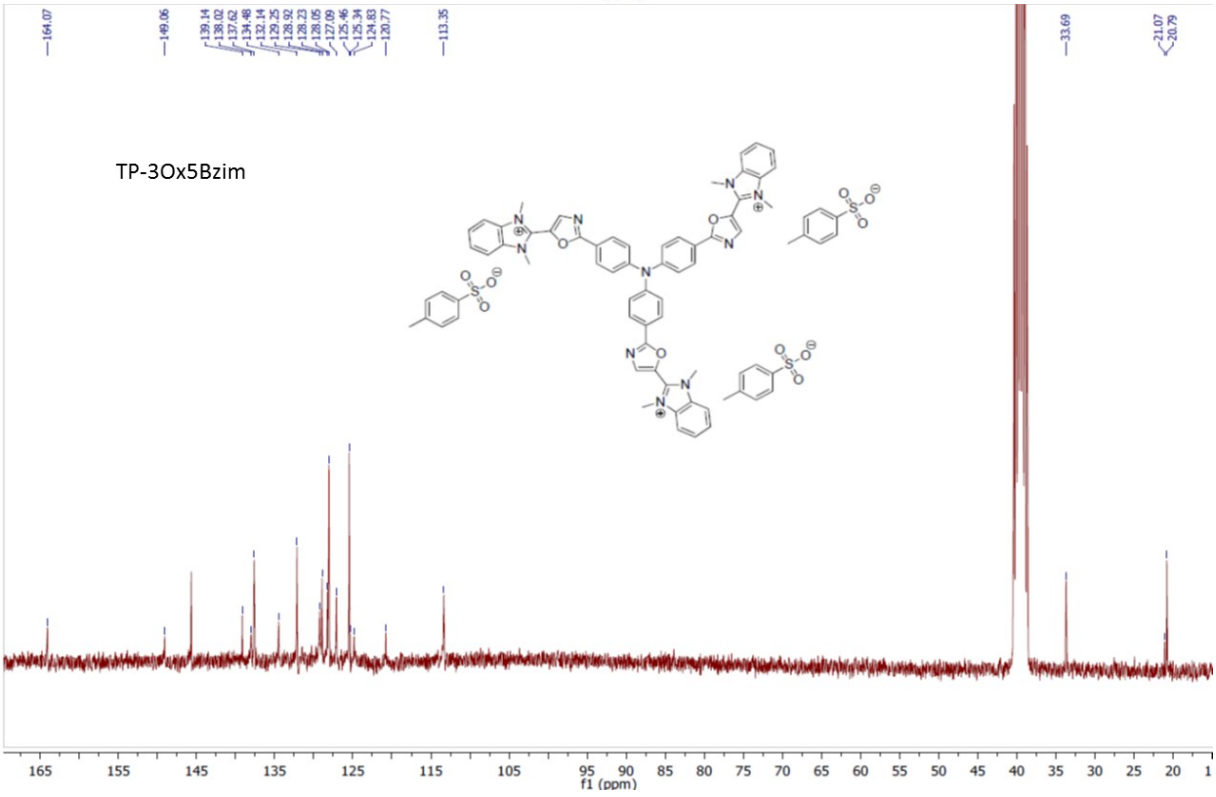
151.51
143.17
142.77
141.75
135.87
127.59
123.64
122.99
120.01
109.54
31.26

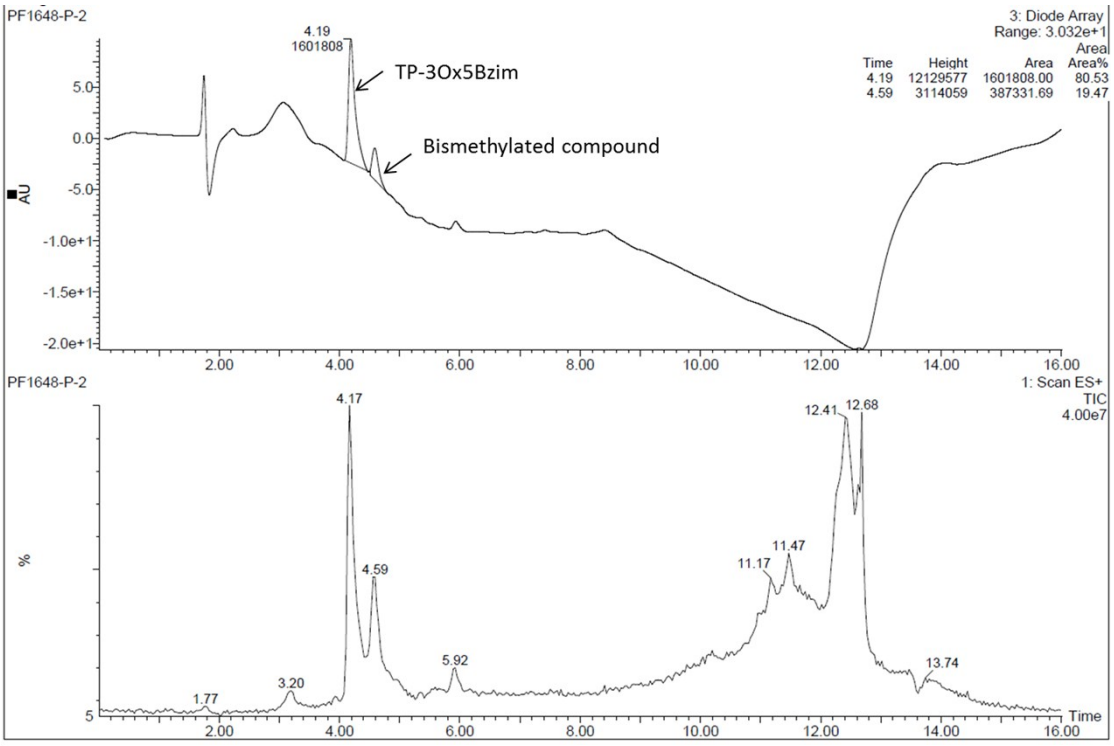


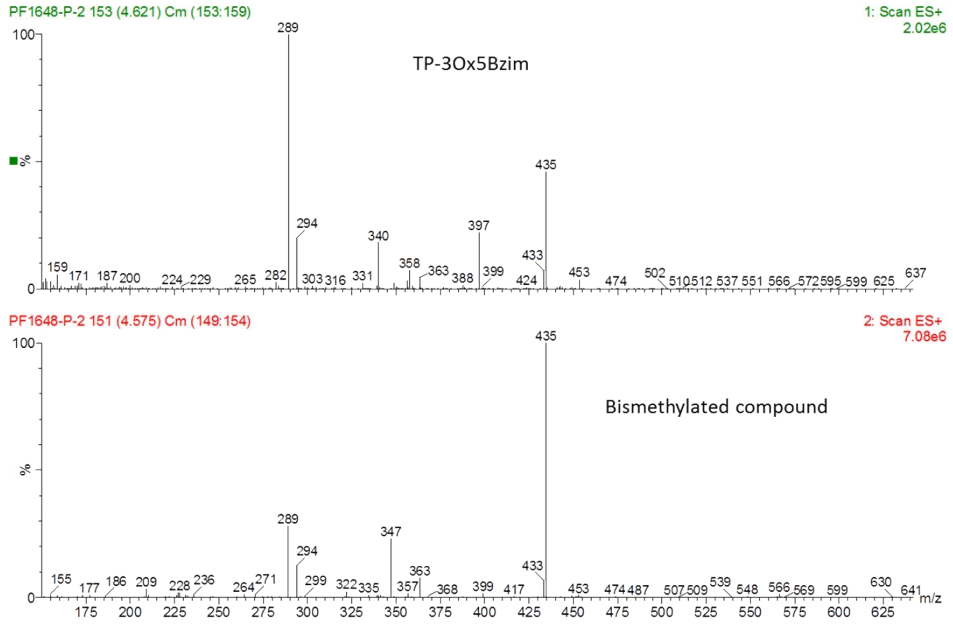
6a

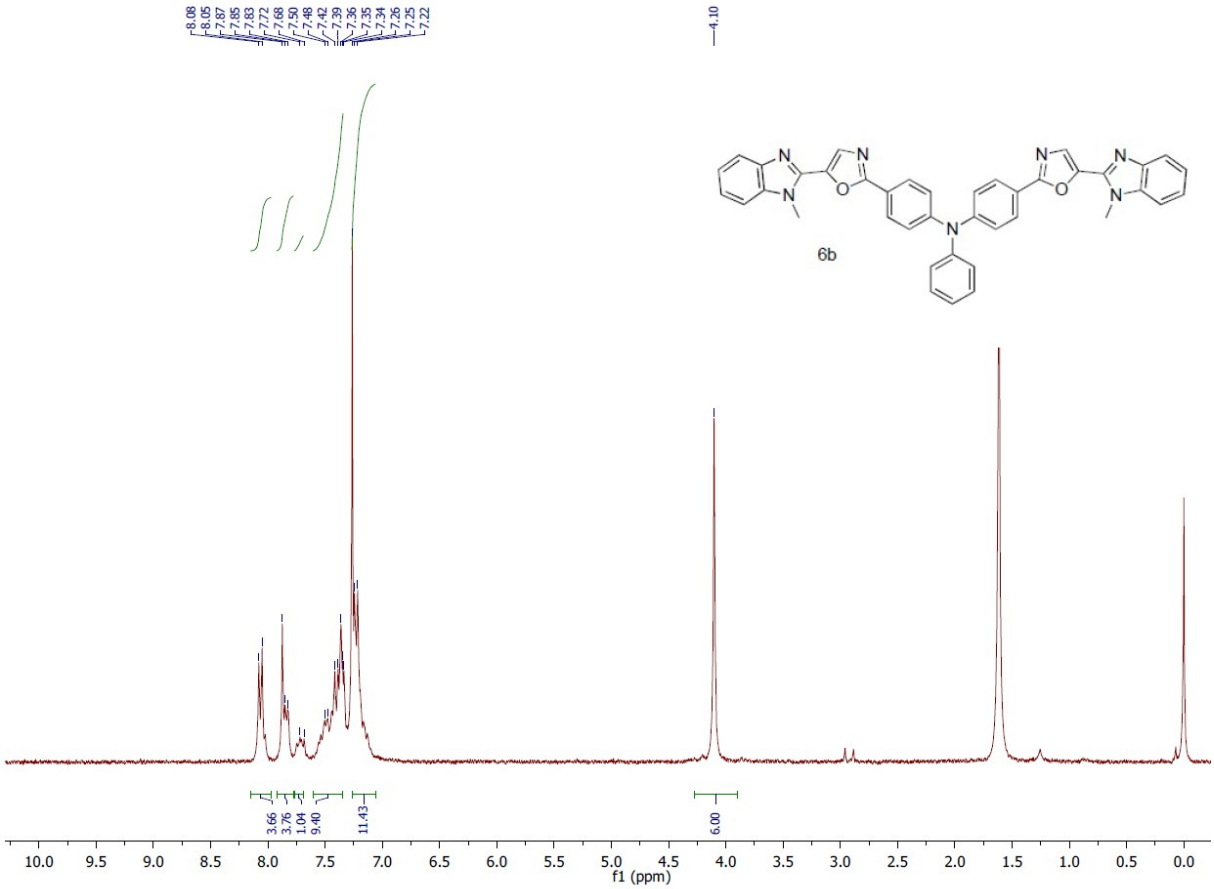


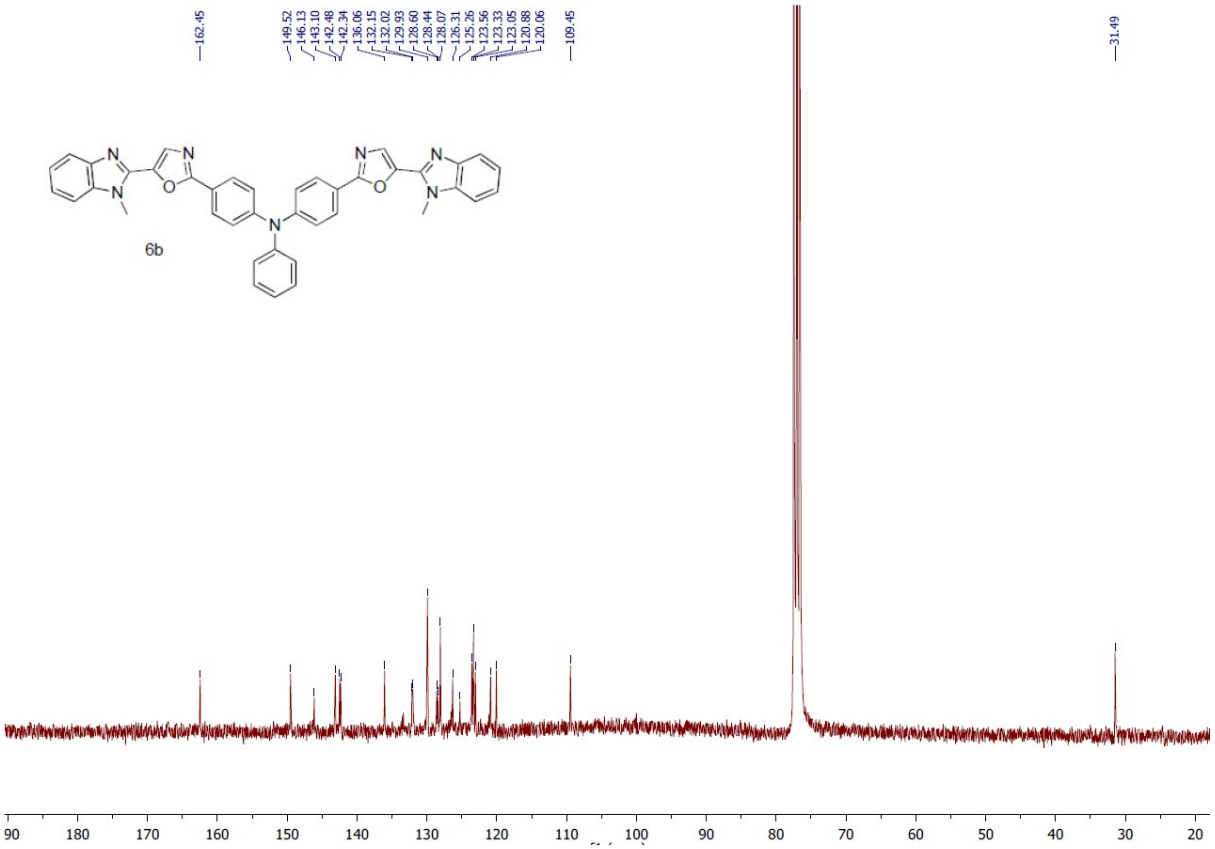

FMB436/10
8.26
8.24
8.16
7.74
7.44
7.42
7.38
7.08
7.06
4.27
3.46
2.48
2.28
2.25
3TsO-
TP-3Ox5Bzim
0.89
4.08
2.46
4.58
3.04
6.00
4.29
f1 (ppm)

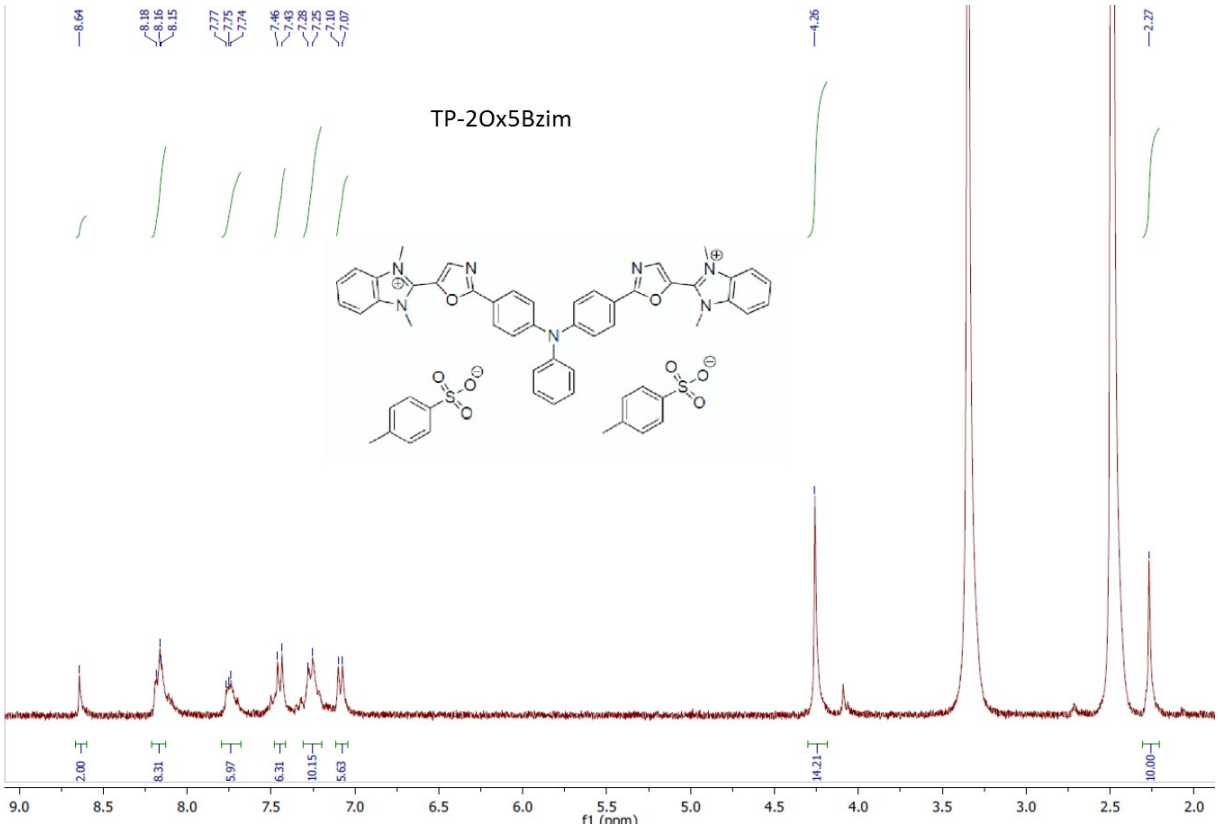

164.07
149.06
139.14
138.02
137.62
134.48
131.14
130.25
128.92
128.23
126.05
127.09
125.46
125.34
124.83
120.77
113.35
33.69
21.07
20.79
TP-3Ox5Bzim
f1 (ppm)

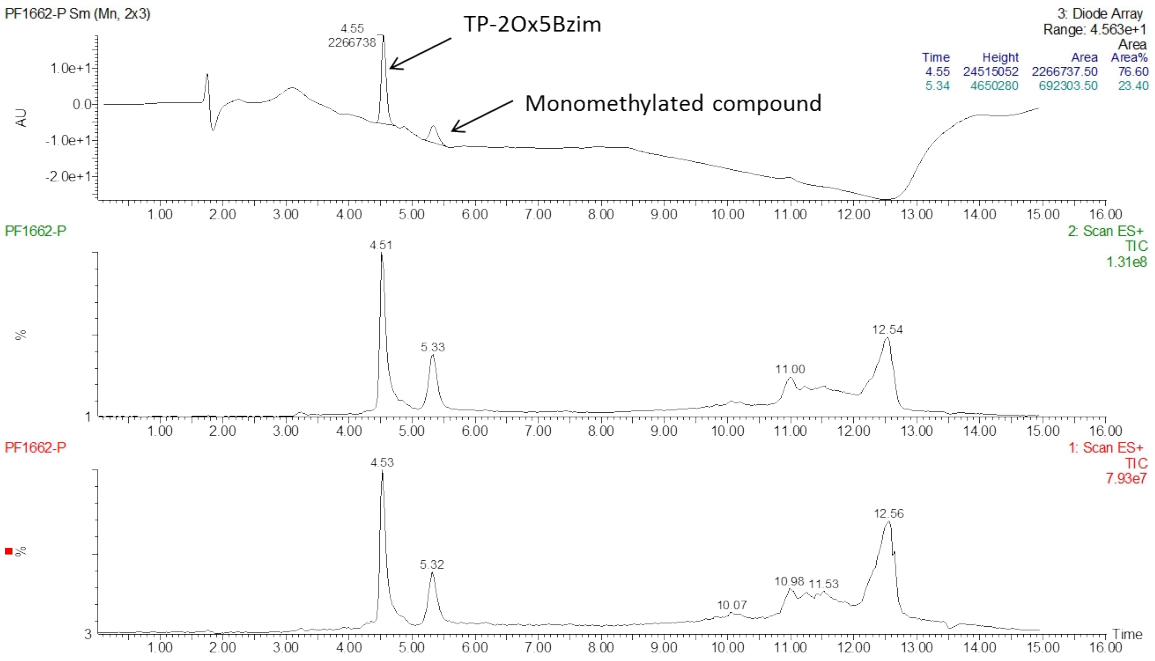

PF1648-P-2
3: Diode Array
Range: 3.032e+1
Time Height Area Area%
4.19 12129577 1601808.00 80.53
4.59 3114059 387331.69 19.47
4.19
1601808
TP-3Ox5Bzim
Bismethylated compound
AU
PF1648-P-2
1: Scan ES+
TIC
4.00e7
%
4.17
12.41
12.68
11.47
11.17
4.59
5.92
13.74
3.20
1.77
Time

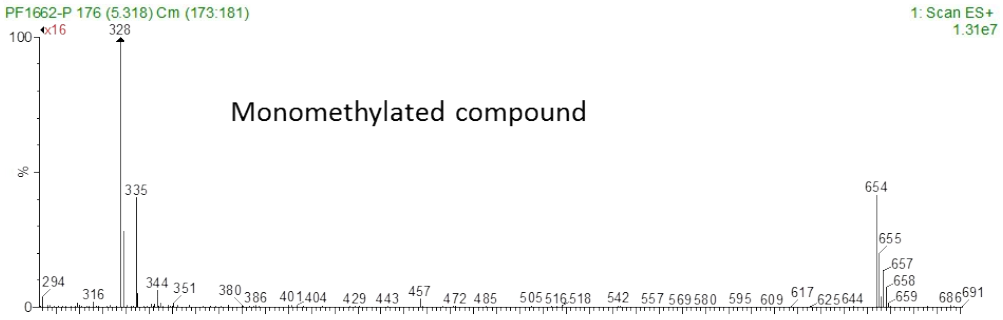

PF1648-P-2 153 (4.621) Cm (153:159)
1: Scan ES+
2.02e6
TP-3Ox5Bzim
PF1648-P-2 151 (4.575) Cm (149:154)
2: Scan ES+
7.08e6
Bismethylated compound
m/z

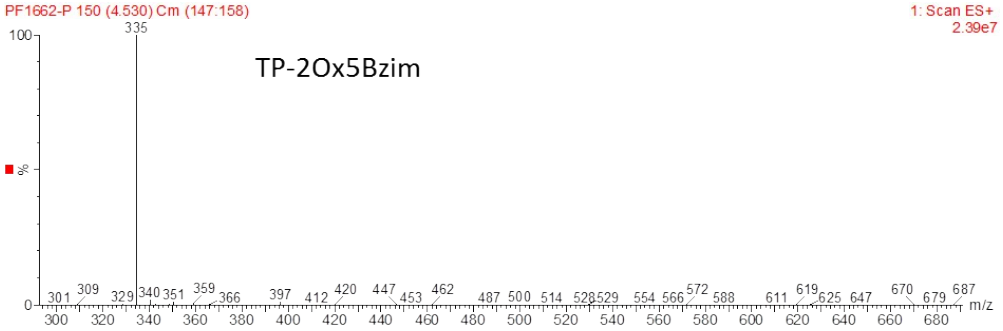

8.08
8.05
7.87
7.85
7.83
7.72
7.68
7.50
7.48
7.42
7.39
7.36
7.35
7.34
7.26
7.25
7.22
4.10
6b
3.66
3.76
1.04
9.40
11.43
6.00
f1 (ppm)


162.45
149.52
146.13
143.10
142.48
142.34
136.06
132.15
132.02
129.93
128.60
128.44
128.07
126.31
125.26
123.56
123.33
123.05
120.88
120.06
109.45
31.49
6b


TP-2Ox5Bzim
8.64
8.18
8.16
8.15
7.77
7.75
7.74
7.46
7.43
7.28
7.25
7.10
7.07
4.26
2.27
2.00
8.31
5.97
6.31
10.15
5.63
14.21
10.00
f1 (ppm)


PF1662-P Sm (Mn, 2x3)
TP-2Ox5Bzim
Monomethylated compound
4.55
2266738
3: Diode Array
Range: 4.563e+1
Area
Time Height Area Area%
4.55 24515052 2266737.50 76.60
5.34 4650280 692303.50 23.40
AU
PF1662-P
2: Scan ES+
TIC
1.31e8
4.51
5.33
11.00
12.54
%
PF1662-P
1: Scan ES+
TIC
7.93e7
4.53
5.32
10.07
10.98
11.53
12.56
Time


PF1662-P 176 (5.318) Cm (173:181)
1: Scan ES+
1.31e7
x16
328
Monomethylated compound
335
654
655
657
658
659
294
316
344
351
380
386
401
404
429
443
457
472
485
505
516
518
542
557
569
580
595
609
617
625
644
686
691
%


PF1662-P 150 (4.530) Cm (147:158)
1: Scan ES+
2.39e7
335
TP-2Ox5Bzim
301
309
329
340
351
359
366
397
412
420
447
453
462
487
500
514
528
529
554
566
572
588
611
619
625
647
670
679
687
m/z
%