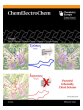
ChemElectroChem

Supporting Information

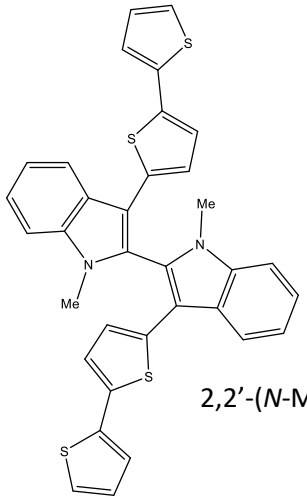


Trópos and *Átropos* Biindole Chiral Electroactive Monomers: A Voltammetry and HPLC Comparative Insight

Serena Arnaboldi, Sara Grecchi, Luca Vaghi, Andrea Penoni, Luca Scapinello, Ivo Franco Buzzi, Roberto Cirilli, Marco Pierini,* Tiziana Benincori,* and Patrizia Romana Mussini*

A. Mass spectra with accurate mass calculations

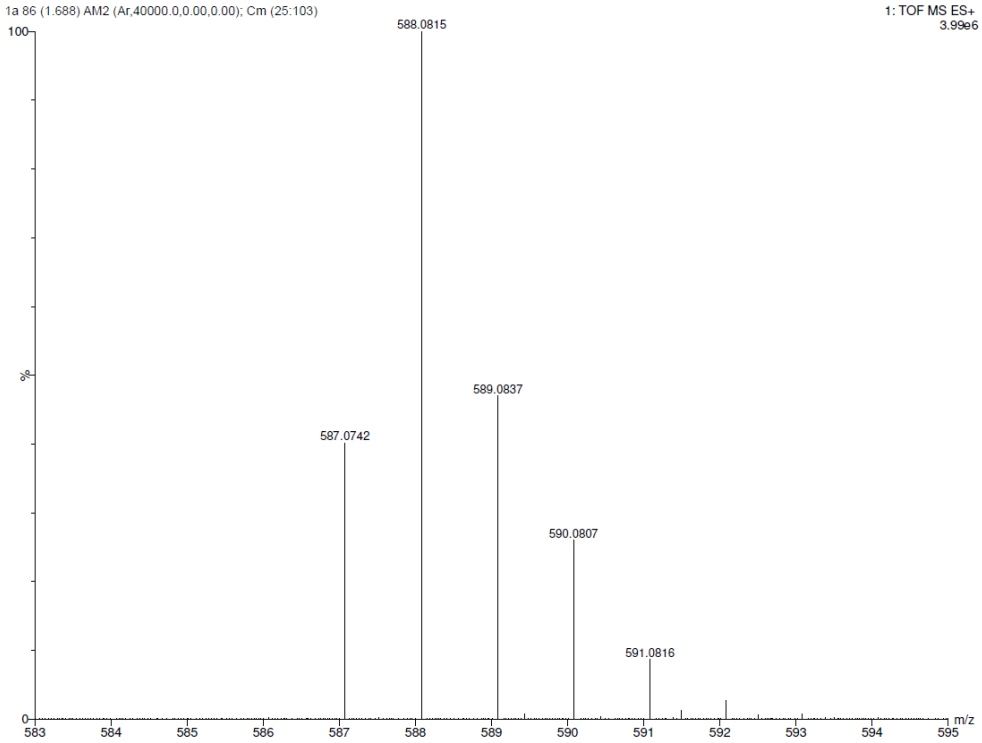
Instrument : Synapt G2-Si QTof mass spectrometer (Waters) - ZsprayTM ESI-probe for electrospray ionization (Waters)
Acquisition : positive polarity full scan mode
Data processing : MassLynxTM V4.2 software (Waters)



Chemical Formula: $C_{34}H_{24}N_2S_4$
Exact Mass: 588,08
Molecular Weight: 588,82

2,2'-(*N*-Me-Ind)$_2$-T$_4$

1a

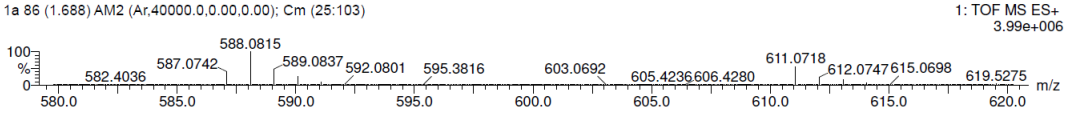


Elemental Composition Report **Page 1**

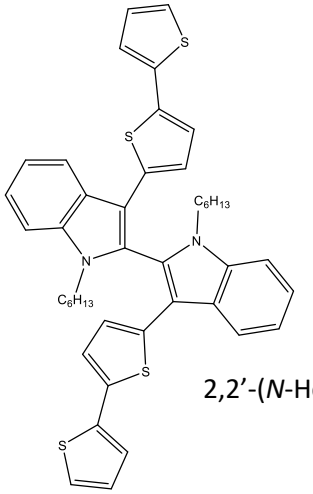
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -2.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 34-34 H: 24-25 N: 2-2 Na: 0-2 S: 4-4

1a 86 (1.688) AM2 (Ar,40000.0,0.00,0.00); Cm (25:103)



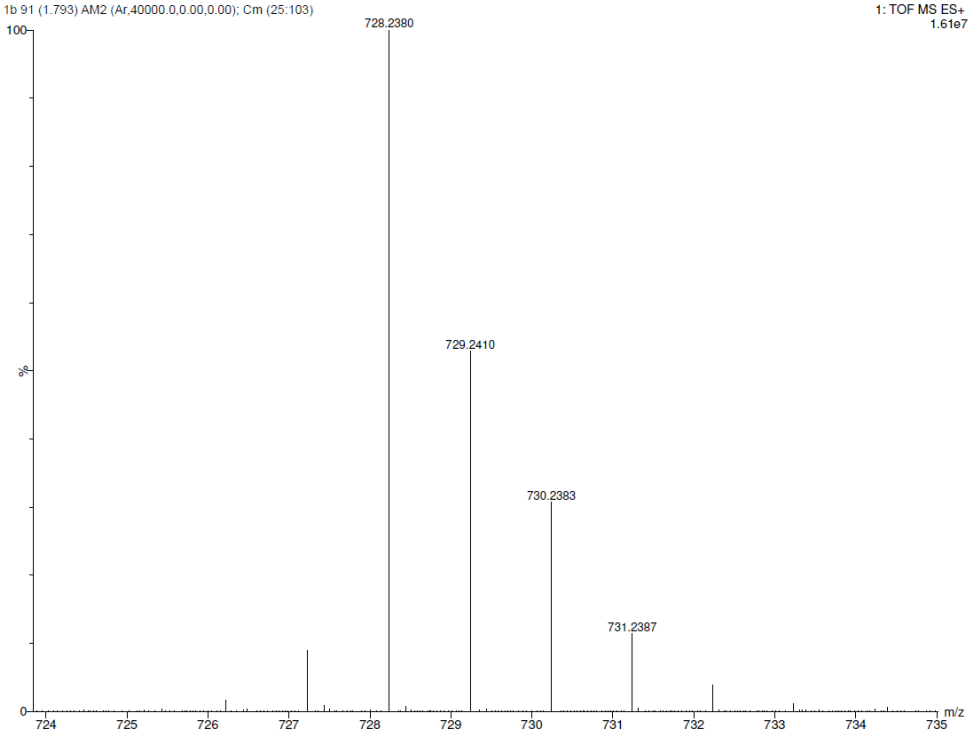
Minimum:				-2.5				
Maximum:		5.0	5.0	200.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
588.0815	588.0822	-0.7	-1.2	24.0	1645.5	n/a	n/a	C34 H24 N2 S4



Chemical Formula: $C_{44}H_{44}N_2S_4$
Exact Mass: 728,24
Molecular Weight: 729,09

2,2'-(*N*-Hex-Ind)$_2$-T$_4$

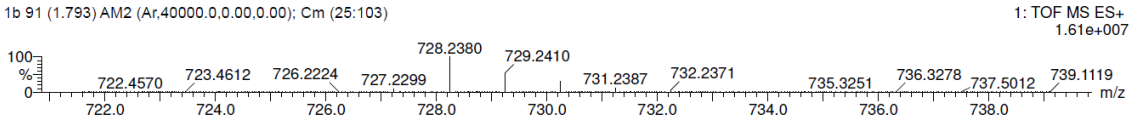
1b



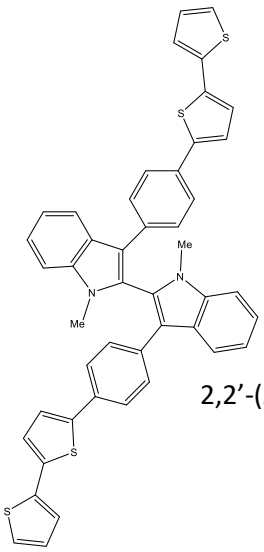
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -2.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 44-44 H: 44-45 N: 2-2 Na: 0-2 S: 4-4



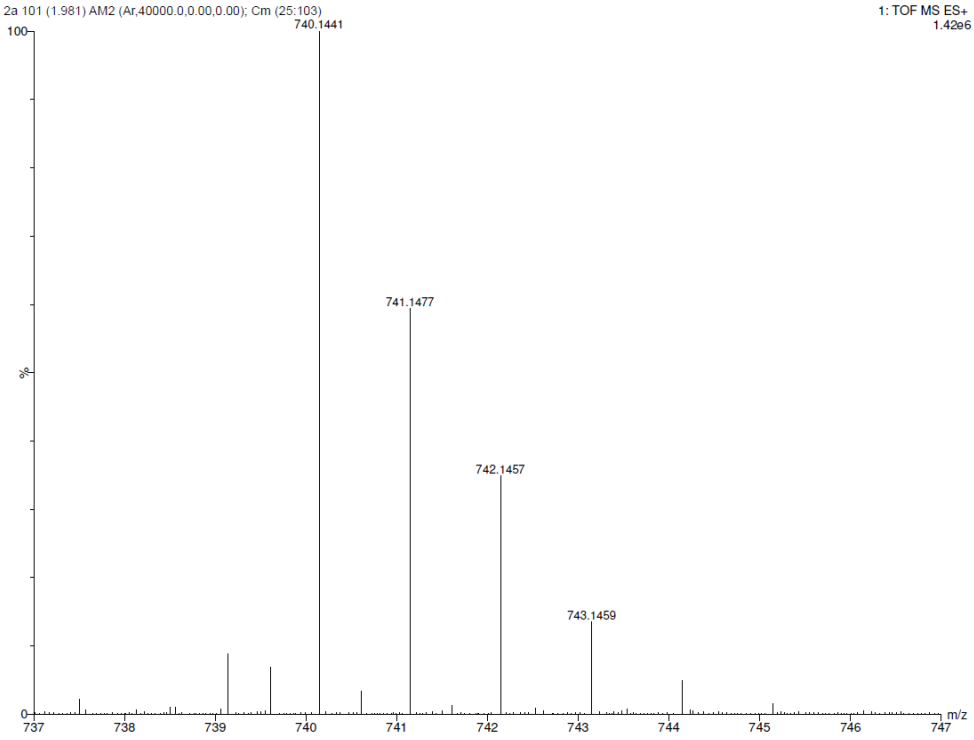
Minimum:				-2.5				
Maximum:		5.0	5.0	200.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
728.2380	728.2387	-0.7	-1.0	24.0	1581.3	n/a	n/a	C44 H44 N2 S4



Chemical Formula: $C_{46}H_{32}N_2S_4$
Exact Mass: 740,14
Molecular Weight: 741,02

2,2'-(*N*-Me-Ind)$_2$-Ph$_2$T$_4$

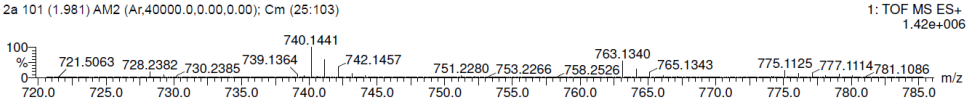
2a



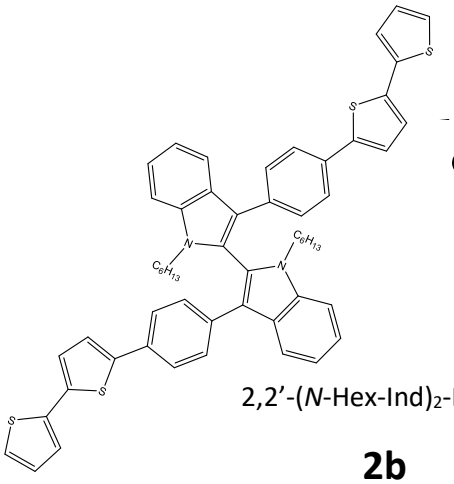
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -2.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 46-46 H: 32-33 N: 2-2 Na: 0-2 S: 4-4



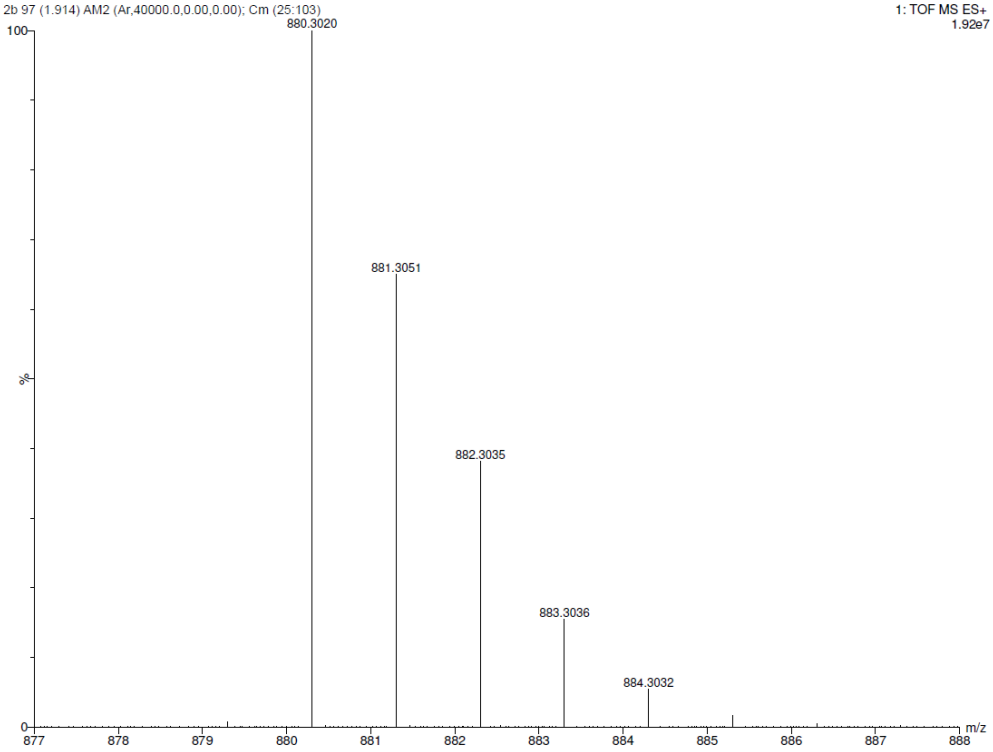
Minimum:				-2.5				
Maximum:		5.0	5.0	200.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
740.1441	740.1448	-0.7	-0.9	32.0	1327.9	n/a	n/a	C46 H32 N2 S4



Chemical Formula: $C_{56}H_{52}N_2S_4$
Exact Mass: 880,30
Molecular Weight: 881,29

2,2'-(*N*-Hex-Ind)$_2$-Ph$_2$T$_4$

2b

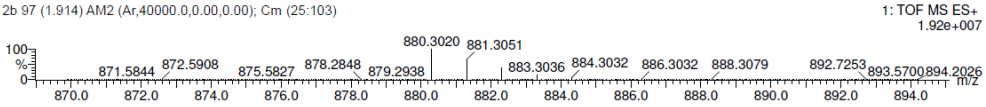


Elemental Composition Report **Page 1**

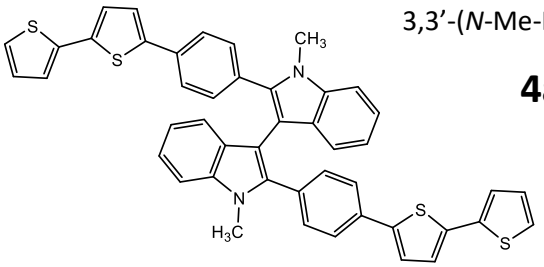
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -2.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 56-56 H: 45-52 N: 2-2 Na: 0-2 S: 4-4

2b 97 (1.914) AM2 (Ar,40000.0,0.00,0.00); Cm (25:103)



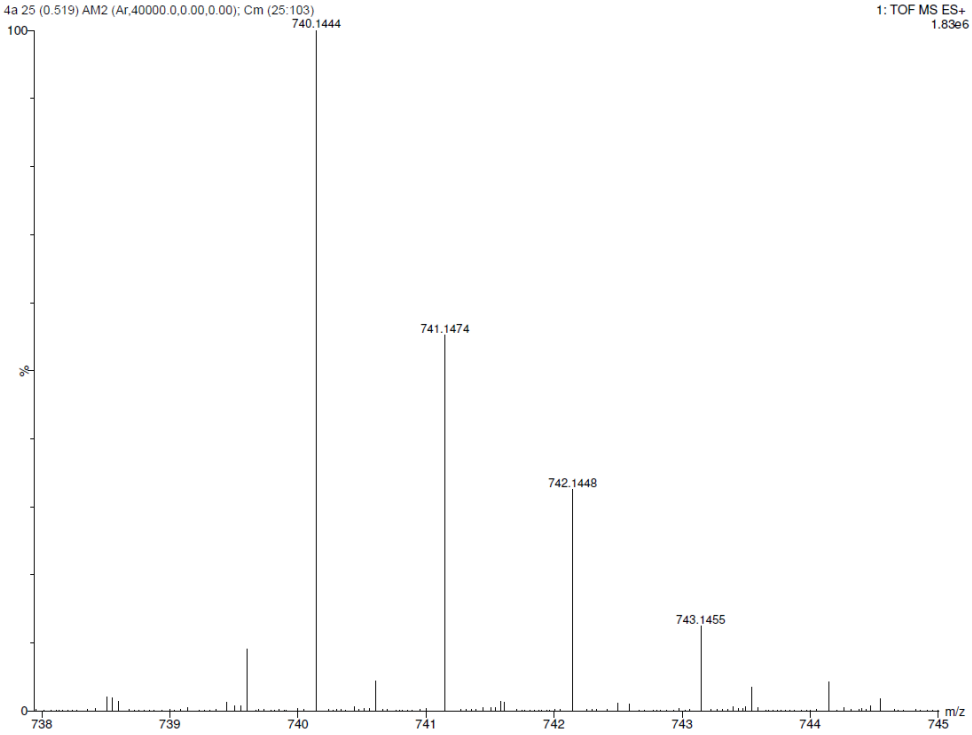
Minimum:			-2.5					
Maximum:		5.0	5.0	200.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
880.3020	880.3013	0.7	0.8	32.0	1227.0	n/a	n/a	C56 H52 N2 S4



3,3'-(*N*-Me-Ind)$_2$-Ph$_2$T$_4$

4a

Chemical Formula: $C_{46}H_{32}N_2S_4$
Exact Mass: 740,14
Molecular Weight: 741,02

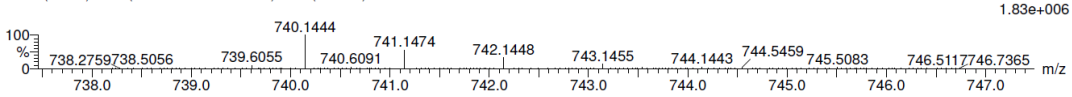


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -2.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

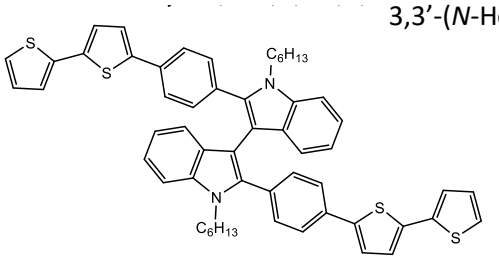
Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 46-46 H: 32-33 N: 2-2 Na: 0-2 S: 4-4

4a 25 (0.519) AM2 (Ar,40000.0,0.00,0.00); Cm (25:103)
1: TOF MS ES+
1.83e+006



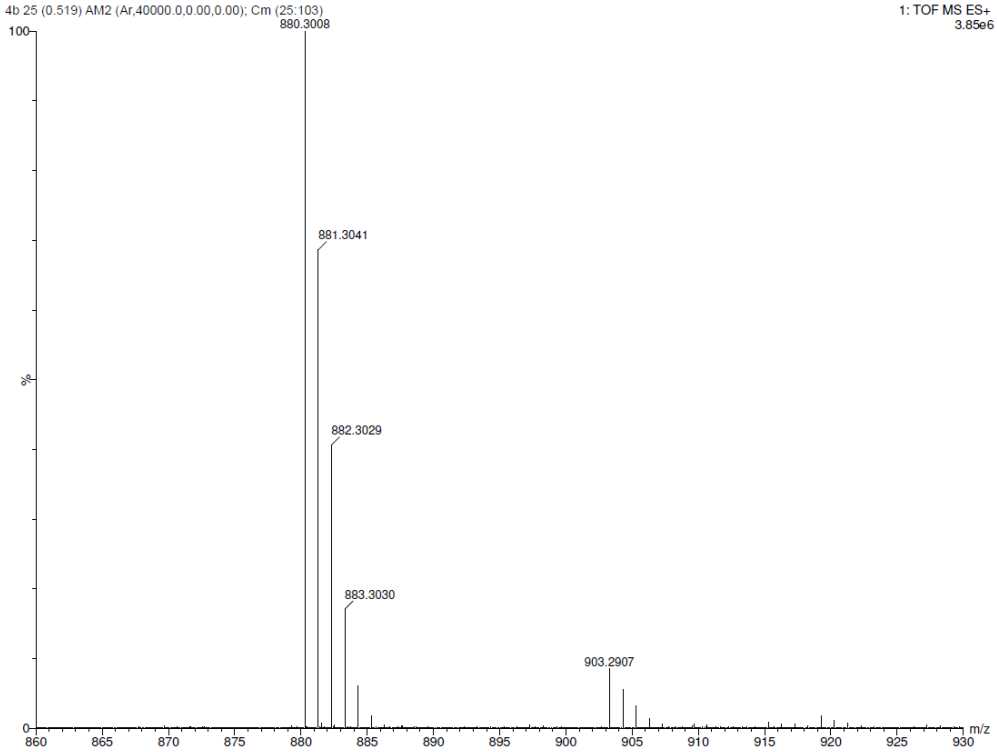
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-2.5				
Maximum:		5.0	5.0	200.0				
740.1444	740.1448	-0.4	-0.5	32.0	1410.8	n/a	n/a	C46 H32 N2 S4

3,3'-(*N*-Hex-Ind)$_2$-Ph$_2$T$_4$



4b

Chemical Formula: $C_{56}H_{52}N_2S_4$
Exact Mass: 880,30
Molecular Weight: 881,29

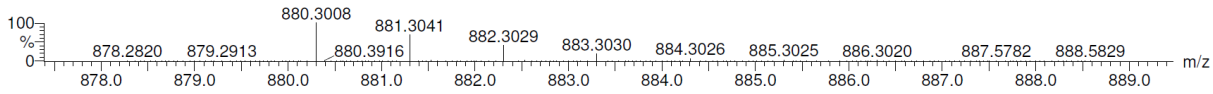


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -2.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 56-56 H: 52-53 N: 2-2 Na: 0-2 S: 4-4

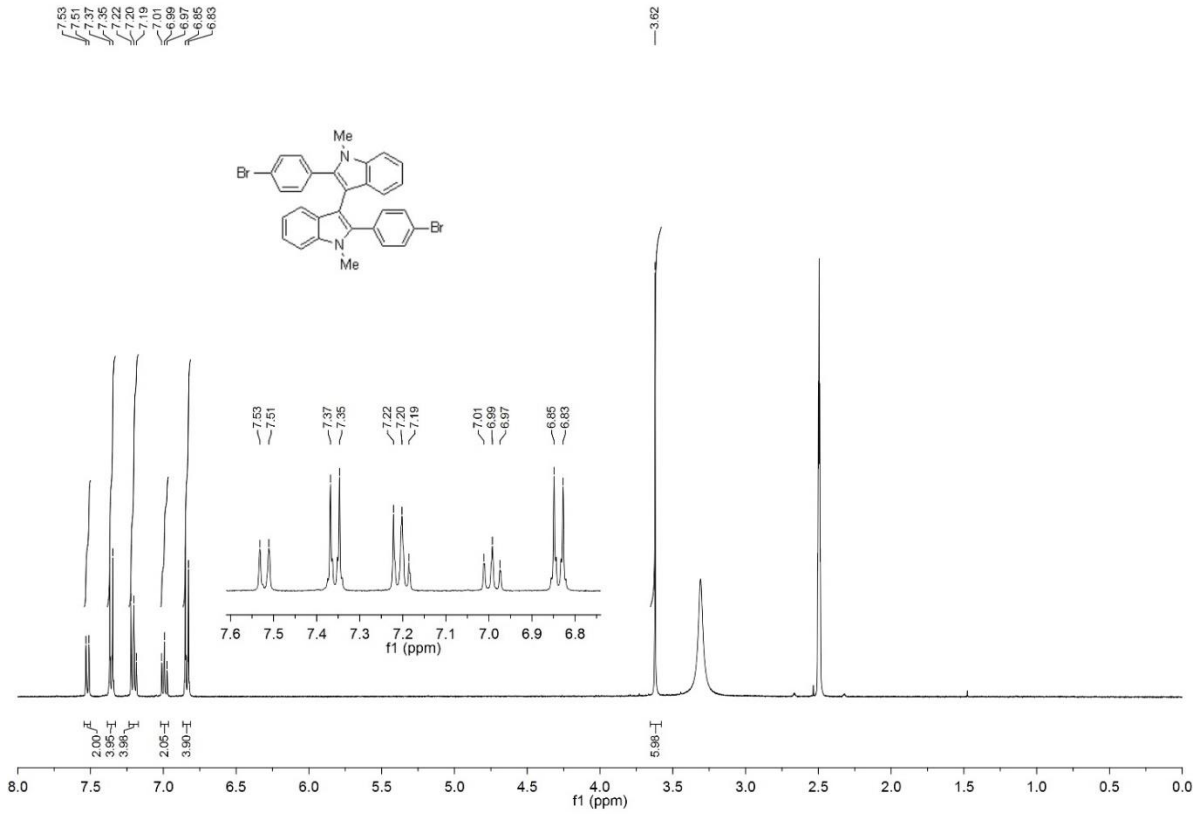
4b 25 (0.519) AM2 (Ar,40000.0,0.00,0.00); Cm (25:103)
1: TOF MS ES+
3.85e+006

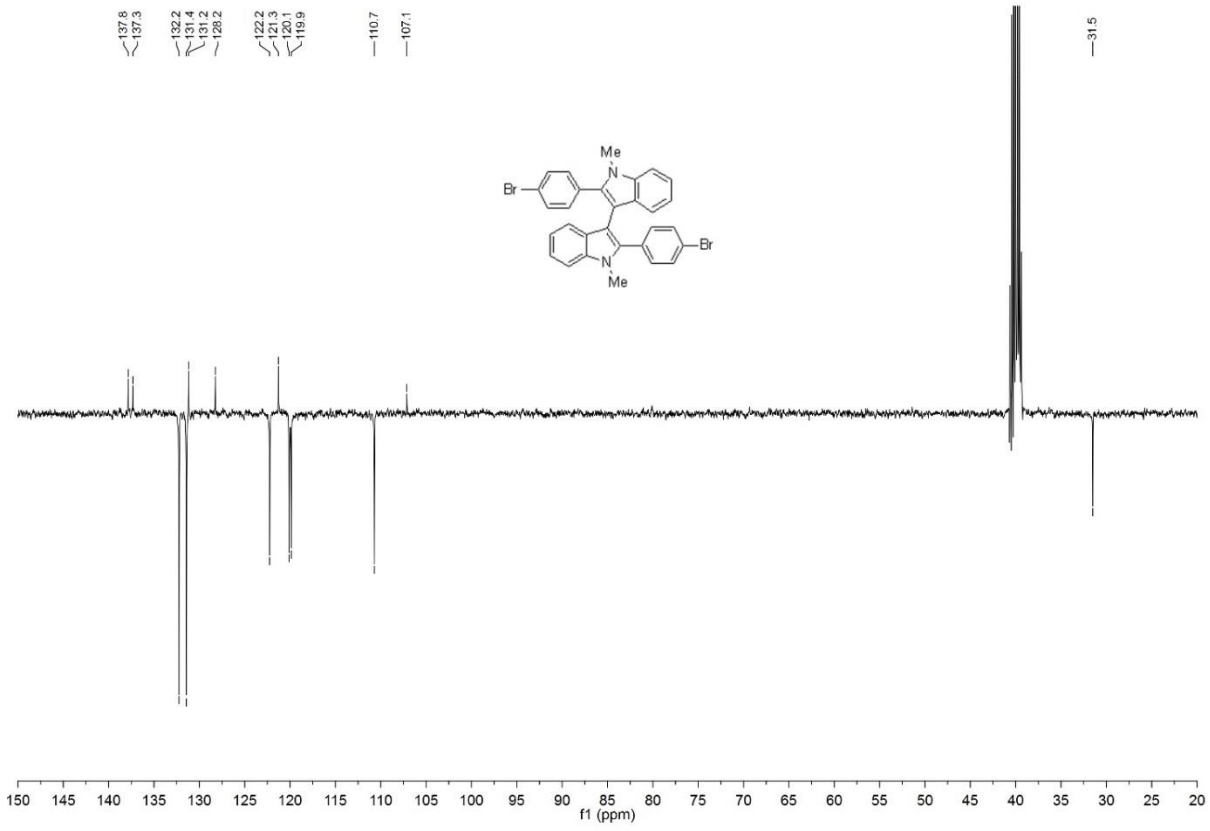


Minimum:				-2.5				
Maximum:		5.0	5.0	200.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
880.3008	880.3013	-0.5	-0.6	32.0	1189.9	n/a	n/a	C56 H52 N2 S4

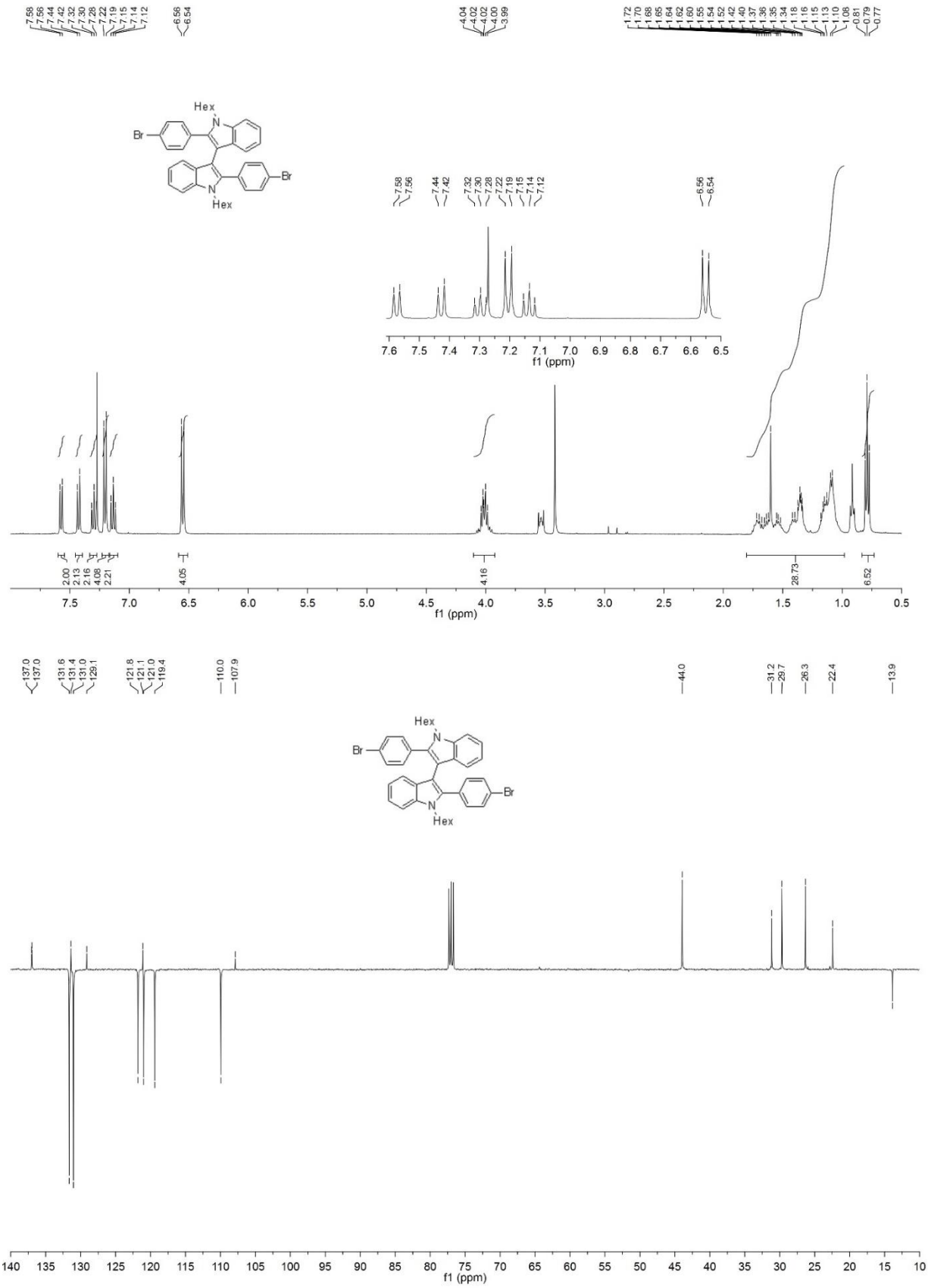
B. ^{1}H NMR and ^{13}C NMR spectra

Compound 11a

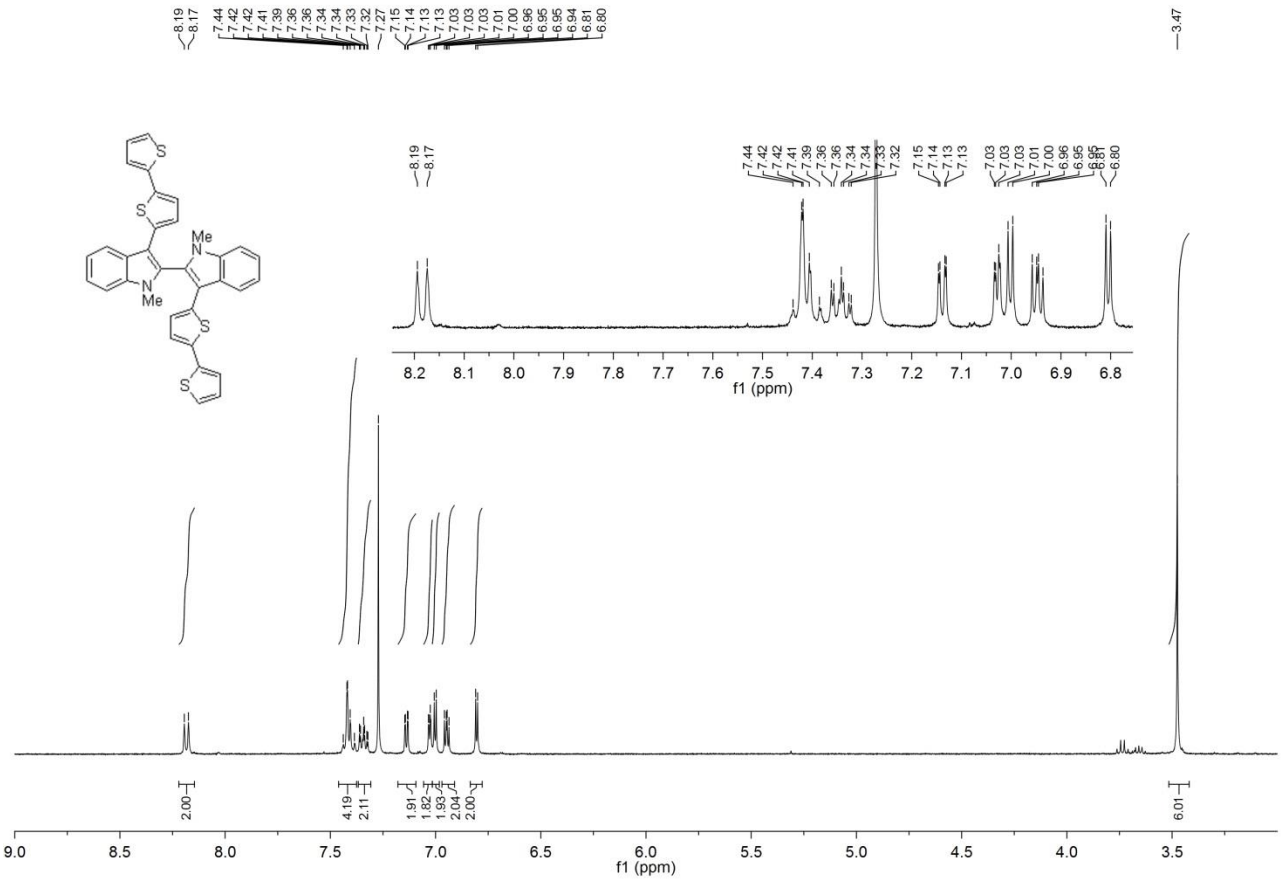




Compound 11b



Compound 1a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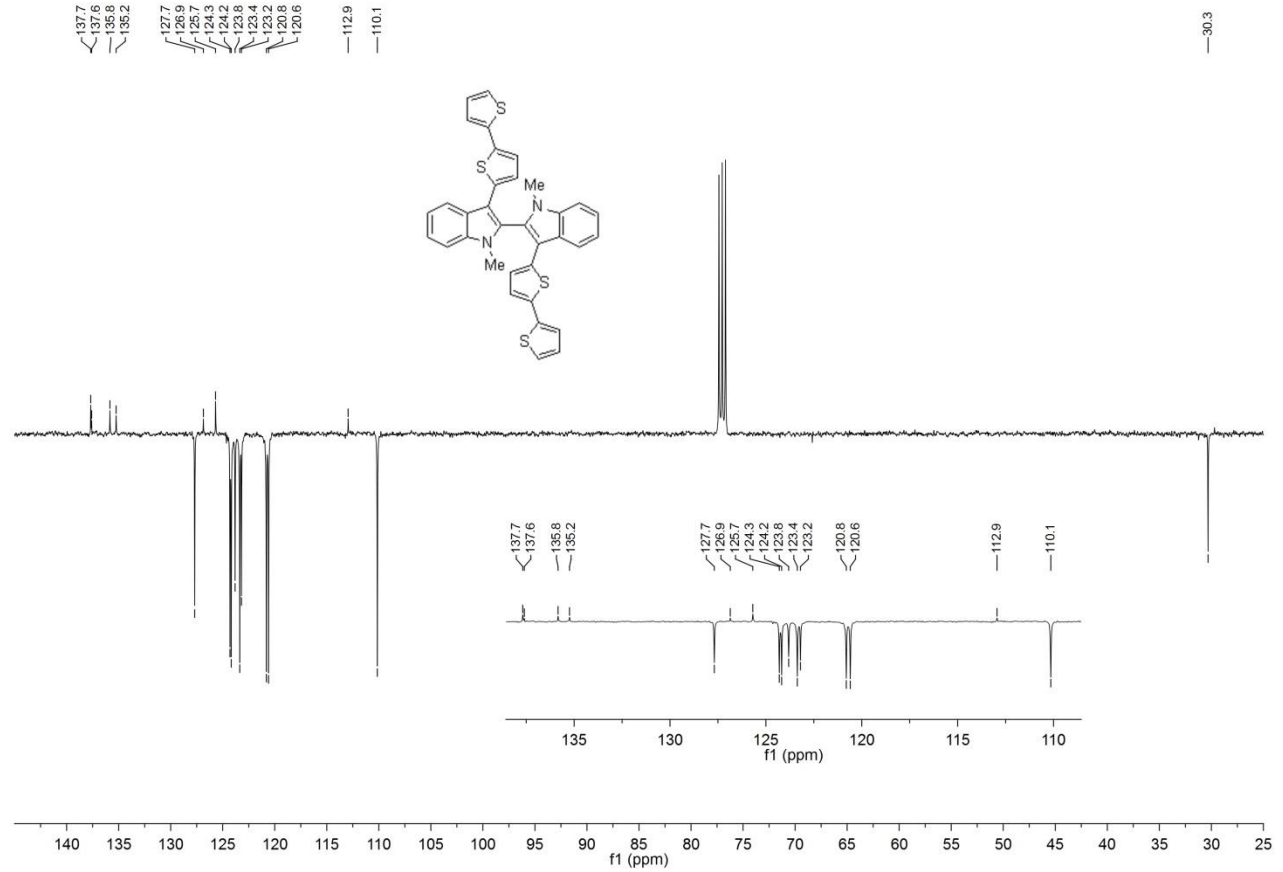
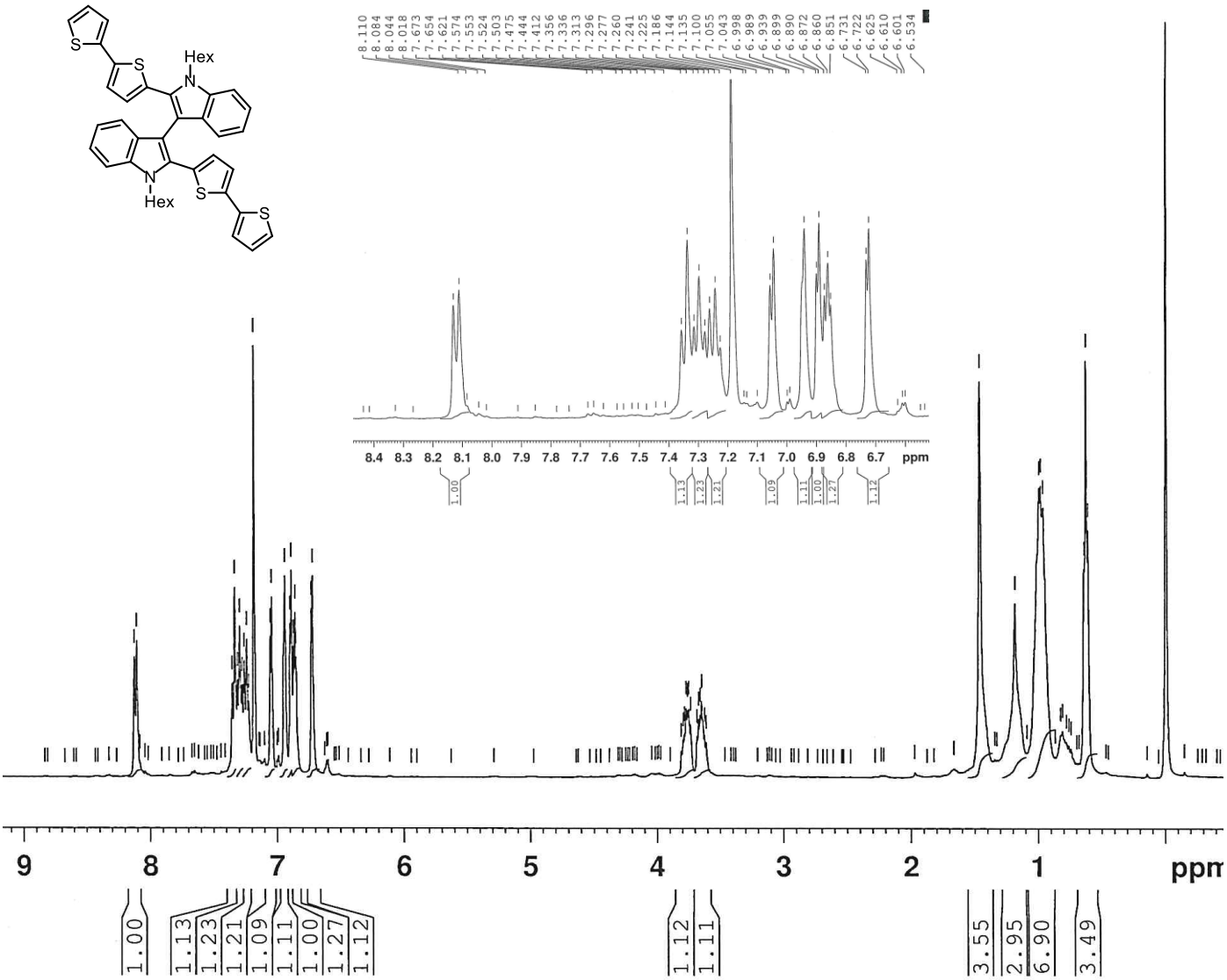
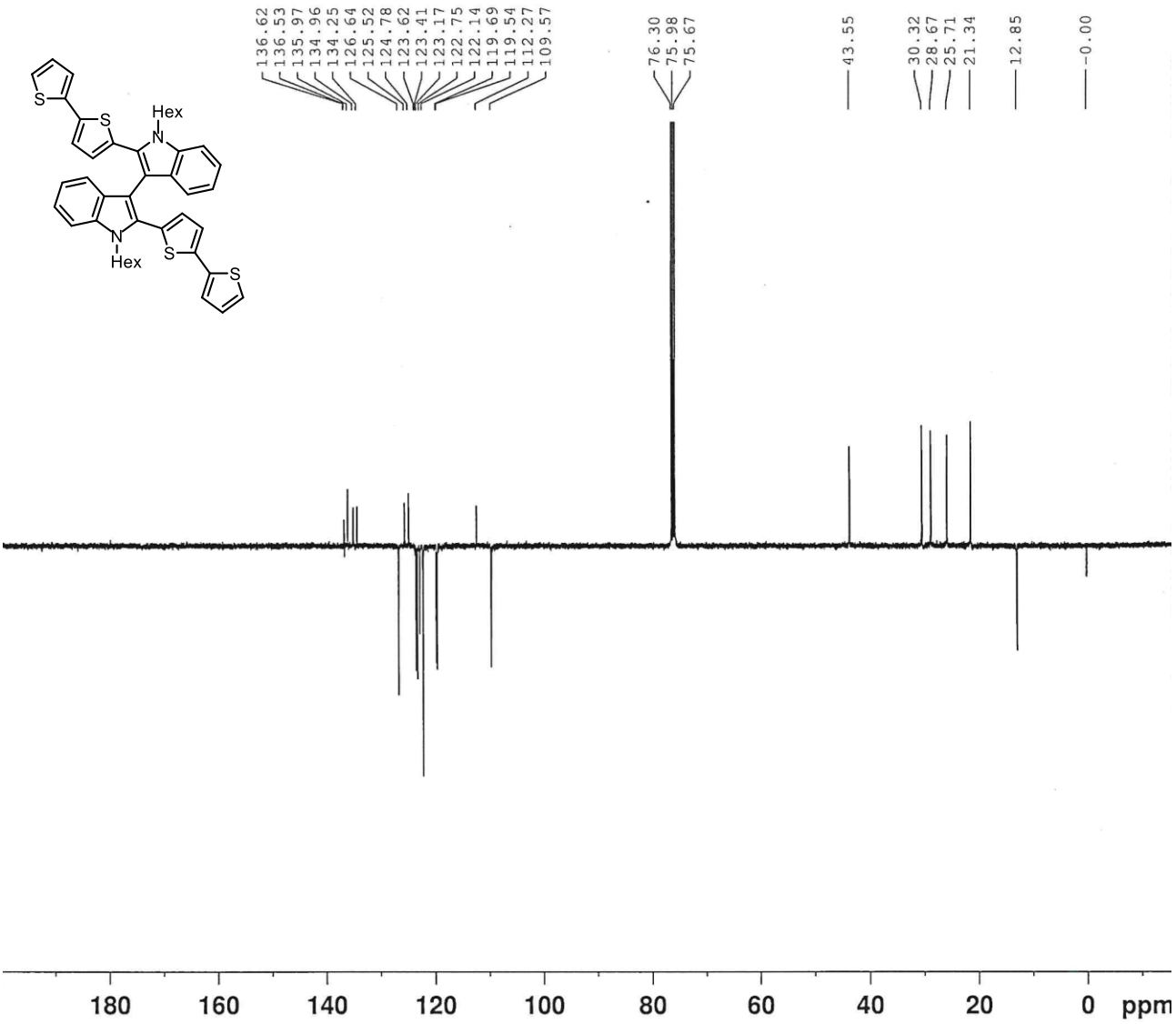
8.17
7.44
7.42
7.42
7.41
7.39
7.36
7.36
7.34
7.34
7.33
7.32
7.27
7.15
7.14
7.13
7.13
7.03
7.03
7.03
7.01
7.00
6.96
6.95
6.94
6.81
6.80
3.47
Me
N
Me
S
f1 (ppm)
2.00
4.19
2.11
1.91
1.82
1.93
2.04
2.00
6.01


137.7
137.6
135.8
135.2
127.7
126.9
125.7
124.3
124.2
123.8
123.4
123.2
120.8
120.6
112.9
110.1
30.3
Me
N
Me
S
f1 (ppm)

Compound 1b


Hex
Hex
S
S
S
S
N
N
8.110
8.084
8.044
8.018
7.673
7.654
7.621
7.574
7.553
7.524
7.503
7.475
7.444
7.412
7.356
7.336
7.313
7.296
7.277
7.260
7.241
7.225
7.186
7.144
7.135
7.100
7.055
7.043
6.998
6.989
6.939
6.899
6.890
6.872
6.860
6.851
6.731
6.722
6.625
6.610
6.601
6.534
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
1.00
1.13
1.23
1.21
1.09
1.11
1.00
1.27
1.12
9 8 7 6 5 4 3 2 1 ppm
1.00
1.13
1.23
1.21
1.09
1.11
1.00
1.27
1.12
1.12
1.11
3.55
2.95
6.90
3.49

Compound 1b


136.62
136.53
135.97
134.96
134.25
126.64
125.52
124.78
123.62
123.41
123.17
122.75
122.14
119.69
119.54
112.27
109.57
76.30
75.98
75.67
43.55
30.32
28.67
25.71
21.34
12.85
-0.00
Hex
Hex
180
160
140
120
100
80
60
40
20
0
ppm

Compounds 2a and 2b

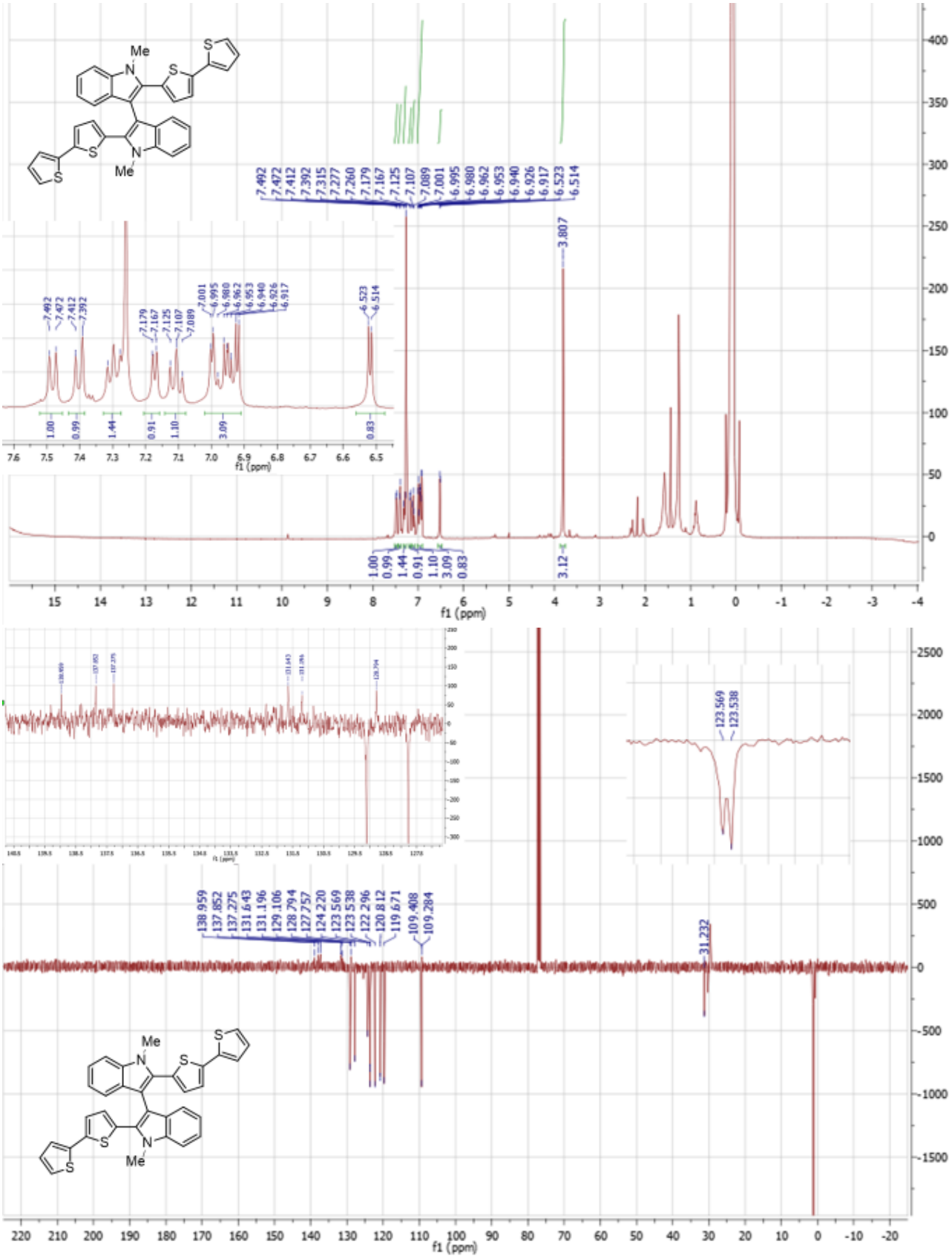
(^{1}H NMR and ^{13}C NMR are available for both monomers in the Supporting Information of

L. Scapinello, S. Grecchi, S. Rossi, F. Arduini, S. Arnaboldi, A. Penoni, R. Cirilli, P.R. Mussini, T. Benincori,

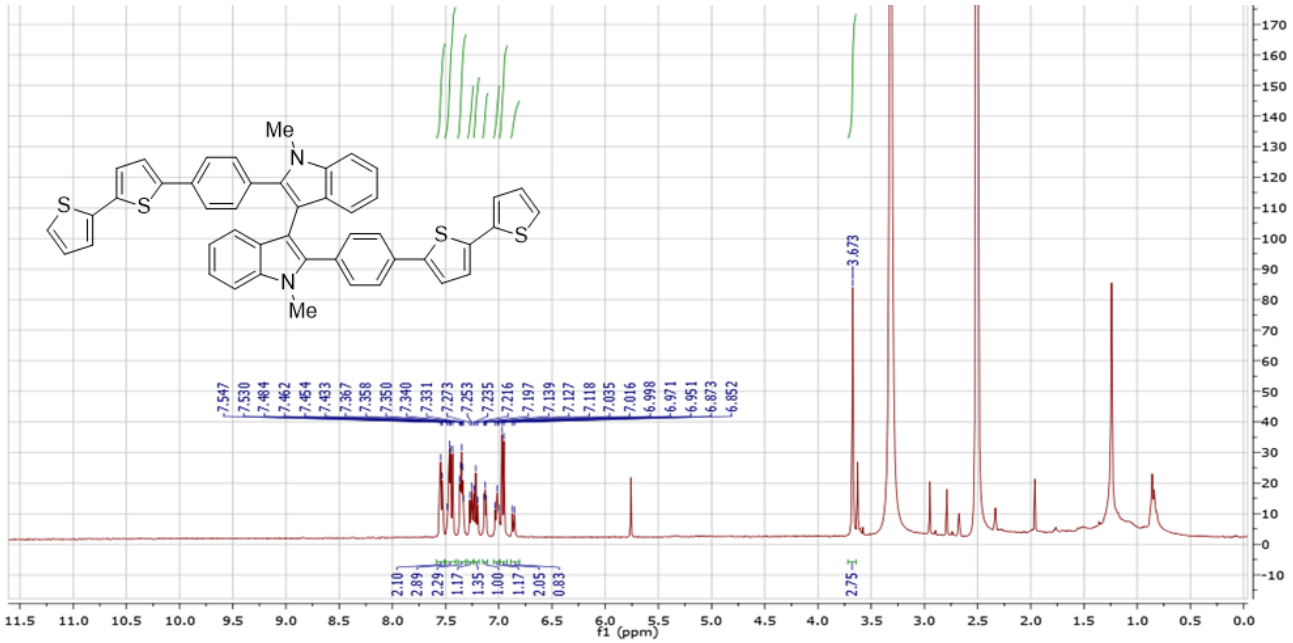
Chem. Eur. J. **2021**, 27, 13190-13202.

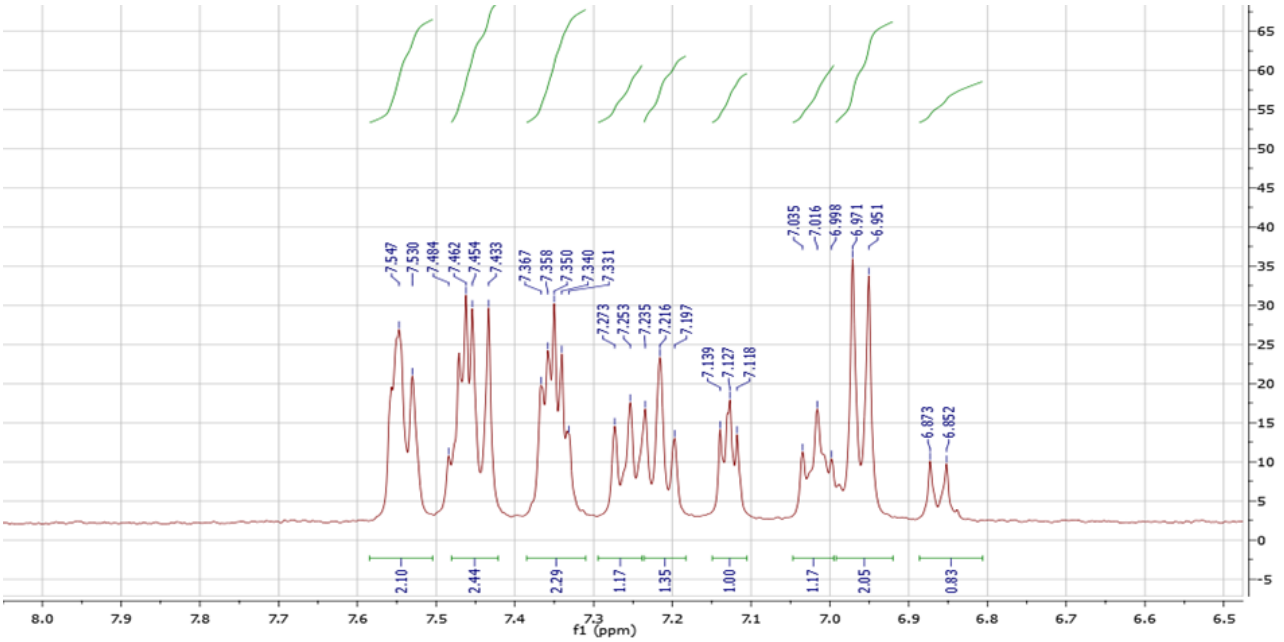
cited in the main paper as reference [6])

Compound 3

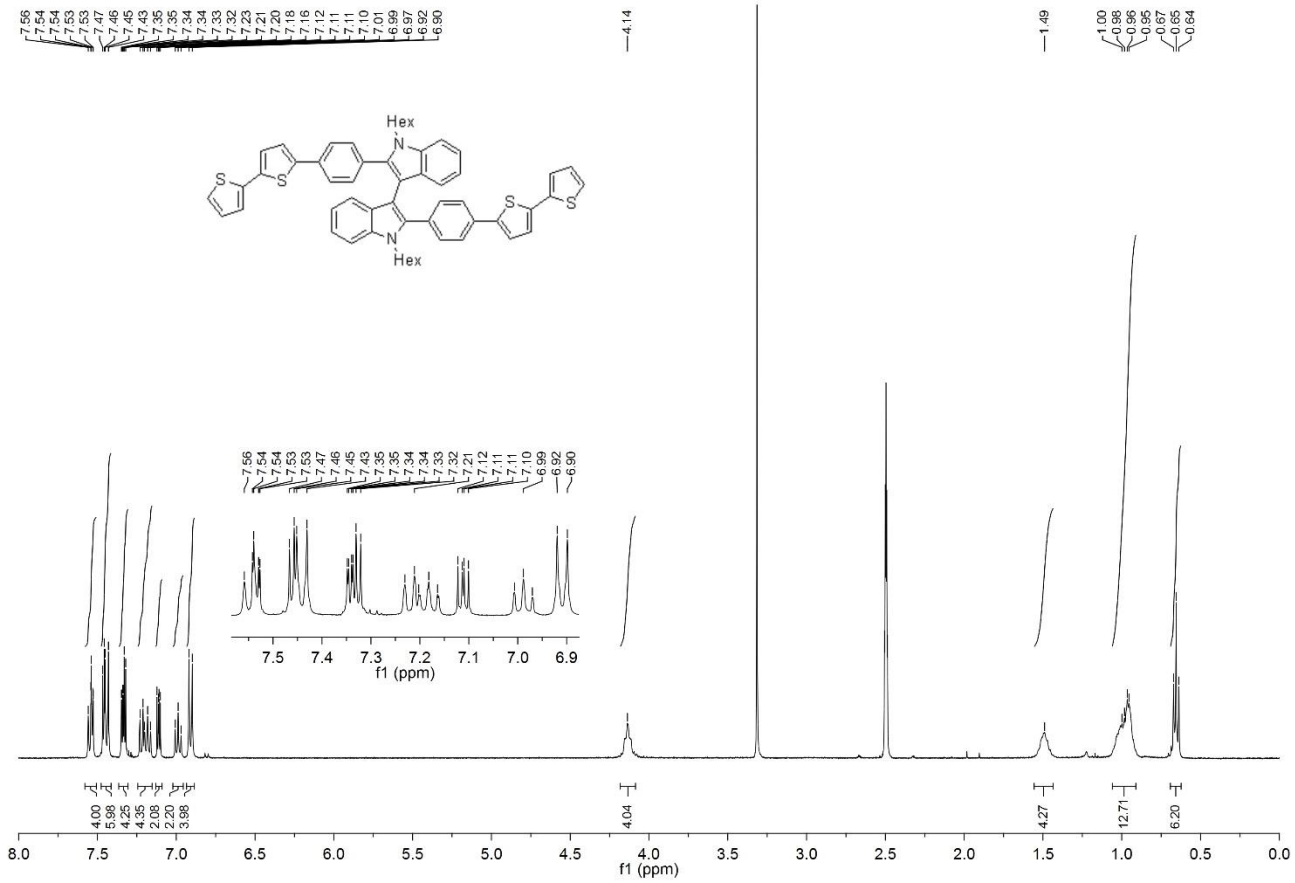

Me
S
N
S
S
N
Me
7.492
7.472
7.412
7.392
7.315
7.277
7.260
7.179
7.167
7.125
7.107
7.089
7.001
6.995
6.980
6.962
6.953
6.940
6.926
6.917
6.523
6.514
3.807
1.00
0.99
1.44
0.91
1.10
3.09
0.83
3.12
f1 (ppm)
123.569
123.538
138.959
137.852
137.275
131.643
131.196
129.106
128.794
127.757
124.220
123.569
123.538
122.296
120.812
119.671
109.408
109.284
31.232

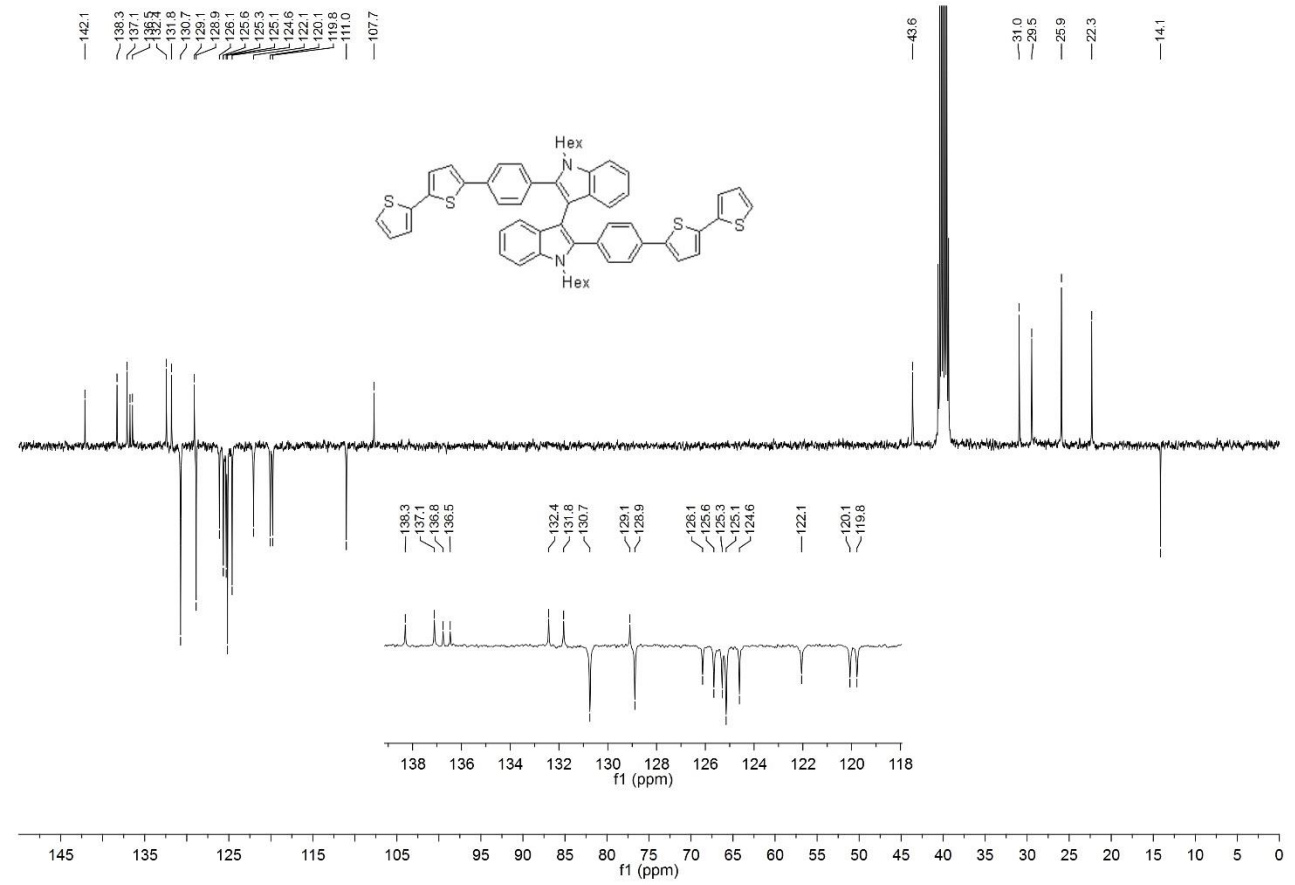
Compound 4a


Me
N
S
S
S
S
N
Me
7.547
7.530
7.484
7.462
7.454
7.433
7.367
7.358
7.350
7.340
7.331
7.273
7.253
7.235
7.216
7.197
7.139
7.127
7.118
7.035
7.016
6.998
6.971
6.951
6.873
6.852
3.673
2.10
2.89
2.29
1.17
1.35
1.00
1.17
2.05
0.83
2.75
f1 (ppm)

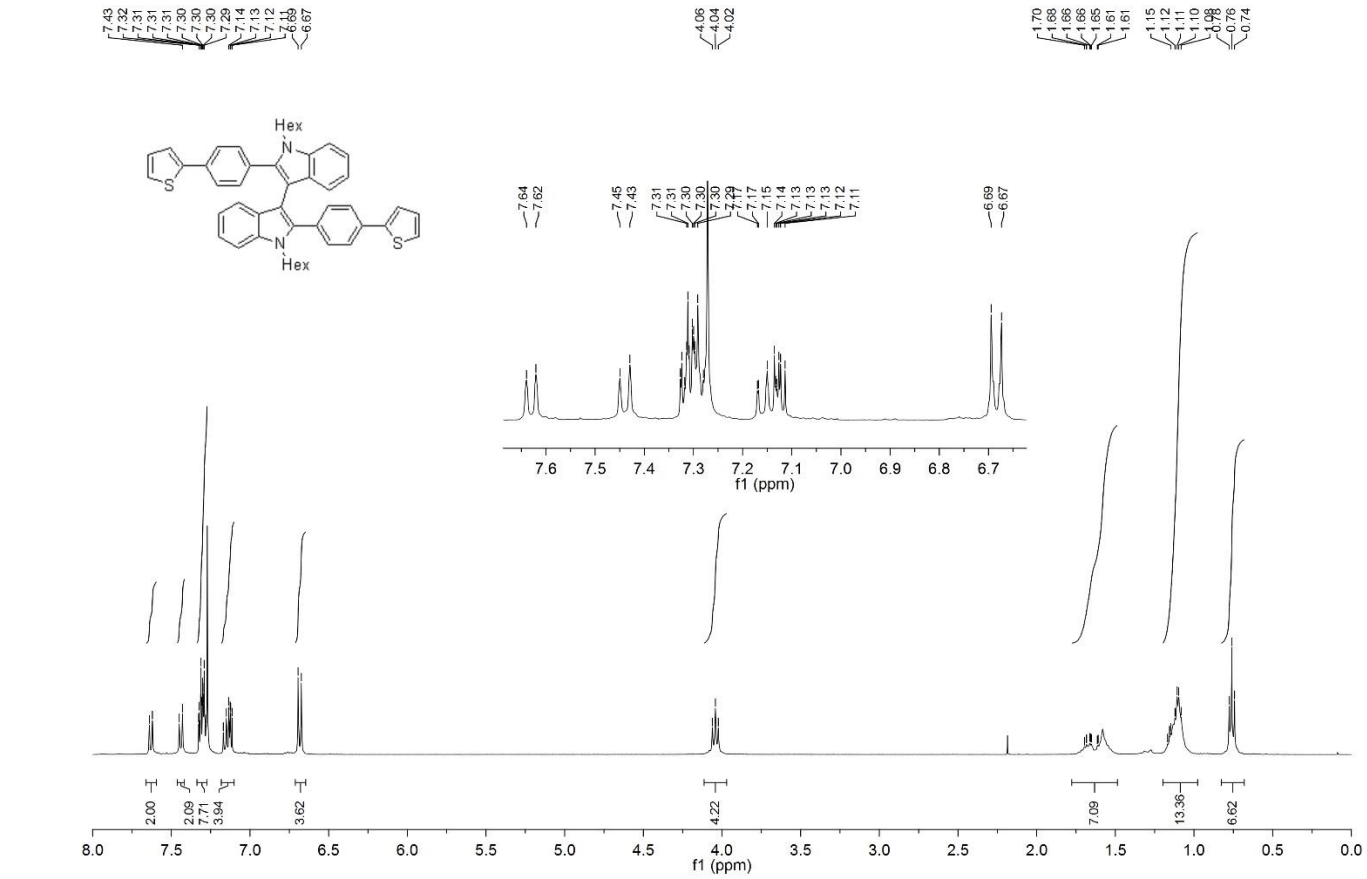

7.547
7.530
7.484
7.462
7.454
7.433
7.367
7.358
7.350
7.340
7.331
7.273
7.253
7.235
7.216
7.197
7.139
7.127
7.118
7.035
7.016
6.998
6.971
6.951
6.873
6.852
2.10
2.44
2.29
1.17
1.35
1.00
1.17
2.05
0.83
f1 (ppm)

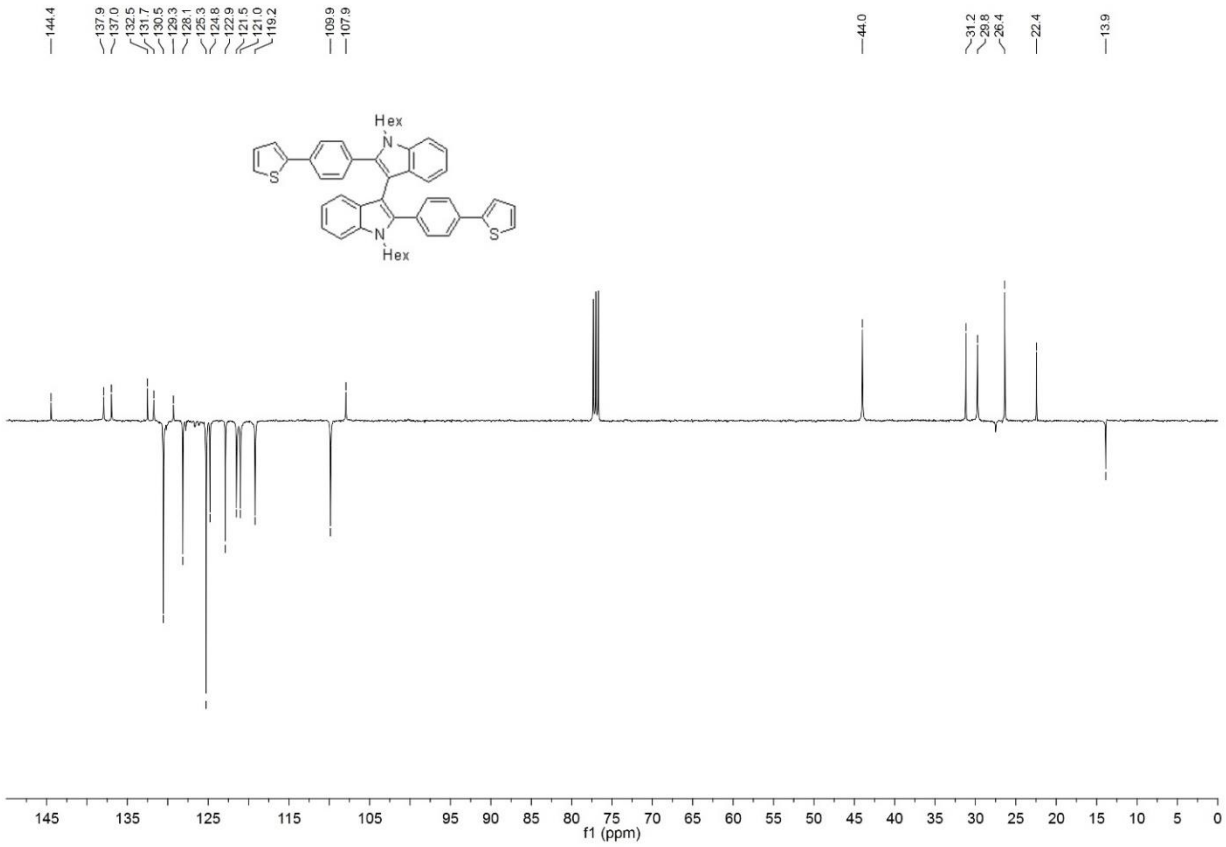
Compound 4b





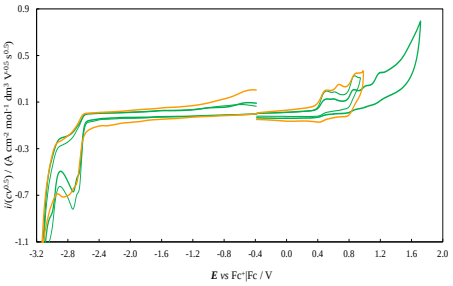
Compound 4c



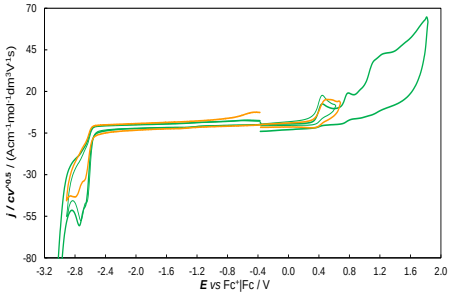


C. Anodic and Cathodic CV patterns in CH_3CN

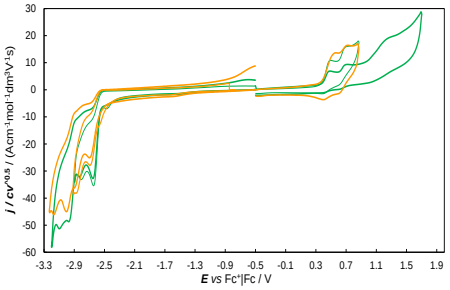
2,2'-Biindole series



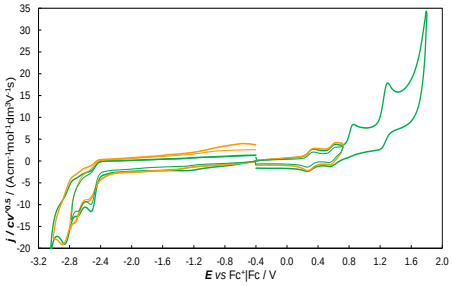
1b



1a

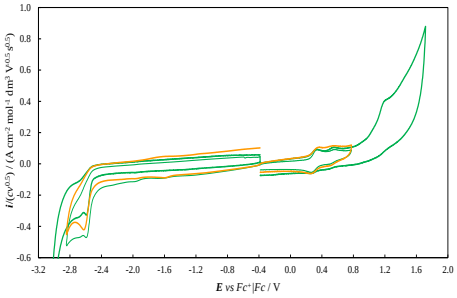


2a

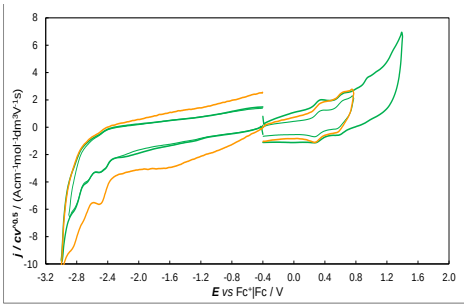


2b

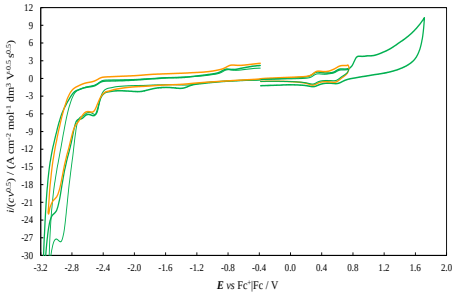
3,3'-Biindole series



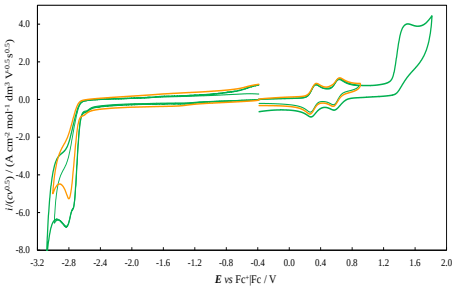
3



4a



4b



4c

A synopsis of normalized 2,2' (left) and 3,3' (right) monomer CV patterns in CH_3CN at 0.2 V/s (or 2 V/s, superimposed orange pattern)). Side by side are 2,2' and 3,3' analogue pairs.