

χ -Shaped bis(areno)-1,4-dihydropyrrolo[3,2-*b*]pyrroles generated by oxidative aromatic coupling

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1. General remarks.

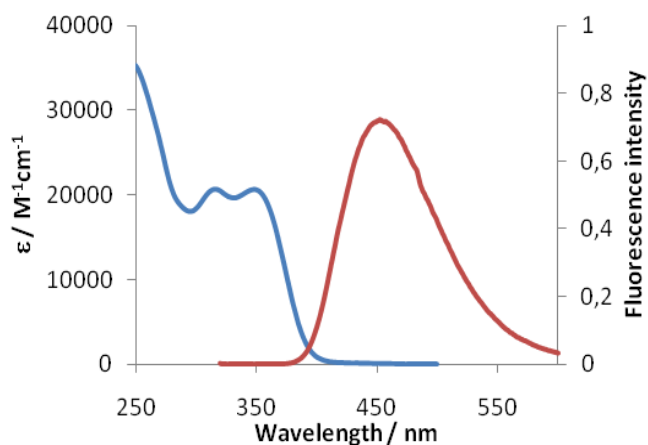
All reagents and solvents were purchased from commercial sources and were used as received unless otherwise noted. Reagent grade solvents (CH_2Cl_2 , hexanes) were distilled prior to use. DMF was dried over magnesium sulfate, then distilled and stored under argon. Transformations with moisture and oxygen sensitive compounds were performed under a stream of argon. The reaction progress was monitored by means of thin layer chromatography (TLC), which was performed on aluminum foil plates, covered with Silica gel 60 F₂₅₄ or Aluminum oxide 60 F₂₅₄ (neutral). Products purification was done by means of column chromatography with Kieselgel 60 or Aluminum oxide. Occasionally, dry column vacuum chromatography (DCVC) for purification of products obtained was performed using Silica gel Type D 5F. The identity and purity of prepared compounds were proved by ^1H NMR and ^{13}C NMR spectrometry as well as by MS-spectrometry (*via* EI-MS or ESI-MS). For HRMS measurements both quadruple and TOF mass analyzer types were used. NMR spectra were measured on 500 MHz, 600 MHz or 400 MHz instruments with TMS as internal standard. All chemical shifts are given in ppm. All melting points for crystalline products were measured with automated melting point apparatus and were given without correction. The absorbance and fluorescence spectra were measured in dichloromethane.

Linear optical measurements

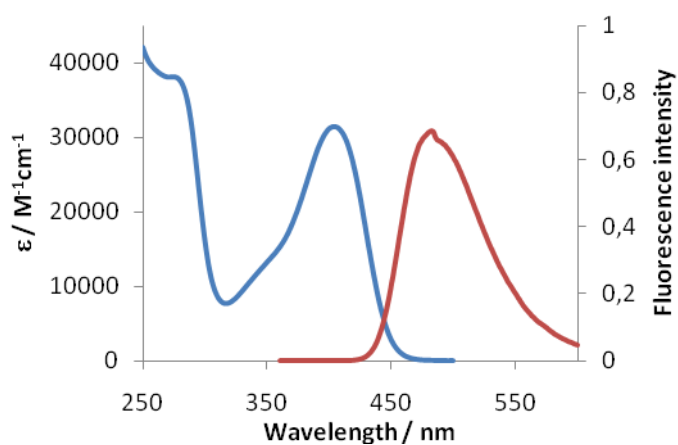
Steady-state fluorescence measurements were performed with dilute solutions (10^{-6}M , optical density < 0.1) contained in standard 1 cm quartz cuvettes at room temperature. Compounds were dissolved in dichloromethane unless otherwise noted. Emission spectra were obtained, for each compound, under excitation at $\lambda=350$ nm. Fluorescence quantum yields were measured by using quinine hemisulphate monohydrate in 0.5M sulfuric acid as a standard.

2. Normalized absorption and emission spectra for synthesized compounds.

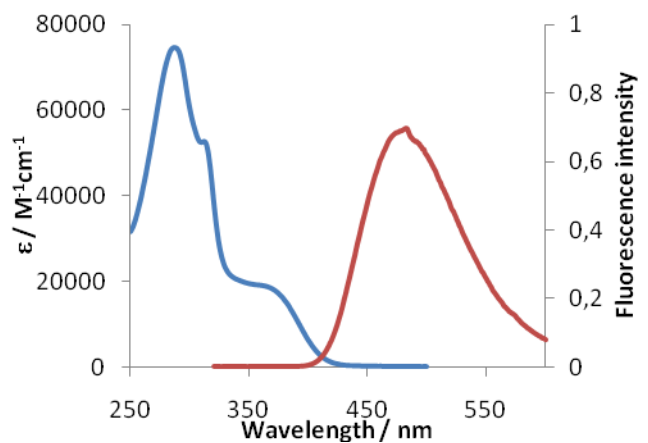
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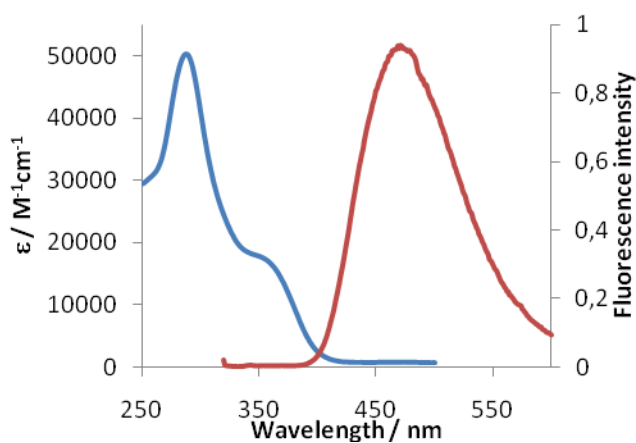
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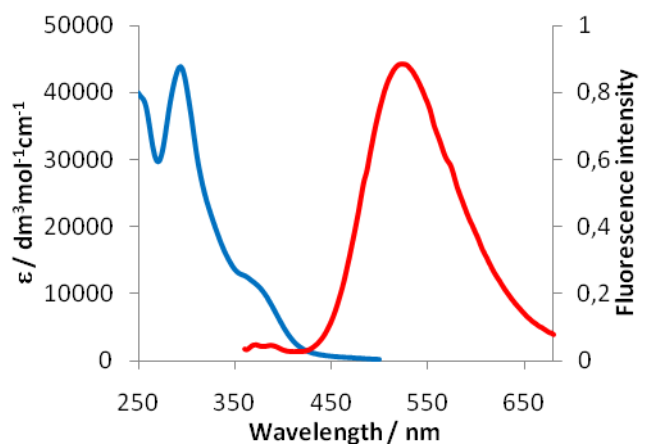
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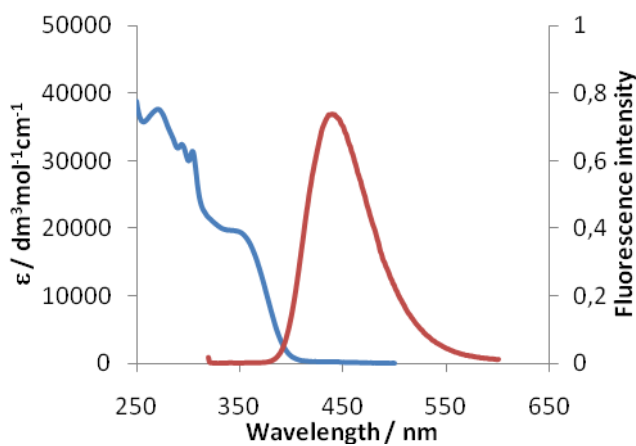
4d

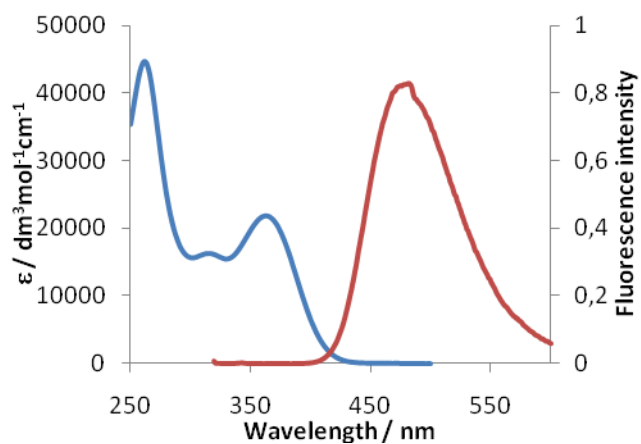
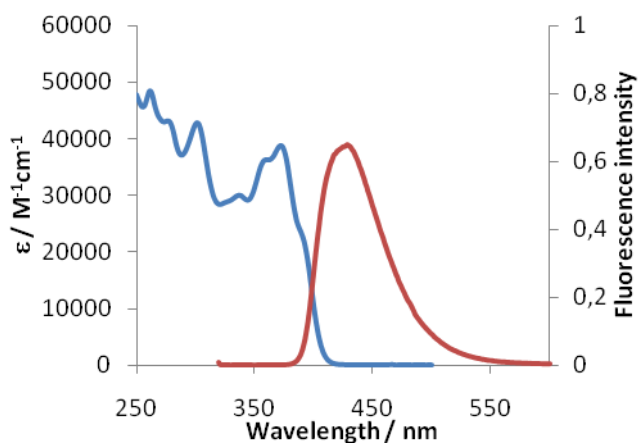
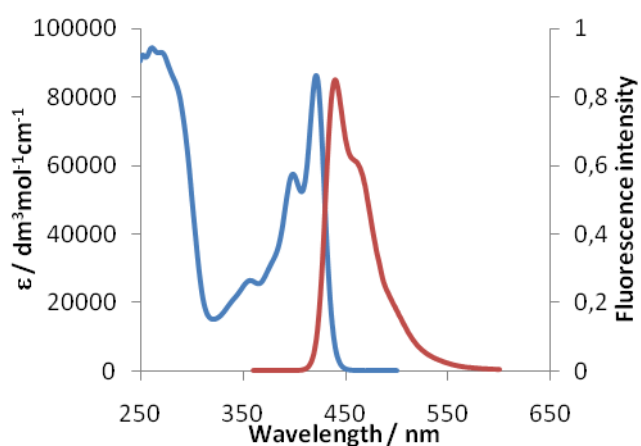
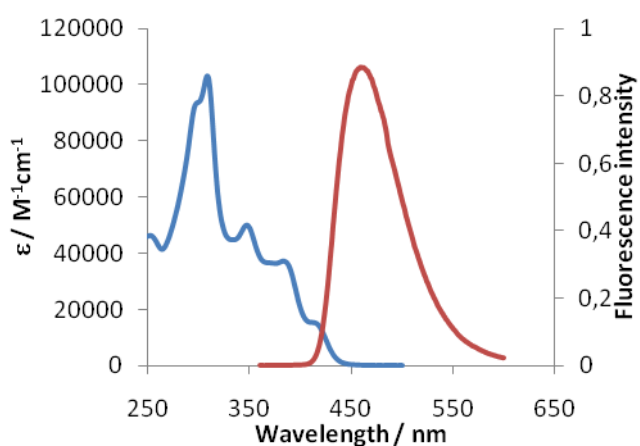
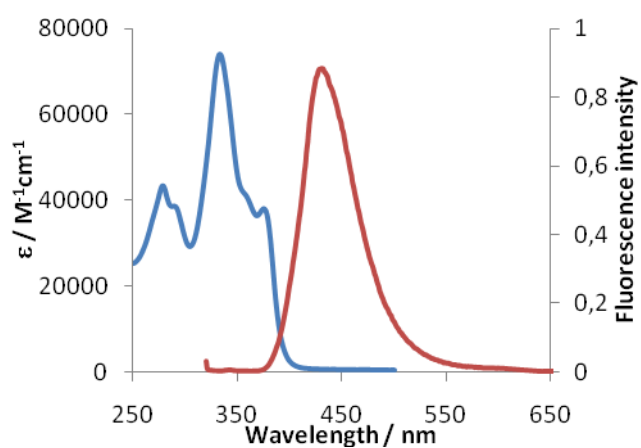
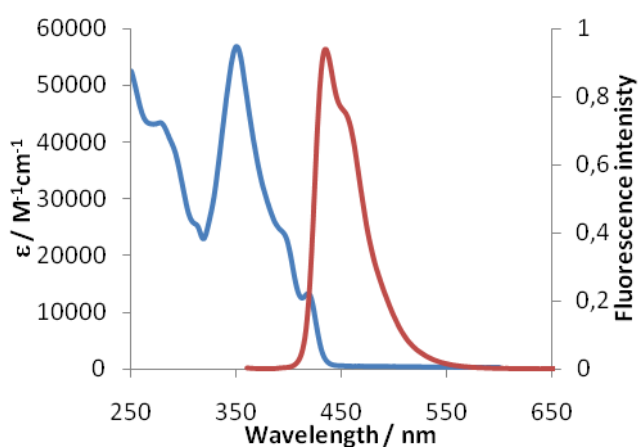


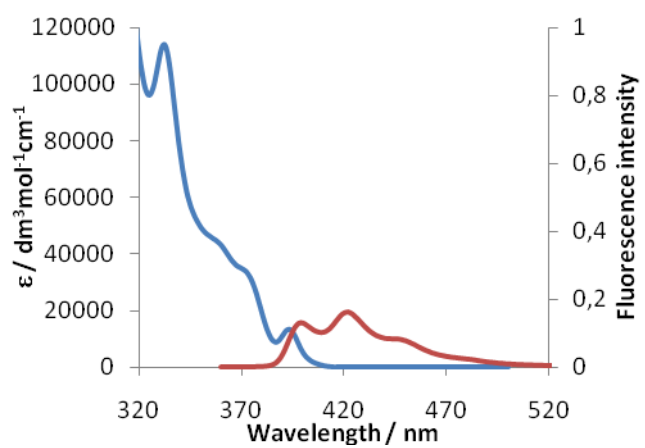
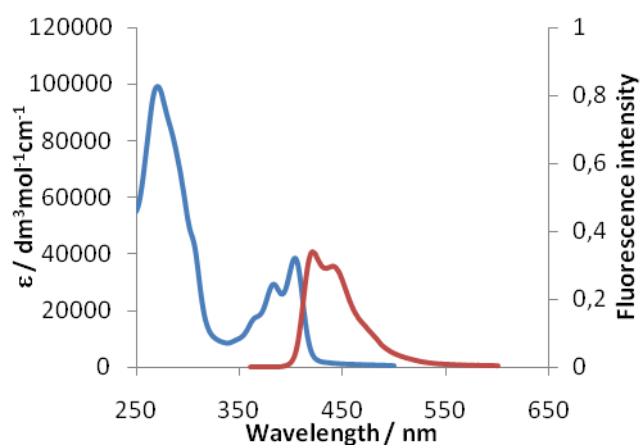
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4f

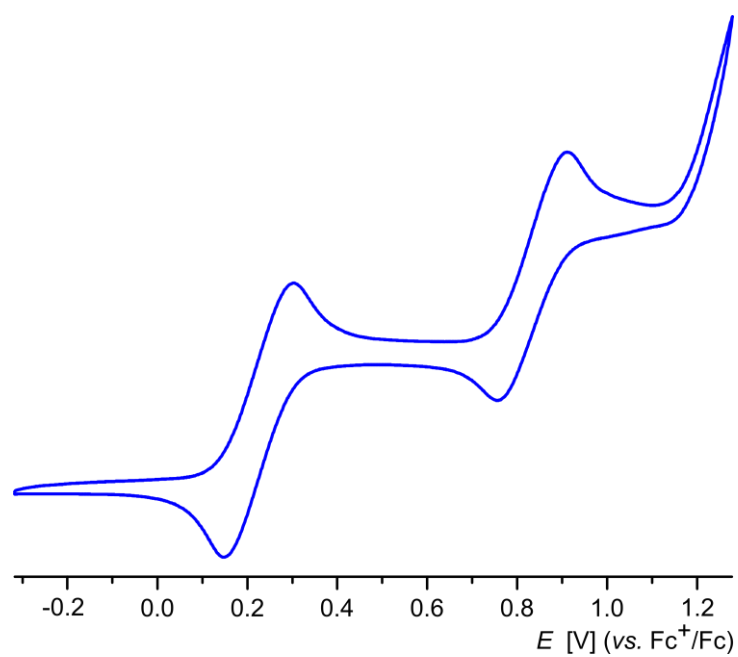


4g**5a****5b****5c****5d****5e**

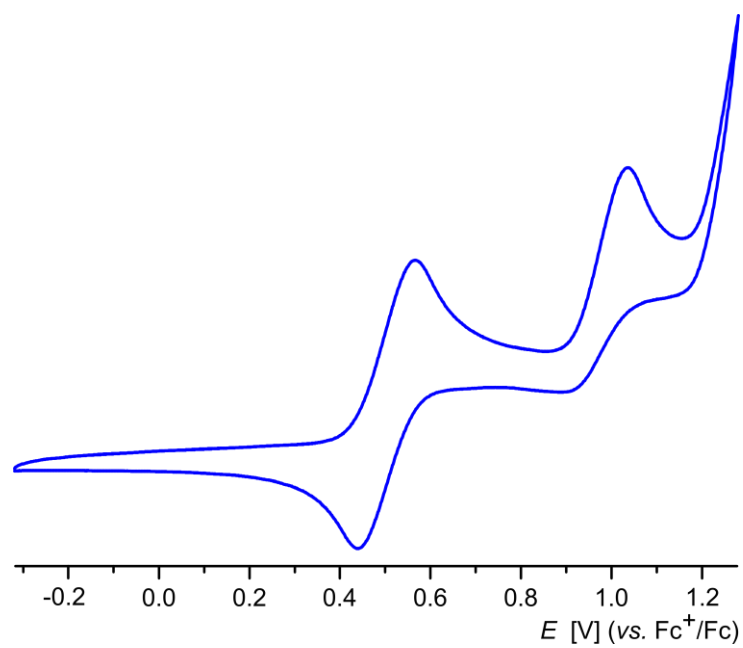
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3. Cyclic voltammetry for selected compounds.

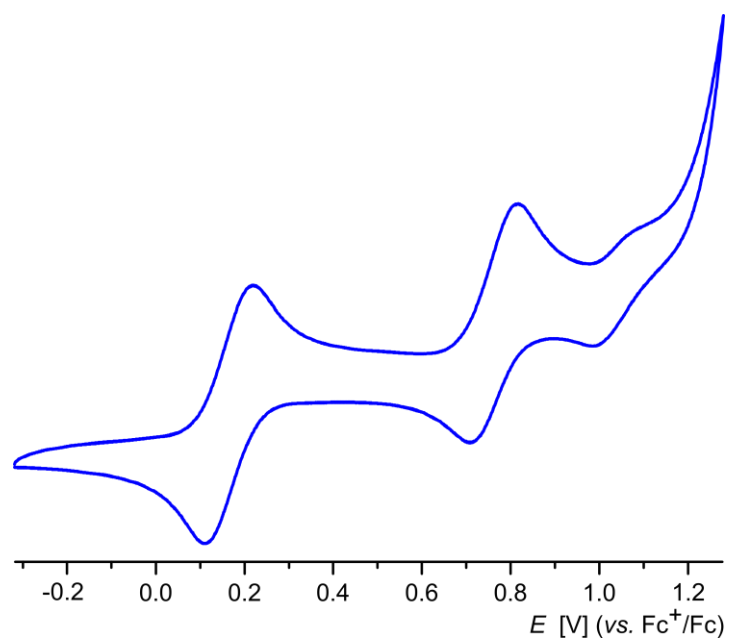
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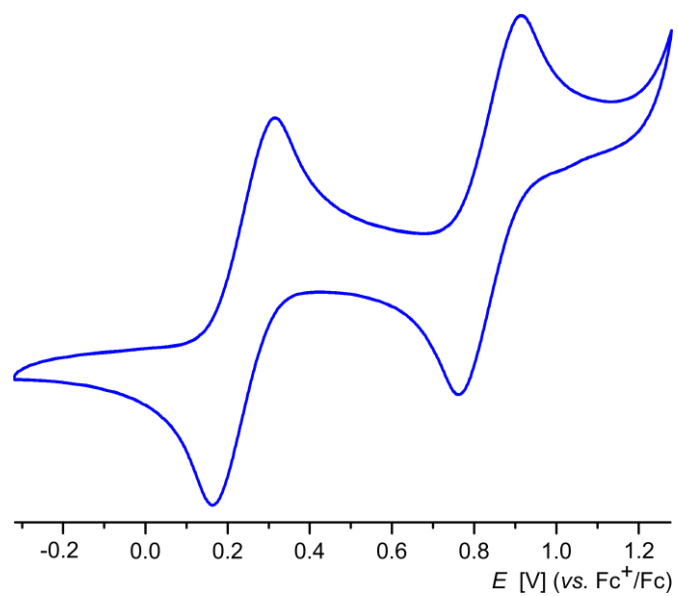
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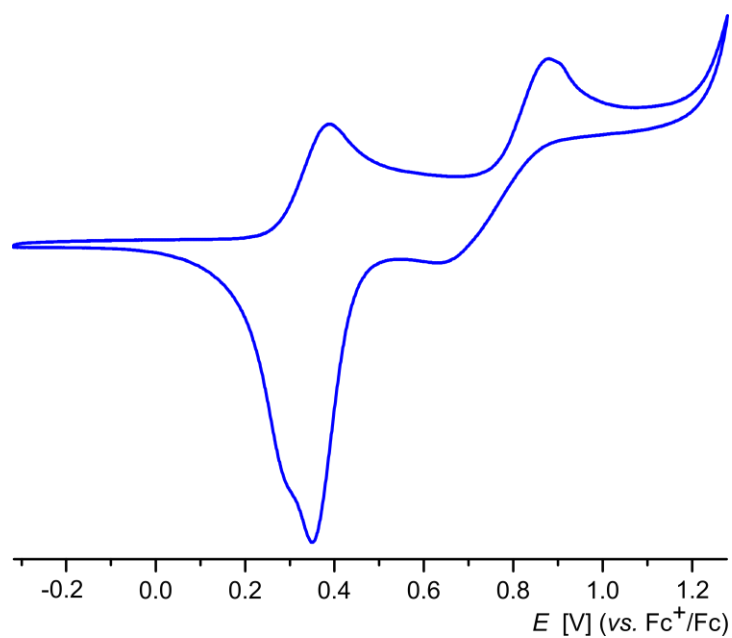
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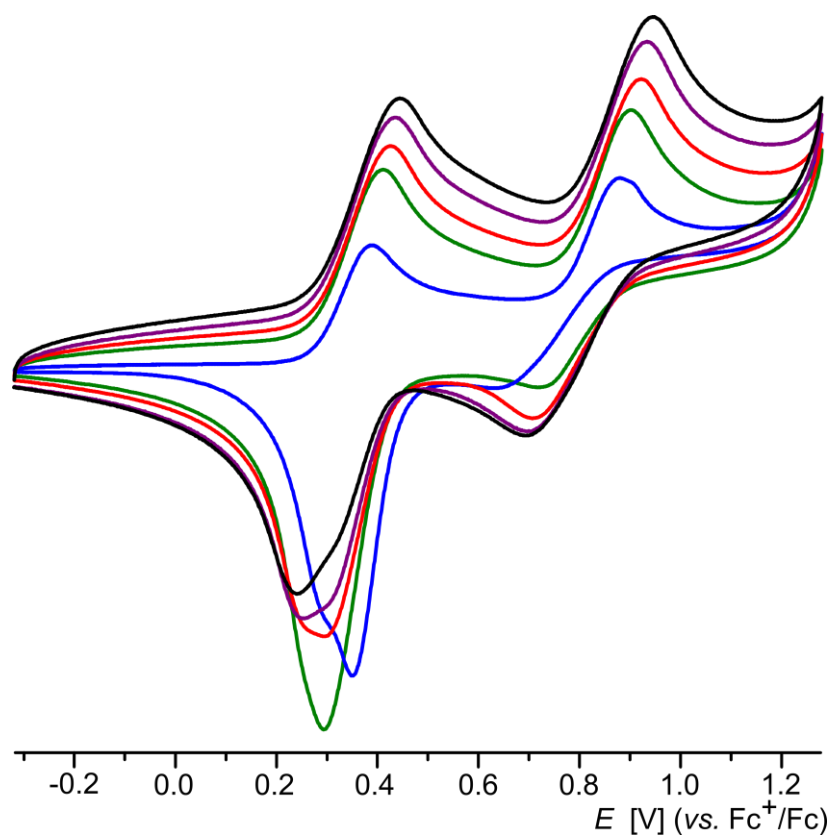
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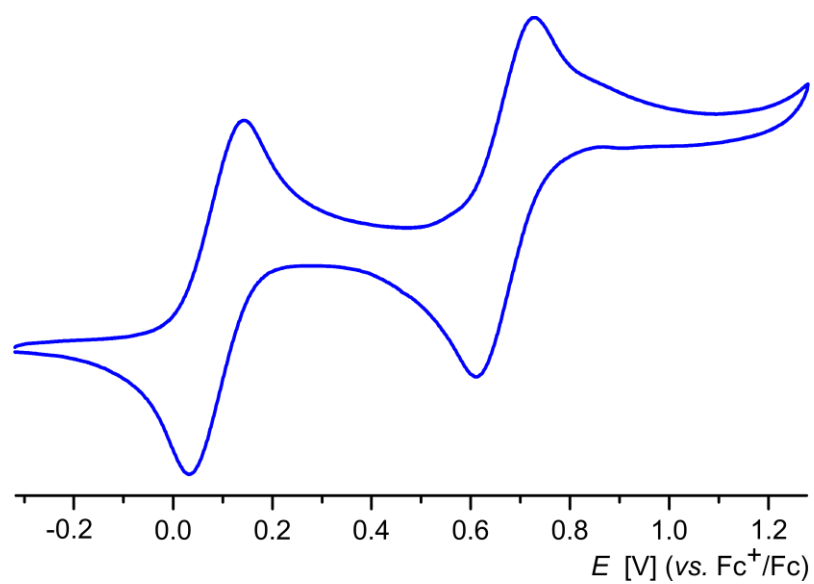
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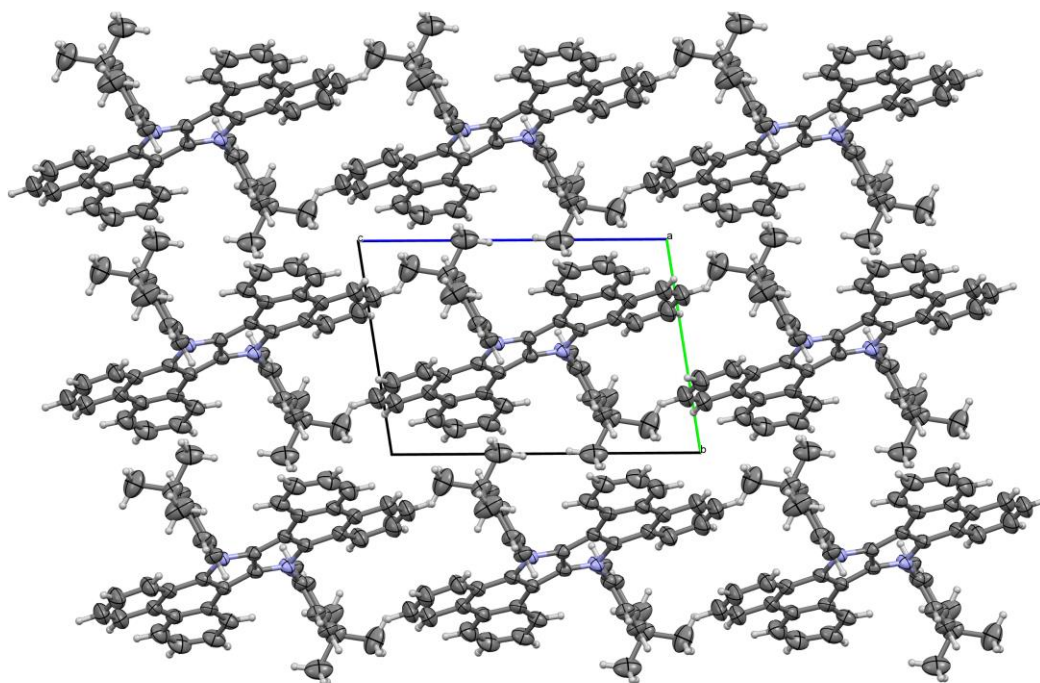
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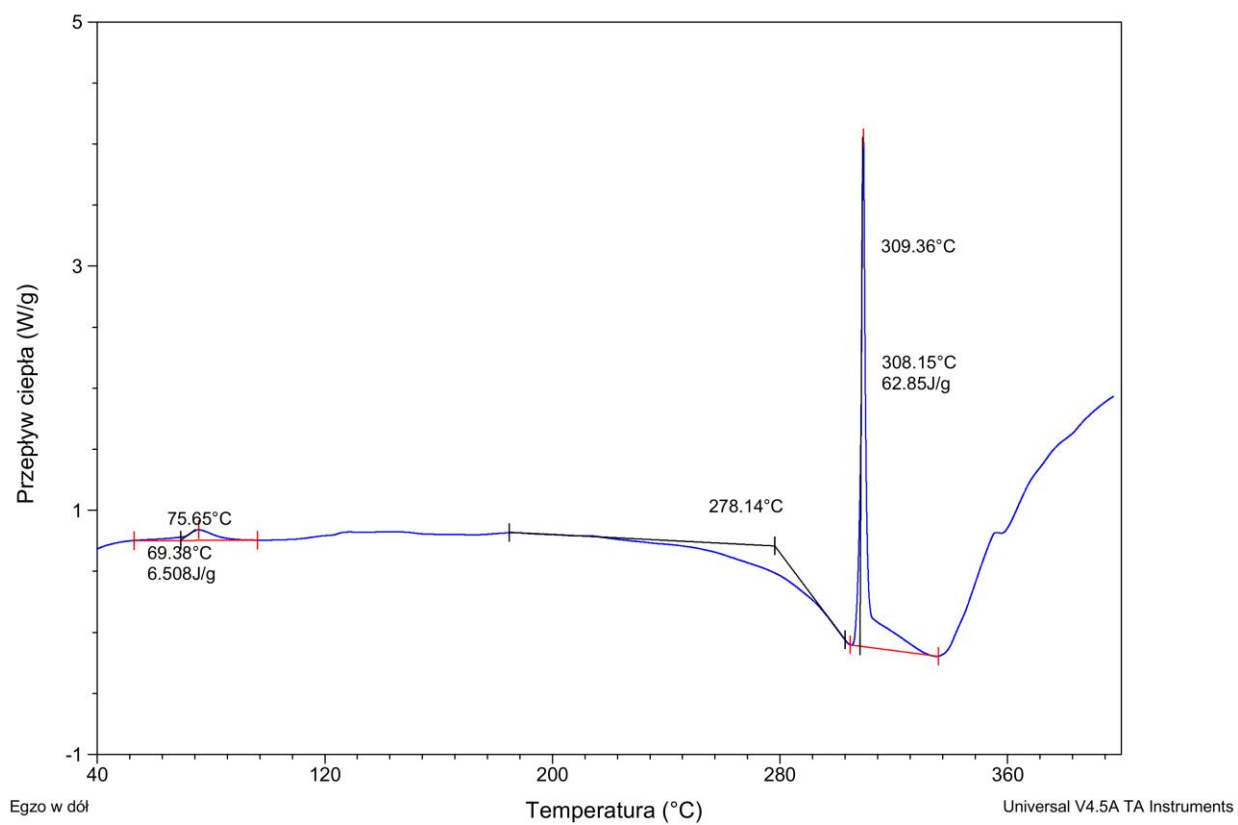
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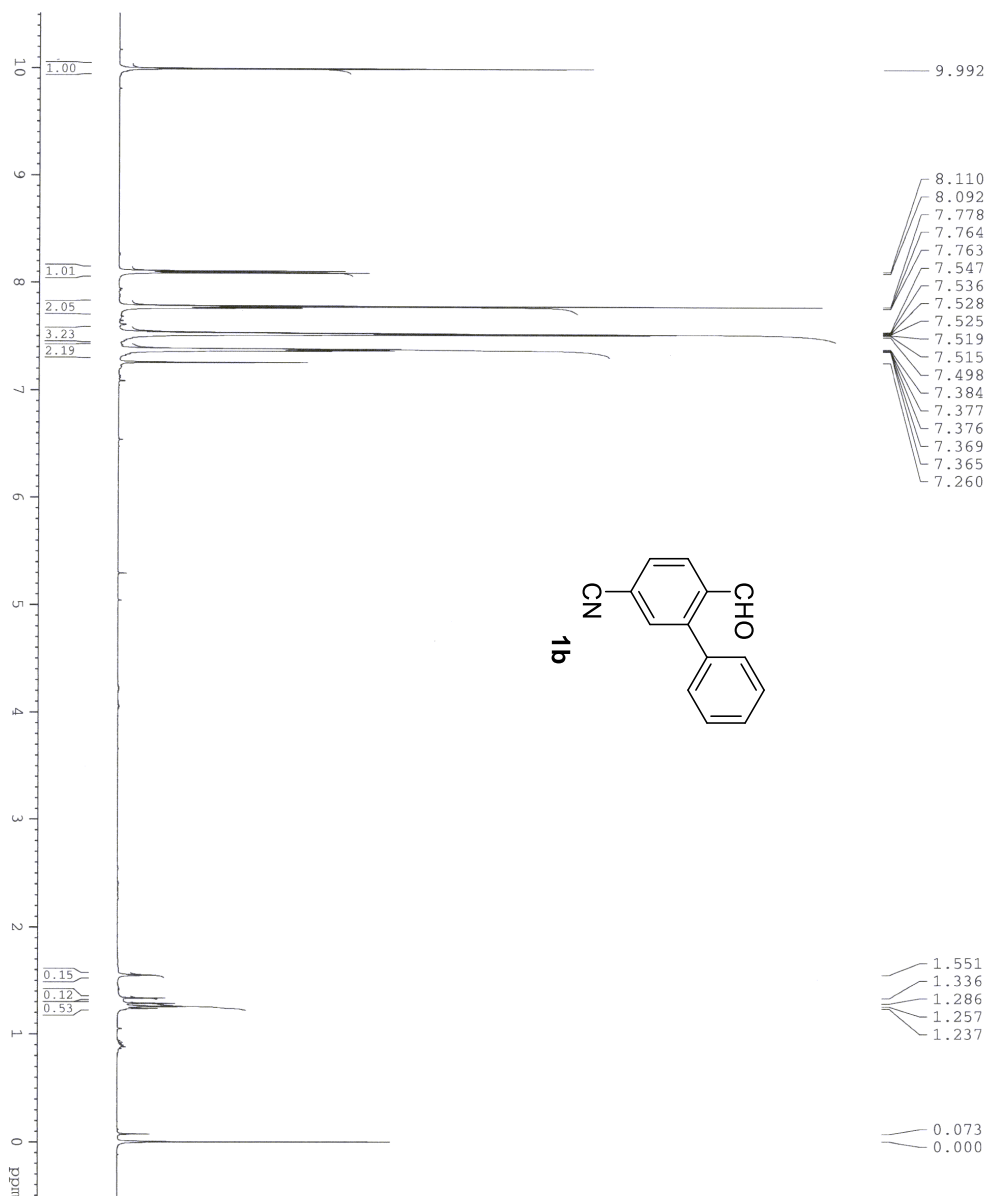
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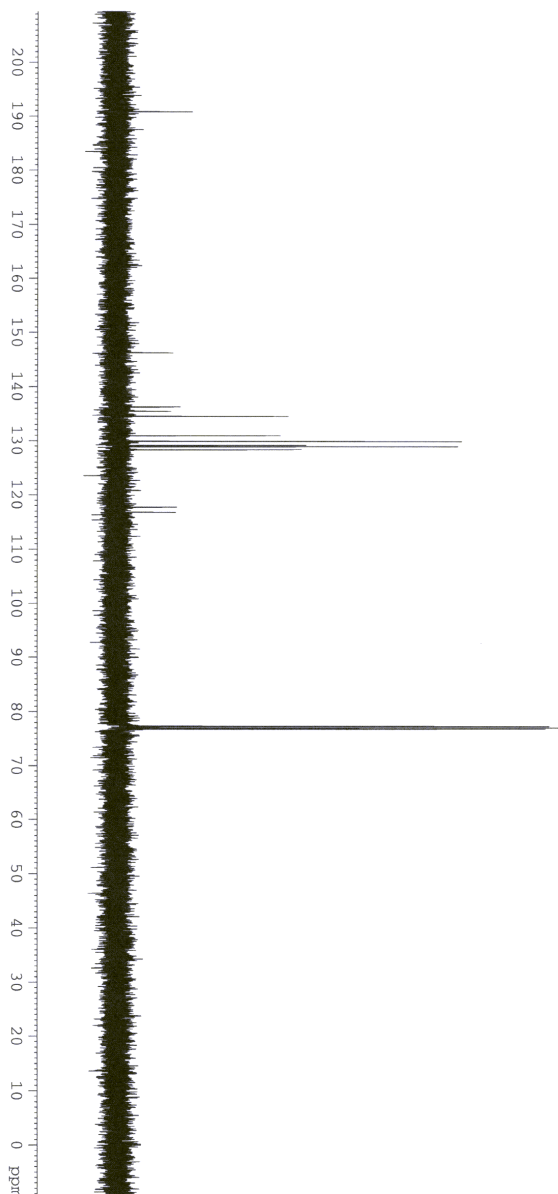
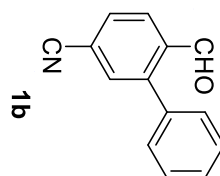
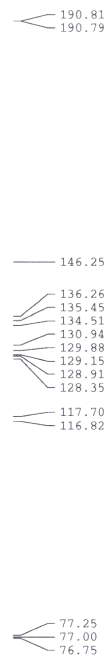
5. Differential Scanning Calorimetry curve for compound 5b.



6. ^1H and ^{13}C NMR spectra of compounds 1b-g, 4a-g and 5a-g.



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TD0 1
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SSB 0
LB 0.00 Hz
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PC 1.00



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Current Data Parameters
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EXPNO     1
PROCNO    1

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PULPROG   zgpg
PROBHD    5 mm TBI 1H/13
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PL1        3.00 dB
SFO1       125.7703643 MHz

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PCPD2      98.00 usec
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PL3        32.00 dB
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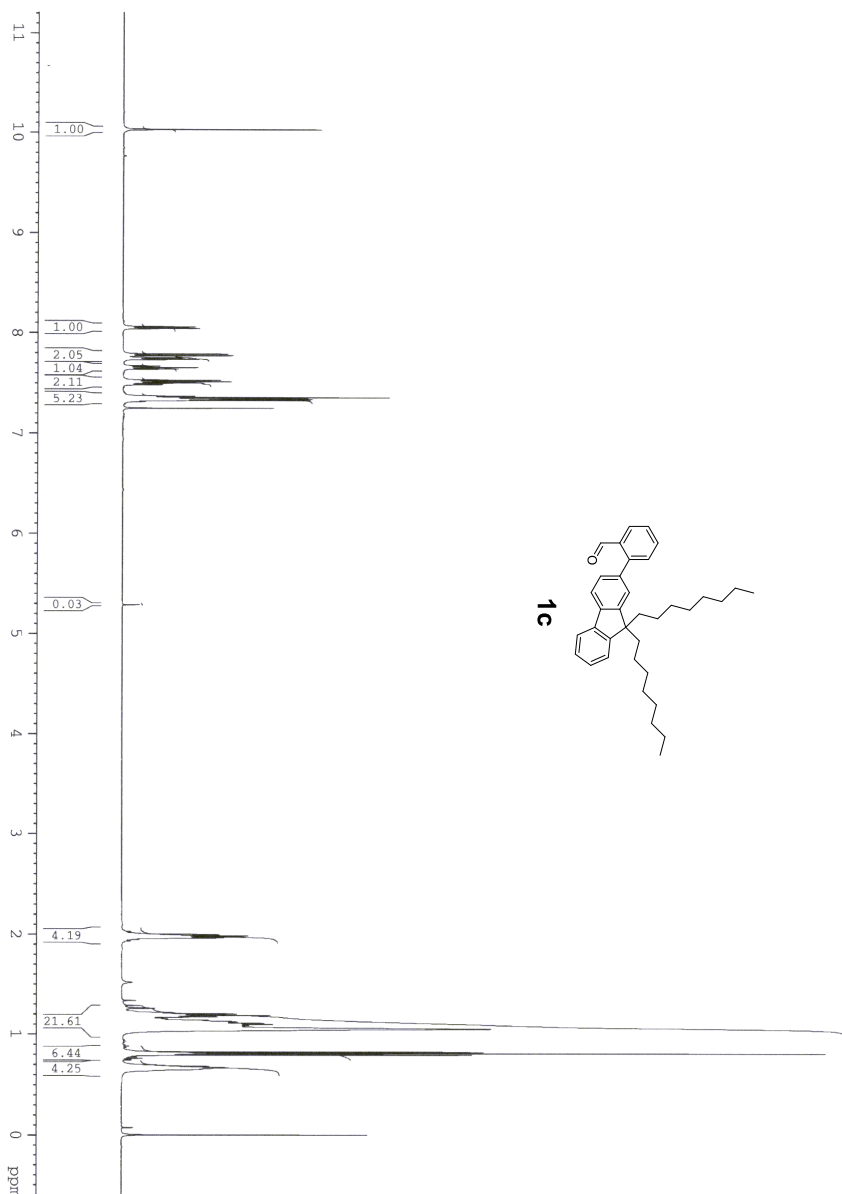
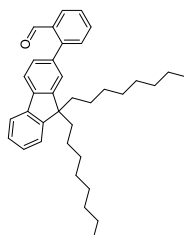
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SFO1 500.1330885 MHz

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PROCNO 1

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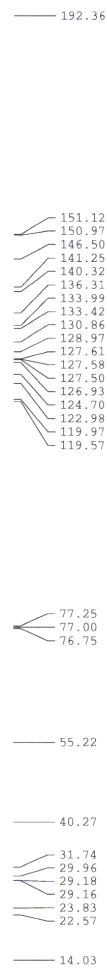
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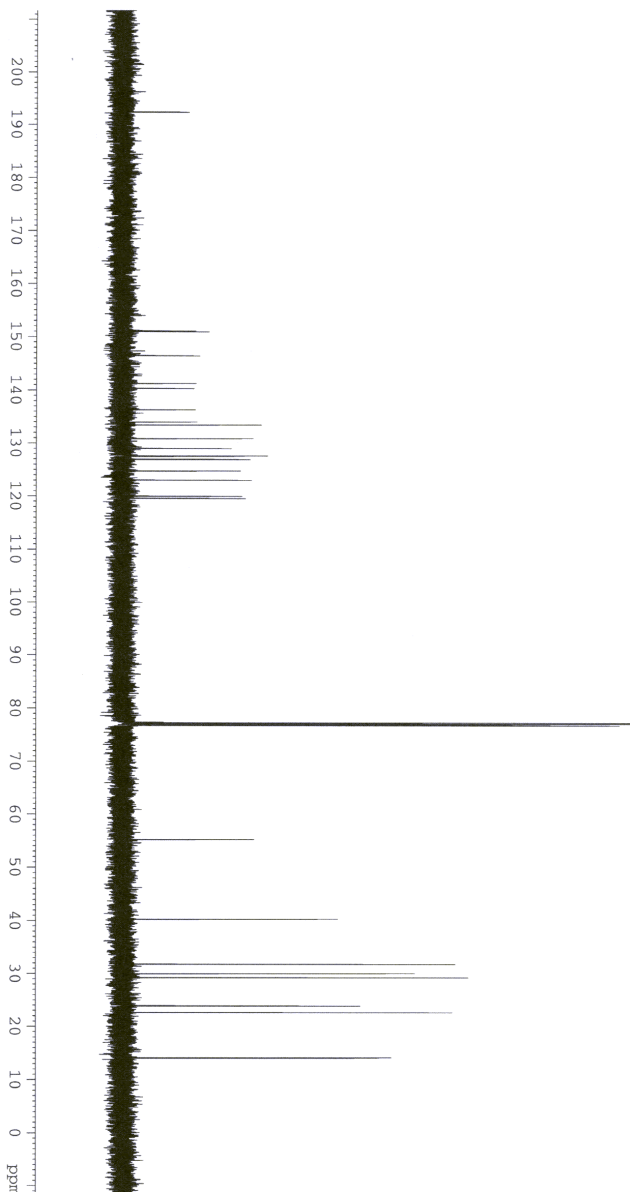
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SSB 0
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GB 0
PC 1.40

F1 - Processing parameters
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1c





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PROCNO 1

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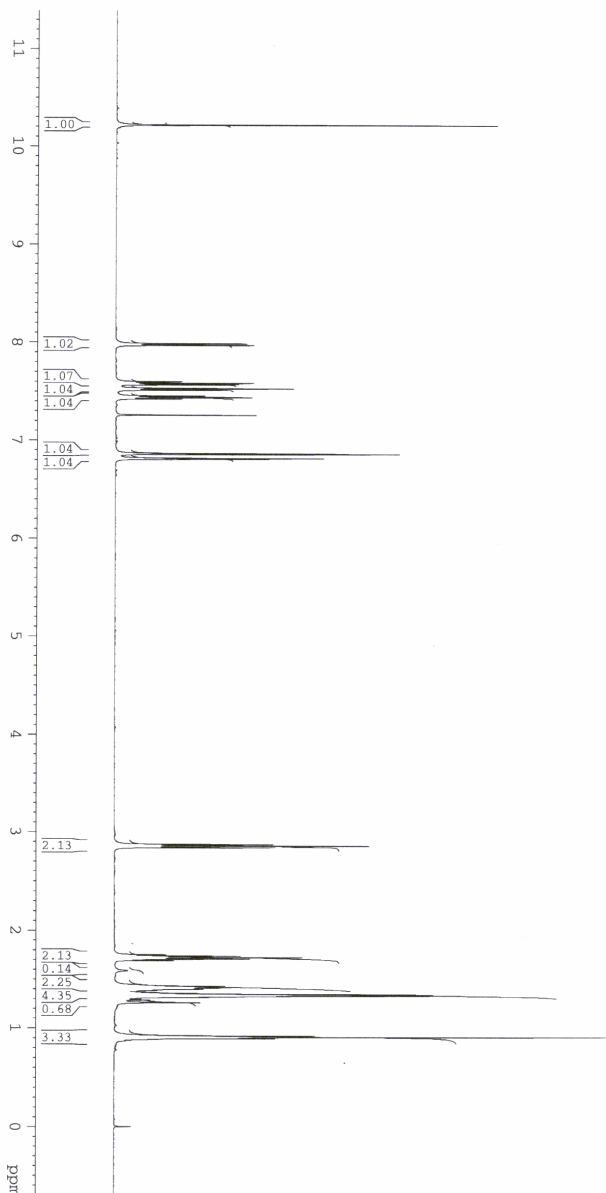
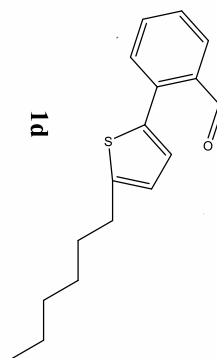
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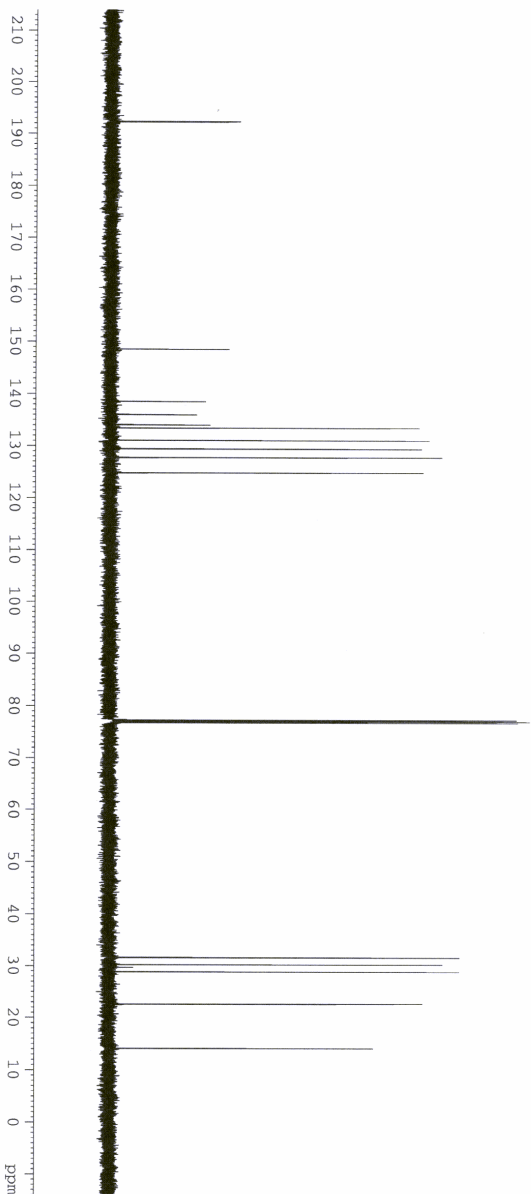
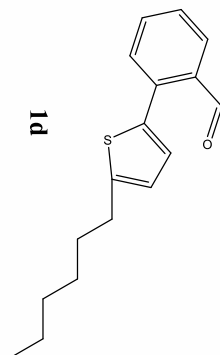
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Current Data Parameters
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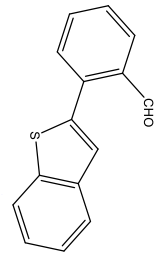
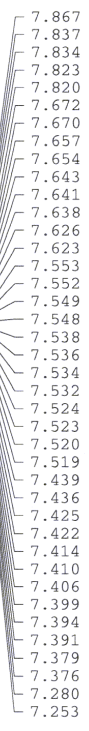
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PL13 32.00 dB
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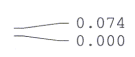
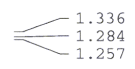
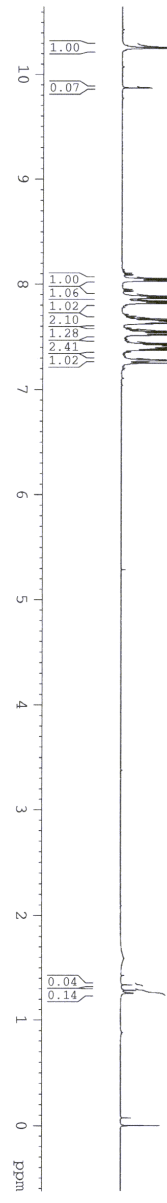
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1c

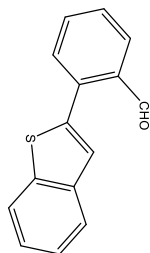


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FIDRES 0.157632 Hz
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RG 287.4
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DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1
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PL1 5.00 dB
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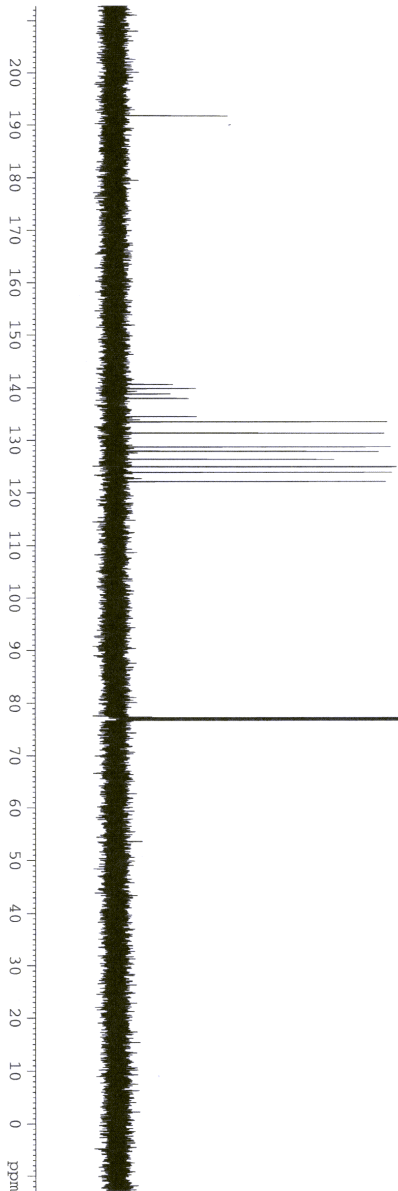
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1c



Current Data Parameters
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PROCNO 1

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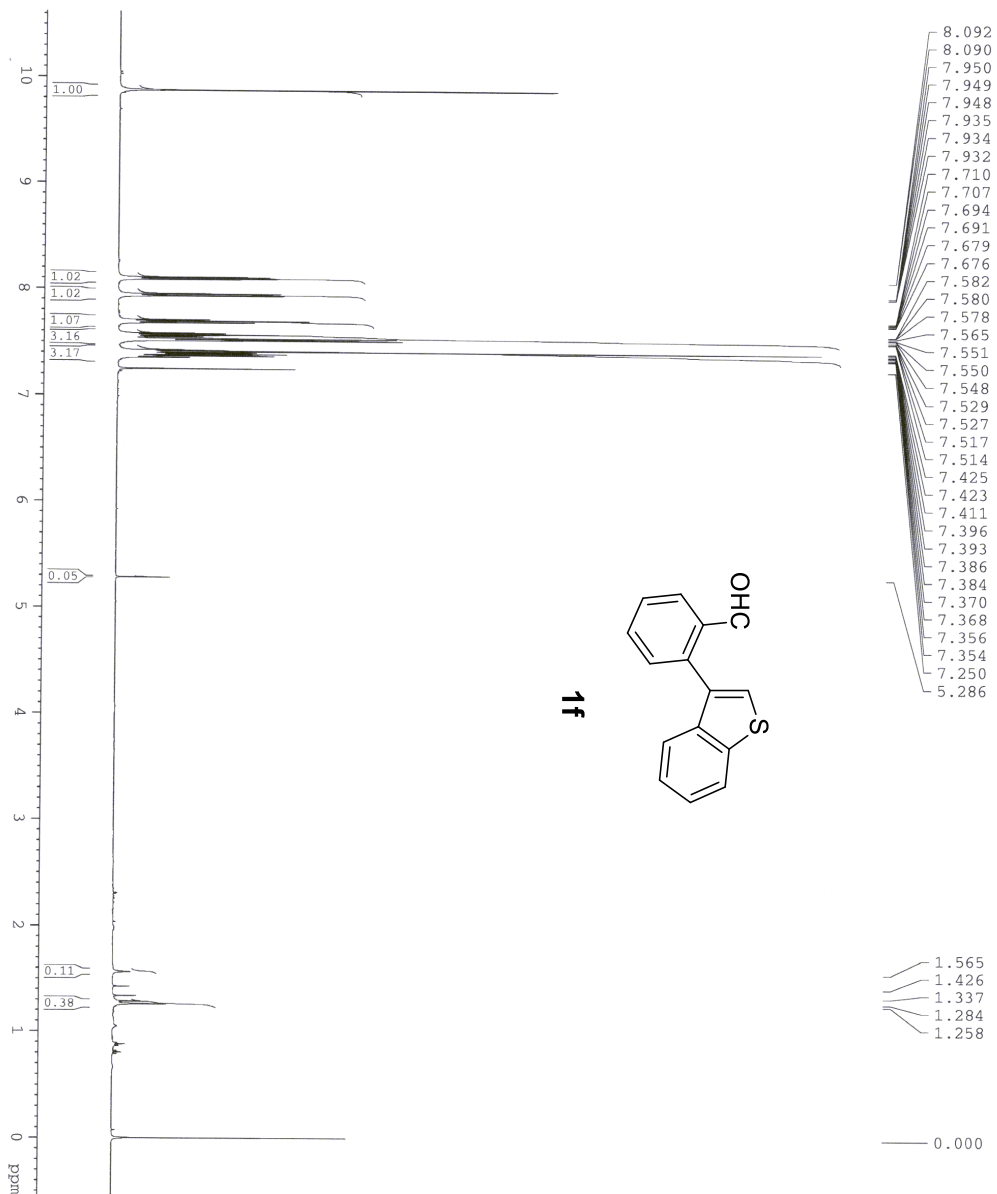
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NUC2 1H
PCPD2 98.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 500.132 MHz
FIDRES 7.812500 Hz
SW 1.992 ppm
FMODE QF

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SF 125.7577942 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

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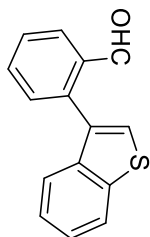
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RG 3.171923 sec
DE 48.400 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300287 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

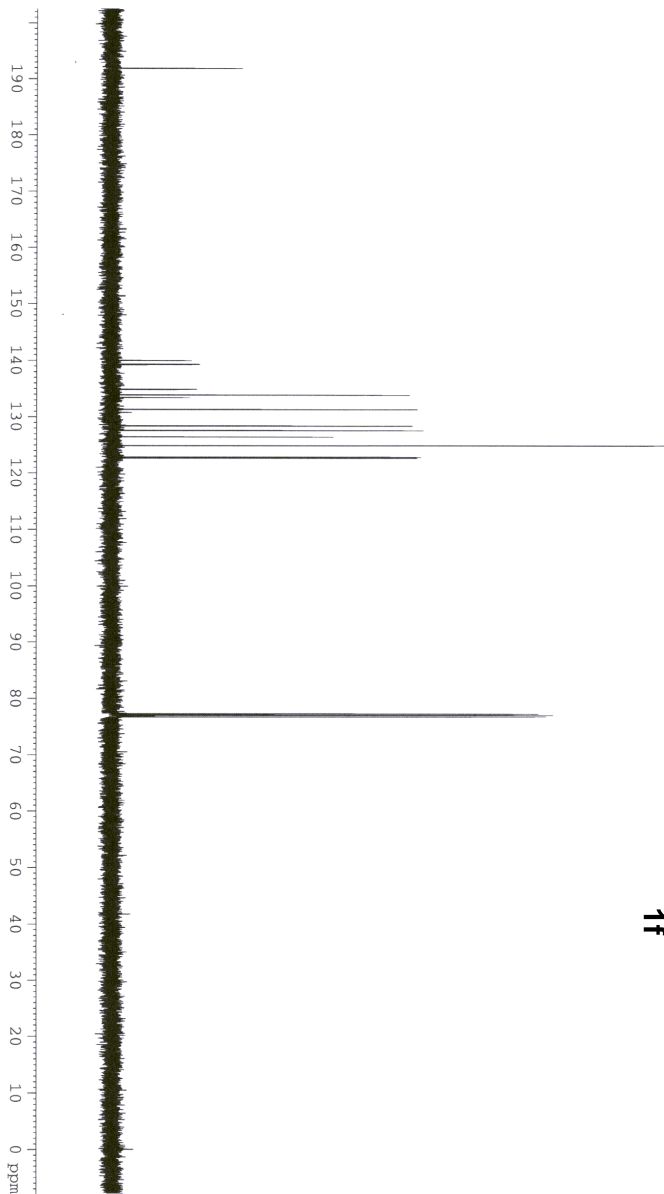
191.91
191.89

139.97
139.34
139.30
134.89
133.89
133.42
131.32
128.41
127.59
126.43
124.89
122.85
122.69

77.25
77.00
76.74



1f



Current Data Parameters
NAME MK215
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140911
Time 12.10
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027508 sec
RG 32768
DW 13.200 usec
DE 7.710 usec
TE 303.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1

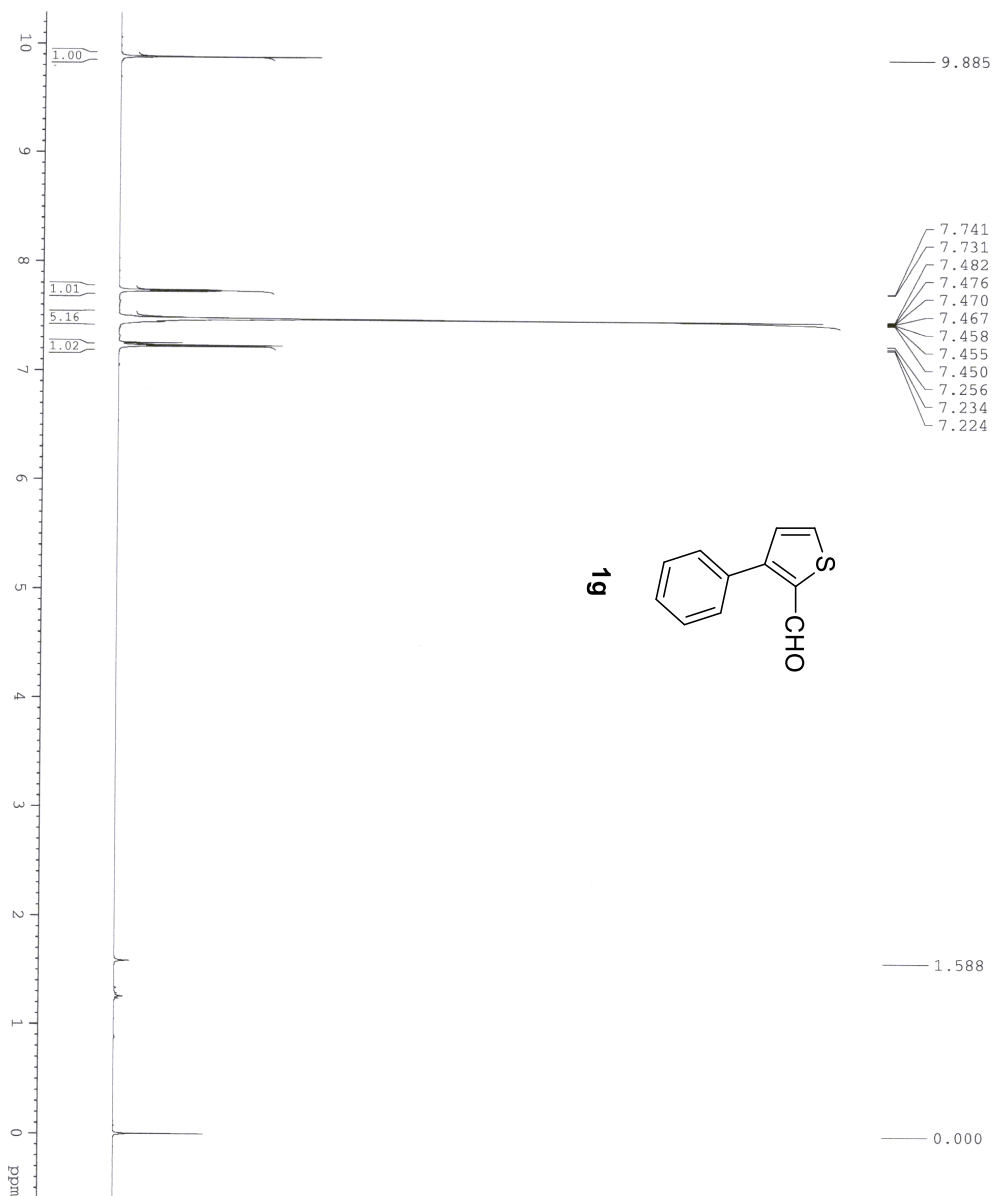
===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -3.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 3.00 dB
PL3 32.00 dB
SFO2 500.1326005 MHz

F1 - Acquisition Parameters
ND0 1
TD 128
SFO1 500.132 MHz
FIDRES 7.81250 Hz
SW 1.599 ppm
FMODE GP

F2 - Processing parameters
SI 262144
SF 125.7577957 MHz
RG 65536
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1



Current Data Parameters
NAME MK209
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140507
Time_ 11.39

INSTRUM 1 PRX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32

DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 181
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300252 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME MK209
EXPNO 2
PROCNO 1

P2 - Acquisition Parameters
Date_ 20140507
Time 12.08
INSTRUM DEX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg
SOLVENT CDCl3
NS 836
DS 4
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027508 sec
RG 327.68
DQ 1533.0 usec
DE 7.10 usec
TE 303.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1

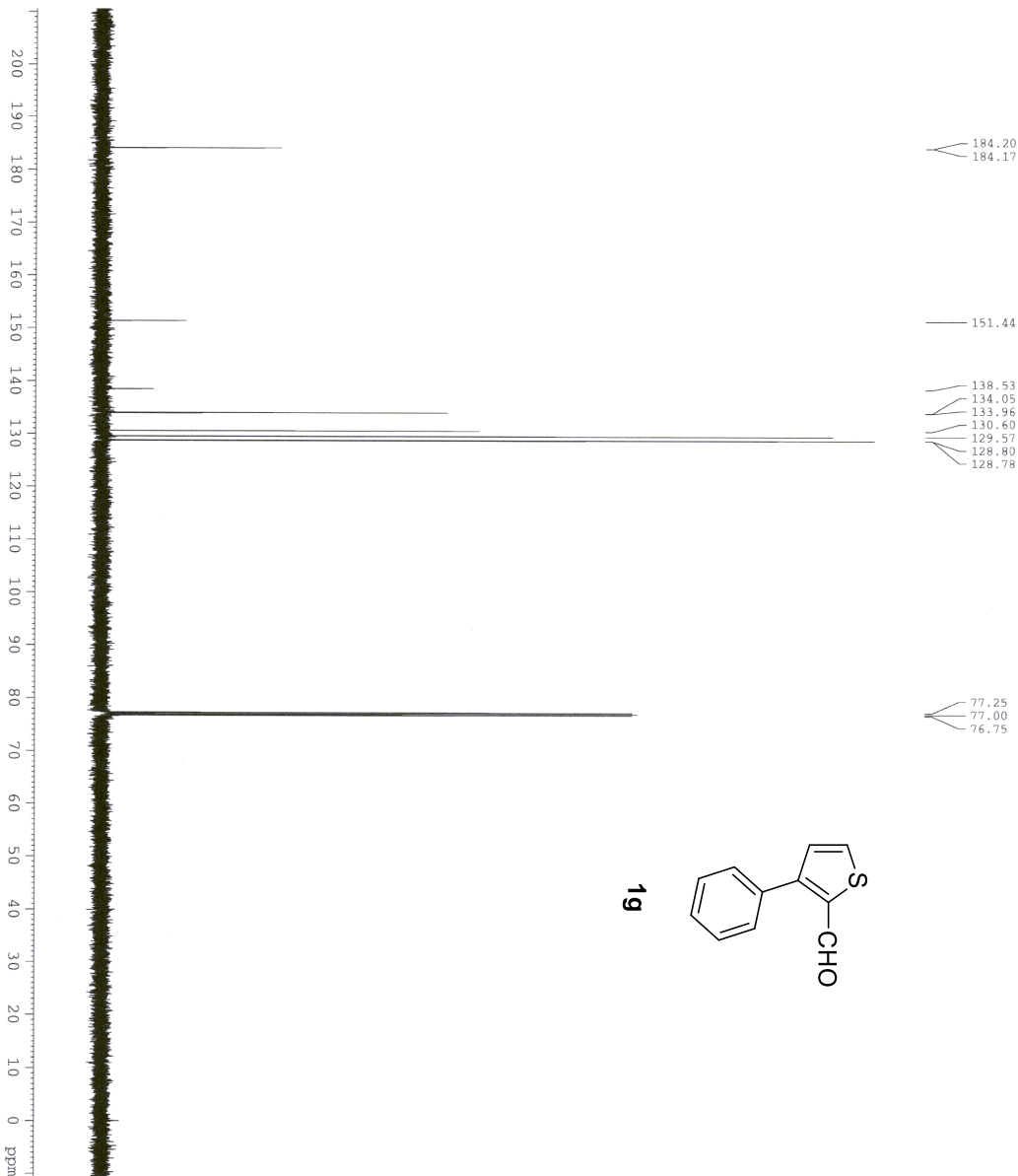
===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 3.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 3.00 dB
PL12 3.00 dB
P11 3.00 dB
SFO2 500.1320005 MHz

P1 - Acquisition parameters
ND0 1
TD 128
SFO1 500.132 MHz
FIDRES 7.81250447
SW 1.999 ppm
P1MODE QF

F2 - Processing parameters
SI 262.44
SF 125.7377949 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

P1 - Processing parameters
SI 1024
MC2 OF
SF 500.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1



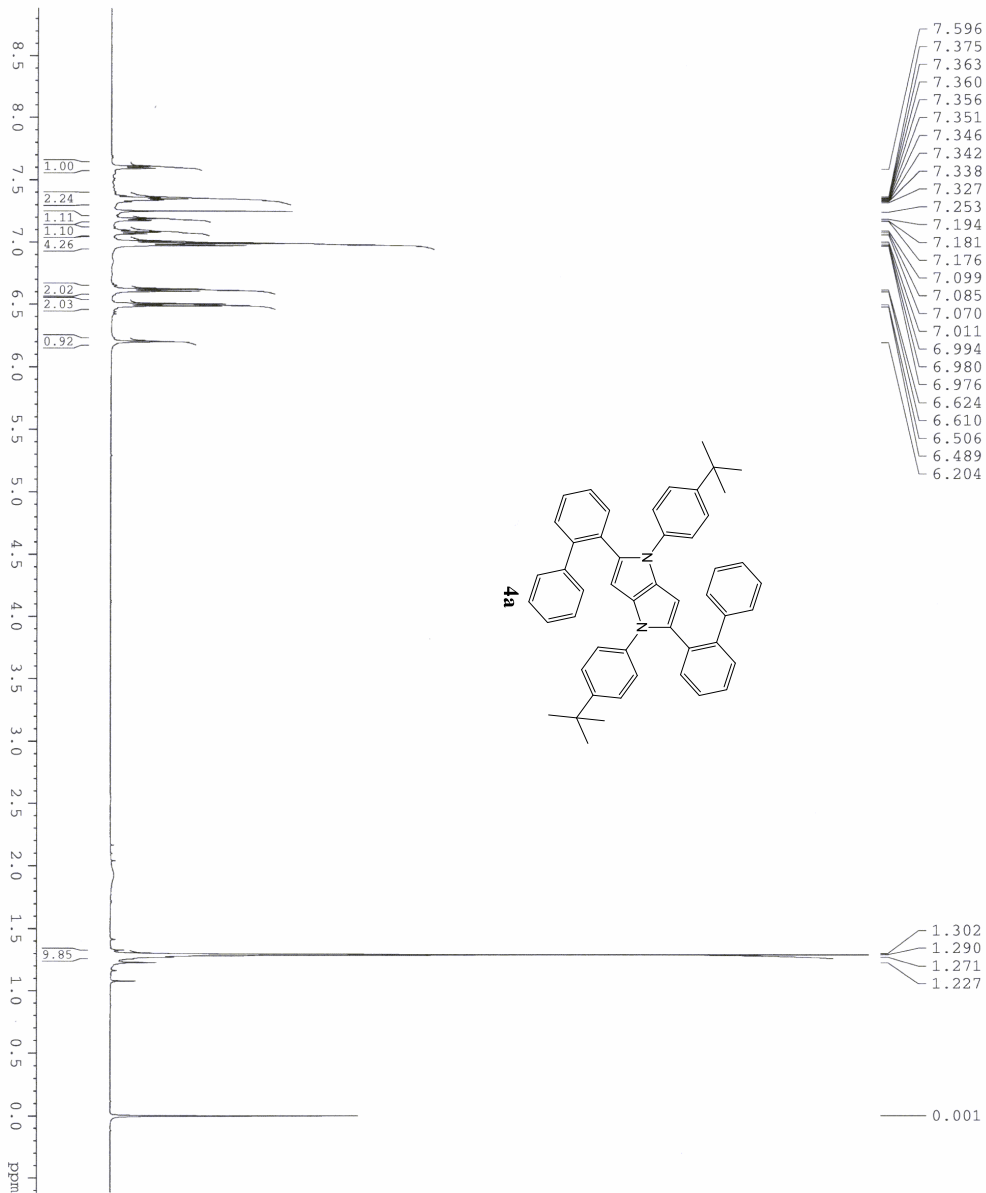


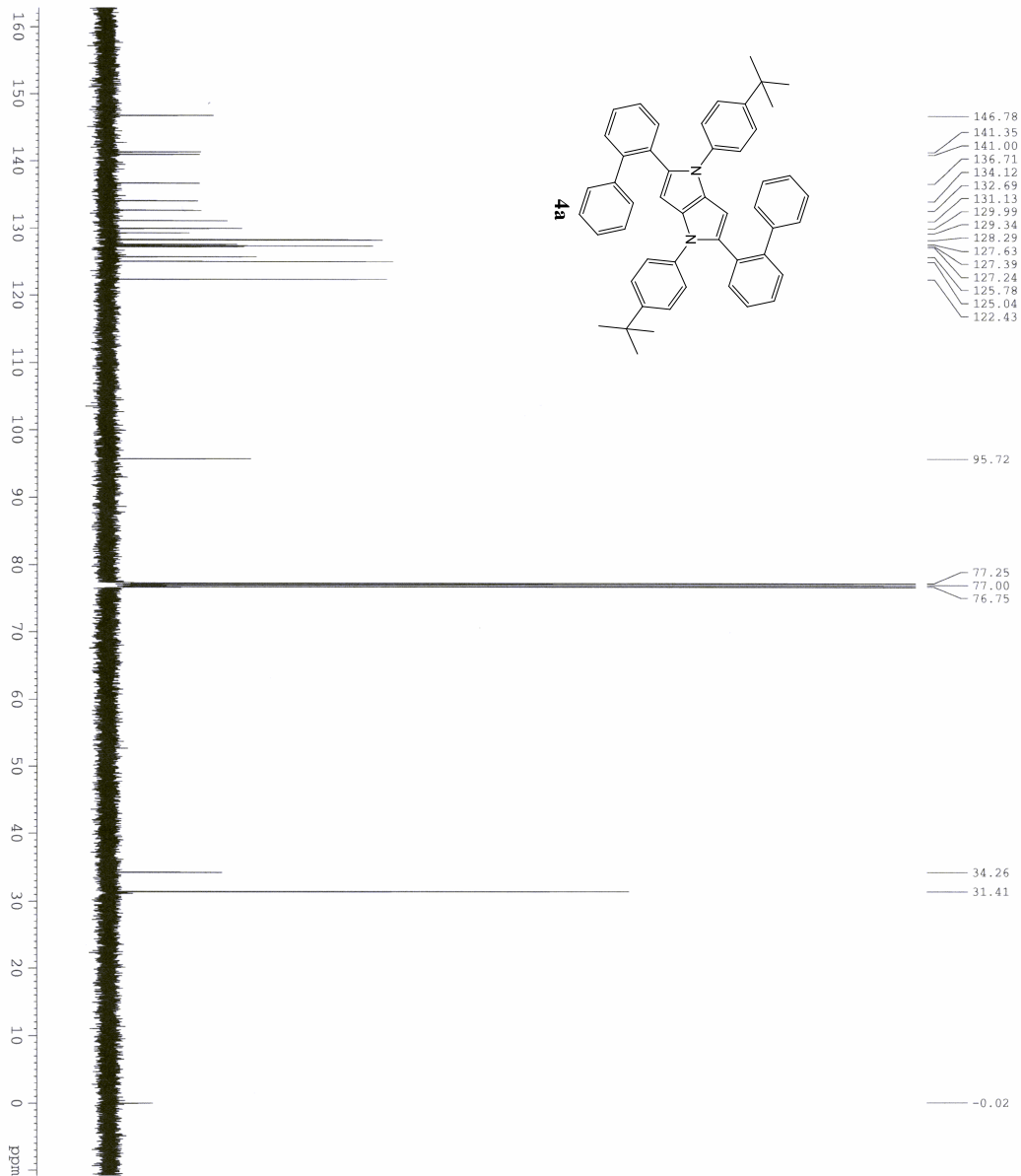
Current Data Parameters
NAME MK188
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140507
Time 13.06
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 287.4
DM 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300271 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00





Current Data Parameters
NAME MK188
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140507
Time 13:50
INSTRUM 13PRX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 2501
DS 4
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027508 sec
RG 32768
DW 15.300 usec
DE 1.100 usec
TE 303.15 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -3.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz

F1 - Acquisition Parameters
ND0 1
TD 128
SF01 500.132 MHz
FIDRES 7.812500 Hz
SFO1 1.999 ppm
P1MODE QF

F2 - Processing Parameters
SI 262144
SF 125.7577925 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

F1 - Processing Parameters
SI 1024
SF 500.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

7.623
7.621
7.607
7.605
7.460
7.458
7.255
7.178
7.163
7.148
7.064
7.048
7.033
6.843
6.826
6.619
6.604
6.434
6.418
6.199

2.540
2.525
2.510

1.595
1.352
1.323
1.312
0.919
0.907
0.893

0.000

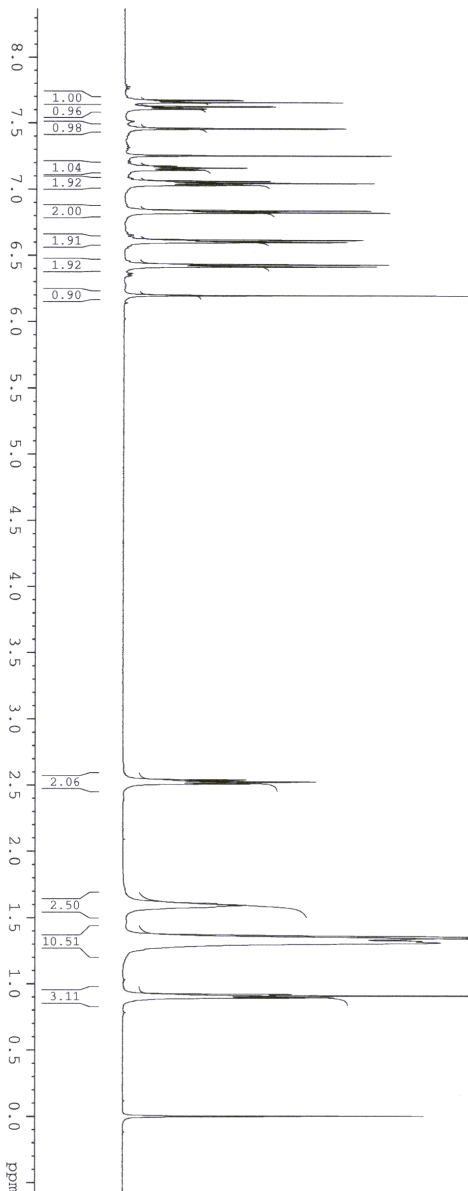
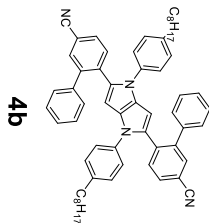


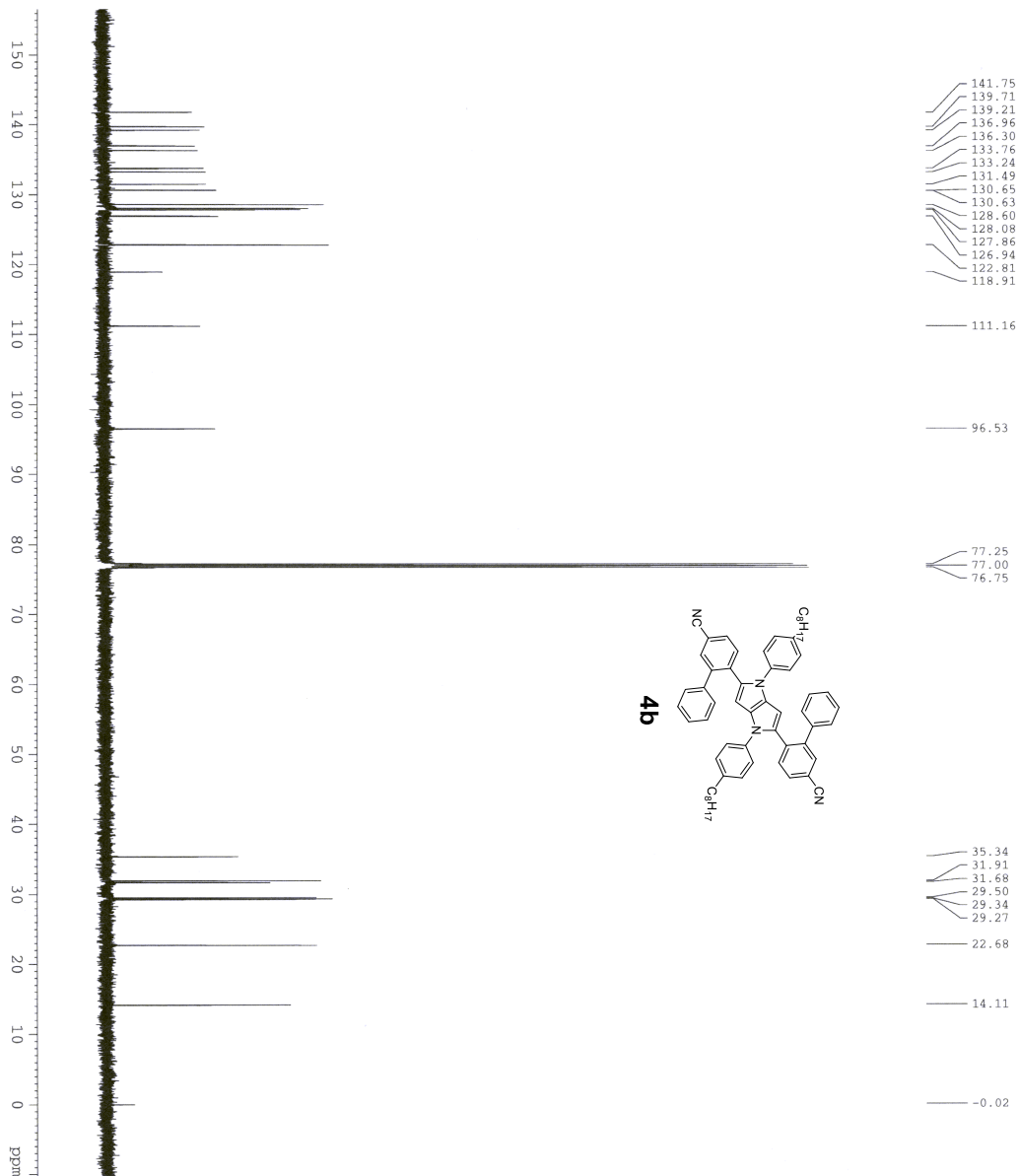
Current Data Parameters
NAME MK250
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140701
Time 15.38
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 32
DS
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 143.7
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
DI 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 2.50 usec
PL1 0.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300260 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME MK250
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110914
 Time_ 11:39
 INSTRUM 1 DRX
 PROBHD 5 mm TBI 1H/13
 PULPROG zgpg
 TD 65536
 FIDRES 0.49853 Hz
 AQ 1.0027508 sec
 RG 32768
 DW 15.300 usec
 DE 32.00 usec
 TE 303.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 DELTA 0.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -3.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CDEPRG2 waltz16
 NUC2 1H
 FCPD2 98.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 22.00 dB
 SFO2 500.1320005 MHz

F1 - Acquisition parameters
 ND0 1
 TD 128
 SF01 500.132 MHz
 FIDRES 7.812500 Hz
 SFO 500.1320005 MHz
 P1 1.392 sec
 P1MODE QF

F2 - Processing parameters
 SI 262144
 SF 125.777925 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 SF 500.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.30 Hz
 GB 0.1

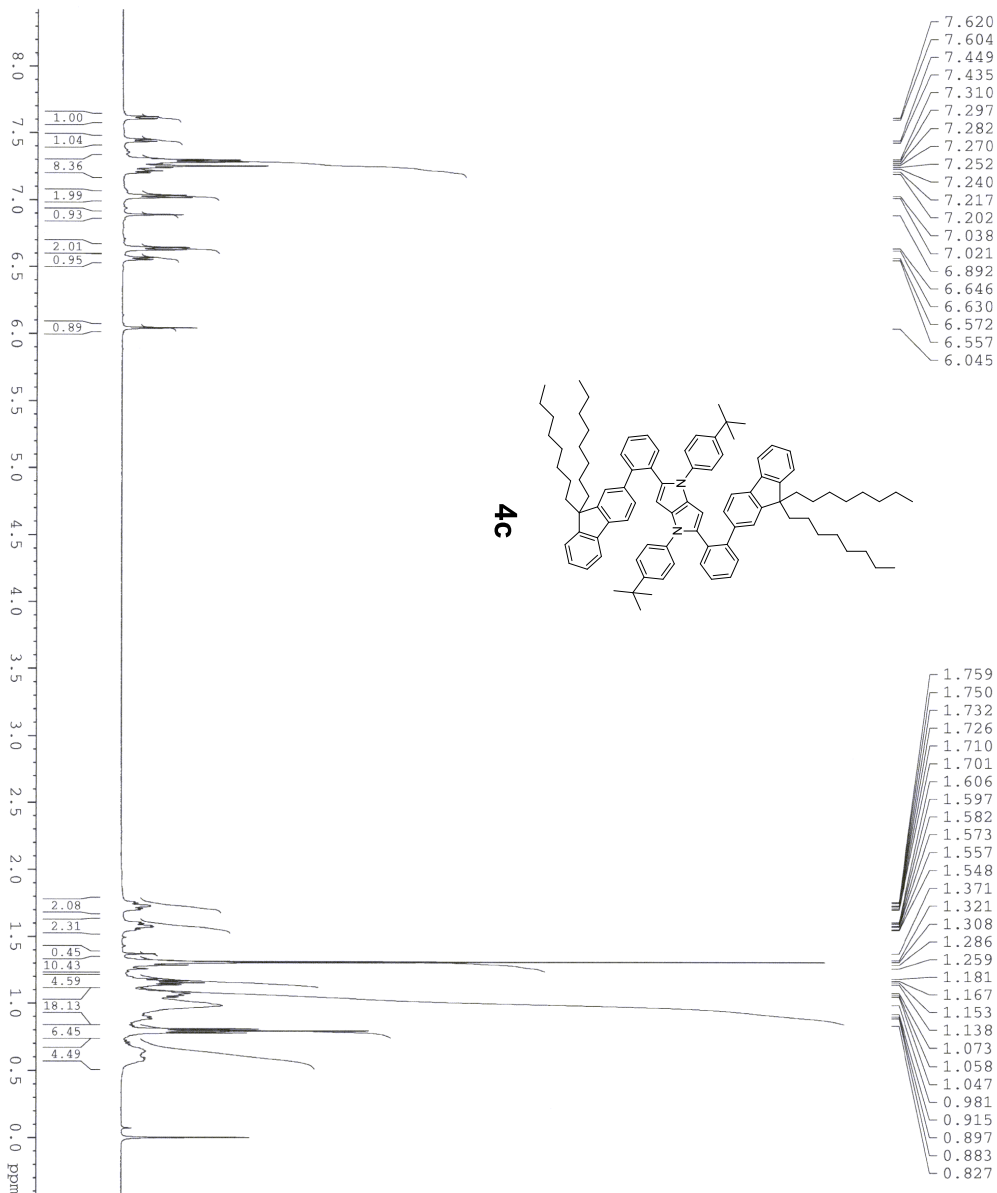


Current Data Parameters
NAME MK216
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140415
Time_ 10.41
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 128
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300278 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



151.08
150.33
146.96
141.67
141.00
140.72
138.62
137.40
134.08
132.42
131.91
130.59
129.96
127.42
127.13
126.71
126.57
126.45
125.23
123.27
123.16
123.03
119.39
118.84

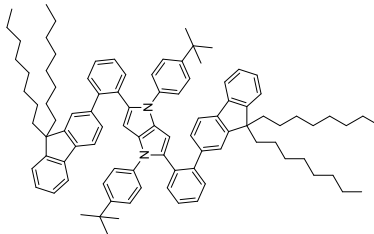
95.87

77.25
77.00
76.75

54.63

39.63
34.32
31.84
31.51
31.46
30.02
29.26
29.18
23.93
22.59

14.05



4c

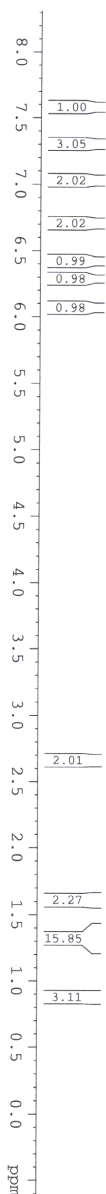
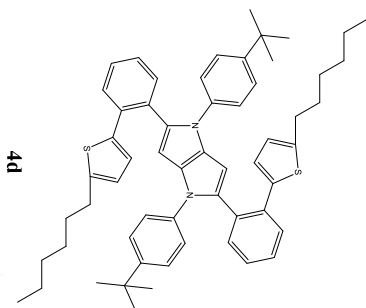
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



Current Data Parameters
NAME RK216
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140415
Time 11.19
INSTRUM 5 mm TBI 1H/13
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1800
DS 4
SWH 32679.738 Hz
FIDRES 0.495653 Hz
RG 1.002353 sec
RG 1.002353 sec
AQ 15.300 sec
DE 7.10 usec
TE 303.0 K
D1 1.0000000 sec
d11 0.1000000 sec
DELTA 0.8999999 sec
TDO 1
===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -10.00 dB
SFO1 125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 -10.00 dB
PL12 23.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz
F1 - Acquisition parameters
TDO 1
TDO 128
SFO1 500.132 MHz
FIDRES 7.812500 Hz
SW 1.999 ppm
PRMODE QF
F2 - Processing parameters
SI 262144
SF 125.7577924 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

7.311
7.305
7.303
7.299
7.296
7.289
7.285
7.282
7.276
7.272
7.270
7.249
7.036
7.032
7.019
6.712
6.695
6.423
6.416
6.286
6.071
6.063

2.680
2.664
2.649
1.639
1.625
1.610
1.595
1.579
1.381
1.368
1.353
1.341
1.318
1.311
1.305
1.298
1.290
1.268
0.890
0.885
0.876
0.862
0.000



Current Data Parameters
NAME MK193
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140317
Time 12.09
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 128
DW 48.400 usec
DE 6.778 usec
TE 303.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.20 usec
PL1 5.00 dB
SFO1 500.130885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300292 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
FC 1.00



146.95
145.95
140.44
136.61
135.14
133.97
132.33
131.63
129.49
129.28
127.73
126.92
124.99
124.96
123.73
122.64

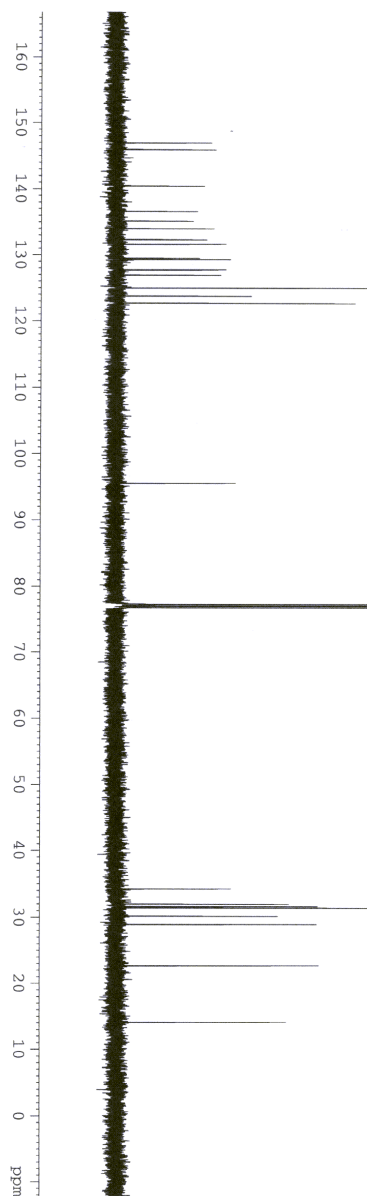
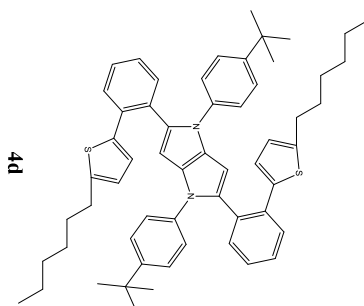
95.52

77.25
77.00
76.75

34.24
31.96
31.61
31.39
30.15
28.93

22.64

14.07



Current Data Parameters
NAME MKI193
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140317
Time 12.21

INSTRUM 5 mm TBI 1H/13
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536

SOLVENT CDCl3
NS 880
DS 4

SWH 32679.728 Hz
FIDRES 0.0002503 Hz
AQ 1.0027503 sec

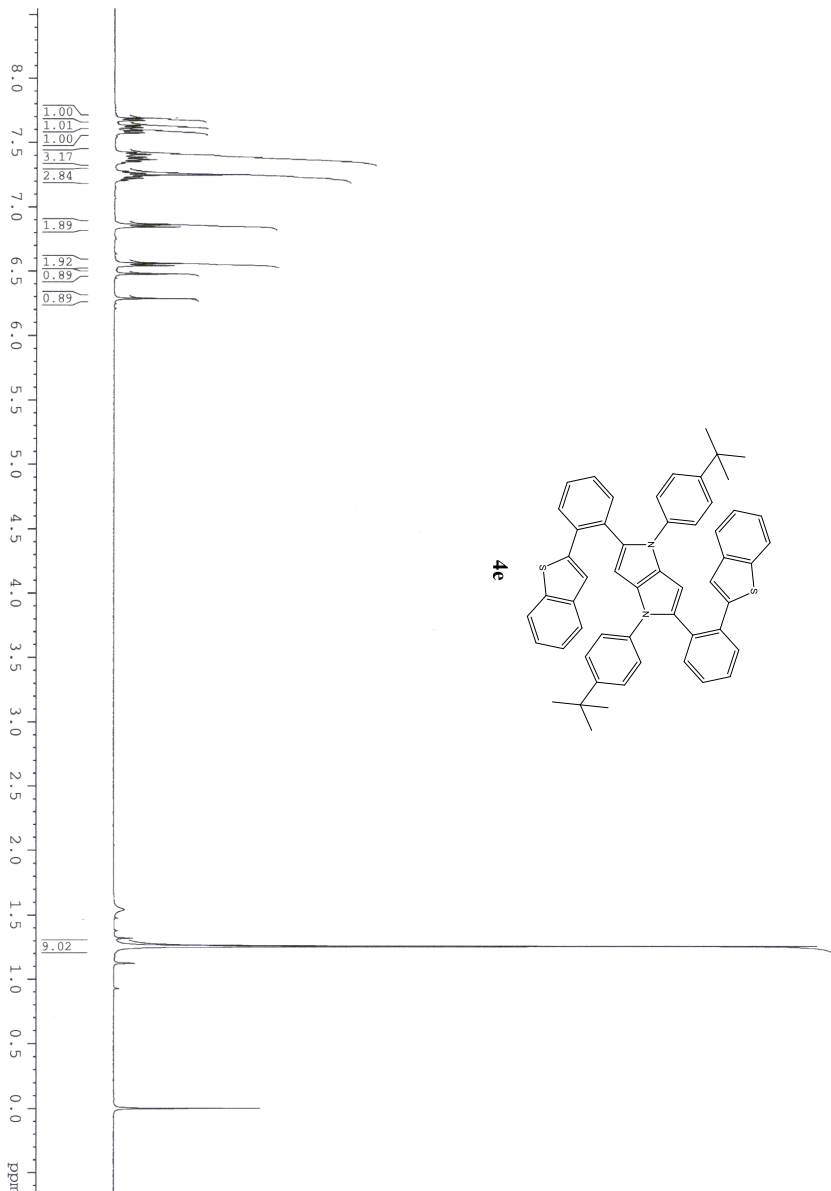
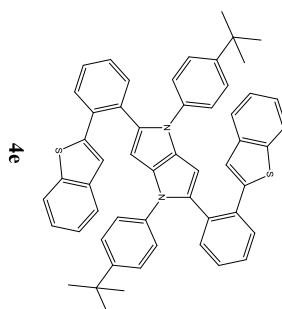
RG 32768
DW 15.300 usec
DE 7.10 usec

TE 303.0 K
D1 1.0000000 sec
d11 0.0000000 sec
DELTA 0.8939998 sec

TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -3.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 98.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz

F1 - Acquisition Parameters
NUC1 13C
TD 128
SFO1 500.132 MHz
FIDRES 7.812500 Hz
SW 1.999 ppm
F2 - Processing Parameters
SI 1024
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
F2 - Processing Parameters
SI 1024
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0.1



Current Data Parameters
NAME MK199-new
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140521
Time 10.29
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SRH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 267.4
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
DL 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300278 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

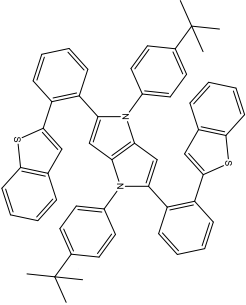


147.18
143.60
140.82
140.20
136.51
134.44
133.65
133.03
131.63
129.98
129.85
128.16
127.84
125.13
123.81
123.63
123.38
122.61
121.93
121.71

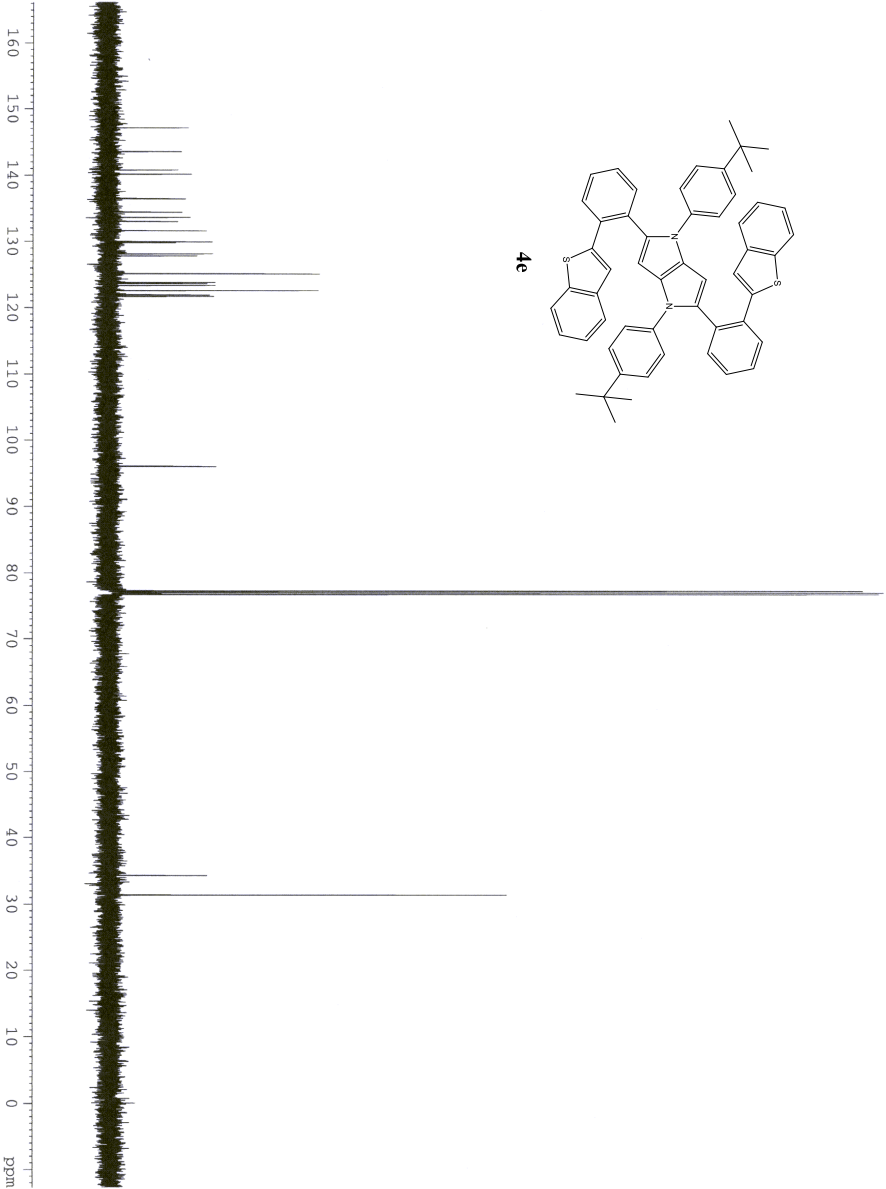
96.03

77.25
77.00
76.75

34.27
31.34



4e



Current Data Parameters
NAME RK19-new
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140521
Time 10.46
INSTRUM 5 mm TBI 1H/13
PROBHD 5mmBBO
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1020
DS 4
SWH 32679.738 Hz
FIDRES 0.149663142
AQ 1.0027508 sec
RG 32768
IW 15.300 usec
DE 7.10 usec
TE 303.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1

==== CHANNEL F1 =====
NUC1 13C
P1 5.00 usec
PL1 -3.00 dB
SFO1 125.7703643 MHz

==== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
P2 98.10 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz

F1 - Acquisition parameters
NUC1 13C
TD 128
SFO1 500.132 MHz
FIDRES 7.812500 Hz
SW 1.999 ppm
PULPROG QF

F2 - Processing parameters
SI 26214
SF 125.7577927 MHz
WDW EM
SSB 0
GB 0.50 Hz
PC 1.40

F1 - Processing parameters
SI 1024
MC2 500.1300000 MHz
WDW SINC
SSB 0
LB 0.30 Hz
GB 0.1



Current Data Parameters
NAME MK251
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

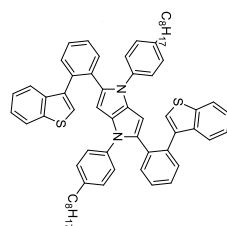
Date_ 20140702
Time 14.06
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

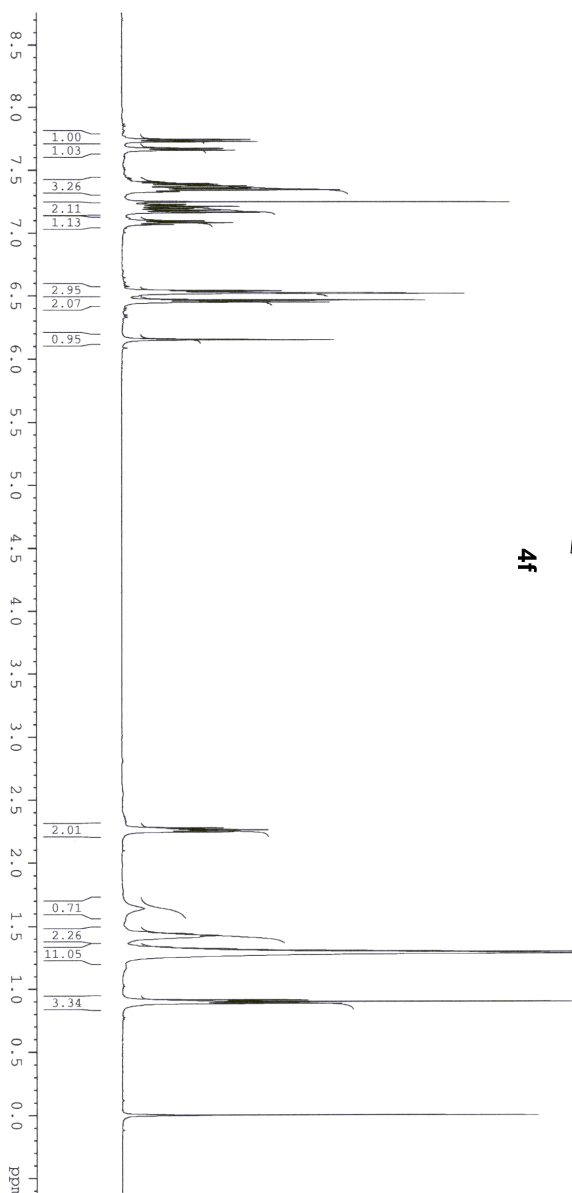
NUC1 1H
P1 2.50 usec
PL1 0.00 dB
SFO1 500.1330885 MHz

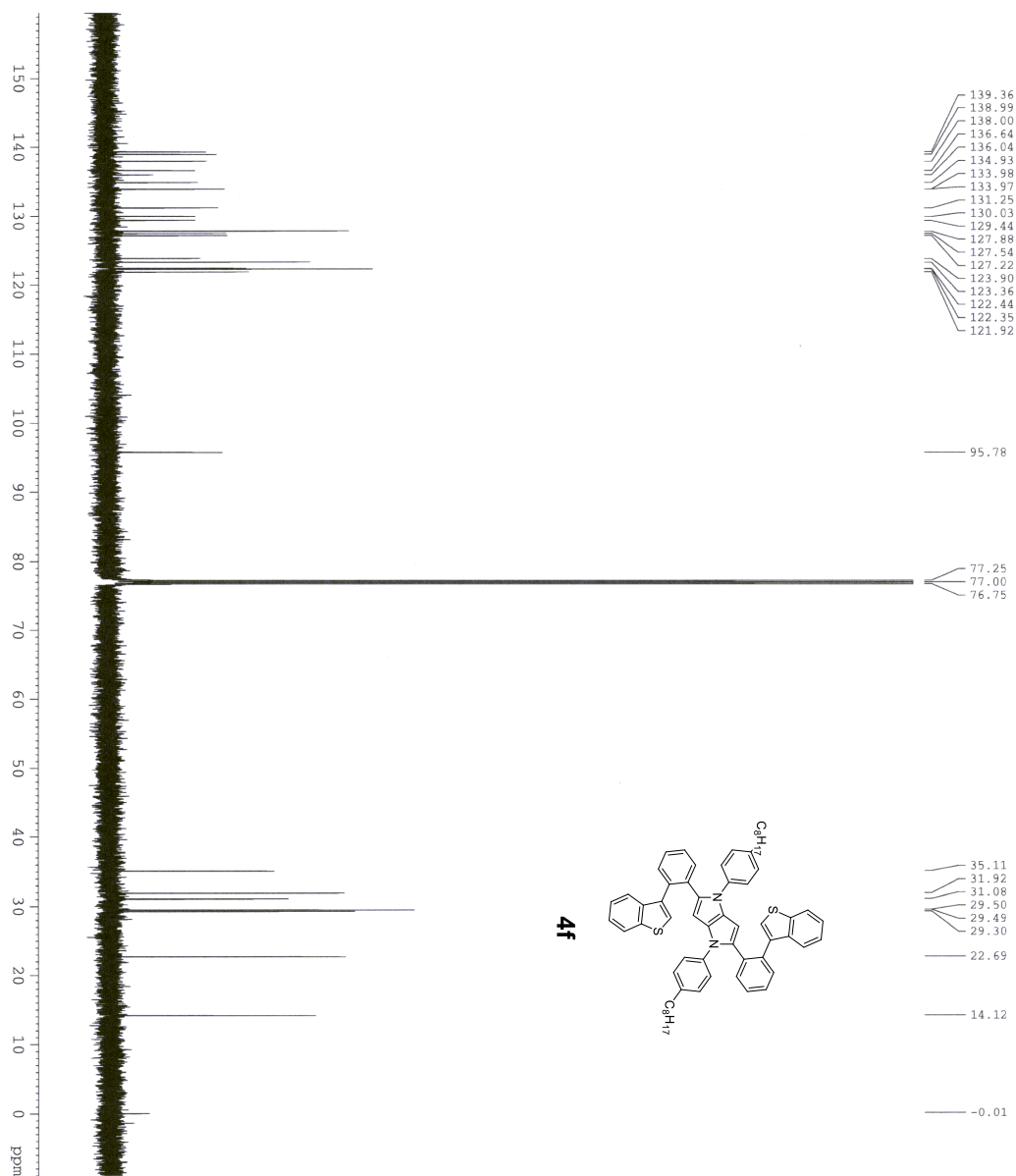
F2 - Processing parameters

SI 32768
SF 500.1300271 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



4f





Current Data Parameters
NAME HK351
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140702
Time 14.42
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2610
DS 4
SWH 32679.733 Hz
FIDRES 0.049653 Hz
AQ 1.0027508 sec
RG 32768
DE 15.300 usec
TE 303.0 K
TD0 1.0000000 sec
d11 0.0300000 sec
DELTA 0.8999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 100.00 usec
PL1 -3.00 dB
SFO1 125.7703643 MHz

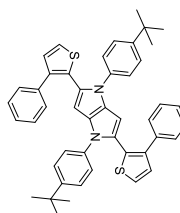
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 98.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz

F1 - Acquisition Parameters
NUC1 128
TD 65536
SFO1 500.132 MHz
FIDRES 7.812500 Hz
SW 1.999 ppm
FNUC1 0F

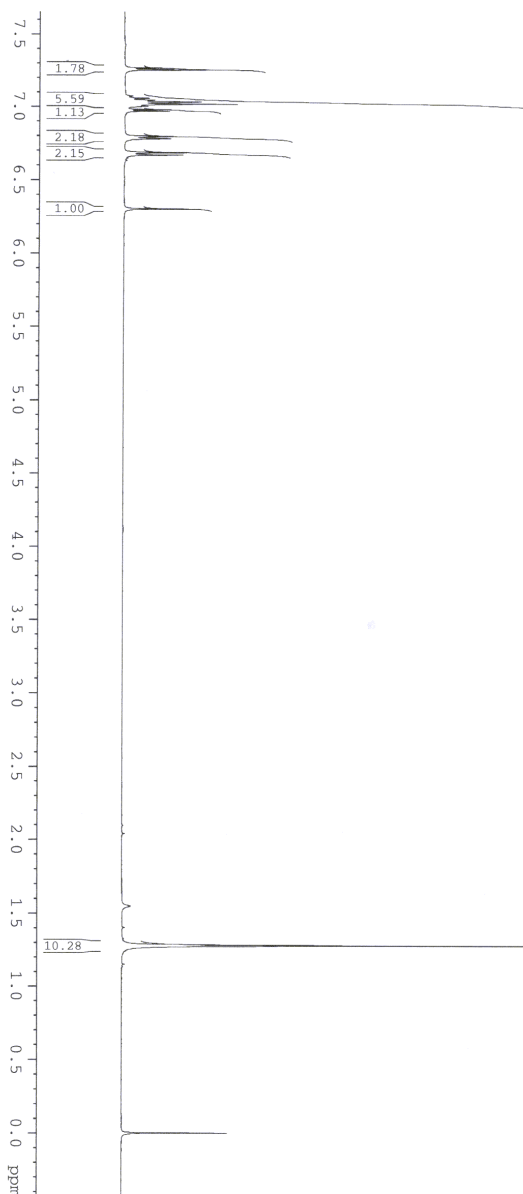
F2 - Processing Parameters
SI 262144
SF 125.7577924 MHz
WDW EM
SSB 0
GB 0.50 Hz
PC 1.40

F1 - Processing Parameters
SI 1024
SF 500.1300000 MHz
WDW EM
SSB 0
GB 0.1 Hz

7.043
7.040
7.033
7.016
7.005
7.002
6.999
6.978
6.967
6.794
6.780
6.777
6.685
6.682
6.668
6.303



4g



1.278
0.000

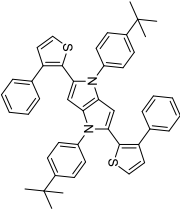
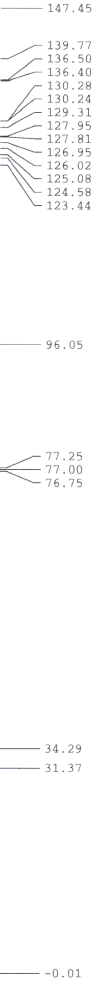


Current Data Parameters
NAME MK212
EXPNO 1
PROCNO 1

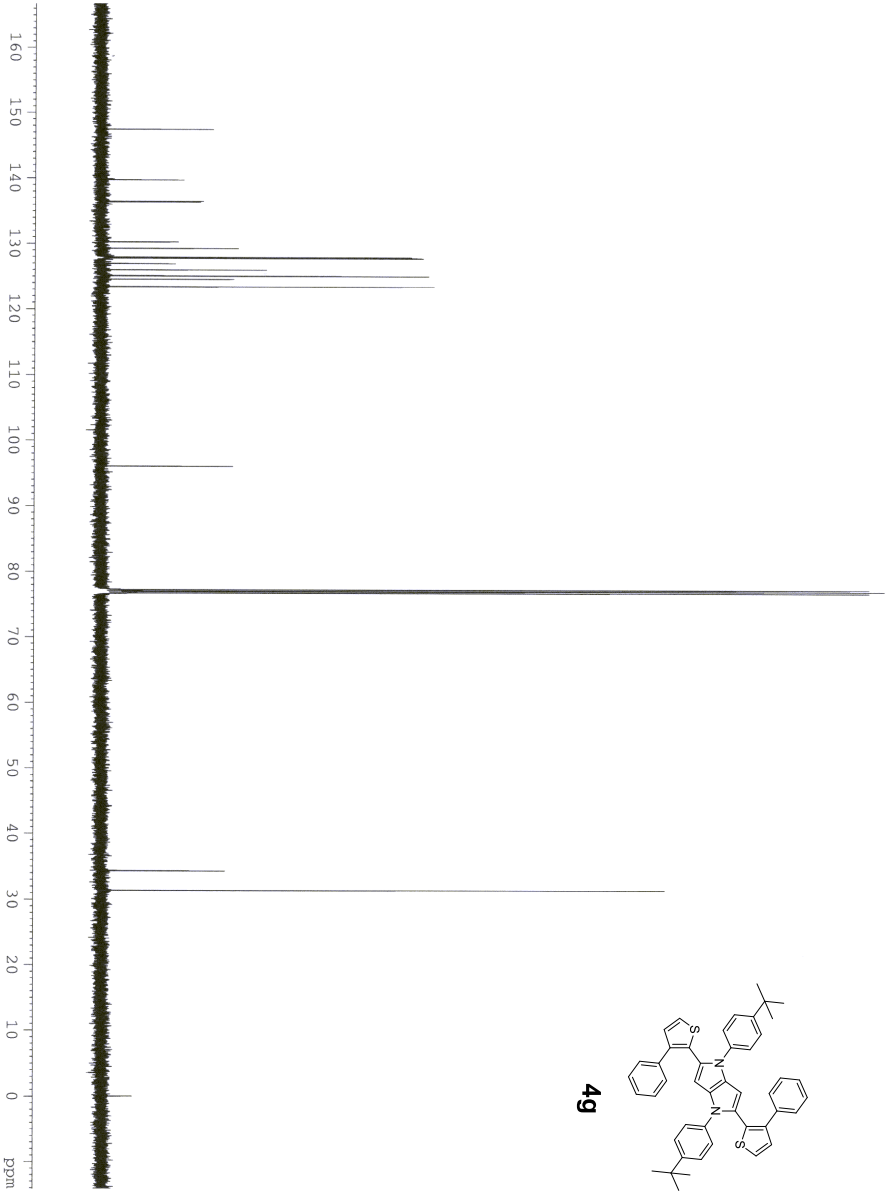
F2 - Acquisition Parameters
Date_ 20140508
Time 10.46
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 287.4
DM 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300278 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



4g



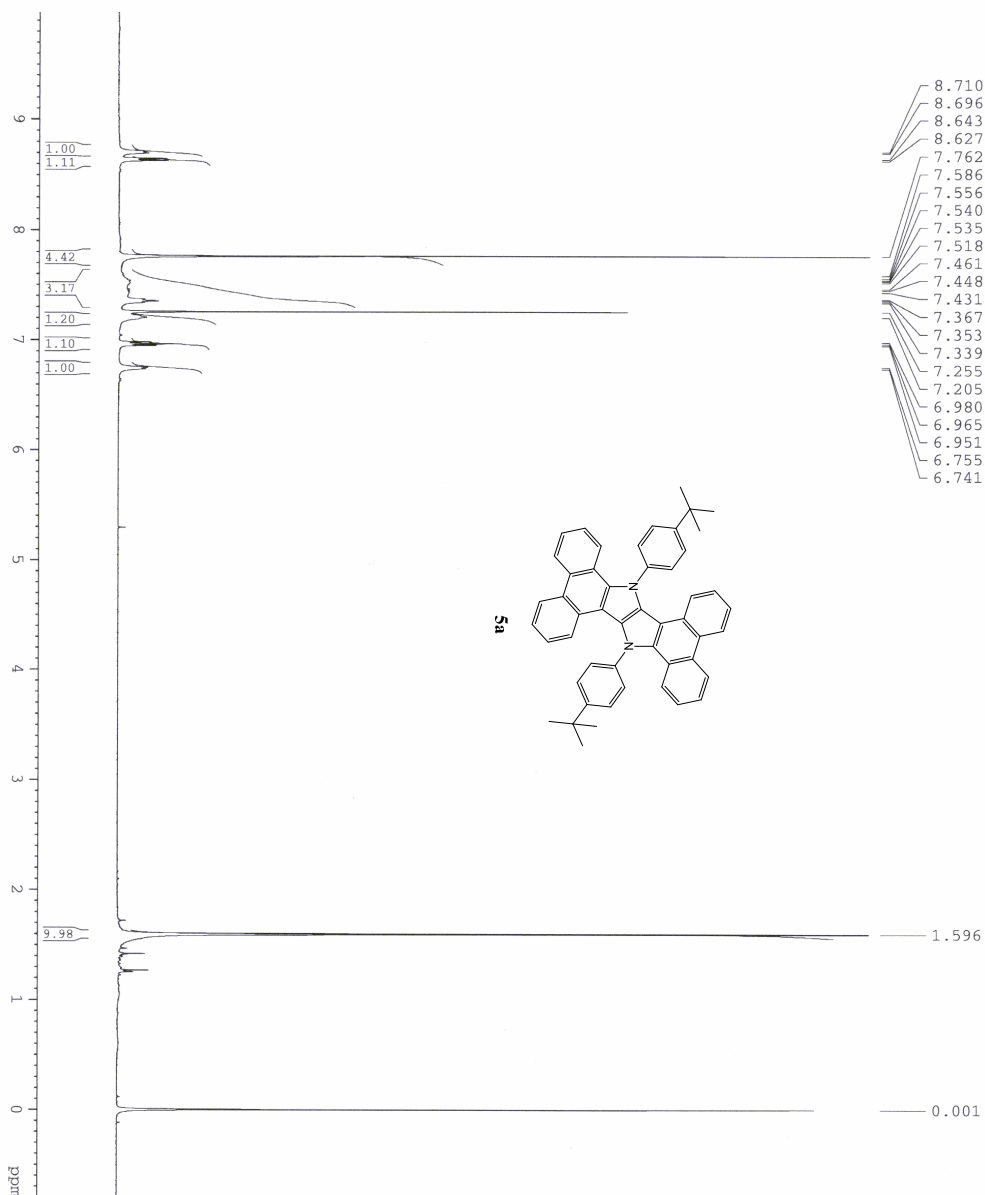
Current Data Parameters
NAME MK212
EXNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140508
Time 11.01
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
FIDRES 0.297
AQ 0.32768
SOLVENT CDCl3
NS 3225
DS 4
SWH 32679.738 Hz
FIDRES 0.45853 Hz
AQ 0.32768 sec
RG 327.68
DE 15.300 usec
TE 303.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.8593939 sec
TD 1
===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -3.00 dB
SFO1 125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 2.00 dB
PL12 2.00 dB
PL13 32.00 dB
SFO2 500.1320005 MHz
F1 - Acquisition parameters
ND0 132
SFO1 500.132 MHz
FIDRES 7.812500 Hz
SW 1.999 ppm
PRMODE QP
F2 - Processing parameters
SI 1024
MC2 500.1300000 MHz
SF 500.1300000 MHz
WDW SINE
SSB 0
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 500.1300000 MHz
SF 500.1300000 MHz
WDW SINE
SSB 0
GB 0.1



Current Data Parameters
NAME WK189-new
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140508
Time 15.15
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 512
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.130885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300265 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



F2 - Acquisition Parameters
Date 20140509

Time	9.07
TIME/DATE	2007

PROBHD 5 mm TBI 1H/13

202100	2929
TD	65536

COLENT	CDCT3
NS	31500

D3	4
SWH	32679.738 Hz

FIDRES	0.498653	Hz
AO	1.0027508	sec

RG	32768
DW	15 300 use

DE 7.10 use
TE 303 0 v

D1	1.000000000 sec
411	0.000000000

DELTA	0.899999998	sec

----- CHANNEL 11 -----	
NUC1	13C

F1	3.00	use
PL1	-3.00	dB

125.7703643 MHz

```
===== CHANNEL f2 =====
CPDPRG2      wa1fz16
```

NUC2	1H
PCPD2	98 00

PL2	3.00 dB
PL1	22.00 dB

PL13 32.00 dB

[illegible]

ND0 1

ID	128
SFO1	500.132 MHz

Field	Frequency (MHz)	Chemical Shift (ppm)
Field	7.812500	Hz
SW	1.999	ppm

FMODE	Q _F
1	0.0000
2	0.0000
3	0.0000
4	0.0000
5	0.0000
6	0.0000
7	0.0000
8	0.0000
9	0.0000
10	0.0000
11	0.0000
12	0.0000
13	0.0000
14	0.0000
15	0.0000
16	0.0000
17	0.0000
18	0.0000
19	0.0000
20	0.0000
21	0.0000
22	0.0000
23	0.0000
24	0.0000
25	0.0000
26	0.0000
27	0.0000
28	0.0000
29	0.0000
30	0.0000
31	0.0000
32	0.0000
33	0.0000
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35	0.0000
36	0.0000
37	0.0000
38	0.0000
39	0.0000
40	0.0000
41	0.0000
42	0.0000
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80	0.0000
81	0.0000
82	0.0000
83	0.0000
84	0.0000
85	0.0000
86	0.0000
87	0.0000
88	0.0000
89	0.0000
90	0.0000
91	0.0000
92	0.0000
93	0.0000
94	0.0000
95	0.0000
96	0.0000
97	0.0000
98	0.0000
99	0.0000
100	0.0000

F2 - Processing parameters
ST 262144

SE	125.7577929 MHz
WITH	TM

SSB 0

[illegible]

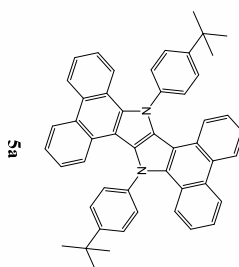
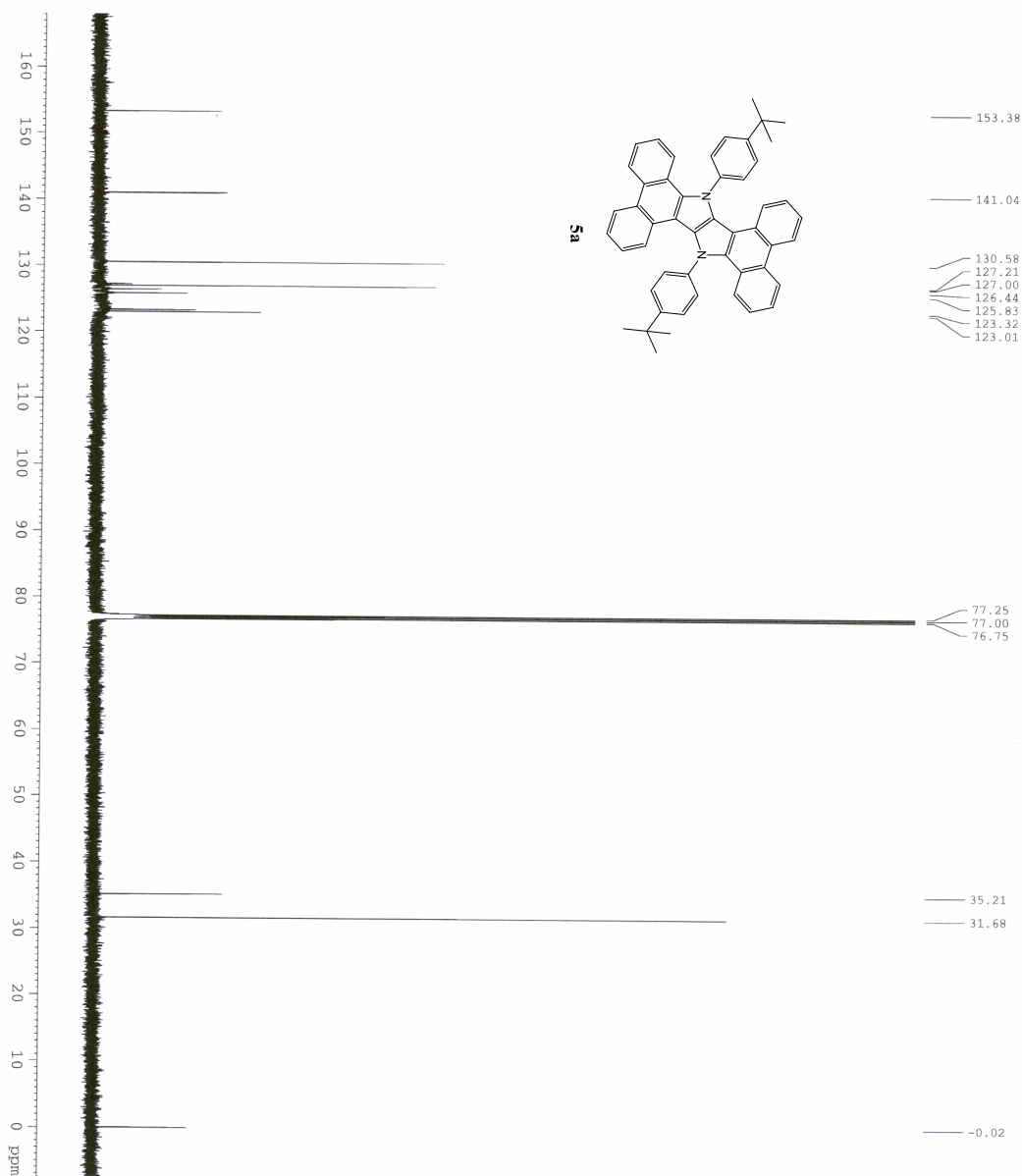
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Processing parameters

MCZ QF
SF 500.1300000 MHz

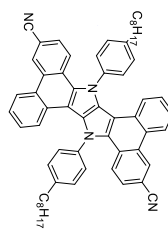
WDW	SINE
SSB	0

LB	0.30 Hz
GB	0.1

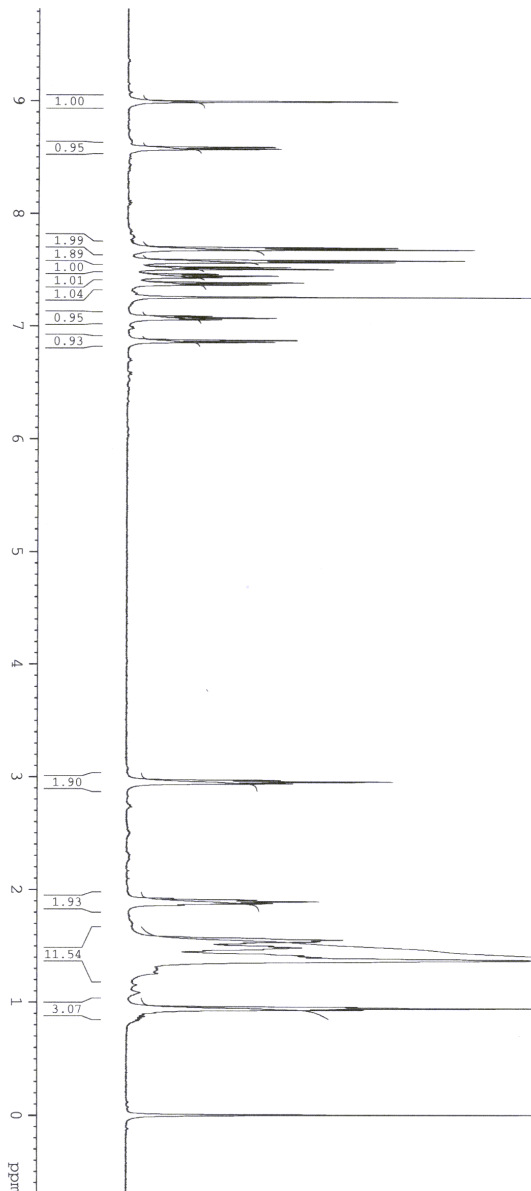


8.996
8.590
8.574
7.697
7.681
7.584
7.569
7.524
7.506
7.461
7.446
7.431
7.385
7.367
7.256
7.087
7.072
7.057
6.875
6.859

2.969
2.954
2.939
1.922
1.907
1.893
1.879
1.863
1.553
1.539
1.525
1.512
1.500
1.485
1.456
1.413
1.399
1.372
1.289
1.255
0.955
0.942
0.929
0.905
0.000



5b

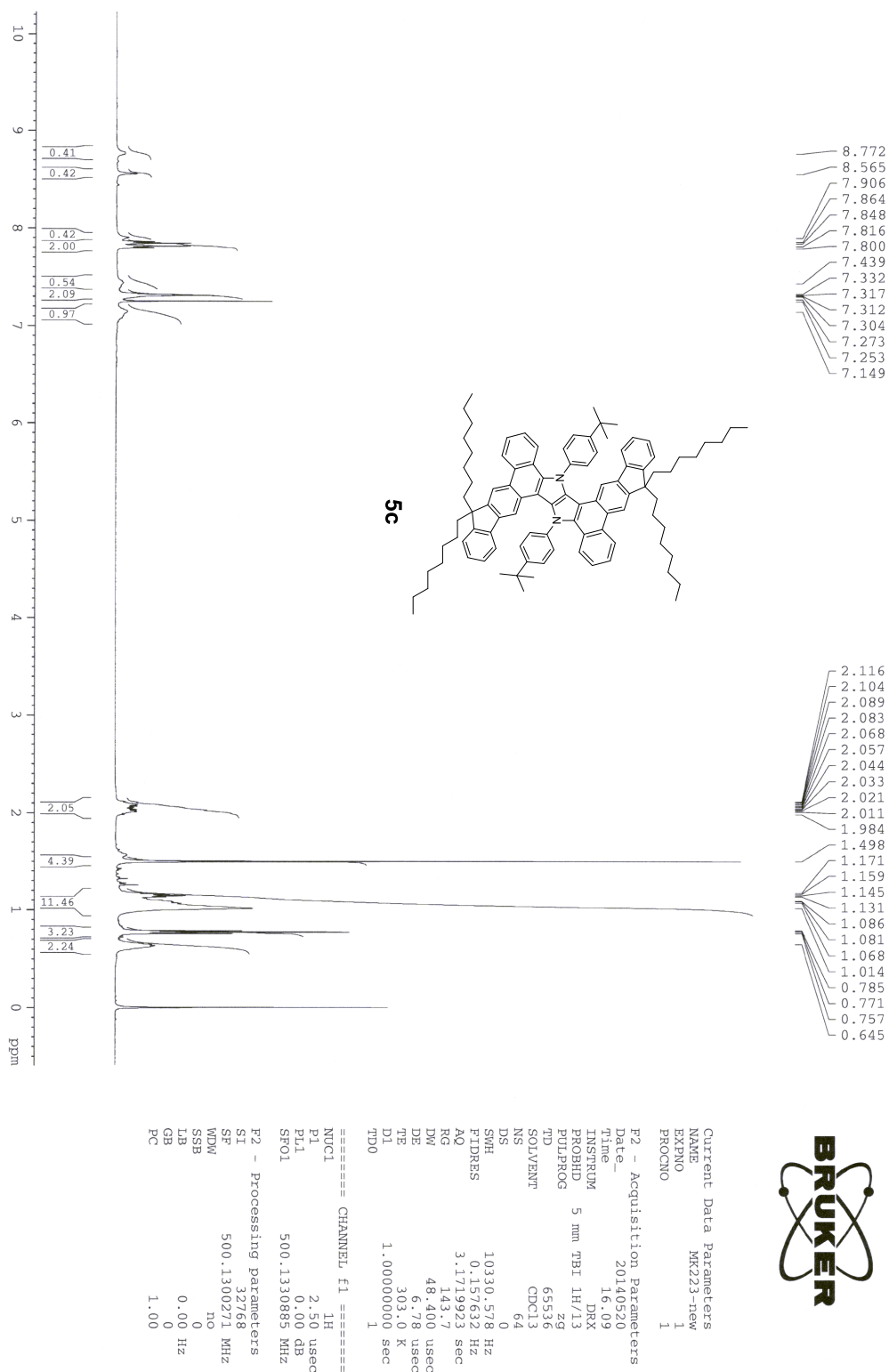


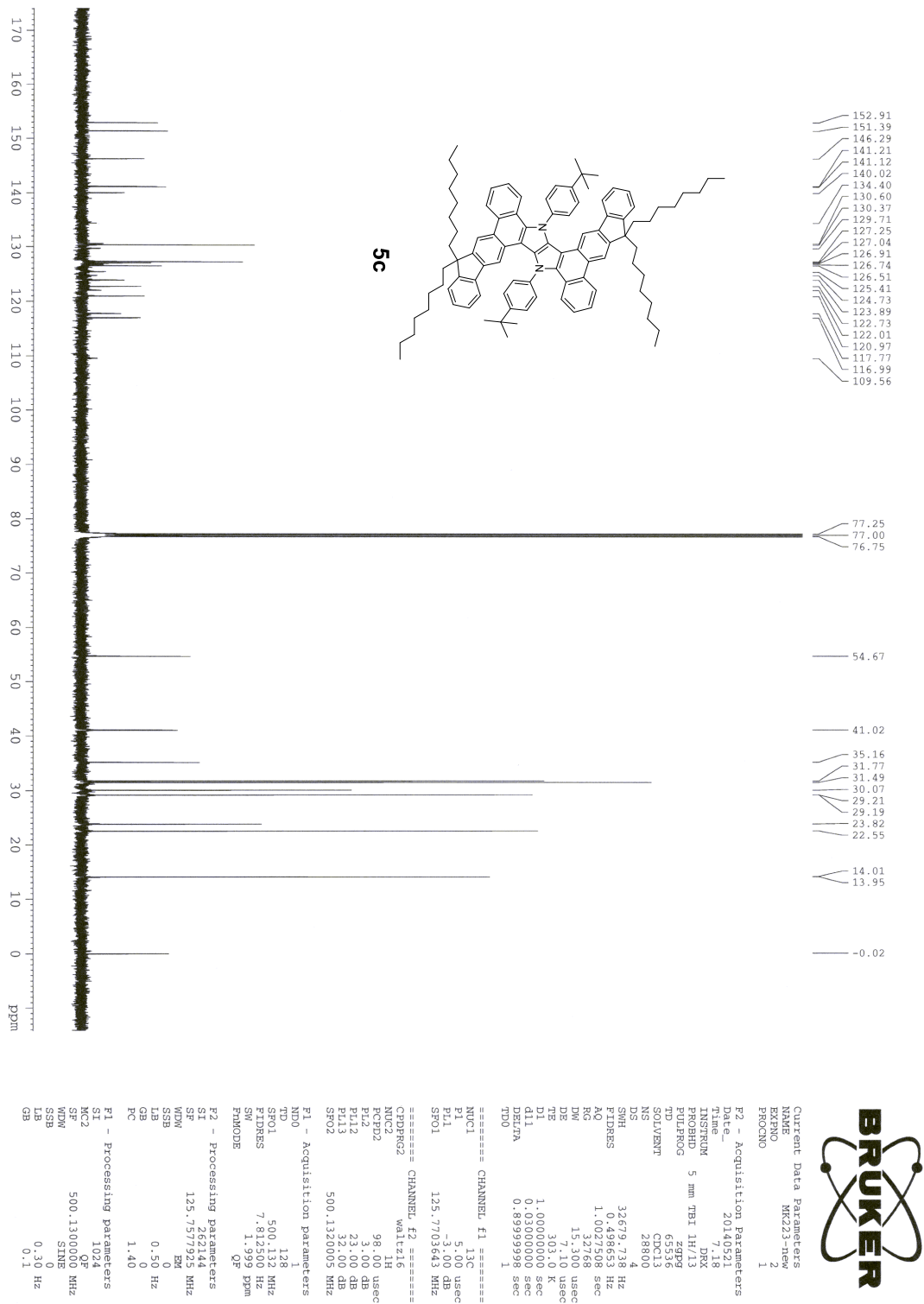
Current Data Parameters
NAME MK252
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140703
Time 14.41
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg
TD 65536
SOLVENT CDCl₃
NS 32
DS 0
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.173923 sec
RG 203.2
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹H
P1 2.50 usec
PL1 0.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300258 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00







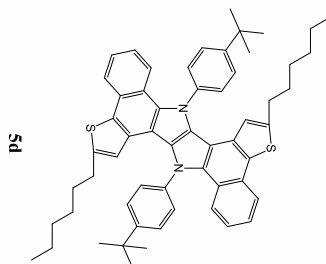
7.775
7.766
7.762
7.745
7.741
7.732
7.728
7.319
7.306
7.301
7.293
7.245
7.082
7.080
7.068
7.065
7.062
7.051
7.048

5.467

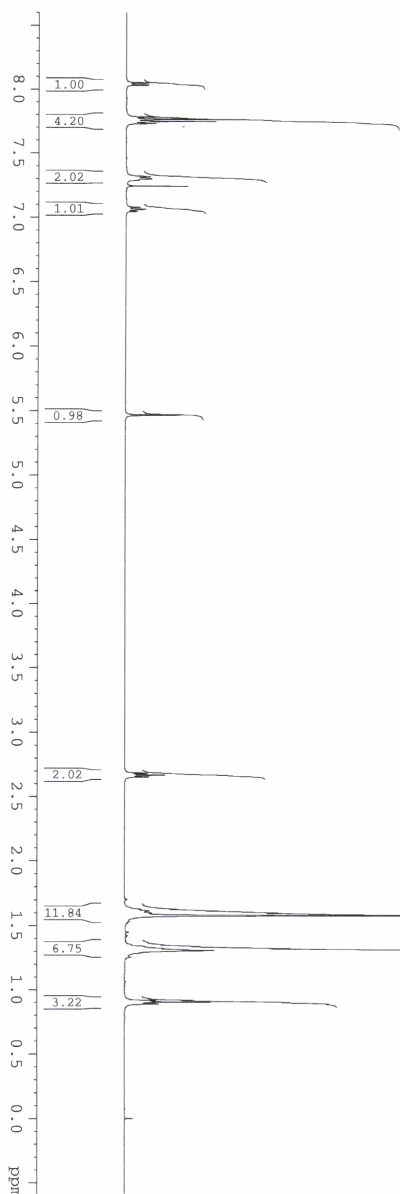
2.684
2.669
2.654

1.628
1.615
1.599
1.593
1.579
1.339
1.335
1.325
1.309
1.285
0.917
0.903
0.889

0.000



5d



Current Data Parameters
NAME MK194
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140317
Time 13.26
INSTRUM 13.DXX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 181
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
TD0 1.00000000 sec
1
===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.130885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300315 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters	
NAME	MK194
EXPNO	2
PROCNO	1

```
F2 - Acquisition Parameters
Date_      20140317
Time_      14 06
```

INSTRUM	DRX
PROBHD	5 mm TBI 1H/13
DIR DRG	

TD	65536
SOLVENT	CDCl ₃
MS	1000

DS	4
SMH	32679.738

1.0027508	AQ
32768	RG

DE	7.10
TE	303.0

DI	1.000000000
d11	0.030000000
DELTA	0.899999998

```
===== CHANNEL f1 =====
```

NUCL	1.30
P1	5.00
PL1	-3.00

```
===== CHANNEL F2 =====
```

CPDPRG2	waltz16
NUC2	1H
PCPD2	98.00

PL2	3.00
PL12	23.00
PL13	32.00

```
SFO2      500.1320005
EI - Acqisition paramete
```

ND0	1
TD	128
SEQ1	500 132

FIDRES	7.812500
SM	1.999
EQMODE	OFF

F2 - Processing parameter
ST 363144

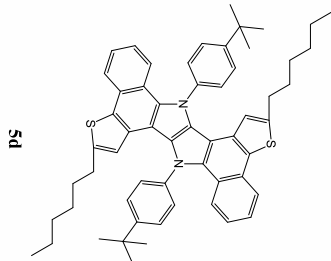
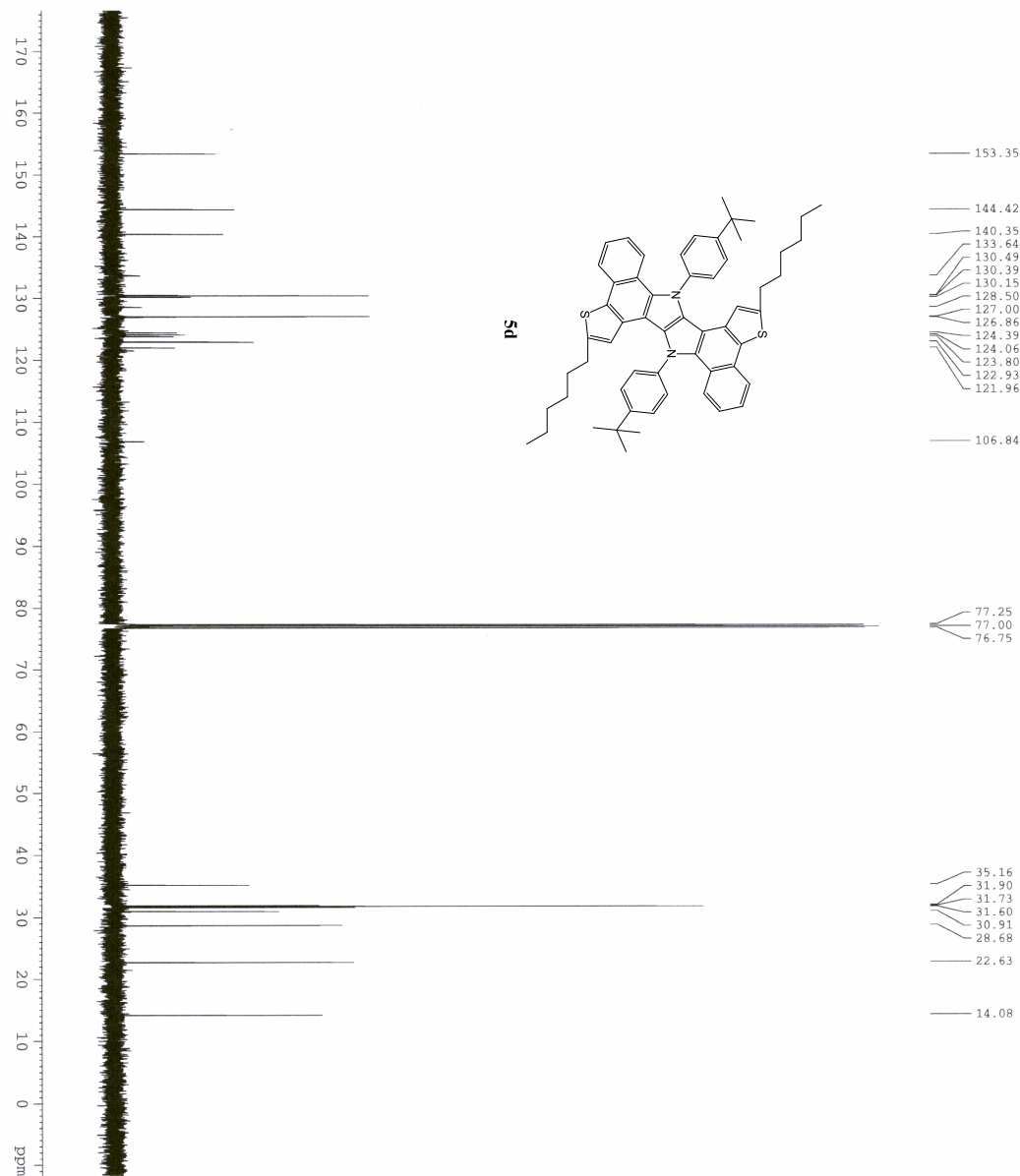
SE 125.7577935
WDW EM
CCP 0

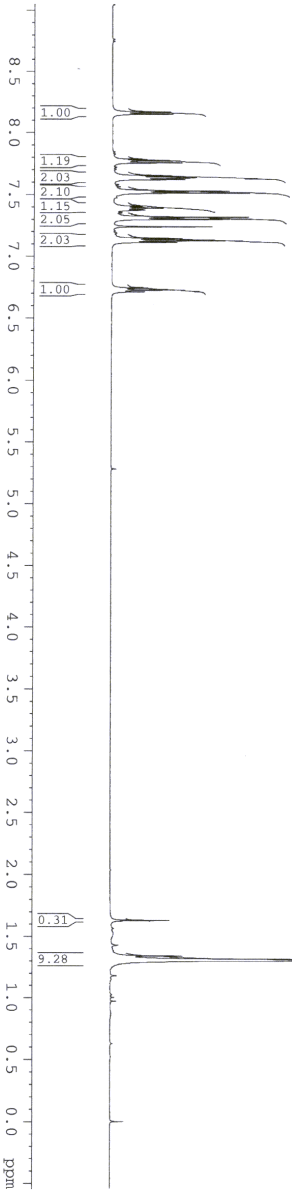
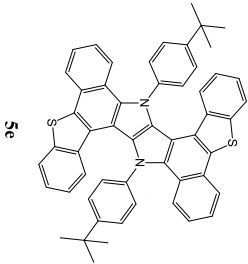
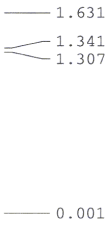
	LB	GB
0.50		
0		

F1 - Processing parameter

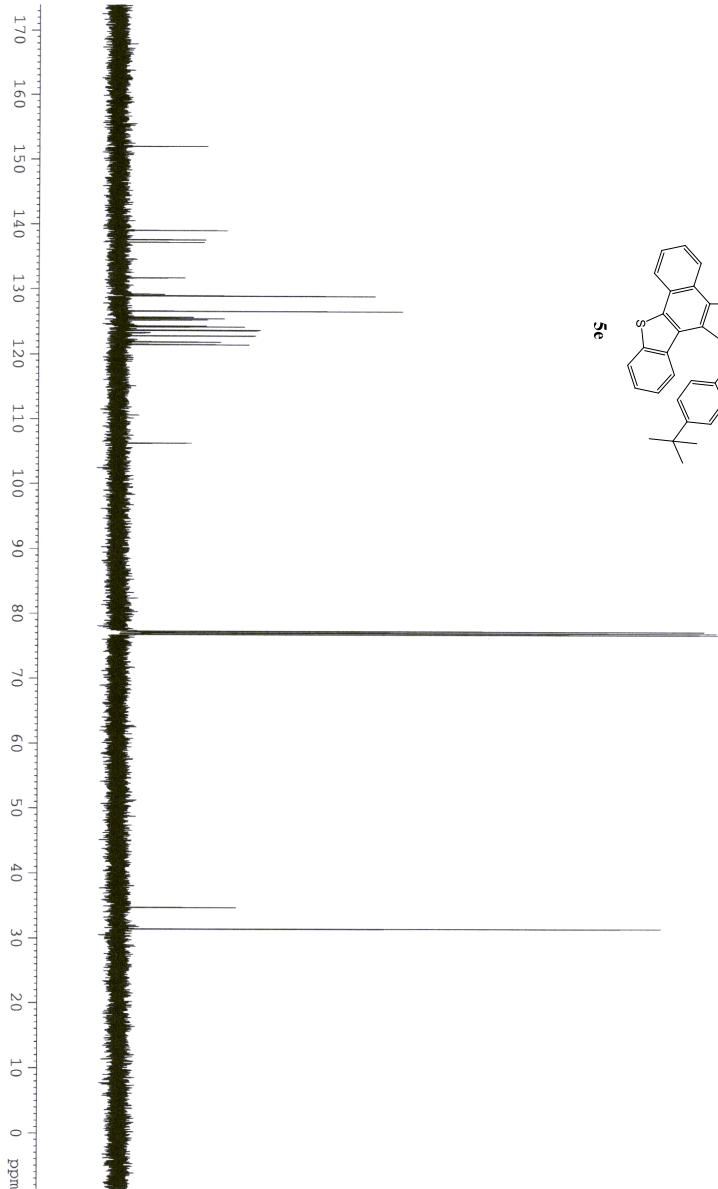
MC2	500.1300000
SE	

Item	Quantity	Unit Price	Total
SSB	0	0.30	0.00
LB	0.30	0.00	0.00





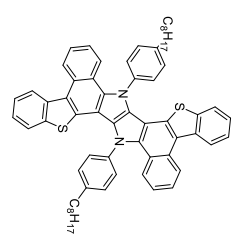
Current Data Parameters
NAME MK200
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140317
Time 12.47
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 181
RW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300318 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



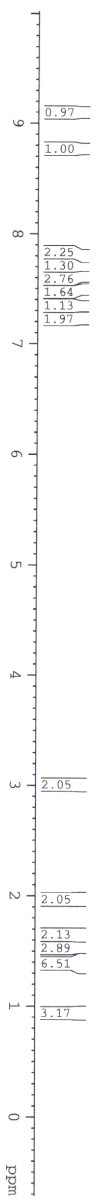
Current Data Parameters
 NAME: 20140317
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20140317
 Time: 13.06
 INSTRUM: spect
 PROBD: 5 mm TBI 1H/13
 PULPROG: zgpg
 TD: 65536
 SOLVENT: CDCl3
 NS: 900
 DS: 4
 SWH: 32679.738 Hz
 FIDRES: 0.498653 Hz
 AQ: 1.0027508 sec
 RG: 32768
 DW: 15.300 usec
 DE: 7.10 usec
 TE: 300.2 K
 D1: 1.0000000 sec
 d11: 0.0300000 sec
 DELTA: 0.8999998 sec
 TD0: 1
 ===== CHANNEL f1 =====
 NUC1: 13C
 P1: 120 usec
 PL1: -3.00 dB
 SFO1: 125.7703643 MHz
 ===== CHANNEL f2 =====
 CDPORG: waltz16
 NUC2: 1H
 P2: 98.00 usec
 PL2: 3.00 dB
 PL12: 23.00 dB
 PL13: 32.00 dB
 SFO2: 500.1320005 MHz
 F1 - Acquisition Parameters
 NUC: 13C
 TD: 128
 SFO1: 500.132 MHz
 FIDRES: 7.812500 Hz
 SW: 1.999 ppm
 FWHMDE: 0P
 F2 - Processing parameters
 SI: 262144
 SF: 125.7577941 MHz
 WDW: EM
 SSB: 0
 LB: 0.50 Hz
 GB: 0
 PC: 1.40
 F1 - Processing parameters
 SI: 1024
 SF: 500.1300000 MHz
 WDW: SDRB
 SSB: 0
 LB: 0.30 Hz
 GB: 0.1

9.102
9.086
8.776
8.759
7.806
7.790
7.700
7.684
7.651
7.616
7.600
7.514
7.499
7.484
7.351
7.337
7.322
7.250
7.234

3.019
3.004
2.989
2.039
2.001
1.986
1.971
1.956
1.941
1.660
1.646
1.631
1.615
1.601
1.559
1.546
1.540
1.530
1.514
1.501
1.448
1.437
1.427
1.410
1.382
1.376
1.368
0.948
0.935



5f

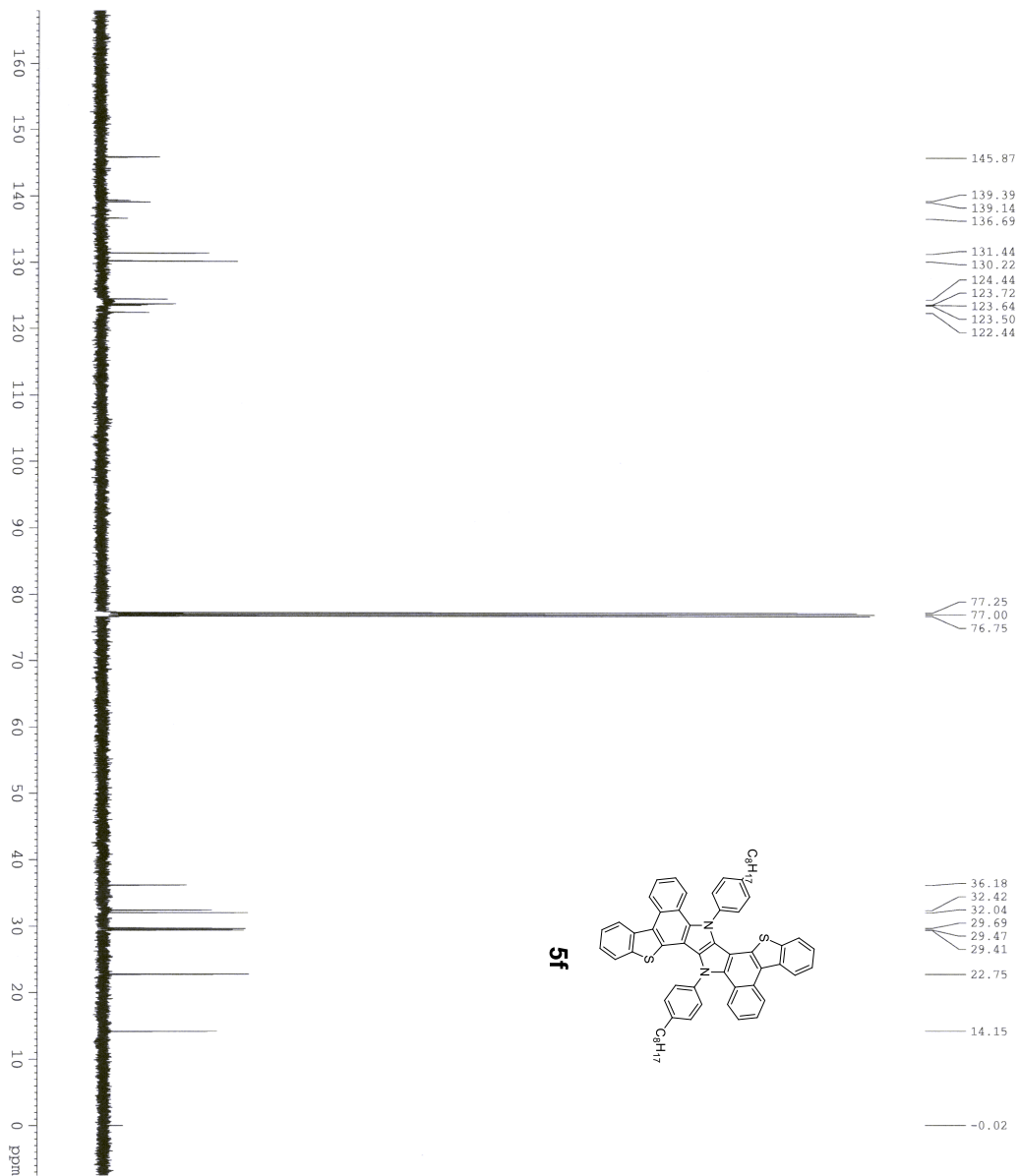


Current Data Parameters
NAME MK253
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140704
Time 10.33
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 181
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 2.50 usec
PL1 0.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300284 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME: 5f
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20140704
Time: 10.49
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zgpg3
TD: 65536
SOLVENT: CDCl3
NS: 4502
DS: 4
SWH: 32679.738 Hz
FIDRES: 0.498653 Hz
AQ: 1.0027508 sec
RG: 32768
DW: 15.300 usec
DE: 7.110 usec
TE: 300.2 K
D1: 1.00000000 sec
d11: 0.03000000 sec
DELTA: 0.89999998 sec
TD0: 1

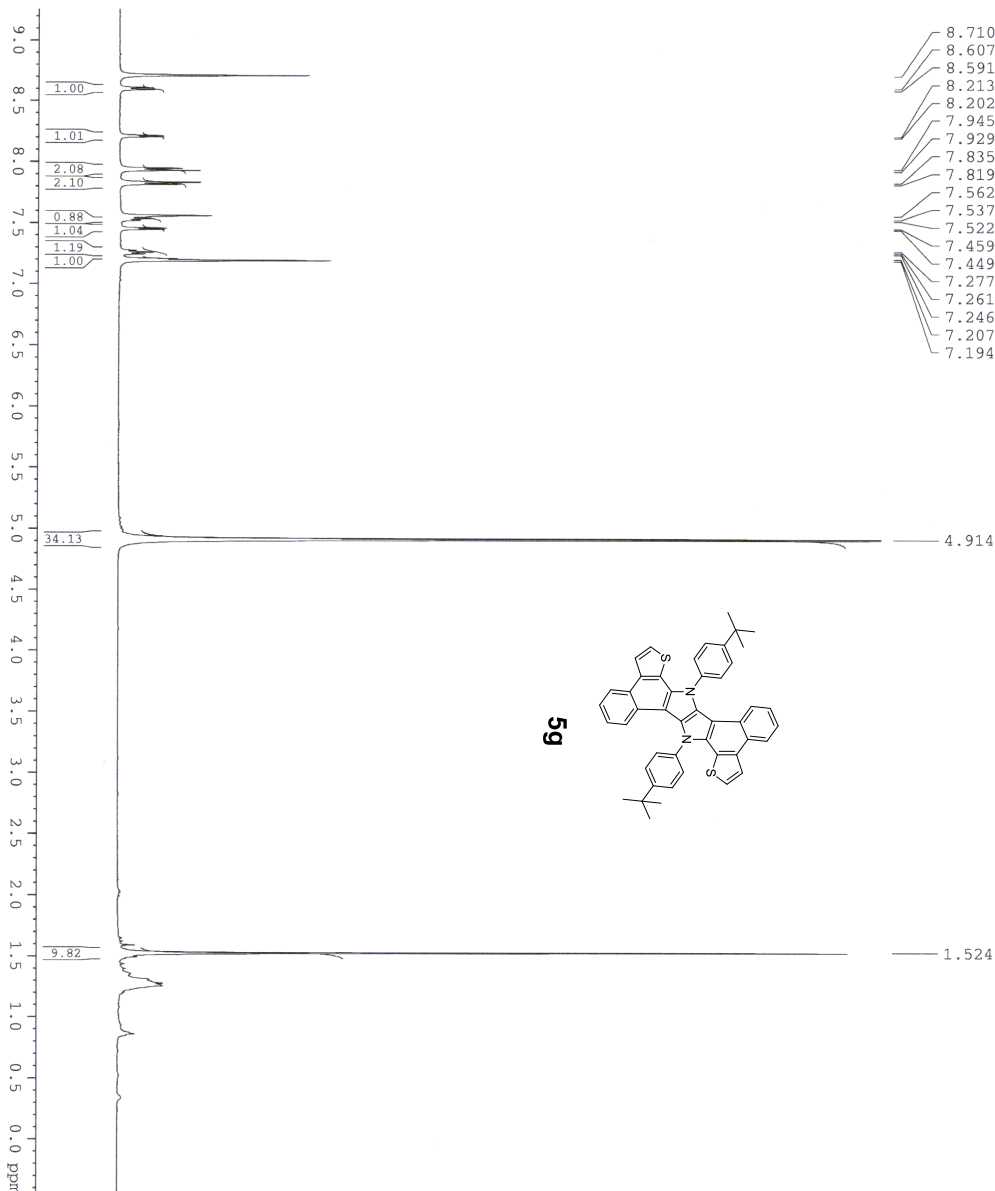
===== CHANNEL f1 =====
NUC1: 13C
P1: 5.00 usec
PL1: -3.00 dB
SFO1: 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
P2: 98.00 usec
PL2: 3.00 dB
PL12: 23.00 dB
PL13: 32.00 dB
SFO2: 500.1320005 MHz
F1 - Acquisition parameters
NUC0: 1
TD: 128
SFO1: 500.132 MHz
FIDRES: 7.812500 Hz
SW: 1.999 ppm
FNUC0: QP

F2 - Processing parameters
SI: 262144
SF: 125.7577929 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.40

F1 - Processing parameters
SI: 1024
RC2: QF
SF: 500.1300000 MHz
WDW: SINE
SSB: 0
LB: 0.30 Hz
GB: 0.1

Pomiar w temp. pokojowej (303 K)



```

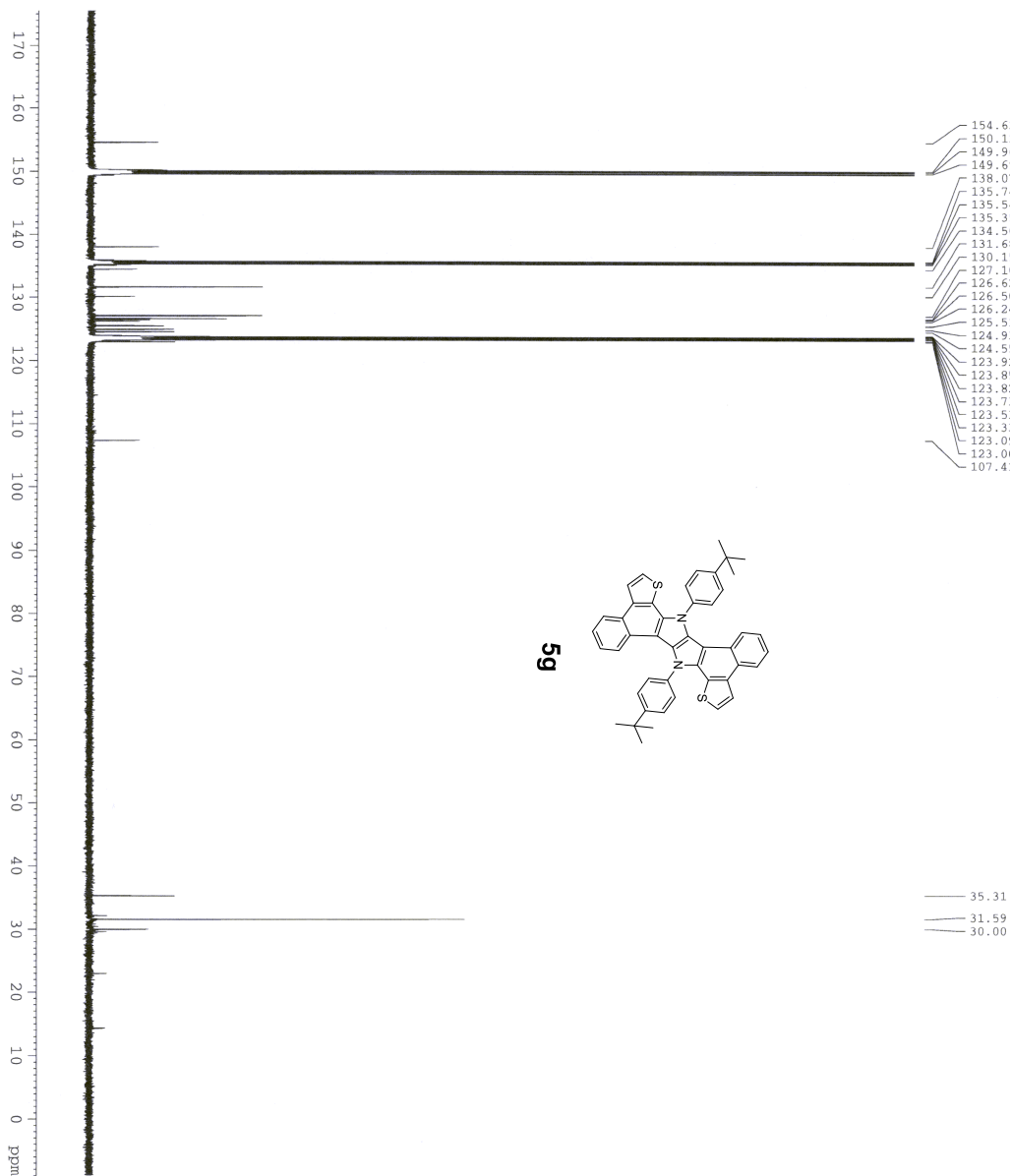
Current Data Parameters
NAME          MK225
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20140521
Time          13.57
INSTRUM       DRX
PROBHD        5 mm TBI 1H/13
PULPROG       zg30
TD            65536
SOLVENT       Pyr
NS            32
DS            0
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            181
DM            48.400 usec
DE            6.78 usec
TE            303.0 K
D1            1.0000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            8.20 usec
PL1           5.00 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI            32768
SF            500.129983 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```

Pomiar w temp. pokojowej (303 K)



Current Data Parameters
 NAME: 5g
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20140521
 Time: 14.15
 INSTRUM: spect
 PROBHD: 5 mm TBI 1H/13
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: Pyr
 NS: 33650
 DS: 4
 SWH: 32679.773 Hz
 FIDRES: 0.4498653 Hz
 AQ: 1.0027508 sec
 RG: 32768
 DW: 15.300 usec
 DE: 7.10 usec
 TE: 300.2 K
 D1: 1.0000000 sec
 d11: 0.0300000 sec
 DELTA: 0.8999998 sec
 TDO: 1
 ===== CHANNEL f1 =====
 NUC1: 13C
 P1: 5.00 usec
 PL1: -3.00 dB
 SFO1: 125.7703643 MHz
 ===== CHANNEL f2 =====
 CDEPRG2: waltz16
 NUC2: 1H
 P2: 98.00 usec
 PL2: 3.00 dB
 PL12: 23.00 dB
 PL13: 32.00 dB
 SFO2: 500.1320005 MHz
 F1 - Acquisition parameters
 NDO: 128
 TD: 128
 SFO1: 500.132 MHz
 FIDRES: 7.812500 Hz
 SW: 1.999 ppm
 F2 - Processing parameters
 SI: 262144
 SF: 125.7577561 MHz
 WDM: EM
 SSB: 0
 GB: 0.50 Hz
 PC: 1.40
 F1 - Processing parameters
 SI: 1024
 SF: 500.1300000 MHz
 WDM: SSB
 SSB: 0
 LB: 0.30 Hz
 GB: 0.1