

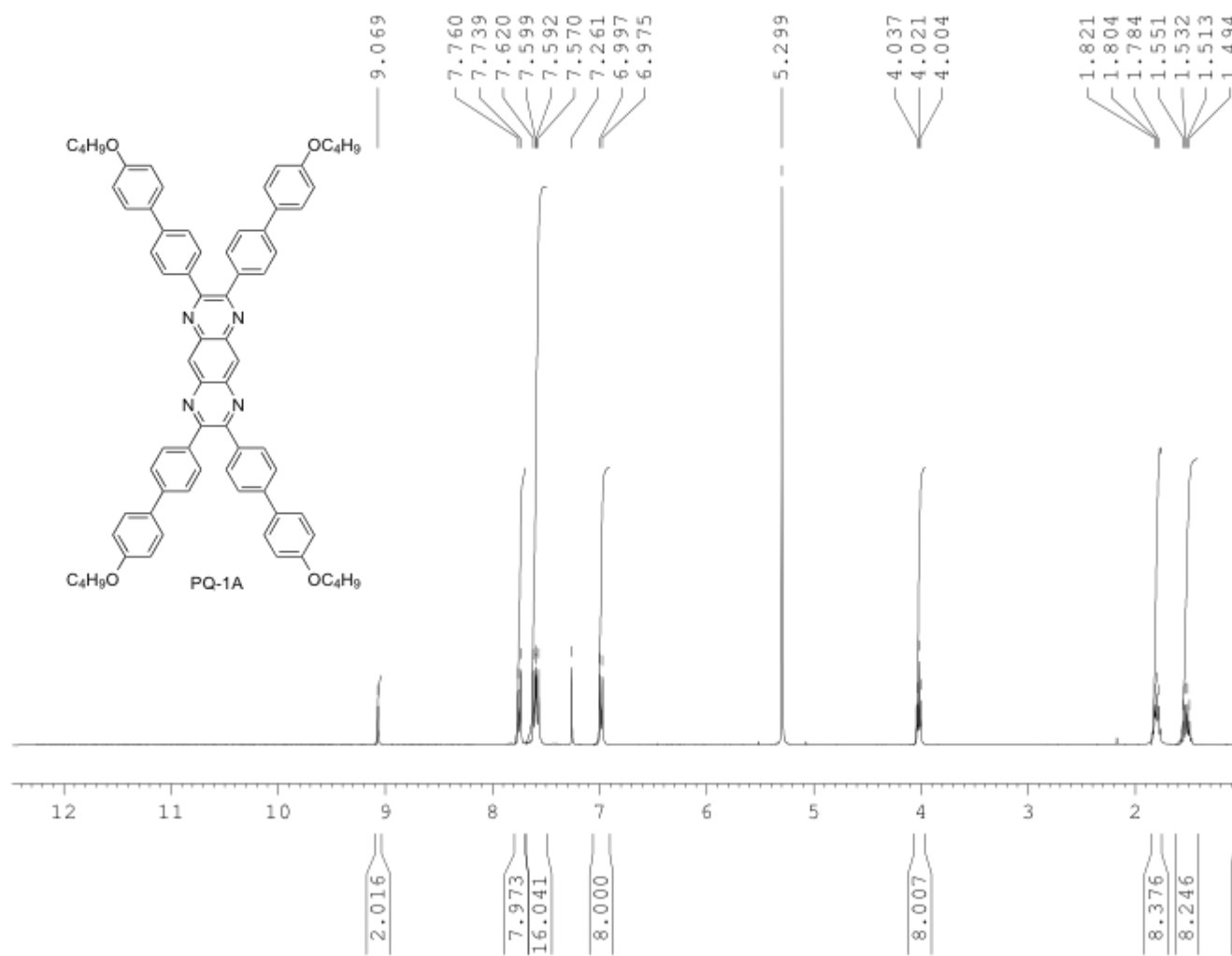
Conjugation and Cross-Conjugation Substituent Effect on Pyrazino[2,3-g]quinoxaline Small Molecules

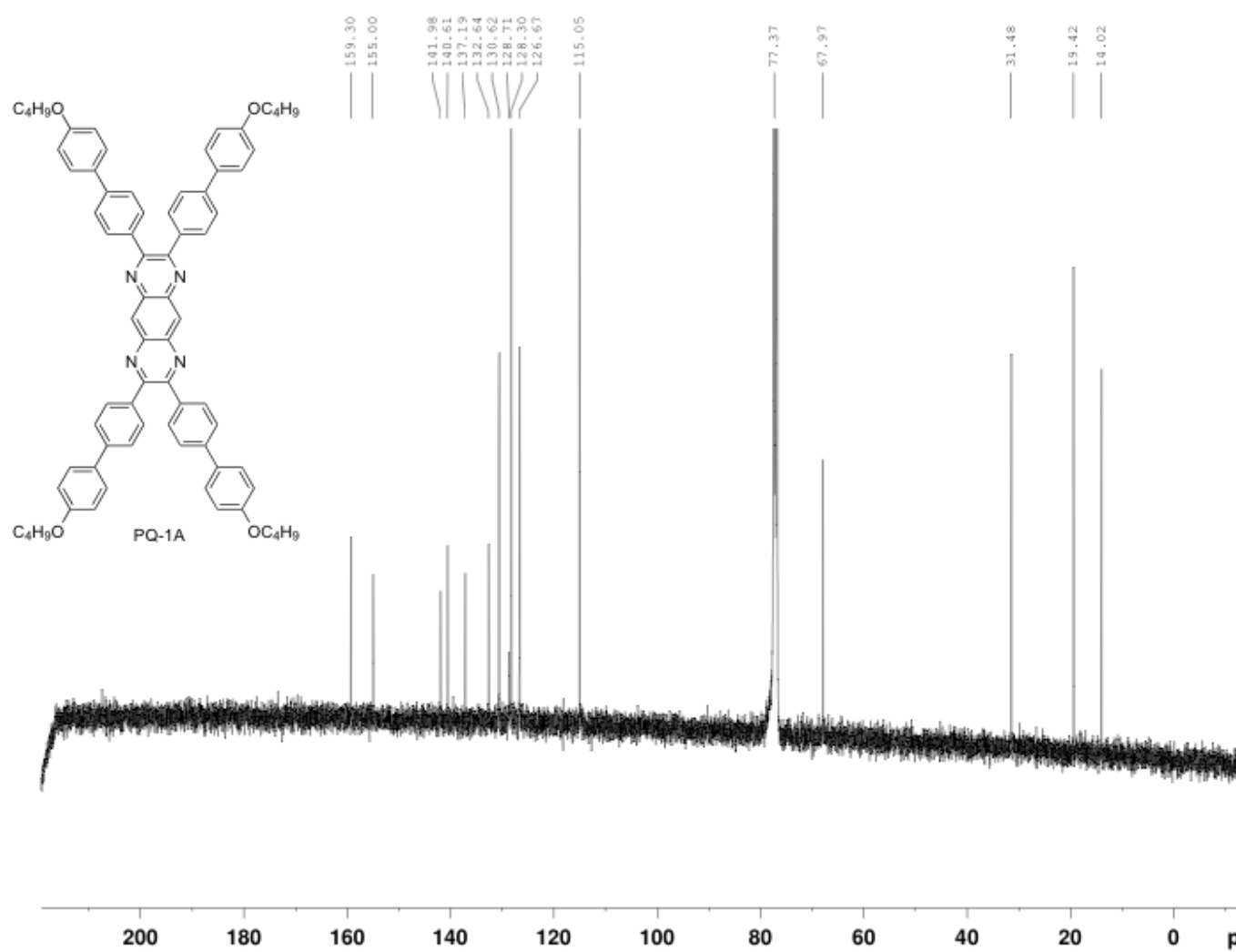
Teck Lip Tam, Feng Zhou, Hairong Li, Chieh Yu Jane Pang, Yeng Ming Lam, Subodh Gautam Mhaisalkar, Haibin Su* and Andrew Clive Grimsdale*

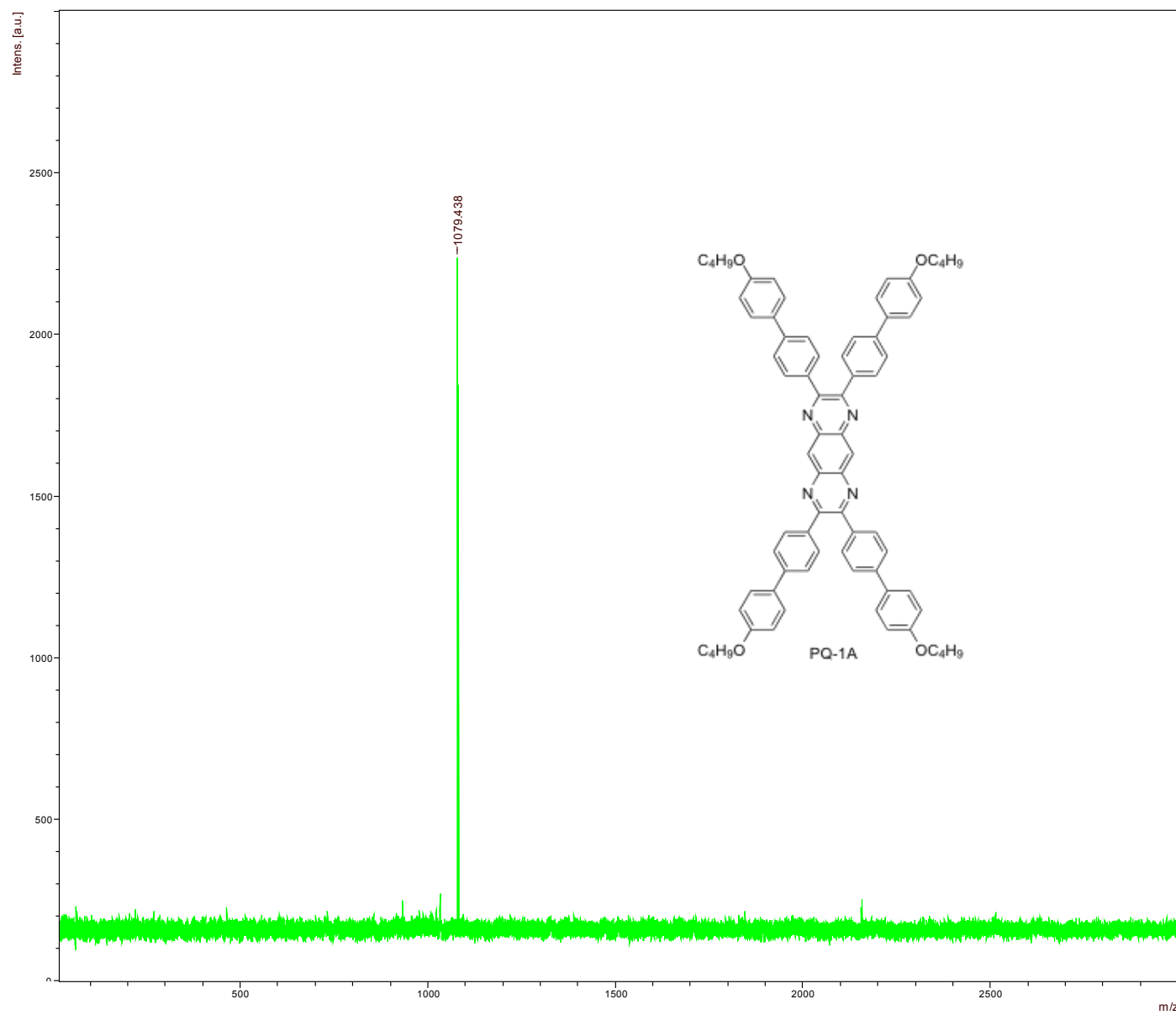
School of Materials Science and Engineering and Energy Research Institute at NTU, Nanyang Technological University, 50 Nanyang Avenue, 639798 Singapore.

**Corresponding Author. Email: hbsu@ntu.edu.sg, ACGrimsdale@ntu.edu.sg*

Supporting document



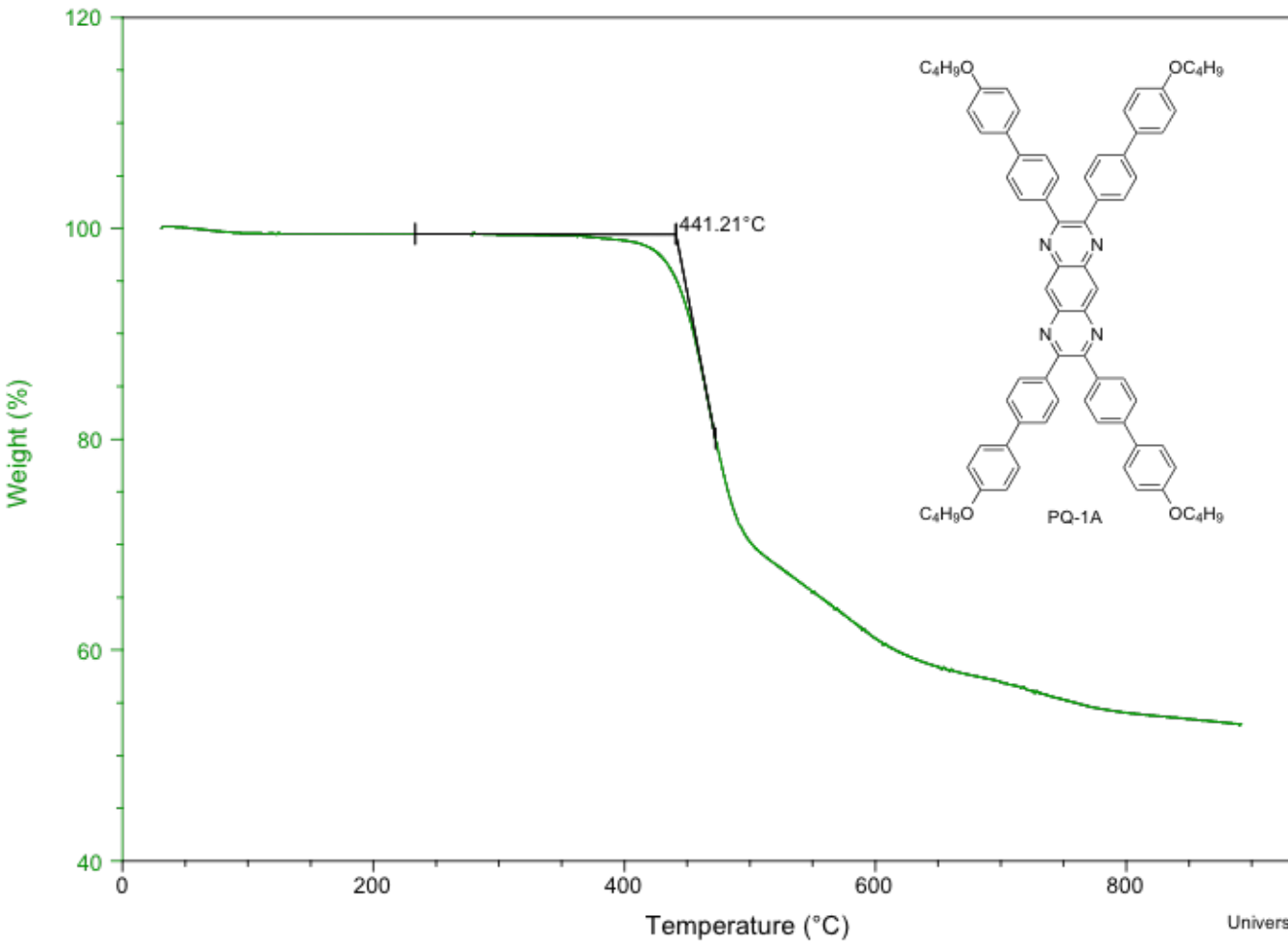




Sample: PQ-4PhPhOBu
Size: 7.5980 mg
Method: Ramp

TGA

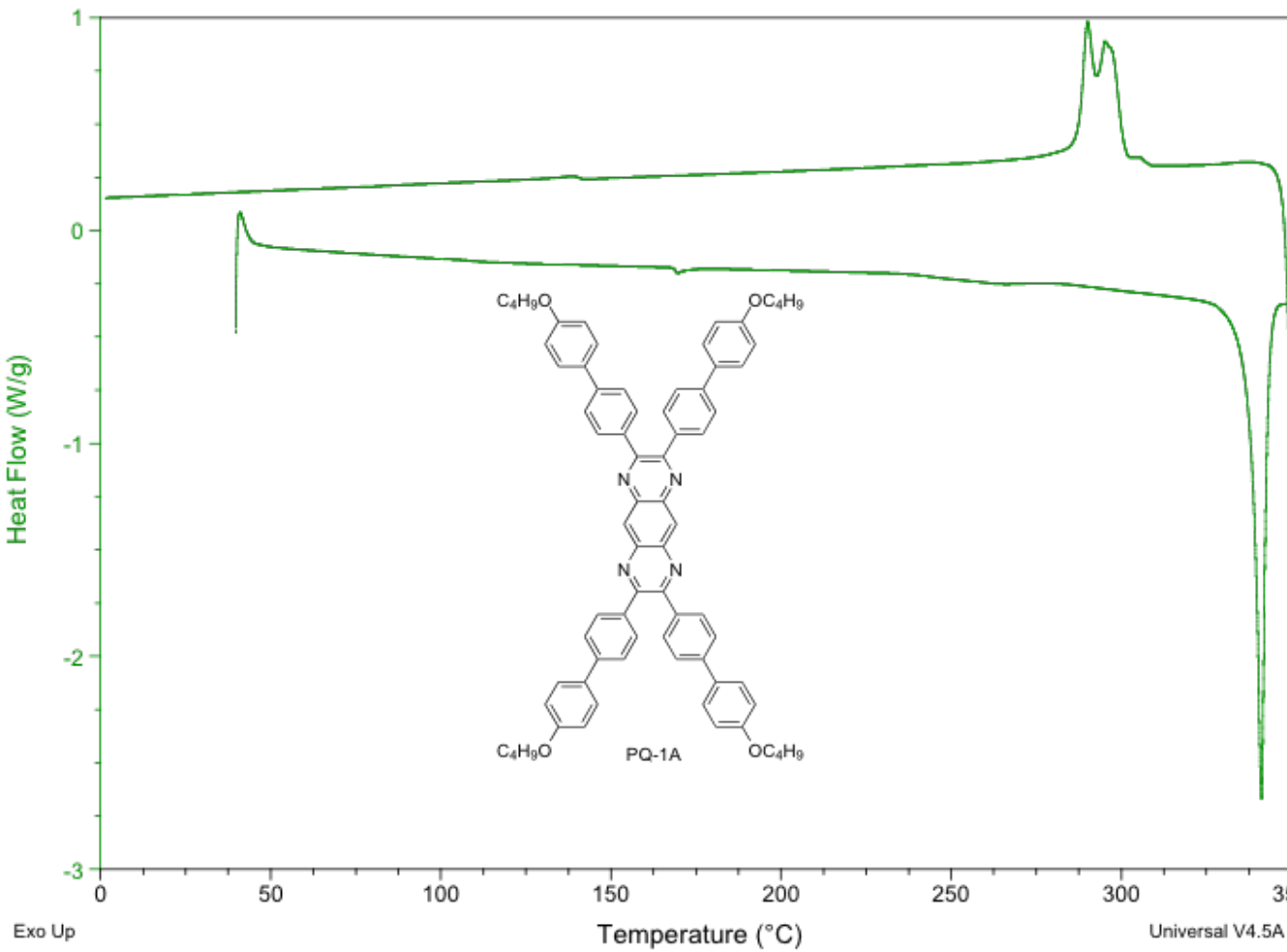
File: D:\RS\TamTL\PQ-4PhPhOBu
Operator: TamTL
Run Date: 20-Mar-2009 19:49
Instrument: TGA Q500 V6.5 Build

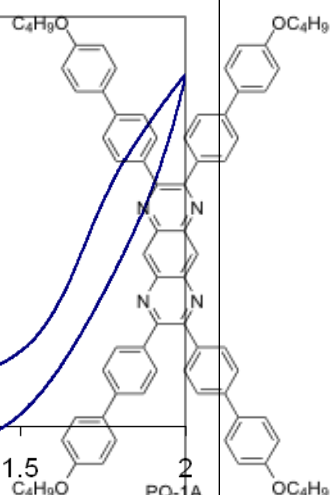
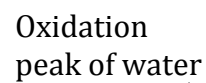


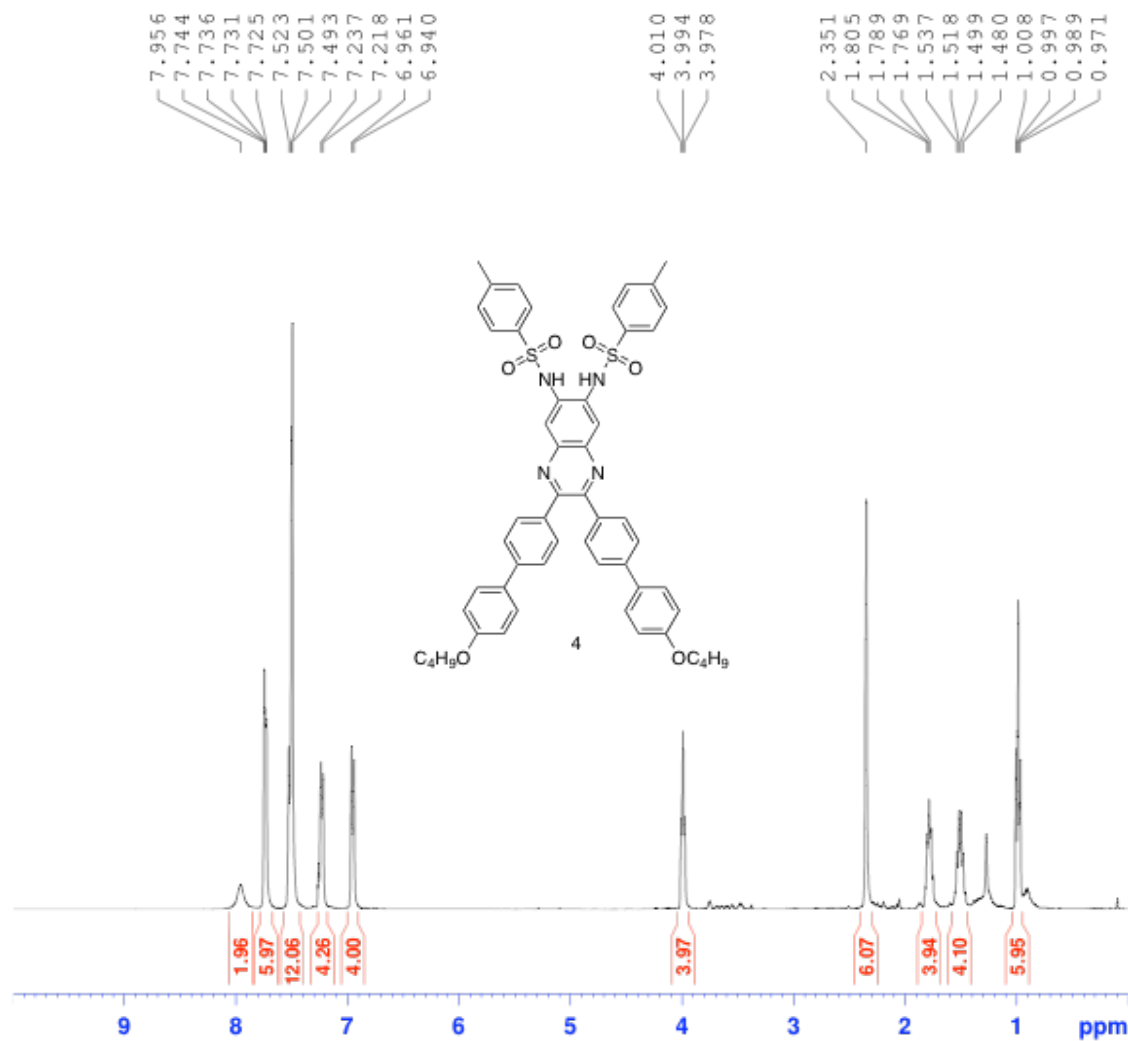
Sample: PQ-4PhPhOBu
Size: 3.4100 mg
Method: TamTL

DSC

File: E:\...TamTL\PQ-4PP\PQ-4PhPhOBu
Operator: TamTL
Run Date: 20-Mar-2009 21:10
Instrument: DSC Q10 V9.6 Build 290





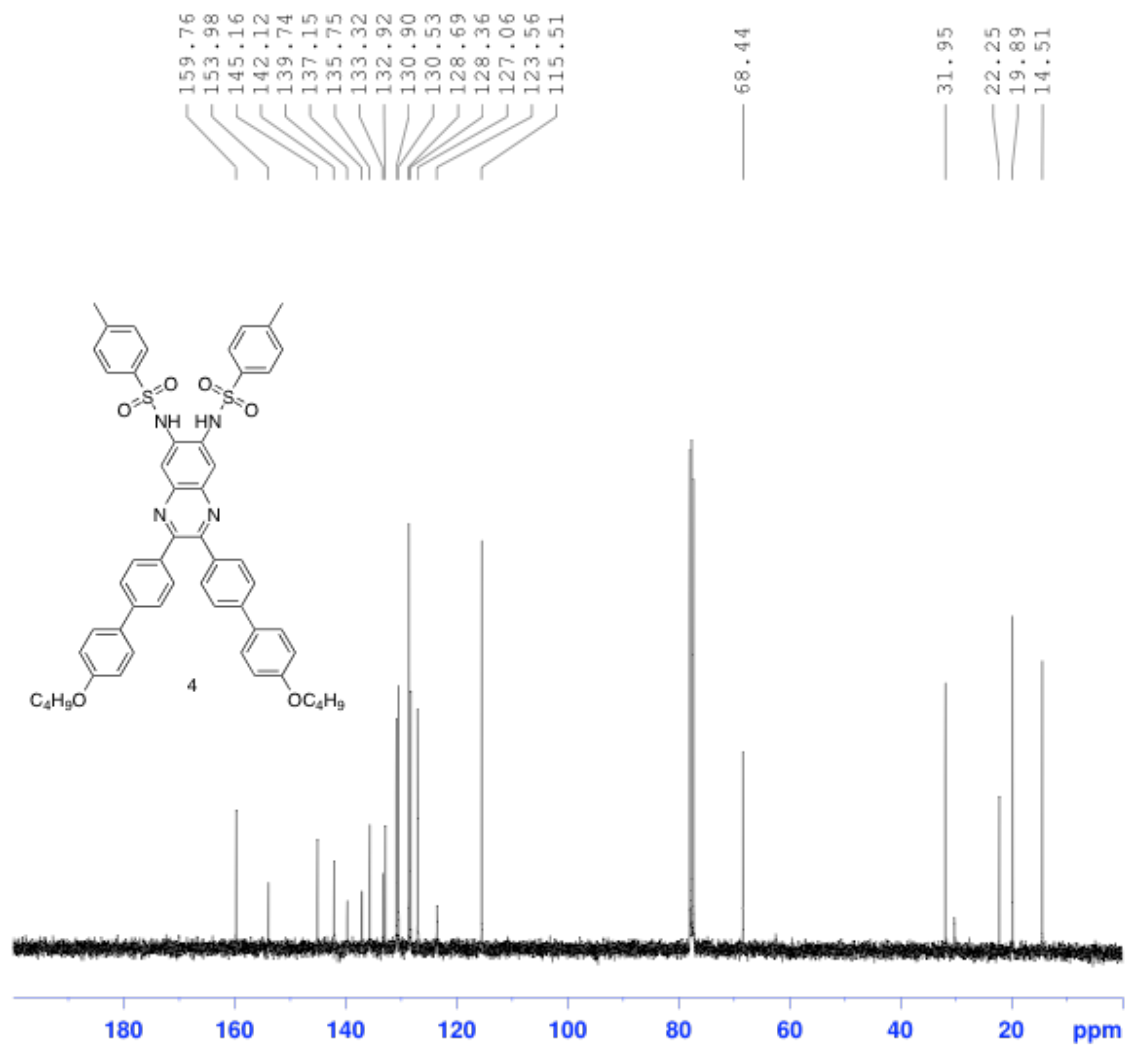


Current Data Parameters
NAME 101
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101118
Time 18:05:11
INSTRUM AVANCE
PROBHD 5 mm PABBO
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 8278.5 Hz
FIDRES 0.126 Hz
AQ 3.9584 s
RG 327.68
DW 60.00 ns
DE 1.90 dB
TE 298.2 K
D1 2.00000 s
TD0

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 μs
PL1 -1.50 dB
SFO1 400.132411 MHz

F2 - Processing parameters
SI 32768
SF 400.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0



Current Data Parameters
NAME 101
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101118
Time 18:00:00
INSTRUM AVANCE
PROBHD 5 mm PABBO
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.133 MHz
FIDRES 0.365 Hz
AQ 1.3664 s
RG 144
DW 20.00 ns
DE 6.00 dB
TE 299.2 K
D1 2.00000 s
d11 0.03000 s
DELTA 1.89999 s
TD0 1

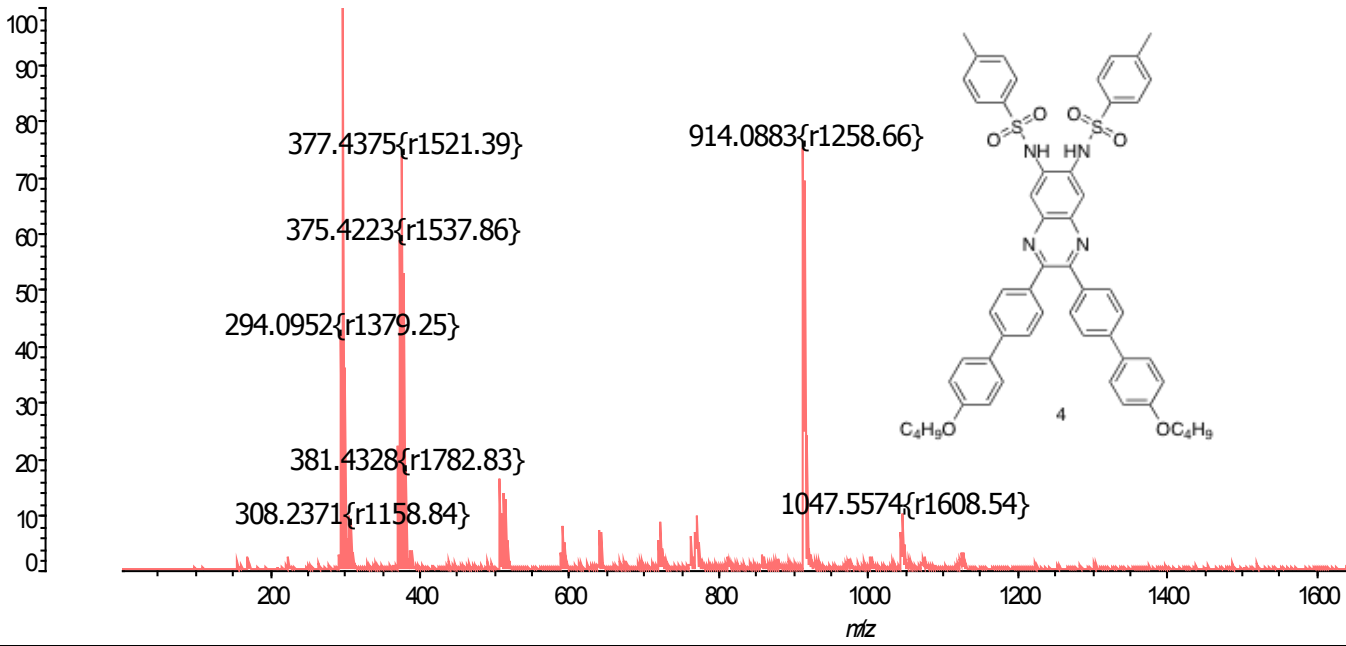
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 ns
PL1 -3.00 dB
SFO1 100.6228 MHz

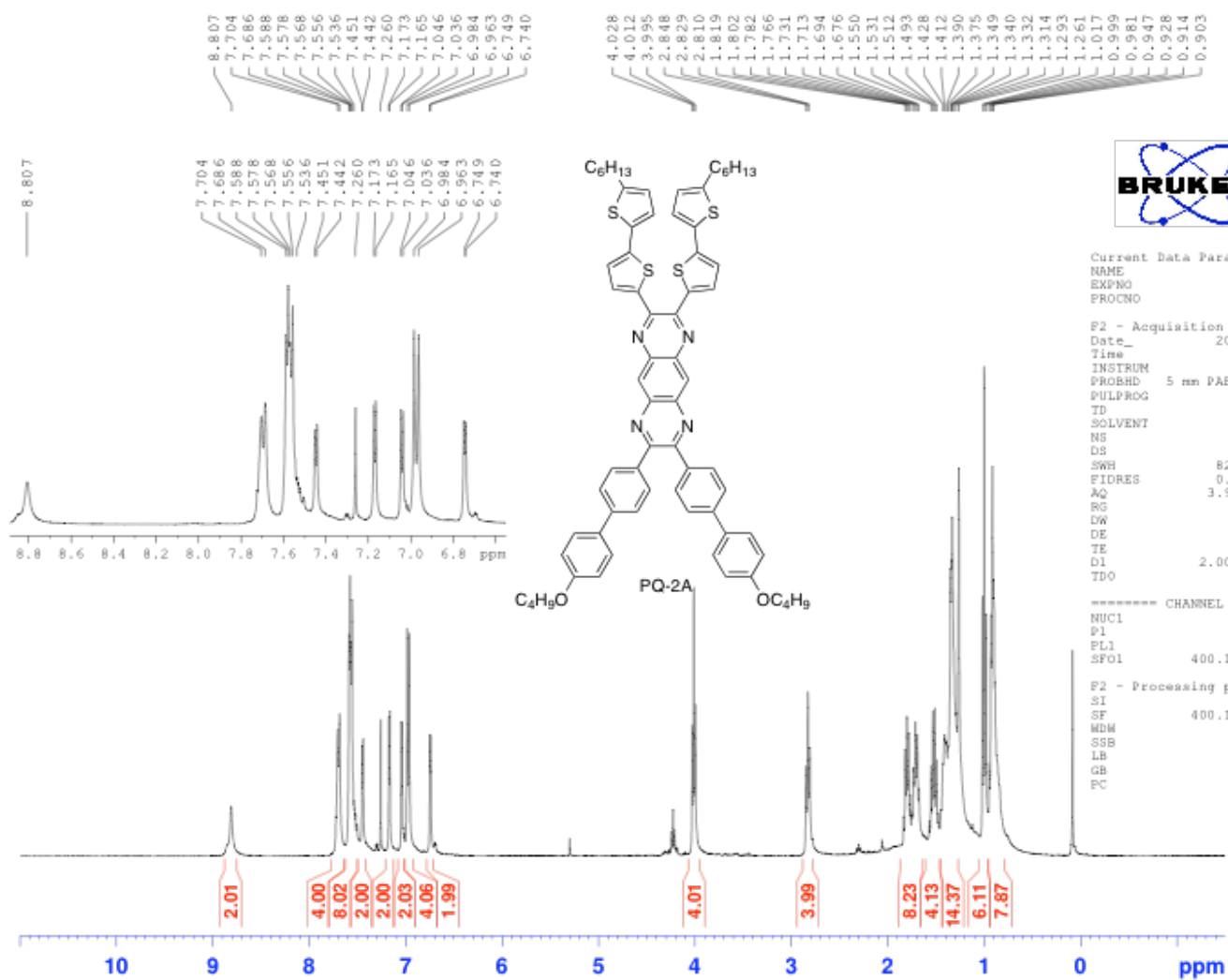
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 ns
PL2 -2.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 400.1316 MHz

F2 - Processing parameters
SI 32768
SF 100.6127 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1

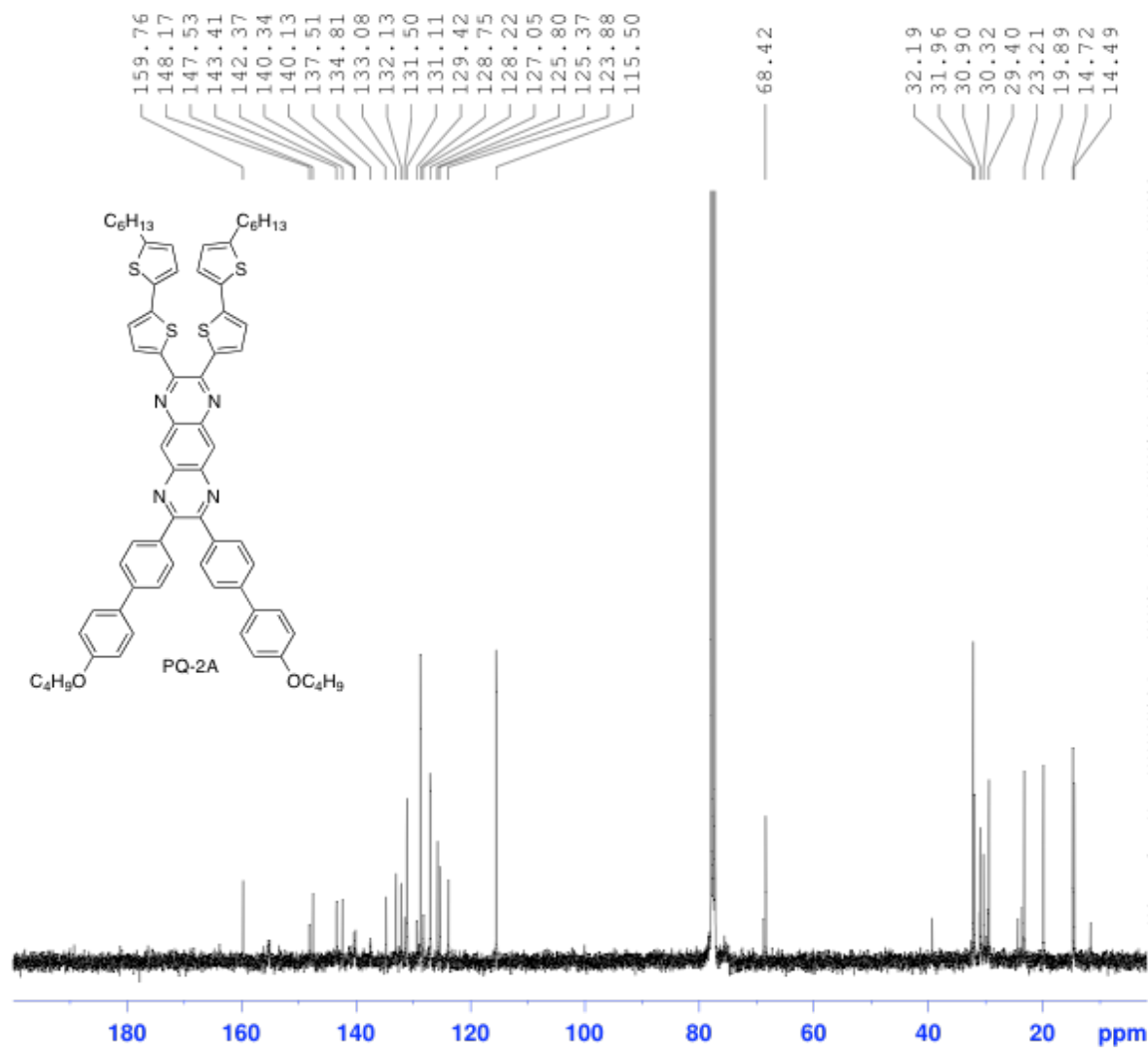
Data: <Untitled>.G24[c] 31 Jan 2011 14:18 Cal: 31 Jan 2011 14:18
Shimadzu Biotech Axima ToF² 2.8.4.200808271B: Mode Reflectron_neg, Power: 80, P.Ext. @916 (bin 71)

%Int. 101 mV[sum= 10090 mV] Profiles 1-100 Smooth Av 5





Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_ 2011
Time
INSTRUM
PROBHD 5 mm PAB
PULPROG
TD
SOLVENT
NS
DS
SWH 82.0
FIDRES 0.1
AQ 3.90
RG
DW
DE
D1 2.00
TDO
===== CHANNEL =====
NUC1
P1
PL1
SF01 400.1
F2 - Processing parameters
SI
SF 400.1
WDW
SSB
LB
GB
PC



Current Data Parameters
NAME: 101
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20101020
Time: 23:00
INSTRUM: AVANCE
PROBHD: 5 mm PABBO
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1024
DS: 4
SWH: 23980 Hz
FIDRES: 0.365 Hz
AQ: 1.366 sec
RG: 256
DW: 20.00 nsec
DE: 1.00 dB
TE: 300.2 K
D1: 2.000000 sec
d11: 0.030000 sec
DELTA: 1.899999 sec
TDO: 0.000000 sec

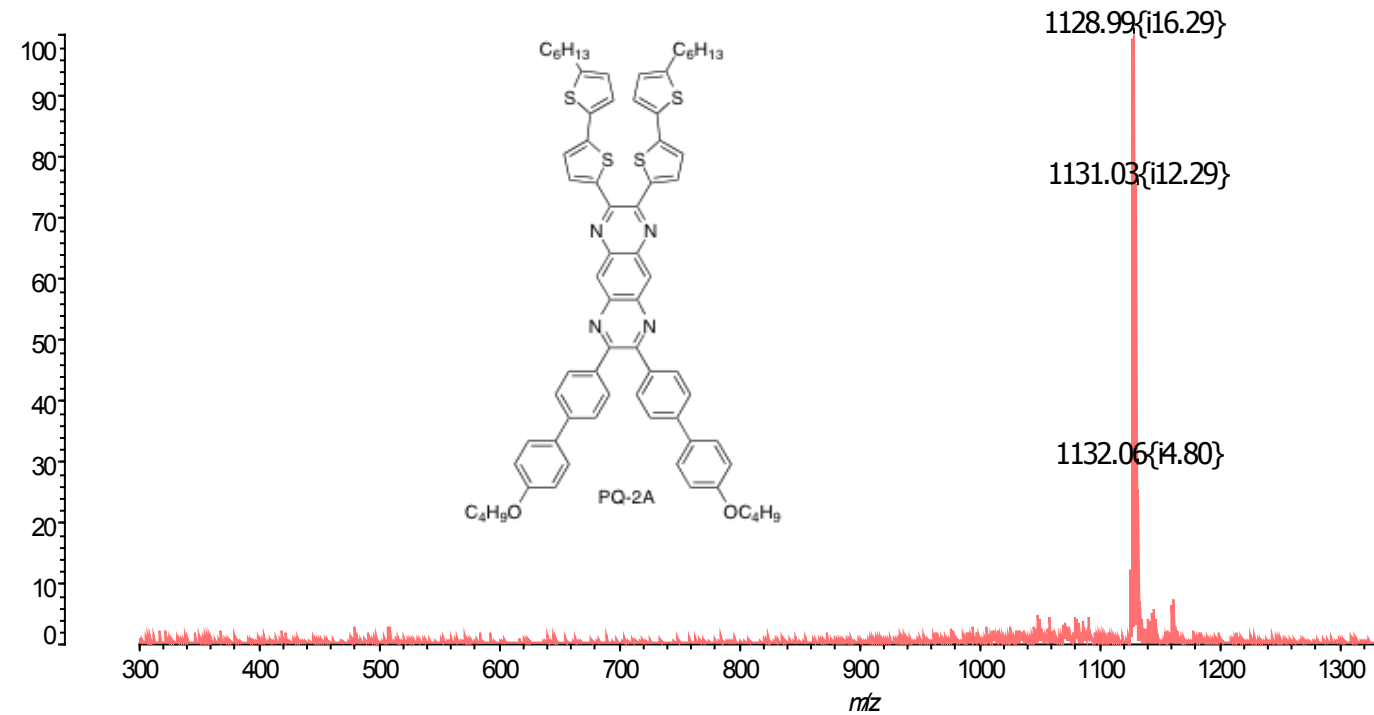
===== CHANNEL f1 =====
NUC1: 13C
P1: 12.00 nsec
PL1: -1.00 dB
SFO1: 100.622500 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 8.00 nsec
PL2: -2.00 dB
PL12: 19.00 dB
PL13: 19.00 dB
SFO2: 400.131400 MHz

F2 - Processing parameters
SI: 32768
SF: 100.612500 MHz
WDM: 1.000000
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

Data: <Untitled>.C16[c] 15 Jan 2011 14:14 Cal: small cal mix pos 12 Jan 2011 16:35
Shimadzu Biotech Axima ToF² 2.8.4.200808271B: Mode Reflectron, Power: 62, P.Ext. @1126 (bin 78)

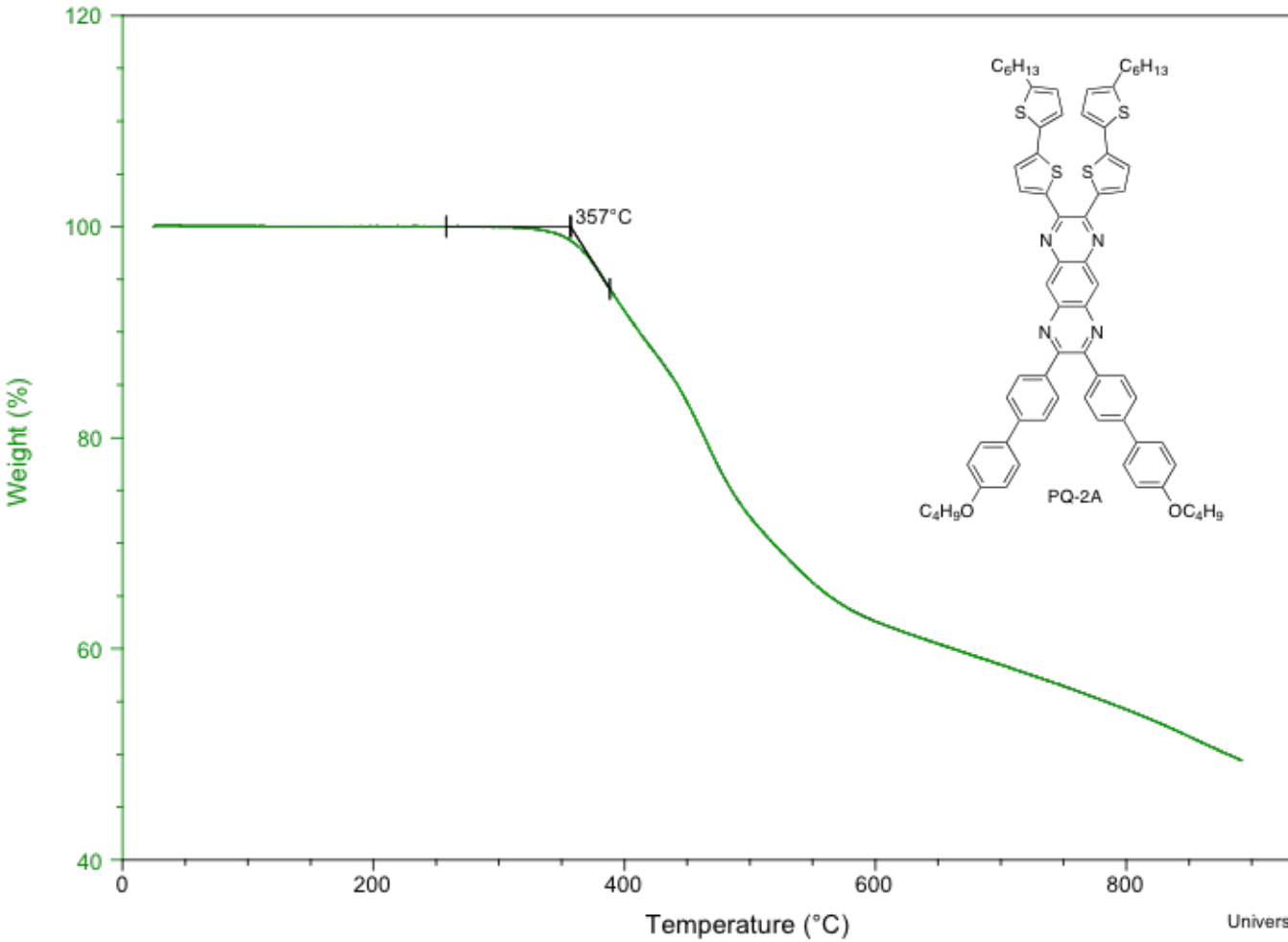
%Int. 16 mV[sum= 3258 mV] Profiles 1-200 Smooth Av 5

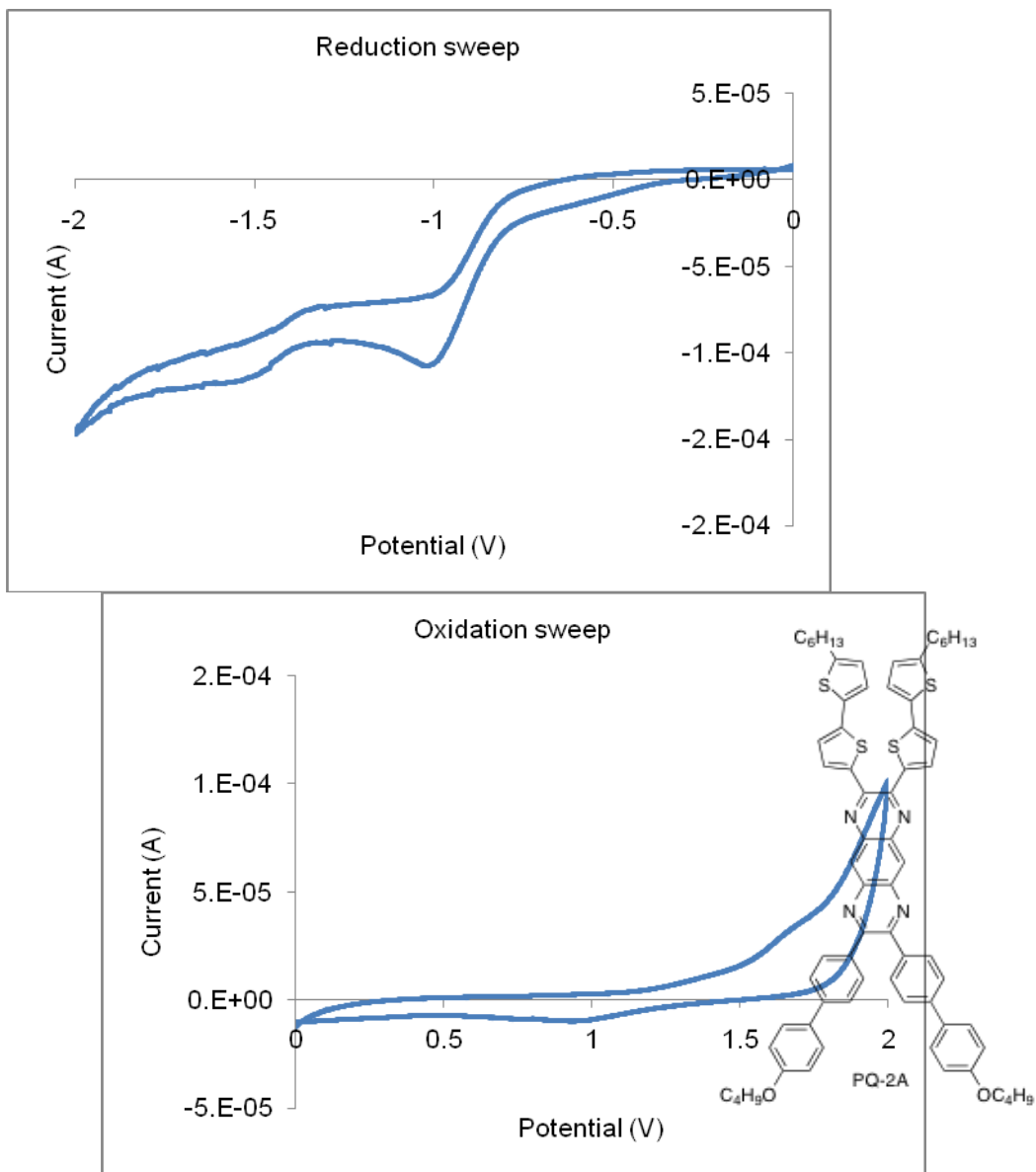


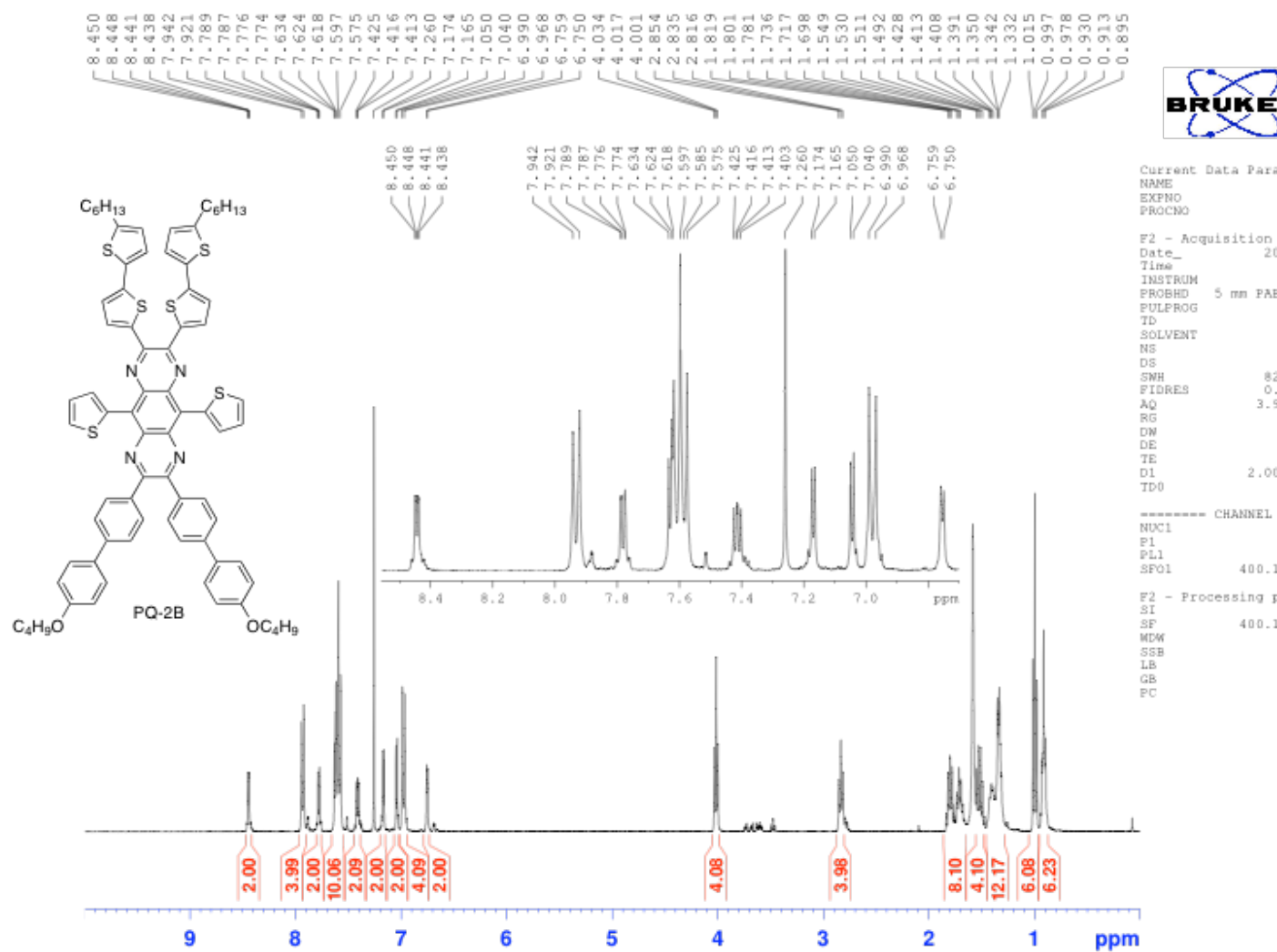
Sample: 2PP-2TT-PQ
Size: 5.4640 mg
Method: Ramp

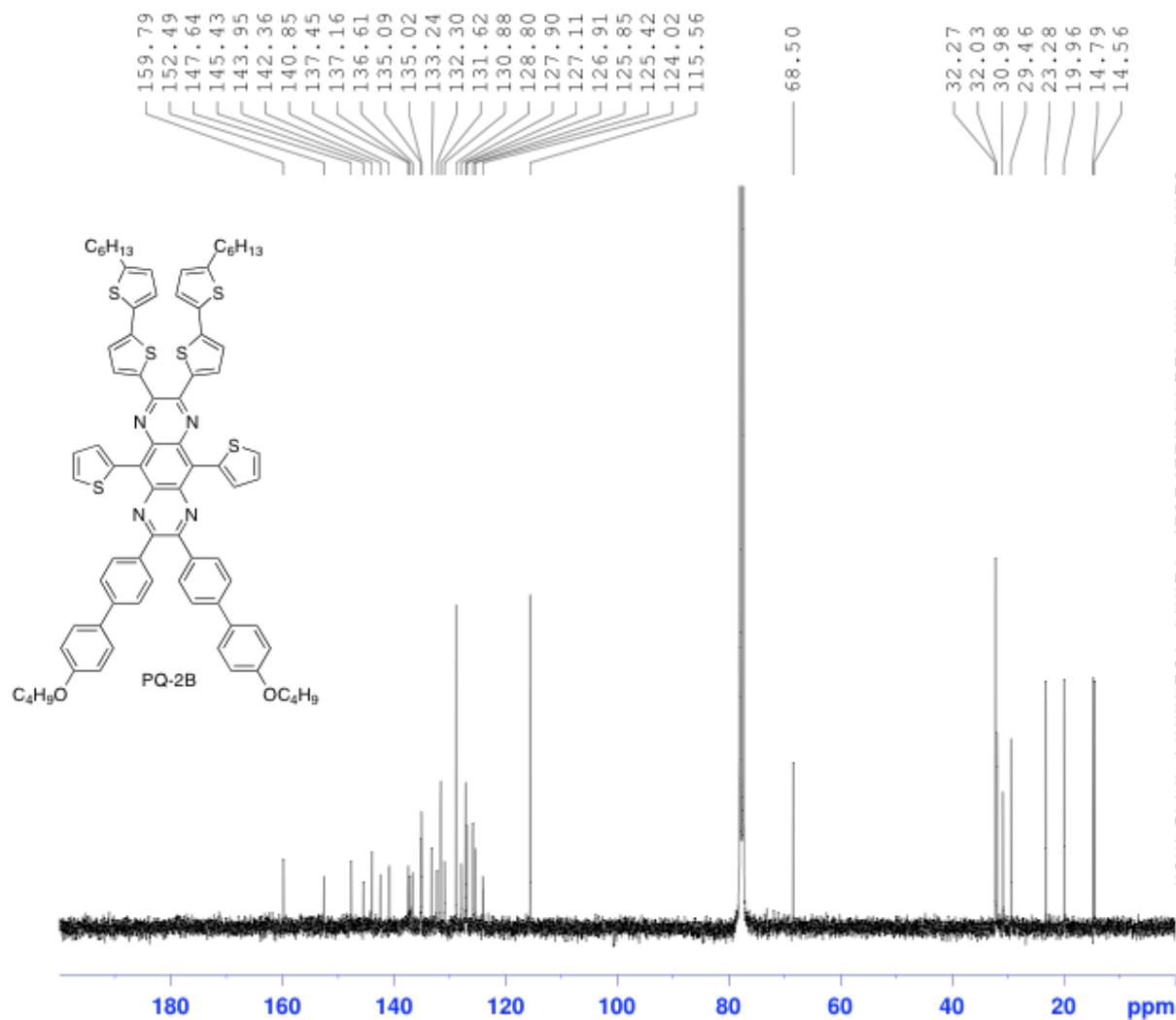
TGA

File: D:\RS\LHR\2PP-2TT-PQ.00
Operator: LHR
Run Date: 13-Jan-2011 18:59
Instrument: TGA Q500 V6.7 Build







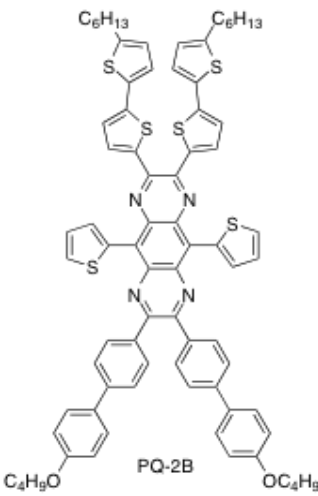
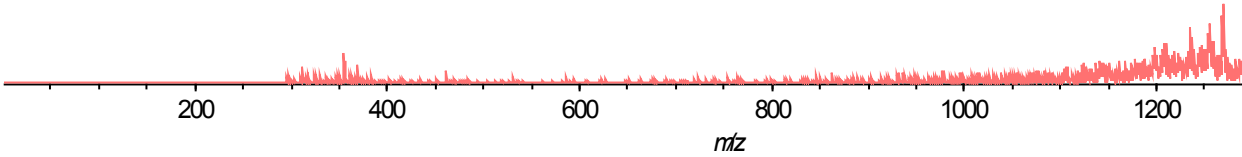


Current Data Parameters
NAME 11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 2011
Time 2
INSTRUM A
PROBHD 5 mm PABBO
PULPROG zgpg30
TD 65536
SOLVENT C
NS 1024
DS 4
SWH 23980.00
FIDRES 0.34
AQ 1.366
RG 256
DM 2048
DE 1.00
TE 298.2
D1 2.00000
d11 0.03000
DELTA 1.8995
TD0
===== CHANNEL f1 =====
NUC1 13C
P1 12.00
PL1 0.00
SFO1 100.622476
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 12.00
PL2 0.00
PL12 0.00
PL13 0.00
SFO2 400.131444
F2 - Processing parameters
SI 32768
SF 100.612500
WDW EM
SSB 0
LB 0.3
GB 0
PC 0

Data: <Untitled>.C12[c] 14 Jan 2011 19:52 Cal: small cal mix pos 12 Jan 2011 16:35
Shimadzu Biotech Axima ToF² 2.8.4.200808271B: Mode Reflectron, Power: 65, P.Ext. @1290 (bin 84)

%Int. 22 mV[sum= 4374 mV] Profiles 1-200 Smooth Av 5

100
90
80
70
60
50
40
30
20
10
0

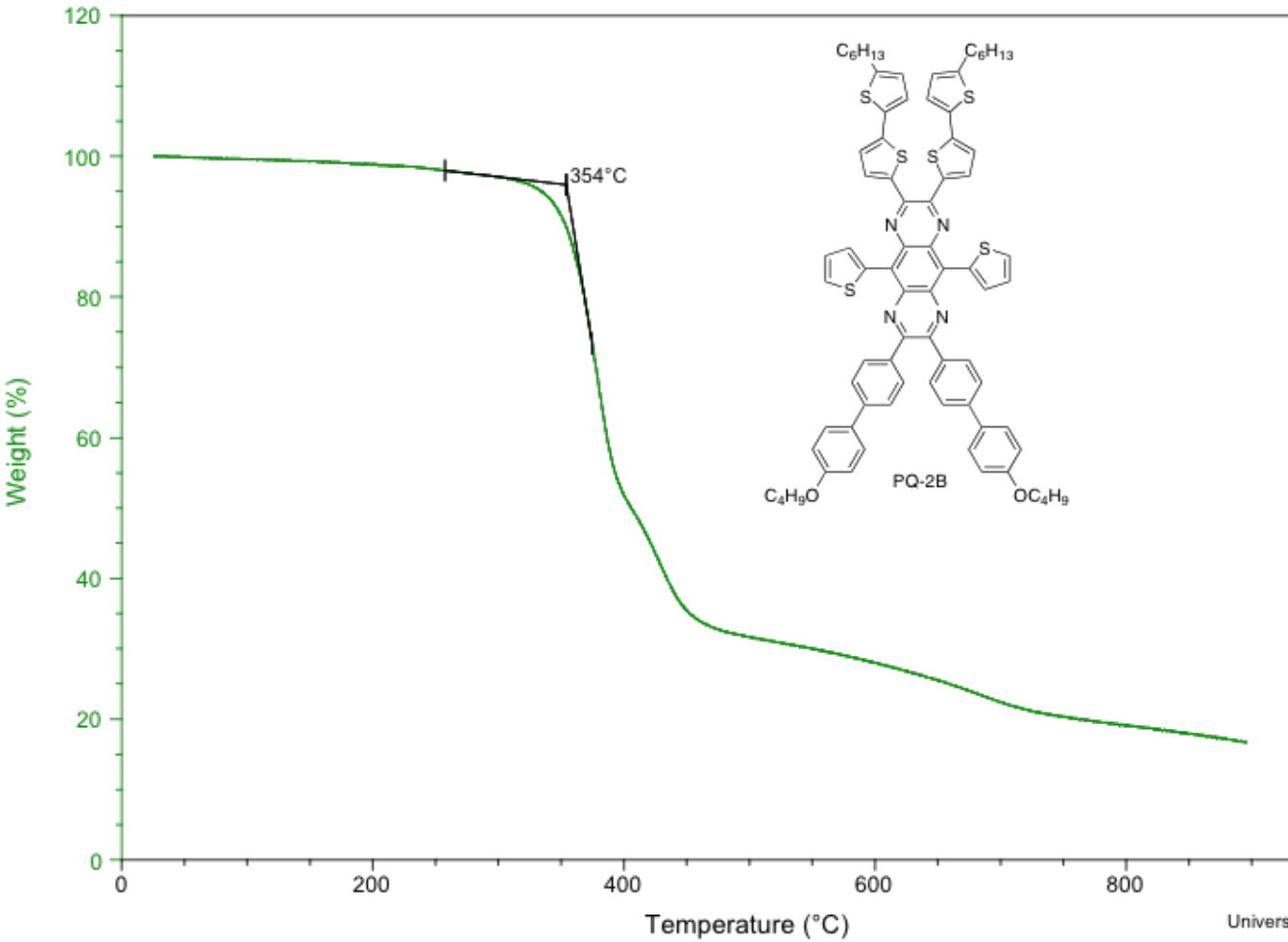


1293.68
1292.68
1294.70
1291.6
1296.7

Sample: 2PP-2TT-2T-PQ
Size: 6.7900 mg
Method: Ramp

TGA

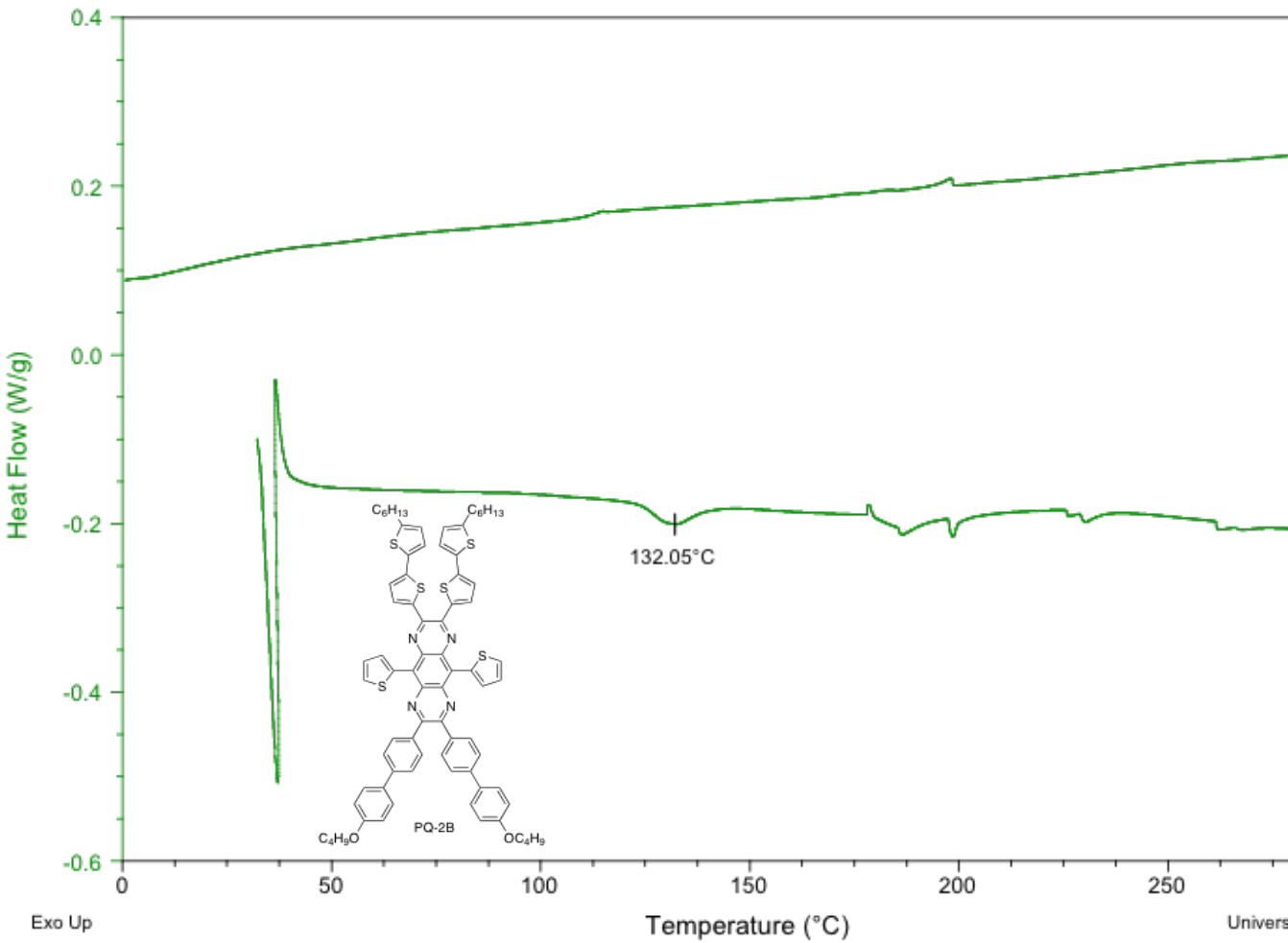
File: D:\RS\LHR\2PP-2TT-2T-PQ
Operator: LHR
Run Date: 21-Jan-2011 16:15
Instrument: TGA Q500 V6.7 Build

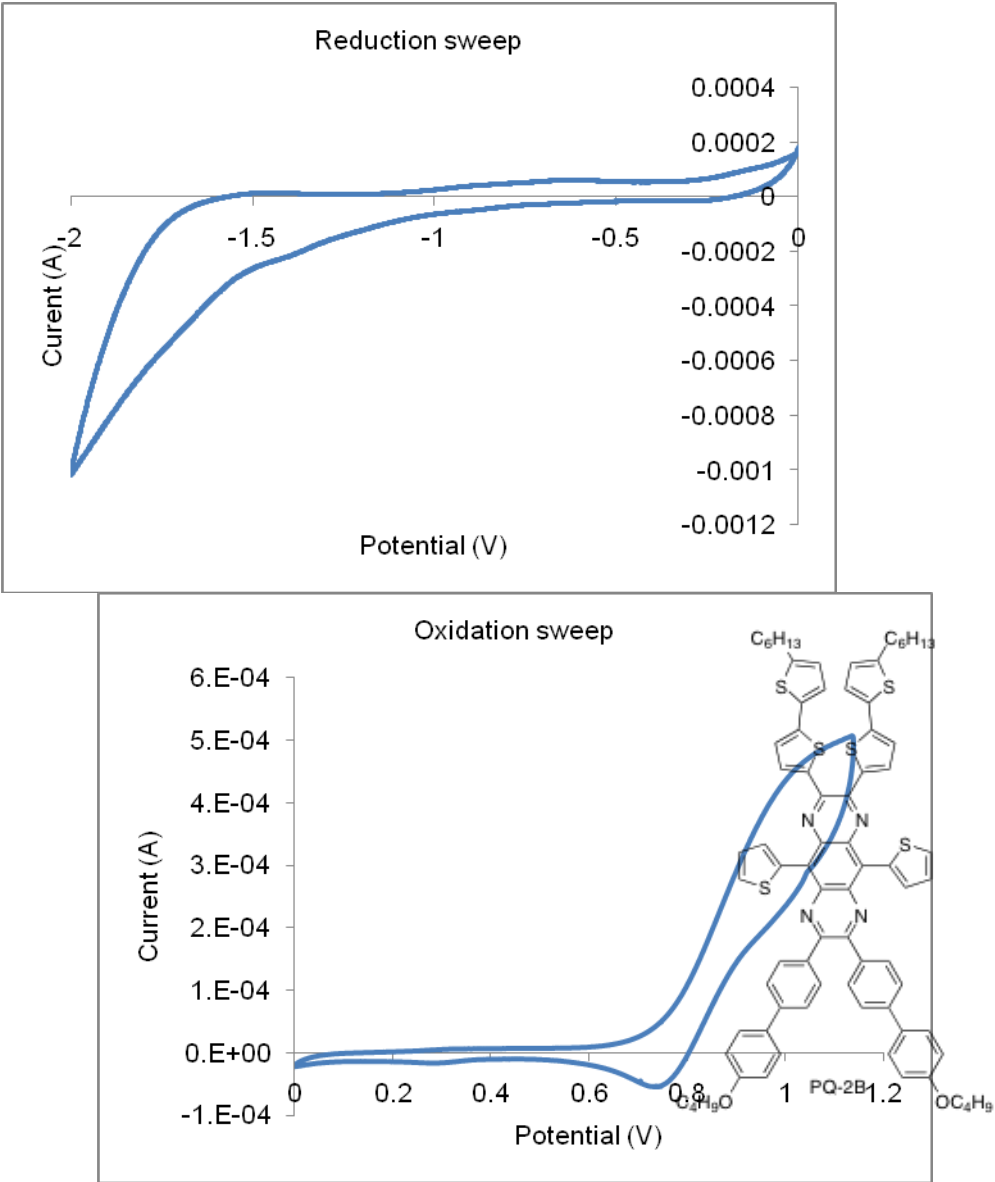


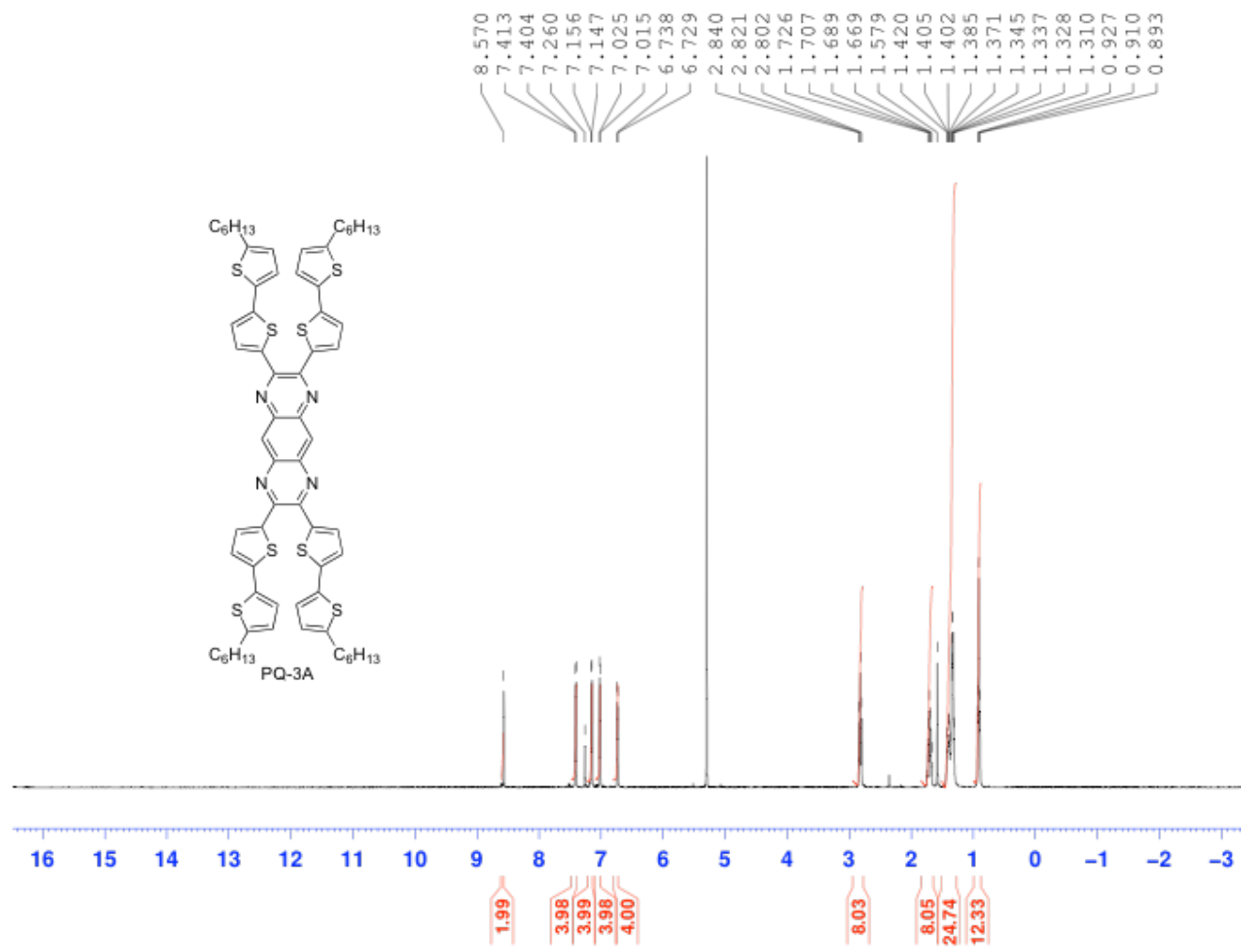
Sample: 2PP-2TT-2T-PQ
Size: 4.2000 mg
Method: TamTL

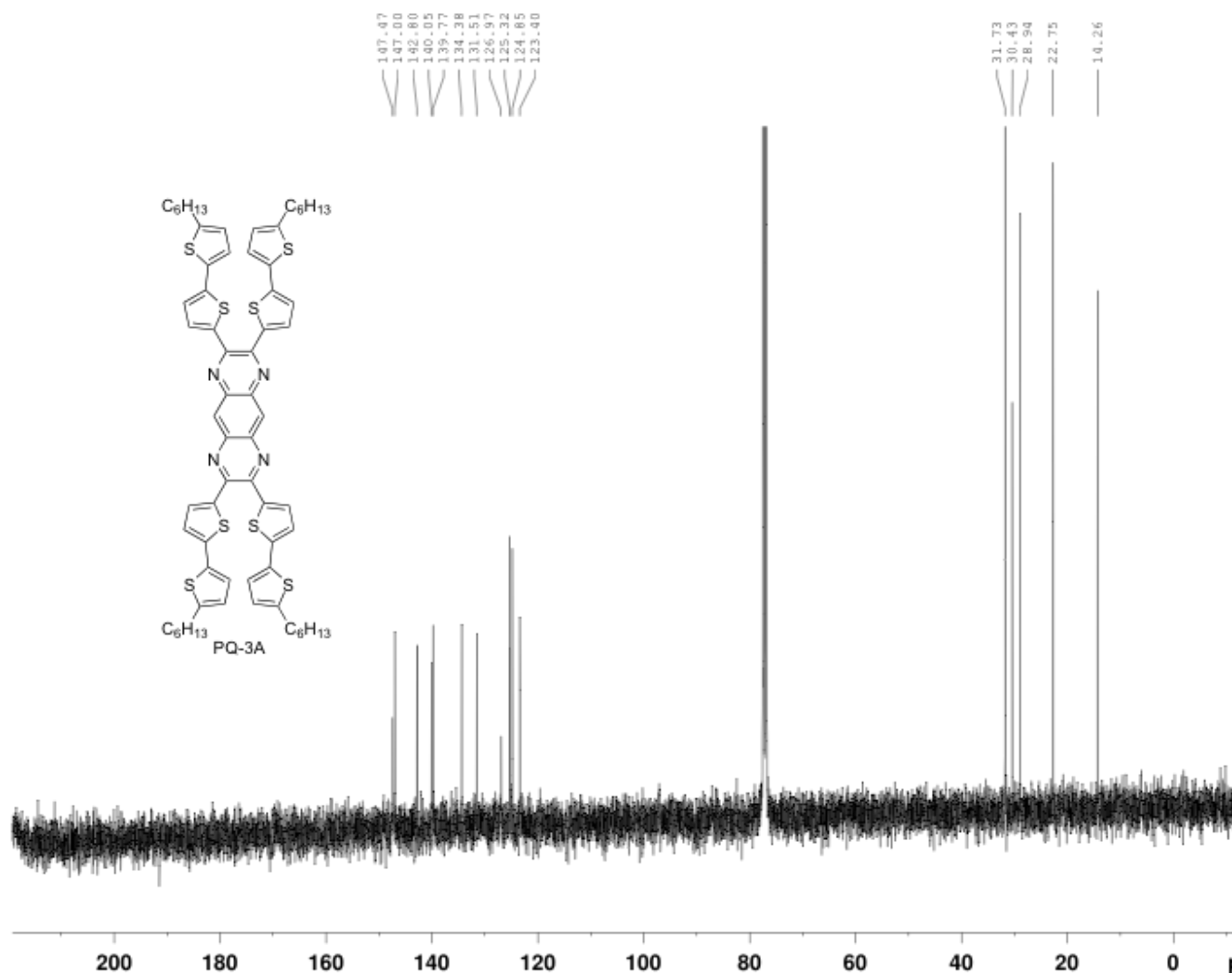
DSC

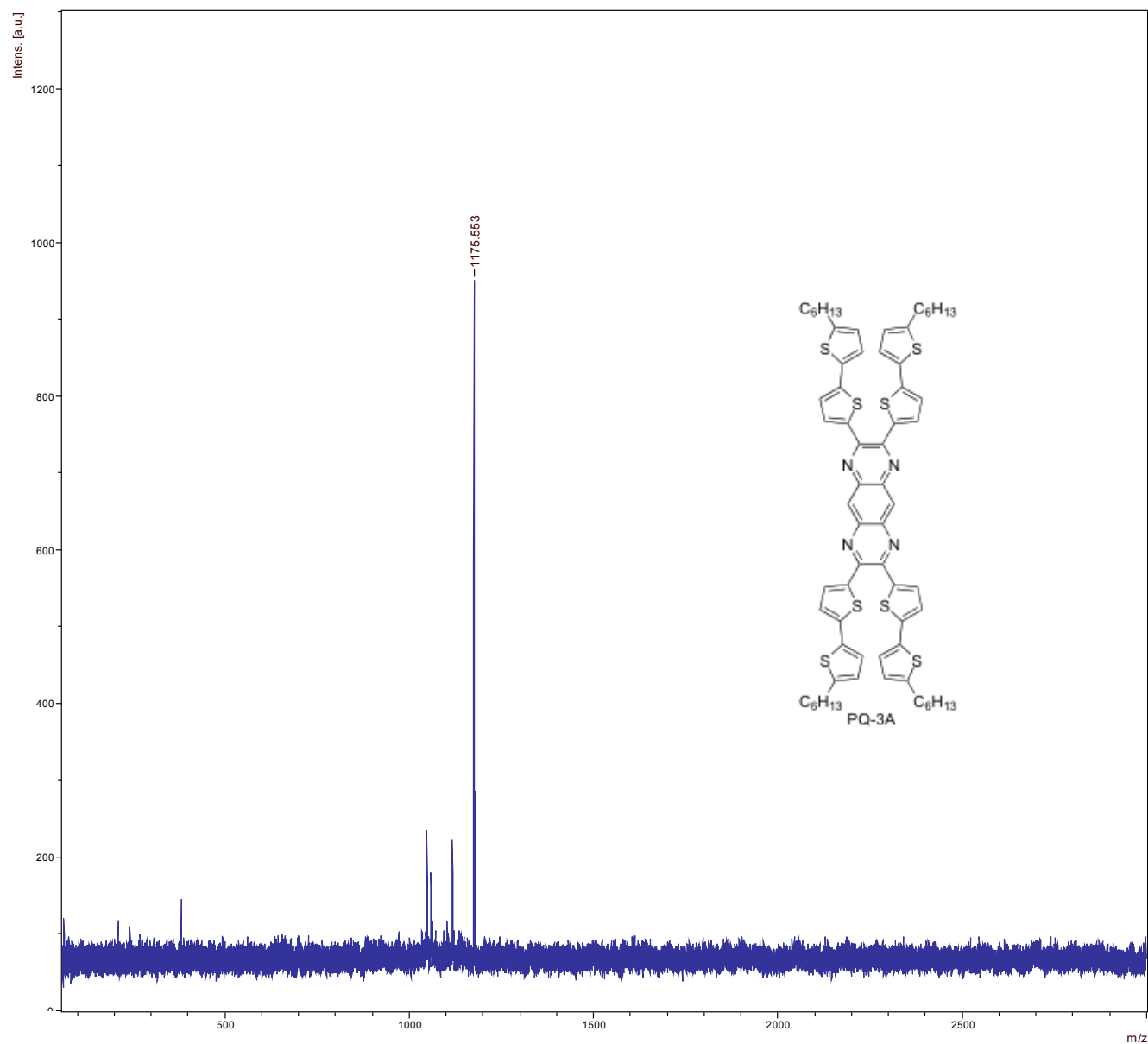
File: E:\LHR\2PP-2TT-2T-PQ.00
Operator: LHR
Run Date: 22-Jan-2011 21:53
Instrument: DSC Q10 V9.9 Build







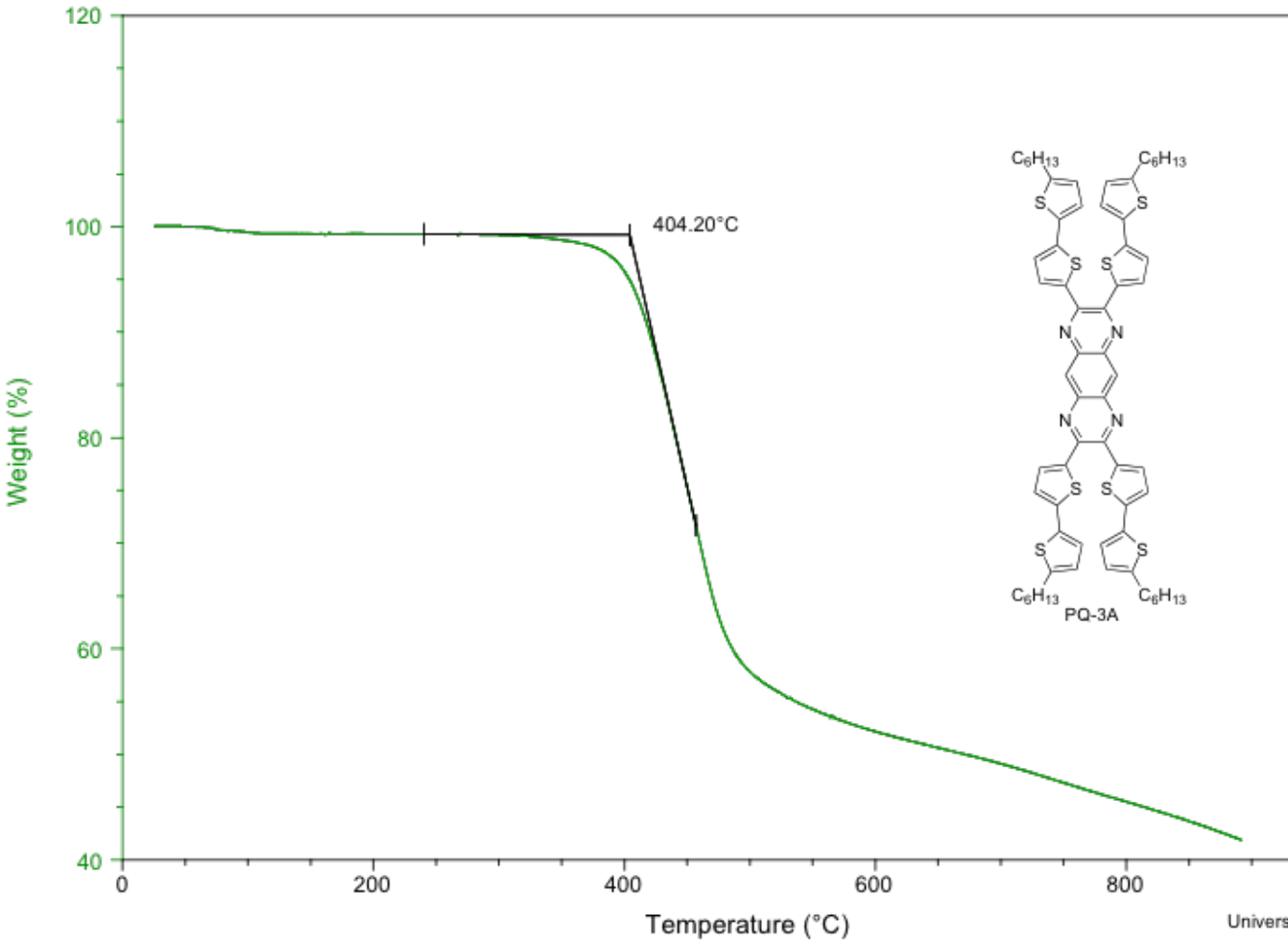




Sample: PQ-4TT
Size: 7.1280 mg
Method: Ramp

TGA

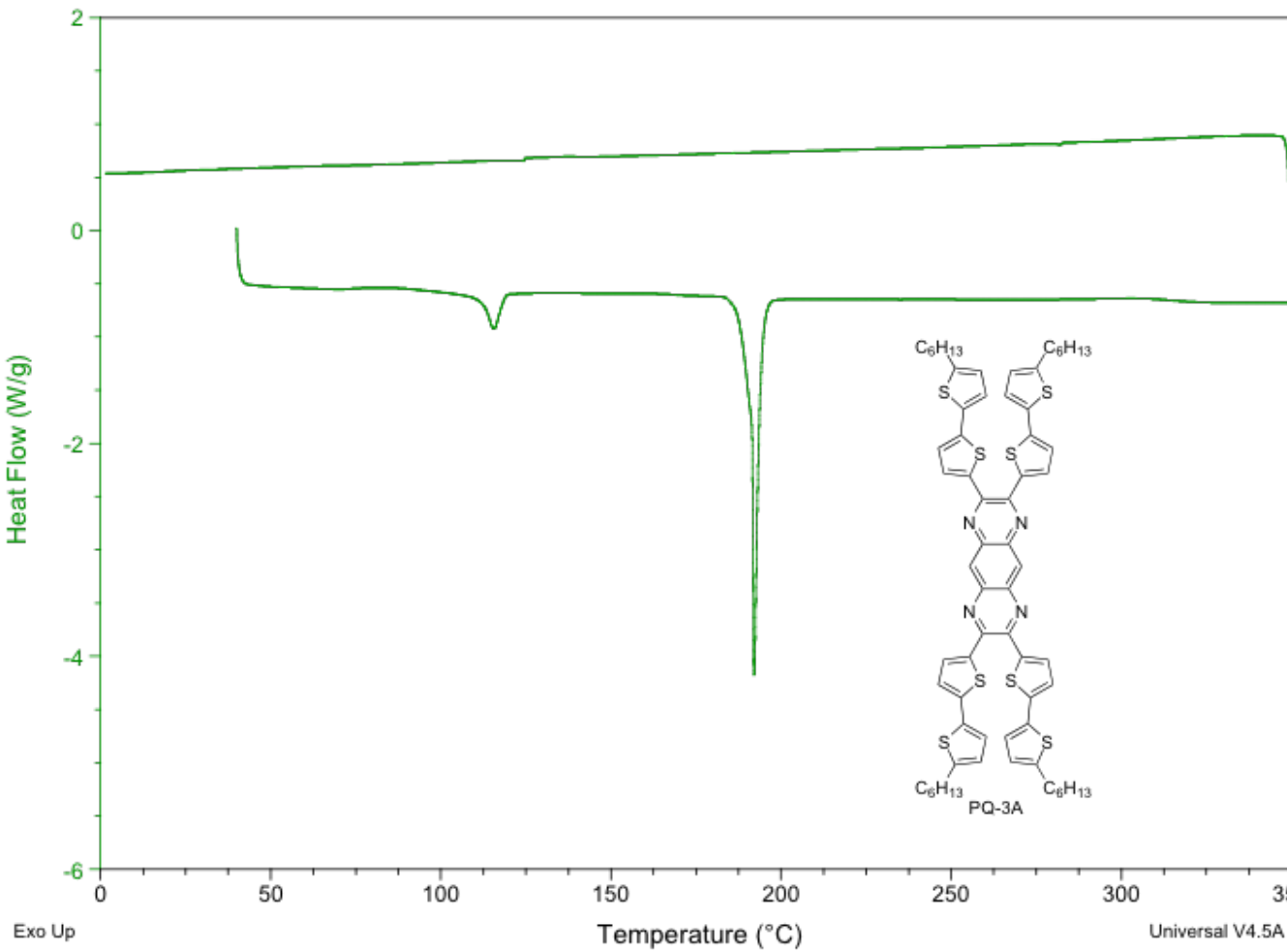
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Operator: TamTL
Run Date: 27-Mar-2009 21:19
Instrument: TGA Q500 V6.5 Build

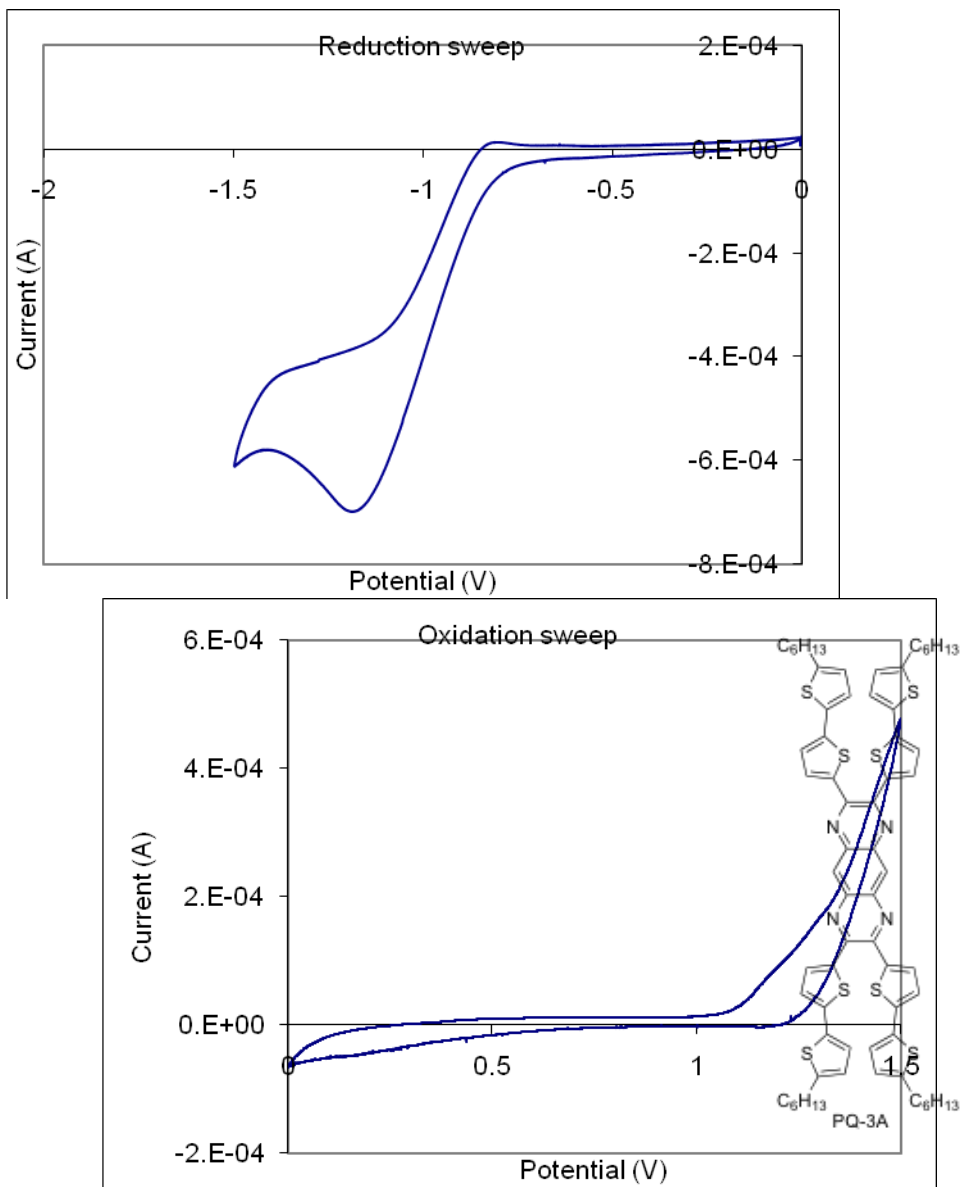


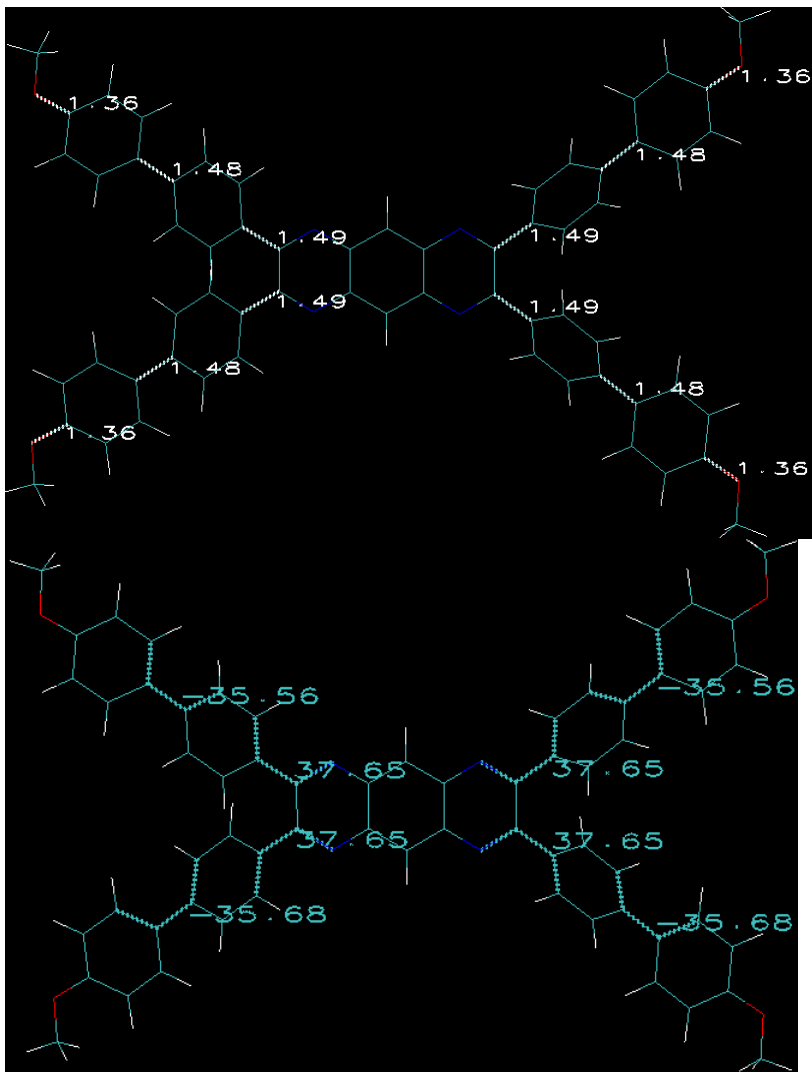
Sample: PQ-4TT
Size: 2.6660 mg
Method: TamTL

DSC

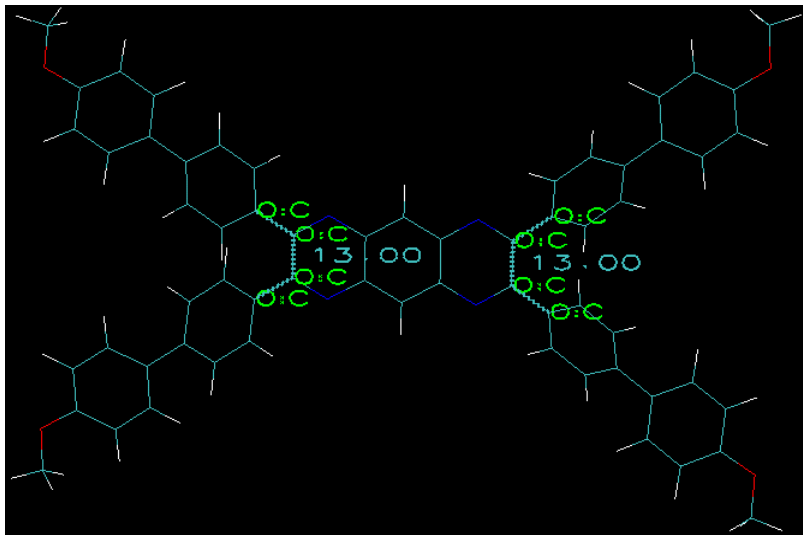
File: E:\RS documents\TamTL\PQ-4TT
Operator: TamTL
Run Date: 24-Apr-2009 17:27
Instrument: DSC Q10 V9.6 Build 290



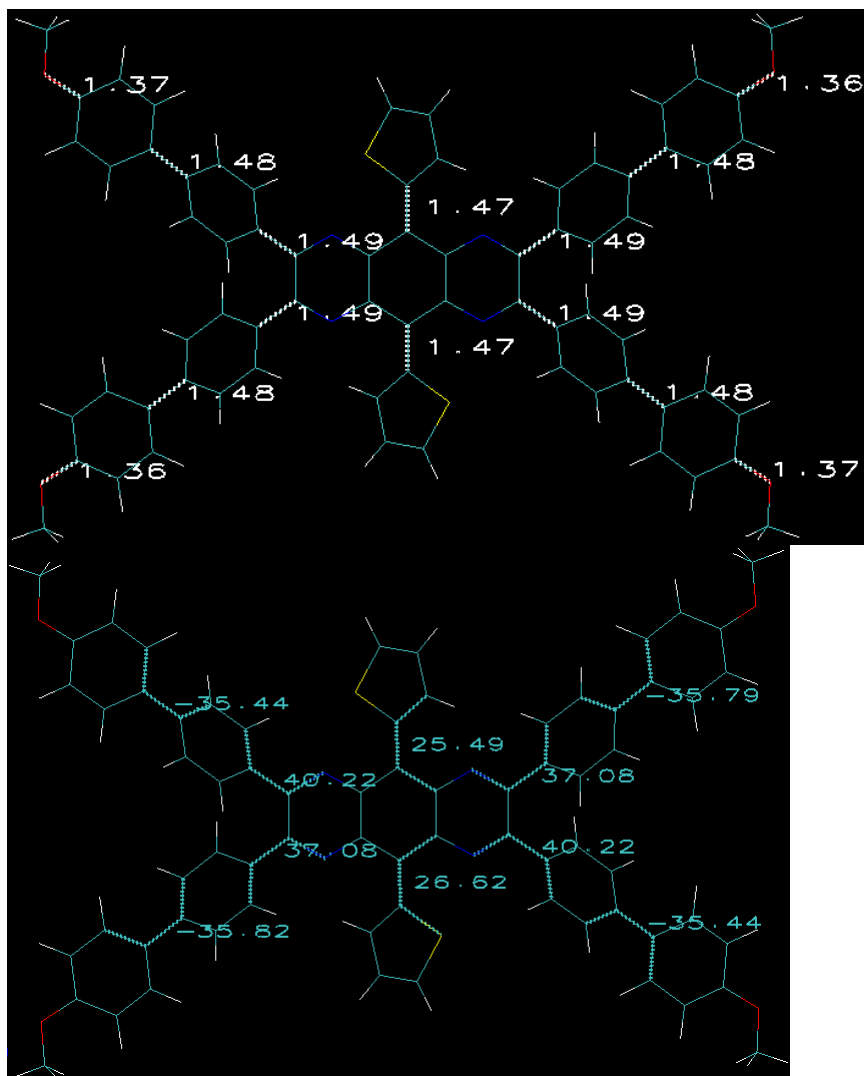




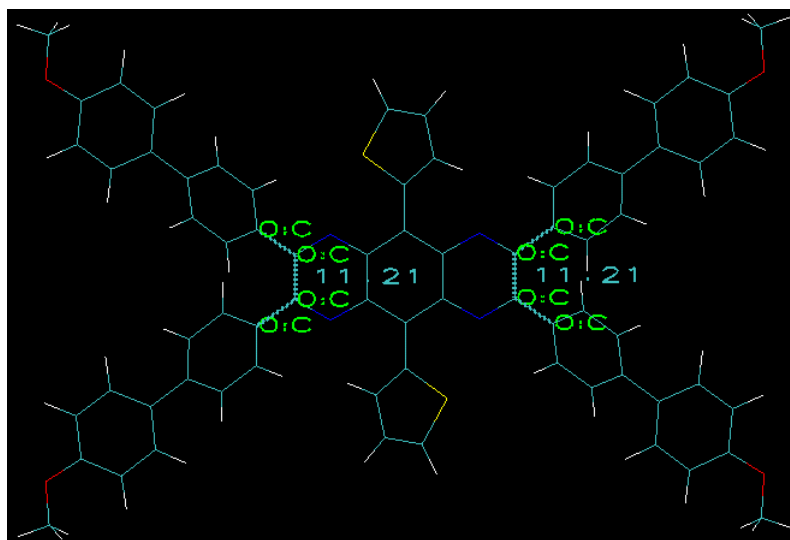
Dihedral angles for PQ-1A



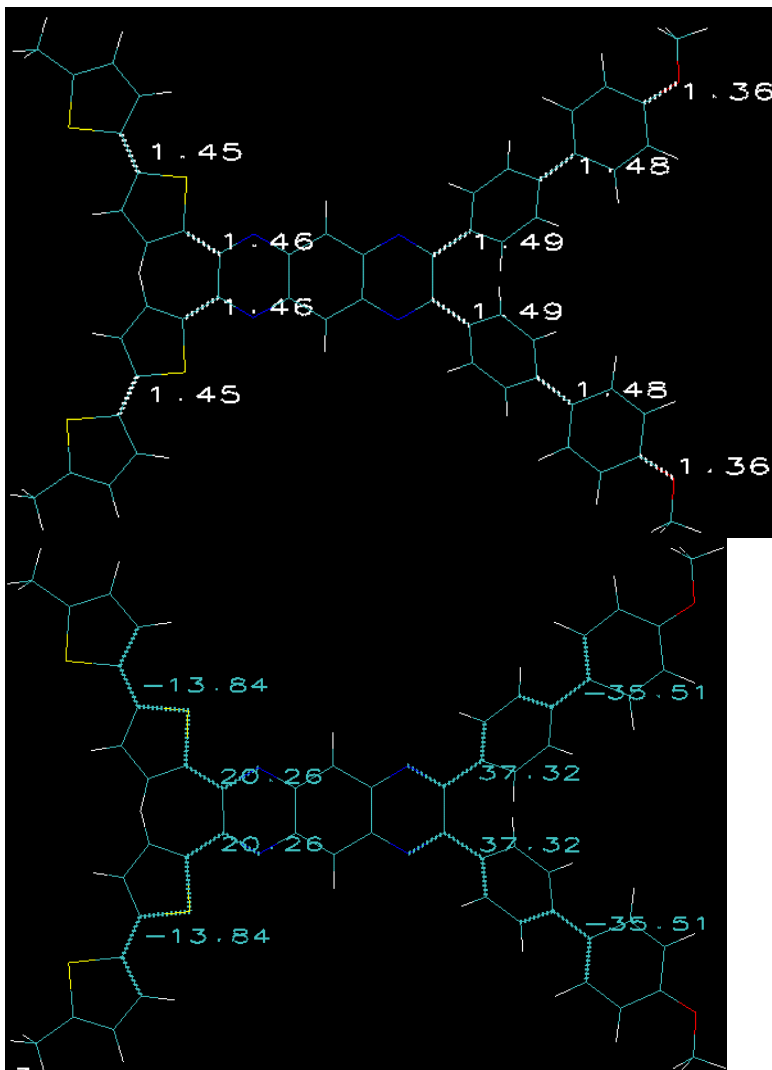
Twist angles and PQ-1A



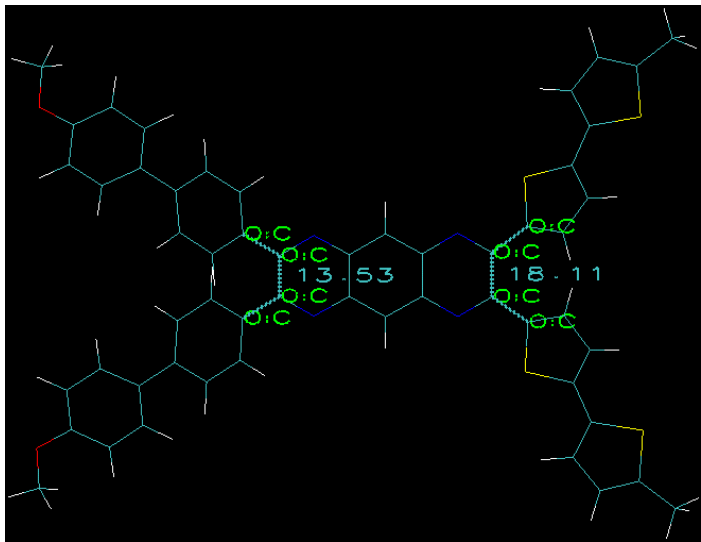
Dihedral angles of PQ-1B.



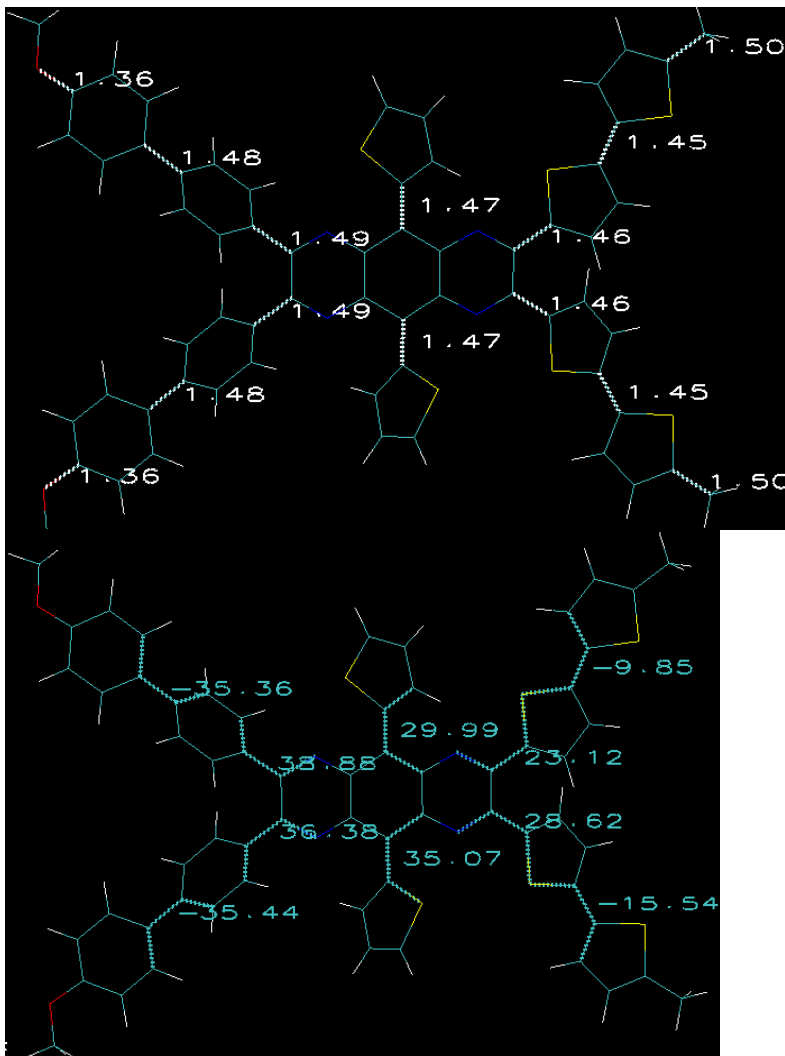
Twist angles of PQ-1B.



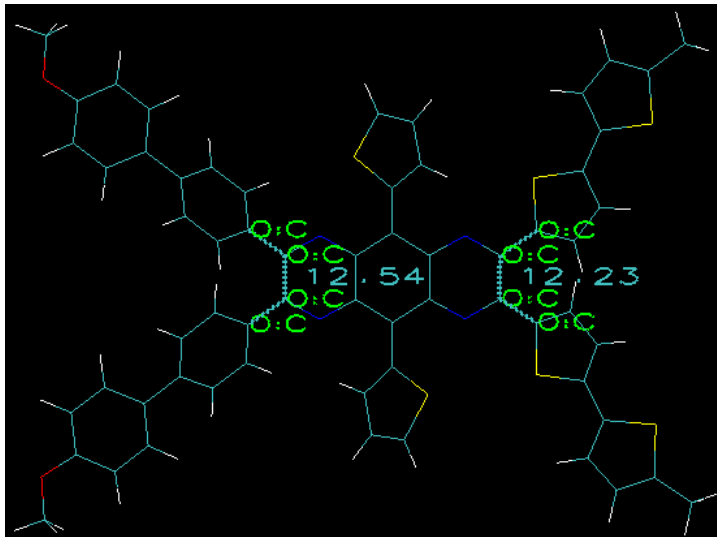
Dihedral angles of PQ-2A.



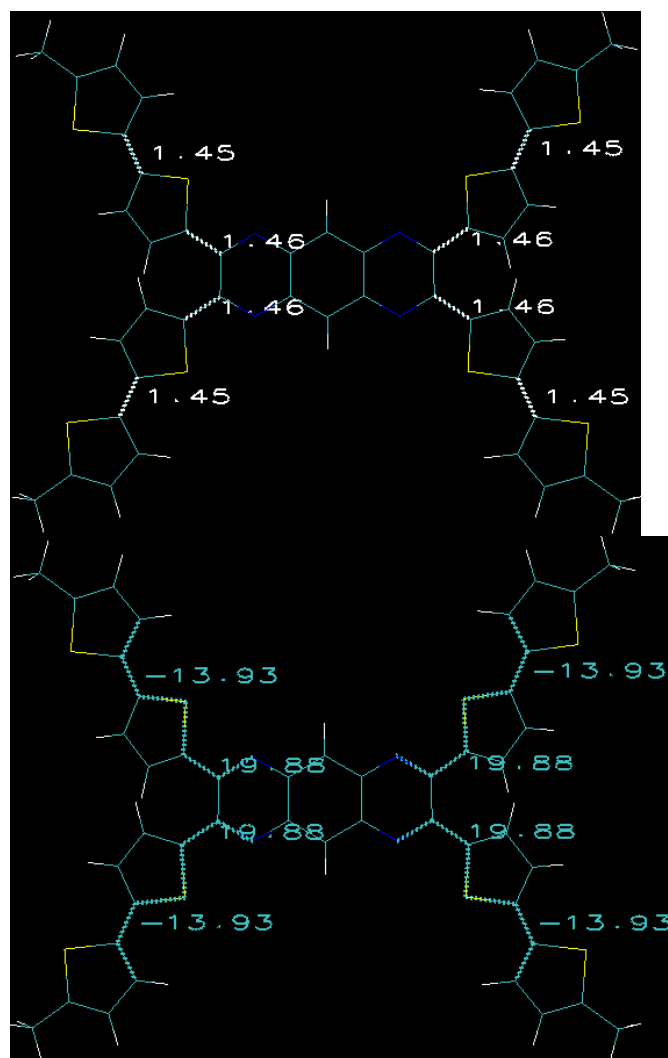
Twist angles of PQ-2A.



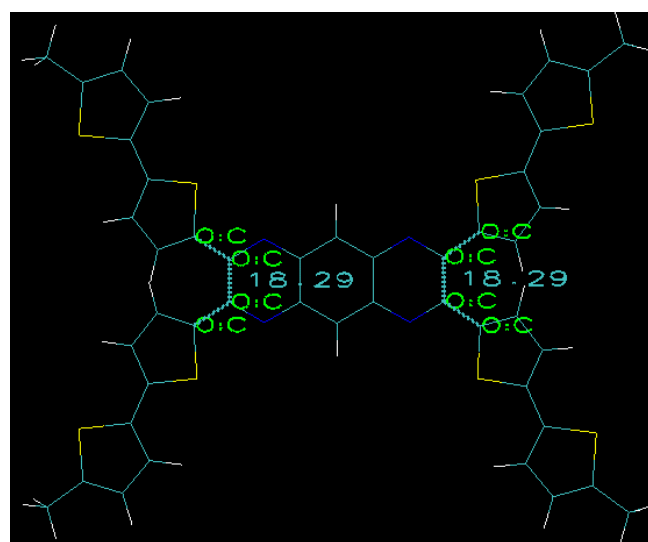
Dihedral angles of PQ-2B.



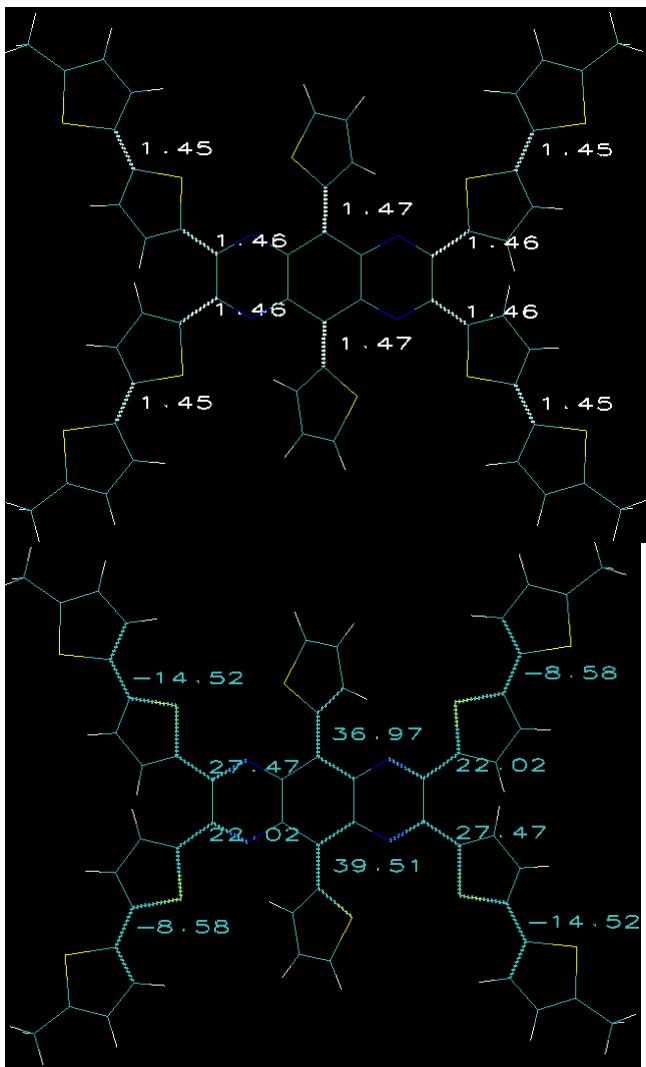
Twist angles of PQ-2B.



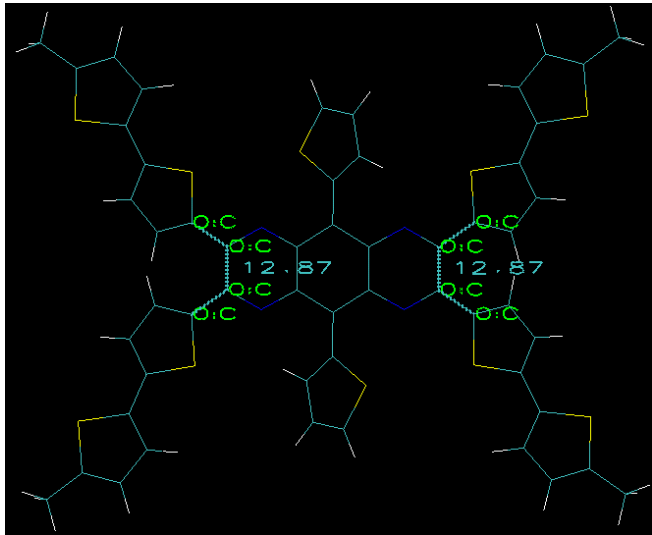
Dihedral angles of PQ-3A.



Twist angles of PQ-3A.



Dihedral angles of PQ-3B.



Twist angles of PQ-3B.