Supporting Information

Synthesis and Structure of Azole-Fused Indeno[2,1-c]Quinolines and their Antimycobacterial properties

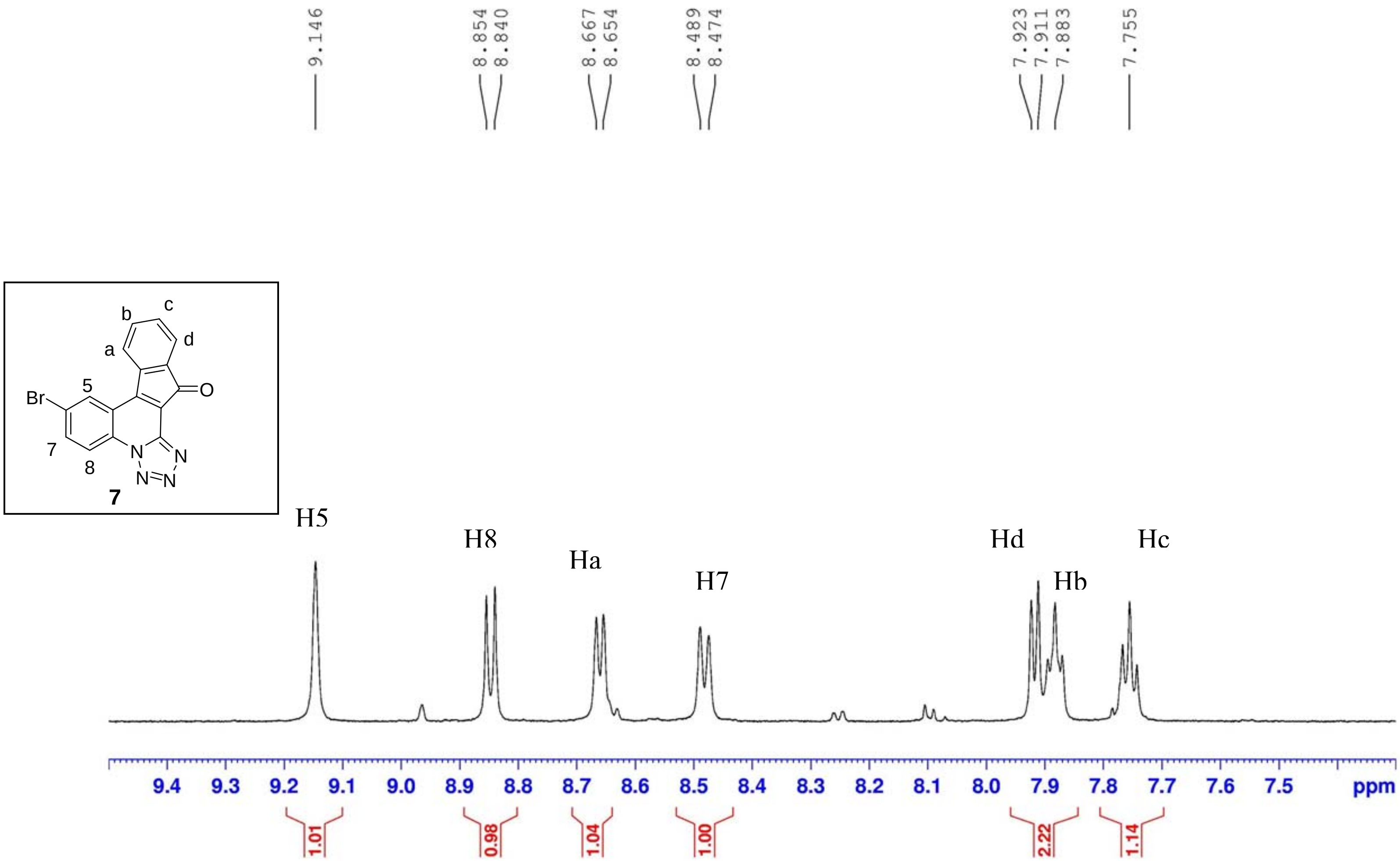
Ram Shankar Upadhayaya[a], Popat D. Shinde[a], Aftab Y. Sayyed[a], Sandip A. Kadam[a], Amit N. Bawane[a], Avijit Poddar[b], Oleksandr Plashkevych[c], Andras Földesi[c] and Jyoti Chattopadhyaya*[,c]

[a]*Institute of Molecular Medicine, Pune 411 057, India.*
[b]*Institute of Molecular Medicine, Calcutta 700 091, India.*

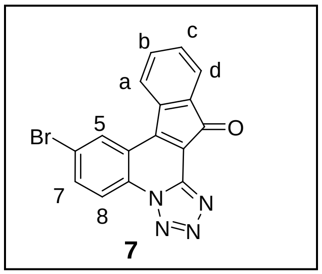
[c] *Bioorganic Chemistry Program, Department of Cell and Molecular Biology, Biomedical Centre, Uppsala University, SE-75123 Uppsala, Sweden.*

** Corresponding Author*
Phone: +46-18-4714577, Fax: +46-18-554495
Email: jyoti@boc.uu.se

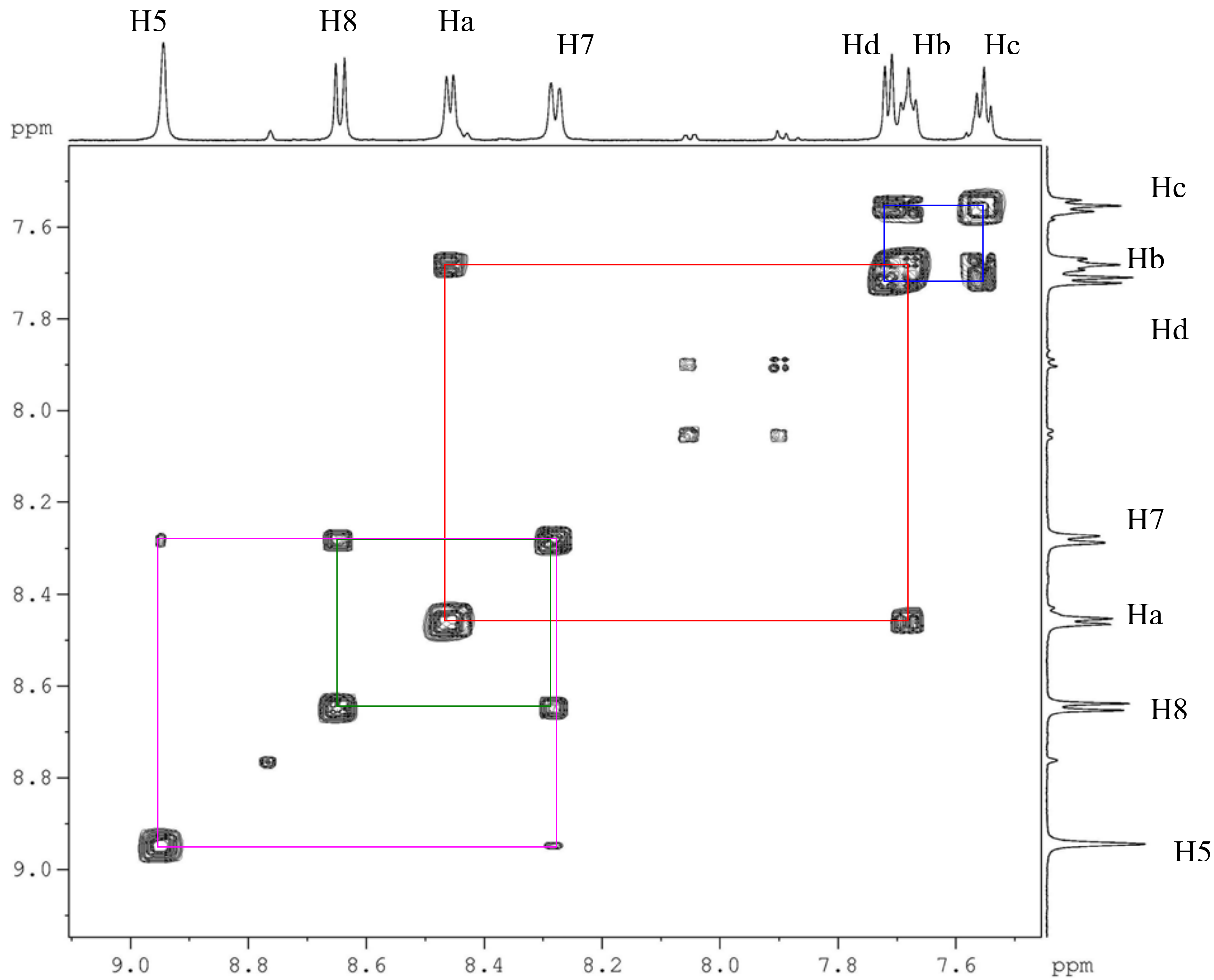
Table of Contents



Br
5
7
8
a
b
c
d
O
N
N
N
N
7
9.146
8.854
8.840
8.667
8.654
8.489
8.474
7.923
7.911
7.883
7.755
H5
H8
Ha
H7
Hd
Hb
Hc
9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
1.01
0.98
1.04
1.00
2.22
1.14



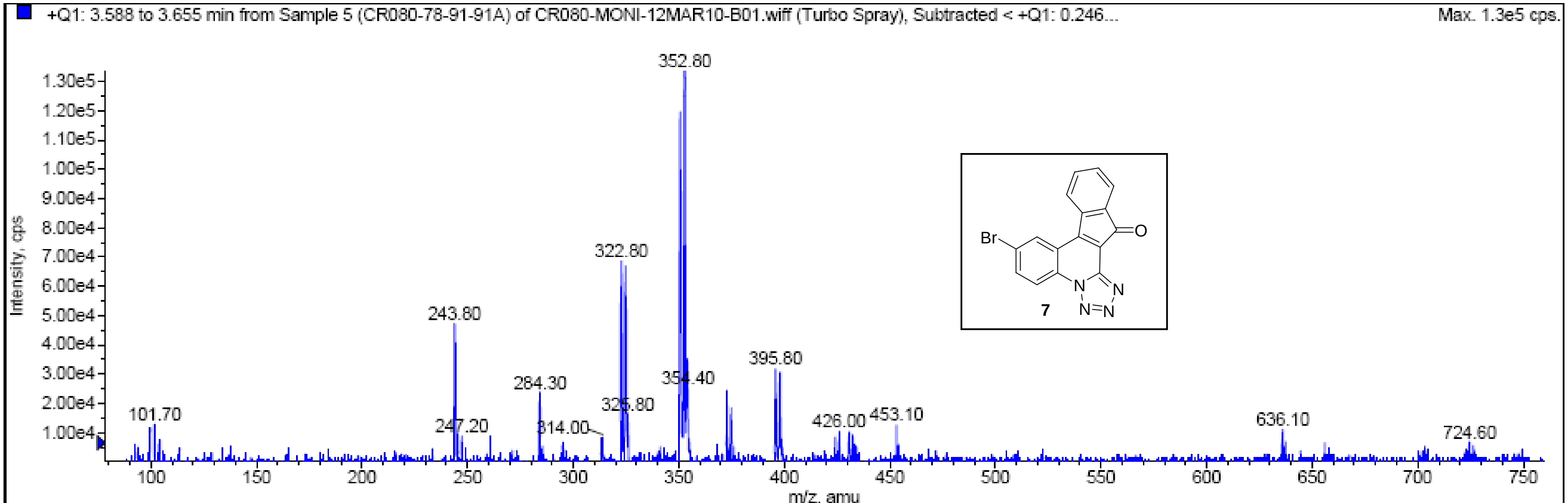
b
c
a
d
Br
5
O
7
8
N
N
N
N
7

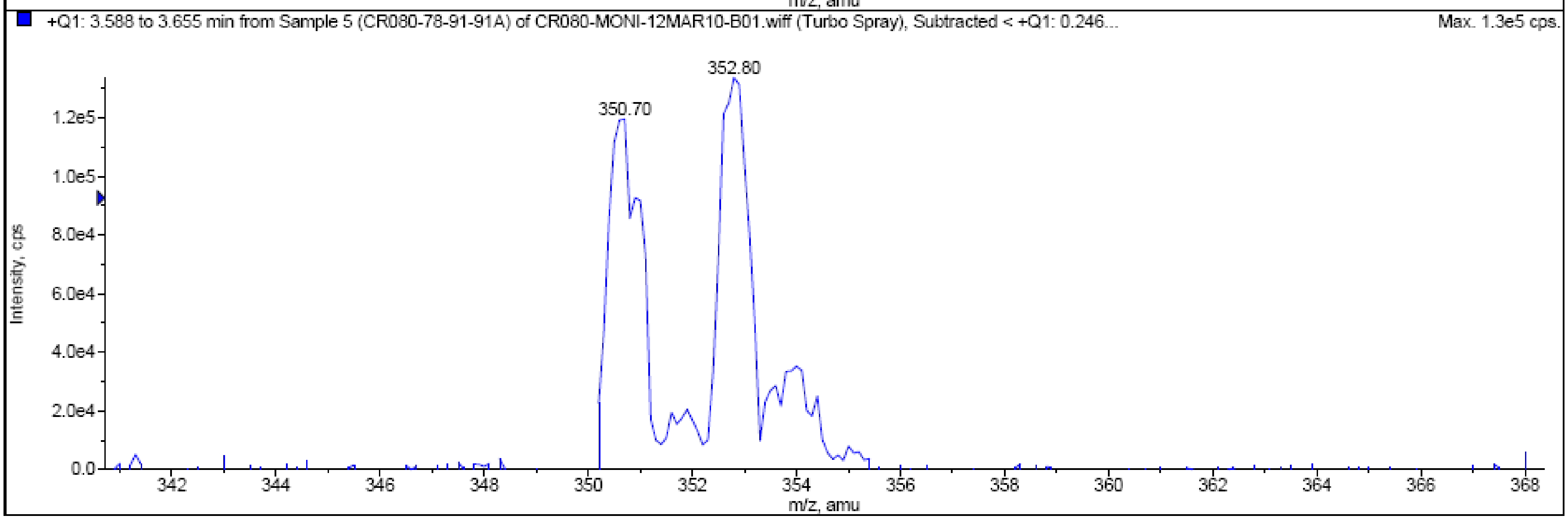


H5
H8
Ha
H7
Hd
Hb
Hc
ppm
7.6
7.8
8.0
8.2
8.4
8.6
8.8
9.0
ppm

INDIA

Sample Name: CR080-78-91-91A Acq. Time: 12:15 Acq. Date: Friday, March 12, 2010





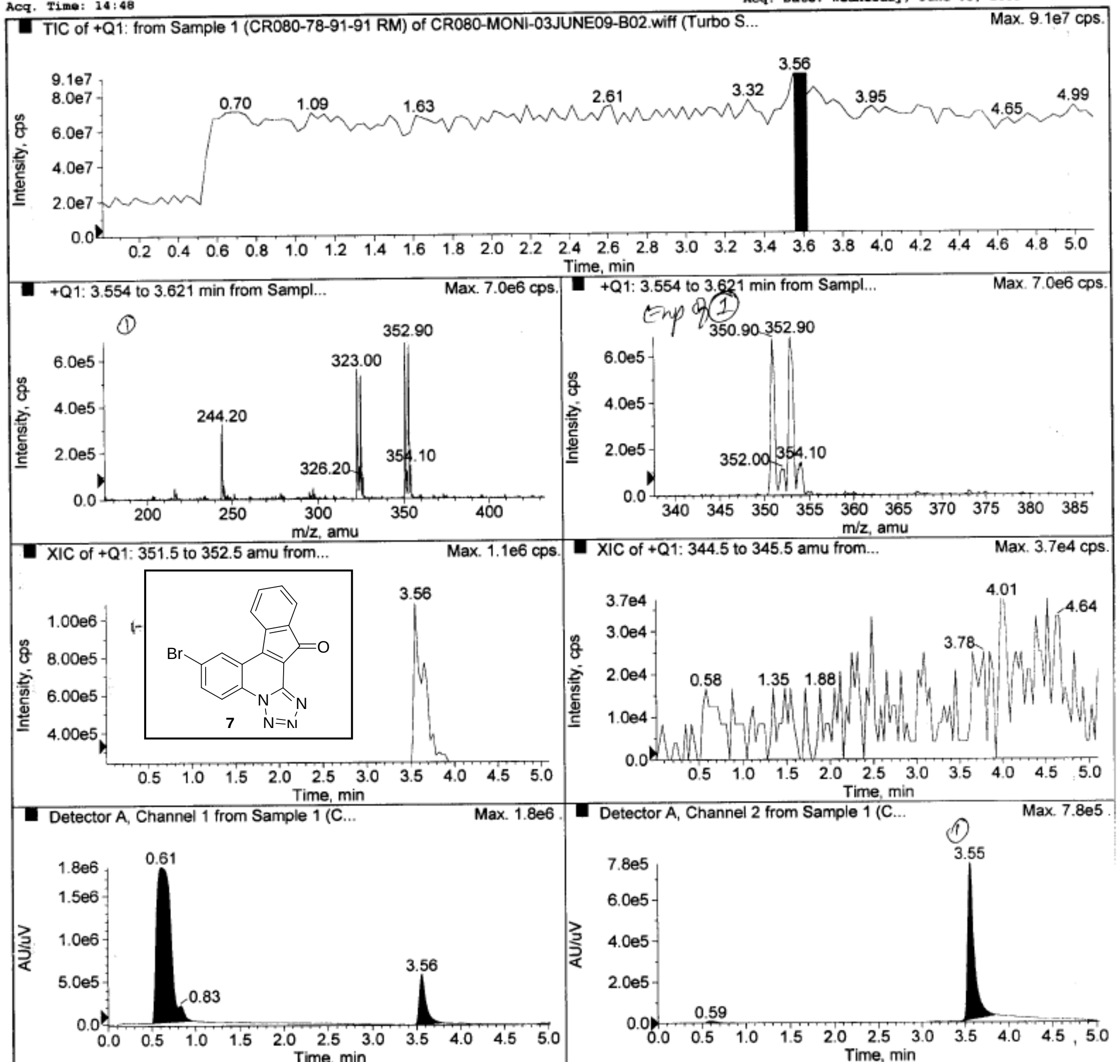
*Sample Comment: [M+H] Expected 351 **Analyzed By : **Checked By :

Sample Name: CR080-78-91-91 RM

CHEMBIOTEK A TCG Lifesciences Enterprise,PUNE

Acq. Time: 14:48

Acq. Date: Wednesday, June 03, 2009



Peak List for "Detector A, Channel 1 from Sample 1 (CR080-78-9

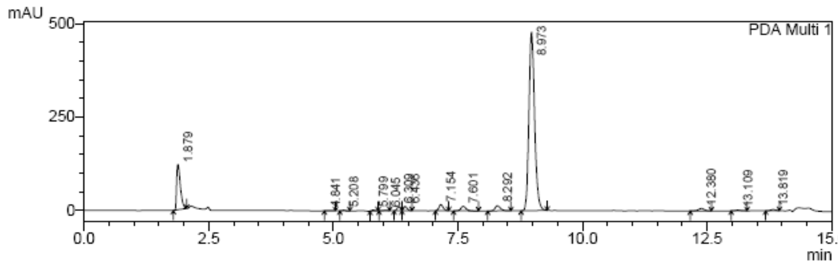
	Time (min)	Area (counts)	%Area	Height
1	0.6134	2.0834e7	85.7984	1.8207e6
2	0.8282	4.1998e5	1.7296	9.5119e4
3	3.5558	3.0285e6	12.4720	5.8564e5

Peak List for "Detector A, Channel 2 from Sample 1 (CR080-78-9

	Time (min)	Area (counts)	%Area	Height
1	0.5948	2.5812e4	0.6102	5497.6043
2	3.5545	4.2043e6	99.3898	7.6826e5

Sample Name : CR080-78-91-91A
Sample ID : CR080-78-91-91A
Column : Gemini C-18 (150 x 4.6 mm)
Vial # : 61
Inj. Volume : 25 uL
Tray # : 1
Acquired by : AVINASH

Data File Name : 15-02-10_CR080-78-91-91A_03.lcd
Method File Name : GENERAL_B2.lcm
Batch File Name : 150210.lcb
Data Acquired : 2/15/2010 2:48:06 PM
Data Processed : 2/15/2010 3:13:10 PM
Ref.No.: DI/A0257/95

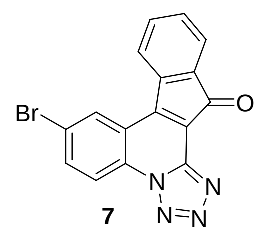


1 PDA Multi 1/246nm 4nm

PeakTable

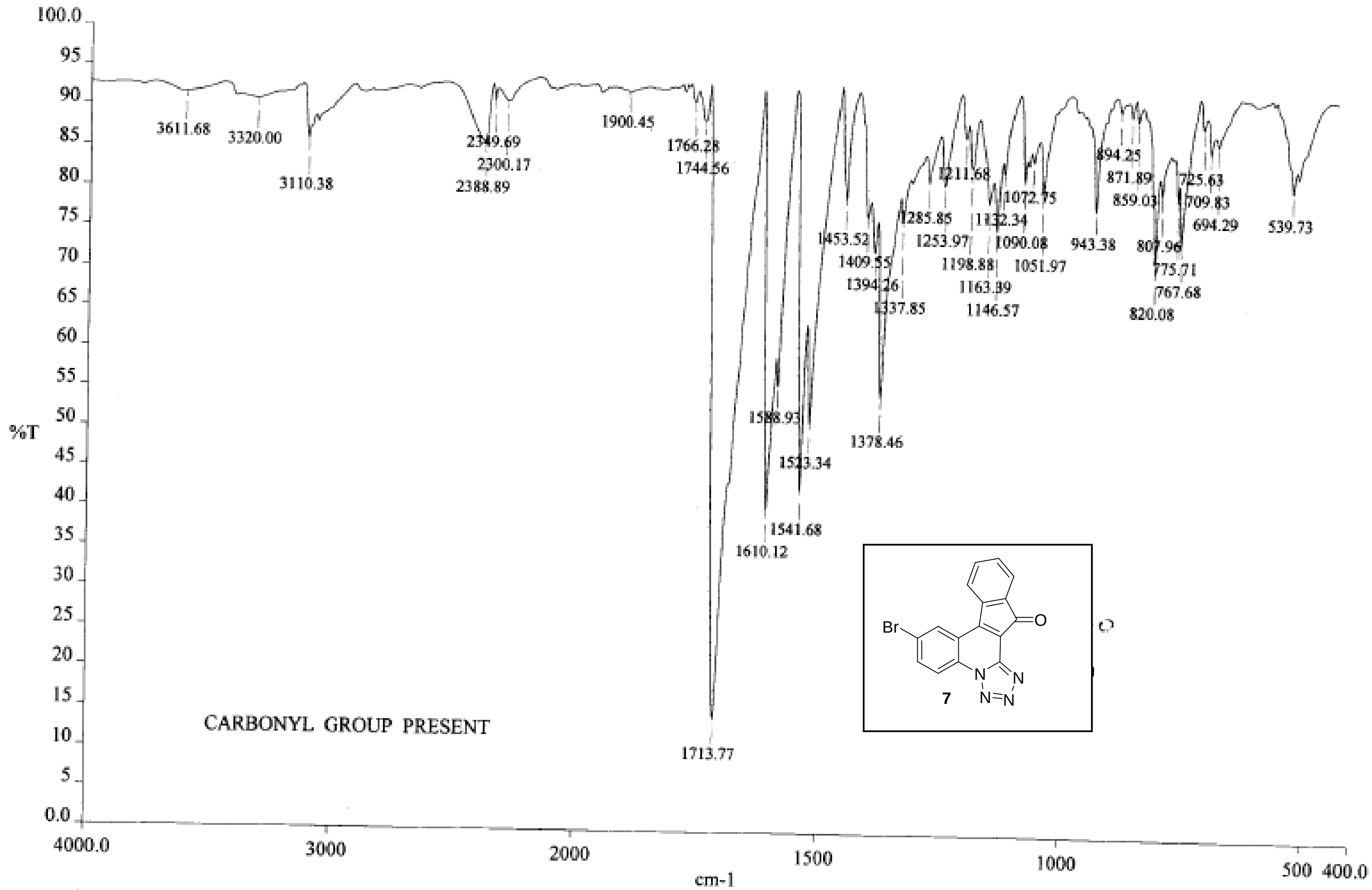
PDA Ch1 246nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	1.88	634154	12.87	121353
2	4.84	1957	0.04	296
3	5.21	7937	0.16	1666
4	5.80	11282	0.23	2390
5	6.04	4739	0.10	752
6	6.31	53977	1.10	11220
7	6.44	59610	1.21	11560
8	7.15	95106	1.93	16623
9	7.60	87951	1.79	12261
10	8.29	101689	2.06	14042
11	8.97	3778861	76.71	478496
12	12.38	53693	1.09	6633
13	13.11	12458	0.25	1831
14	13.82	22763	0.46	3460
Total		4926178	100.00	682582

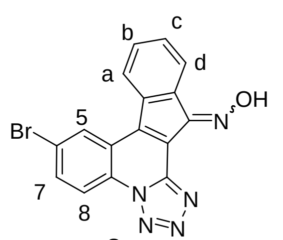


7

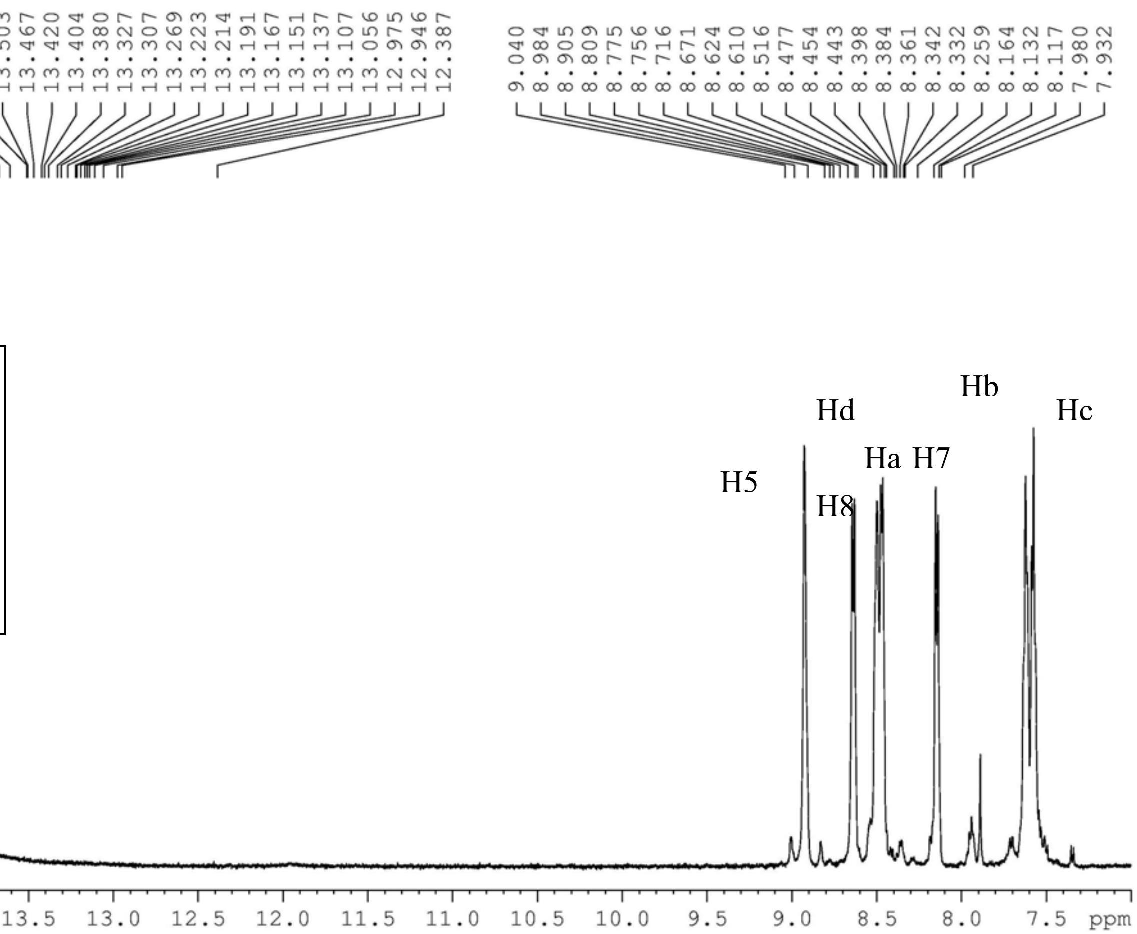
C:\LabSolutions\Data\Project1\HPLC-02\FEB-10\15-02-10_CR080-78-91-91A_03.lcd

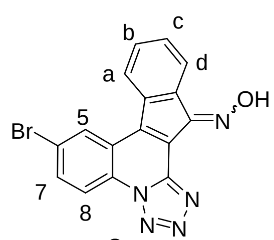


100.0
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0.0
%T
4000.0
3000
2000
1500
1000
500 400.0
cm-1
3611.68
3320.00
3110.38
2349.69
2300.17
2388.89
1900.45
1766.28
1744.56
1713.77
1610.12
1588.93
1541.68
1523.34
1453.52
1409.55
1394.26
1378.46
1337.85
1285.85
1253.97
1211.68
1198.88
1163.39
1146.57
1132.34
1090.08
1072.75
1051.97
943.38
894.25
871.89
859.03
820.08
807.96
775.71
767.68
725.63
709.83
694.29
539.73
CARBONYL GROUP PRESENT
Br
O
N
7

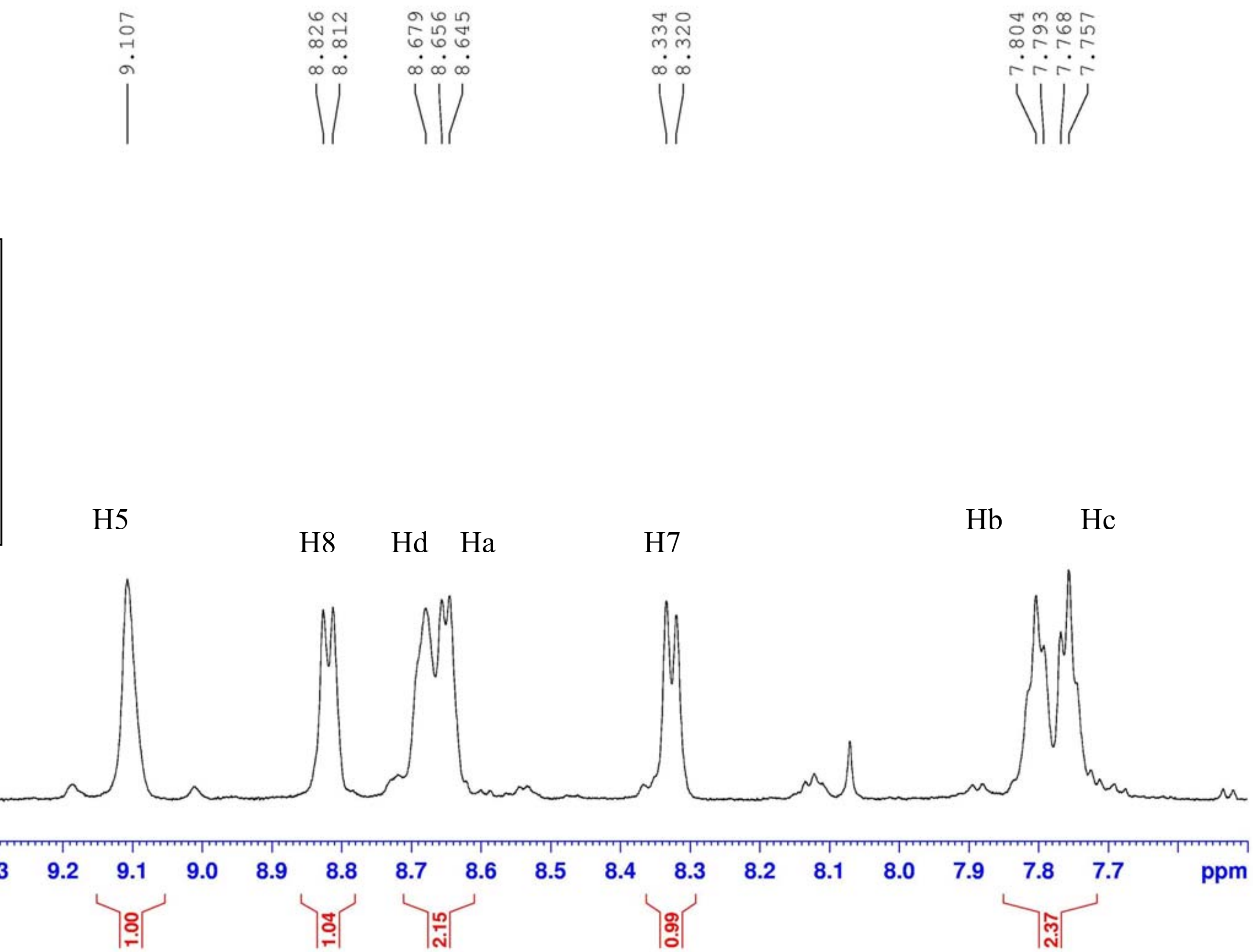

a
b
c
d
5
7
8
Br
N
N
N
N
N
OH

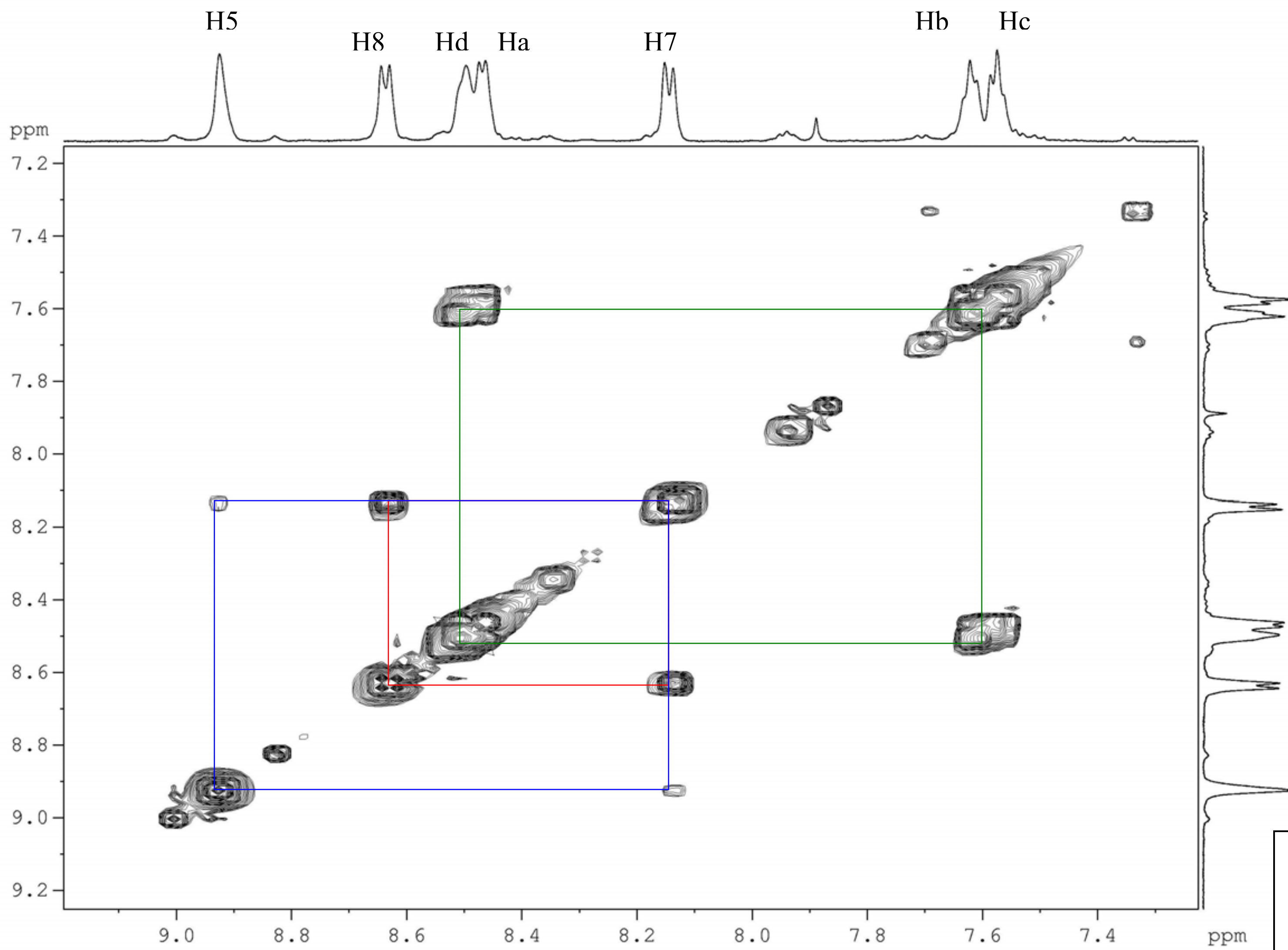
8

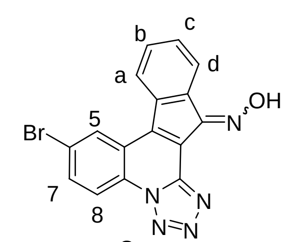

13.840
13.803
13.762
13.757
13.704
13.676
13.608
13.509
13.503
13.467
13.420
13.404
13.380
13.327
13.307
13.269
13.223
13.214
13.191
13.167
13.151
13.137
13.107
13.056
12.975
12.946
12.387
9.040
8.984
8.905
8.809
8.775
8.756
8.716
8.671
8.624
8.610
8.516
8.477
8.454
8.443
8.398
8.384
8.361
8.342
8.332
8.259
8.164
8.132
8.117
7.980
7.932
H5
Hd
H8
Ha
H7
Hb
Hc
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
ppm

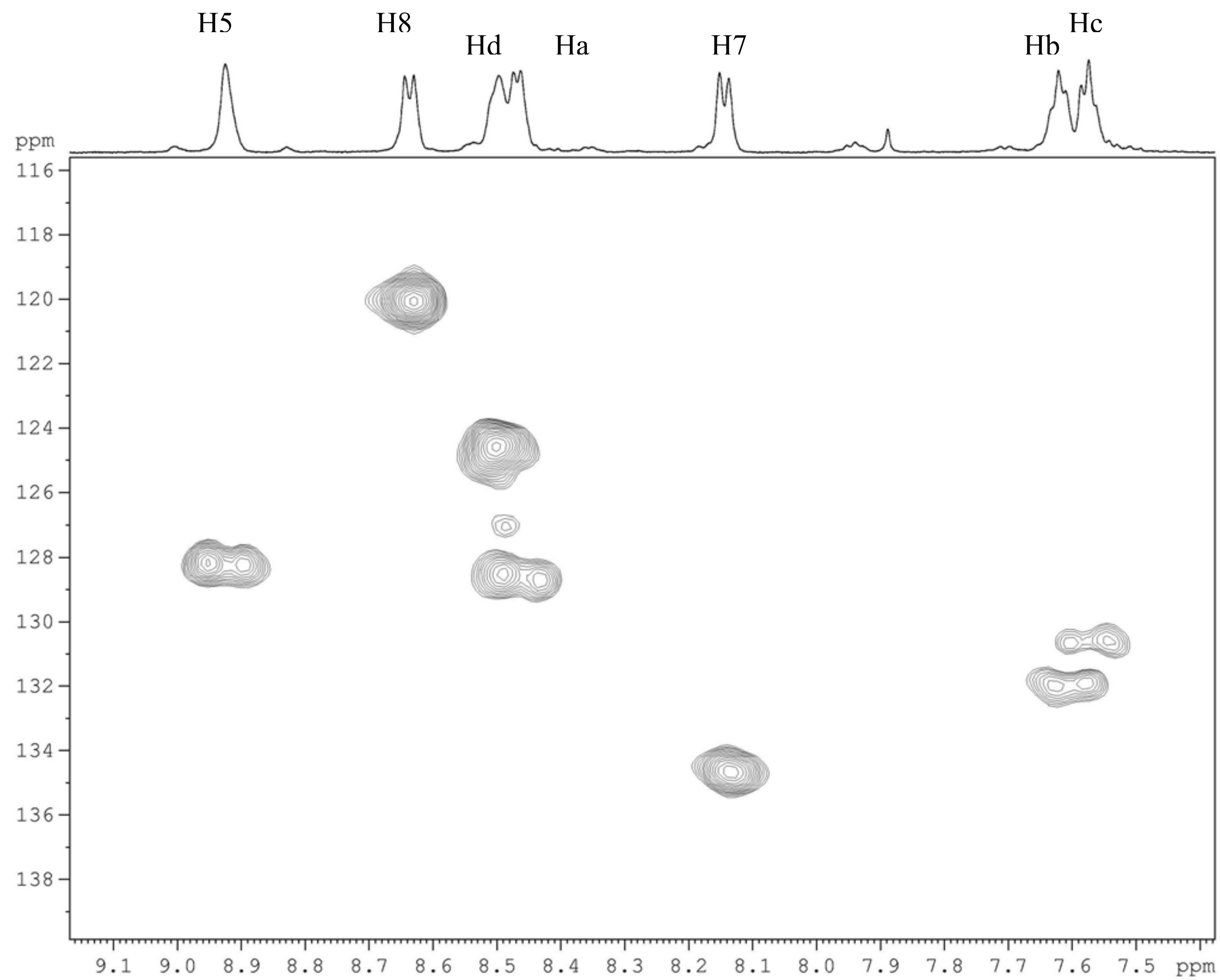

b
c
a
d
OH
N
Br
5
7
8
N
N
N
N

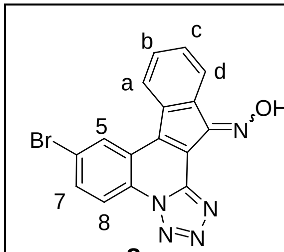
8


9.107
8.826
8.812
8.679
8.656
8.645
8.334
8.320
7.804
7.793
7.768
7.757
H5
H8
Hd
Ha
H7
Hb
Hc
9.4
9.3
9.2
9.1
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
ppm
1.00
1.04
2.15
0.99
2.37

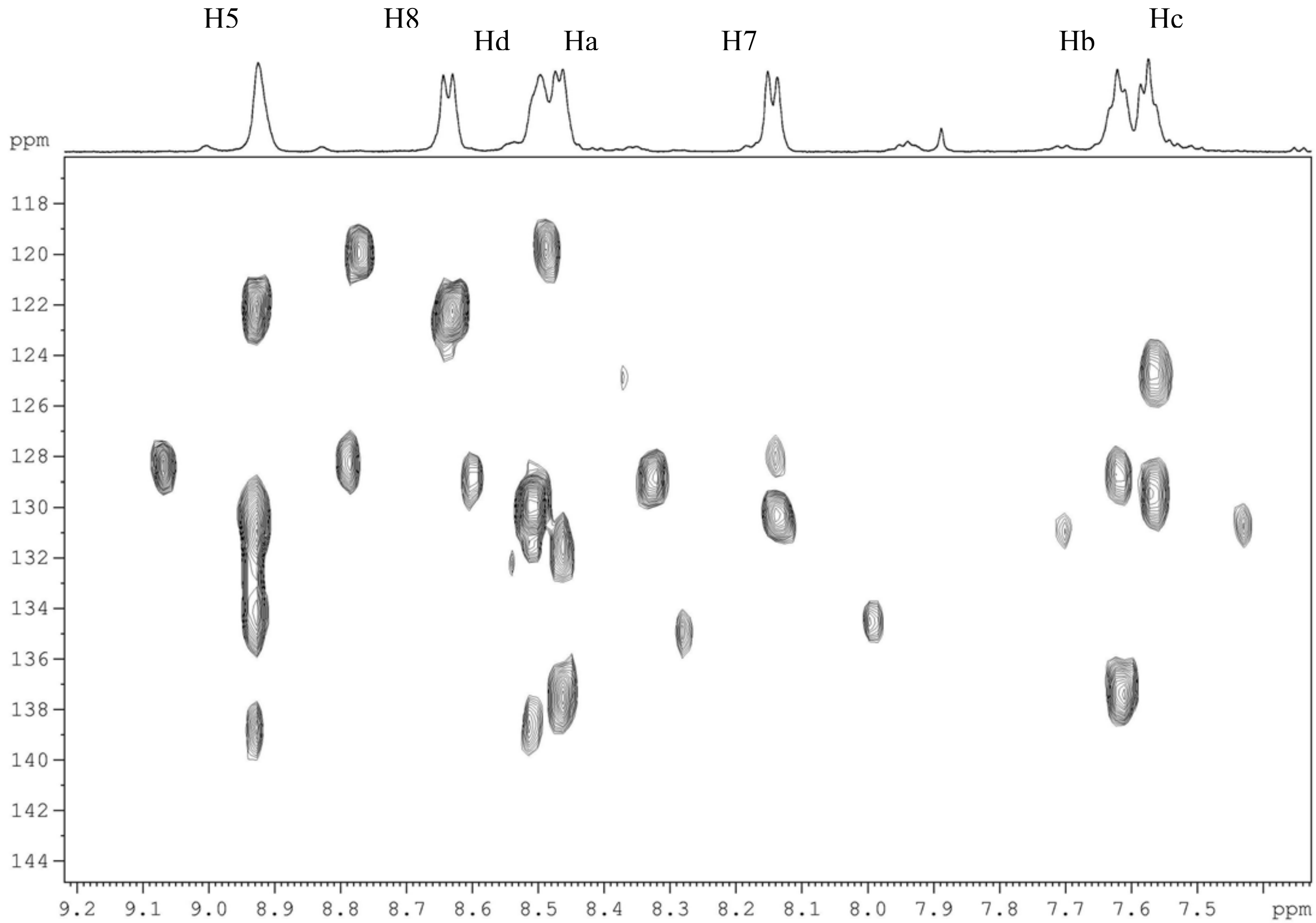

H5
H8
Hd
Ha
H7
Hb
Hc
ppm
7.2
7.4
7.6
7.8
8.0
8.2
8.4
8.6
8.8
9.0
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
ppm
Hc
Hb
H7
Ha
Hd
H8
H5

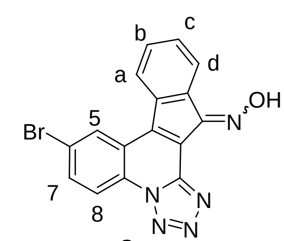

b
c
a
d
5
Br
OH
N
7
8
N
N
N
N
8


H5
H8
Hd
Ha
H7
Hb
Hc
ppm
116
118
120
122
124
126
128
130
132
134
136
138
9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm


b
c
a
d
OH
N
Br
5
7
8
N
N
N
N

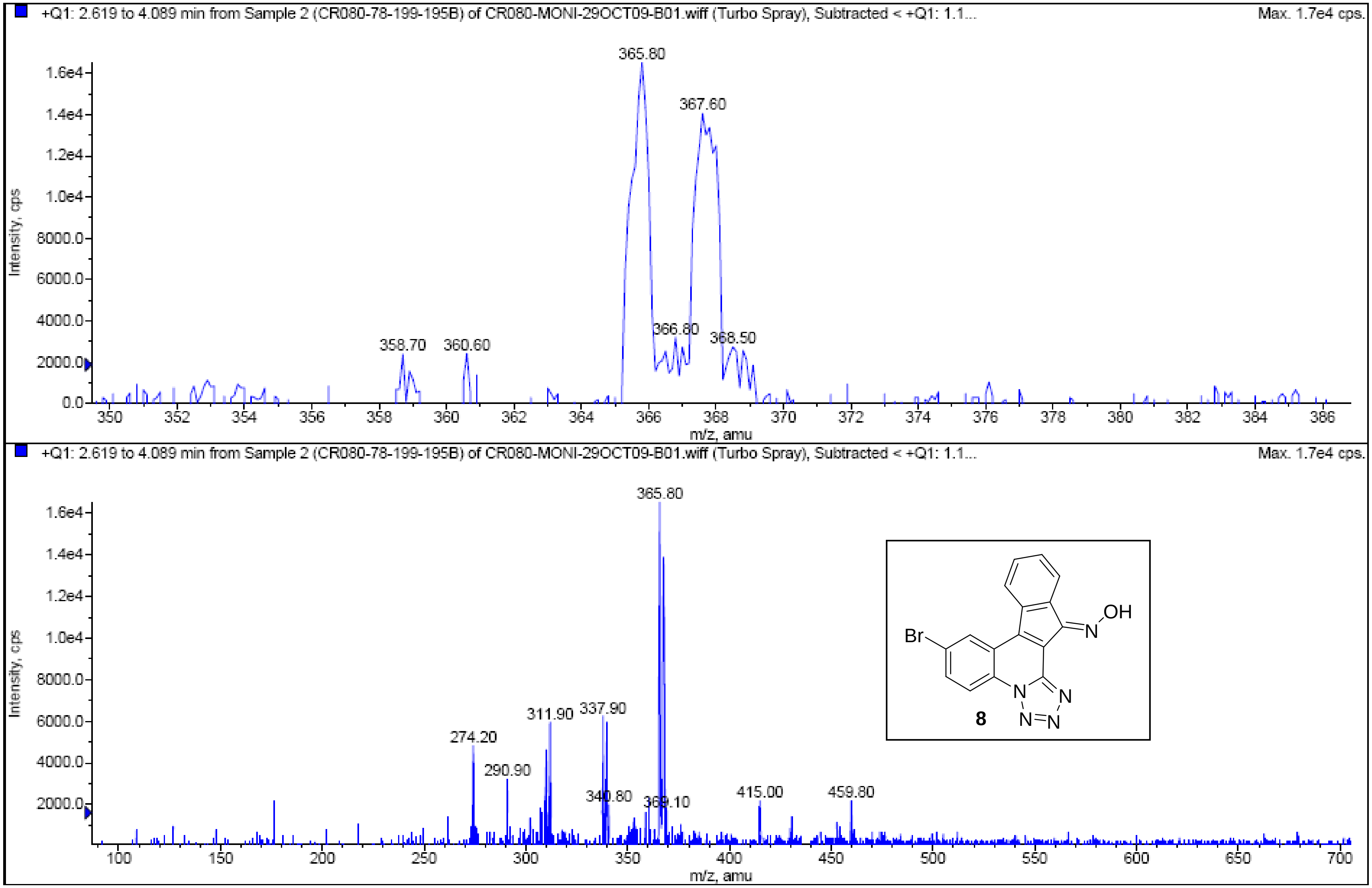
8


H5
H8
Hd
Ha
H7
Hb
Hc
ppm
118
120
122
124
126
128
130
132
134
136
138
140
142
144
9.2
9.1
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
ppm

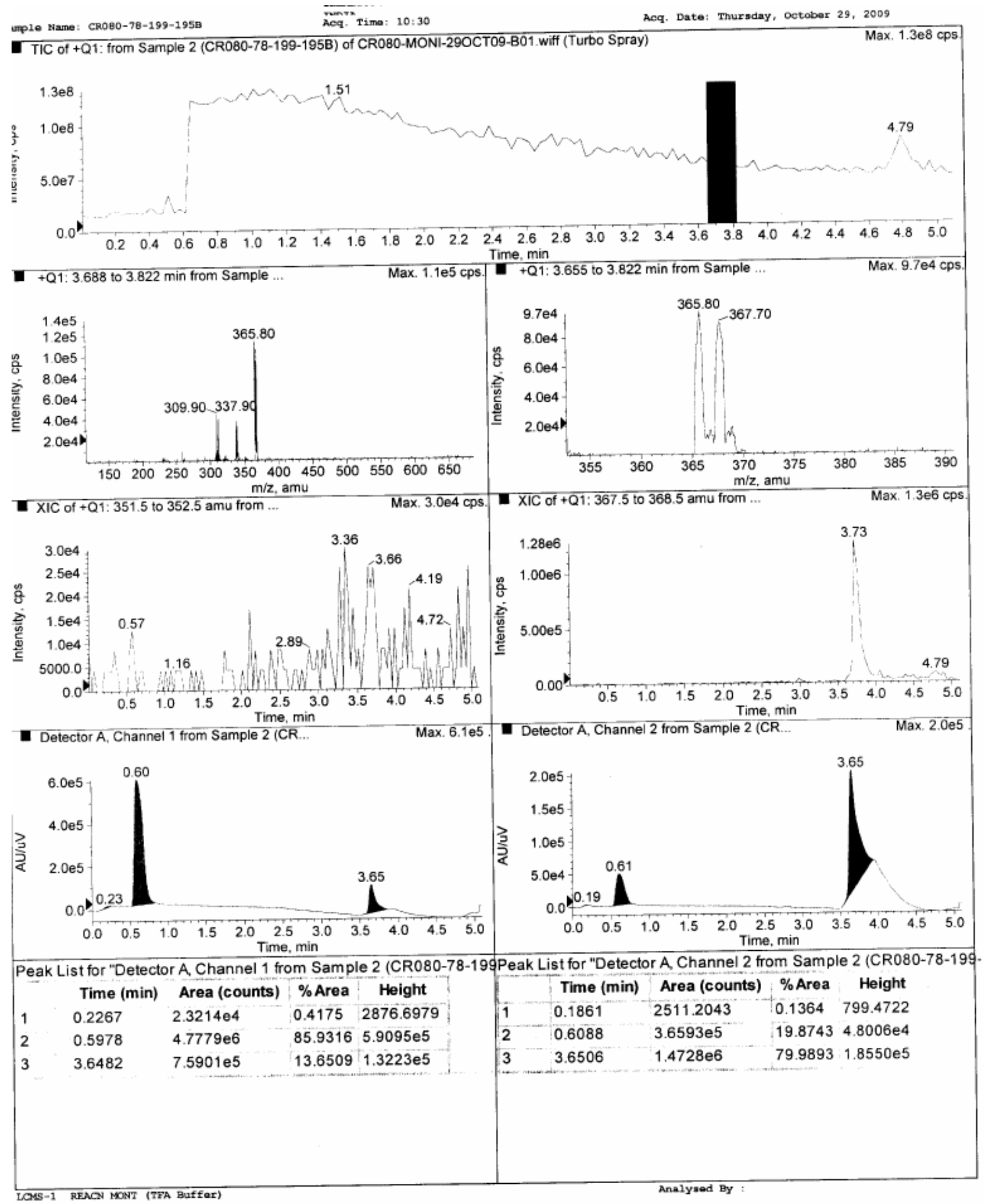

b
c
d
a
OH
N
5
Br
7
8
N
N
N
N

8

Sample Name: CR080-78-199-195B Acq. Time: 10:30 Acq. Date: Thursday, October 29, 2009



*Sample Comment: [M+H]366 Expected **Analyzed By : **Checked By :



Peak List for "Detector A, Channel 1 from Sample 2 (CR080-78-199

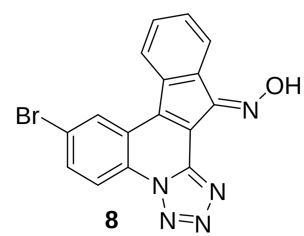
	Time (min)	Area (counts)	%Area	Height
1	0.2267	2.3214e4	0.4175	2876.6979
2	0.5978	4.7779e6	85.9316	5.9095e5
3	3.6482	7.5901e5	13.6509	1.3223e5

Peak List for "Detector A, Channel 2 from Sample 2 (CR080-78-199-

	Time (min)	Area (counts)	%Area	Height
1	0.1861	2511.2043	0.1364	799.4722
2	0.6088	3.6593e5	19.8743	4.8006e4
3	3.6506	1.4728e6	79.9893	1.8550e5

LCMS-1 REACN MONT (TFA Buffer)

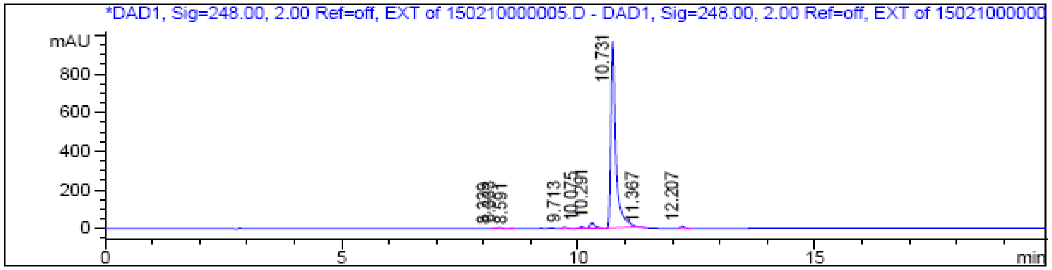
Analysed By :



8

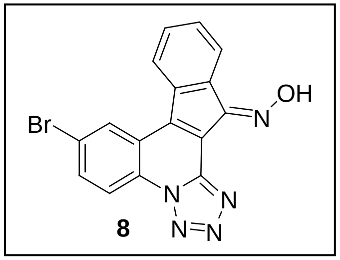
==
Sample:CR080-78-199-195 B ->
Column: XTERRA RP(250X4.6)mm 5µ

Injection date : Mon, 15. Feb. 2010 Location : Vial 22
Sample Name : CR080-78-199-195 B Inj. No. : 1
Acq Operator : BHUSHAN Inj. Vol. : 3 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _1.M
Last Changed : Mon, 15. Feb. 2010,
Acq. Method : C:\Chem32\2\DATA\FEB-10\150210A 2010-02-15 08-51-54\
UPLC_GENARAL_GRAD _1.M
Method ref : DI/A0257/92

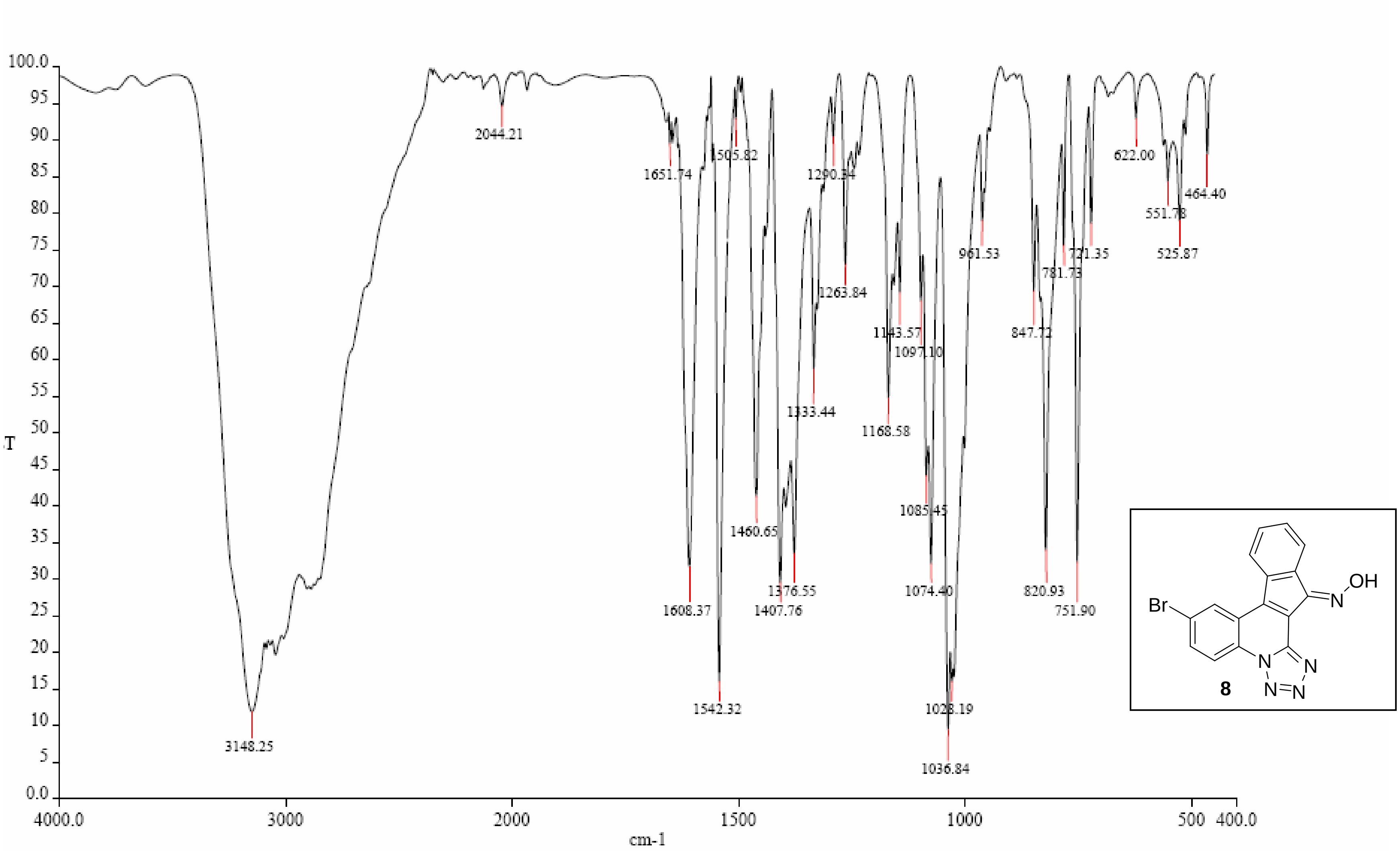


DAD1, Sig=248.00, 2.00 Ref=off, EXT

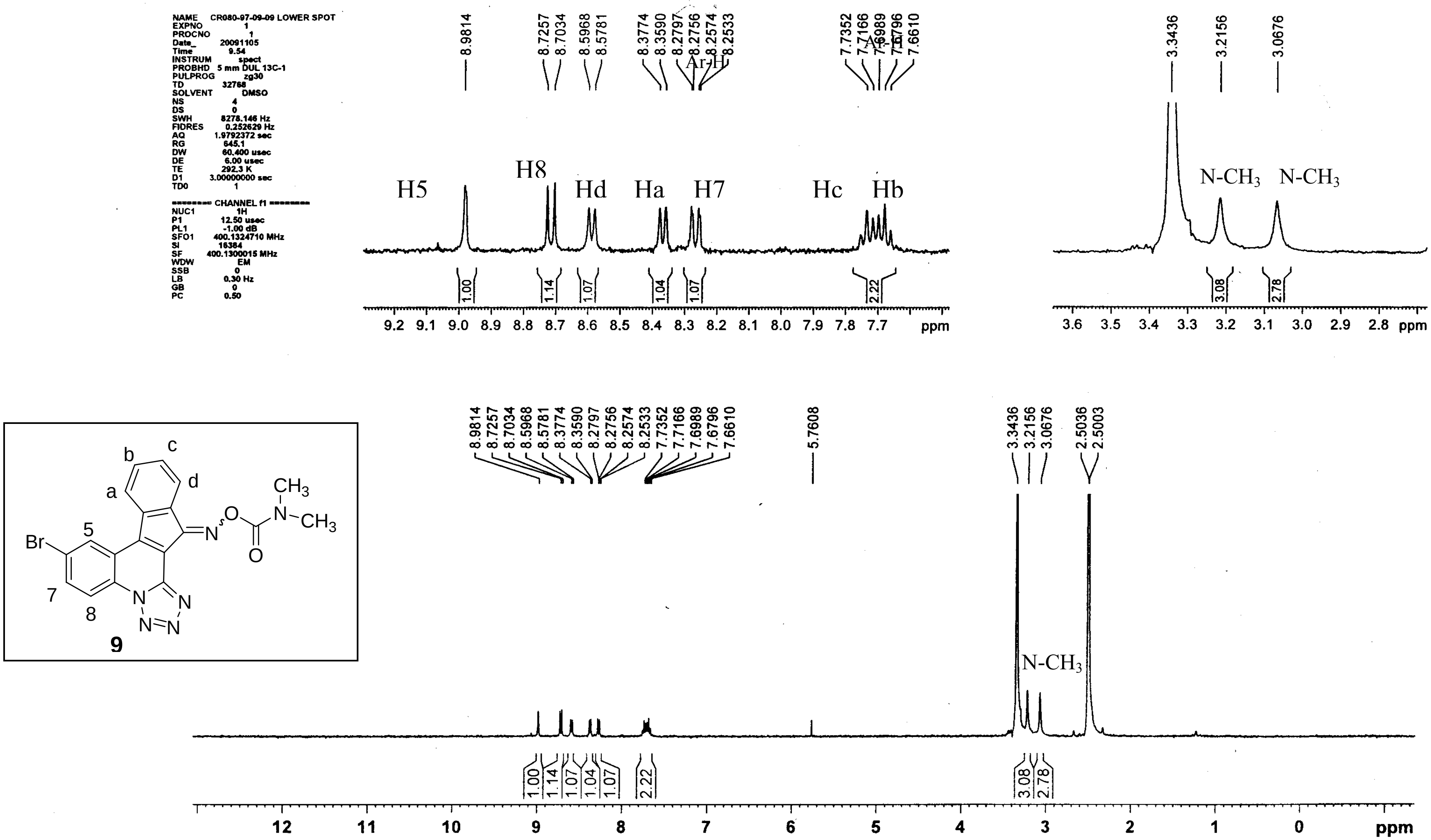
Peak #	RT (Min)	Width (Min)	Area	Area %
1	8.229	0.070	5.980	0.080
2	8.333	0.083	31.004	0.416
3	8.591	0.078	6.119	0.082
4	9.713	0.096	45.518	0.611
5	10.075	0.086	48.980	0.657
6	10.291	0.127	208.882	2.802
7	10.731	0.121	7.020e3	94.185
8	11.367	0.074	8.972	0.120
9	12.207	0.106	78.009	1.047

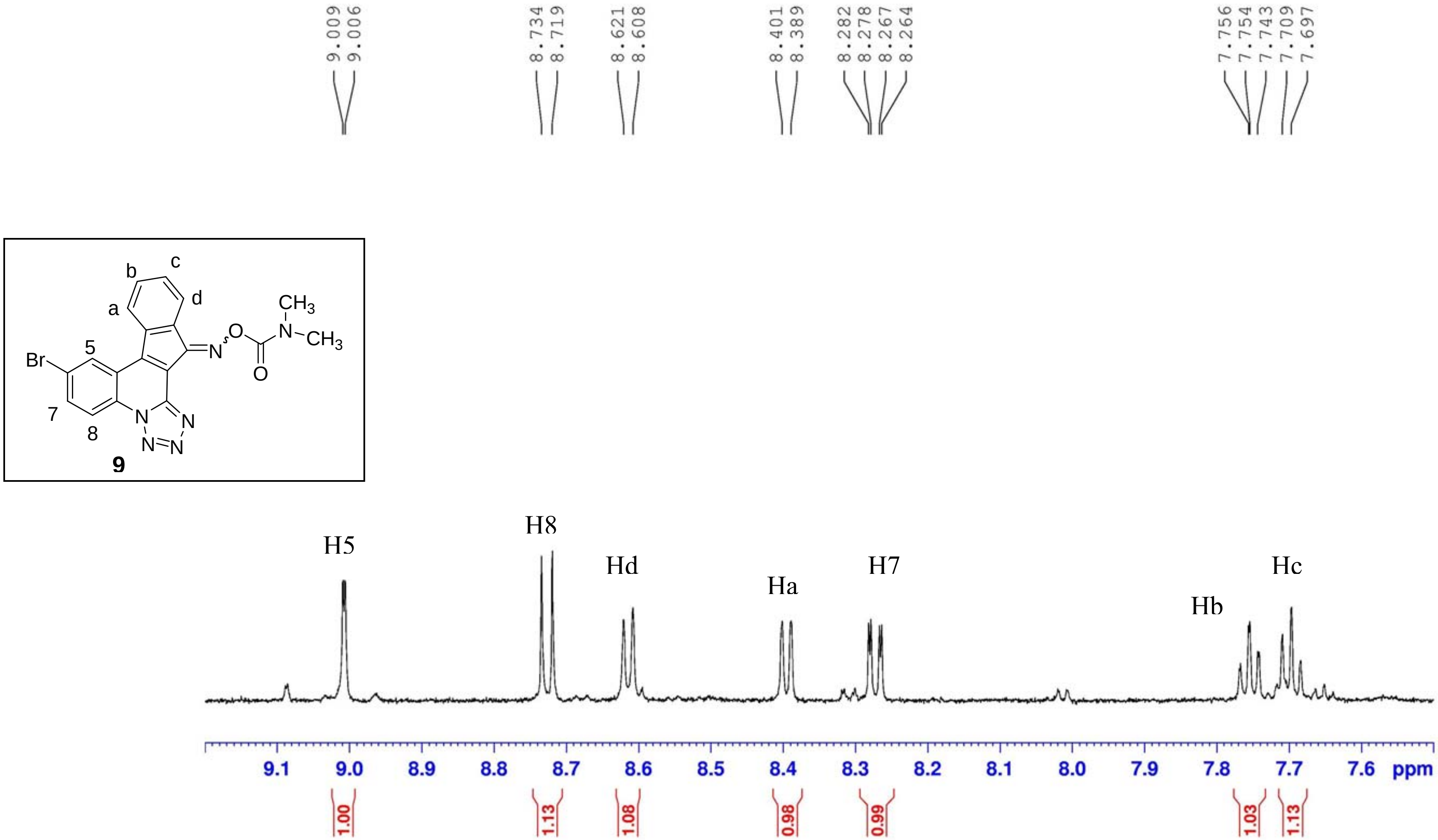


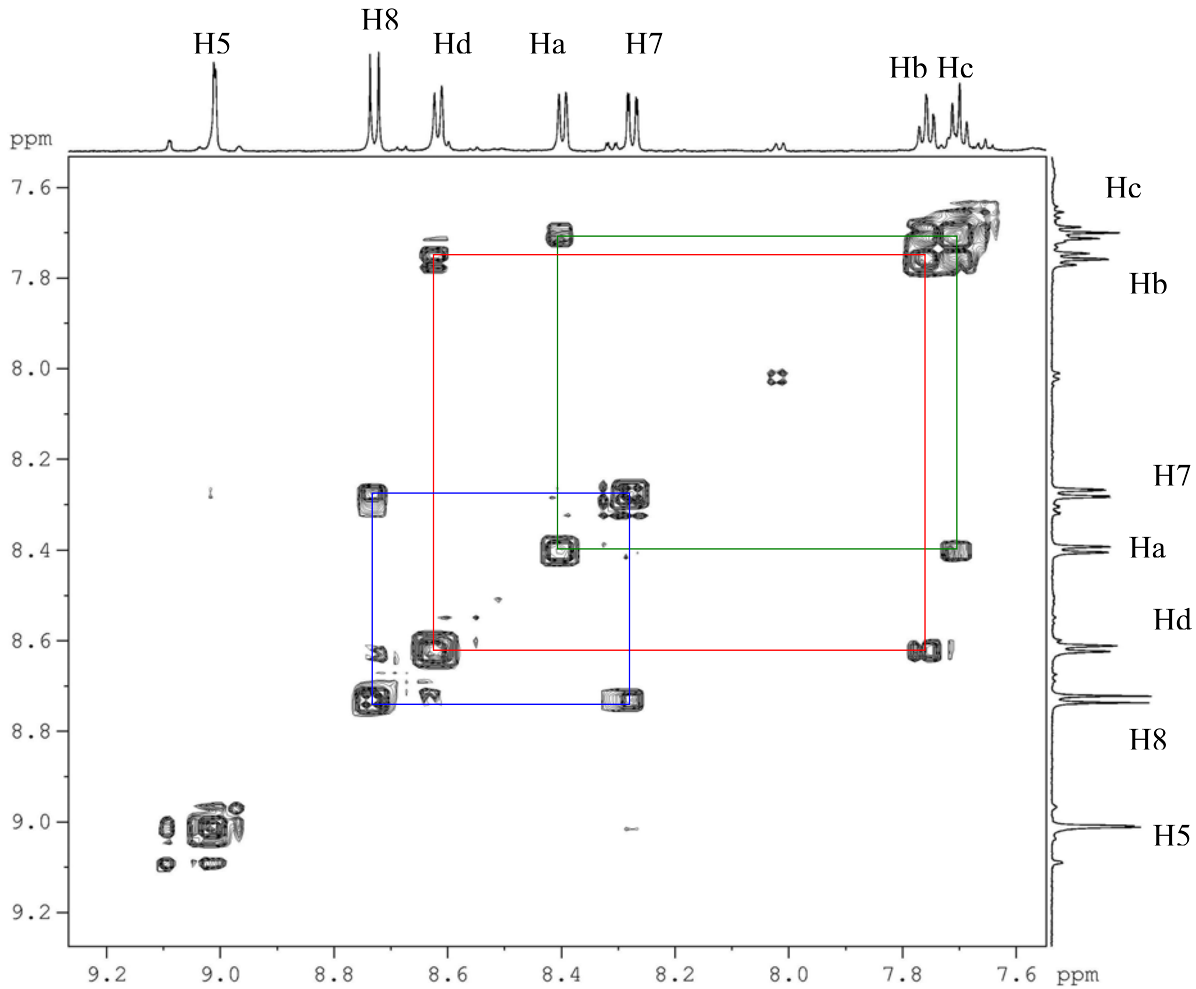
==
*** End of Report***

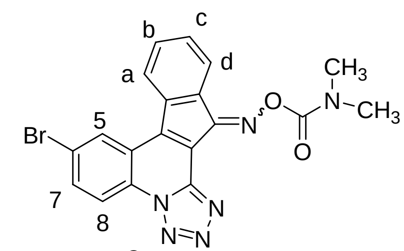


%T
cm-1
3148.25
2044.21
1651.74
1608.37
1542.32
1505.82
1460.65
1407.76
1376.55
1333.44
1290.34
1263.84
1168.58
1143.57
1097.10
1085.45
1074.40
1036.84
1028.19
961.53
847.72
820.93
781.73
751.90
721.35
622.00
551.78
525.87
464.40
Br
N
OH
8

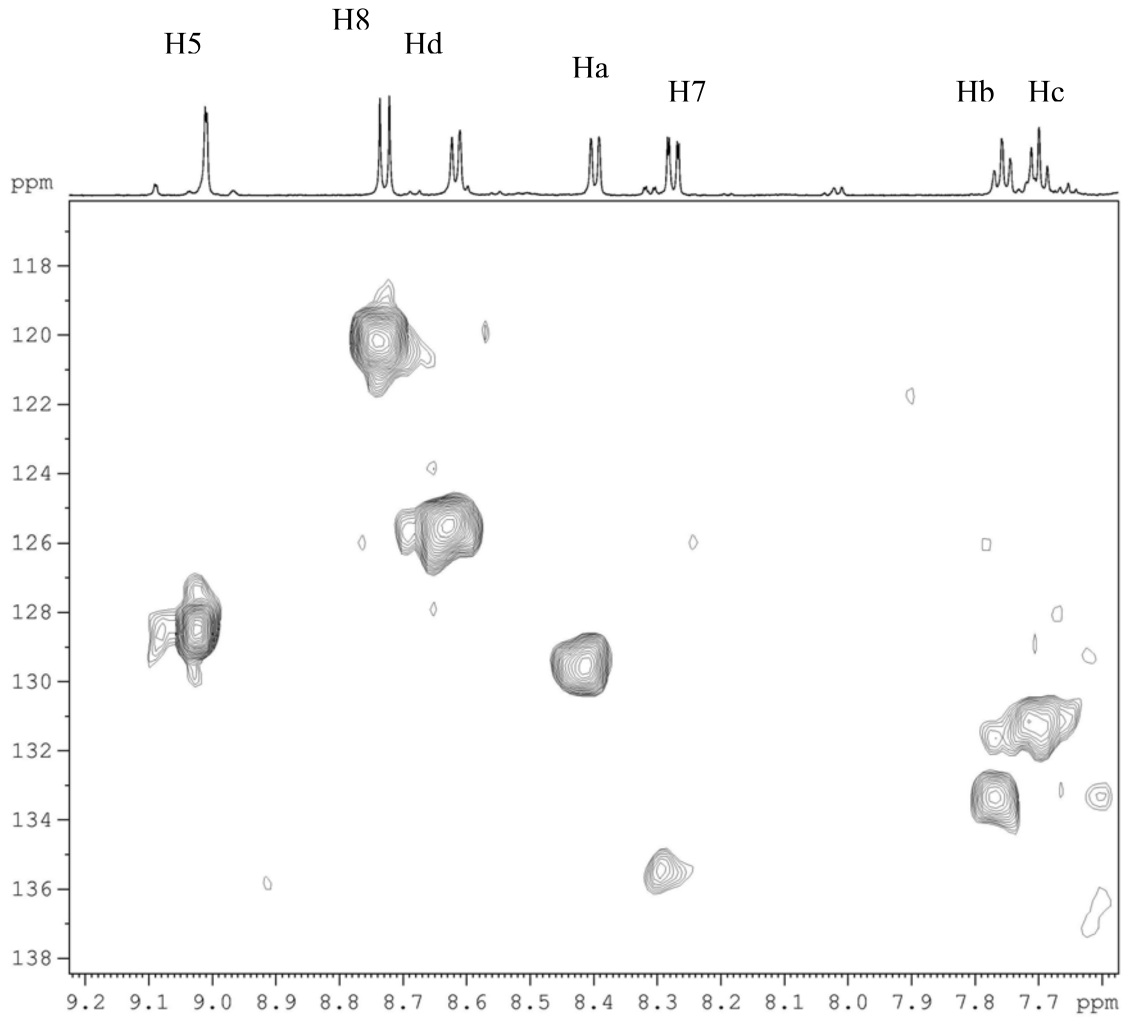

NAME CR080-97-09-09 LOWER SPOT
SOLVENT DMSO
H5
H8
Hd
Ha
H7
Hc
Hb
Ar-H
N-CH$_3$
N-CH$_3$
N-CH$_3$
ppm
9

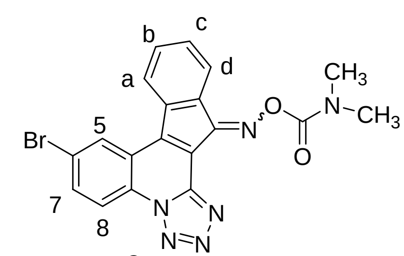

9.009
9.006
8.734
8.719
8.621
8.608
8.401
8.389
8.282
8.278
8.267
8.264
7.756
7.754
7.743
7.709
7.697
b
c
d
a
5
Br
7
8
9
H5
H8
Hd
Ha
H7
Hb
Hc
9.1
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
ppm
1.00
1.13
1.08
0.98
0.99
1.03
1.13


H5
H8
Hd
Ha
H7
Hb Hc
ppm
7.6
7.8
8.0
8.2
8.4
8.6
8.8
9.0
9.2
9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 ppm
Hc
Hb
H7
Ha
Hd
H8
H5

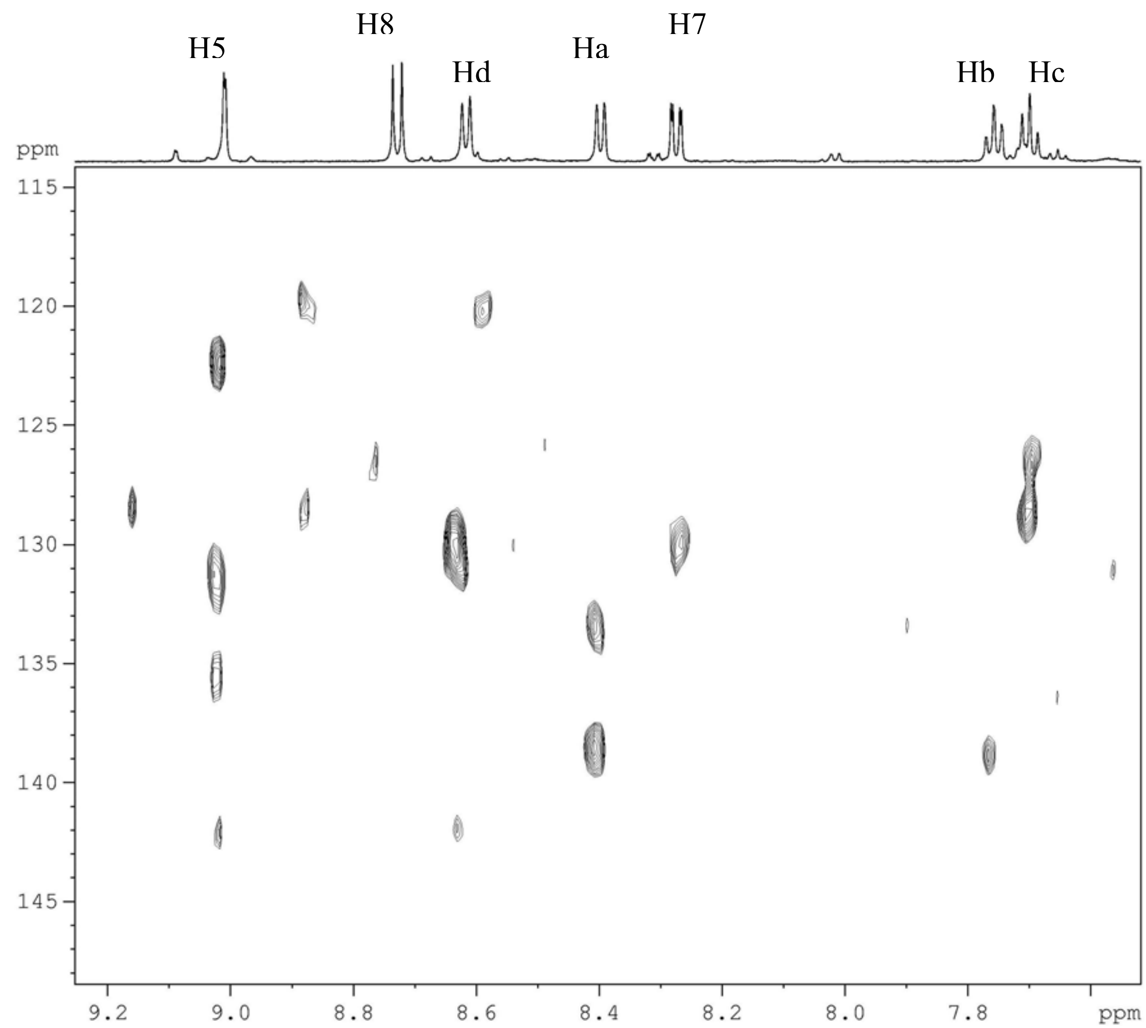

b
c
d
a
5
Br
7
8
N
O
CH3
N
CH3
O
N
N
N
N

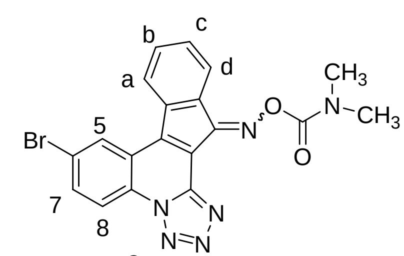
9


H5
H8
Hd
Ha
H7
Hb
Hc
ppm
118
120
122
124
126
128
130
132
134
136
138
9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 ppm

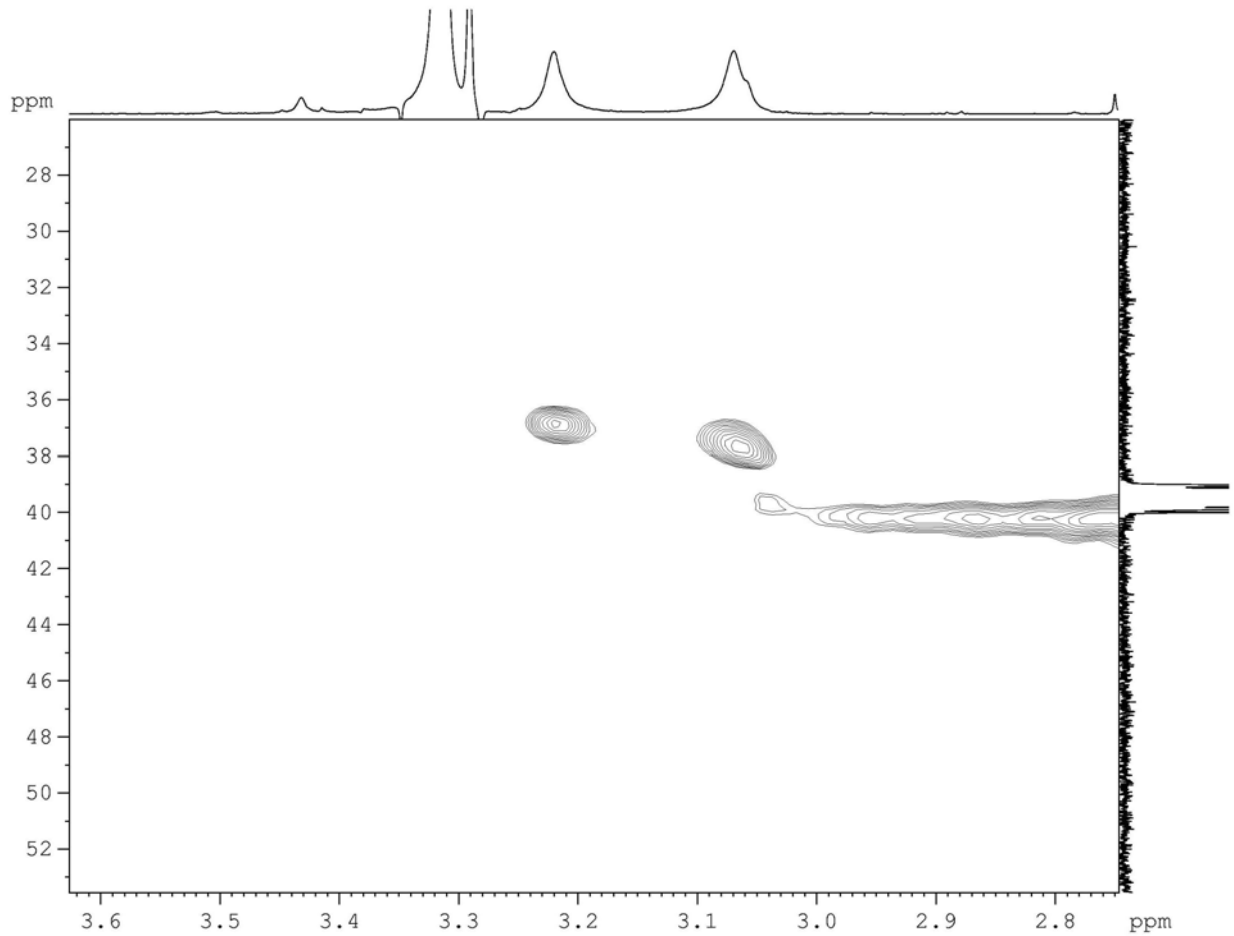

b
c
d
a
5
Br
7
8
N
N
N
N
O
N
CH3
N
CH3
O

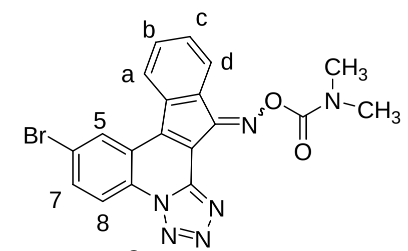
9


H5
H8
Hd
Ha
H7
Hb
Hc
ppm
115
120
125
130
135
140
145
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
ppm


b
c
a
d
CH3
O
N
N
CH3
5
Br
O
7
N
N
8
N
N

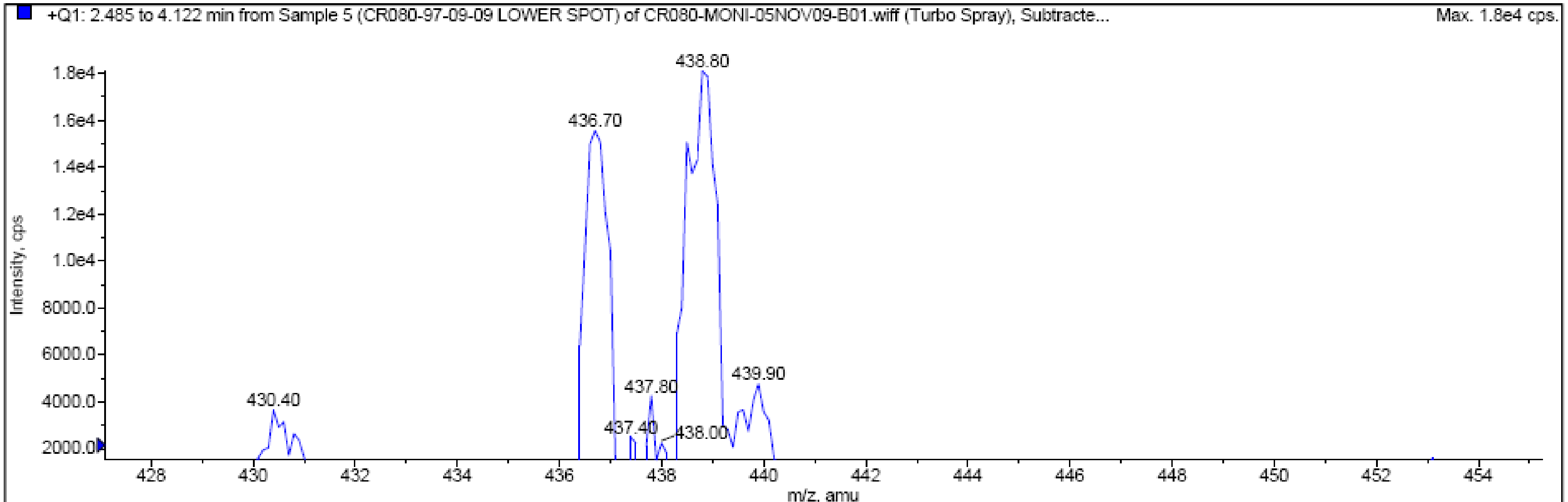
9

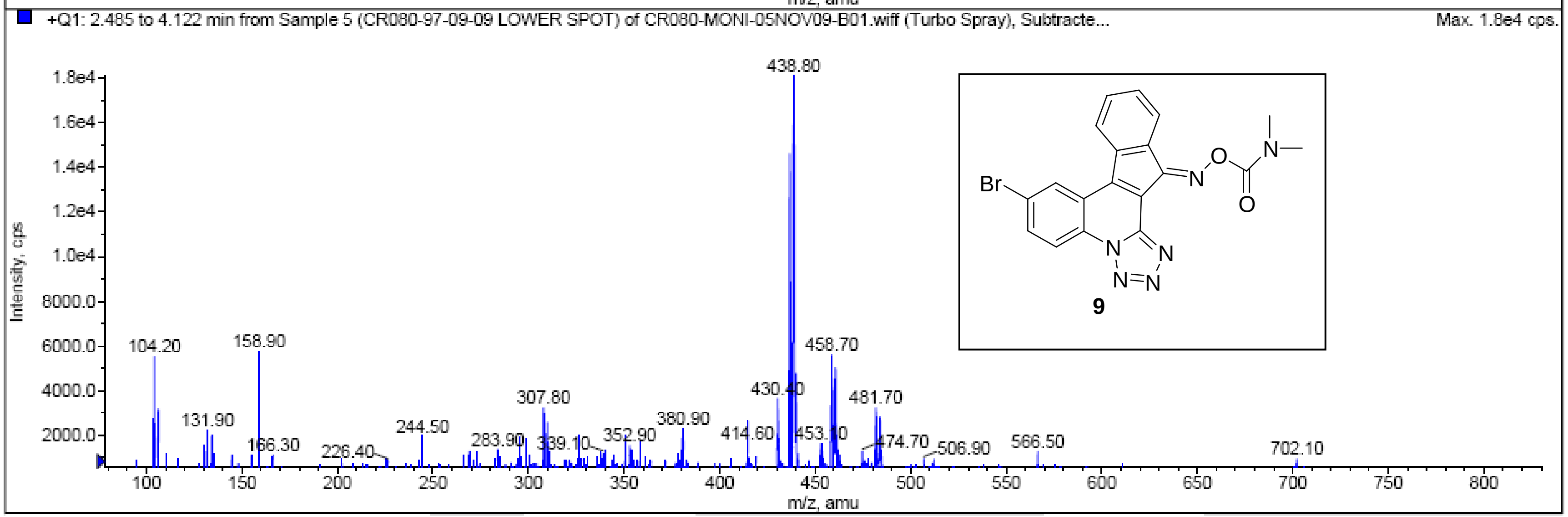

ppm
28
30
32
34
36
38
40
42
44
46
48
50
52
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
ppm



9

Sample Name: CR080-97-09-09 LOWER SPOT   Acq. Time: 11:08   Acq. Date: Thursday, November 05, 2009

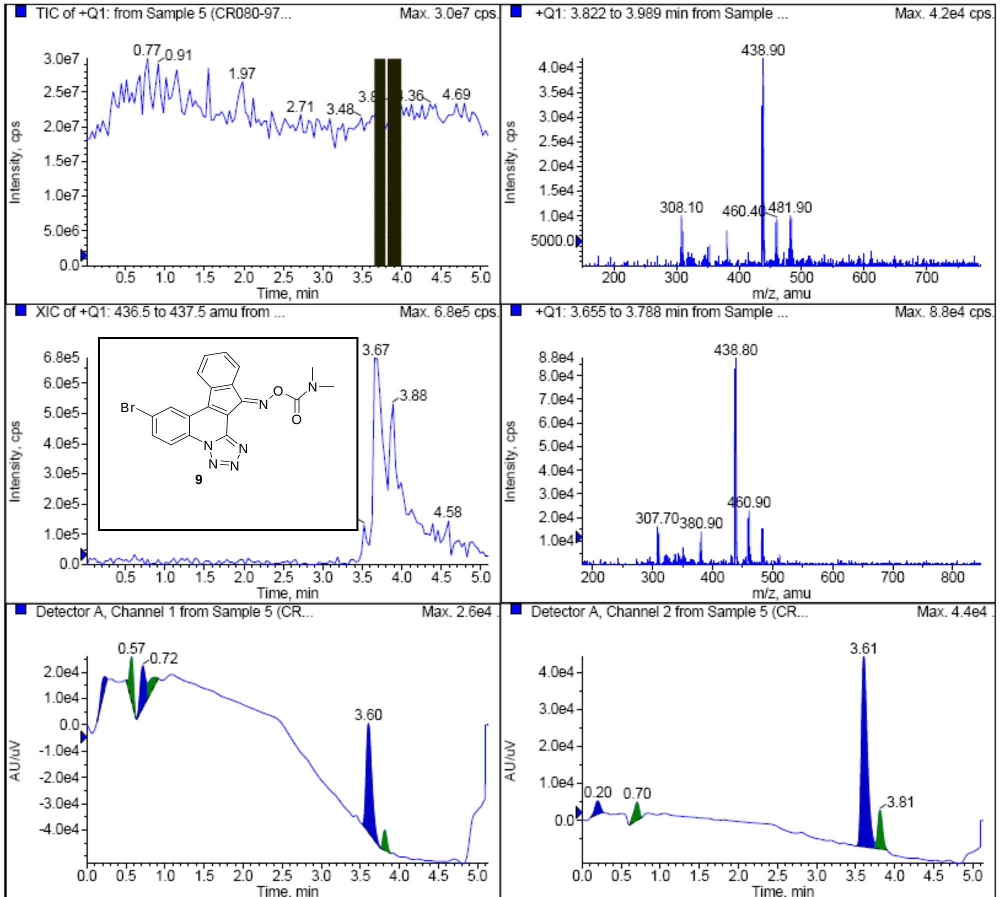




9

*Sample Comment: [M+H] 437 Expected   **Analyzed By :   **Checked By :

Sample Name: CR080-97-09-09 LOWER SPOT   Acq. Time: 11:08   Acq. Date: Thursday, November 05, 2009



Peak List for "Detector A, Channel 1 from Sample 5 (CR080-97-09-

	Time (min)	Area (counts)	%Area	Height
1	0.2265	2.5414e4	6.1011	4781.6726
2	0.5714	5.5330e4	13.2829	1.6848e4
3	0.7163	7.3242e4	17.5829	1.5801e4
4	0.8681	3.0647e4	7.3574	3046.4484
5	3.6042	2.0575e5	49.3930	4.1310e4
6	3.8133	2.6171e4	6.2827	7587.3881

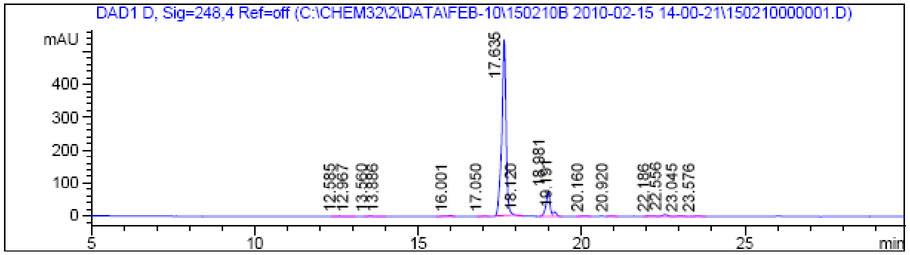
Peak List for "Detector A, Channel 2 from Sample 5 (CR080-97-09-

	Time (min)	Area (counts)	%Area	Height
1	0.2003	1.6291e4	4.7171	3544.7317
2	0.7041	2.2472e4	6.5070	4851.3842
3	3.6068	2.6447e5	76.5789	5.1266e4
4	3.8127	4.2123e4	12.1970	1.0432e4

LCMS-1 REACN MONT (TFA Buffer)   PEAK MERGED   Analysed By :

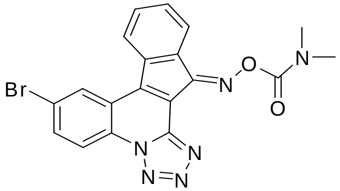
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

```
================================================================================
Sample:CR080-97-09-09LOWER SPOT                                                ->
Column: XTERRA RP (250X4.6)mm 5µ
Injection date  : Mon, 15. Feb. 2010             Location   :     Vial 23
Sample Name     : CR080-97-09-09LOWER SPOT       Inj. No.   :           1
Acq Operator    : BHUSHAN                        Inj. Vol.  :       30 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _59.M
Last Changed    : Mon, 15. Feb. 2010,
Acq. Method     : C:\Chem32\2\DATA\FEB-10\150210B 2010-02-15 14-00-21\
                  UPLC_GENARAL_GRAD _59.M
Method ref      :DI/A0257/93
```



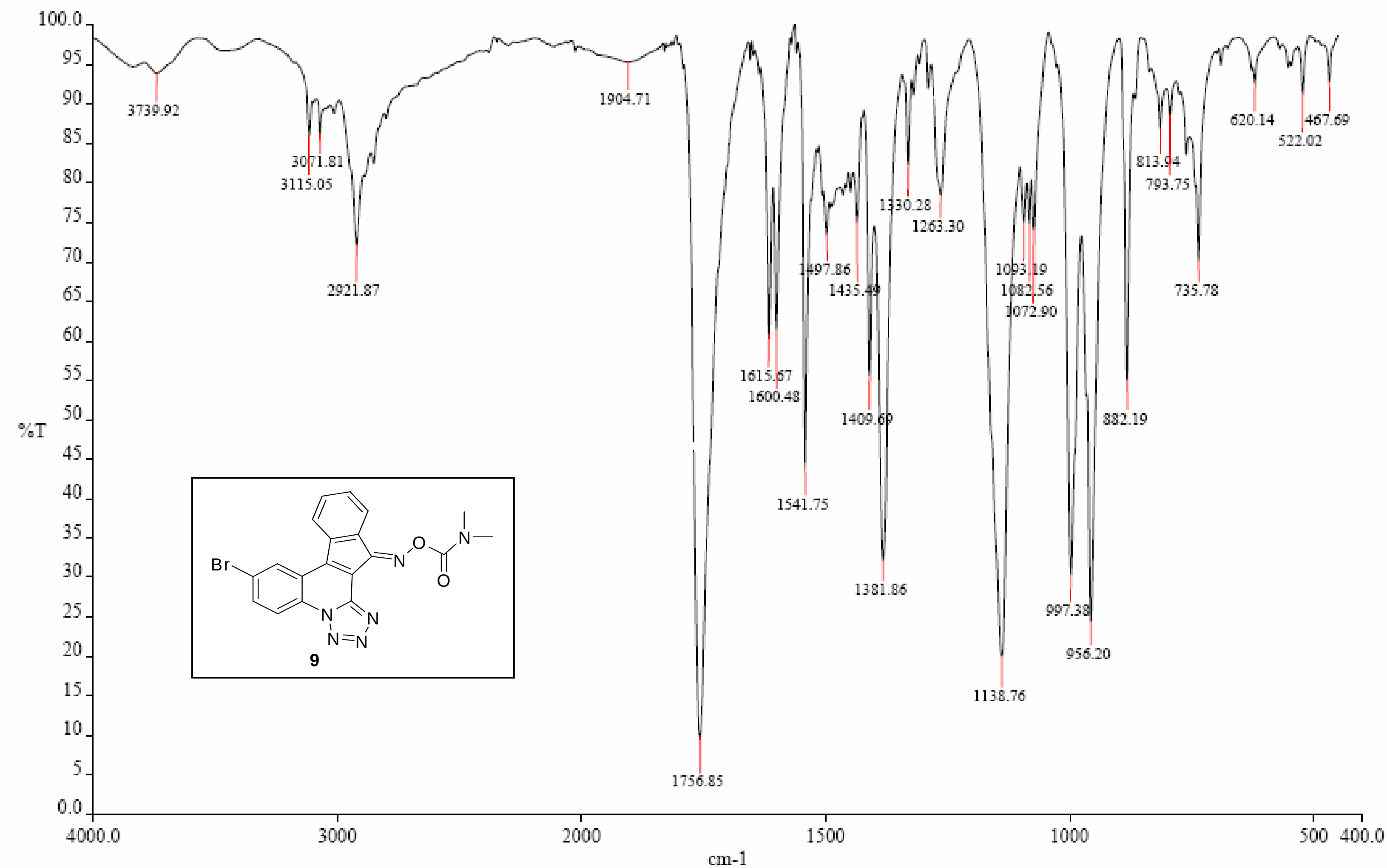
DAD1 D, Sig=248,4 Ref=off

Peak #	RT (Min)	Width (Min)	Area	Area %
1	12.585	0.116	7.906	0.138
2	12.967	0.179	8.916	0.156
3	13.560	0.130	13.794	0.241
4	13.886	0.176	6.247	0.109
5	16.001	0.249	36.225	0.633
6	17.050	0.152	10.309	0.180
7	17.635	0.149	4.794e3	83.818
8	18.120	0.098	8.469	0.148
9	18.981	0.137	628.046	10.980
10	19.191	0.123	102.312	1.789
11	20.160	0.185	14.205	0.248
12	20.920	0.159	9.286	0.162
13	22.186	0.146	7.670	0.134
14	22.556	0.160	50.485	0.883
15	23.045	0.164	12.655	0.221
16	23.576	0.229	9.063	0.158

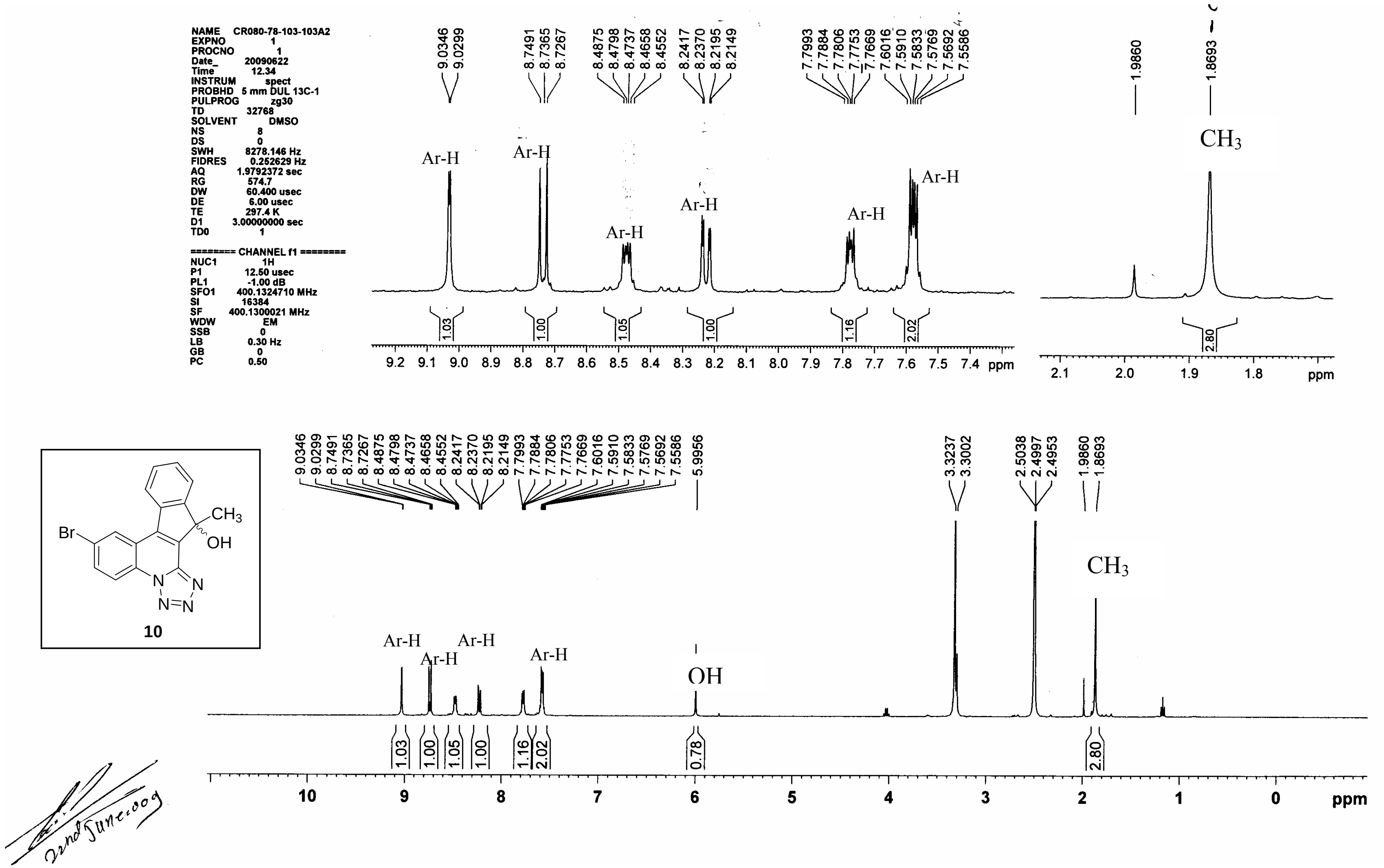


9

```
================================================================================
                         *** End of Report***
```

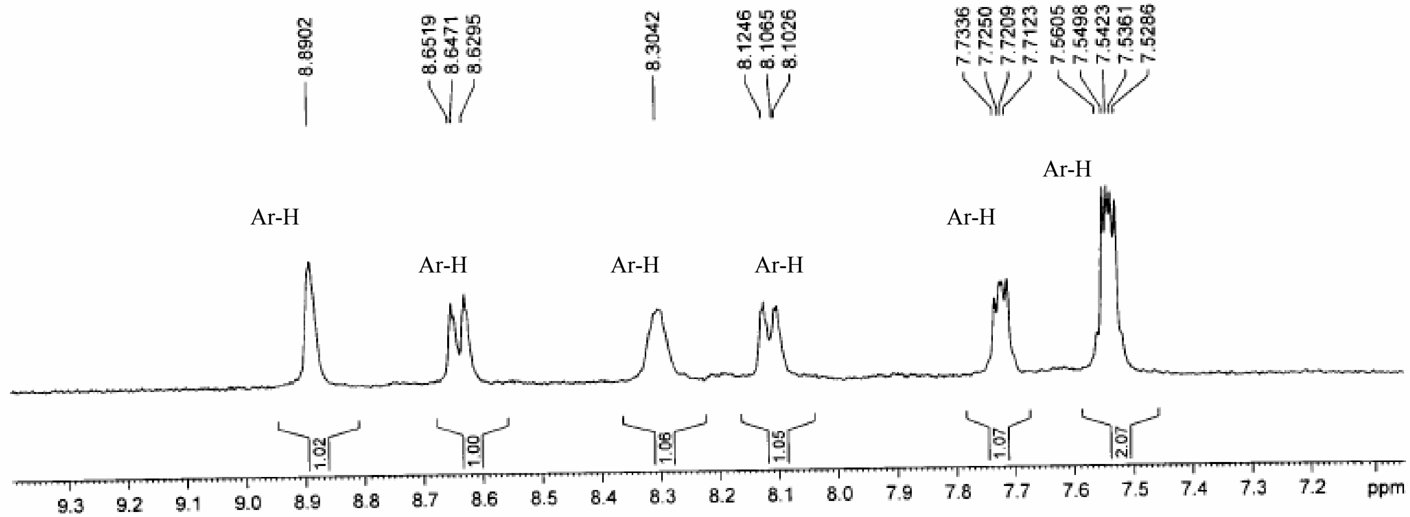


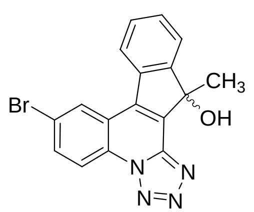
100.0
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0.0
%T
4000.0
3000
2000
1500
1000
500
400.0
cm-1
3739.92
3071.81
3115.05
2921.87
1904.71
1756.85
1615.67
1600.48
1541.75
1497.86
1435.49
1409.69
1381.86
1330.28
1263.30
1138.76
1093.19
1082.56
1072.90
997.38
956.20
882.19
813.94
793.75
735.78
620.14
522.02
467.69
Br
O
N
N
N
N
N
N
O
9


NAME CR080-78-103-103A2
EXPNO 1
PROCNO 1
Date_ 20090622
Time 12.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 297.4 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
9.0346 9.0299 8.7491 8.7365 8.7267 8.4875 8.4798 8.4737 8.4658 8.4552 8.2417 8.2370 8.2195 8.2149 7.7993 7.7884 7.7806 7.7753 7.7669 7.6016 7.5910 7.5833 7.5769 7.5692 7.5586
1.9860 1.8693
Ar-H
CH3
1.03 1.00 1.05 1.00 1.16 2.02 2.80
9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
2.1 2.0 1.9 1.8 ppm
5.9956 3.3237 3.3002 2.5038 2.4997 2.4953
OH
0.78
10 9 8 7 6 5 4 3 2 1 0 ppm
Br
CH3
OH
N
10

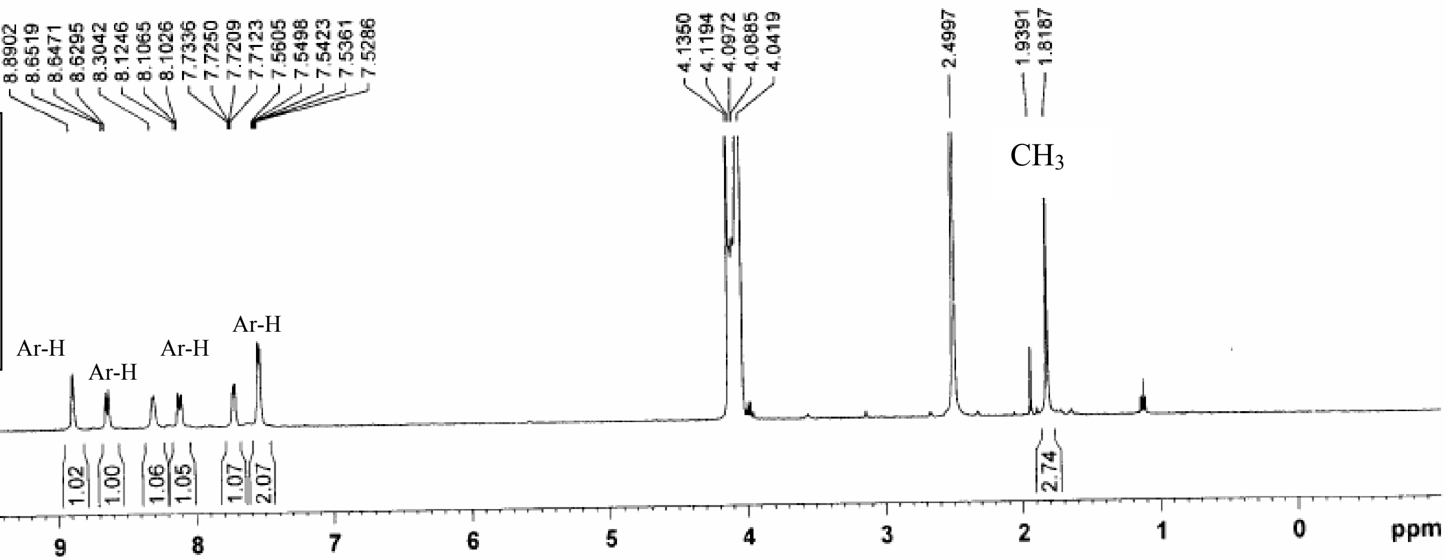
NAME CR080-78-103-103A2
EXPNO 2
PROCNO 1
Date_ 20090623
Time 18.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 292.4 K
D1 3.00000000 sec
TD0 1

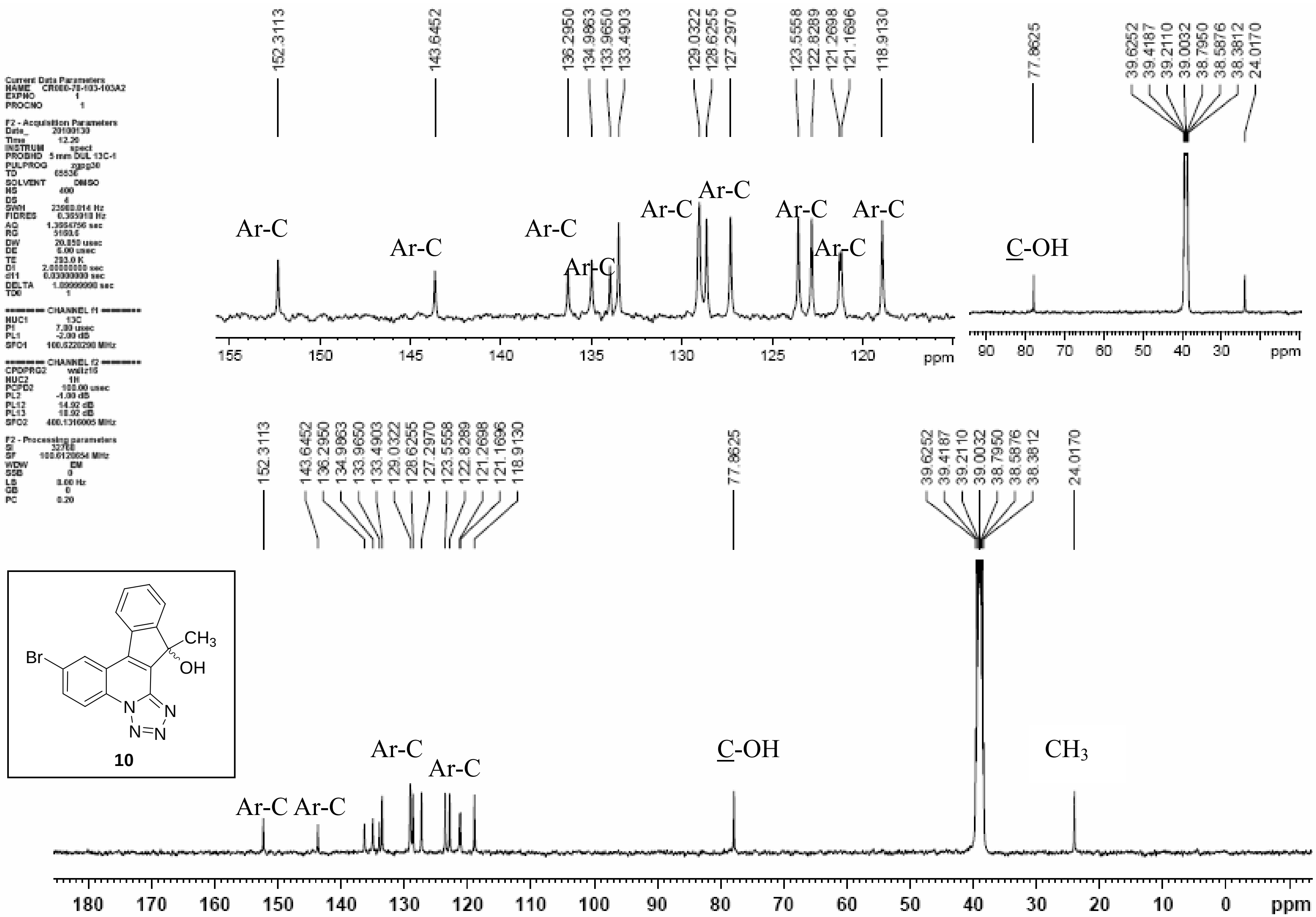
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50



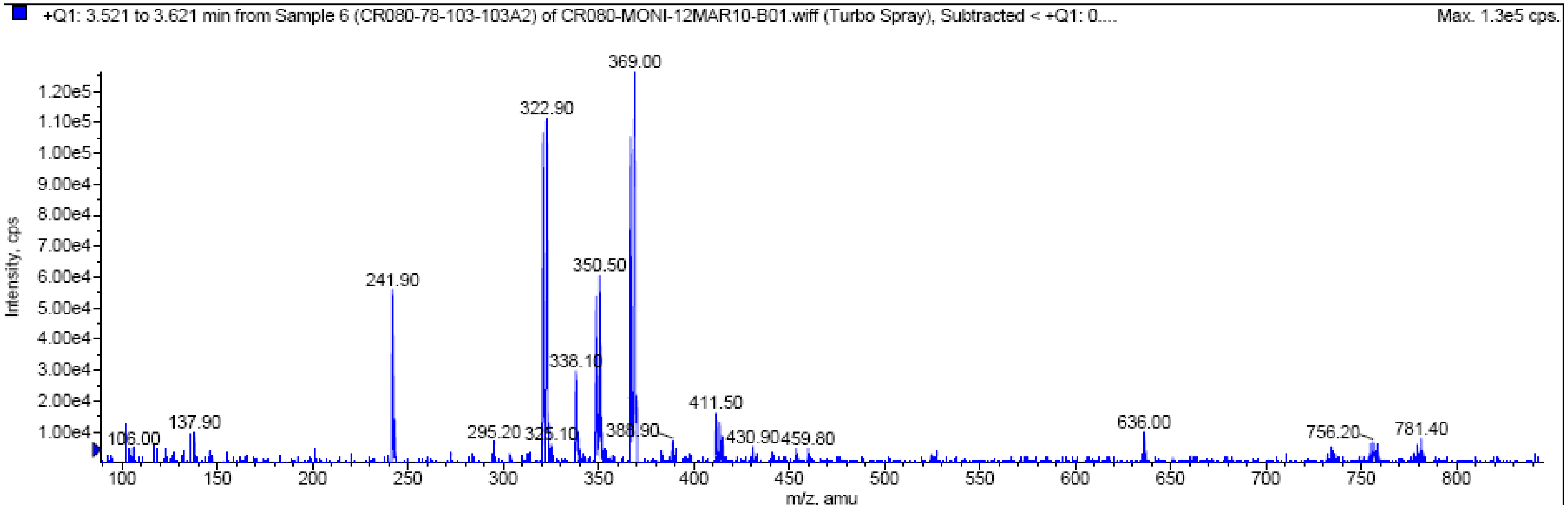


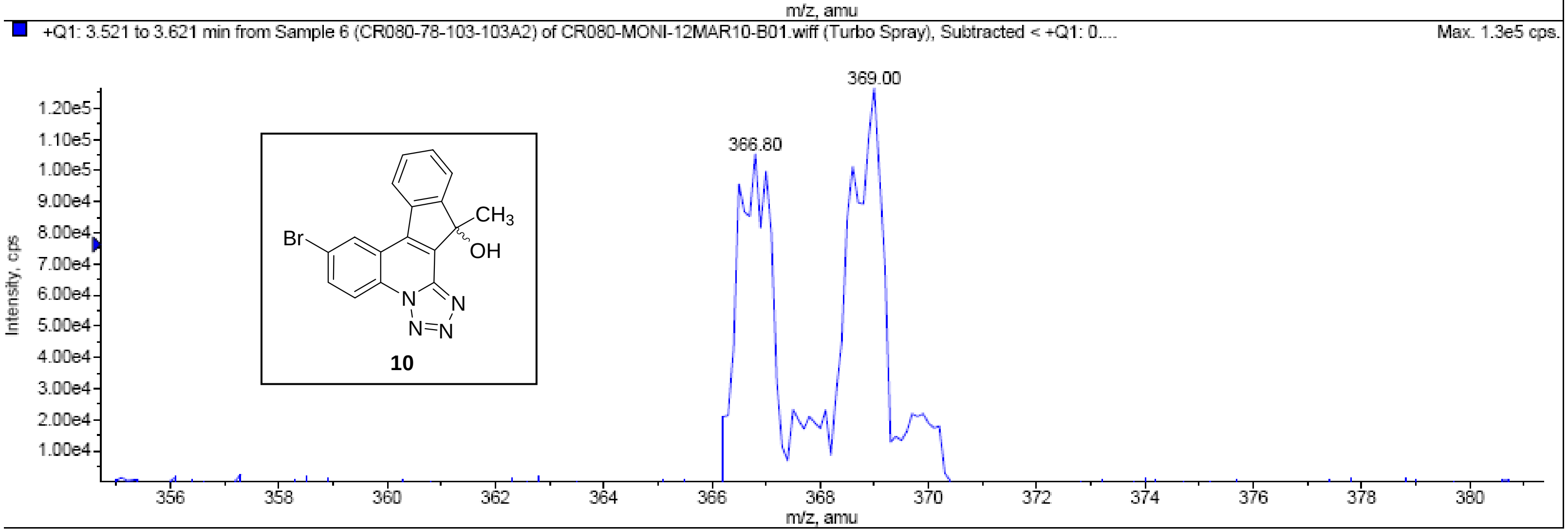
10



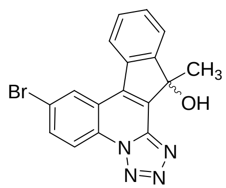

152.3113
143.6452
136.2950
134.9863
133.9650
133.4903
129.0322
128.6255
127.2970
123.5558
122.8289
121.2698
121.1696
118.9130
77.8625
39.6252
39.4187
39.2110
39.0032
38.7950
38.5876
38.3812
24.0170
Ar-C
C-OH
CH3
Br
CH3
OH
N
10
ppm

Sample Name: CR080-78-103-103A2 INDIA Acq. Time: 12:21 Acq. Date: Friday, March 12, 2010

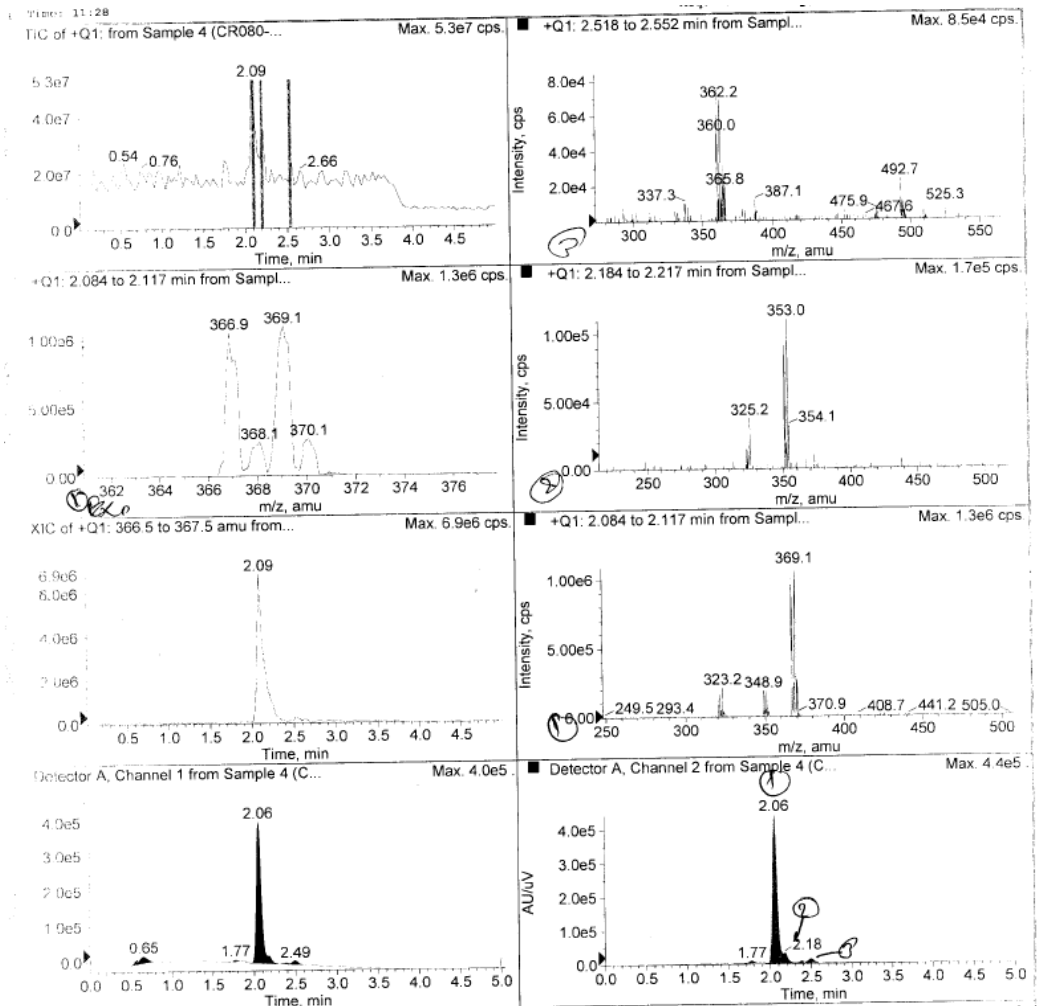




*Sample Comment: [M+H] Expected 367 **Analyzed By : **Checked By :



10



Peak List for "Detector A, Channel 1 from Sample 4 (CR080-78-1

Time (min)	Area (counts)	% Area	Height
0.6532	1.6637e5	8.2272	2.0038e4
1.7714	2.3808e4	1.1773	7368.5984
2.0572	1.7666e6	87.3612	4.0132e5
2.3805	1.5872e4	0.7849	4108.7069
2.4919	4.9531e4	2.4493	1.0487e4

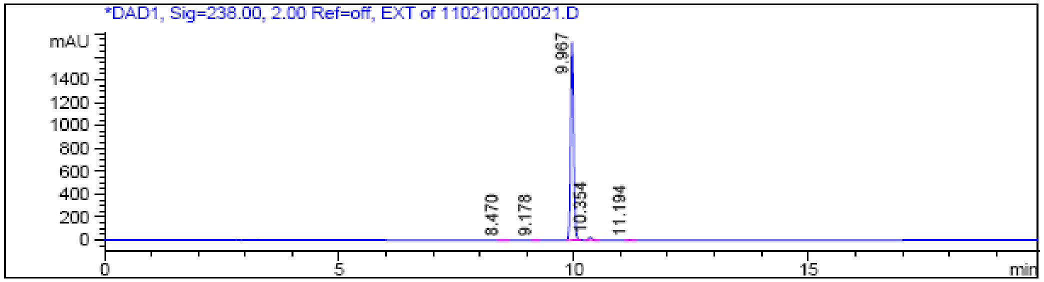
Peak List for "Detector A, Channel 2 from Sample 4 (CR080-78-1

	Time (min)	Area (counts)	% Area	Height
1	1.7734	1.9157e4	0.9386	5866.5226
2	2.0576	1.8720e6	91.7187	4.4124e5
3	2.1754	7.8583e4	3.8501	2.0268e4
4	2.3817	1.9746e4	0.9674	5158.9867
5	2.4959	5.1542e4	2.5252	1.1378e4

2 ReactionMonitoring in TFA

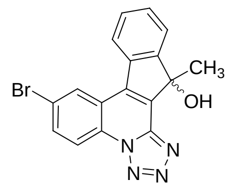
Analyzed By :

```
===========================================================================
Sample:CR080-78-103-103 A2                                                  ->
Column: XTERRA RP(250X4.6)mm 5µ
Injection date  : Thu, 11. Feb. 2010            Location   :     Vial 24
Sample Name     : CR080-78-103-103 A2           Inj. No.   :           1
Acq Operator    : BHUSHAN                       Inj. Vol.  :        3 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _1.M
Last Changed    : Thu, 11. Feb. 2010,
Acq. Method     : C:\Chem32\2\DATA\FEB-10\110210E 2010-02-11 16-18-57\
                  UPLC_GENARAL_GRAD _1.M
Method ref      : DI/A0257/88
```



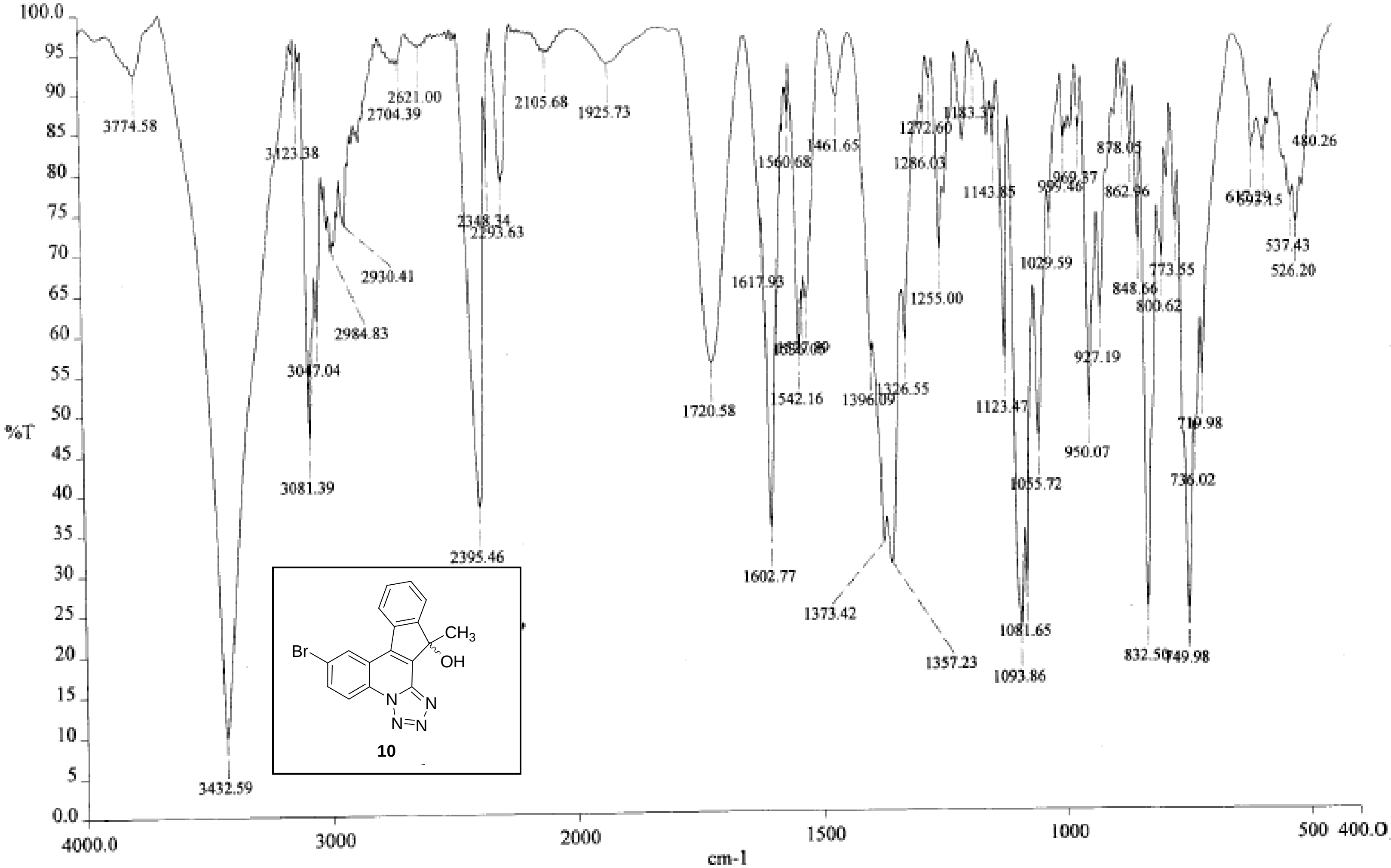
DAD1, Sig=238.00, 2.00 Ref=off, EXT

Peak #	RT (Min)	Width (Min)	Area	Area %
1	8.470	0.075	12.580	0.154
2	9.178	0.075	7.401	0.091
3	9.967	0.077	7.971e3	97.810
4	10.354	0.080	129.704	1.592
5	11.194	0.112	28.745	0.353

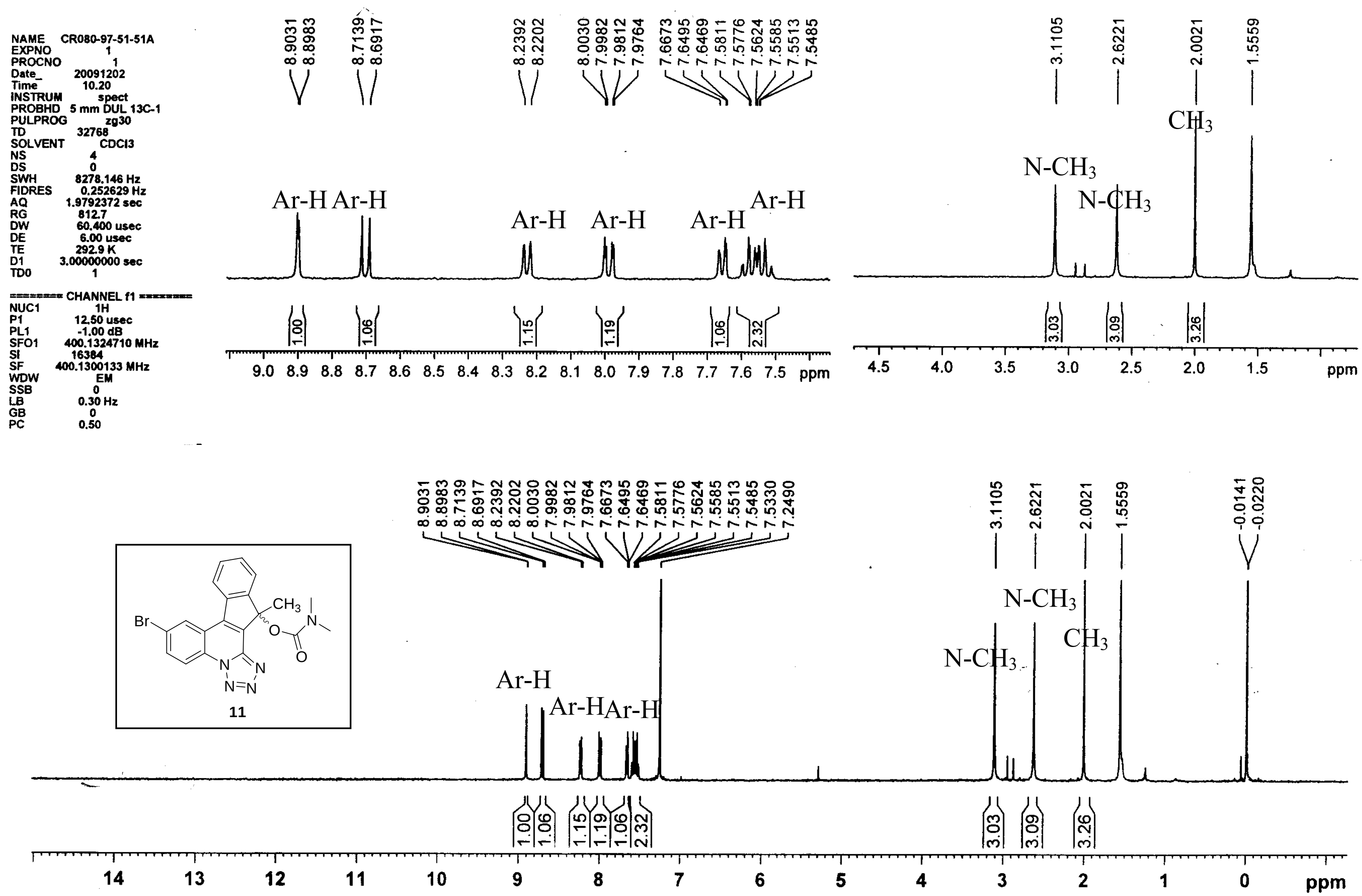


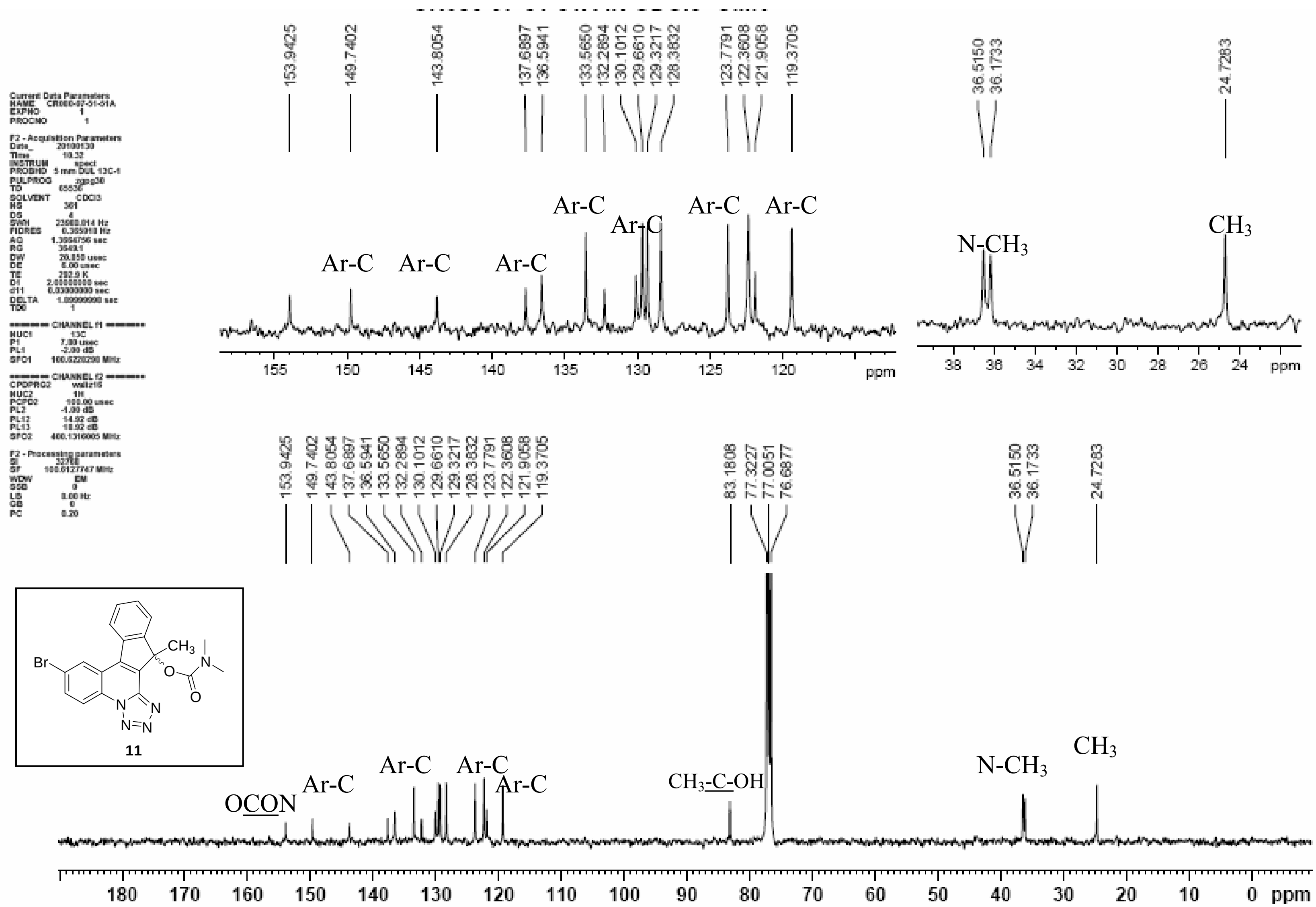
10

*** End of Report***



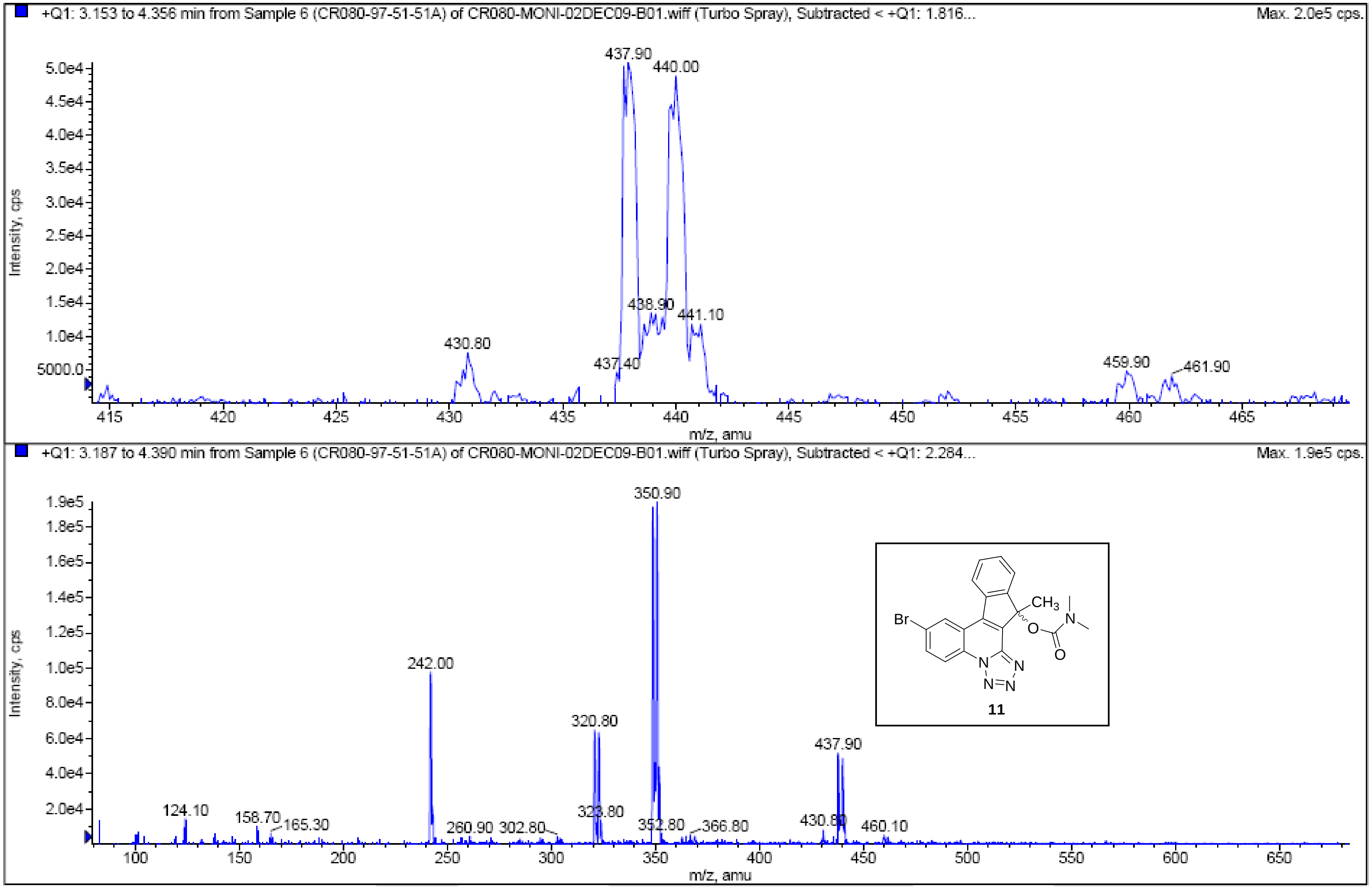
%T
cm-1
4000.0
3000
2000
1500
1000
500
400.0
3432.59
3774.58
3123.38
3081.39
3047.04
2984.83
2930.41
2704.39
2621.00
2395.46
2348.34
2293.63
2105.68
1925.73
1720.58
1617.93
1602.77
1560.68
1542.16
1461.65
1396.09
1373.42
1357.23
1326.55
1286.03
1272.60
1255.00
1183.37
1143.85
1123.47
1093.86
1081.65
1055.72
1029.59
999.46
969.57
950.07
927.19
878.05
862.96
848.66
832.50
800.62
773.55
749.98
736.02
719.98
537.43
526.20
480.26
Br
CH3
OH
N
10


NAME CR080-97-51-51A
EXPNO 1
PROCNO 1
Date_ 20091202
Time 10.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 812.7
DW 60.400 usec
DE 6.00 usec
TE 292.9 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
Ar-H
N-CH3
CH3
ppm
11


153.9425
149.7402
143.8054
137.6897
136.5941
133.5650
132.2894
130.1012
129.6610
129.3217
128.3832
123.7791
122.3608
121.9058
119.3705
36.5150
36.1733
24.7283
Ar-C
CH3
N-CH3
83.1808
77.3227
77.0051
76.6877
OCON
CH3-C-OH
Br
O
N
11
ppm

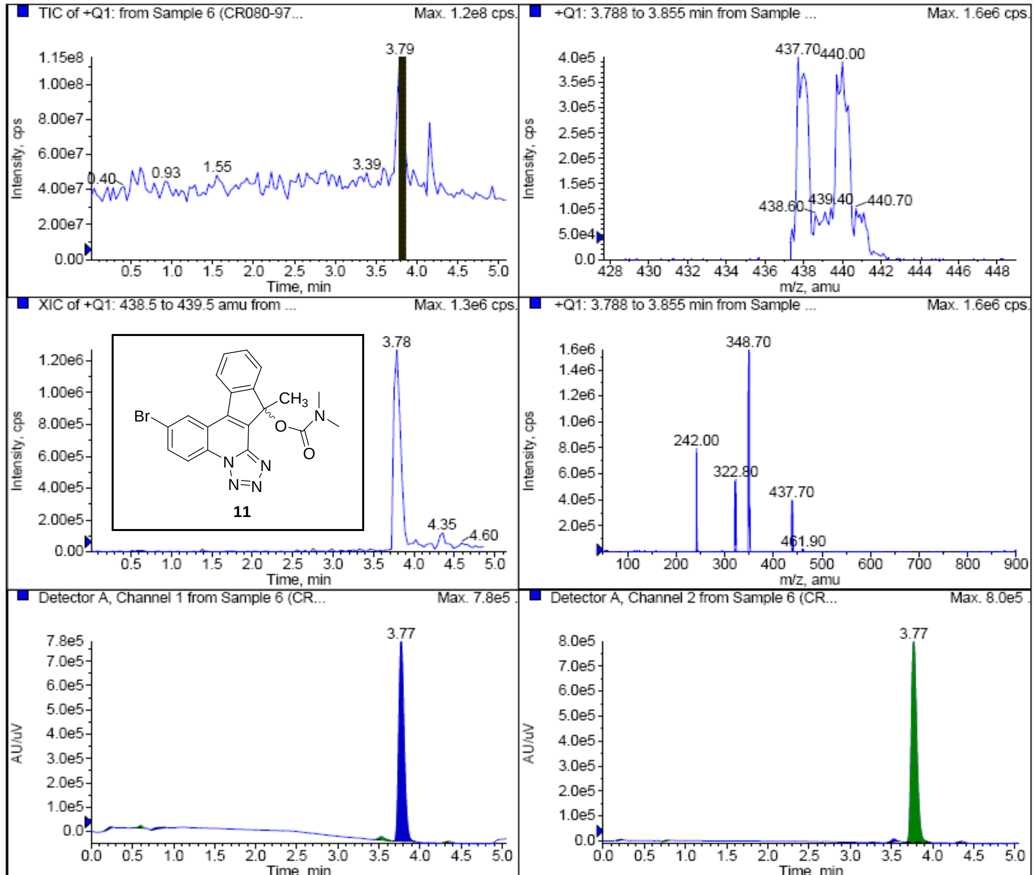
INDIA

Sample Name: CR080-97-51-51A Acq. Time: 11:21 Acq. Date: Wednesday, December 02, 2009



*Sample Comment: [M+H] 438 Expected **Analyzed By : **Checked By :

Sample Name: CR080-97-51-51A Acq. Time: 11:21 Acq. Date: Wednesday, December 02, 2009



Peak List for "Detector A, Channel 1 from Sample 6 (CR080-97-51-

	Time (min)	Area (counts)	% Area	Height
1	0.2436	1.3881e4	0.3695	2459.5995
2	0.6013	2.6760e4	0.7123	9830.7255
3	0.8708	3.0907e4	0.8227	1804.4309
4	3.5277	6.6379e4	1.7670	1.3350e4
5	3.7698	3.6125e6	96.1618	8.1976e5
6	4.3522	6262.8132	0.1667	1326.0400

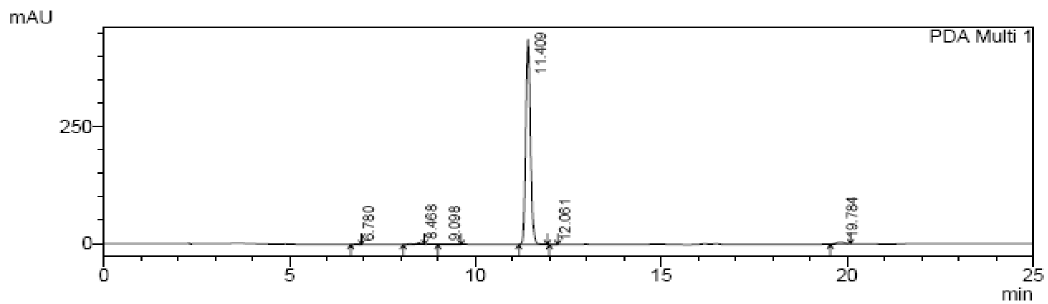
Peak List for "Detector A, Channel 2 from Sample 6 (CR080-97-51-

	Time (min)	Area (counts)	% Area	Height
1	0.2199	3071.4114	0.0834	1059.8488
2	0.7886	5245.4871	0.1424	1106.8128
3	3.5293	3.9271e4	1.0658	1.0568e4
4	3.7704	3.6312e6	98.5494	8.0196e5
5	4.3519	5863.1002	0.1591	1211.8792

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

Sample Name : CR080-97-51-51A
Sample ID : CR080-97-51-51A
Column : Gemini C-18 (150 x 4.6 mm)
Vial # : 57
Inj. Volume : 4 uL
Tray # : 1
Acquired by : AVINASH

Data File Name : 11-02-10_CR080-97-51-51A_04.lcd
Method File Name : GENERAL_B2.lcm
Batch File Name : 130210.lcb
Data Acquired : 2/13/2010 3:36:00 PM
Data Processed : 2/13/2010 4:01:03 PM
Ref.No.: DI/A0257/90

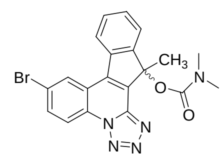


1 PDA Multi 1/242nm 4nm

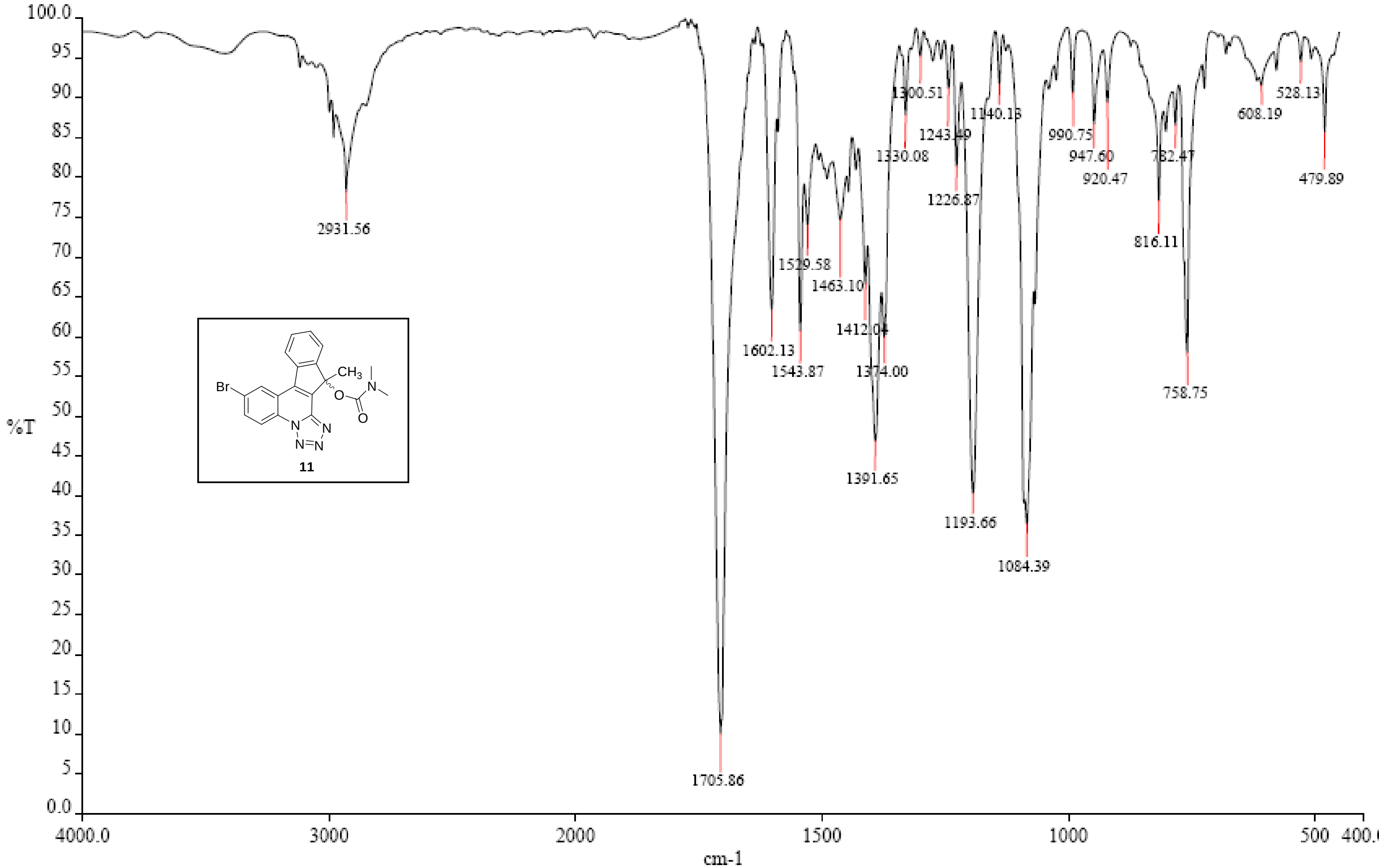
PeakTable

PDA Ch1 242nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	6.78	3076	0.08	490
2	8.47	38385	0.98	3979
3	9.10	8800	0.22	508
4	11.41	3811649	97.09	437964
5	12.06	785	0.02	121
6	19.78	63090	1.61	4027
Total		3925785	100.00	447089



11



Spectrum Name: CR080-97-51-51A.sp

Analyst: GANESH

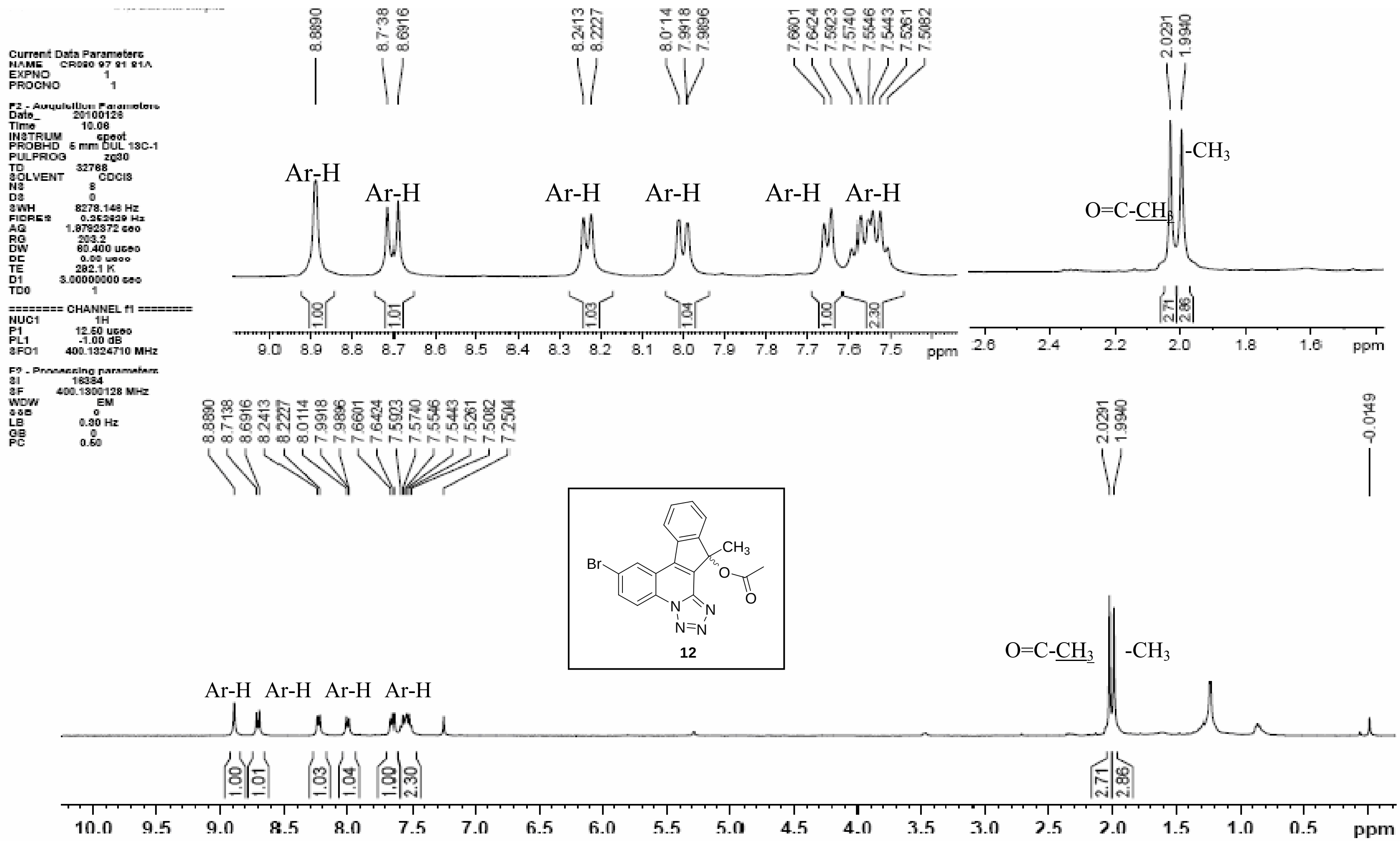
Accumulations: 16

Time: 10:04:53 AM

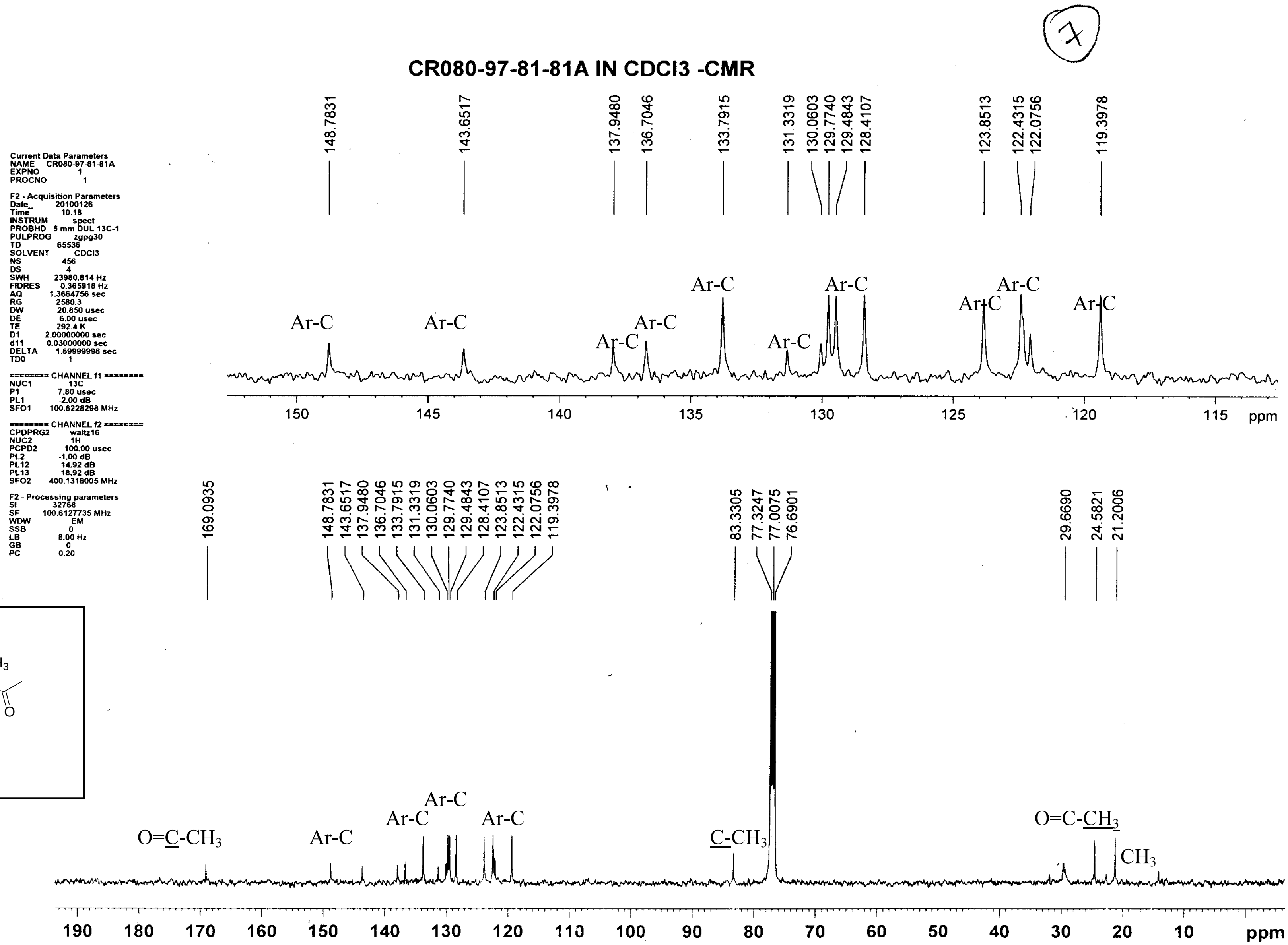
Description: CR080-97-51-51A IN KBr

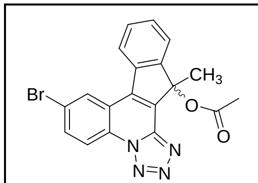
Resolution: 4.00 cm-1

Date: 2/3/2010



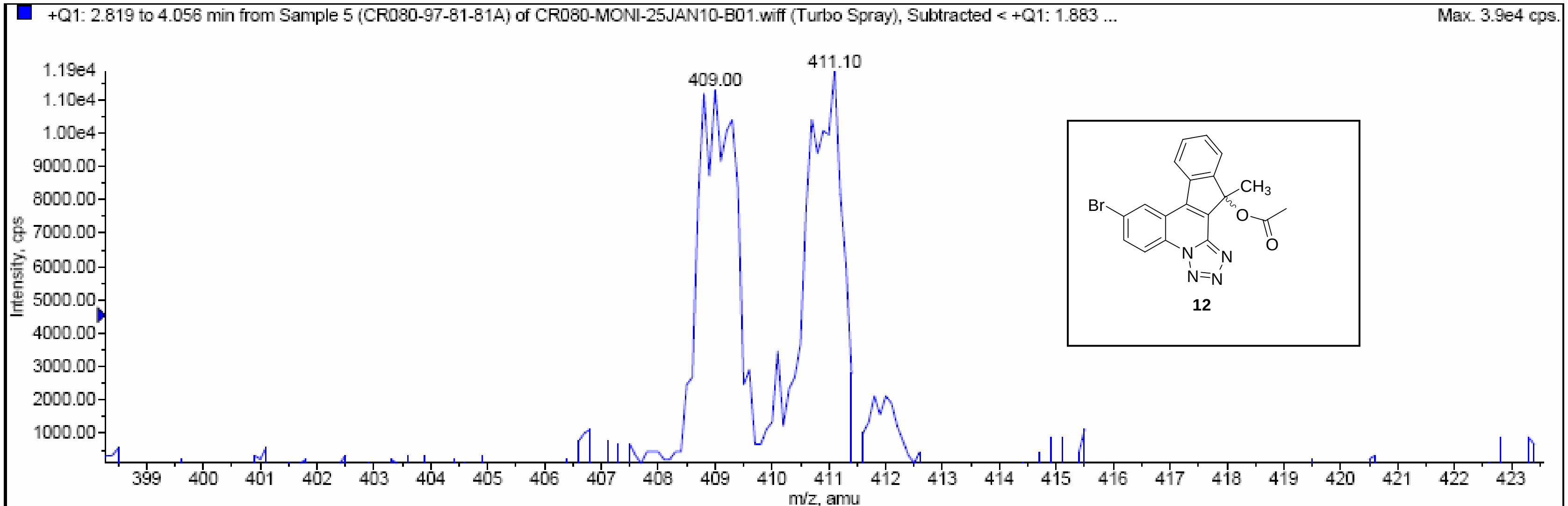
Current Data Parameters
8.8890
8.7138
8.6916
8.2413
8.2227
8.0114
7.9918
7.9896
7.6601
7.6424
7.5923
7.5740
7.5546
7.5443
7.5261
7.5082
7.2504
2.0291
1.9940
-0.0149
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
O=C-CH3
-CH3
1.00
1.01
1.03
1.04
1.00
2.30
2.71
2.86
Br
CH3
O
N
12
ppm

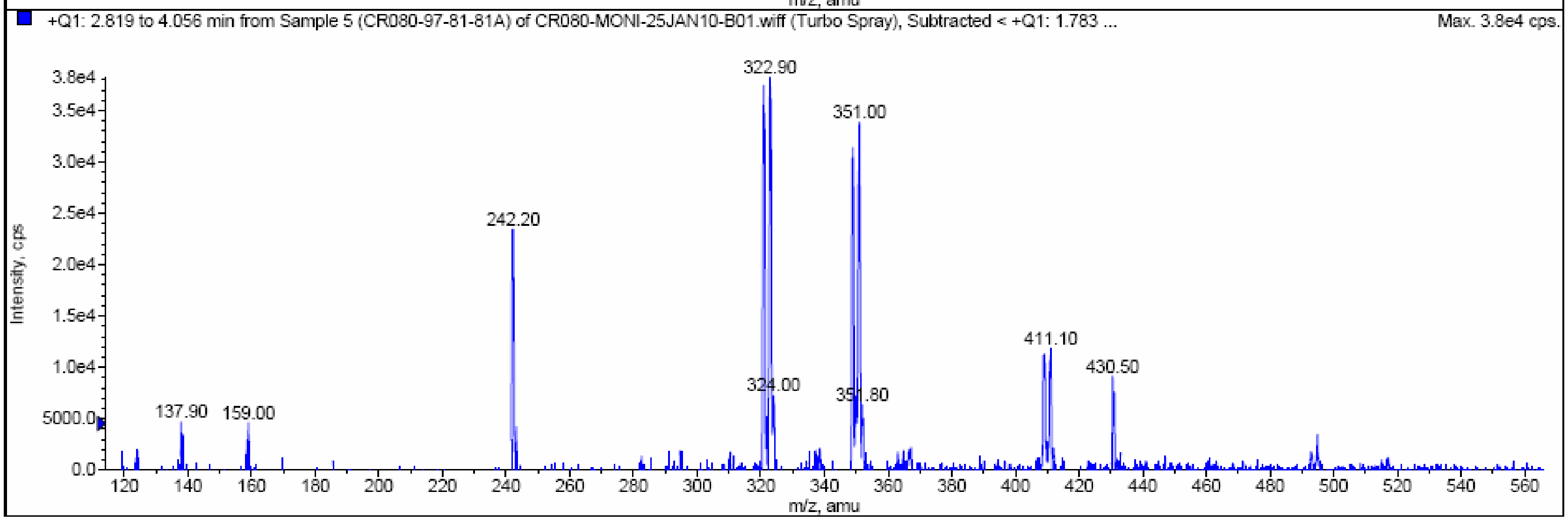

CR080-97-81-81A IN CDCl3 -CMR
Current Data Parameters
NAME CR080-97-81-81A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100126
Time 10.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 456
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2580.3
DW 20.850 usec
DE 6.00 usec
TE 292.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.92 dB
PL13 18.92 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127735 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 0.20
148.7831
143.6517
137.9480
136.7046
133.7915
131.3319
130.0603
129.7740
129.4843
128.4107
123.8513
122.4315
122.0756
119.3978
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
150
145
140
135
130
125
120
115
ppm
169.0935
148.7831
143.6517
137.9480
136.7046
133.7915
131.3319
130.0603
129.7740
129.4843
128.4107
123.8513
122.4315
122.0756
119.3978
83.3305
77.3247
77.0075
76.6901
29.6690
24.5821
21.2006
O=C-CH3
Ar-C
Ar-C
Ar-C
Ar-C
C-CH3
O=C-CH3
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Br
CH3
O
O
N
N
N
N

12

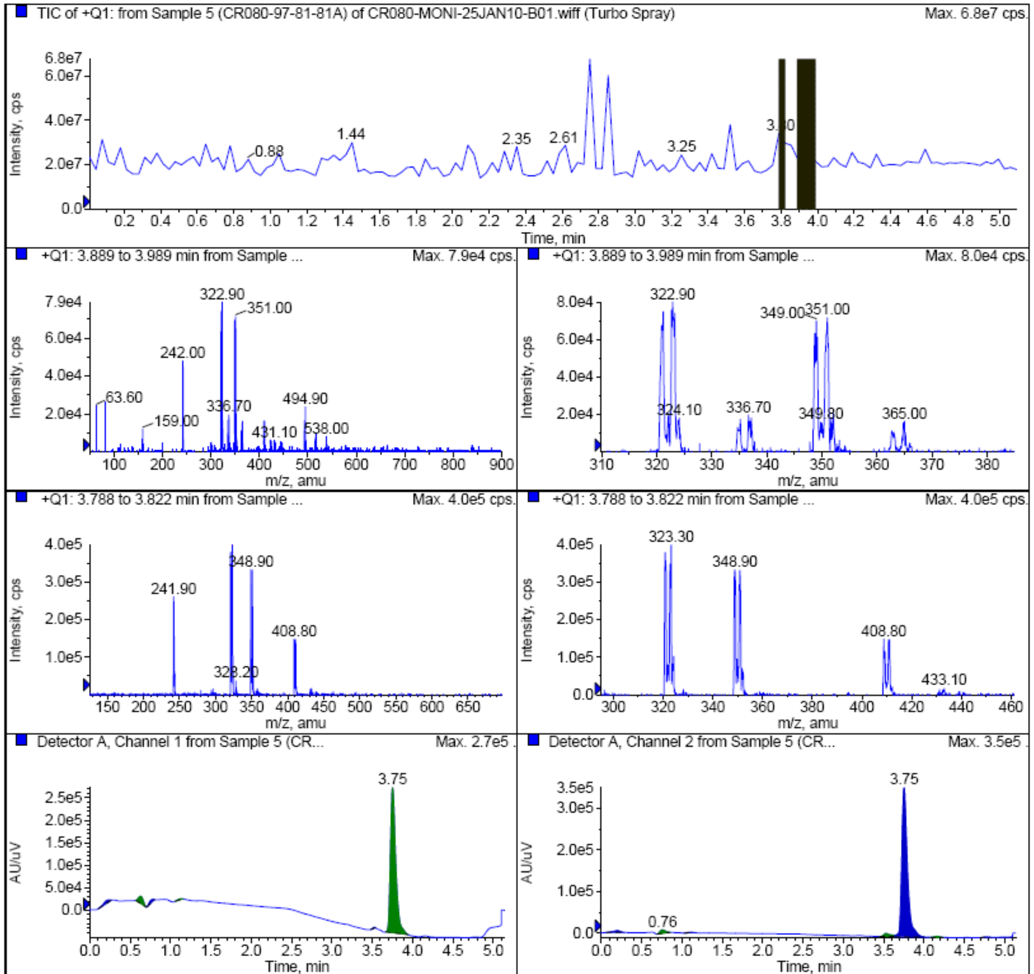
Sample Name: CR080-97-81-81A   Acq. Time: 10:36   Acq. Date: Monday, January 25, 2010





*Sample Comment: [M+H]409   Expected   **Analyzed By :   **Checked By :

Sample Name: CR080-97-81-81A Acq. Time: 10:36 Acq. Date: Monday, January 25, 2010



Peak List for "Detector A, Channel 1 from Sample 5 (CR080-97-81-

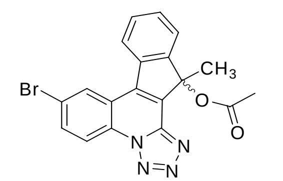
	Time (min)	Area (counts)	%Area	Height
1	0.2417	2.6066e4	1.6493	3236.9711
2	0.6275	6.5509e4	4.1449	1.5835e4
3	0.7832	1.9888e4	1.2584	3447.9606
4	1.1388	6934.9241	0.4388	1239.7454
5	3.5273	3045.8599	0.1927	1453.2988
6	3.7517	1.4590e6	92.3158	3.2225e5

Peak List for "Detector A, Channel 2 from Sample 5 (CR080-97-81-

	Time (min)	Area (counts)	%Area	Height
1	0.1973	2.7965e4	1.5362	4341.0894
2	0.7570	3.9939e4	2.1939	8606.0930
3	1.1050	3584.9029	0.1969	864.0747
4	3.5296	4.2728e4	2.3472	7324.8247
5	3.7537	1.6905e6	92.8629	3.5741e5
6	4.1595	1.0864e4	0.5968	2469.0353
7	4.7745	4844.5106	0.2661	1226.2988

LCMS-1 REACN MONT (TFA Buffer) PEAK MERGED PLEASE GIVE EXACT MASS Analysed By :

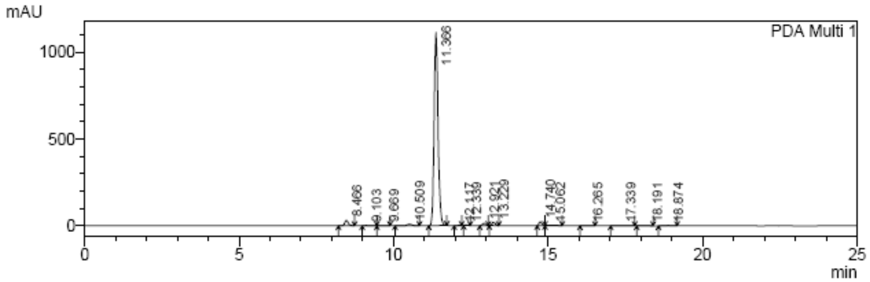
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

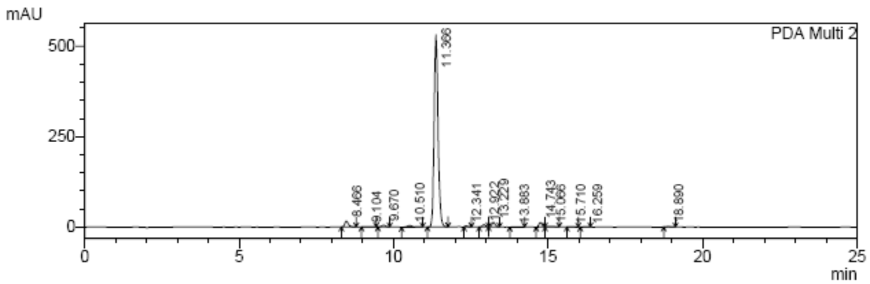


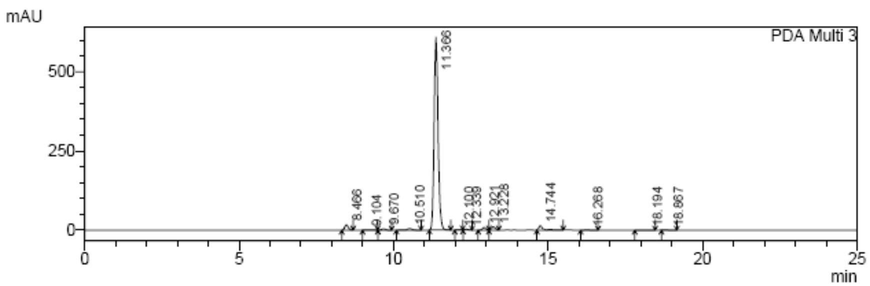
12

Sample Name : CR080-97-81-81A
Sample ID : CR080-97-81-81A
Column : Gemini C-18 (150 x 4.6 mm)
Vial # : 60
Inj. Volume : 4 uL
Tray # : 1
Acquired by : AVINASH

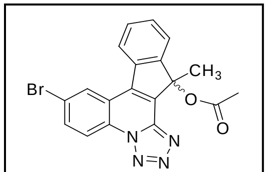
Data File Name : 11-02-10_CR080-97-81-81A_04.lcd
Method File Name : GENERAL_B2.lcm
Batch File Name : 130210.lcb
Data Acquired : 2/13/2010 6:11:59 PM
Data Processed : 2/13/2010 6:37:01 PM
Ref.No.: DI/A0257/91







1 PDA Multi 1/242nm 4nm
2 PDA Multi 2/220nm 4nm
3 PDA Multi 3/260nm 4nm



12

PDA Ch1 242nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	8.47	239135	2.24	30905
2	9.10	15125	0.14	1668
3	9.67	19700	0.18	2150
4	10.51	96383	0.90	8833
5	11.37	9795432	91.84	1112000
6	12.12	7310	0.07	977
7	12.34	23531	0.22	3559
8	12.92	90624	0.85	13432
9	13.23	137545	1.29	19655
10	14.74	145995	1.37	21516
11	15.06	43265	0.41	2331
12	16.27	11761	0.11	1019
13	17.34	11675	0.11	579
14	18.19	9189	0.09	591
15	18.87	19111	0.18	1485
Total		10665781	100.00	1220699

PeakTable

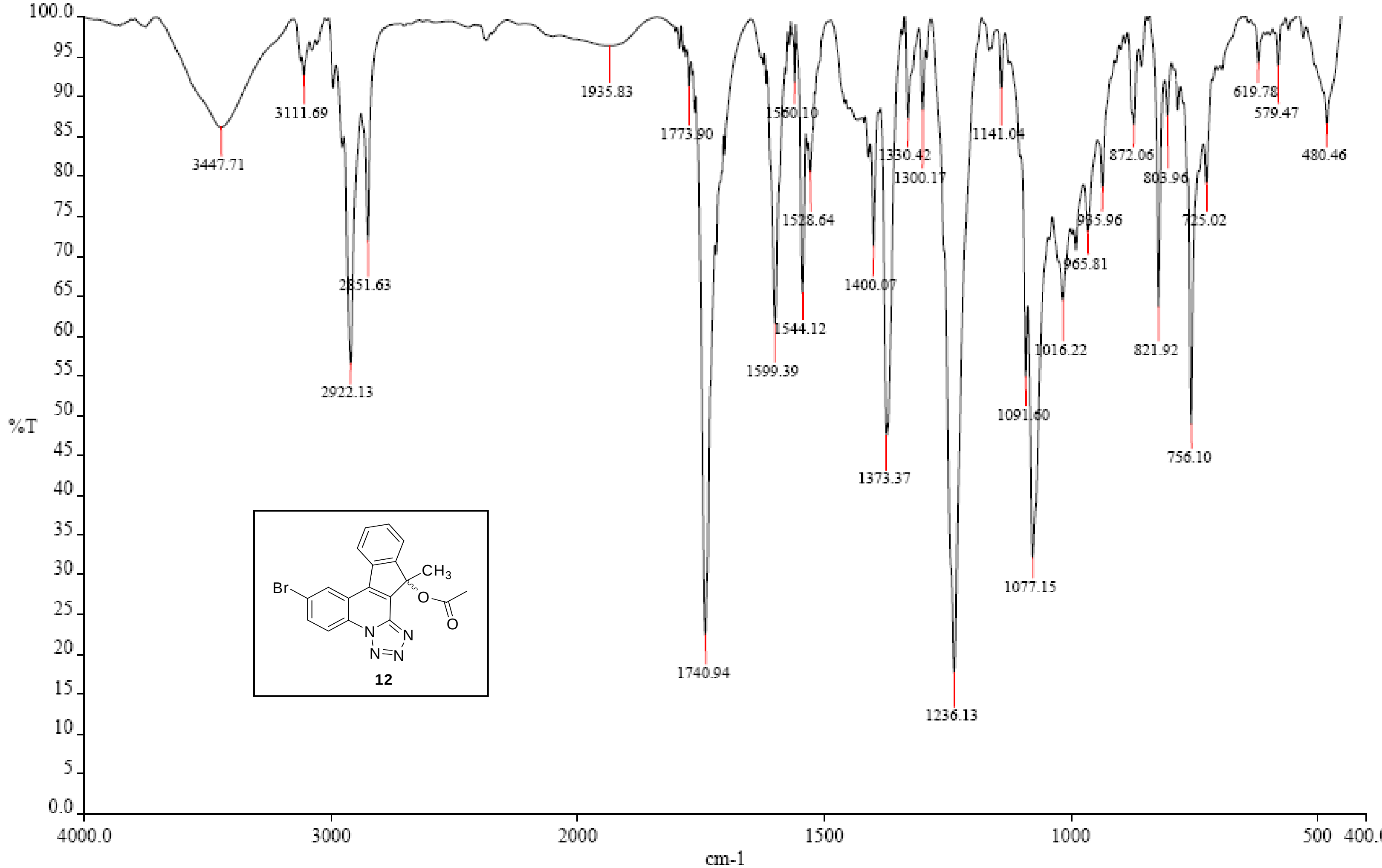
PDA Ch2 220nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	8.47	129262	2.46	16333
2	9.10	13426	0.26	939
3	9.67	44532	0.85	5108
4	10.51	54266	1.03	4564
5	11.37	4705517	89.72	530597
6	12.34	16268	0.31	2497
7	12.92	42297	0.81	6163
8	13.23	91486	1.74	12665
9	13.88	11086	0.21	1022
10	14.74	88703	1.69	12578
11	15.07	22844	0.44	1507
12	15.71	6730	0.13	677
13	16.26	8042	0.15	760
14	18.89	10272	0.20	902
Total		5244731	100.00	596314

PeakTable

PDA Ch3 260nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	8.47	127488	2.15	16586
2	9.10	9426	0.16	934
3	9.67	33843	0.57	3851
4	10.51	51663	0.87	4856
5	11.37	5392938	91.03	608664
6	12.10	6931	0.12	853
7	12.34	17416	0.29	2283
8	12.92	58850	0.99	8083
9	13.23	80398	1.36	10680
10	14.74	123673	2.09	13895
11	16.27	7930	0.13	576
12	18.19	5575	0.09	323
13	18.87	8118	0.14	695
Total		5924251	100.00	672278



Spectrum Name: CR080-97-81-81A.sp

Analyst: GANESH

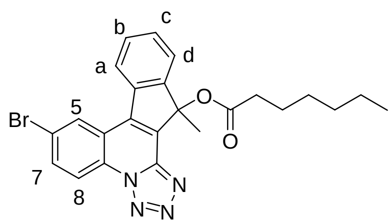
Accumulations: 16

Time: 10:45:32 AM

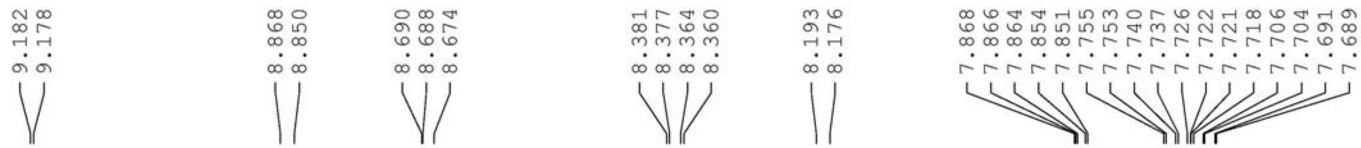
Description: CR080-97-81-81A IN KBr

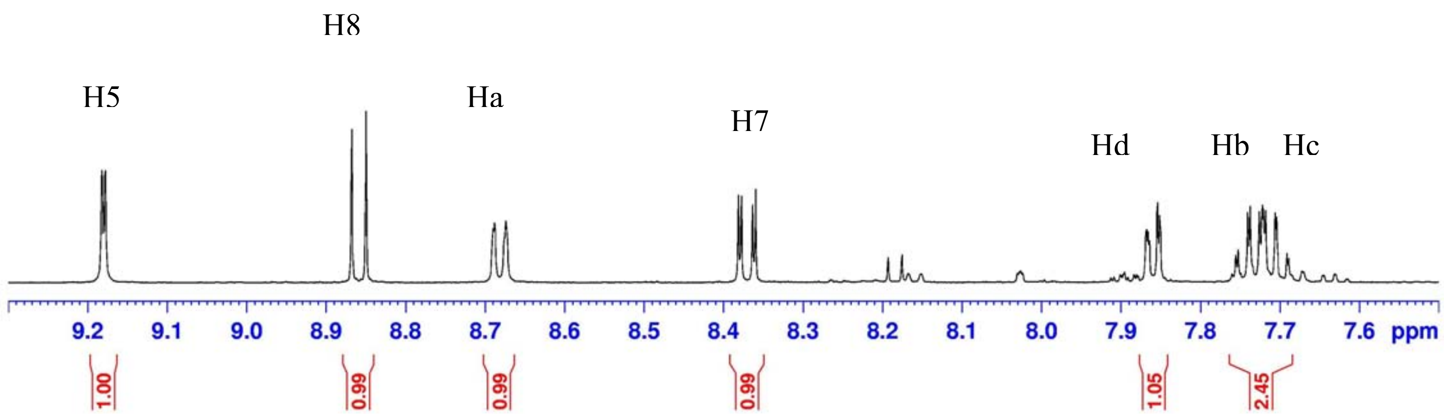
Resolution: 4.00 cm-1

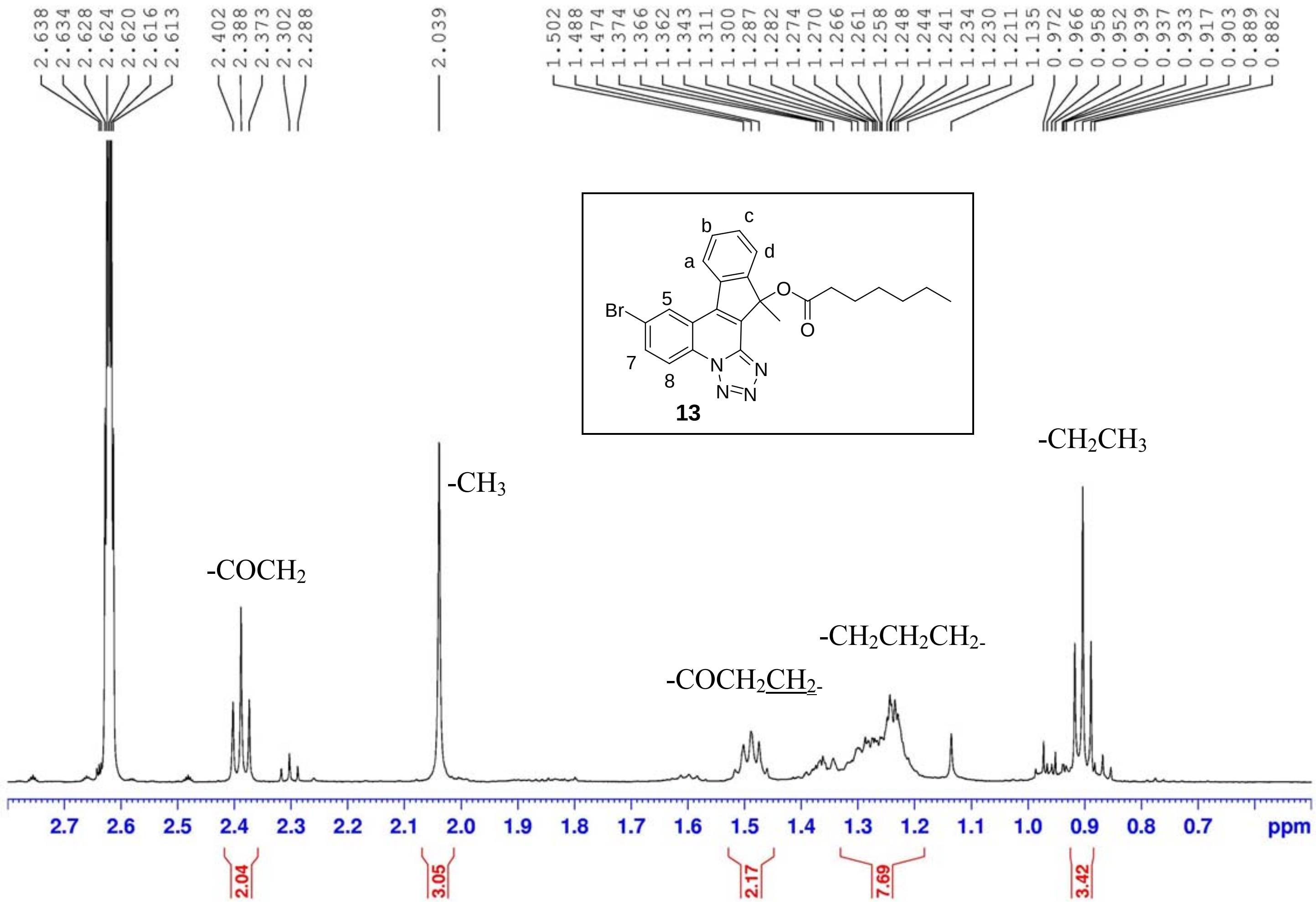
Date: 1/25/2010


Br
a
b
c
d
5
7
8
O
O
N
N
N
N

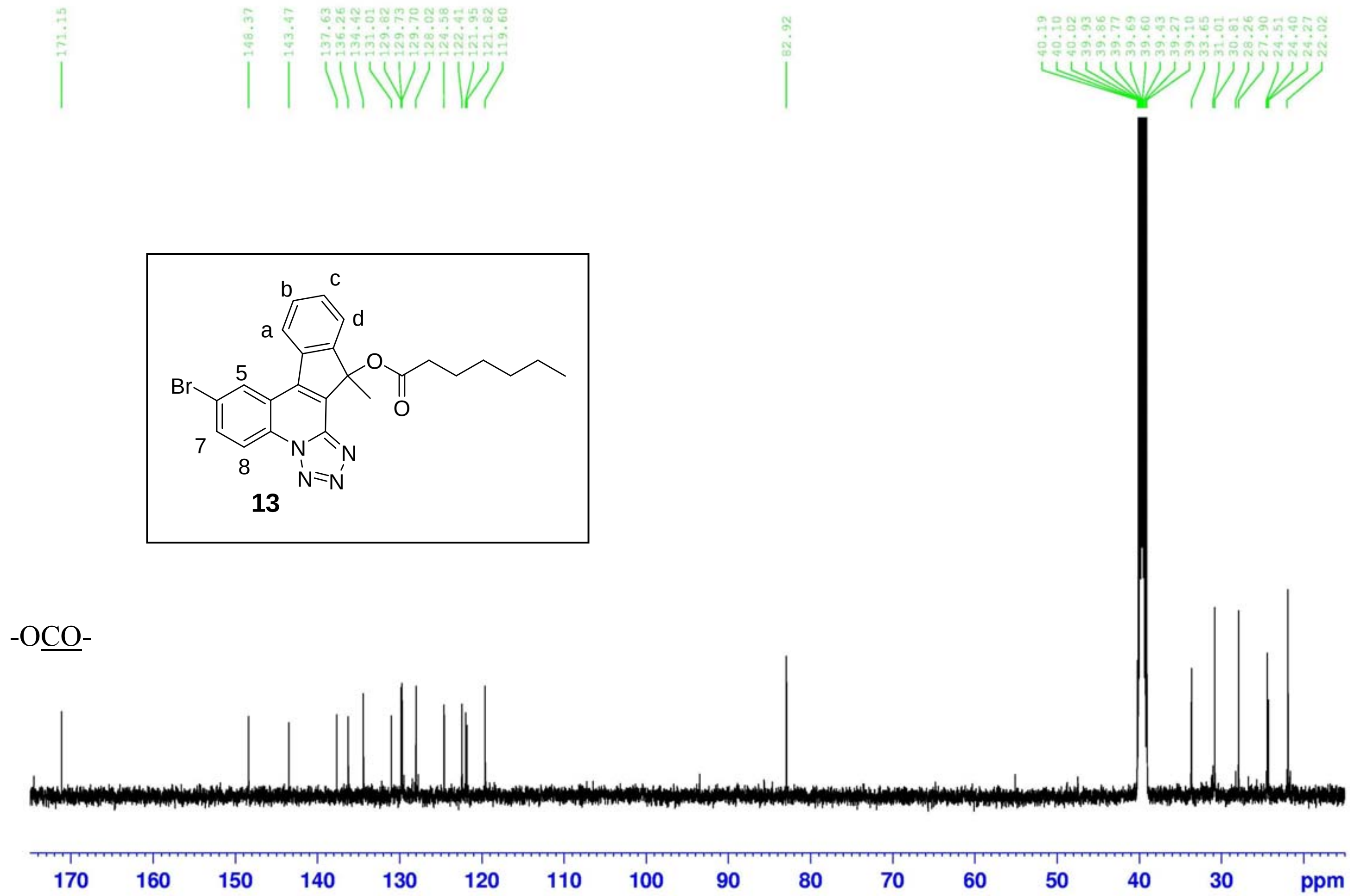
13


9.182
9.178
8.868
8.850
8.690
8.688
8.674
8.381
8.377
8.364
8.360
8.193
8.176
7.868
7.866
7.864
7.854
7.851
7.755
7.753
7.740
7.737
7.726
7.722
7.721
7.718
7.706
7.704
7.691
7.689

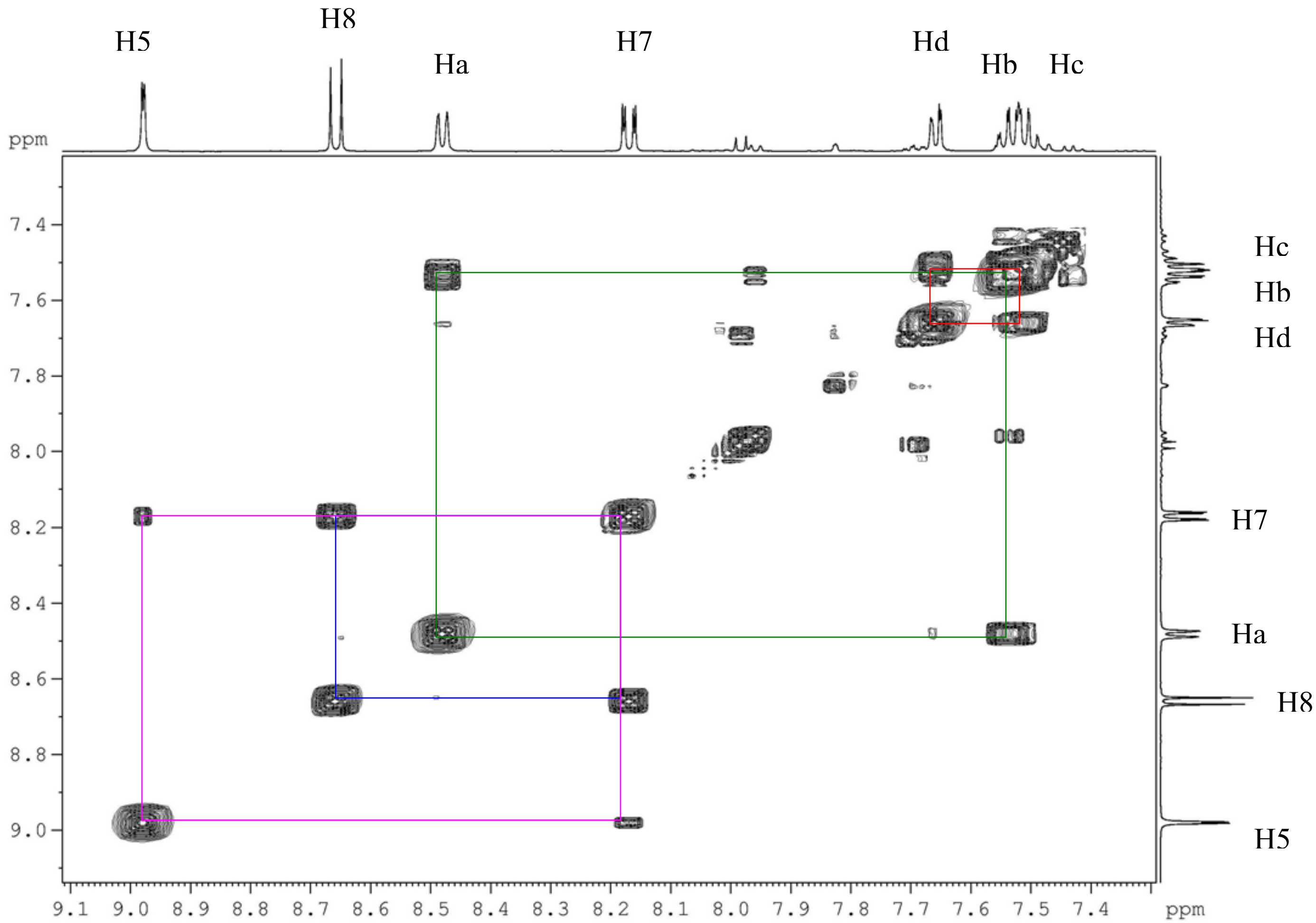

H8
H5
Ha
H7
Hd
Hb
Hc
9.2
9.1
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
ppm
1.00
0.99
0.99
0.99
1.05
2.45

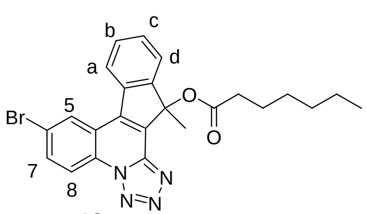


2.638
2.634
2.628
2.624
2.620
2.616
2.613
2.402
2.388
2.373
2.302
2.288
2.039
1.502
1.488
1.474
1.374
1.366
1.362
1.343
1.311
1.300
1.287
1.282
1.274
1.270
1.266
1.261
1.258
1.248
1.244
1.241
1.234
1.230
1.211
1.135
0.972
0.966
0.958
0.952
0.939
0.937
0.933
0.917
0.903
0.889
0.882
13
-COCH2
-CH3
-COCH2CH2-
-CH2CH2CH2-
-CH2CH3
ppm
2.04
3.05
2.17
7.69
3.42

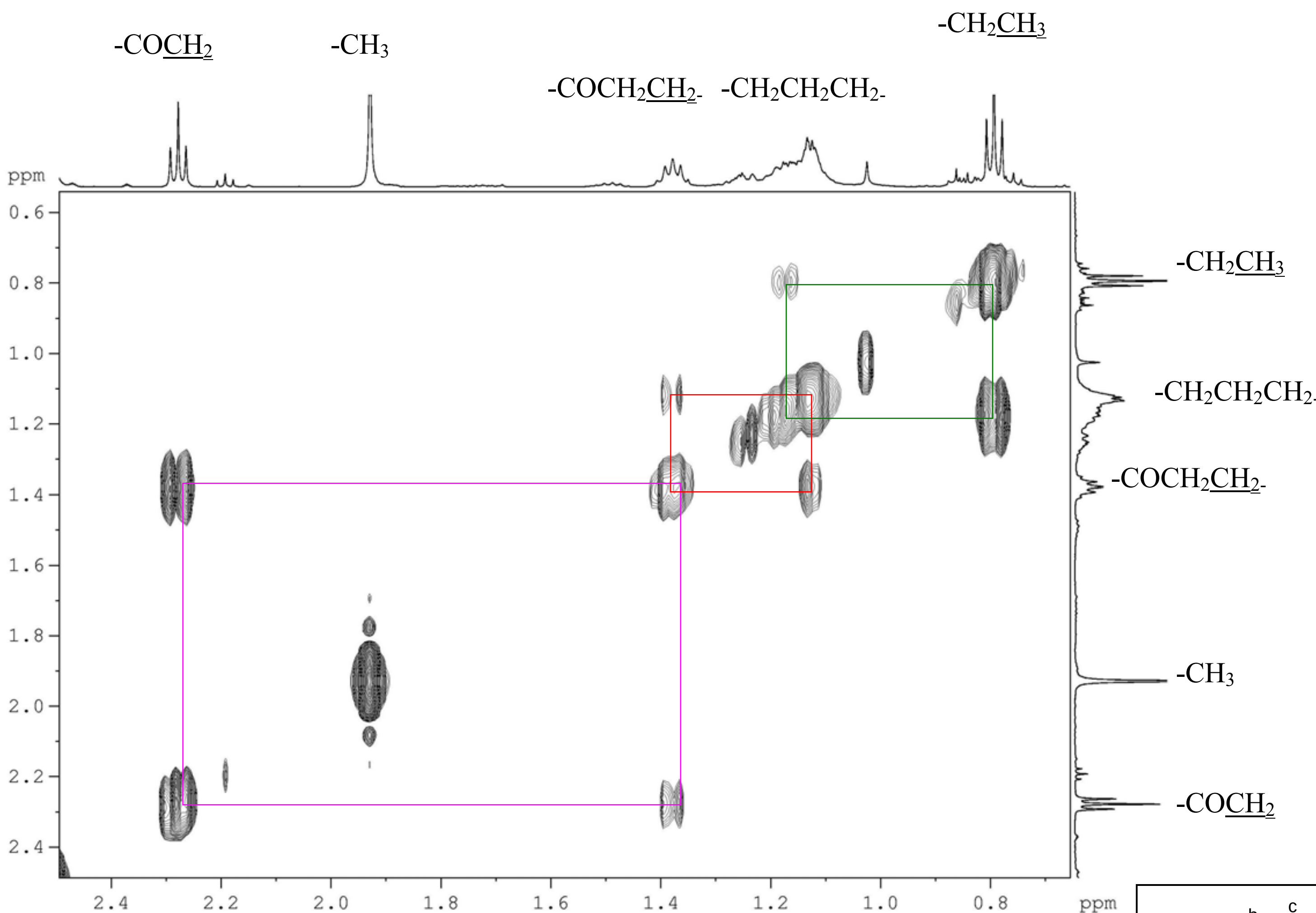


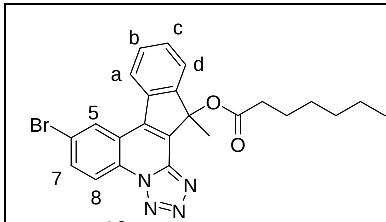
171.15
148.37
143.47
137.63
136.26
134.42
131.01
129.82
129.73
129.70
128.02
124.58
122.41
121.95
121.82
119.60
82.92
40.19
40.10
40.02
39.93
39.86
39.77
39.69
39.60
39.43
39.27
39.10
33.65
31.01
30.81
28.26
27.90
24.51
24.40
24.27
22.02
-OCO-
Br
13
ppm


H5
H8
Ha
H7
Hd
Hb
Hc
ppm
7.4
7.6
7.8
8.0
8.2
8.4
8.6
8.8
9.0
9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
Hc
Hb
Hd
H7
Ha
H8
H5

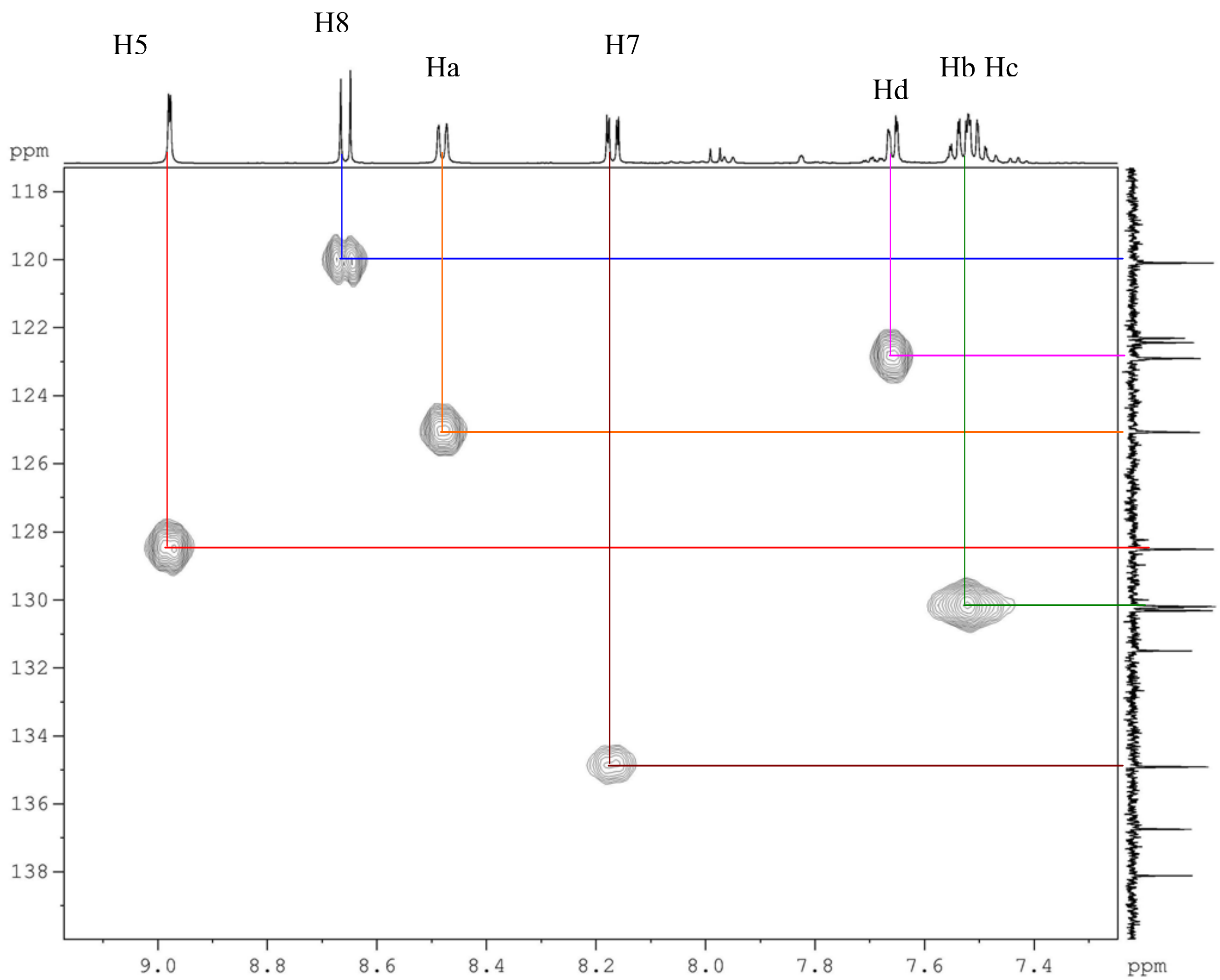

Br
5
7
8
a
b
c
d
O
O
N
N
N
N

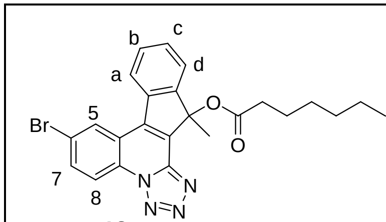
13


-COCH2
-CH3
-COCH2CH2-
-CH2CH2CH2-
-CH2CH3
ppm
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
ppm
-CH2CH3
-CH2CH2CH2-
-COCH2CH2-
-CH3
-COCH2

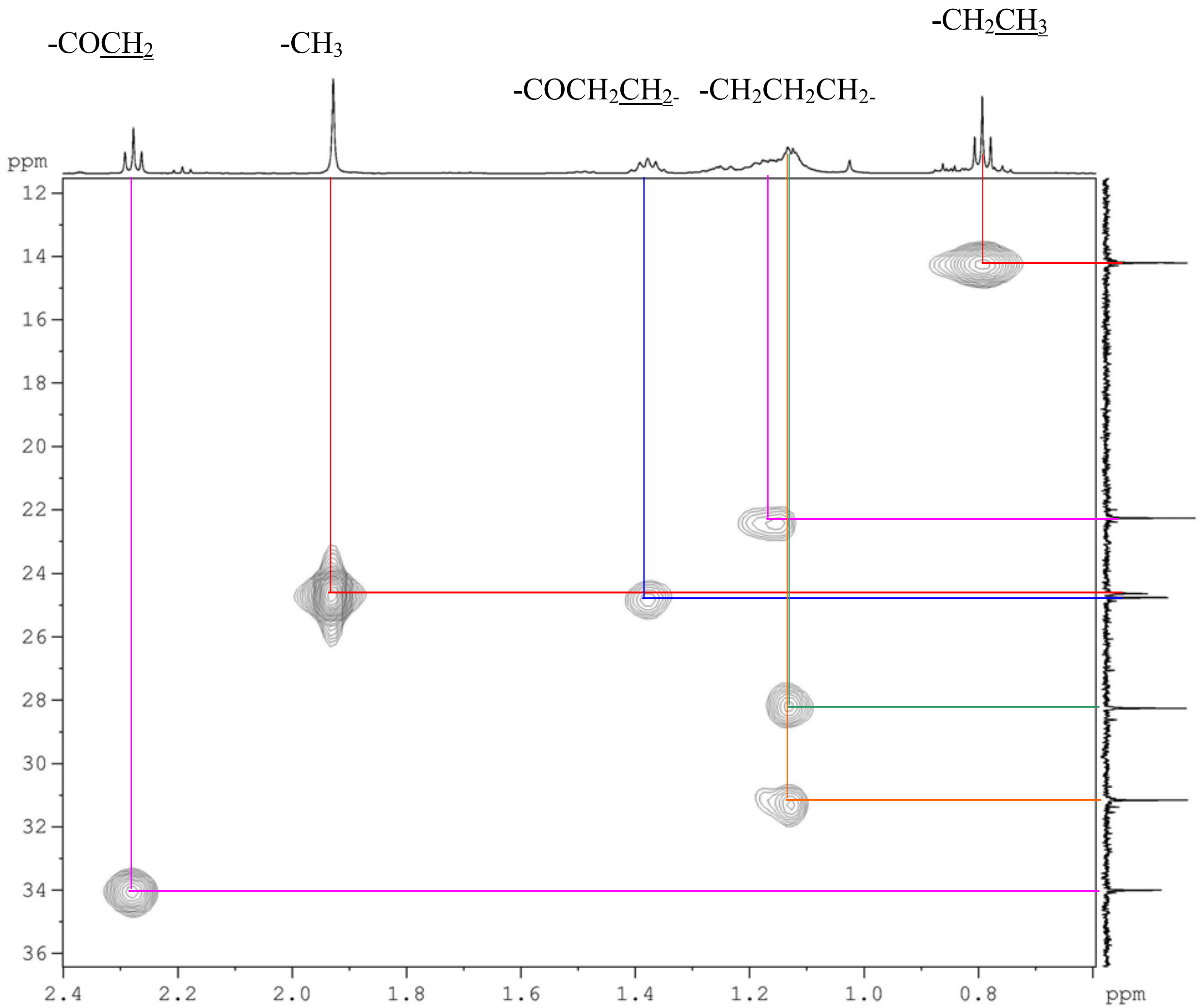

a
b
c
d
5
7
8
Br
O
O
N
N
N
N

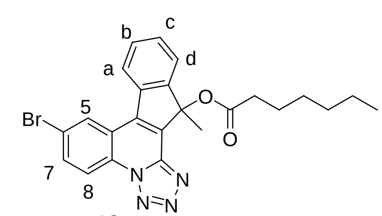
13


H5
H8
Ha
H7
Hd
Hb Hc
ppm
118
120
122
124
126
128
130
132
134
136
138
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
ppm

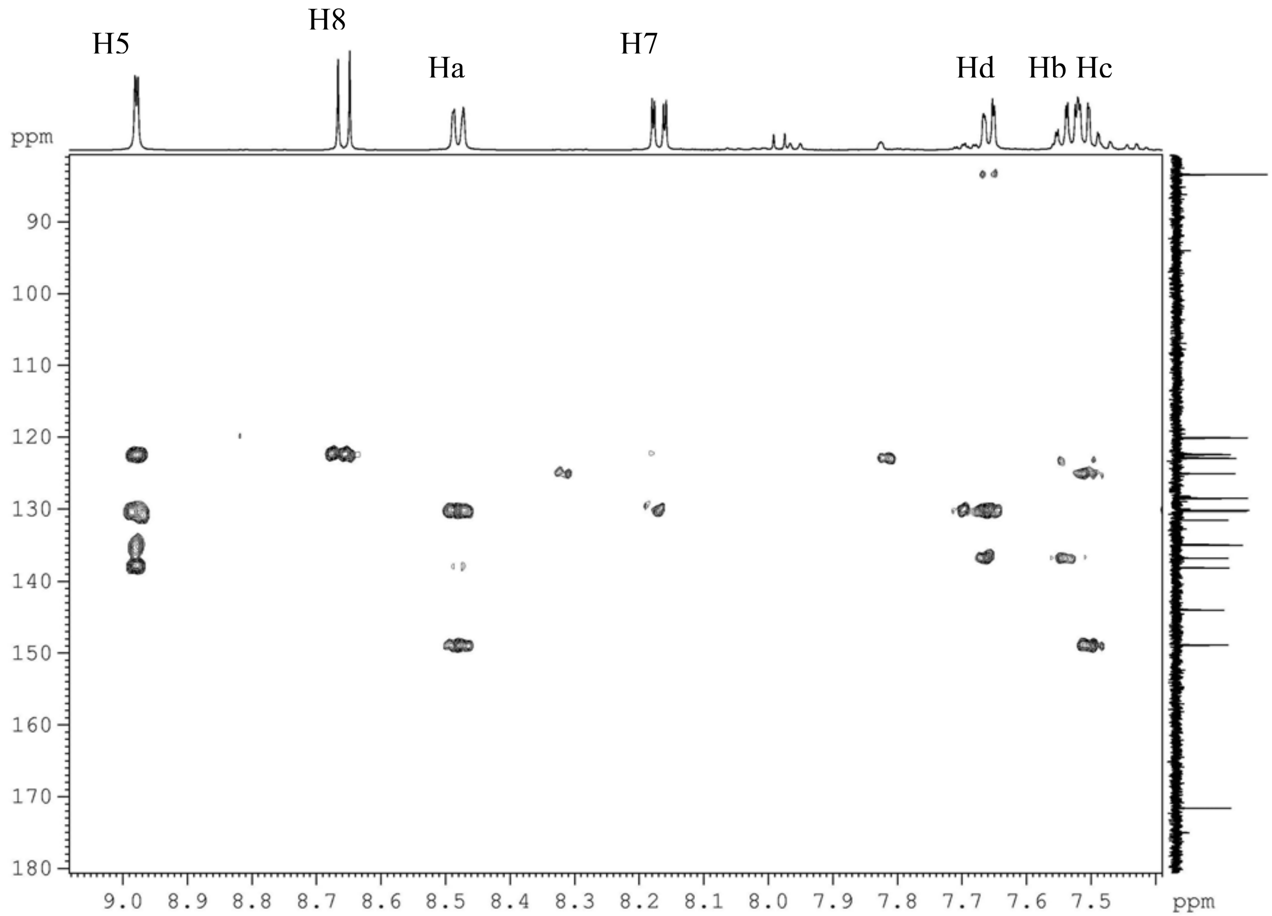

b
c
a
d
O
Br
5
O
7
8
N
N
N
N

13

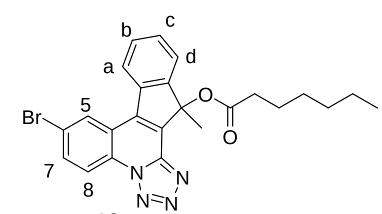

-COCH2
-CH3
-COCH2CH2-
-CH2CH2CH2-
-CH2CH3
ppm
12
14
16
18
20
22
24
26
28
30
32
34
36
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
ppm


b
c
a
d
Br
5
O
O
7
8
N
N
N
N

13

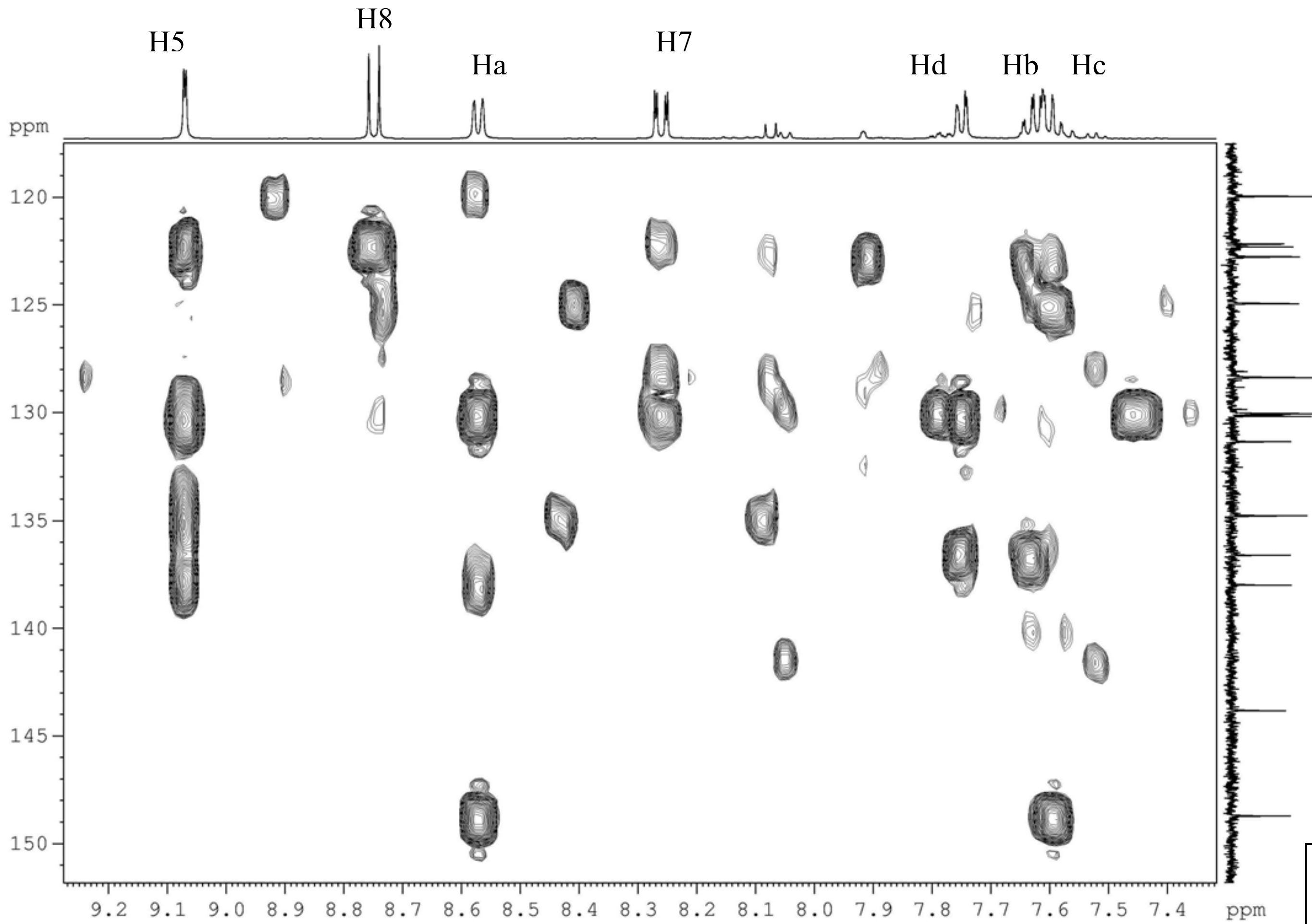


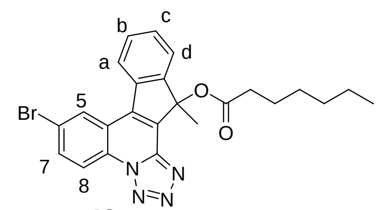
H5
H8
Ha
H7
Hd
Hb Hc
ppm
90
100
110
120
130
140
150
160
170
180
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
ppm

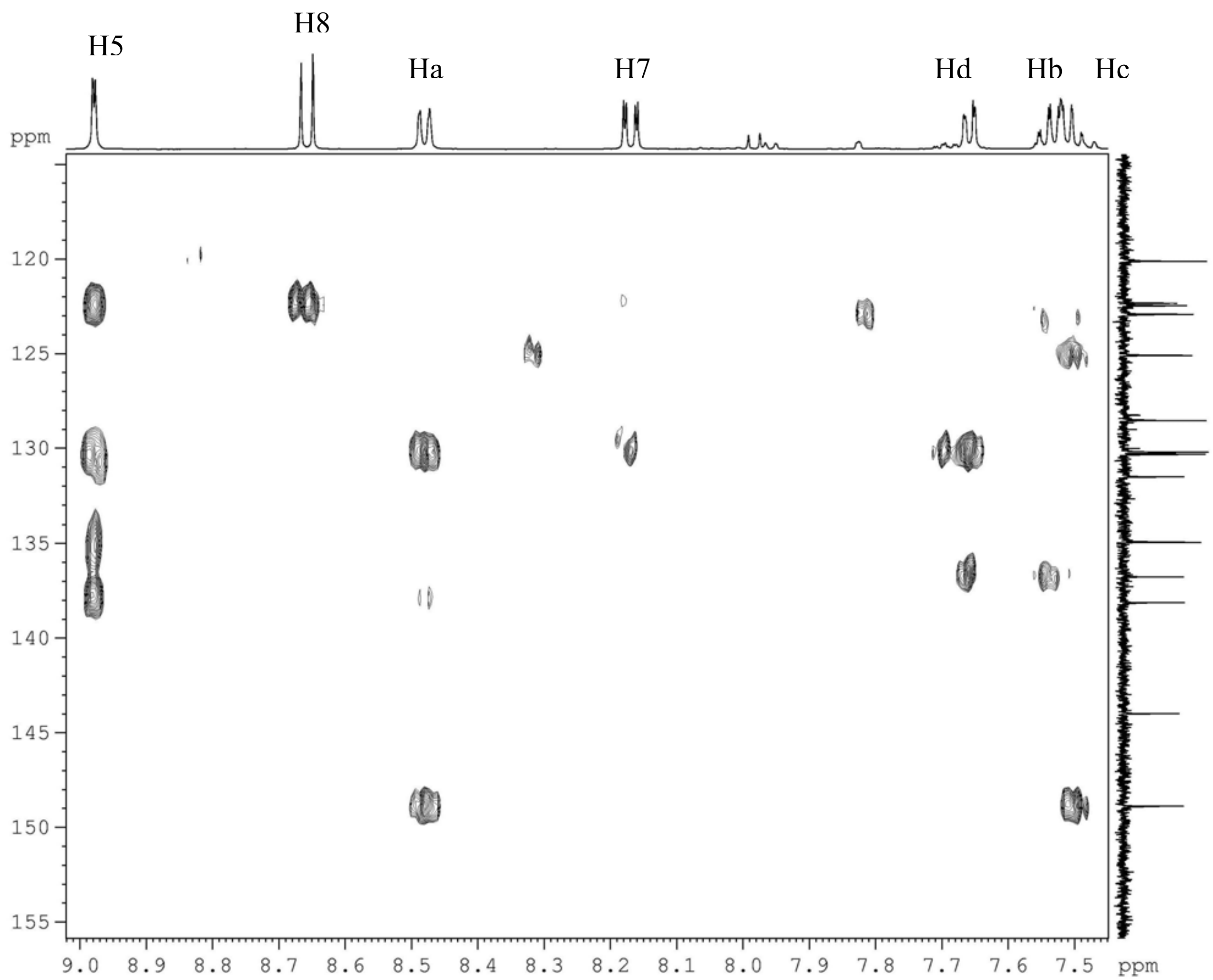


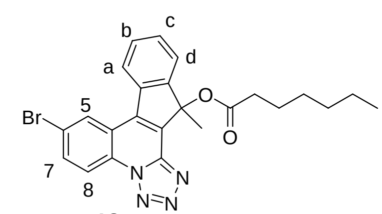
a
b
c
d
Br
5
7
8
O
O
N
N
N
N

13

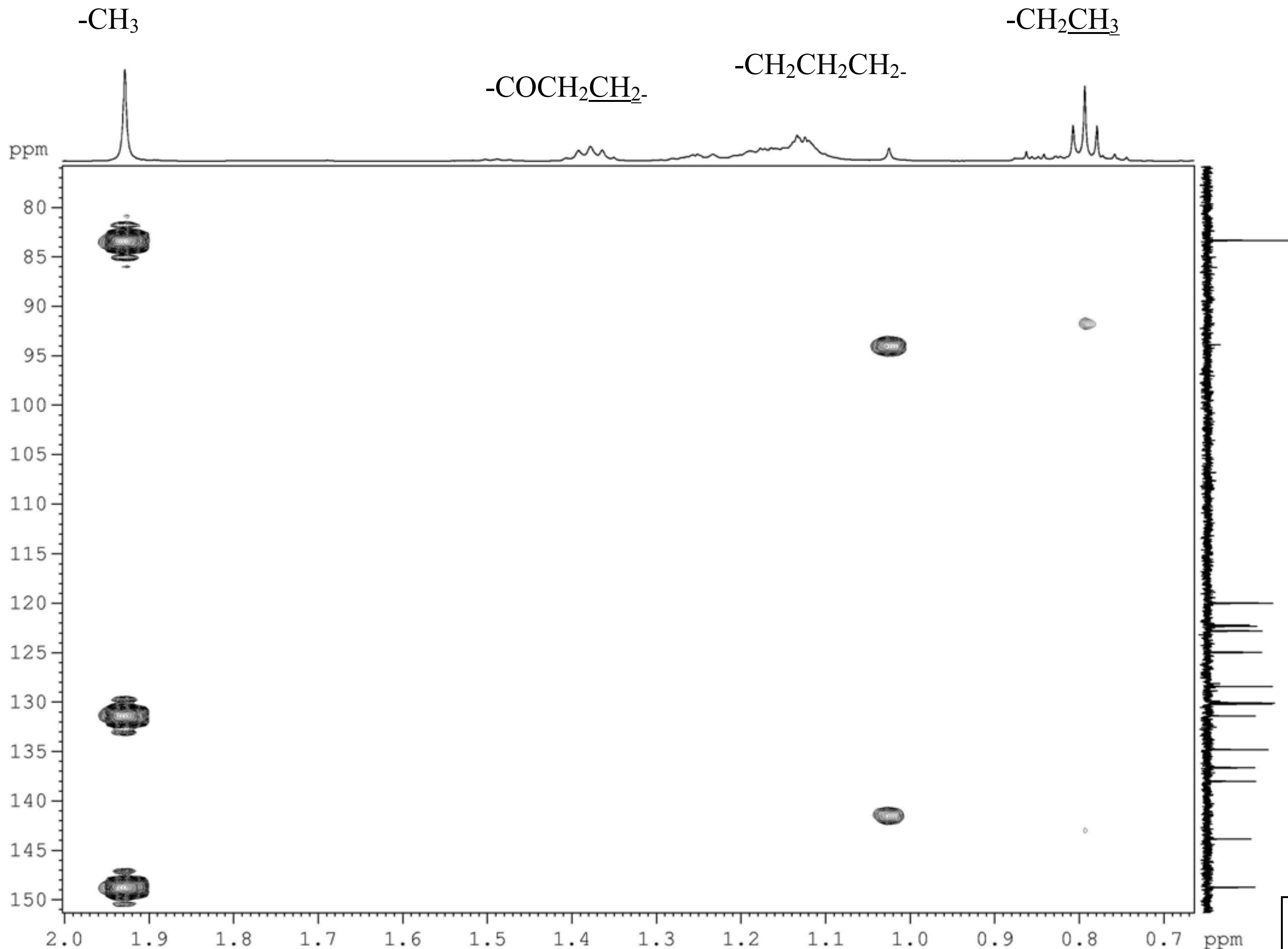

H5
H8
Ha
H7
Hd
Hb
Hc
ppm
120
125
130
135
140
145
150
9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
ppm

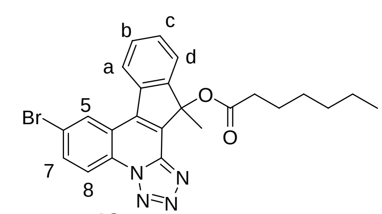

a
b
c
d
5
7
8
Br
O
O
N
N
N
N
13


H5
H8
Ha
H7
Hd
Hb
Hc
ppm
120
125
130
135
140
145
150
155
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
ppm

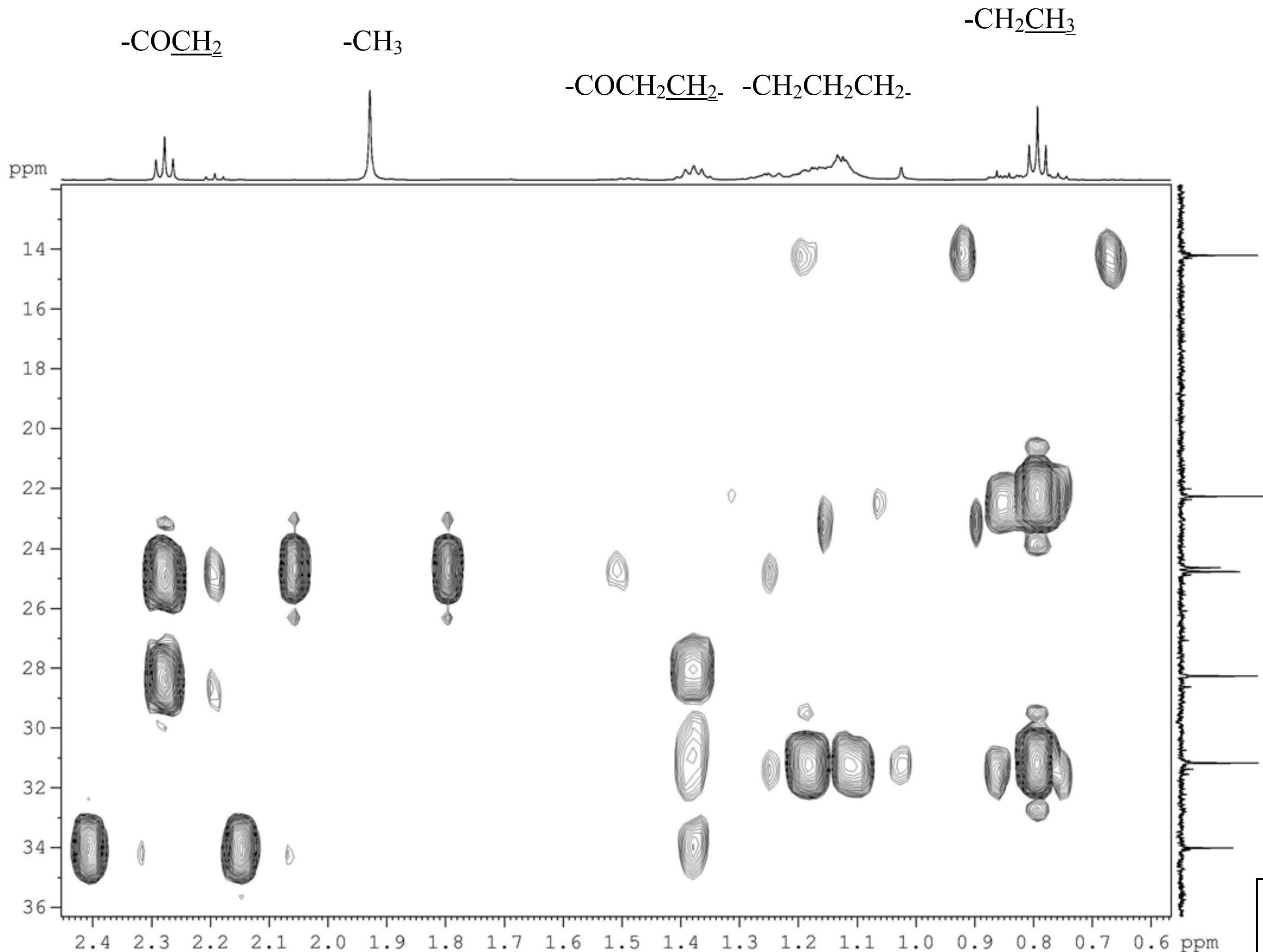

b
c
a
d
Br
5
7
8
O
O
N
N
N
N

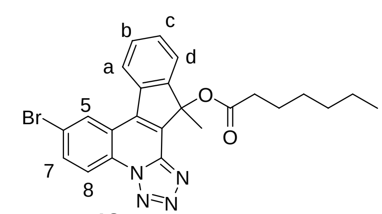
13


-CH3
-COCH2CH2-
-CH2CH2CH2-
-CH2CH3
ppm
80
85
90
95
100
105
110
115
120
125
130
135
140
145
150
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
ppm


b
c
d
a
O
Br
5
O
7
8
N
N
N
N

13

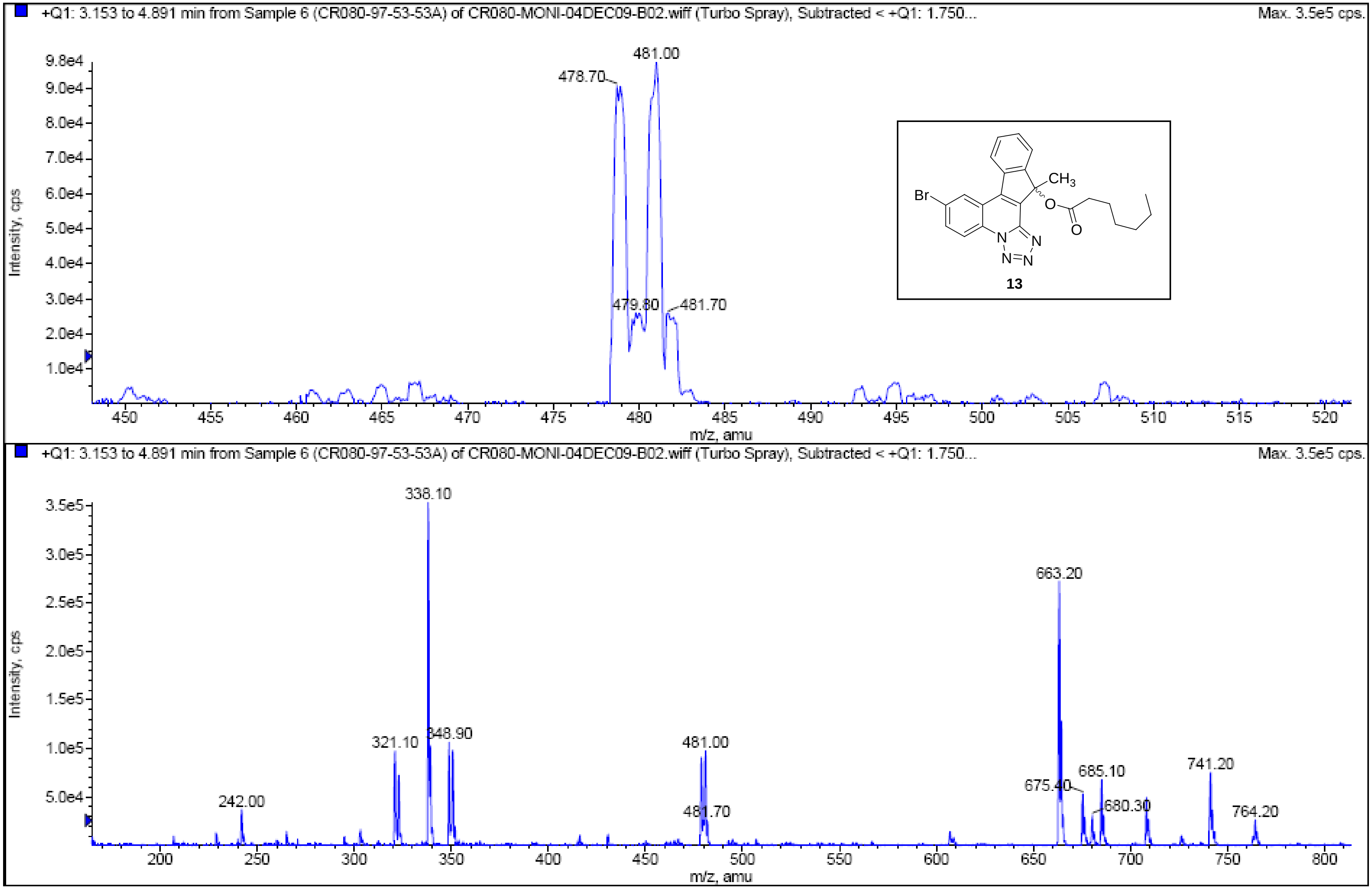

-COCH2
-CH3
-COCH2CH2-
-CH2CH2CH2-
-CH2CH3
ppm
14
16
18
20
22
24
26
28
30
32
34
36
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
ppm


b
c
a
d
O
5
Br
O
7
8
N
N
N
N

13

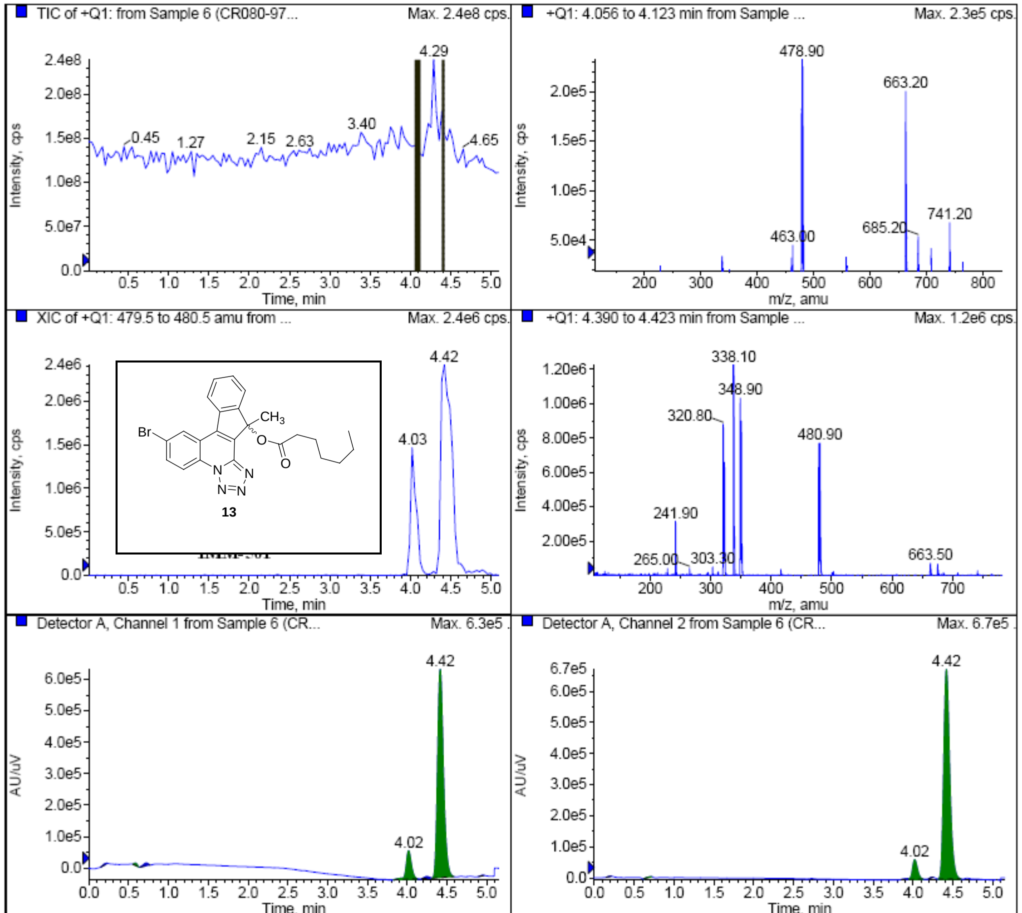
INDIA

Sample Name: CR080-97-53-53A Acq. Time: 15:20 Acq. Date: Friday, December 04, 2009



*Sample Comment: [M+H] 480 Expected **Analyzed By : **Checked By :

Sample Name: CR080-97-53-53A   Acq. Time: 15:20   Acq. Date: Friday, December 04, 2009



Peak List for "Detector A, Channel 1 from Sample 6 (CR080-97-53-

	Time (min)	Area (counts)	%Area	Height
1	0.2221	1.0097e4	0.2606	2068.1318
2	0.5832	1.8688e4	0.4824	7374.1384
3	0.7210	3.4376e4	0.8873	8704.5195
4	4.0207	4.0995e5	10.5814	9.0225e4
5	4.2487	2.4120e4	0.6226	5662.2632
6	4.4176	3.3733e6	87.0690	6.6245e5
7	4.9575	3746.0716	0.0967	1071.9310

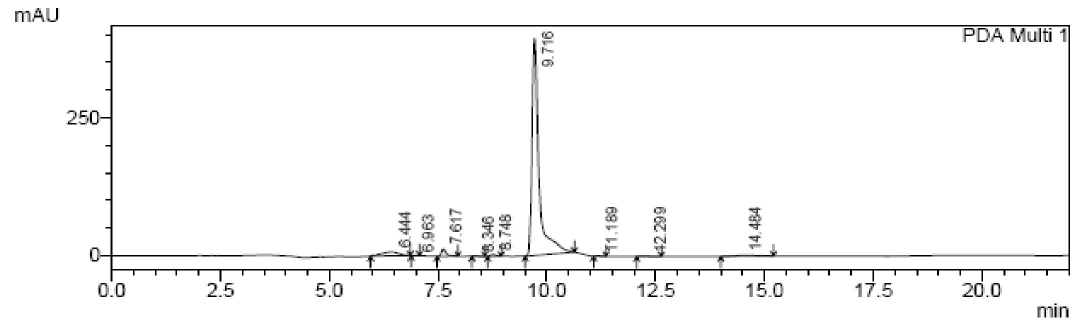
Peak List for "Detector A, Channel 2 from Sample 6 (CR080-97-53-5

	Time (min)	Area (counts)	%Area	Height
1	0.2037	2733.6839	0.0725	954.6030
2	0.7117	7949.8087	0.2107	1161.9433
3	3.9303	1.1425e4	0.3028	2808.9083
4	4.0191	2.6394e5	6.9958	6.2609e4
5	4.2405	3388.6255	0.0898	1331.3241
6	4.4170	3.4833e6	92.3284	6.7416e5

LCMS-1 REACN MONT (TFA Buffer)   Analysed By :

Sample Name : CR080-97-53-53A
Sample ID : CR080-97-53-53A
Column : Gemini C-18 (150 x 4.6 mm)
Vial # : 58
Inj. Volume : 1 uL
Tray # : 1
Acquired by : AVINASH

Data File Name : 15-02-10_CR080-97-53-53A_06.lcd
Method File Name : GENERAL_B1.lcm
Batch File Name : 150210.lcb
Data Acquired : 2/15/2010 1:23:16 PM
Data Processed : 2/15/2010 1:45:20 PM
Ref.No.: DI/A0257/94

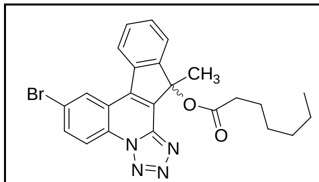


1 PDA Multi 1/242nm 4nm

PeakTable

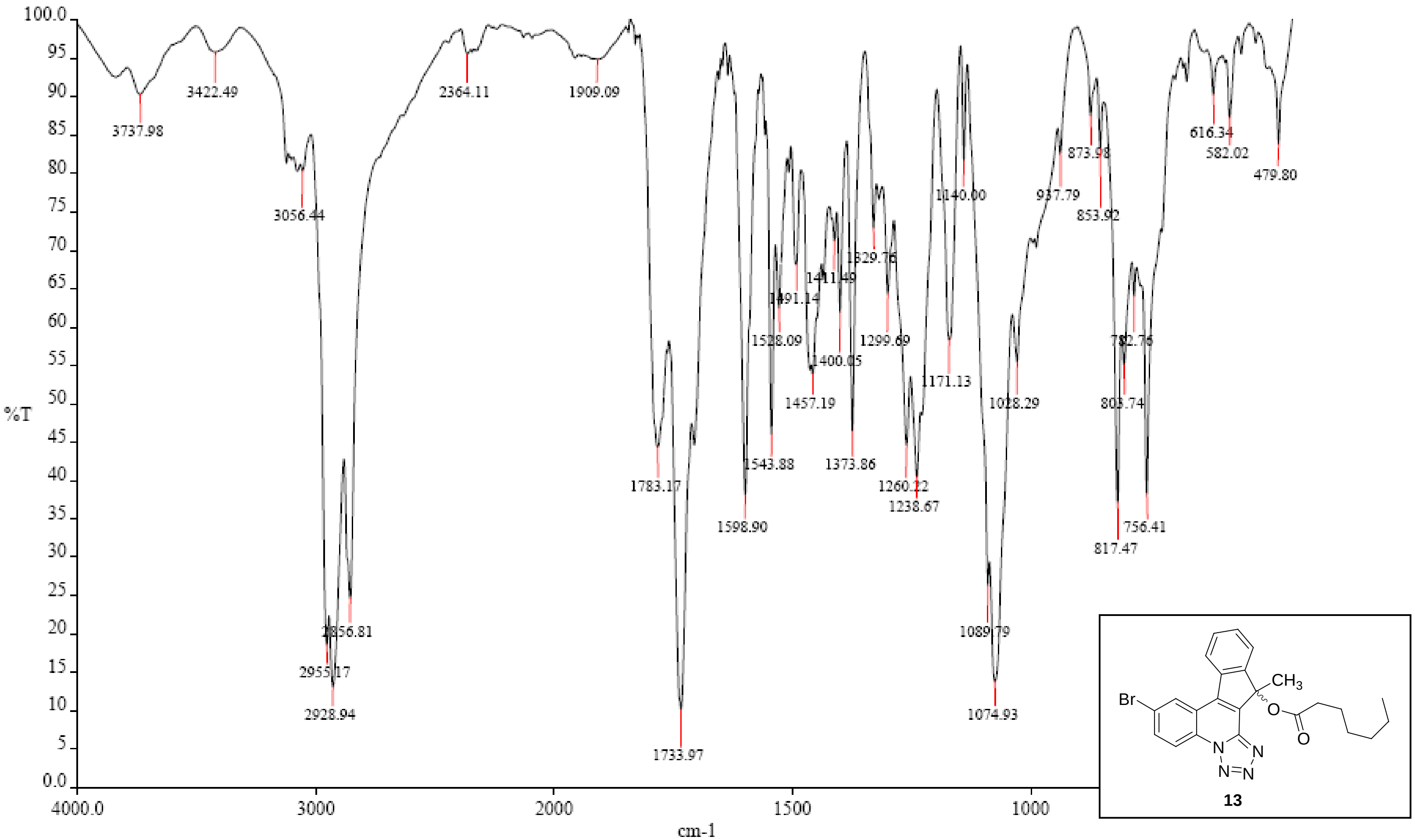
PDA Ch1 242nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	6.44	202832	4.23	7133
2	6.96	3518	0.07	752
3	7.62	103626	2.16	13846
4	8.35	4318	0.09	646
5	8.75	27218	0.57	3593
6	9.72	4375879	91.31	392648
7	11.19	7426	0.15	886
8	12.30	7291	0.15	580
9	14.48	60431	1.26	1872
Total		4792539	100.00	421956



13

CHEMBIOTEK A TCG Lifesciences Enterprises, PUNE



Spectrum Name: CR080-97-53-53A.sp

Analyst: GANESH

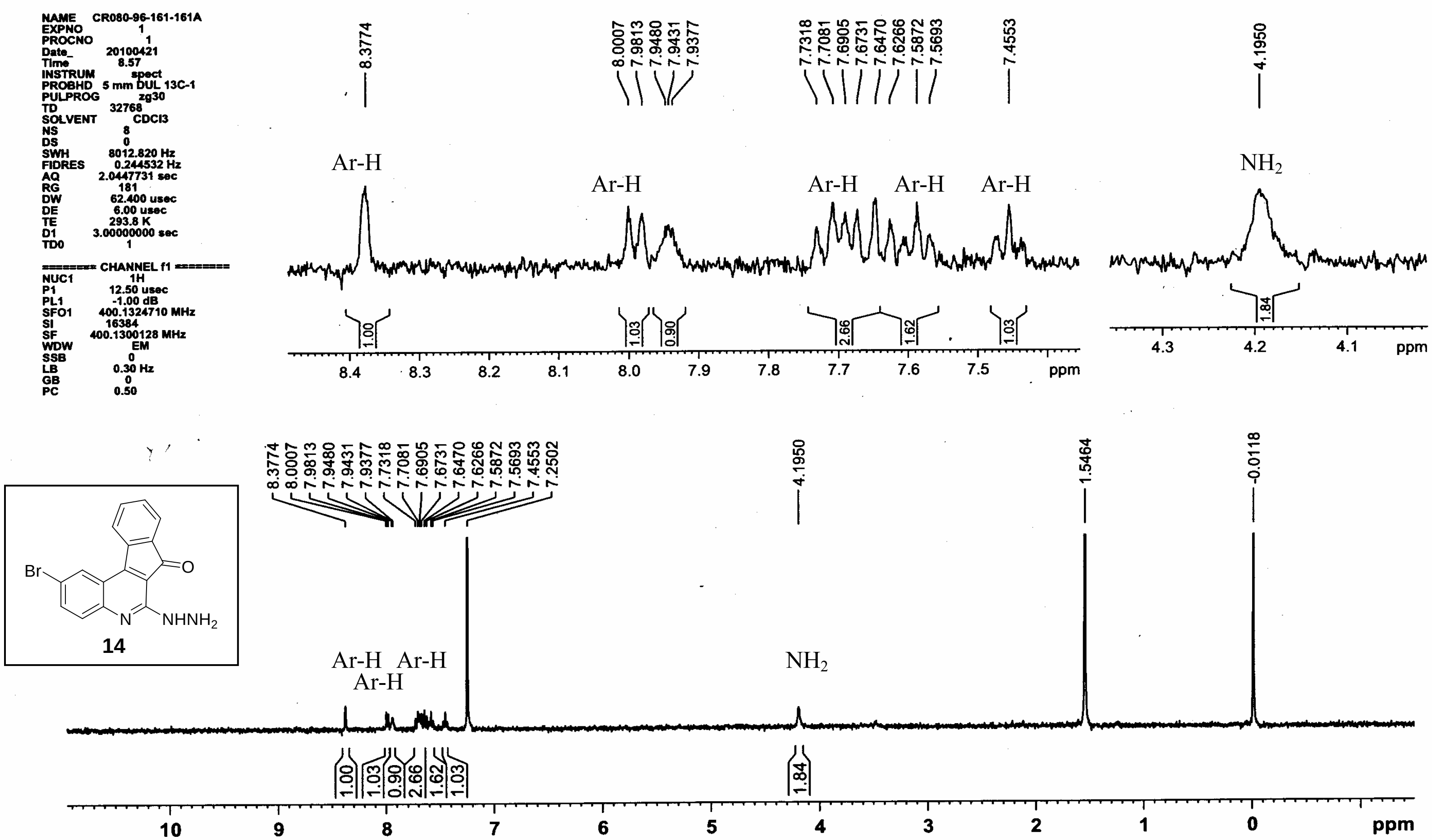
Accumulations: 16

Time: 10:30:35 AM

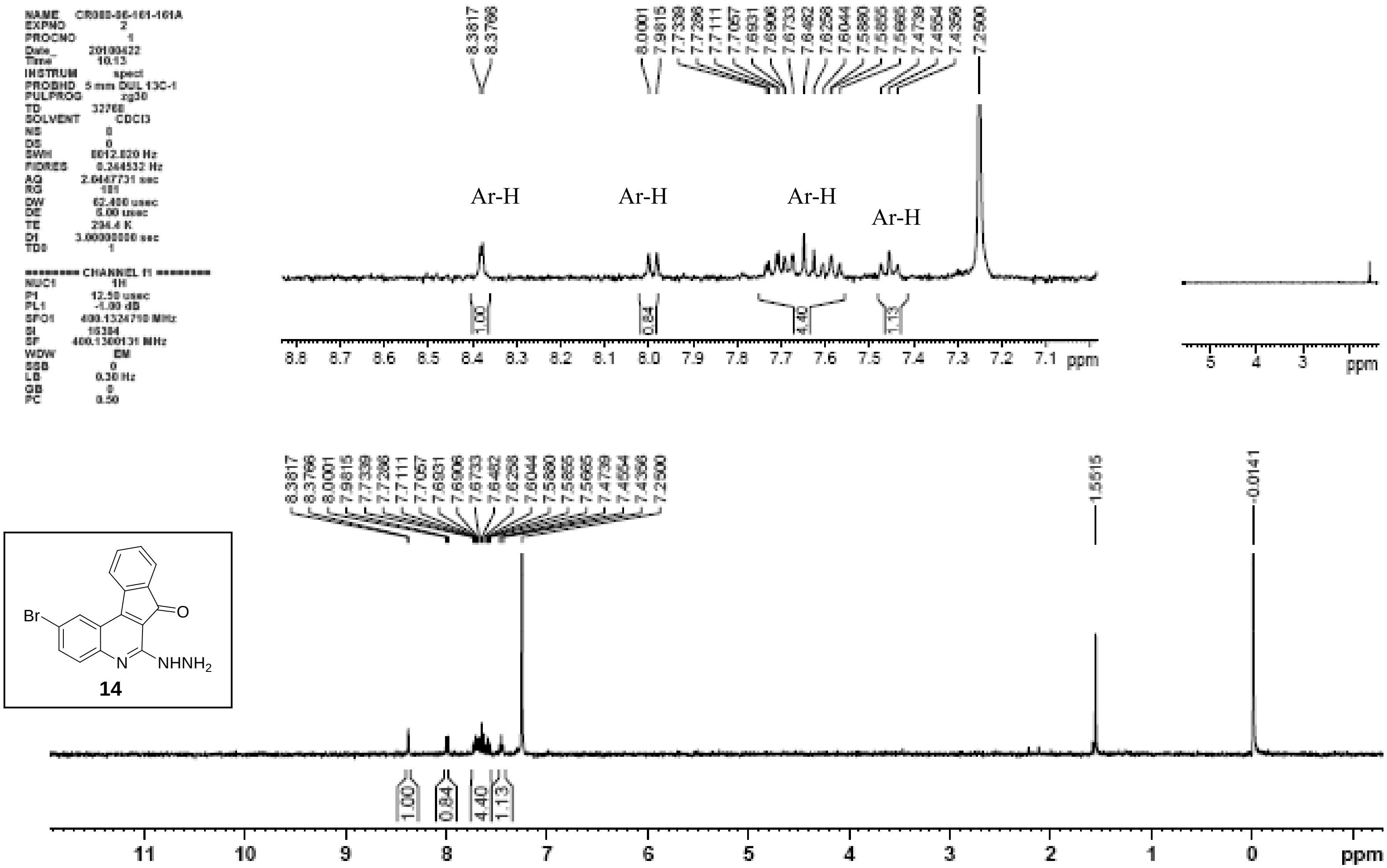
Description: CR080-97-53-53A IN KBr

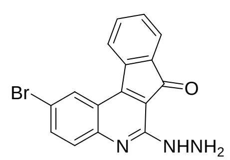
Resolution: 4.00 cm-1

Date: 2/3/2010

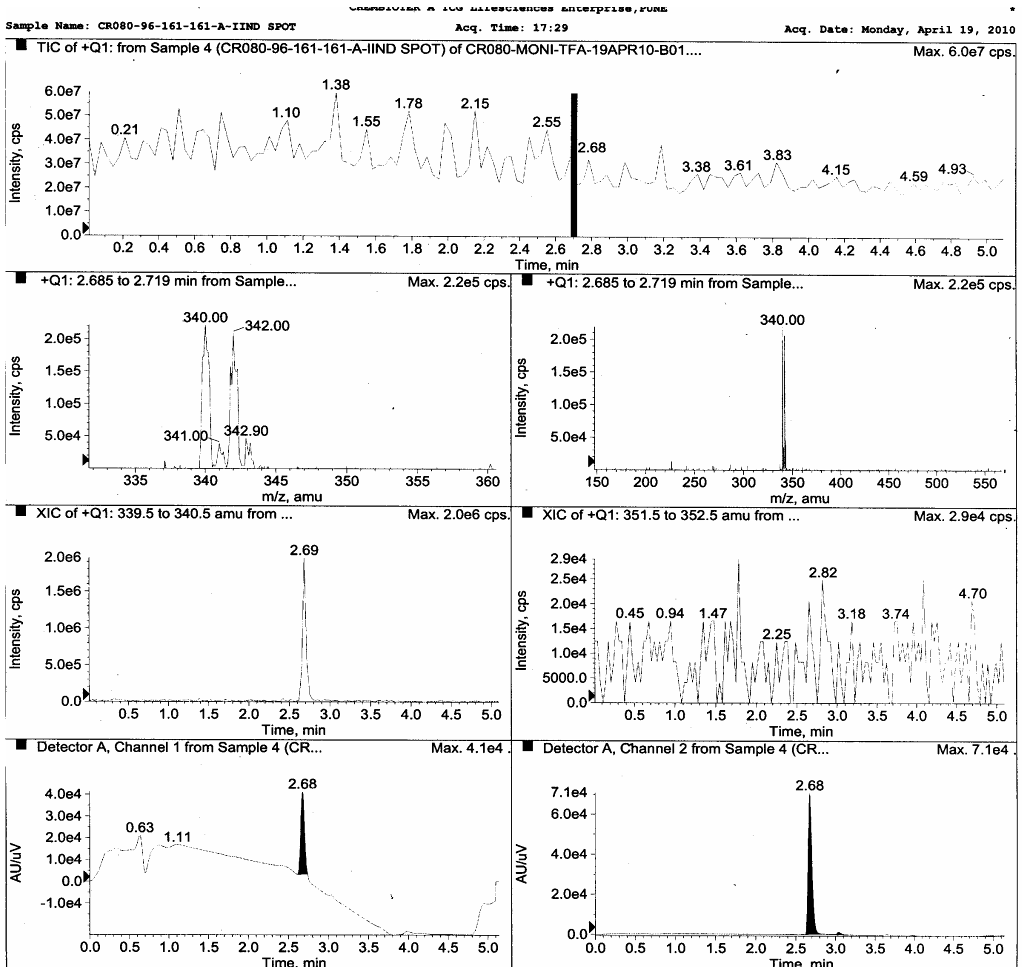


Analysed by: Yogita


Ar-H
Ar-H
Ar-H
Ar-H
Br
O
N
NHNH2
14
ppm



14



Peak List for "Detector A, Channel 1 from Sample 4 (CR080-96-161

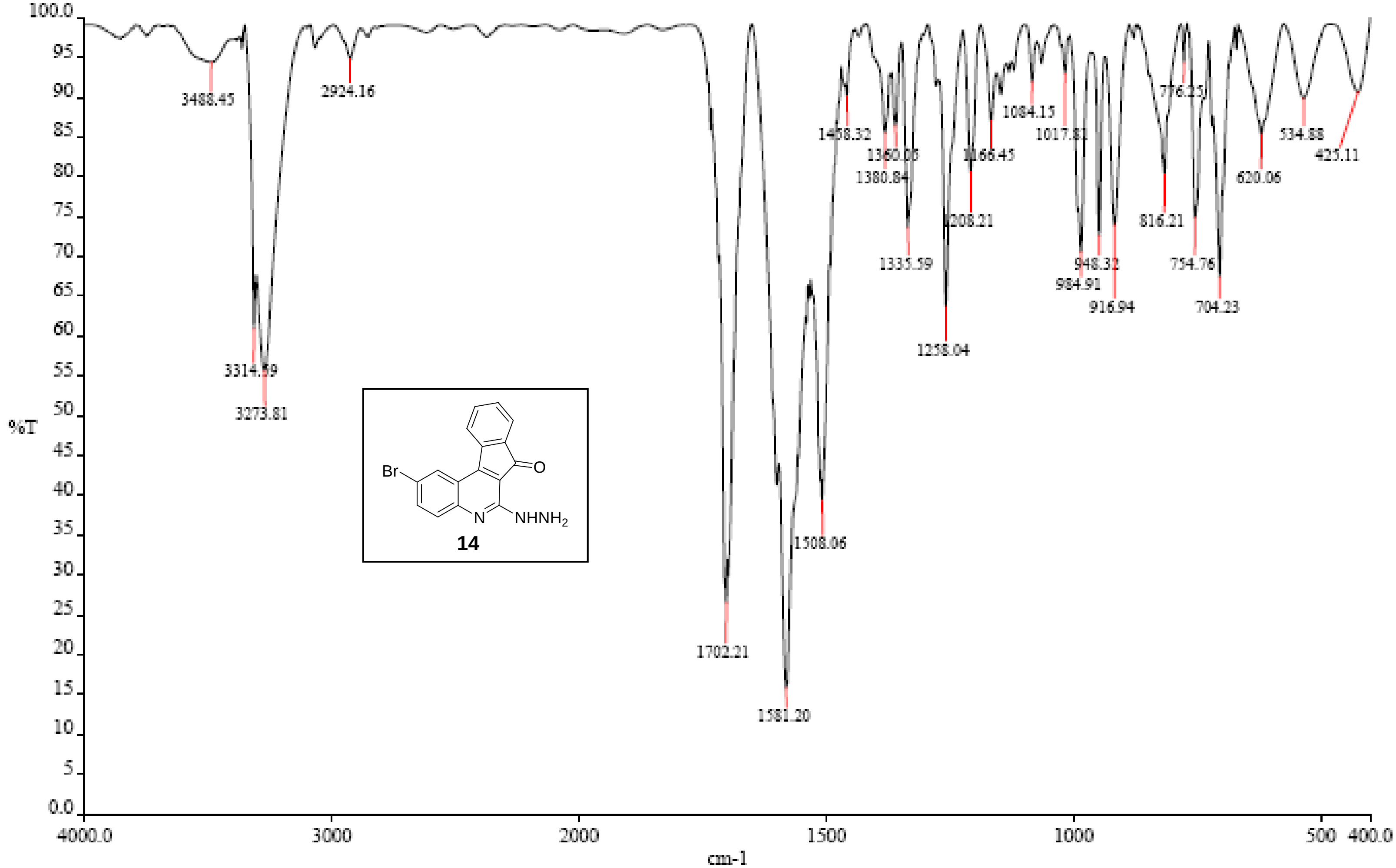
	Time (min)	Area (counts)	%Area	Height
1	2.6802	1.2621e5	100.000	3.8425e4

Peak List for "Detector A, Channel 2 from Sample 4 (CR080-96-161-

	Time (min)	Area (counts)	%Area	Height
1	2.6752	2.3972e5	96.9652	7.0659e4
2	3.0425	4433.2904	1.7932	1229.8433
3	3.9743	1508.2804	0.6101	405.5891
4	4.9362	1561.2646	0.6315	265.1650

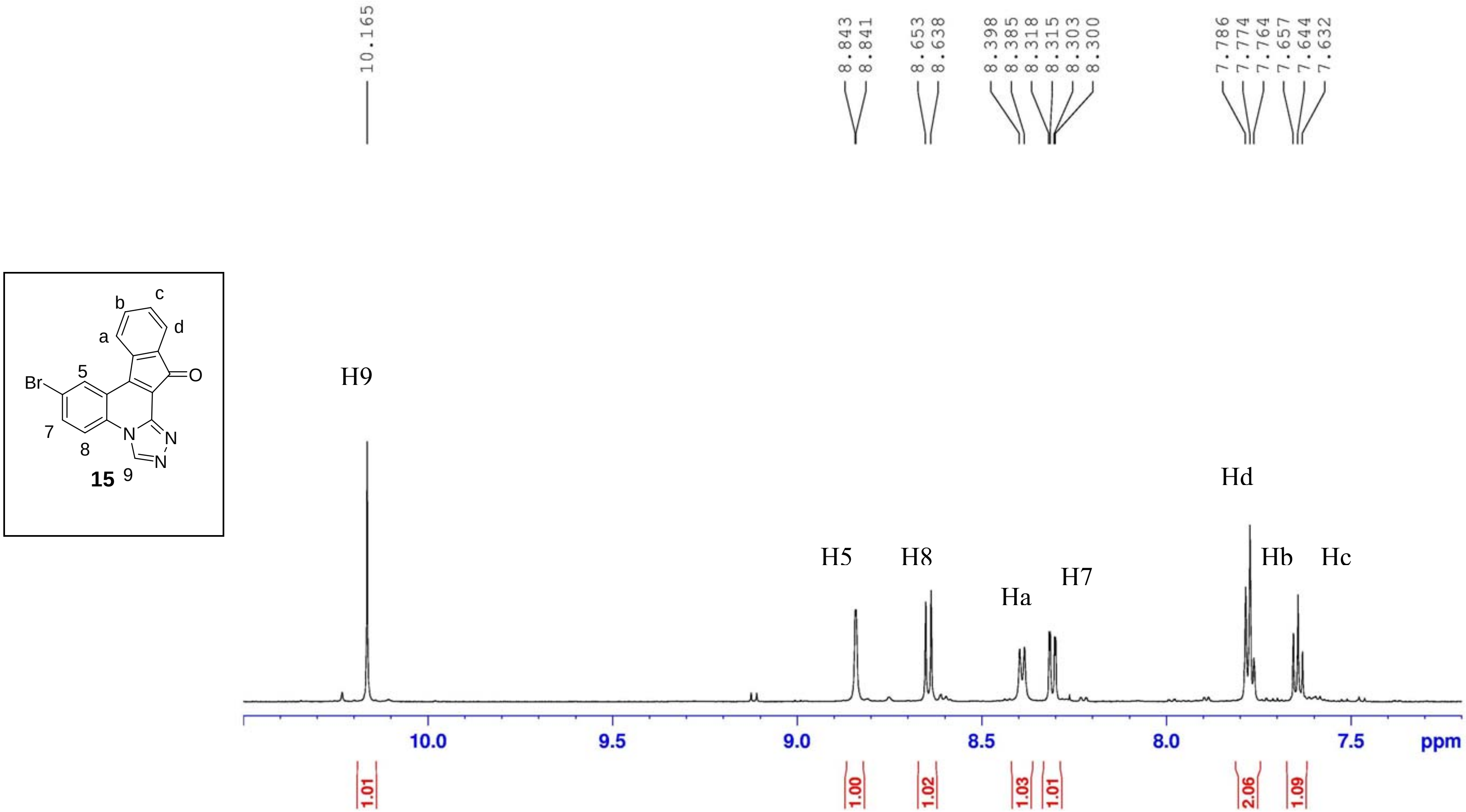
LCMS 2 Reaction Monitoring (TFA Buffer) Analyzed By :

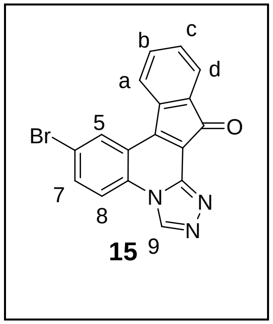
*Channel 1 at wavelength 220 nm , Channel 2 at wavelength 260 nm



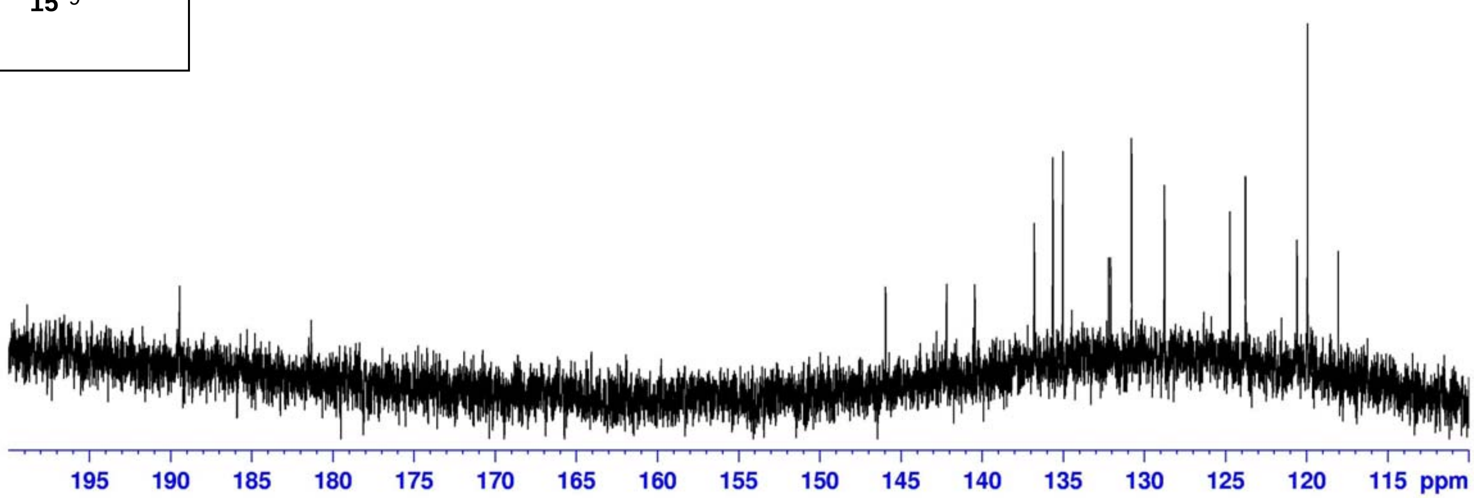
Spectrum Name: CR080-96-161-161A.sp Analyst: GANESH Accumulations: 16 Time: 9:22:49 AM

Description: CR080-96-161-161A IN Kbr Resolution: 4.00 cm-1 Date: 4/23/2010

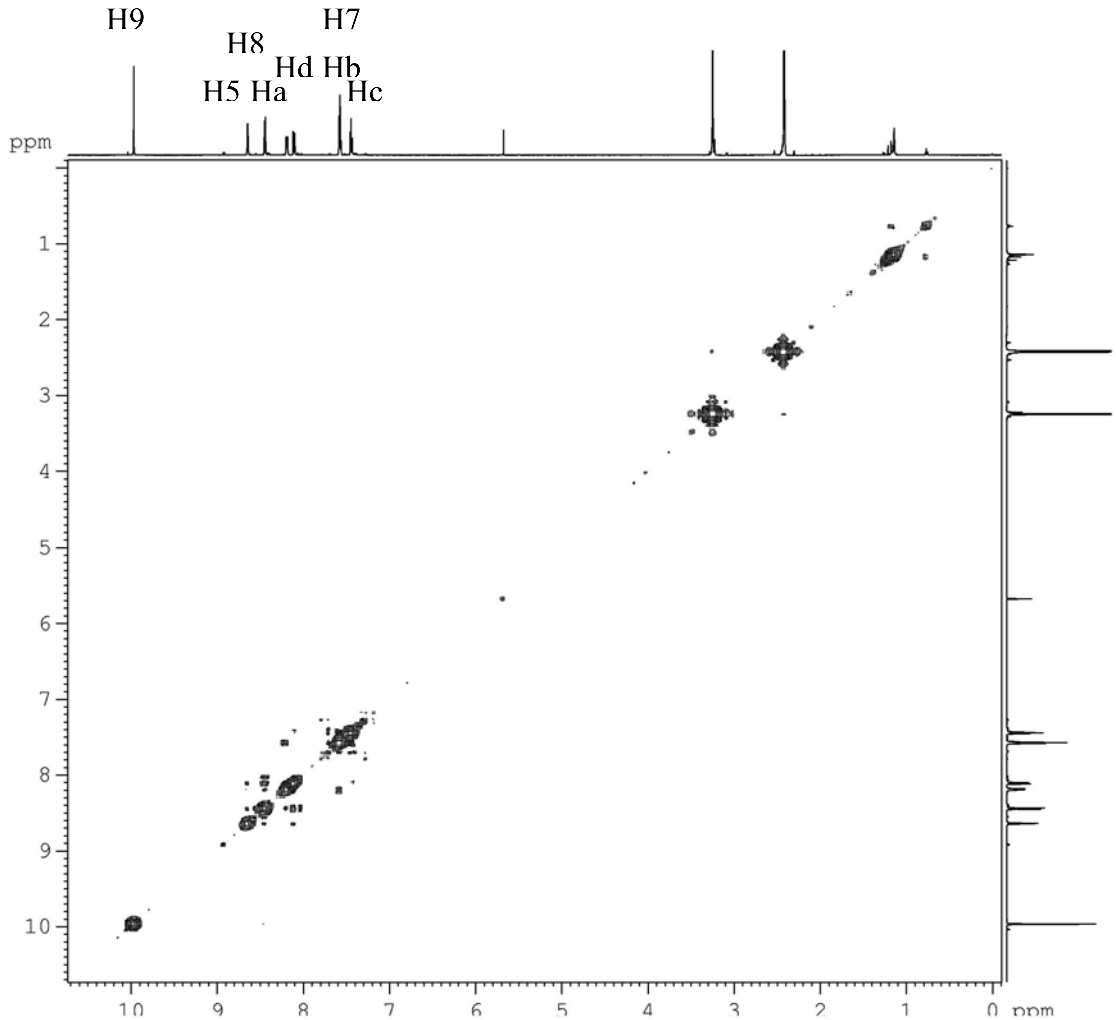

10.165
8.843
8.841
8.653
8.638
8.398
8.385
8.318
8.315
8.303
8.300
7.786
7.774
7.764
7.657
7.644
7.632
H9
H5
H8
Ha
H7
Hd
Hb
Hc
10.0
9.5
9.0
8.5
8.0
7.5
ppm
1.01
1.00
1.02
1.03
1.01
2.06
1.09
Br
O
N
N
N
a
b
c
d
5
7
8
9
15

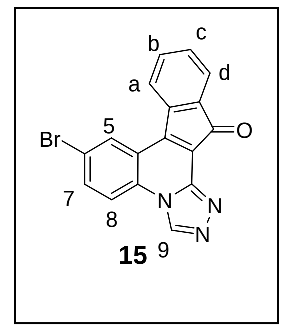


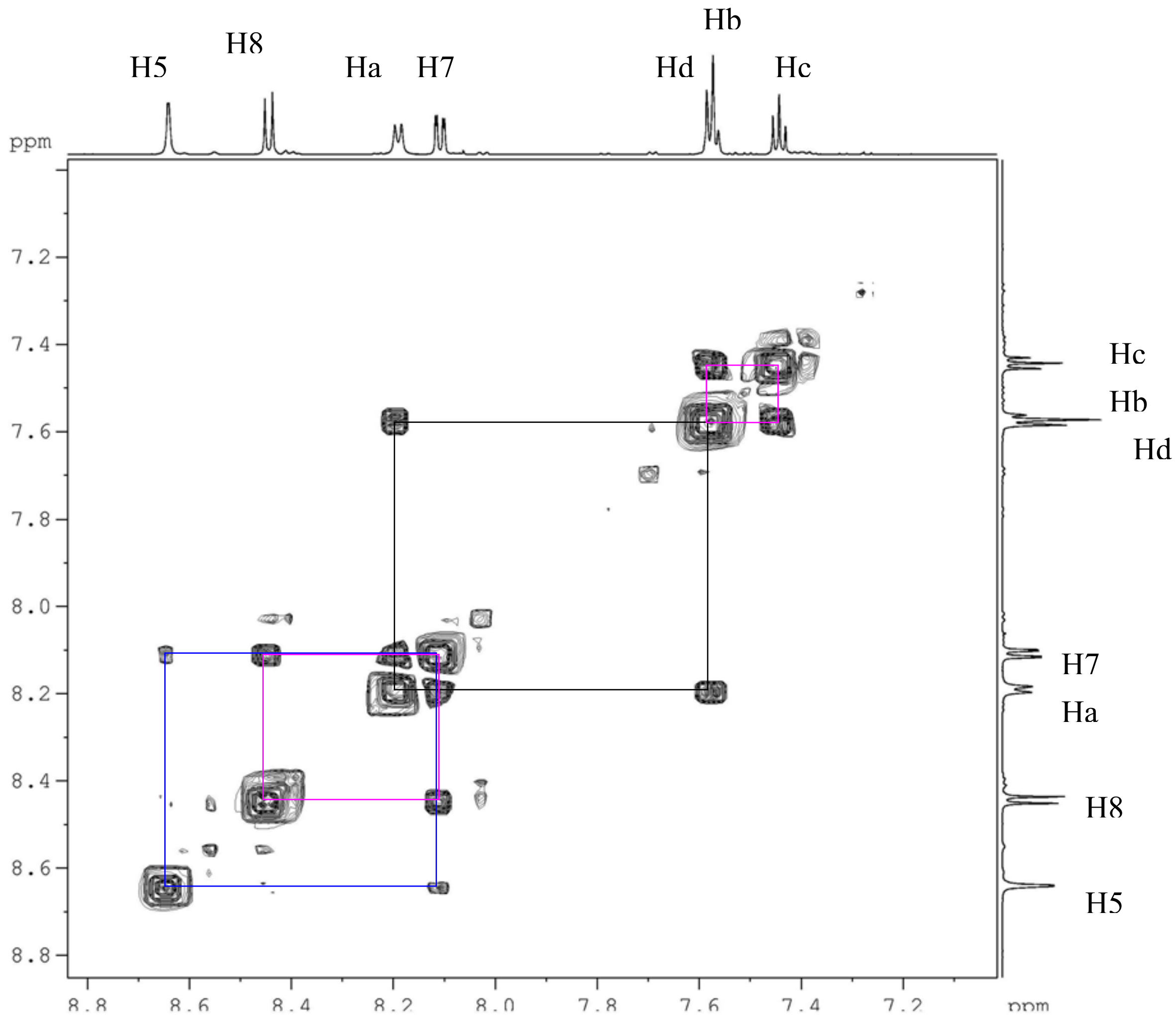
b
c
d
a
5
Br
O
7
N
N
8
N
15
9

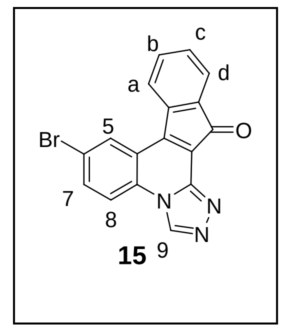


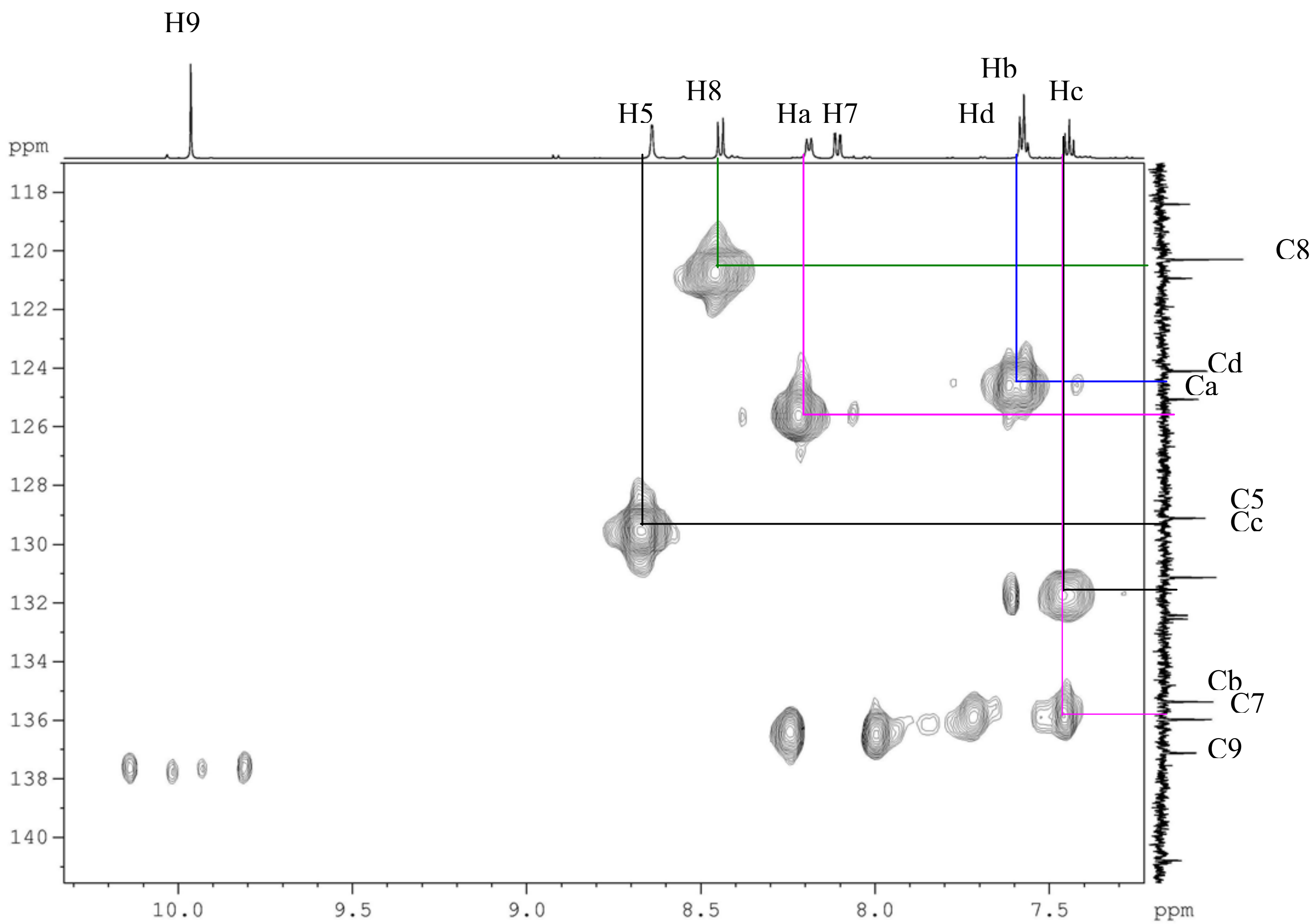
136.80
135.65
135.04
130.80
128.78
124.74
123.78
119.97
195
190
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
ppm

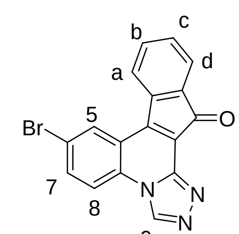

H9
H8
H7
Hd Hb
H5 Ha
Hc
ppm
1
2
3
4
5
6
7
8
9
10
10 9 8 7 6 5 4 3 2 1 0 ppm


b
c
d
a
5
Br
O
N
N
N
7
8
9
15

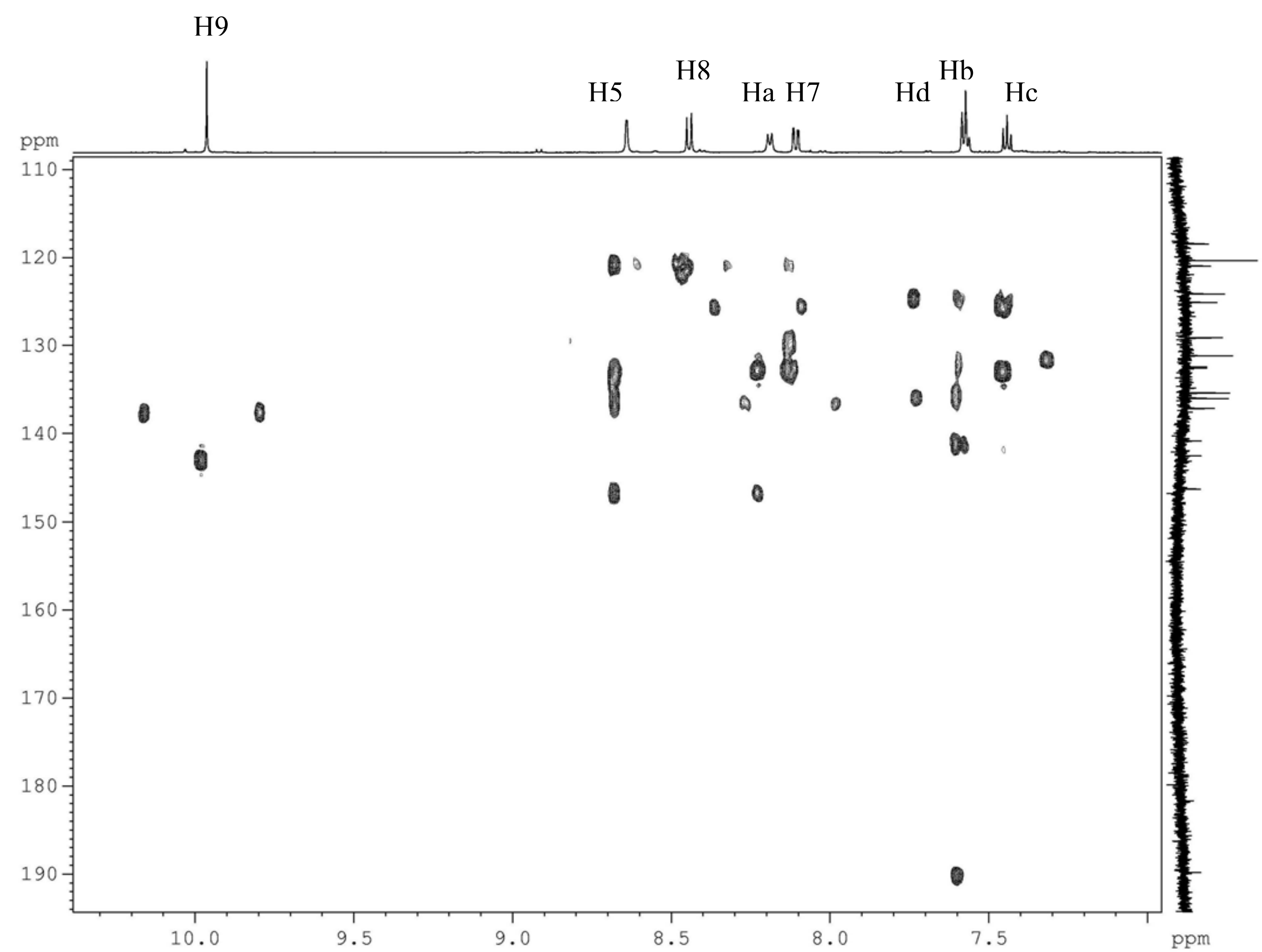

H5
H8
Ha
H7
Hd
Hb
Hc
ppm
7.2
7.4
7.6
7.8
8.0
8.2
8.4
8.6
8.8
Hc
Hb
Hd
H7
Ha
H8
H5

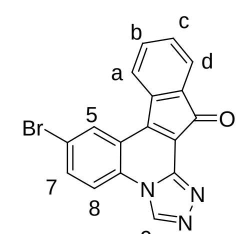

Br
5
7
8
a
b
c
d
O
N
N
N
9
15


H9
H8
H5
Ha
H7
Hd
Hb
Hc
ppm
118
120
122
124
126
128
130
132
134
136
138
140
10.0
9.5
9.0
8.5
8.0
7.5
ppm
C8
Cd
Ca
C5
Cc
Cb
C7
C9

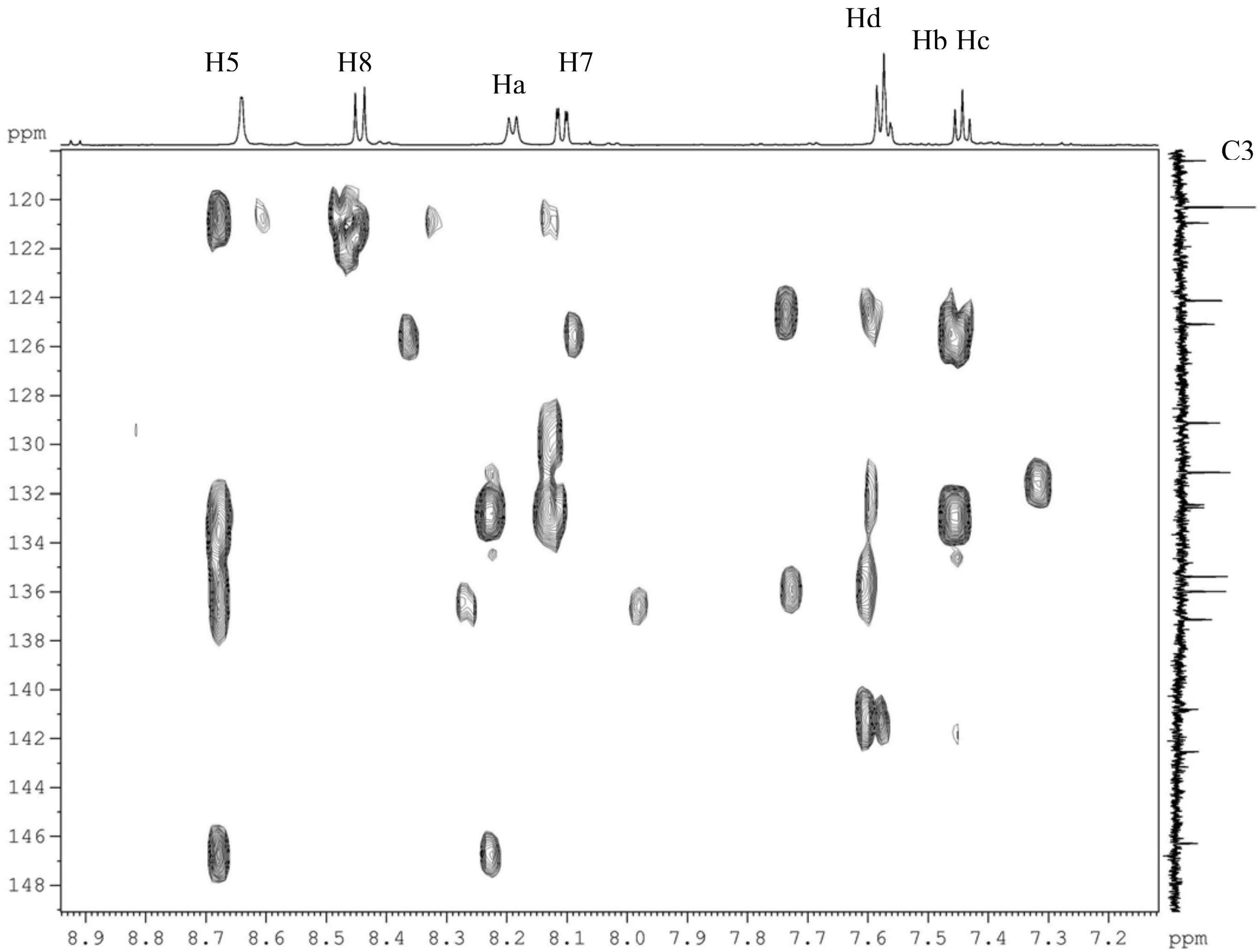

Br
5
a
b
c
d
O
7
8
N
N
N
9

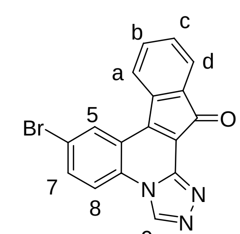
15


H9
H5
H8
Ha H7
Hd
Hb
Hc
ppm
110
120
130
140
150
160
170
180
190
10.0
9.5
9.0
8.5
8.0
7.5
ppm

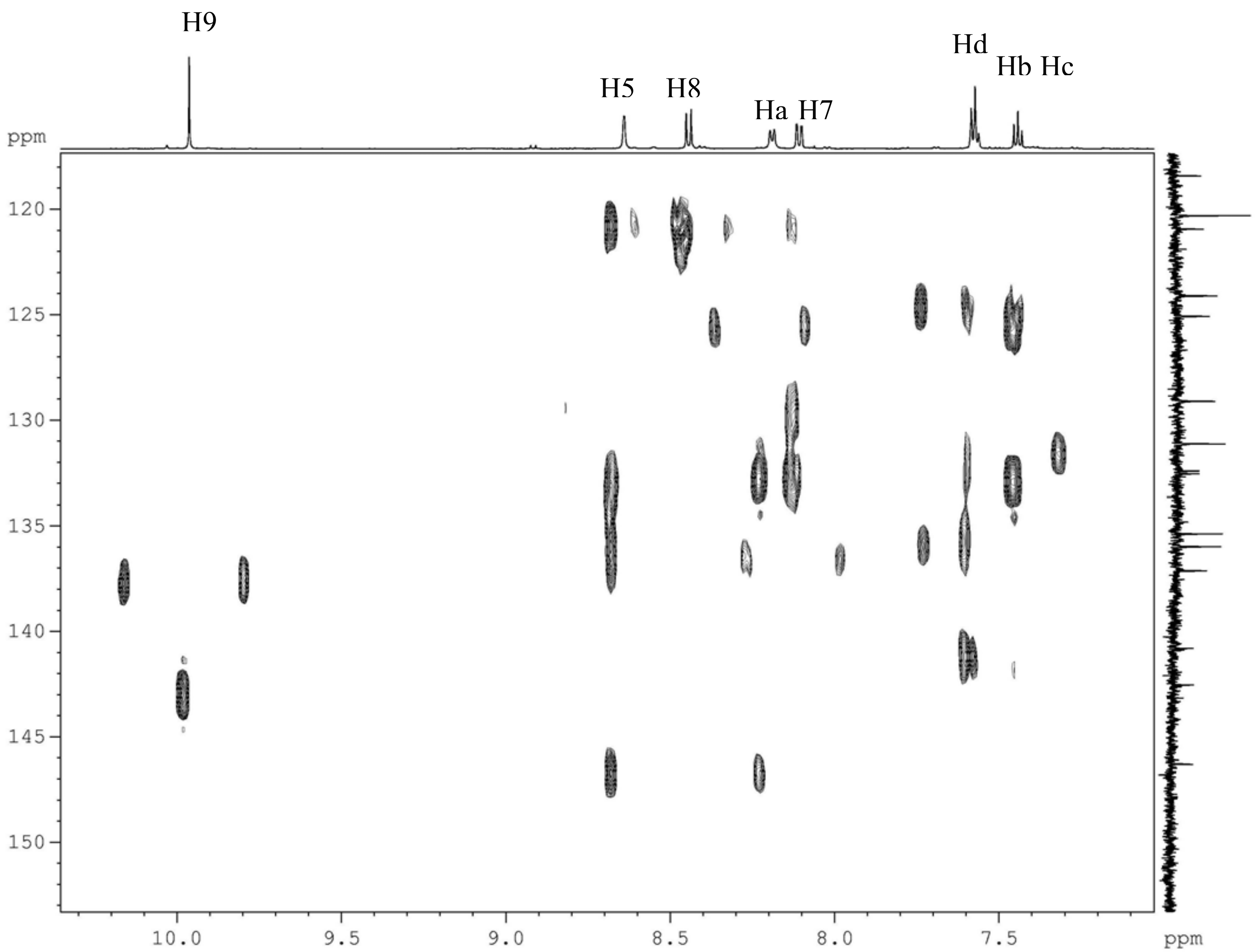

b
c
a
d
Br
5
O
7
8
N
N
N
9

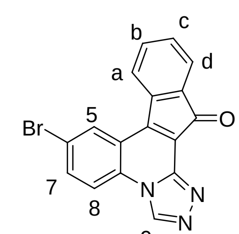
15


H5
H8
Ha
H7
Hd
Hb Hc
C3
ppm
120
122
124
126
128
130
132
134
136
138
140
142
144
146
148
8.9 8.8 8.7 8.6 8.5 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
ppm


b
c
a
d
5
Br
O
7
8
N
N
N
9

15


H9
H5
H8
Ha
H7
Hd
Hb
Hc
ppm
120
125
130
135
140
145
150
10.0
9.5
9.0
8.5
8.0
7.5
ppm

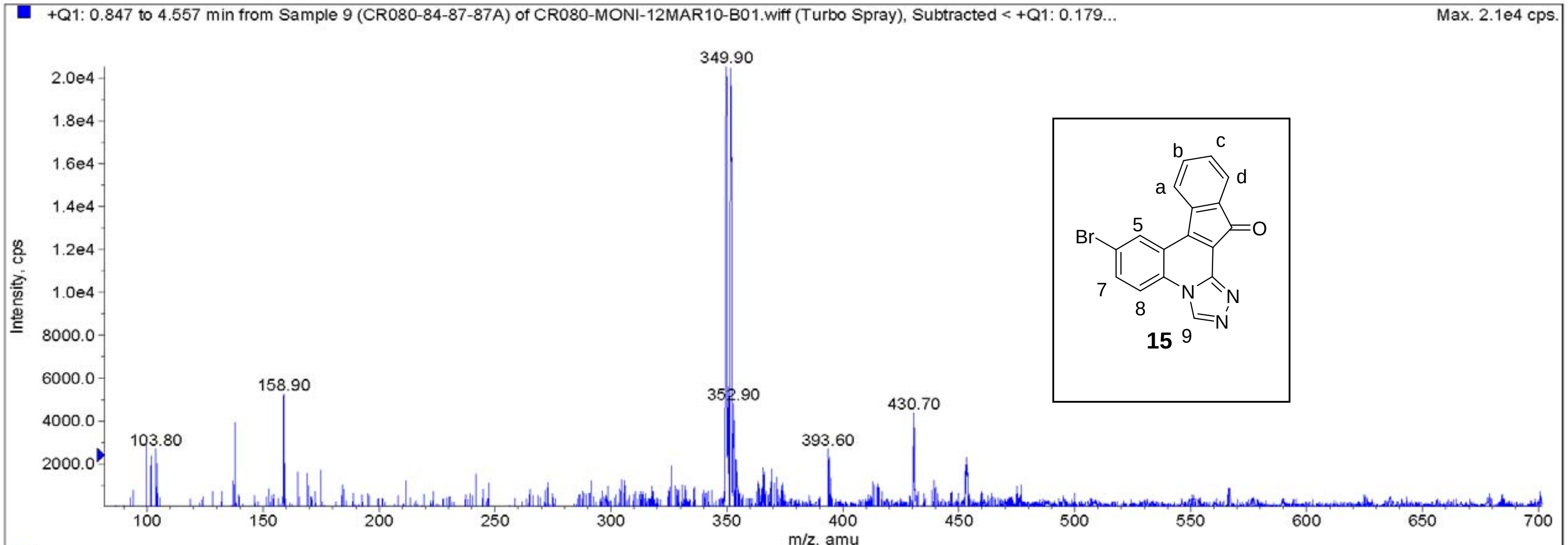

b
c
a
d
Br
5
O
7
8
N
N
N
9

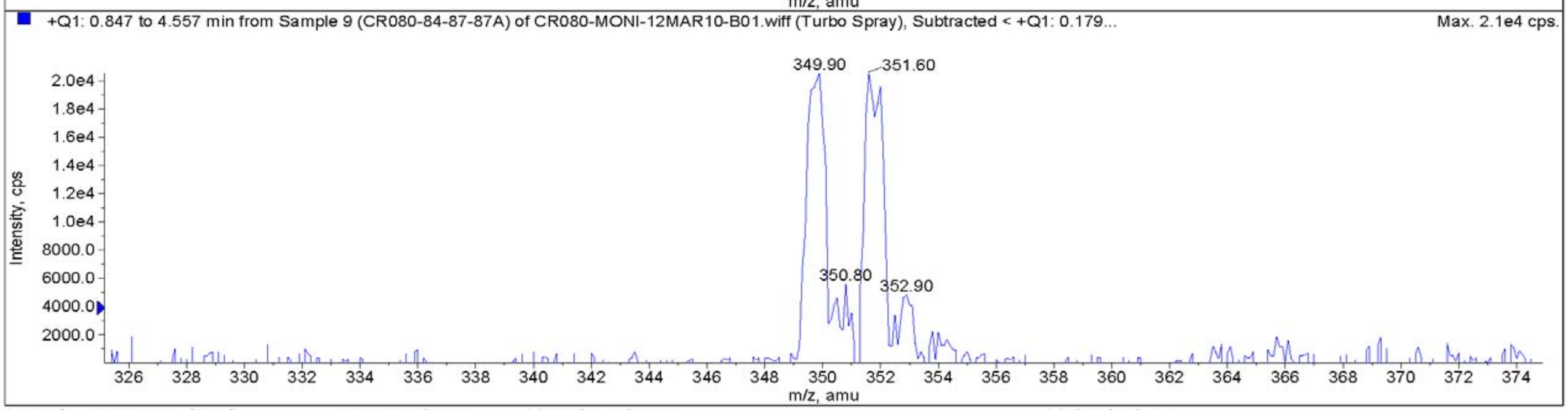
15

*

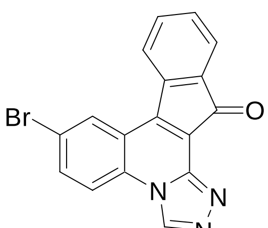
INDIA

Sample Name: CR080-84-87-87A   Acq. Time: 13:23   Acq. Date: Friday, March 12, 2010

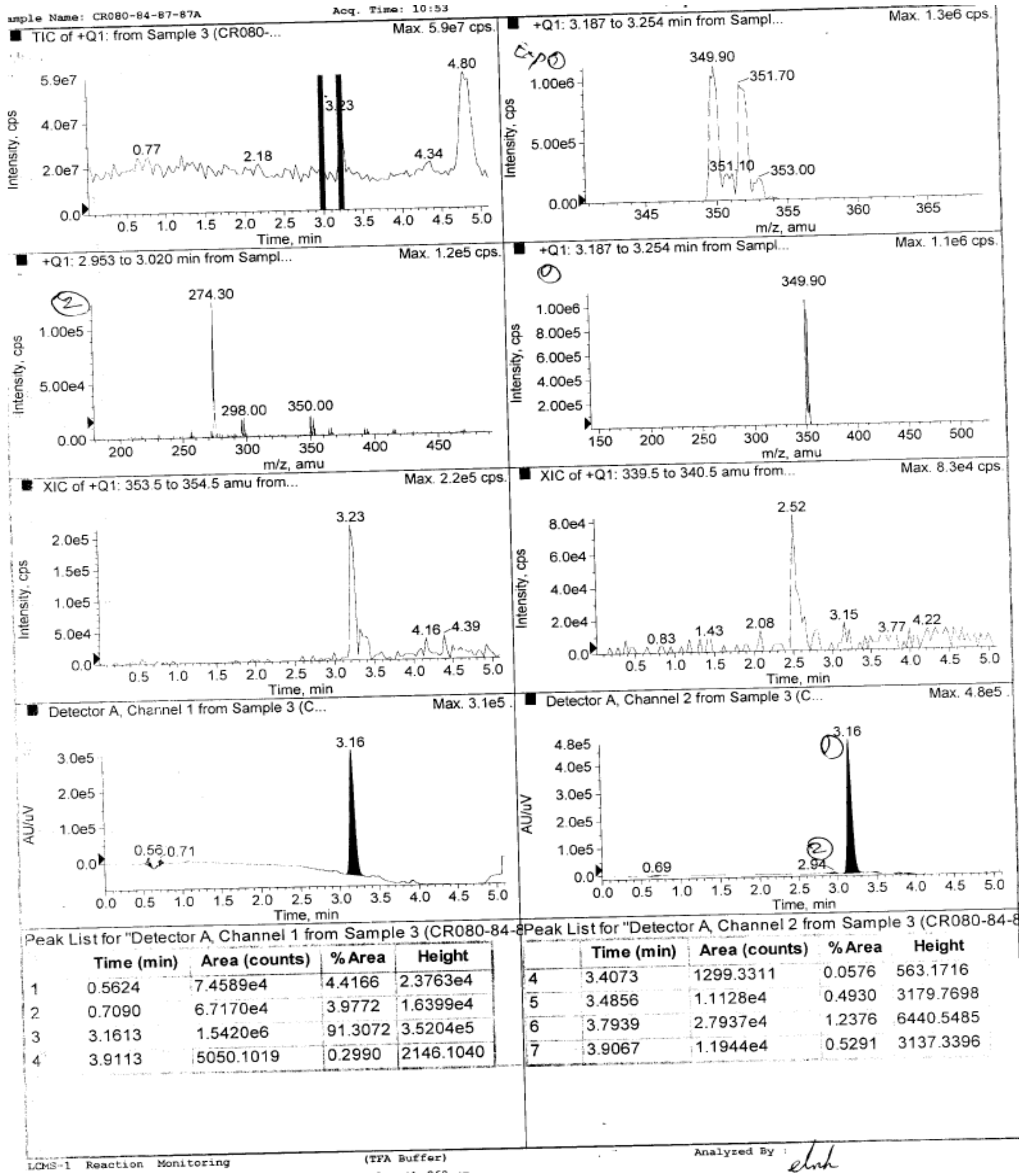




*Sample Comment: [M+H]   Expected 350   **Analyzed By :   **Checked By :



15



Peak List for "Detector A, Channel 1 from Sample 3 (CR080-84-8

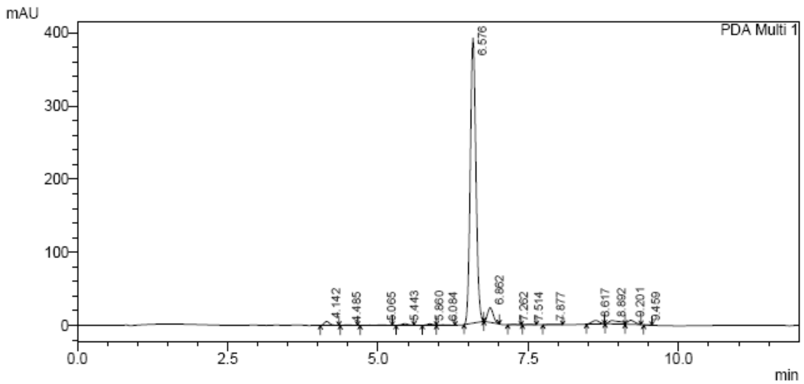
	Time (min)	Area (counts)	% Area	Height
1	0.5624	7.4589e4	4.4166	2.3763e4
2	0.7090	6.7170e4	3.9772	1.6399e4
3	3.1613	1.5420e6	91.3072	3.5204e5
4	3.9113	5050.1019	0.2990	2146.1040

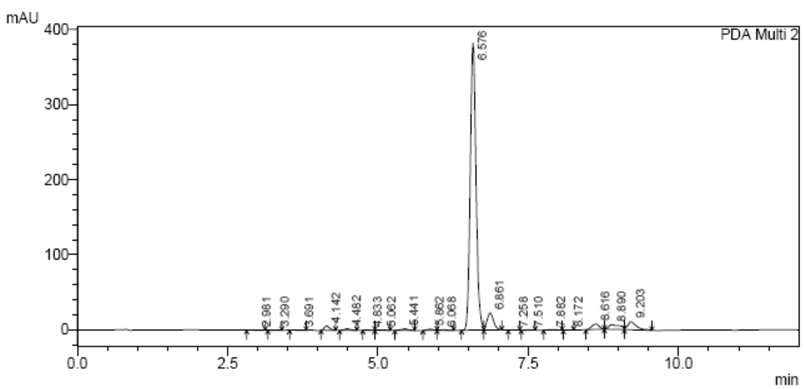
Peak List for "Detector A, Channel 2 from Sample 3 (CR080-84-8

	Time (min)	Area (counts)	% Area	Height
4	3.4073	1299.3311	0.0576	563.1716
5	3.4856	1.1128e4	0.4930	3179.7698
6	3.7939	2.7937e4	1.2376	6440.5485
7	3.9067	1.1944e4	0.5291	3137.3396

Sample Name : CR080-84-87-87A
Sample ID : CR080-84-87-87A
Column : Gemini C-18 (50 x 4.6 mm) 5u
Vial # : 47
Inj. Volume : 6 uL
Tray # : 2
Acquired by : AVINASH

Data File Name : 05031021.lcd
Method File Name : GENERAL-A.lcm
Batch File Name : 050310.lcb
Data Acquired : 3/5/2010 4:25:22 PM
Data Processed : 3/5/2010 4:37:29 PM
Ref.No.:NP/A0011/53





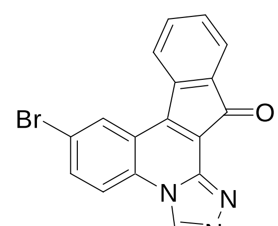
1 PDA Multi 1/263nm 4nm
2 PDA Multi 2/244nm 4nm

PeakTable
PDA Ch1 263nm 4nm

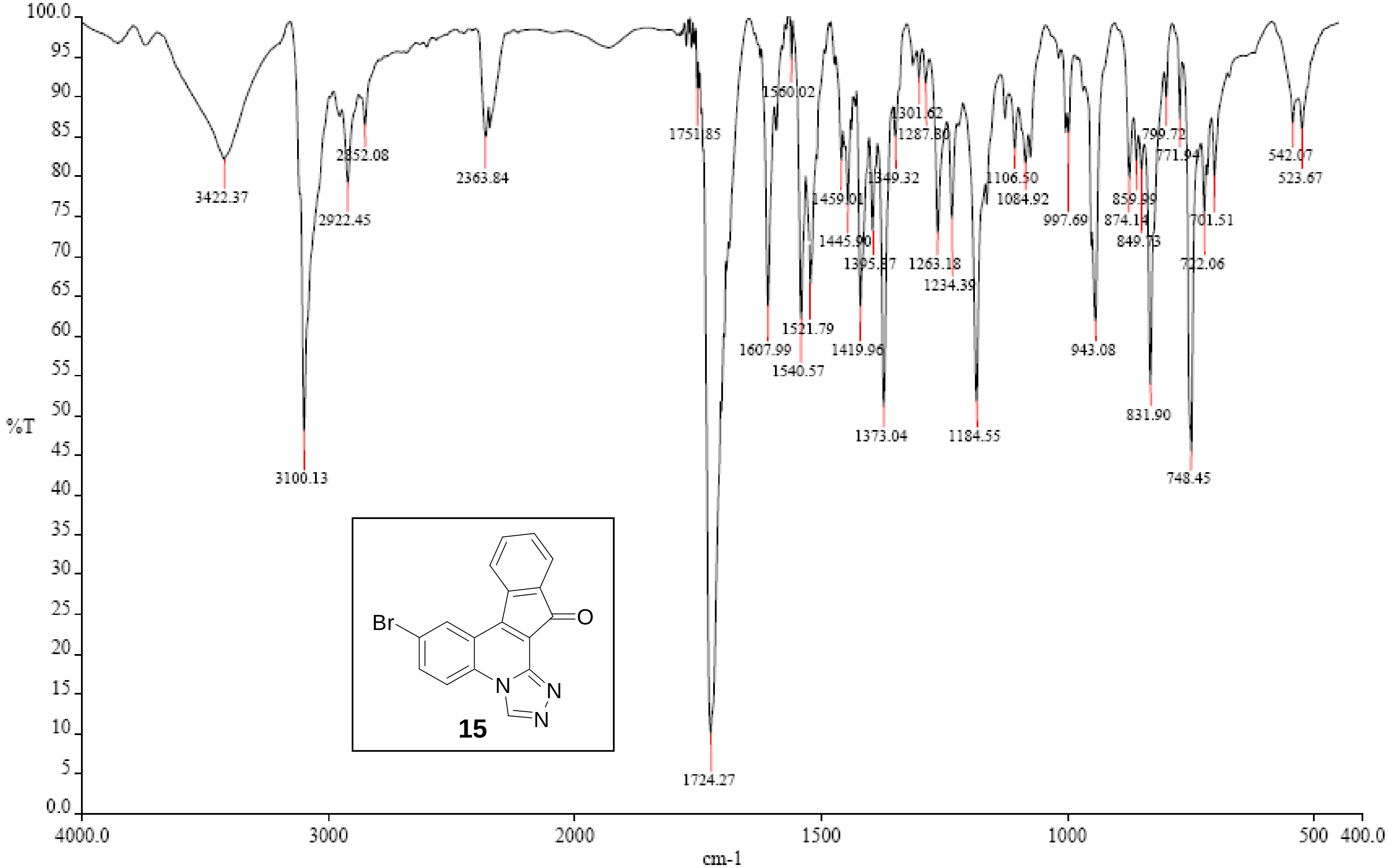
Peak#	Ret. Time	Area	Area %	Height
1	4.14	33361	1.15	5426
2	4.48	4262	0.15	614
3	5.06	7544	0.26	724
4	5.44	14605	0.50	2121
5	5.86	12304	0.42	1806
6	6.08	5419	0.19	522
7	6.58	2540919	87.23	389831
8	6.86	129594	4.45	20022
9	7.26	3256	0.11	467
10	7.51	4566	0.16	736
11	7.88	5400	0.19	488
12	8.62	40701	1.40	4832
13	8.89	62481	2.14	4655
14	9.20	47218	1.62	5628
15	9.46	1260	0.04	303
Total		2912891	100.00	438174

PeakTable
PDA Ch2 244nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	2.98	3854	0.13	400
2	3.29	3725	0.12	559
3	3.69	4615	0.15	540
4	4.14	34984	1.14	5862
5	4.48	13886	0.45	2049
6	4.83	1148	0.04	209
7	5.06	3400	0.11	562
8	5.44	14494	0.47	1971
9	5.86	9514	0.31	1569
10	6.07	3930	0.13	509
11	6.58	2538376	82.62	382074
12	6.86	170149	5.54	22795
13	7.26	2798	0.09	439
14	7.51	4984	0.16	779
15	7.88	6869	0.22	700
16	8.17	675	0.02	128
17	8.62	60921	1.98	7162
18	8.89	84746	2.76	6218
19	9.20	109320	3.56	10869
Total		3072388	100.00	445395



15



Spectrum Name: CR080-84-87-87A.sp

Analyst: GANESH

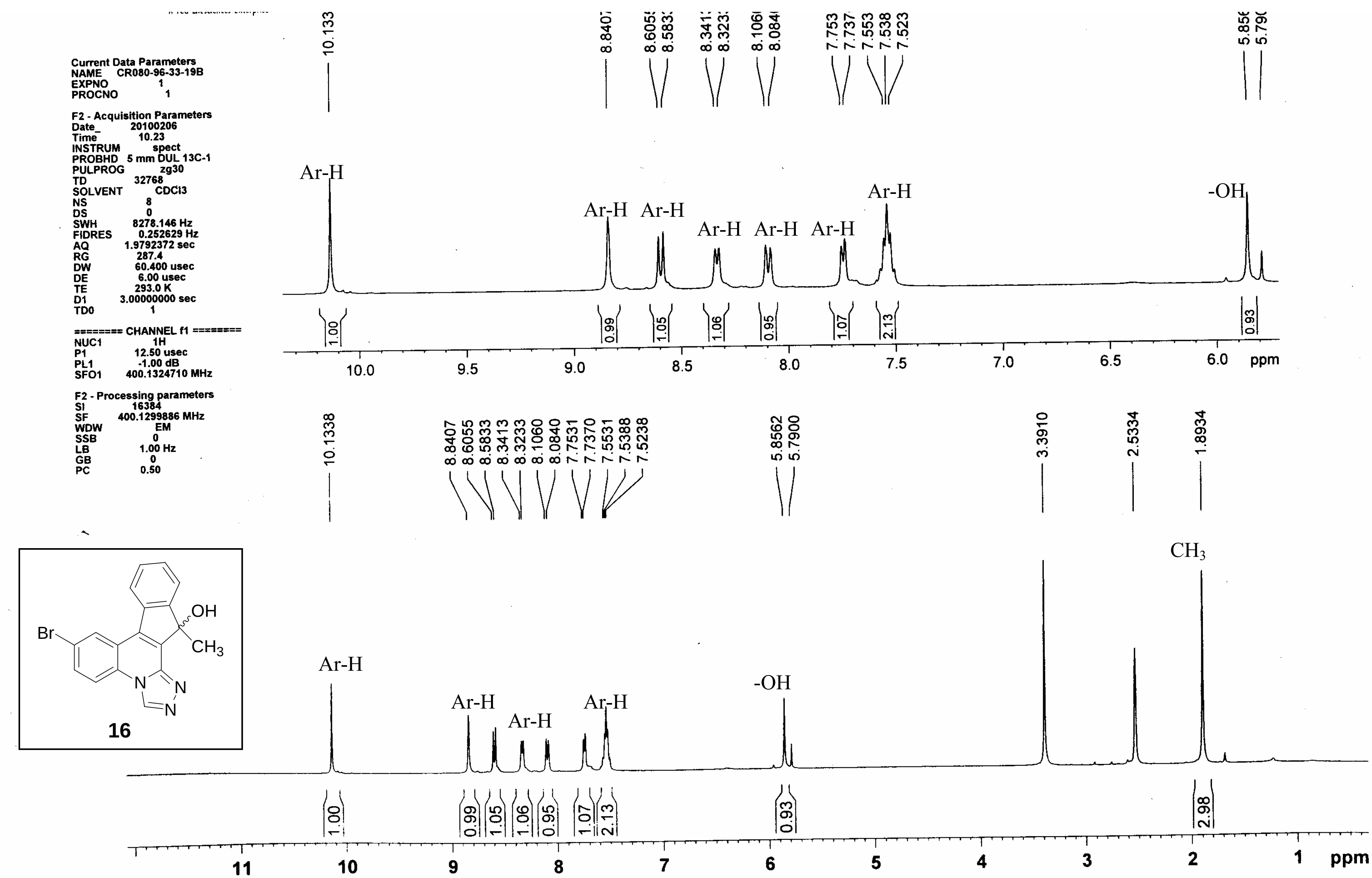
Accumulations: 16

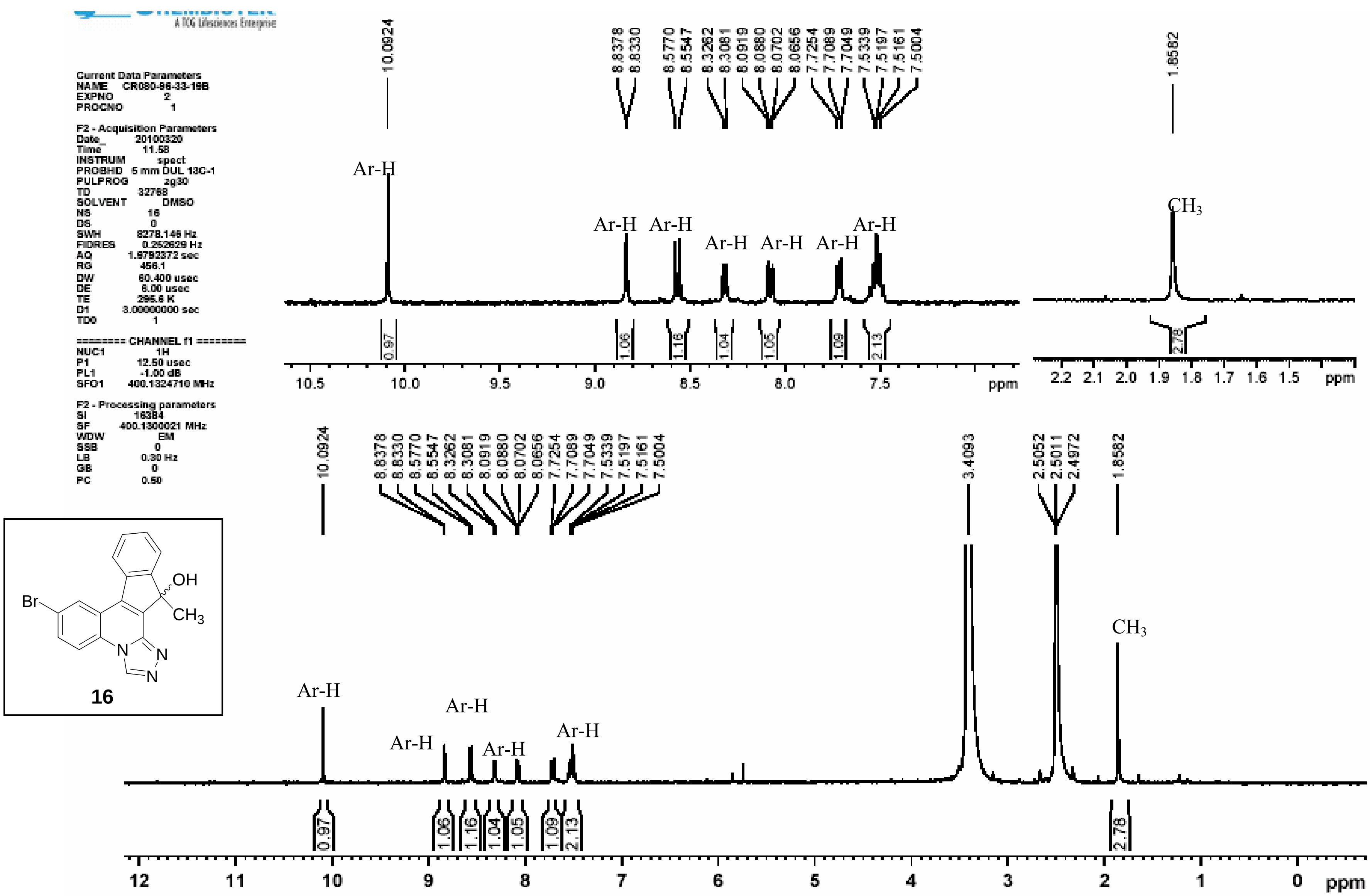
Time: 4:42:44 PM

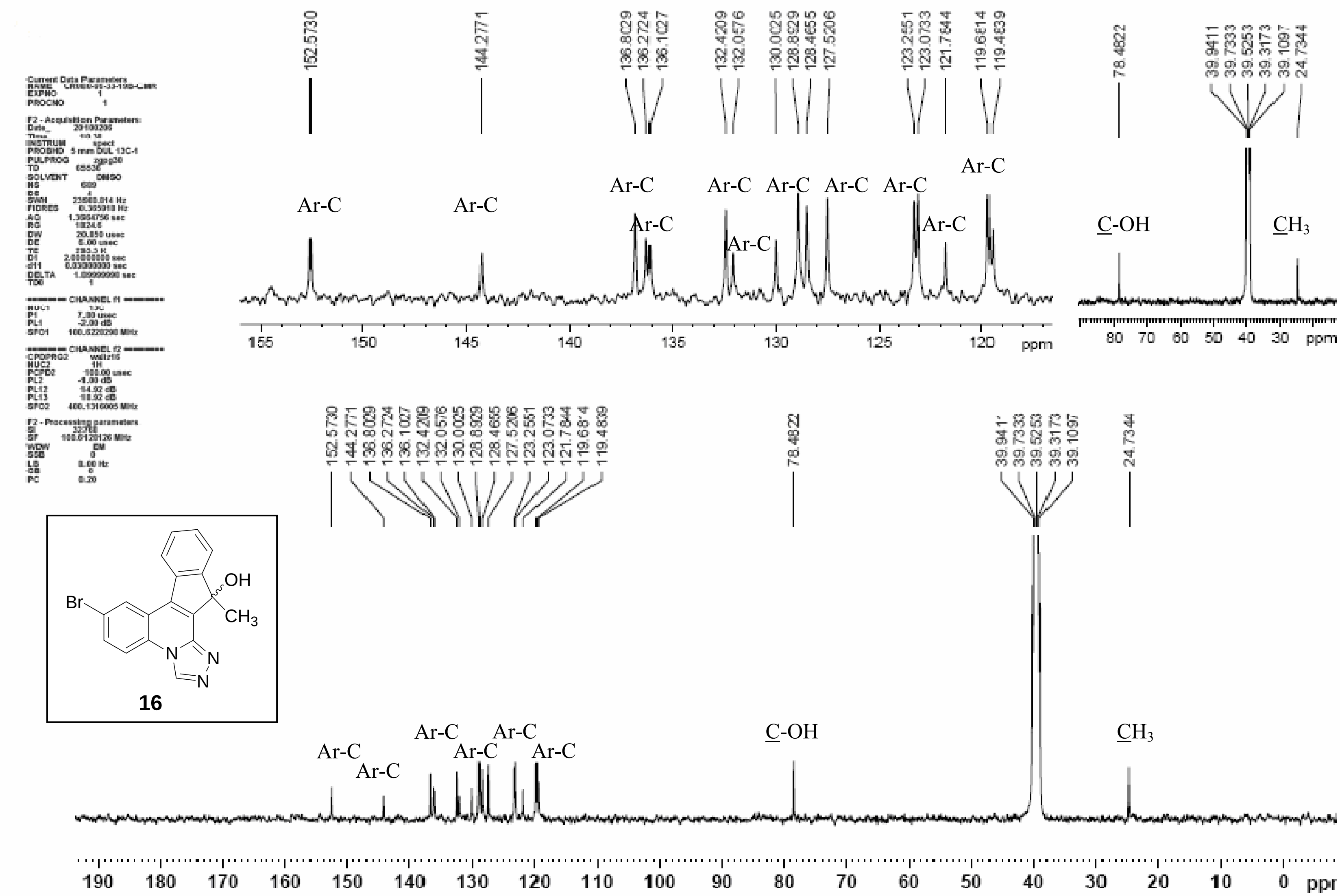
Description: CR080-84-87-87A IN KBr

Resolution: 4.00 cm-1

Date: 2/5/2010


Current Data Parameters
NAME CR080-96-33-19B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100206
Time 10.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 293.0 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1299886 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50
Ar-H
-OH
CH3
ppm
Br
OH
CH3
N
16


A TCG Lifesciences Enterprise
Current Data Parameters
NAME CR080-96-33-19B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100320
Time 11.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 295.6 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
10.0924
8.8378
8.8330
8.5770
8.5547
8.3262
8.3081
8.0919
8.0880
8.0702
8.0656
7.7254
7.7089
7.7049
7.5339
7.5197
7.5161
7.5004
3.4093
2.5052
2.5011
2.4972
1.8582
Ar-H
CH3
0.97
1.06
1.16
1.04
1.05
1.09
2.13
2.78
ppm
Br
OH
CH3
N
16

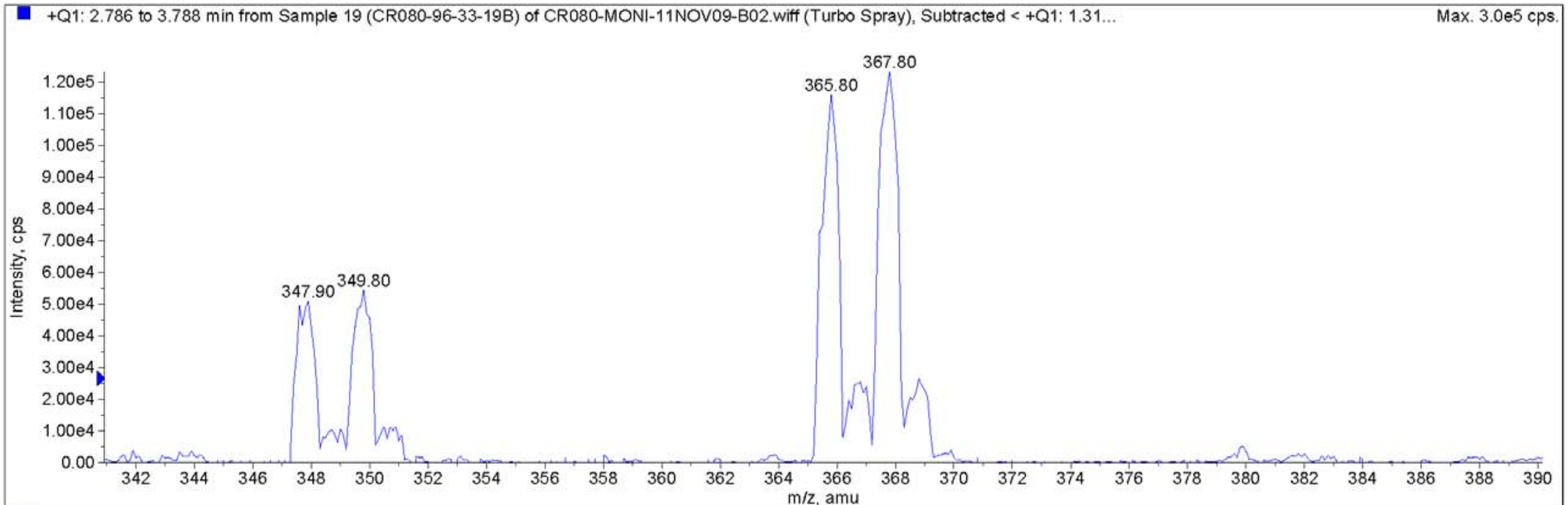


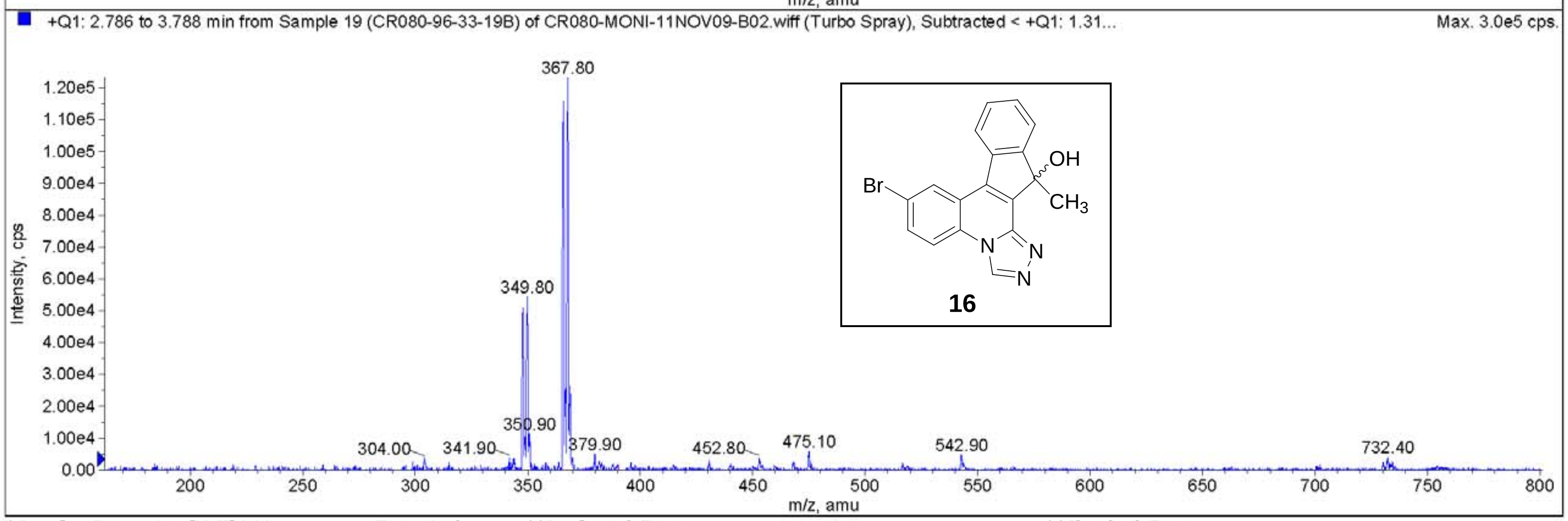
152.5730
144.2771
136.8029
136.2724
136.1027
132.4209
132.0576
130.0025
128.8929
128.4655
127.5206
123.2551
123.0733
121.7844
119.6814
119.4839
78.4822
39.9411
39.7333
39.5253
39.3173
39.1097
24.7344
Ar-C
C-OH
CH3
OH
Br
N
16
ppm

*

INDIA

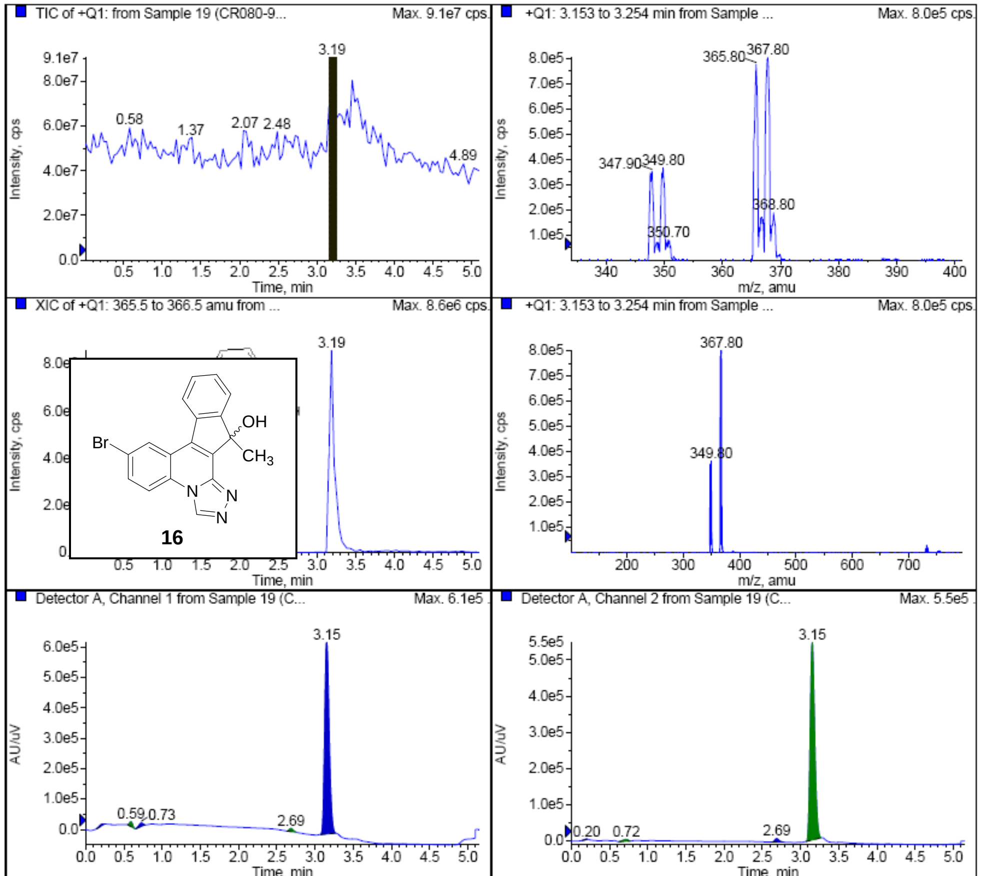
Sample Name: CR080-96-33-19B Acq. Time: 18:38 Acq. Date: Wednesday, November 11, 2009





*Sample Comment: [M+H]366 Expected **Analyzed By : **Checked By :

Sample Name: CR080-96-33-19B Acq. Time: 18:38 Acq. Date: Wednesday, November 11, 2009



Peak List for "Detector A, Channel 1 from Sample 19 (CR080-96-33

	Time (min)	Area (counts)	%Area	Height
1	0.2284	1.6182e4	0.6007	2729.7931
2	0.5906	4.2547e4	1.5794	1.5293e4
3	0.7287	3.8782e4	1.4397	1.0618e4
4	2.6855	3.4256e4	1.2716	1.0332e4
5	3.1523	2.5621e6	95.1086	6.2997e5

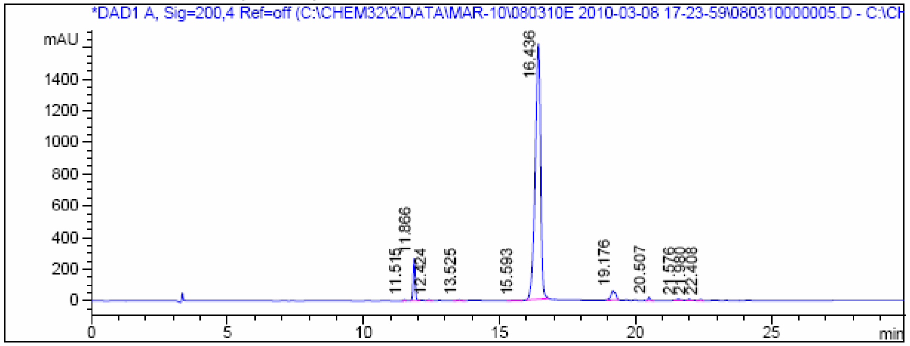
Peak List for "Detector A, Channel 2 from Sample 19 (CR080-96-33

	Time (min)	Area (counts)	%Area	Height
1	0.2008	2505.6703	0.1101	876.6607
2	0.7178	2.3234e4	1.0209	4913.7550
3	2.6881	3.2489e4	1.4276	9216.3112
4	3.1537	2.2176e6	97.4414	5.4463e5

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

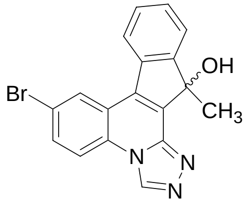
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

```
=========================================================================
SAMPLE: CR080-96-33-19 B                                              ->
Column: GEMINI-C18(250X4.6)mm 5µ
Injection date  : Mon, 8. Mar. 2010               Location    :     Vial 11
Sample Name     : CR080-96-33-19 B                Inj. No.    :          1
Acq Operator    : GANESH Z                        Inj. Vol.   :       20 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _2_3.M
Last Changed    : Mon, 8. Mar. 2010,
Acq. Method     : C:\Chem32\2\DATA\MAR-10\080310E 2010-03-08 17-23-59\
                  UPLC_GENARAL_GRAD _2_3.M
Method ref      : NP/A0011/58
```



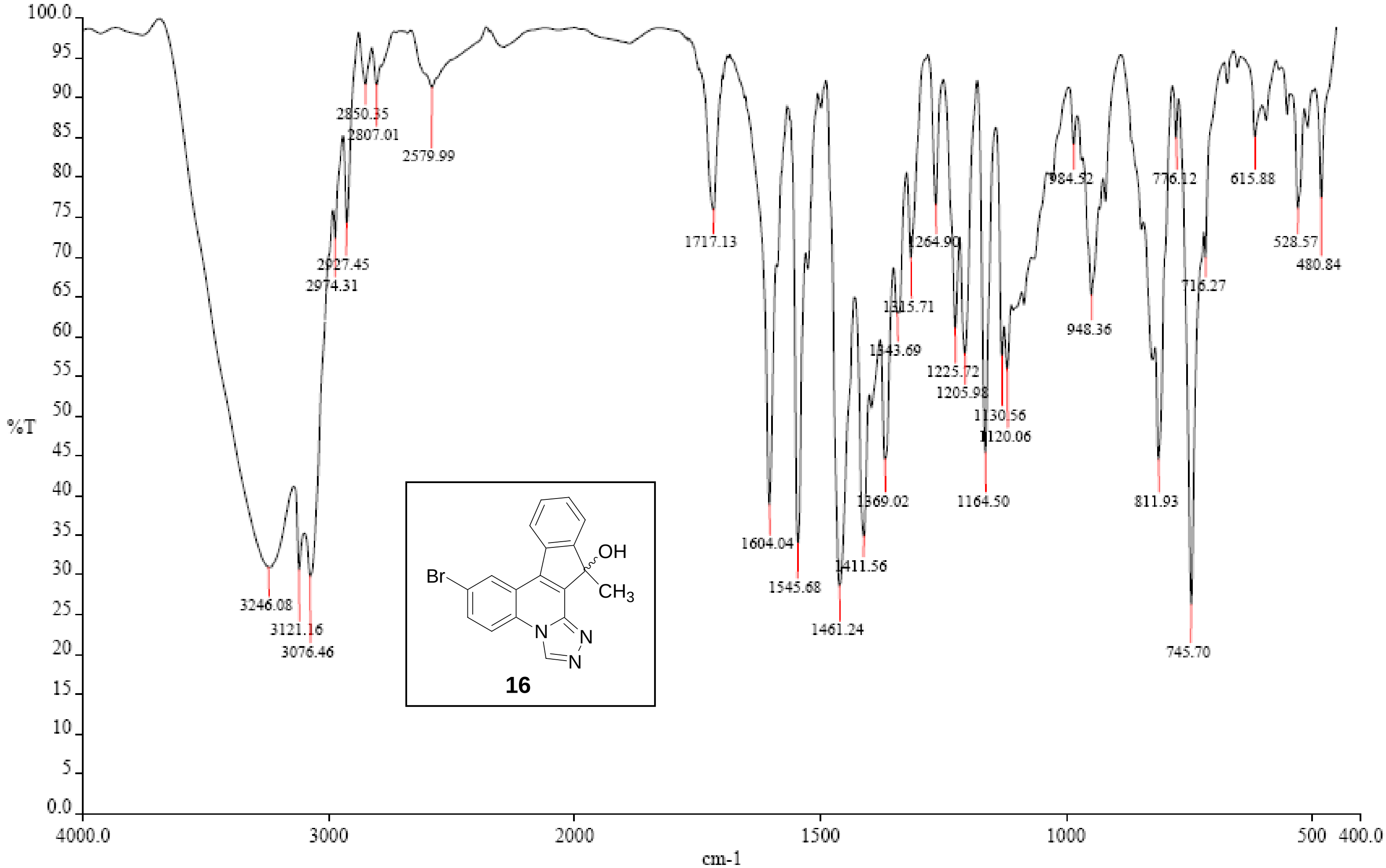
DAD1 A, Sig=200,4 Ref=off

Peak #	RT (Min)	Width (Min)	Area	Area %
1	11.515	0.067	26.724	0.110
2	11.866	0.085	1.355e3	5.564
3	12.424	0.116	30.074	0.123
4	13.525	0.191	40.173	0.165
5	15.593	0.254	33.581	0.138
6	16.436	0.226	2.193e4	90.047
7	19.176	0.200	679.650	2.790
8	20.507	0.088	110.934	0.455
9	21.576	0.120	61.662	0.253
10	21.980	0.092	48.290	0.198
11	22.408	0.091	38.001	0.156



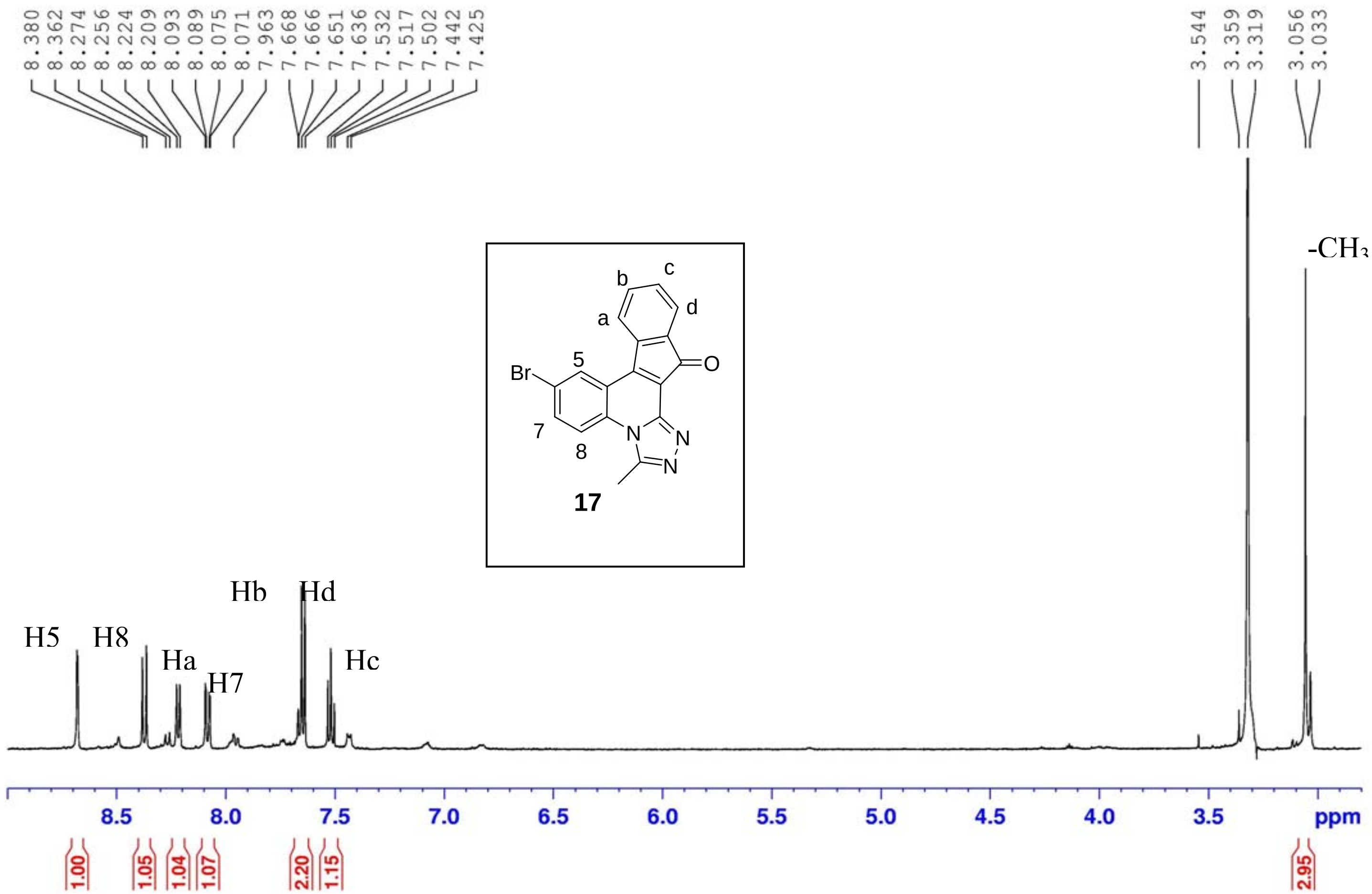
16

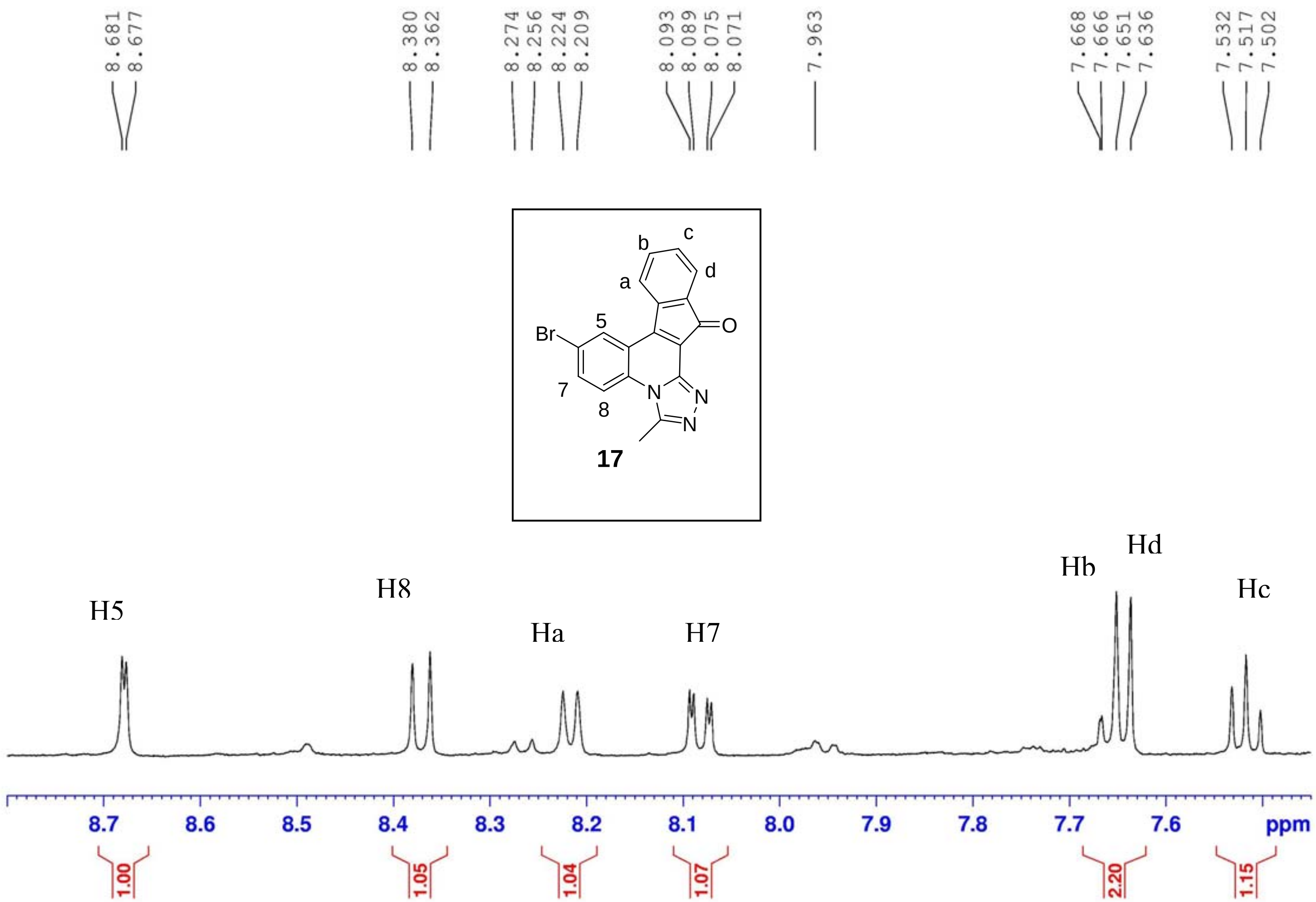
```
=========================================================================
                          *** End of Report***
```

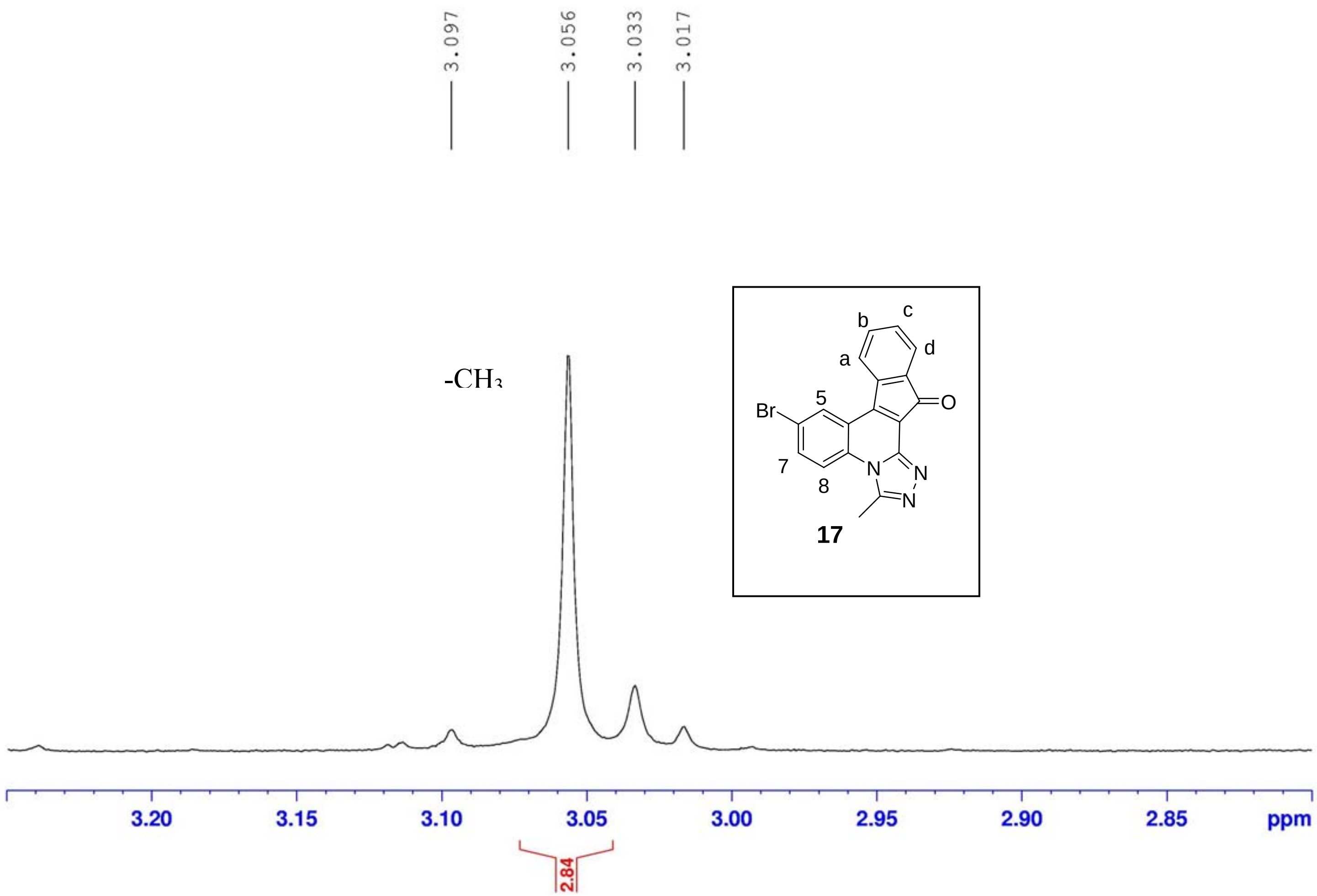


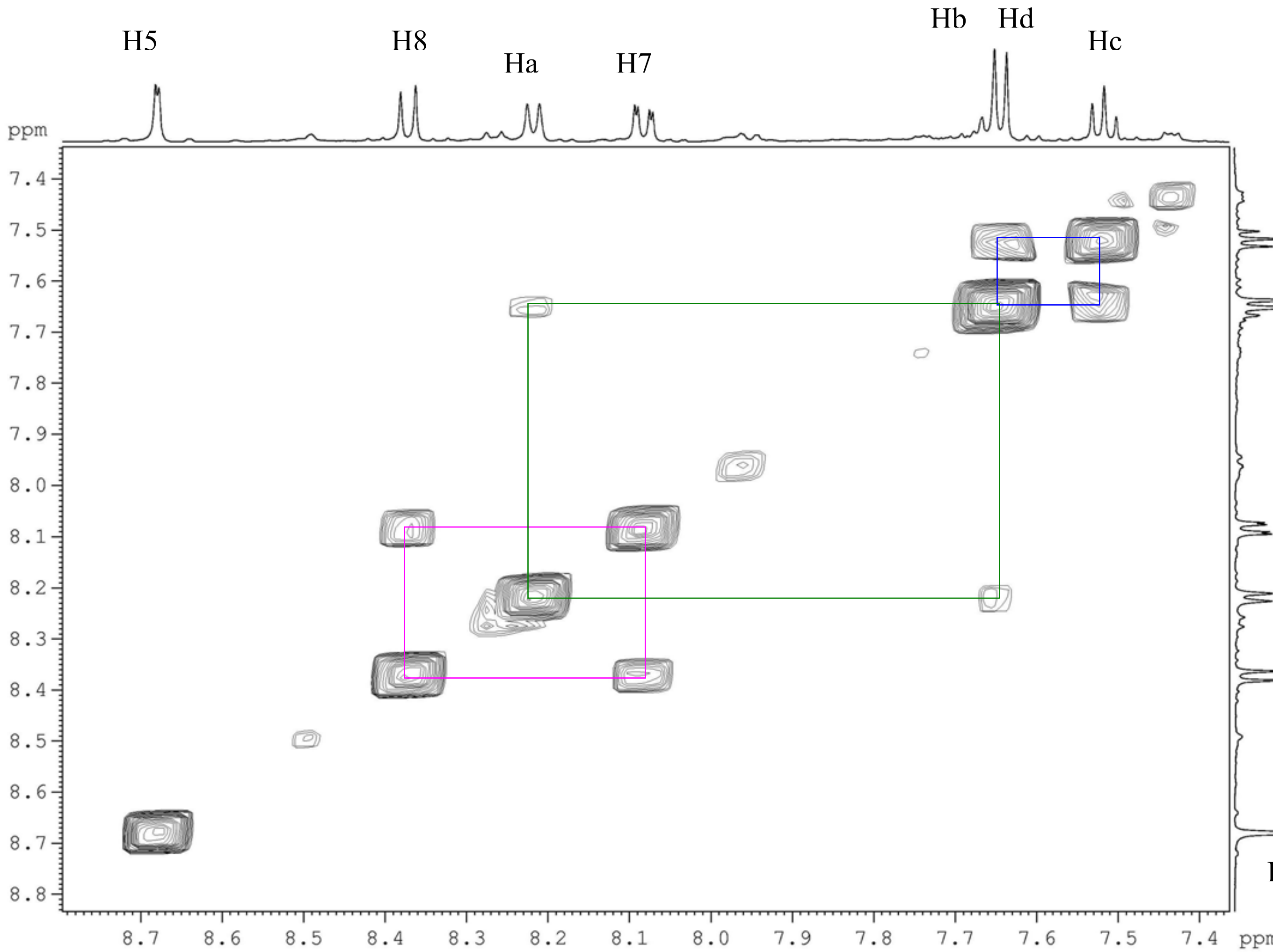
Spectrum Name: CR080-96-33-19B.sp | Analyst: GANESH | Accumulations: 16 | Time: 10:40:37 AM

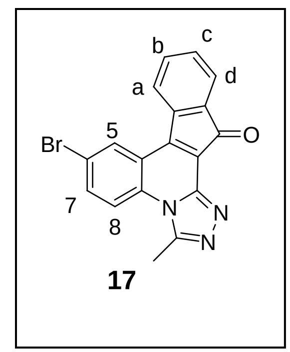
Description: CR080-96-33-19B IN KBr | Resolution: 4.00 cm-1 | Date: 2/10/2010

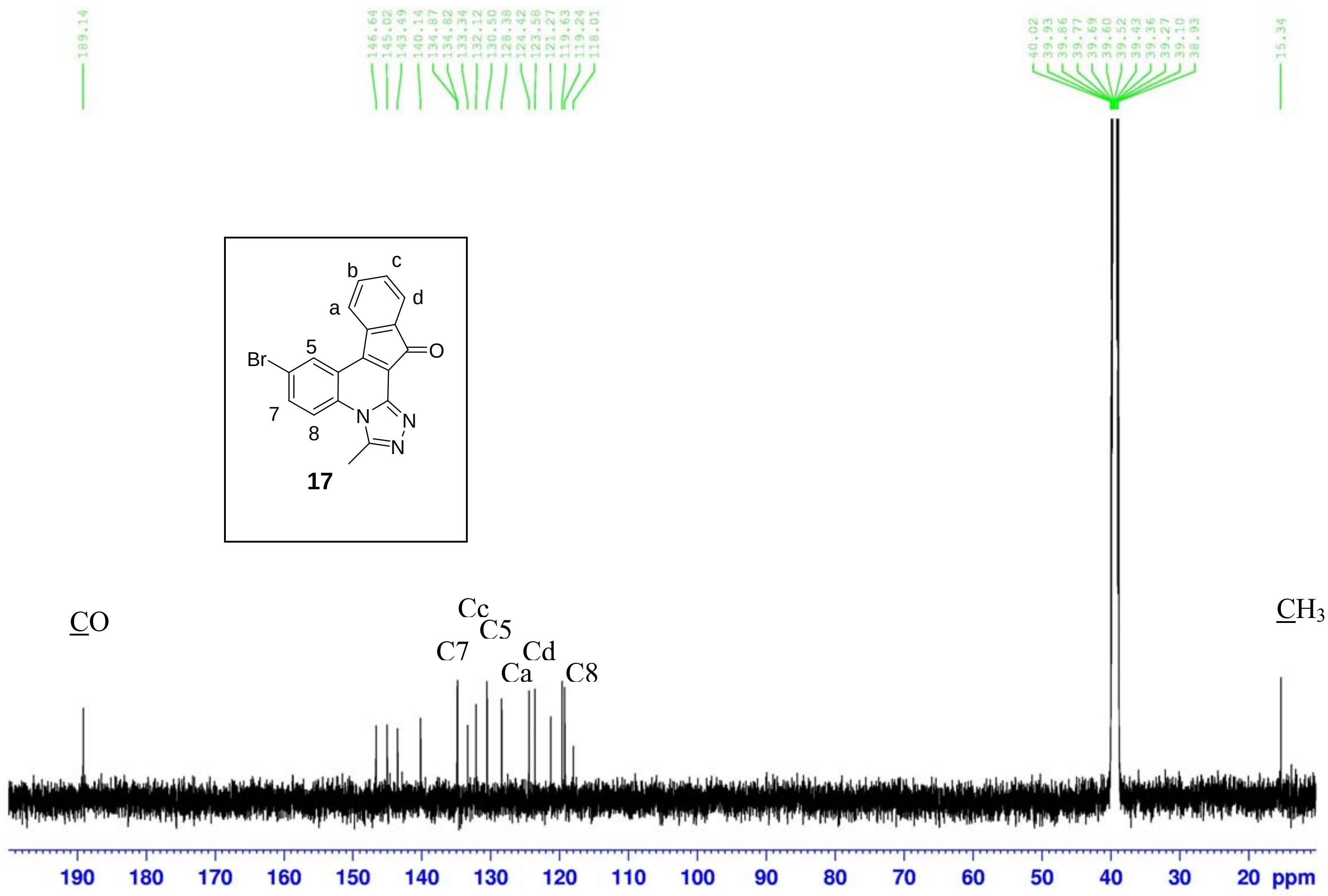

8.380
8.362
8.274
8.256
8.224
8.209
8.093
8.089
8.075
8.071
7.963
7.668
7.666
7.651
7.636
7.532
7.517
7.502
7.442
7.425
3.544
3.359
3.319
3.056
3.033
-CH3
b
c
a
d
Br
5
O
7
N
N
8
N
17
Hb
Hd
H5
H8
Ha
H7
Hc
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
ppm
1.00
1.05
1.04
1.07
2.20
1.15
2.95


8.681
8.677
8.380
8.362
8.274
8.256
8.224
8.209
8.093
8.089
8.075
8.071
7.963
7.668
7.666
7.651
7.636
7.532
7.517
7.502
b
c
a
d
Br
5
O
7
8
N
N
N
17
H5
H8
Ha
H7
Hb
Hd
Hc
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
ppm
1.00
1.05
1.04
1.07
2.20
1.15

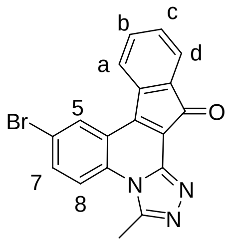

3.097
3.056
3.033
3.017
-CH3
b
c
a
d
Br
5
O
7
8
N
N
N
17
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
ppm
2.84


H5
H8
Ha
H7
Hb
Hd
Hc
ppm
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
8.6
8.7
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
Hc
Hd
Hb
H7
Ha
H8
H5

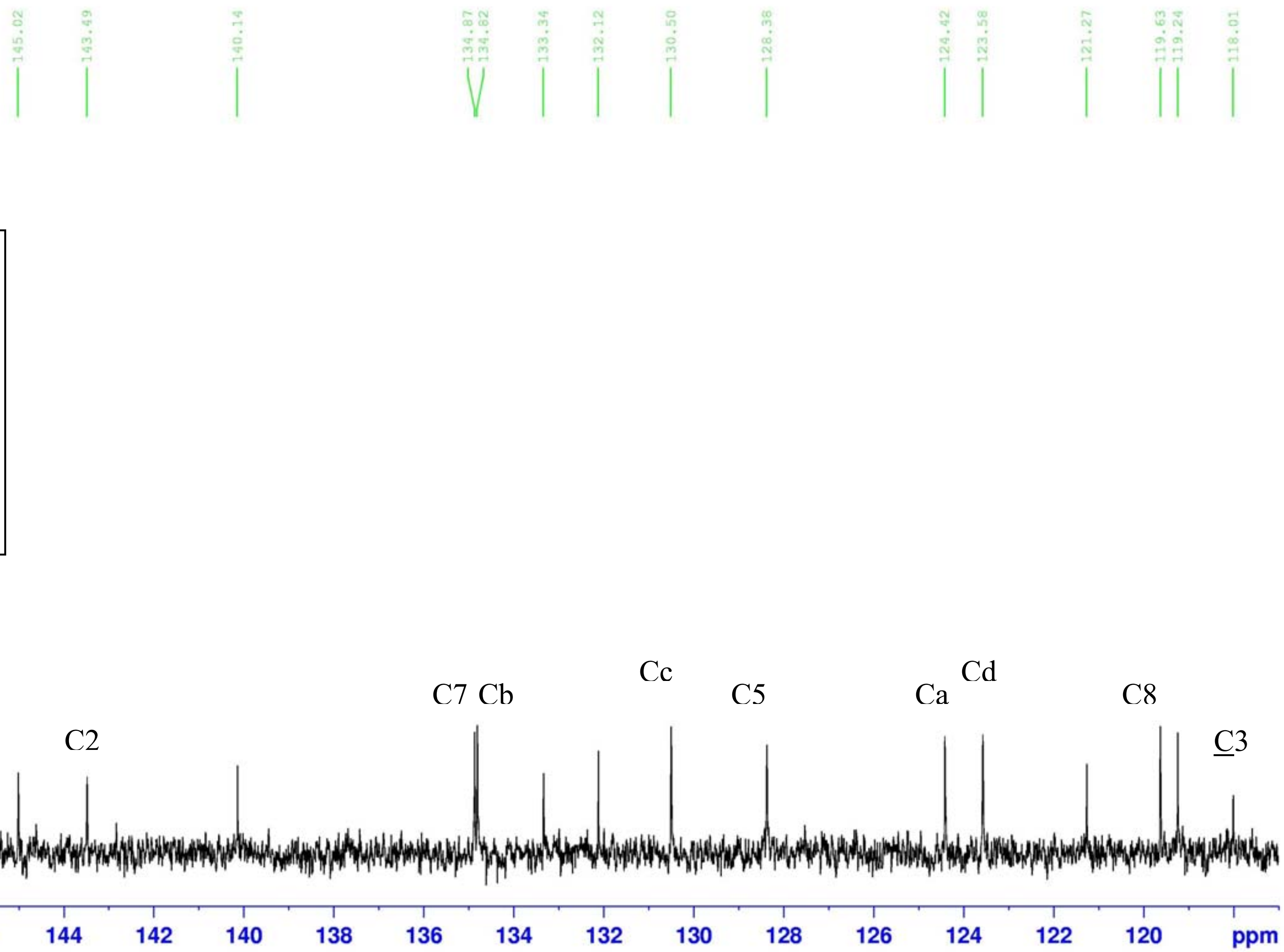

b
c
a
d
Br
5
O
7
8
N
N
N
17

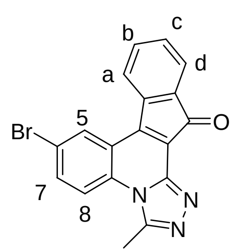


189.14
146.64
145.02
143.49
140.14
134.87
134.82
133.34
132.12
130.50
128.38
124.42
123.58
121.27
119.63
119.24
118.01
40.02
39.93
39.86
39.77
39.69
39.60
39.52
39.43
39.36
39.27
39.10
38.93
15.34
b
c
a
d
5
Br
O
7
N
N
8
N
17
CO
Cc
C5
C7
Cd
Ca
C8
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

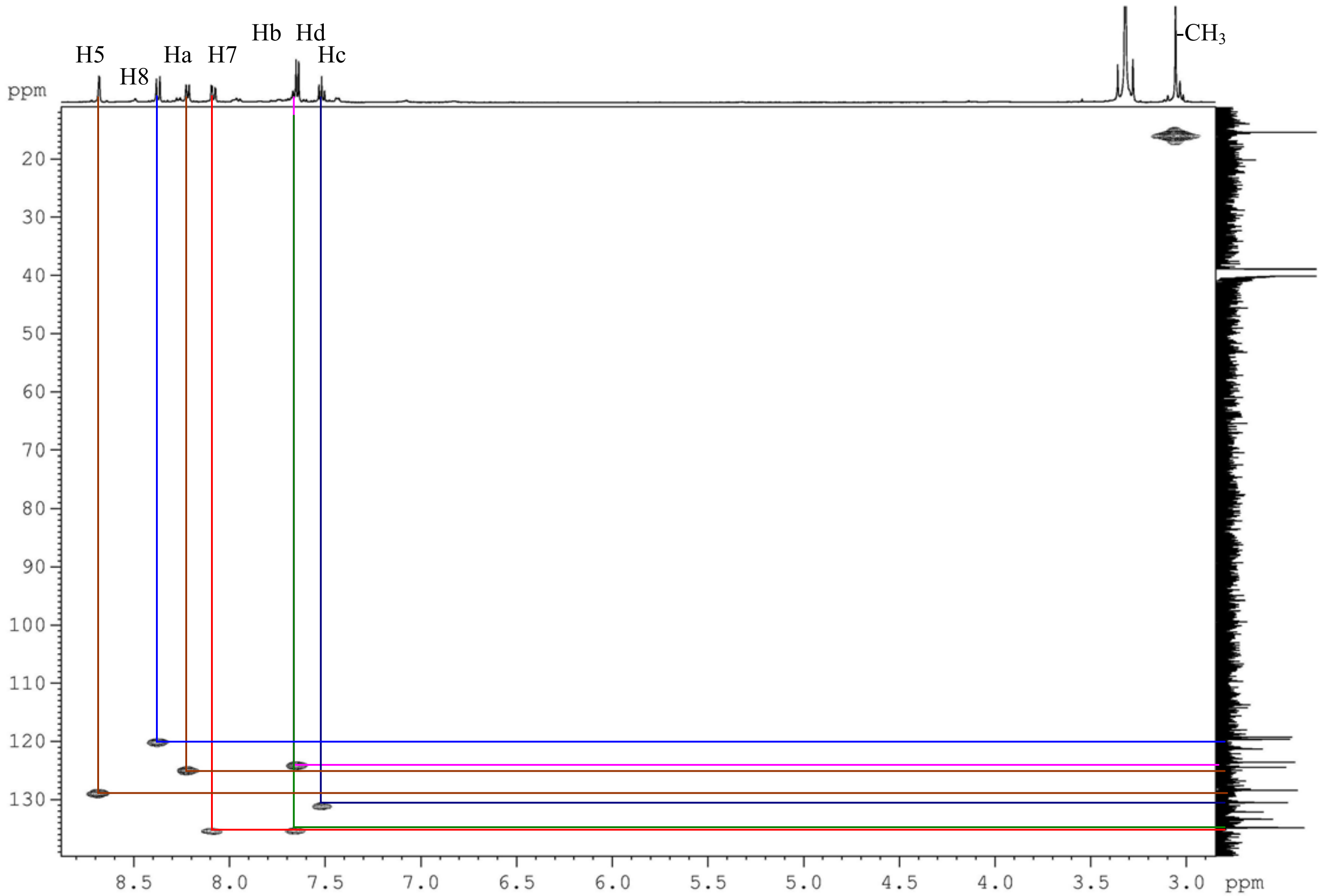

b
c
a
d
Br
5
O
7
8
N
N
N

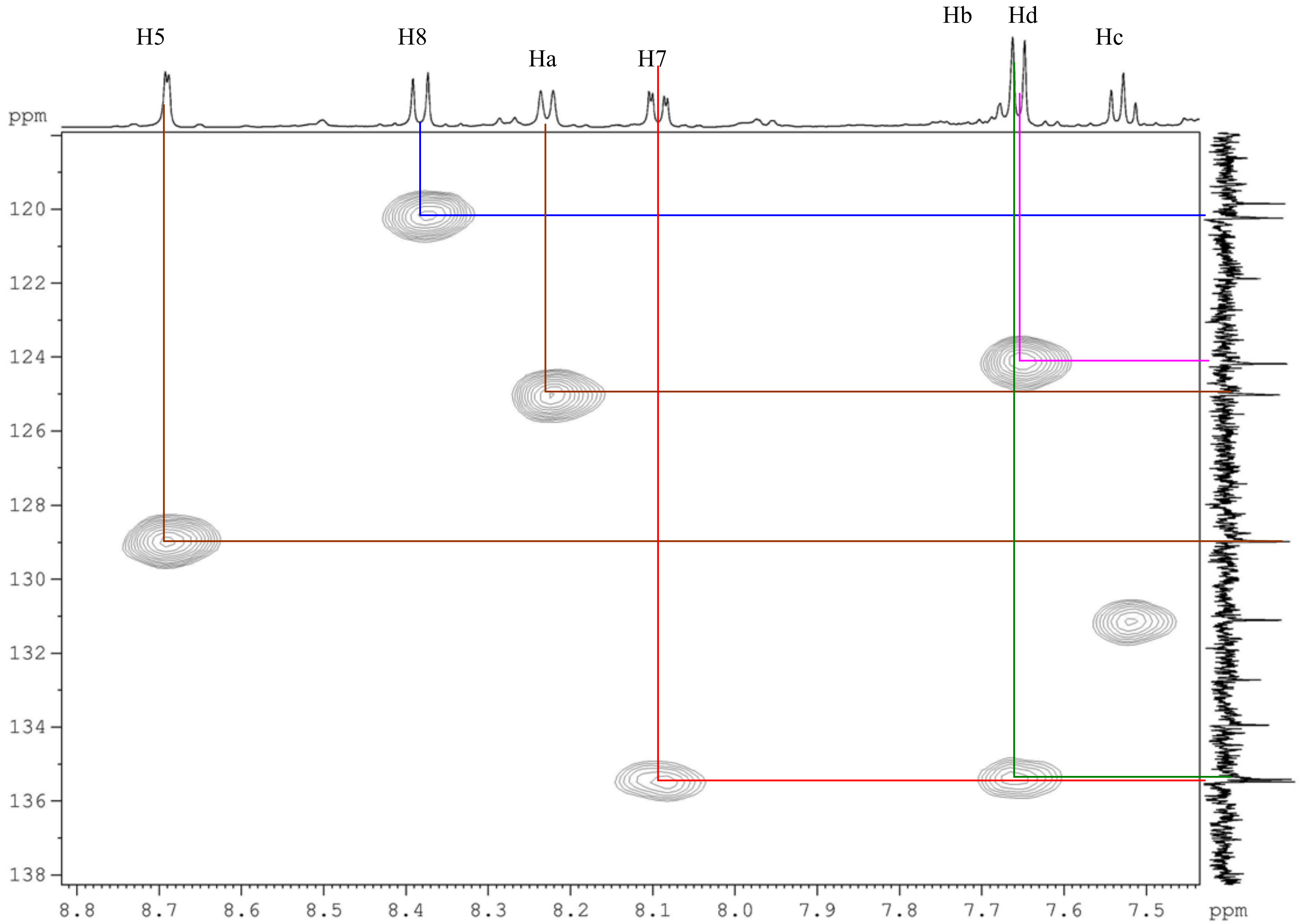
17

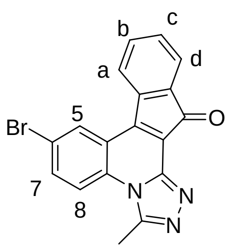

146.64
145.02
143.49
140.14
134.87
134.82
133.34
132.12
130.50
128.38
124.42
123.58
121.27
119.63
119.24
118.01
C2
C7 Cb
Cc
C5
Ca
Cd
C8
C3
146
144
142
140
138
136
134
132
130
128
126
124
122
120
ppm


b
c
a
d
5
Br
O
7
8
N
N
N

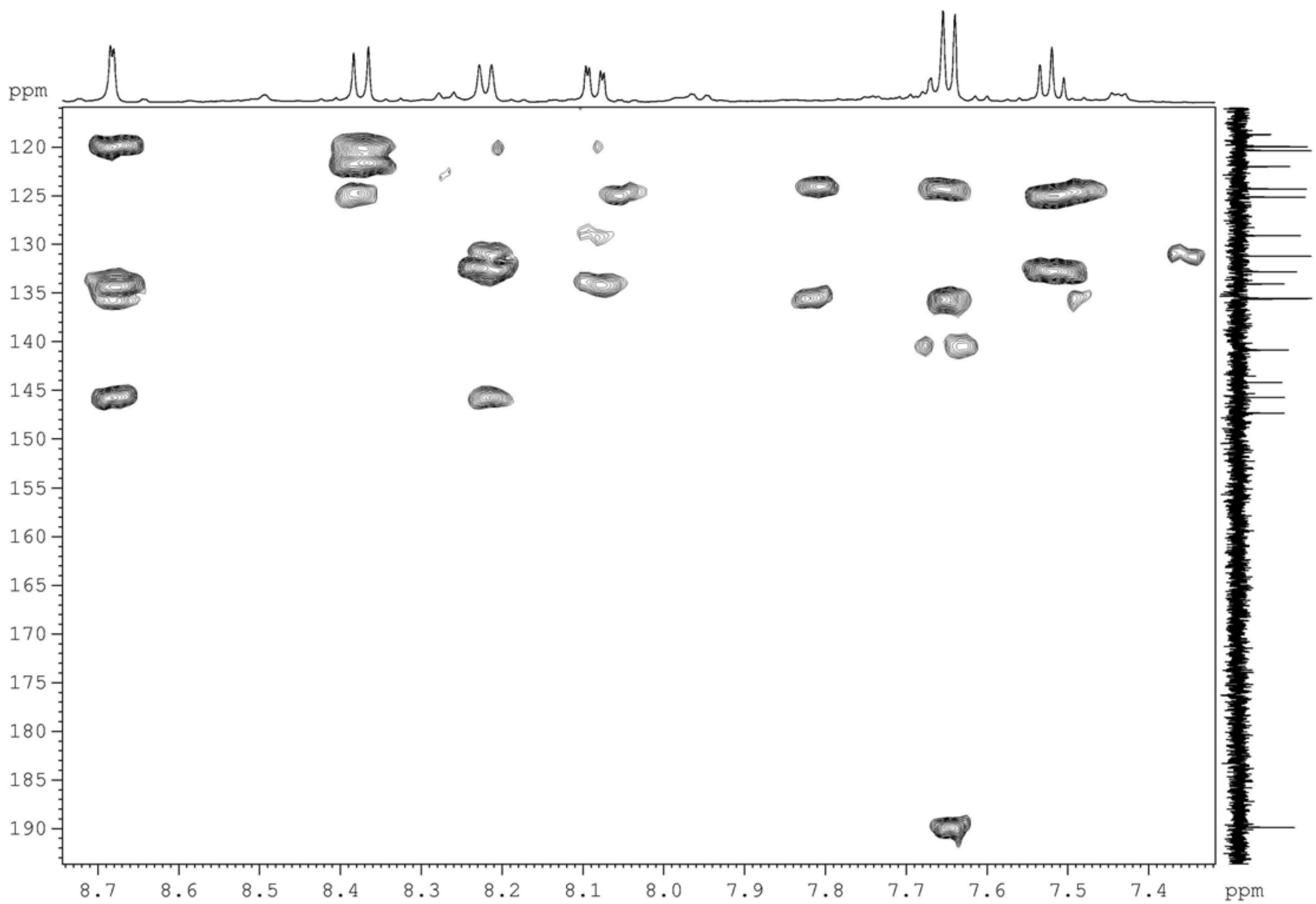
17

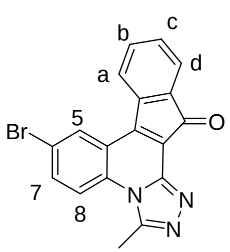

H5
H8
Ha
H7
Hb
Hd
Hc
-CH3
ppm
20
30
40
50
60
70
80
90
100
110
120
130
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm


H5
H8
Ha
H7
Hb
Hd
Hc
ppm
120
122
124
126
128
130
132
134
136
138
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
ppm

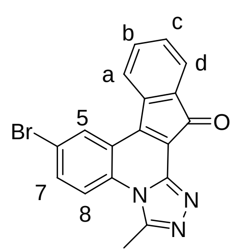

b
c
a
d
5
O
Br
7
N
N
8
N

17

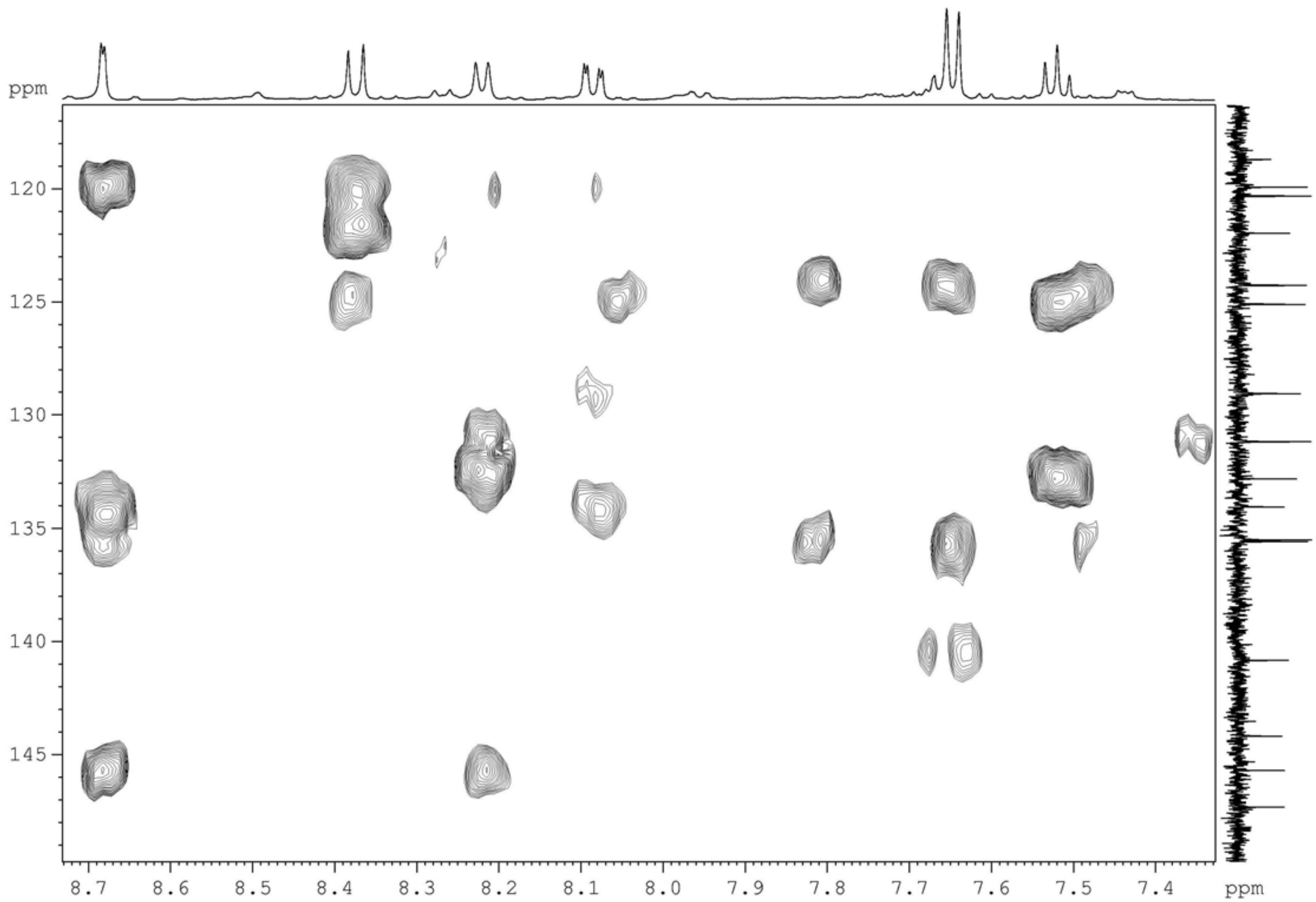

ppm
120
125
130
135
140
145
150
155
160
165
170
175
180
185
190
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm

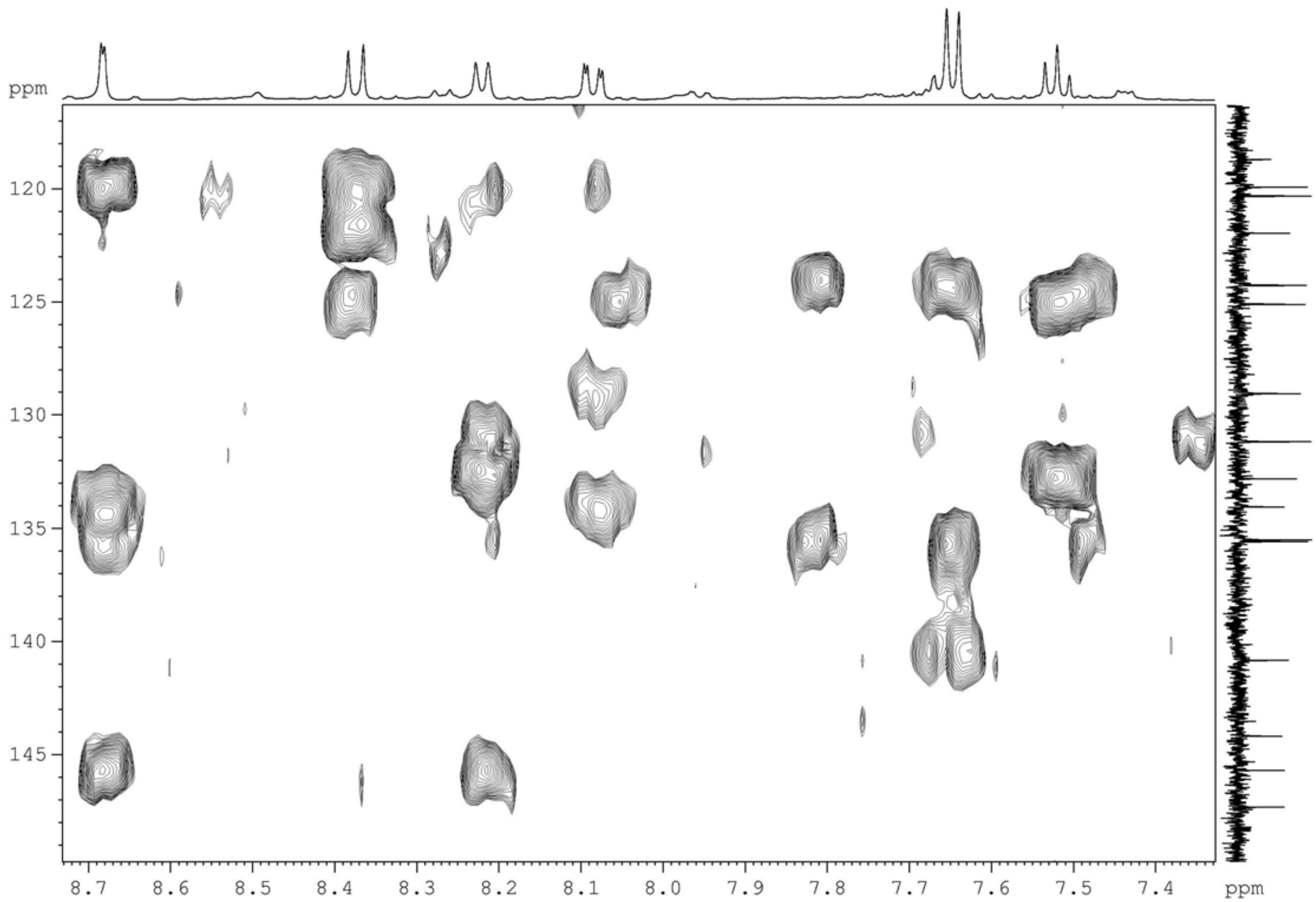

b
c
a
d
5
Br
O
7
N
N
8
N

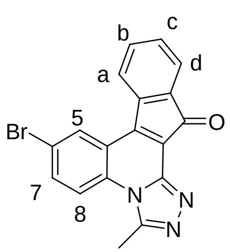
17


b
c
a
d
Br
5
O
7
8
N
N
N

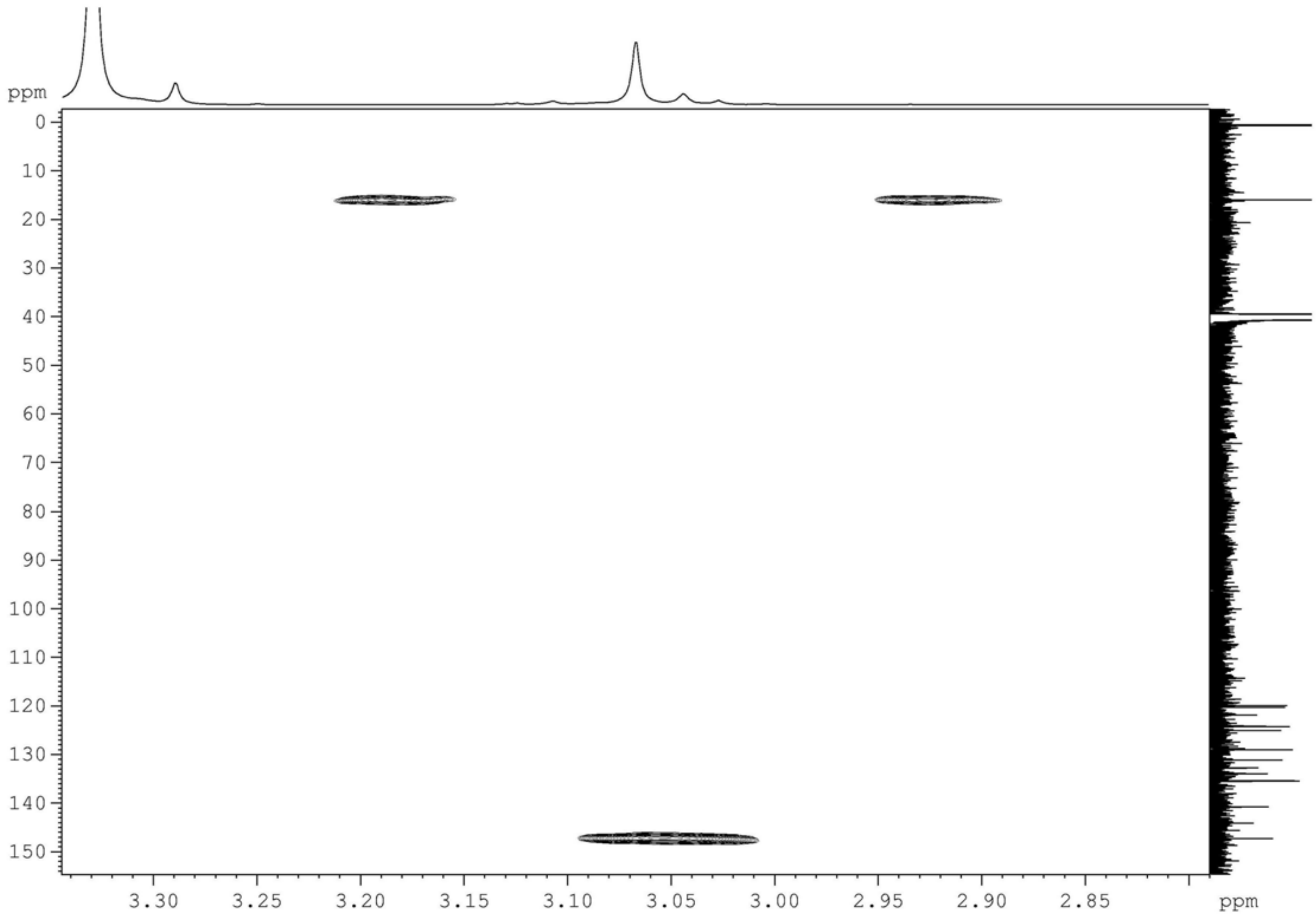
17


ppm
120
125
130
135
140
145
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
ppm

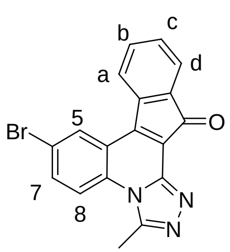

ppm
120
125
130
135
140
145
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm


b
c
a
d
Br
5
O
7
8
N
N
N

17



ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
3.30
3.25
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
ppm



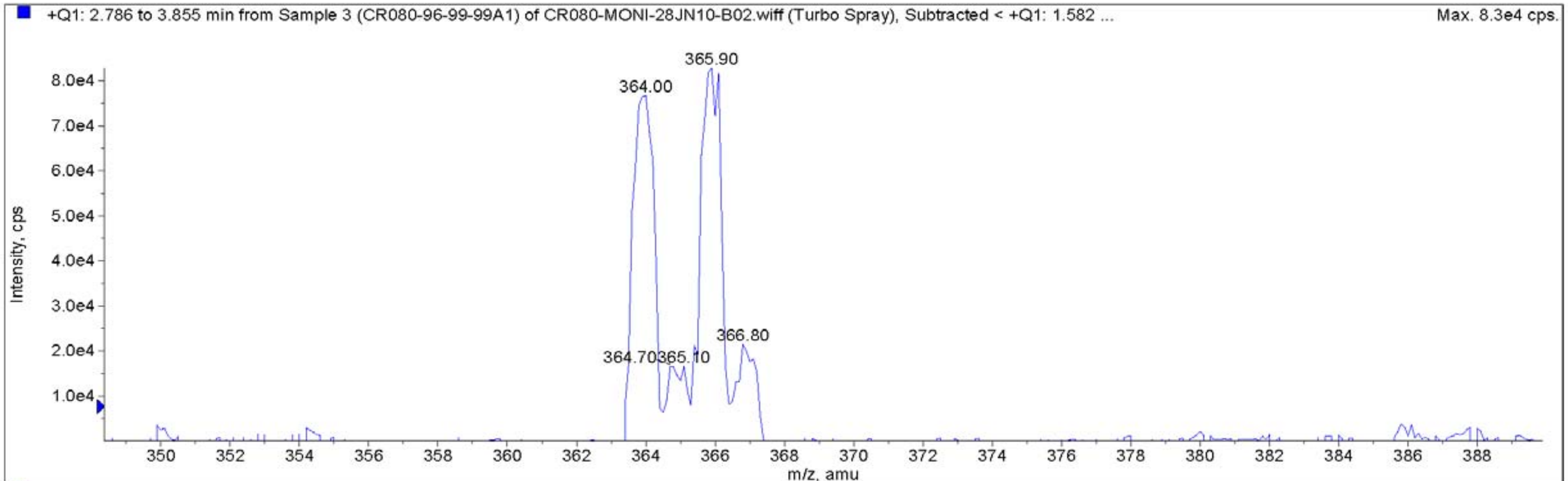
b
c
a
d
5
O
Br
7
8
N
N
N

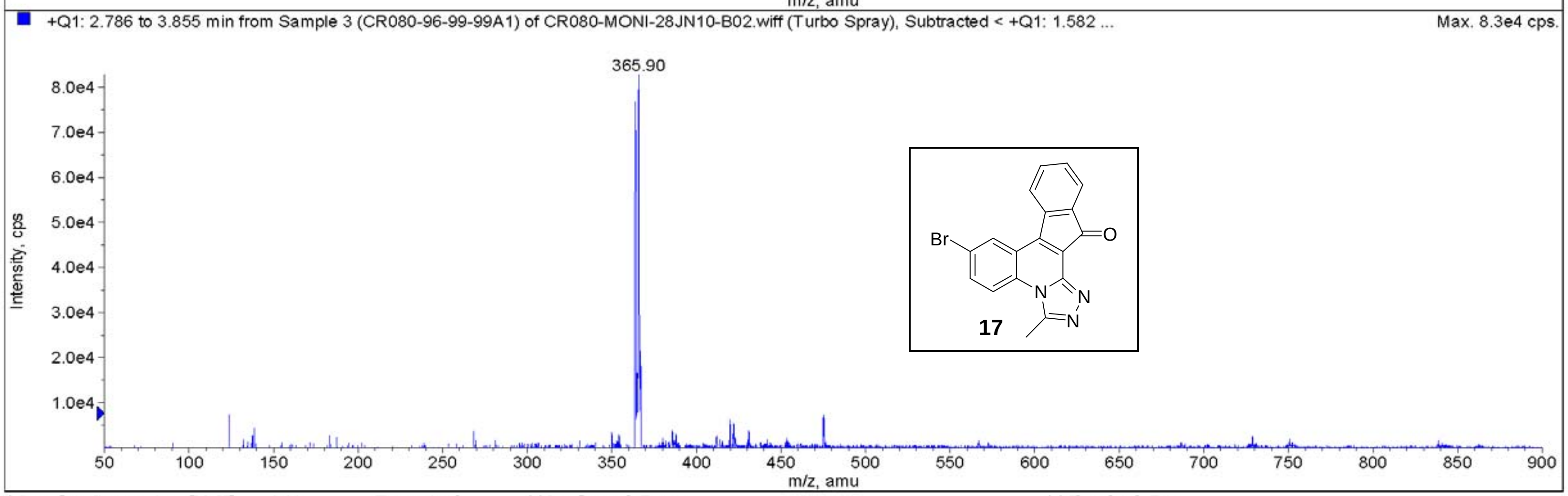
17

*

INDIA

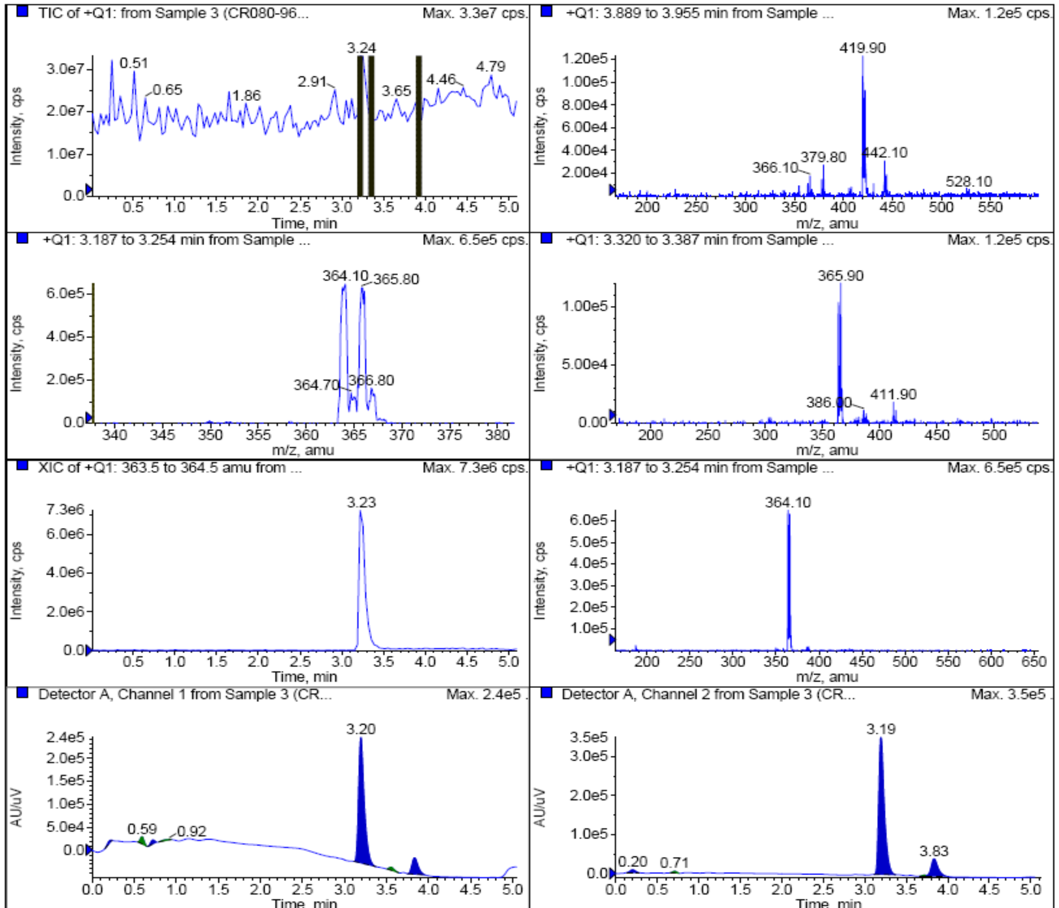
Sample Name: CR080-96-99-99A1 Acq. Time: 15:21 Acq. Date: Thursday, January 28, 2010





*Sample Comment: [M+H] 364 Expected **Analyzed By : **Checked By :

Sample Name: CR080-96-99-99A1 Acq. Time: 15:21 Acq. Date: Thursday, January 28, 2010



Peak List for "Detector A, Channel 1 from Sample 3 (CR080-96-99-

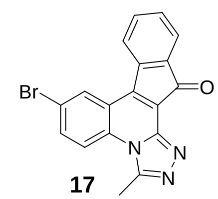
	Time (min)	Area (counts)	% Area	Height
1	0.2212	1.4871e4	0.9488	2973.5358
2	0.5909	4.7847e4	3.0527	1.5575e4
3	0.7209	2.7269e4	1.7398	8533.2895
4	0.9183	1.1528e4	0.7355	952.2236
5	3.1952	1.2609e6	80.4437	2.7206e5
6	3.5520	2.7181e4	1.7342	6733.3221
7	3.8343	1.7783e5	11.3455	3.5538e4

Peak List for "Detector A, Channel 2 from Sample 3 (CR080-96-99-

	Time (min)	Area (counts)	% Area	Height
1	0.2024	3.1745e4	1.6483	7509.7079
2	0.7076	1.5375e4	0.7983	4740.3948
3	3.1936	1.6252e6	84.3812	3.5180e5
4	3.7211	8004.4767	0.4156	2456.2077
5	3.8343	2.4569e5	12.7567	4.4151e4

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm



17

===

SAMPLE: CR080-96-99-99A1 ->

Column: PUROSPHERE-RP18(250X4.6)mm 5µ

Injection date : Thu, 11. Mar. 2010 Location : Vial 16

Sample Name : CR080-96-99-99A1 Inj. No. : 1

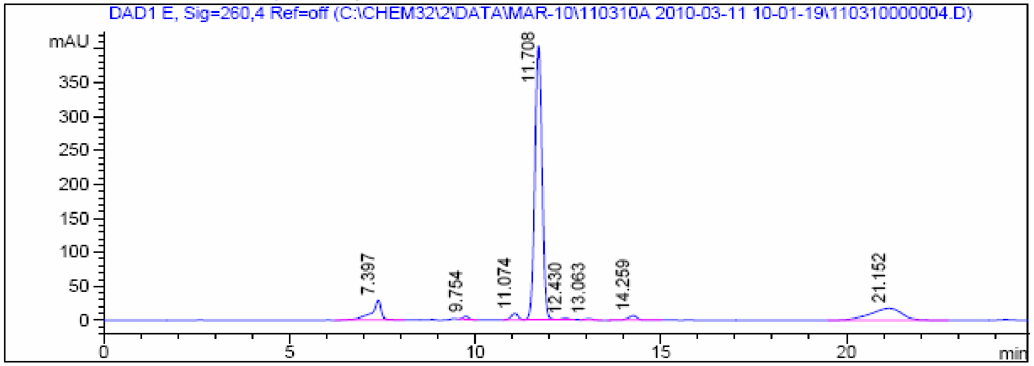
Acq Operator : BHUSHAN Inj. Vol. : 15 µl

Analysis Method : C:\CHEM32\2\METHODS\UPLC__ISO_50_50.M

Last Changed : Thu, 11. Mar. 2010,

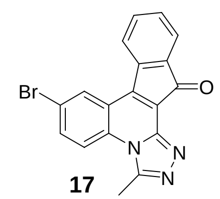
Acq. Method : C:\Chem32\2\DATA\MAR-10\110310A 2010-03-11 10-01-19\UPLC__ISO_50_50.M

Method ref : NP/A0011/59



DAD1 E, Sig=260,4 Ref=off

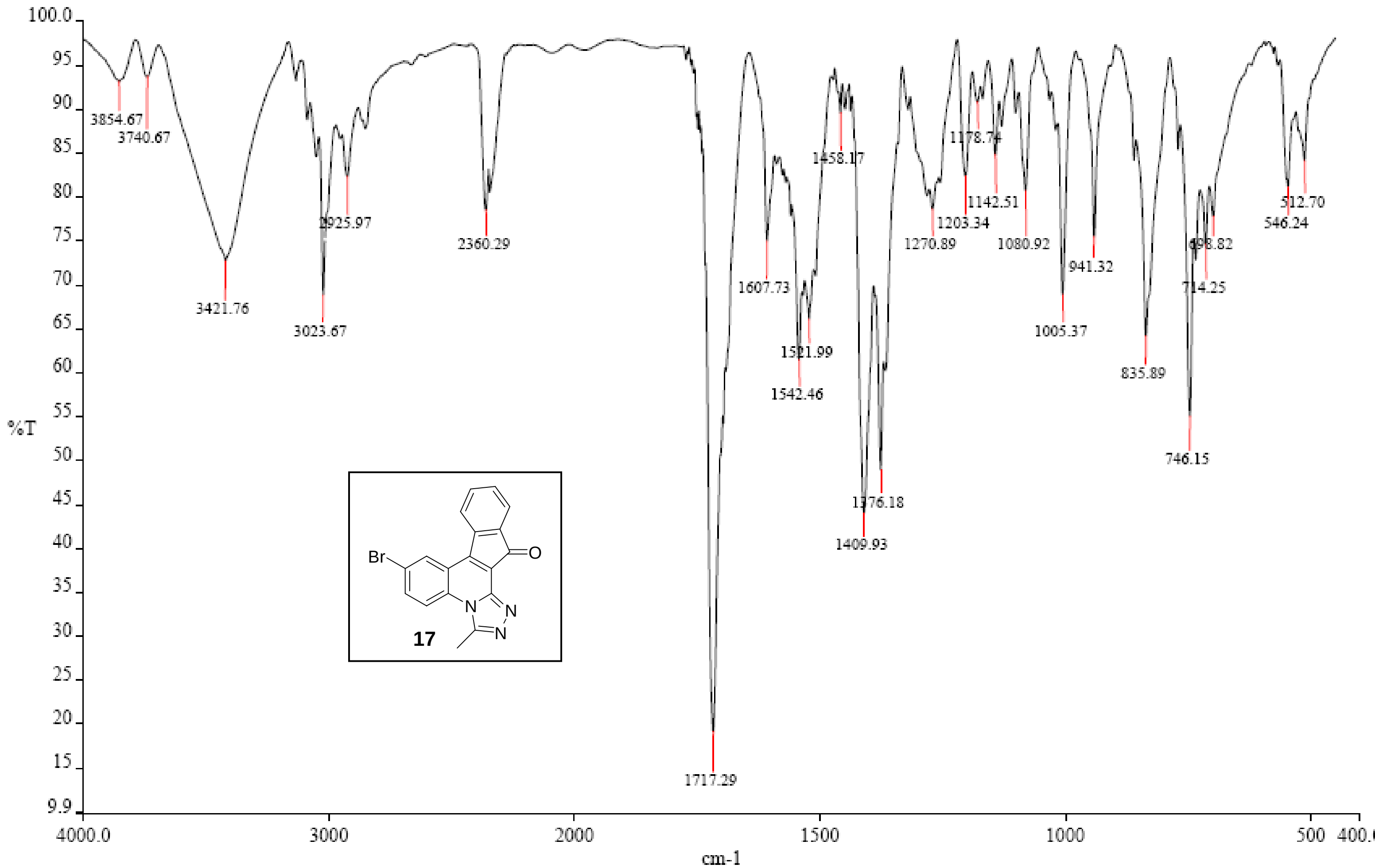
Peak #	RT (Min)	Width (Min)	Area	Area %
1	7.397	0.243	519.218	7.160
2	9.754	0.172	46.034	0.635
3	11.074	0.207	116.083	1.601
4	11.708	0.208	5.404e3	74.526
5	12.430	0.190	23.078	0.318
6	13.063	0.193	20.430	0.282
7	14.259	0.258	107.350	1.480
8	21.152	0.875	1.015e3	13.998



17

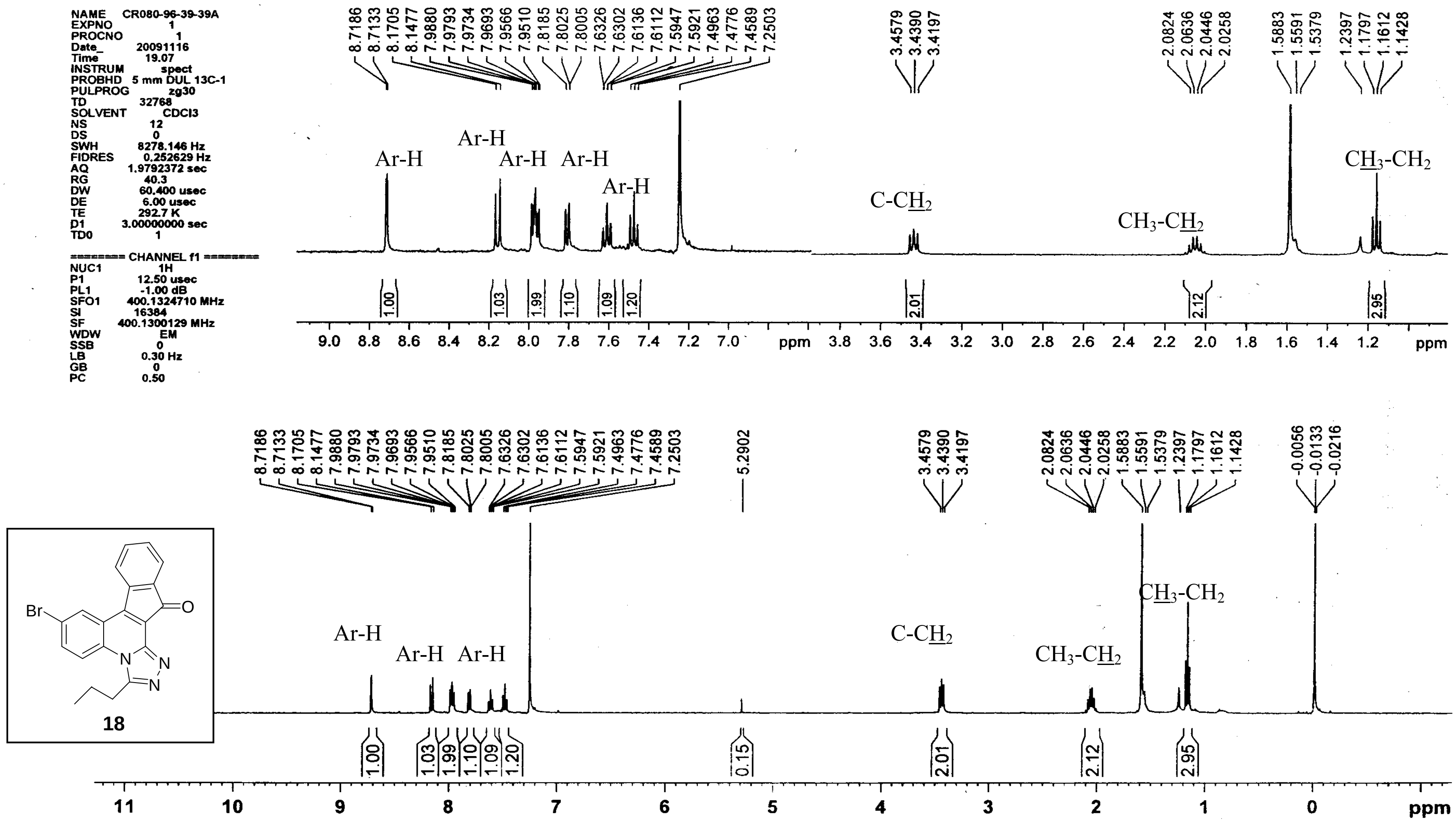
===

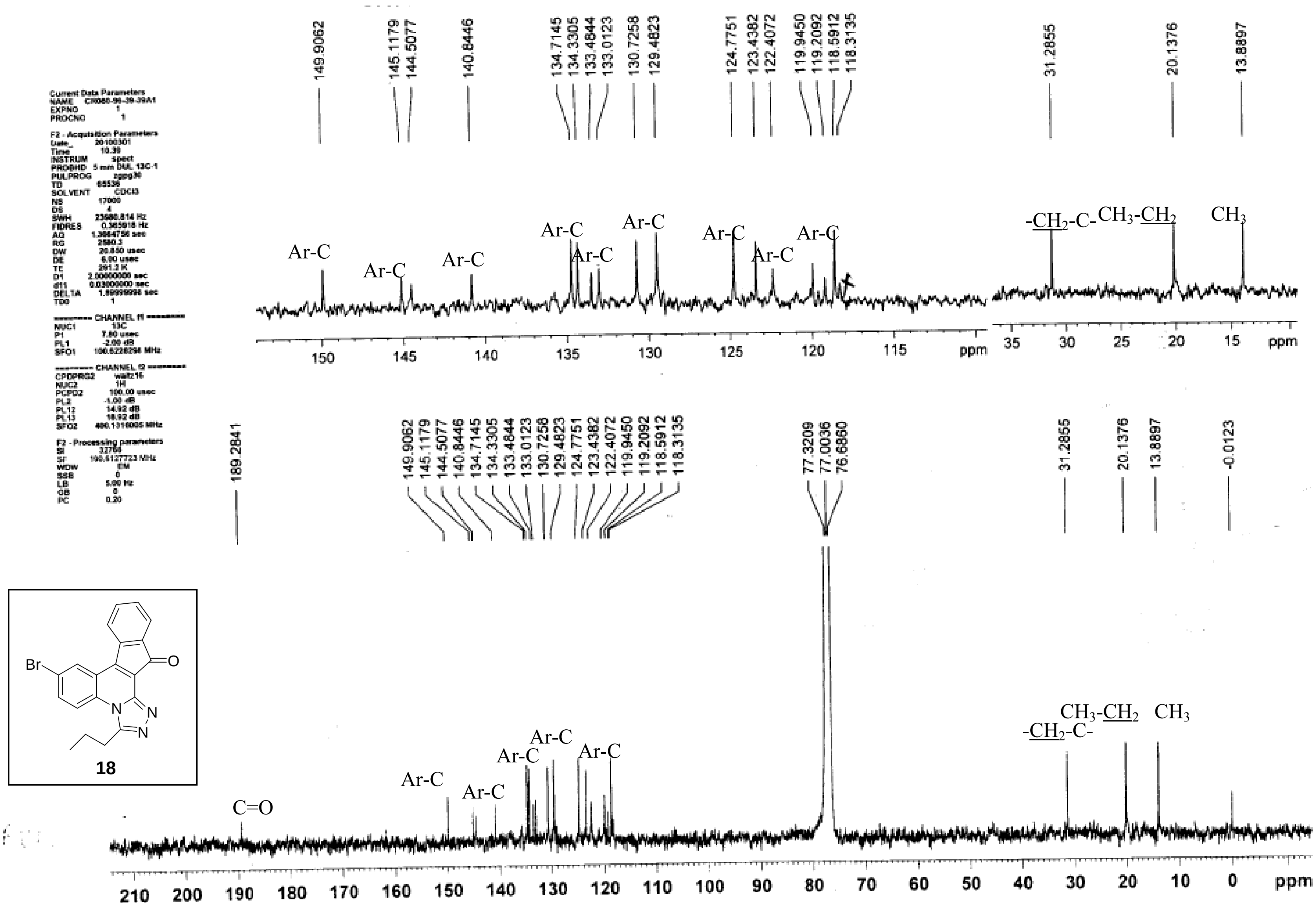
*** End of Report***

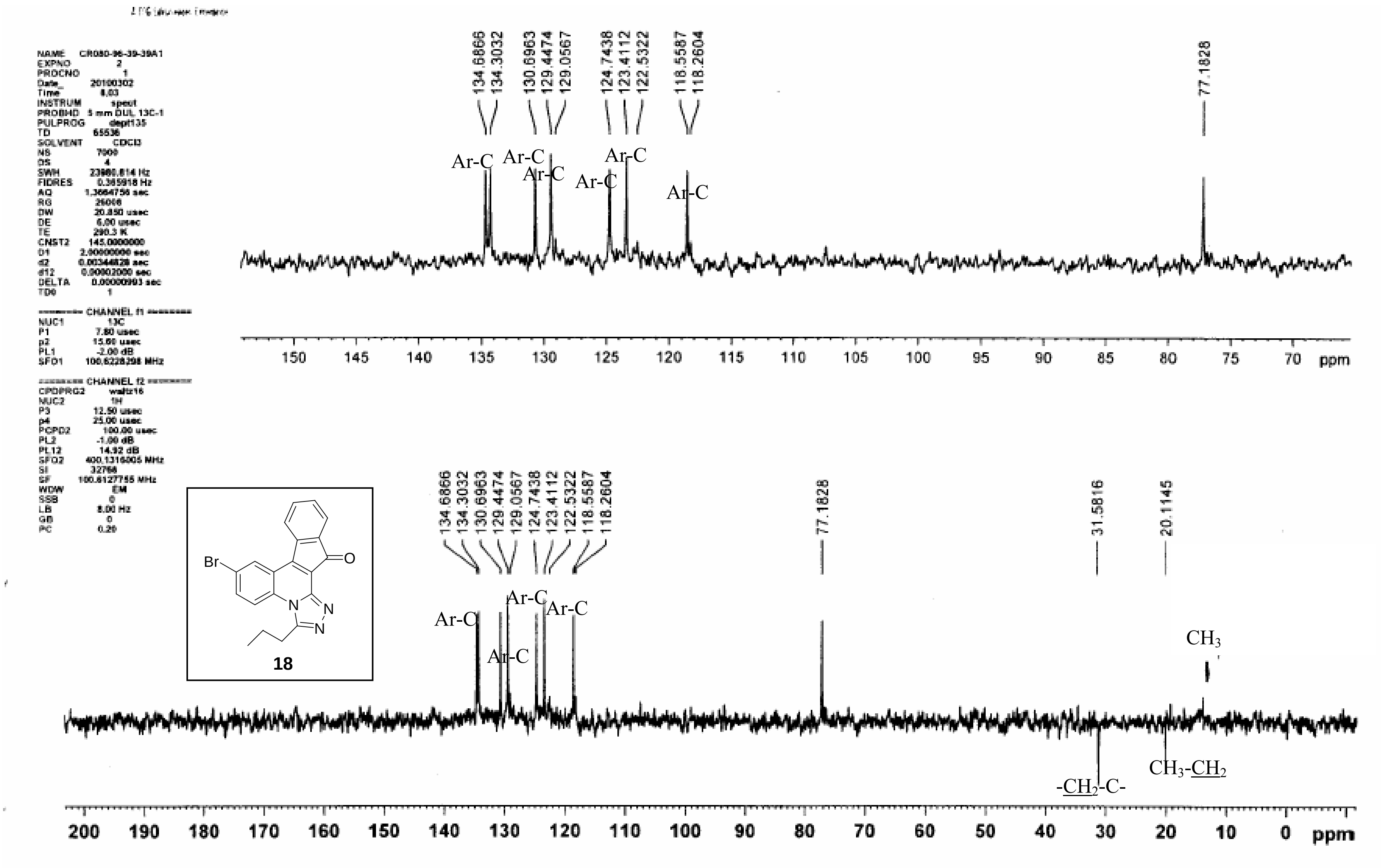


Spectrum Name: CR080-96-99-99A.sp Analyst: GANESH Accumulations: 16 Time: 1:02:38 PM

Description: CR080-96-99-99A IN KBr Resolution: 4.00 cm-1 Date: 2/5/2010

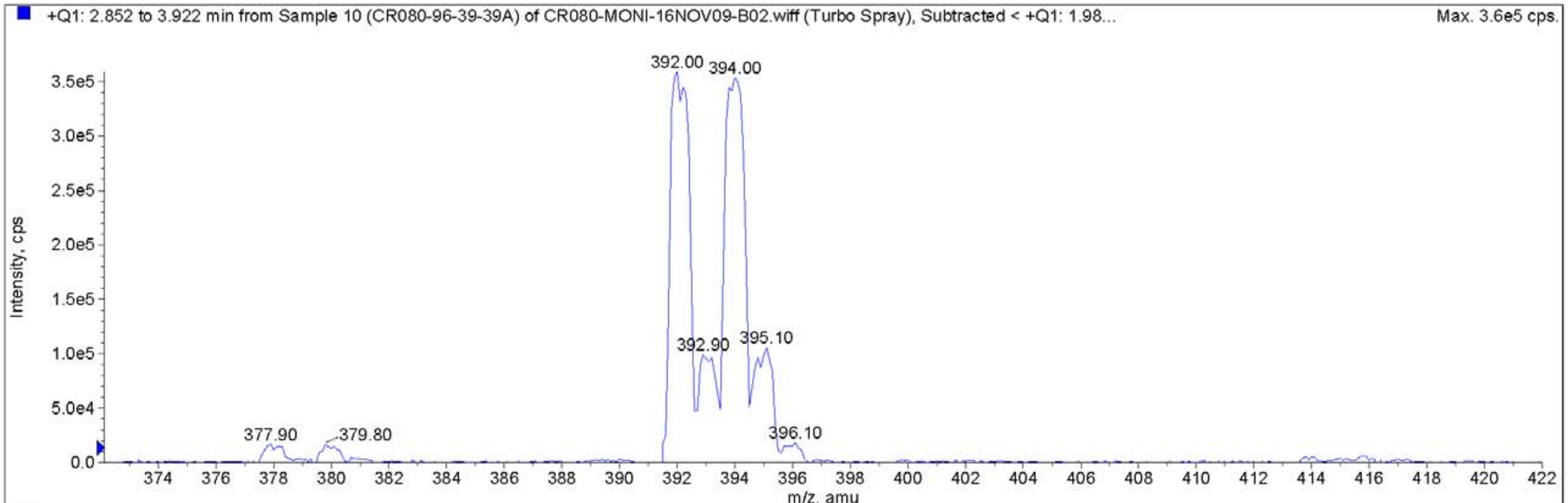

NAME CR080-96-39-39A
EXPNO 1
PROCNO 1
Date_ 20091116
Time 19.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 40.3
DW 60.400 usec
DE 6.00 usec
TE 292.7 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
8.7186 8.7133 8.1705 8.1477 7.9880 7.9793 7.9734 7.9693 7.9566 7.9510 7.8185 7.8025 7.8005 7.6326 7.6302 7.6136 7.6112 7.5947 7.5921 7.4963 7.4776 7.4589 7.2503
3.4579 3.4390 3.4197
2.0824 2.0636 2.0446 2.0258
1.5883 1.5591 1.5379
1.2397 1.1797 1.1612 1.1428
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
C-CH2
CH3-CH2
CH3-CH2
1.00
1.03
1.99
1.10
1.09
1.20
2.01
2.12
2.95
ppm
5.2902
-0.0056 -0.0133 -0.0216
0.15
Br
N
N
N
O
18

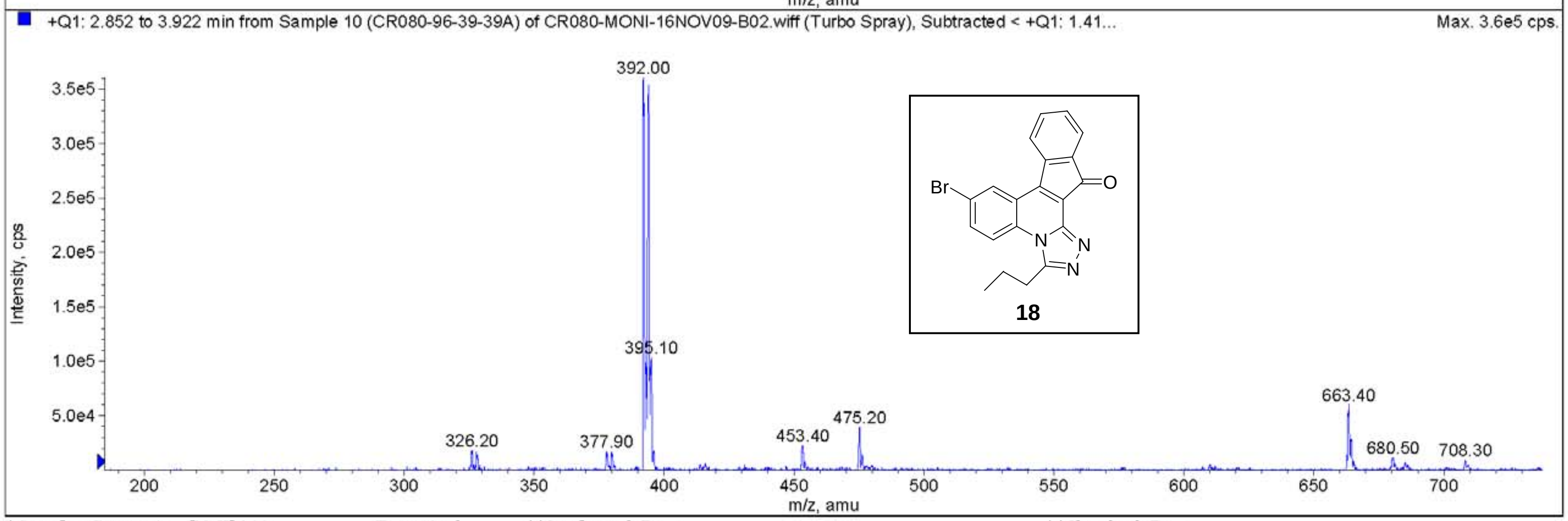

149.9062
145.1179
144.5077
140.8446
134.7145
134.3305
133.4844
133.0123
130.7258
129.4823
124.7751
123.4382
122.4072
119.9450
119.2092
118.5912
118.3135
31.2855
20.1376
13.8897
189.2841
77.3209
77.0036
76.6860
-0.0123
Ar-C
C=O
-CH2-C-
CH3-CH2
CH3
ppm
Br
O
N
N
N
18


NAME CR080-96-39-39A1
EXPNO 2
PROCNO 1
Date_ 20100302
Time 8.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 7000
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 26008
DW 20.850 usec
DE 6.00 usec
TE 290.3 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000903 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 7.80 usec
p2 15.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 12.50 usec
p4 25.00 usec
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.92 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 0.20
134.6866
134.3032
130.6963
129.4474
129.0567
124.7438
123.4112
122.5322
118.5587
118.2604
77.1828
31.5816
20.1145
Ar-C
CH3
-CH2-C-
CH3-CH2
Br
O
N
18
ppm

*

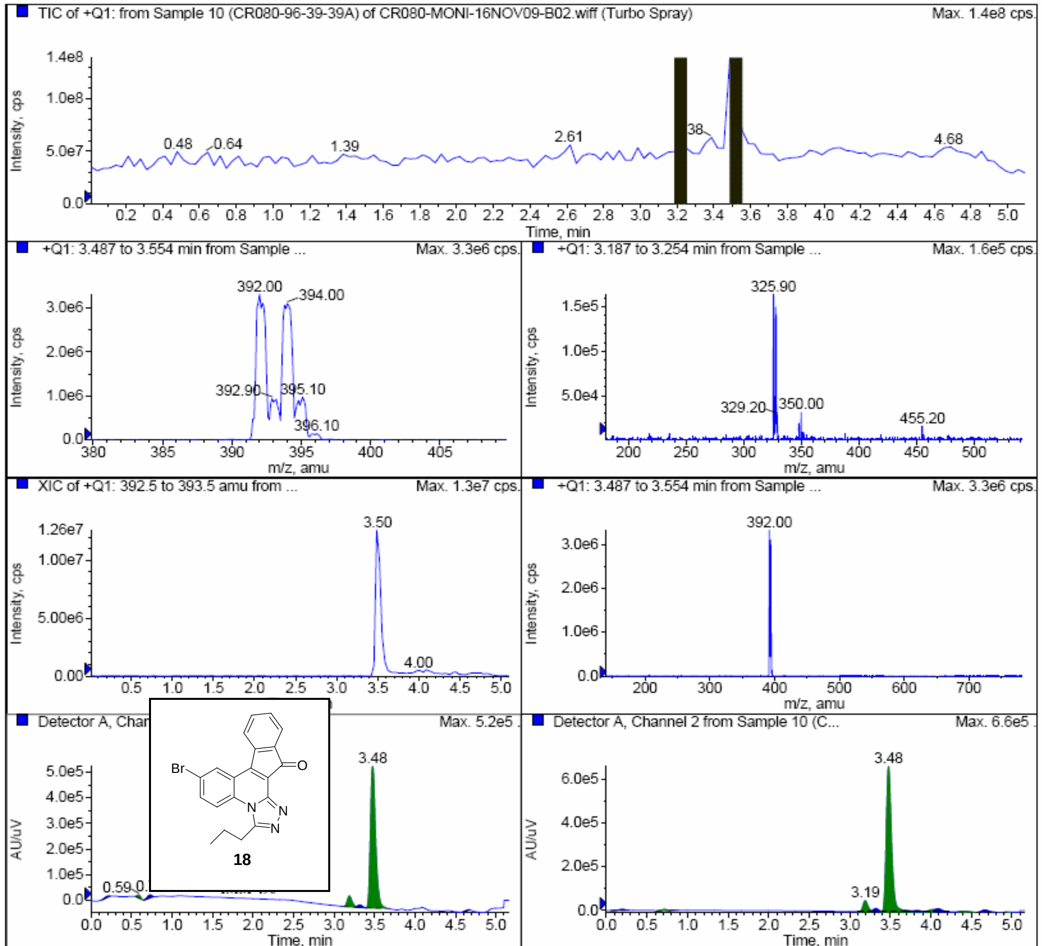
Sample Name: CR080-96-39-39A   Acq. Time: 19:49   Acq. Date: Monday, November 16, 2009





*Sample Comment: [M+H]392   Expected   **Analyzed By :   **Checked By :

Sample Name: CR080-96-39-39A Acq. Time: 19:49 Acq. Date: Monday, November 16, 2009



Peak List for "Detector A, Channel 1 from Sample 10 (CR080-96-39

	Time (min)	Area (counts)	%Area	Height
1	0.2199	1.5650e4	0.5804	2885.5159
2	0.5854	3.1729e4	1.1767	1.1446e4
3	0.7283	4.4141e4	1.6371	1.1932e4
4	3.1892	1.6793e5	6.2283	4.2234e4
5	3.3177	3.9042e4	1.4480	9899.6632
6	3.4774	2.3916e6	88.6997	5.5154e5
7	4.6650	6198.2488	0.2299	1657.1961

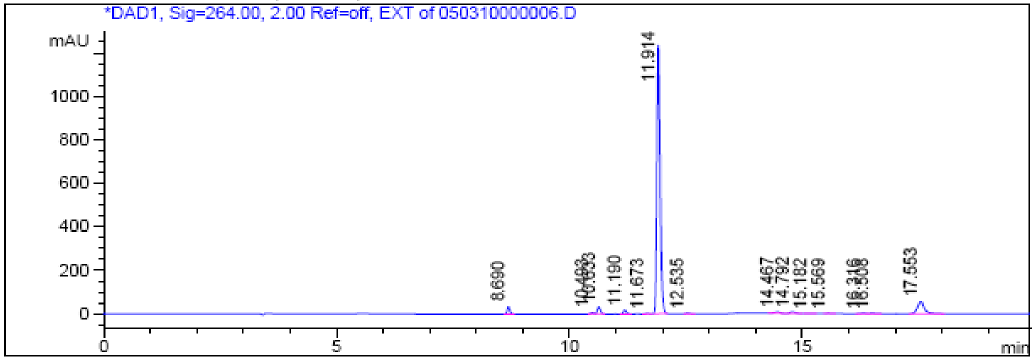
Peak List for "Detector A, Channel 2 from Sample 10 (CR080-96-39-

	Time (min)	Area (counts)	%Area	Height
1	0.1956	2.2211e4	0.6324	4249.1929
2	0.7174	2.7979e4	0.7966	5671.8634
3	0.8567	2886.5774	0.0822	546.7729
4	3.1906	2.0133e5	5.7323	4.9338e4
5	3.3191	6.0928e4	1.7347	1.4381e4
6	3.4781	2.9466e6	83.8944	6.6170e5
7	3.8298	4.2246e4	1.2028	5013.9989

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

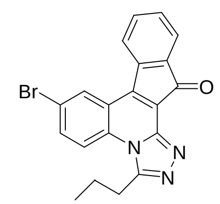
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

```
================================================================================
SAMPLE: CR080-96-39-39 A                                                      ->
Column: GEMINI-C18(250X4.6)mm 5µ
Injection date  : Fri, 5. Mar. 2010              Location   :     Vial 14
Sample Name     : CR080-96-39-39 A               Inj. No.   :           1
Acq Operator    : BHUSHAN                        Inj. Vol.  :       10 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _1.M
Last Changed    : Mon, 8. Mar. 2010,
Acq. Method     : C:\Chem32\2\DATA\MAR-10\050310E 2010-03-05 16-35-20\
                  UPLC_GENARAL_GRAD _1.M
Method ref      : NP/A0011/56
```



DAD1, Sig=264.00, 2.00 Ref=off, EXT

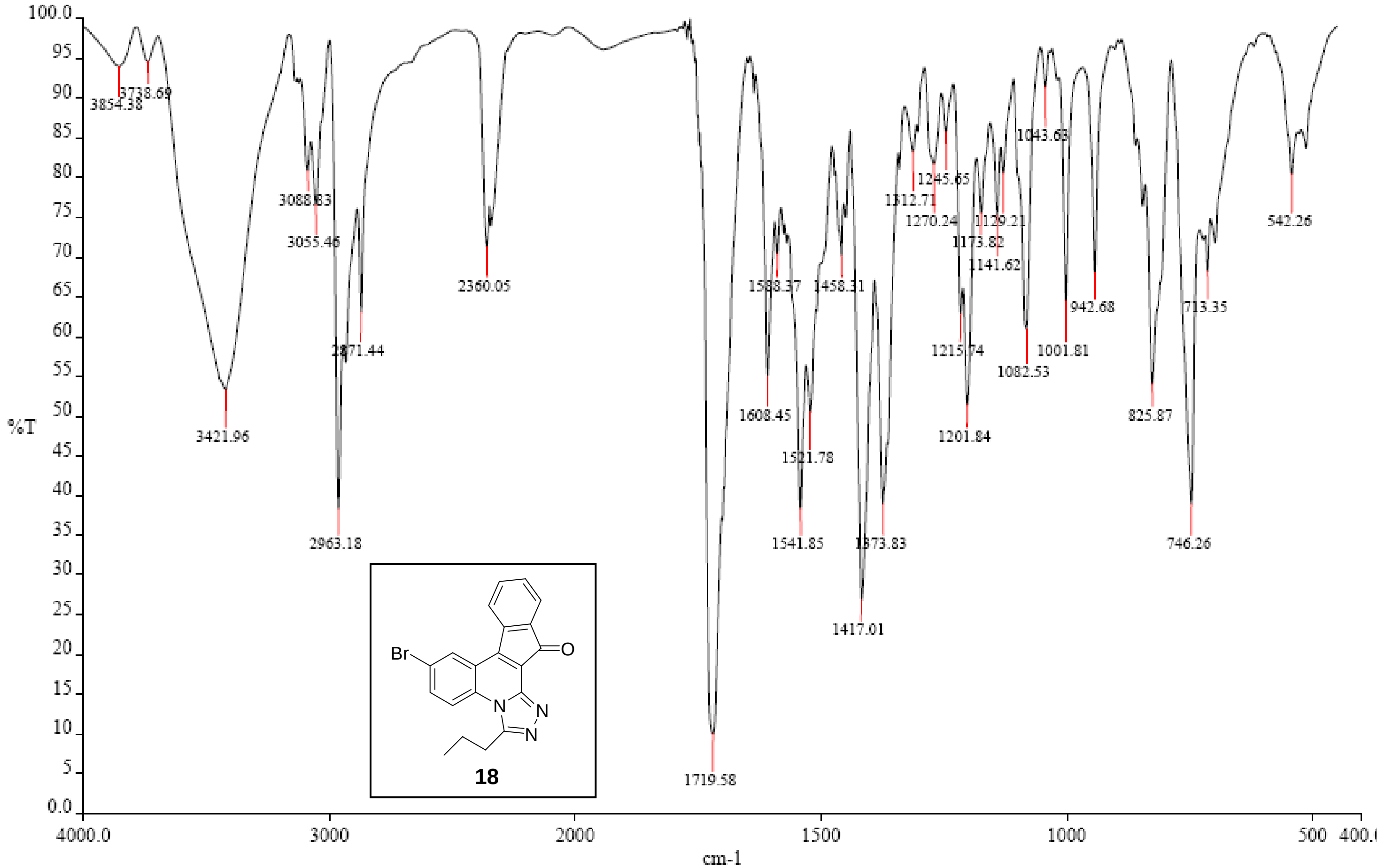
Peak #	RT (Min)	Width (Min)	Area	Area %
1	8.690	0.064	137.043	1.939
2	10.493	0.062	23.326	0.330
3	10.633	0.073	145.084	2.052
4	11.190	0.077	88.321	1.249
5	11.673	0.087	12.239	0.173
6	11.914	0.080	5.907e3	83.565
7	12.535	0.094	20.460	0.289
8	14.467	0.128	44.996	0.637
9	14.792	0.126	57.948	0.820
10	15.182	0.144	6.538	0.092
11	15.569	0.114	10.059	0.142
12	16.316	0.135	20.007	0.283
13	16.508	0.145	20.341	0.288
14	17.553	0.175	575.369	8.140



18

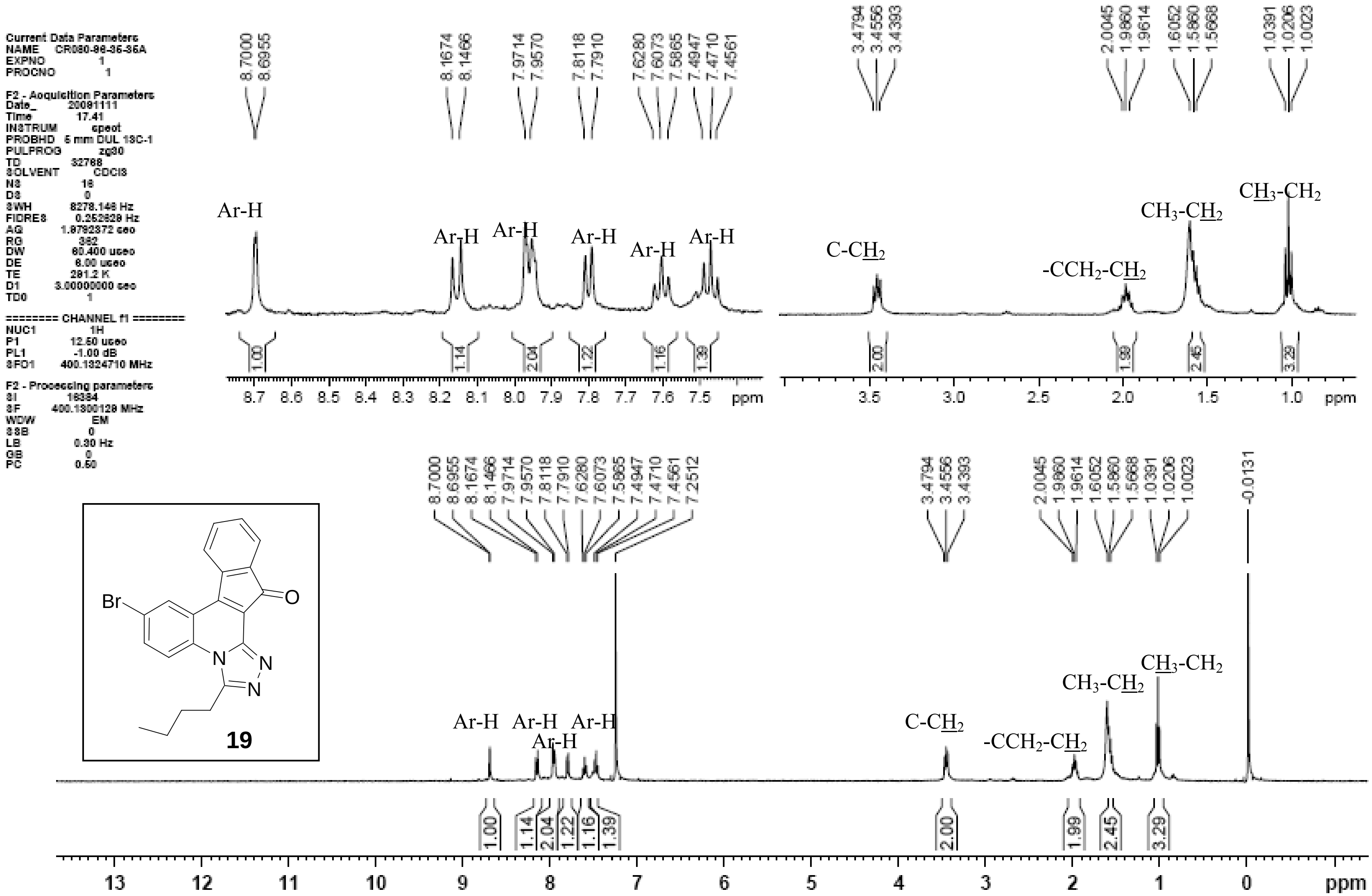
==

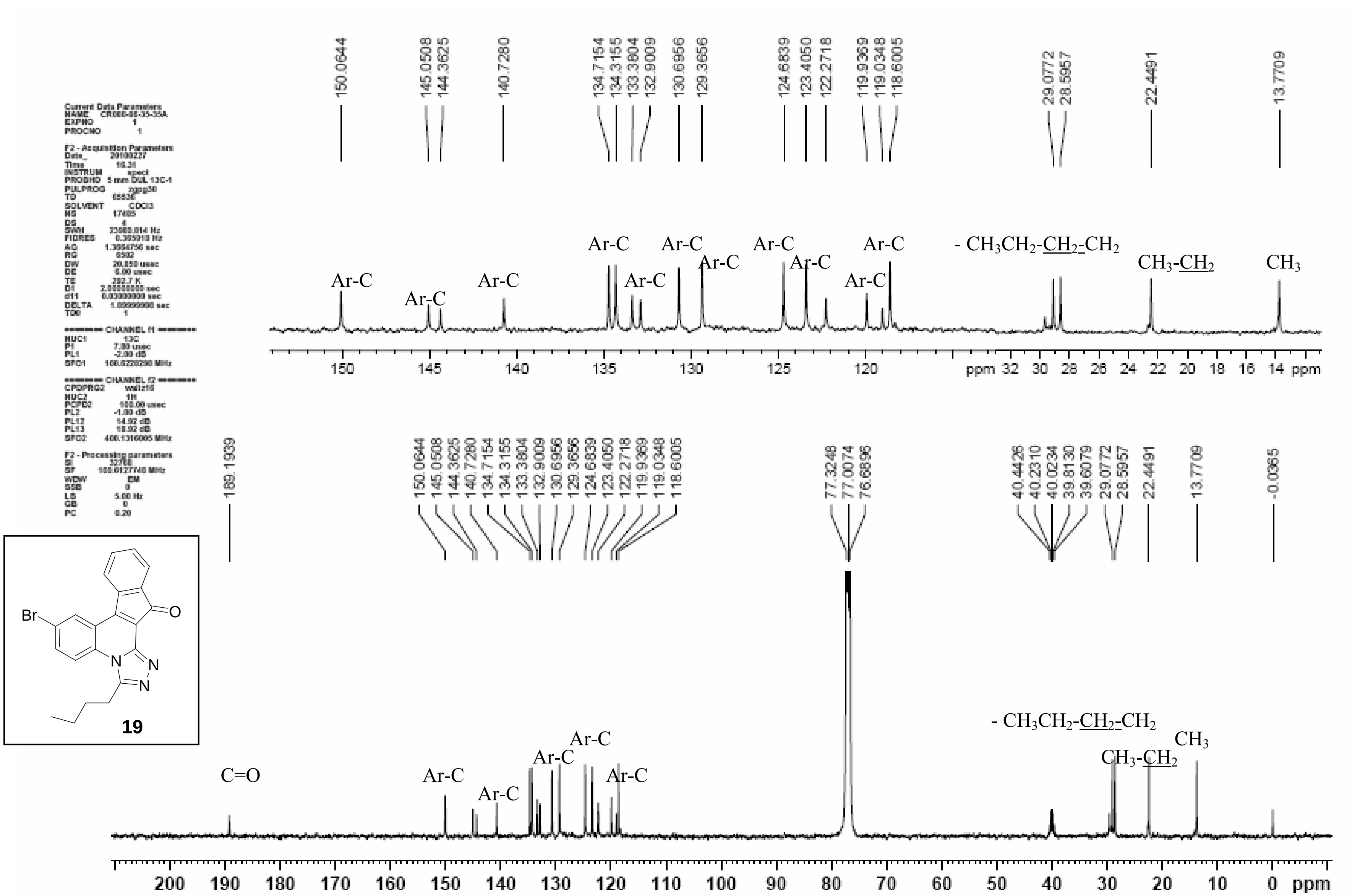
*** End of Report***

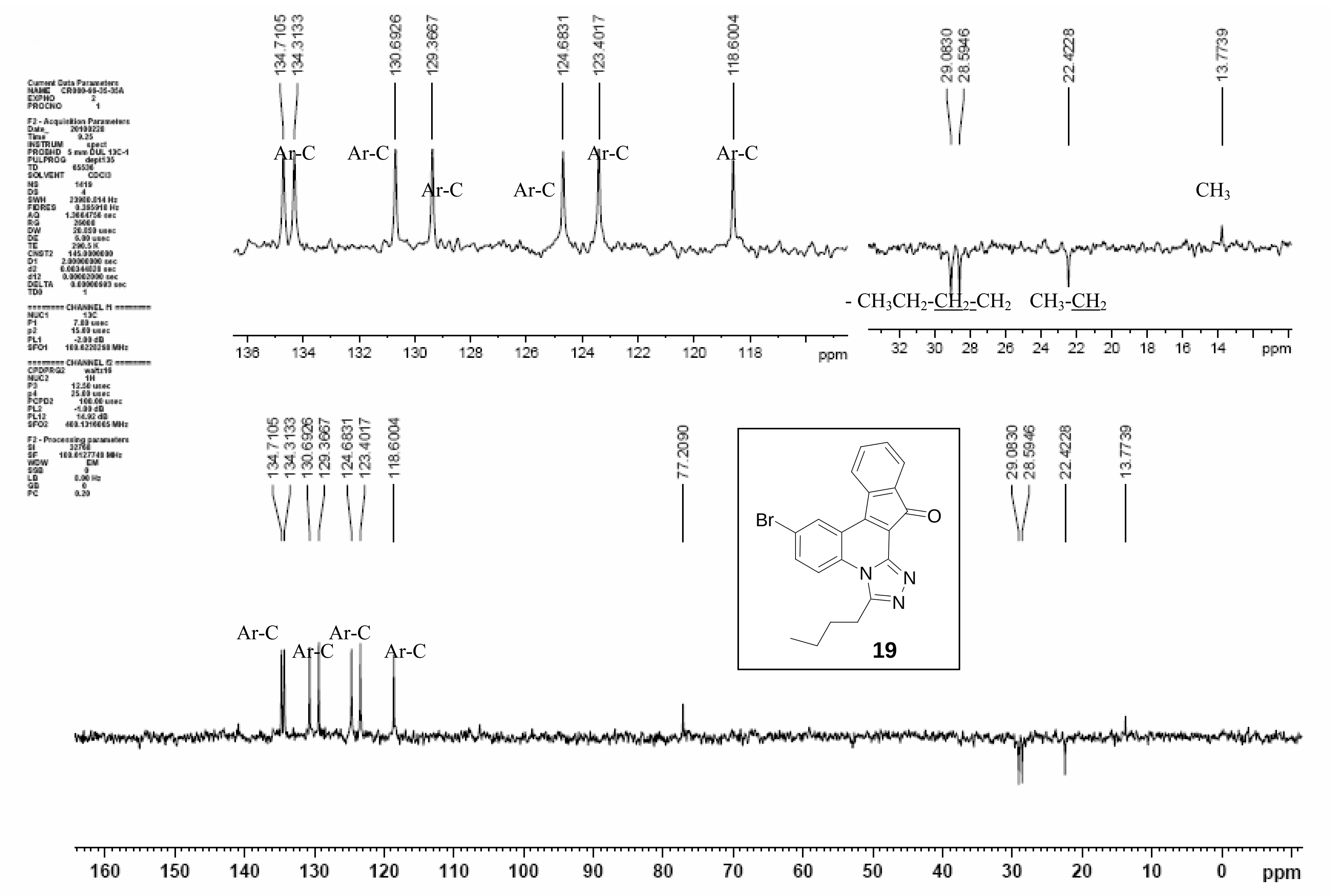


Spectrum Name: CR080-96-39-39A.sp Analyst: GANESH Accumulations: 16 Time: 5:49:57 PM

Description: CR080-96-39-39A IN KBr Resolution: 4.00 cm-1 Date: 2/5/2010


Current Data Parameters
NAME CR080-86-36-36A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081111
Time 17.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252628 Hz
AQ 1.9792372 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
Ar-H
C-CH2
-CCH2-CH2
CH3-CH2
CH3-CH2
Br
O
N
N
N
19
ppm

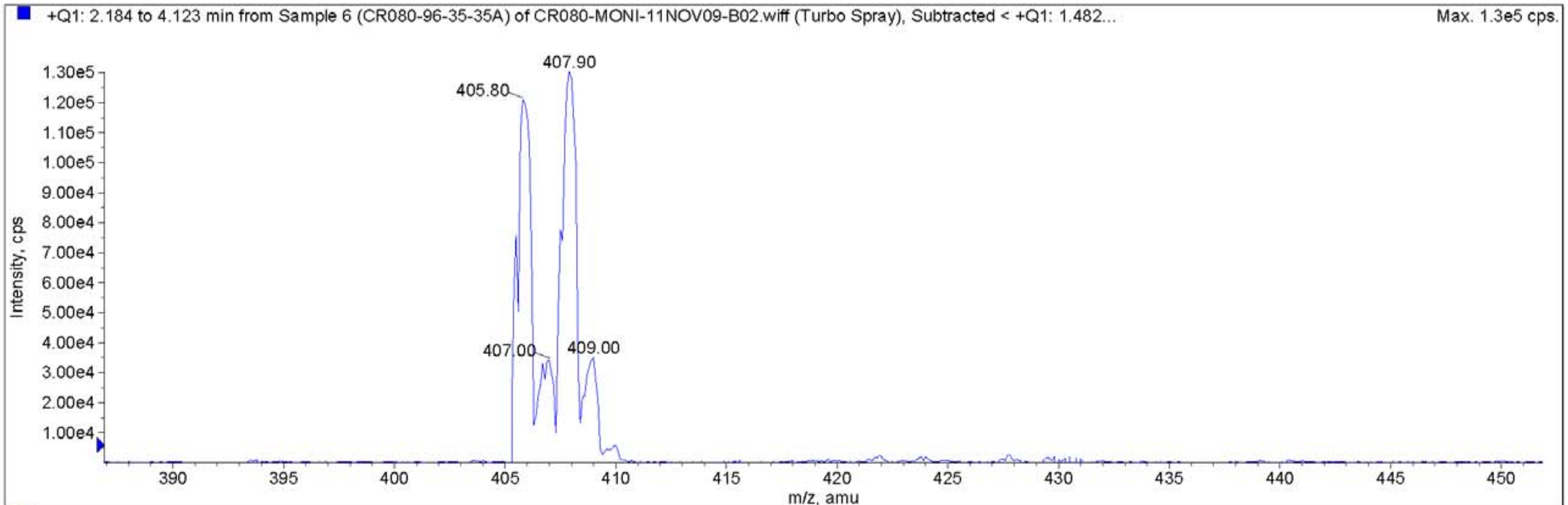

150.0644
145.0508
144.3625
140.7280
134.7154
134.3155
133.3804
132.9009
130.6956
129.3656
124.6839
123.4050
122.2718
119.9369
119.0348
118.6005
29.0772
28.5957
22.4491
13.7709
Ar-C
- CH3CH2-CH2-CH2
CH3-CH2
CH3
ppm
189.1939
77.3248
77.0074
76.6896
40.4426
40.2310
40.0234
39.8130
39.6079
-0.0365
C=O
Br
O
N
19
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

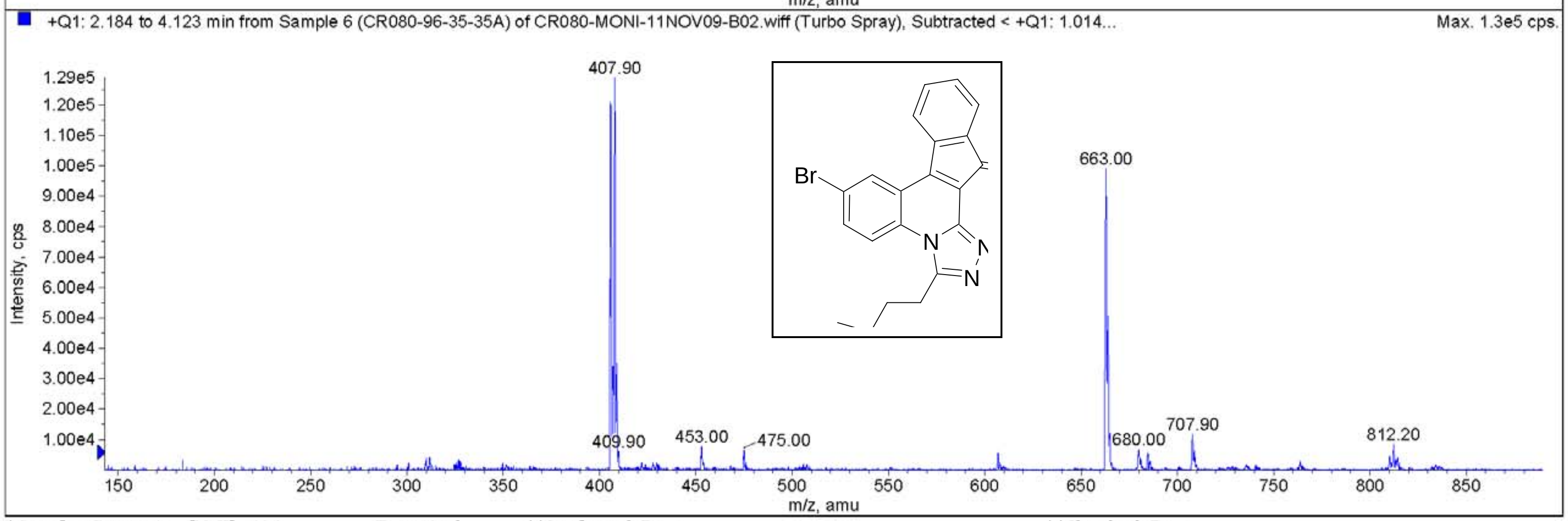

134.7105
134.3133
130.6926
129.3667
124.6831
123.4017
118.6004
29.0830
28.5946
22.4228
13.7739
77.2090
Ar-C
CH3
- CH3CH2-CH2-CH2
CH3-CH2
Br
O
N
19
ppm

*

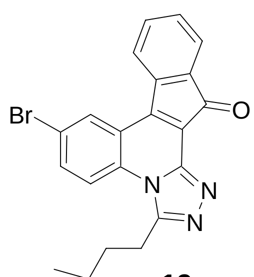
INDIA

Sample Name: CR080-96-35-35A Acq. Time: 15:15 Acq. Date: Wednesday, November 11, 2009



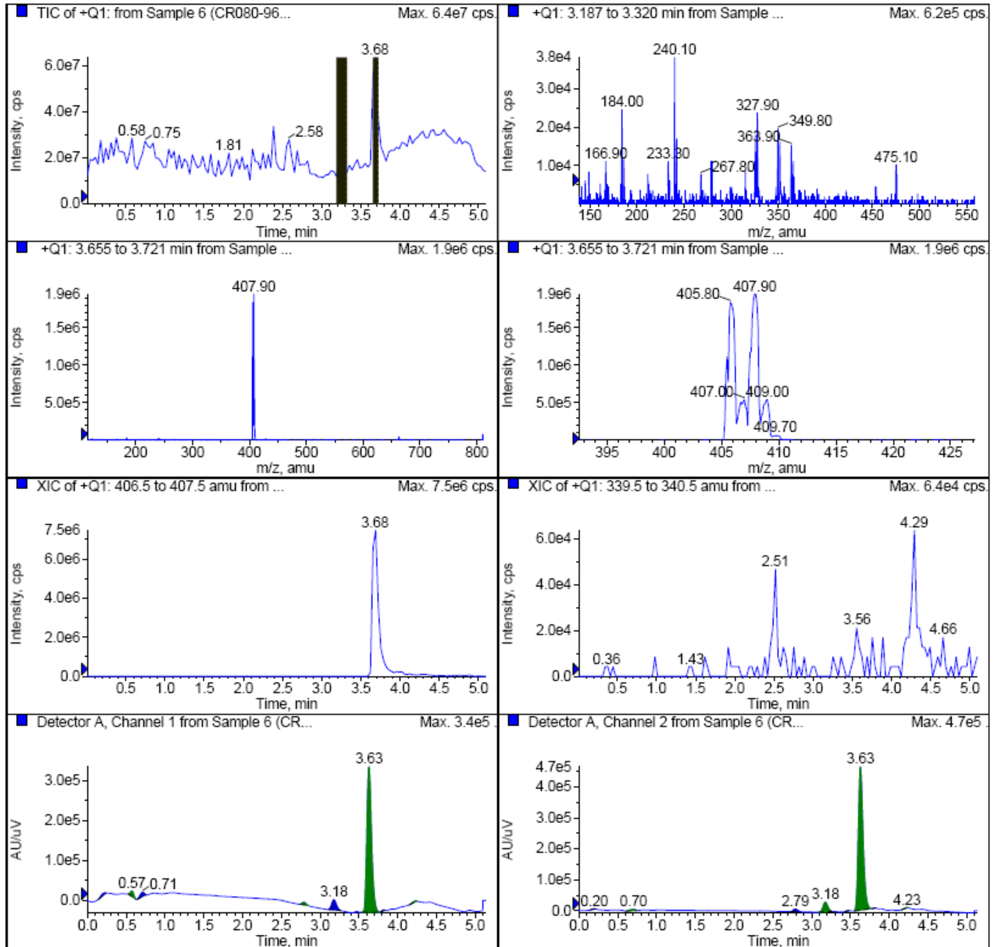


*Sample Comment: [M+H] 406 Expected **Analyzed By : **Checked By :



19

Sample Name: CR080-96-35-35A　　Acq. Time: 15:15　　Acq. Date: Wednesday, November 11, 2009



Peak List for "Detector A, Channel 1 from Sample 6 (CR080-96-35-

	Time (min)	Area (counts)	%Area	Height
4	2.7893	2.0217e4	1.1491	6252.1247
5	3.1773	1.0515e5	5.9768	2.5466e4
6	3.6308	1.5266e6	86.7720	3.6518e5
7	3.8214	3394.3915	0.1929	1486.3814
8	4.2372	8609.3228	0.4894	1730.3281

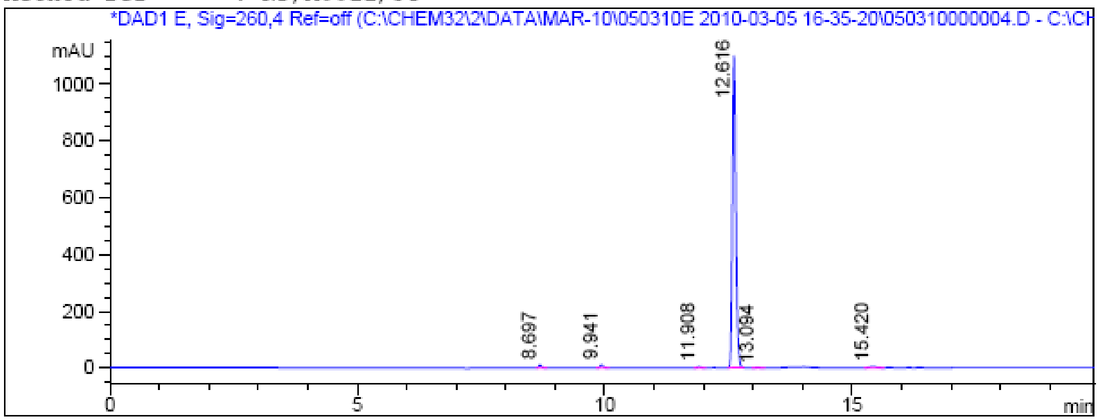
Peak List for "Detector A, Channel 2 from Sample 6 (CR080-96-35-

	Time (min)	Area (counts)	%Area	Height
3	2.7899	2.7466e4	1.2813	8011.5475
4	3.1777	1.2962e5	6.0472	3.0764e4
5	3.4739	2637.0729	0.1230	1032.5532
6	3.6300	1.9525e6	91.0882	4.6398e5
7	3.8166	1573.8917	0.0734	852.1187
8	4.2298	5265.7844	0.2457	1319.6463

LCMS-1 REACN MONT (TFA Buffer)　　Analysed By :

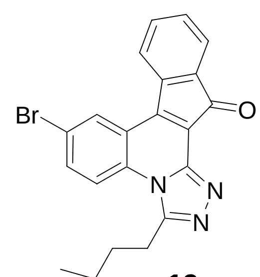
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

```
================================================================================
SAMPLE: CR080-96-35-35 A                                                      ->
Column: GEMINI-C18(250X4.6)mm 5µ
Injection date  : Fri, 5. Mar. 2010             Location   :    Vial 13
Sample Name     : CR080-96-35-35 A              Inj. No.   :          1
Acq Operator    : BHUSHAN                       Inj. Vol.  :      10 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _1.M
Last Changed    : Sun, 7. Mar. 2010,
Acq. Method     : C:\Chem32\2\DATA\MAR-10\050310E 2010-03-05 16-35-20\
                  UPLC_GENARAL_GRAD _1.M
Method ref      : NP/A0011/54
```



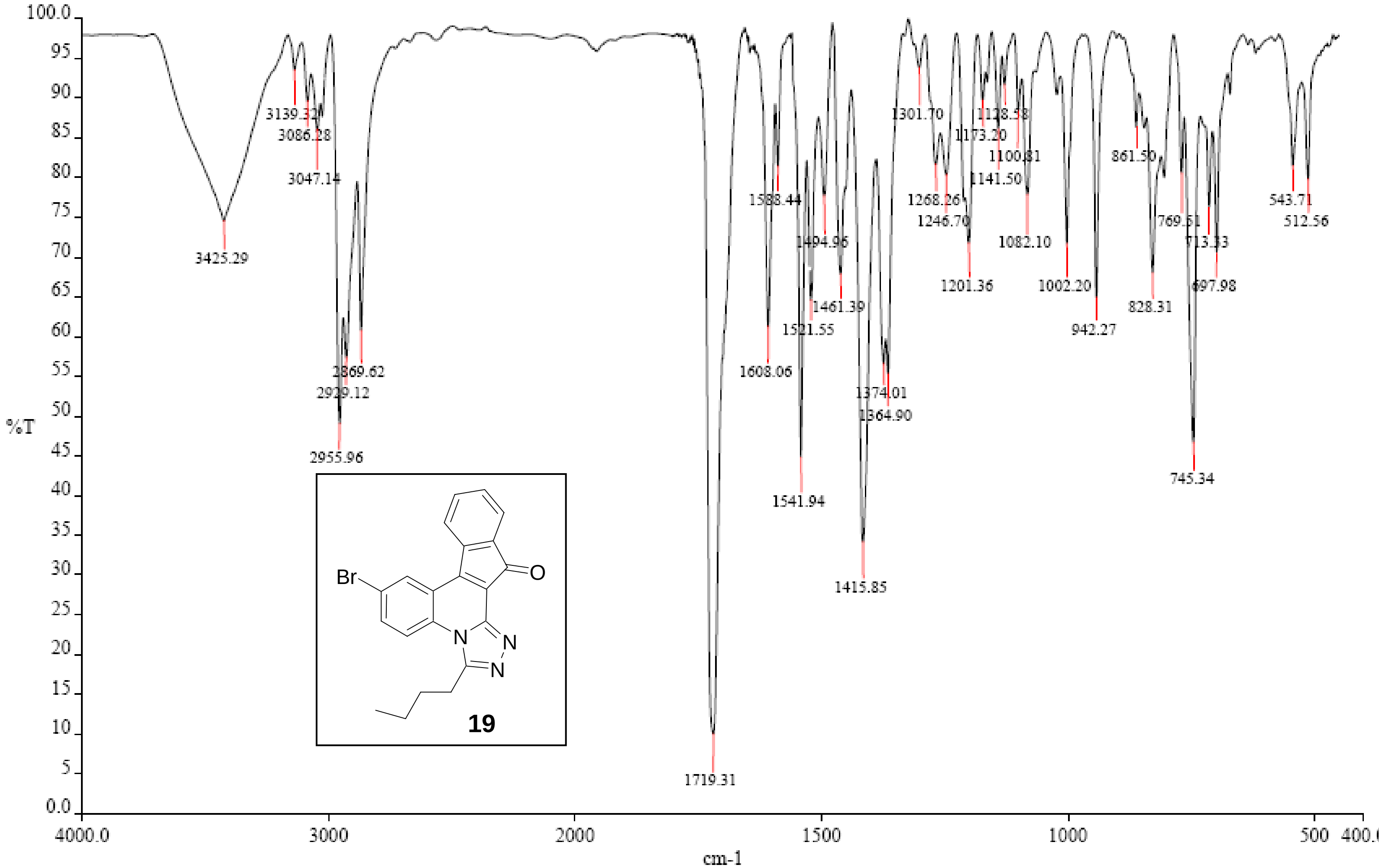
DAD1 E, Sig=260,4 Ref=off

Peak #	RT (Min)	Width (Min)	Area	Area %
1	8.697	0.067	43.694	0.800
2	9.941	0.074	50.746	0.930
3	11.908	0.080	22.490	0.412
4	12.616	0.080	5.289e3	96.888
5	13.094	0.101	9.533	0.175
6	15.420	0.147	43.441	0.796



19

```
================================================================================
*** End of Report***
```



Spectrum Name: CR080-96-35-35A.sp

Analyst: GANESH

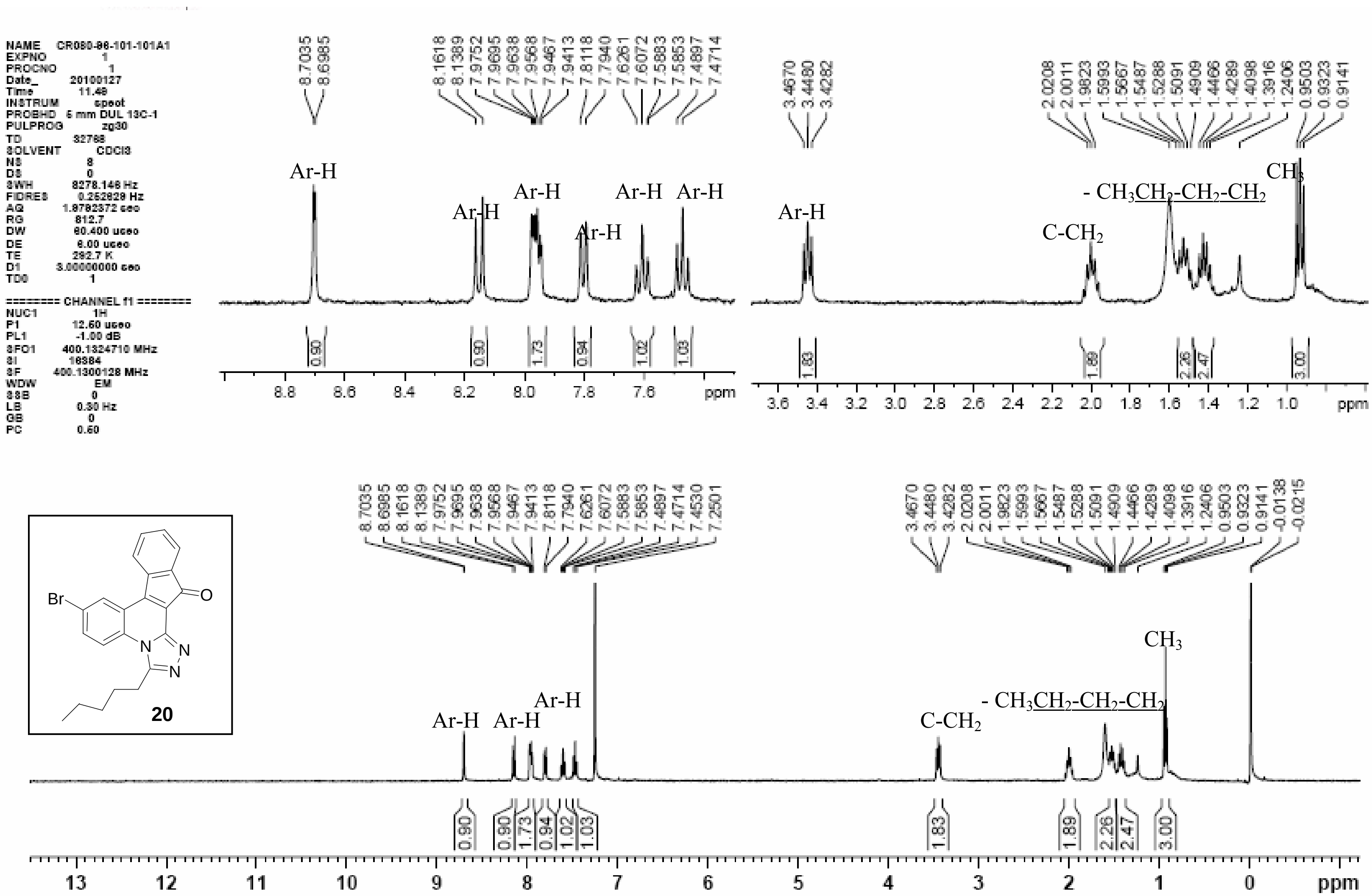
Accumulations: 16

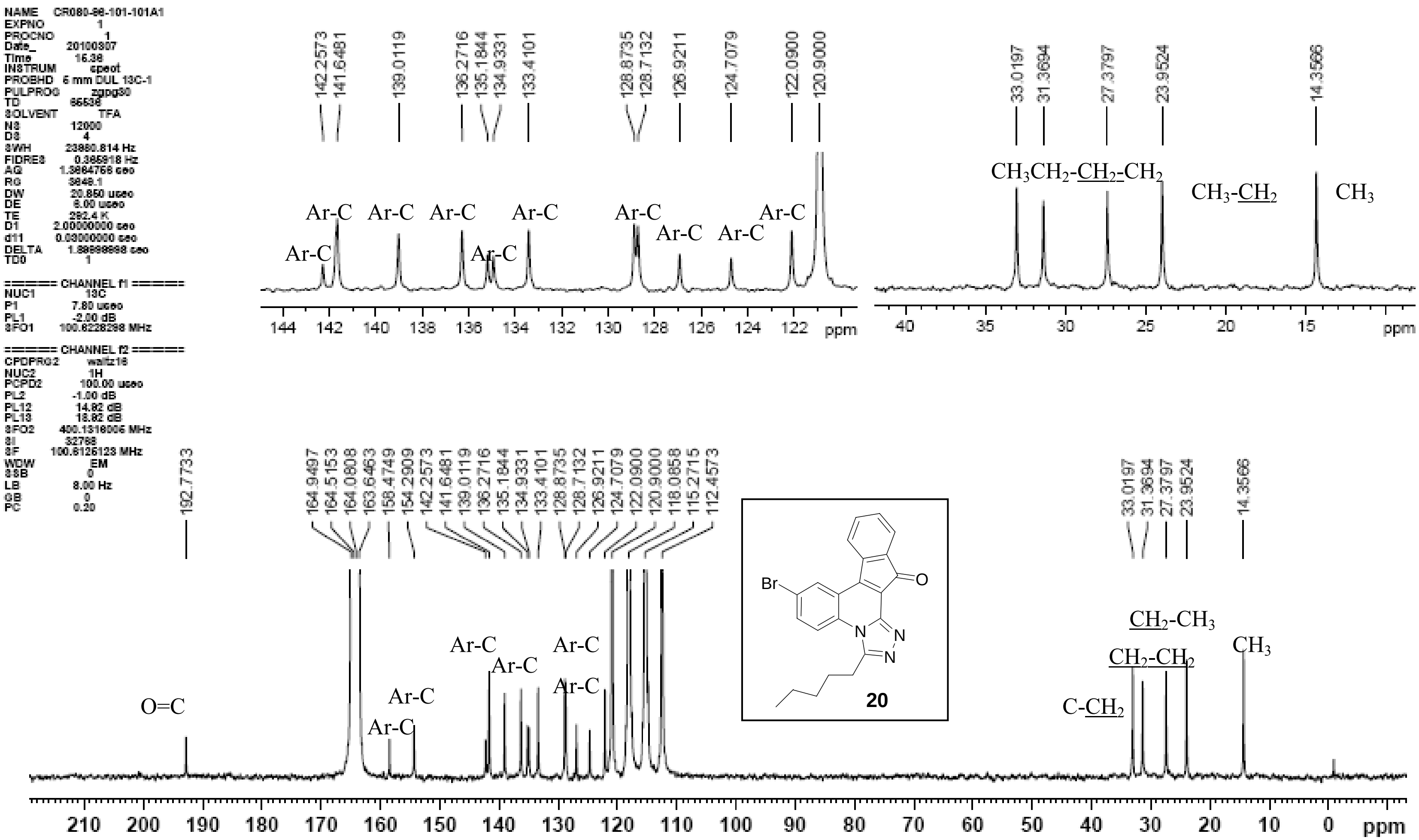
Time: 10:18:07 AM

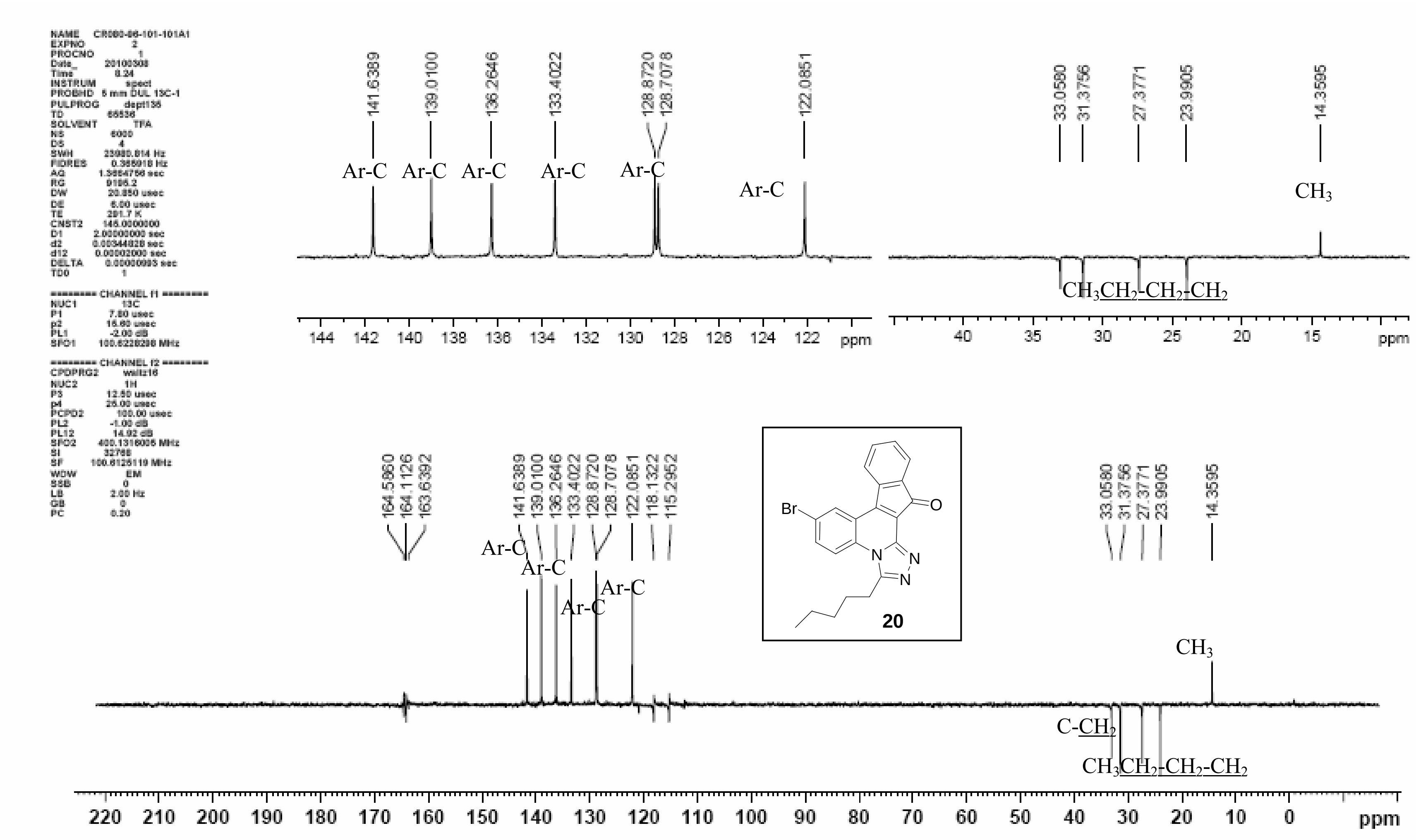
Description: CR080-96-35-35A IN KBr

Resolution: 4.00 cm-1

Date: 2/10/2010


NAME CR080-96-101-101A1
EXPNO 1
PROCNO 1
Date_ 20100127
Time 11.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.252628 Hz
AQ 1.9792372 sec
RG 812.7
DW 60.400 usec
DE 6.00 usec
TE 292.7 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
C-CH2
- CH3CH2-CH2-CH2
CH3
CH3
Br
O
N
N
N
20
ppm

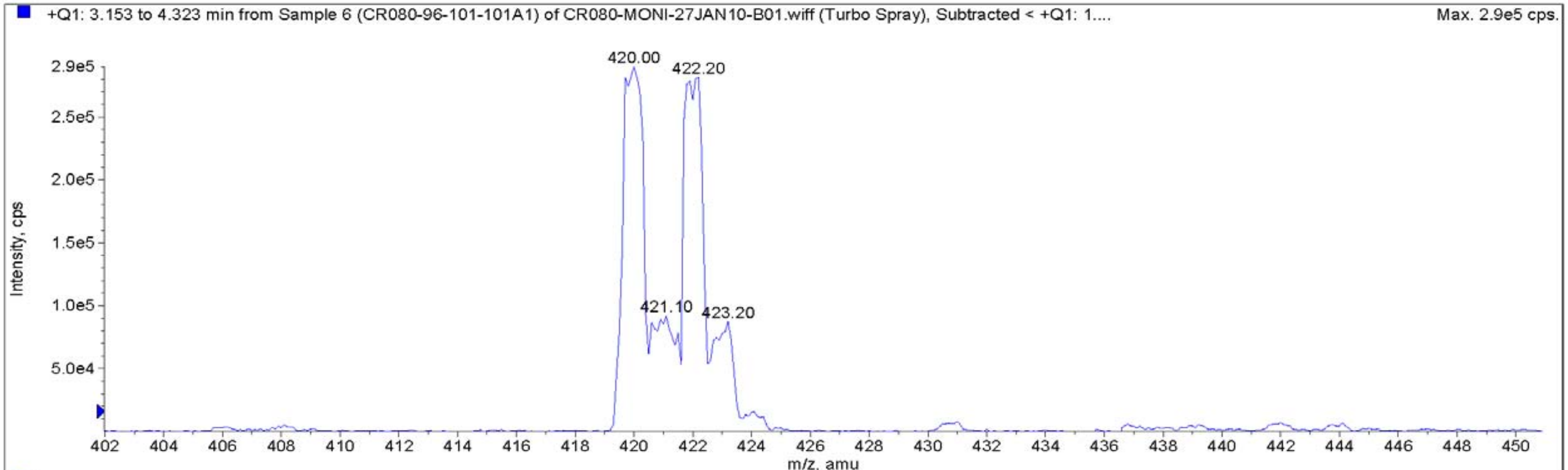

NAME CR080-98-101-101A1
EXPNO 1
PROCNO 1
Date_ 20100307
SOLVENT TFA
NS 12000
CHANNEL f1
NUC1 13C
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
SFO2 400.1316006 MHz
142.2573 141.6481 139.0119 136.2716 135.1844 134.9331 133.4101 128.8735 128.7132 126.9211 124.7079 122.0900 120.9000
Ar-C
33.0197 31.3694 27.3797 23.9524 14.3566
CH3CH2-CH2-CH2
CH3-CH2
CH3
192.7733
164.9497 164.5153 164.0808 163.6463 158.4749 154.2909 142.2573 141.6481 139.0119 136.2716 135.1844 134.9331 133.4101 128.8735 128.7132 126.9211 124.7079 122.0900 120.9000 118.0858 115.2715 112.4573
O=C
C-CH2
CH2-CH2
CH2-CH3
Br
O
N
20
ppm

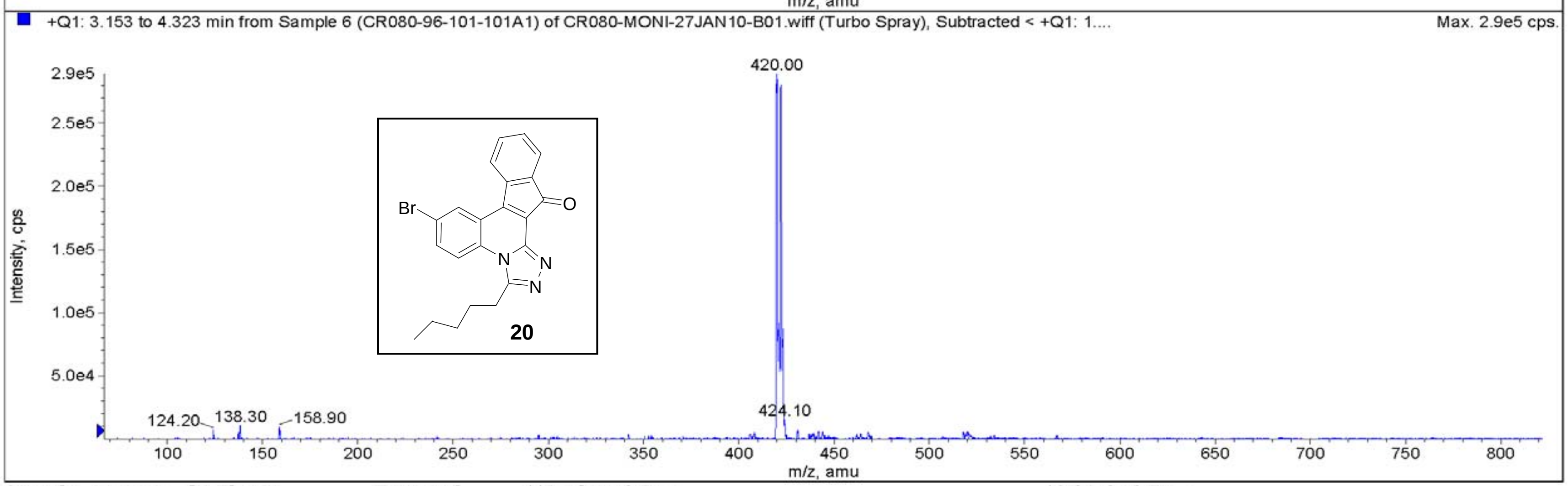


*

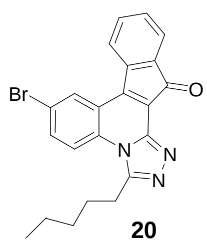
INDIA

Sample Name: CR080-96-101-101A1 Acq. Time: 13:11 Acq. Date: Wednesday, January 27, 2010



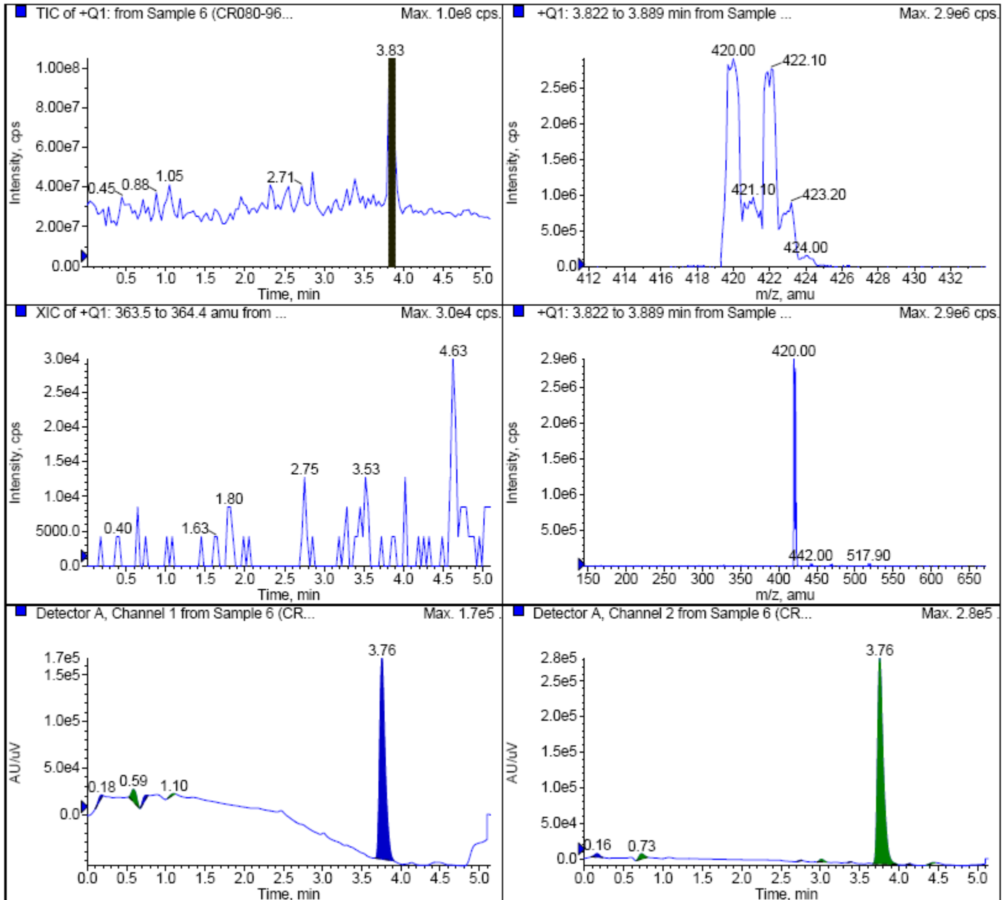


*Sample Comment: [M+H] 420 Expected **Analyzed By : **Checked By :



20

Sample Name: CR080-96-101-101A1 Acq. Time: 13:11 Acq. Date: Wednesday, January 27, 2010



Peak List for "Detector A, Channel 1 from Sample 6 (CR080-96-101

	Time (min)	Area (counts)	%Area	Height
1	0.1825	1.2445e4	1.1092	2507.9324
2	0.5874	6.0706e4	5.4106	1.3183e4
3	0.7542	1.7437e4	1.5542	2927.9639
4	1.1028	5925.4056	0.5281	1086.4141
5	3.7581	1.0255e6	91.3979	2.1588e5

Peak List for "Detector A, Channel 2 from Sample 6 (CR080-96-101

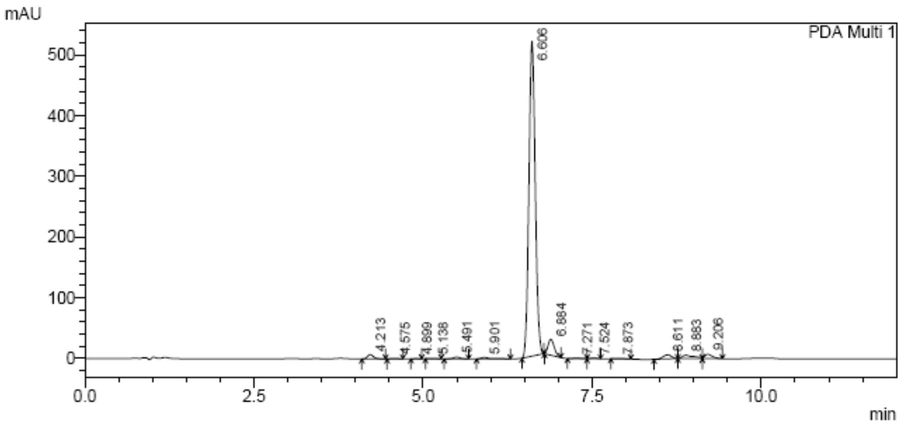
	Time (min)	Area (counts)	%Area	Height
1	0.1605	2.1085e4	1.4096	4879.6883
2	0.7280	3.2566e4	2.1772	7316.2624
3	2.7534	1275.4333	0.0853	509.3171
4	3.0142	1.3621e4	0.9107	3898.6749
5	3.3877	946.8859	0.0633	475.4406
6	3.7566	1.4214e6	95.0252	2.8874e5
7	4.1375	1089.5715	0.0728	461.2059
8	4.4458	3827.4378	0.2559	643.6293

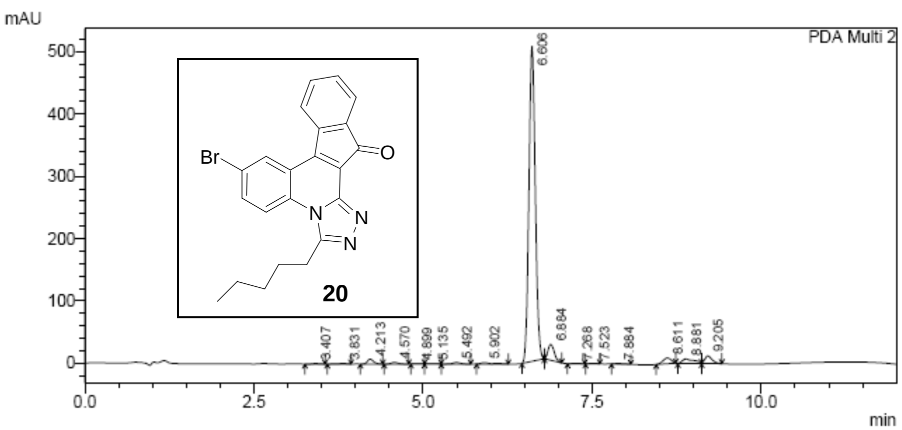
LCMS-1 REACN MONT (TFA Buffer) Analysed By :

Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

Sample Name : CR080-96-101-101A1
Sample ID : CR080-96-101-101A1
Column : Gemini C-18 (50 x 4.6 mm) 5u
Vial # : 47
Inj. Volume : 8 uL
Tray # : 2
Acquired by : AVINASH

Data File Name : 05031019.lcd
Method File Name : GENERAL-A.lcm
Batch File Name : 050310.lcb
Data Acquired : 3/5/2010 3:59:20 PM
Data Processed : 3/5/2010 4:11:24 PM
Ref.No.:NP/A0011/52





1 PDA Multi 1/263nm 4nm
2 PDA Multi 2/244nm 4nm

PeakTable

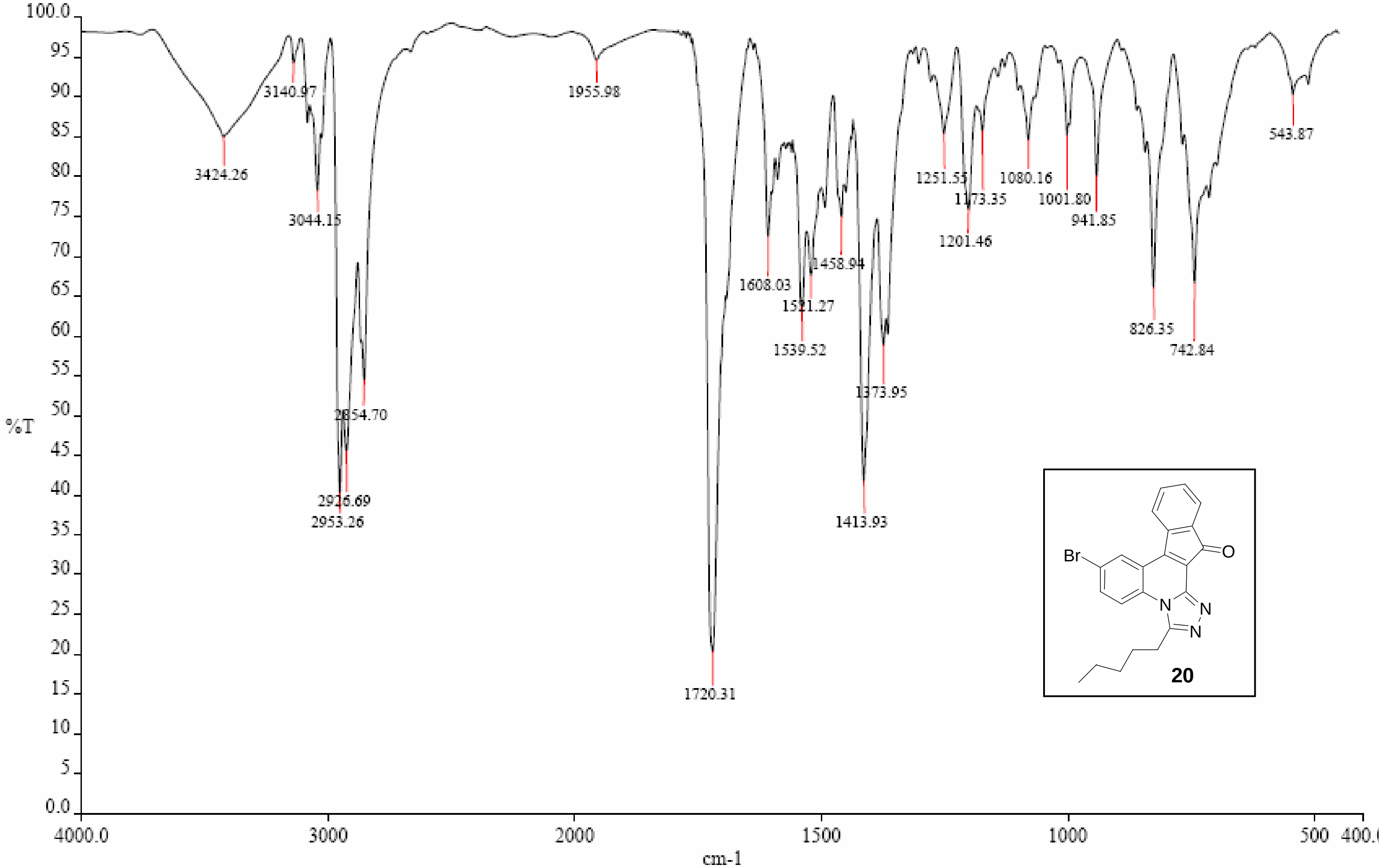
PDA Ch1 263nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	4.21	45077	1.17	7223
2	4.57	5288	0.14	779
3	4.90	1369	0.04	246
4	5.14	5182	0.13	833
5	5.49	20524	0.53	2897
6	5.90	21766	0.57	2319
7	6.61	3377885	87.96	519168
8	6.88	165707	4.31	26200
9	7.27	4079	0.11	623
10	7.52	5512	0.14	937
11	7.87	6584	0.17	604
12	8.61	56892	1.48	6625
13	8.88	69056	1.80	5559
14	9.21	55366	1.44	7054
Total		3840286	100.00	581066

PeakTable

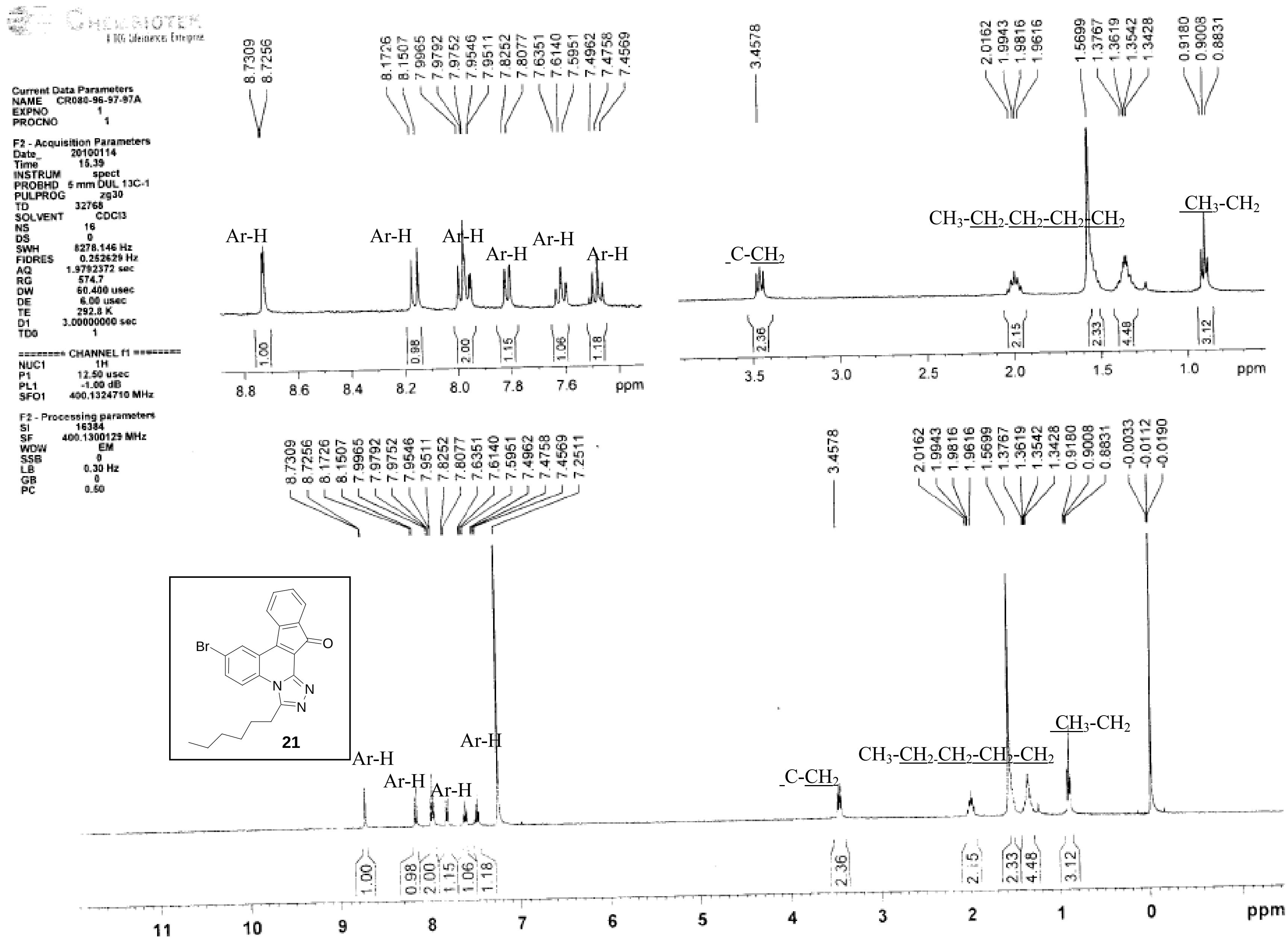
PDA Ch2 244nm 4nm

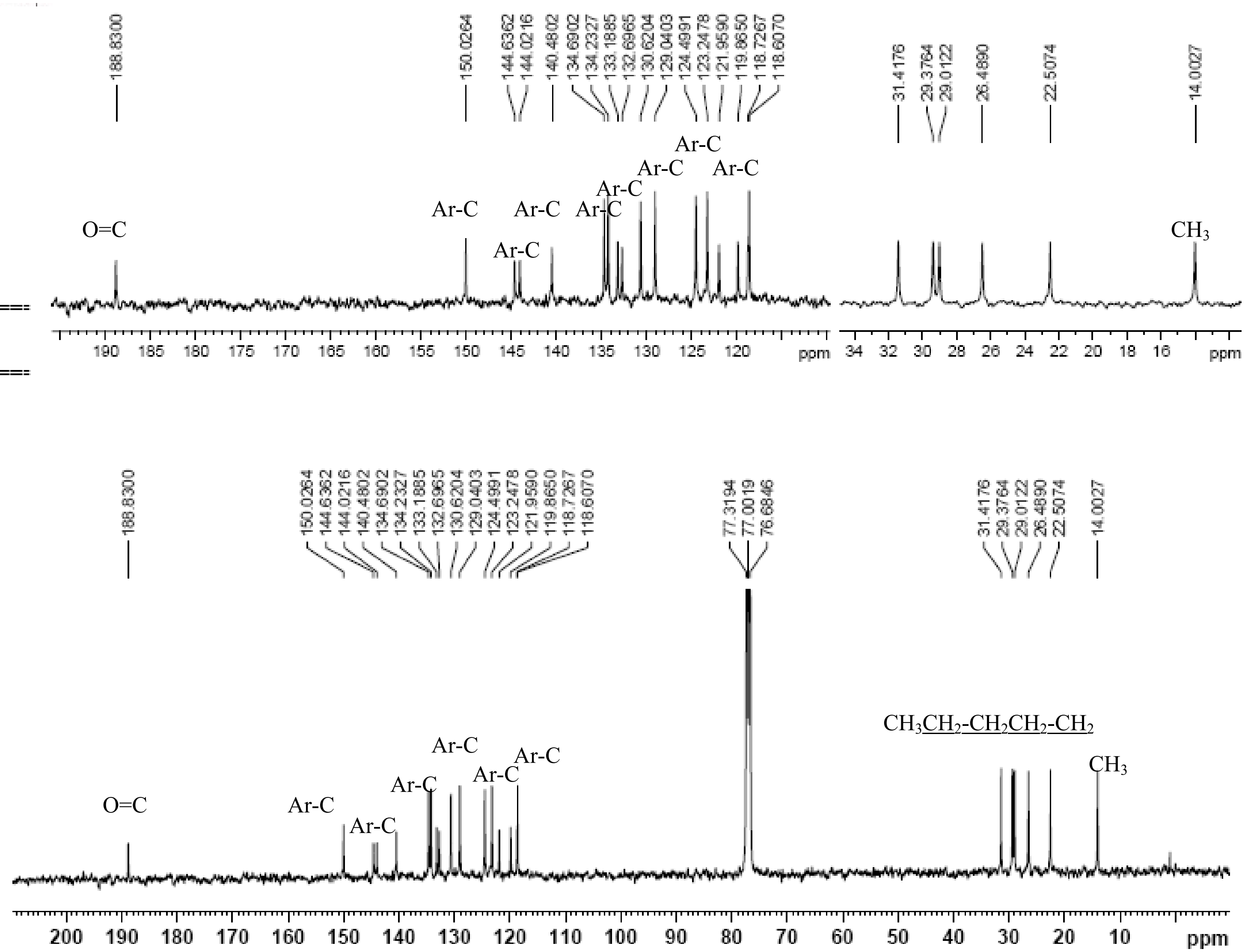
Peak#	Ret. Time	Area	Area %	Height
1	3.41	5474	0.14	968
2	3.83	7299	0.19	715
3	4.21	48642	1.25	7842
4	4.57	17775	0.46	2652
5	4.90	1554	0.04	306
6	5.13	4286	0.11	726
7	5.49	19027	0.49	2623
8	5.90	24325	0.63	2313
9	6.61	3308844	85.22	506293
10	6.88	161467	4.16	25504
11	7.27	4317	0.11	664
12	7.52	5705	0.15	973
13	7.88	8033	0.21	859
14	8.61	77998	2.01	9379
15	8.88	93792	2.42	7424
16	9.21	94113	2.42	12453
Total		3882650	100.00	581695



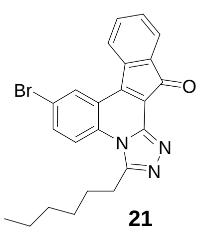
Spectrum Name: CR080-96-101-101A1.sp | Analyst: GANESH | Accumulations: 16 | Time: 10:02:49 AM

Description: CR080-96-101-101A1 IN KBr | Resolution: 4.00 cm-1 | Date: 2/10/2010

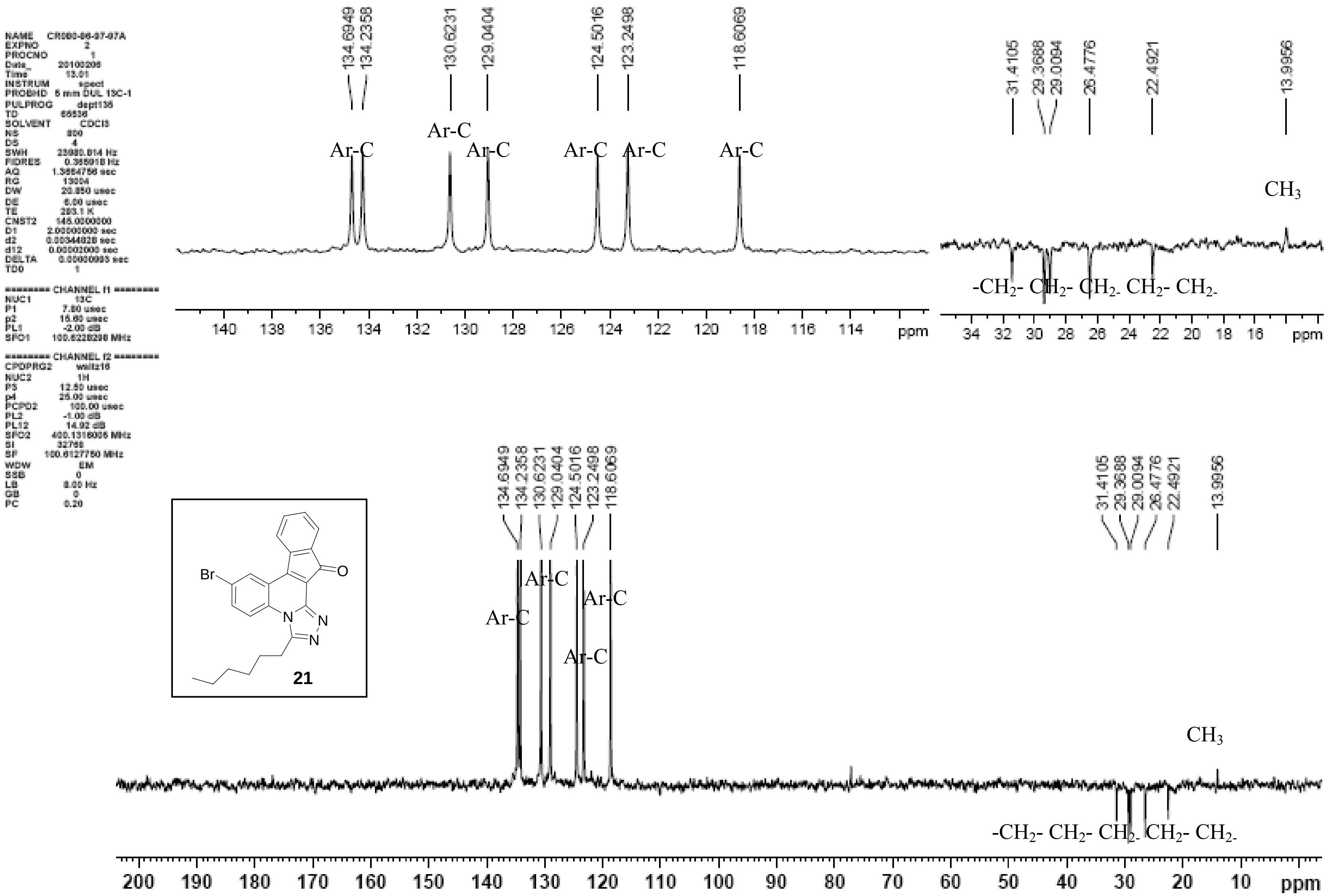

Current Data Parameters
NAME CR080-96-97-97A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100114
Time 15.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 292.8 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
Ar-H
C-CH2
CH3-CH2-CH2-CH2-CH2
CH3-CH2
Br
O
N
21
ppm



NAME CR080-96-97-97A
EXPNO 1
PROCNO 1
Date_ 20100208
Time 12.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 10321.3
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
====== CHANNEL f1 ======
NUC1 13C
P1 7.80 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
====== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.82 dB
PL13 18.82 dB
SFO2 400.1316006 MHz
SI 32768
SF 100.6127749 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 0.20
188.8300
150.0264
144.6362
144.0216
140.4802
134.6902
134.2327
133.1885
132.6965
130.6204
129.0403
124.4991
123.2478
121.9590
119.8650
118.7267
118.6070
77.3194
77.0019
76.6846
31.4176
29.3764
29.0122
26.4890
22.5074
14.0027
O=C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
CH_3
CH_3CH_2-CH_2CH_2-CH_2
ppm



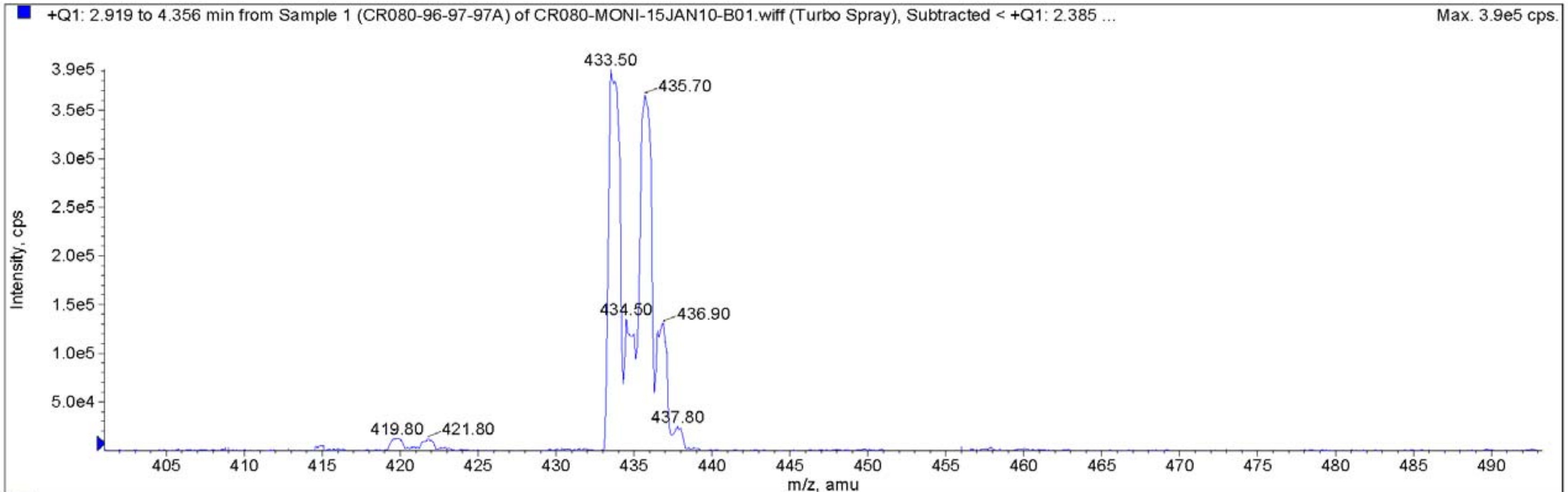
21

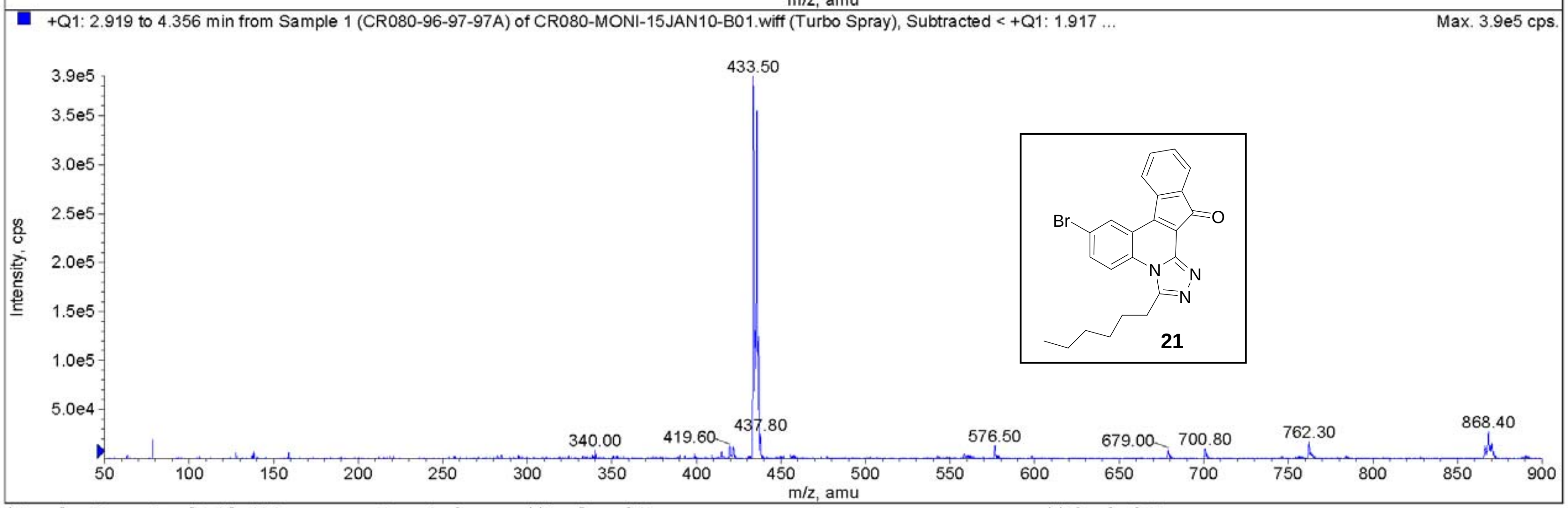

NAME CR080-06-07-07A
EXPNO 2
PROCNO 1
Date_ 20100206
Time 13.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 13004
DW 20.850 usec
DE 6.00 usec
TE 293.1 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000093 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
p2 15.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 12.50 usec
p4 25.00 usec
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.92 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127750 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 0.20
134.6949
134.2358
130.6231
129.0404
124.5016
123.2498
118.6069
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
140 138 136 134 132 130 128 126 124 122 120 118 116 114 ppm
31.4105
29.3688
29.0094
26.4776
22.4921
13.9956
CH$_3$
-CH$_2$- CH$_2$- CH$_2$- CH$_2$- CH$_2$-
34 32 30 28 26 24 22 20 18 16 ppm
Br
O
N
N
N
21
134.6949
134.2358
130.6231
129.0404
124.5016
123.2498
118.6069
31.4105
29.3688
29.0094
26.4776
22.4921
13.9956
Ar-C
Ar-C
Ar-C
Ar-C
CH$_3$
-CH$_2$- CH$_2$- CH$_2$- CH$_2$- CH$_2$-
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

*

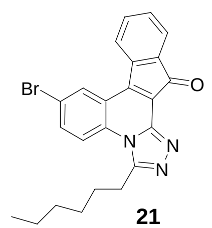
INDIA

Sample Name: CR080-96-97-97A Acq. Time: 10:00 Acq. Date: Friday, January 15, 2010



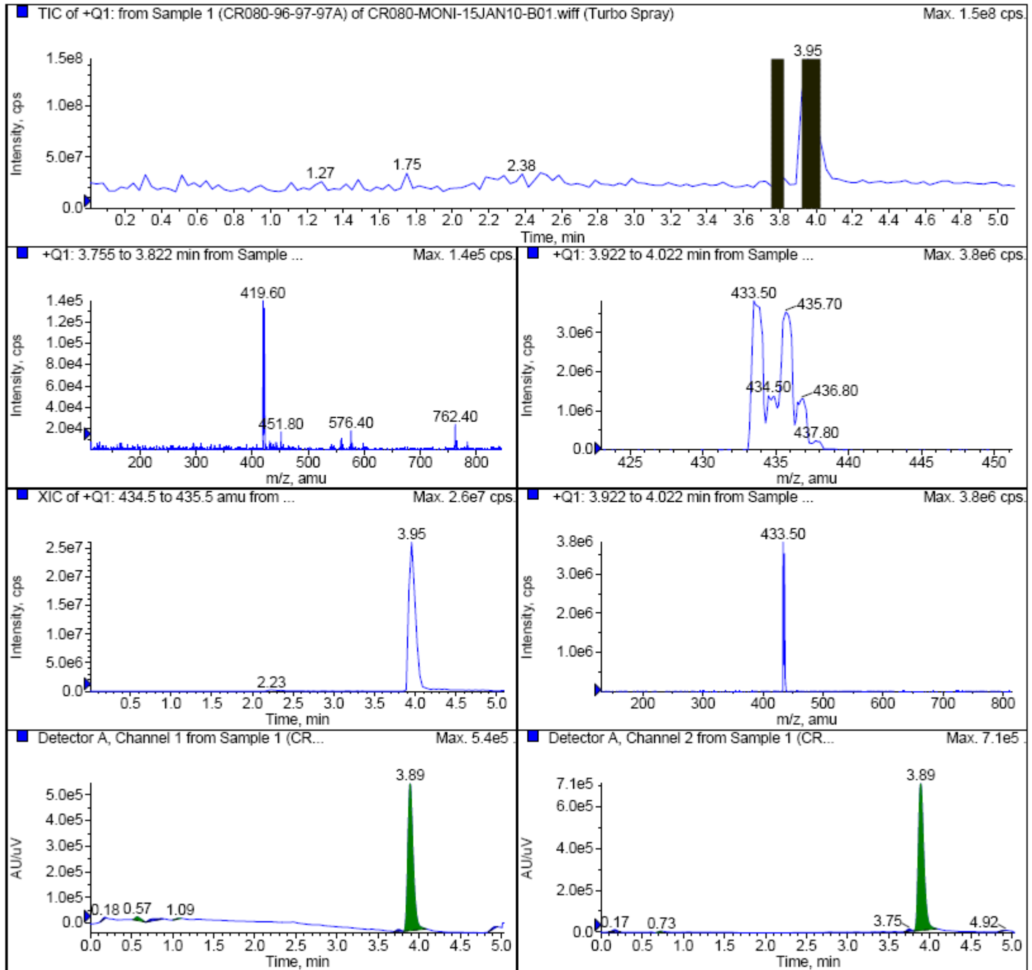


*Sample Comment: [M+H] 434 Expected **Analyzed By : **Checked By :



21

Sample Name: CR080-96-97-97A Acq. Time: 10:00 Acq. Date: Friday, January 15, 2010



Peak List for "Detector A, Channel 1 from Sample 1 (CR080-96-97-

	Time (min)	Area (counts)	%Area	Height
1	0.1768	1.0174e4	0.3769	2917.6786
2	0.5689	6.1903e4	2.2935	1.3867e4
3	0.8642	5.1125e4	1.8942	1514.3005
4	1.0890	6723.4059	0.2491	1296.9450
5	3.7519	2.4455e4	0.9061	7168.7077
6	3.8915	2.5243e6	93.5257	5.7261e5
7	4.9390	2.0363e4	0.7544	2855.1379

Peak List for "Detector A, Channel 2 from Sample 1 (CR080-96-97-

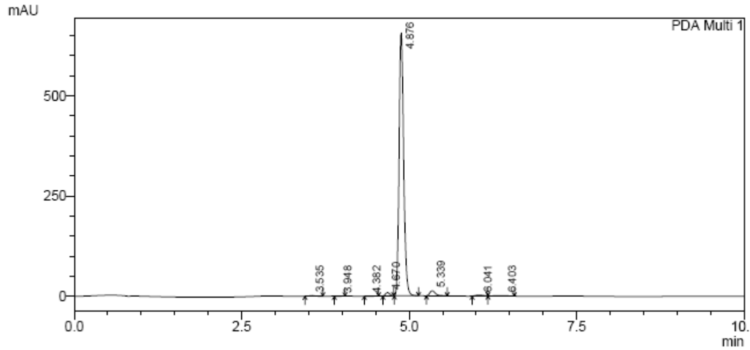
	Time (min)	Area (counts)	%Area	Height
1	0.1658	3.7296e4	1.1489	9617.5762
2	0.7338	5820.7035	0.1793	1490.6523
3	3.7501	3.6354e4	1.1199	1.0238e4
4	3.8912	3.1613e6	97.3846	6.9874e5
5	4.9226	5429.6115	0.1673	1168.5468

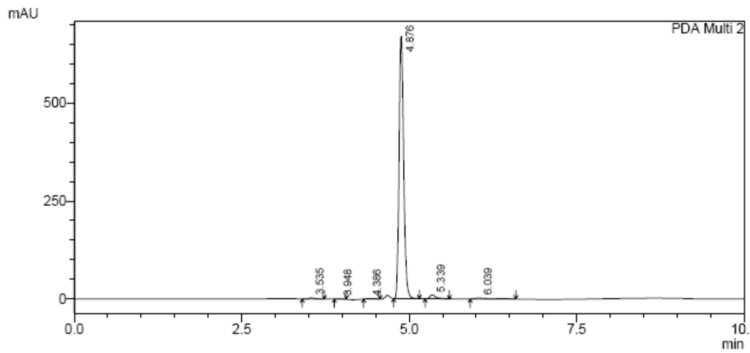
LCMS-1 REACN MONT (TFA Buffer) Analysed By :

Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

Sample Name : CR080-96-97-97A
Sample ID : CR080-96-97-97A
Column : Gemini C-18 (50 x 4.6 mm) 5u
Vial # : 49
Inj. Volume : 2 uL
Tray # : 2
Acquired by : AVINASH

Data File Name : 05031016.lcd
Method File Name : GENERAL.lcm
Batch File Name : 050310.lcb
Data Acquired : 3/5/2010 3:32:40 PM
Data Processed : 3/5/2010 3:45:28 PM
Ref.No.:NP/A0011/51





1 PDA Multi 1/244nm 4nm
2 PDA Multi 2/264nm 4nm

PeakTable

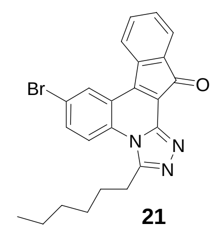
PDA Ch1 244nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	3.54	6772	0.21	1513
2	3.95	1437	0.04	333
3	4.38	1527	0.05	235
4	4.67	37319	1.14	8574
5	4.88	3125584	95.32	655590
6	5.34	78146	2.38	12929
7	6.04	15889	0.48	2235
8	6.40	12322	0.38	1097
Total		3278996	100.00	682505

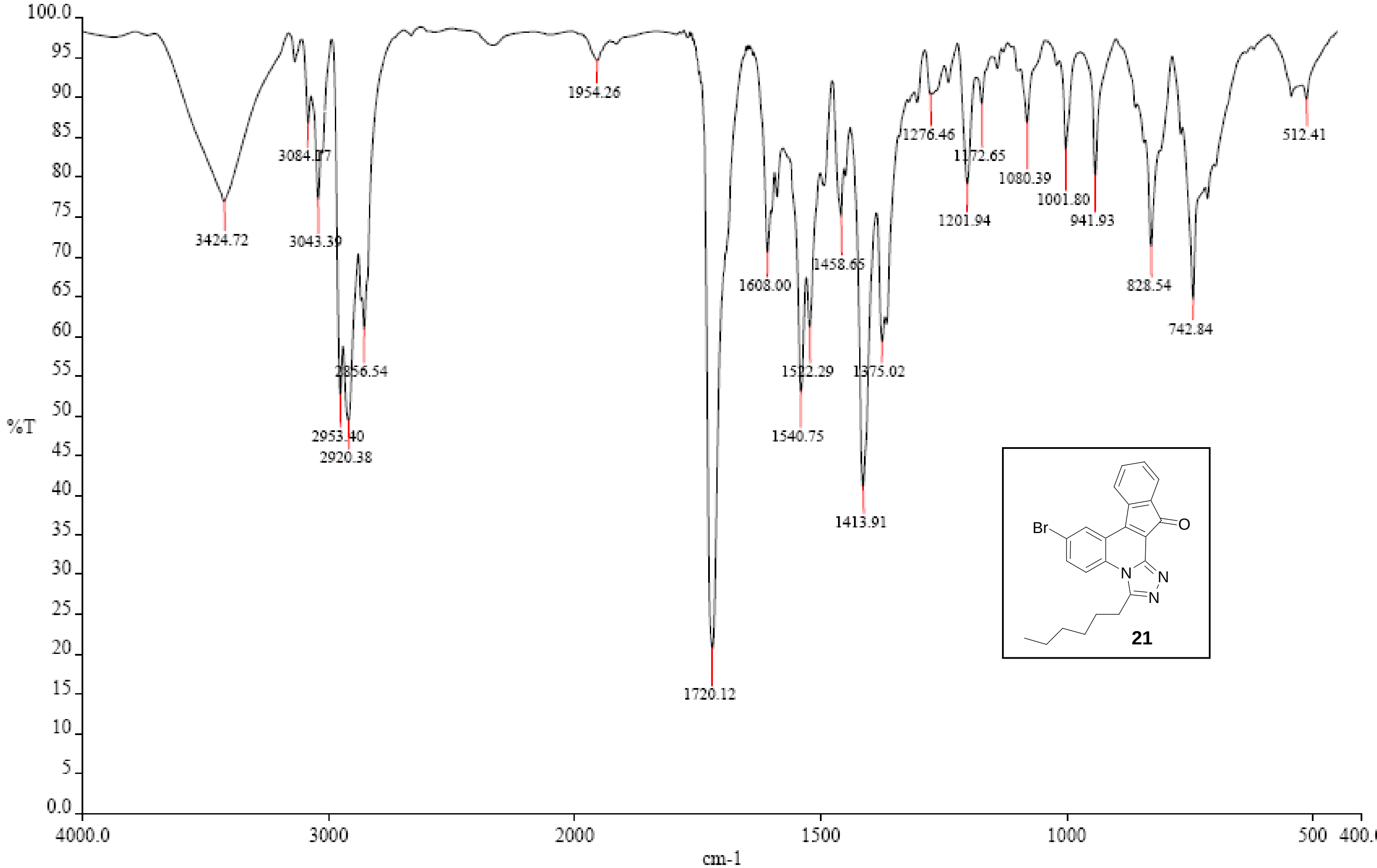
PeakTable

PDA Ch2 264nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	3.54	12391	0.37	2841
2	3.95	1352	0.04	301
3	4.39	1919	0.06	262
4	4.88	3199471	96.64	670681
5	5.34	61963	1.87	9787
6	6.04	33620	1.02	2057
Total		3310716	100.00	685929

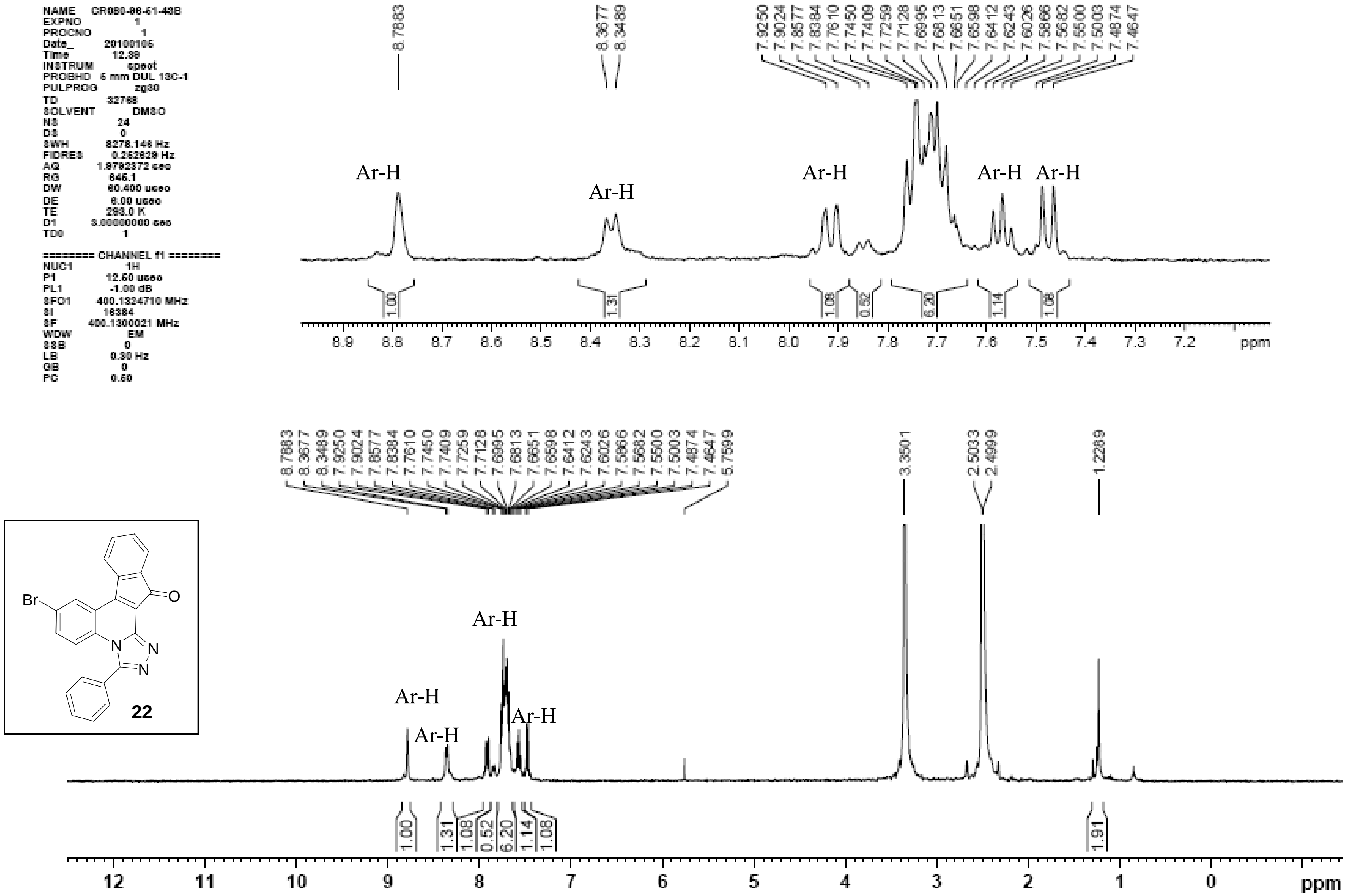


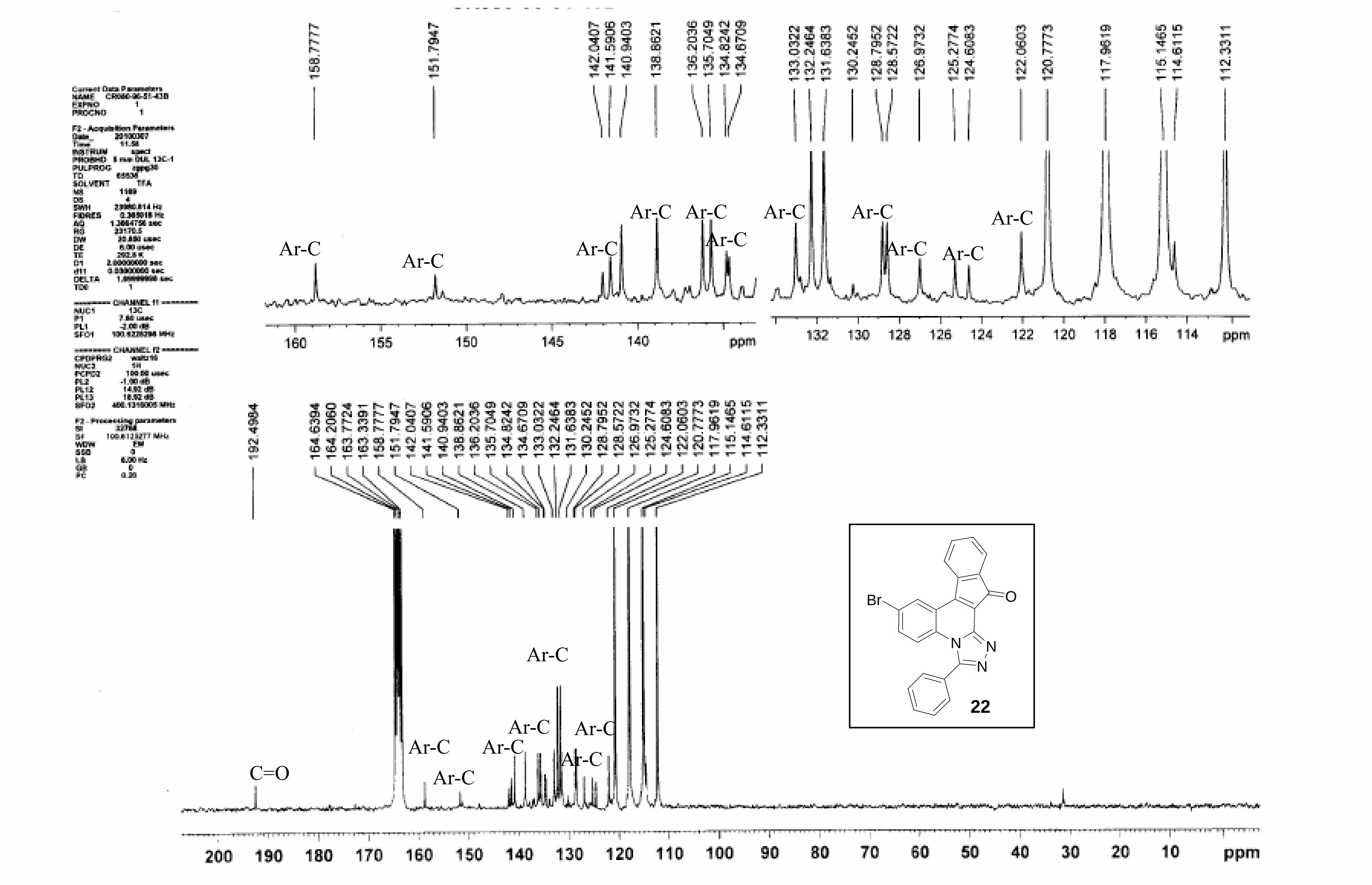
21



Spectrum Name: CR080-96-97-97A.sp　Analyst: GANESH　Accumulations: 16　Time: 12:19:02 PM

Description: CR080-96-97-97A IN KBr　Resolution: 4.00 cm-1　Date: 2/10/2010

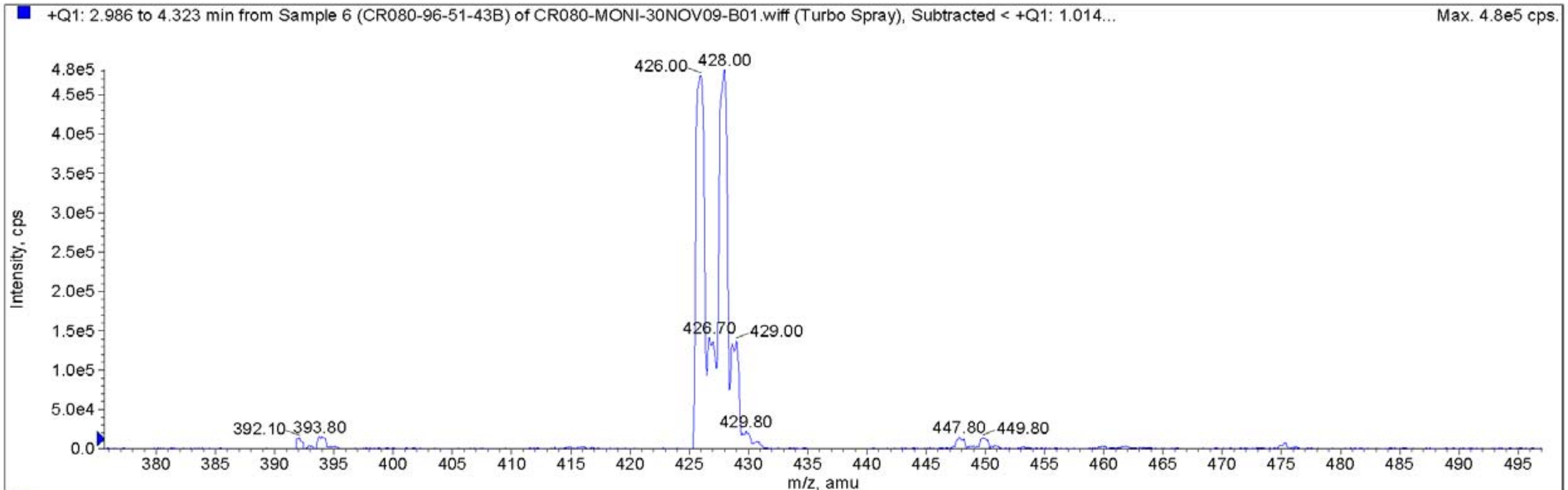

NAME CR080-86-61-43B
EXPNO 1
PROCNO 1
Date_ 20100106
Time 12.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 24
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 645.1
DW 60.400 usec
DE 6.00 usec
TE 293.0 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60
Ar-H
Br
O
N
22
ppm

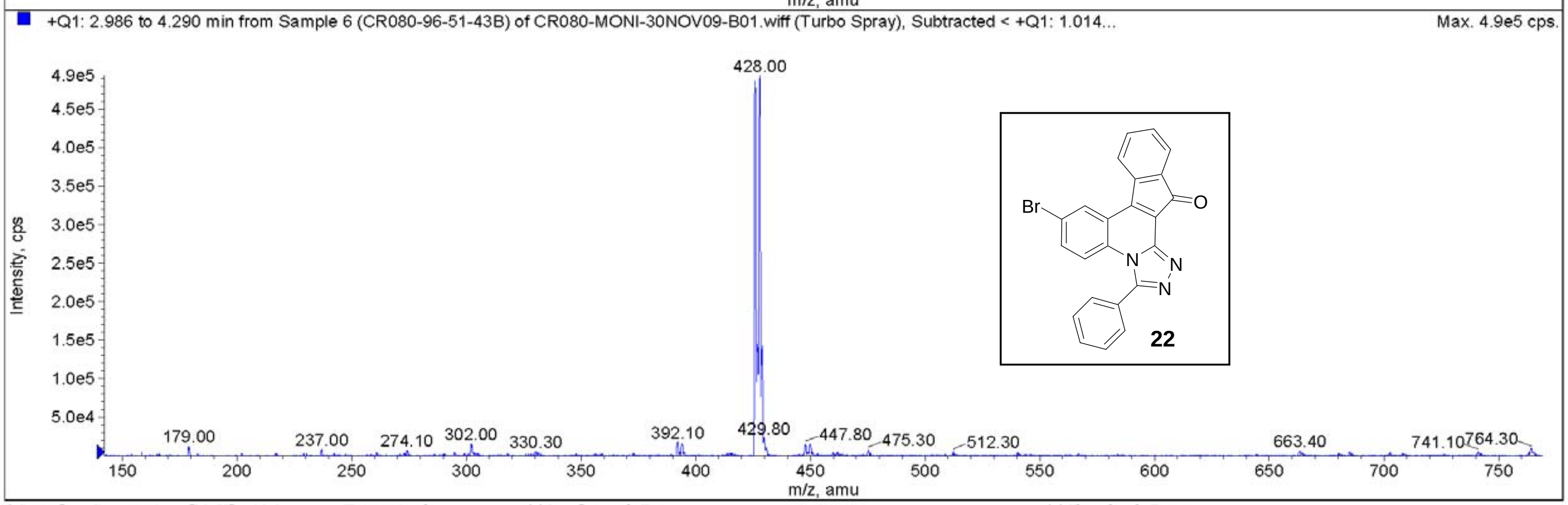

Ar-C
C=O
Br
O
N
N
N
22

*

INDIA

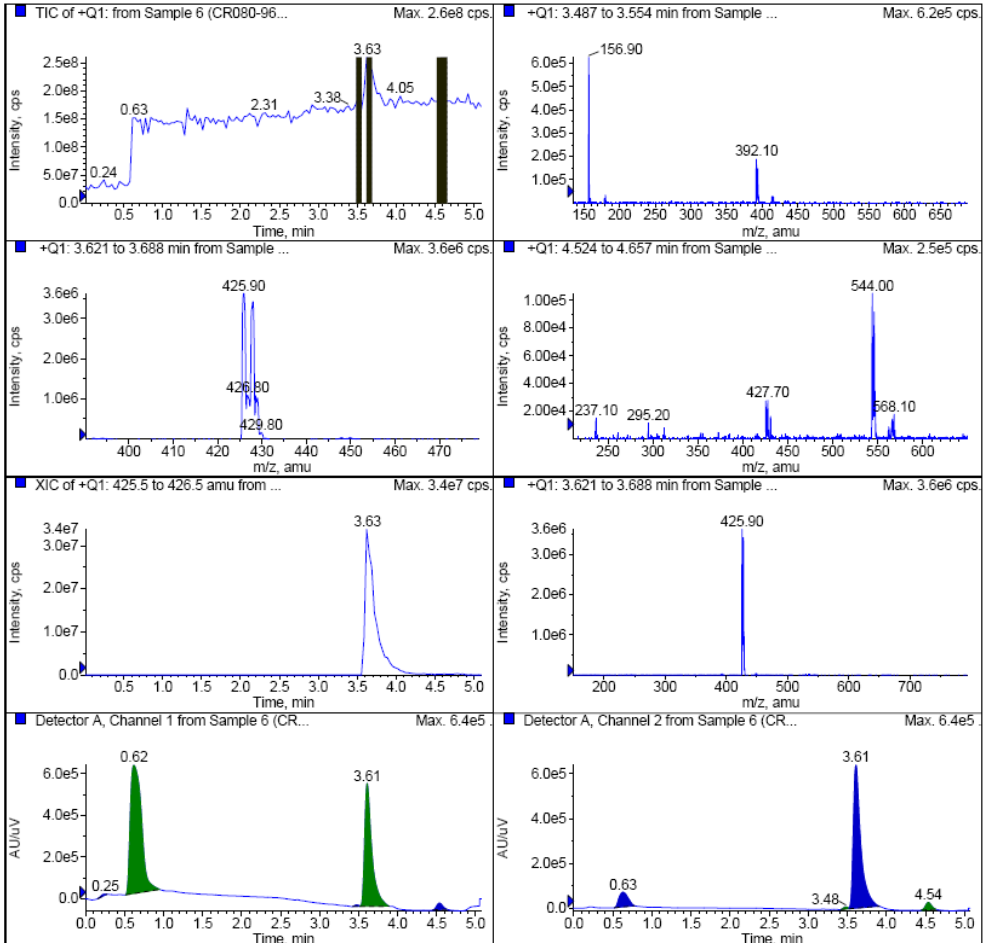
Sample Name: CR080-96-51-43B Acq. Time: 10:31 Acq. Date: Monday, November 30, 2009





*Sample Comment: [M+H] 426 Expected **Analyzed By : **Checked By :

Sample Name: CR080-96-51-43B   Acq. Time: 10:31   Acq. Date: Monday, November 30, 2009



Peak List for "Detector A, Channel 1 from Sample 6 (CR080-96-51-

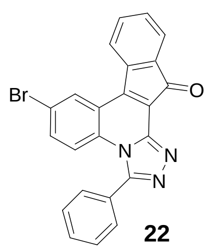
	Time (min)	Area (counts)	% Area	Height
2	0.6173	6.0369e6	60.4763	6.1442e5
3	3.4743	2.4657e4	0.2470	7075.7050
4	3.6091	3.7350e6	37.4161	5.8903e5
5	4.5360	1.5732e5	1.5760	3.0972e4

Peak List for "Detector A, Channel 2 from Sample 6 (CR080-96-51-4

	Time (min)	Area (counts)	% Area	Height
2	3.4795	3.7941e4	0.7760	9893.1836
3	3.6097	4.1709e6	85.3086	6.3796e5
4	4.5364	1.6538e5	3.3826	3.2105e4

LCMS-1 REACN MONT (TFA Buffer)   Analysed By :

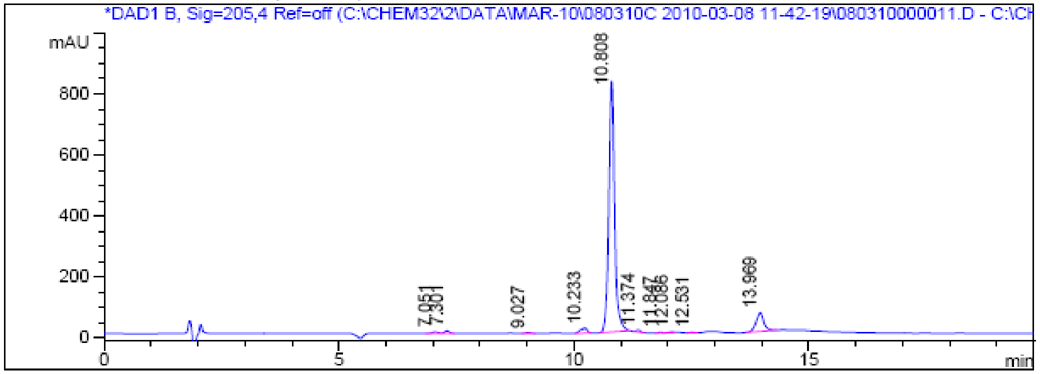
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm



22

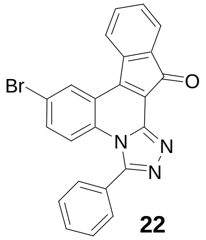
==
SAMPLE: CR080-96-51-43 B ->
Column: **GEMINI**-C18(150X4.6)mm 5µ

Injection date : Mon, 8. Mar. 2010 Location : Vial 16
Sample Name : CR080-96-51-43 B Inj. No. : 1
Acq Operator : GANESH Z Inj. Vol. : 10 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _33.M
Last Changed : Mon, 8. Mar. 2010,
Acq. Method : C:\Chem32\2\DATA\MAR-10\080310C 2010-03-08 11-42-19\
UPLC_GENARAL_GRAD _33.M
Method ref : NP/A0011/57



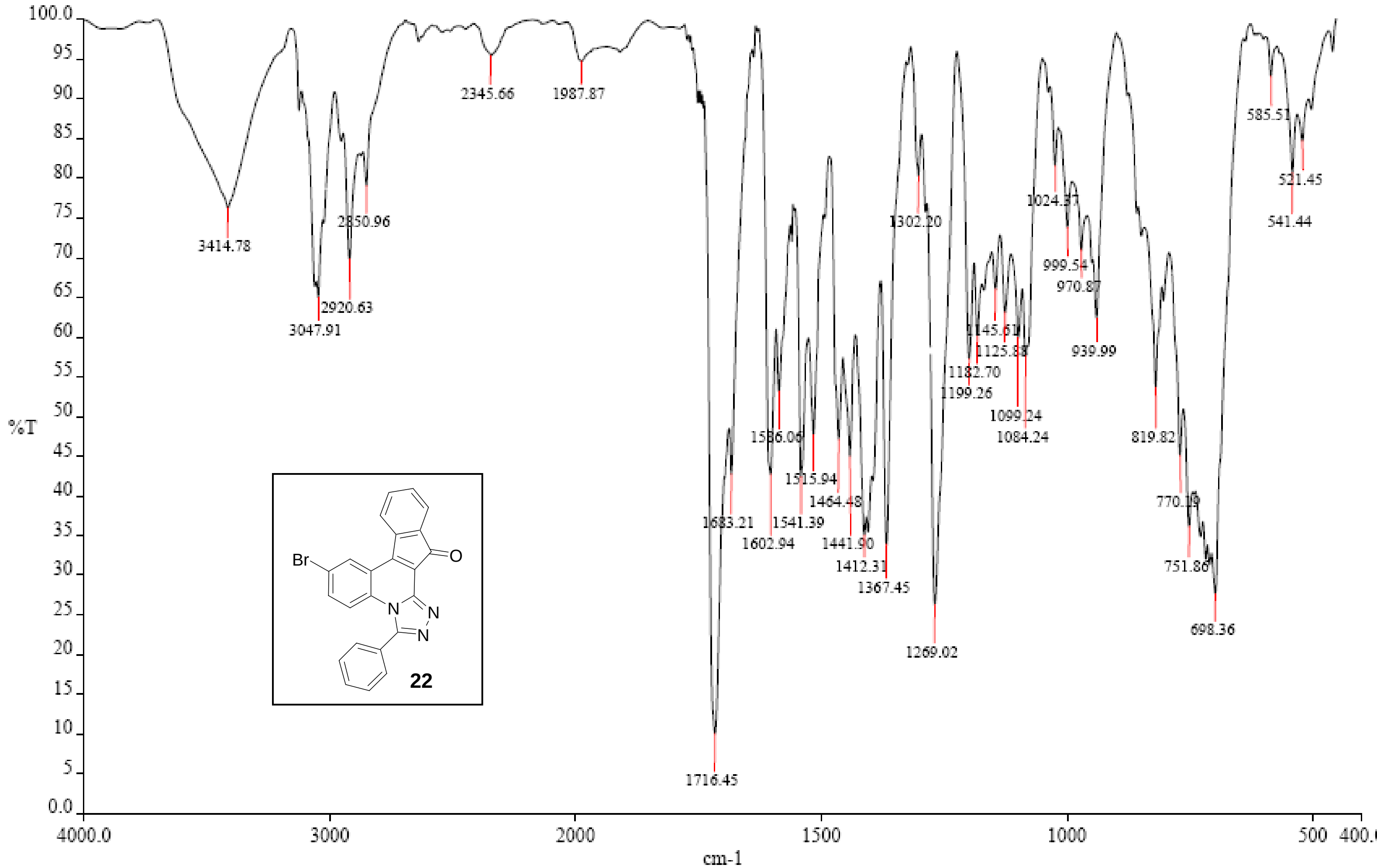
DAD1 B, Sig=205,4 Ref=off

Peak #	RT (Min)	Width (Min)	Area	Area %
1	7.051	0.141	38.844	0.477
2	7.301	0.113	53.580	0.658
3	9.027	0.164	24.842	0.305
4	10.233	0.168	166.695	2.047
5	10.808	0.143	7.086e3	87.001
6	11.374	0.109	39.993	0.491
7	11.847	0.077	14.607	0.179
8	12.086	0.134	15.508	0.190
9	12.531	0.117	10.940	0.134
10	13.969	0.190	693.677	8.517



22

==
*** End of Report***



Spectrum Name: CR080-96-51-43B.sp

Analyst: GANESH

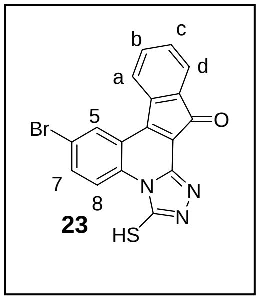
Accumulations: 16

Time: 2:48:26 PM

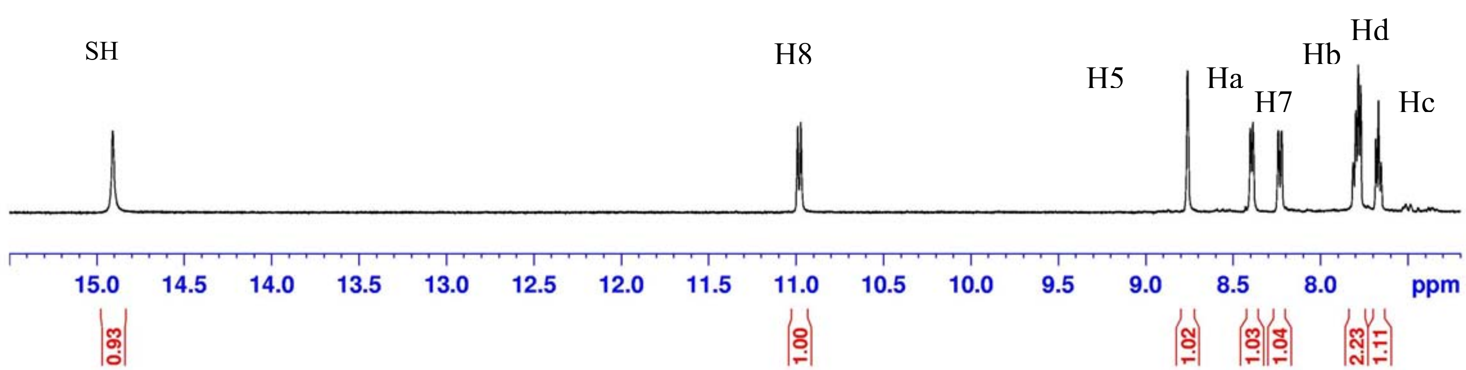
Description: CR080-96-51-43B IN KBr

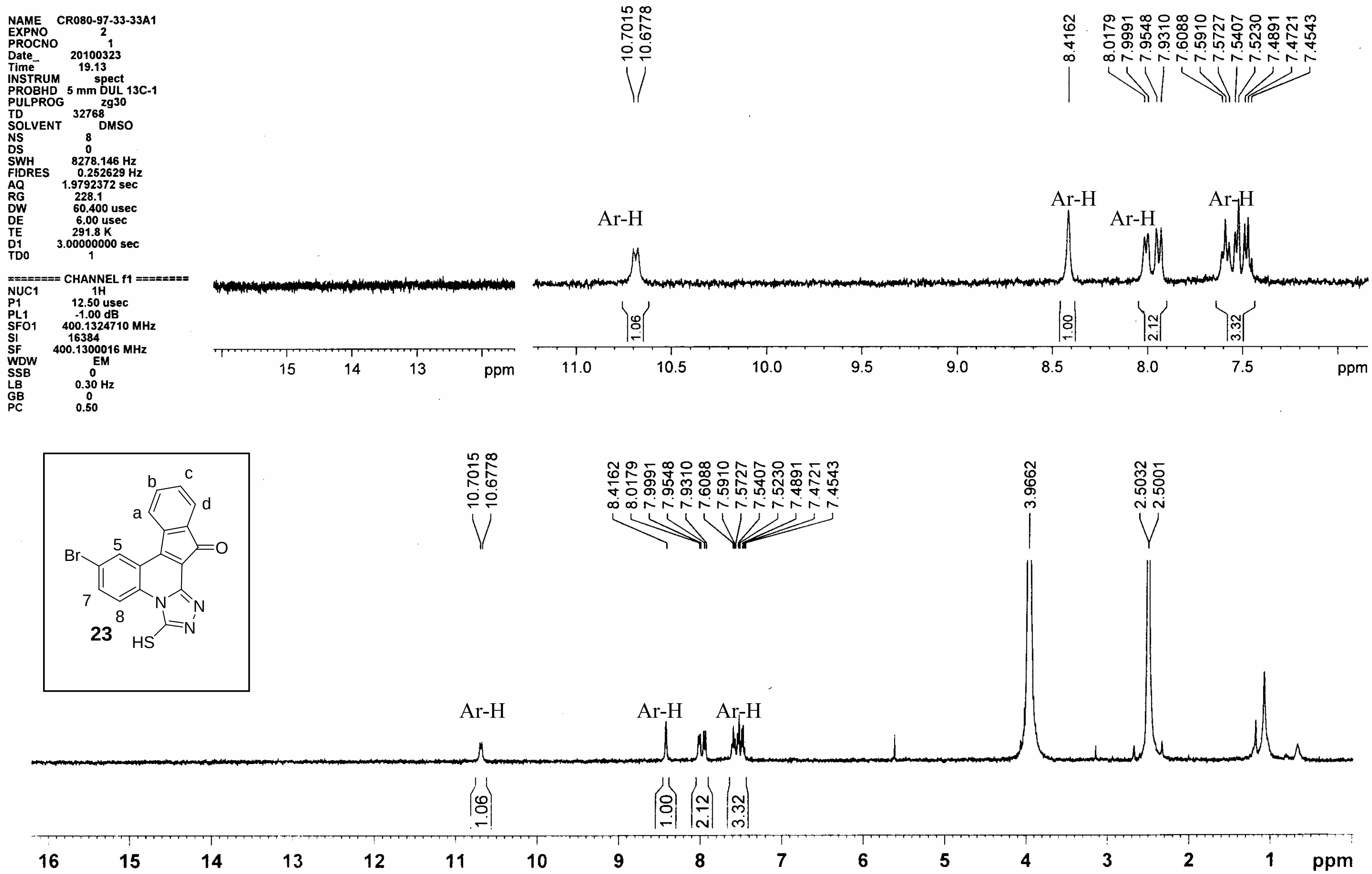
Resolution: 4.00 cm-1

Date: 2/10/2010

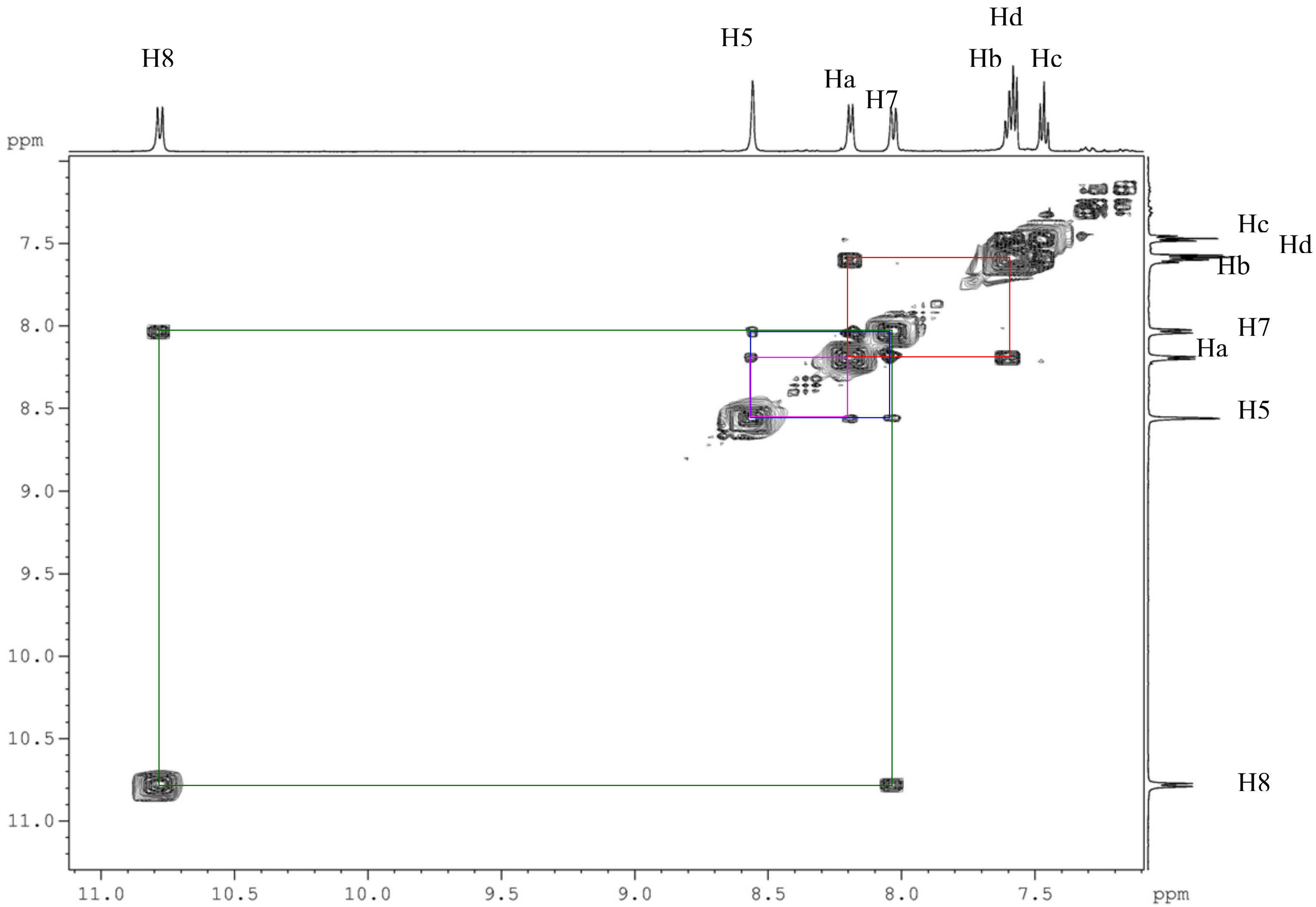

b
c
a
d
5
Br
O
7
8
N
N
N
HS

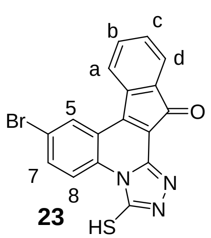
23


10.991
10.972
8.760
8.401
8.386
8.241
8.222
7.813
7.798
7.784
7.771
7.683
7.668
SH
H8
H5
Ha
H7
Hb
Hd
Hc
15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
ppm
0.93
1.00
1.02
1.03
1.04
2.23
1.11

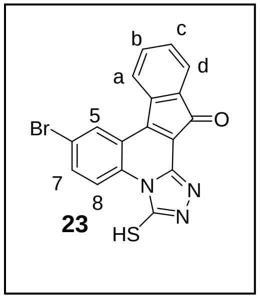


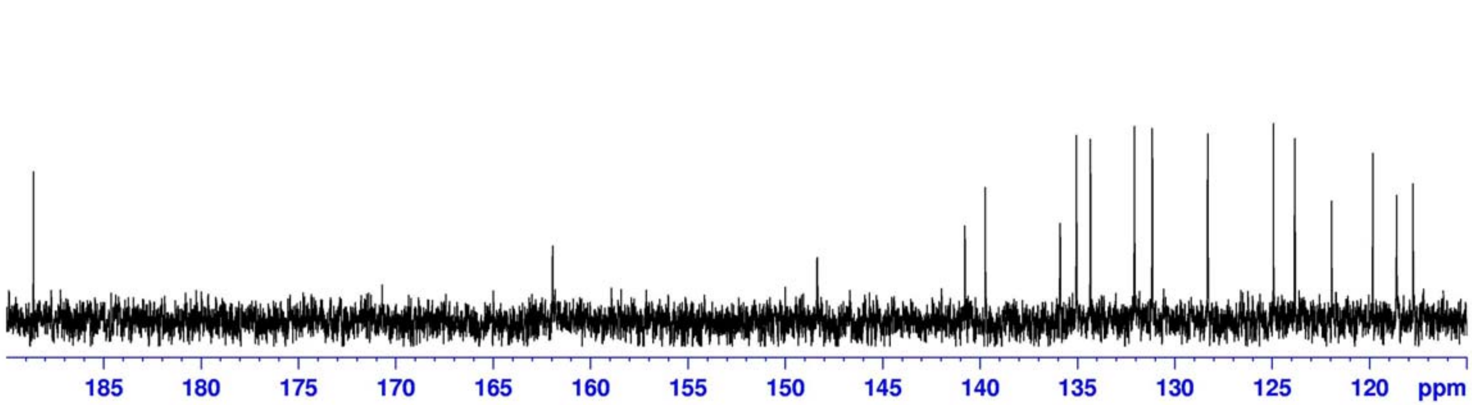
NAME CR080-97-33-33A1
EXPNO 2
PROCNO 1
Date_ 20100323
Time 19.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 228.1
DW 60.400 usec
DE 6.00 usec
TE 291.8 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
10.7015
10.6778
8.4162
8.0179
7.9991
7.9548
7.9310
7.6088
7.5910
7.5727
7.5407
7.5230
7.4891
7.4721
7.4543
3.9662
2.5032
2.5001
Ar-H
Ar-H
Ar-H
Ar-H
1.06
1.00
2.12
3.32
ppm
23
Br
HS


H8
H5
Ha
H7
Hd
Hb
Hc
ppm
7.5
8.0
8.5
9.0
9.5
10.0
10.5
11.0
Hc
Hd
Hb
H7
Ha
H5
H8
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
ppm

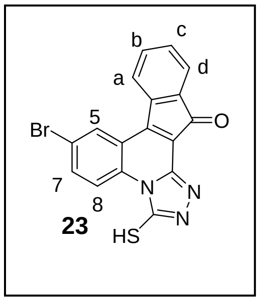

b
c
d
a
5
O
Br
7
8
N
N
N
HS

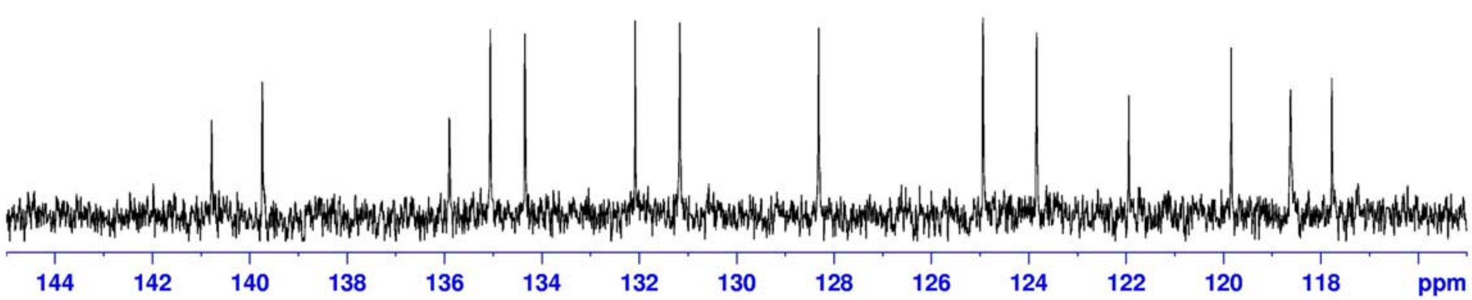
23

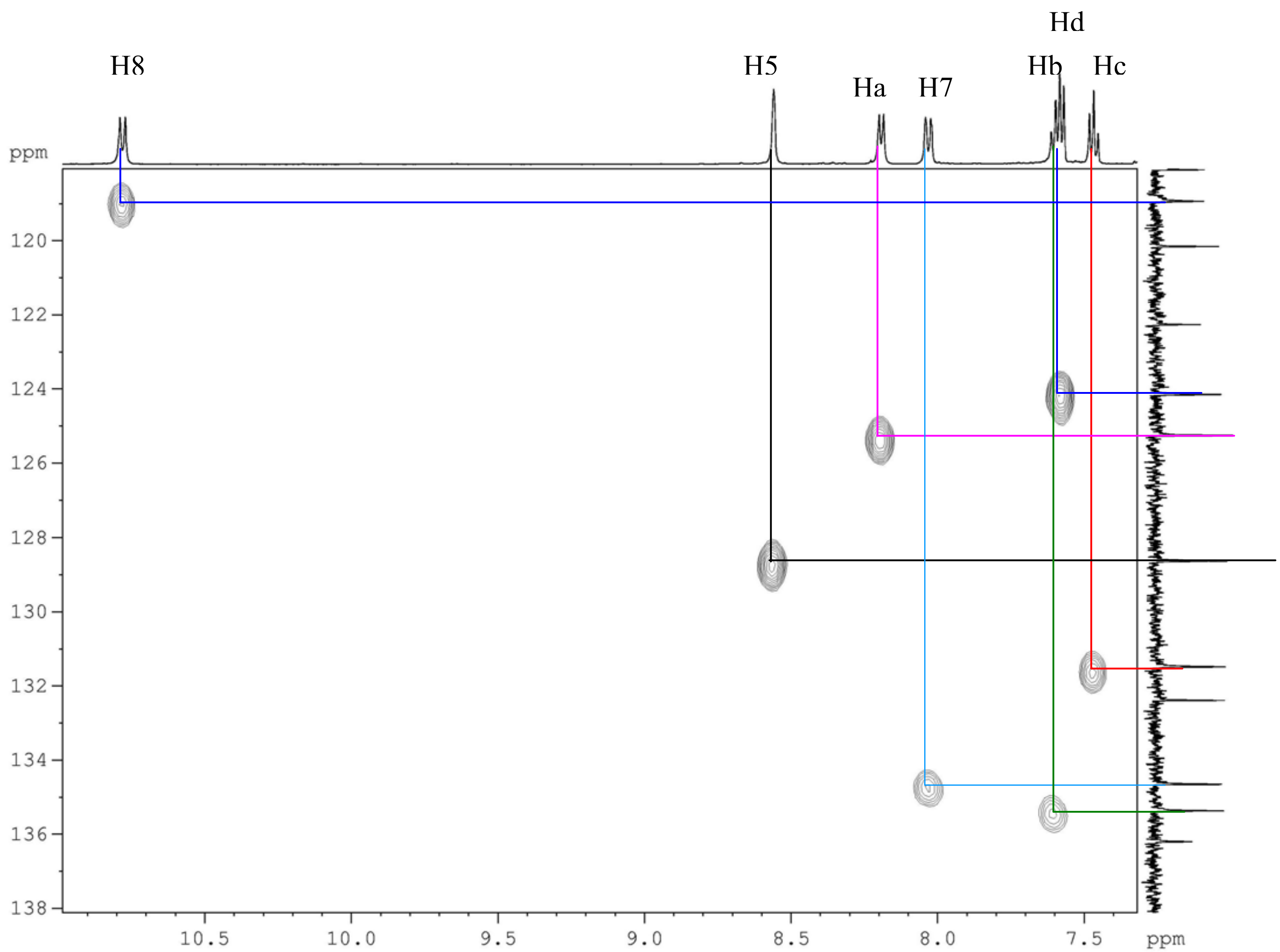

b
c
a
d
Br
5
O
7
8
N
N
N
23
HS

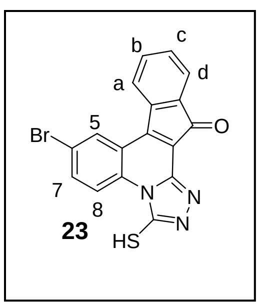

188.61
161.94
148.38
140.79
139.75
135.90
135.06
134.35
132.08
131.18
128.32
124.94
123.85
121.96
119.85
118.63
117.78
185
180
175
170
165
160
155
150
145
140
135
130
125
120
ppm

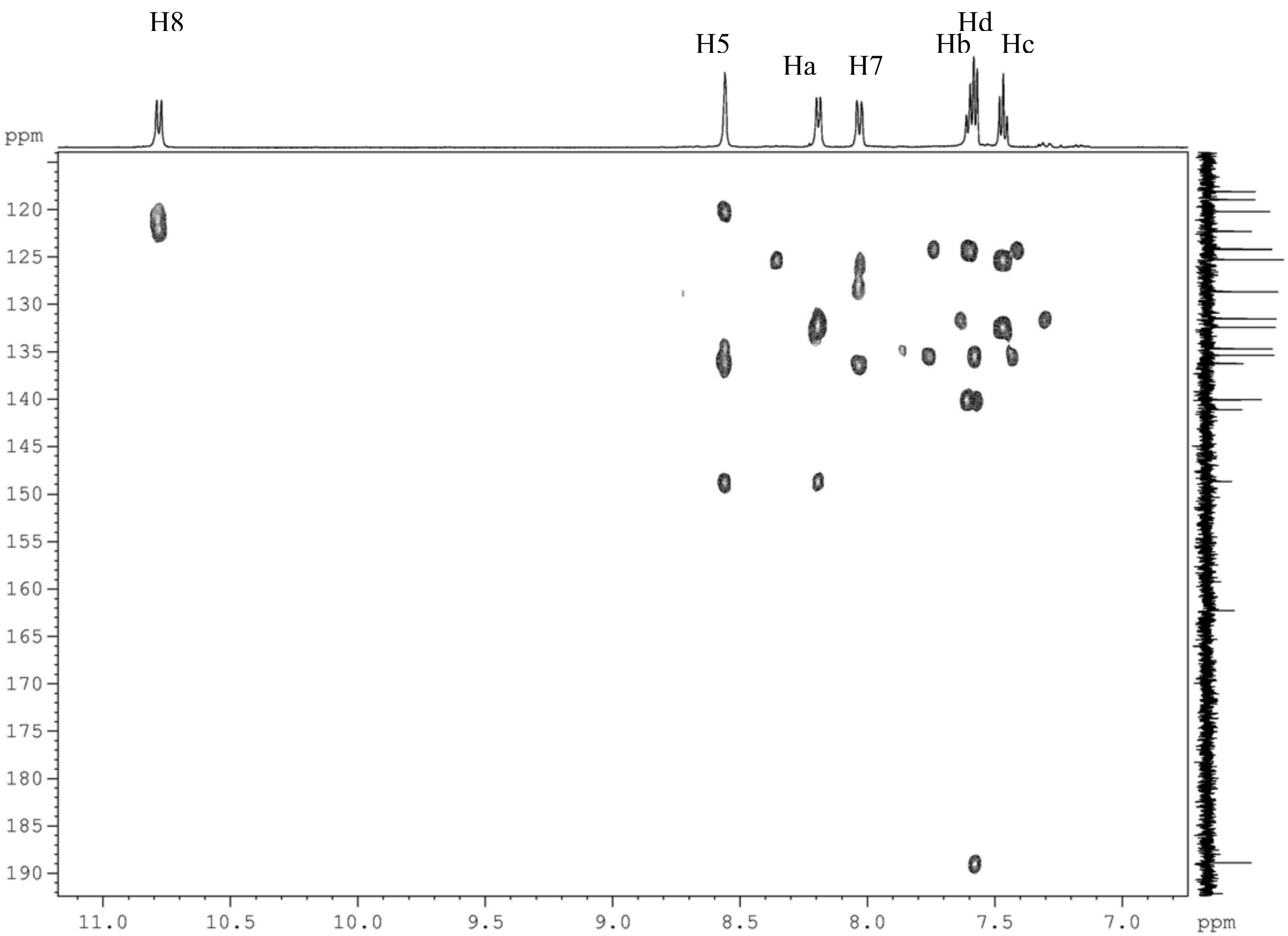

140.79
139.75
135.90
135.06
134.35
132.08
131.18
128.32
124.94
123.85
121.96
119.85
118.63
117.78

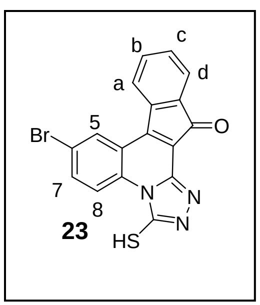

b
c
a
d
Br
5
O
7
8
N
N
N
HS
23

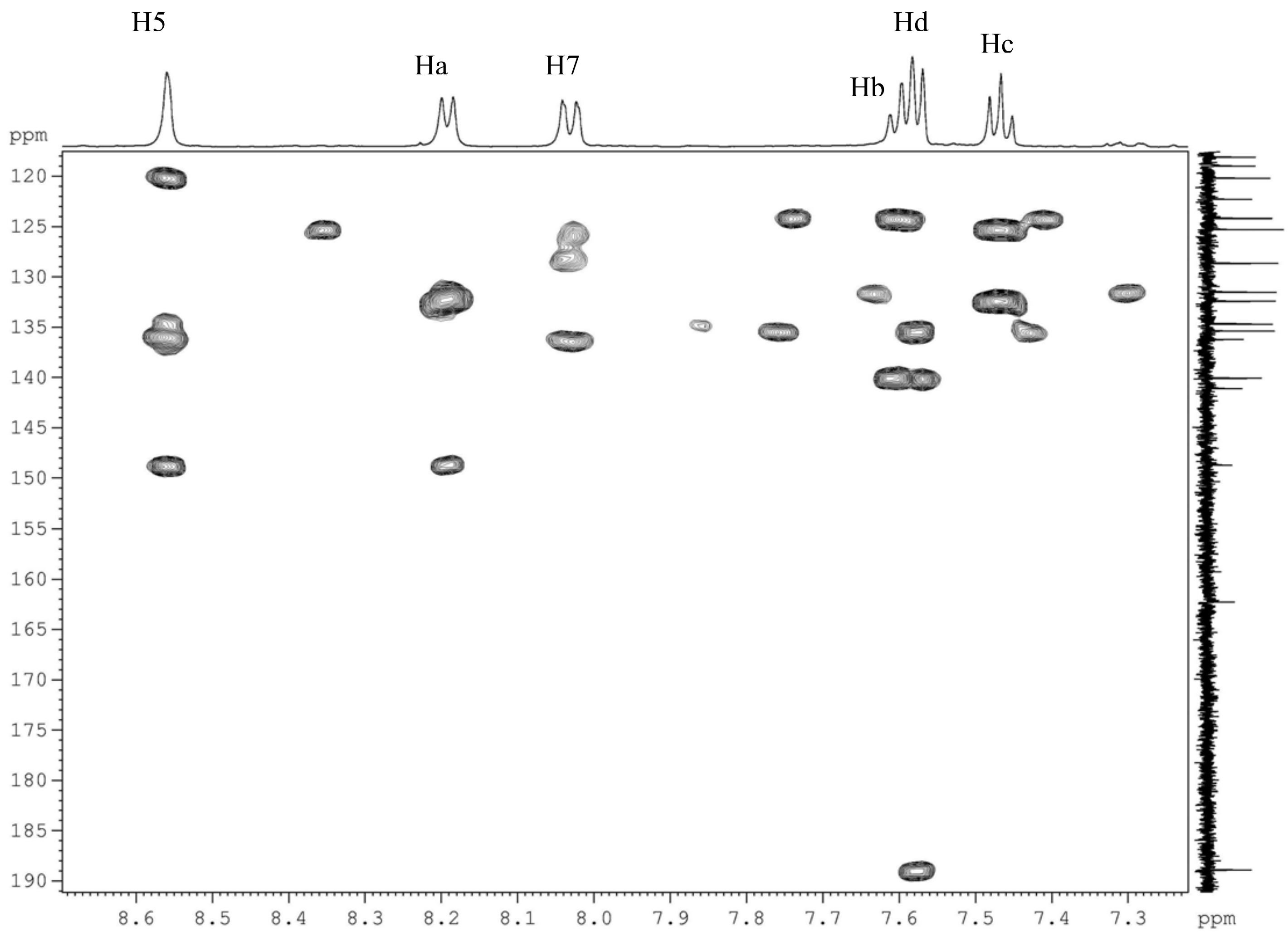

144
142
140
138
136
134
132
130
128
126
124
122
120
118
ppm

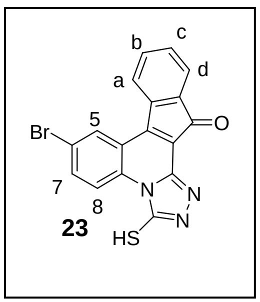

H8
H5
Ha
H7
Hd
Hb
Hc
ppm
120
122
124
126
128
130
132
134
136
138
10.5
10.0
9.5
9.0
8.5
8.0
7.5
ppm

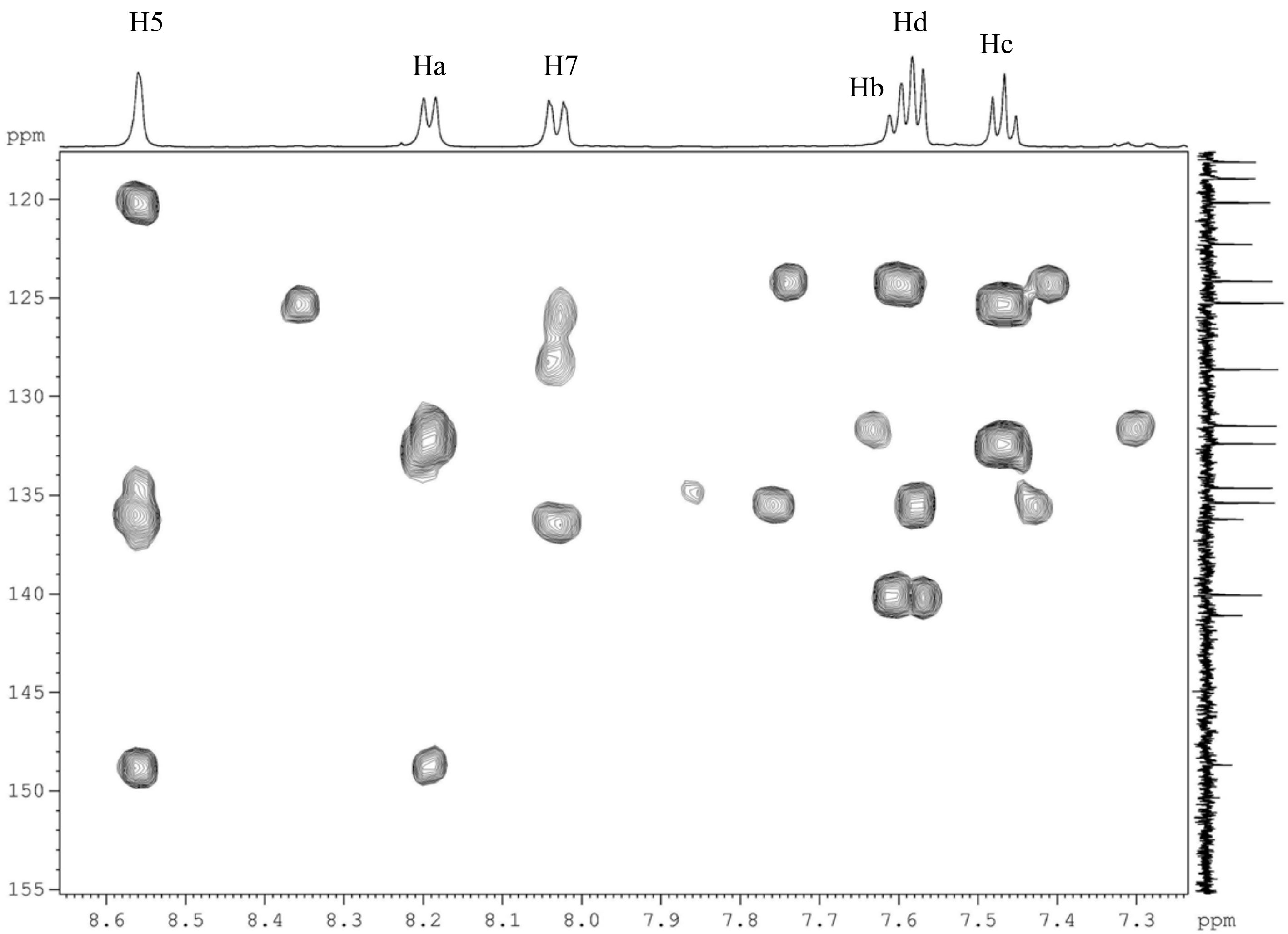

b
c
a
d
5
Br
O
7
8
N
N
N
HS
23

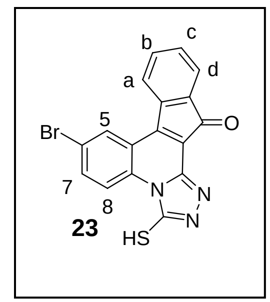

H8
H5
Ha
H7
Hb
Hd
Hc
ppm
120
125
130
135
140
145
150
155
160
165
170
175
180
185
190
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
ppm

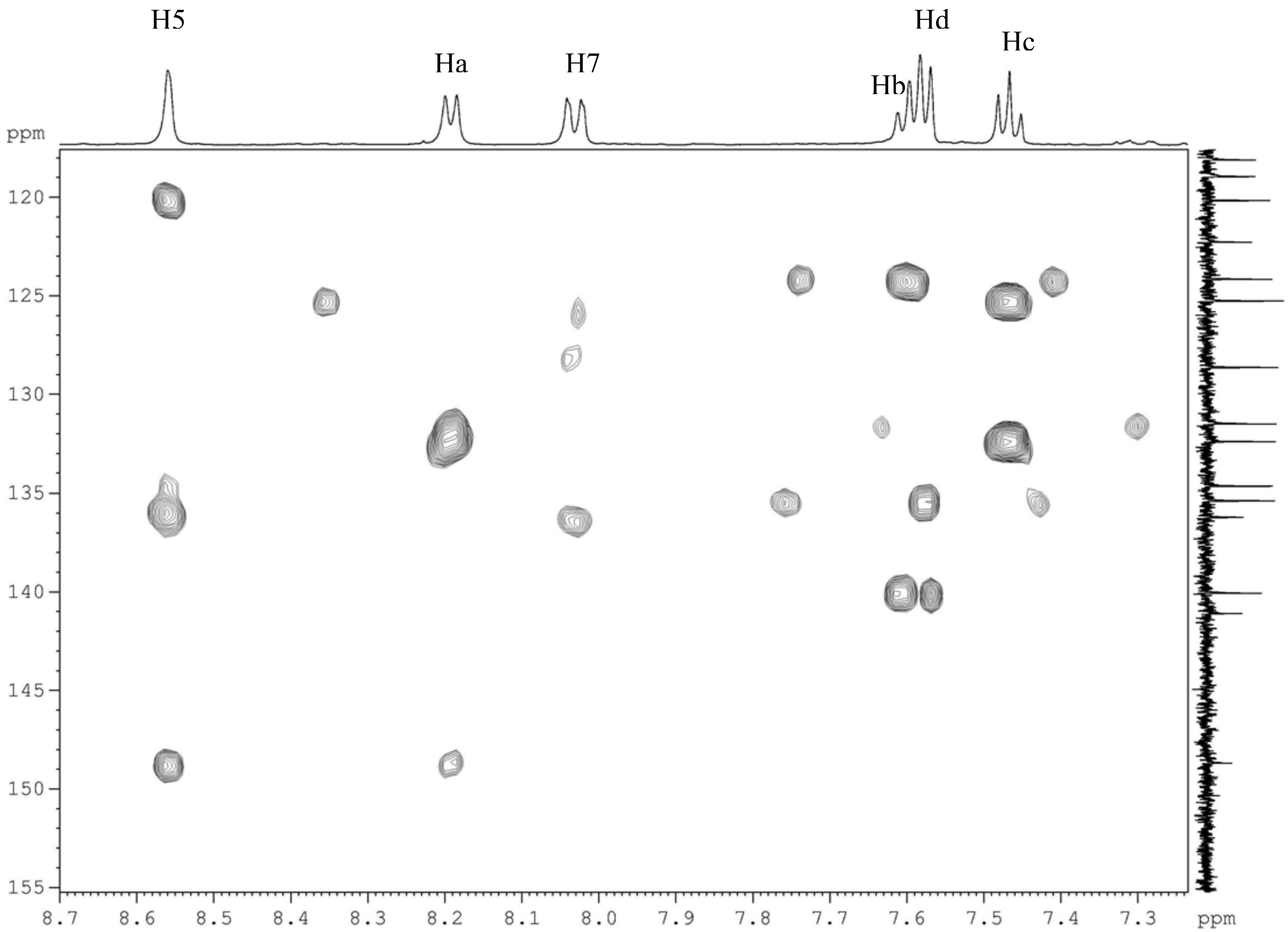

b
c
d
a
5
Br
O
7
8
N
N
N
HS
23

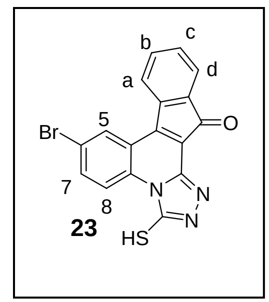

H5
Ha
H7
Hd
Hb
Hc
ppm
120
125
130
135
140
145
150
155
160
165
170
175
180
185
190
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm


b
c
a
d
Br
5
O
7
8
N
N
N
23
HS


H5
Ha
H7
Hb
Hd
Hc
ppm
120
125
130
135
140
145
150
155
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm


b
c
a
d
5
Br
O
7
8
N
N
N
23
HS

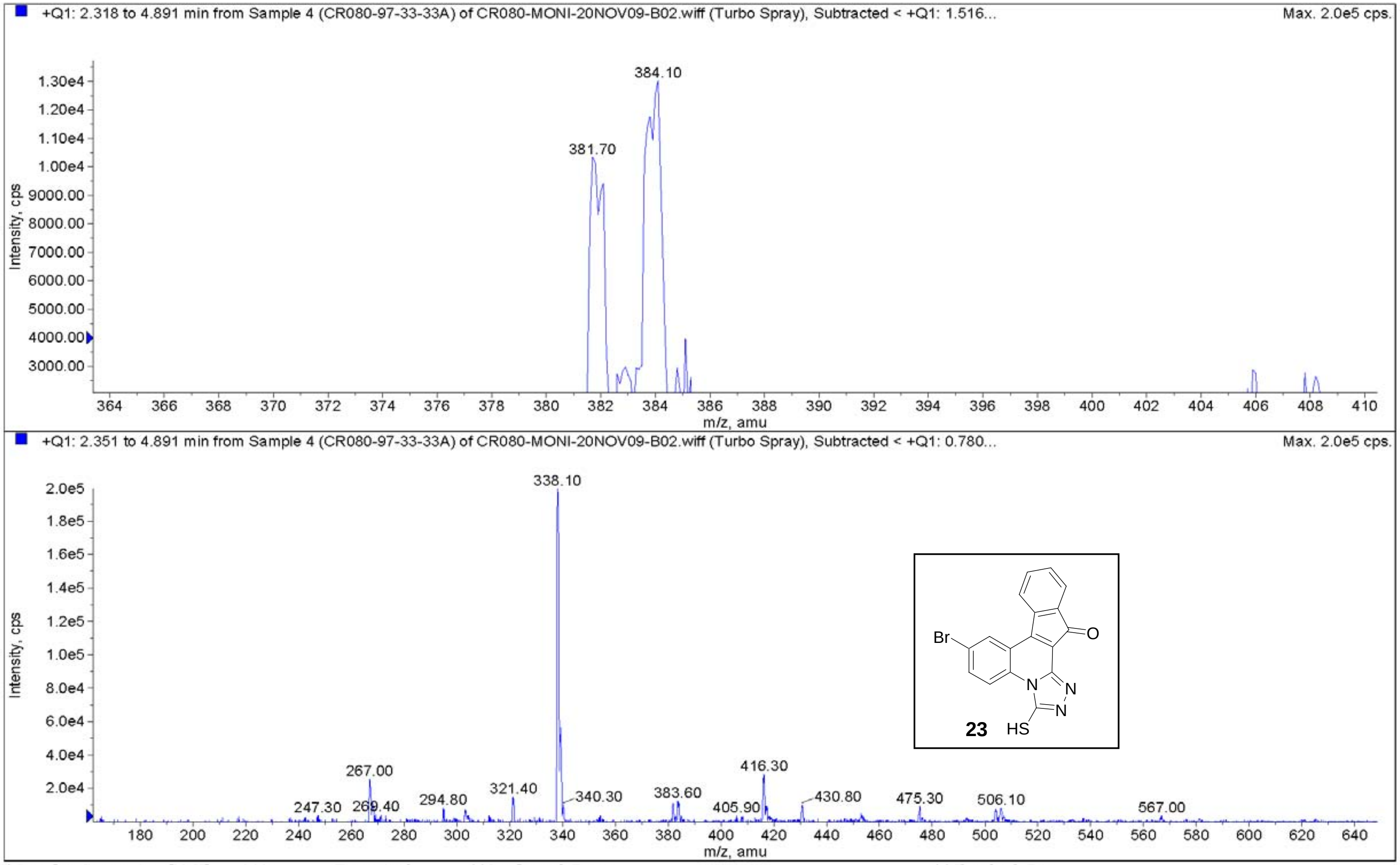

H5
Ha
H7
Hb
Hd
Hc
ppm
120
125
130
135
140
145
150
155
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm


b
c
a
d
Br
5
O
7
N
N
8
N
HS
23

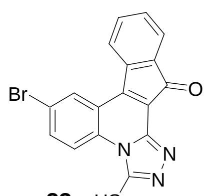
*

INDIA

Sample Name: CR080-97-33-33A Acq. Time: 15:37 Acq. Date: Friday, November 20, 2009

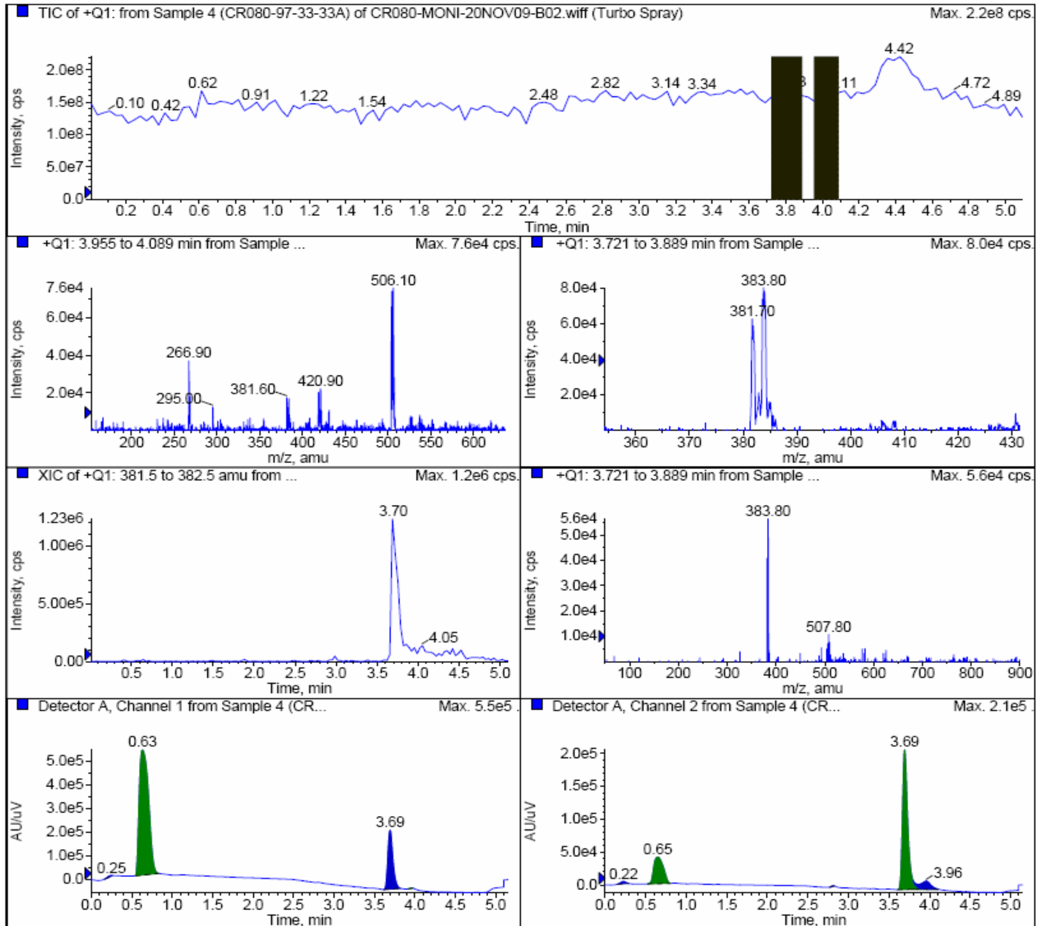


*Sample Comment: [M+H] 382 Expected **Analyzed By : **Checked By :



23

Sample Name: CR080-97-33-33A Acq. Time: 15:37 Acq. Date: Friday, November 20, 2009



Peak List for "Detector A, Channel 1 from Sample 4 (CR080-97-33-

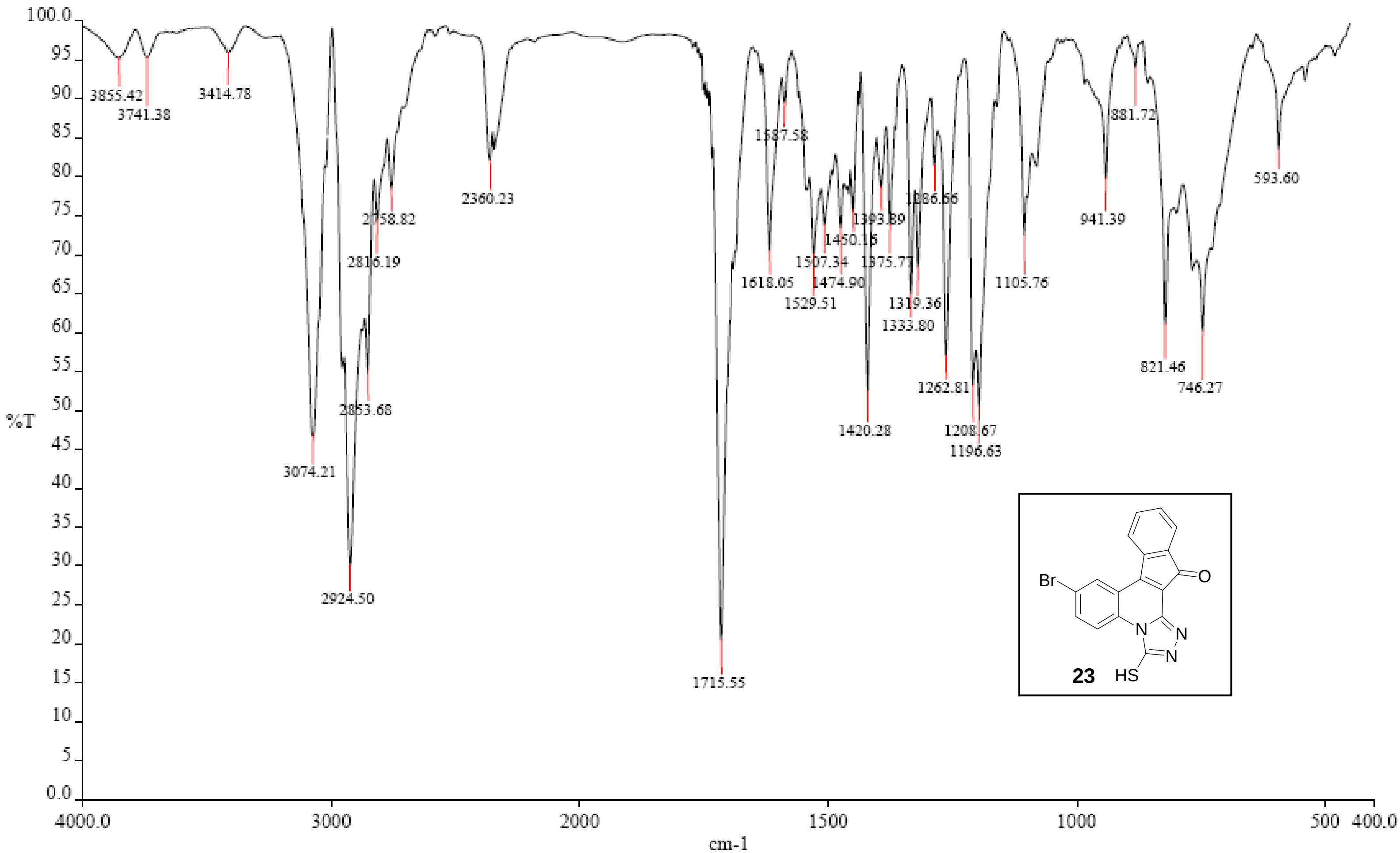
	Time (min)	Area (counts)	%Area	Height
2	0.6335	4.2336e6	79.7072	5.2696e5
3	3.6949	1.0599e6	19.9540	2.4799e5
4	3.9639	2813.5490	0.0530	1211.7812

Peak List for "Detector A, Channel 2 from Sample 4 (CR080-97-33-

	Time (min)	Area (counts)	%Area	Height
3	2.8136	1412.1798	0.1001	660.8329
4	3.6933	9.5910e5	67.9760	2.1202e5
5	3.9609	1.0863e5	7.6993	1.2210e4

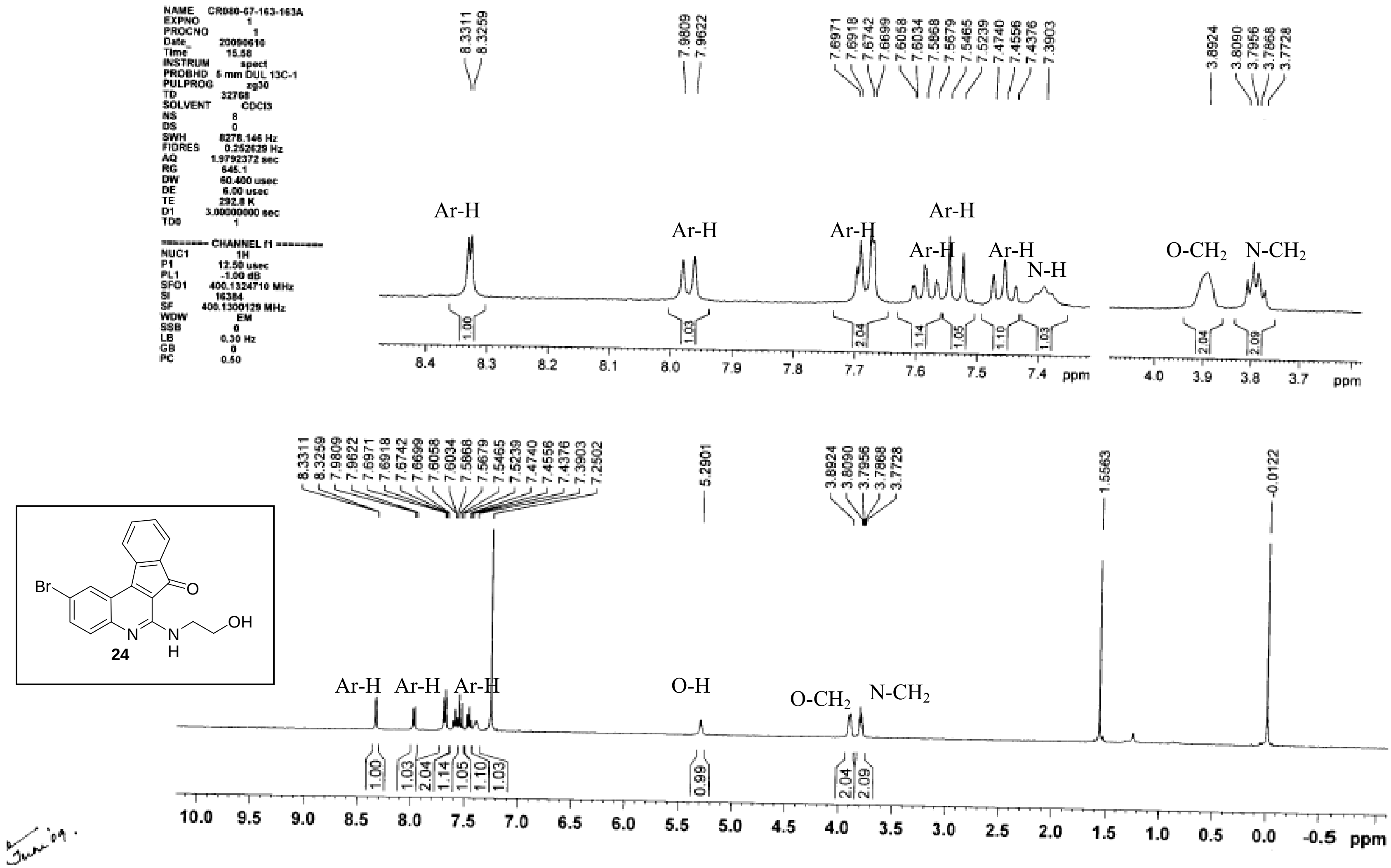
LCMS-1 REACN MONT (TFA Buffer) Analysed By :

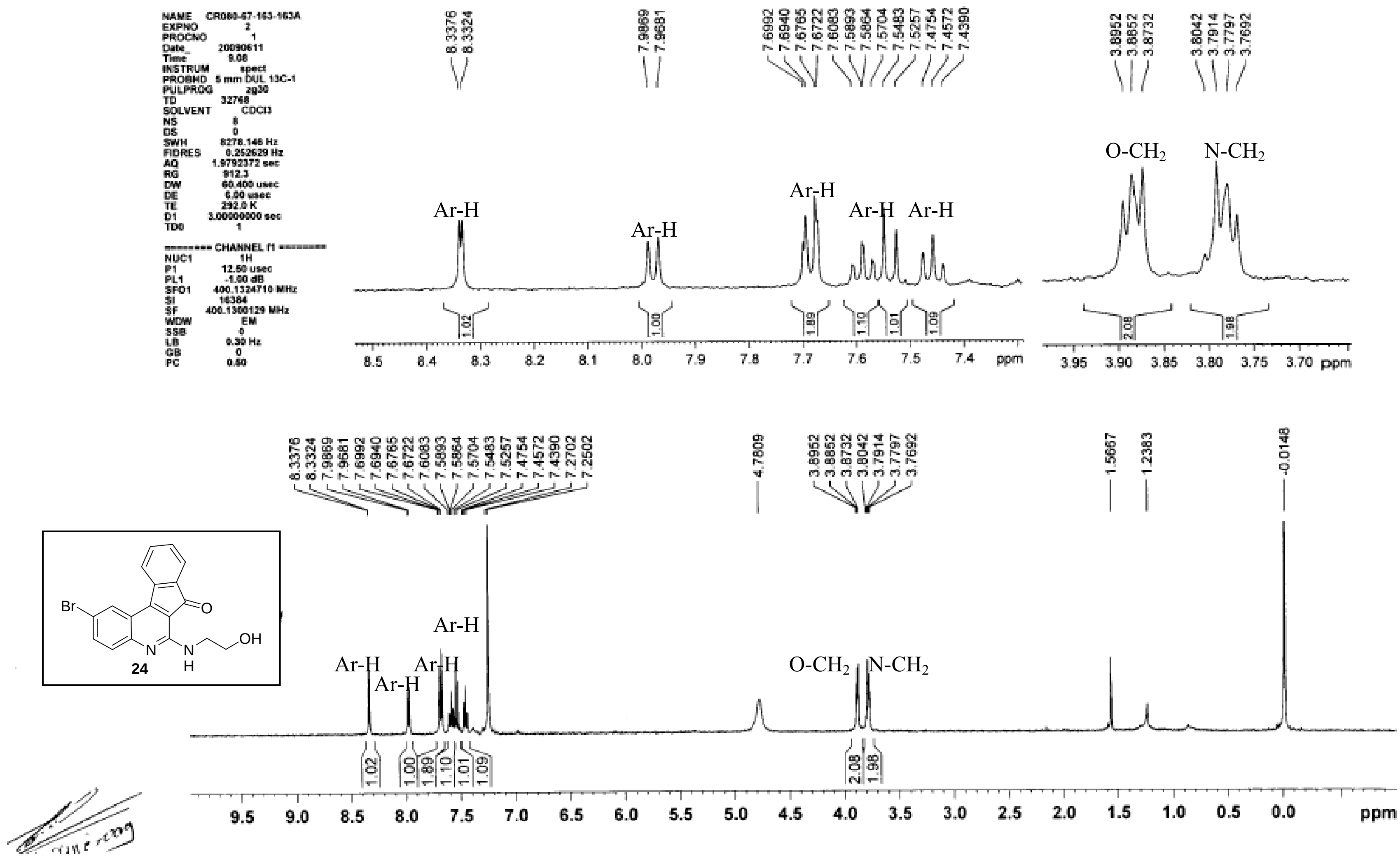
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm



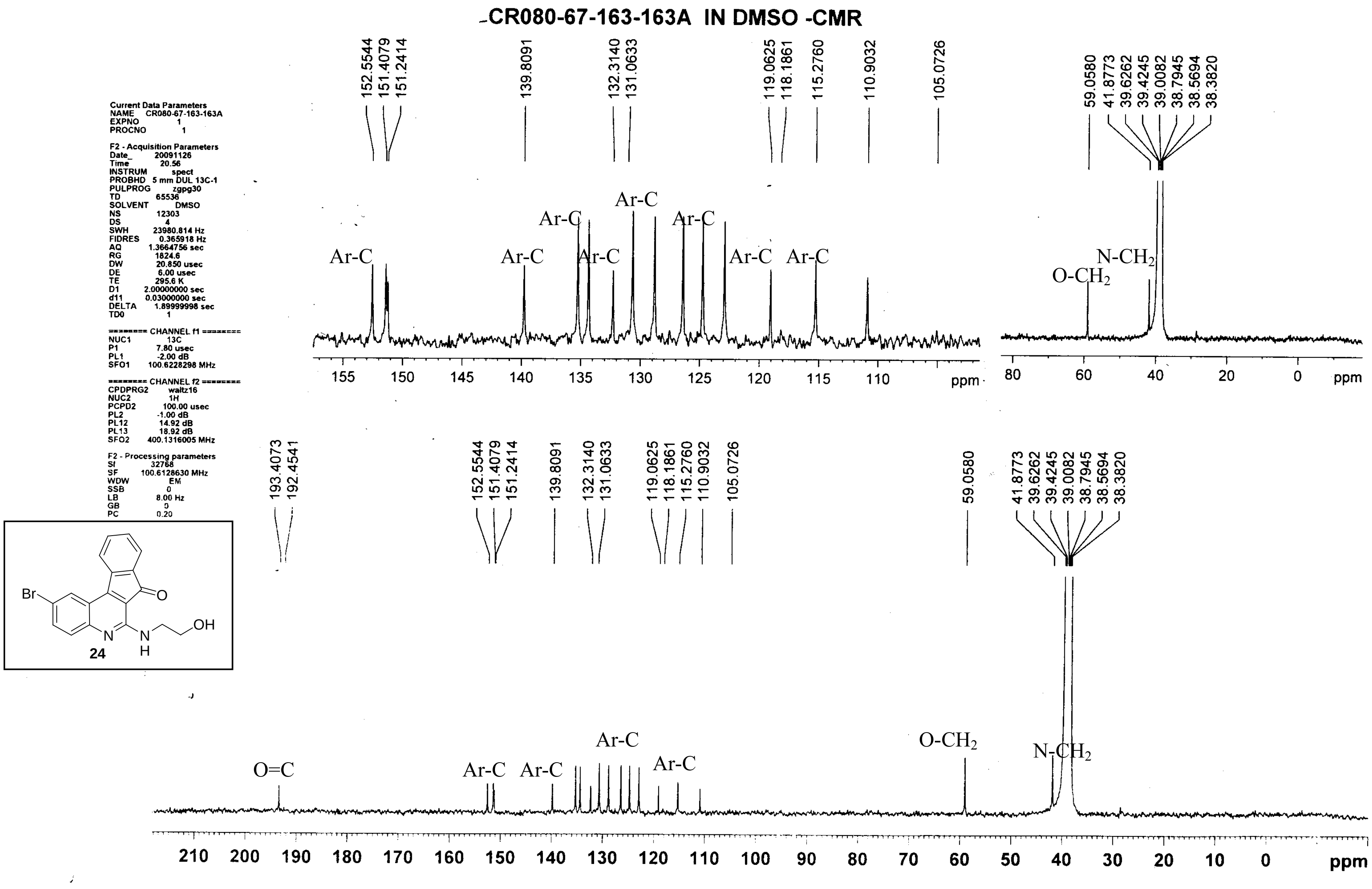
Spectrum Name: CR080-97-33-33A.sp Analyst: GANESH Accumulations: 16 Time: 1:17:39 PM

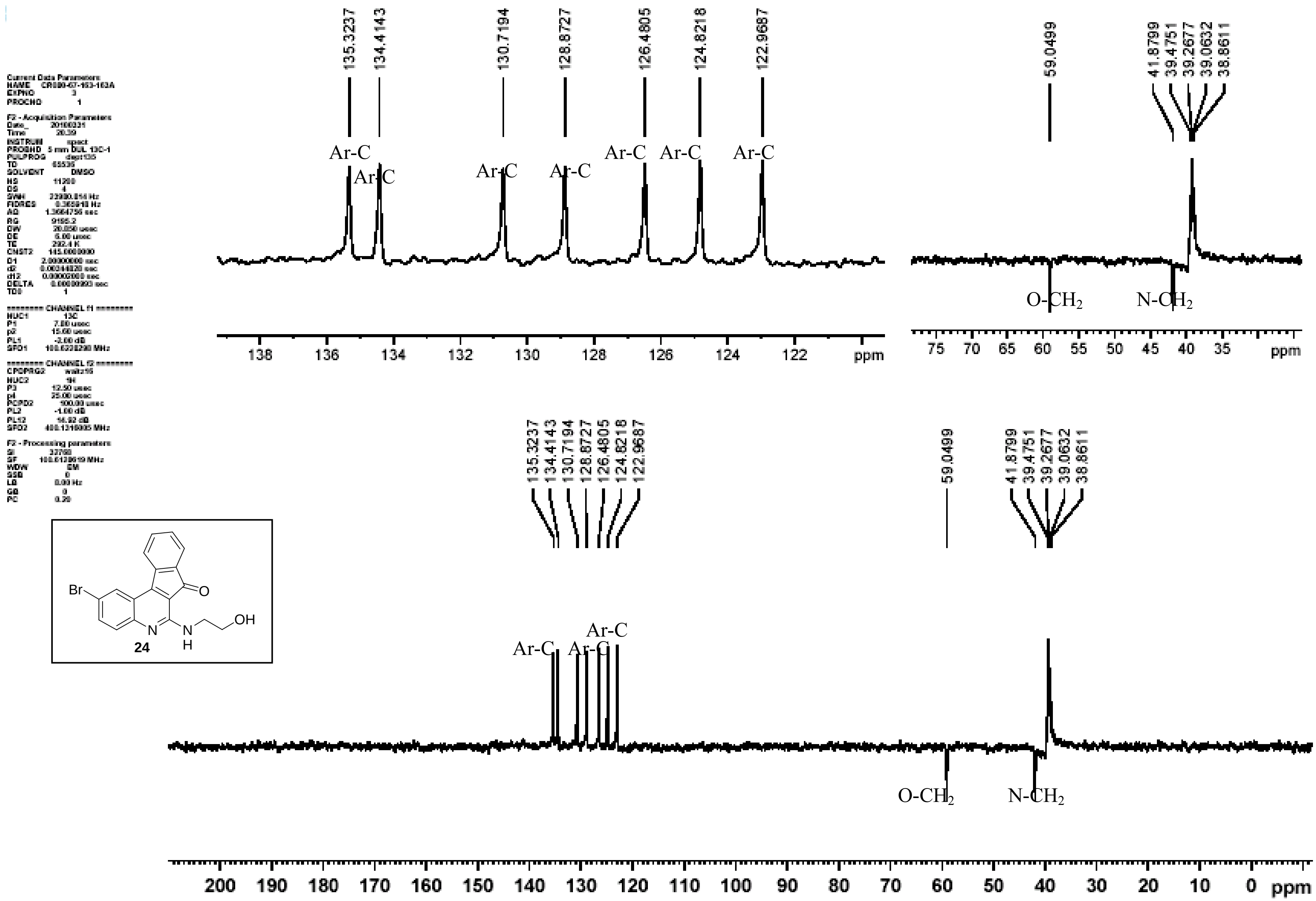
Description: CR080-97-33-33A IN KBr Resolution: 4.00 cm-1 Date: 2/5/2010


NAME CR080-67-163-163A
SOLVENT CDCl3
SFO1 400.1324710 MHz
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
N-H
O-CH2
N-CH2
Br
O
N
N
H
OH
24
Ar-H
Ar-H
Ar-H
O-H
O-CH2
N-CH2
ppm



NAME CR080-67-163-163A
EXPNO 2
PROCNO 1
Date_ 20090611
SOLVENT CDCl3
Ar-H
O-CH$_2$
N-CH$_2$
Br
N
N
H
OH
O
24
ppm

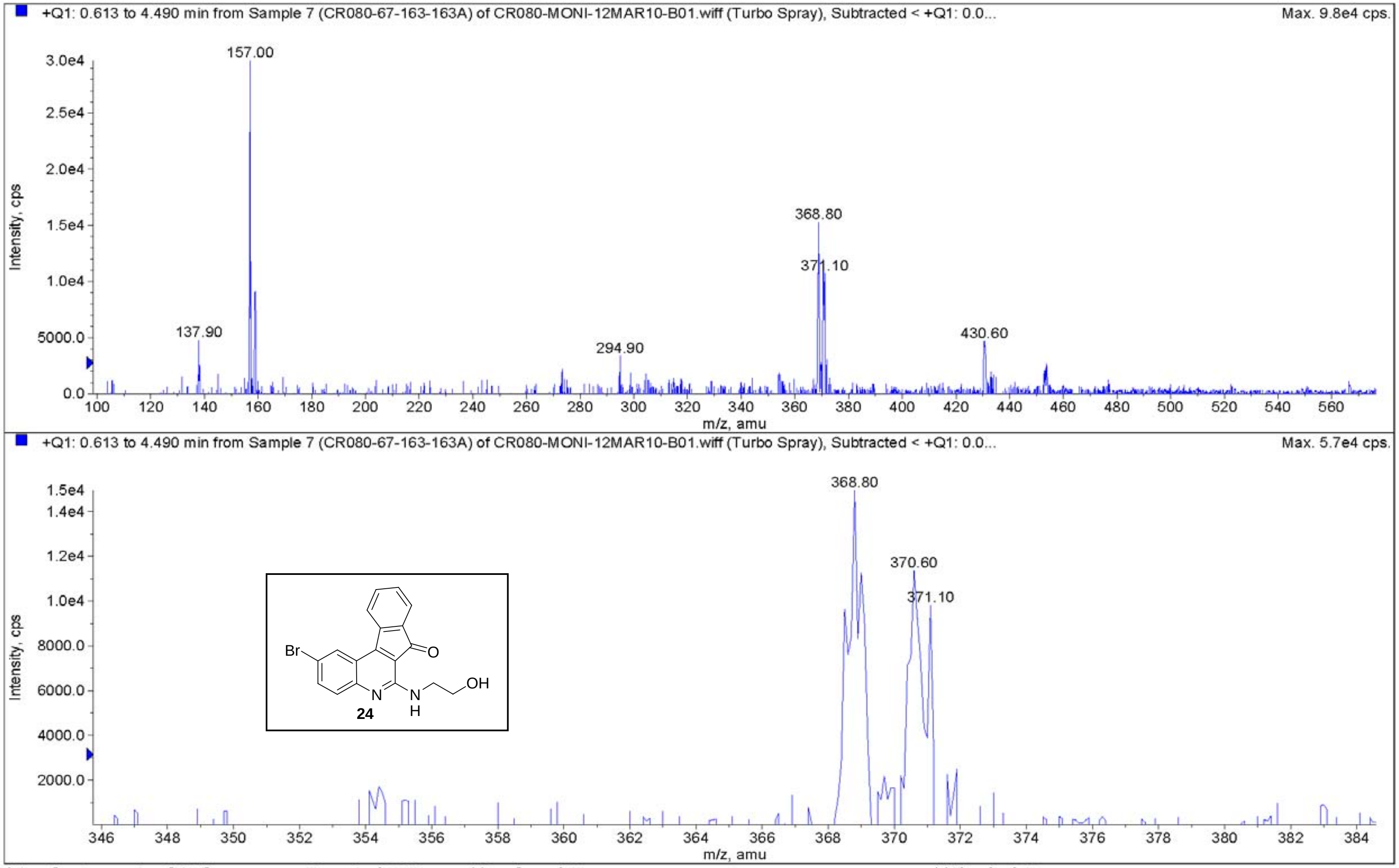

CR080-67-163-163A IN DMSO -CMR
Current Data Parameters
NAME CR080-67-163-163A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091126
Time 20.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12303
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.92 dB
PL13 18.92 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128630 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 0.20
Br
O
N
N
H
OH
24
193.4073
192.4541
152.5544
151.4079
151.2414
139.8091
132.3140
131.0633
119.0625
118.1861
115.2760
110.9032
105.0726
59.0580
41.8773
39.6262
39.4245
39.0082
38.7945
38.5694
38.3820
O=C
Ar-C
Ar-C
Ar-C
Ar-C
O-CH2
N-CH2
ppm


Current Data Parameters
Ar-C
O-CH2
N-CH2
135.3237
134.4143
130.7194
128.8727
126.4805
124.8218
122.9687
59.0499
41.8799
39.4751
39.2677
39.0632
38.8611
ppm
Br
O
N
N
H
OH
24

*

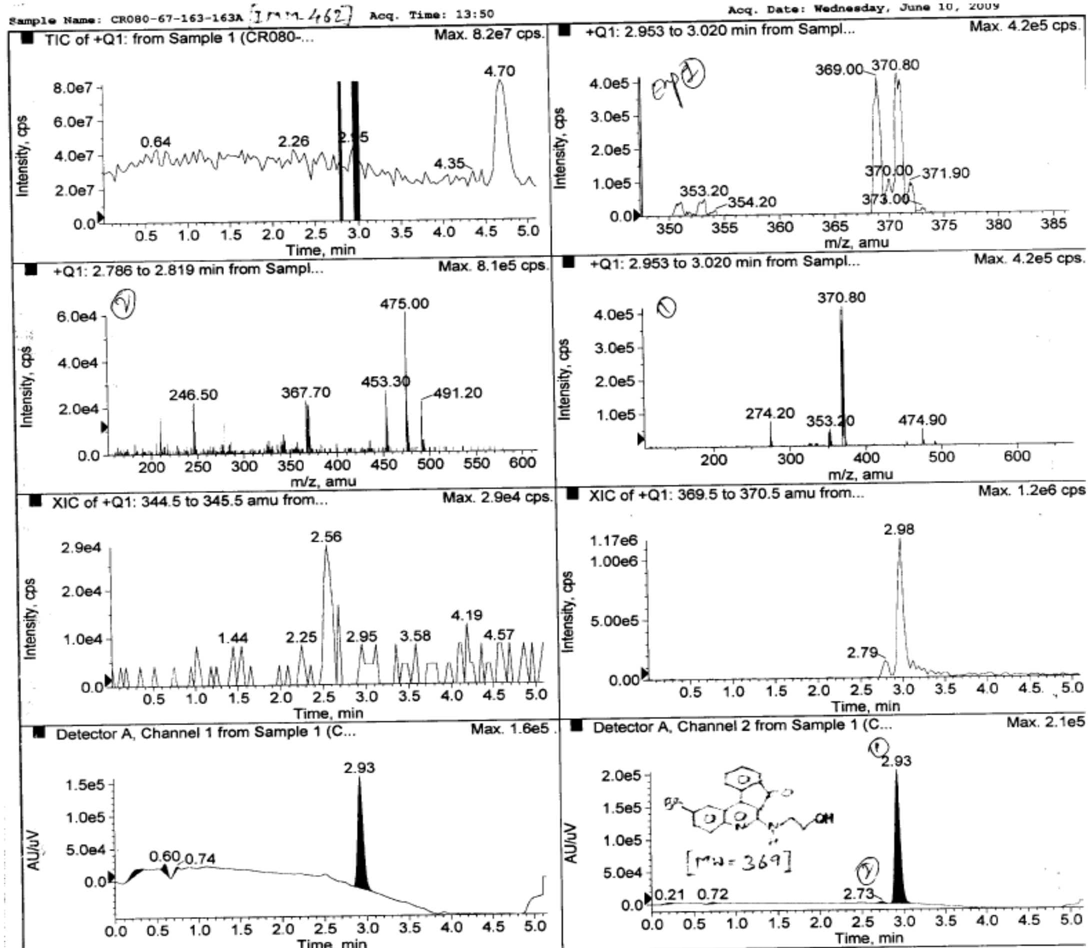
INDIA

Sample Name: CR080-67-163-163A   Acq. Time: 12:27   Acq. Date: Friday, March 12, 2010



*Sample Comment: [M+H]   Expected 369   **Analyzed By :   **Checked By :

Sample Name: CR080-67-163-163A [IMM-462] Acq. Time: 13:50 Acq. Date: Wednesday, June 10, 2009



	Time (min)	Area (counts)	% Area	Height
1	0.3231	6.2168e4	6.8468	2110.8398
2	0.5962	5.0731e4	5.5872	1.4327e4
3	0.7439	1.1911e4	1.3118	2865.3704
4	2.9297	7.8319e5	86.2542	1.7317e5

Peak List for "Detector A, Channel 1 from Sample 1 (CR080-67-1

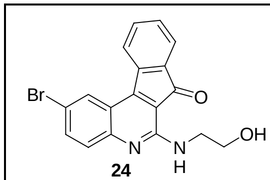
	Time (min)	Area (counts)	% Area	Height
1	0.2142	1.0920e4	1.0989	2103.3701
2	0.7234	1.0999e4	1.1069	2576.3264
3	2.7335	1.5328e4	1.5426	3030.4582
4	2.9303	9.5643e5	96.2516	2.0715e5

Peak List for "Detector A, Channel 2 from Sample 1 (CR080-67

LCMS-1 Reaction Monitoring (TFA Buffer)

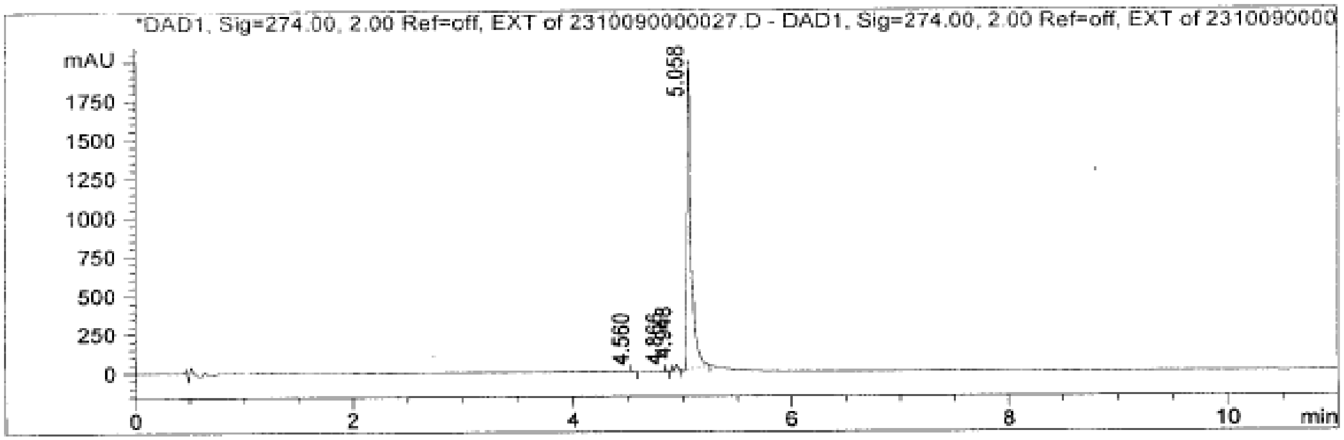
Channel 1 at wavelength 220 nm, Channel 2 at wavelength 260 nm

Analyzed By : 10/06/2009



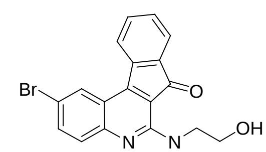
24

Sample:CR080-67-163-163A ->
Column: ZORBAX SB-C18(50X4.6)mm 1.8µ
Injection date : Fri, 23. Oct. 2009 Location : Vial 21
Sample Name : CR080-67-163-163A Inj. No. : 1
Acq Operator : GANESH Z Inj. Vol. : 10 µl
Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _25.M
Last Changed : Fri, 23. Oct. 2009,
Acq. Method :C:\Chem32\2\DATA\OCT-09\231009E 2009-10-23 11-54-41\
UPLC_GENARAL_GRAD _25.M
Method ref : DI/A0257/45



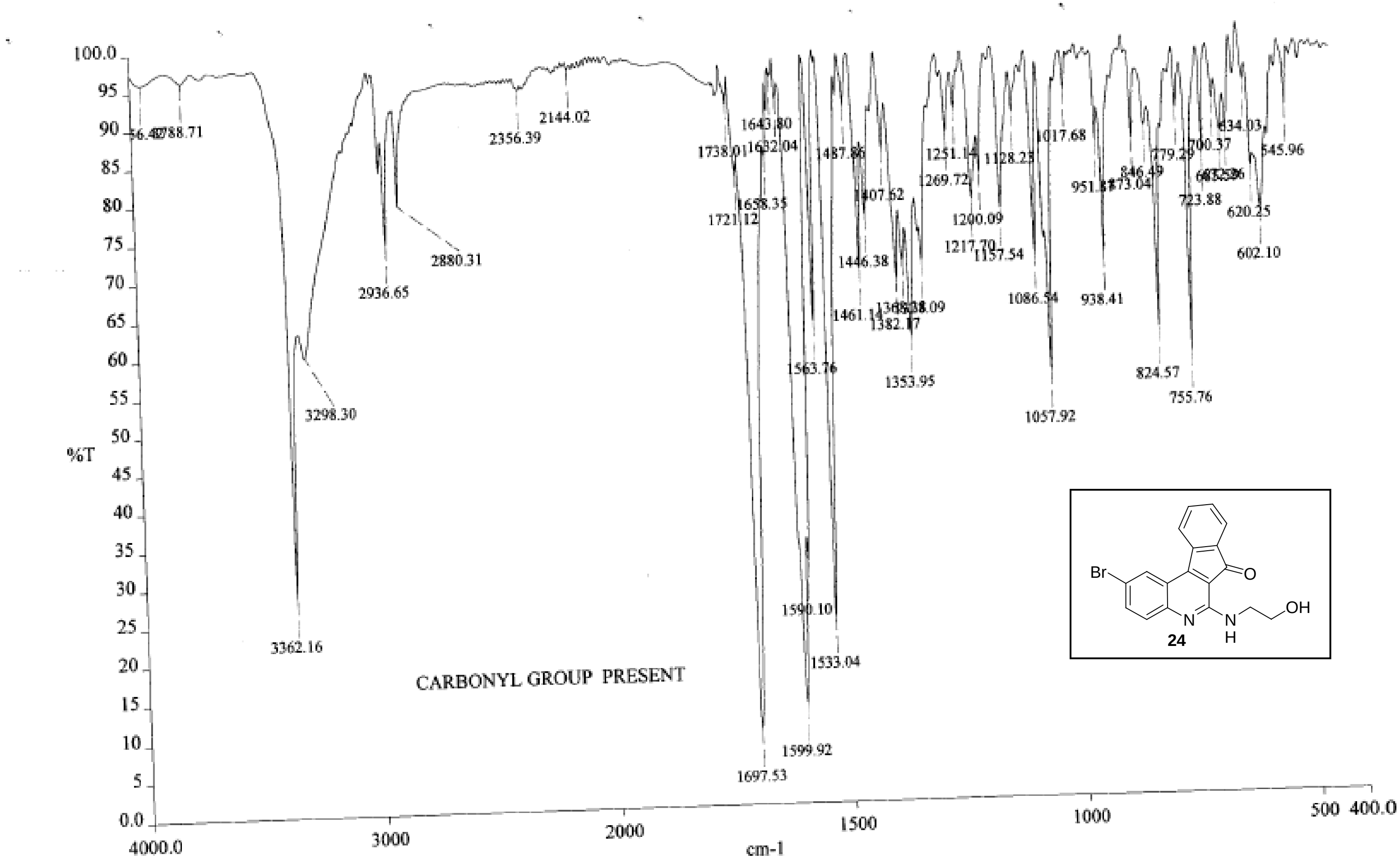
DAD1, Sig=274.00, 2.00 Ref=off, EXT

Peak #	RT (Min)	Width (Min)	Area	Area %
1	4.560	0.044	14.392	0.272
2	4.866	0.027	12.573	0.238
3	4.948	0.030	76.562	1.446
4	5.058	0.043	5189.865	98.044



24

*** End of Report***



Spectrum Name: CR080-67-163-163A.sp

Description: CR080-67-163-163A IN KBr

Analyst : GANESH Z

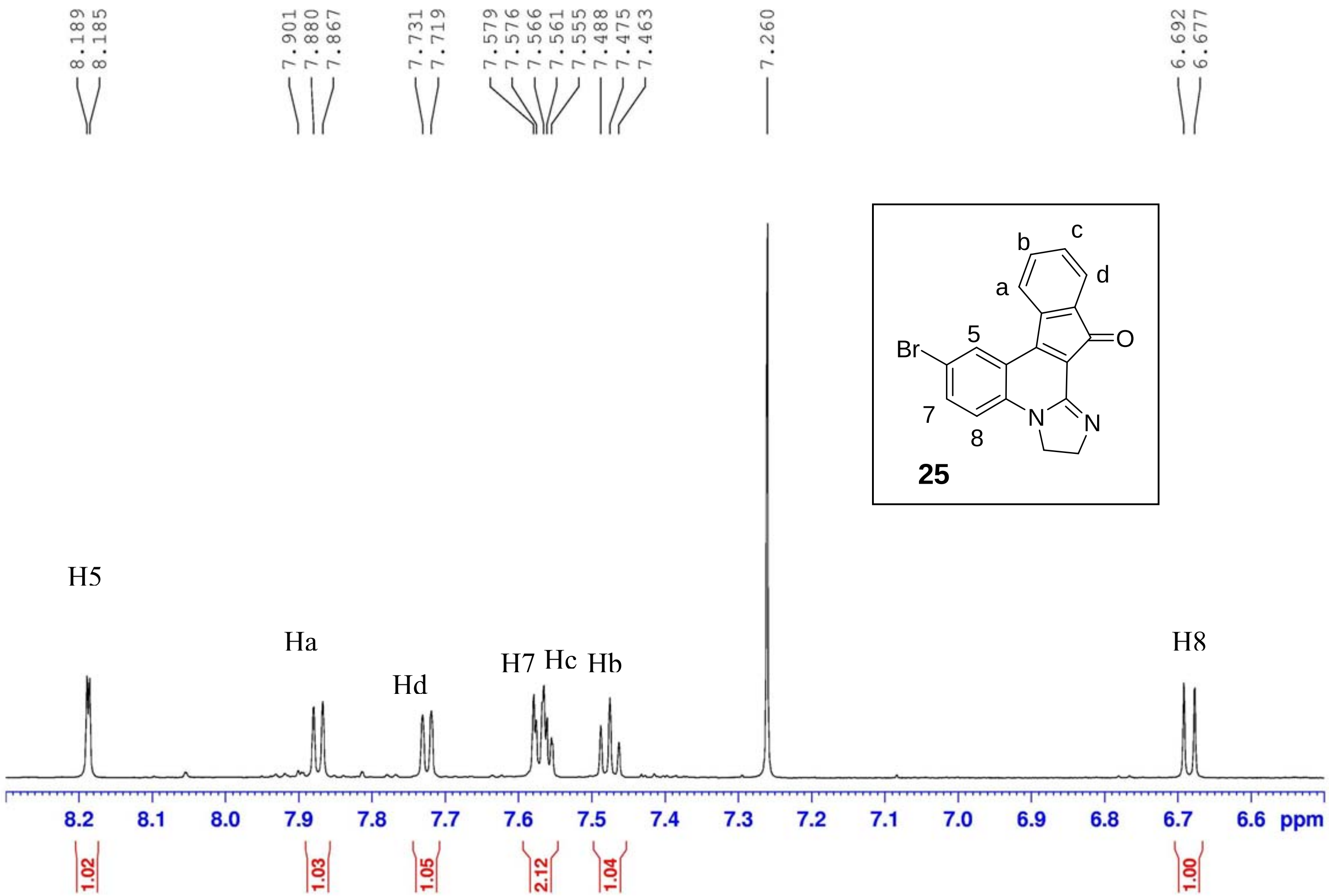
Accumulations: 16

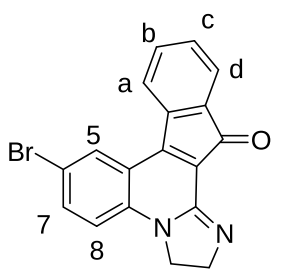
Resolution: 4.00 cm-1

Time: 5:21:48 AM

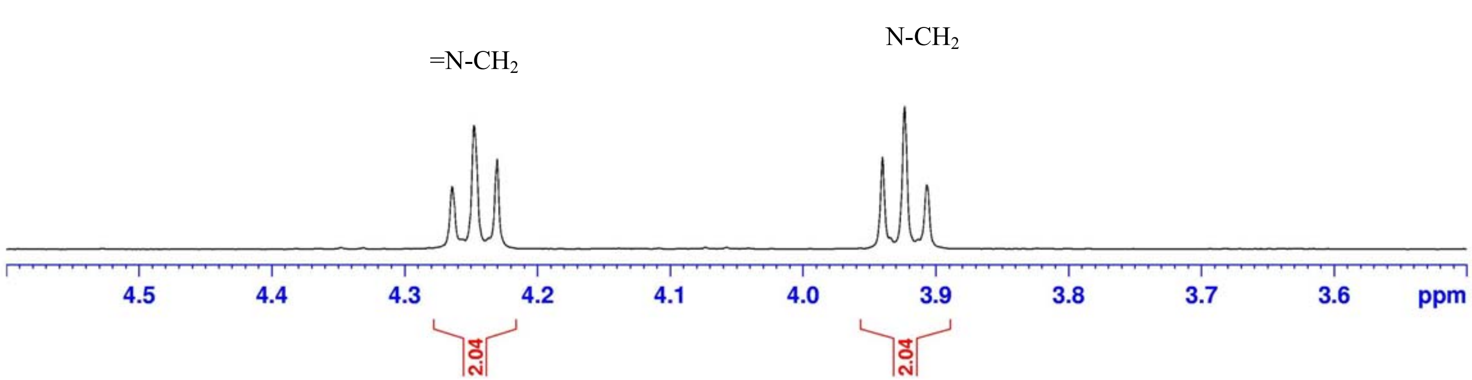
Date: 7/6/2009

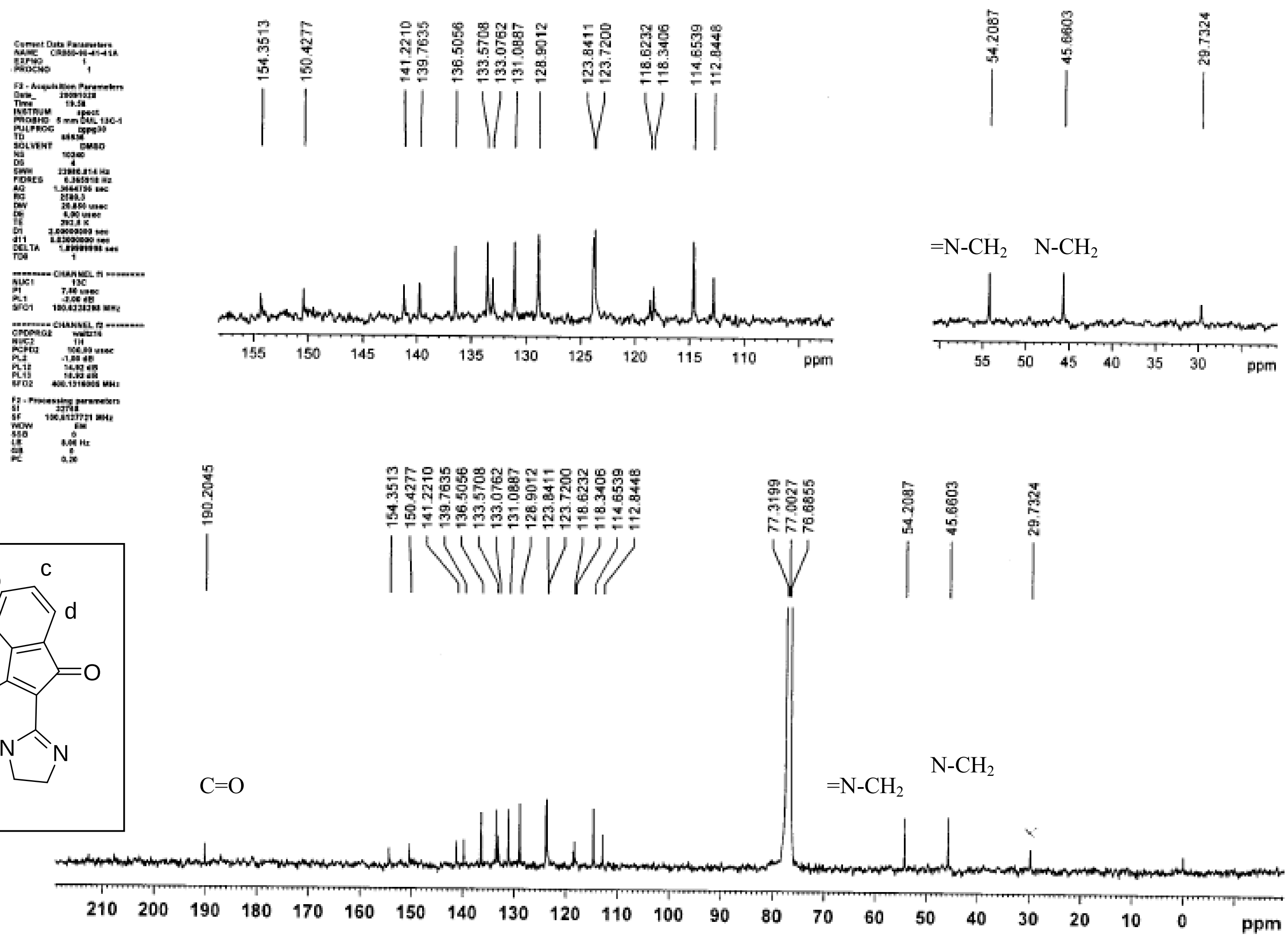
06 JUL 2009


8.189
8.185
7.901
7.880
7.867
7.731
7.719
7.579
7.576
7.566
7.561
7.555
7.488
7.475
7.463
7.260
6.692
6.677
b
c
a
d
5
Br
O
7
N
N
8
25
H5
Ha
Hd
H7
Hc
Hb
H8
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
6.6
ppm
1.02
1.03
1.05
2.12
1.04
1.00

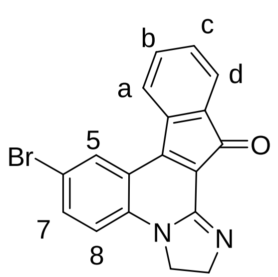


25


4.264
4.257
4.248
4.230
3.940
3.923
3.913
3.907
=N-CH2
N-CH2
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
ppm
2.04
2.04

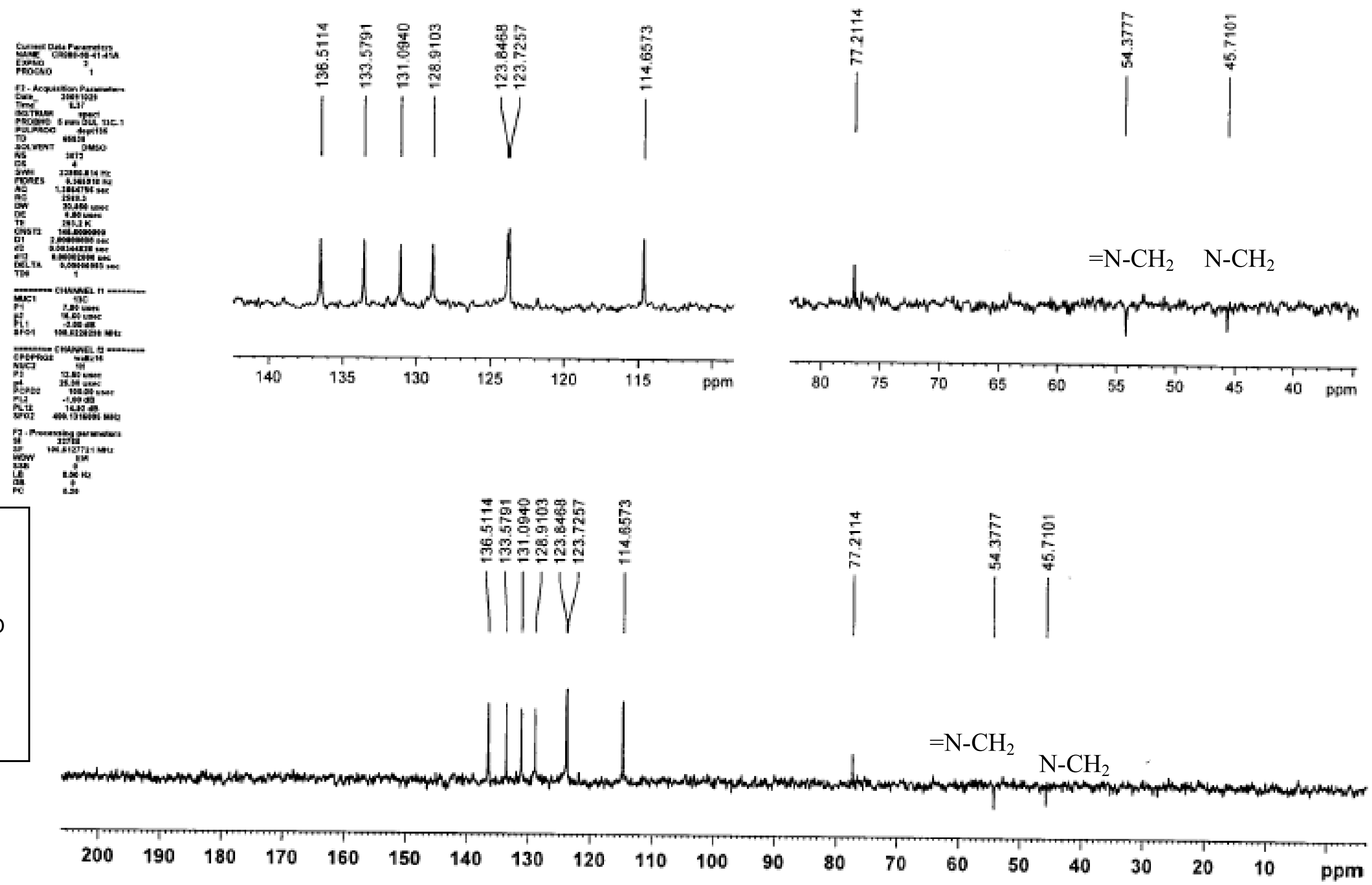


154.3513
150.4277
141.2210
139.7635
136.5056
133.5708
133.0762
131.0887
128.9012
123.8411
123.7200
118.6232
118.3406
114.6539
112.8448
54.2087
45.6603
29.7324
=N-CH2
N-CH2
ppm
190.2045
77.3199
77.0027
76.6855
C=O
=N-CH2
N-CH2
ppm

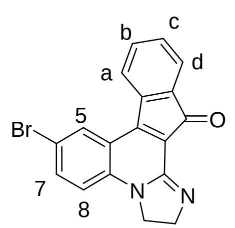


a
b
c
d
5
7
8
Br
O
N
N

25

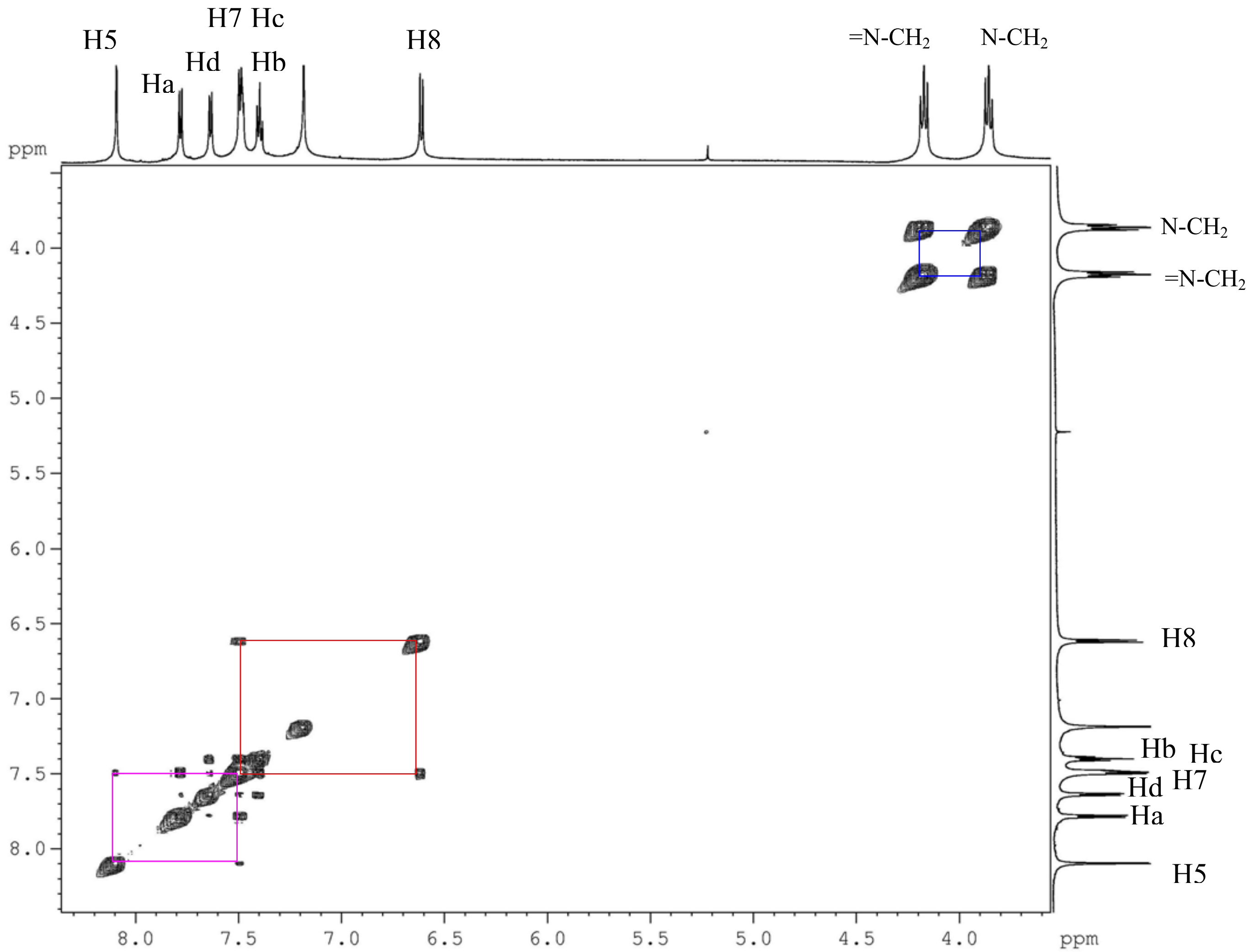


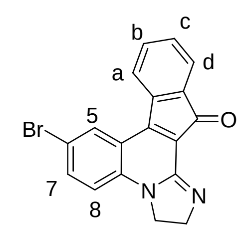
136.5114
133.5791
131.0940
128.9103
123.8468
123.7257
114.6573
77.2114
54.3777
45.7101
=N-CH2
N-CH2
ppm



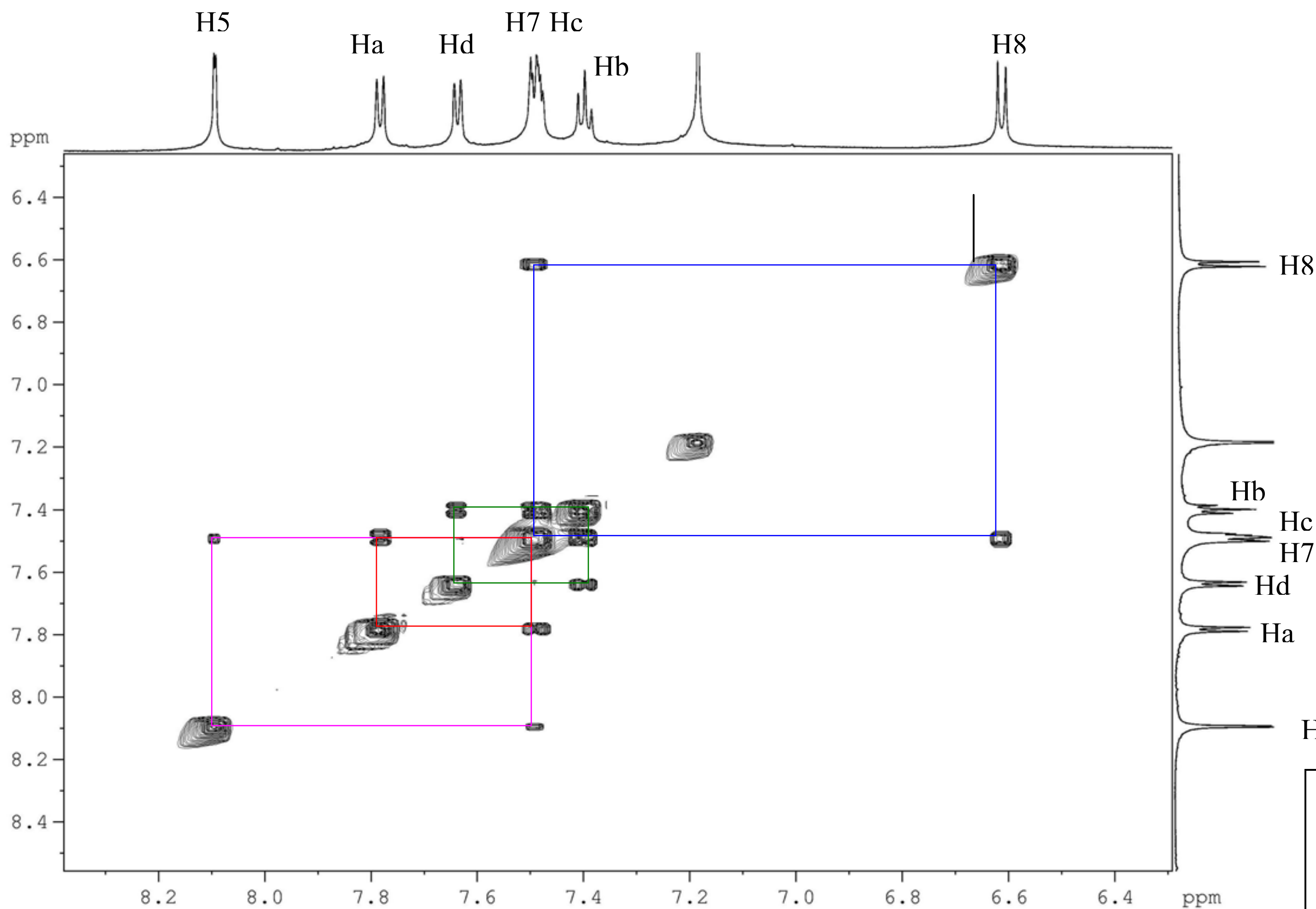
Br
5
7
8
a
b
c
d
O
N
N

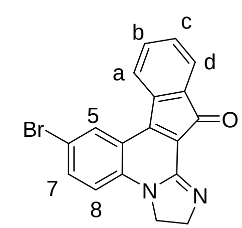
25


H5
Ha
Hd
H7 Hc
Hb
H8
=N-CH2
N-CH2
ppm
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
N-CH2
=N-CH2
H8
Hb Hc
Hd H7
Ha
H5

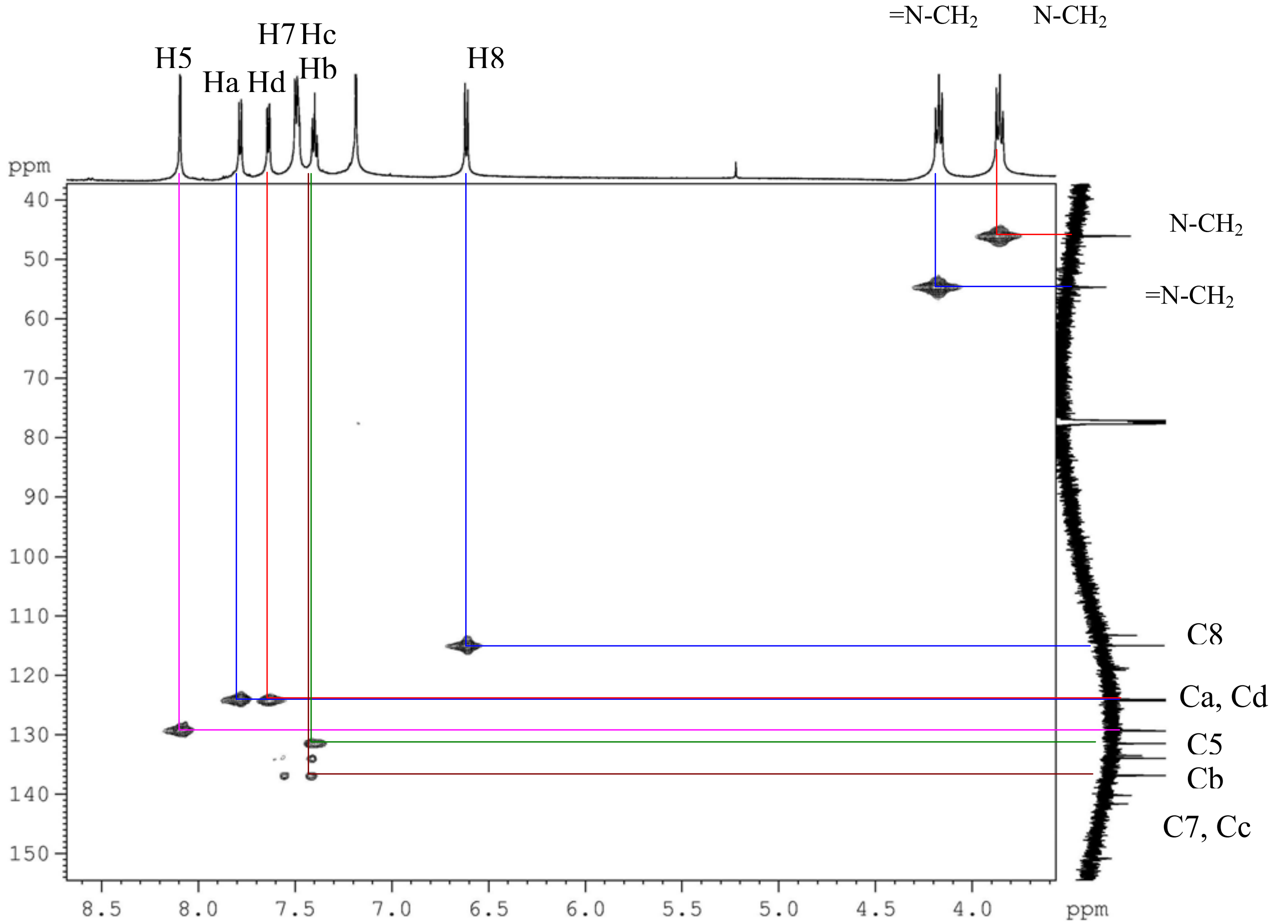

b
c
a
d
5
Br
O
7
8
N
N

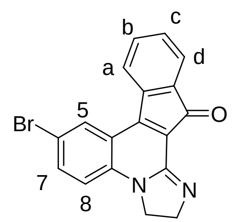
25


H5
Ha
Hd
H7 Hc
Hb
H8
ppm
6.4
6.6
6.8
7.0
7.2
7.4
7.6
7.8
8.0
8.2
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
ppm
H8
Hb
Hc
H7
Hd
Ha
H5

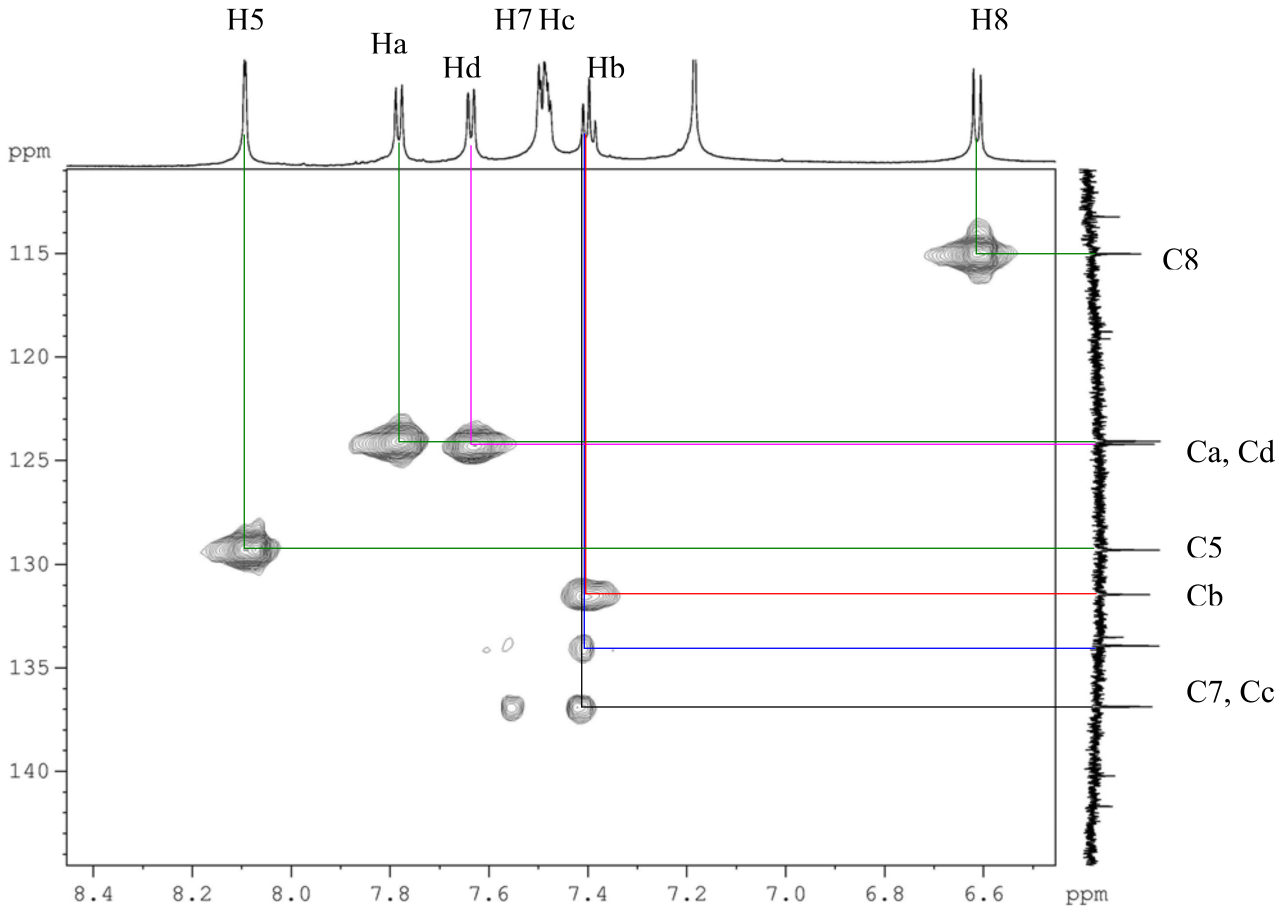

Br
5
7
8
a
b
c
d
N
N
O

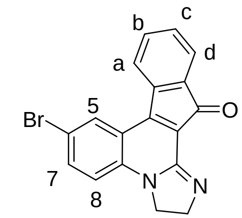
25


H5
Ha
Hd
H7
Hc
Hb
H8
=N-CH$_2$
N-CH$_2$
ppm
N-CH$_2$
=N-CH$_2$
C8
Ca, Cd
C5
Cb
C7, Cc
40
50
60
70
80
90
100
110
120
130
140
150
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm

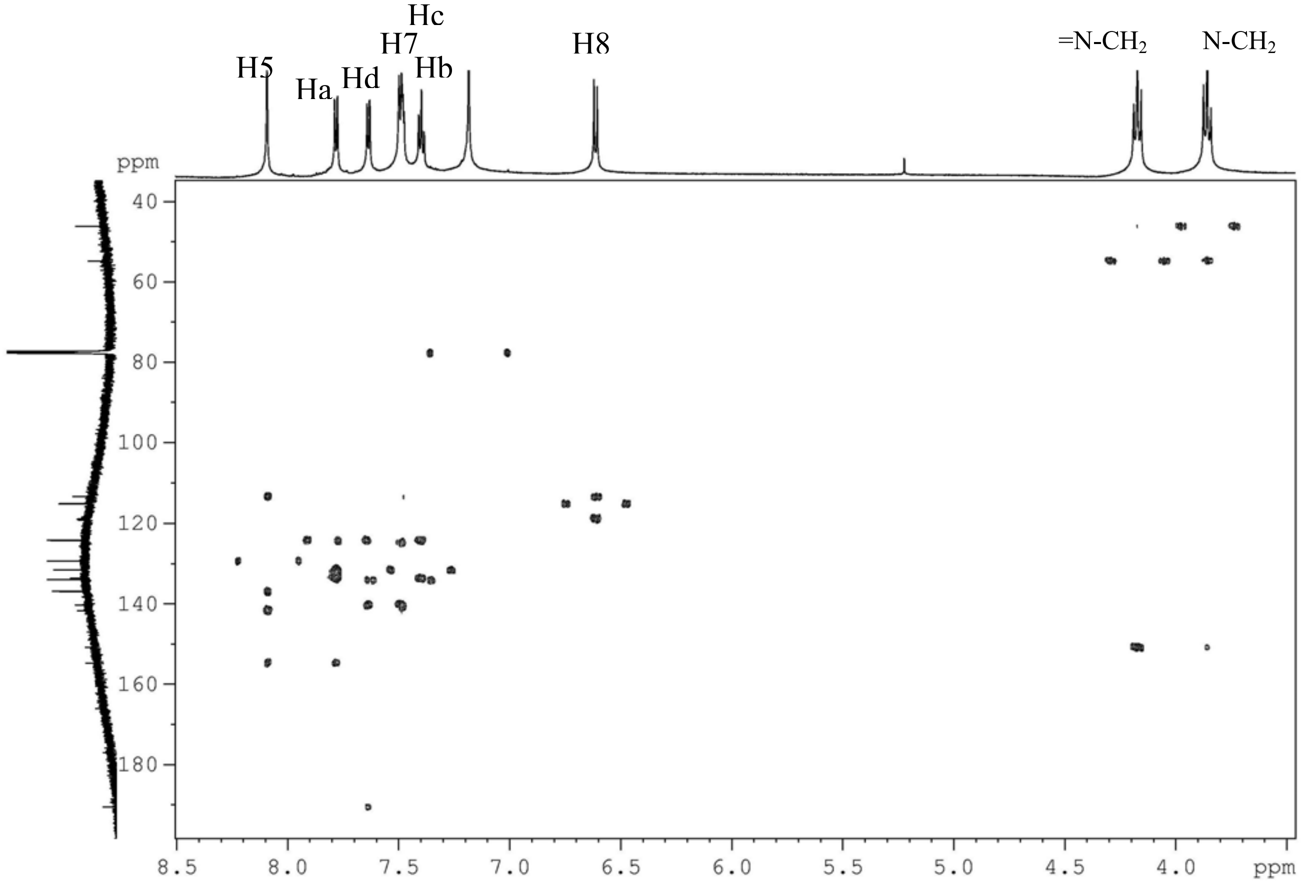

b
c
d
a
5
O
Br
7
N
N
8

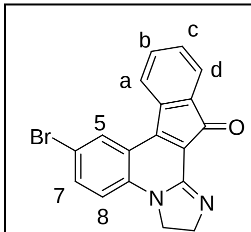
25


H5
Ha
Hd
H7 Hc
Hb
H8
ppm
C8
Ca, Cd
C5
Cb
C7, Cc
115
120
125
130
135
140
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm

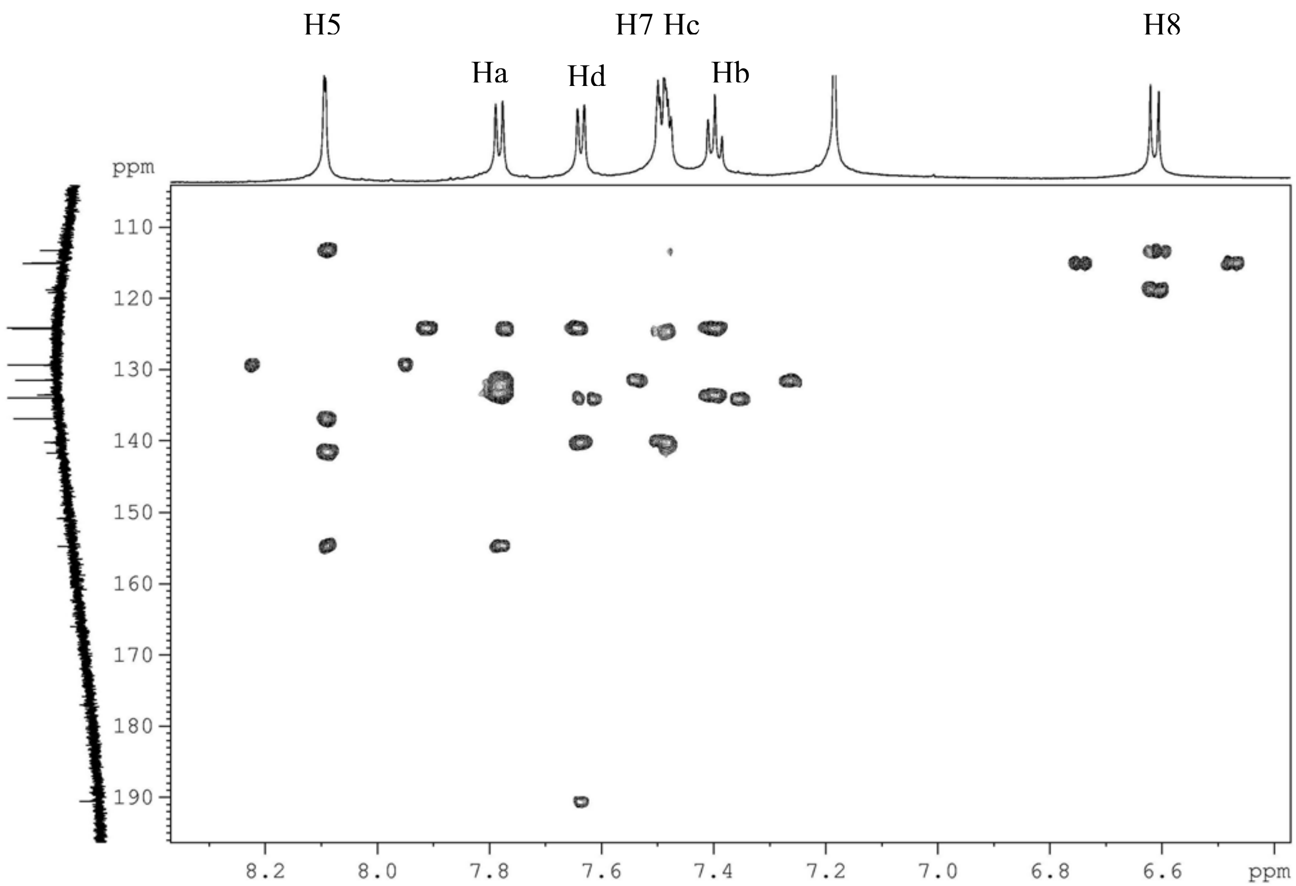

b
c
a
d
Br
5
O
7
N
N
8

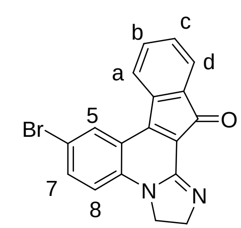
25


H5
Ha
Hd
H7
Hc
Hb
H8
=N-CH$_2$
N-CH$_2$
ppm
40
60
80
100
120
140
160
180
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm

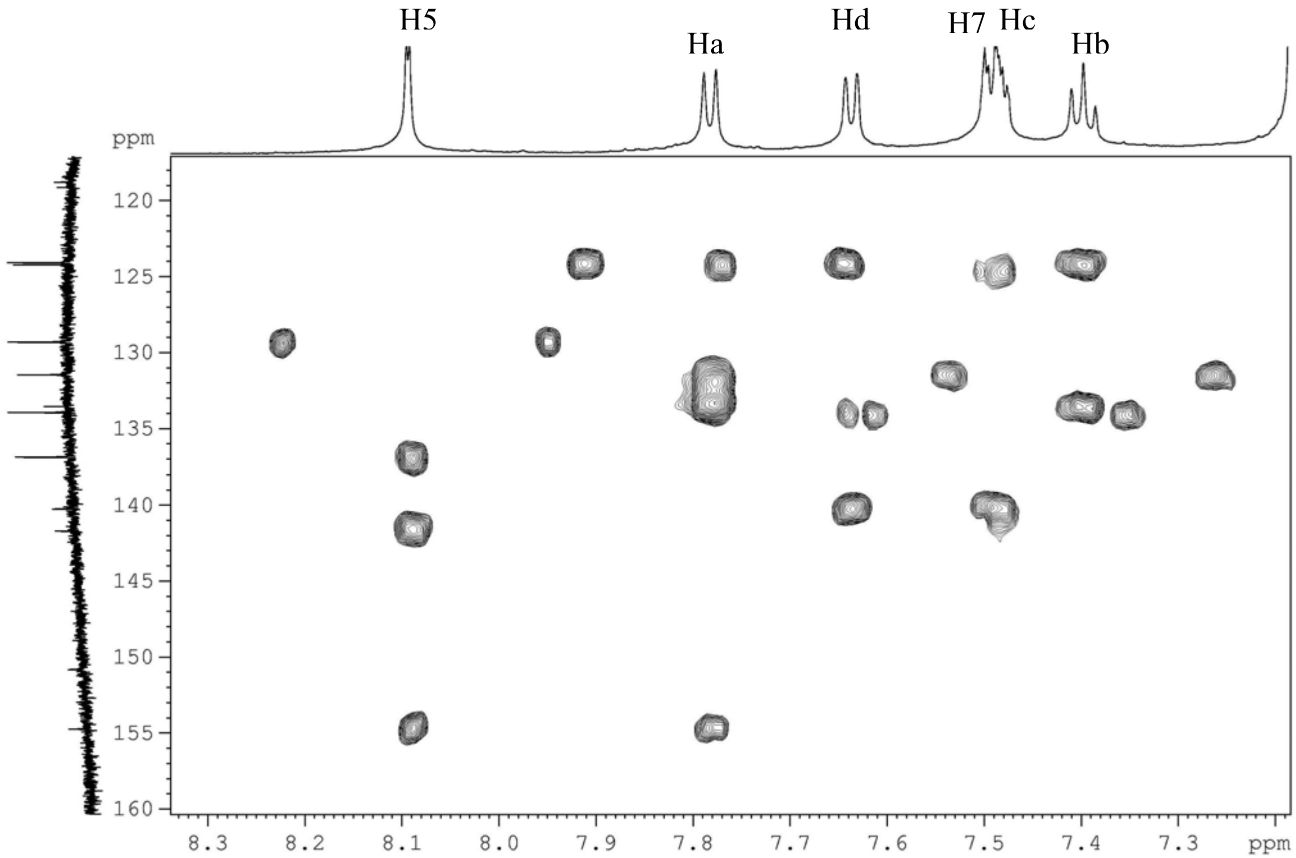

b
c
a
d
5
Br
O
7
8
N
N

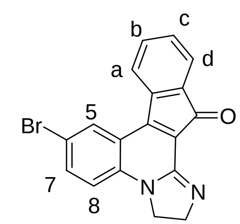
25


H5
Ha
Hd
H7 Hc
Hb
H8
ppm
110
120
130
140
150
160
170
180
190
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm

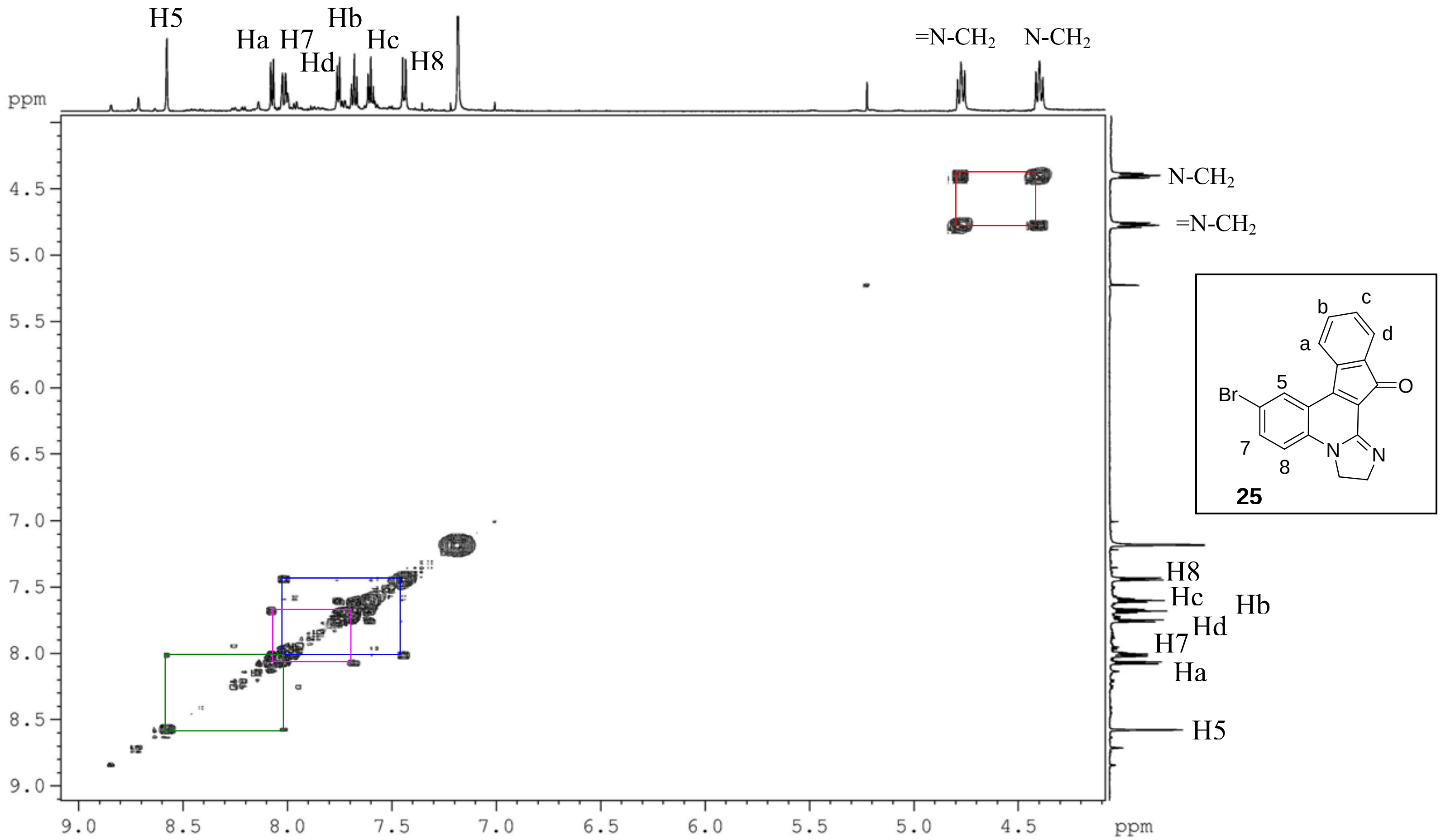

b
c
a
d
Br
5
O
7
8
N
N

25

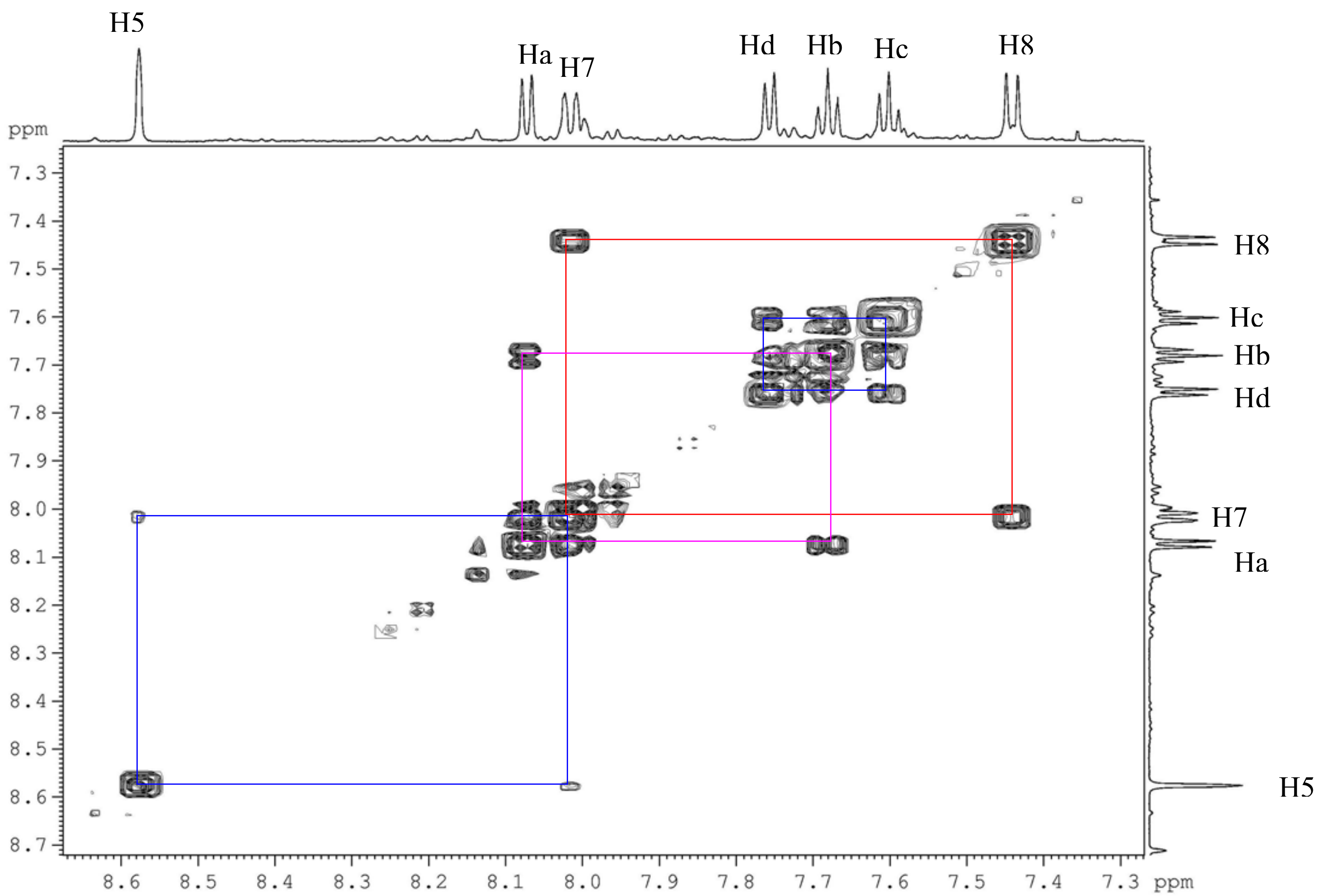

H5
Ha
Hd
H7
Hc
Hb
ppm
120
125
130
135
140
145
150
155
160
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm

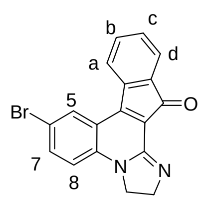

b
c
d
a
5
Br
O
7
8
N
N

25



H5
Ha
H7
Hd
Hb
Hc
H8
=N-CH$_2$
N-CH$_2$
ppm
N-CH$_2$
=N-CH$_2$
Br
5
7
8
a
b
c
d
O
N
N
25
H8
Hc
Hb
Hd
H7
Ha
H5

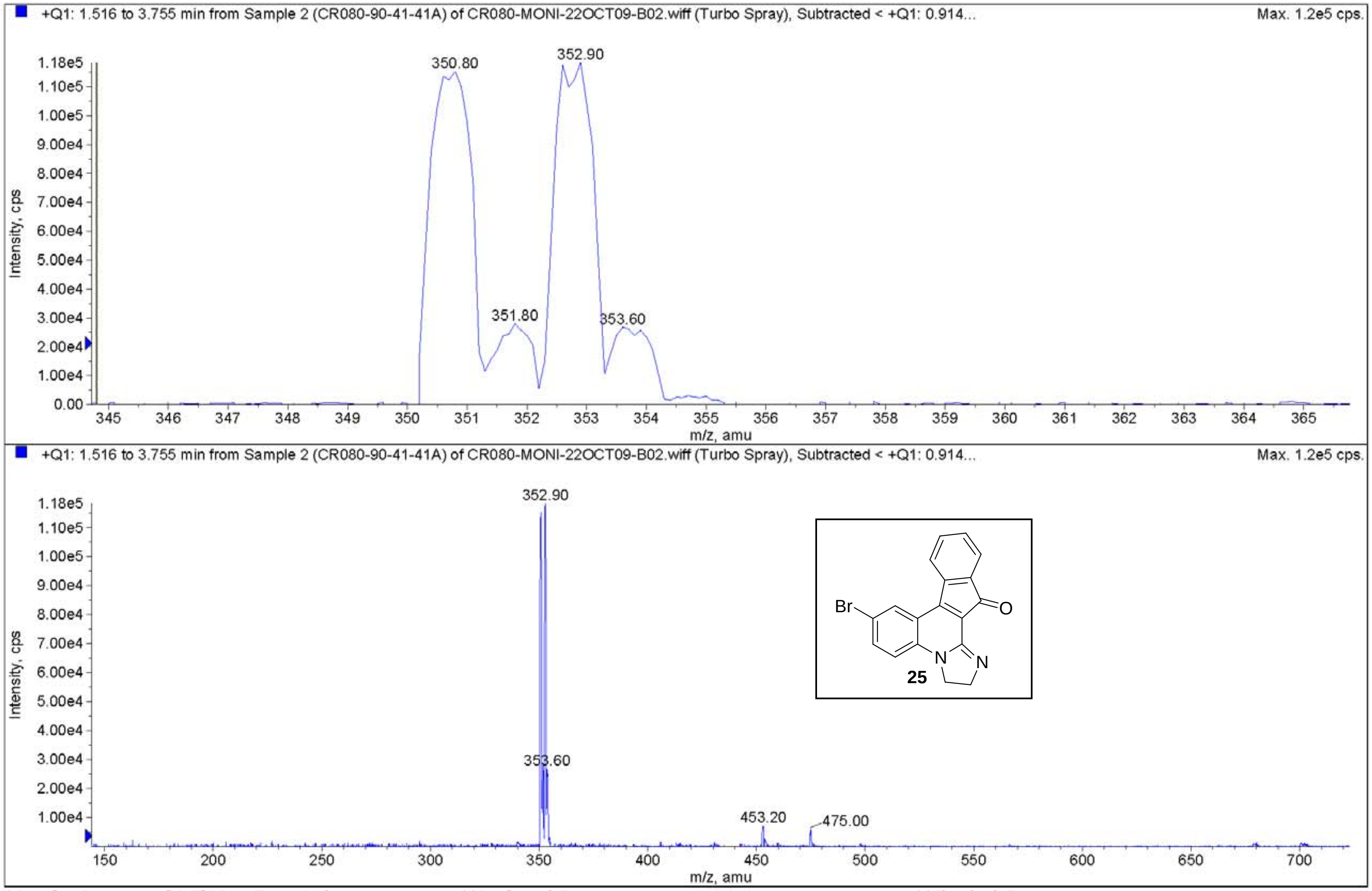

H5
Ha
H7
Hd
Hb
Hc
H8
ppm
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
8.6
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3 ppm
H8
Hc
Hb
Hd
H7
Ha
H5


b
c
a
d
Br
5
O
7
8
N
N
25

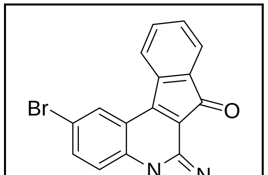
*

INDIA

Sample Name: CR080-90-41-41A   Acq. Time: 15:32   Acq. Date: Thursday, October 22, 2009

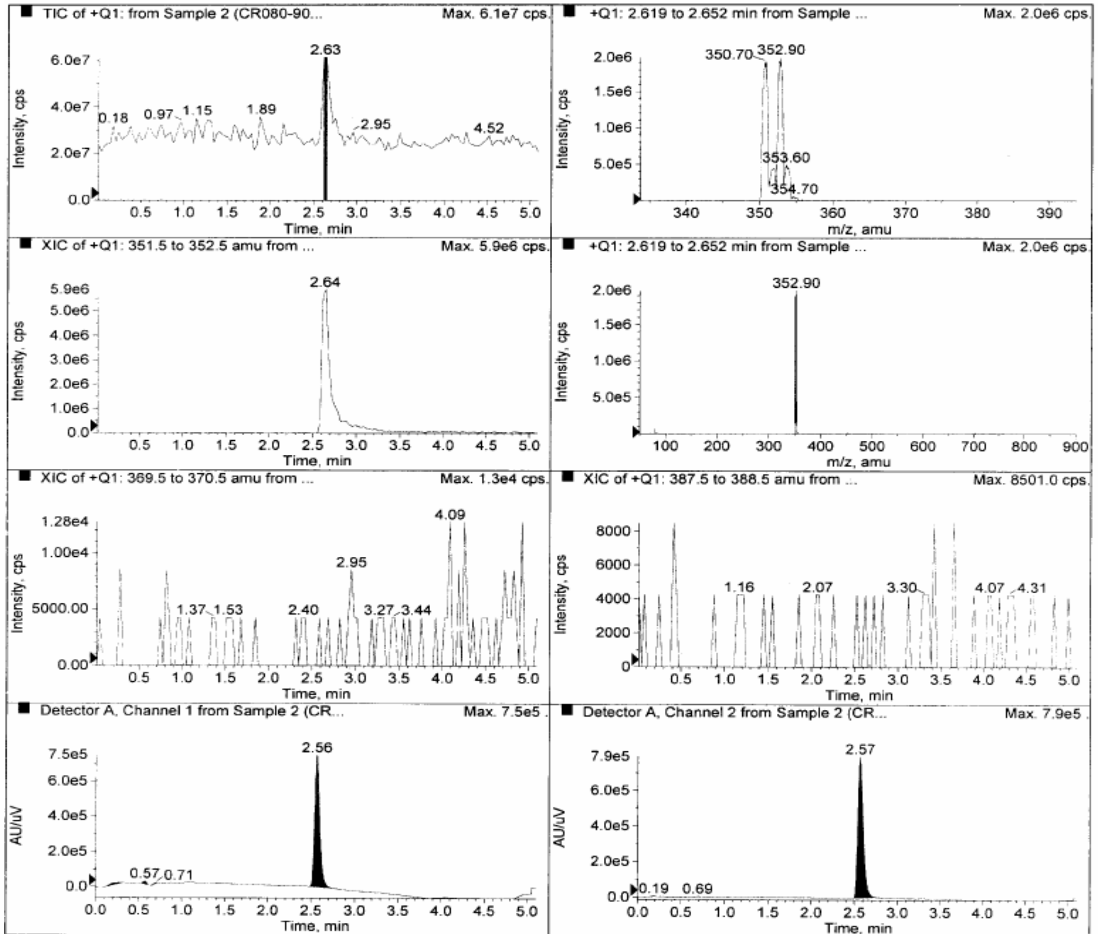


*Sample Comment: [M+H]351 Expected   **Analyzed By :   **Checked By :



25

Sample Name: CR080-90-41-41A Acq. Time: 15:32 Acq. Date: Thursday, October 22, 2009



Peak List for "Detector A, Channel 1 from Sample 2 (CR080-90-41-

	Time (min)	Area (counts)	%Area	Height
2	0.5710	5.5280e4	1.6366	1.9162e4
3	0.7070	1.0311e4	0.3052	3196.1749
4	2.5643	3.2437e6	96.0301	7.5053e5

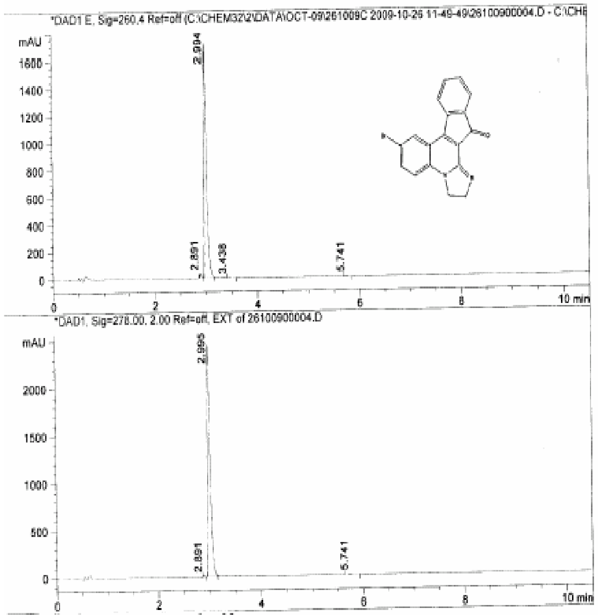
Peak List for "Detector A, Channel 2 from Sample 2 (CR080-90-41-4

	Time (min)	Area (counts)	%Area	Height
2	0.6939	1987.9664	0.0565	894.3511
3	2.5655	3.5131e6	99.7913	7.9201e5
4	3.2862	2152.8718	0.0612	818.0143

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

Sample:CR080-90-41-41A
Column: ZORBAX SB-C18(50X4.6)mm 1.8µ
Injection date :Mon, 26. Oct. 2009 Location : Vial 13
Sample Name :CR080-90-41-41A Inj. No. : 1
Acq Operator :BHUSHAN Inj. Vol. : 5 µl
Analysis Method :C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _5.M
Last Changed :Wed, 21. Oct. 2009,
Acq. Method :C:\Chem32\2\DATA\OCT-09\261009C 2009-10-26 11-49-49\
UPLC_GENARAL_GRAD _5.M
Method ref : DI/A0257/44



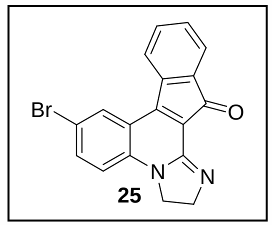
DAD1 E, Sig=260,4 Ref=off

Peak #	RT (Min)	Width (Min)	Area	Area %
1	2.891	0.032	56.220	0.960
2	2.994	0.056	5776.617	98.623
3	3.438	0.061	7.964	0.136
4	5.741	0.069	16.446	0.281

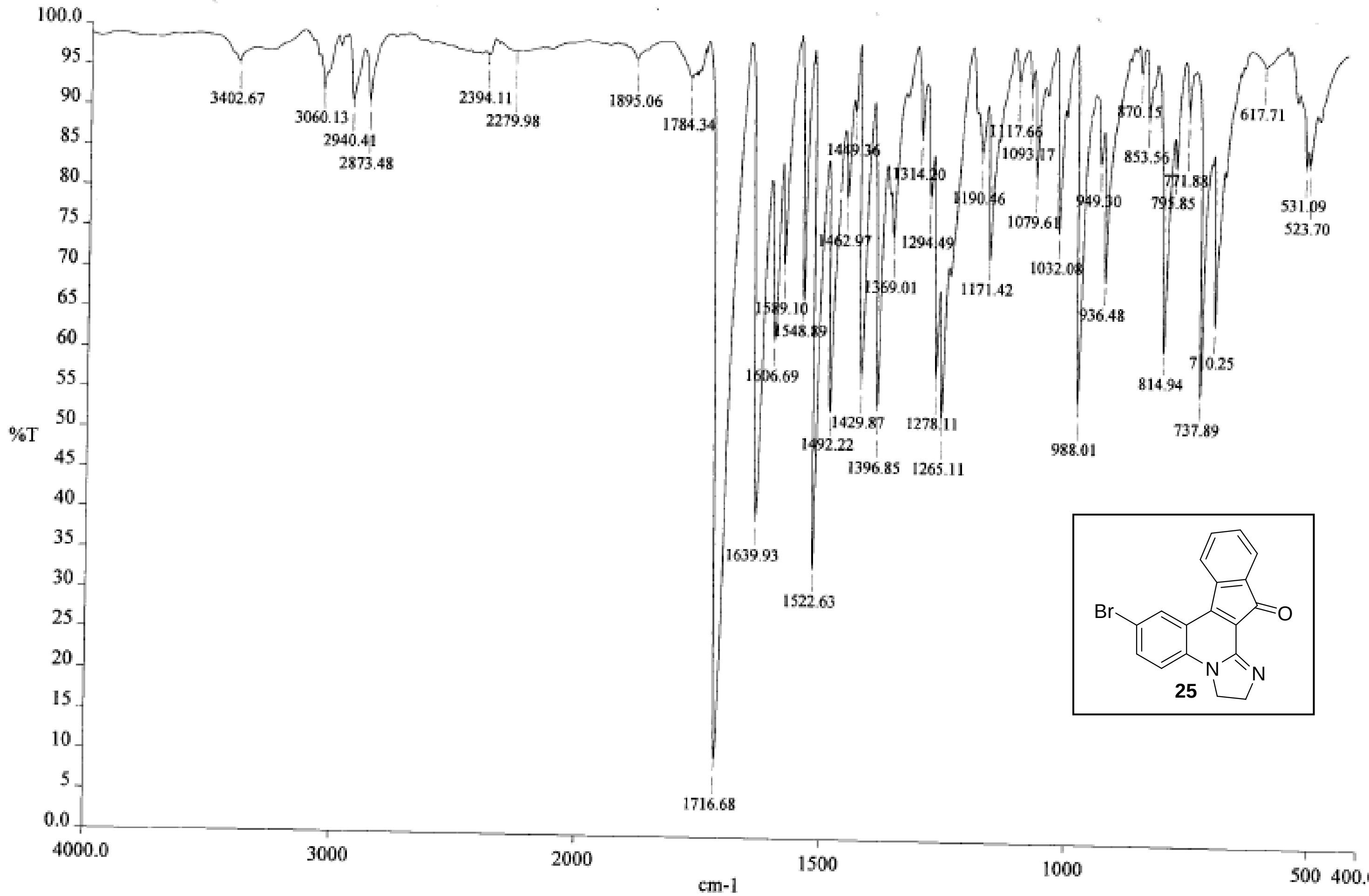
DAD1, Sig=278.00, 2.00 Ref=off, EXT

Peak #	RT (Min)	Width (Min)	Area	Area %
1	2.891	0.029	17.050	0.197
2	2.995	0.058	8586.340	99.424
3	5.741	0.085	32.673	0.378

*** End of Report***



25



Spectrum Name: CR080-67-183-183A1.sp

Description: CR080-67-183-183A1 IN KBr

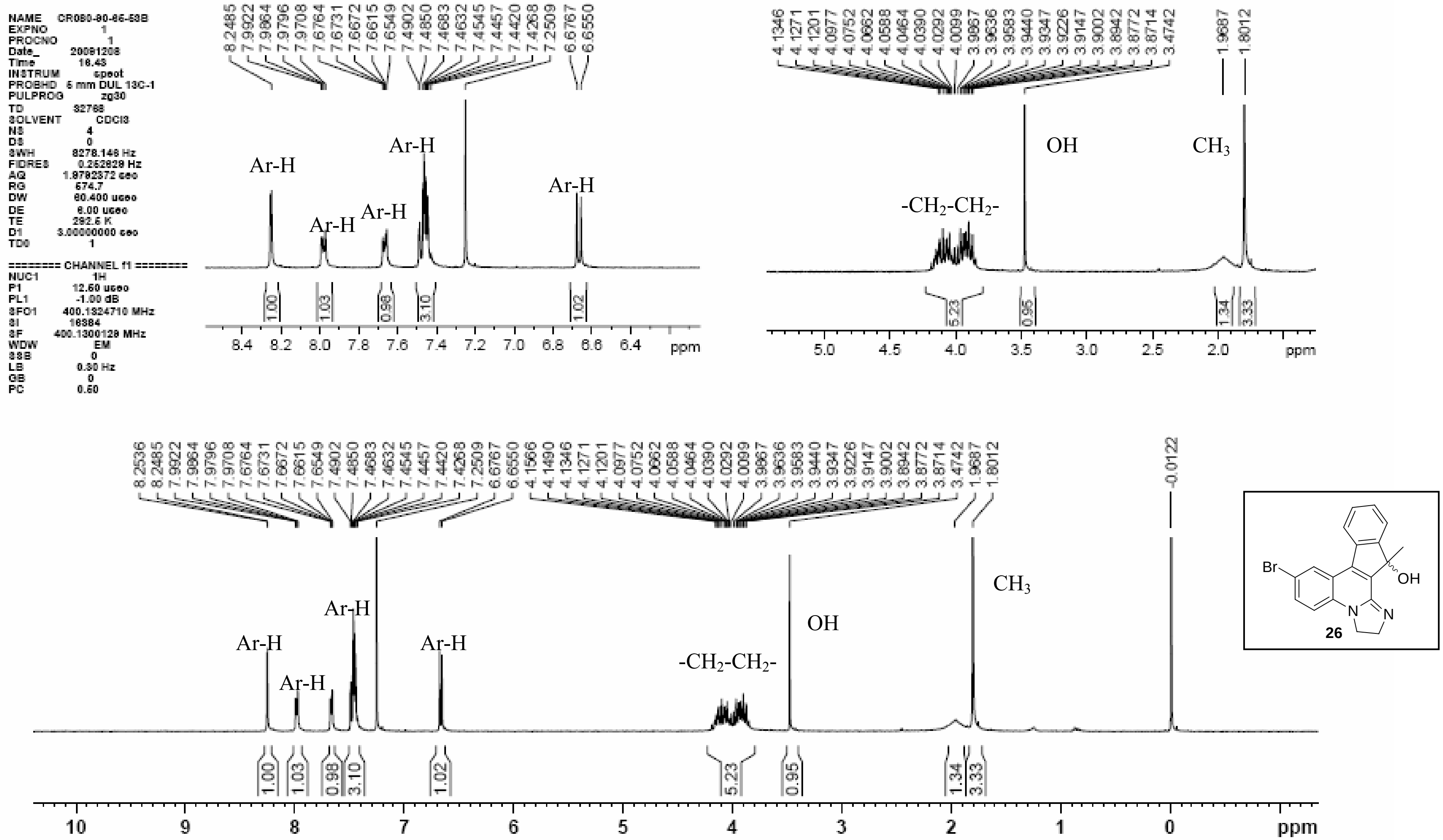
Analyst : GANESH Z

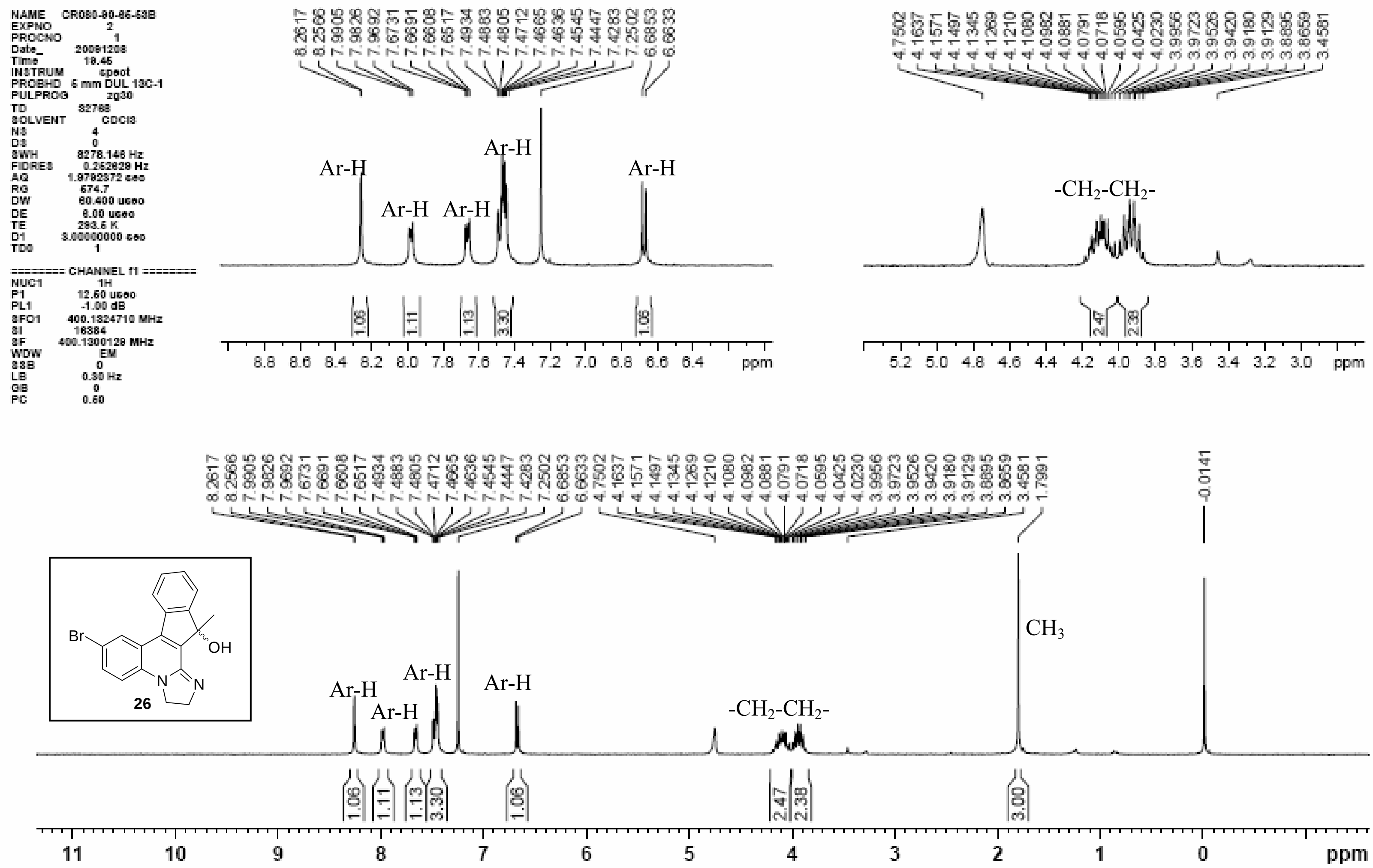
Accumulations: 16

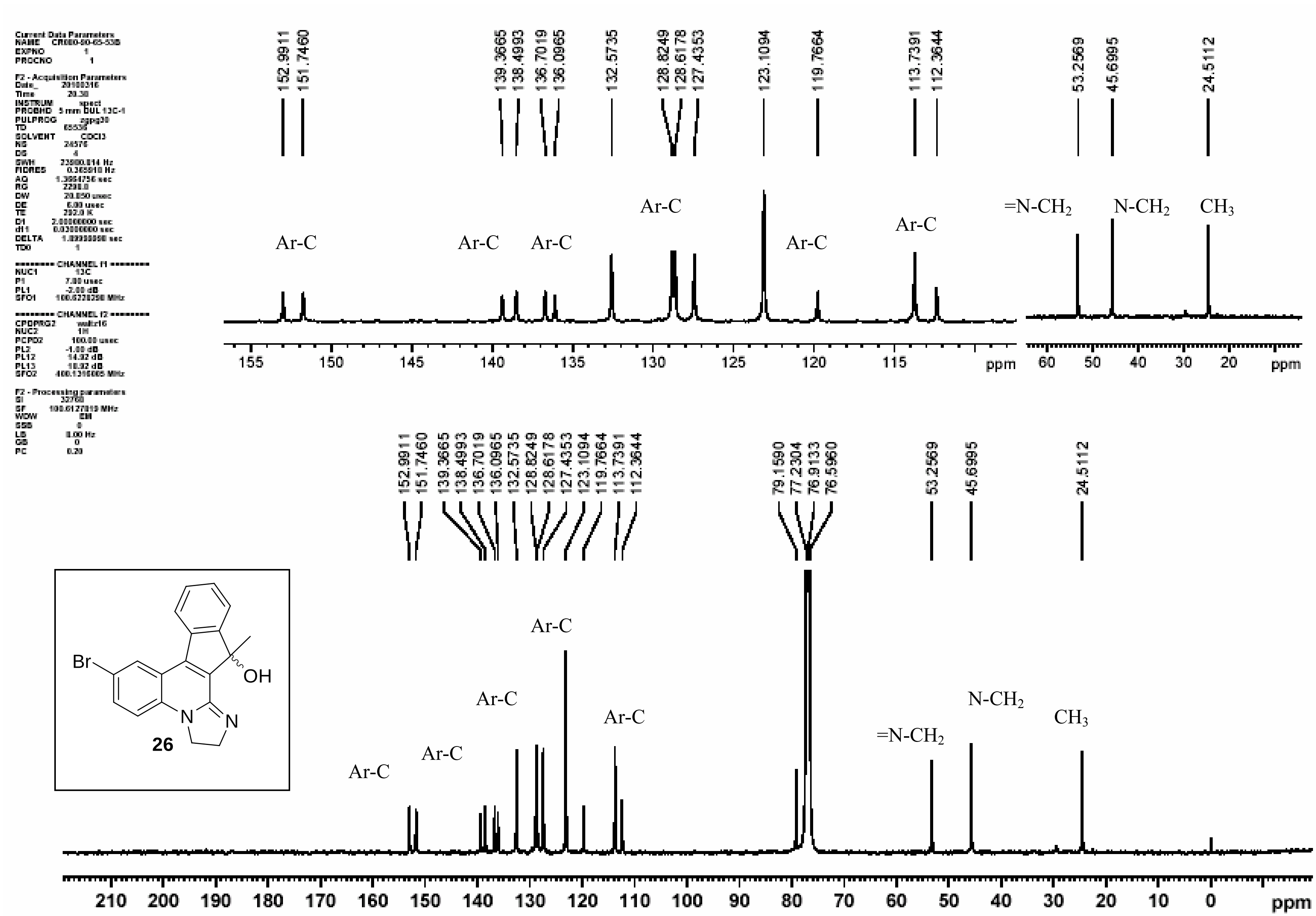
Resolution: 4.00 cm-1

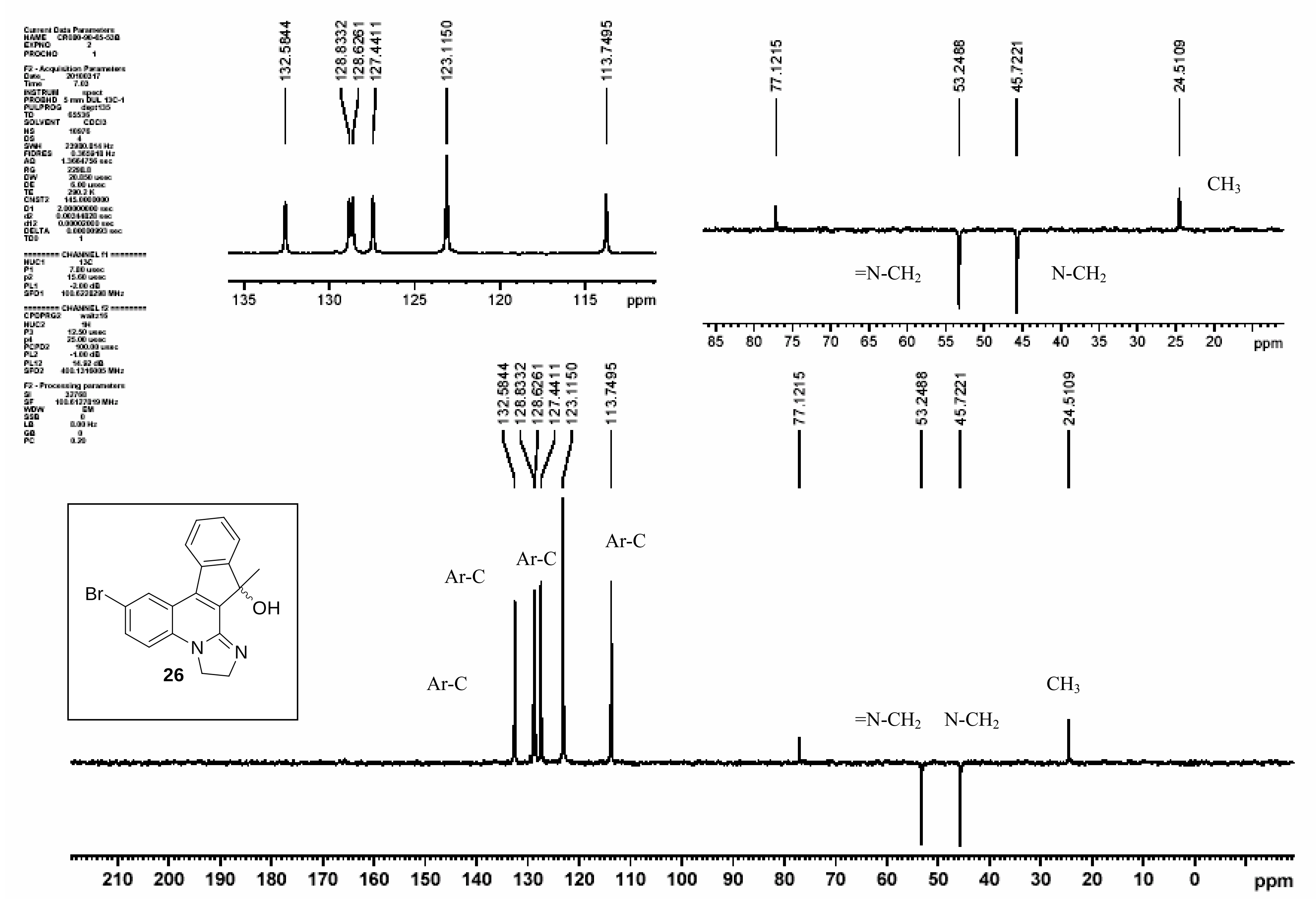
Time: 4:30:59 PM

Date: 7/8/2009


NAME CR090-90-66-53B
EXPNO 1
PROCNO 1
Date_ 20091208
Time 16.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8278.146 Hz
FIDRES 0.252628 Hz
AQ 1.9792372 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 292.5 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
-CH2-CH2-
OH
CH3
ppm
Br
OH
N
N
26


NAME CR080-90-86-53B
EXPNO 2
PROCNO 1
Date_ 20091208
Time 18.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 293.6 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
-CH2-CH2-
CH3
Br
OH
N
N
26
ppm

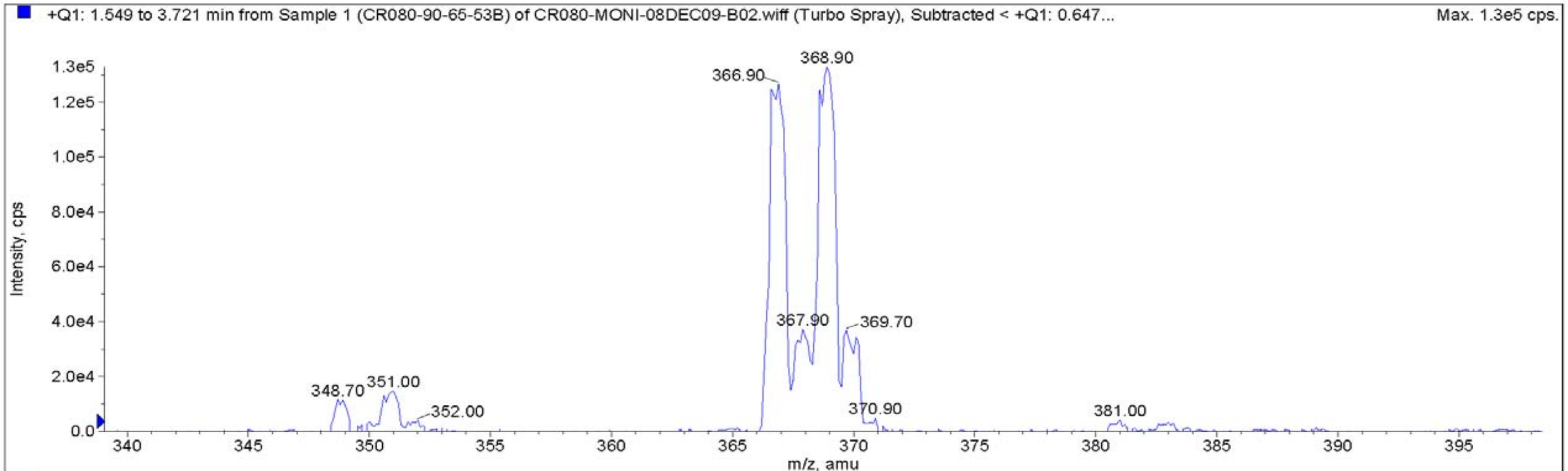

152.9911
151.7460
139.3665
138.4993
136.7019
136.0965
132.5735
128.8249
128.6178
127.4353
123.1094
119.7664
113.7391
112.3644
53.2569
45.6995
24.5112
79.1590
77.2304
76.9133
76.5960
Ar-C
=N-CH2
N-CH2
CH3
ppm
Br
OH
N
26

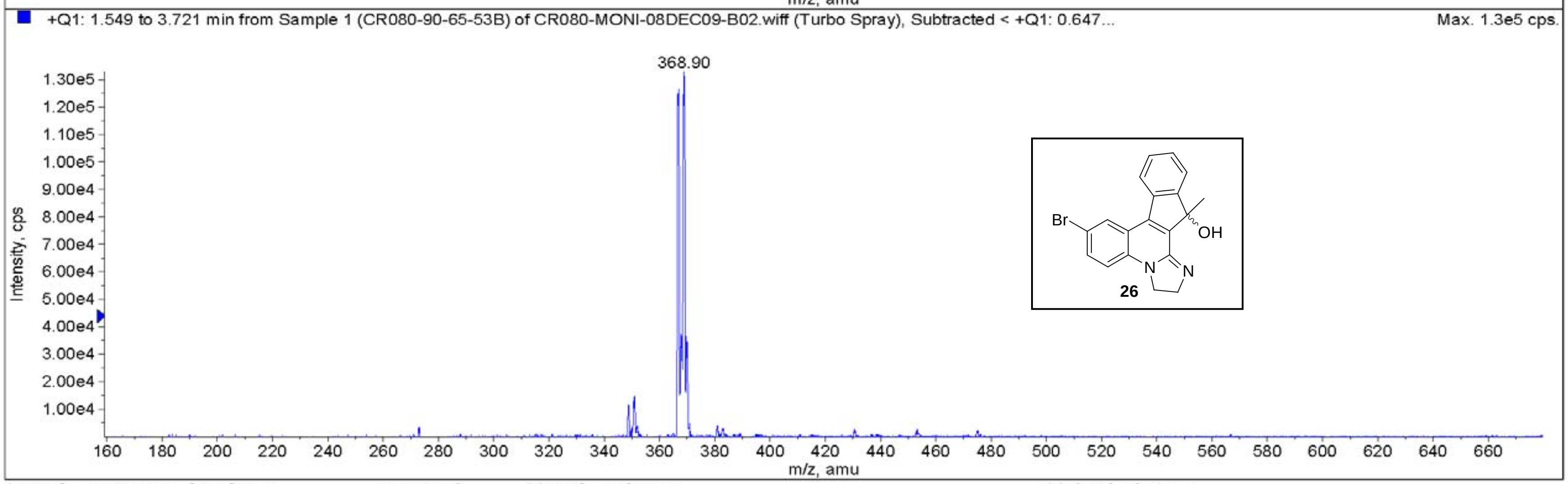

132.5844
128.8332
128.6261
127.4411
123.1150
113.7495
77.1215
53.2488
45.7221
24.5109
CH3
=N-CH2
N-CH2
Ar-C
Br
OH
N
26
ppm

*

INDIA

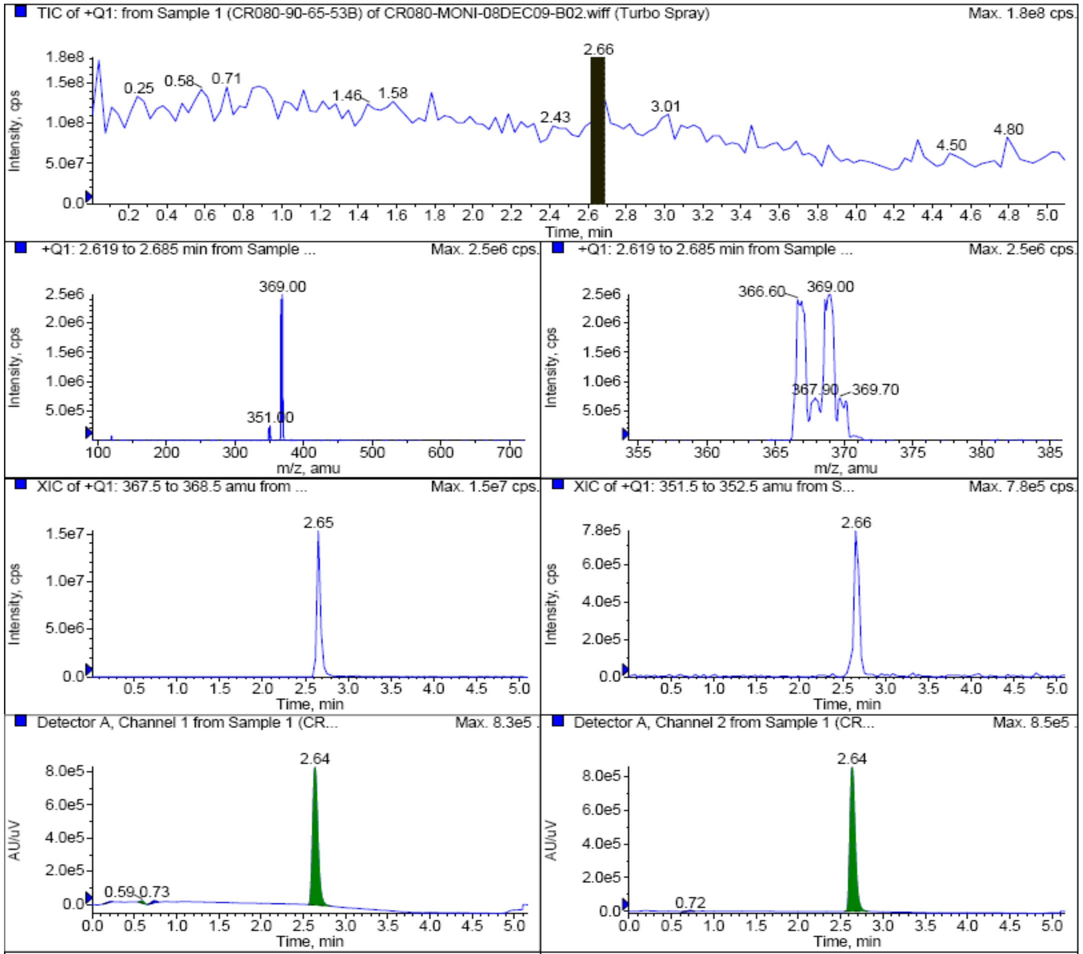
Sample Name: CR080-90-65-53B Acq. Time: 16:38 Acq. Date: Tuesday, December 08, 2009

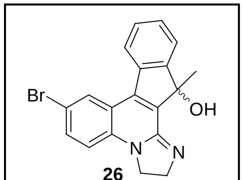




*Sample Comment: [M+H]367 Expected **Analyzed By : **Checked By :

Sample Name: CR080-90-65-53B Acq. Time: 16:38 Acq. Date: Tuesday, December 08, 2009





26

Peak List for "Detector A, Channel 1 from Sample 1 (CR080-90-65-

	Time (min)	Area (counts)	% Area	Height
2	0.5873	4.1746e4	1.1596	1.4379e4
3	0.7333	5.3065e4	1.4740	1.3802e4
4	2.6378	3.4912e6	96.9735	8.2786e5

Peak List for "Detector A, Channel 2 from Sample 1 (CR080-90-65-

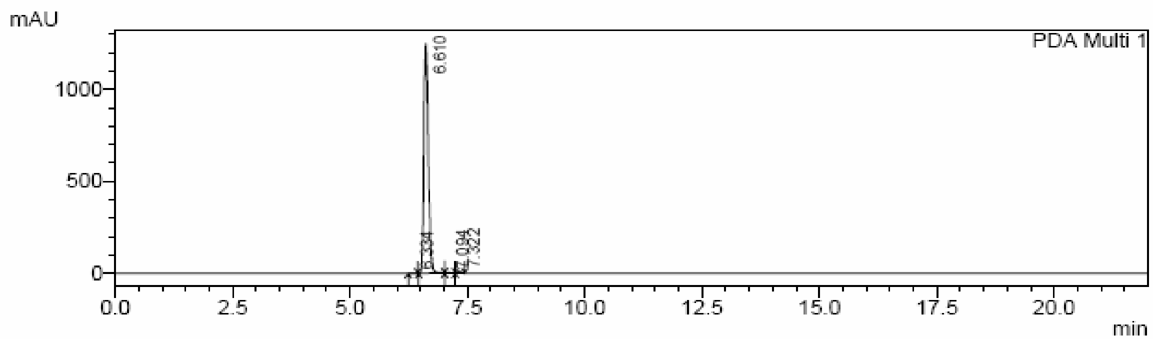
	Time (min)	Area (counts)	% Area	Height
1	0.7224	2.7191e4	0.7458	5739.3274
2	2.6367	3.6186e6	99.2542	8.5385e5

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

Sample Name : CR080-90-65-53B
Sample ID : CR080-90-65-53B
Column : Xterra RP-18 (250 x 4.6 mm) 5u
Vial # : 22
Inj. Volume : 2 uL
Tray # : 2
Acquired by : AVINASH

Data File Name : 17-02-10_CR080-90-65-53B_01.lcd
Method File Name : GENERAL_B11.lcm
Batch File Name : 170210.lcb
Data Acquired : 2/18/2010 3:32:59 AM
Data Processed : 2/18/2010 4:03:02 AM
Ref.No.: DI/A0257/97

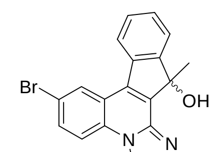


1 PDA Multi 1/252nm 4nm

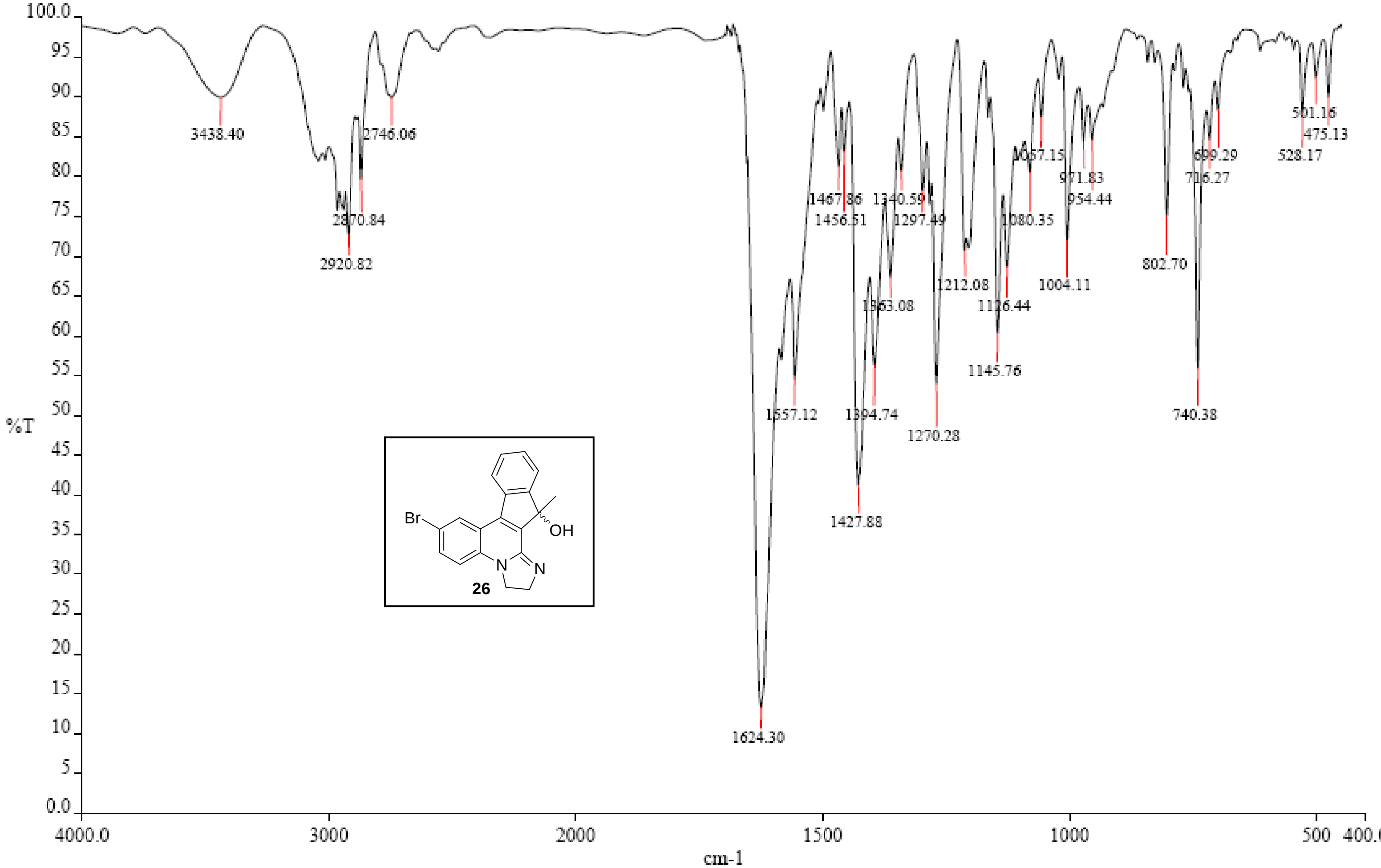
PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	6.33	3095	0.04	563
2	6.61	7980395	99.14	1247755
3	7.09	14101	0.18	1716
4	7.32	52185	0.65	9224
Total		8049776	100.00	1259258



26



Spectrum Name: CR080-90-65-53B.sp

Analyst: GANESH

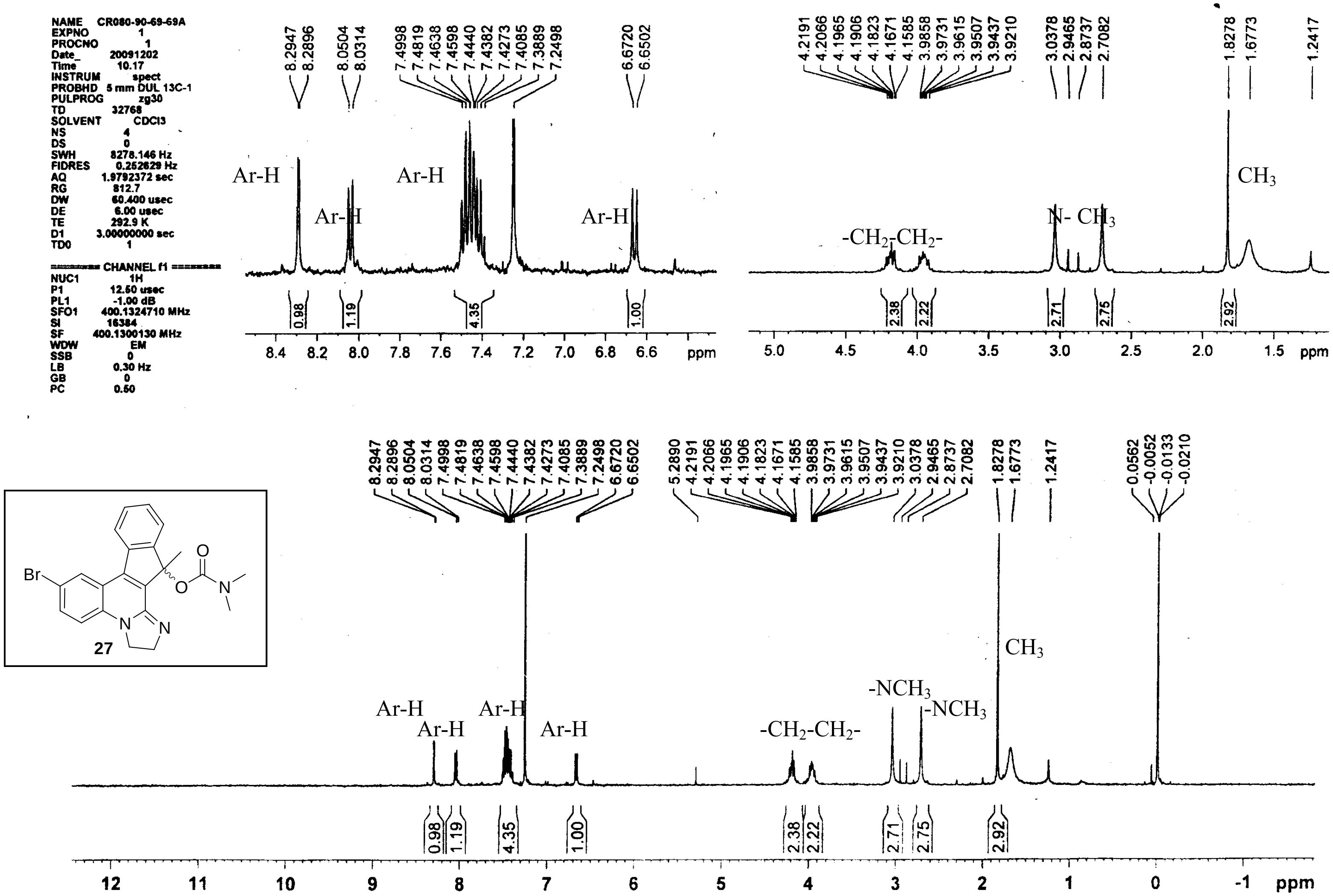
Accumulations: 16

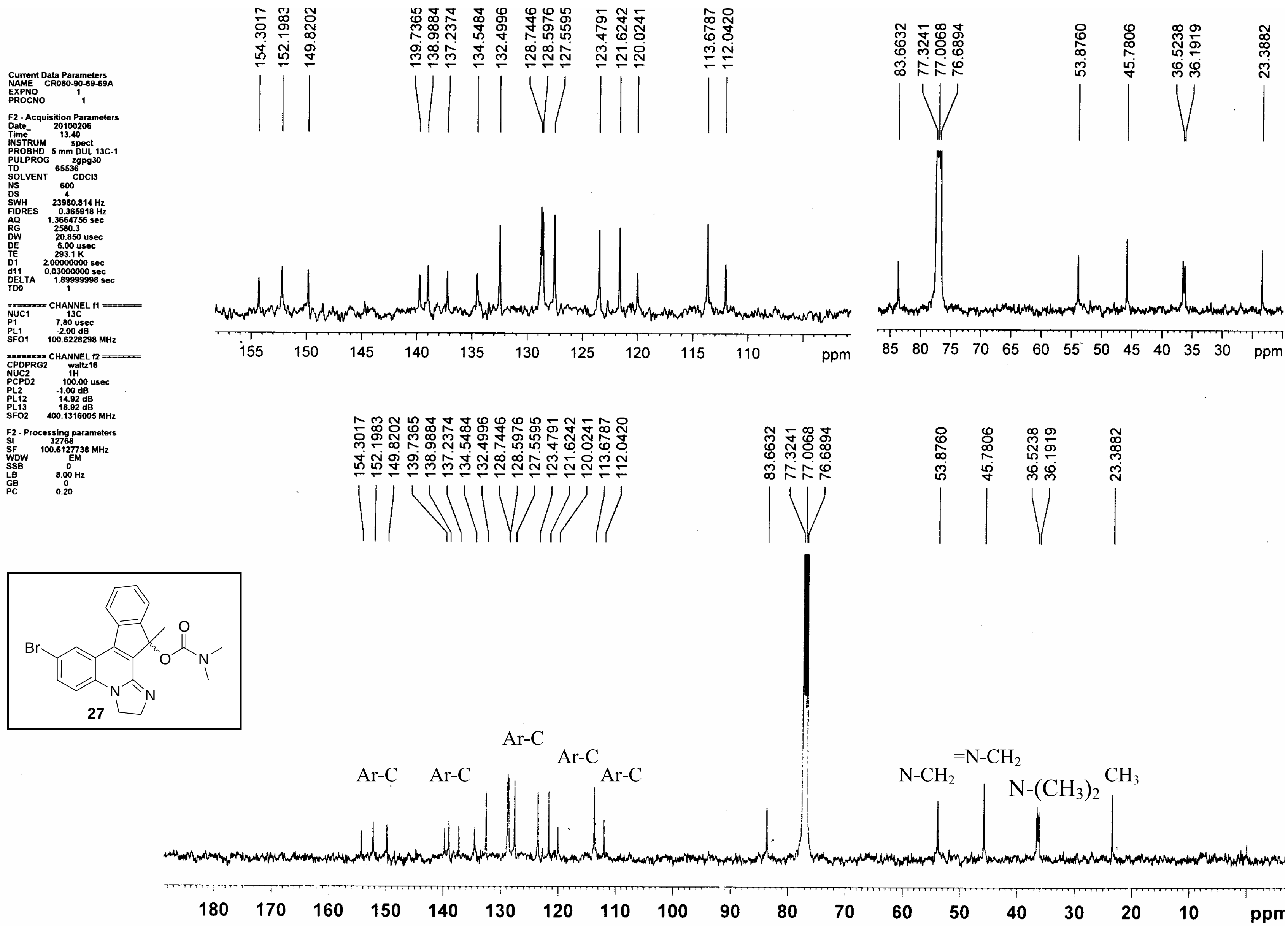
Time: 11:15:50 AM

Description: CR080-90-65-53B IN KBr

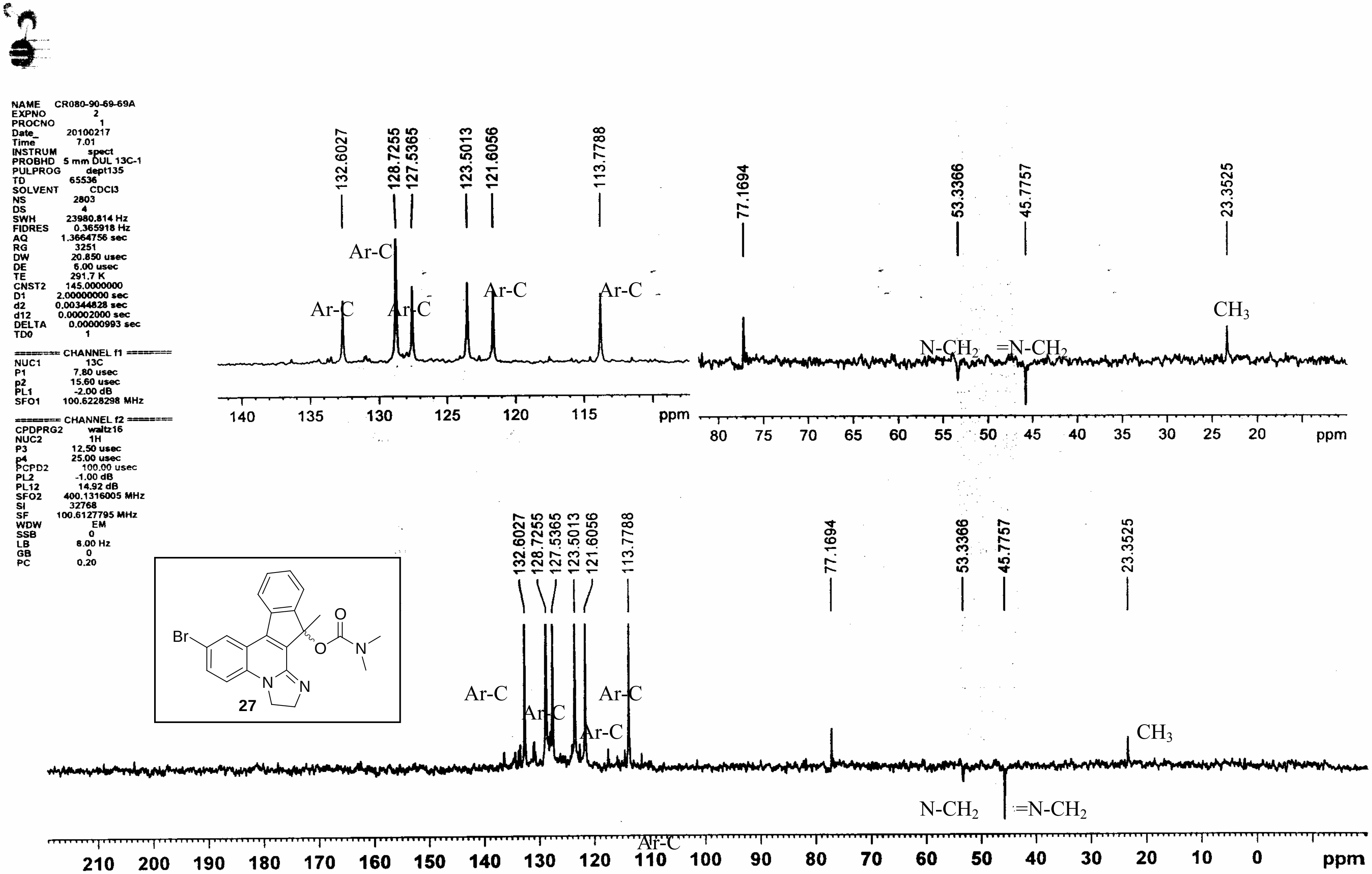
Resolution: 4.00 cm-1

Date: 2/5/2010


NAME CR080-90-69-69A
EXPNO 1
PROCNO 1
Date_ 20091202
Time 10.17
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 812.7
DW 60.400 usec
DE 6.00 usec
TE 292.9 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.50
8.2947 8.2896 8.0504 8.0314 7.4998 7.4819 7.4638 7.4598 7.4440 7.4382 7.4273 7.4085 7.3889 7.2498 6.6720 6.6502
Ar-H
Ar-H
Ar-H
Ar-H
0.98 1.19 4.35 1.00
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 ppm
4.2191 4.2066 4.1965 4.1906 4.1823 4.1671 4.1585 3.9858 3.9731 3.9615 3.9507 3.9437 3.9210 3.0378 2.9465 2.8737 2.7082 1.8278 1.6773 1.2417
CH3
N- CH3
-CH2-CH2-
2.38 2.22 2.71 2.75 2.92
5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
Br
O
O
N
N
N
27
8.2947 8.2896 8.0504 8.0314 7.4998 7.4819 7.4638 7.4598 7.4440 7.4382 7.4273 7.4085 7.3889 7.2498 6.6720 6.6502 5.2890 4.2191 4.2066 4.1965 4.1906 4.1823 4.1671 4.1585 3.9858 3.9731 3.9615 3.9507 3.9437 3.9210 3.0378 2.9465 2.8737 2.7082 1.8278 1.6773 1.2417 0.0562 -0.0052 -0.0133 -0.0210
CH3
-NCH3
-NCH3
Ar-H
Ar-H
Ar-H
Ar-H
-CH2-CH2-
0.98 1.19 4.35 1.00 2.38 2.22 2.71 2.75 2.92
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm


Current Data Parameters
NAME CR080-90-69-69A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100206
Time 13.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2580.3
DW 20.850 usec
DE 6.00 usec
TE 293.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.80 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.92 dB
PL13 18.92 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127738 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 0.20
154.3017
152.1983
149.8202
139.7365
138.9884
137.2374
134.5484
132.4996
128.7446
128.5976
127.5595
123.4791
121.6242
120.0241
113.6787
112.0420
83.6632
77.3241
77.0068
76.6894
53.8760
45.7806
36.5238
36.1919
23.3882
ppm
Br
O
N
N
N
O
27
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
N-CH2
=N-CH2
N-(CH3)2
CH3
ppm

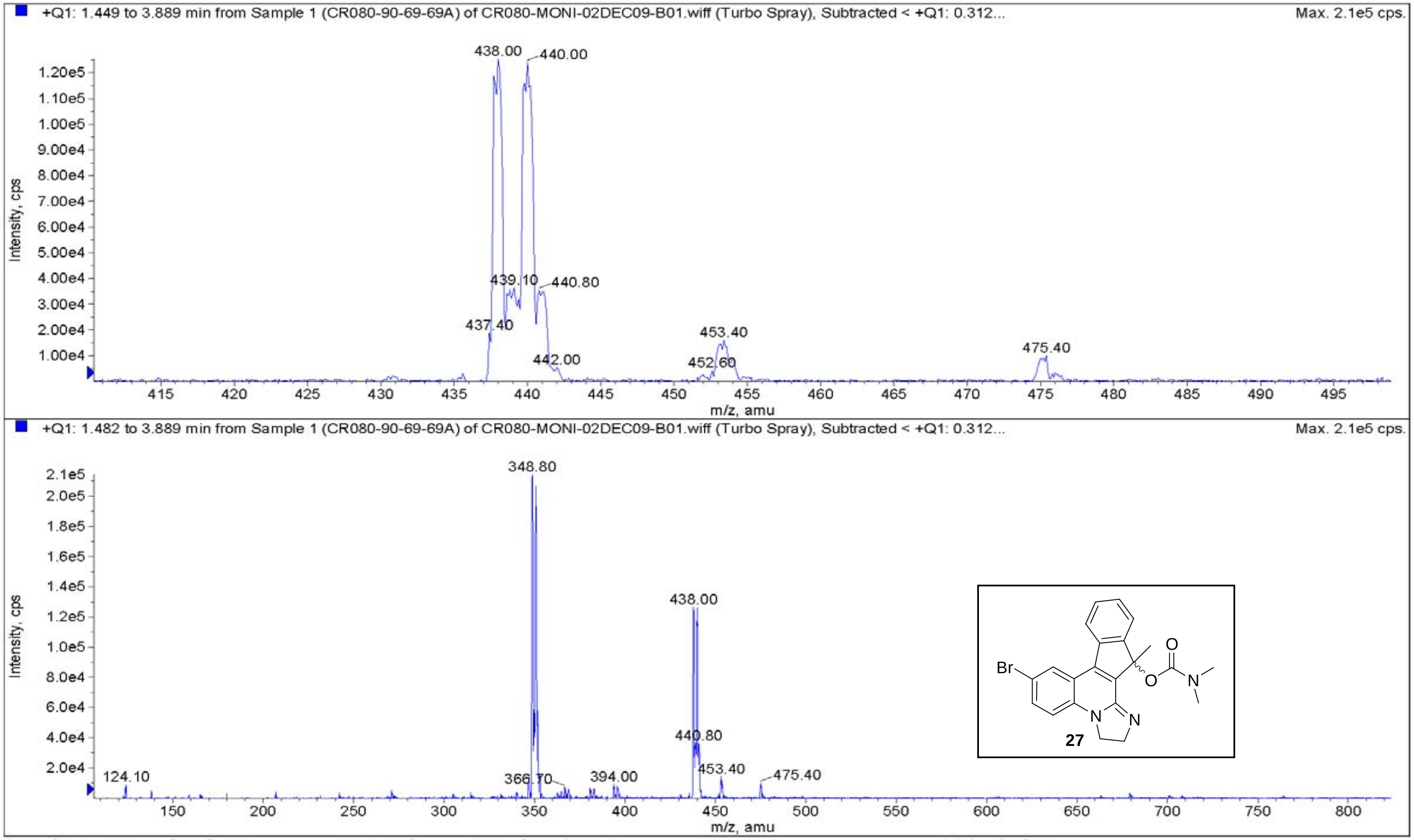
(27)



Analysed by: Yogita

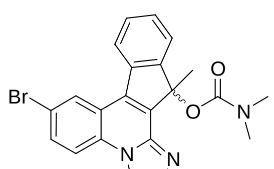
*

Sample Name: CR080-90-69-69A Acq. Time: 10:29 Acq. Date: Wednesday, December 02, 2009

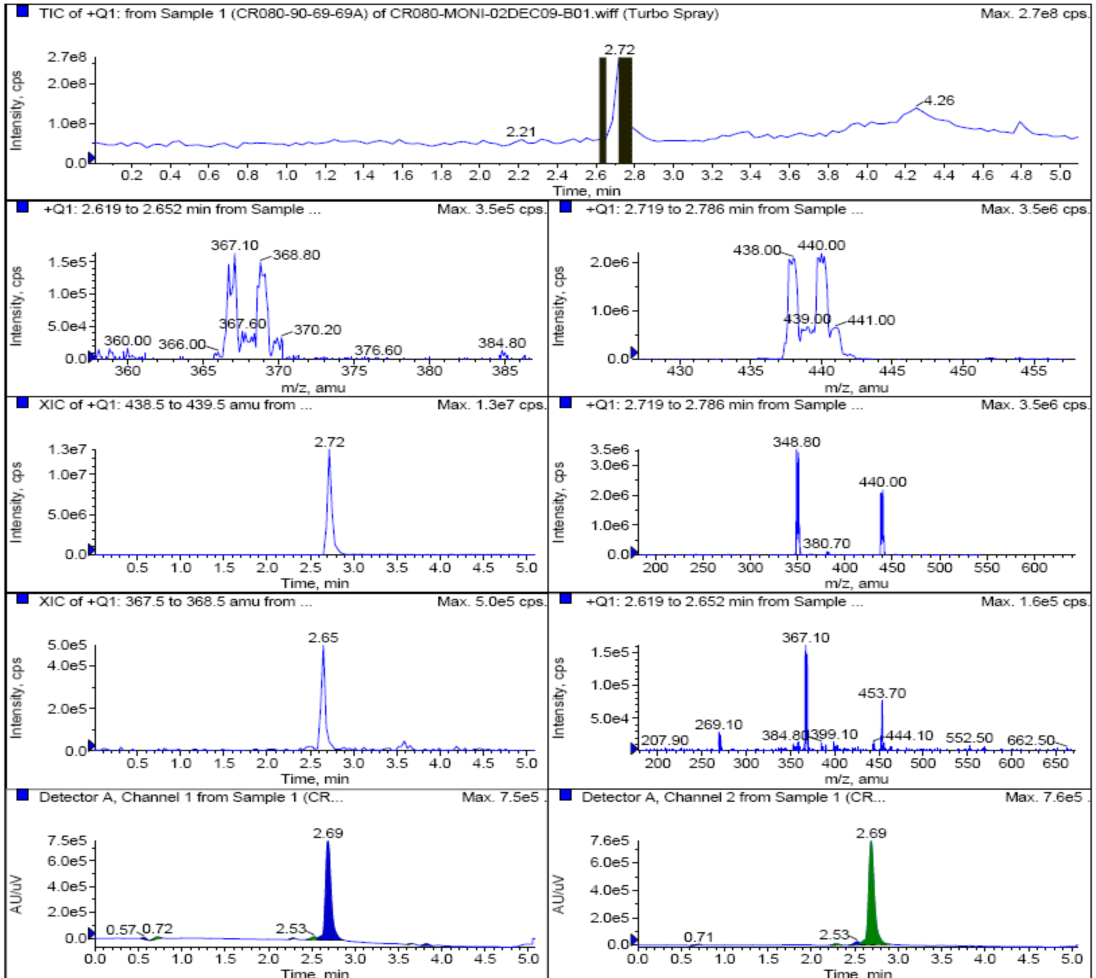


*Sample Comment: [M+H] 438 Expected **Analyzed By : **Checked By :

Sample Name: CR080-90-69-69A   Acq. Time: 10:29   Acq. Date: Wednesday, December 02, 2009



27



Peak List for "Detector A, Channel 1 from Sample 1 (CR080-90-69-

	Time (min)	Area (counts)	%Area	Height
1	0.5651	2.9263e4	0.8025	1.0150e4
2	0.7194	6.5053e4	1.7840	1.5700e4
3	2.2831	6348.2182	0.1741	2705.2257
4	2.5262	1.0511e5	2.8826	2.2843e4
5	2.6869	3.3844e6	92.8139	7.6305e5
6	3.6549	5621.9603	0.1542	2036.7344

Peak List for "Detector A, Channel 2 from Sample 1 (CR080-90-69-

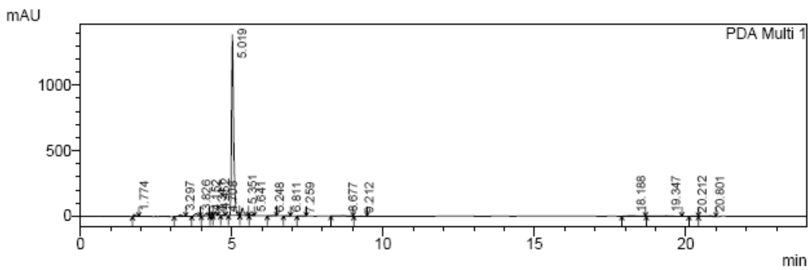
	Time (min)	Area (counts)	%Area	Height
1	0.7060	6496.5548	0.1793	1594.4783
2	2.2852	4.0229e4	1.1102	1.0801e4
3	2.5275	1.0285e5	2.8384	2.3857e4
4	2.6886	3.4740e6	95.8721	7.5658e5

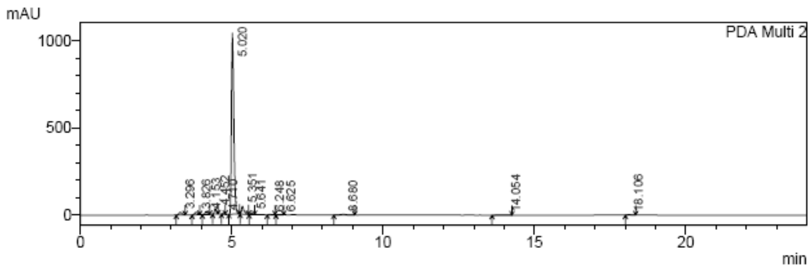
LCMS-1 REACN MONT (TFA Buffer)PEAK MERGED   Analysed By :

Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm

Sample Name : CR080-90-69-69A
Sample ID : CR080-90-69-69A
Column : Xterra RP-18 (150 x 4.6 mm) 5u
Vial # : 53
Inj. Volume : 1 uL
Tray # : 1
Acquired by : VISHAL

Data File Name : 07-01-2010_CR080-90-69-69A_07.lcd
Method File Name : GENERAL_B1.lcm
Batch File Name : 07-01-2010.lcb
Data Acquired : 1/7/2010 2:46:10 PM
Data Processed : 1/7/2010 3:10:08 PM
Ref.No.: DI/A0257/84





1 PDA Multi 1/200nm 4nm
2 PDA Multi 2/252nm 4nm

PeakTable

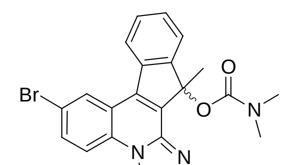
PDA Ch1 200nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	1.77	75640	0.94	15376
2	3.30	90352	1.13	13629
3	3.83	124462	1.55	18675
4	4.15	104525	1.31	18912
5	4.34	15819	0.20	3788
6	4.45	117919	1.47	26412
7	4.71	25822	0.32	5779
8	5.02	6594694	82.37	1377696
9	5.35	310478	3.88	56713
10	5.64	33575	0.42	7536
11	6.25	12408	0.15	1385
12	6.81	16178	0.20	3206
13	7.26	11390	0.14	1308
14	8.68	52312	0.65	3580
15	9.21	10800	0.13	836
16	18.19	126536	1.58	5193
17	19.35	157137	1.96	4077
18	20.21	35339	0.44	3458
19	20.80	90998	1.14	4991
Total		8006384	100.00	1572550

PeakTable

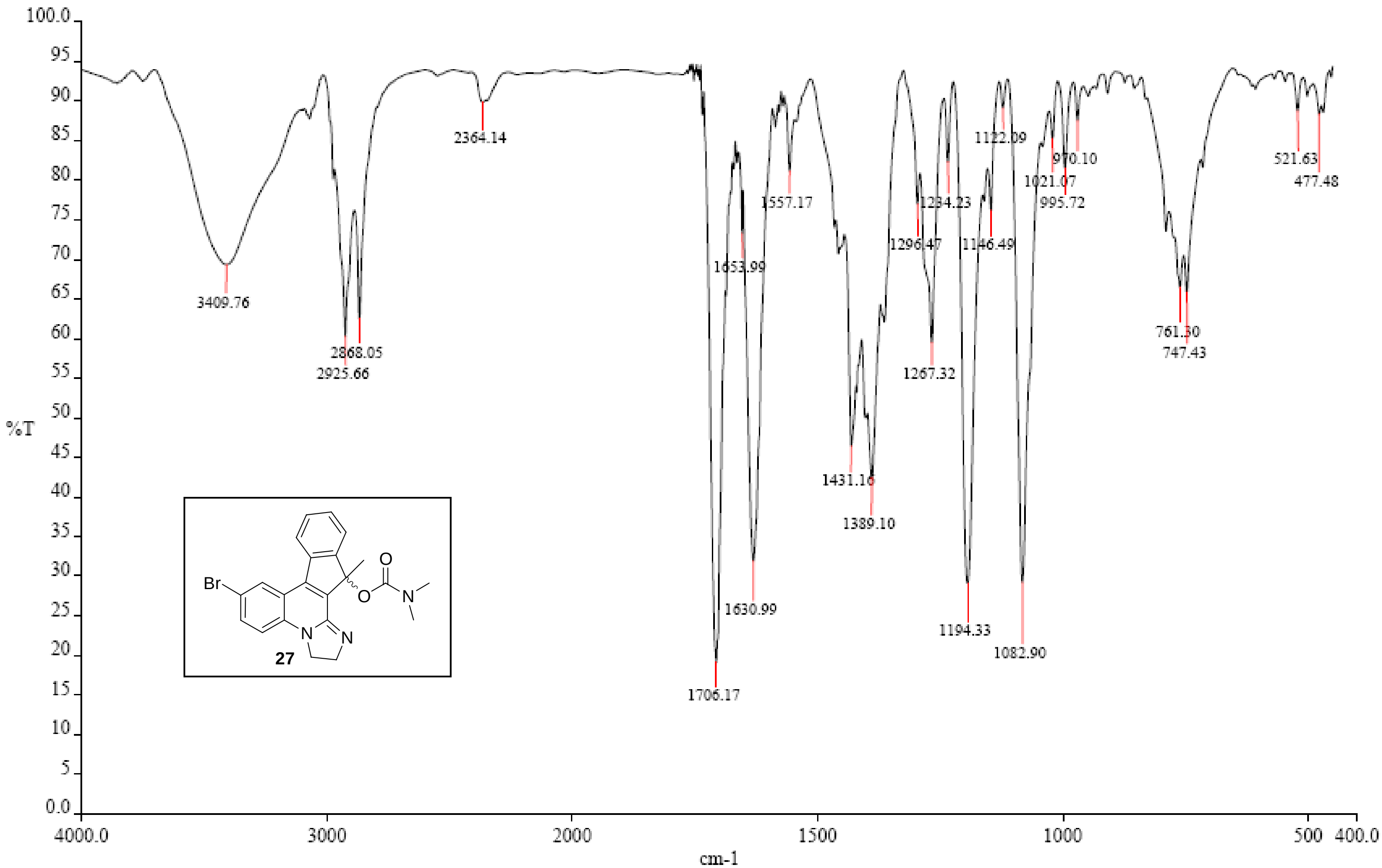
PDA Ch2 252nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	3.30	103804	1.60	15388
2	3.83	96307	1.48	14946
3	4.15	91270	1.41	17503
4	4.45	138058	2.13	31548
5	4.71	16736	0.26	4168
6	5.02	5632554	86.73	1036381
7	5.35	254781	3.92	44996
8	5.64	44804	0.69	10046
9	6.25	13407	0.21	2160
10	6.63	12615	0.19	1784
11	8.68	58133	0.90	4513
12	14.05	18306	0.28	1063
13	18.11	13327	0.21	2265
Total		6494103	100.00	1186762



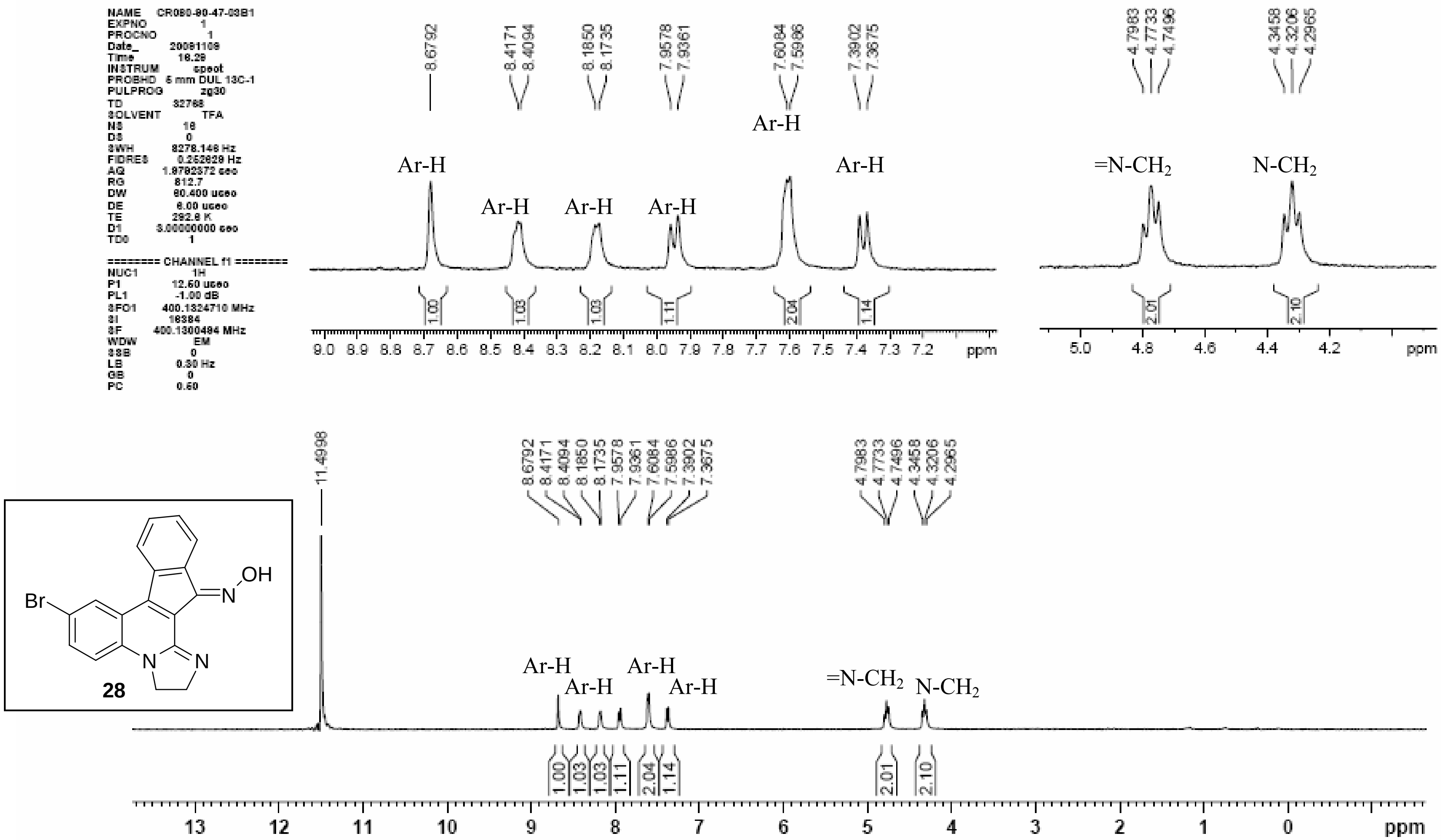
27

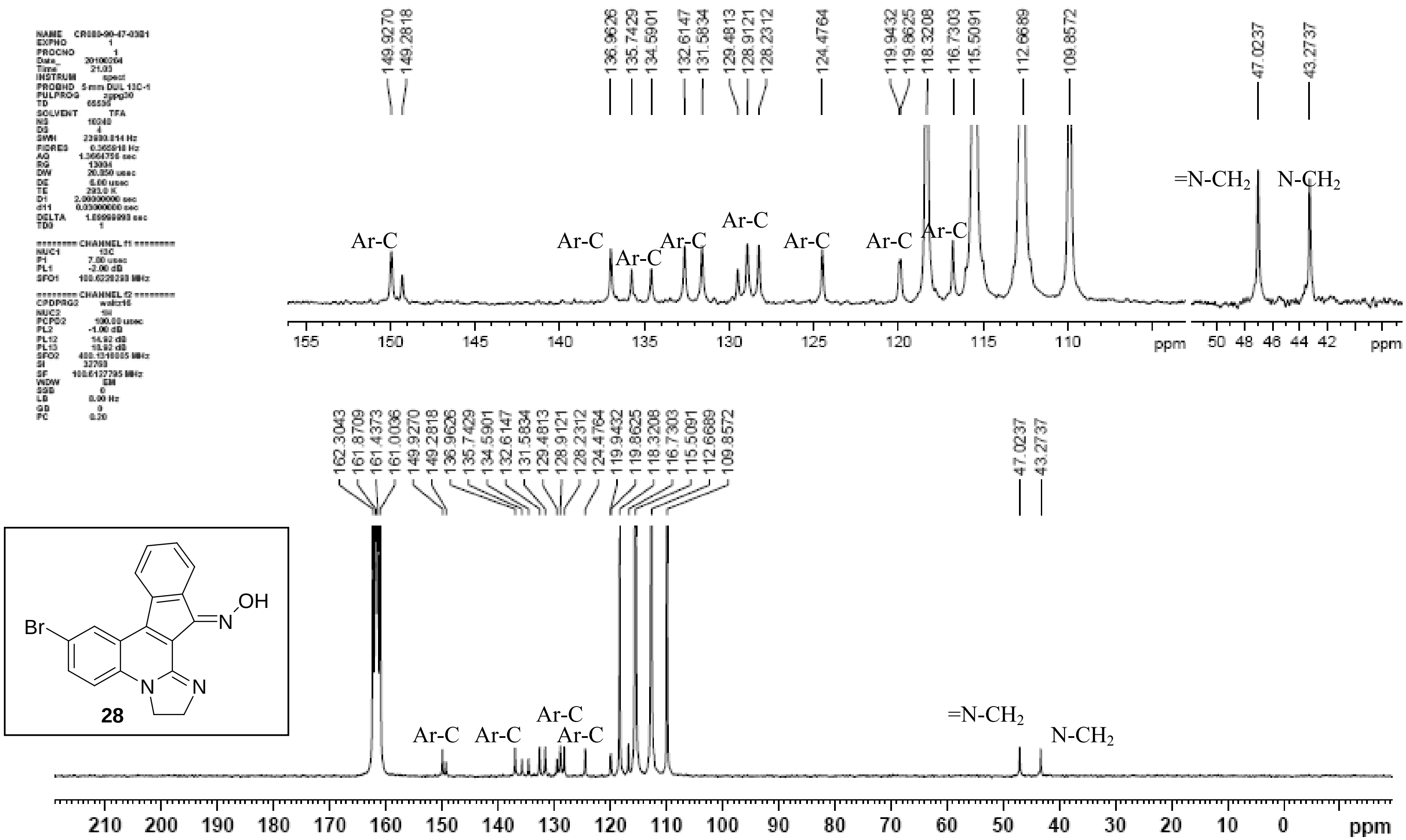
C:\LabSolutions\Data\Project1\HPLC-01\JAN-10\07-01-2010_CR080-90-69-69A_07.lcd



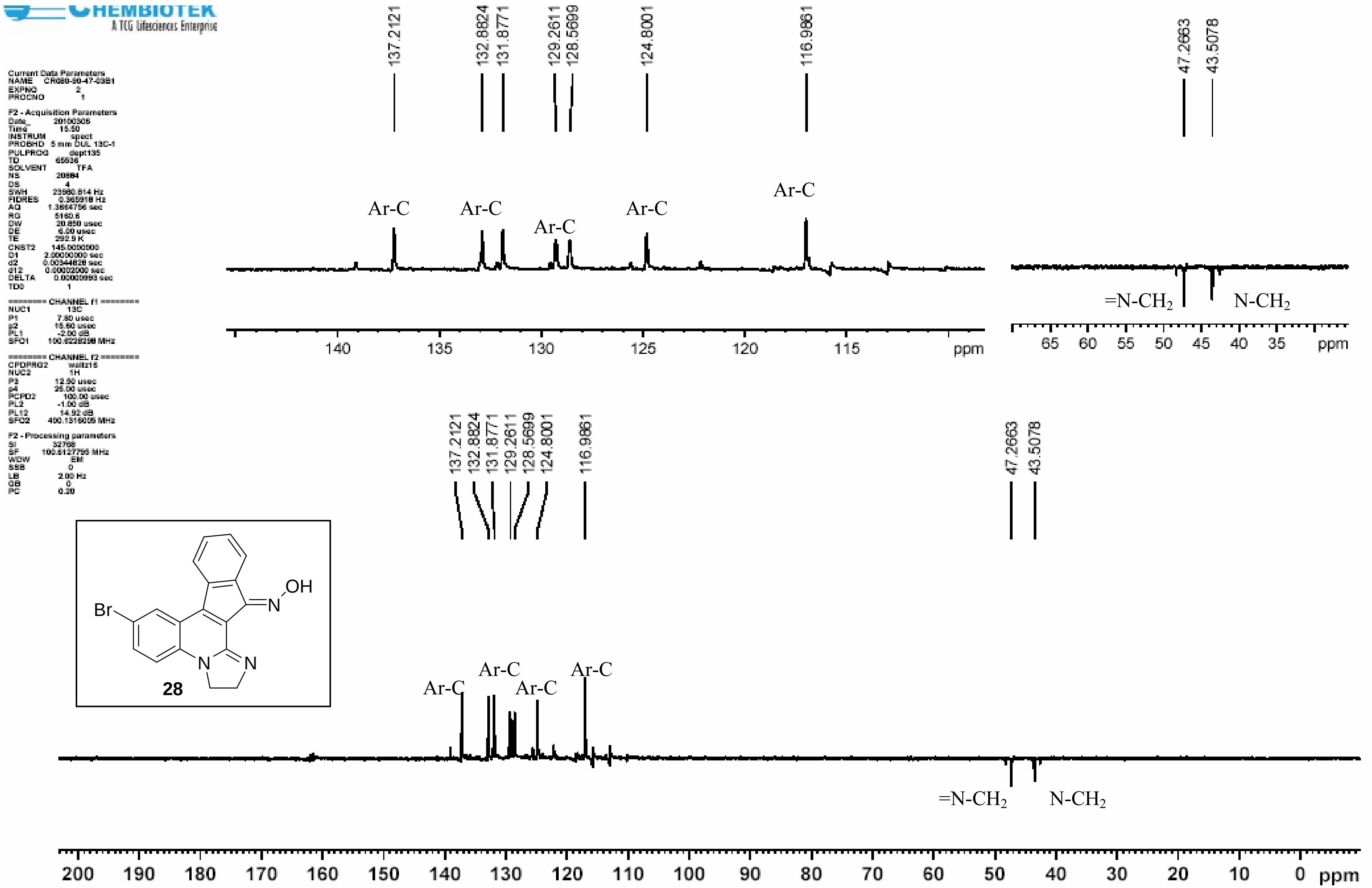
Spectrum Name: CR080-90-69-69A.sp | Analyst: GANESH | Accumulations: 16 | Time: 11:32:02 AM

Description: CR080-90-69-69A IN KBr | Resolution: 4.00 cm-1 | Date: 2/5/2010


Ar-H
=N-CH$_2$
N-CH$_2$
Br
OH
N
28
ppm



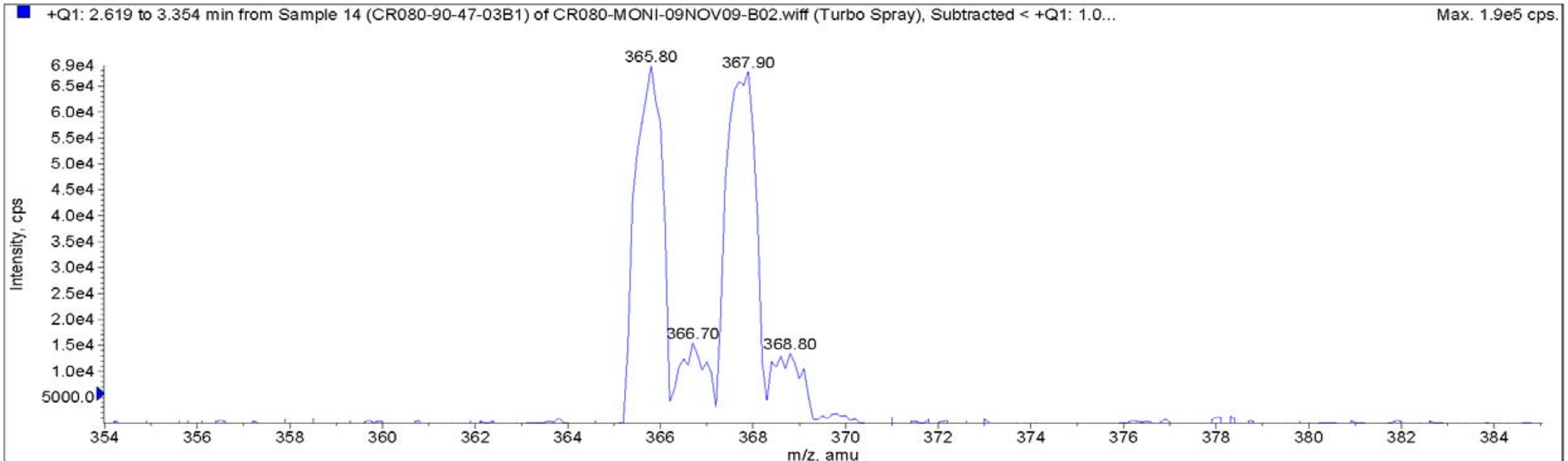
Analysed by: Yogita

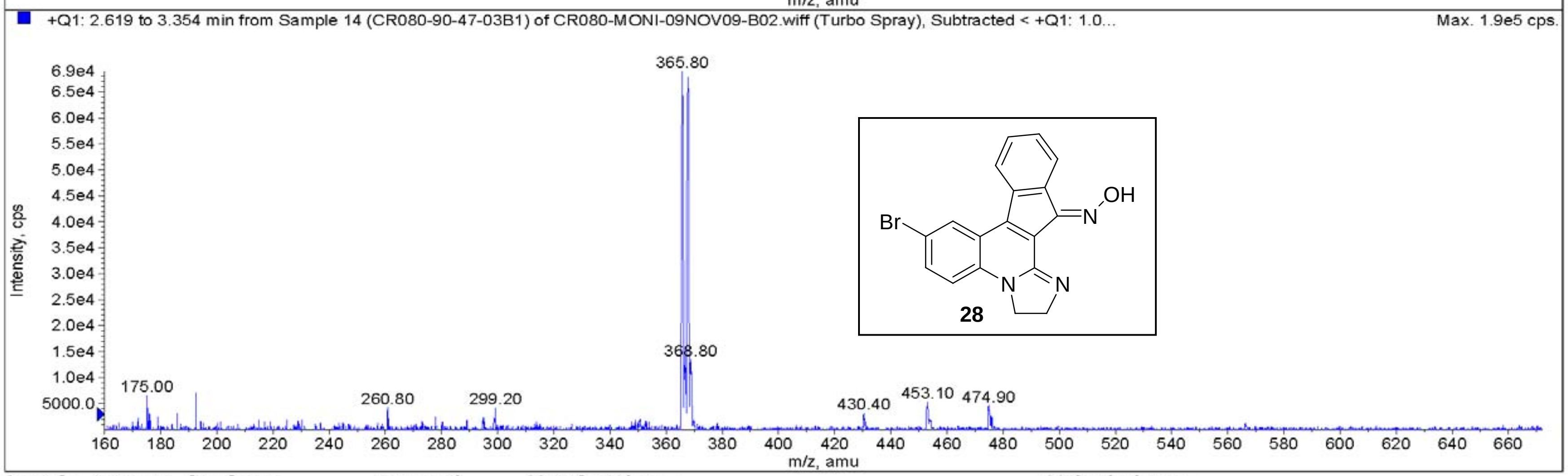


CHEMBIOTEK
A TCG Lifesciences Enterprise
137.2121
132.8824
131.8771
129.2611
128.5699
124.8001
116.9861
47.2663
43.5078
Ar-C
Ar-C
Ar-C
Ar-C
Ar-C
=N-CH2
N-CH2
Br
OH
N
N
N
28
ppm

*

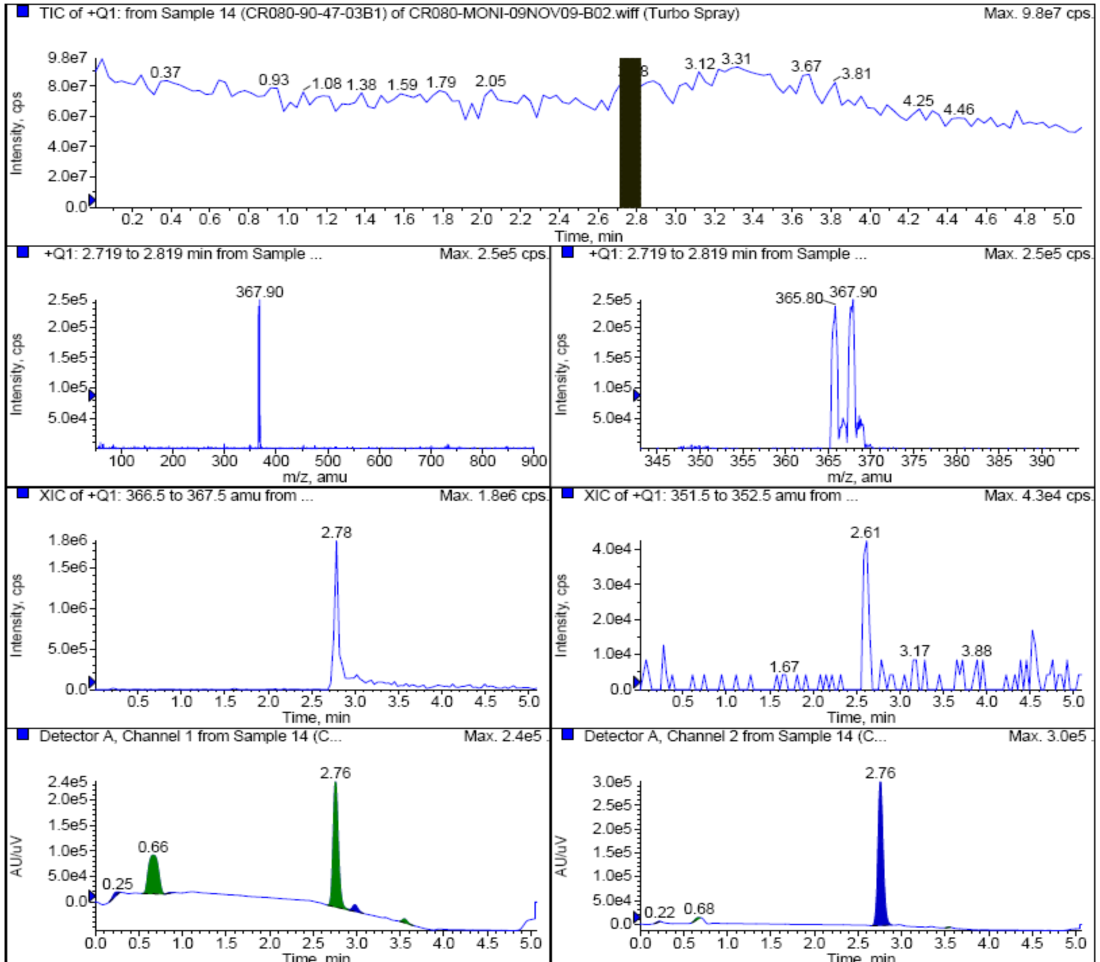
Sample Name: CR080-90-47-03B1 Acq. Time: 18:53 Acq. Date: Monday, November 09, 2009





*Sample Comment: [M+H] 366 Expected **Analyzed By : **Checked By :

Sample Name: CR080-90-47-03B1 Acq. Time: 18:53 Acq. Date: Monday, November 09, 2009



Peak List for "Detector A, Channel 1 from Sample 14 (CR080-90-47

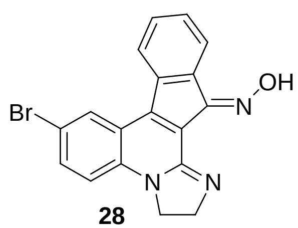
	Time (min)	Area (counts)	% Area	Height
3	0.8812	6425.9238	0.3764	1229.2909
4	2.7553	1.0024e6	58.7187	2.4521e5
5	2.9767	5.3742e4	3.1481	1.2835e4
6	3.5454	2.8991e4	1.6982	7484.5389

Peak List for "Detector A, Channel 2 from Sample 14 (CR080-90-47

	Time (min)	Area (counts)	% Area	Height
2	0.6752	1.0913e4	0.8992	1808.9480
3	2.7573	1.1986e6	98.7618	3.0097e5
4	3.5470	1320.5049	0.1088	617.3673

LCMS-1 REACN MONT (TFA Buffer) Analysed By :

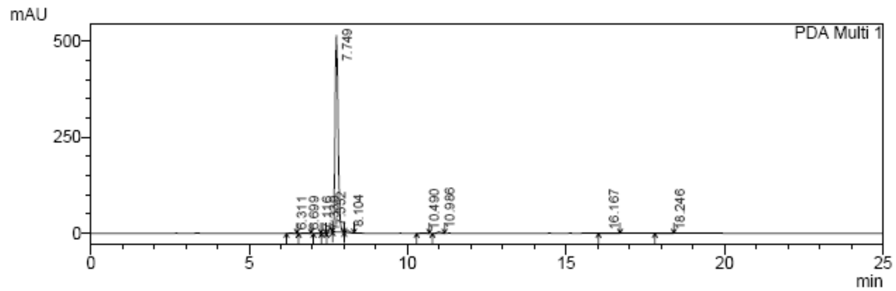
Channel 1 at wavelength 220nm, Channel 2 at wavelength 260 nm



28

Sample Name : CR080-90-47-03B1
Sample ID : CR080-90-47-03B1
Column : Xterra RP-18 (250 x 4.6 mm) 5u
Vial # : 23
Inj. Volume : 4 uL
Tray # : 2
Acquired by : AVINASH

Data File Name : 17-02-10_CR080-90-47-03B1_02.lcd
Method File Name : GENERAL_B11.lcm
Batch File Name : 170210.lcb
Data Acquired : 2/18/2010 5:05:56 AM
Data Processed : 2/18/2010 5:35:59 AM
Ref.No.: DI/A0257/98

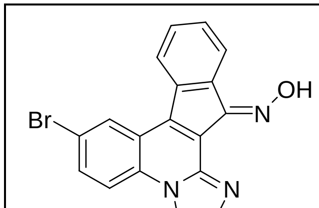


1 PDA Multi 1/252nm 4nm

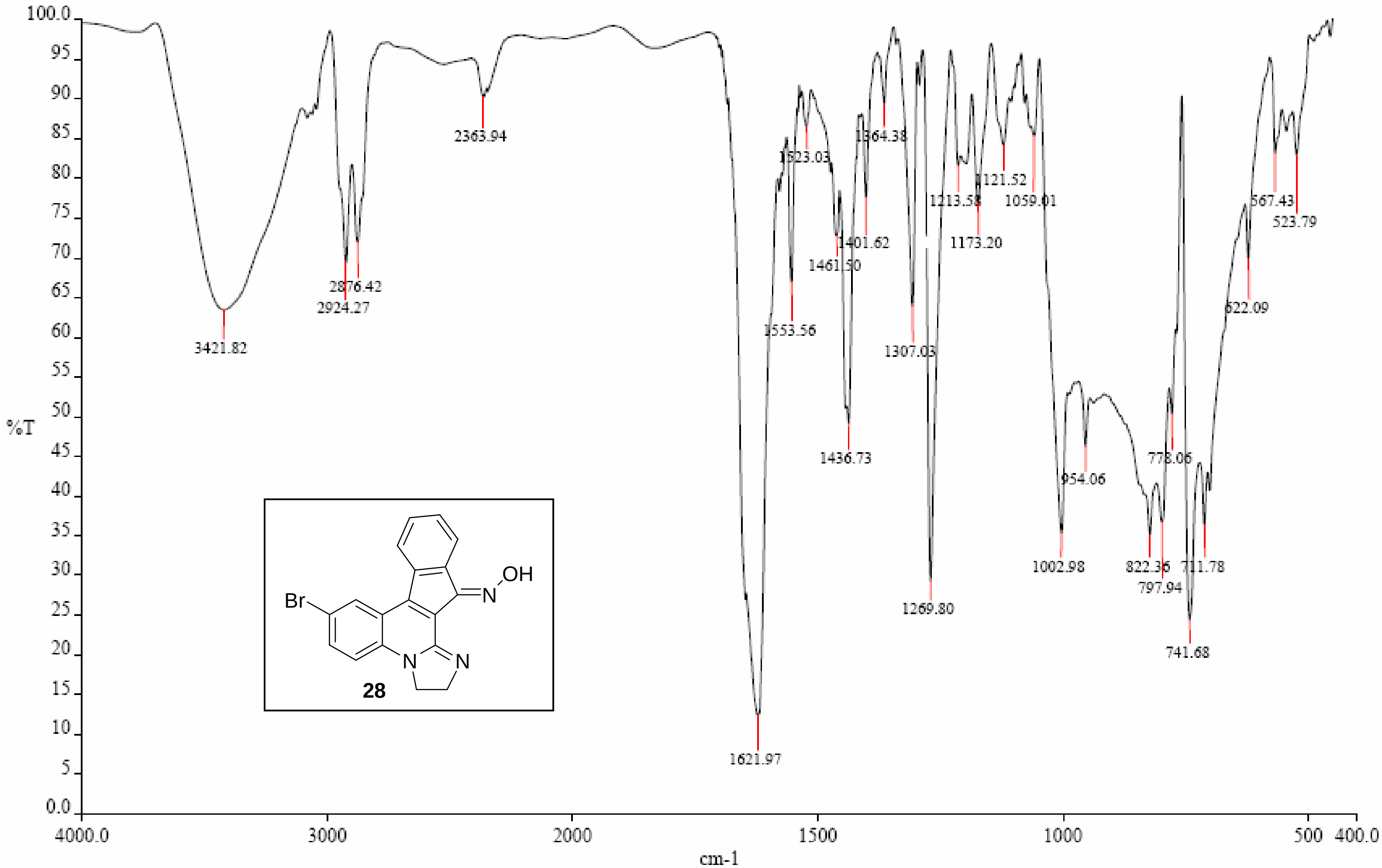
PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %	Height
1	6.31	3452	0.10	534
2	6.70	3362	0.10	319
3	7.12	1029	0.03	153
4	7.34	729	0.02	160
5	7.55	50295	1.45	9915
6	7.75	3328354	96.02	511507
7	8.10	36183	1.04	5768
8	10.49	7190	0.21	885
9	10.99	28623	0.83	3718
10	16.17	3454	0.10	328
11	18.25	3510	0.10	132
Total		3466182	100.00	533419

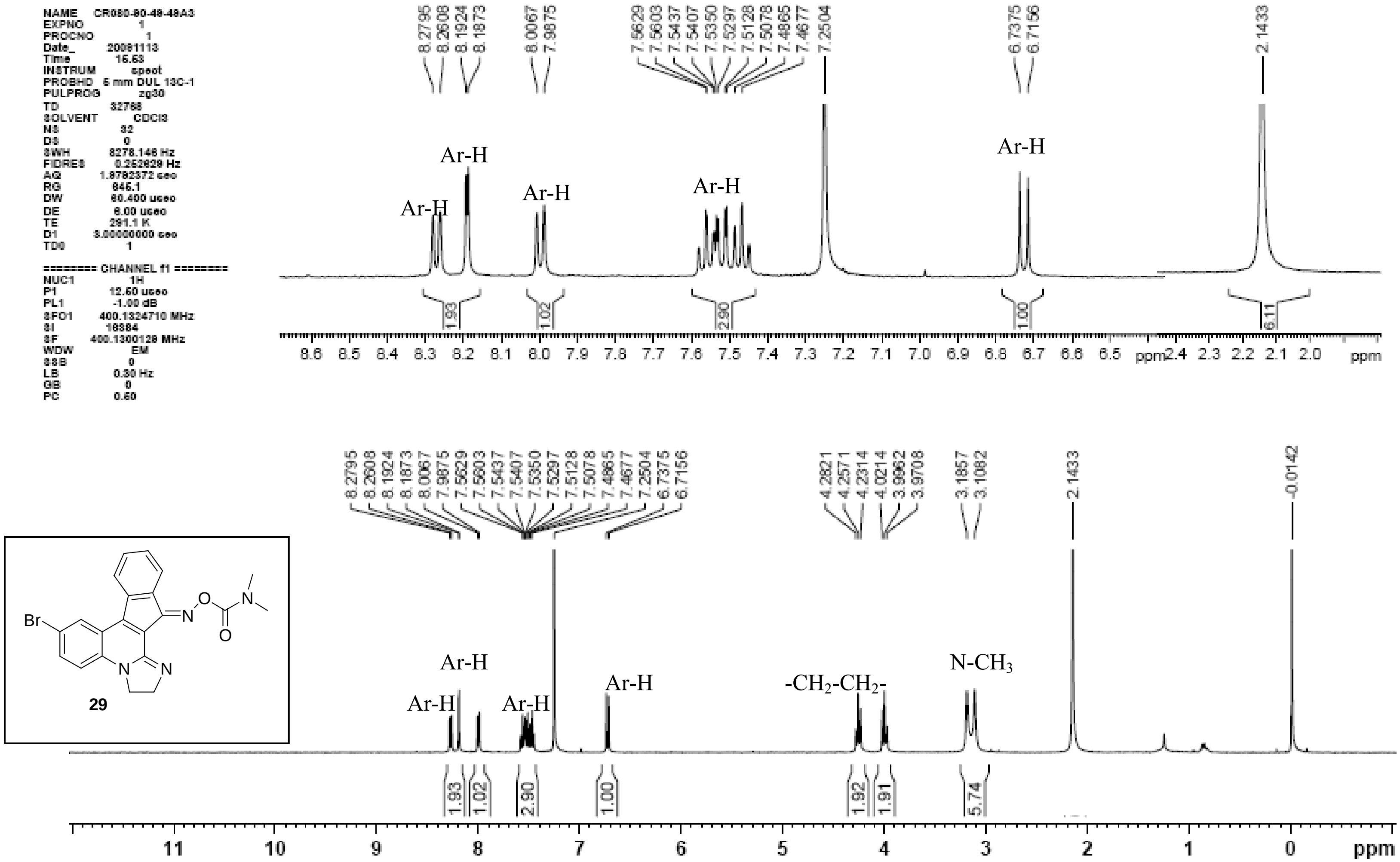


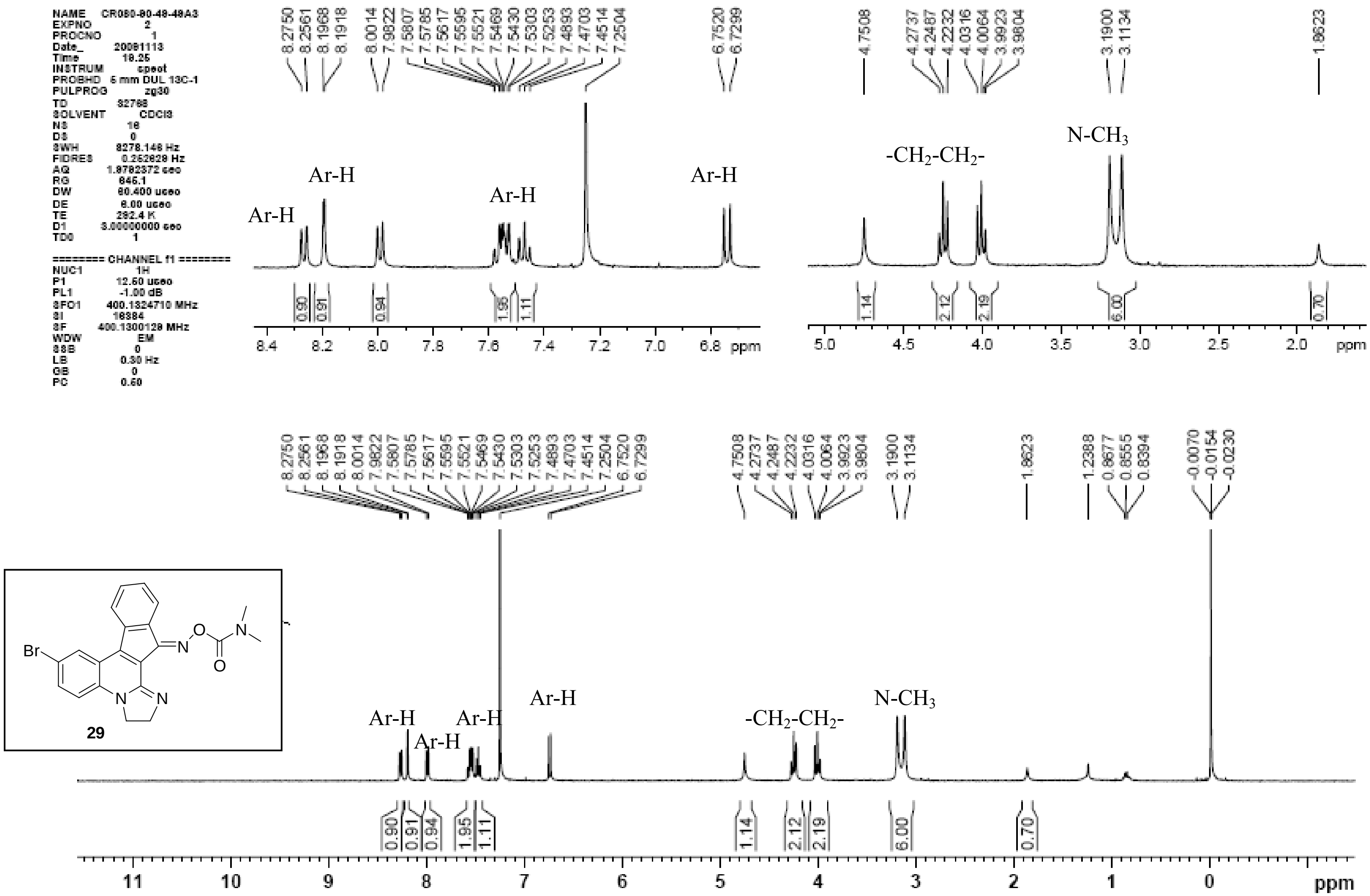
28

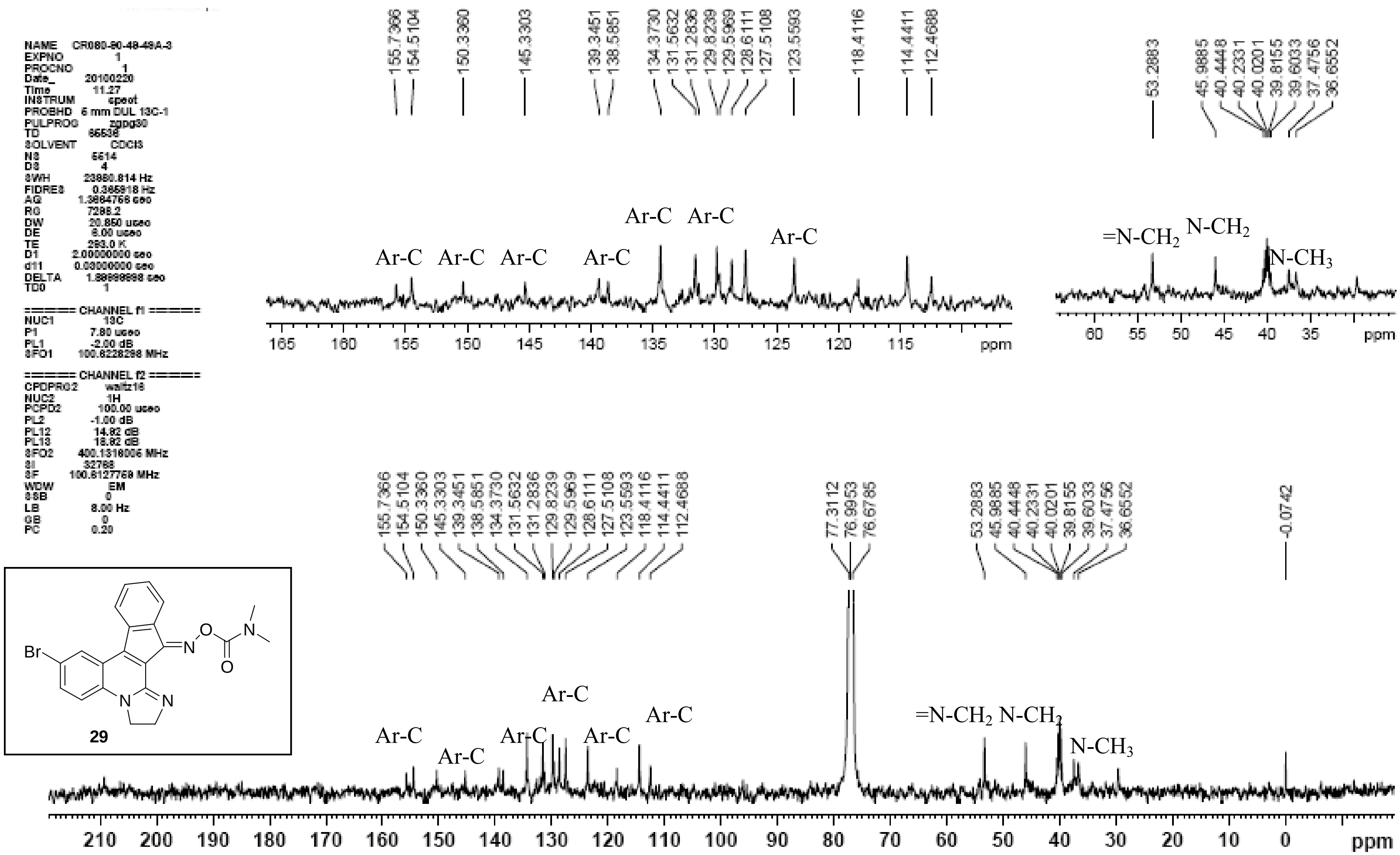


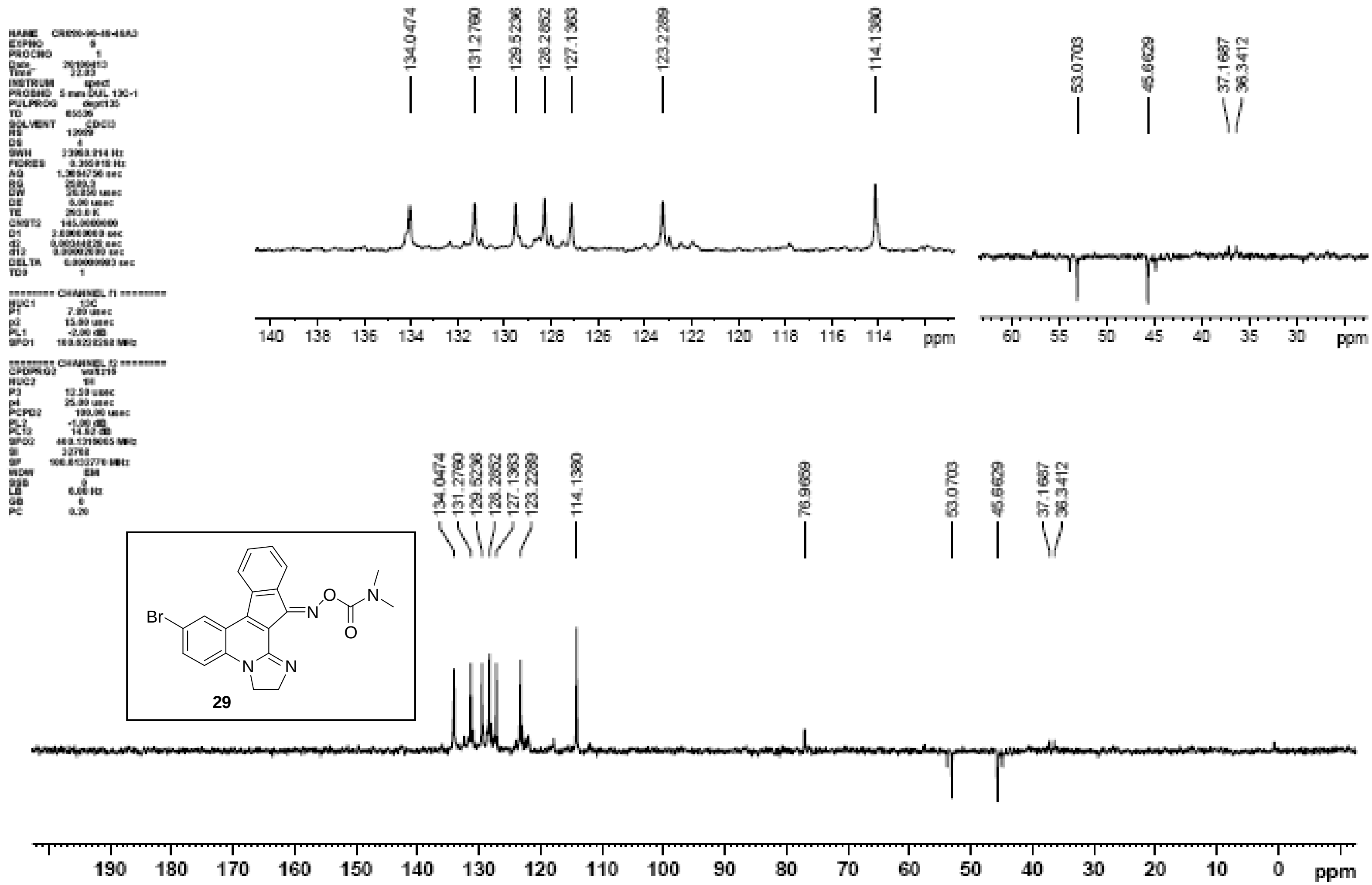
Spectrum Name: CR080-90-47-03B1.sp Analyst: GANESH Accumulations: 16 Time: 10:01:14 AM

Description: CR080-90-47-03B1 IN KBr Resolution: 4.00 cm-1 Date: 2/5/2010

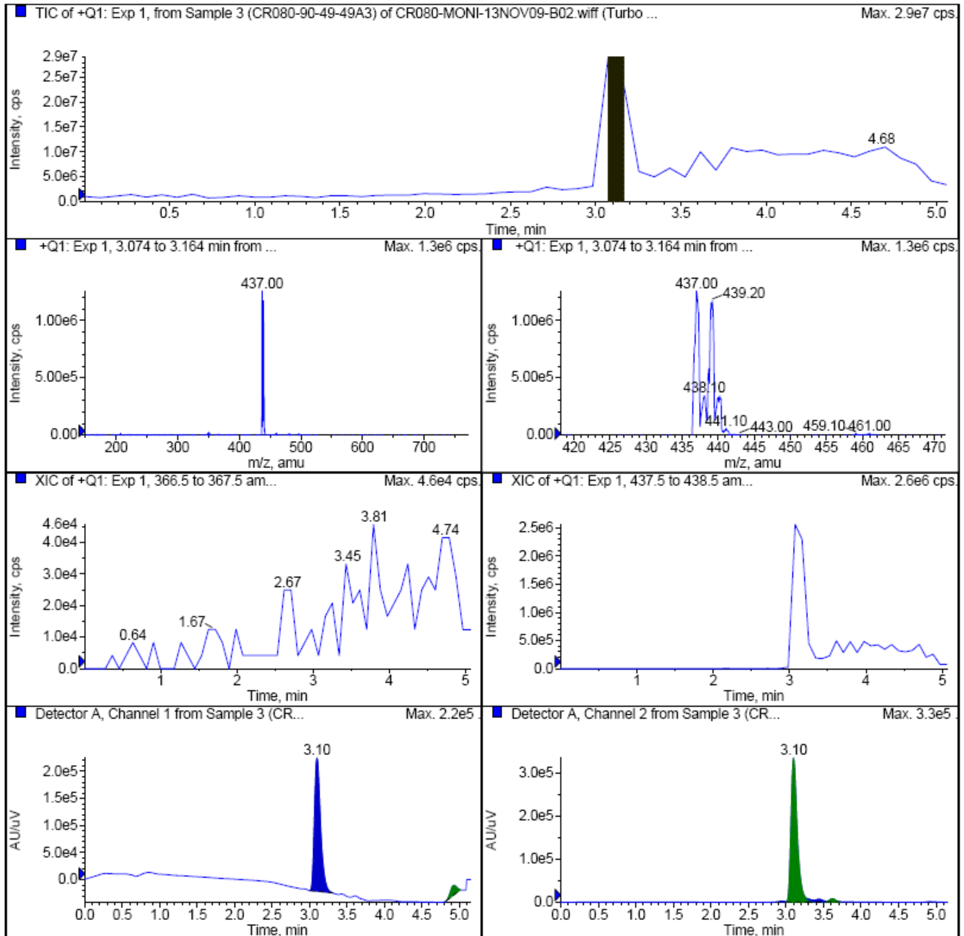

NAME CR080-80-48-48A3
EXPNO 1
PROCNO 1
Date_ 20091113
Time 15.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 645.1
DW 60.400 usec
DE 6.00 usec
TE 291.1 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60
Ar-H
Ar-H
Ar-H
Ar-H
Ar-H
-CH2-CH2-
N-CH3
ppm
29

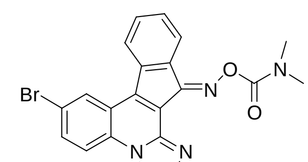

NAME CR080-80-48-48A3
EXPNO 2
PROCNO 1
Date_ 20081113
Time 18.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252628 Hz
AQ 1.9792372 sec
RG 645.1
DW 60.400 usec
DE 6.00 usec
TE 292.4 K
D1 3.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60
Ar-H
Ar-H
Ar-H
Ar-H
-CH2-CH2-
N-CH3
ppm
Br
N
O
29


NAME CR080-90-48-49A-3
EXPNO 1
PROCNO 1
Date_ 20100220
Time 11.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5614
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 7298.2
DW 20.850 usec
DE 6.00 usec
TE 293.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======= CHANNEL f1 =======
NUC1 13C
P1 7.80 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======= CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 14.82 dB
PL13 16.82 dB
SFO2 400.1316006 MHz
SI 32768
SF 100.6127759 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20
155.7366 154.5104 150.3360 145.3303 139.3451 138.5851 134.3730 131.5632 131.2836 129.8239 129.5969 128.6111 127.5108 123.5593 118.4116 114.4411 112.4688
77.3112 76.9953 76.6785
53.2883 45.9885 40.4448 40.2331 40.0201 39.8155 39.6033 37.4756 36.6552
-0.0742
Ar-C
=N-CH2
N-CH2
N-CH3
ppm
Br
N
O
29


134.0474
131.2760
129.5236
128.2852
127.1363
123.2289
114.1380
53.0703
45.6629
37.1687
36.3412
76.9659
ppm
Br
N
O
29

Sample Name: CR080-90-49-49A3 Acq. Time: 17:03 Acq. Date: Friday, November 13, 2009





29

Peak List for "Detector A, Channel 1 from Sample 3 (CR080-90-49-

	Time (min)	Area (counts)	%Area	Height
1	3.1015	1.3896e6	93.0984	2.4608e5
2	4.9305	1.0301e5	6.9016	1.7544e4

Peak List for "Detector A, Channel 2 from Sample 3 (CR080-90-49-4

	Time (min)	Area (counts)	%Area	Height
1	2.9454	9563.8300	0.4653	2232.7391
2	3.1014	1.9567e6	95.2029	3.3436e5
3	3.4388	4.9591e4	2.4129	6016.7544
4	3.6190	3.9438e4	1.9189	7507.8208

LCMS 2 Reaction Monitoring (NH4OAc Buffer) Analyzed By :

*Channel 1 at wavelength 220 nm . Channel 2 at wavelength 260 nm

===

Sample:CR080-90-49-49A3 ->

Column:GEMINI-C18(150X4.6)mm 5µ

Injection date : Tue, 17. Nov. 2009 Location : Vial 15

Sample Name : CR080-90-49-49A3 Inj. No. : 1

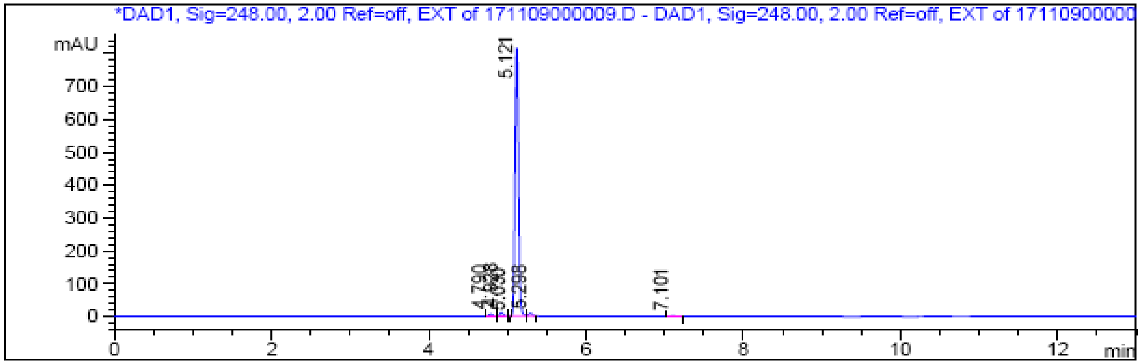
Acq Operator : PRAKASH Inj. Vol. : 5 µl

Analysis Method : C:\CHEM32\2\METHODS\UPLC_GENARAL_GRAD _G1.M

Last Changed : Wed, 18. Nov. 2009,

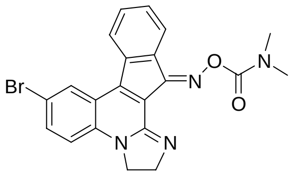
Acq. Method :C:\Chem32\2\DATA\NOV-09\171109F 2009-11-17 17-19-25\UPLC_GENARAL_GRAD _G1.M

Method ref :DI/A0257/50



DAD1, Sig=248.00, 2.00 Ref=off, EXT

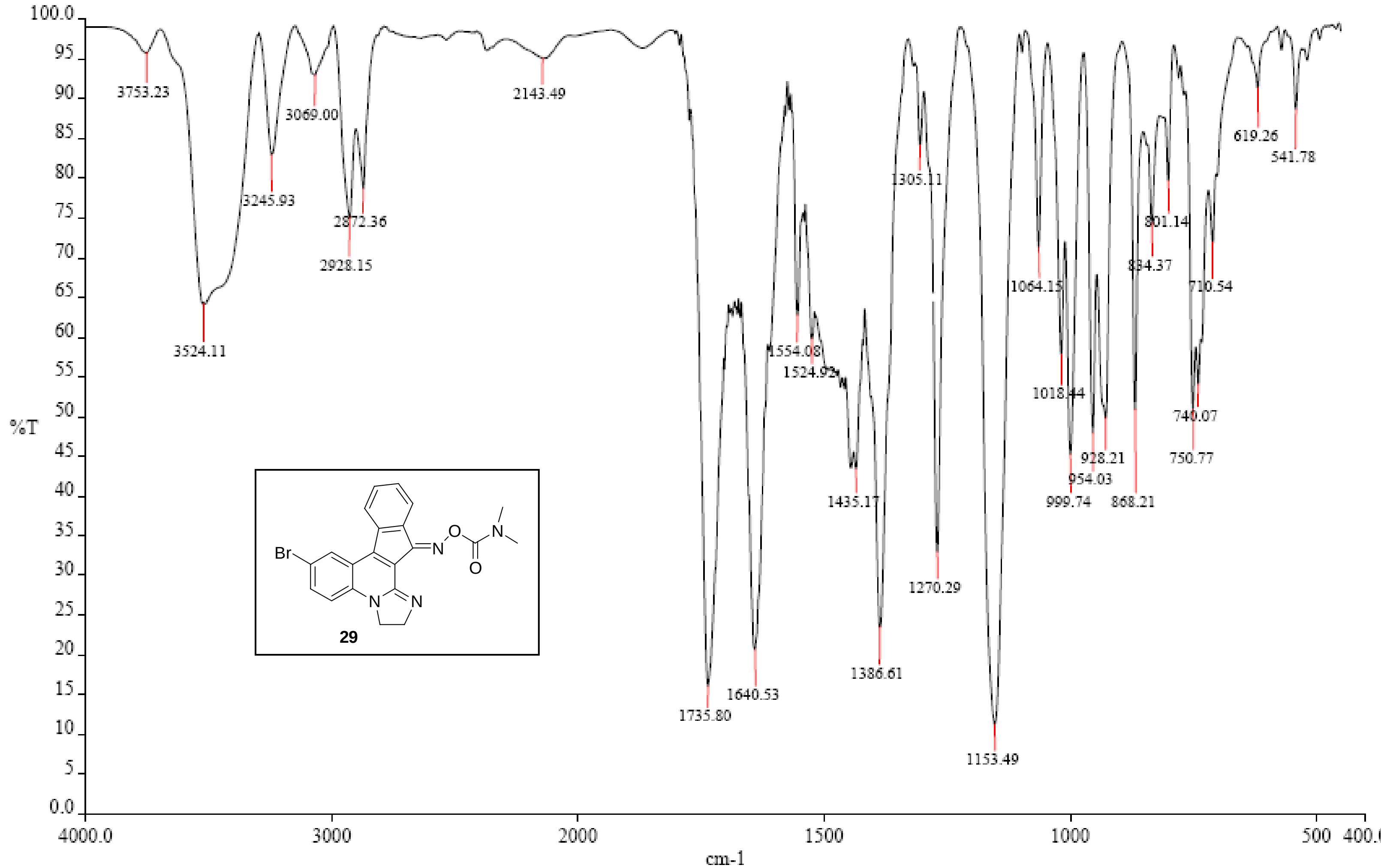
Peak #	RT (Min)	Width (Min)	Area	Area %
1	4.790	0.047	20.452	0.828
2	4.928	0.048	33.080	1.339
3	5.030	0.023	0.458	0.019
4	5.121	0.048	2385.486	96.560
5	5.298	0.046	22.999	0.931
6	7.101	0.070	7.986	0.323



29

===

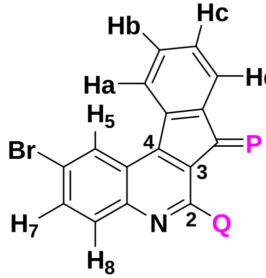
*** End of Report***



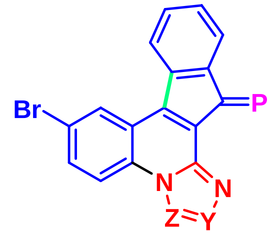
Spectrum Name: CR080-90-49-49A3.sp   Analyst: GANESH   Accumulations: 16   Time: 10:15:44 AM

Description: CR080-90-49-49A3 IN KBr   Resolution: 4.00 cm-1   Date: 2/5/2010

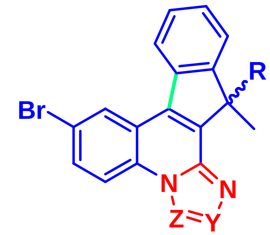
Table S1: Comparison of Chemical shift values (δ) of quinoline ring protons after formation of fused ring system¶



2b : P = O, Q = Methoxy
2c : P = O, Q = Trifluoromethyl
2d : P = O, Q = Imodazol-1-yl
2e : P = O, Q = 1H-Pyrazol-1-yl
2f : P = O, Q = 4-(2-Pyridyl)-piperazin-1-yl
2g : P = NOH, Q = Imidazol-1-yl
2h : P = NOH, Q = 4-(2-Pyridyl)-piperazin-1-yl
6 : P = O, Q = Cl

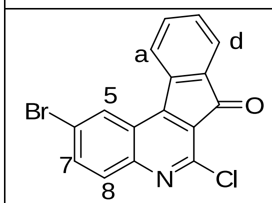
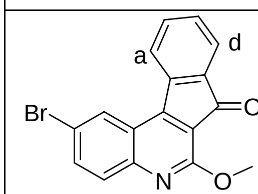


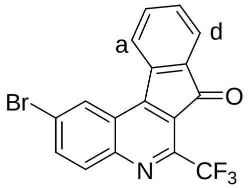
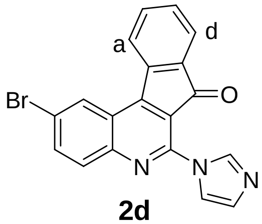
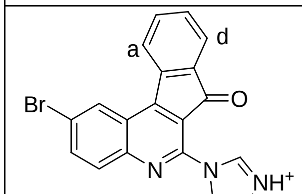
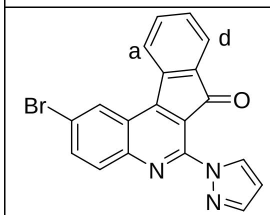
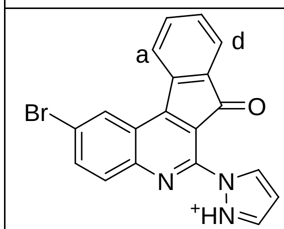
7 : Y=Z=N, P=O
8 : Y=Z=N, P=NOH
9 : Y=Z=N, P= N-O-C(=O)-N(CH_3)$_2$
15 : Y=N; Z=CH, P=O
17 : Y=N; Z=(C-CH_3), P=O
23 : Y=NH; Z=(C=S), P=O
25 : Y=Z=CH_2, P=O
28 : Y=Z=CH_2, P=NOH

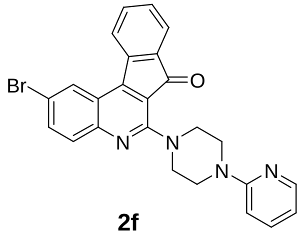
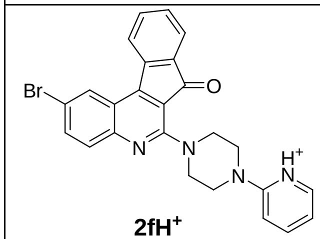
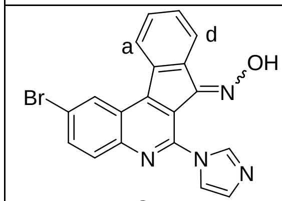
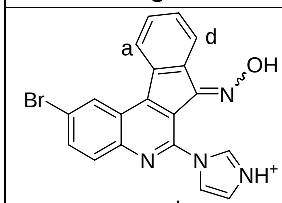
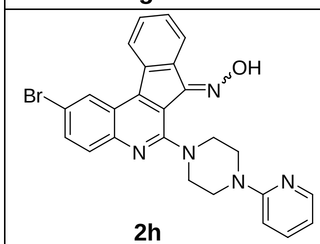


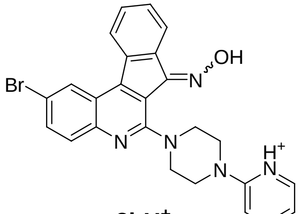
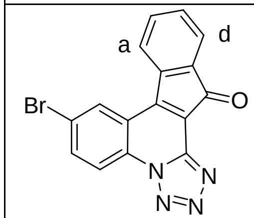
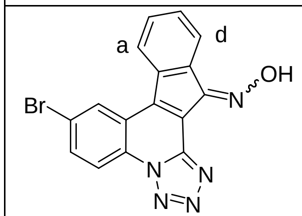
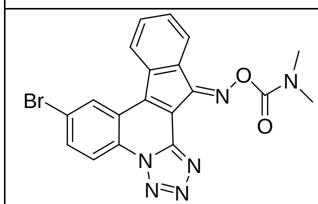
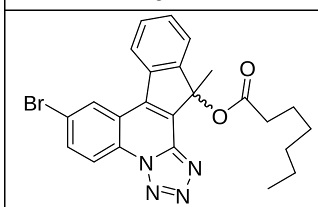
13:Y=Z=N, R=O-C(=O)(CH$_2$)$_5$CH$_3$

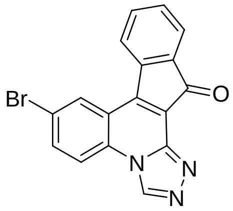
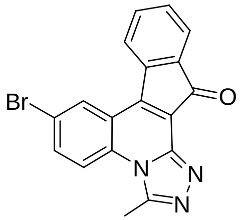
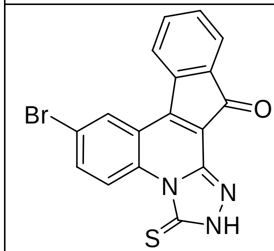
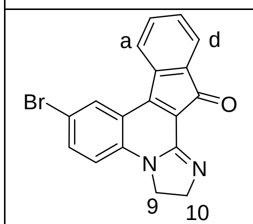
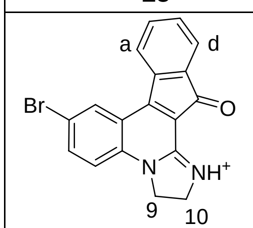
27:Y=Z=CH$_2$, R=O- C(=O)-N(CH$_3$)$_2$

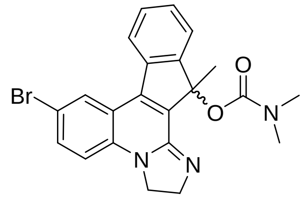
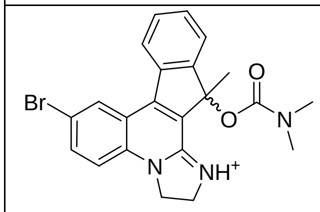
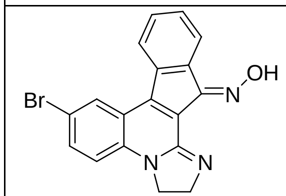
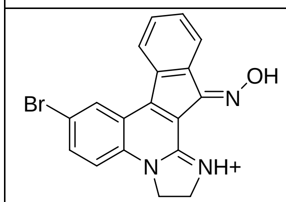
Structure	H_5	H_7	H_8	Ha	Hb	Hc	Hd	Other signals
 **6**	9.00 (*d*, *J* = 1.9Hz)	8.27 (*dd*, *J* = 1.9, 9.1 Hz)	8.12 (*d*, *J* = 9.1 Hz)	8.66 (*d*, *J* = 7.6Hz)	7.90 (*m*)	7.78 (*t*, *J* = 7.4 Hz)	7.90 (*m*)	
 **2b**	8.66 (*d*, *J* = 1.9Hz)	7.95 (*dd*, *J* = 1.9, 9.1 Hz)	7.77 (*d*, *J* = 9.1 Hz)	8.34 (*d*, *J* = 7.6Hz)	7.70 (*t*, *J* = 7.6 Hz)	7.58 (*t*, *J* = 7.6 Hz)	7.66 (*d*, *J* = 7.2 Hz)	4.08 (*s*) CH_3

 **2c**	8.89 (*d*, *J* = 1.9Hz)	8.20 (*dd*, *J* = 1.9, 9.1 Hz)	8.14 (*d*, *J* = 9.1 Hz)	8.51 (*d*, *J* = 7.6Hz)	7.78 (*dt*, *J* = 1.1, 7.6 Hz)	7.66 (*t*, *J* = 7.4 Hz)	7.76 (*d*, *J* = 6.8 Hz)	
 **2d**	8.90 (*d*, *J* = 1.9Hz)	8.13 (*dd*, *J* = 1.9, 8.8 Hz)	8.01 (*d*, *J* = 8.8 Hz)	8.55 (*d*, *J* = 7.6Hz)	7.80 (*dt*, *J* = 1.3, 7.6 Hz)	7.67 (*t*, *J* = 7.6 Hz)	7.78 (*d*, *J* = 7.6 Hz)	8.44 (*t*, *J* = 1 Hz) H2', 7.89 (*t*, *J* = 1.3 Hz) H5', 7.13 (*t*) H4'
 **2dH$^+$**	9.01 (*d*, *J* = 1.9Hz)	8.24 (*dd*, *J* = 1.9, 9.1 Hz)	8.11 (*d*, *J* = 9.1 Hz)	8.65 (*d*, *J* = 7.6 Hz)	7.85 (*dt*, *J* = 1.3, 7.6, Hz)	7.71 (*t*, *J* = 7.4 Hz)	7.82 (*d*, *J* = 7.3 Hz)	9.85 (*t*, *J* = 1.3 Hz) H2', 8.35 (*t*, *J* = 1.7 Hz) H5', 7.98 (*t*) H4'
 **2e**	8.88 (*d*, *J* = 1.9 Hz)	8.11 (*dd*, *J* = 1.9, 8.8 Hz)	8.01 (*d*, *J* = 8.8 Hz)	8.51 (*d*, *J* = 7.6 Hz)	7.78 (*dt*, *J* = 7.6,1.3 Hz)	7.65 (*t*, *J* = 7.4 Hz)	7.72 (*d*, *J* = 7.3 Hz)	8.42 (*d*, *J* = 2.5 Hz) H3', 7.84 (*d*, *J* = 1.6 Hz) H5', 6.59 (*dd*) H4'
 **2eH$^+$**	8.85 (*br. s*)	8.07 (*d*, *J* = 8.8 Hz)	7.97 (*d*, 8.8 Hz)	8.49 (*d*, 7.6Hz)	7.75 (*dt*, *J* = 7.6 Hz, 1.3 Hz)	7.61 (*t*, *J* = 7.4 Hz)	7.69 (*d*, *J* = 7.3 Hz)	8.41 (*s*) H3', 7.83 (*s*) H5', 6.57 (*d*) H4'

 **2f**	8.62 (*d*, *J* = 2 Hz)	7.86 (*dd*, *J* = 2 , 9.1 Hz)	7.66 (*d*, *J* = 9.1 Hz)	8.33 (*d*, *J* = 7.6 Hz)	7.70 (*t*, *J* = 7.3 Hz)	7.57 (*t*, *J* = 7.3Hz)	7.67 (*d*, *J* = 7.6 Hz)	8.15 (*dd*, *J* = 1.7, 4.7 Hz), 7.56 (*ddd*, *J* = 1.9, 6.9, 8.8 Hz), 6.89 (*d*, *J* = 8.5 Hz), 6.67 (*dd*, *J* = 6.9, 4.7 Hz), 3.72 (*s*, 8H)
 **2fH$^+$**	8.65 (*d*, *J* = 2 Hz)	7.90 (*dd*, *J* = 2, 9.1 Hz)	7.69 (*d*, *J* = 9.1 Hz)	8.37 (*d*, *J* = 7.6 Hz)	7.71 (*t*, *J* = 7.3 Hz)	7.57 (*t*, *J* = 7.3Hz)	7.68 (*d*, *J* = 7.3 Hz)	8.07 (*dt*, J = 1.9, 6.9 Hz), 8.06 (*d*, *J* = 6.9 Hz), 7.51 (*d*, *J* = 9.1 Hz), 7.00 (*t*, *J* = 7.3 Hz), 3.94-3.84 (*m*, 8H)
 **2g**	9.05 (*br*. *s*)	8.16-8.11 (*m*)	8.16-8.11 (*m*)	8.74 (*d*, *J* = 7.9 Hz)	7.77 (*t*, *J* = 7.6 Hz)	7.73 (*t*, *J* = 7.6 Hz)	8.57 (*d*, *J* = 7.6 Hz)	9.67 (*br*. *s*), 8.25 (*t*, *J* = 1.6 Hz), 7.90 (*br*. *s*) H2,5&4 Im, 13.43 (OH)
 **2gH$^+$**	9.06 (*br*. *s*)	8.18-8.12 (*m*)	8.18-8.12 (*m*)	8.75 (*d*, *J* = 7.9 Hz)	7.77 (*t*, *J* = 7.6 Hz)	7.74 (*t*, *J* = 7.6 Hz)	8.57 (*d*, *J* = 7.6 Hz)	9.83 (*t*, *J* = 1.5 Hz), 8.30 (*t*, *J* = 1.7 Hz), 7.98 (*t*, *J* = 1.5 Hz) H2,5&4 Im, 13.43 (OH)
 **2h**	8.72 (*br*. *s*)	7.76 (*s*)	7.76 (*s*)	8.43 (*d*, *J* = 7.6 Hz)	7.57 (*t*, *J* = 7.6 Hz)	7.52 (*t*, *J* = 7.4 Hz)	8.73 (*d*, *J* = 7.6 Hz)	8.06 (*dd*, *J* = 1,6, 4.4 Hz), 7.34 (*br*. *t*, *J* = 7.6 Hz), 6.68 (*d*, *J* = 8.2 Hz), 6.59 (*dd*, *J* = 5.0, 6.9 Hz), 3.70-3.60 (*m*, 8H)

 **2hH+**	8.77 (*d*, *J* = 1.9 Hz)	7.88 (*d*, *J* = 8.8 Hz)	7.84 (*dd*, *J* = 1.9, 8.8 Hz)	8.51 (*d*, *J* = 7.6 Hz)	7.68 (*dt*, *J* = 1.3, 7.6 Hz)	7.63 (*t*, *J* = 7.3 Hz)	8.61	8.14-8.07 (*m*, 2H), 7.53 (*d*, *J* = 9.5 Hz), 7.02 (*t*, *J* = 6.6 Hz), 3.95-3.74 (*m*, 8H)
 **7**	9.15 (*s*)	8.48 (*d*, *J* = 8.7 Hz)	8.85 (*d*, *J* = 8.7 Hz)	8.66 (*d*, *J* = 7.6 Hz)	7.88 (*m*)	7.76 (*t*, *J* = 7.2 Hz)	7.92 (*d*, *J* = 7.2 Hz)	
 **8**	9.11 (*br. s*)	8.33 (*d*, *J* = 8.7 Hz)	8.82 (*d*, *J* = 8.4 Hz)	8.65-8.70(*m*)	7.78-7.82 (*m*, *J* = 6.4, 6.8 , Hz)	7.72-7.77 (*m*, *J* = 6.8 Hz, 6.4 Hz)	8.65 (*d*, *J* = 6.4 Hz)	13.82 (*br. s*)
 **9**	9.01 (*d*, *J* = 1.9 Hz)	8.27 (*d*, *J* = 1.9 Hz, 9.1 Hz)	8.73 (*d*, *J* = 9.1 Hz)	8.61 (*d*, *J* = 7.6 Hz)	7.76 (*t*, *J* = 7.6 Hz)	7.70 (*d*, *J* = 7.6 Hz)	8.40 (*d*, *J* = 7.6 Hz)	3.22 (*s*); 3.07 (*s*)
 **13**	9.18 (*d*, *J* = 2 Hz)	8.38 (*dd*, *J* = 2.0, 9.1 Hz)	8.86 (*d*, *J* = 9.1 Hz)	8.68 (*d*, *J* = 7.6 Hz)	7.69-7.76 (*m*)	7.69-7.76 (*m*)	7.87 (*m*)	0.90 (*t*, *J* = 7.1 Hz); 1.18-1.35 (*m*); 1.49 (*quint*, *J* = 6.9 Hz); 2.04 (*s*); 2.39 (*t*, *J* = 7.3 Hz)

 **15**	8.84 (*d*)	8.31 (*d*, *J* = 9.1 Hz)	8.65 (*d*, *J* = 9.1 Hz)	8.39 (*d*, *J* = 7.6 Hz)	7.77 (*t*, *J* = 7.6 Hz)	7.64 (*t*, *J* = 7.2 Hz)	7.78 (*d*, *J* = 6.6 Hz)	10.17 (s, 1H) H9
 **17**	8.68 (*d*, *J* = 2.1 Hz)	8.08 (*dd*, *J* = 2.1, 9.1 Hz)	8.37 (*d*, *J* = 9.1 Hz)	8.22 (*d*, *J* = 7.6 Hz)	7.65 (*t* *J* = 7.6 Hz)	7.52 (*t*, *J* = 7.3 Hz)	7.64 (*d*, *J* = 7.3 Hz)	3.06 (s, 3H)
 **23**	8.76 (*s*, 1H)	8.23 (*d*, *J* = 9.1 Hz)	10.98 (*d*, *J* = 9.1 Hz)	8.39 (*d*, *J* = 7.6 Hz)	7.80 (*t*, *J* = 7.6 Hz)	7.67 (*t*, *J* = 7.5 Hz)	7.78 (*d*, *J* = 6.6 Hz)	14.93 (*s*)
 **25**	8.19 (*d*, *J* = 1.9 Hz)	7.57 (*m*)	6.68 (*d*, J = 9.1 Hz)	7.87 (*d*, *J* = 7.6 Hz)	7.48 (*m*)	7.56 (*t*, *J* = 7.6 Hz)	7.73 (*d*, *J* = 7.2 Hz)	4.26 (*t*, *J* = 10.2 Hz), 3.93 (*t*, *J* = 10.2 Hz)
 **25H+**	8.65 (*s*)	8.10 (*d*, *J* = 9.1 Hz)	7.52 (*d*, *J* = 9.1 Hz)	8.15 (*d*, *J* = 7.6 Hz)	7.76 (*d*, *J* = 7.6 Hz)	7.67 (*t*, *J* = 7.4 Hz)	7.83 (*d*, *J* = 7.2 Hz)	4.86 (*dd*, *J* = 9.1, 10.6 Hz); 4.49 (*dd*, *J* = 9.1, 10.6 Hz)

 **27**	8.28 (*d*, *J* = 2.3 Hz)	7.63 (*dd*, *J* = 2.3, 8.7 Hz)	6.94 (*d*, *J* = 8.7 Hz)	8.16 (*d*, *J* = 7.6 Hz)	7.48 (*dt*, *J* = 1.1,7.6 Hz)	7.44 (*t*, *J* = 7.2 Hz)	7.55 (*d*, *J* = 7.2 Hz)	4.08-3.93 (*m*, 4H), 2.95 & 2.59 (2x*br. s*, 2x3H), 1.73 (*s*, 3H)
 **27H⁺**	8.87 (*d*, *J* = 1.9 Hz)	8.15 (*dd*, *J* = 1.9, 8.8 Hz)	7.76 (*d*, *J* = 8.8 Hz)	8.57 (*d*, *J* = 7.6 Hz)	7.67 (*t*, *J* = 7.3 Hz)	7.63 (*t*, *J* = 7.6 Hz)	7.74 (*d*, *J* = 7.3 Hz)	4.90-4.77 (*m*, 2H), 4.29-4.19 (*m*, 2H), 3.05 & 2.63 (2x*br. s*, 2x3H), 1.84 (*s*, 3H), 9.97 (*s*, 1H)
 **28**	8.46 (*d*, *J* = 2.2 Hz)	7.76 (*dd*, *J* = 2.2, 8.8 Hz)	7.16 (*d*, *J* = 8.8 Hz)	8.31 (*m*)	7.55 (*m*)	7.55 (*m*)	8.00 (*m*)	4.38 (*t*, *J* = 10.1 Hz, 2H), 4.10 (*t*, *J* = 10.1 Hz, 2H), 15.58 (*s*, OH)
 **28H⁺**	8.74 (*br. s*)	8.11 (*d*, *J* = 9.1 Hz)	7.73 (*d*, *J* = 9.1 Hz)	8.56 (*m*)	7.67 (*t*, *J* = 7.3 Hz)	7.63 (*t*, *J* = 7.6 Hz)	8.45 (*m*)	4.78 (*t*, *J* = 9.5 Hz, 2H), 4.20 (*t*, *J* = 9.5 Hz, 2H), 9.23 (*s*, OH)

Synthesis of compounds **2b**, **2d**, **2g**, **2h** and **2f** and their analytical data has been given in reference **14** of manuscript.

2c Unpublished result

¶ We have used arbitrary systematic position numbering of protons for the sake of easier comparison within the same structural scaffold.

The IUPAC nomenclature of compounds is used throughout text in the Experimental section.

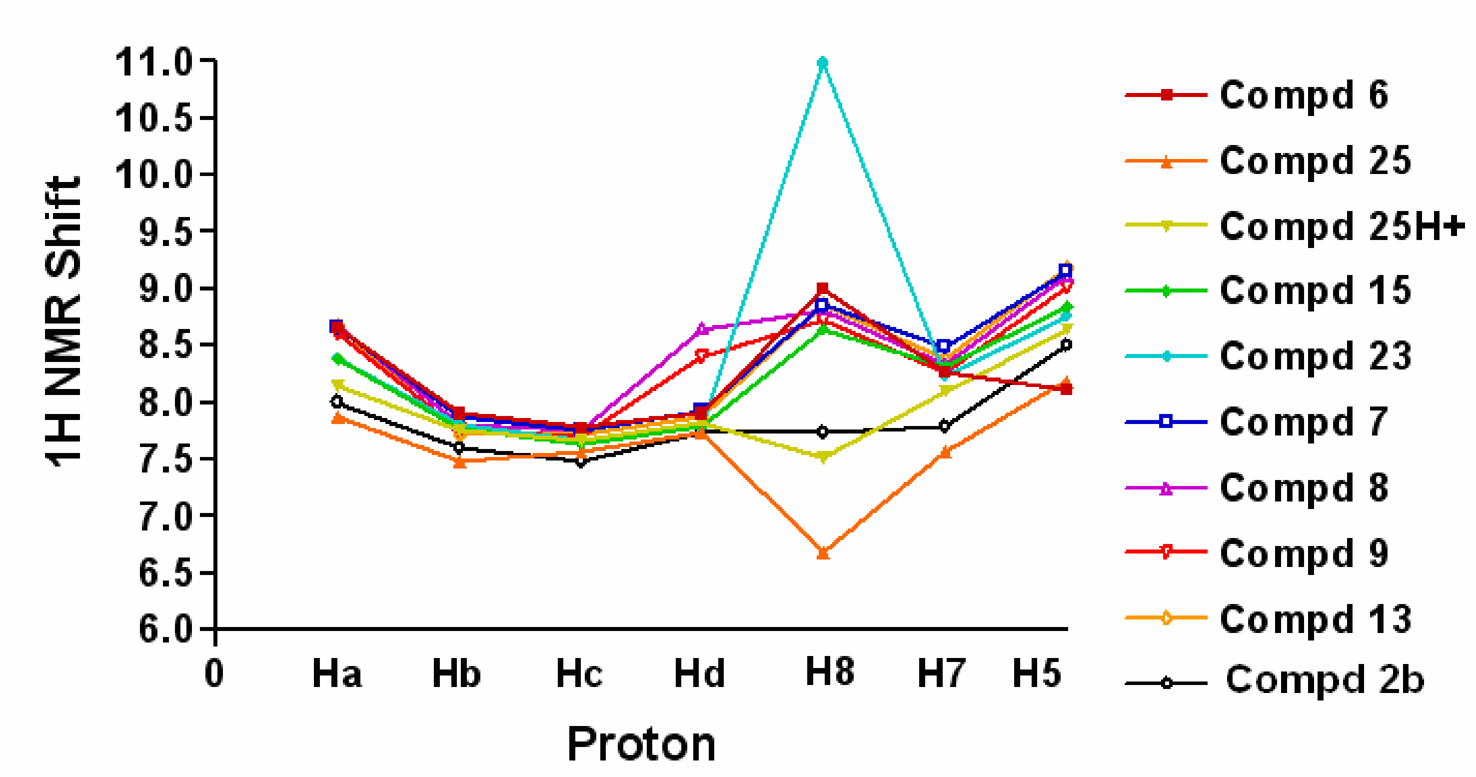


Figure S1: Plot of aromatic ^{1}H Chemical shifts for various fused azoles. Maximum variation of proton shifts is observed for aromatic protons H8, Hd and H7 (shown in the square box).

Computational details: All geometry optimizations have been carried out using closed-shell Hartree-Fock method[1] and 6-31G(d,p) basis set[2] as it is implemented in Gaussian 03.[3] Then GIAO nuclear magnetic shielding tensors were calculated using the same method and basis set as the one employed during the geometry optimizations. Isotopic shielding part of the GIAO nuclear magnetic shielding tensors[4] have employed to calculated proton NMR chemical shifts relative to TMS (see Table S3). The TMS reference signal for proton chemical shifts was found located at 32.3355 ppm. Chemical shifts have been calculated as follows: δ (calc) = Isotropic Shielding(TMS) – Isotropic Shielding(proton).

1 *Ab initio* studies and comparison of theoretical proton chemical shifts with those of experimentals.

1.1 *Thiol-thione tautomerism of compound 23*

Our energy calculations have showed that thione tautomeric form of compound **23** is more stable than thiol form by 16.95 kcal/mol. Calculated proton chemical shifts for both forms are found to be almost identical (see Table S2) with exceptions of proton associated with the tautomerization (proton in position **A**, Table S2) and proton interacting with the mercapto part of **23** (proton in position **8**, Table S2). Comparison of experimental and theoretical proton chemical shifts (see Table S2) suggests that thione form is indeed the only tautomeric form present in solution. Thus the calculated chemical shift of proton in position **8** (11.10 ppm) in the thione form is found to be within 0.12 ppm from the experimental value of 10.98 ppm while in thiol form the theoretical value is 8.39 ppm (2.59 ppm from the experimental δ). Calculated chemical shift of proton in position **A** in thione form is also much closer to experimental value than the one in thiol (9.54 ppm versus 5.58 ppm) but is still quite far from the experimental value of 14.93 ppm. This difference suggests that proton in position **A** is probably involved in interaction with solvent which is not taken into account in our theoretical calculations.

1.2 ***Ab intio simulation of proton chemical shifts***

The assignment of experimental NMR spectra has been confirmed via *ab initio* simulations of proton chemical shifts (see Calculations details in computational part). A good agreement (standard error 0.37 ppm, Figure 2) between experimental and theoretical values has been obtained for the aromatic and aliphatic protons of all compounds (see Figure 2 as well as Table S3). However, the fast exchanging protons of hydroxyl groups in compounds **8**, **2g**, **2gH+** as well as proton in position **A** of compound **23** are not reproduced well missing the target 13 to 14 ppm chemical shift by almost 7 ppm (Table S3). Taking into account generally good reproducibility of experimental values by the computational technique employed (see Figure 2), such large deviation cannot be explained by deficiencies in technique *per se* and can probably be attributed to strong interactions of these protons with solvent which has not been taken into account in the gas phase calculations employed. Calculated chemical shifts of protons in position **d** of all compounds under investigation have also shown quite large 0.5-1.2 ppm deviation from the experimental values (see Table S3) which suggests presence of interactions unaccounted for by the theoretical model employed.

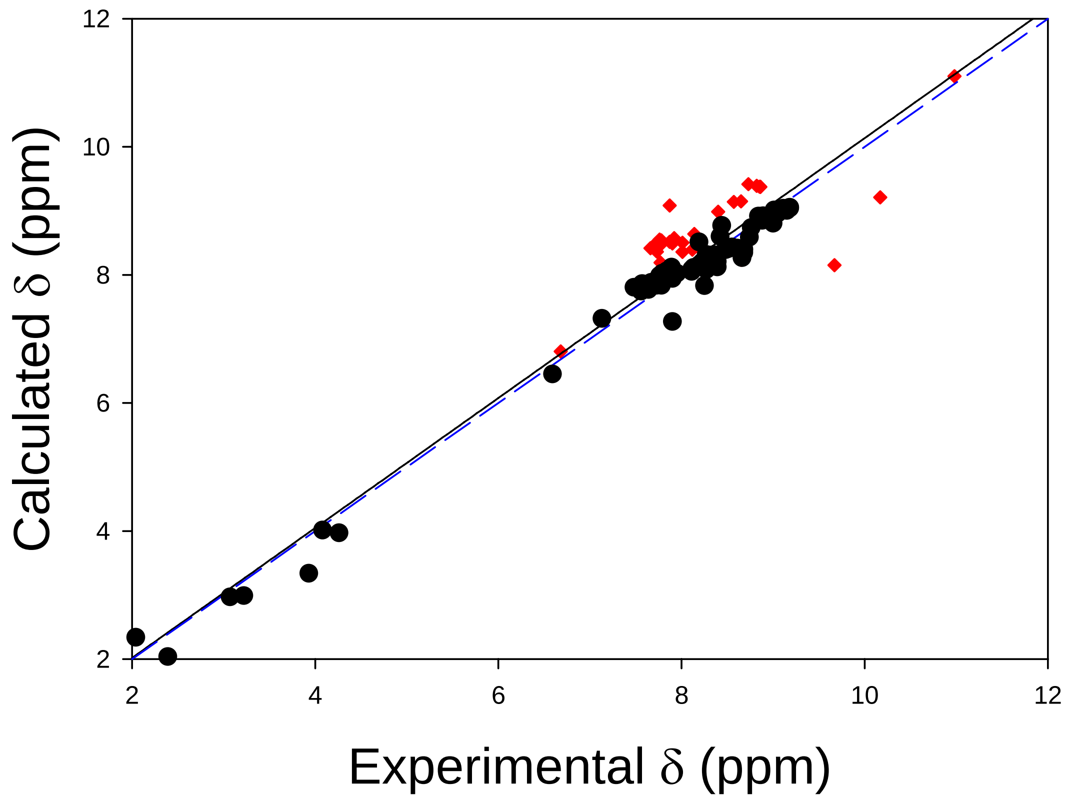
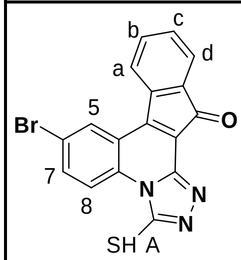
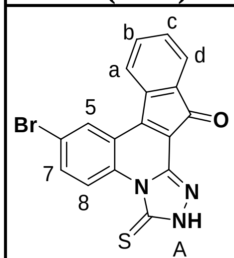


Figure S2. Comparison between theoretical and experimental proton chemical shifts of all protons (excluding hydroxyl protons of **8** and **2g** as well as proton in position **A** of compound **23**) in all compounds investigated (Table S3). Linear regression $y = (1.0146 \pm 0.0179)\,x - (0.0120 \pm 0.1405)$, $R = 0.982$, $R^2 = 0.965$, standard error of estimate = 0.37 ppm. Excluding from this statistics the aromatic protons in positions **8** and **d** as well as imidazole proton in position **A** of compound **2g** (red diamonds) significantly improves statistical parameters (linear regression $y = (1.0121 \pm 0.0105)\,x - (-0.0940 \pm 0.0809)$, $R = 0.995$, $R^2 = 0.991$, standard error of estimate = 0.21 ppm). The fact that these protons can spacially interact with C2-substituents in the series via solvent suggests a presence of additional interactions with the solvent which are not accounted for in the theoretical model employed. Blue dashed line represents ideal 1 to 1 correspondence between theoretical and experimental values.

Table S2. Hartree-Fock energy of thiol and thione tautomeric forms[a,b,c] of compound **23** as well as calculated (relative to TMS) and experimental chemical shifts[b] of aromatic protons (ppm) in compound **23.**

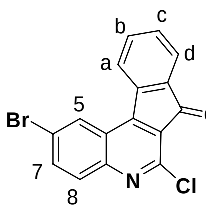
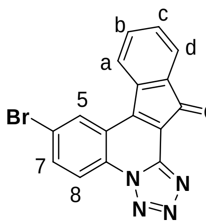
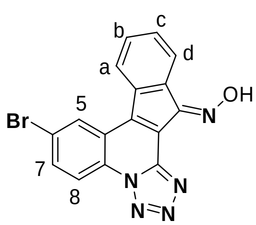
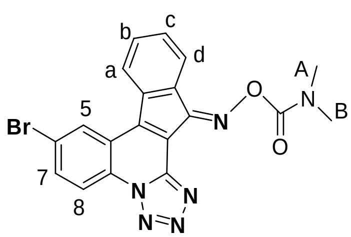
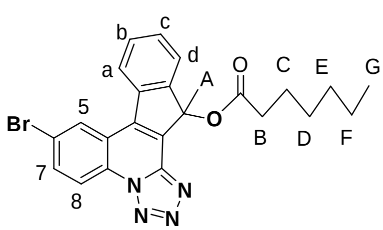
	HF energy (a.u.)	**$\delta(H_5)$**	**$\delta(H_7)$**	**$\delta(H_8)$**	**$\delta(H_a)$**	**$\delta(H_b)$**	**$\delta(H_c)$**	**$\delta(H_d)$**
 **23 (thiol)**	-3854.02610644	8.76 (8.89) Δ=0.13	8.23 (8.21) Δ0.02	10.98 (8.39) Δ=2.59	8.39 (8.12) Δ=0.27	7.80 (7.89) Δ=0.09	7.67 (7.77) Δ=0.10	7.78 (8.49) Δ=0.71
 **23 (thione)**	-3854.05312372	8.76 (8.74) Δ=0.02	8.23 (8.20) Δ=0.03	10.98 (11.10) Δ=0.12	8.39 (8.21) Δ=0.18	7.80 (7.93) Δ=0.13	7.67 (7.83) Δ=0.16	7.78 (8.48) Δ=0.70

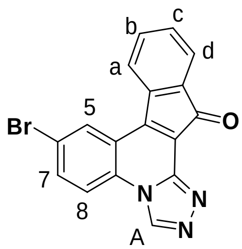
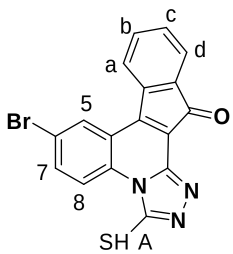
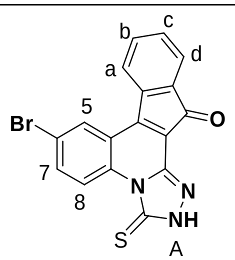
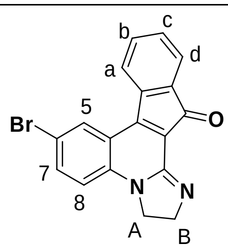
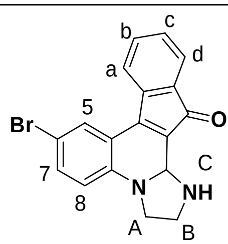
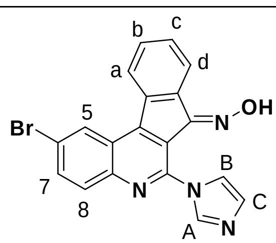
[a]The chemical shifts in parenthesis are from the *ab initio* calculations.

[b]Δ is a difference between experimental and calculated values (ppm).

[c]ΔE = -0.02701728 a.u. = -16.95 kcal/mol, which means **23** (thione) is stabilized by 16.95 kcal/mol over **23** (thiol).

Table S3: Comparison between theoretical and experimental chemical shifts

Sr. No.	Structure	Proton position	δ (exp), ppm	δ (calc), ppm	Δ = δ(exp) - δ(calc), ppm
6		5	9.00	8.80	0.20
		7	8.27	8.08	0.19
		8	8.12	8.39	-0.27
		a	8.66	8.34	0.32
		b	7.90	7.94	-0.04
		c	7.78	7.84	-0.06
		d	7.90	8.49	-0.59
7		5	9.15	9.00	0.15
		7	8.48	8.39	0.09
		8	8.85	9.38	-0.53
		a	8.66	8.27	0.39
		b	7.88	7.96	-0.08
		c	7.76	7.87	-0.11
		d	7.92	8.57	-0.65
8		5	9.01	9.01	0.00
		7	8.33	8.28	0.05
		8	8.82	9.39	-0.57
		a	8.68	8.40	0.28
		b	7.80	7.95	-0.15
		c	7.76	7.88	-0.12
		d	8.65	9.15	-0.50
		OH	13.82	7.09	6.73
9		5	9.01	9.01	0.00
		7	8.27	8.31	-0.04
		8	8.73	9.42	-0.69
		a	8.61	8.42	0.20
		b	7.76	7.99	-0.23
		c	7.70	7.84	-0.14
		d	8.40	8.99	-0.59
		A	3.07	2.97	0.10
		B	3.22	2.99	0.23
13		5	9.18	9.05	0.13
		7	8.38	8.29	0.09
		8	8.86	9.37	-0.51
		a	8.68	8.35	0.33
		b	7.73	7.88	-0.16
		c	7.73	7.84	-0.12
		d	7.87	9.08	-1.21
		A	2.04	2.34	-0.30
		B	2.39	2.04	0.35
		C	1.49	1.53	-0.04
		D	1.27 (1.18-1.35)	0.93	0.33
		E	1.27 (1.18-1.35)	1.14	0.12
		F	1.27 (1.18-1.35)	1.15	0.12
		G	0.90	0.95	-0.05

15		5	8.84	8.91	-0.07
		7	8.31	8.21	0.10
		8	8.65	8.23	0.42
		a	8.39	8.12	0.27
		b	7.77	7.89	-0.12
		c	7.64	7.77	-0.13
		d	7.78	8.51	-0.73
		A	10.17	9.21	0.96
23 (thiol form)		5	8.76	8.89	-0.13
		7	8.23	8.21	0.02
		8	10.98	8.39	2.59
		a	8.39	8.12	0.27
		b	7.80	7.89	-0.09
		c	7.67	7.77	-0.10
		d	7.78	8.49	-0.71
		A	14.93	5.58	9.35
23 **(thione form, more stable)**		5	8.76	8.74	0.02
		7	8.23	8.20	0.03
		8	10.98	11.10	-0.12
		a	8.39	8.21	0.18
		b	7.80	7.93	-0.13
		c	7.67	7.83	-0.16
		d	7.78	8.48	-0.70
		A	14.93	9.536	5.39
25		5	8.17	8.51	-0.34
		7	7.57	7.86	-0.29
		8	6.68	6.80	-0.12
		a	7.89	8.05	-0.16
		b	7.57	7.80	-0.23
		c	7.46	7.75	-0.29
		d	7.73	8.36	-0.63
		A	3.92	3.34	0.58
		B	4.25	3.97	0.28
25 H+		5	8.65	9.25	-0.60
		7	8.10	8.76	-0.66
		8	7.52	7.57	-0.05
		a	8.15	8.62	-0.47
		b	7.76	8.36	-0.60
		c	7.67	8.43	-0.76
		d	7.83	8.82	-0.99
		A	4.86	4.41	0.45
		B	4.49	4.21	0.28
		C	-	6.73	-
2g		5	9.05	8.96/8.96	0.09/0.09
		7	8.11	8.05/8.04	0.06/0.07
		8	8.16	8.44/8.42	-0.28/-0.26
		a	8.74	8.59/8.59	0.15/0.15
		b	7.77	8.00/8.00	-0.23/-0.23
		c	7.73	7.89/7.90	-0.16/-0.17
		d	8.57	9.14/9.15	-0.57/-0.58
		A	9.67	8.45/8.15	1.22/1.52

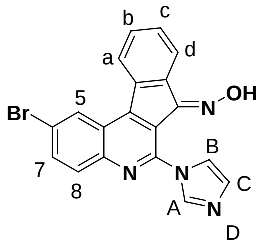
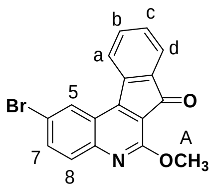
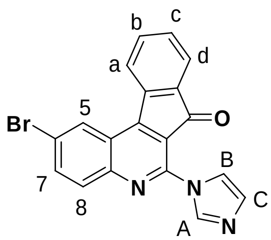
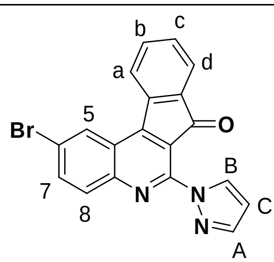
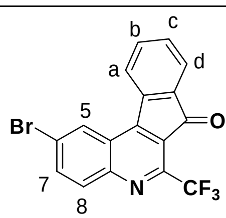
		B	8.25	7.50/7.83	0.75/0.42
		C	7.90	7.23/7.27	0.67/0.63
		OH	13.43	6.44/6.48	6.99/6.95
2g H+		5	9.06	9.25	-0.19
		7	8.15	8.50	-0.35
		8	8.15	8.47	-0.32
		a	8.75	8.83	-0.08
		b	7.77	8.36	-0.59
		c	7.74	8.29	-0.55
		d	8.57	9.28	-0.71
		A	7.98	8.41	-0.43
		B	9.83	9.34	0.49
		C	8.30	9.16	-0.86
		D	13.43	6.46	6.97
2b		5	8.66	8.76	-0.10
		7	7.95	8.02	-0.07
		8	7.77	8.19	-0.42
		a	8.34	8.31	0.03
		b	7.70	7.89	-0.19
		c	7.58	7.79	-0.21
		d	7.66	8.42	-0.76
		A	4.08	4.01	0.07
2d		5	8.90	8.87	0.03
		7	8.13	8.11	0.02
		8	8.01	8.36	-0.35
		a	8.55	8.43	0.12
		b	7.80	8.00	-0.20
		c	7.67	7.88	-0.21
		d	7.78	8.54	-0.76
		A	8.44	8.77	-0.33
		B	7.89	8.12	-0.23
		C	7.13	7.32	-0.19
2e		5	8.90	8.87	0.03
		7	8.13	8.11	0.02
		8	8.01	8.36	-0.35
		a	8.55	8.43	0.12
		b	7.80	8.00	-0.20
		c	7.67	7.88	-0.21
		d	7.78	8.54	-0.76
		A	7.84	8.06	-0.22
		B	8.42	8.60	-0.18
		C	6.59	6.45	0.14
2c		5	8.89	8.92	-0.03
		7	8.20	8.16	0.04
		8	8.14	8.64	-0.50
		a	8.51	8.41	0.10
		b	7.78	7.99	-0.21
		c	7.66	7.87	-0.21
		d	7.76	8.55	-0.79

Table S4. Coordinates, charge, multiplicity, Hartree-Fock energy and dipole moment of *ab initio* optimized geometries (HF/6-31G**, Gaussian 03).

Compound 6

Charge = 0 Multiplicity = 1
C,0,2.8321931156,-0.3539189876,0.0001501645
C,0,2.9056053728,-1.7657535663,0.0012153337
C,0,1.7614997579,-2.4922835998,0.0015944185
C,0,0.4953369331,-1.8527663348,0.0010105859
C,0,0.4307432081,-0.4434296756,0.0001151986
C,0,1.6441732963,0.2951614289,-0.0003822407
C,0,-0.8735941104,0.1178225207,-0.0002080945
C,0,-1.9618938651,-0.7197704298,-0.0006451507
C,0,-1.7597109082,-2.115926438,-0.0003887429
N,0,-0.5957282278,-2.6535667933,0.000816634
C,0,-1.3550495041,1.5370077913,0.0001312069
C,0,-2.7492440943,1.5090408507,-0.0005111458
C,0,-3.2211478661,0.092397202,-0.0010721999
O,0,-4.3488120441,-0.2777590361,-0.001558295
Cl,0,-3.1157194747,-3.1907555048,0.0000072416
C,0,-0.7054317893,2.7548467321,0.0013695015
C,0,-2.8537753288,3.8765813488,0.0006192099
C,0,-3.5119932421,2.6500293798,-0.0002921291
H,0,1.777963683,-3.5654690114,0.0023117374
H,0,-3.4177256151,4.7916527318,0.0007340403
H,0,-4.5846367036,2.584829923,-0.0008161826
Br,0,4.4465412433,0.6383757844,-0.0007433574
H,0,3.8651940481,-2.2461841863,0.0016581501
H,0,1.6341203189,1.3625673132,-0.0014550378
H,0,0.3613349522,2.8444797842,0.0024307023
C,0,-1.4719923372,3.9198258183,0.0015077274
H,0,-0.9716810099,4.8716701691,0.002499054

HF=-3768.686413
RMSD=6.219e-009
Dipole =1.0156339,1.6672115,0.0008983
PG=C01 [X(C16H7Br1Cl1N1O1)]

Compound 7

Charge = 0 Multiplicity = 1
C,0,-2.7546423812,-0.211321651,0.0301817128
C,0,-2.8608595116,-1.6013872744,0.0045938737
C,0,-1.7244253663,-2.3669670465,-0.0243731759
C,0,-0.4790968458,-1.7417665378,-0.027751935
C,0,-0.3510963872,-0.3457086034,-0.0023178356
C,0,-1.534716591,0.407920594,0.0269862453
C,0,0.9914188179,0.2221703118,-0.0080475764
C,0,2.0806958966,-0.579992122,-0.0371896005
C,0,1.9320981158,-2.0009533558,-0.0628024104
N,0,0.6836766345,-2.4919802425,-0.0567459169
C,0,1.4510556106,1.6542933034,0.0140273104
C,0,2.8483953621,1.646712965,-0.0036707184
C,0,3.3331874557,0.2347426361,-0.0371300736
O,0,4.4557628738,-0.1449517814,-0.0584983975

N,0,2.7594395824,-3.0051799111,-0.0924304918
C,0,0.788683952,2.8623856056,0.0458835204
C,0,2.920999511,4.01559428,0.0415186265
C,0,3.5949507302,2.7953502971,0.0093133967
H,0,-1.7761707248,-3.4378319267,-0.044458224
H,0,3.4738316749,4.9372718473,0.0524973491
H,0,4.6683306056,2.7441040382,-0.0051681794
Br,0,-4.3300456313,0.8374457994,0.0700545265
H,0,-3.8275490205,-2.0669758121,0.007604584
H,0,-1.5007450866,1.4737154276,0.047185071
H,0,-0.2782735774,2.9446630267,0.0608823728
C,0,1.5416197065,4.039420711,0.0593249412
H,0,1.0272772793,4.9834250821,0.0841704199
N,0,0.7690182894,-3.8247037347,-0.0835657969
N,0,1.9948918514,-4.0941825534,-0.1041024299

HF=-3472.4876487
RMSD=4.911e-009
Dipole=-2.0009017,2.5810999,0.0749247
PG=C01 [X(C16H7Br1N4O1)]

Compound 8

Charge = 0 Multiplicity = 1
C,0,-3.0030838179,-0.2478445663,0.039511649
C,0,-3.1048994734,-1.6370444626,0.013903926
C,0,-1.9624294829,-2.3938401885,-0.017766694
C,0,-0.7218625018,-1.7602797899,-0.0237401007
C,0,-0.5976756806,-0.3650713535,0.0016933905
C,0,-1.7864435263,0.3795506425,0.033784192
C,0,0.7446560631,0.2093235518,-0.0069287041
C,0,1.8385802222,-0.5870496283,-0.0387831751
C,0,1.6922544754,-2.010561627,-0.0644389952
N,0,0.4465868622,-2.5053367491,-0.0556049822
C,0,1.2070264541,1.6288575735,0.0141484161
C,0,2.61217113,1.6308512131,-0.0066823921
C,0,3.0685563212,0.2229486386,-0.0411481553
N,0,4.2064840429,-0.3091058692,-0.0685939816
N,0,2.5226588864,-3.0141963739,-0.0963613958
C,0,0.5270089849,2.8314892037,0.0479803934
C,0,2.6327203632,4.0112996104,0.0399791371
C,0,3.3296854104,2.8086252511,0.0058904601
H,0,-2.0064905153,-3.4651035957,-0.0380422504
H,0,3.1740756385,4.9400972884,0.0502838072
H,0,4.399943413,2.7957432071,-0.0102531321
Br,0,-4.5838250993,0.7950194802,0.0832039243
H,0,-4.0689086111,-2.1079069096,0.0189576972
H,0,-1.7616264875,1.4452750832,0.0542010492
H,0,-0.5411465359,2.8903377826,0.0649885729
C,0,1.2516942126,4.0188182636,0.0606434721
H,0,0.7225076976,4.9545905562,0.0869798023
N,0,0.5350581935,-3.8366149803,-0.0828077573
N,0,1.7618773849,-4.104338331,-0.1063463177
O,0,5.2292307072,0.578291381,-0.0663820545
H,0,6.0052657043,0.0416658648,-0.0884763341

HF=-3527.4606282
RMSD=5.653e-009
Dipole=-0.5696856,2.1381979,0.0503419
PG=C01 [X(C16H8Br1N5O1)]

Compound 9

Charge = 0 Multiplicity = 1
C,0,-4.2900581858,-0.2404878818,0.074473012
C,0,-4.425679385,-1.6222083728,0.1918538627
C,0,-3.3023941946,-2.4050655225,0.2545006973
C,0,-2.0462340782,-1.8049680374,0.2005163769
C,0,-1.8881067556,-0.4179969584,0.0846663328
C,0,-3.0582542492,0.3538522397,0.0213776593
C,0,-0.5312734318,0.11881887,0.0341087966
C,0,0.5425024942,-0.7024483081,0.0832400182
C,0,0.3620700062,-2.1174058281,0.2124420101
N,0,-0.8973113525,-2.5762135132,0.2624320702
C,0,-0.0358235802,1.5242827921,-0.069990371
C,0,1.3691532245,1.494339749,-0.0800315665
C,0,1.7937645691,0.0754943208,0.0074620921
N,0,2.9108728117,-0.4988394312,0.0102523807
N,0,1.1651255344,-3.1369904773,0.3121626037
C,0,-0.6902210279,2.7377465843,-0.150082508
C,0,1.4377526889,3.8695056603,-0.2596295486
C,0,2.1083989043,2.6536483712,-0.1773861106
H,0,-3.3725748085,-3.4713334727,0.3439379408
H,0,1.9991753749,4.7831074814,-0.3357057927
H,0,3.1776134009,2.6221472614,-0.1922872057
Br,0,-5.8445142075,0.8380571327,-0.0144525385
H,0,-5.401099525,-2.0672259122,0.231658655
H,0,-3.0083968447,1.4146658776,-0.0714590785
H,0,-1.7566239338,2.819596228,-0.1433329164
C,0,0.0583558644,3.9072765297,-0.2437671077
H,0,-0.4519235363,4.8517015114,-0.3060802095
N,0,-0.8434355478,-3.9027929914,0.3931635932
N,0,0.3762309392,-4.2015002406,0.4194230113
O,0,3.9544087868,0.3837830081,0.0031404877
C,0,5.1127268632,-0.1573723108,-0.4645275142
N,0,6.1760545179,0.5630052991,-0.0495295807
C,0,6.1074543437,1.6921047241,0.8558116757
C,0,7.4801552637,0.2577648882,-0.6049186629
O,0,5.1428843575,-1.10956004,-1.1700014354
H,0,5.2137945615,1.6530061033,1.4559837599
H,0,6.1330353127,2.637019224,0.3173714385
H,0,6.9648898219,1.659633806,1.518234131
H,0,7.8743592576,1.1189955483,-1.1375257167
H,0,7.3956185011,-0.5726945877,-1.2850431586
H,0,8.1732902018,-0.0023720306,0.1889311681

HF=-3773.3083721
RMSD=5.117e-009
Dipole=-0.5776884,3.4349931,0.4627808
PG=C01 [X(C19H13Br1N6O2)]

Compound 13

Isomer 1

Charge = 0 Multiplicity = 1
C,0,-4.7836692929,-0.1983297716,-1.2972301773
C,0,-4.7783617447,-1.5486436696,-1.6389824322
C,0,-3.7068064421,-2.3268873696,-1.2847974938
C,0,-2.6450196932,-1.7529481699,-0.5897175321
C,0,-2.6318024978,-0.3977241886,-0.2341455916
C,0,-3.742291582,0.3702158937,-0.6134680207
C,0,-1.4719854482,0.1192300392,0.4932905347
C,0,-0.4470764674,-0.6910273413,0.8168462336
C,0,-0.4791757038,-2.0691349684,0.4438399595
N,0,-1.5491971919,-2.5188267155,-0.2218510501
C,0,-1.148704238,1.4857426868,0.9945286615
C,0,0.1110445558,1.4331187731,1.6032761846
C,0,0.6657833003,0.0137554173,1.5597669534
O,0,1.8020581936,-0.1269596787,0.6996843055
N,0,0.3375638536,-3.0713755098,0.6165164433
C,0,-1.8473015287,2.6802272536,0.9635063308
C,0,-0.0361581045,3.7512417486,2.1372339364
C,0,0.6678460444,2.5527862932,2.1816188815
H,0,-3.6712732551,-3.3694393009,-1.5338247969
H,0,0.389169366,4.634893834,2.5783067762
H,0,1.6318873273,2.5016920671,2.6477189165
Br,0,-6.264841319,0.8746424309,-1.7903545638
H,0,-5.6052544374,-1.973202983,-2.1747510986
H,0,-3.7922824722,1.4087931495,-0.3768049797
H,0,-2.8165681192,2.7691028247,0.5184555922
C,0,-1.2782803919,3.8112667032,1.5352134524
H,0,-1.8178388297,4.7411928093,1.5099618624
N,0,-1.3685747364,-3.8212844508,-0.4563265655
N,0,-0.2560403437,-4.1156745186,0.0466868195
C,0,3.0211470984,0.2992738717,1.0115230075
C,0,4.0057754279,-0.1037524983,-0.0579874158
C,0,5.4318102068,0.3579877229,0.2238980838
O,0,3.288494492,0.9131230788,1.9942081313
C,0,6.4057206014,-0.0665594549,-0.8759832066
C,0,0.9010119826,-0.6030283299,2.9399027346
H,0,3.6392878822,0.2955769285,-1.0000270376
H,0,3.9487442495,-1.1847256093,-0.1525033418
H,0,5.7557826756,-0.044384614,1.1790808104
H,0,5.4444531554,1.4387114158,0.3312935625
H,0,6.0730812691,0.3378469729,-1.8312656963
H,0,6.384155112,-1.1504512088,-0.9807221614
C,0,7.8417218544,0.3862673548,-0.6091761877
C,0,8.8222871372,-0.0344259567,-1.7047861579
C,0,10.2550289681,0.4206785964,-1.4320627519
H,0,-0.0361765702,-0.6141890939,3.4849890081
H,0,1.6261446594,-0.035390211,3.5018042084
H,0,1.2504888553,-1.6222785801,2.8287497385
H,0,8.1747743384,-0.0182803643,0.345533202
H,0,7.863748316,1.4701434686,-0.5042296448
H,0,8.4908071786,0.3702181911,-2.6593211099
H,0,8.8016420427,-1.1175370966,-1.8096122091
H,0,10.6282223324,0.0040492924,-0.5005464626
H,0,10.3151720807,1.5029655525,-1.3563811186

H,0,10.9253322018,0.1070448238,-2.226461231

HF=-3859.6739138
RMSD=4.372e-009
Dipole=-0.8192255,1.5281333,-0.307326
PG=C01 [X(C24H23Br1N4O2)]

Isomer 2

Charge = 0 Multiplicity = 1
C,0,-4.6382289576,-0.2509237662,1.7405099546
C,0,-4.5806776669,-1.597053397,2.0938183707
C,0,-3.5352131721,-2.3641150571,1.6489125252
C,0,-2.5516514703,-1.7832284095,0.8519597828
C,0,-2.5921005562,-0.4320932957,0.4831641557
C,0,-3.673856317,0.3244054358,0.9567974804
C,0,-1.5131310212,0.0928114306,-0.3546003835
C,0,-0.5108576827,-0.7065945807,-0.7645272799
C,0,-0.4872537903,-2.0806765468,-0.3763760929
N,0,-1.4835286054,-2.5377504536,0.3909576103
C,0,-1.2586454122,1.4579814631,-0.8973843603
C,0,-0.060645008,1.4161325477,-1.6208614286
C,0,0.5169378234,0.0052890965,-1.6153542342
N,0,0.3248099372,-3.0732556677,-0.6145446405
C,0,-1.9690095266,2.6428678869,-0.8128303031
C,0,-0.2917409035,3.7258391197,-2.1615133124
C,0,0.4228667288,2.5368807089,-2.2598031873
H,0,-3.4608984855,-3.4031587853,1.9039698715
H,0,0.0772552807,4.6103311631,-2.6491646399
H,0,1.3397828393,2.4940124677,-2.8135766787
Br,0,-6.0830141466,0.8065952547,2.3590110259
H,0,-5.3475035671,-2.0270865419,2.7087163399
H,0,-3.7613913948,1.3593963815,0.7153599105
H,0,-2.8936119644,2.7232643628,-0.279814749
C,0,-1.4728726812,3.7752701628,-1.4464416445
H,0,-2.021545763,4.6977953569,-1.3798967891
N,0,-1.2622145592,-3.8347664556,0.6206122523
N,0,-0.1971767467,-4.119204689,0.0187306256
O,0,1.7306526426,-0.1096868688,-0.8639956638
C,0,2.9086816178,0.3302035973,-1.2926445371
C,0,3.9947596225,-0.0465609953,-0.3157837456
C,0,5.381159382,0.4318815094,-0.7344110771
O,0,3.0739031742,0.9365268045,-2.3021254396
C,0,6.459680719,0.0338724856,0.2739845298
H,0,3.9630942166,-1.127058871,-0.2052913233
H,0,3.7118001993,0.3584739983,0.6522572819
H,0,5.3674096109,1.5113529722,-0.8535921751
H,0,5.6206653346,0.0230162611,-1.7114968472
H,0,6.4643282251,-1.048926046,0.391377815
H,0,6.2115118617,0.4446328132,1.251964606
C,0,7.8575474933,0.5037238105,-0.130422265
C,0,0.6315246039,-0.6237878211,-3.0051877443
C,0,8.94222664,0.1096008324,0.8730662238
C,0,10.3362846731,0.5815233021,0.4630110199
H,0,7.8533368786,1.5865121694,-0.2480523342
H,0,8.1061905356,0.0928490328,-1.1078730176
H,0,1.2924470141,-0.0524638366,-3.638071058
H,0,-0.3521671985,-0.6542217507,-3.4601616566

H,0,1.0050952997,-1.6367064075,-2.9169934366
H,0,8.9477360287,-0.9723976644,0.9905079445
H,0,8.6951644377,0.52066387,1.8501741551
H,0,10.3728012235,1.6635839997,0.3708147954
H,0,10.6272322165,0.1592575517,-0.4949112159
H,0,11.0823747572,0.286667846,1.1945505045

HF=-3859.6739138
RMSD=4.372e-009
Dipole=-0.8103326,1.5200273,0.367354
PG=C01 [X(C24H23Br1N4O2)]|

Compound 15

Charge = 0 Multiplicity = 1
C,0,-2.7653725384,-0.1913512223,0.0306524043
C,0,-2.8847954436,-1.5749886312,0.0061271348
C,0,-1.7509931619,-2.3493242168,-0.0223779792
C,0,-0.4922263176,-1.7529429206,-0.026673808
C,0,-0.3602275773,-0.3549183459,-0.0021263831
C,0,-1.5331443069,0.4086651479,0.0267040331
C,0,0.9850780934,0.2143751165,-0.0081275274
C,0,2.0679669698,-0.5883729145,-0.0363346947
C,0,1.9338023199,-2.0157230364,-0.061164209
N,0,0.661935164,-2.5272331836,-0.0552965419
C,0,1.4419010495,1.6484964783,0.0126804329
C,0,2.8391836808,1.6407798075,-0.0047566975
C,0,3.3222483424,0.2280455199,-0.0368229147
O,0,4.4462122639,-0.1473567829,-0.0577436858
N,0,2.8043095252,-2.964880784,-0.0892996474
C,0,0.7828285437,2.8584554347,0.0431152329
C,0,2.9166734985,4.0099957989,0.0380014218
C,0,3.5876162189,2.7877305642,0.0071493973
H,0,-1.8445431115,-3.4177534271,-0.0412845452
H,0,3.4711019265,4.9307773255,0.0481333267
H,0,4.6609282792,2.7335812333,-0.0071395432
Br,0,-4.3257531648,0.880312453,0.0700790553
H,0,-3.8542531117,-2.0348922844,0.0094310253
H,0,-1.4844687465,1.4737114006,0.0461642974
H,0,-0.2837992674,2.9450143608,0.0578105195
C,0,1.5378647682,4.0348503692,0.0554899483
H,0,1.0241631455,4.9793912328,0.0792487941
C,0,0.8651662092,-3.8782340908,-0.0825942078
N,0,2.1188958285,-4.1347881536,-0.1025765348
H,0,0.0851278258,-4.6068297362,-0.0866217606

HF=-3456.5228163
RMSD=4.870e-009
Dipole=-2.5890061,1.6114949,0.0613891
PG=C01 [X(C17H8Br1N3O1)]

Compound 23

Thiol form

Charge = 0 Multiplicity = 1
C,0,-2.7498096995,0.267081408,0.0361160337
C,0,-2.8816811233,-1.1111117979,0.0133987089
C,0,-1.7558631393,-1.9009119132,-0.0133896668
C,0,-0.4847849435,-1.3327509049,-0.0179654057
C,0,-0.3460975507,0.069618392,0.0051641851
C,0,-1.5075233328,0.8465276964,0.0321041314
C,0,0.9934166715,0.650164468,0.0001198368
C,0,2.0754022719,-0.1480630522,-0.0263684117
C,0,1.9485233744,-1.5737861579,-0.0500996283
N,0,0.6776375298,-2.1165952941,-0.0451316344
C,0,1.4460085766,2.0867040472,0.0204040666
C,0,2.8436491711,2.0804690057,0.0043110919
C,0,3.3296422048,0.6690478981,-0.0262251133
O,0,4.4543847334,0.2962207115,-0.0456644234
N,0,2.8425527789,-2.4926615677,-0.0765575974
C,0,0.7877130897,3.2973690329,0.0494071903
C,0,2.9215128597,4.4496312157,0.0453823015
C,0,3.5921590546,3.2272495503,0.0160546029
H,0,-1.8877547805,-2.96081568,-0.0305224889
H,0,3.4758225921,5.3704832184,0.0553451979
H,0,4.6654582977,3.1725657609,0.0028088293
Br,0,-4.2932772267,1.3612814405,0.0729927644
H,0,-3.8538638697,-1.5650360322,0.0165571671
H,0,-1.4409807643,1.9100227236,0.0500262008
H,0,-0.2785260154,3.386532592,0.0632325342
C,0,1.5428837301,4.4738201958,0.0616041791
H,0,1.0286159757,5.41807893,0.0842330039
C,0,0.9305427419,-3.466970909,-0.0718733108
N,0,2.1935305008,-3.6805347653,-0.0901123973
S,0,-0.2427893503,-4.7816596008,-0.0817362175
H,0,0.6952738285,-5.7158816674,-0.1095896778

HF=-3854.0261064
RMSD=4.565e-009
Dipole=-2.1563163,1.403344,0.0493519
PG=C01 [X(C17H8Br1N3O1S1)]|

Thione form

Charge = 0 Multiplicity = 1
C,0,-2.7599825159,0.2489170144,0.0212177502
C,0,-2.8872638383,-1.1278969522,0.0056421774
C,0,-1.7611271928,-1.9220099825,-0.0113492481
C,0,-0.4951832908,-1.3477860193,-0.0129331286
C,0,-0.3589314576,0.0555607929,0.0030323265
C,0,-1.5180946899,0.8322589967,0.0199681676
C,0,0.9782405443,0.6448963799,0.0013090502
C,0,2.066387779,-0.1432822039,-0.0156294497
C,0,1.9469248742,-1.5703571897,-0.0321980209
N,0,0.6767039797,-2.1356867728,-0.0303096612
C,0,1.4255620399,2.0839361192,0.0160401378
C,0,2.8236251265,2.0835483419,0.0066464989
C,0,3.3154288434,0.674337715,-0.0139465585
O,0,4.4410595554,0.3010550967,-0.0260336683
N,0,2.8616715943,-2.4563729806,-0.0492746639
C,0,0.7608819731,3.2910644968,0.0354503466
C,0,2.8894691318,4.452501629,0.0354208584

C,0,3.5669251673,3.2335749198,0.0158298043
H,0,-1.8632618879,-2.9847035041,-0.023388752
H,0,3.4392915031,5.3760139375,0.0431080066
H,0,4.6404914325,3.1847632421,0.0080249313
Br,0,-4.3036843215,1.3434858478,0.0444718908
H,0,-3.8583956752,-1.5842785354,0.006650573
H,0,-1.4538120604,1.895690111,0.0321835518
H,0,-0.3055290807,3.3749822221,0.043747794
C,0,1.5106789103,4.4709416619,0.0449567804
H,0,0.9922046471,5.4128721505,0.0600966023
C,0,0.857107404,-3.5029925987,-0.0481935693
N,0,2.1771997547,-3.6205945023,-0.0587287332
S,0,-0.2073480588,-4.8043037648,-0.0565999901
H,0,2.6541347197,-4.49162377,-0.0724618263

HF=-3854.0531237
RMSD=8.709e-009
Dipole=-0.3412225,2.4638613,0.0323475
PG=C01 [X(C17H8Br1N3O1S1)]|

Compound 25

Charge = 0 Multiplicity = 1
C,0,-2.7882386501,-0.1234294834,0.0349727118
C,0,-2.9010909136,-1.504944916,0.0111520027
C,0,-1.7689392851,-2.2848937345,-0.0181981483
C,0,-0.4993277426,-1.6979336474,-0.0243760224
C,0,-0.3841875537,-0.2905262128,-0.0002489829
C,0,-1.5512520512,0.4725378809,0.0293689448
C,0,0.9650923942,0.2657562216,-0.0081107194
C,0,2.0468878673,-0.5391539176,-0.036908009
C,0,1.9305103753,-1.9836968681,-0.0616252466
N,0,0.6260029492,-2.4693389837,-0.0533185681
C,0,1.4236614644,1.7002726142,0.0116836681
C,0,2.8193012813,1.6896011668,-0.006767483
C,0,3.2984580884,0.2730316134,-0.0386183084
O,0,4.4279412744,-0.0899923399,-0.0599358478
N,0,2.8440234613,-2.8476679109,-0.0894543909
C,0,0.7653688927,2.9113513851,0.0419203171
C,0,2.9006662222,4.0581352013,0.0346449402
C,0,3.5699239873,2.8352454786,0.0039633858
H,0,-1.8668875792,-3.3526641864,-0.036395101
H,0,3.4565733326,4.978270142,0.0438973105
H,0,4.643117543,2.7790329069,-0.0111060707
Br,0,-4.3496844379,0.9524359859,0.0755939394
H,0,-3.8703708208,-1.9666336428,0.0156233256
H,0,-1.5010513202,1.5378392307,0.048317033
H,0,-0.3010119904,2.9987004734,0.0572351096
C,0,1.521457836,4.0863896407,0.0531167229
H,0,1.009666612,5.0320127587,0.0767069919
C,0,0.6845762786,-3.9245280184,-0.0805857768
C,0,2.2162805601,-4.1602803127,-0.1051909971
H,0,0.1854659869,-4.3140016824,-0.9614838859
H,0,0.2088159295,-4.346025189,0.7984929187
H,0,2.5214475723,-4.7041818664,-0.9924607196
H,0,2.5445806836,-4.7362260182,0.7531247034

HF=-3441.7125376
RMSD=8.244e-009
Dipole=-1.5758249,0.1144842,0.022368
PG=C01 [X(C18H11Br1N2O1)]

Compound 25 H+

Charge = 1 Multiplicity = 1
C,0,-2.8183252567,-0.1203978507,0.0463851809
C,0,-2.8972196284,-1.5149008551,0.0188301416
C,0,-1.7560958941,-2.2744731801,-0.0167501332
C,0,-0.5058364283,-1.6532151424,-0.0255827934
C,0,-0.4111806399,-0.2455073856,0.0019572544
C,0,-1.6022503506,0.5008916332,0.0381409622
C,0,0.9079183735,0.333872481,-0.0089323748
C,0,2.0026898669,-0.4836637506,-0.0449769913
C,0,1.866752335,-1.8767031746,-0.0714596717
N,0,0.6486879225,-2.4159462817,-0.0614805571
C,0,1.4006171082,1.7457236793,0.0119313842
C,0,2.8038429167,1.7131898988,-0.0130209284
C,0,3.2602978649,0.2969193756,-0.0504725633
O,0,4.3635723021,-0.1497625178,-0.0789162164
N,0,2.807890574,-2.792942141,-0.1066728454
C,0,0.7527094333,2.9618609498,0.0484523669
C,0,2.9025191713,4.0795481565,0.0345096746
C,0,3.5652975319,2.8517286745,-0.0024956646
H,0,-1.8366368104,-3.3436367773,-0.0375415184
H,0,3.4676900672,4.9931884233,0.0437297155
H,0,4.6379050397,2.7934290671,-0.022252135
Br,0,-4.4002508009,0.9010631384,0.0950574589
H,0,-3.8577765038,-1.9938083088,0.0255950462
H,0,-1.5686390446,1.5674625024,0.0596671364
H,0,-0.3132298853,3.0569211914,0.0689220247
C,0,1.5229232547,4.1268539271,0.0593622924
H,0,1.0253617423,5.0787882745,0.0877813883
C,0,0.733191258,-3.8871559747,-0.0932860602
C,0,2.2587222599,-4.1441054746,-0.1252032755
H,0,0.2351979283,-4.2658617223,-0.9747693378
H,0,0.2659584901,-4.3021935017,0.7886798815
H,0,2.5613404764,-4.6672729405,-1.0216490625
H,0,2.5919954175,-4.703841518,0.7376483895
H,0,3.7755441638,-2.5528613585,-0.1187518449

HF=-3442.1415096
RMSD=5.212e-009
Dipole=1.2767589,-2.3448734,-0.0708537
PG=C01 [X(C18H12Br1N2O1)]

Compound 2g

Charge = 0 Multiplicity = 1
C,0,-3.4139534617,-0.1682739282,0.1962565909
C,0,-3.4076773197,-1.5769454835,0.093721865
C,0,-2.2226732944,-2.2276820993,-0.0041958103

C,0,-0.9978051412,-1.5121942737,-0.003479443
C,0,-1.0123720643,-0.1086648362,0.1041709047
C,0,-2.2661163367,0.5509856167,0.2021541839
C,0,0.2598134006,0.5282224676,0.0649242291
C,0,1.3967374889,-0.2307450909,-0.0776823573
C,0,1.2841175081,-1.647276529,-0.1060614277
N,0,0.137771135,-2.2382552418,-0.08169261
C,0,0.6463186909,1.9653423689,0.0921820576
C,0,2.0289757338,2.0518824829,-0.1160867083
C,0,2.5584498846,0.6760092226,-0.2696548261
N,0,3.7020900537,0.2555265201,-0.5758433833
N,0,2.3998047495,-2.4980650867,-0.1645230734
C,0,-0.089791382,3.1190176612,0.2938933877
C,0,1.9243627098,4.4247110763,0.056938378
C,0,2.6752630868,3.2728141238,-0.1397643288
H,0,-2.1759348793,-3.2974320489,-0.0816350444
H,0,2.4099195381,5.3839090642,0.0448602265
H,0,3.7311074031,3.3308968433,-0.3020937989
Br,0,-5.0818904404,0.724869216,0.3243060096
H,0,-4.3366002594,-2.1142598919,0.0940474438
H,0,-2.3235303944,1.6140499647,0.2712593183
H,0,-1.1436551955,3.1027182984,0.4777042307
C,0,0.5609784831,4.3461671986,0.2736611739
H,0,-0.007822705,5.2449276276,0.4318905455
C,0,3.5456041482,-2.4782698085,0.6101910102
C,0,4.1973947891,-3.6170820849,0.3230149373
N,0,3.4972259175,-4.3555348646,-0.6060632725
C,0,2.4383939655,-3.6768344034,-0.8515457529
H,0,3.7728129615,-1.6747029485,1.2723385745
H,0,5.1286812236,-3.9602183825,0.7228913382
H,0,1.6496479745,-3.9548105802,-1.5177203359
O,0,4.6201794065,1.2360255208,-0.7755384664
H,0,5.4057361659,0.7734939546,-1.0189171132

HF=-3588.4210539
RMSD=5.458e-009
Dipole=-0.0307091,2.0660834,0.2518793
PG=C01 [X(C19H11Br1N4O1)]

Compound 2gH+

Charge = 1 Multiplicity = 1
C,0,-3.4376962199,-0.1497917312,0.2215476191
C,0,-3.4262739095,-1.5633608778,0.1514472138
C,0,-2.2437622364,-2.2172233756,0.0570631911
C,0,-1.0235153438,-1.4969764658,0.0283884306
C,0,-1.035059497,-0.0867281774,0.1016214177
C,0,-2.2906681102,0.5709611974,0.1984969604
C,0,0.2285153099,0.5610589164,0.0473244863
C,0,1.3763648906,-0.1982371532,-0.0681112148
C,0,1.2422408882,-1.5933047552,-0.0898951863
N,0,0.1191275824,-2.2147336443,-0.0539710093
C,0,0.6190182374,1.9953847048,0.0471673967
C,0,2.009632429,2.0756247581,-0.1229361792
C,0,2.54637382,0.7006760171,-0.224977449
N,0,3.7021964942,0.2556885064,-0.4430796763

N,0,2.3786007931,-2.4774135735,-0.1662189845
C,0,-0.1228882854,3.1537327826,0.1862165576
C,0,1.9009152284,4.4506854019,-0.0272563105
C,0,2.6586916043,3.2938841373,-0.1640602281
H,0,-2.2006911002,-3.2886038476,0.0065530938
H,0,2.3864511825,5.408942943,-0.05485244
H,0,3.7188809168,3.3496499133,-0.295800835
Br,0,-5.0993559847,0.7346359832,0.3486134183
H,0,-4.3544038938,-2.1012450162,0.1749163221
H,0,-2.3488694709,1.6345959059,0.2495772095
H,0,-1.1826406196,3.1461829219,0.3304367616
C,0,0.5311112632,4.3792804065,0.1472235969
H,0,-0.0407848705,5.2826600413,0.256109085
C,0,3.5063983112,-2.4963582109,0.6381001427
C,0,4.2049217091,-3.5883021062,0.3097547519
N,0,3.4920980526,-4.2228834964,-0.6914275326
C,0,2.4007049318,-3.5391217599,-0.9418859773
H,0,3.6994160664,-1.7351018142,1.357603873
H,0,5.1256578648,-3.9739194767,0.6874905986
H,0,1.6407010742,-3.7962515465,-1.6472827123
O,0,4.6407646903,1.221057091,-0.5998752087
H,0,5.4407774069,0.7629960584,-0.8014758317
H,0,3.7525368041,-5.0665290215,-1.154237995

HF=-3588.8237819
RMSD=7.051e-009
Dipole=4.6452388,-3.7795648,-0.7429579
PG=C01 [X(C19H12Br1N4O1)]

Compound 2b

Charge = 0 Multiplicity = 1
C,0,-2.8124827911,-0.1866511805,0.0161225686
C,0,-2.9427105787,-1.590696118,-0.0062719526
C,0,-1.8285485564,-2.3660595086,-0.0267325077
C,0,-0.5353160958,-1.7872486632,-0.0260048412
C,0,-0.4169309658,-0.3813957138,-0.0035996538
C,0,-1.5943473383,0.4074937688,0.0176020201
C,0,0.9147172172,0.1278587127,-0.0042988851
C,0,1.9627070945,-0.7484178755,-0.0256429537
C,0,1.715396296,-2.1477646535,-0.0469942074
N,0,0.5221217648,-2.6352767044,-0.0470768178
C,0,1.4562981634,1.526740354,0.0148813913
C,0,2.8487684062,1.4373636163,0.0042961888
C,0,3.2552827809,-0.0028658035,-0.0219361761
O,0,4.366634294,-0.422207996,-0.0360637395
O,0,2.7674846295,-2.9400459377,-0.0670192208
C,0,0.8603077987,2.7705613615,0.038819851
C,0,3.054437474,3.7987459091,0.0412073219
C,0,3.6590108413,2.5440089644,0.016924591
H,0,-1.8961433332,-3.4373282034,-0.0439800151
H,0,3.6580409128,4.6883199735,0.0516846776
H,0,4.7279751271,2.4329713216,0.0080977367
Br,0,-4.3828836516,0.8775481101,0.0446889196
H,0,-3.9207818485,-2.032976778,-0.0069067499
H,0,-1.5361552974,1.4736926564,0.035037803
H,0,-0.2018983162,2.9053994176,0.0477695096

C,0,1.6766957843,3.9021747016,0.0518229715
H,0,1.2179013639,4.8746812189,0.0705246233
C,0,2.5652189718,-4.338475788,-0.088535223
H,0,2.0138109029,-4.6334107016,-0.9710008164
H,0,2.0253322384,-4.6621976468,0.7909570016
H,0,3.5540153033,-4.7705992159,-0.1020575716

HF=-3423.6905686
RMSD=8.253e-009
Dipole=-0.5022873,0.5041672,0.0112763
PG=C01 [X(C17H10Br1N1O2)]

Compound 2d

Charge = 0 Multiplicity = 1
C,0,-3.2110980415,-0.0992350338,0.146798779
C,0,-3.2071045236,-1.5104976955,0.0409476045
C,0,-2.027791918,-2.1696402235,-0.0510121668
C,0,-0.7959395847,-1.4617029565,-0.0413784487
C,0,-0.809280255,-0.0561496061,0.0657868946
C,0,-2.0608832031,0.612227532,0.159002544
C,0,0.4613642142,0.5706470758,0.0416207933
C,0,1.6028930089,-0.1948290096,-0.0681189417
C,0,1.4884549646,-1.6102222089,-0.124183448
N,0,0.3319126437,-2.1921306836,-0.1181736537
C,0,0.8398228204,2.0207236096,0.062036742
C,0,2.2198047187,2.0946757971,-0.1036001202
C,0,2.7833691121,0.7193815246,-0.21009517
O,0,3.9286633709,0.452506228,-0.3881607863
N,0,2.5858517723,-2.4712322032,-0.2054636149
C,0,0.1169558944,3.1879836543,0.2077197252
C,0,2.1701719344,4.4603074142,0.0003971296
C,0,2.9021560872,3.2851321167,-0.1407183057
H,0,-1.9884349942,-3.2393967611,-0.1298676601
H,0,2.6679060502,5.4127279116,-0.0226652746
H,0,3.9684307408,3.2956587229,-0.2737151244
Br,0,-4.8762642375,0.7969624787,0.2712586152
H,0,-4.1388695214,-2.0430988599,0.0349919291
H,0,-2.1097433451,1.6754112913,0.2355615904
H,0,-0.9433040089,3.2032759368,0.351834791
C,0,0.799819019,4.40347594,0.1747010099
H,0,0.2420803824,5.3158029861,0.2884322435
C,0,3.8463271721,-2.3712370664,0.3672304181
C,0,4.4480487085,-3.5451616798,0.1237984074
N,0,3.6130662289,-4.3856791159,-0.5828393802
C,0,2.5263018916,-3.7314433904,-0.7437039519
H,0,4.1838738051,-1.4929958453,0.8628982102
H,0,5.4346584742,-3.8463639267,0.4070483007
H,0,1.6471771256,-4.0780787771,-1.2413246728

HF=-3533.4539629
RMSD=8.752e-009
Dipole=-1.2295682,2.3341505,0.4290611
PG=C01 [X(C19H10Br1N3O1)]

Compound 2e

Charge = 0 Multiplicity = 1
C,0,-3.0626403782,-1.008425992,0.0162591648
C,0,-2.6581183911,-2.364521498,-0.0229229471
C,0,-1.338247833,-2.6658074769,-0.0349451329
C,0,-0.3561846687,-1.6386002319,-0.0077573588
C,0,-0.7696714208,-0.2901447316,0.0309963593
C,0,-2.1620031837,0.0000096718,0.0412511084
C,0,0.2724980737,0.668841613,0.0376667909
C,0,1.5835278925,0.247226833,0.0207601557
C,0,1.8700296332,-1.1425337172,0.0069073981
N,0,0.9320711151,-2.027910085,-0.0057523078
C,0,0.2377090453,2.1671259637,0.0067659515
C,0,1.5539088751,2.6151910161,-0.0763764893
C,0,2.478403718,1.445750103,-0.0759987629
O,0,3.6654818851,1.4958202753,-0.1399205755
N,0,3.1863810649,-1.6300331477,0.0004978947
C,0,-0.7859757041,3.0922079439,0.042965499
C,0,0.8489031335,4.8768421572,-0.0991356006
C,0,1.8836719779,3.9463582773,-0.1310405467
H,0,-0.9928347871,-3.6815504709,-0.0657792787
H,0,1.0667450725,5.9286228365,-0.1409217071
H,0,2.9130063322,4.24816225,-0.196360594
Br,0,-4.9172849564,-0.6157521928,0.0319012477
H,0,-3.4019011779,-3.137937248,-0.0435850683
H,0,-2.5113629308,1.008186656,0.0675956743
H,0,-1.817585057,2.8162913085,0.1148993267
C,0,-0.4622376555,4.4479502287,-0.0110787565
H,0,-1.255938307,5.1730253342,0.0168562899
C,0,4.2420519505,-1.2238180504,0.750874362
C,0,5.2526269077,-2.0940155128,0.522658188
C,0,4.7058304396,-3.0204314185,-0.4029256968
N,0,3.4766240385,-2.7454881575,-0.6945955309
H,0,4.1904279162,-0.358918317,1.3720309577
H,0,6.2354922438,-2.0769476655,0.9431220396
H,0,5.1850410888,-3.865381478,-0.8556292142

HF= -3533.42936975
HF=-3533.4293698|
RMSD=9.021e-009
Dipole=-0.7143412,1.496856,0.5894937
PG=C01 [X(C19H10Br1N3O1)]

Compound 2c

Charge = 0 Multiplicity = 1
C,0,-3.1179834437,-0.052030197,0.156271184
C,0,-3.2001301068,-1.4608139089,0.0726723508
C,0,-2.0605306189,-2.1872171477,-0.0308506319
C,0,-0.7937955639,-1.5501153482,-0.0559622021
C,0,-0.7205361237,-0.1440473354,0.0279458896
C,0,-1.9285414275,0.5951564492,0.1358116751
C,0,0.5847685707,0.4151464226,-0.0039467081
C,0,1.6651266084,-0.4239048413,-0.1113810184
C,0,1.4654168576,-1.8204715787,-0.1881939148
N,0,0.2923567785,-2.3495280456,-0.1612262493

C,0,1.0704333622,1.8315412402,0.0593929446
C,0,2.4628644538,1.8026830022,-0.0135204385
C,0,2.9268852078,0.3891845985,-0.1253093003
O,0,4.0493113267,0.0127340352,-0.2062620659
C,0,2.6348890655,-2.7842433534,-0.3083611831
C,0,0.4268405743,3.0475169479,0.167821937
C,0,2.5771555874,4.1655399309,0.1276685183
C,0,3.2294750686,2.9406307775,0.018160917
H,0,-2.0813410153,-3.2584391739,-0.0965366868
H,0,3.1441325395,5.0783109745,0.1555528732
H,0,4.3005009311,2.8746613295,-0.0406044923
Br,0,-4.724286195,0.9415003414,0.3003536396
H,0,-4.1610847731,-1.93793373,0.0920850982
H,0,-1.9141000652,1.660467776,0.201509466
H,0,-0.6381982369,3.1383568663,0.2277203808
C,0,1.1974783892,4.2096143802,0.2007717082
H,0,0.7015574003,5.1600632723,0.2851580716
F,0,3.4410909959,-2.6709655379,0.7300543931
F,0,3.3316587642,-2.5379421891,-1.401512494
F,0,2.2315461527,-4.0320028793,-0.3654899199

HF=-3645.4038559
RMSD=5.418e-009
Dipole=-1.3094064,1.853069,0.1824836
PG=C01 [X(C17H7Br1F3N1O1)]

References:

1 C. C. J. Roothan, *Rev. Mod. Phys*. 1951, **23**, 69-89.

2 R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys*. 1971, **54**, 724-728.

3 Gaussian 03, Revision B.02, J. A. Pople *et. al.*, Gaussian, Inc., Pittsburgh PA, **2003**.

4 K. Ruud, T. Helgaker, K. L. Bak, P. Jørgensen, H. J. A. Jensen, *J. Chem. Phys.* 1993, **99**, 3847-3859.