

# **Facile construction of densely functionalized thiopyrano[2,3-*b*]quinolines *via* three-component reactions catalyzed by L-proline**

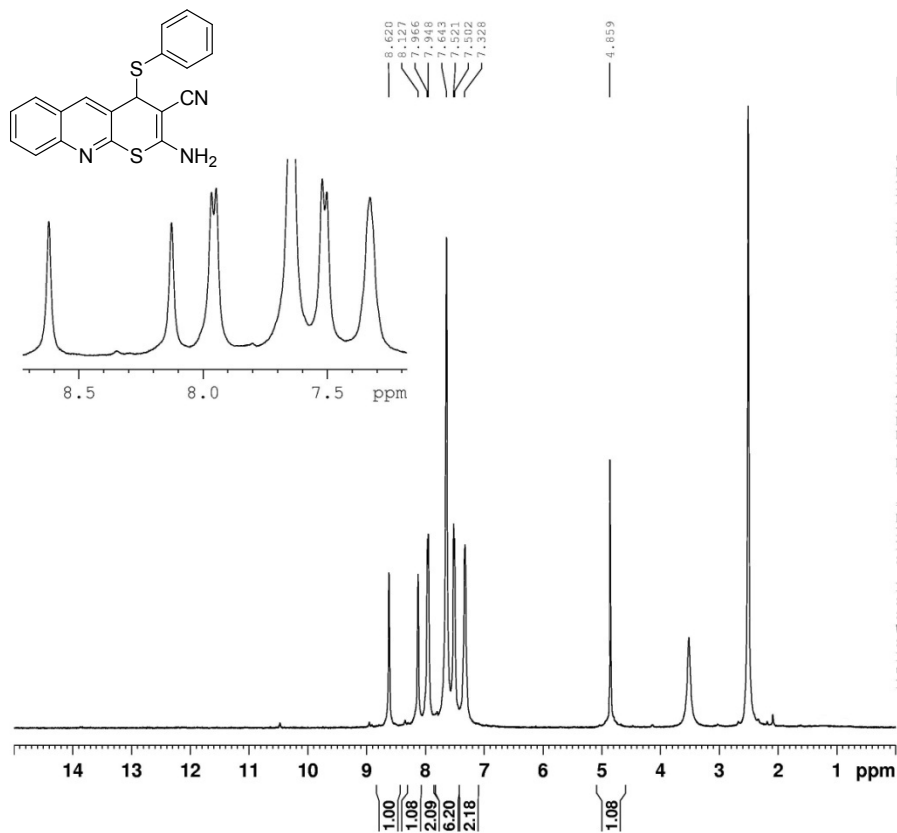
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*Department of Chemistry, Sardar Patel University, Vallabh vidyanagar 388120, India*

## **Supporting information**

- 1.  $^1\text{H}$  NMR of Compounds**
- 2. Mass spectra**

# <sup>1</sup>H NMR of Compound 4a



Current Data Parameters  
NAME MPP  
EXPNO 736  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130716  
Time 14.07  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 362  
DW 60.400 usec  
DE 6.00 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 15.00 usec  
PL1 -6.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

## Mass spectra of 4a

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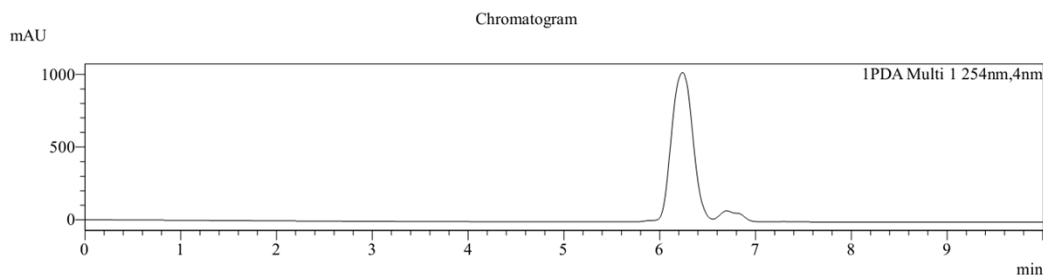
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### <Sample Information>

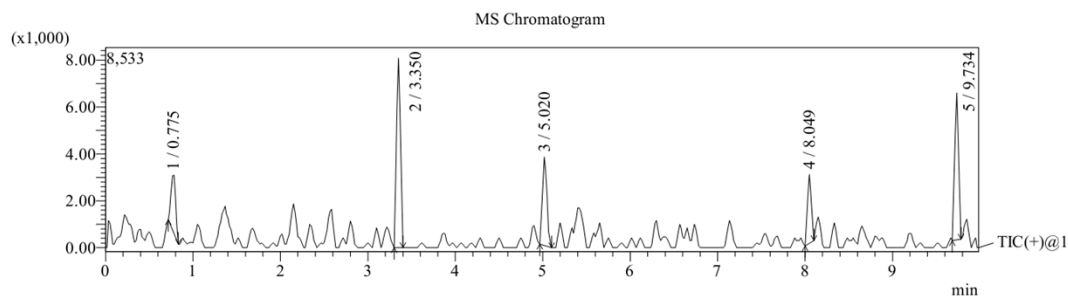
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Sample ID : TM 3b  
Vial # : 1-19  
Injection Volume : 0.5 uL  
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Date Processed : 20-01-2014 12:03:49

Sample Type : Unknown  
Acquired by : System Administrator  
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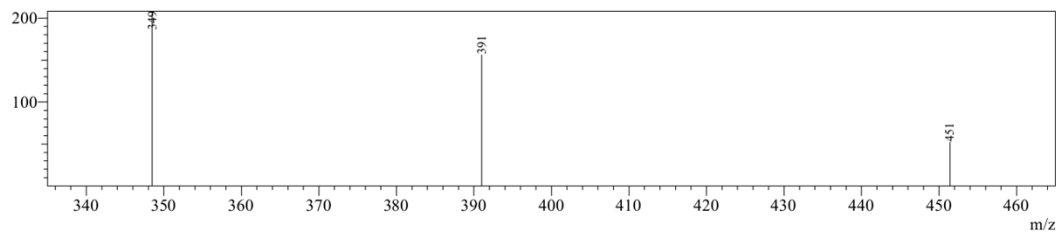
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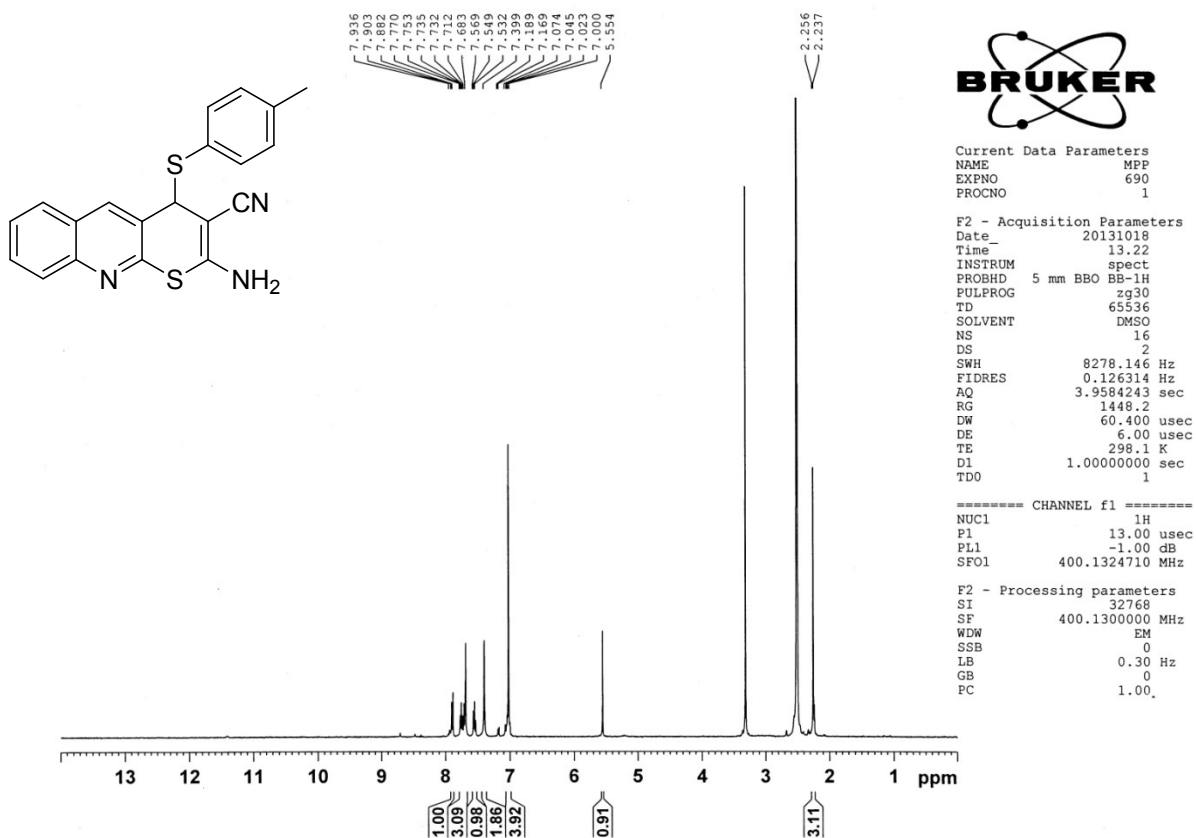
Line#:1 R.Time:----(Scan#;----)  
MassPeaks:3  
Spectrum Mode:Averaged 2.667-2.967(161-179) Base Peak:349(208)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 348.00



Line#:1 R.Time:----(Scan#;----)  
MassPeaks:3  
Spectrum Mode:Averaged 2.667-2.967(161-179) Base Peak:349(208)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 348.00

Sr. No.	m/z	Absolute Intensity	Relative Intensity
1	348.50	208	100.00
2	391.00	156	75.00
3	451.40	52	25.00

# <sup>1</sup>H NMR of Compound 4b



## Mass spectra of 4b

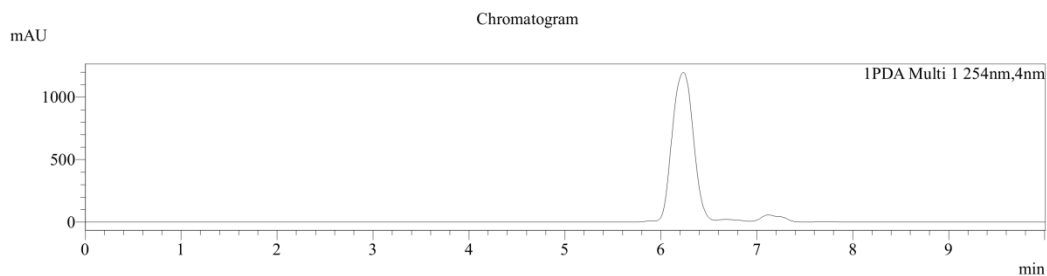
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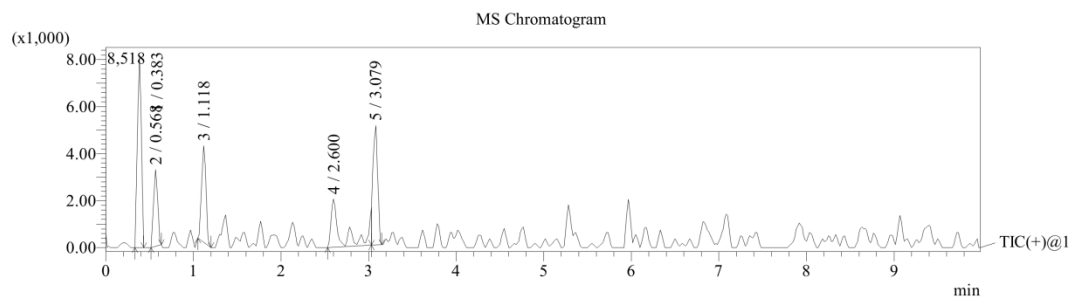
### <Sample Information>

Sample Name	: TM 6b	Sample Type	: Unknown
Sample ID	: TM 6b		
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Injection Volume	: 0.5 uL		
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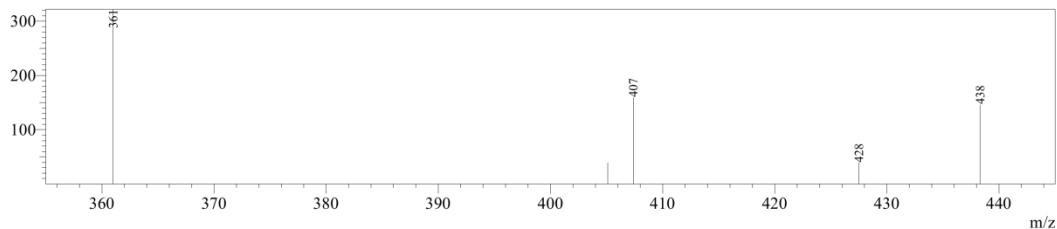
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### <MS>



Line#:1 R.Time:----(Scan#:----)  
MassPeaks:5  
Spectrum Mode:Averaged 2.483-2.833(150-171) Base Peak:361(322)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 361.05



Line#:1 R.Time:----(Scan#:----)  
MassPeaks:5  
Spectrum Mode:Averaged 2.483-2.833(150-171) Base Peak:361(322)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 361.05

Sr. No.	m/z	Absolute Intensity	Relative Intensity
1	361.00	322	100.00
2	405.10	39	12.11
3	407.40	159	49.38
4	427.50	39	12.11
5	438.30	146	45.34

## Mass spectra of 4c

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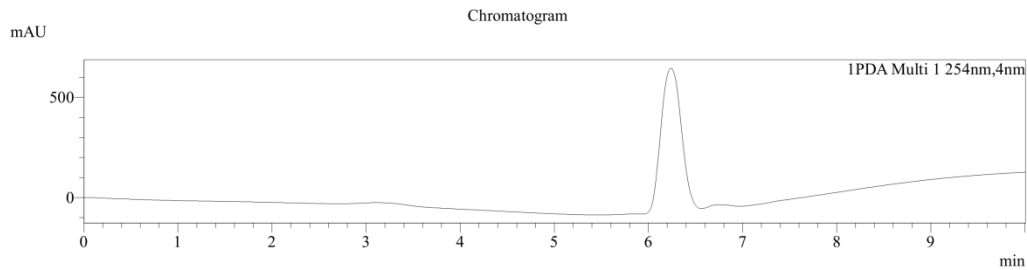
21-01-2014 10:25:06 Page 1 / 1

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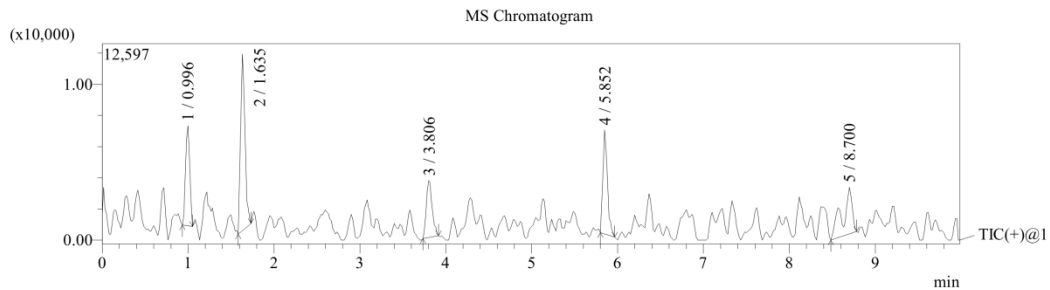
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Sample ID : TM 2  
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Injection Volume : 0.5 uL  
Date Acquired : 20-01-2014 11:17:34  
Date Processed : 20-01-2014 11:30:33

Sample Type : Unknown  
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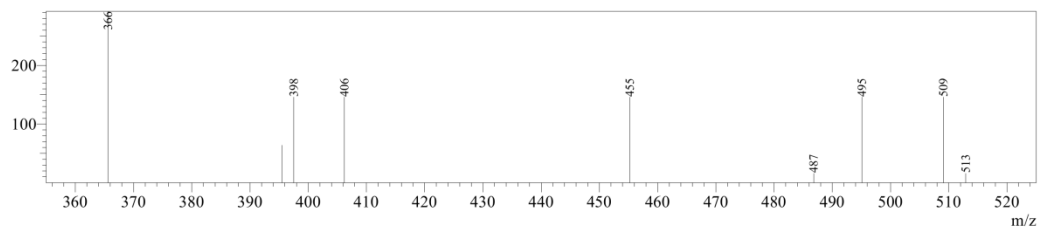


### <MS>



### MS Spectrum

Line#:1 R.Time:----(Scan#:-)----  
MassPeaks:9  
Spectrum Mode:Averaged 7.517-7.783(452-468) Base Peak:366(292)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 365.00

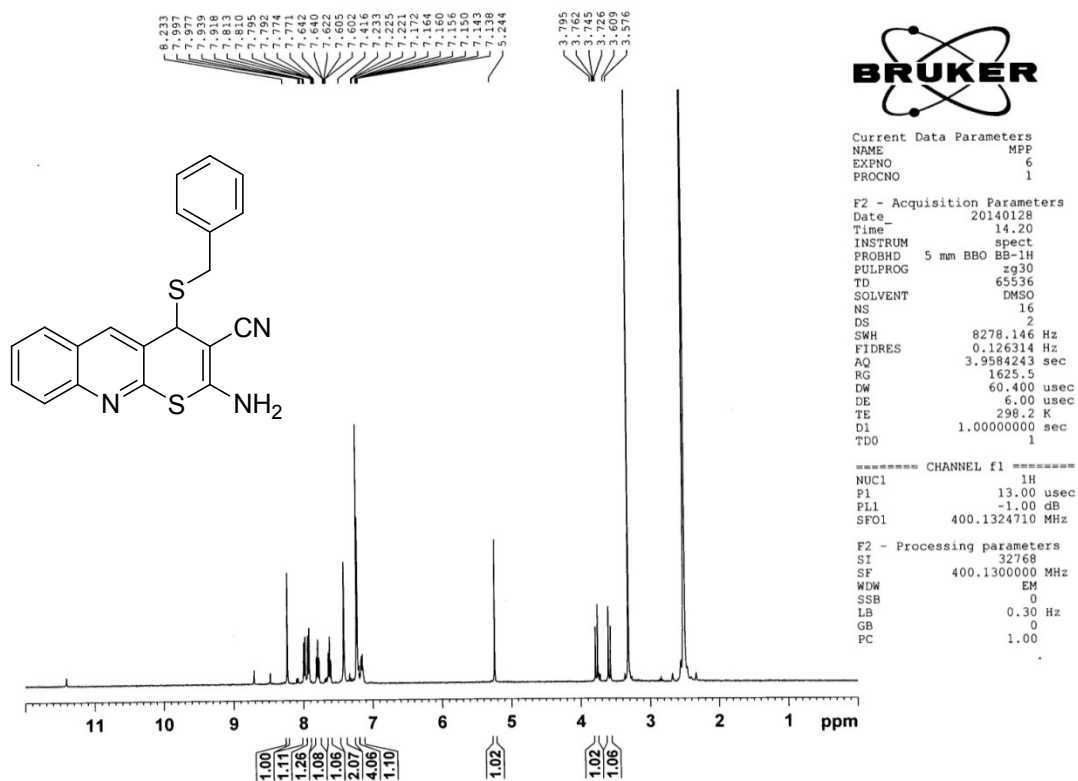


### MS Spectrum

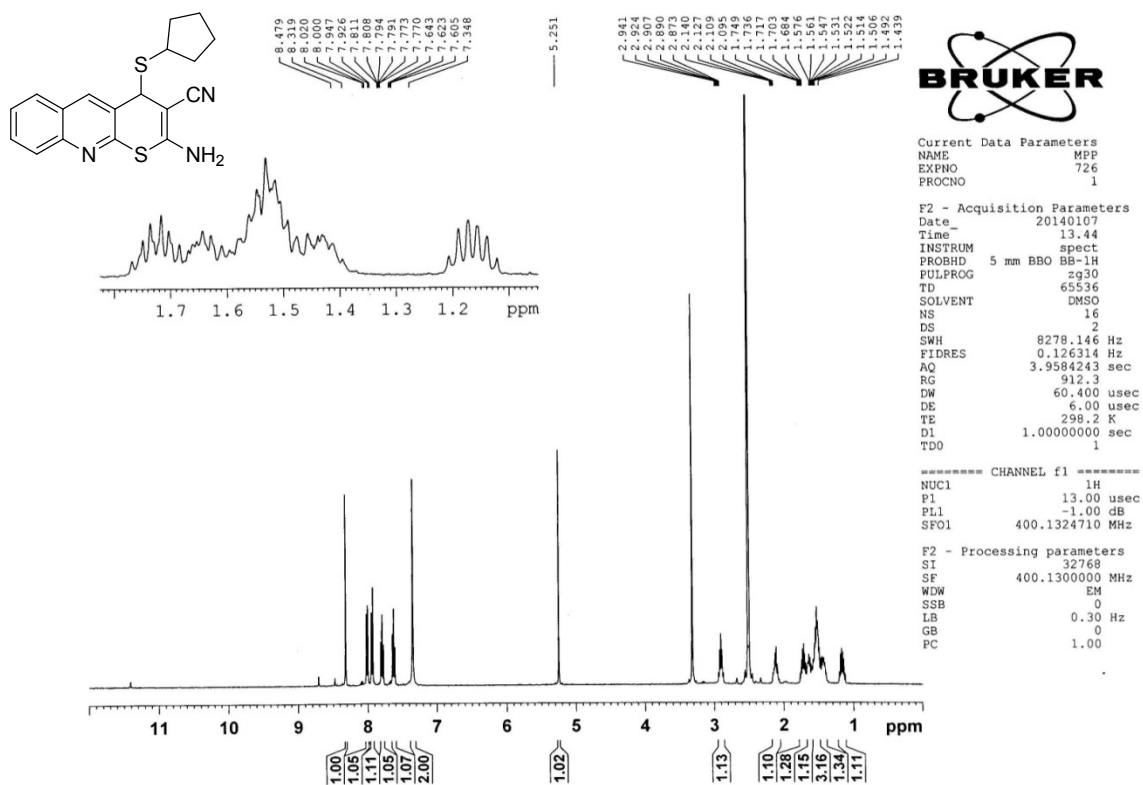
Line#:1 R.Time:----(Scan#:-)----  
MassPeaks:9  
Spectrum Mode:Averaged 7.517-7.783(452-468) Base Peak:366(292)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 365.00

Sr. No.	m/z	Absolute Intensity	Relative Intensity
1	365.60	292	100.00
2	395.50	64	21.92
3	397.50	146	50.00
4	406.20	146	50.00
5	455.20	146	50.00
6	486.80	16	5.48
7	495.10	146	50.00
8	509.10	146	50.00
9	512.90	16	5.48

# <sup>1</sup>H NMR of Compound 4d

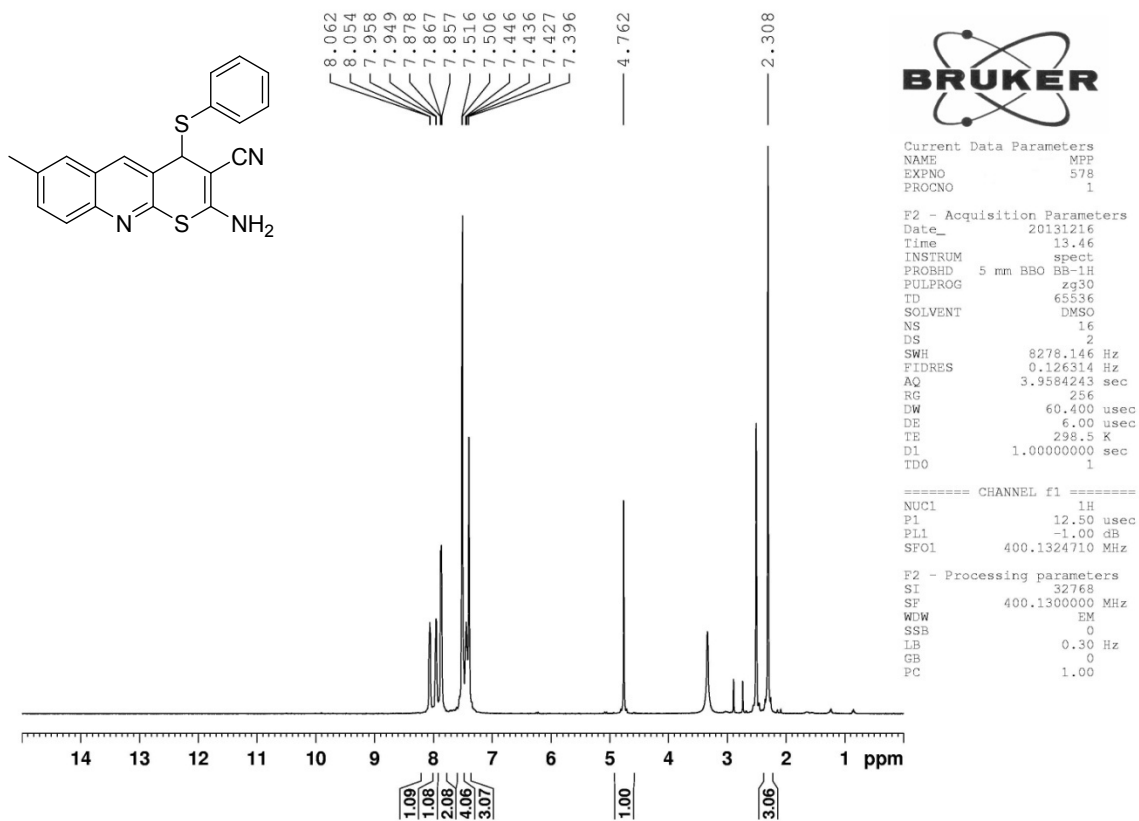


# <sup>1</sup>H NMR of Compound 4e

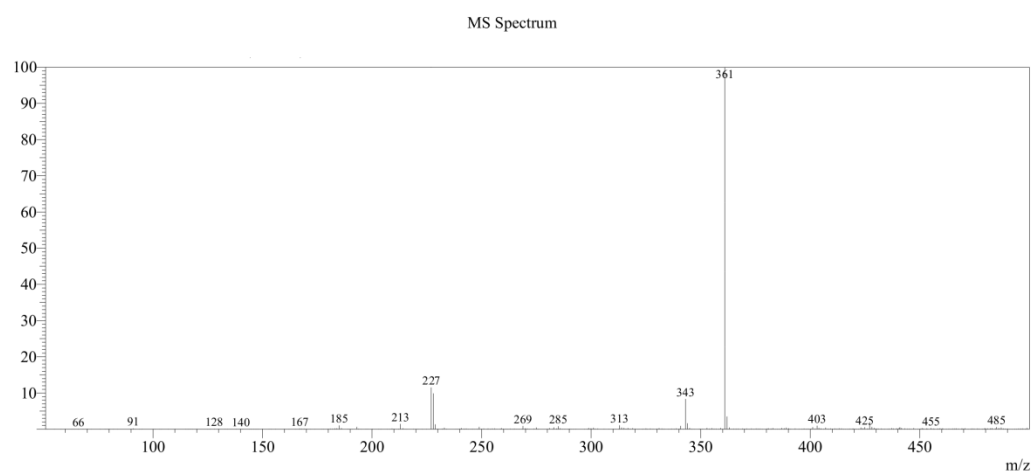




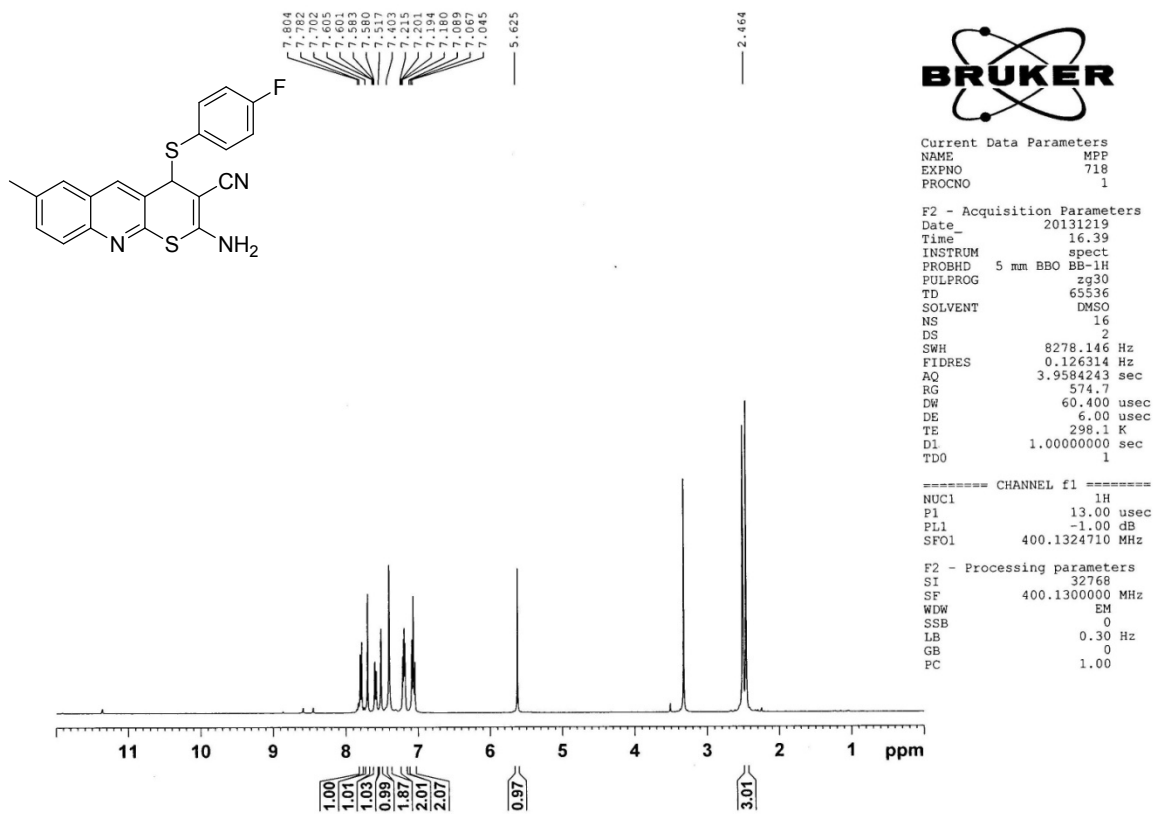
# <sup>1</sup>H NMR of Compound 4g



## Mass spectra of 4g



# <sup>1</sup>H NMR of Compound 4i



## Mass spectra of 4i

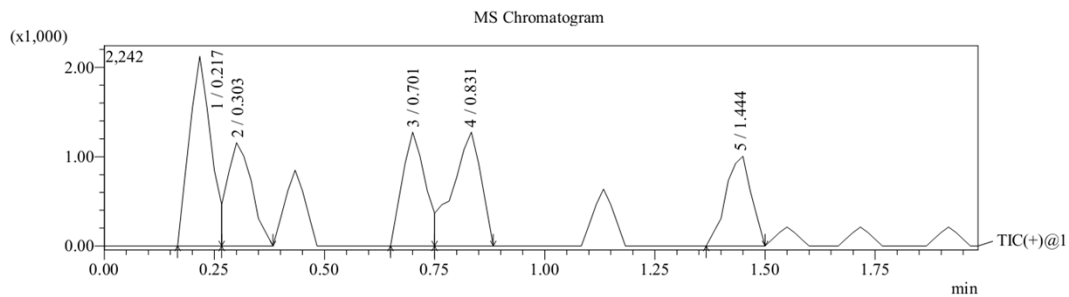
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### <Sample Information>

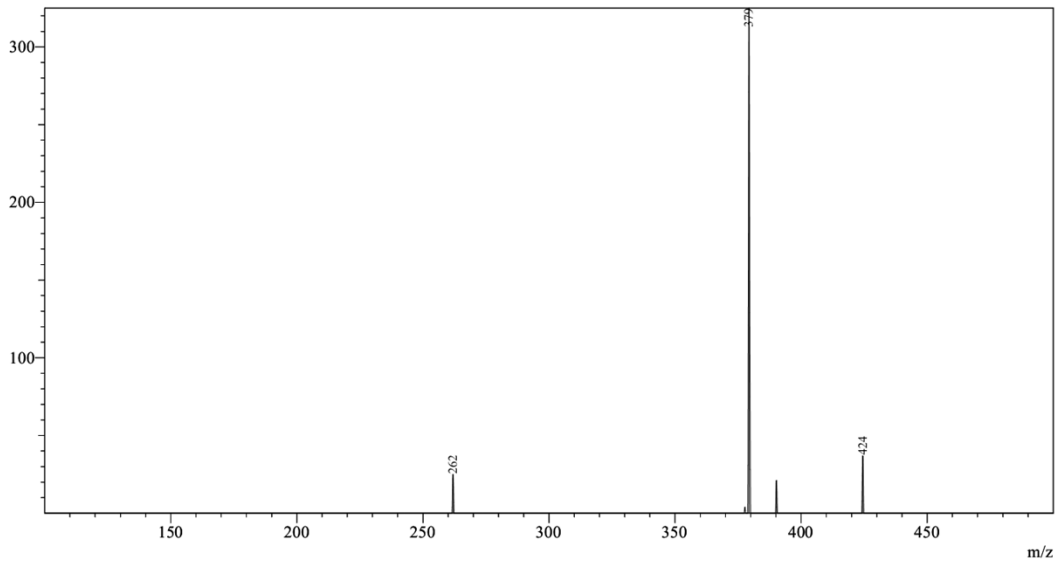
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Sample ID	: TN-10		
Vial #	: 1-7		
Injection Volume	: 0.1 uL		
Date Acquired	: 26-12-2013 16:05:36	Acquired by	: System Administrator
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### <MS Chromatogram>



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MassPeaks:4  
Spectrum Mode:Averaged 0.250-0.667(16-41) Base Peak:379(325)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 378.40

MS Spectrum



MS Spectrum

Line#:1 R.Time:----(Scan#----)  
MassPeaks:4  
Spectrum Mode:Averaged 0.250-0.667(16-41) Base Peak:379(325)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 378.40

Sr. No.	m/z	Absolute Intensity	Relative Intensity
1	261.90	25	7.69
2	379.30	325	100.00
3	390.20	21	6.46
4	424.40	37	11.38

# Mass spectra of 4k

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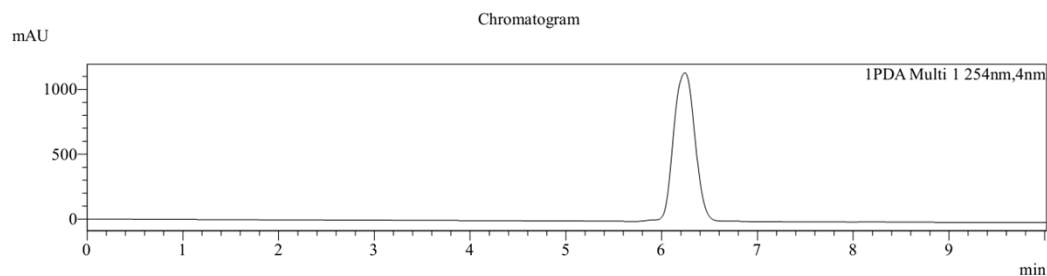
21-01-2014 10:30:12 Page 1 / 1

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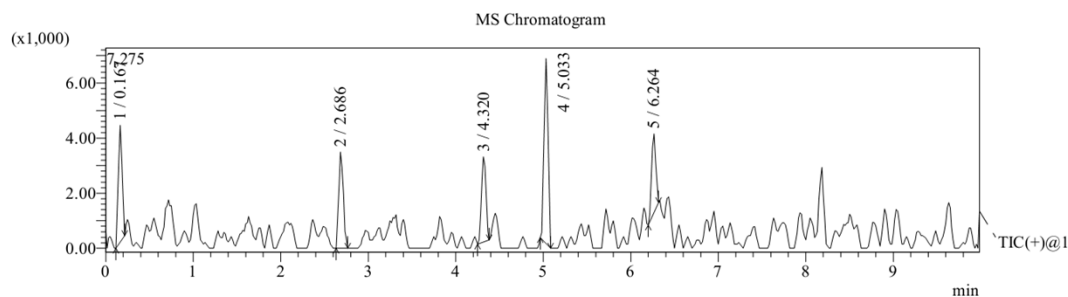
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Sample ID : TM 6a  
Vial # : 1-20  
Injection Volume : 0.5 uL  
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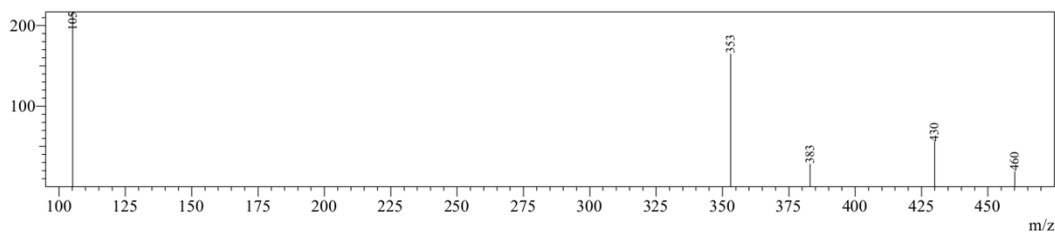
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## <MS>



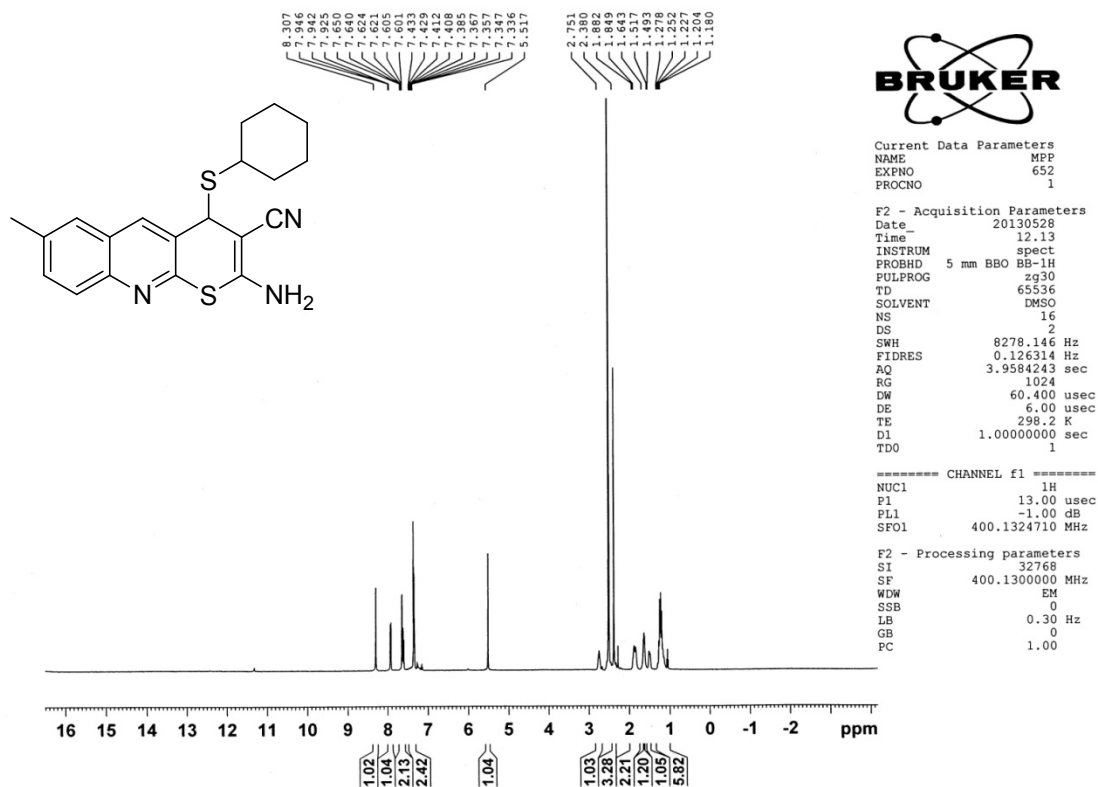
Line#:1 R.Time:---(Scan#;---)  
MassPeaks:5  
Spectrum Mode:Averaged 5.800-5.983(349-360) Base Peak:105(217)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 353.10



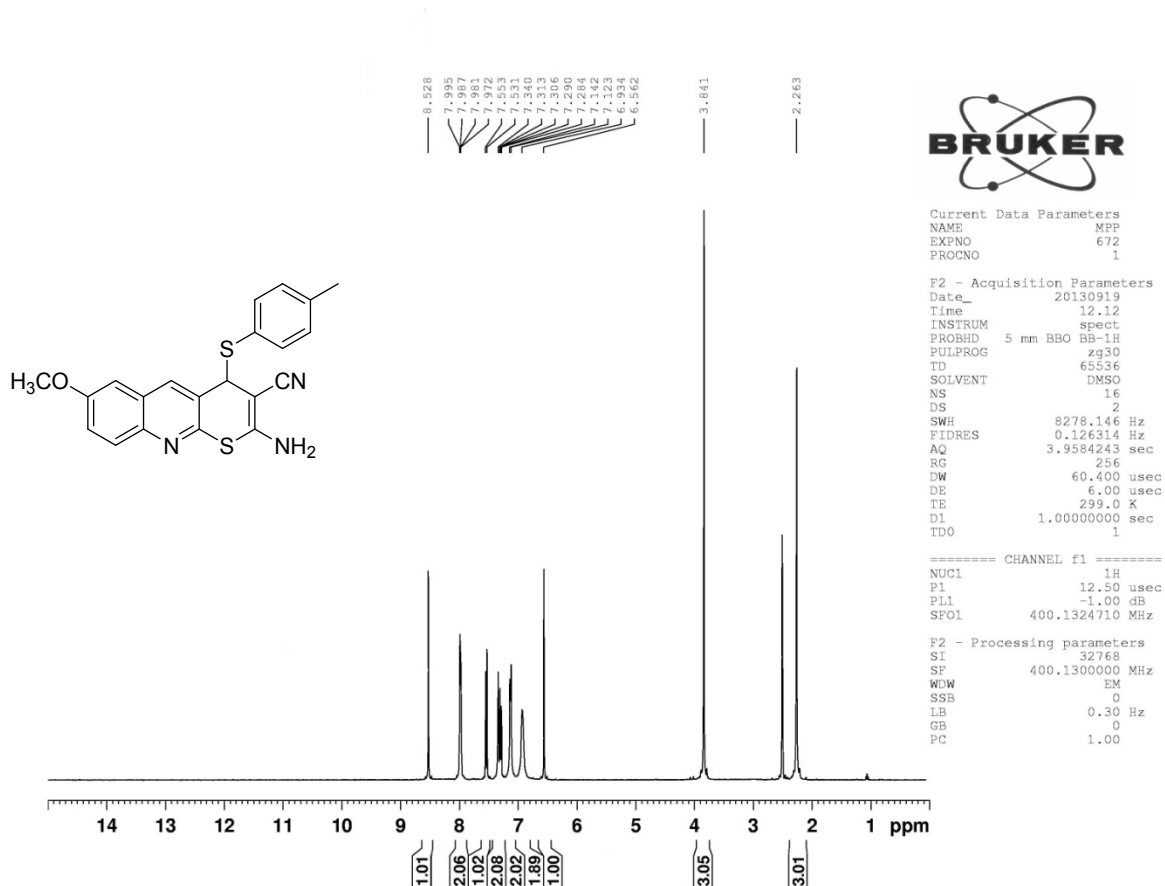
Line#:1 R.Time:---(Scan#;---)  
MassPeaks:5  
Spectrum Mode:Averaged 5.800-5.983(349-360) Base Peak:105(217)  
BG Mode:None Segment 1 - Event 1  
Precursor Ion Scan:m/z 353.10

Sr. No.	m/z	Absolute Intensity	Relative Intensity
1	105.10	217	100.00
2	353.00	165	76.04
3	383.00	28	12.90
4	430.00	56	25.81
5	460.10	19	8.76

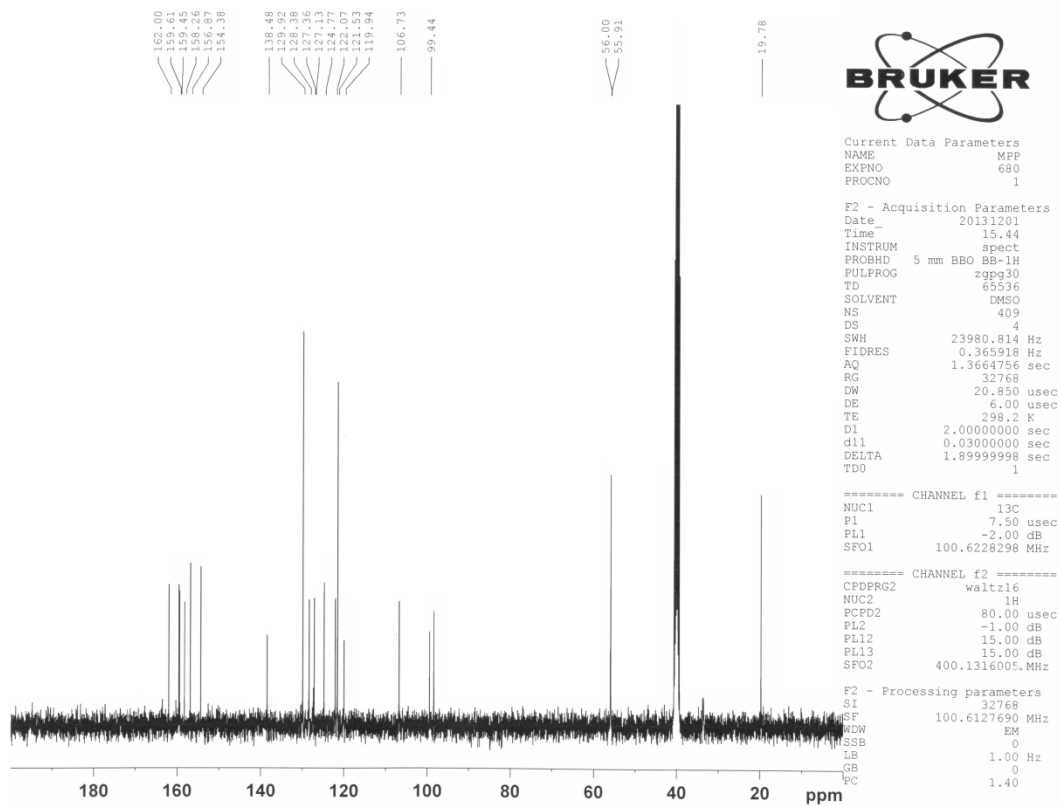
# <sup>1</sup>H NMR of Compound 4l



# <sup>1</sup>H NMR of Compound 4m



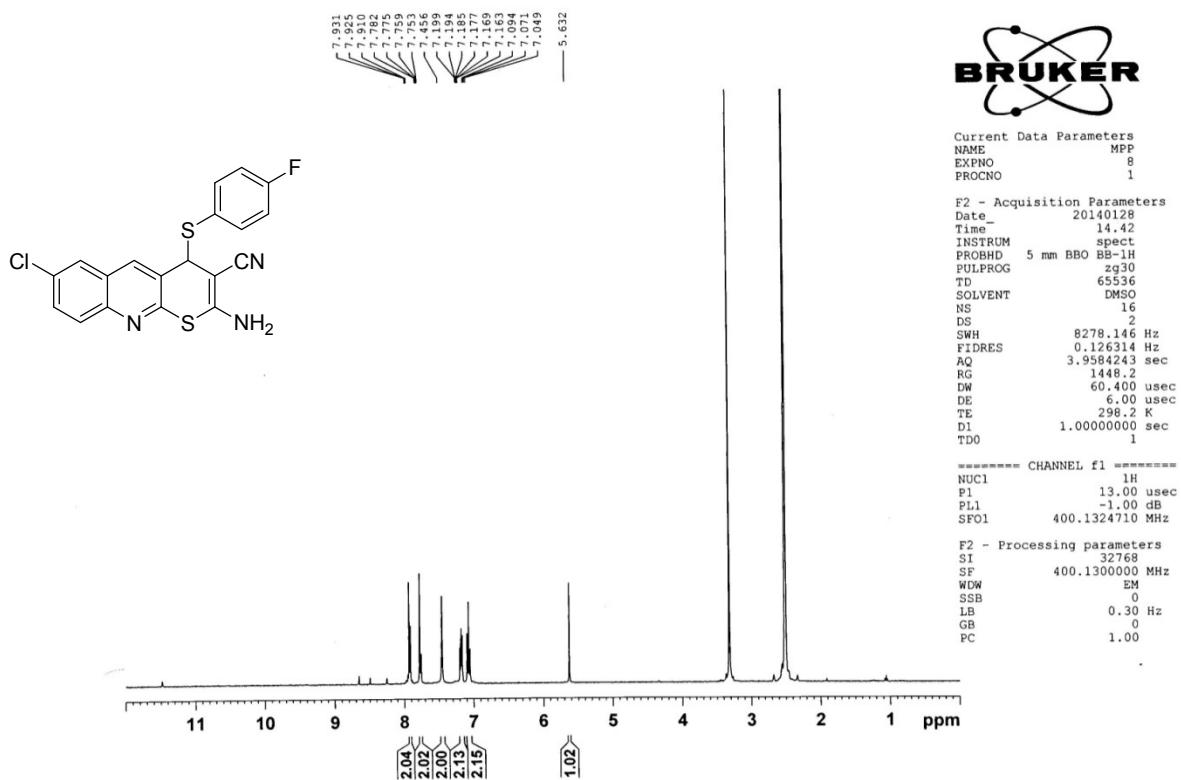
## <sup>13</sup>C NMR of Compound 4m







# <sup>1</sup>H NMR of Compound 4o



# Mass spectra of 4o

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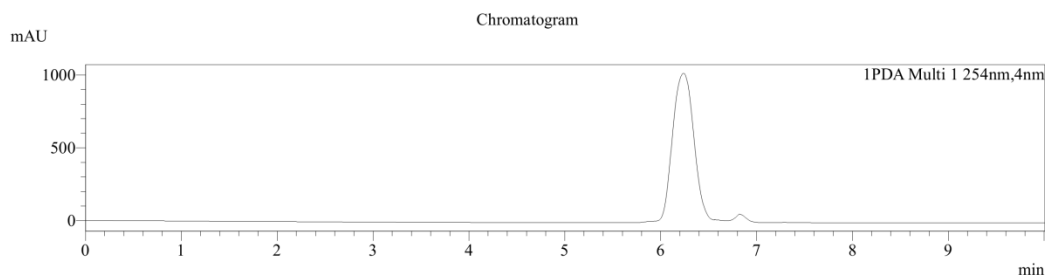
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## <Sample Information>

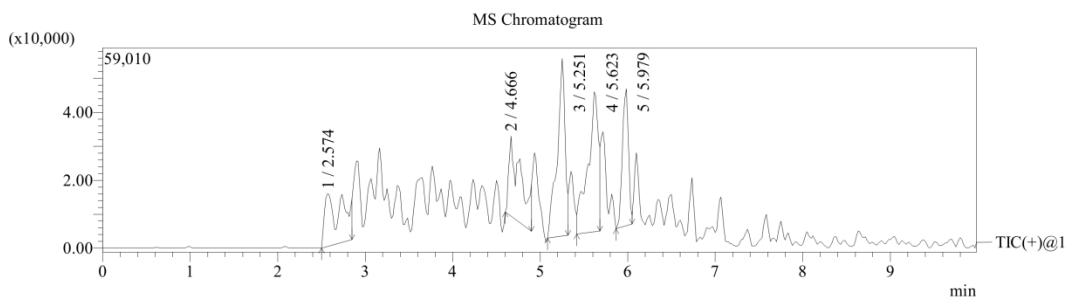
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Sample ID : TM 15  
Vial # : 1-16  
Injection Volume : 0.5 uL  
Date Acquired : 20-01-2014 11:01:28  
Date Processed : 20-01-2014 11:15:06

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Processed by : System Administrator

## <LC>



## <MS>



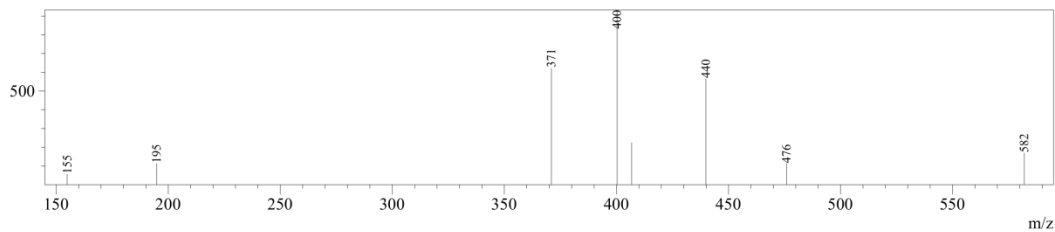
Line#:1 R.Time:----(Scan#----)

MassPeaks:8

Spectrum Mode:Averaged 8.417-8.767(506-527) Base Peak:400(933)

BG Mode:None Segment 1 - Event 1

Precursor Ion Scan:m/z 400.00



Line#:1 R.Time:----(Scan#----)

MassPeaks:8

Spectrum Mode:Averaged 8.417-8.767(506-527) Base Peak:400(969)

BG Mode:None Segment 1 - Event 1

Precursor Ion Scan:m/z 400.00

Sr. No.	m/z	Absolute Intensity	Relative Intensity
1	154.90	56	6.00
2	194.90	113	12.11
3	370.90	622	66.67
4	400.25	933	100.00
5	406.80	225	24.12
6	439.90	566	60.66
7	475.80	113	12.11
8	582.00	169	18.11