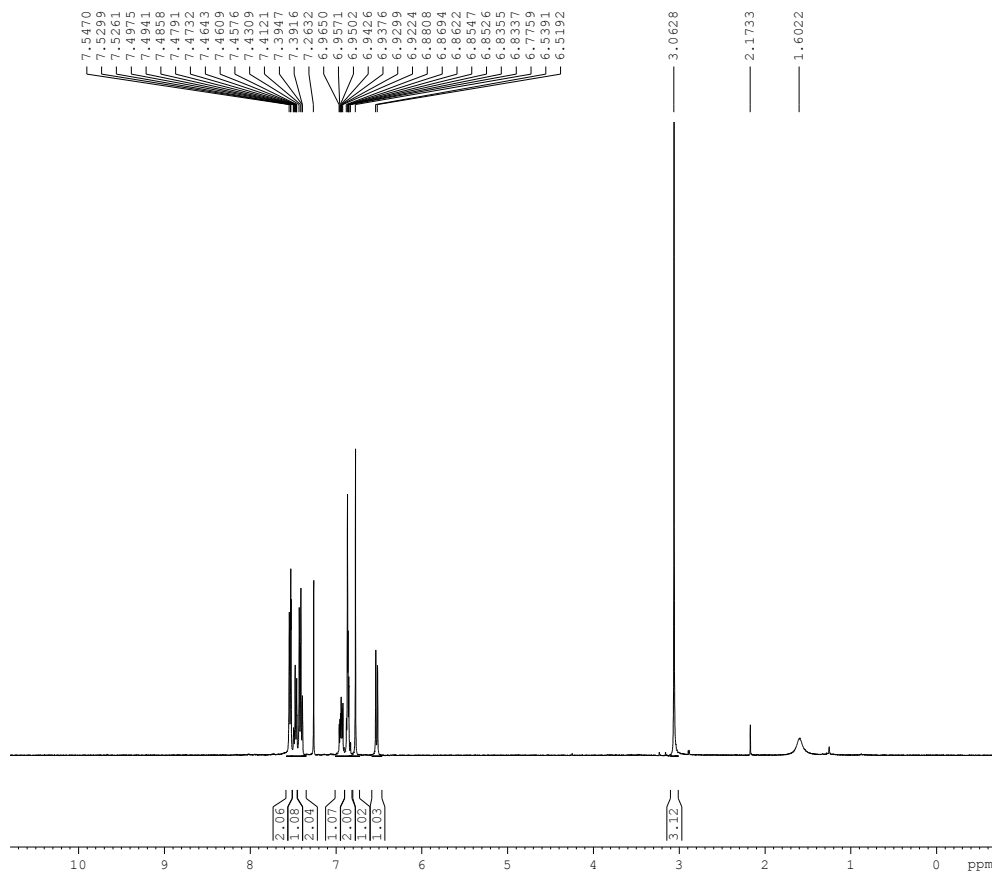


S-1



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Mar21-2013  
EXPNO 240  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130321  
Time 14.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7263477 sec  
RG 456  
DW 41.600 usec  
DE 6.00 usec  
TE 295.1 K  
D1 1.00000000 sec  
TD0 1

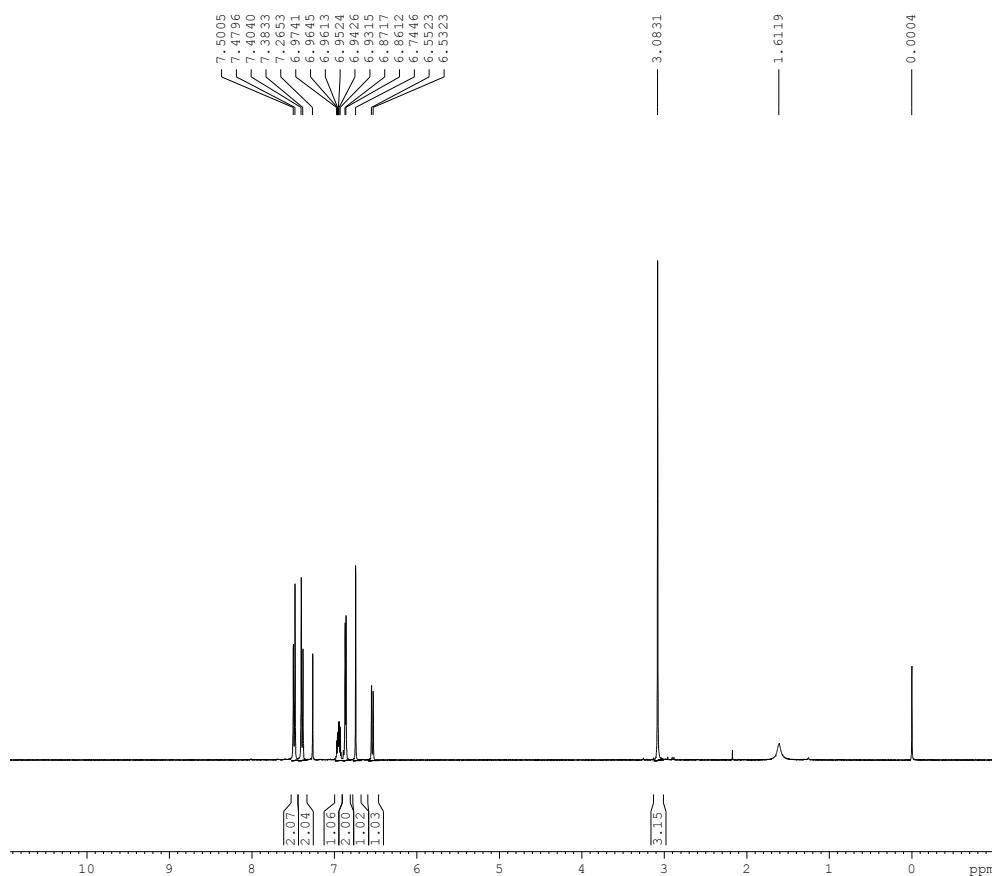
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NUC1 1H  
P1 10.90 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.130083 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

avtar\_saifpu@yahoo.co.in

<sup>1</sup>H NMR of (4-Methyl-4H-benzo[b][1,4]thiazin-2-yl)(phenyl)methanone **3(a)**

S-II



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME April-2013-Administrator  
EXPNO 250  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130412  
Time\_ 1.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7263477 sec  
RG 512  
DW 41.600 usec  
DE 6.00 usec  
TE 292.1 K  
D1 1.0000000 sec  
TDO 1

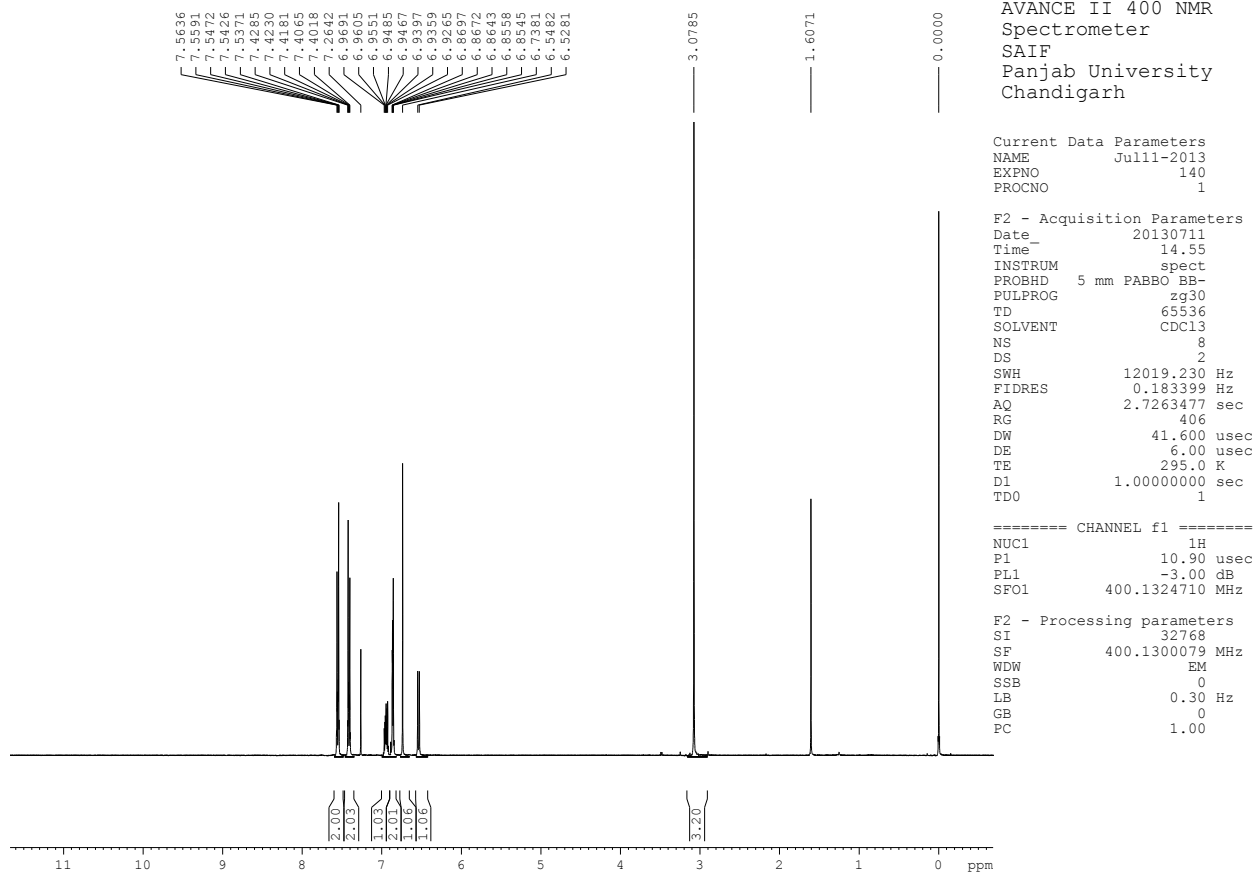
==== CHANNEL f1 =====  
NUC1 1H  
P1 10.90 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1281069 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-Chlorophenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone 3(b)**

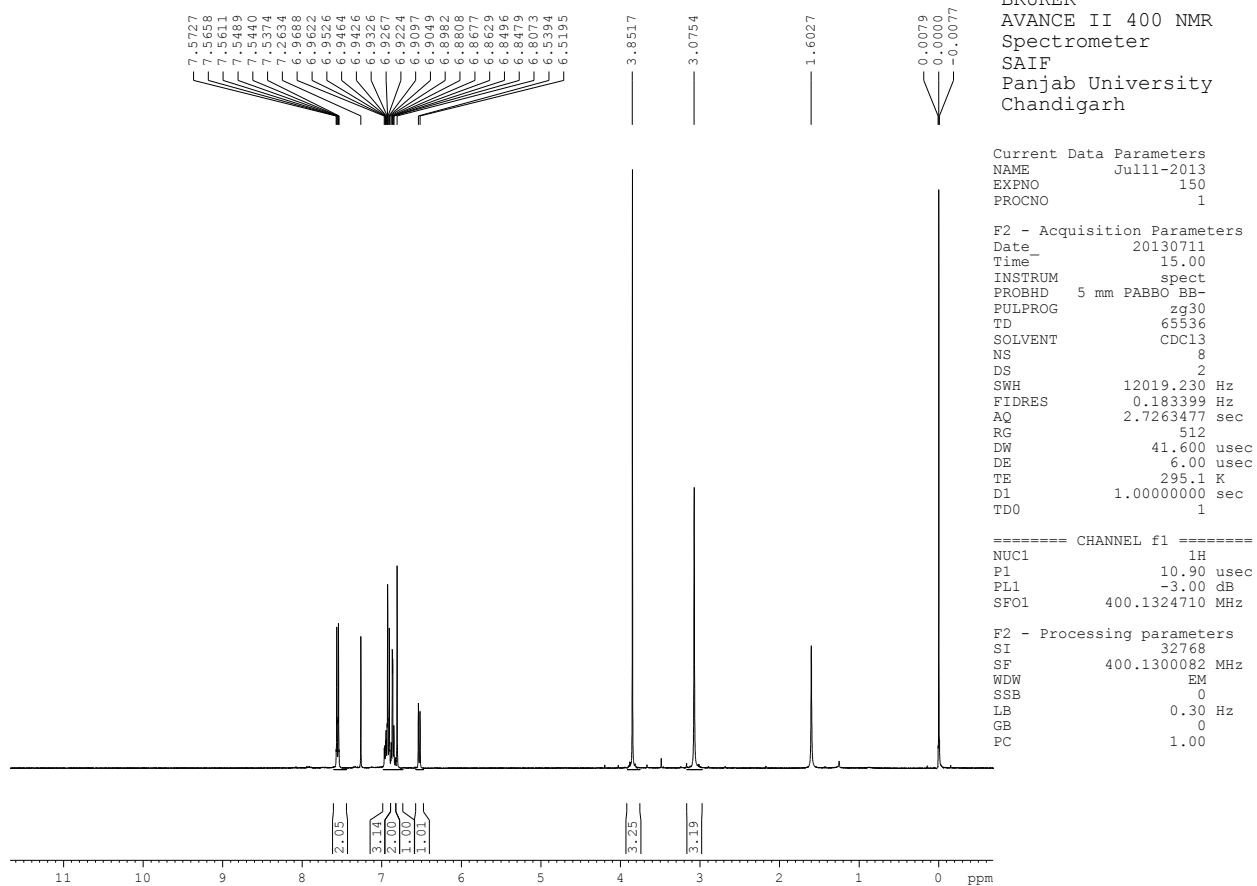
S-III



avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-Bromophenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone 3(c)**

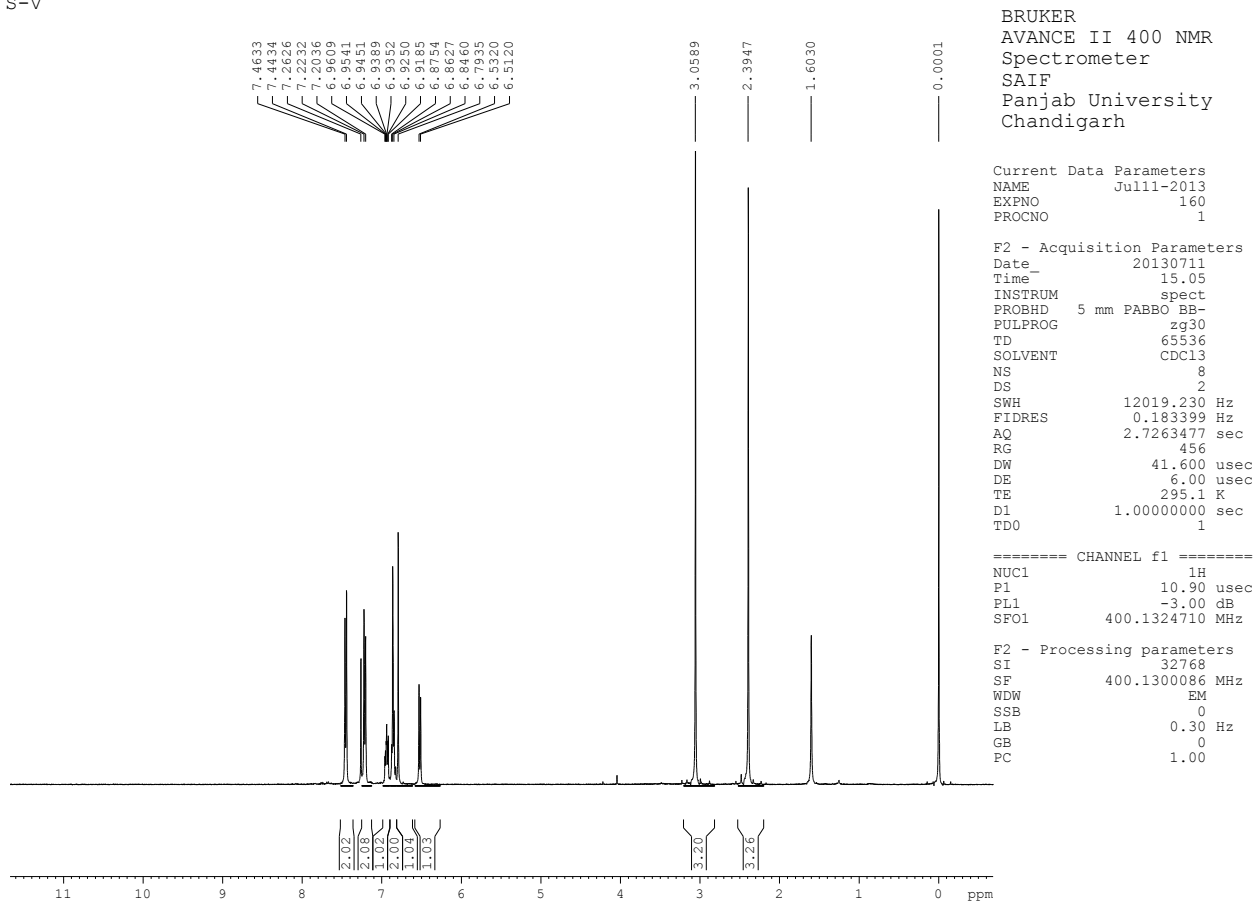
S-IV



avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-Methoxyphenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone 3(d)**

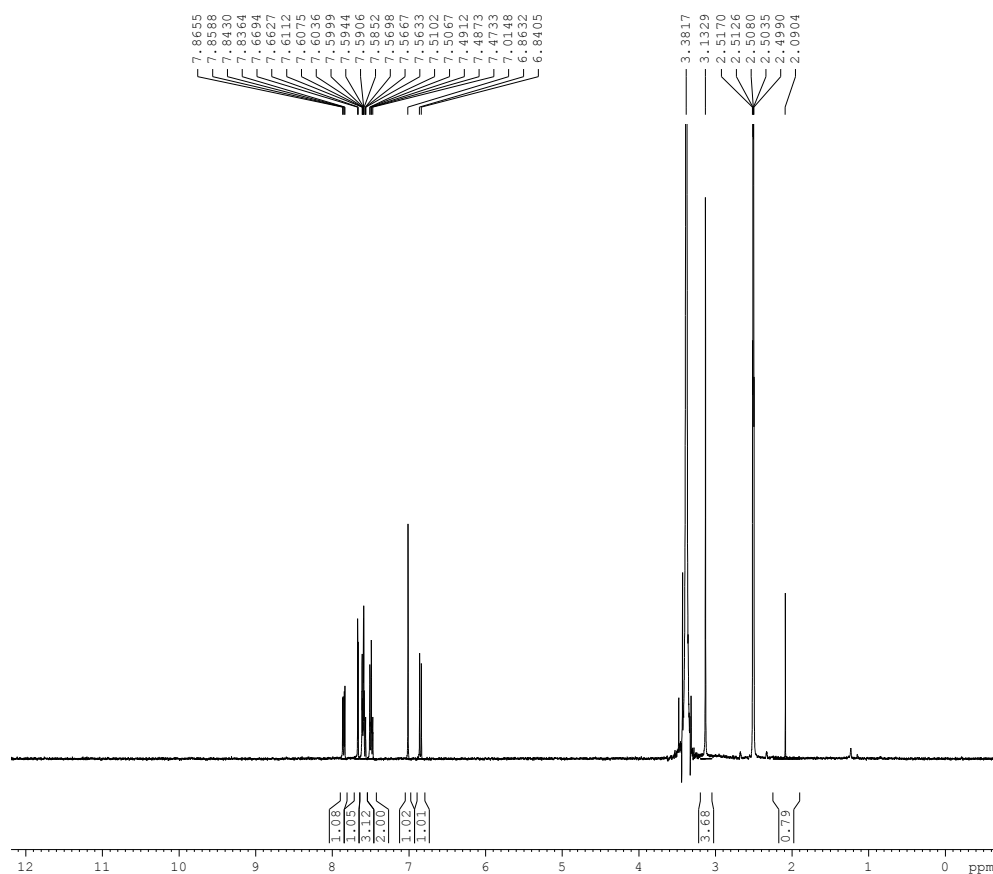
S-V



avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-Methylphenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone 3(e)**

BN-1



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Feb06-2015  
EXPNO 370  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150208  
Time\_ 21.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7263477 sec  
RG 362  
DW 41.600 usec  
DE 6.00 usec  
TE 294.1 K  
D1 1.00000000 sec  
TD0 1

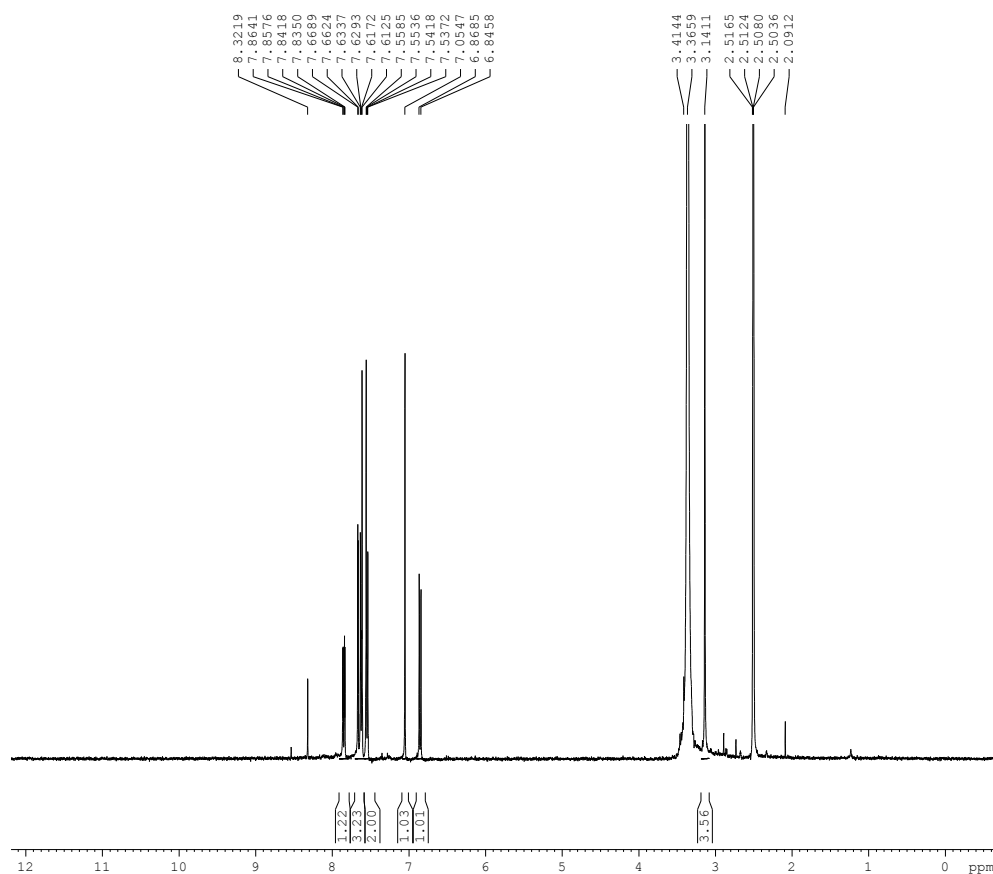
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PL1 -3.00 dB  
SFO1 400.1324710 MHz

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

avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)(phenyl)methanone (3f)**

BN-2



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Feb06-2015  
EXPNO 380  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150208  
Time\_ 22.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7263477 sec  
RG 456  
DW 41.600 usec  
DE 6.00 usec  
TE 294.1 K  
D1 1.00000000 sec  
TD0 1

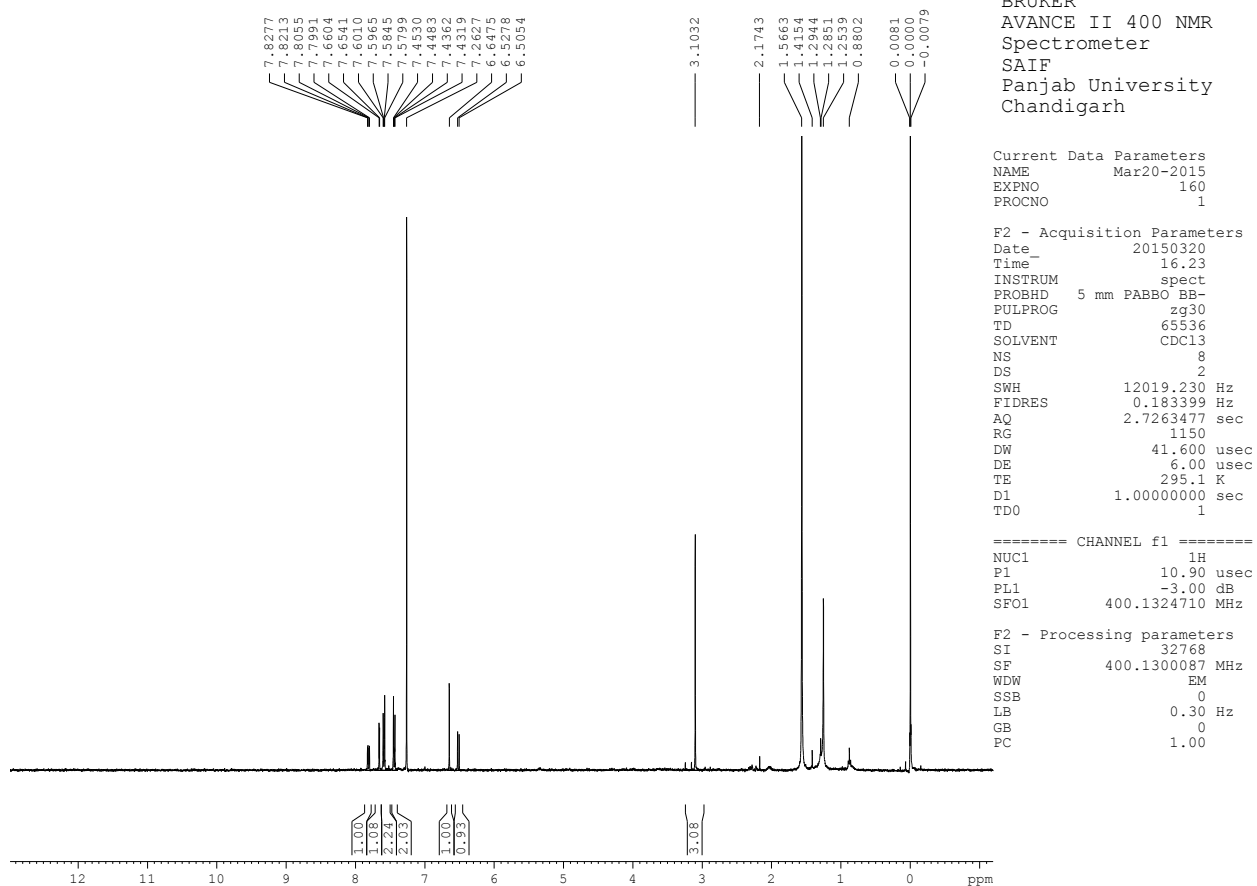
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.90 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

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

avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-chlorophenyl)(4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)methanone (3g)**

BN-4

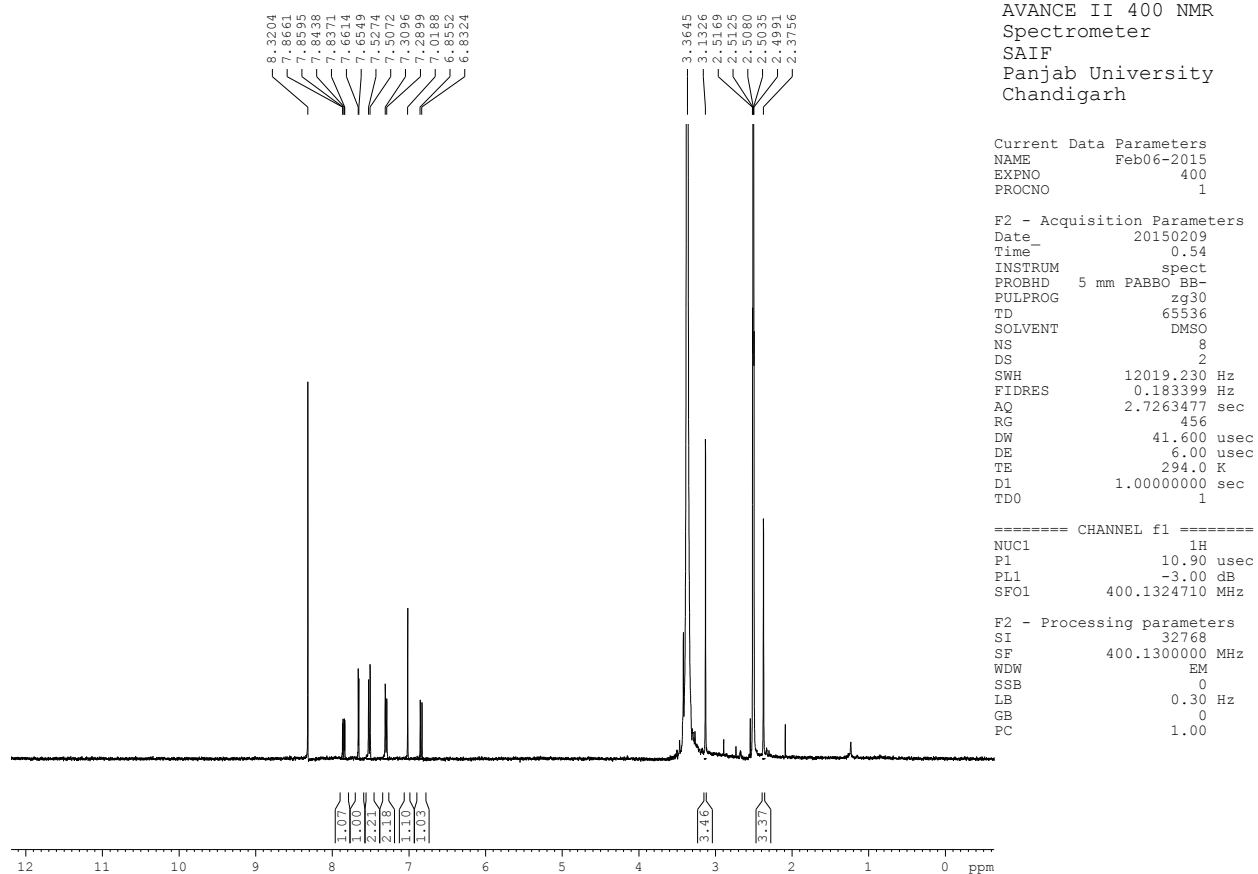


avtar\_saifpu@yahoo.co.in

**<sup>1</sup>H NMR of (4-bromophenyl)(4-methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl) methanone (3h)**



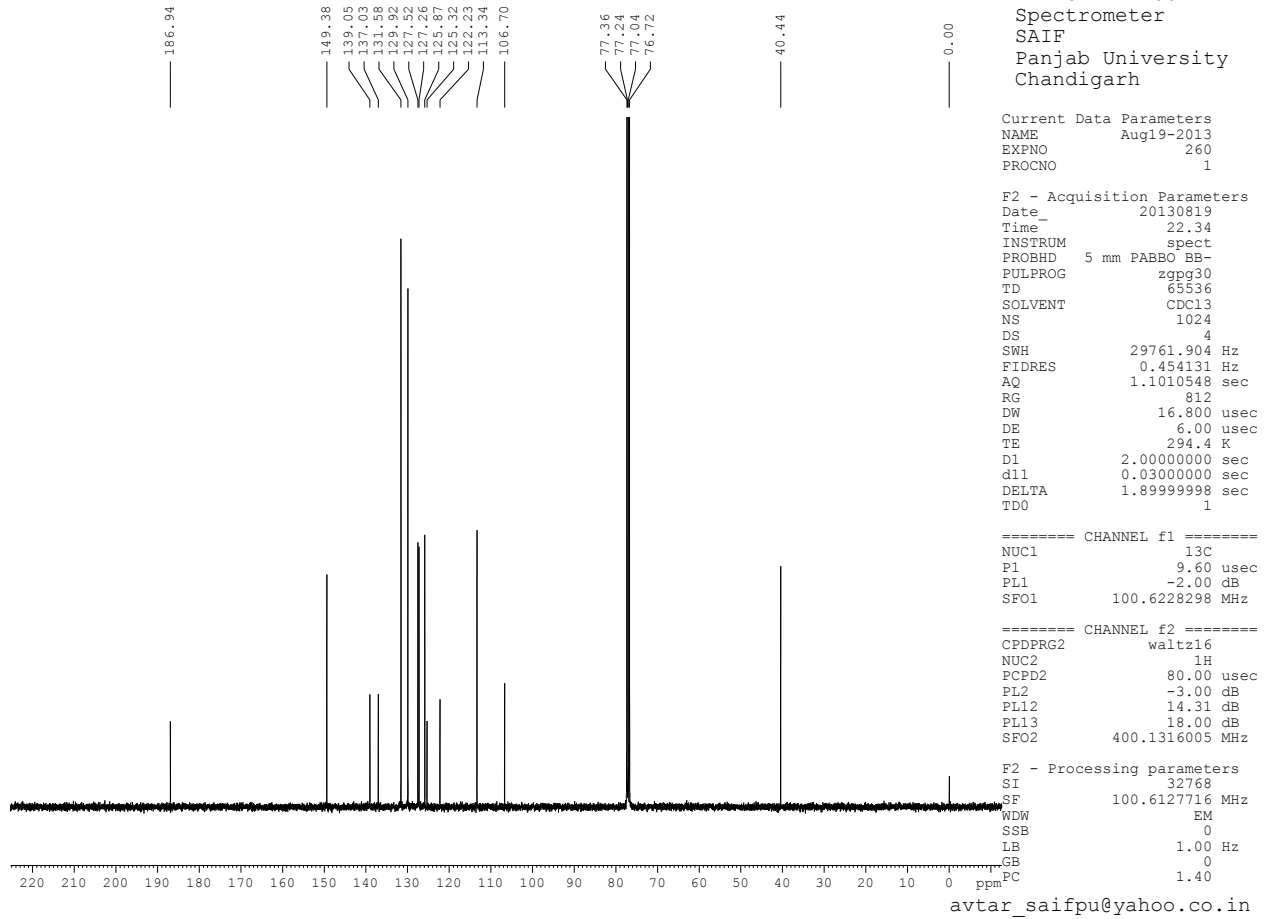
BN-4



avtar\_saifpu@yahoo.co.in

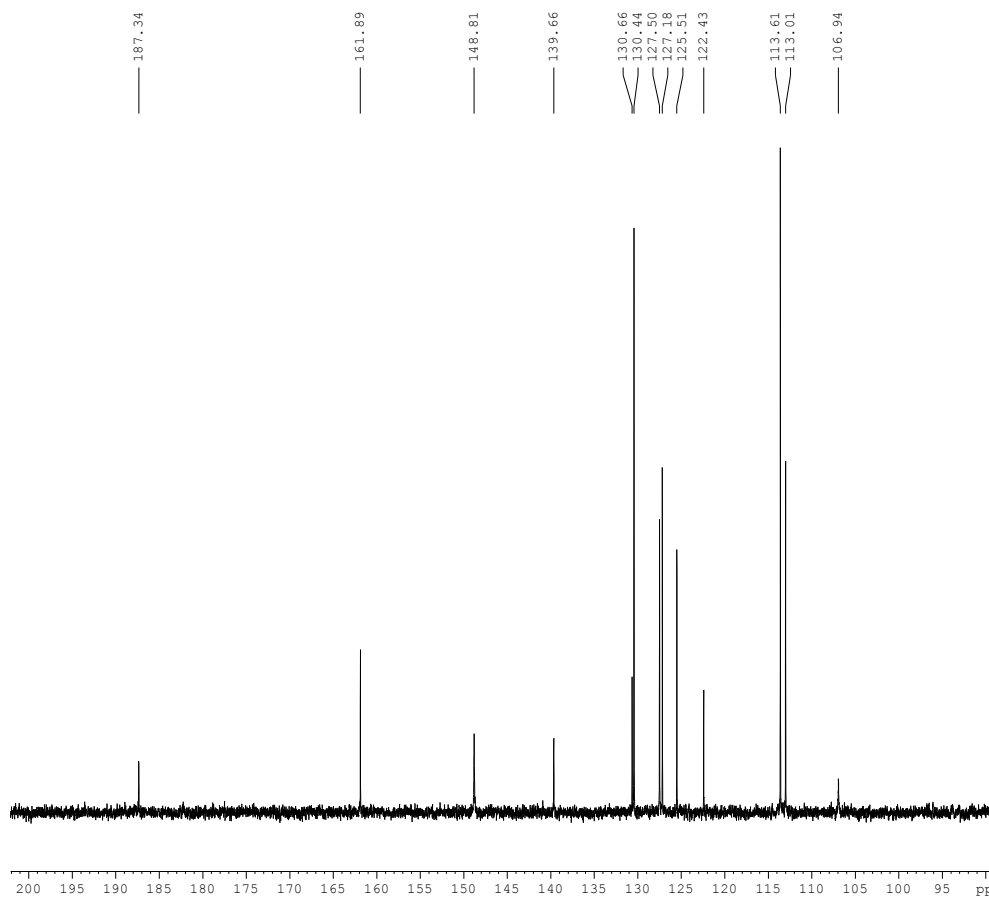
**<sup>1</sup>H NMR of (4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)(p-tolyl)methanone (3i)**

S-III



<sup>13</sup>C NMR of (4-Chlorophenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone **3(b)**

S-IV



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Aug19-2013  
EXPNO 250  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 20130819  
Time 21.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 812  
DW 16.800 usec  
DE 6.00 usec  
TE 294.5 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -2.00 dB  
SFO1 100.6228298 MHz

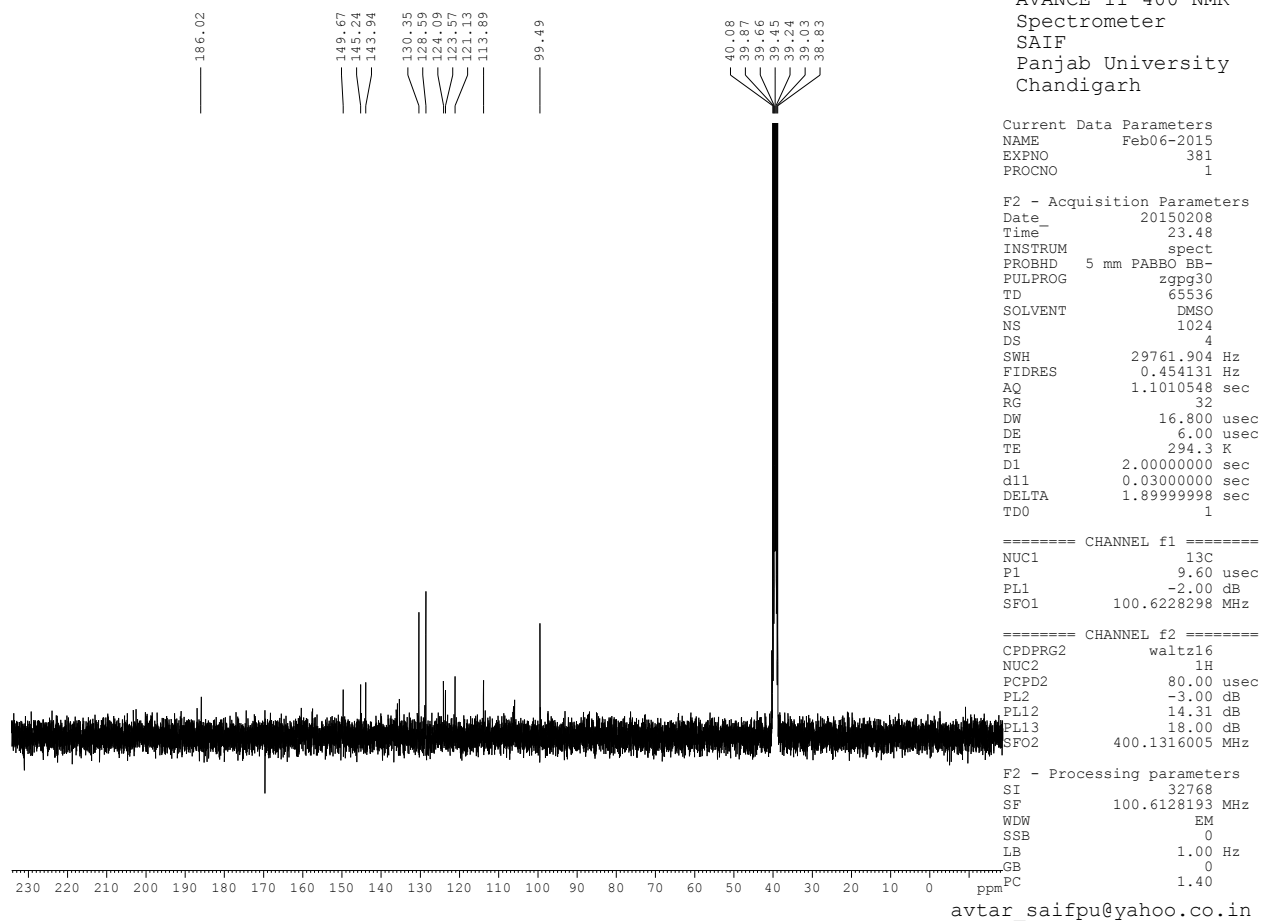
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.31 dB  
PL13 18.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127708 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

avtar\_saifpu@yahoo.co.in

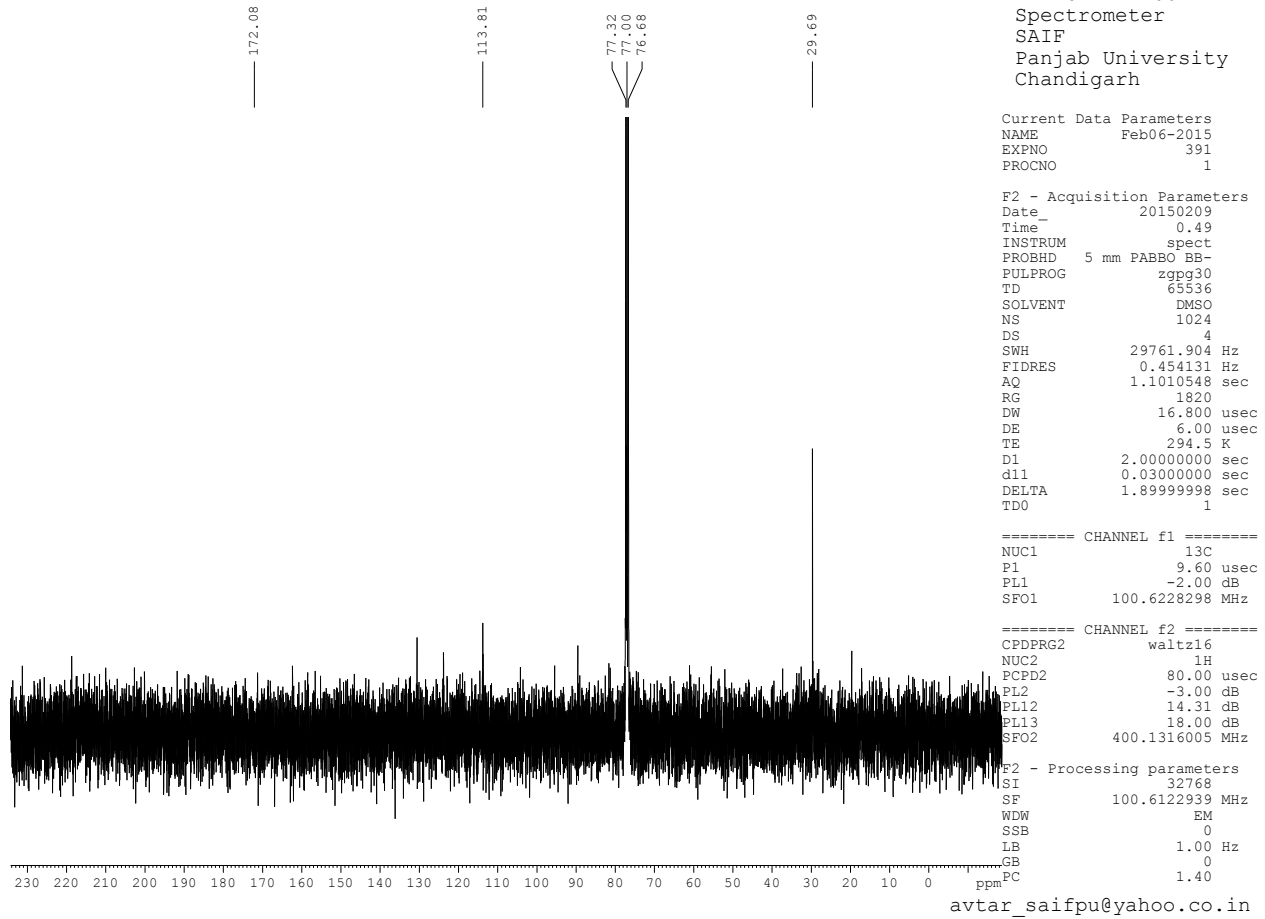
**<sup>13</sup>C NMR of (4-Bromophenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone 3(d)**

BN-2



**<sup>13</sup>C NMR of (4-chlorophenyl)(4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)methanone (3g)**

BN-3



**<sup>13</sup>C NMR of (4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)(p-tolyl)methanone (3h)**

## Mass Spectra

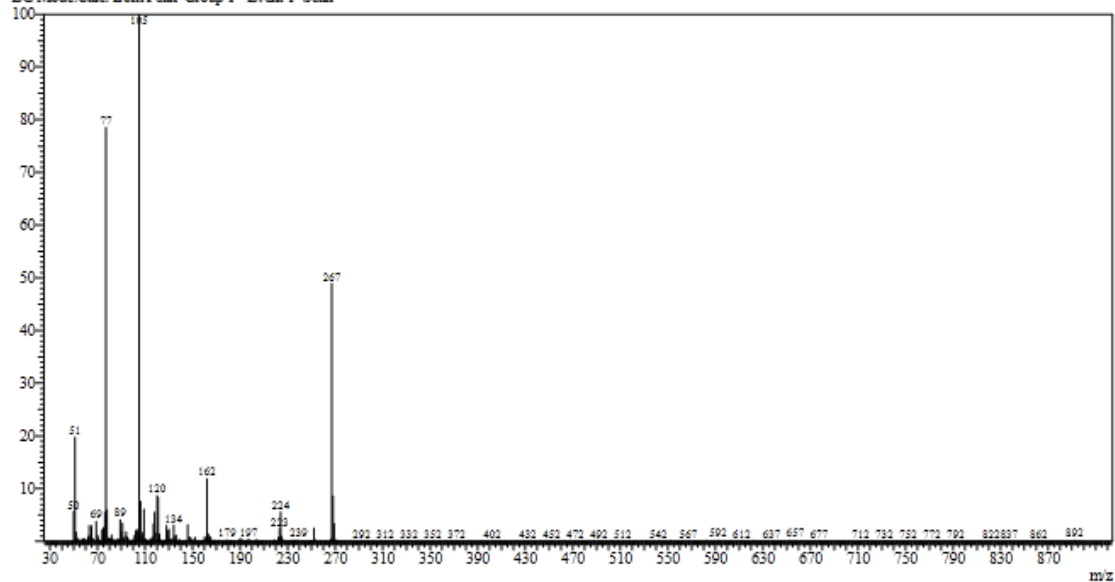
Spectrum

Line#: 1 R. Time: 6.215(Scan#: 1144)

MassPeaks: 419

RawMode: Averaged 6.210-6.220(1143-1145) BasePeak: 105(107139)

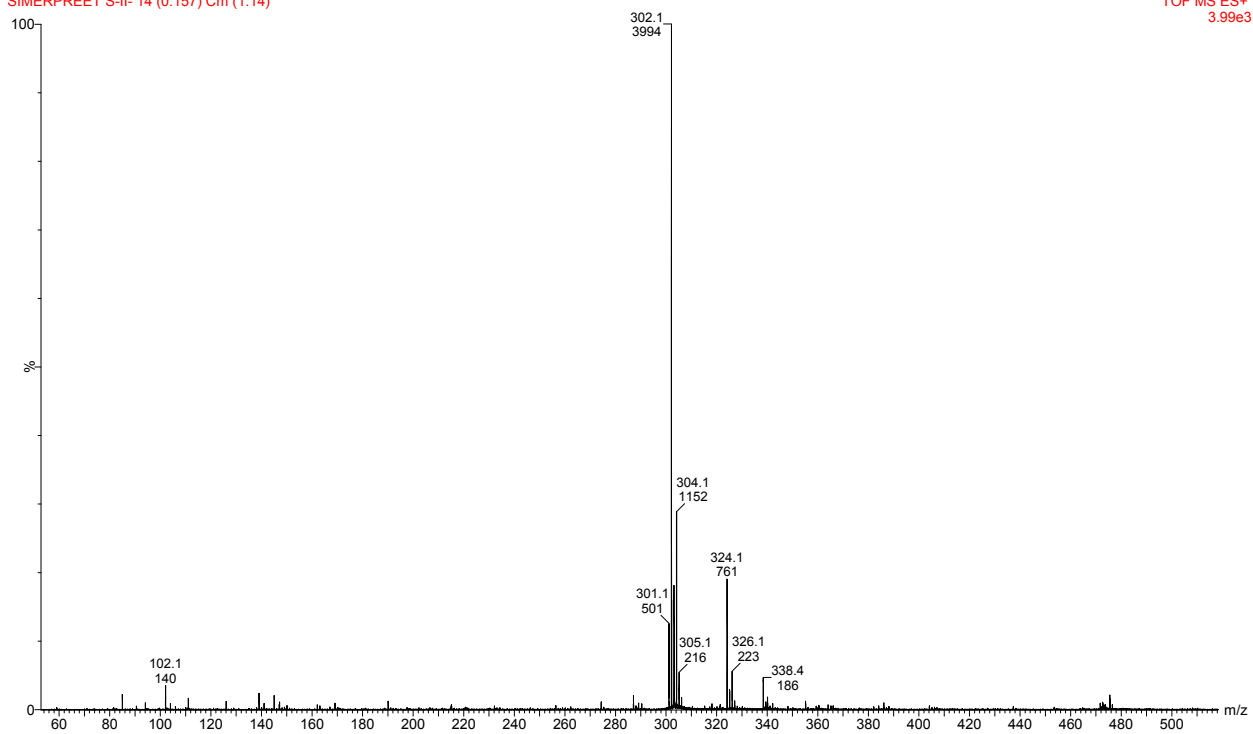
EGMode: Calc. from Peak Group 1 - Event 1 Scan



*Mass spectra of (4-Methyl-4H-benzo[b][1,4]thiazin-2-yl)(phenyl)methanone (3a)*

WATERS, Q-TOF MICROMASS (LC-MS)  
SIMERPREET S-II- 14 (0.157) Cm (1:14)

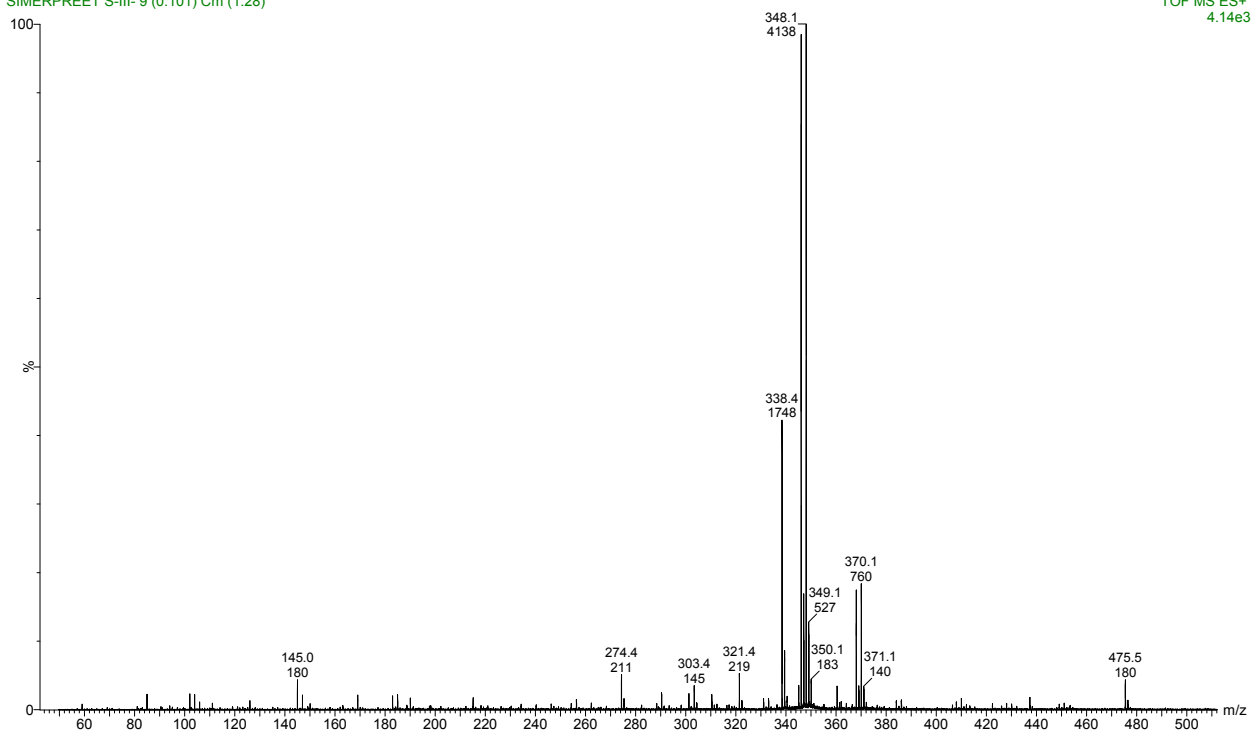
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH  
TOF MS ES+  
3.99e3



Mass spectra of (4-Chlorophenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone 3(b)

WATERS, Q-TOF MICROMASS (LC-MS)  
SIMERPREET S-III-9 (0.101) Cm (1:28)

SAIF/CIL, PANJAB UNIVERSITY, CHANDIGARH  
TOF MS ES+  
4.14e3



Mass spectra of (4-Bromophenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone **3(c)**



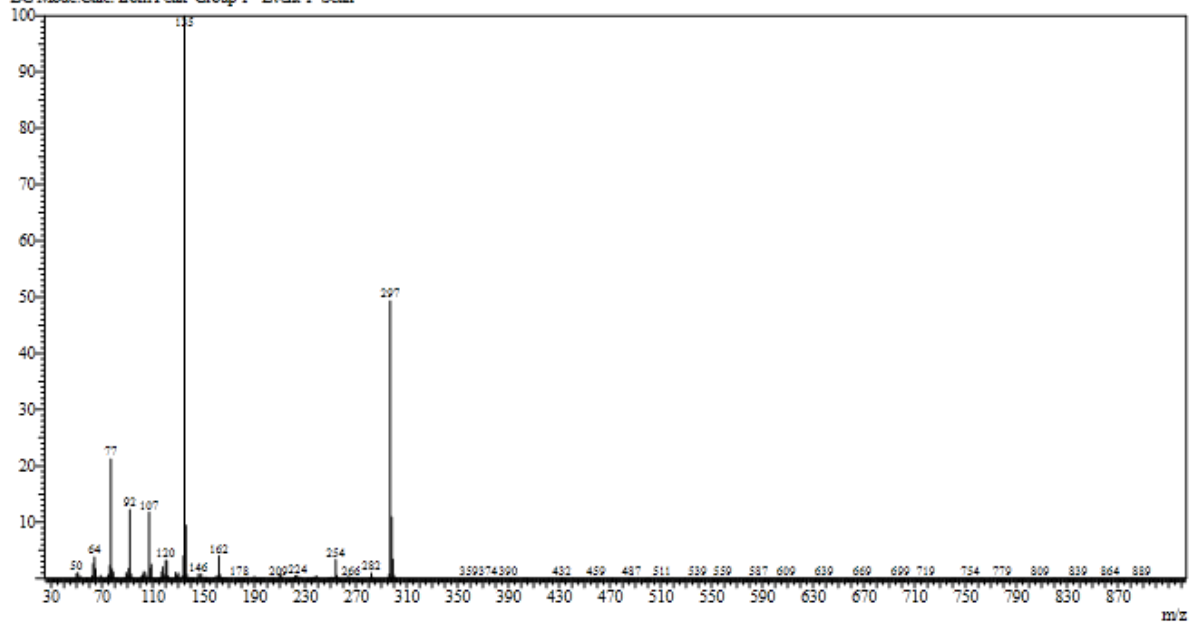
Spectrum

Line# 1 R.Time:6.855(Scan#:1272)

MassPeaks:325

RawMode:Averaged 6.850-6.860(1271-1273) BasePeak:135(3756830)

BGMode:Calc. from Peak Group 1 - Event 1 Scan



Mass spectra of *(4-Methoxyphenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone (3d)*

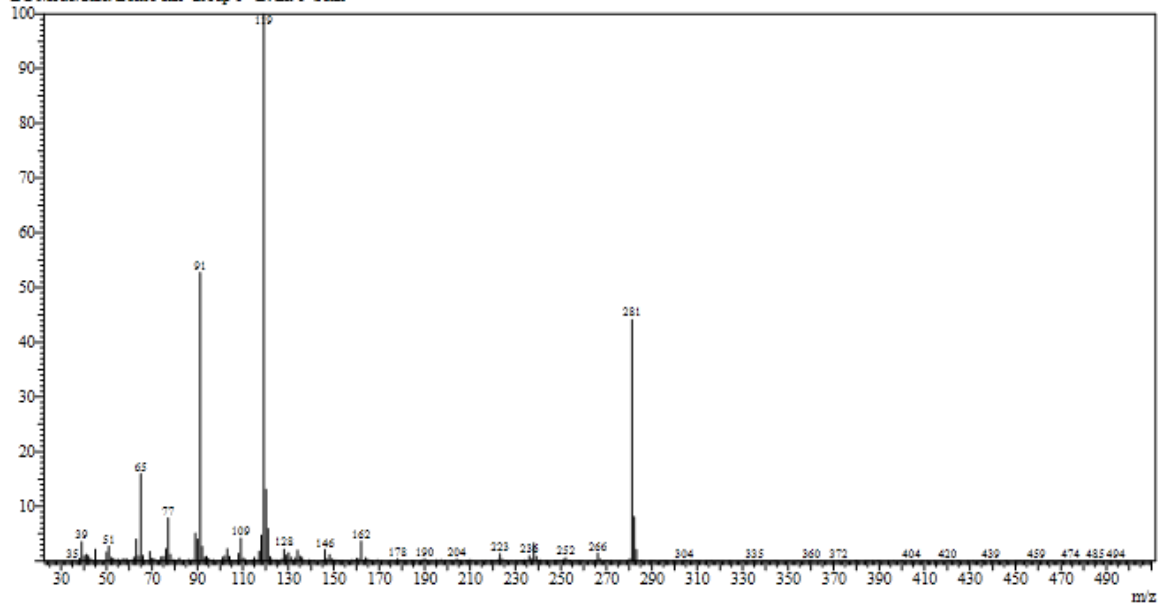
Spectrum

Line# 1 R.Time:8.560(Scan#:1113)

MassPeaks:298

RawMode:Averaged 8.555-8.565(1112-1114) BasePeak:119(27553)

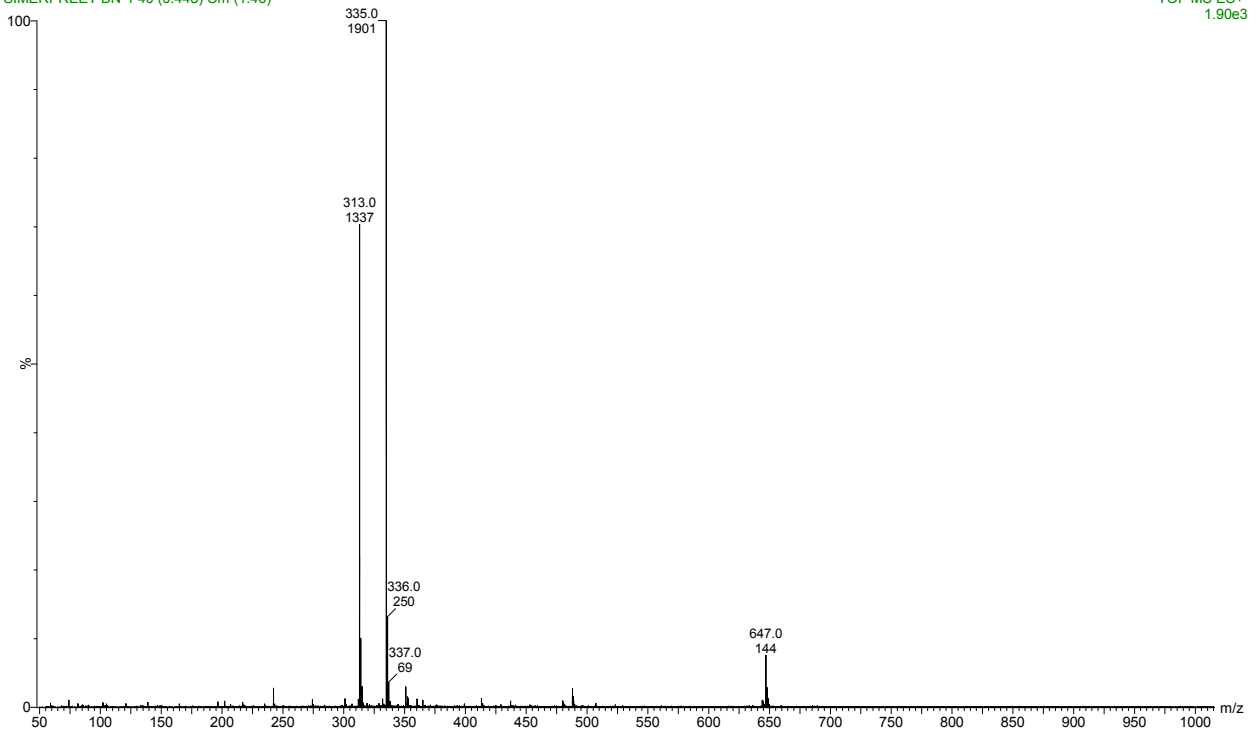
BGMode:Calc. from Peak Group 1 - Event 1 Scan



Mass spectra of *(4-Methylphenyl)(4-methyl-4H-benzo[b][1,4]thiazin-2-yl)methanone (3e)*

WATERS, Q-TOF MICROMASS (LC-MS)  
SIMERPREET BN-1 40 (0.448) Cm (1:46)

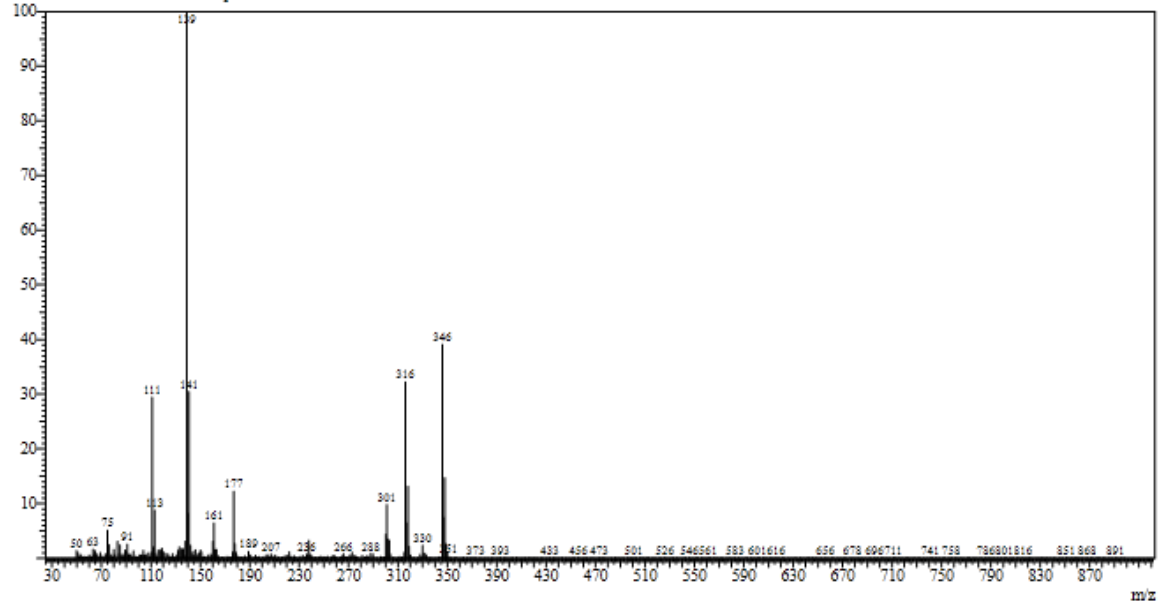
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH  
TOF MS ES+  
1.90e3



Mass spectra of (4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)(phenyl)methanone (3f)

Spectrum

Line#: 1 R. Time: 10.950 (Scan#: 2091)  
Mass Peaks: 513  
Raw Mode: Averaged 10.945-10.955 (2090-2092) Base Peak: 139 (75106)  
BGM Mode: Calc. from Peak Group 1 - Event 1 Scan



Mass spectra of *(4-chlorophenyl)(4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)methanone* (3g)

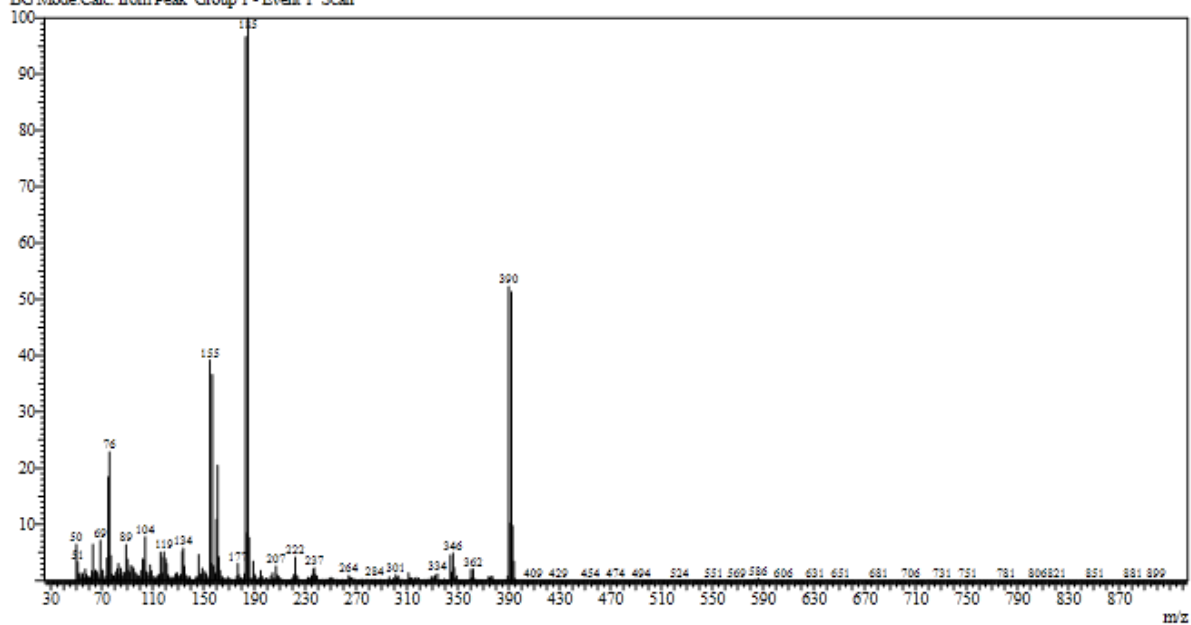
Spectrum

Line# 1 R.Time: 8.970 (Scan#: 1695)

MassPeaks: 536

RawMode: Averaged 8.965-8.975 (1694-1696) BasePeak: 185 (216814)

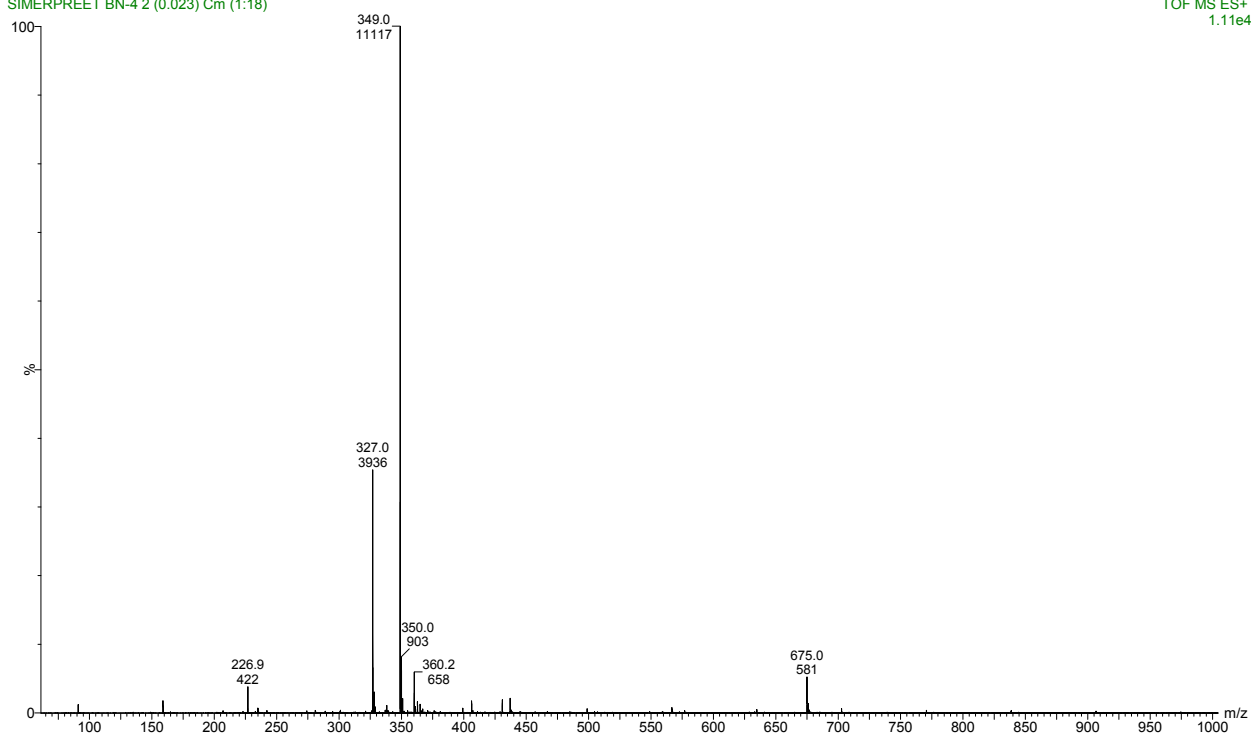
BG Mode: Calc. from Peak Group 1 - Event 1 Scan



Mass spectra of *(4-bromophenyl)(4-methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl) methanone (3h)*

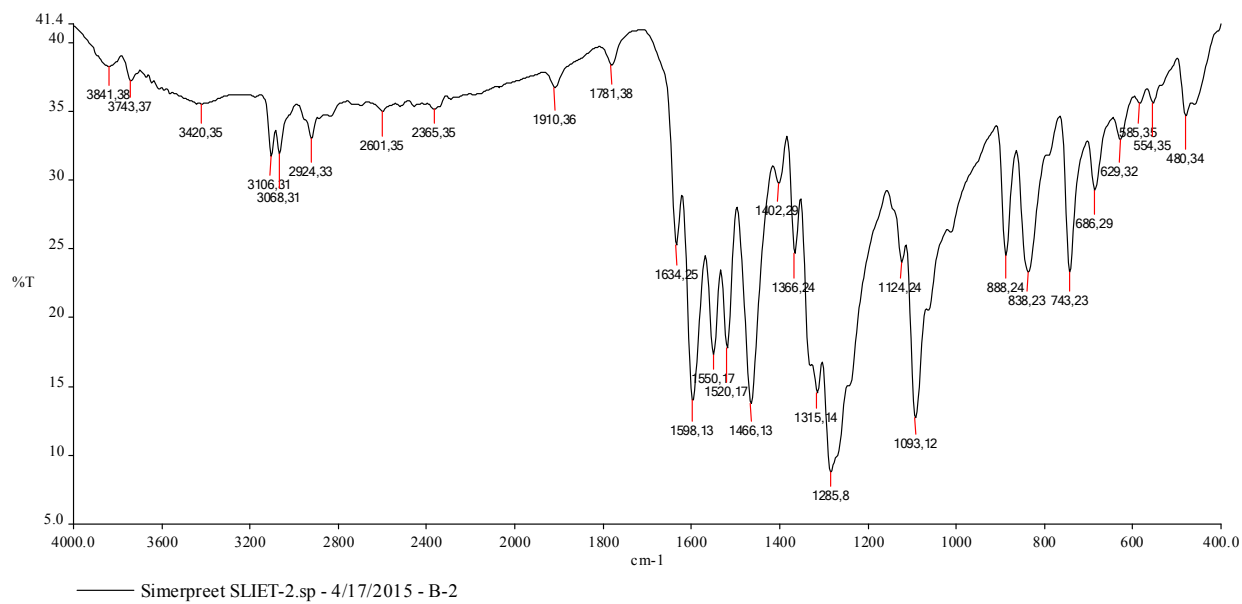
WATERS, Q-TOF MICROMASS (LC-MS)  
SIMERPREET BN-4 2 (0.023) Cm (1:18)

SAIF/CIL, PANJAB UNIVERSITY, CHANDIGARH  
TOF MS ES+  
1.11e4



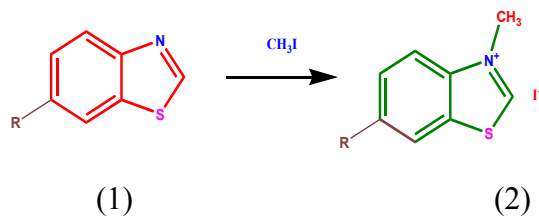
*Mass spectra of (4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)(p-tolyl)methanone (3i)*

RC SAIF PU, Chandigarh



IR spectra of (4-chlorophenyl)(4-Methyl-7-nitro-4H-benzo[b][1,4]thiazin-2-yl)methanone (3g)

**Scheme.** Synthesis of N-methyl 1,3-benzothiazolium iodide (2)



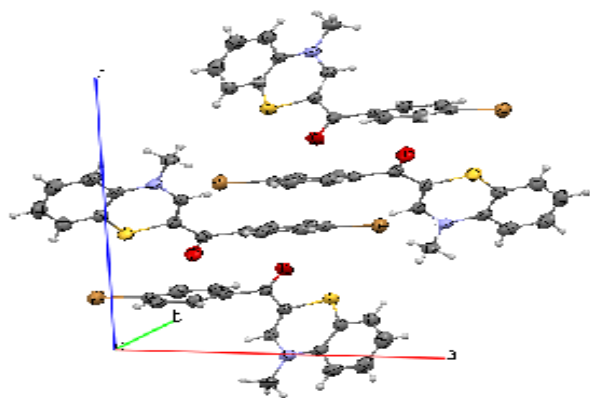


Figure 4. Crystal packing arrangement along a,b,c coordinates

Table: Comparison of conventional and ultrasonication method

S.no	Compounds	Conventional Time/ Yield	Ultrasonication Time/Yield	PTC
1.	3(a)	4 hrs/ 40%	25 mins/ 70%	35 mins
2.	3(b)	4 hrs/ 40%	25 mins/ 72%	35 mins
3.	3(c)	4 hrs/ 42%	30 mins/ 75%	40 mins
4.	3(d)	4hrs 30 mins/ 45%	30 mins/ 72%	40 mins
5.	3(e)	4 hrs 15 mins/ 42%	30 mins/ 78%	38 mins
6.	3(f)	4 hrs/ 41%	25 mins/ 76%	35mins
7.	3(g)	4 hrs 10 mins/ 44%	25 mins/ 78%	40mins
8.	3(h)	4hrs 30 mins/ 46%	30 mins/ 82%	30 mins
9.	3(i)	4 hrs 15 mins/ 43%	30 mins/ 80%	40 mins