

On Water Catalyst-Free Synthesis of Benzo[d]Imidazo[2,1-b] Thiazoles and Novel N-Alkylated 2-Aminobenzo[d]oxazoles Under Microwave Irradiation

Narasimharao Mukku, and Barnali Maiti*

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Vellore-632014, India.

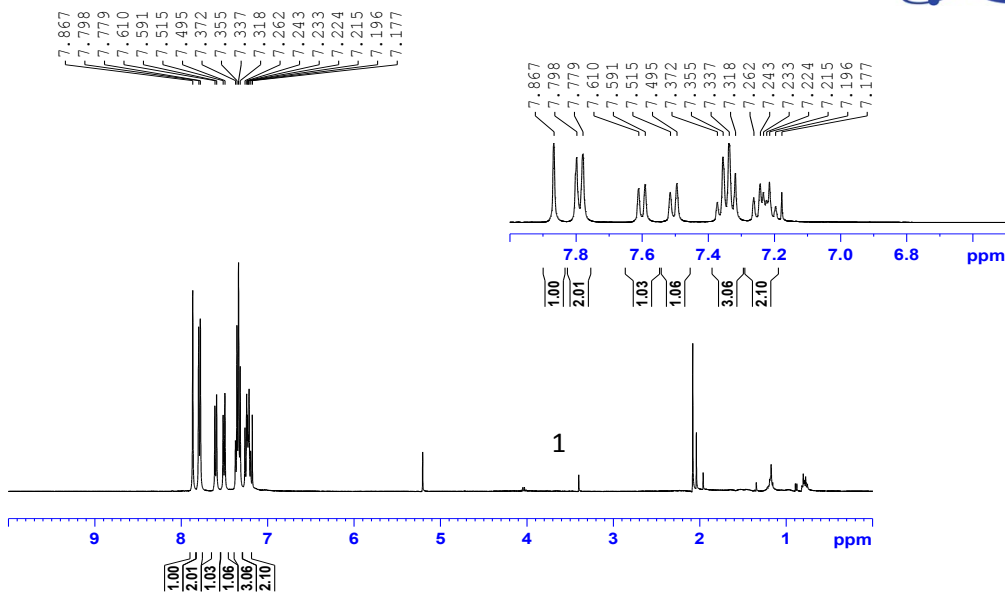
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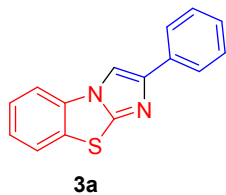
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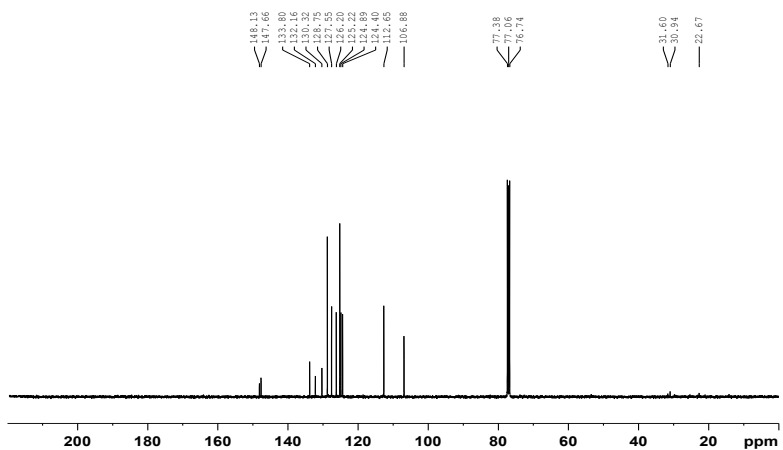
1. Characterization data of compound 3a-5f.....2-37
2. Supporting data for microwave reaction.....38

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NS-A-1





Signature SIF VIT VELLORE
NS-A-1

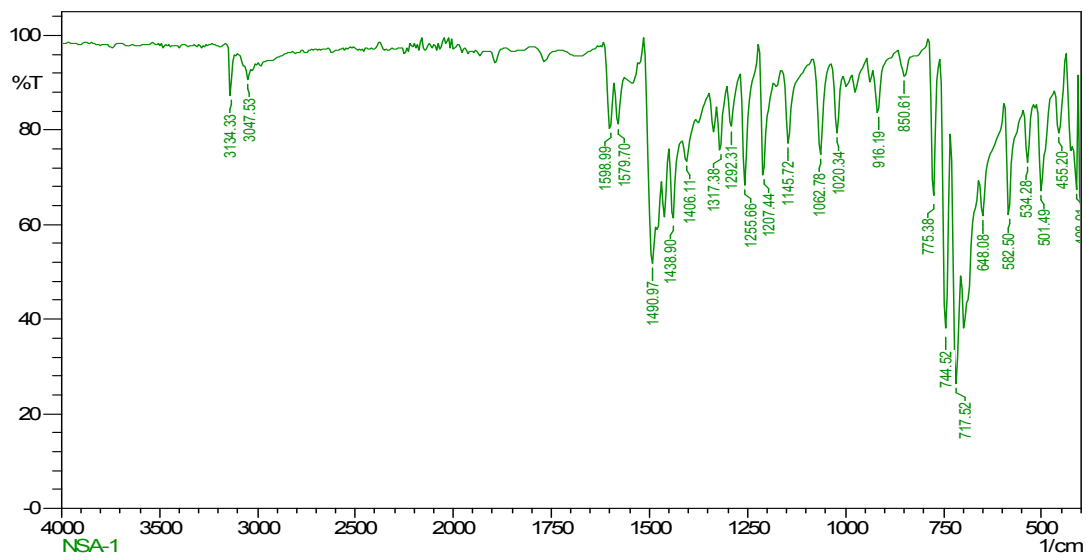
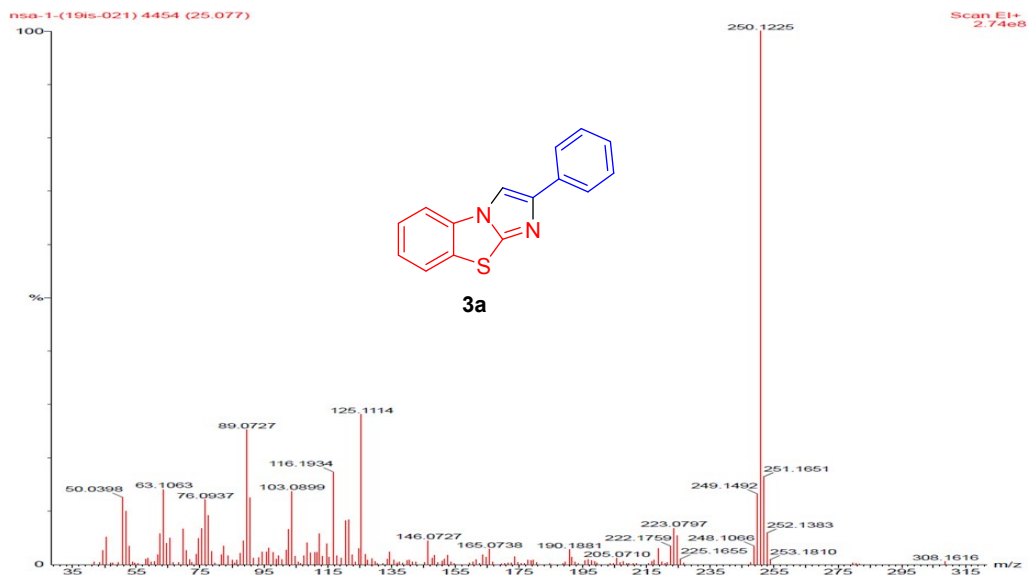


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DE 6.50 usec
TE 300.0 K
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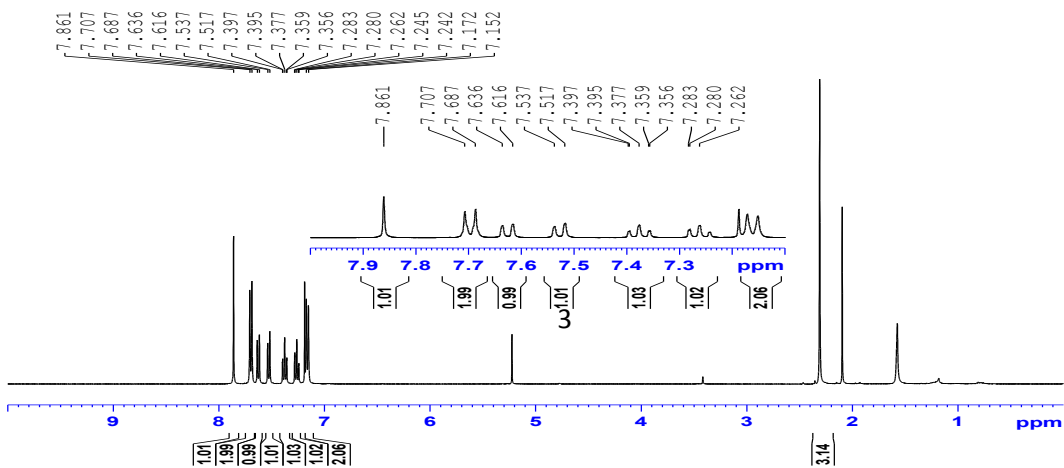
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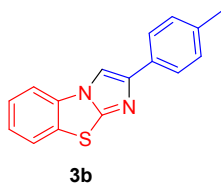
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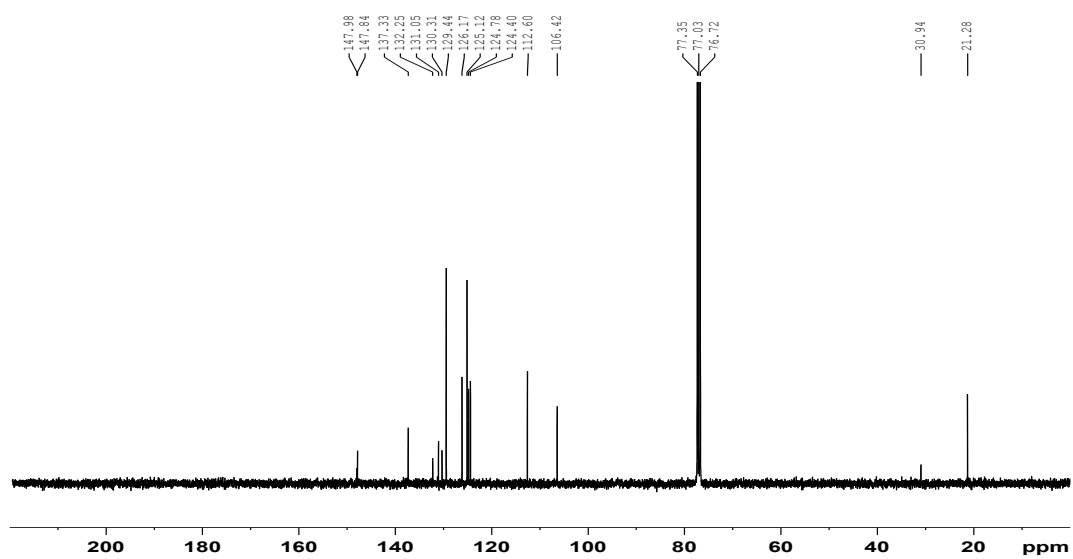
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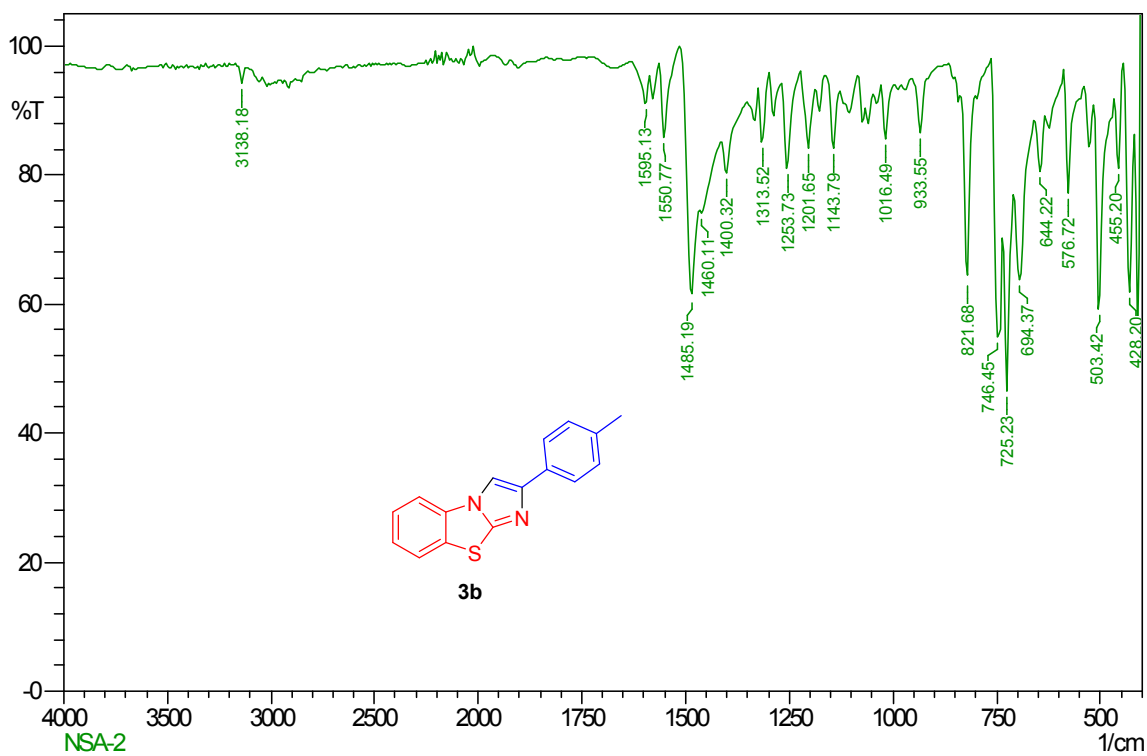




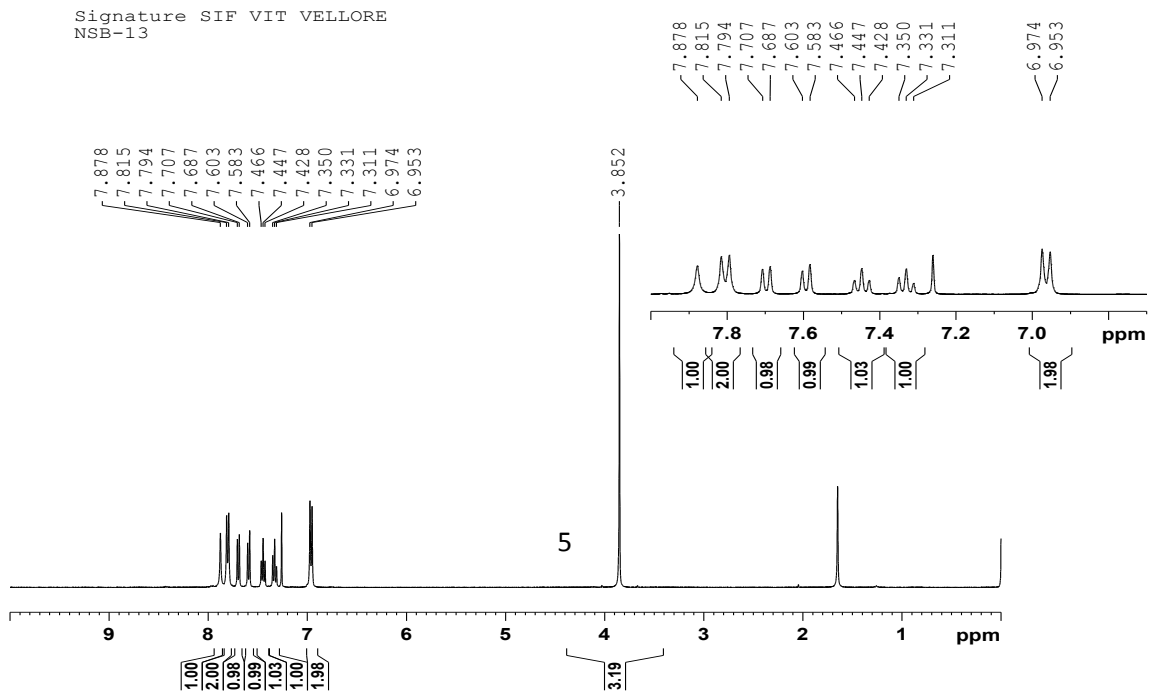
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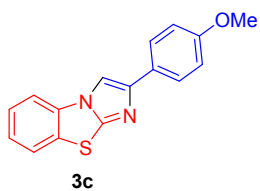


¹H and ¹³C NMR spectrum of compound 3b in CDCl₃

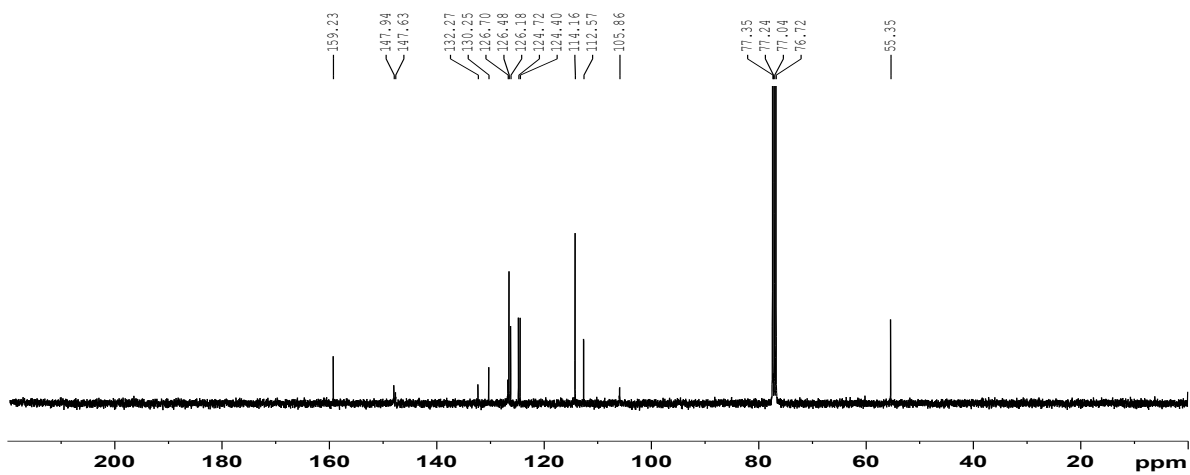


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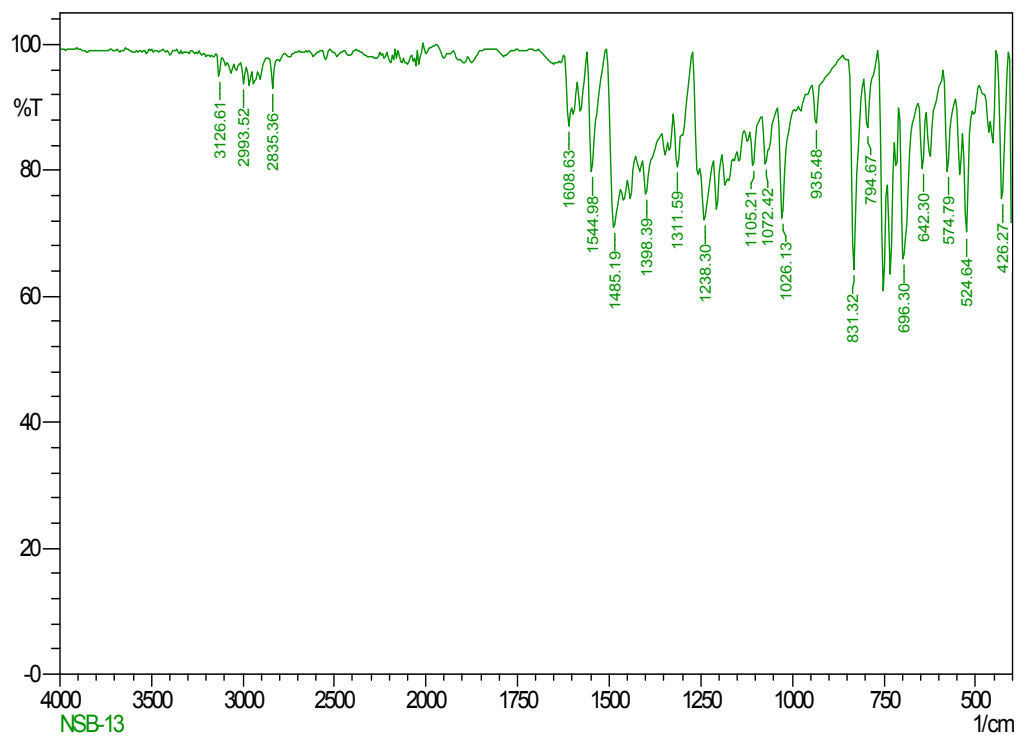
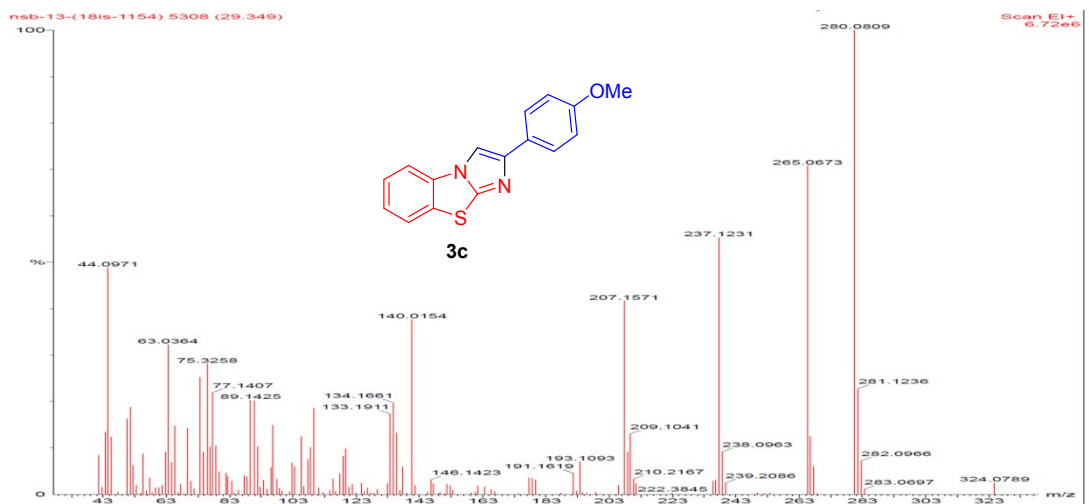




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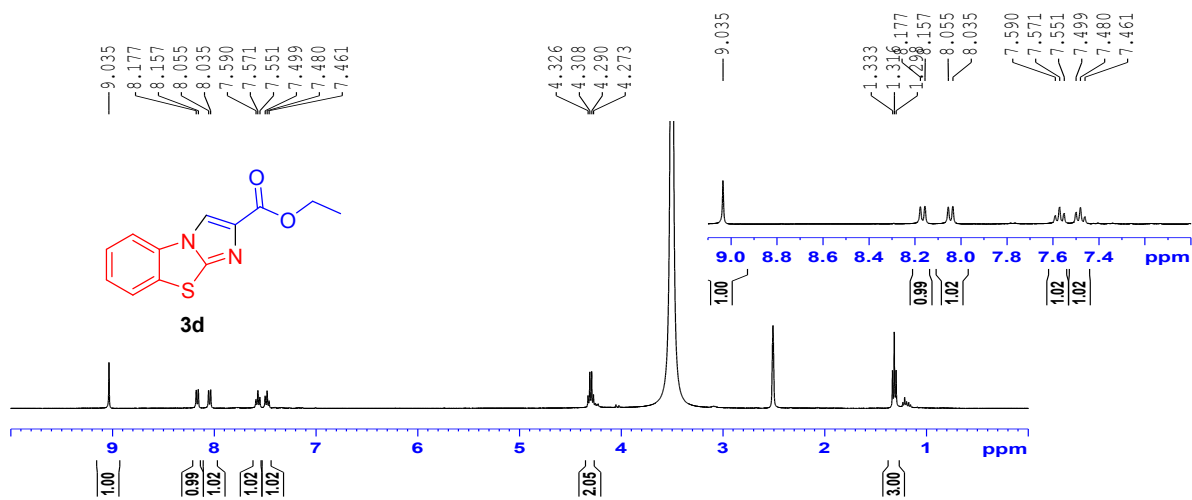


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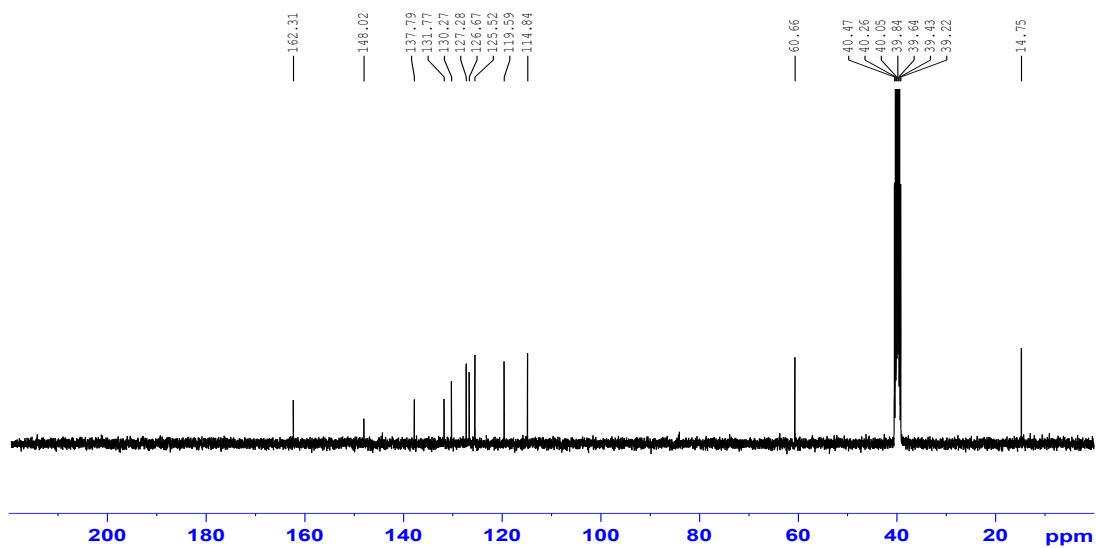


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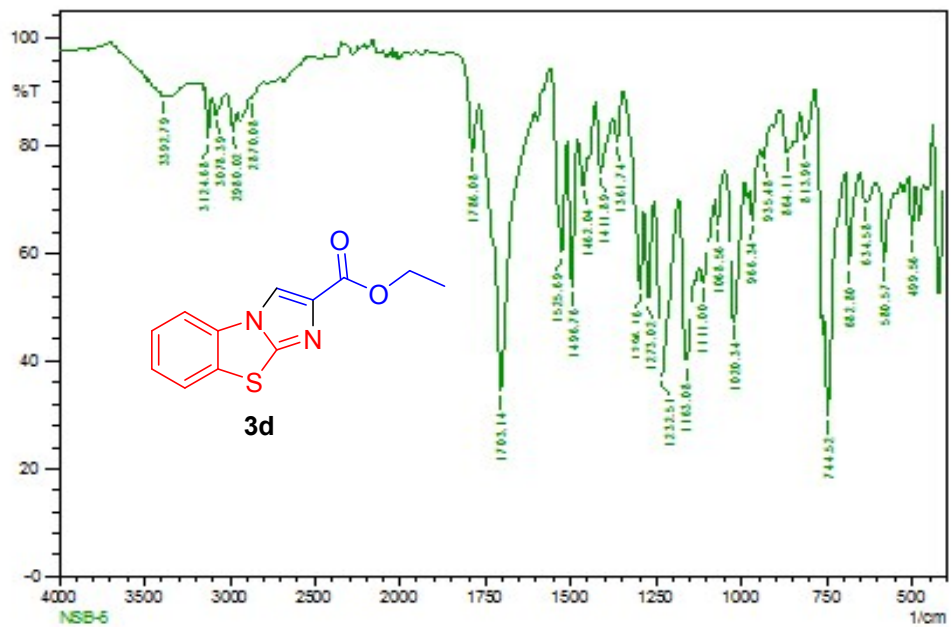
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Signature SIF VIT VELLORE
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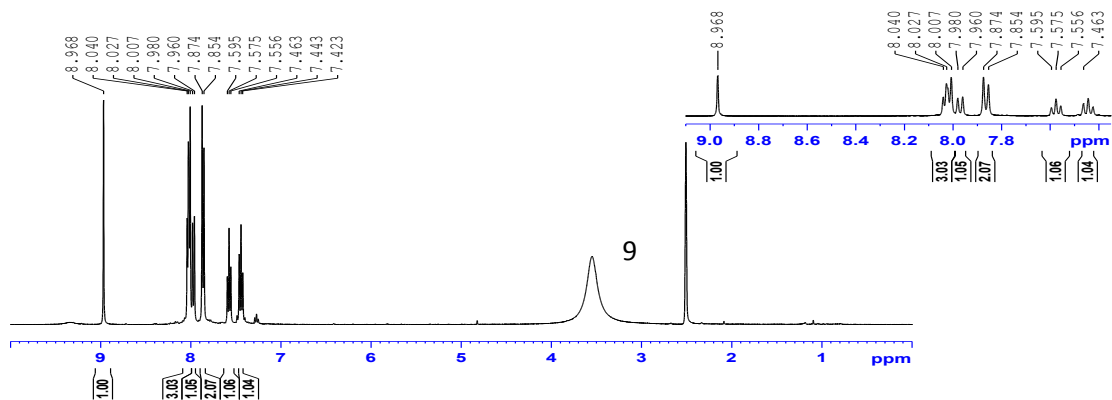


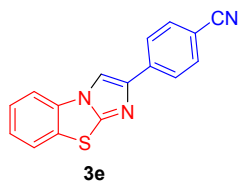
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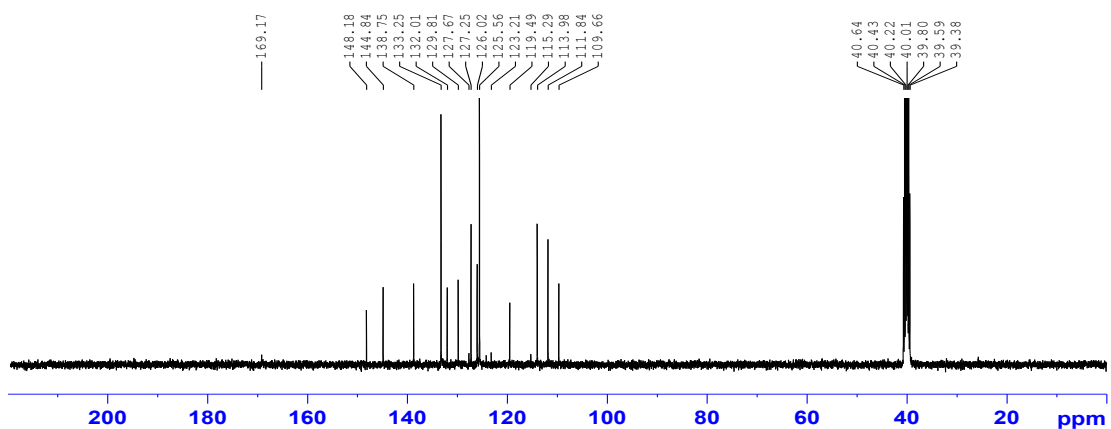
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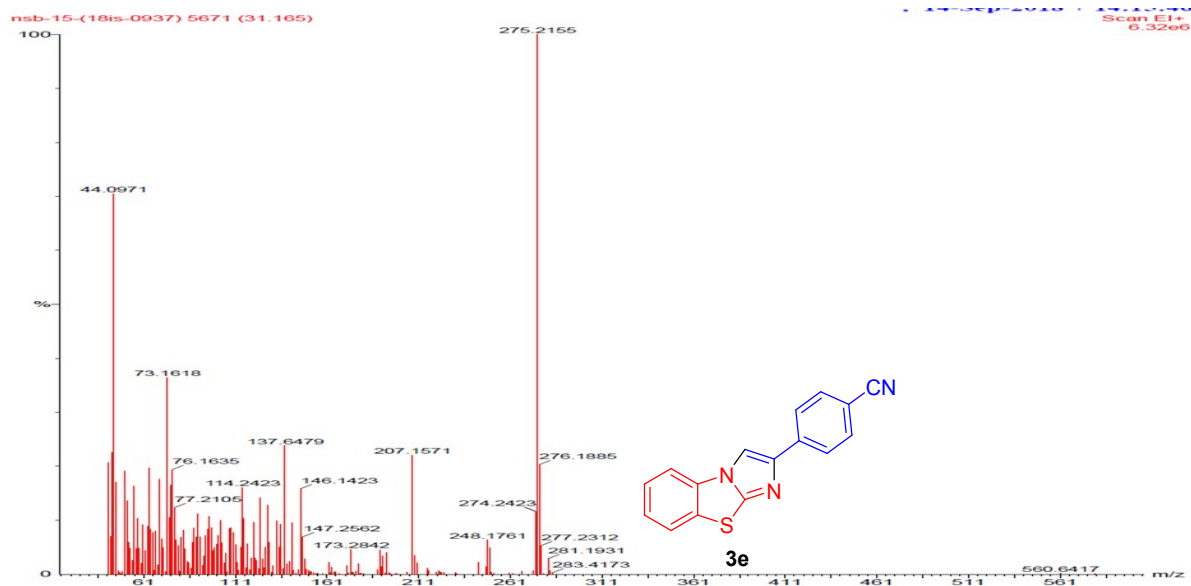


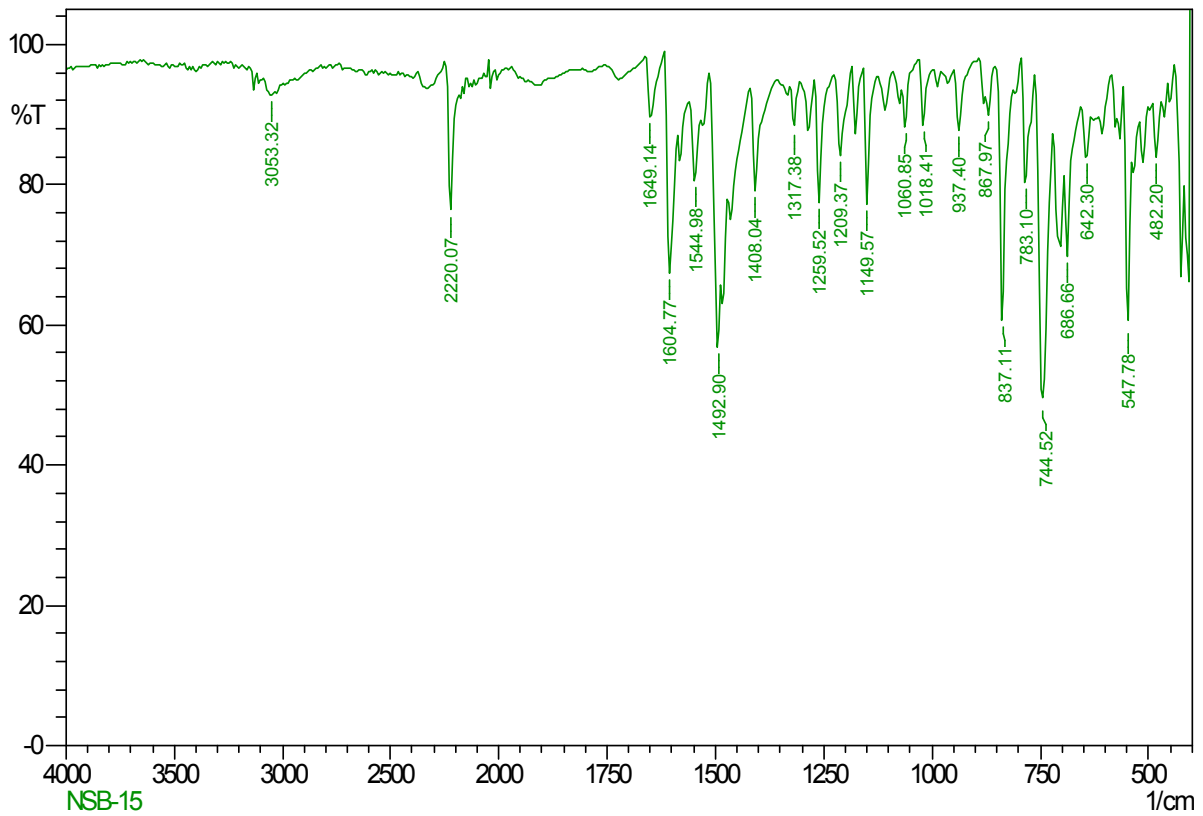


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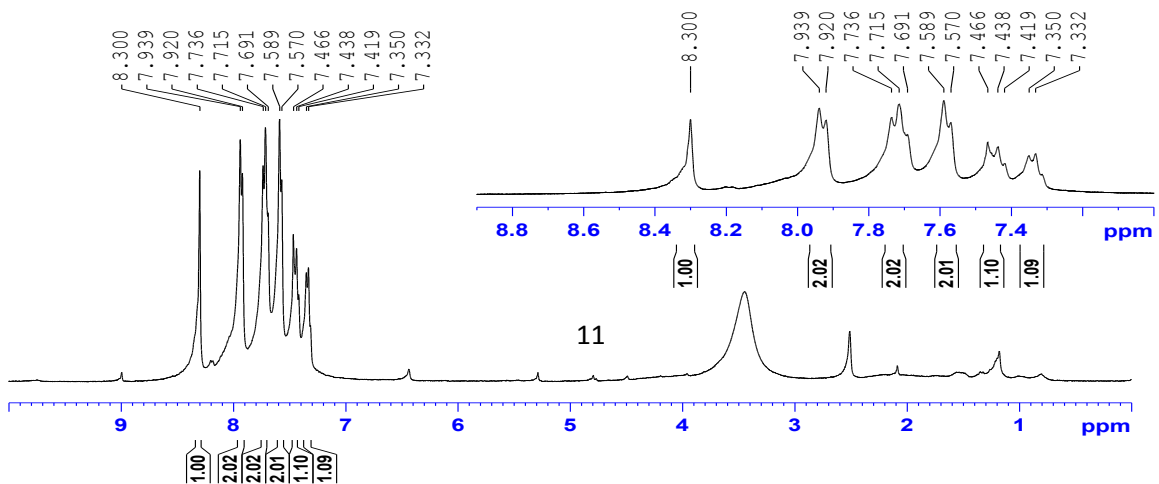
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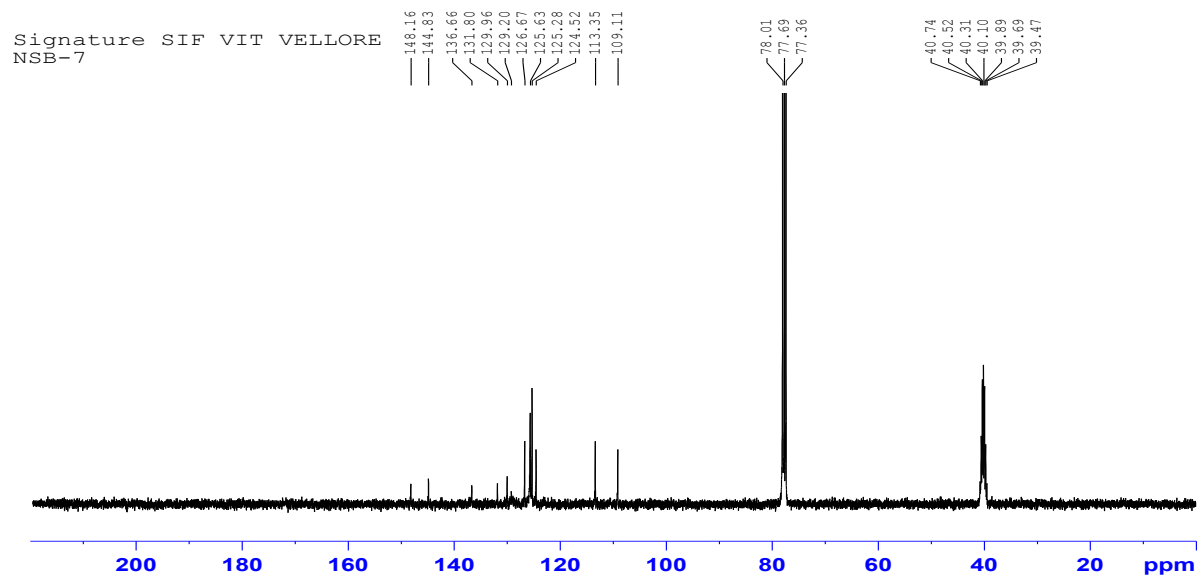
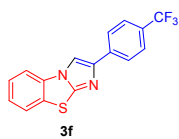




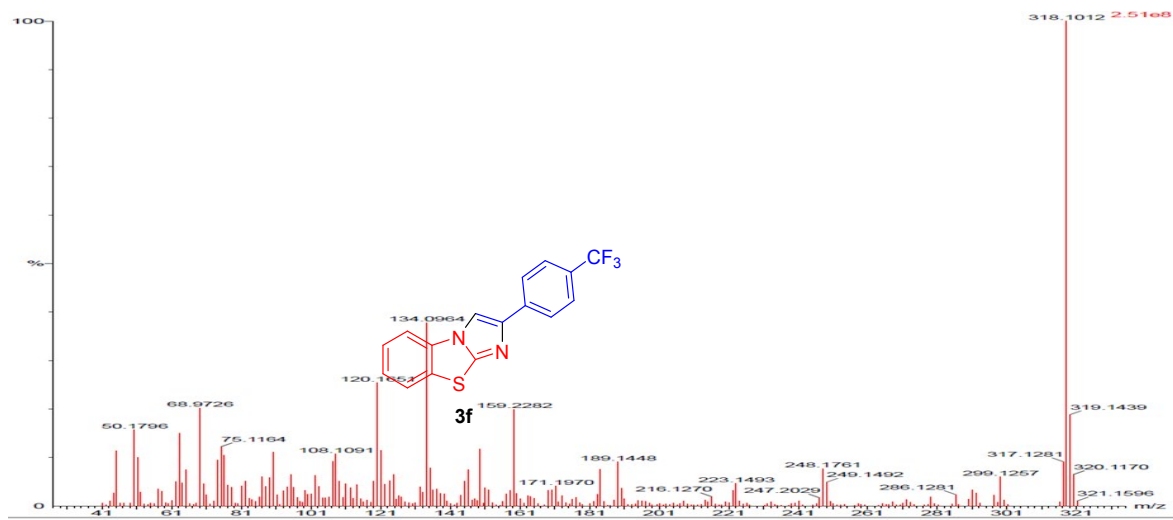
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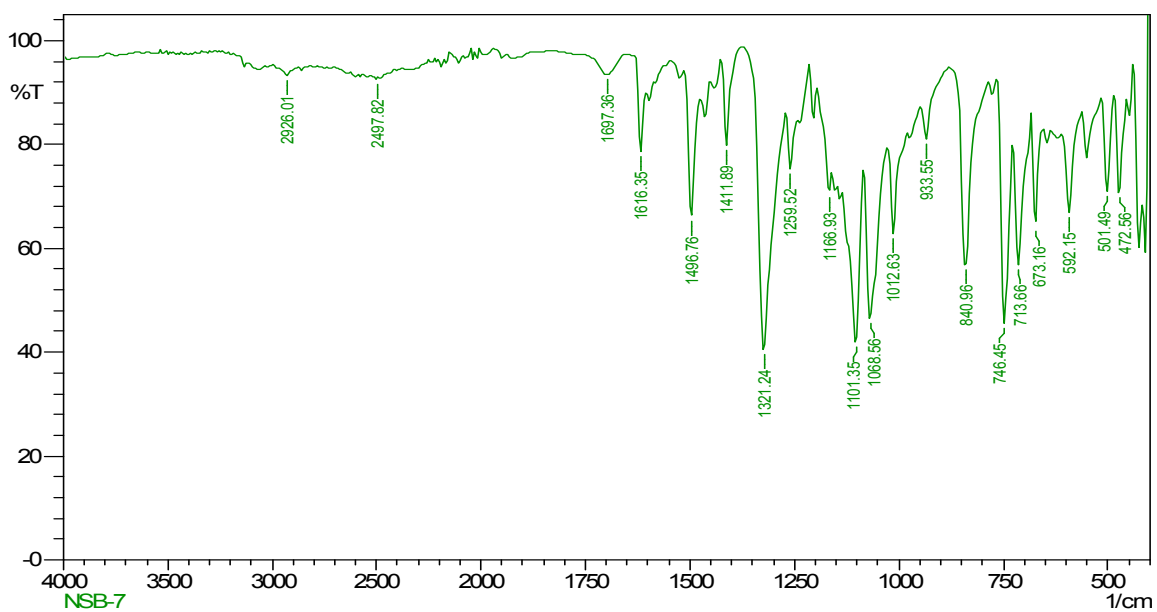
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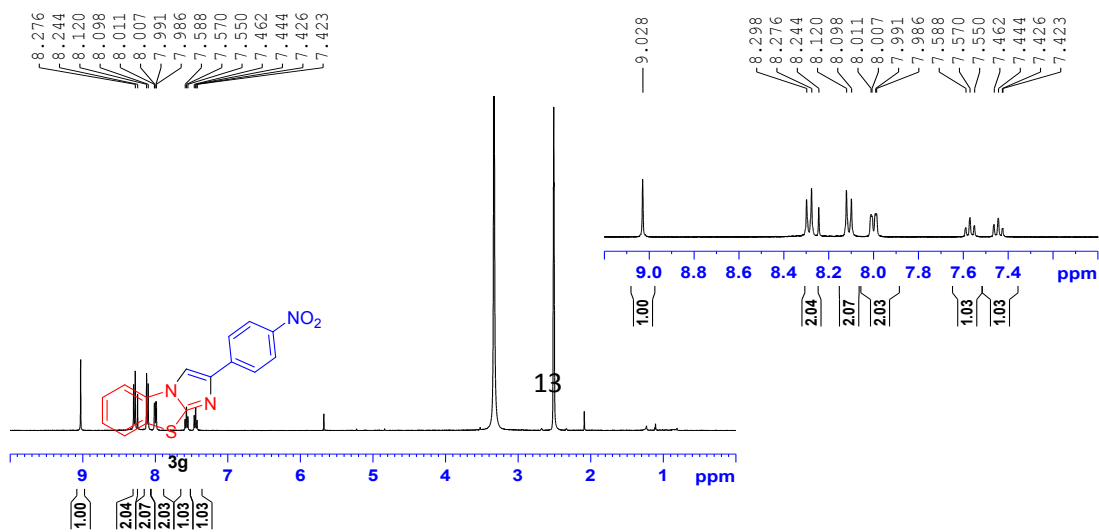
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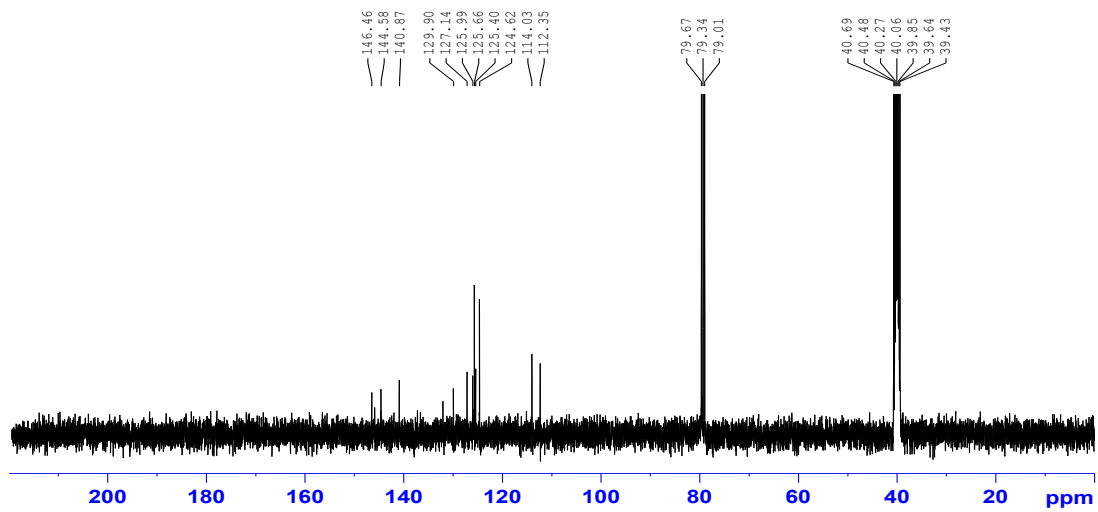


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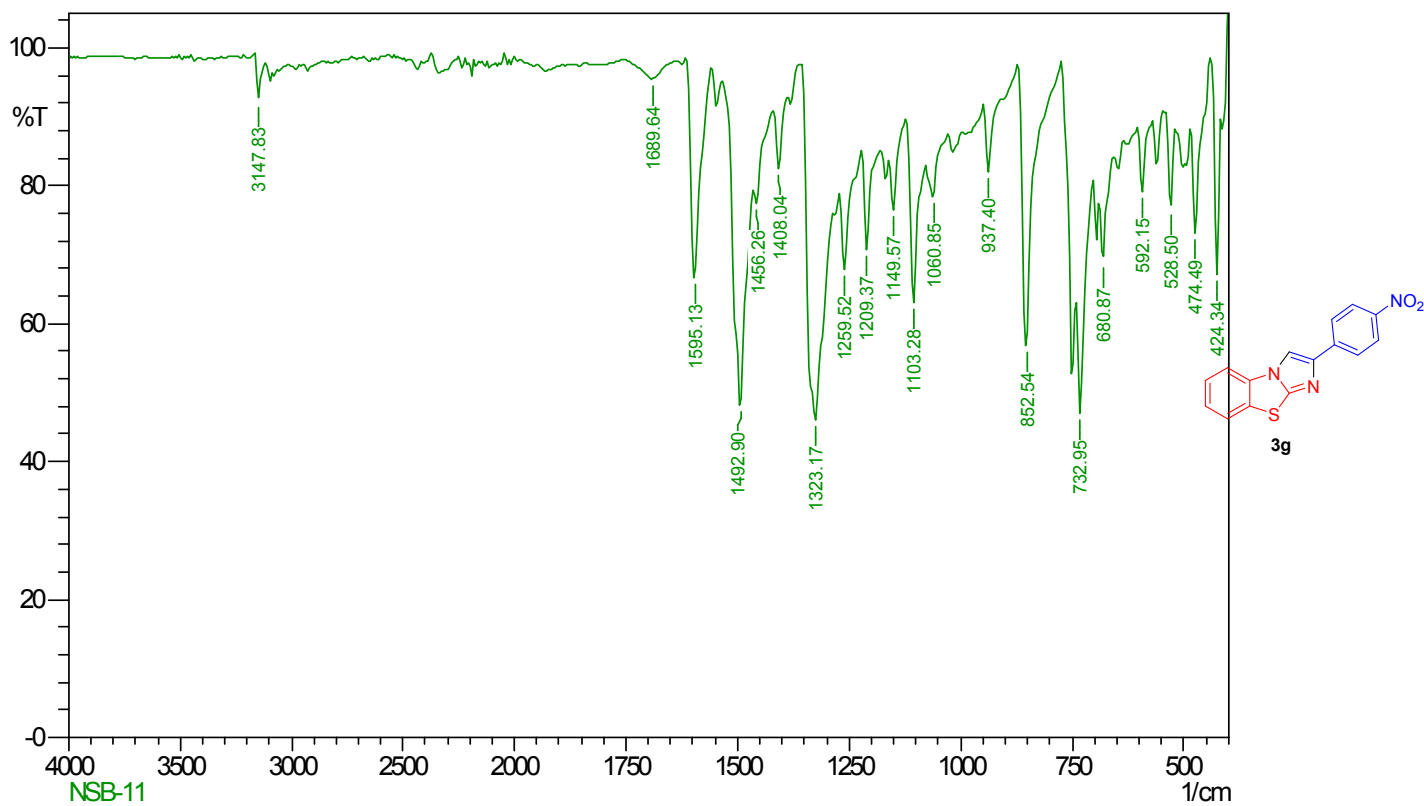
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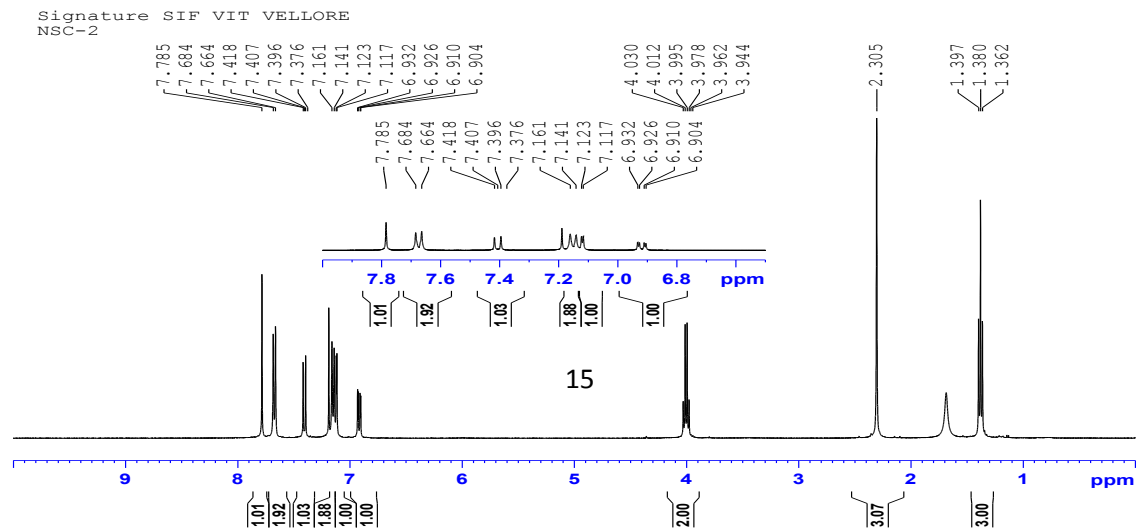
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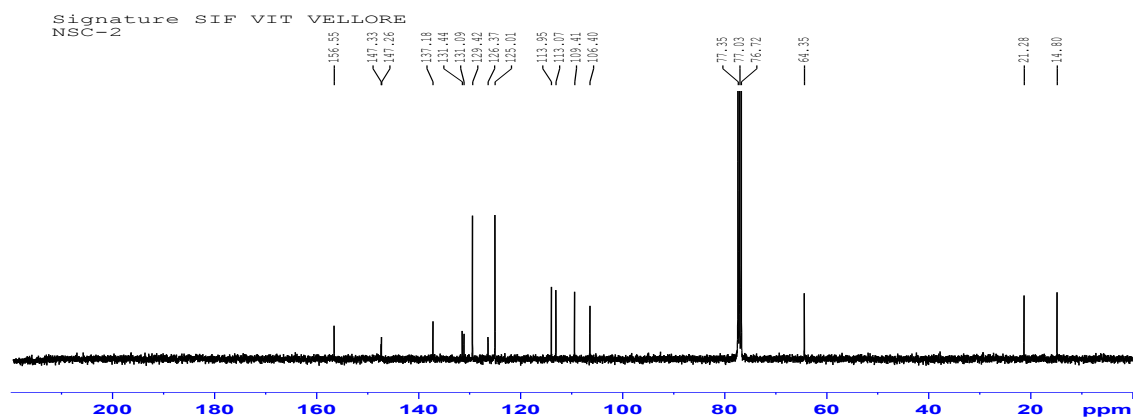
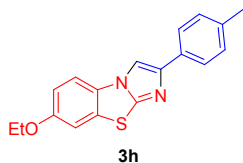


¹H and ¹³C NMR spectrum of compound 3g in CDCl₃

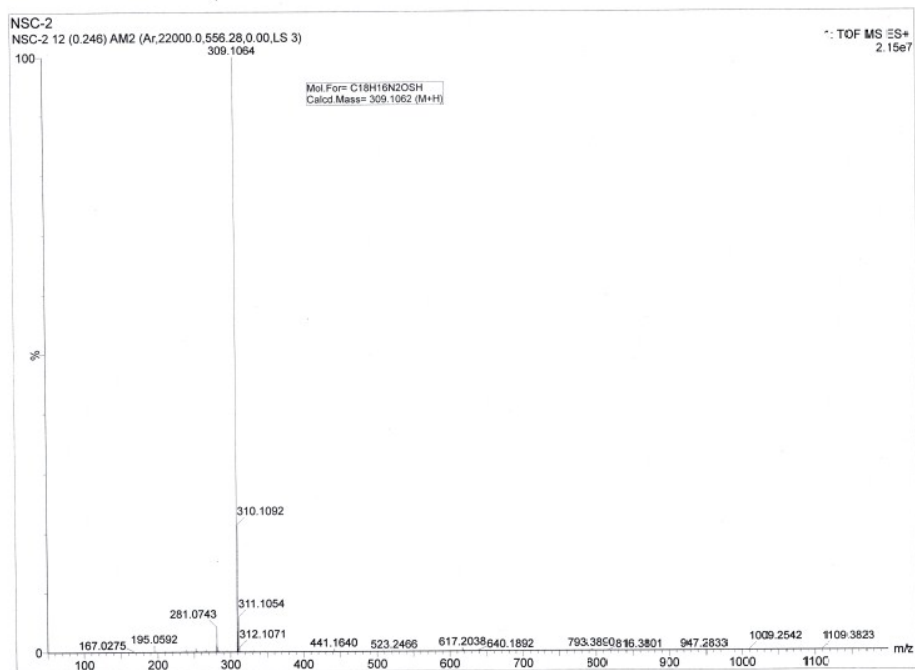


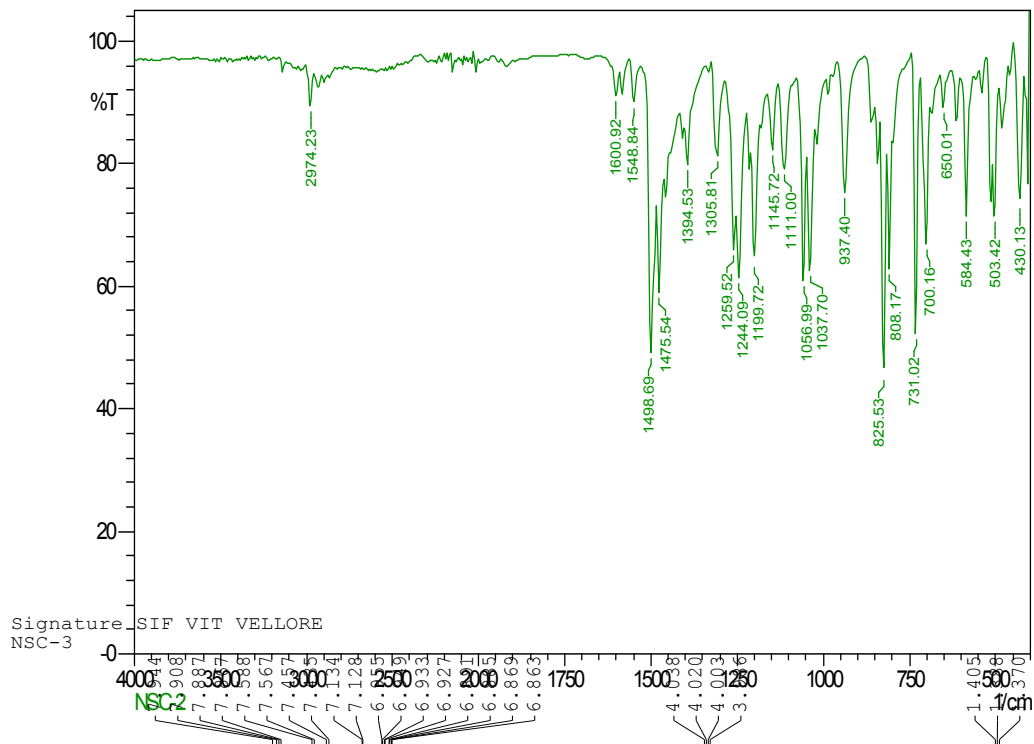
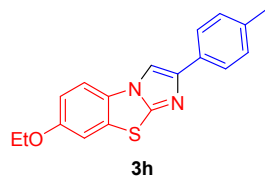
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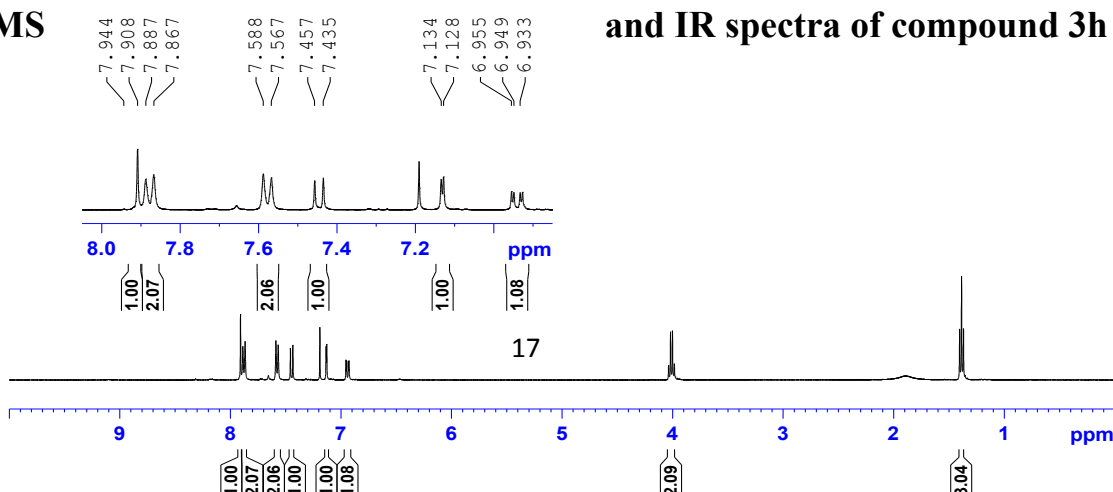


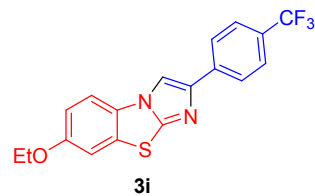
^1H and ^{13}C NMR spectrum of compound 3h in CDCl_3



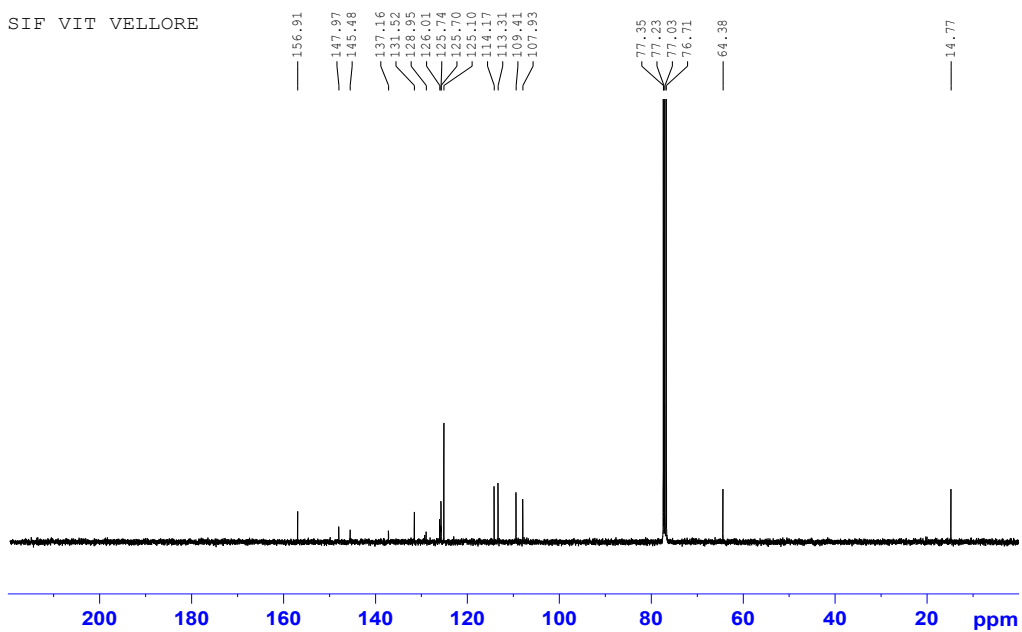


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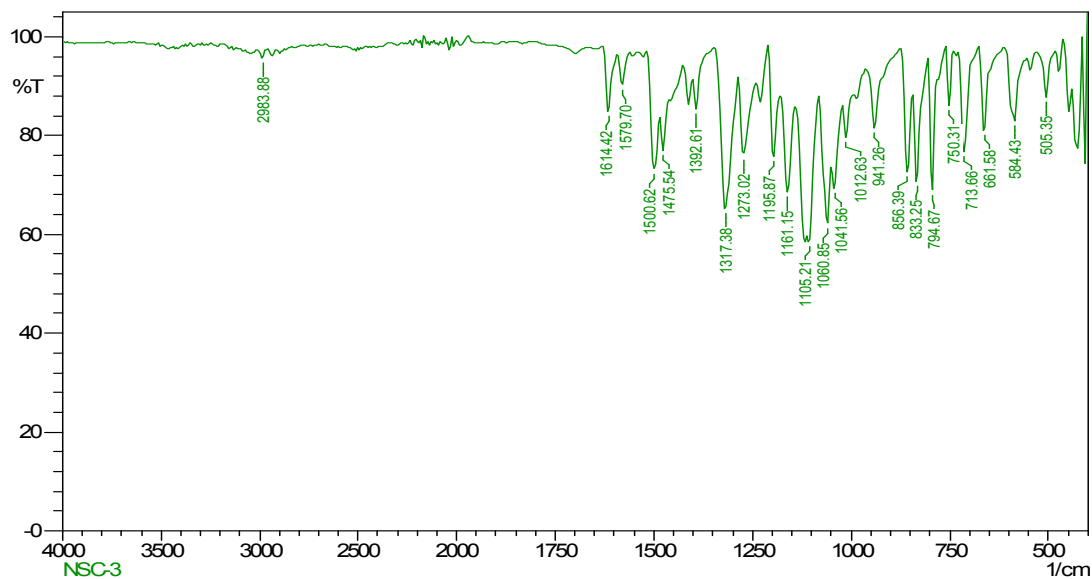
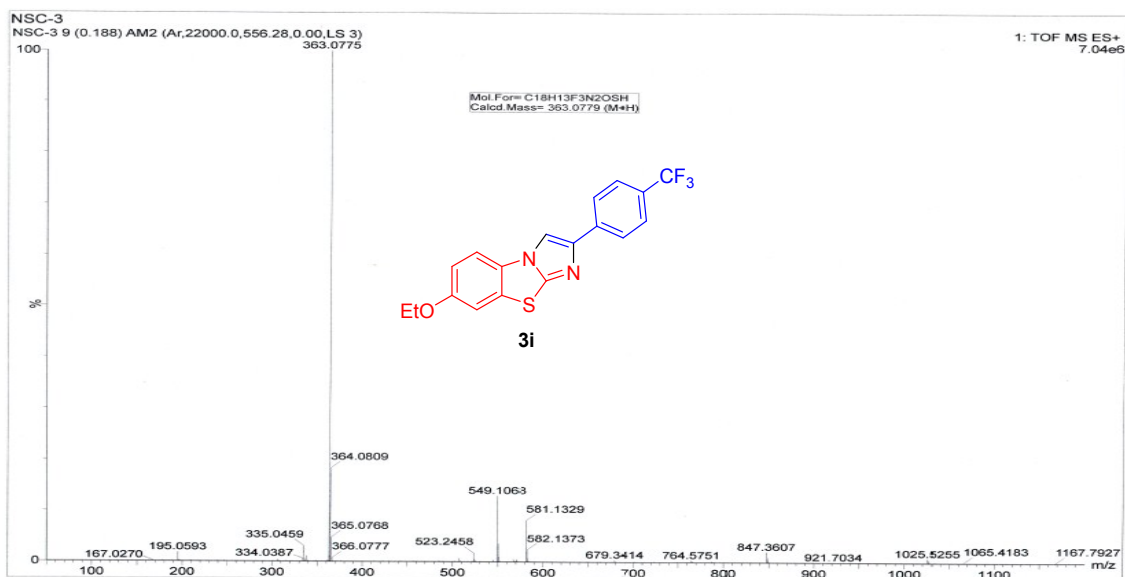




Signature SIF VIT VELLORE
NSC-3



¹H and ¹³C NMR spectrum of compound 3i in CDCl₃

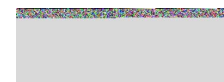


Signature SIF VIT VELLORE



HR MS

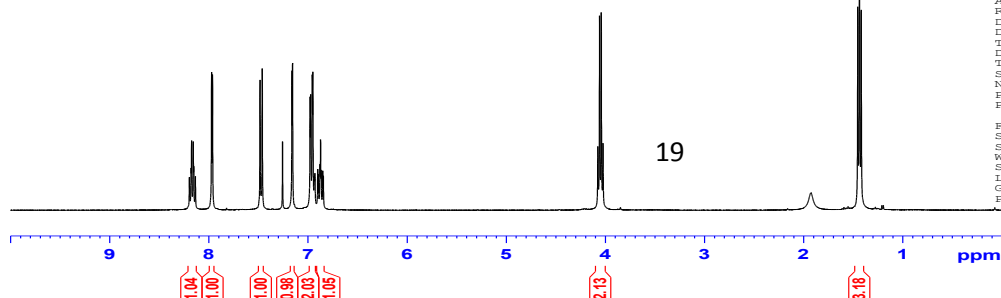
and IR spectra of compound 3i

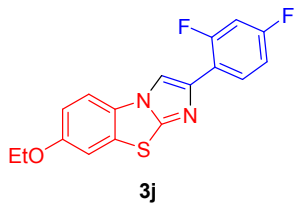


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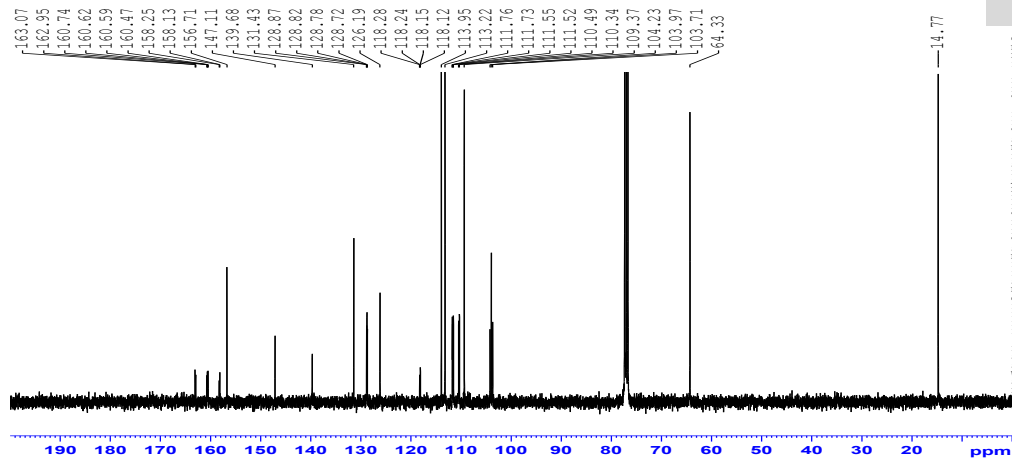
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NUC1 1H
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Signature SIF VIT VELLORE
NSC-9

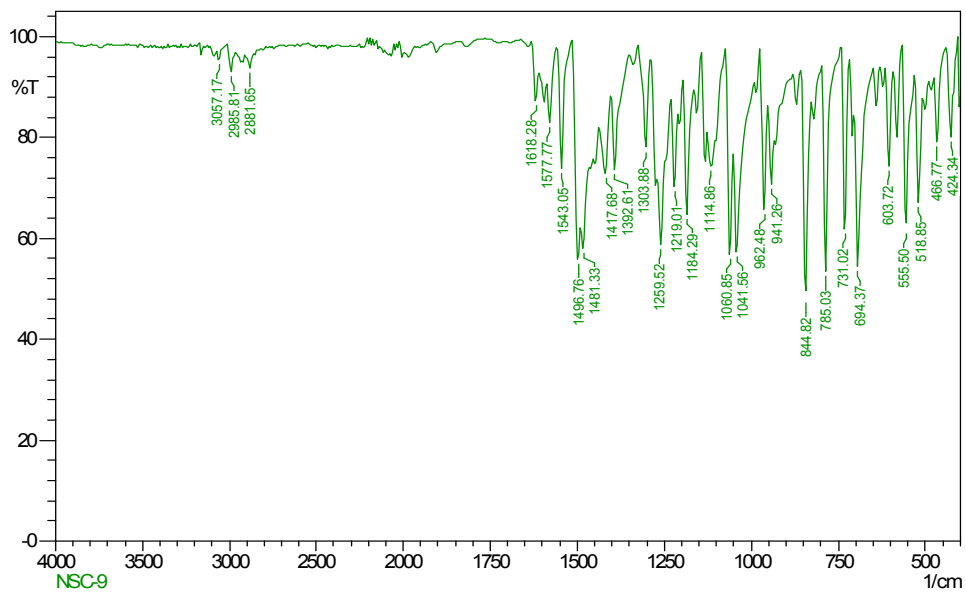
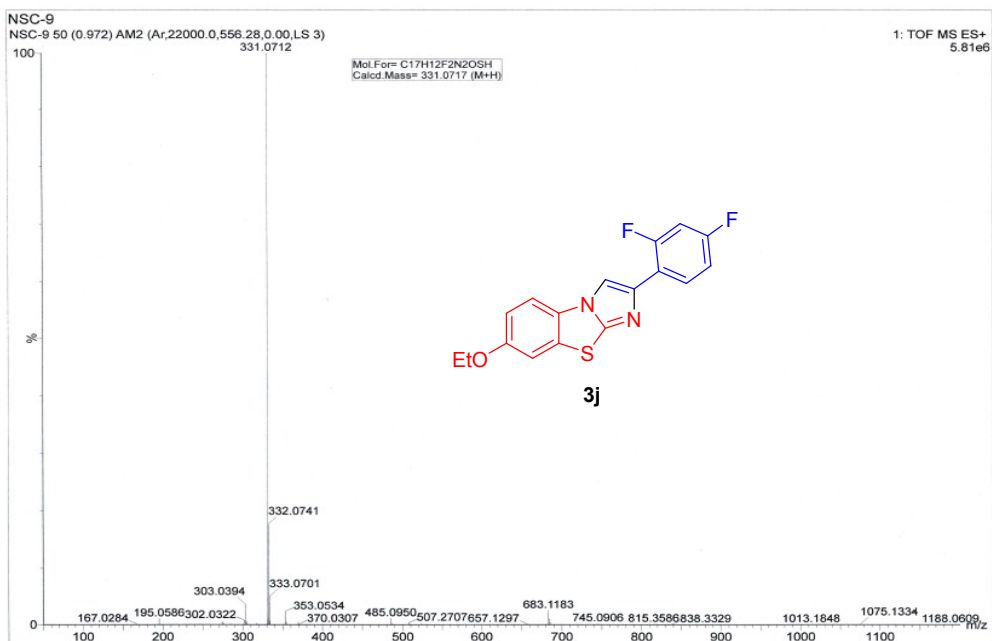


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TE            301.6 K
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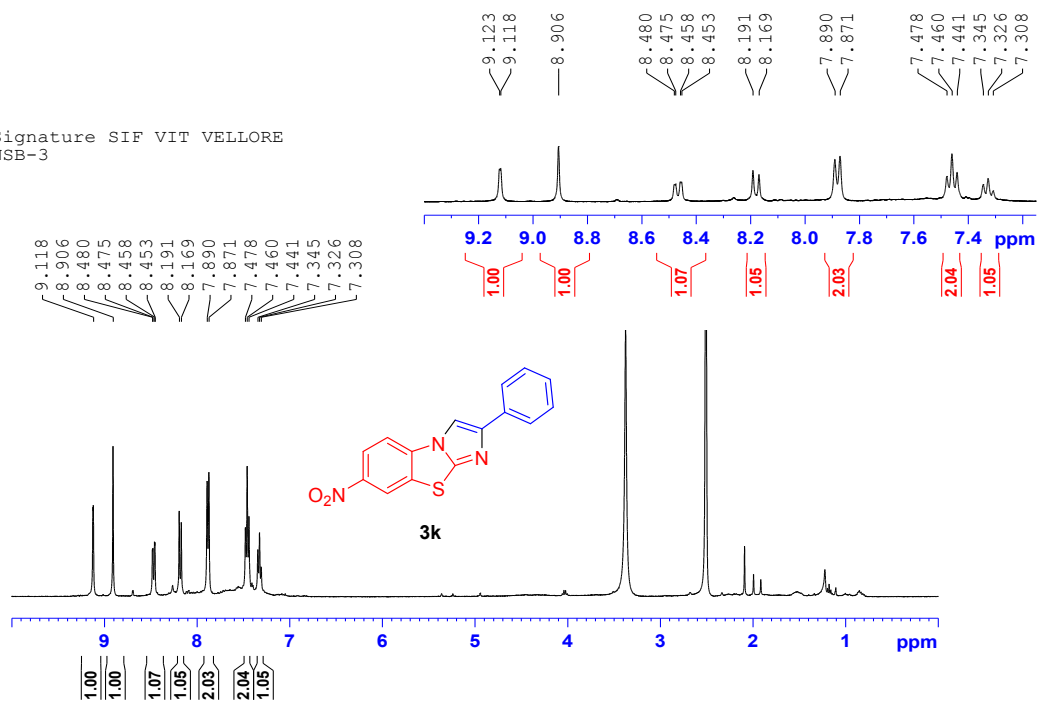
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^1H and ^{13}C NMR spectrum of compound 3j in CDCl_3

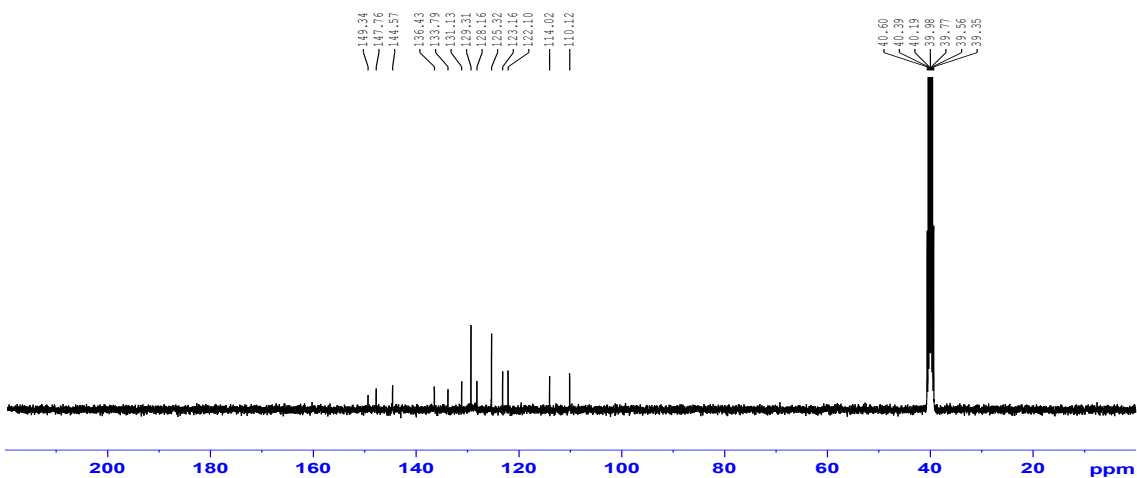


HR MS and IR spectra of compound 3j

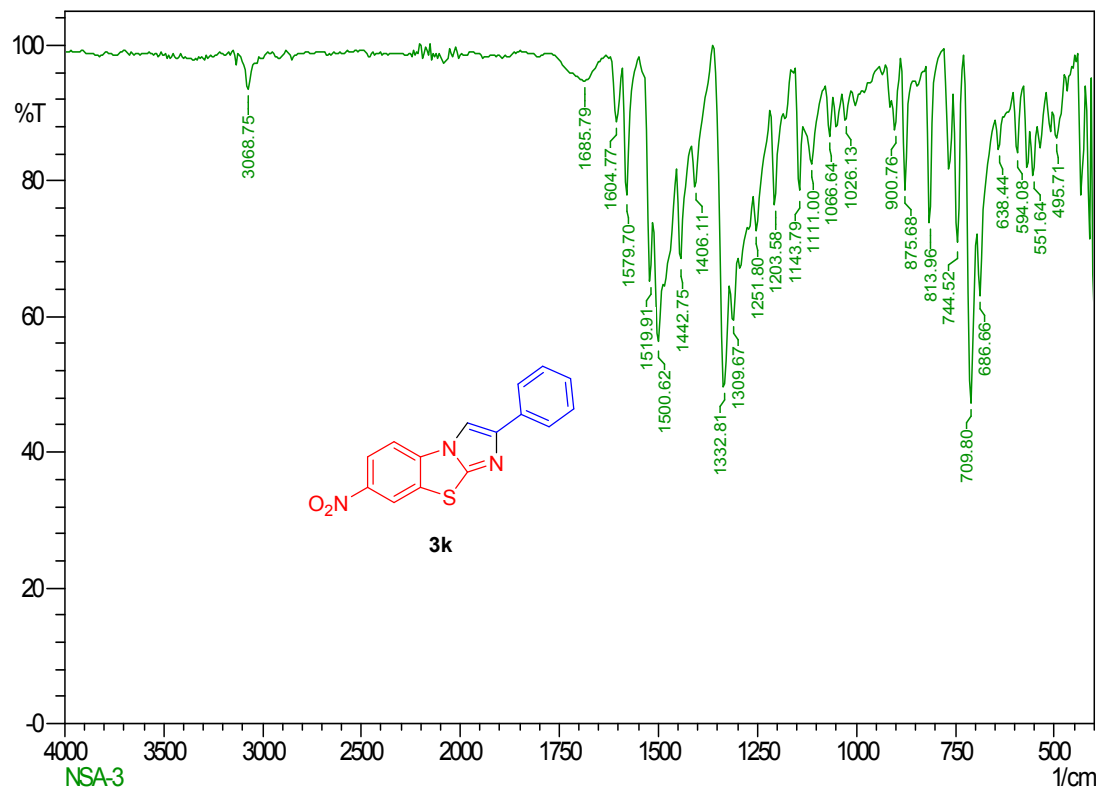
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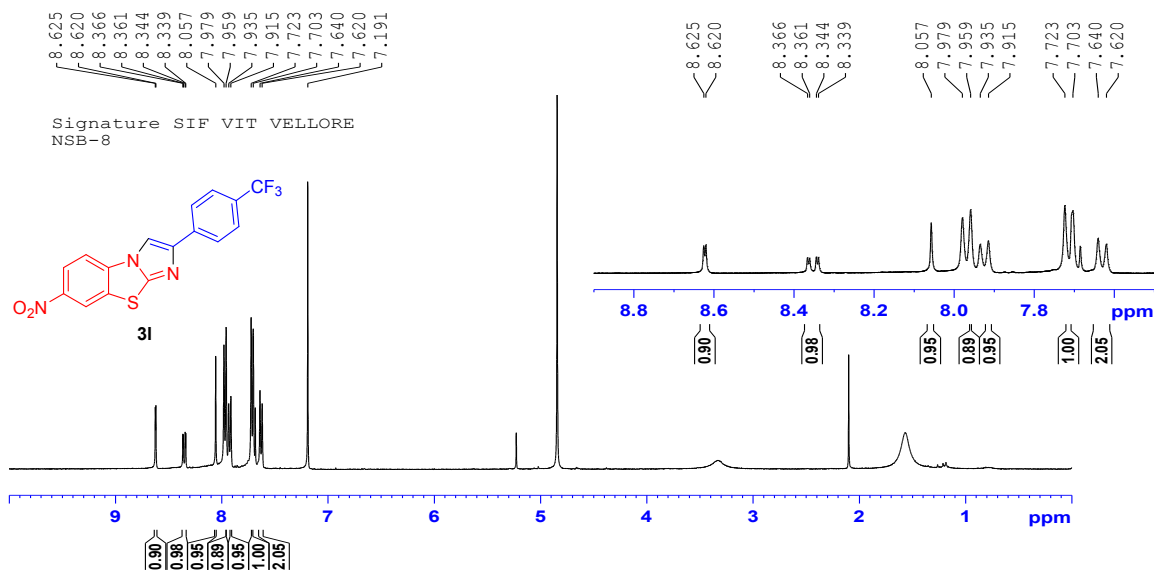
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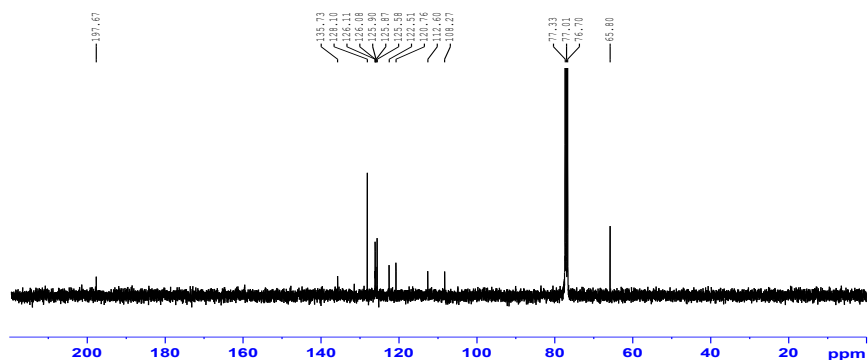
¹H and ¹³C NMR spectrum of compound 3k in CDCl₃



IR spectra of compound 3k



Signature SIF VIT VELLORE
NSB-8



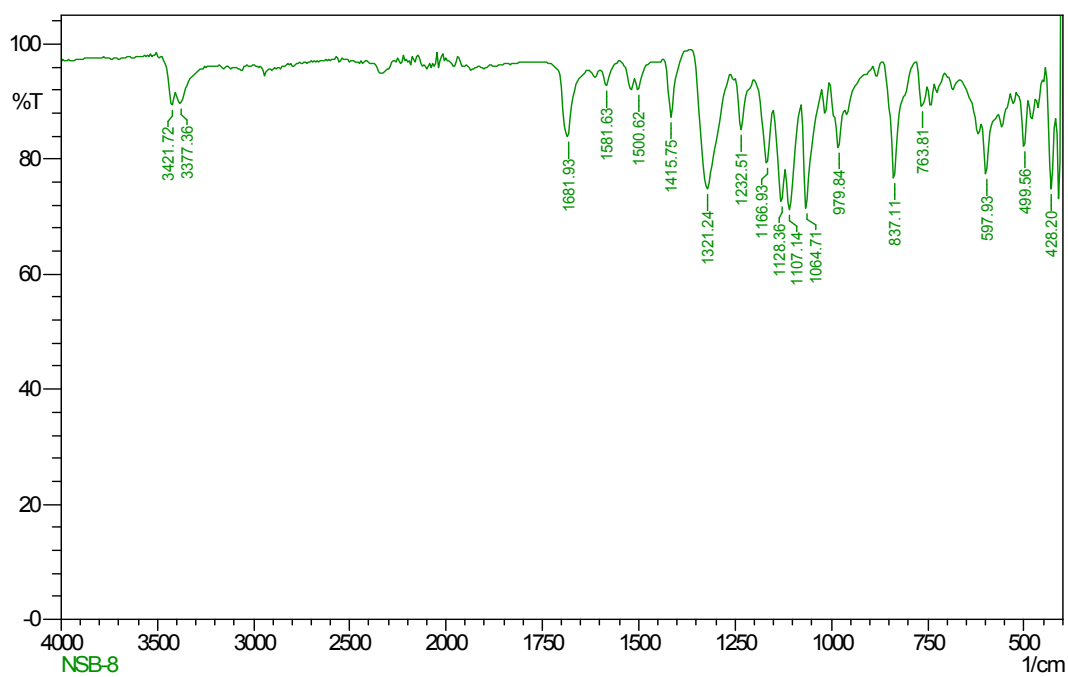
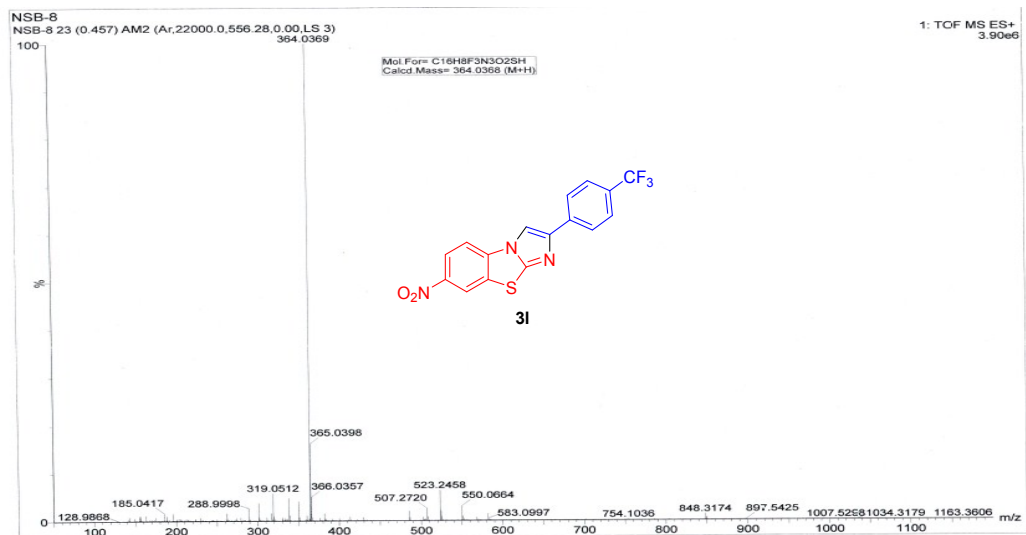
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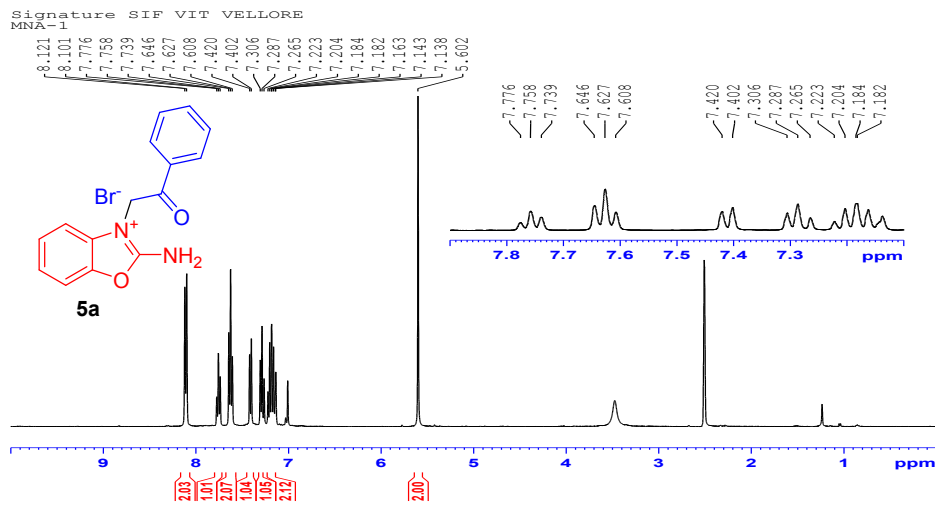
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¹H and ¹³C NMR spectrum of compound 3l in CDCl₃



HR MS and IR spectra of compound 31

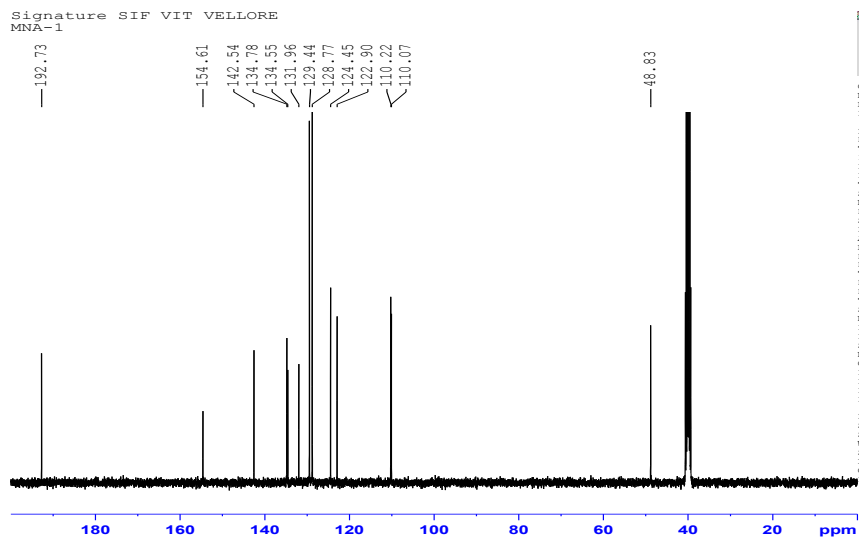


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FIDRES   0.244532 Hz
AQ       4.089445 sec
RG       127.79
DW       62.400 usec
DE       6.50 usec
TE       297.8 K
D1       1.00000000 sec
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F1       14.00 usec
FLW1     16.00000000 W

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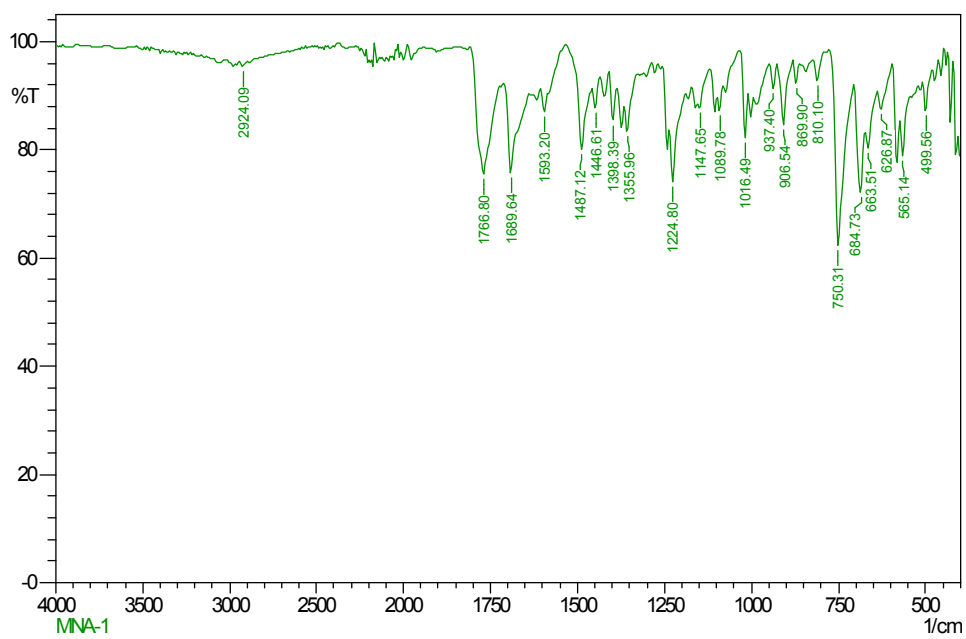
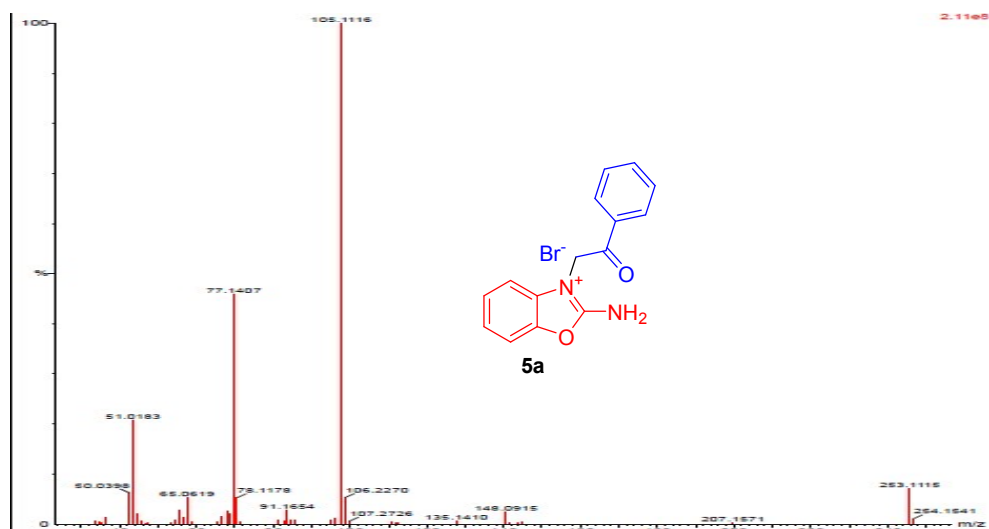
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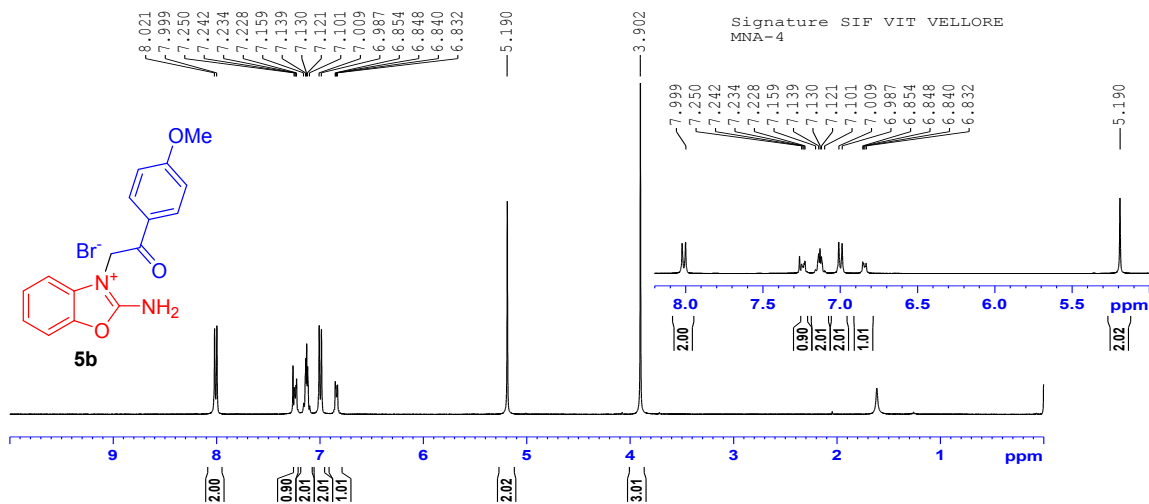
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FIDRES   0.733596 Hz
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DW       20.800 usec
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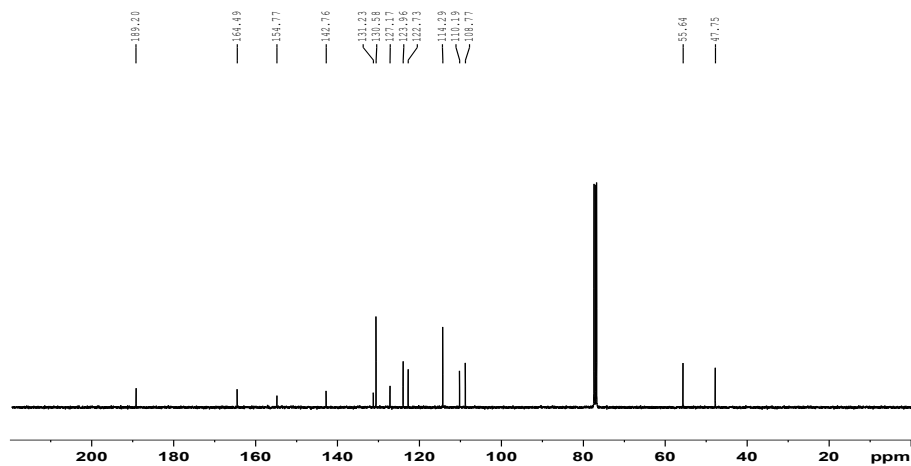
¹H and ¹³C NMR spectrum of compound 5a in CDCl₃



GC MS and IR spectra of compound 5a



Signature SIF VIT VELLORE
MNA-4

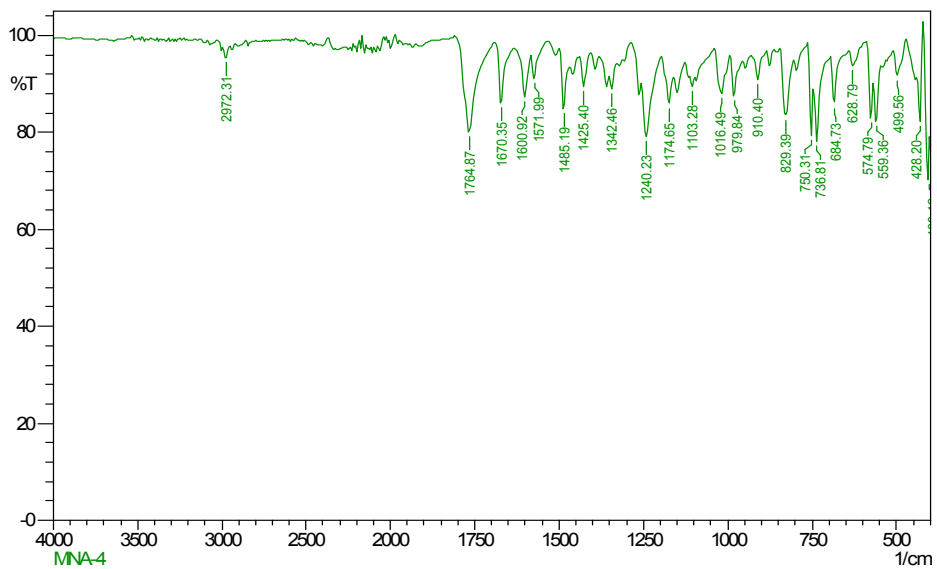
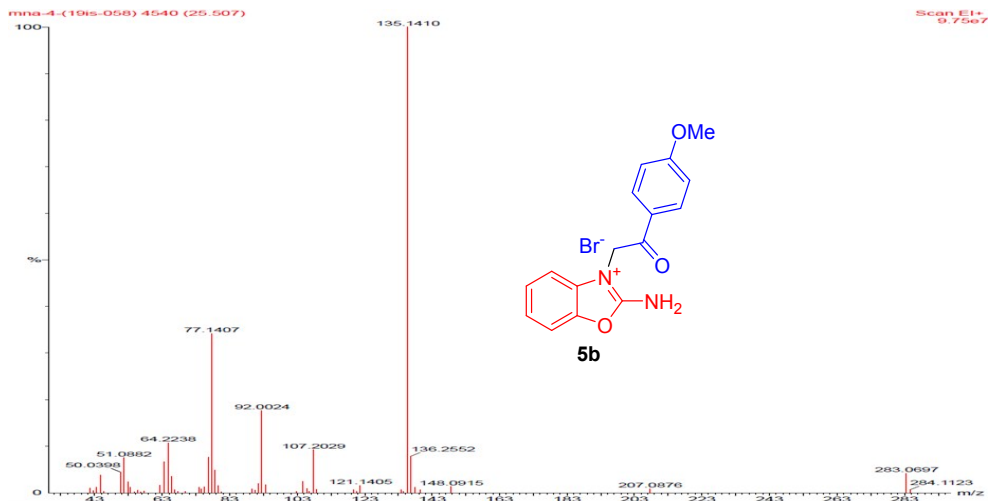


Current Data Parameters
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EXPNO 14
PROCNO 1

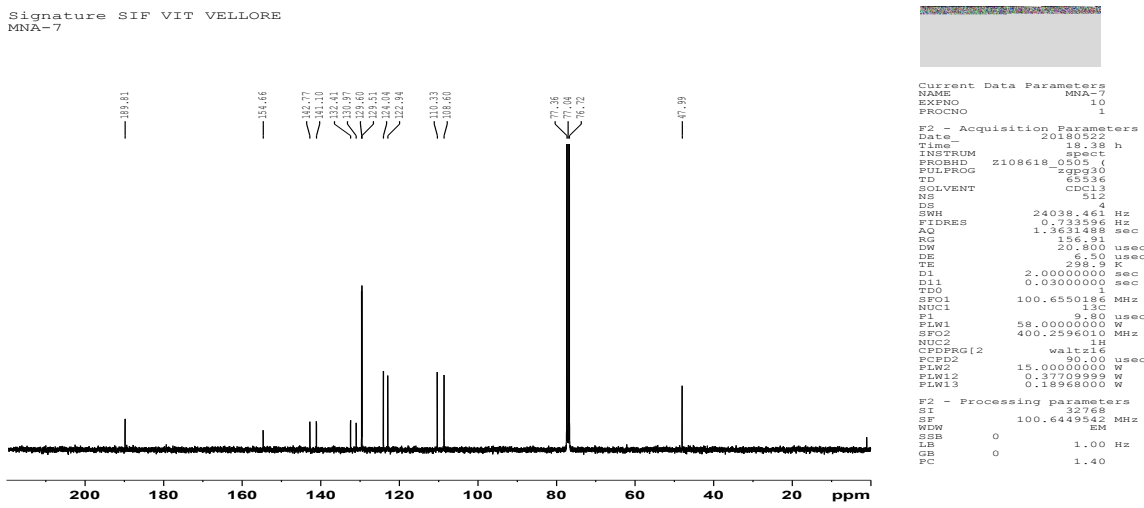
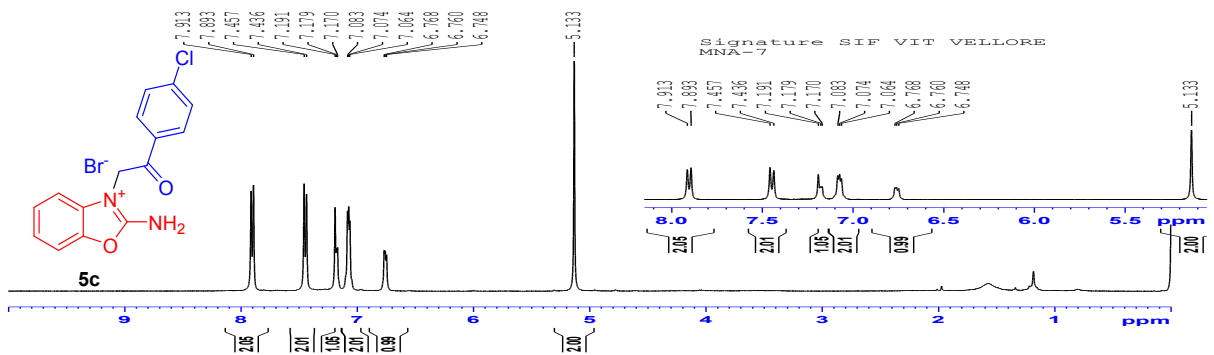
F2 - Acquisition Parameters
Date_ 20180522
Time_ 19.46 h
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PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 100.6550186 MHz
SFO1 13C
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
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F2 - Processing parameters
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SF 100.6449542 MHz
WDW EM
SSB 0
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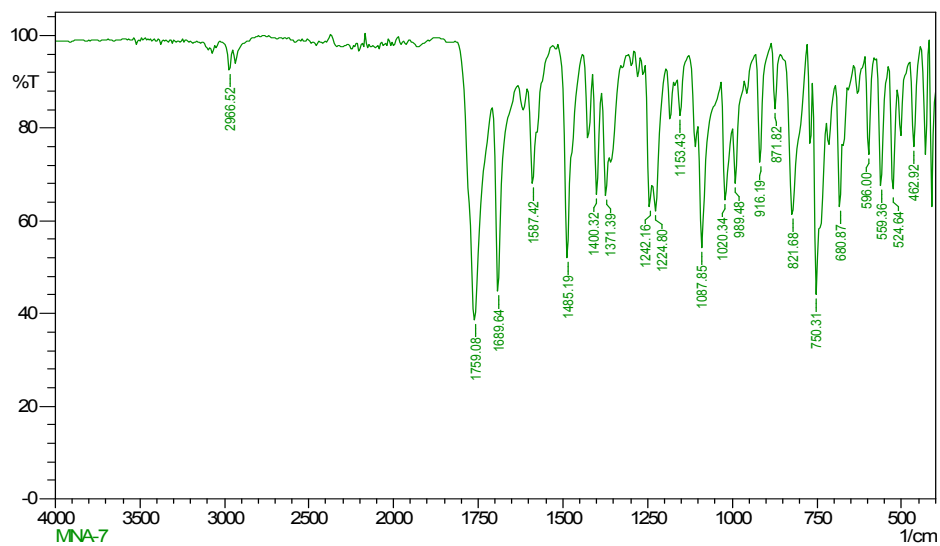
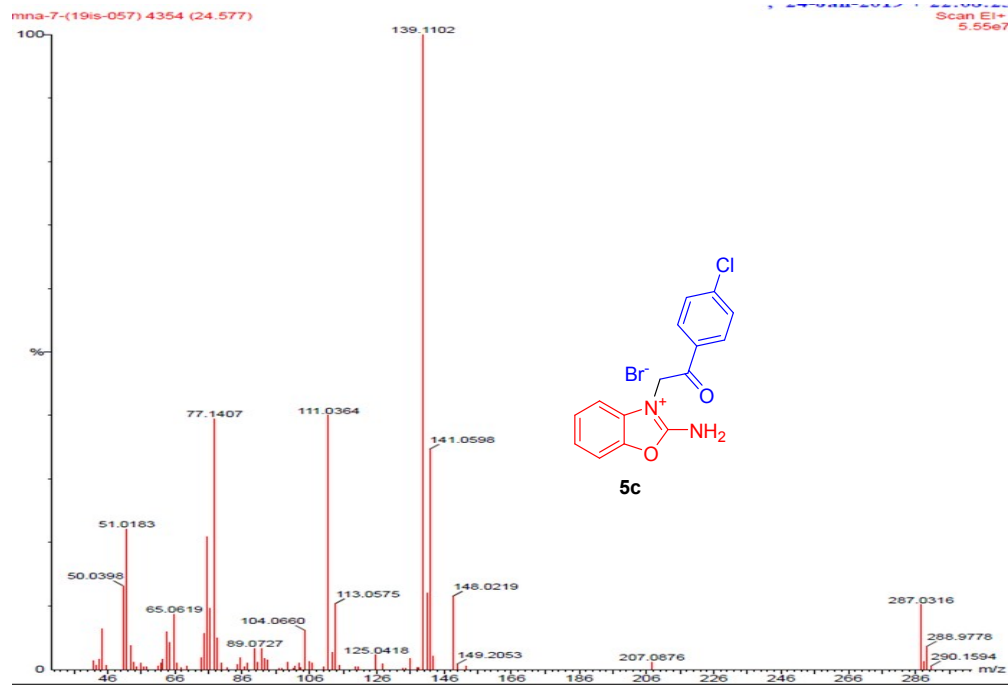
¹H and ¹³C NMR spectrum of compound 5b in CDCl₃



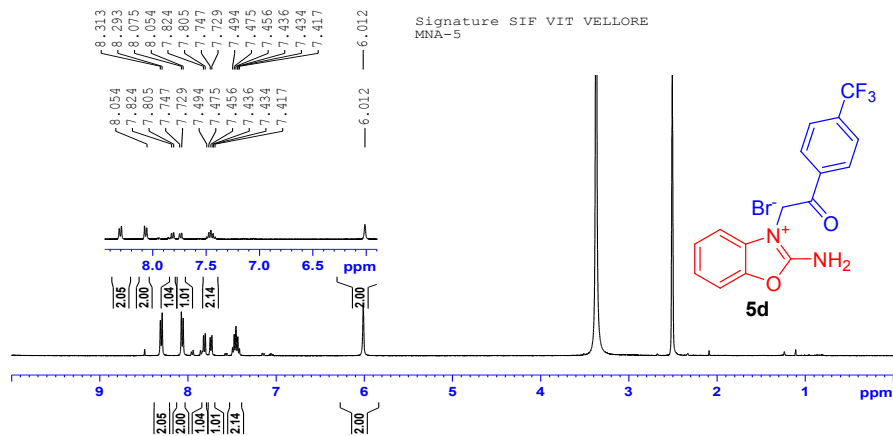
GC MS and IR spectra of compound 5b



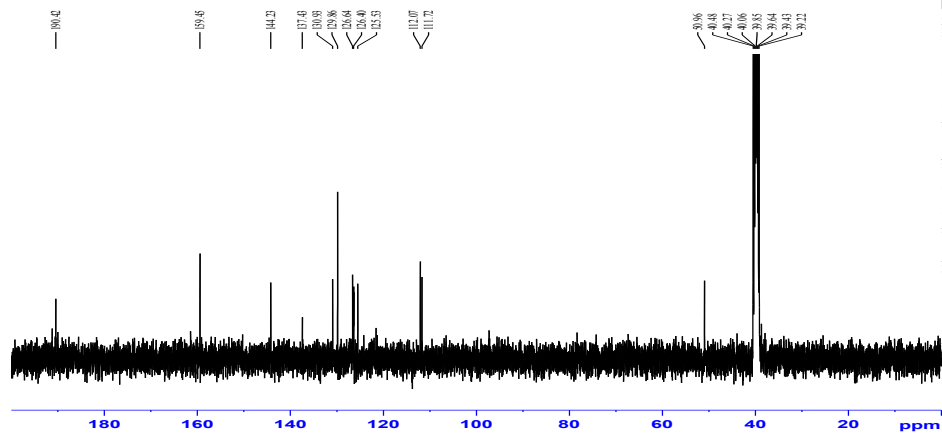
¹H and ¹³C NMR spectrum of compound 5c in CDCl₃



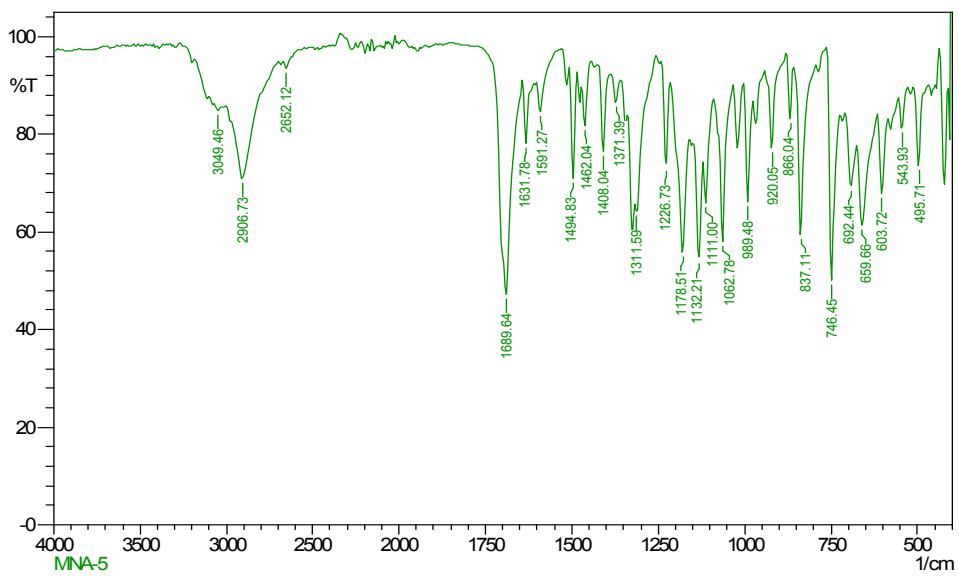
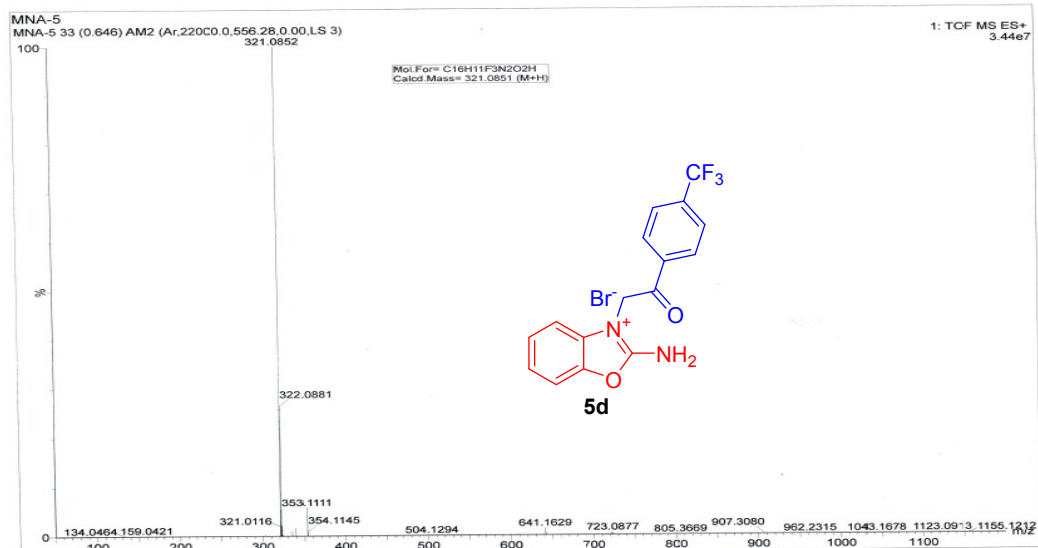
GC MS and IR spectra of compound 5c



Signature SIF VIT VELLORE
MNA-5

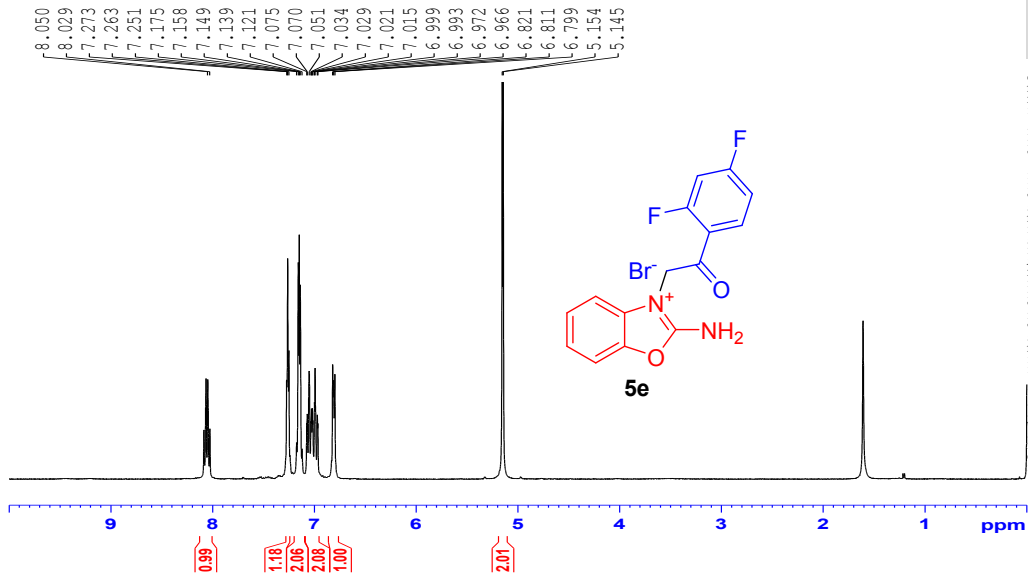


^1H and ^{13}C NMR spectrum of compound 5d in CDCl_3



GC MS and IR spectra of compound 5d

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MNA-6



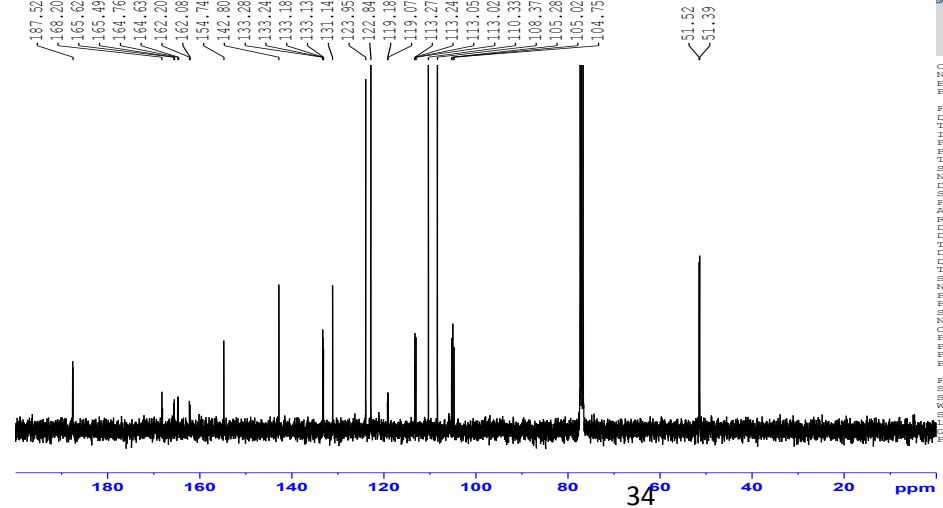
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Current Data Parameters
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EXPNO    11
PROCNO   1

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PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        4.0894465 sec
RG         175.97
DW         62.400 usec
DE         6.50 usec
TE         298.4 K
TD0        1.0000000 sec
SFO1      400.2604716 MHz
NUC1      1H
P1         14.27 usec
PLW1      15.00000000 W

F2 - Processing parameters
SI         65536
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Signature SIF VIT VELLORE
MNA-6



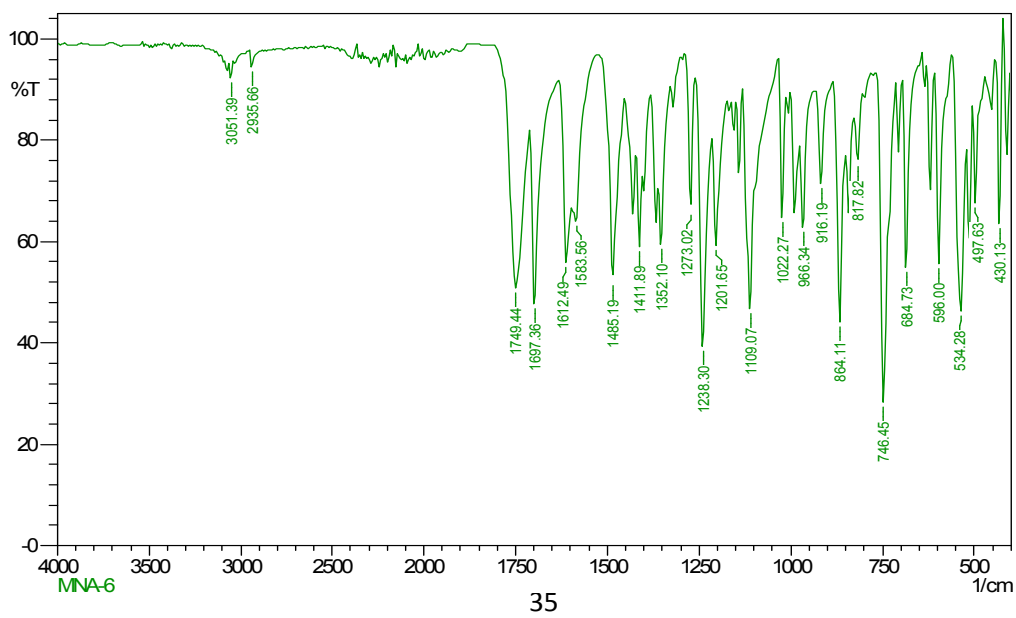
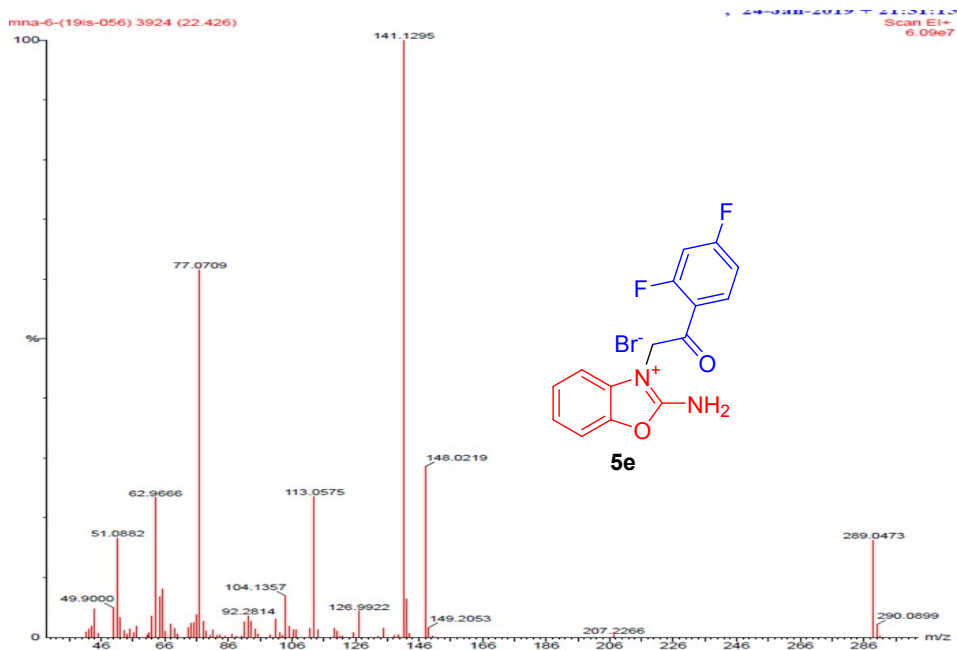
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Current Data Parameters
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PROCNO   1

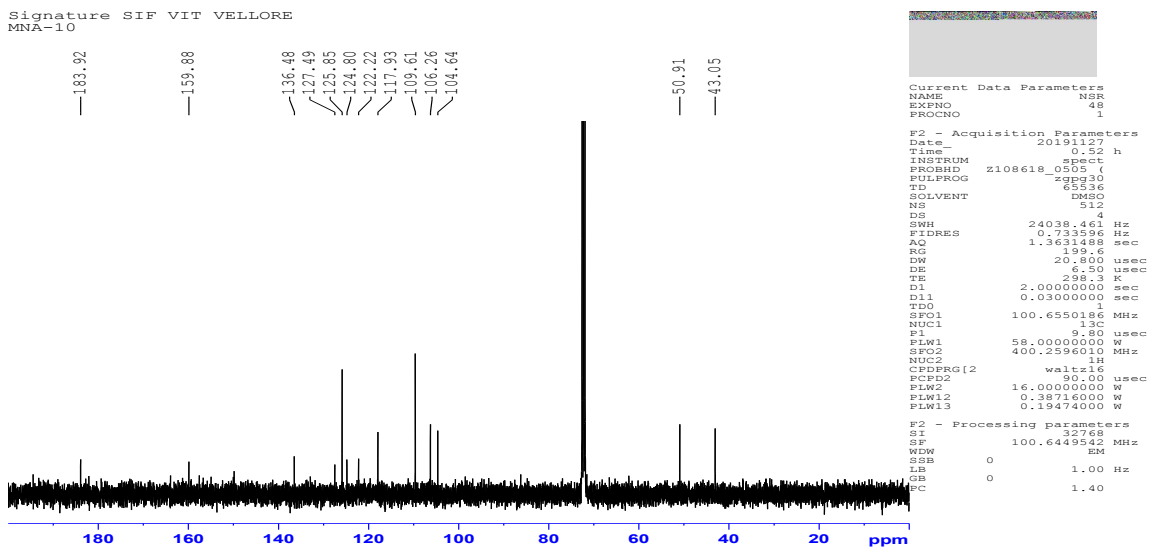
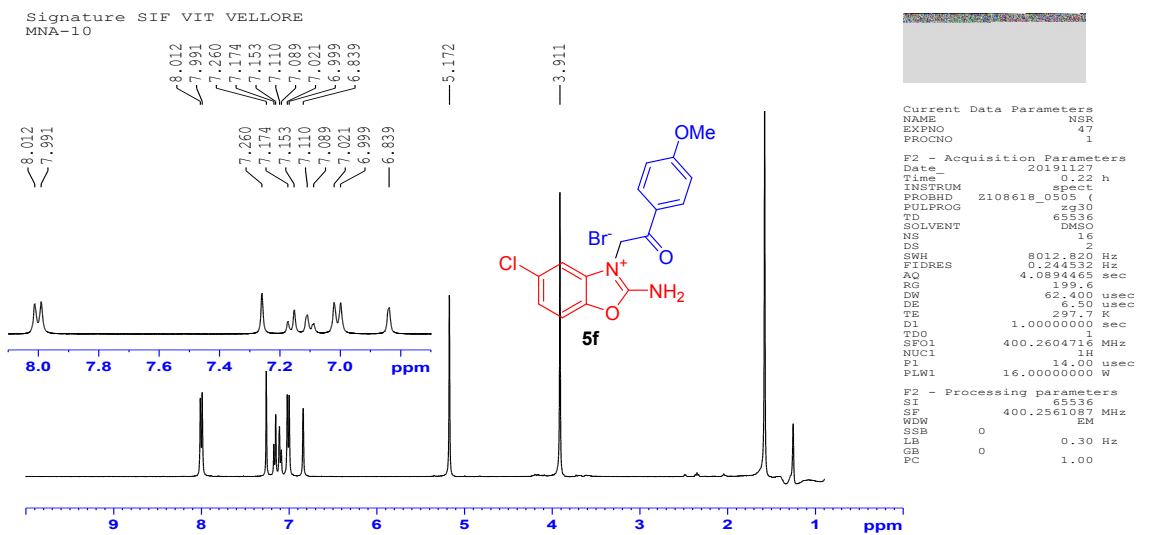
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Time     19.12 h
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PROBHD   z108618_0505 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        12
DS        4
SWH       24038.461 Hz
FIDRES    0.732596 Hz
AQ        1.3631488 sec
RG         156.91
DW         20.800 usec
DE         6.50 usec
TE         299.1 K
TD0        2.0000000 sec
D11        0.03000000 sec
SFO1      100.6550186 MHz
NUC1      13C
P1         9.80 usec
PLW1      58.00000000 W
SFO2      400.2596010 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      15.00000000 W
PLW12     0.37709999 W
PLW13     0.18968000 W

F2 - Processing parameters
SI         32768
SF         100.6449542 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
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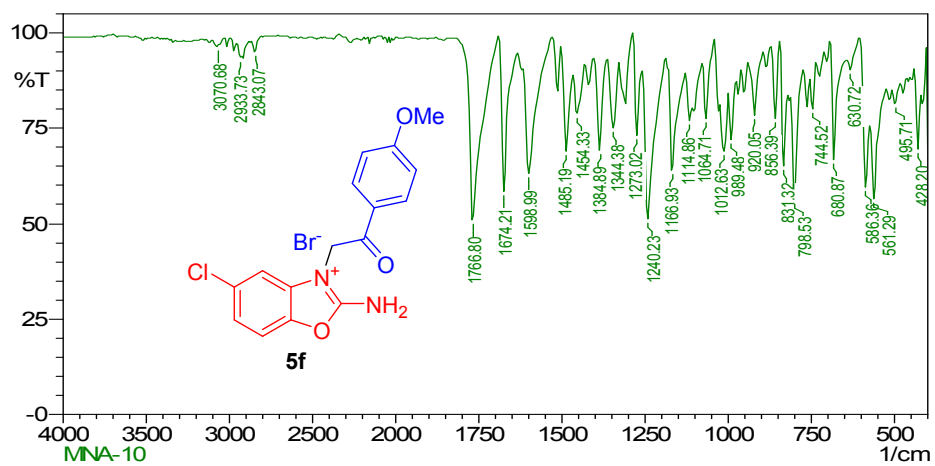
^1H and ^{13}C NMR spectrum of compound 5e in CDCl_3



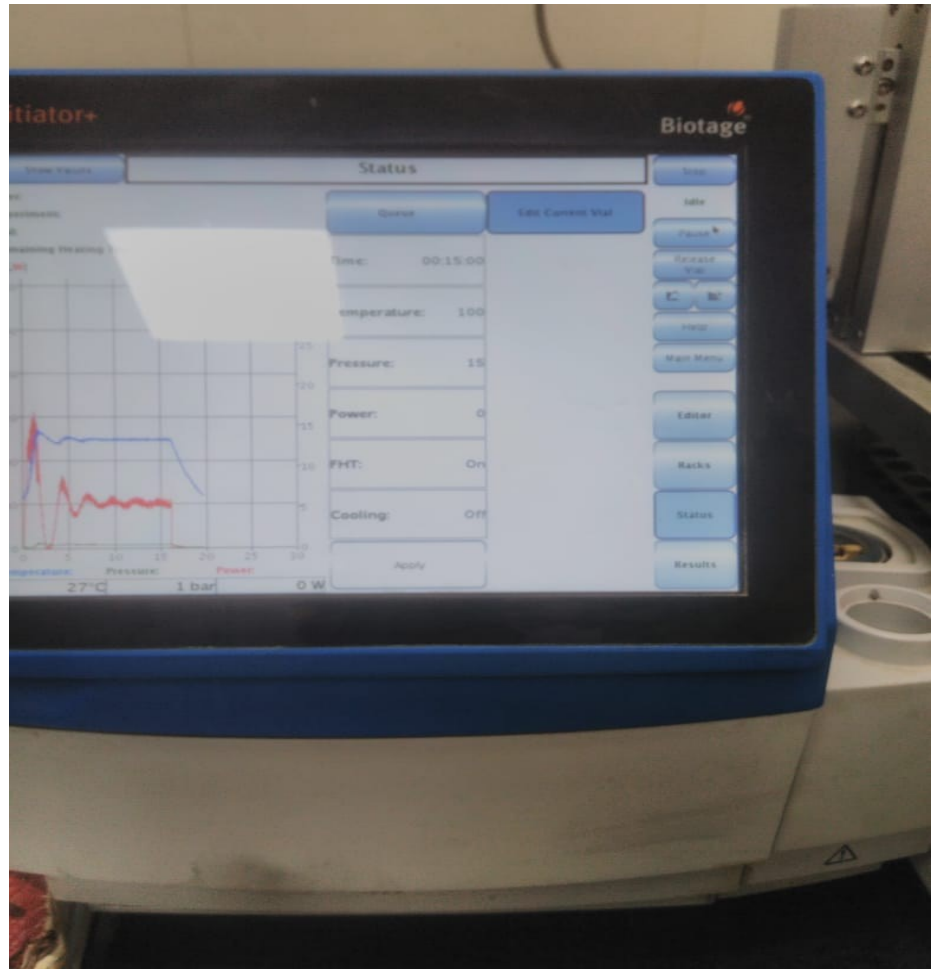
GC MS and IR spectra of compound 5e



^1H and ^{13}C NMR spectrum of compound **5f** in CDCl_3



IR spectra of compound **5f**



**Microwave reactions were carried in Biotage instrument, 2011 model, SW version: 4.1.3.
Build 11768**