

Supporting Information

**Iodine mediated synthesis of indazolo-quinazolinones *via* a multi-component reaction**

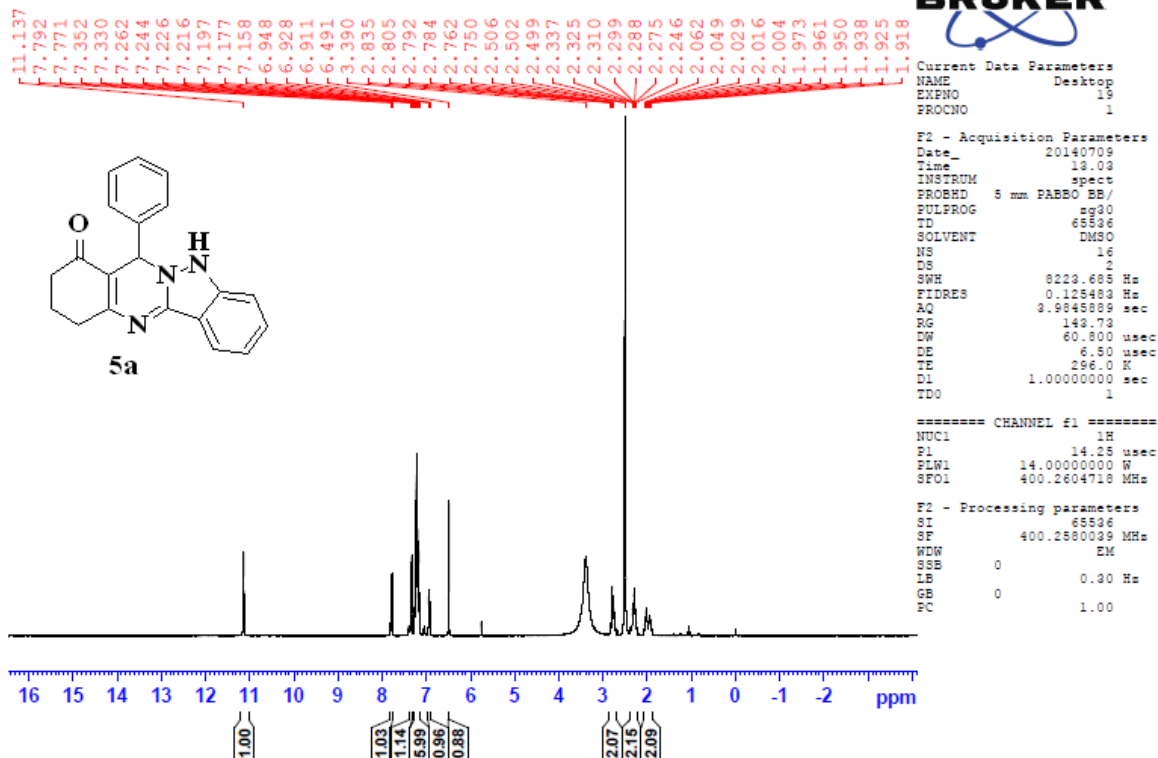
Jeyakannu Palaniraja and Selvaraj Mohana Roopan\*

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VIT University, Vellore, Tamil Nadu-632014, India. Email: mohanaroopan.s@gmail.com;  
Fax: +91-416-224-3092; Tel: +0416-220-2352.

Copies of <sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS of [5(a-l) & 6(a-f)]

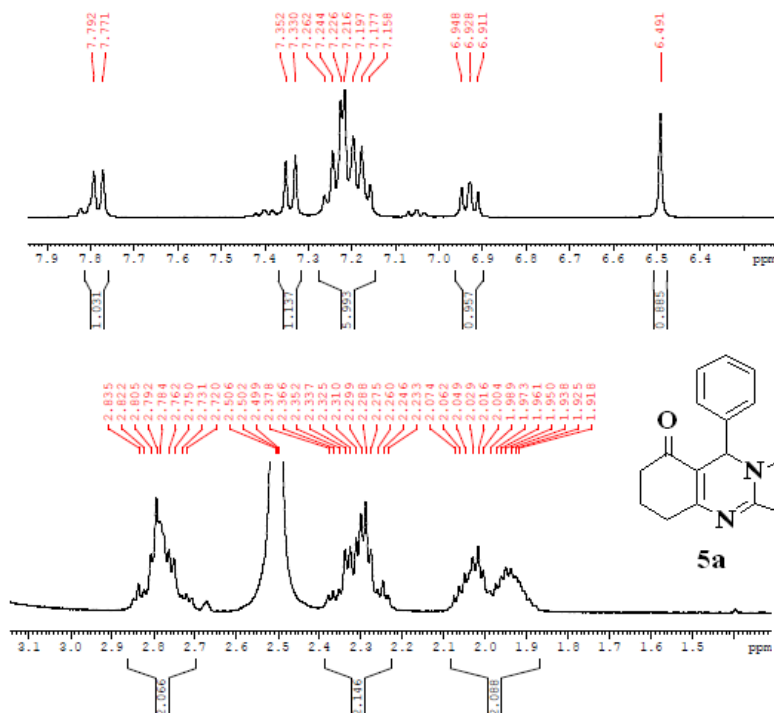
<sup>1</sup>H NMR spectrum of compound (5a):

Signature SIF VIT VELLORE  
JPR-174-P1



# Expanded <sup>1</sup>H NMR spectrum of compound (5a):

Signature SIF VIT VELLORE  
JPR-174-P1



Current Data Parameters  
NAME Desktop  
EXPNO 19  
PROCNO 1

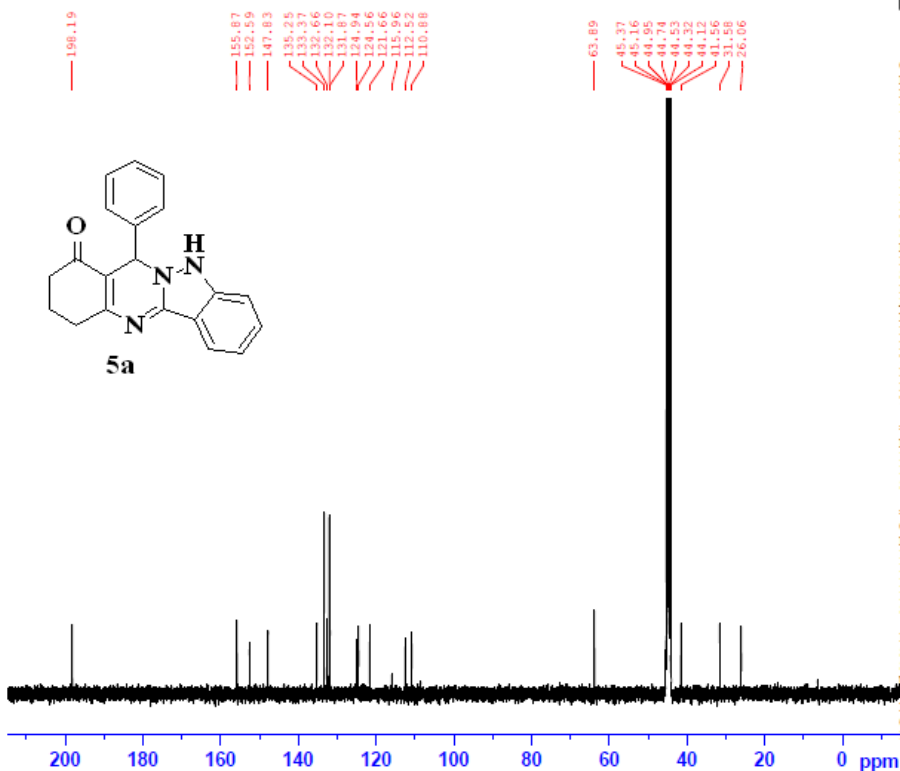
F2 - Acquisition Parameters  
Date\_ 20140709  
Time 19.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8223.695 Hz  
FIDRES 0.128483 Hz  
AQ 3.9845889 sec  
RG 142.73  
DW 60.800 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
PLW1 14.00000000 W  
SFO1 400.2604718 MHz

F2 - Processing parameters  
SI 65536  
SF 400.2580039 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C NMR spectrum of compound (5a):

Signature SIF VIT VELLORE  
JPR-174-P



```
Current Data Parameters
NAME      Desktop
EXPNO    12
PROCNO   1

F2 - Acquisition Parameters
Date_    20140708
Time     11.52
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       156.91
DW       20.800 usec
DE       6.80 usec
TE       296.8 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     13C
P1       9.80 usec
PLW1     58.00000000 W
SFO1     100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PLW2     14.00000000 W
PLW12    0.35097000 W
PLW13    0.28428999 W
SFO2     400.2596010 MHz

F2 - Processing parameters
SI       32768
SF       100.6250182 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
FC       1.40
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### <sup>13</sup>C NMR - DEPT 135 spectrum of compound (5a):

Signature SIF VIT VELLORE  
JPR-174-P

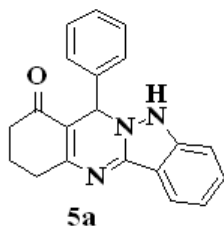
133.37  
132.66  
132.10  
131.88  
124.93  
124.56  
121.66

63.89

45.42  
44.79  
44.59  
44.57  
41.56

31.58

26.06



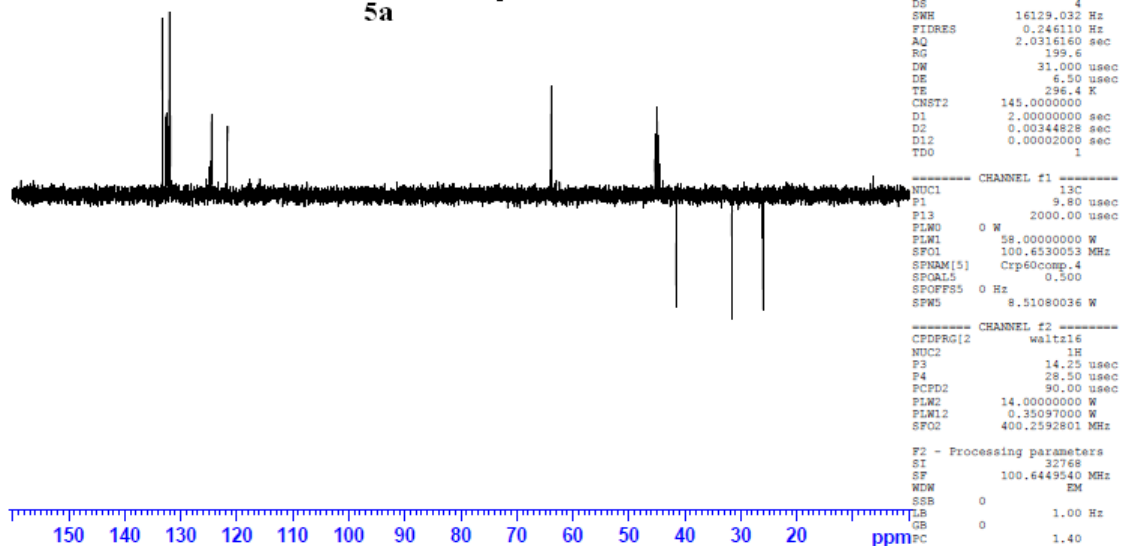
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EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
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INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptsp135  
TD 65536  
SOLVENT cdcl3  
NS 256  
DS 4  
SWH 16129.032 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DE 6.50 usec  
TE 296.4 K  
CNST2 145.0000000  
D1 2.00000000 sec  
D2 0.0034828 sec  
D12 0.00002000 sec  
TDO 1

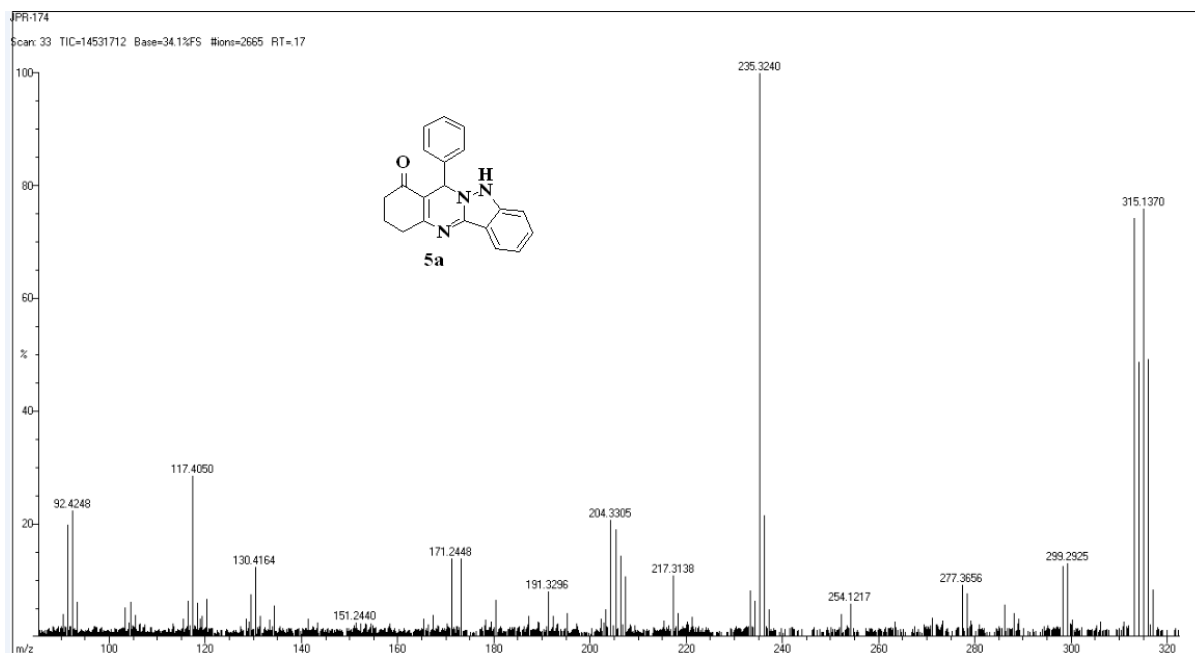
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P13 2000.00 usec  
PLW0 0 W  
PLW1 58.00000000 W  
SFO1 100.6230053 MHz  
SFXNAM[5] Crp60comp.4  
SFOAL5 0.500  
SFOFF5 0 Hz  
SFW5 8.51080036 W

CHANNEL f2 -----  
CFDPRG[2] waltz16  
NUC2 1H  
P3 14.25 usec  
P4 28.50 usec  
PCPD2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.35097000 W  
SFO2 400.2592801 MHz

F2 - Processing parameters  
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SF 100.6449540 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

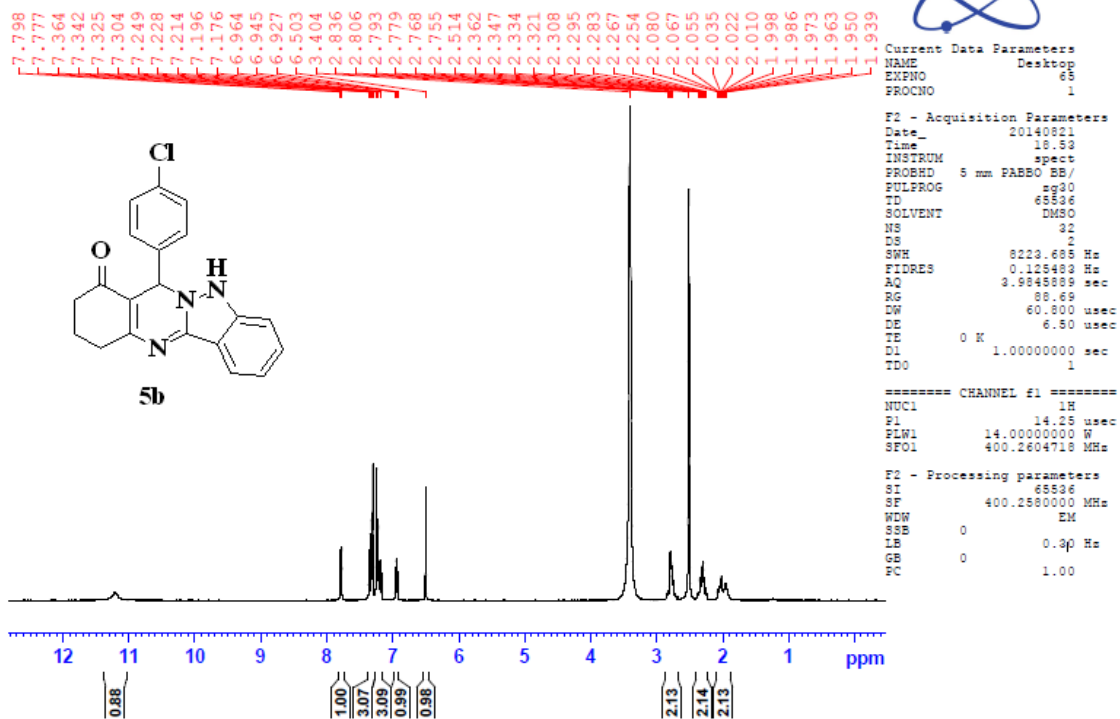


### HRMS spectrum of compound (5a):



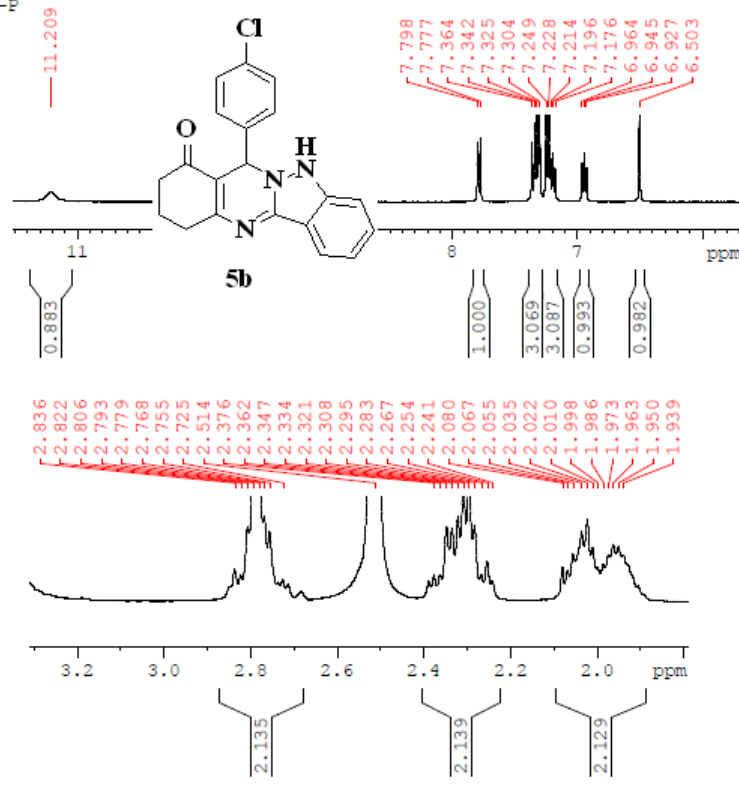
# <sup>1</sup>H NMR spectrum of compound (5b):

Signature SIF VIT VELLORE  
JPR-198-P



# Expanded <sup>1</sup>H NMR spectrum of compound (5b):

Signature SIF VIT VELLORE  
JPR-198-P



Current Data Parameters  
 NAME Desktop  
 EXPNO 65  
 PROCNO 1

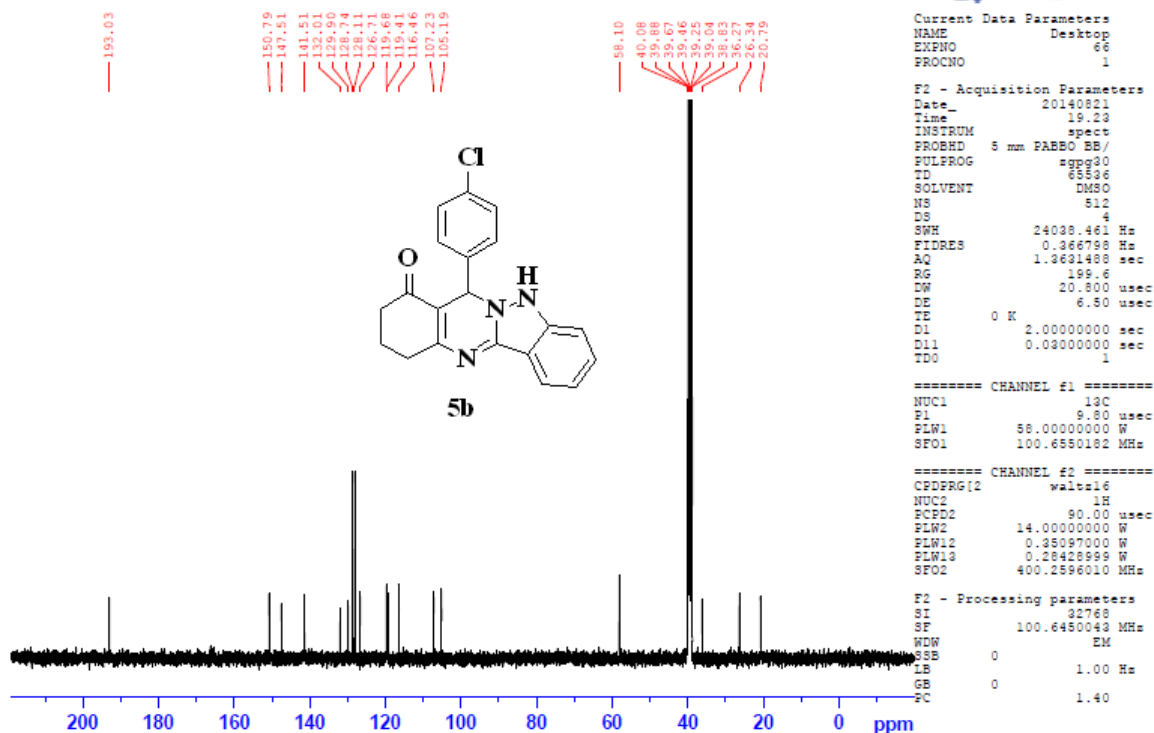
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 Time 18.53  
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 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.128483 Hz  
 AQ 3.9845889 sec  
 RG 88.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.26 usec  
 PLW1 14.00000000 W  
 SF01 400.2604718 MHz

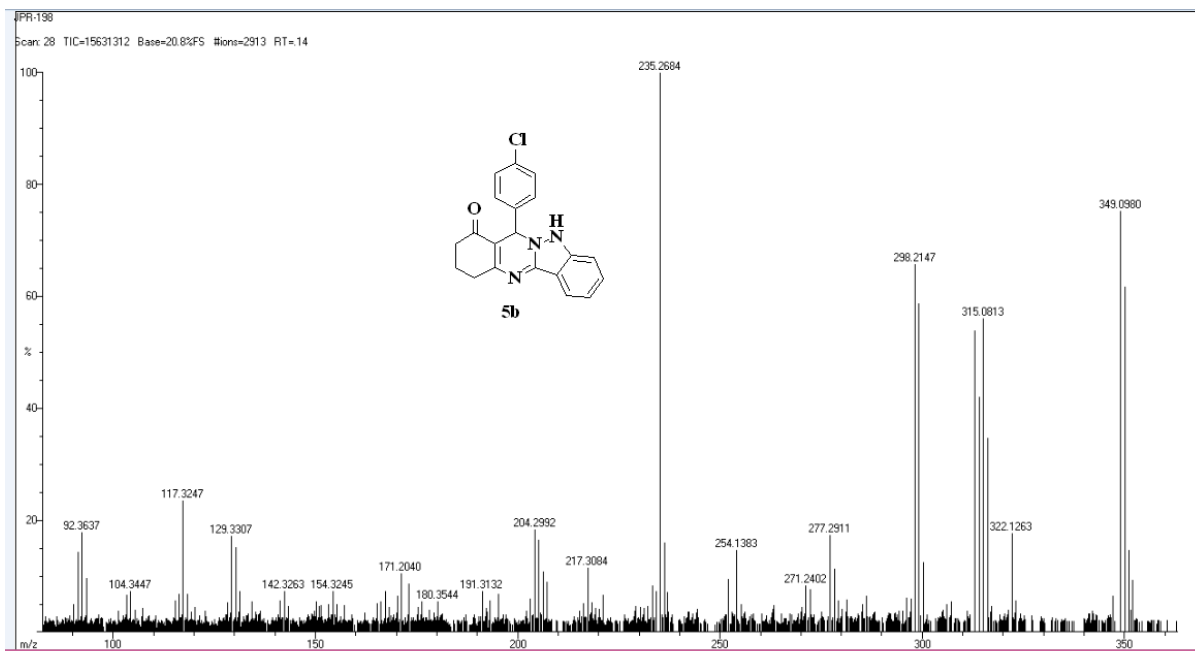
F2 - Processing parameters  
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 SF 400.2580000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 FC 1.00

# <sup>13</sup>C NMR spectrum of compound (5b):

Signature SIF VIT VELLORE  
JPR-198-P



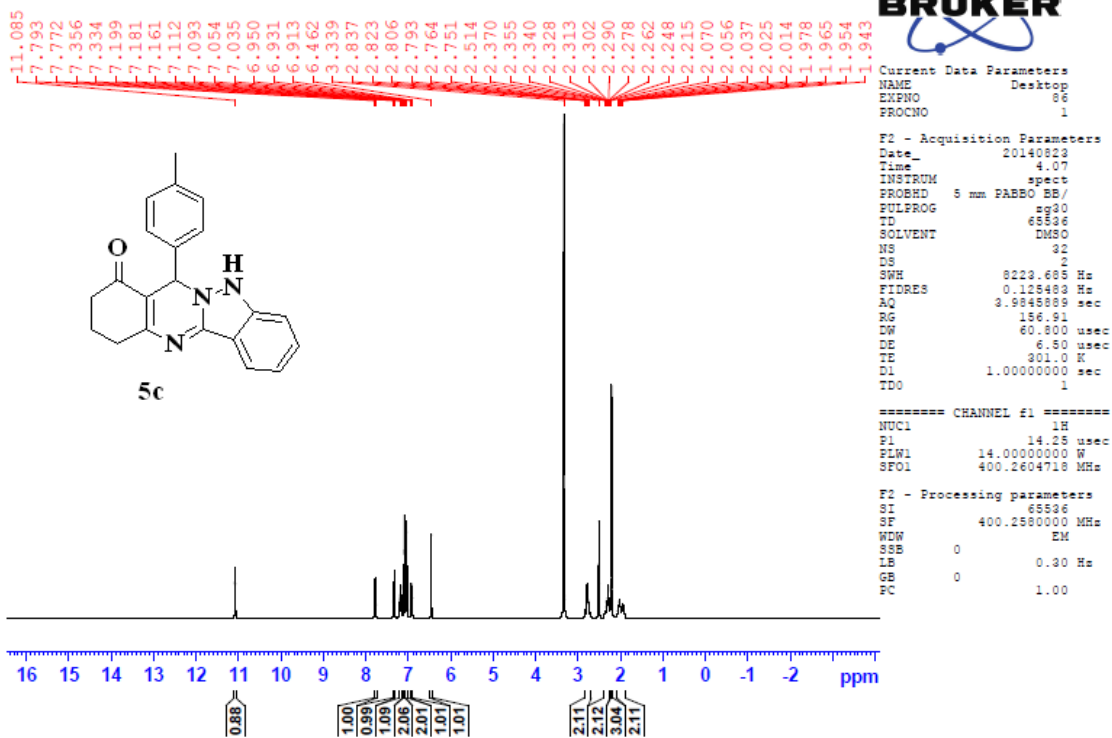
# HRMS spectrum of compound (5b):



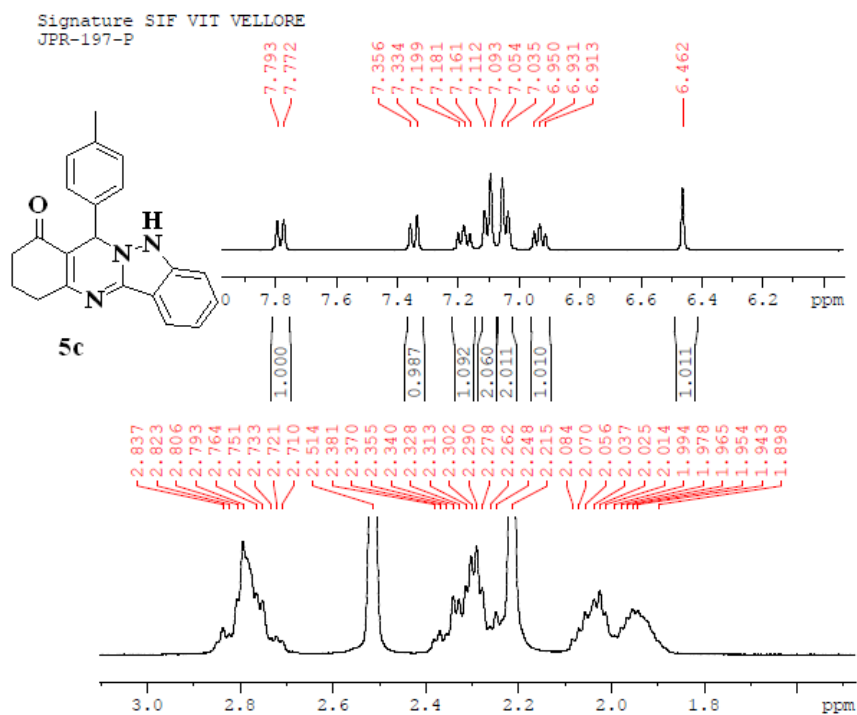


**<sup>1</sup>H NMR spectrum of compound (5c):**

Signature SIF VIT VELLORE  
JPR-197-P



### Expanded <sup>1</sup>H NMR spectrum of compound (5c):



Current Data Parameters

NAME	Desktop
EXPNO	06
PROCNO	1

F2 - Acquisition Parameters

Date_	20140823
Time	4.07
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	32
DS	2
SWH	8223.688 Hz
FIDRES	0.125483 Hz
AQ	3.9845889 sec
RG	156.91
DW	60.800 usec
DE	6.50 usec
TE	301.0 K
D1	1.00000000 sec
TD0	1

===== CHANNEL f1 =====

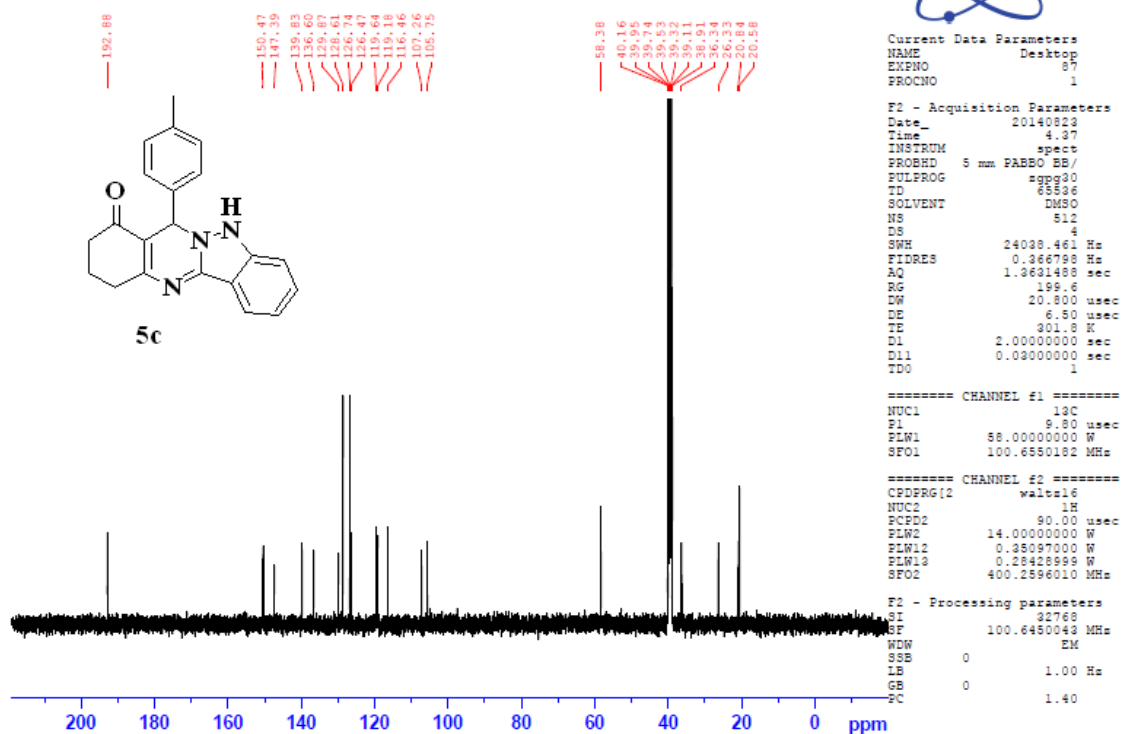
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F1	14.25 usec
PLW1	14.00000000 W
SFO1	400.2604718 MHz

F2 - Processing parameters

SI	65536
SF	400.2580000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

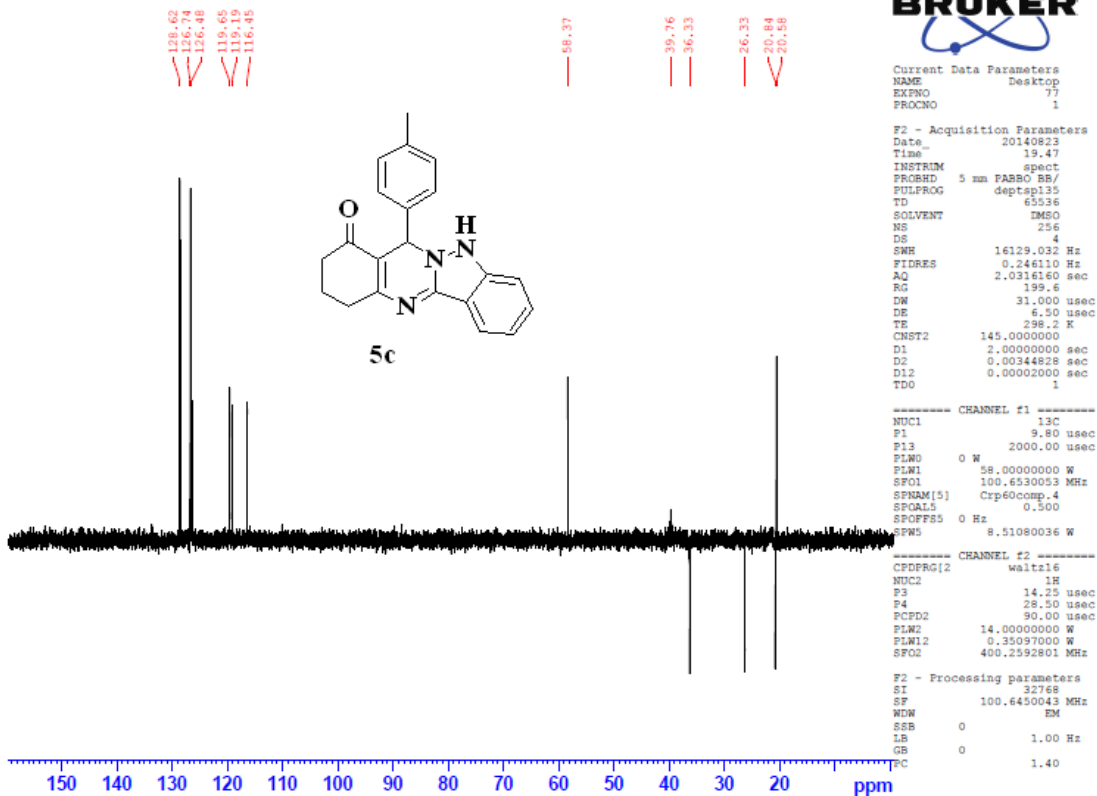
# <sup>13</sup>C NMR spectrum of compound (5c):

Signature SIF VIT VELLORE  
JPR-197-P

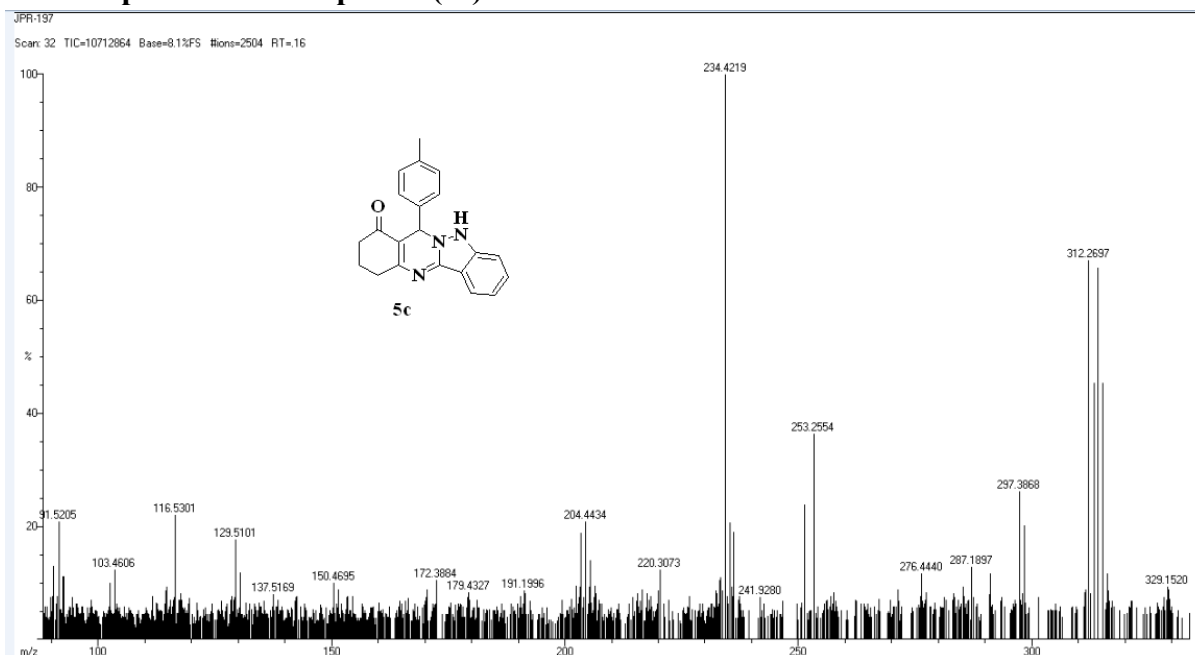


### <sup>13</sup>C NMR - DEPT 135 spectrum of compound (5c):

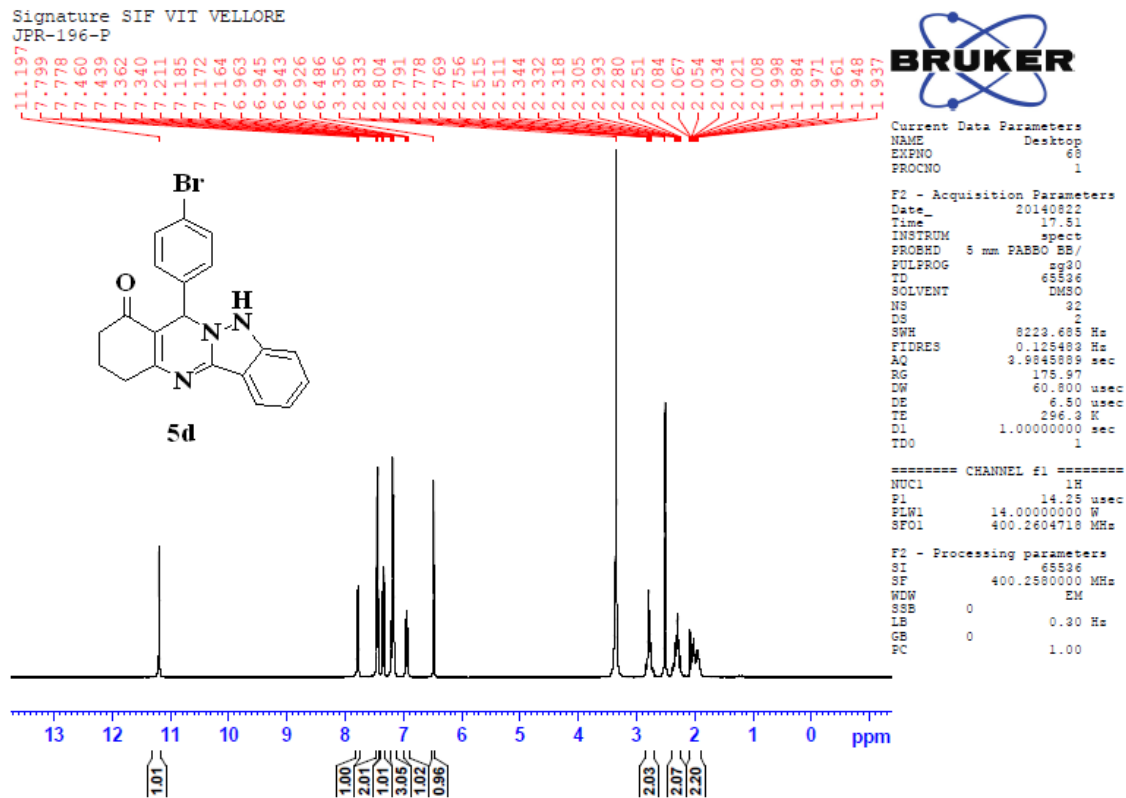
Signature SIF VIT VELLORE  
JPR-197-P



### HRMS spectrum of compound (5c):

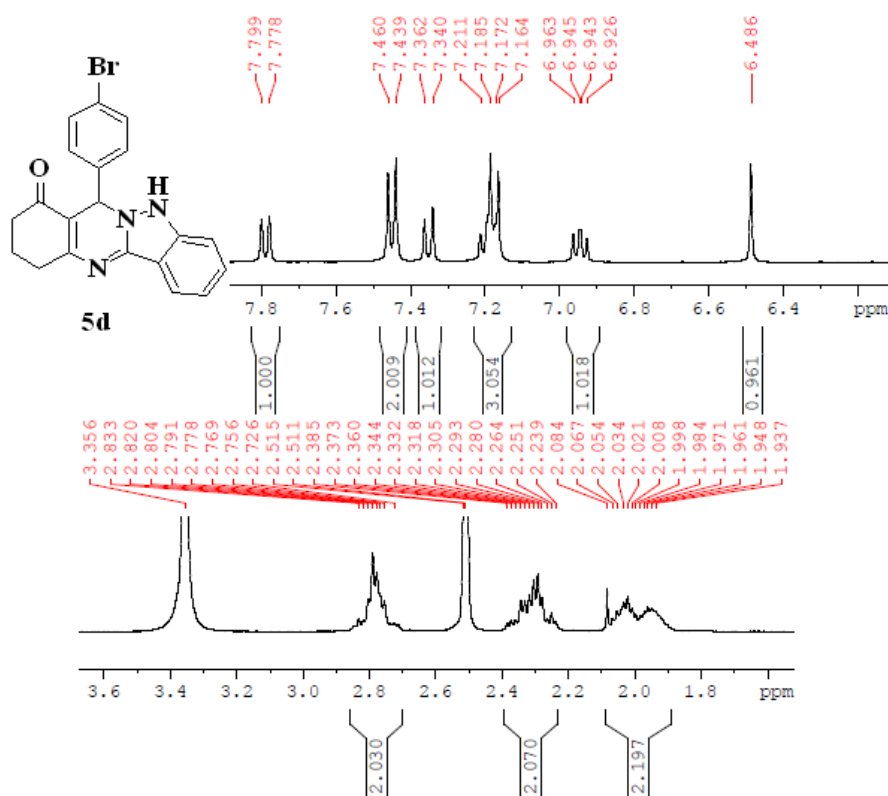


**<sup>1</sup>H NMR spectrum of compound (5d):**



## Expanded <sup>1</sup>H NMR spectrum of compound (5d):

Signature SIF VIT VELLORE  
JPR-196-P



Current Data Parameters  
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 EXPNO 68  
 PROCNO 1

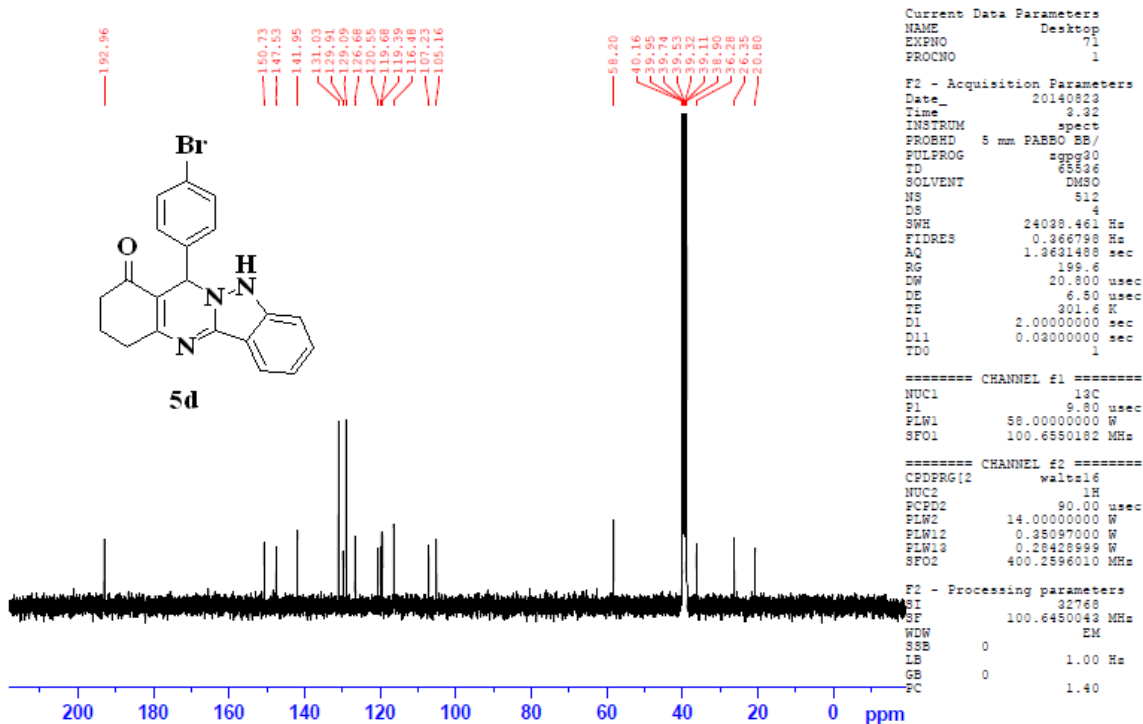
F2 - Acquisition Parameters  
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 Time 17.51  
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 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 8223.688 Hz  
 FIDRES 0.126483 Hz  
 AQ 3.9845889 sec  
 RG 178.97  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.25 usec  
 PL1 14.00000000 W  
 SP1 400.2604718 MHz

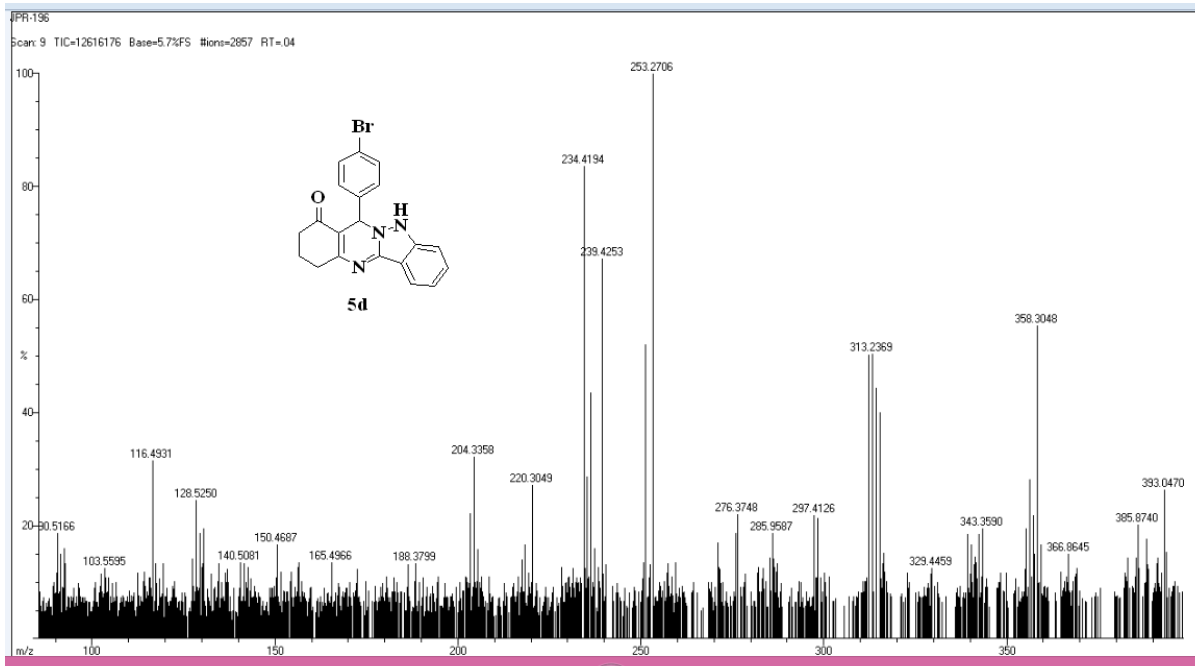
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 SF 400.2600000 MHz  
 WDW EM  
 GB 0  
 LB 0.30 Hz  
 GB 0  
 FC 1.00

### <sup>13</sup>C NMR spectrum of compound (5d):

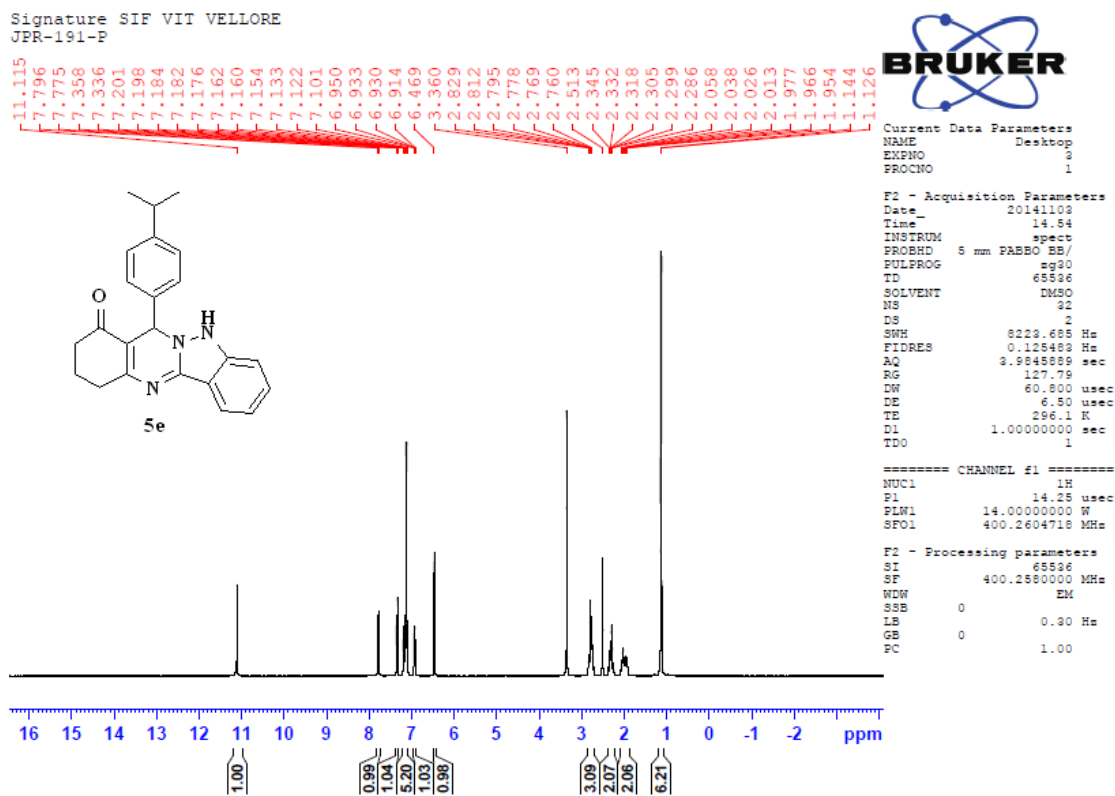
Signature SIF VIT VELLORE  
JPR-196-P



### HRMS spectrum of compound (5d):



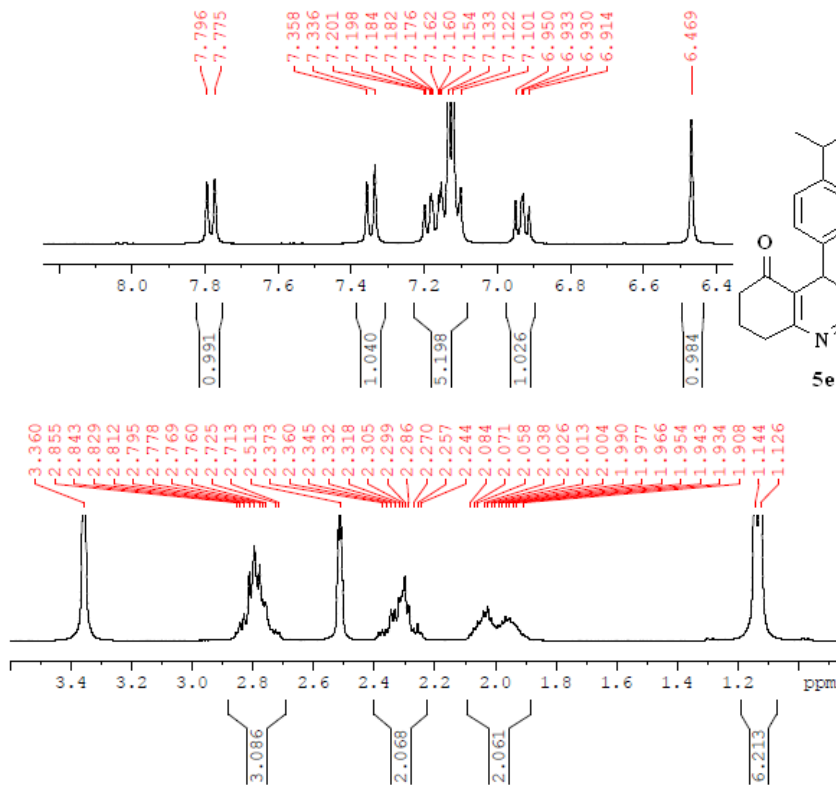
# <sup>1</sup>H NMR spectrum of compound (5e):





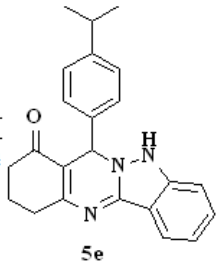
# Expanded <sup>1</sup>H NMR spectrum of compound (5e):

Signature SIF VIT VELLORE  
JPR-191-P



Current Data Parameters  
NAME Desktop  
EXPNO 3  
PROCNO 1

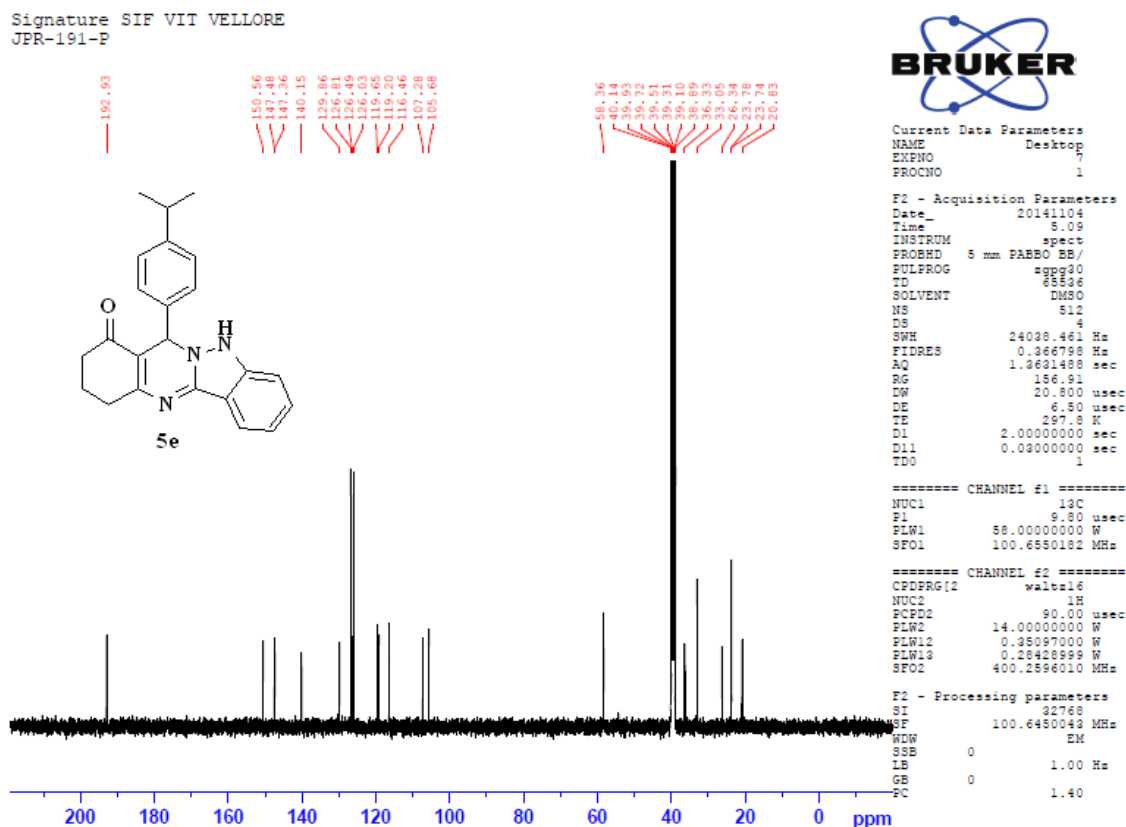
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20141103  
14.54  
spect  
nm PARBO BB/  
ag30  
65536  
DMSO  
22  
2  
8223.685 Hz  
0.125483 Hz  
3.9845888 sec  
17.75  
60.800 usec  
6.80 usec  
296.1 K  
1.00000000 sec  
TDU 1



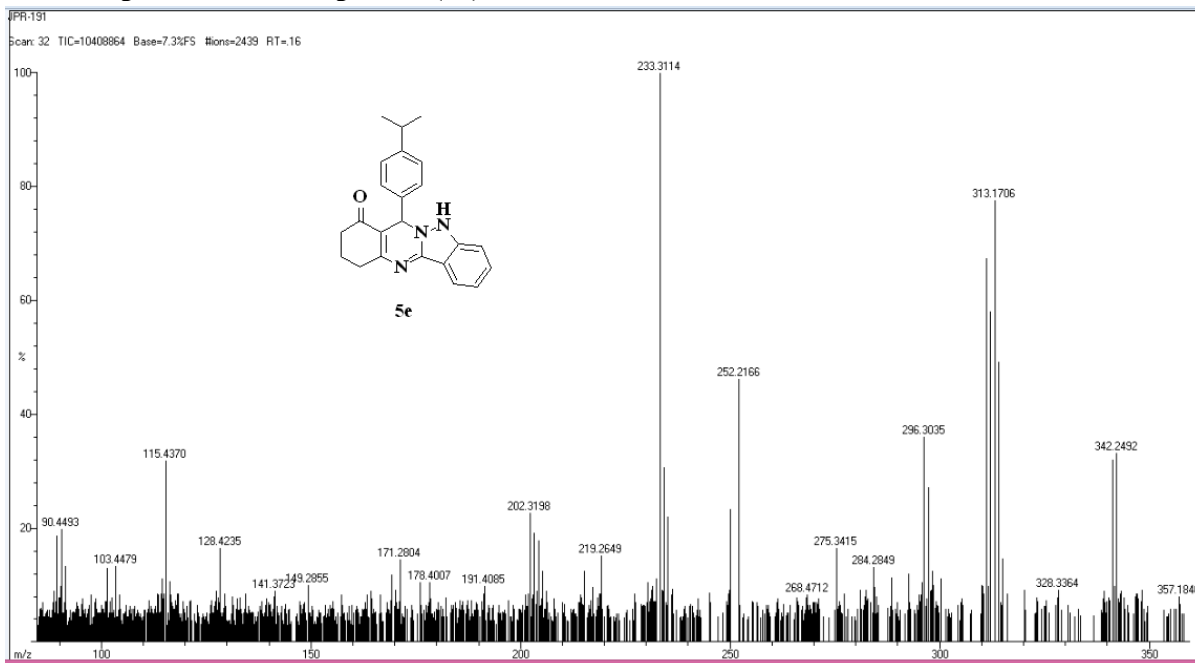
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P1 14.28 usec  
PLW1 14.0000000 W  
SFO1 400.2604718 MHz

F0 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### <sup>13</sup>C NMR spectrum of compound (5e):

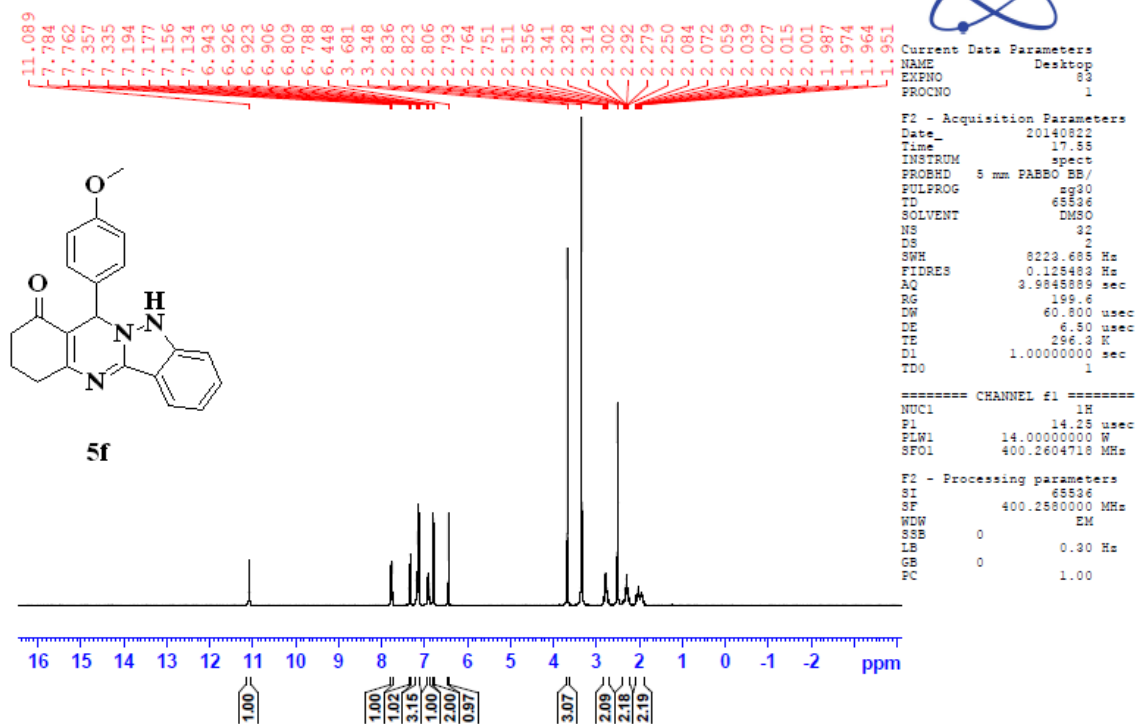


### HRMS spectrum of compound (5e):



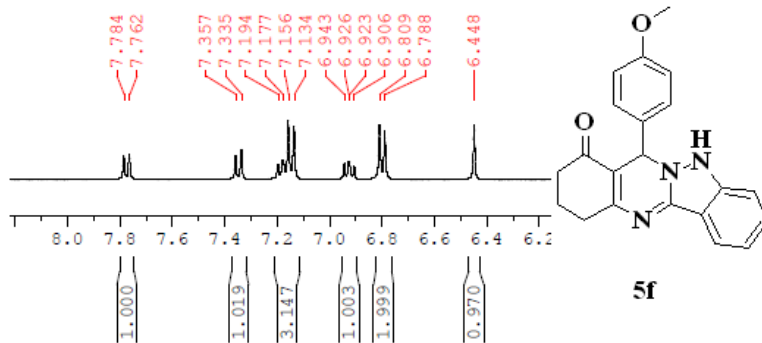
# <sup>1</sup>H NMR spectrum of compound (5f):

Signature SIF VIT VELLORE  
JPR-193-P



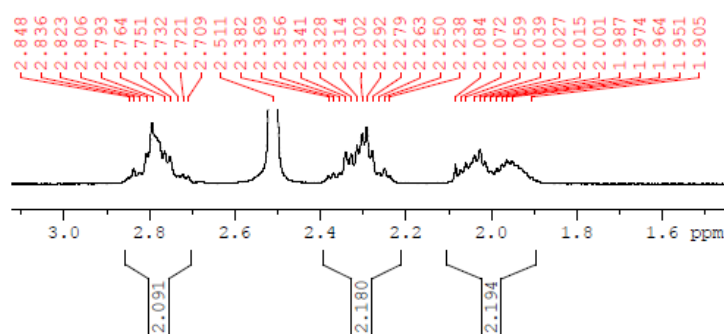
# Expanded <sup>1</sup>H NMR spectrum of compound (5f):

Signature SIF VIT VELLORE  
JPR-193-P



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PROCNO   1

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Time     17.55
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PROBHD   5 mm FASBO BB/
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        32
DS        2
SWH       8223.685 Hz
FIDRES    0.125489 Hz
AQ         3.9845889 sec
RG         199.6
DW         60.800 usec
DE         6.50 usec
TE         296.3 K
D1         1.00000000 sec
TDO        1
```

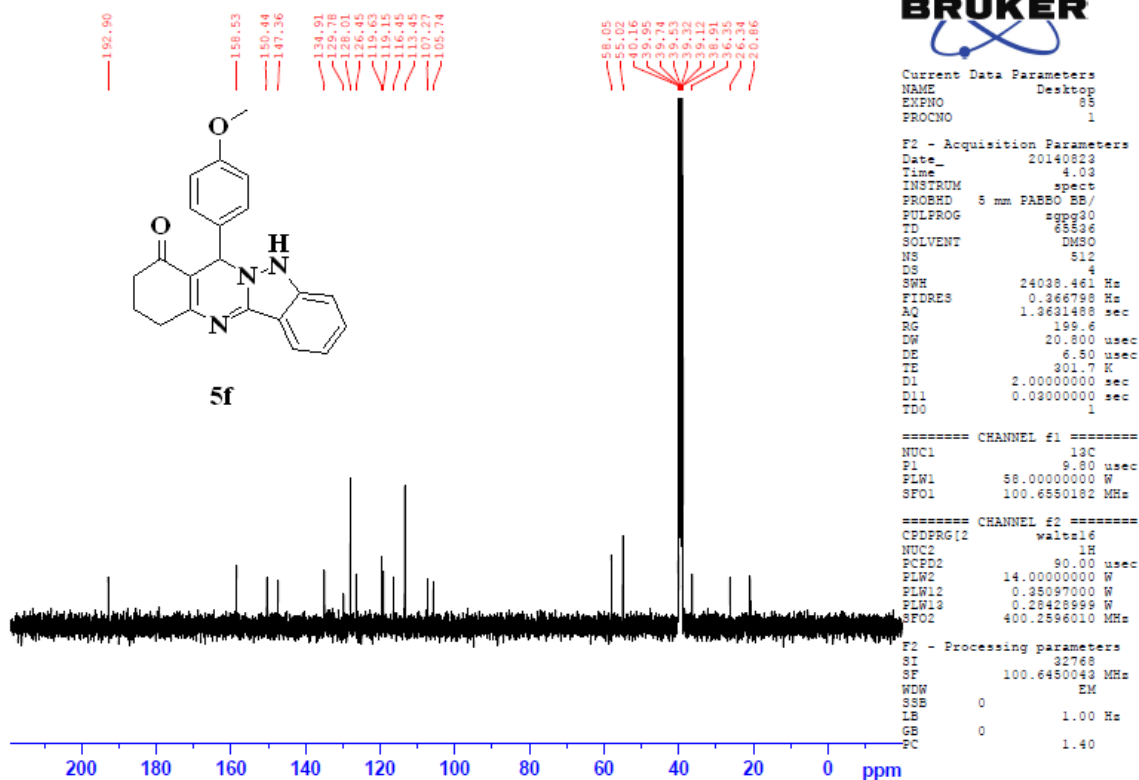


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P1       14.25 usec
PLW1     14.00000000 W
SFO1     400.2604718 MHz

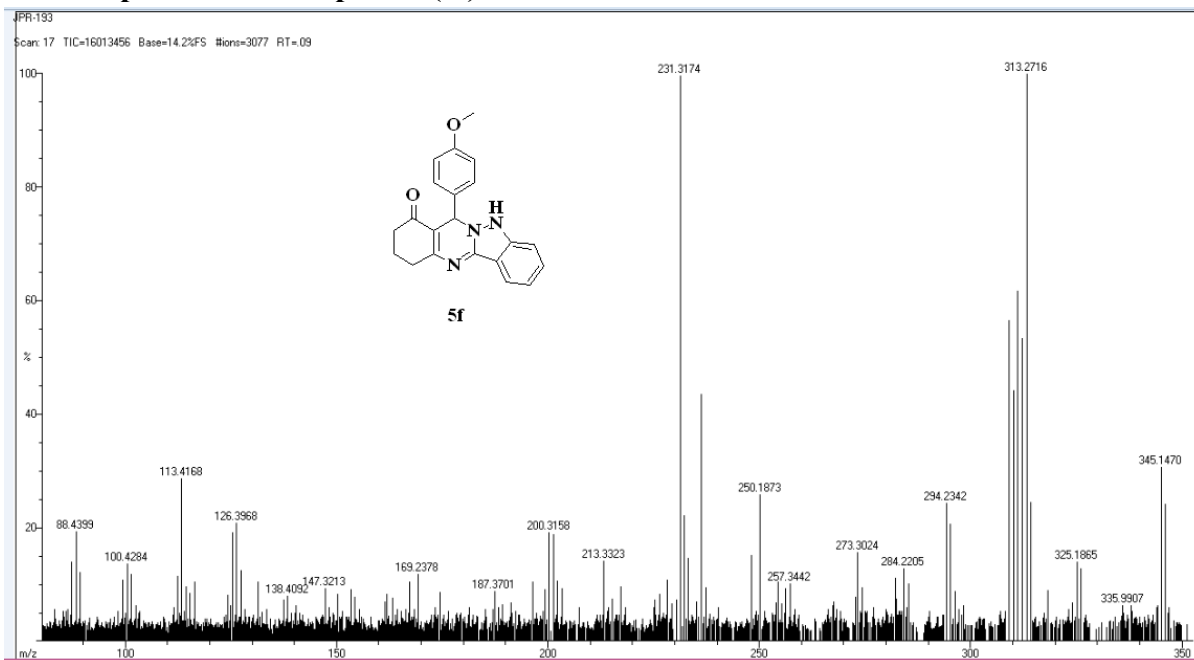
F2 - Processing parameters
SI        65536
SF        400.2580000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
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PC        1.00
```

### <sup>13</sup>C NMR spectrum of compound (5f):

Signature SIF VIT VELLORE  
JPR-193-P

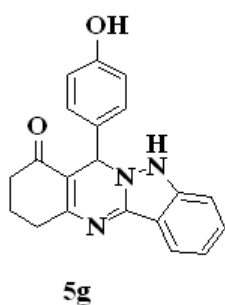
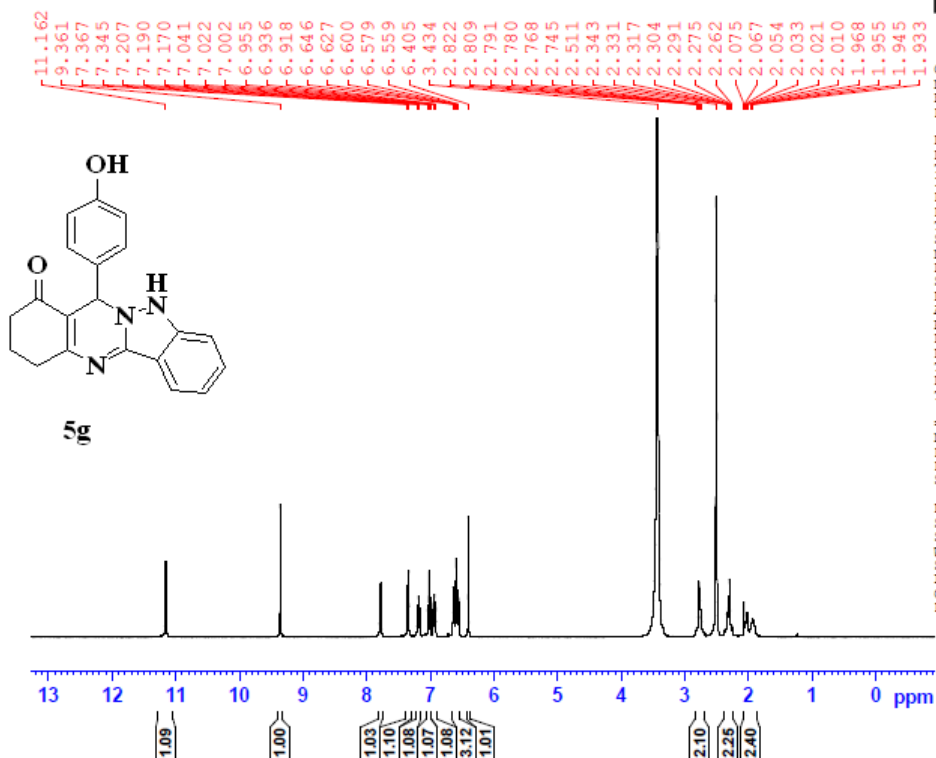


### HRMS spectrum of compound (5f):



**<sup>1</sup>H NMR spectrum of compound (5g):**

Signature SIF VIT VELLORE  
JFR-01-003-P



Current Data Parameters  
NAME Desktop  
EXPNO 67  
PROCNO 1

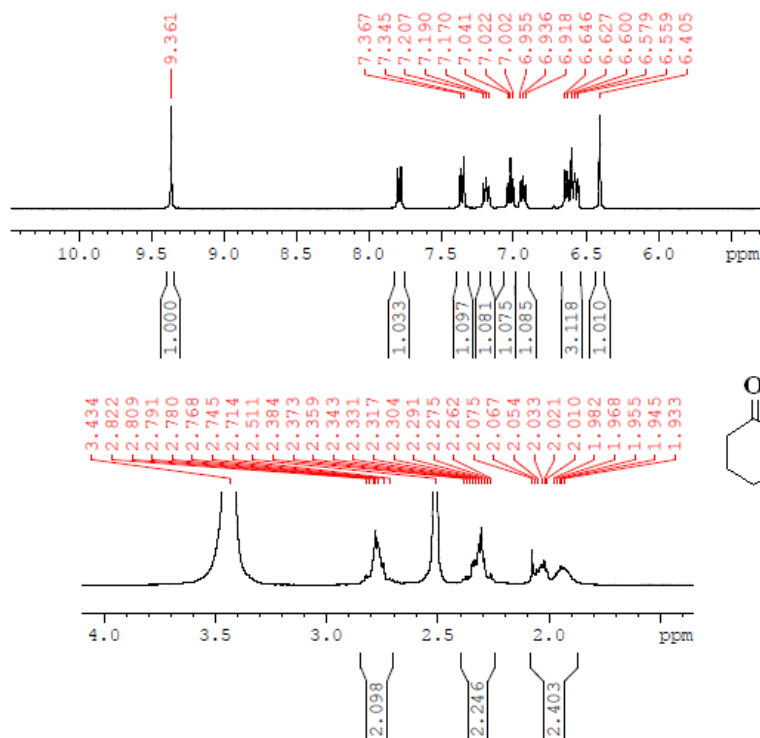
F2 - Acquisition Parameters  
Date\_ 20140822  
Time 17.46  
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PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 32  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125493 Hz  
AQ 3.9845889 sec  
RG 77.73  
DW 60.800 usec  
DE 6.50 usec  
TE 296.3 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
PLW1 14.00000000 W  
SF01 400.2604718 MHz

F2 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

## Expanded <sup>1</sup>H NMR spectrum of compound (5g):

Signature SIF VIT VELLORE  
JPR-01-003-P



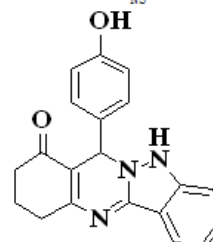
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EXPNO 67  
PROCNO 1

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Time 17.46  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 32

822.685 Hz  
0.125483 Hz  
3.9845983 sec  
77.73  
60.800 usec  
6.50 usec  
296.3 K  
1.00000000 sec  
1

NNEL f1 =====  
1H  
14.25 usec  
14.00000000 W  
400.2604718 MHz

ing parameters  
65536  
400.2580000 MHz  
EM  
0.30 Hz  
1.00

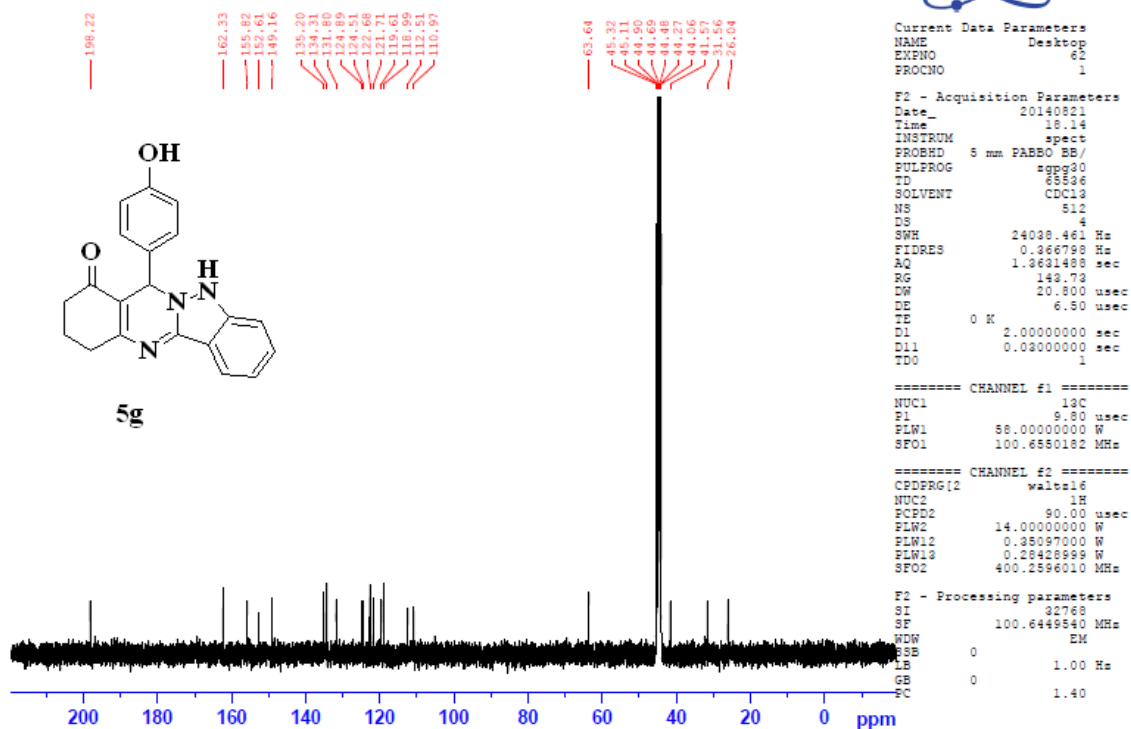


5g

0.30 Hz  
1.00

# <sup>13</sup>C NMR spectrum of compound (5g):

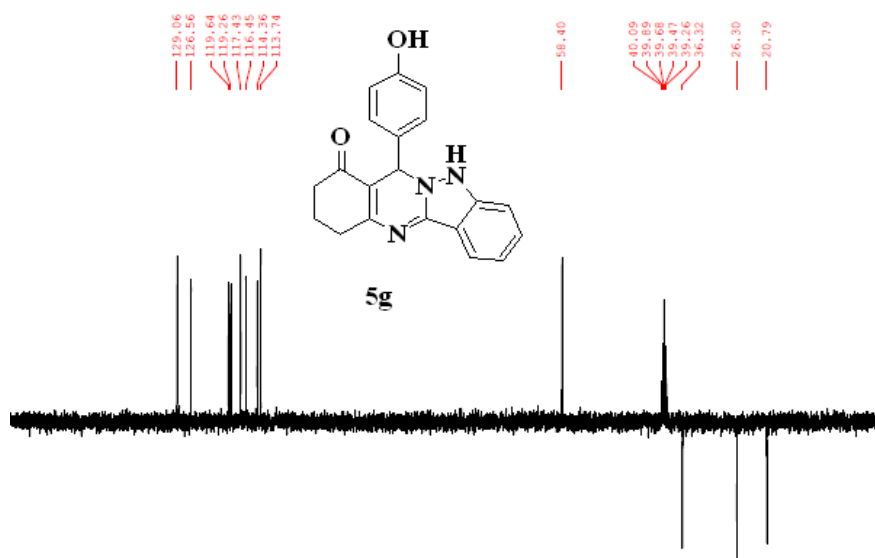
Signature SIF VIT VELLORE  
JPR-01-003-P





### <sup>13</sup>C NMR - DEPT 135 spectrum of compound (5g):

Signature SIF VIT VELLORE  
JPR-01-003-P



Current Data Parameters  
NAME Desktop  
EXPNO 82  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140823  
Time\_ 20.44  
INSTRUM spect  
PROBHD 5 mm PABO BB/  
PULPROG deptsp135  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 4  
SWH 16129.032 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316160 sec  
RG 199.6  
DW 31.000 usec  
DE 6.50 usec  
TE 298.1 K  
CMST2 145.0000000 sec  
D1 2.0000000 sec  
D2 0.0034828 sec  
D12 0.0000200 sec  
TDO 1

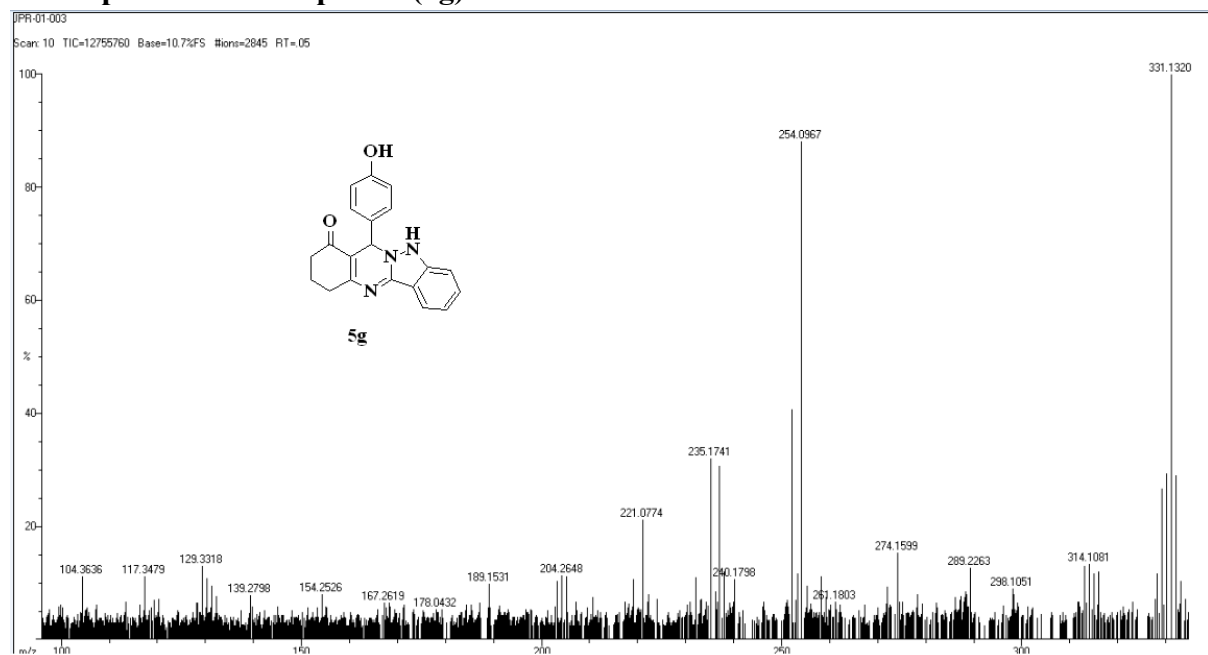
----- CHANNEL f1 -----  
NUC1 13C  
P1 9.80 usec  
PL1 2000.00 usec  
PLW0 0 W  
PLM1 58.0000000 W  
SFO1 100.6250053 MHz  
SFO1(5) Crp60comp.4  
SFOAL5 0.500  
SFOFF5 0 Hz  
SFO5 8.51080036 W

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
P3 14.25 usec  
P4 28.50 usec  
PCPD2 90.00 usec  
PLM2 14.0000000 W  
PLM12 0.35097000 W  
SFO2 400.2592801 MHz

F2 - Processing parameters  
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SF 100.6450043 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

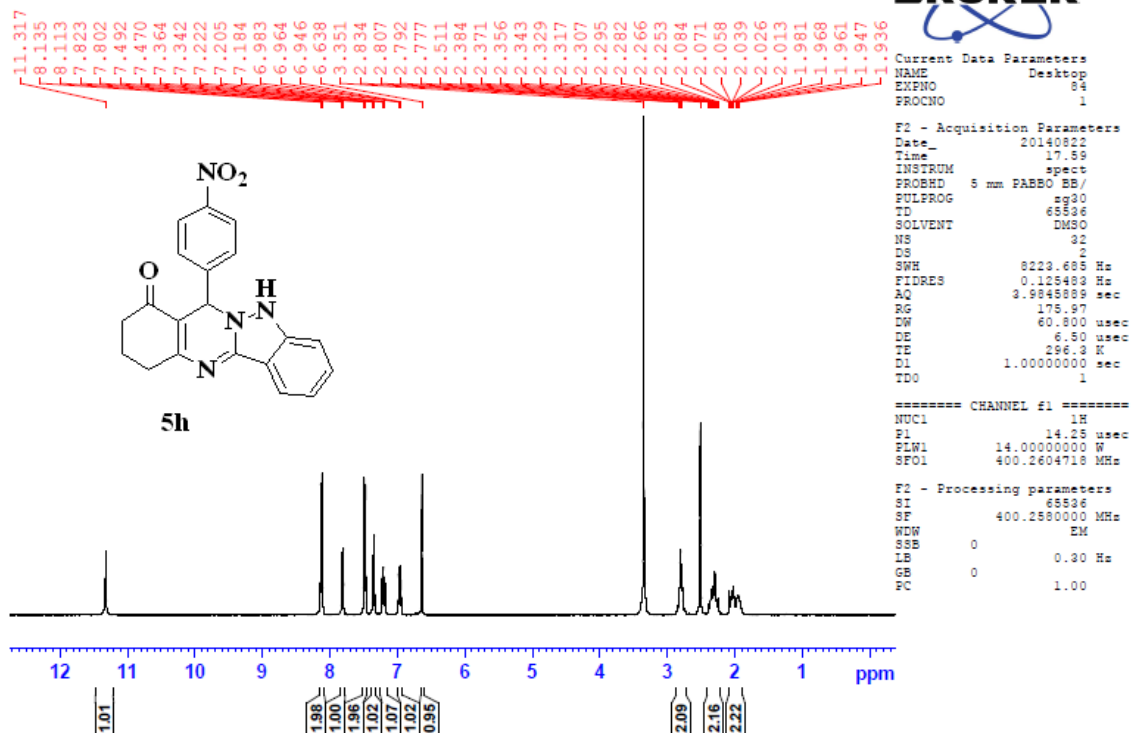
H

### RMS spectrum of compound (5g):



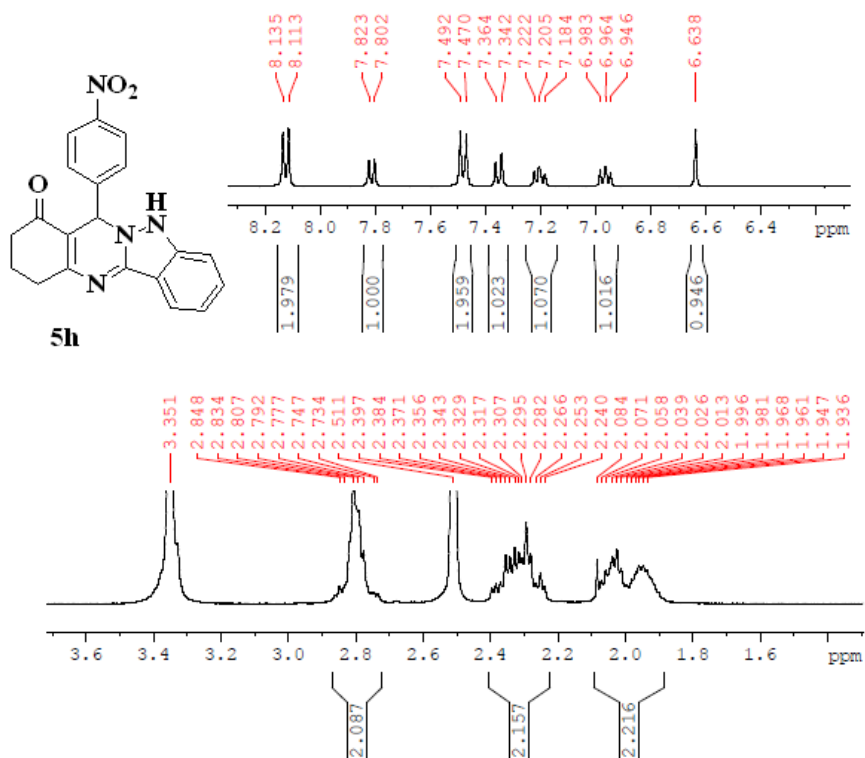
**<sup>1</sup>H NMR spectrum of compound (5h):**

Signature SIF VIT VELLORE  
JPR-194-P



## Expanded <sup>1</sup>H NMR spectrum of compound (5h):

Signature SIF VIT VELLORE  
JPR-194-P



```

Current Data Parameters
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EXPNO    84
PROCNO   1

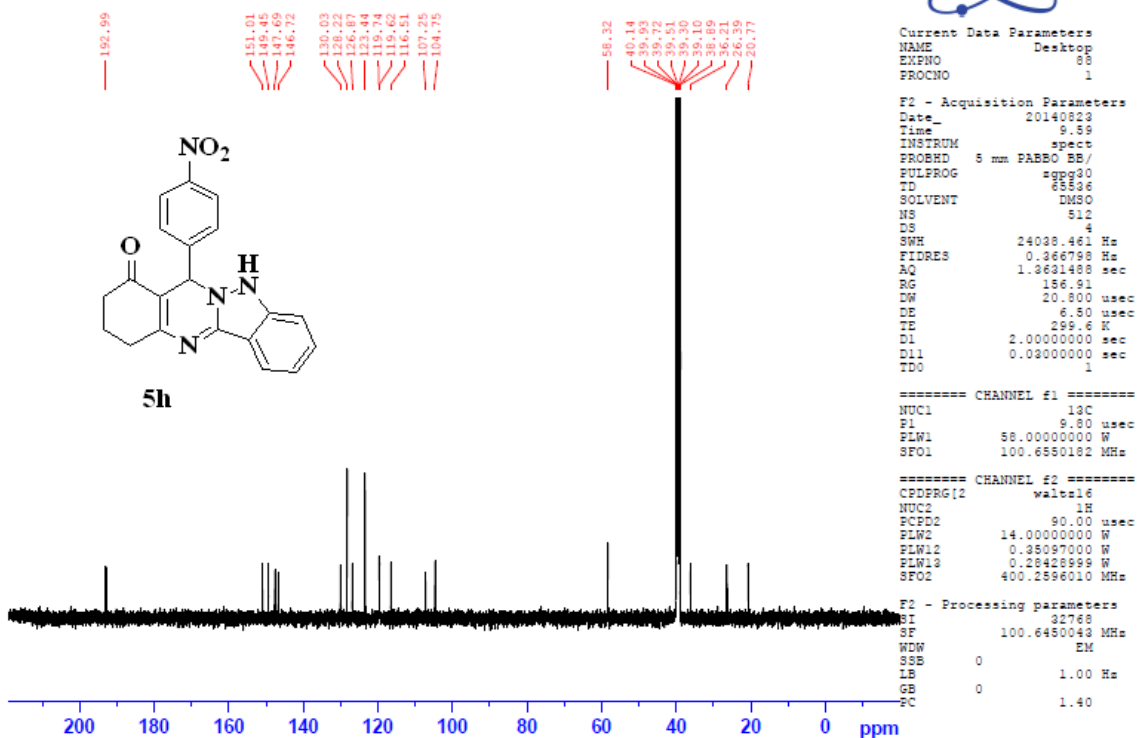
F2 - Acquisition Parameters
Date_    20140822
Time     17.59
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        32
DS        2
SWH       8229.695 Hz
FIDRES    0.125493 Hz
AQ        3.9845889 sec
RG         175.97
DW         60.800 usec
DE         6.50 usec
TE        296.3 K
D1         1.0000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      1H
P1        14.25 usec
PL1       14.00000000 W
SFO1      400.2604718 MHz

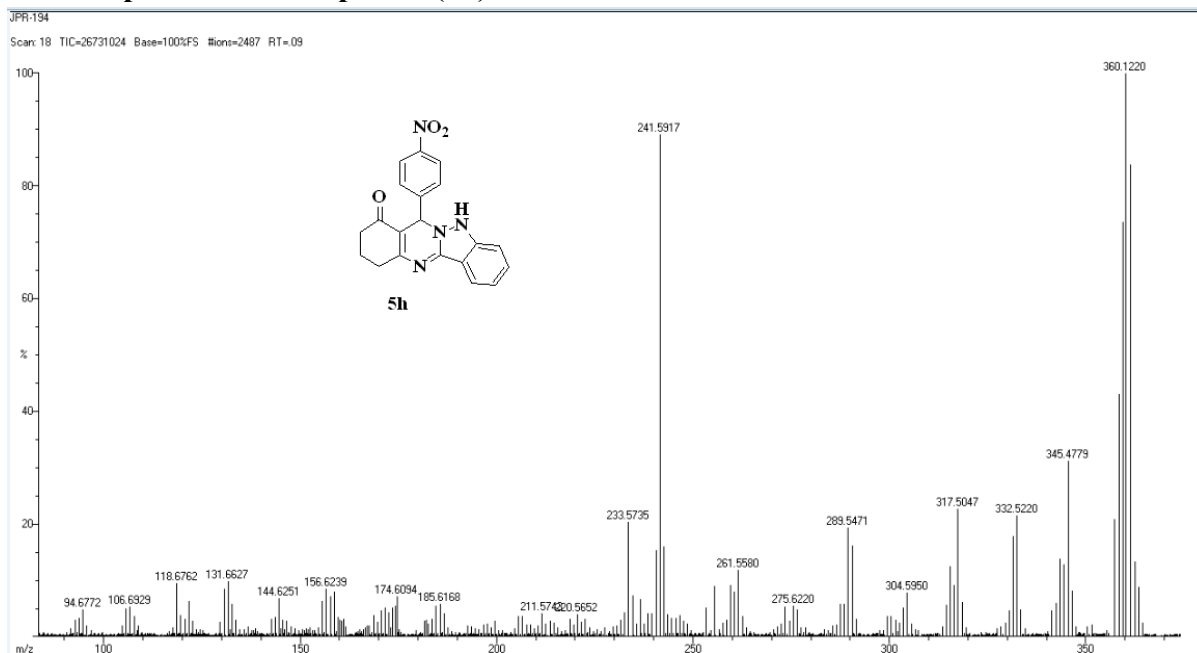
F2 - Processing parameters
SI        65536
SF        400.2600000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
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### <sup>13</sup>C NMR spectrum of compound (5h):

Signature SIF VIT VELLORE  
JPR-194-P

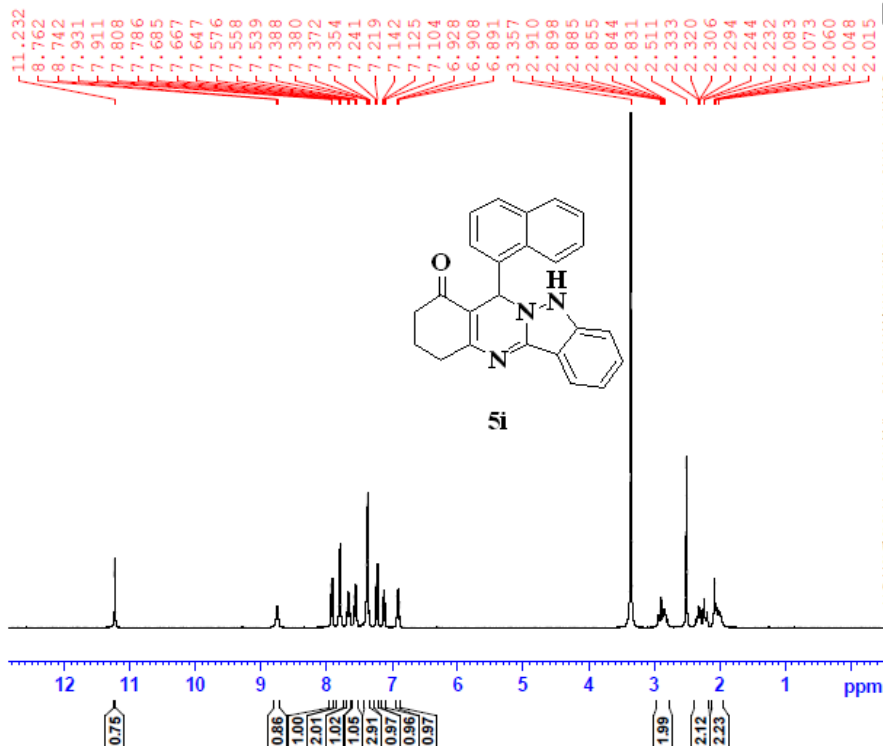


### HRMS spectrum of compound (5h):



# <sup>1</sup>H NMR spectrum of compound (5i):

Signature SIF VIIT VELLORE  
JPR-01-008-P



Current Data Parameters  
NAME Desktop  
EXPNO 60  
PROCNO 1

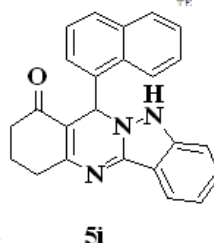
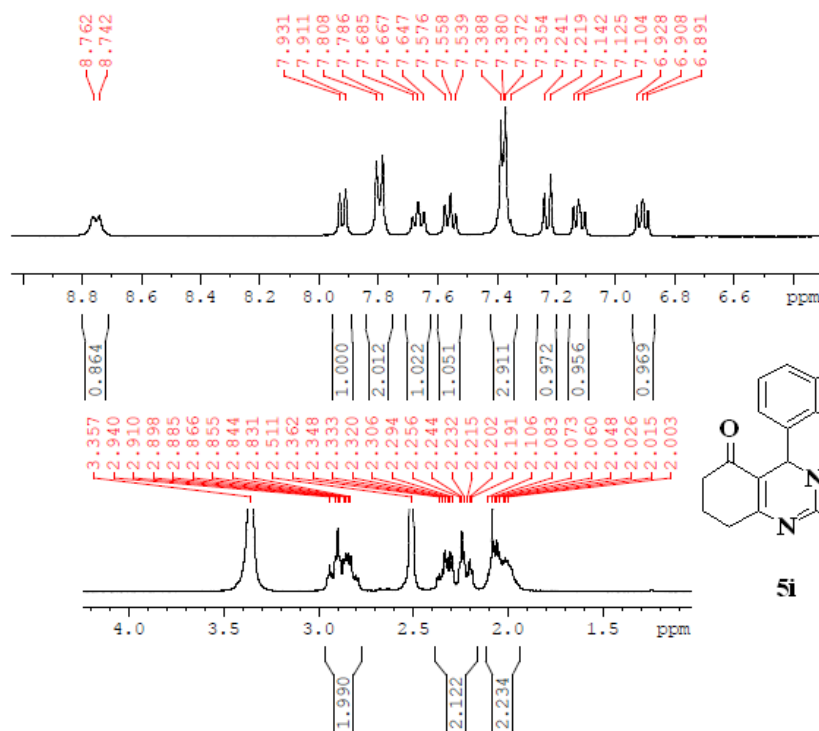
F2 - Acquisition Parameters  
Date\_ 20140822  
Time 17.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg  
TD 65536  
SOLVENT DMSO  
NS 32  
DS 2  
SWH 8223.655 Hz  
FIDRES 0.123493 Hz  
AQ 3.9345899 sec  
RG 156.91  
DM 60.800 usec  
DE 6.50 usec  
TE 296.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
PLW1 14.00000000 W  
SFO1 400.2604718 MHz

F2 - Processing parameters  
SI 65536  
SF 400.2604718 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

## Expanded <sup>1</sup>H NMR spectrum of compound (5i):

Signature SIF VIT VELLORE  
JPR-01-008-P



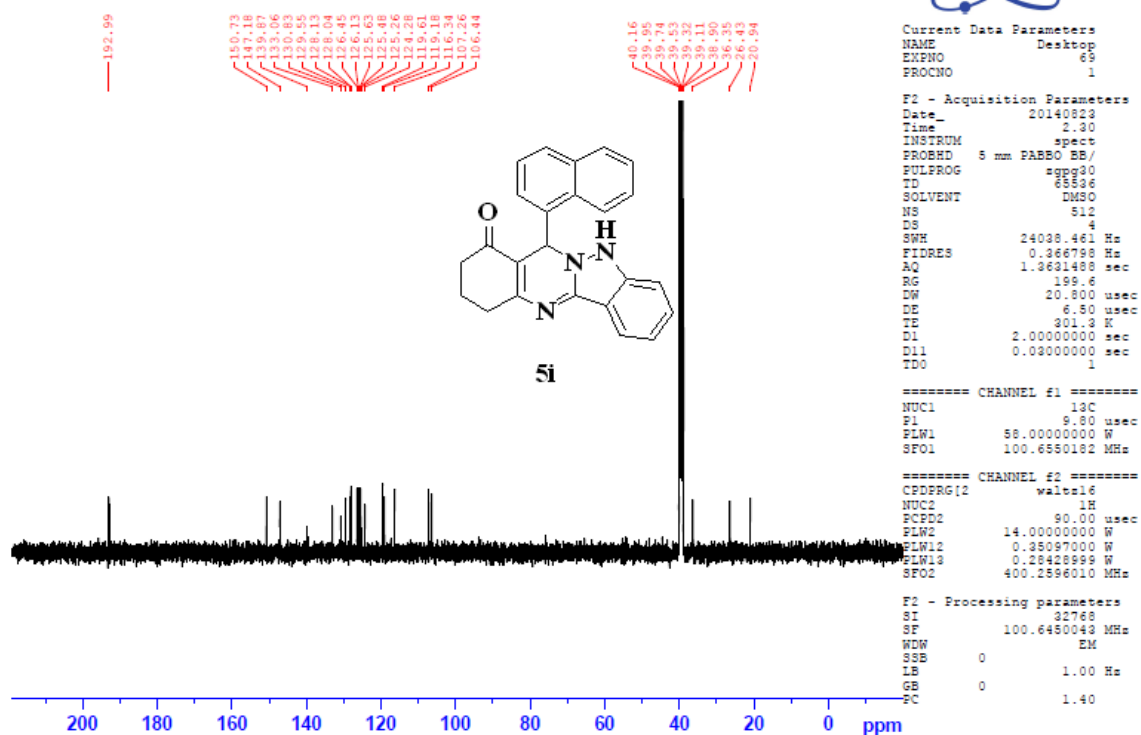
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Current Data Parameters
NAME      Desktop
EXPNO    63
PROCNO   1

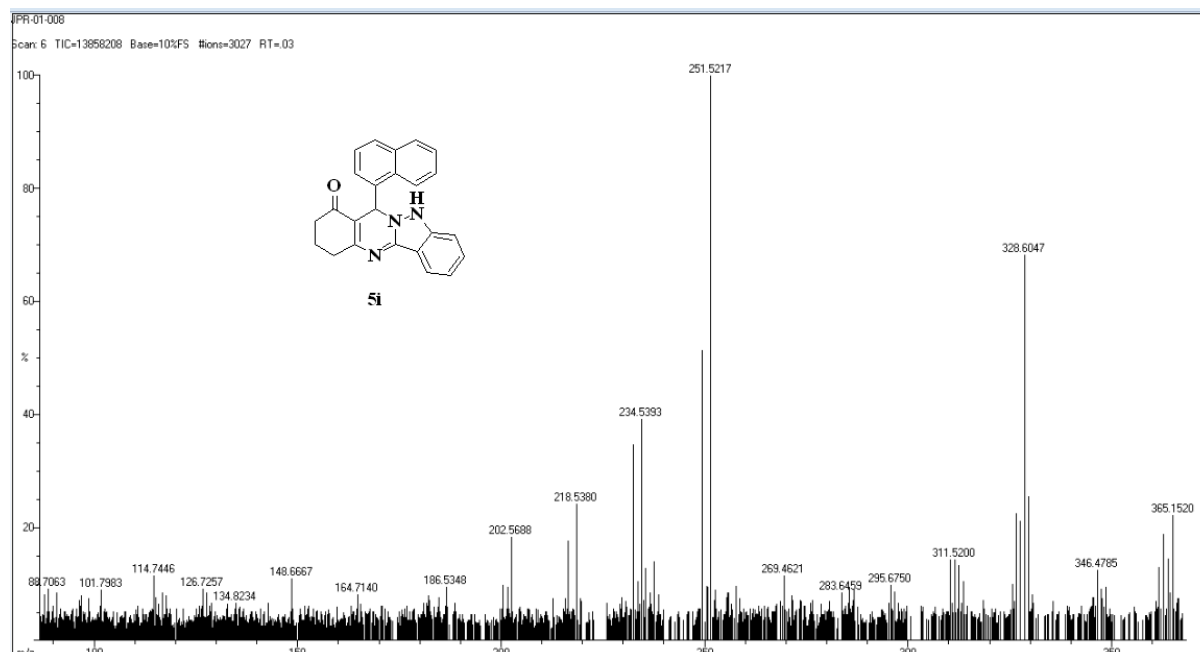
F2 - Acquisition Parameters
Date_    20140822
Time     17.42
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg
TD       65536
SOLVENT  DMSO
NS       32
DS       2
SWH      8229.665 Hz
FIDRES   0.125493 Hz
AQ       3.9845889 sec
RG       156.81
DW       60.800 usec
DE       6.50 usec
TE       296.3 K
PRF      1.00000000 sec
===== CHANNEL f1 =====
NUC1      1H
P1        14.25 usec
PL1       14.00000000 W
FREQ1    400.2604718 MHz
===== Processing parameters =====
SI        65536
SF        400.2600000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
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### <sup>13</sup>C NMR spectrum of compound (5i):

Signature SIF VIT VELLORE  
JPR-01-008-P

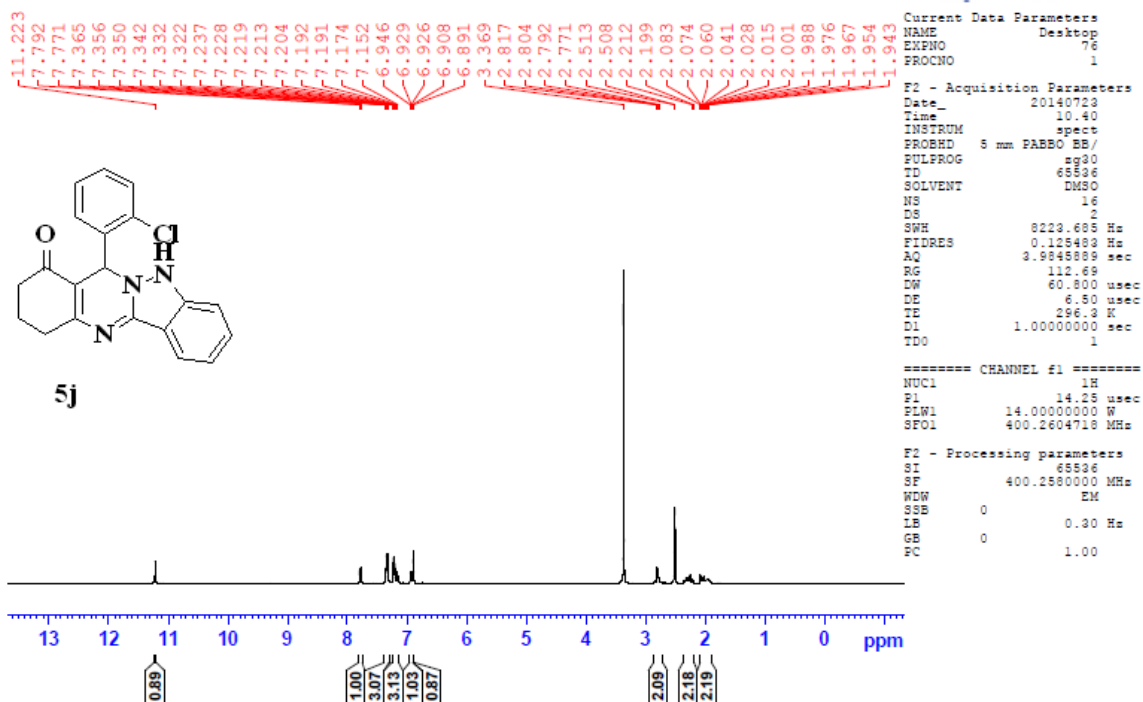


### HRMS spectrum of compound (5i):



# <sup>1</sup>H NMR spectrum of compound (5j):

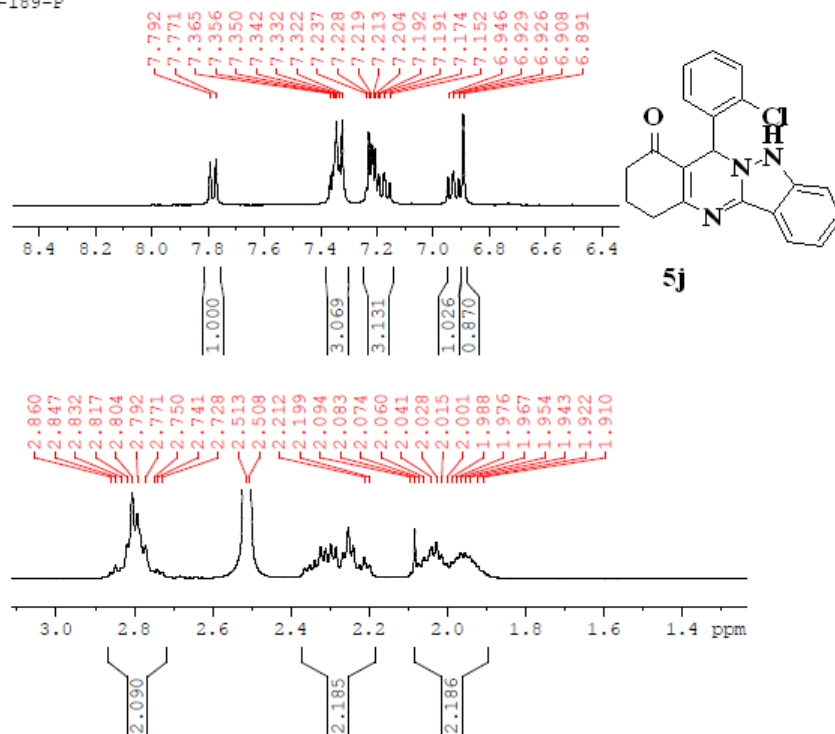
Signature SIF VIT VELLORE  
JPR-189-P





## Expanded <sup>1</sup>H NMR spectrum of compound (5j):

Signature SIF VIT VELLORE  
JPR-189-P



Current Data Parameters

NAME	Desktop
EXFNO	76
PROCNO	1

F2 - Acquisition Parameters

Date_	20140728
Time	10.40
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.688 Hz
FIDRES	0.129488 Hz
AQ	3.9945889 sec
RG	112.68
DW	60.800 usec
DE	6.50 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

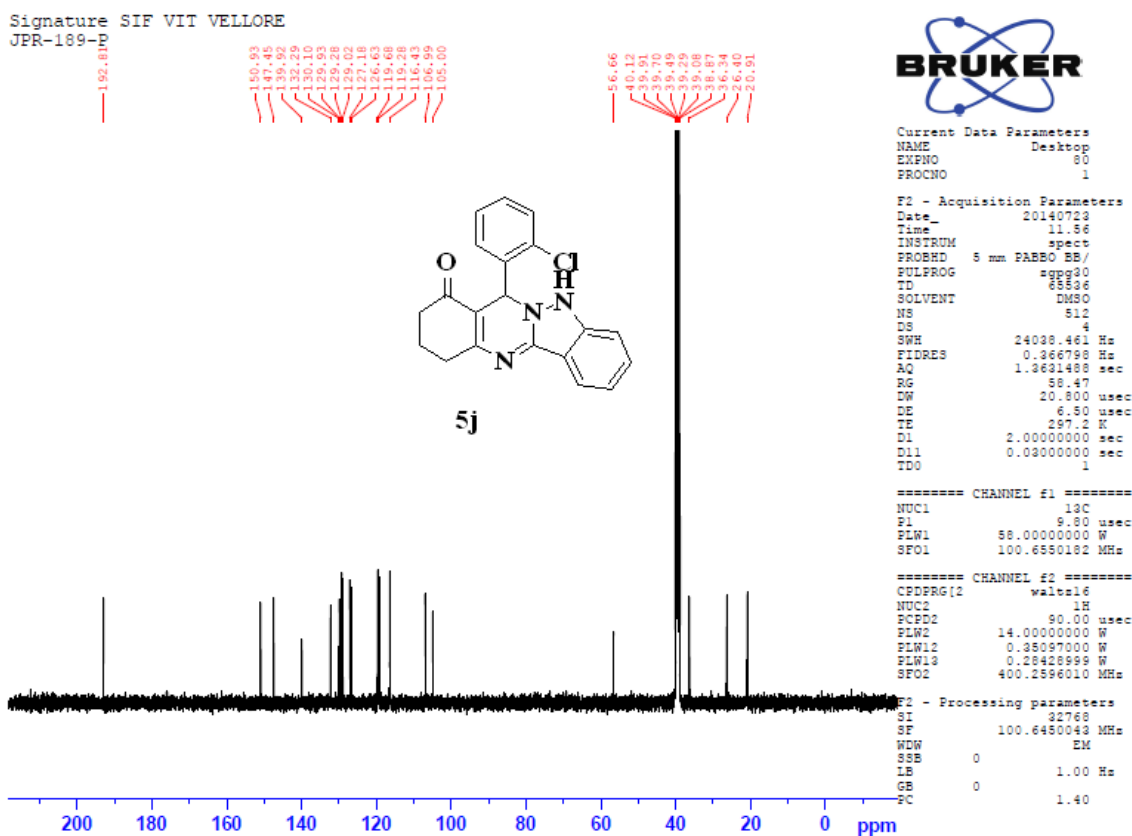
==== CHANNEL f1 =====

NUC1	1H
F1	14.25 usec
PLN1	14.00000000 W
SFO1	400.2604718 MHz

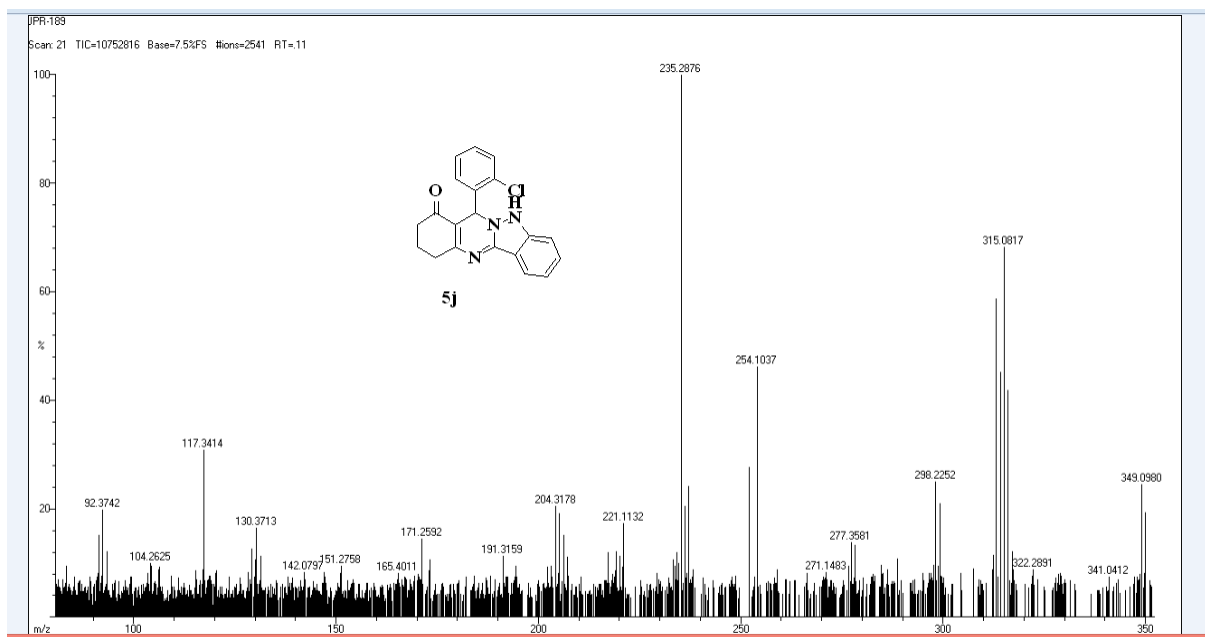
F2 - Processing parameters

SI	65536
SF	400.2580000 MHz
WDW	EM
SSE	0
LE	0.30 Hz
GB	0
EC	1.00

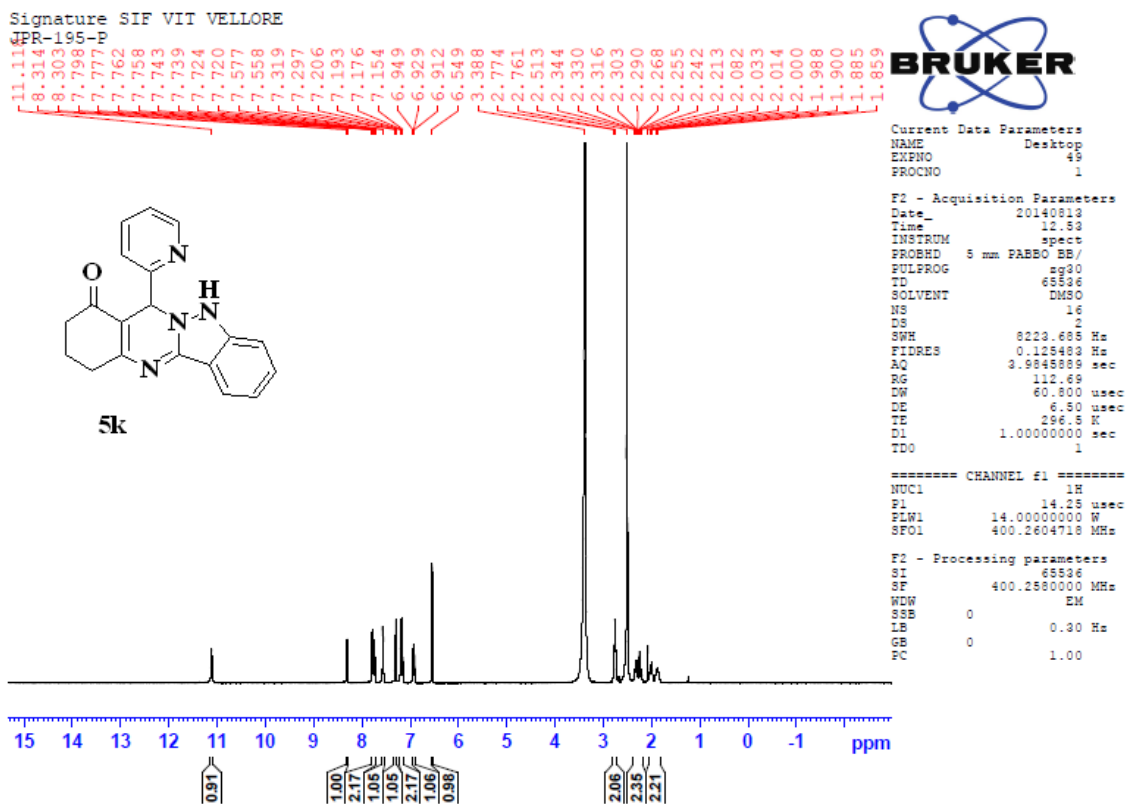
### <sup>13</sup>C NMR spectrum of compound (5j):



### HRMS spectrum of compound (5j):

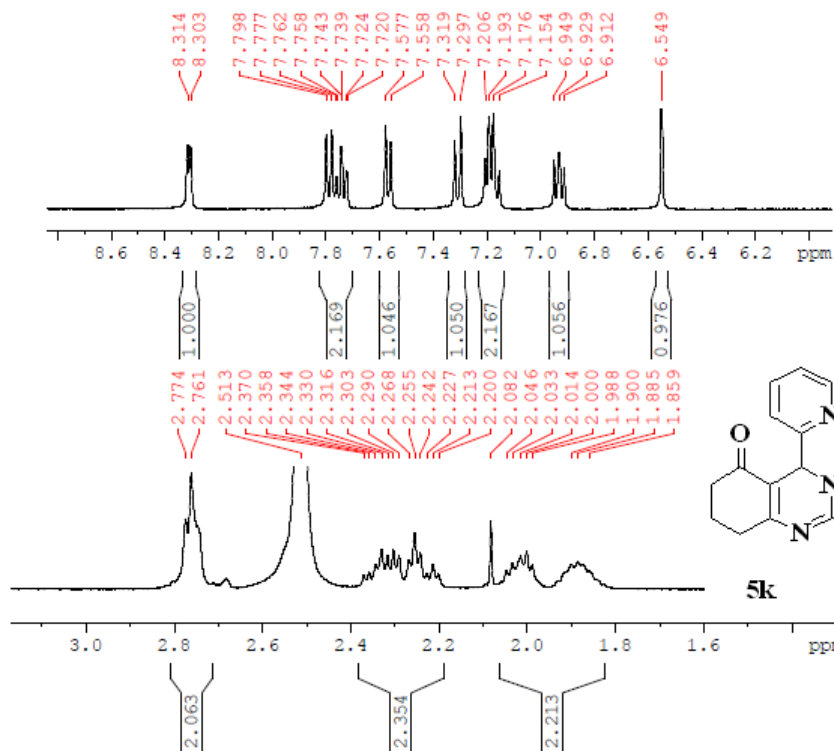


**<sup>1</sup>H NMR spectrum of compound (5k):**



# Expanded <sup>1</sup>H NMR spectrum of compound (5k):

Signature SIF VIT VELLORE  
JPR-195-P



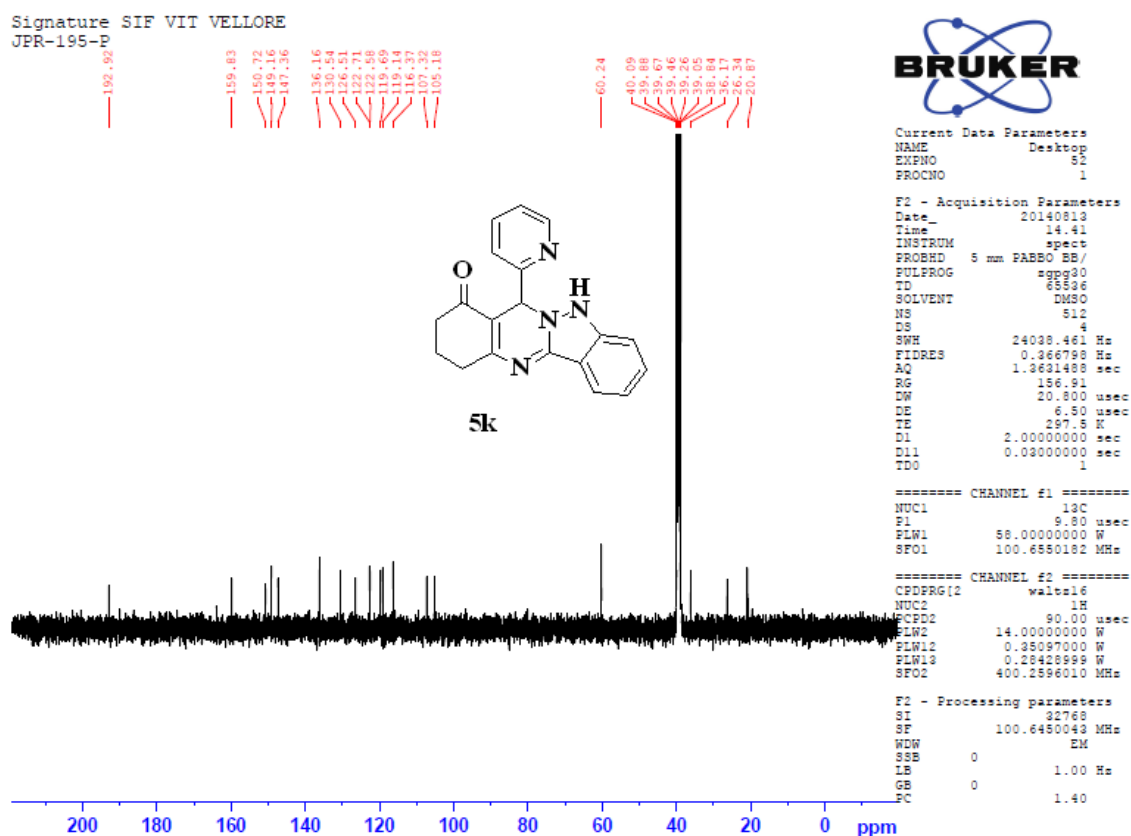
Current Data Parameters  
 NAME Desktop  
 EXPNO 49  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20140813  
 Time 12.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8223.688 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9845889 sec  
 RG 112.69  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.3 K  
 1.00000000 sec

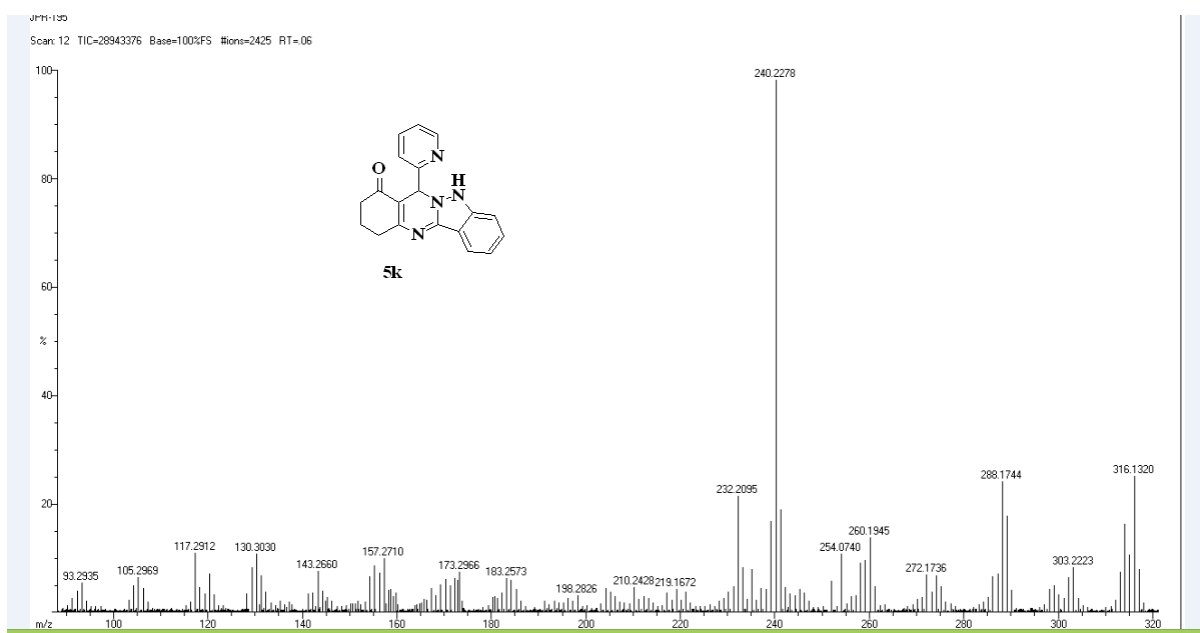
=== CHANNEL f1 =====  
 1H  
 14.25 usec  
 14.00000000 W  
 400.2604718 MHz

Processing parameters  
 65536  
 400.2580000 MHz  
 EM  
 0 0.30 Hz  
 0 1.00

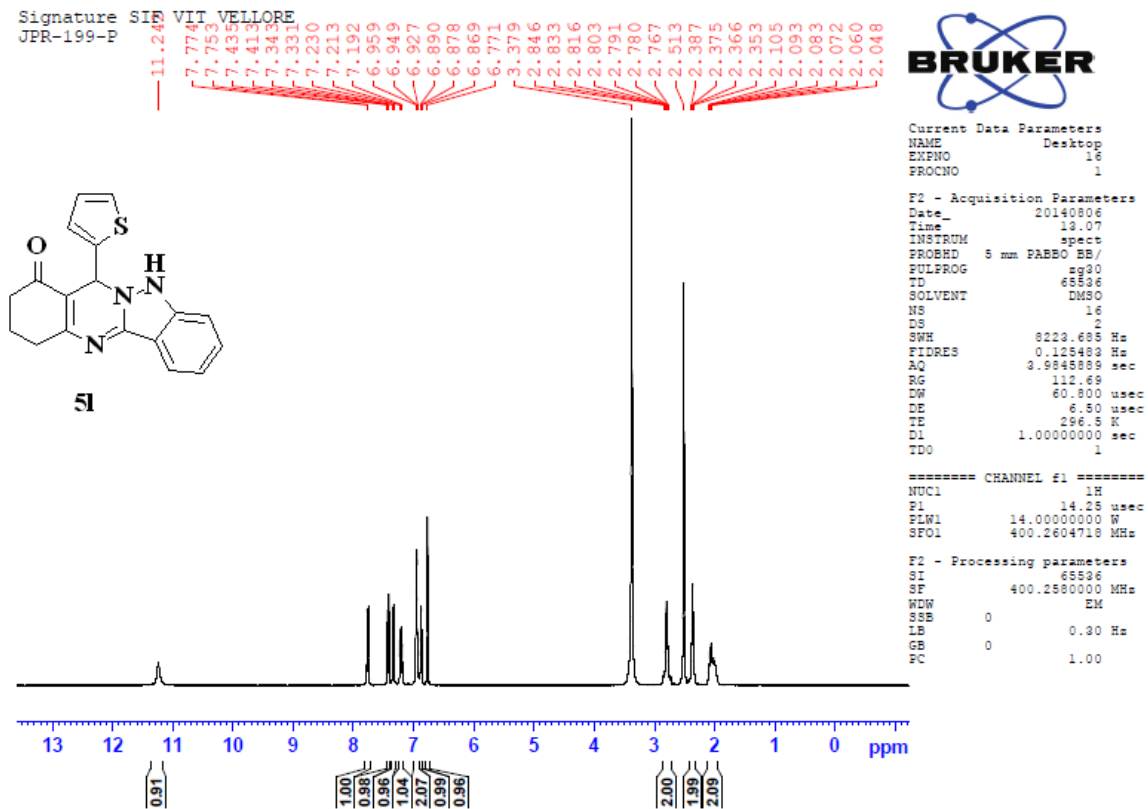
### <sup>13</sup>C NMR spectrum of compound (5k):



### HRMS spectrum of compound (5k):

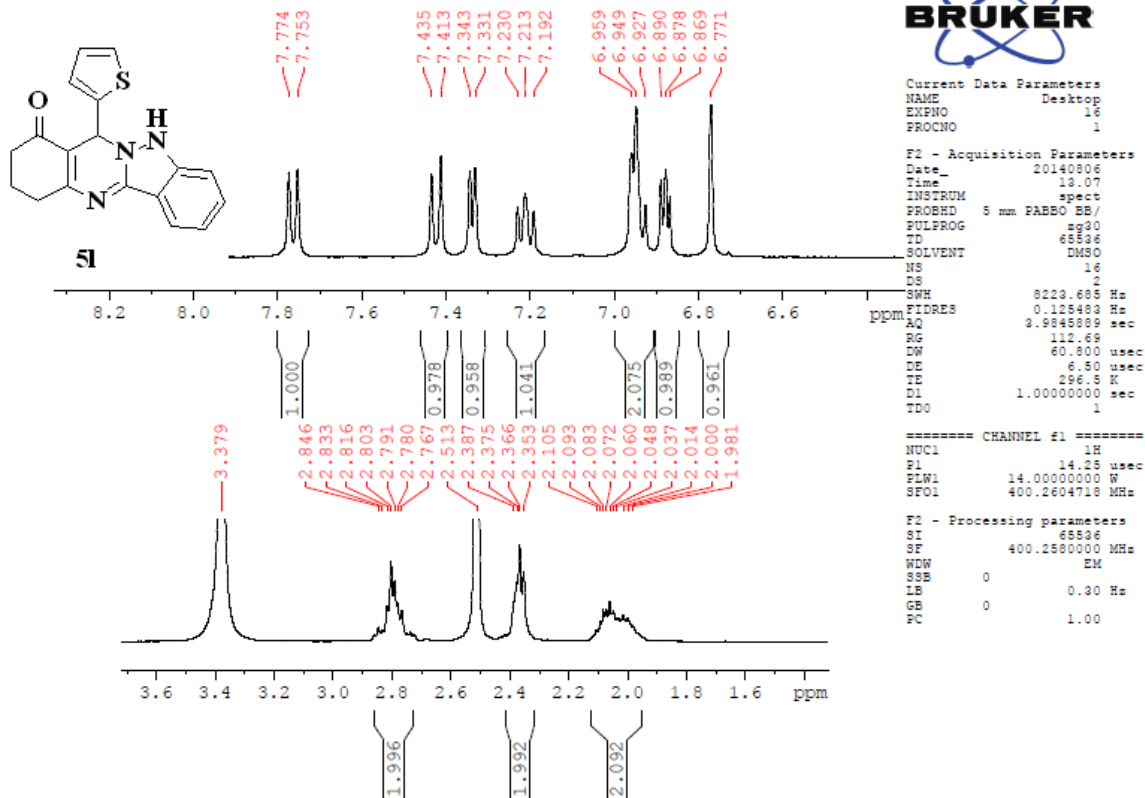


**<sup>1</sup>H NMR spectrum of compound (5l):**



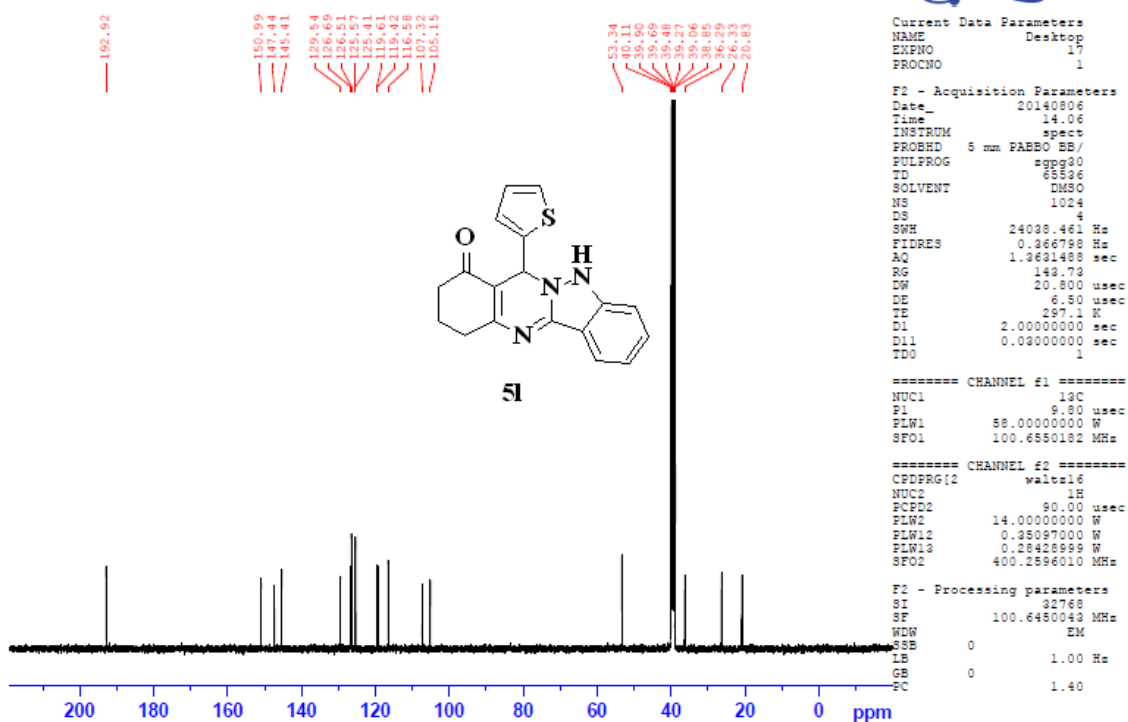
### Expanded <sup>1</sup>H NMR spectrum of compound (5l):

Signature SIF VIT VELLORE  
JPR-199-P

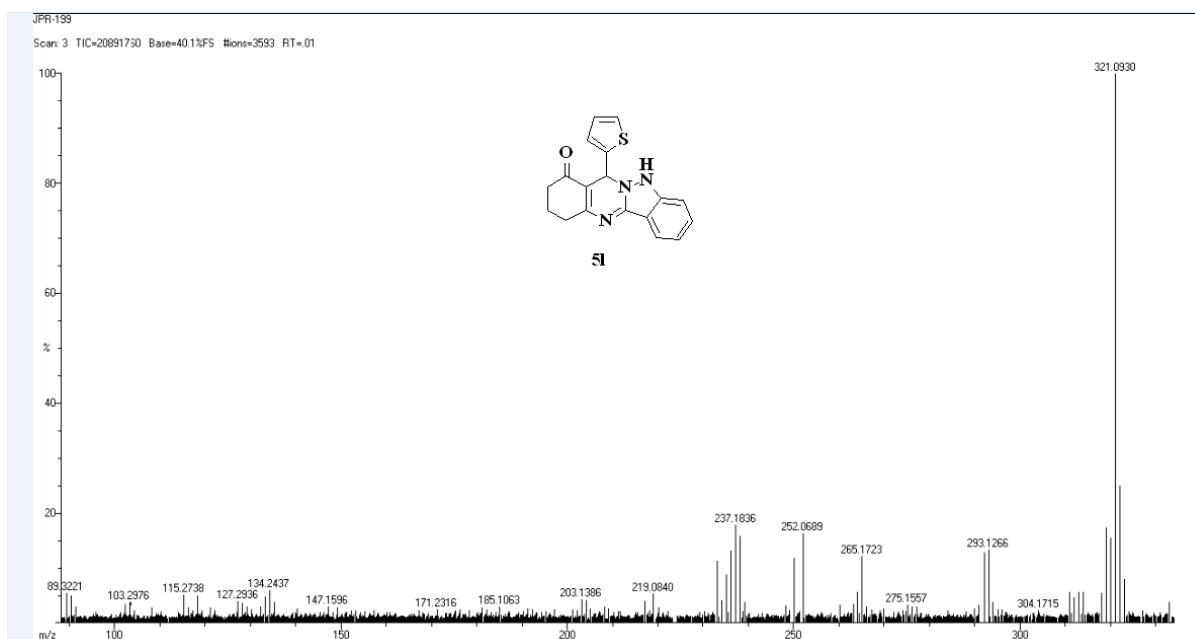


### <sup>13</sup>C NMR spectrum of compound (5I):

Signature SIF VIT VELLORE  
JPR-199-P



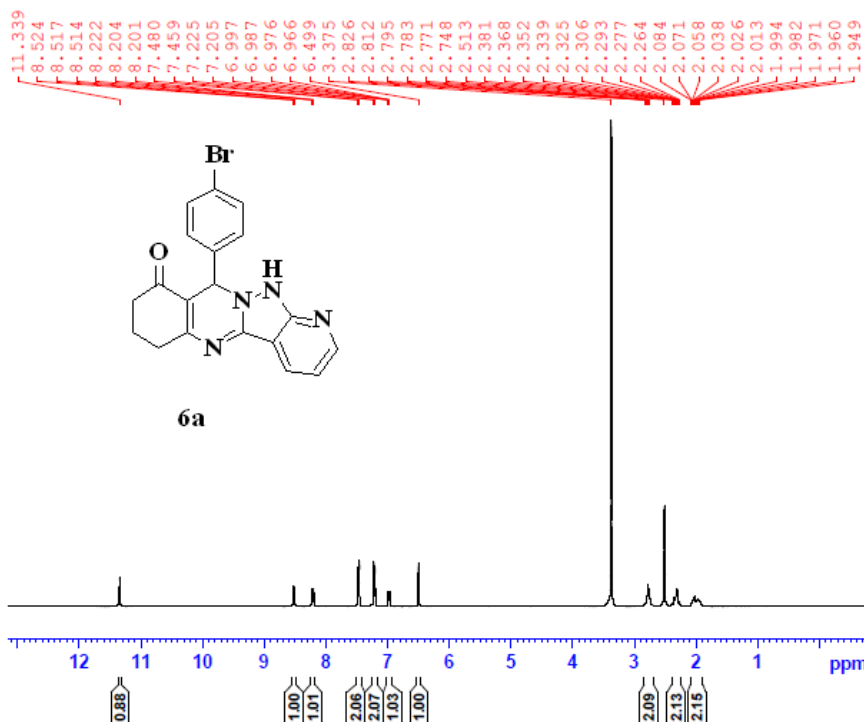
### HRMS spectrum of compound (5I):





**<sup>1</sup>H NMR spectrum of compound (6a):**

Signature SIF VIT VELLORE  
JPR-01-002-P



Current Data Parameters  
NAME Desktop  
EXPNO 109  
PROCNO 1

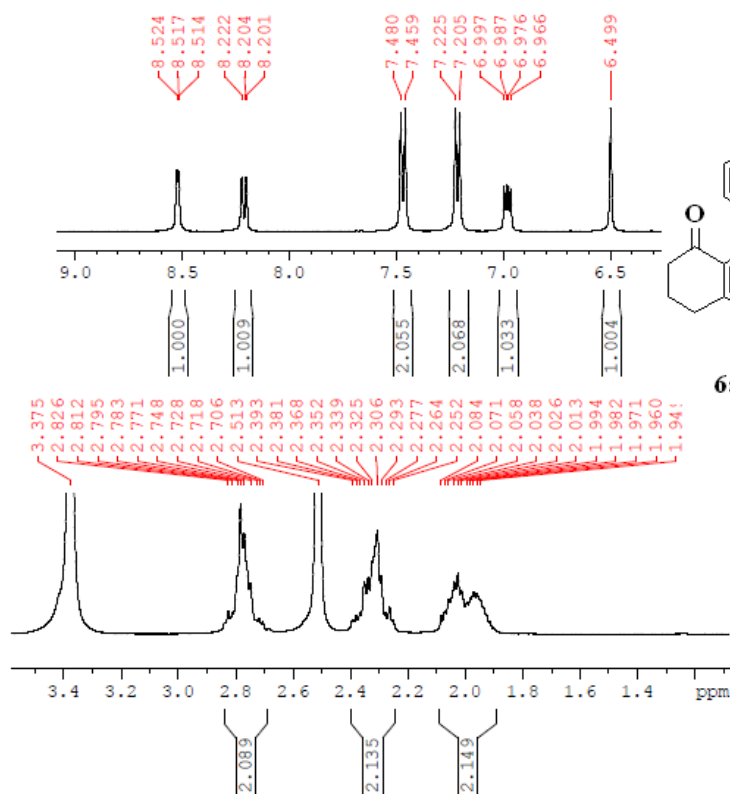
F2 - Acquisition Parameters  
Date\_ 20140731  
Time 13.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
FULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8223.686 Hz  
FIDRES 0.125483 Hz  
AQ 3.9345009 sec  
RG 112.69  
DM 60.800 usec  
DE 6.50 usec  
TE 296.6 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
PLW1 14.00000000 W  
SFO1 400.2604718 MHz

F2 - Processing parameters  
SI 65536  
SF 400.2600000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
FC 1.00

## Expanded <sup>1</sup>H NMR spectrum of compound (6a):

Signature SIF VIT VELLORE  
JPR-01-002-P



Current Data Parameters  
NAME Desktop  
EXPNO 109  
XCNO 1

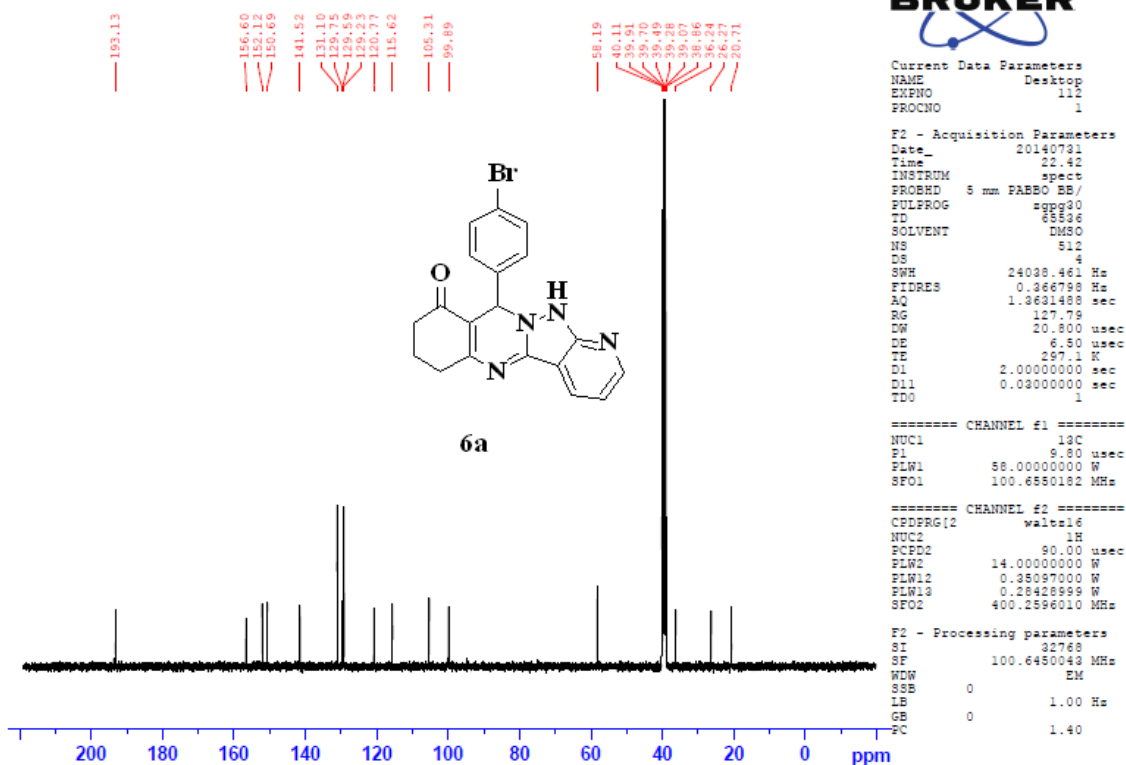
- Acquisition Parameters  
se\_ 20140731  
sc 13.23  
SRUM spect  
XRD 5 mm PABBO BB/  
LPROG zg30  
LVENT 65536  
DMSO 16

F2 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

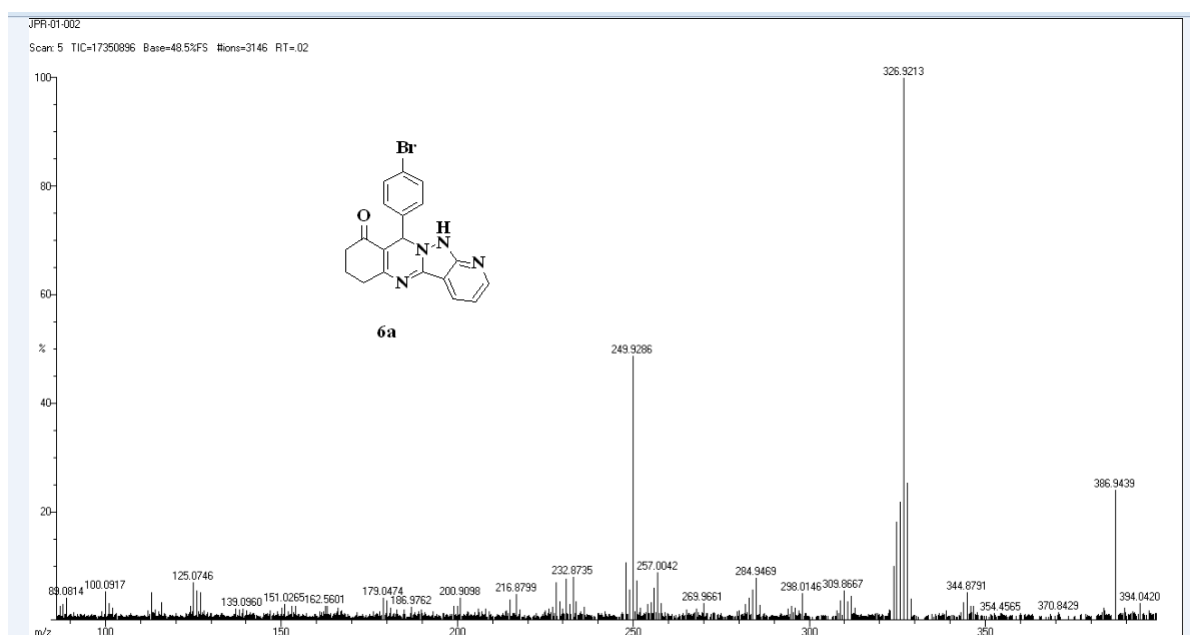
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
PLW1 14.00000000 W  
SFO1 400.2604718 MHz

### <sup>13</sup>C NMR spectrum of compound (6a):

Signature SIF VIT VELLORE  
JPR-01-002-P

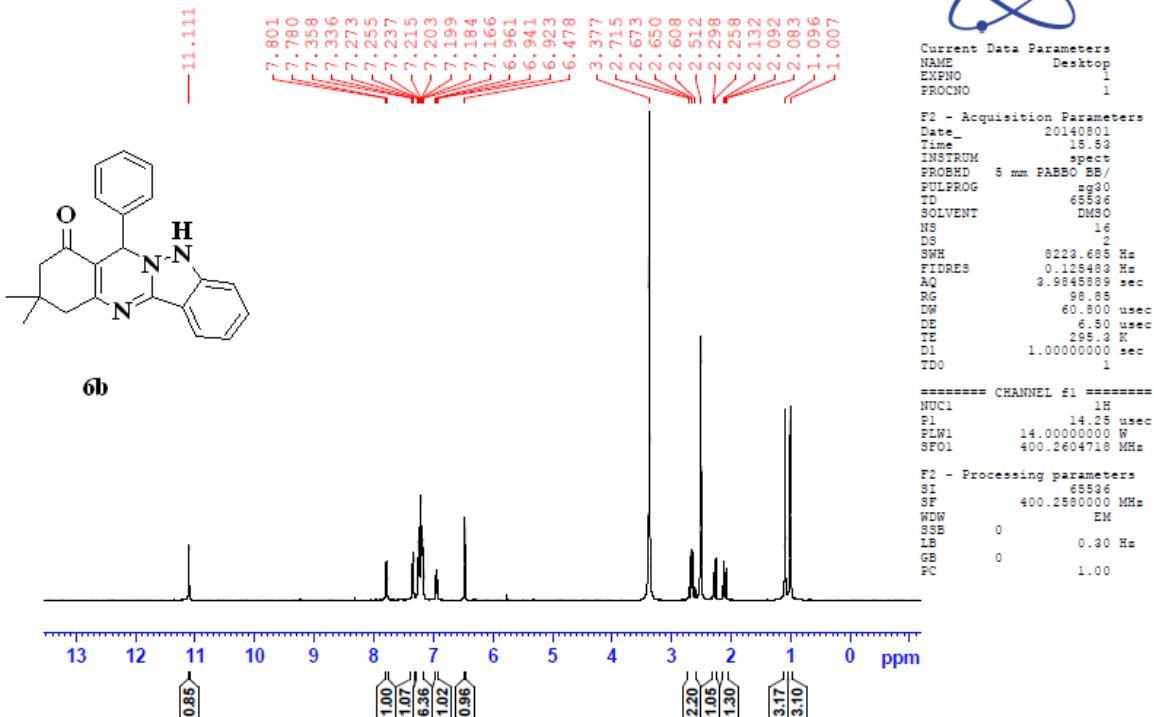


### HRMS spectrum of compound (6a):



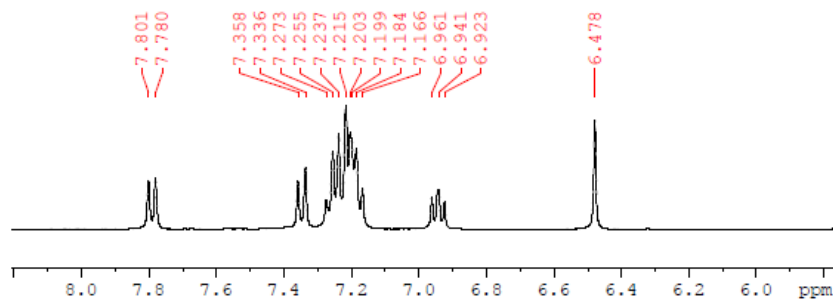
**<sup>1</sup>H NMR spectrum of compound (6b):**

Signature SIF VIT VELLORE  
JPR-202-P



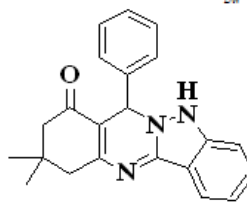
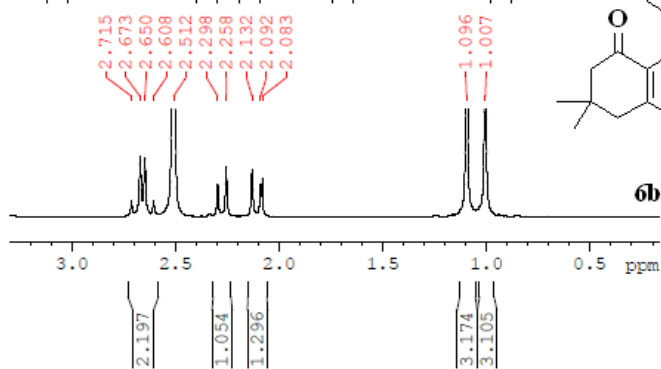
# Expanded <sup>1</sup>H NMR spectrum of compound (6b):

Signature SIF VIT VELLORE  
JPR-202-P



Current Data Parameters  
NAME Desktop  
EXNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140801  
Time 15.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8223.688 Hz  
FIDRES 0.125489 Hz  
AQ 3.9848889 sec  
RG 88.88  
RG 88.88  
DW 60.800 usec  
6.50 usec  
295.3 K  
1.00000000 sec  
1

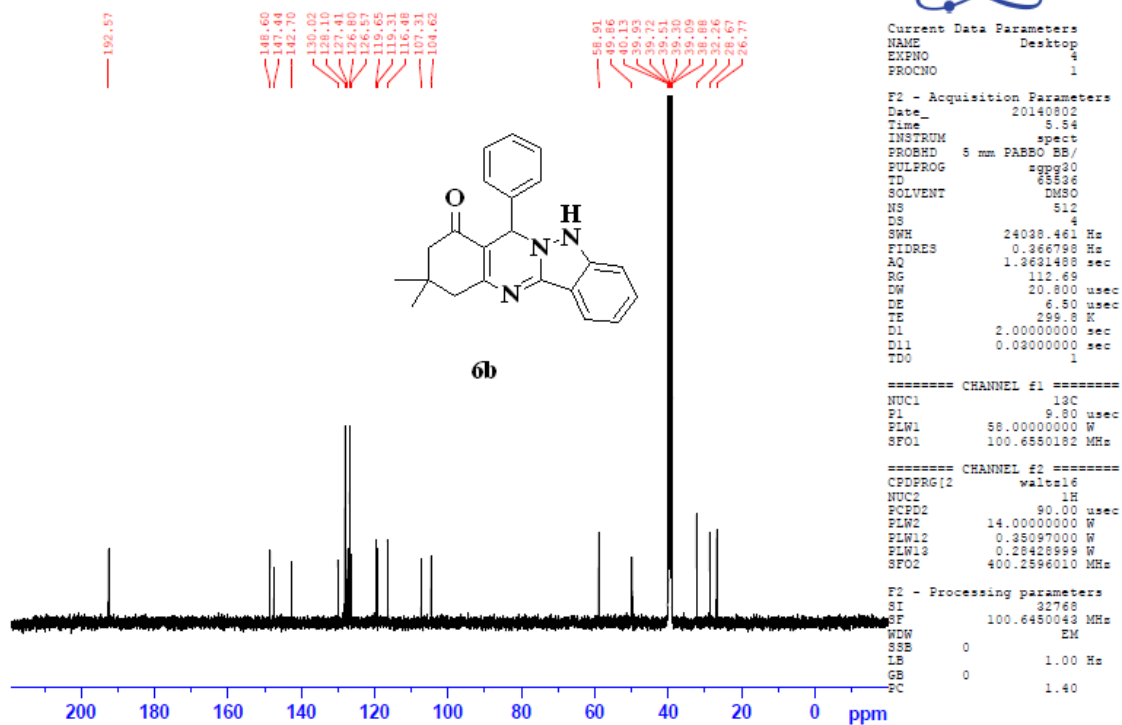


==== CHANNEL f1 =====  
1H  
14.25 usec  
14.00000000 W  
400.2604718 MHz

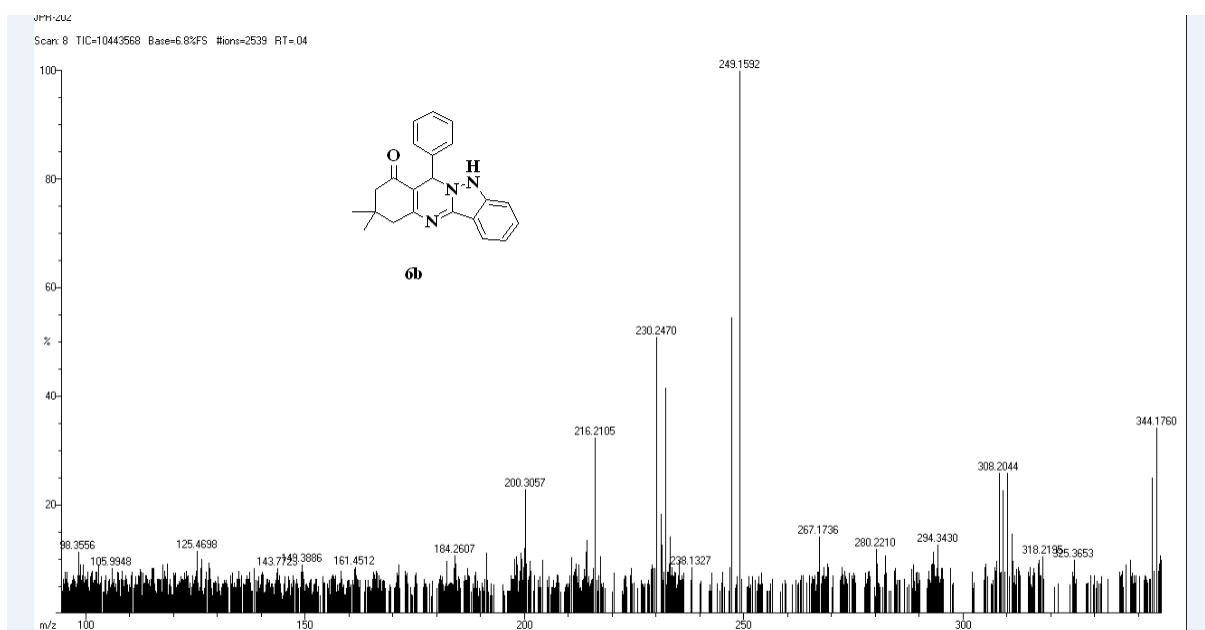
Processing parameters  
65536  
400.2580000 MHz  
EM  
0 0.30 Hz  
0 1.00

### <sup>13</sup>C NMR spectrum of compound (6b):

Signature SIF VIT VELLORE  
JPR-202-P

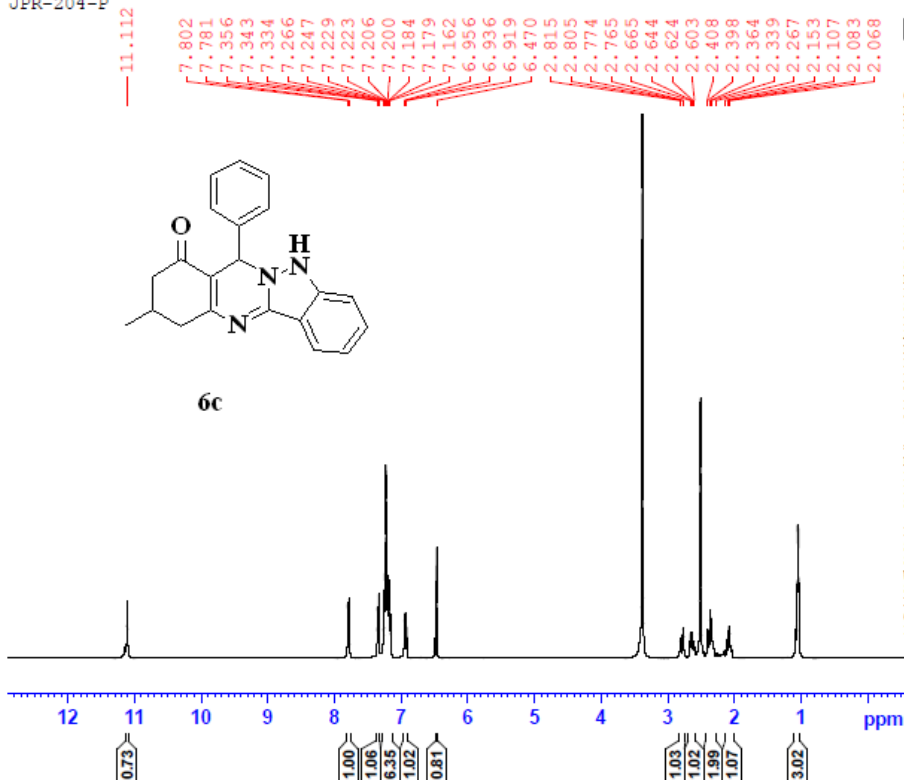
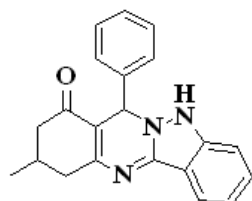


### HRMS spectrum of compound (6b):



**<sup>1</sup>H NMR spectrum of compound (6c):**

Signature SIF VIT VELLORE  
JPR-204-P



Current Data Parameters  
NAME Desktop  
EXFNO 3  
PROCNO 1

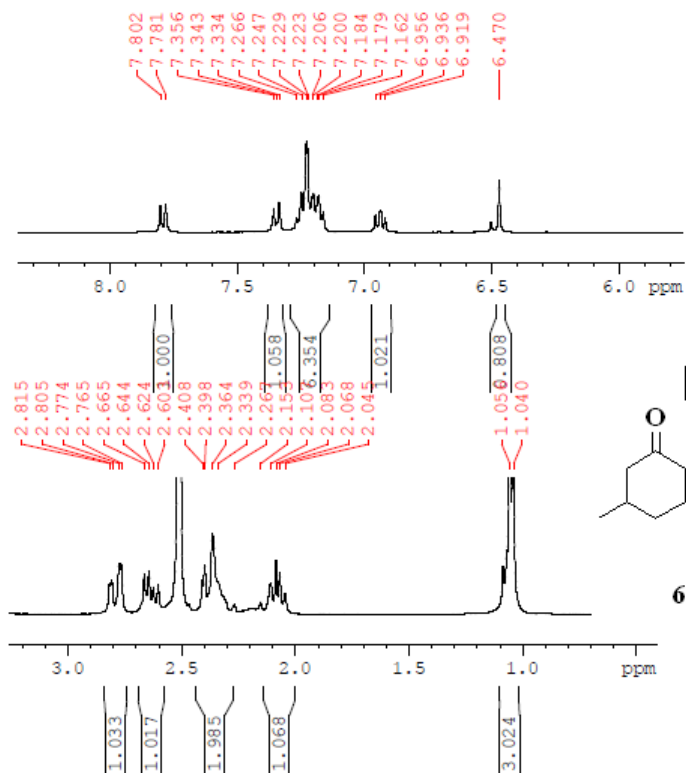
F2 - Acquisition Parameters  
Date\_ 20140801  
Time 16.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8228.698 Hz  
FIDRES 0.125493 Hz  
AQ 3.9845889 sec  
RG 88.68  
DW 60.800 usec  
DE 6.50 usec  
TE 295.4 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
PLW1 14.00000000 W  
SFO1 400.2604718 MHz

F2 - Processing parameters  
SI 65536  
SF 400.2580000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### Expanded <sup>1</sup>H NMR spectrum of compound (6c):

Signature SIF VIT VELLORE  
JPR-204-P

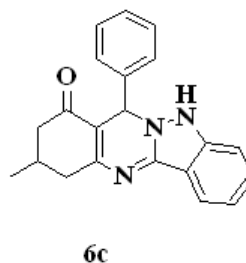


Current Data Parameters  
NAME Desktop  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140801  
Time 16.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8223.688 Hz  
FIDRES 0.125489 Hz  
AQ 3.9845009 sec  
RG 88.69  
W 60.800 usec  
E 6.50 usec  
E 295.4 K  
l 1.000000000 sec  
DO 1

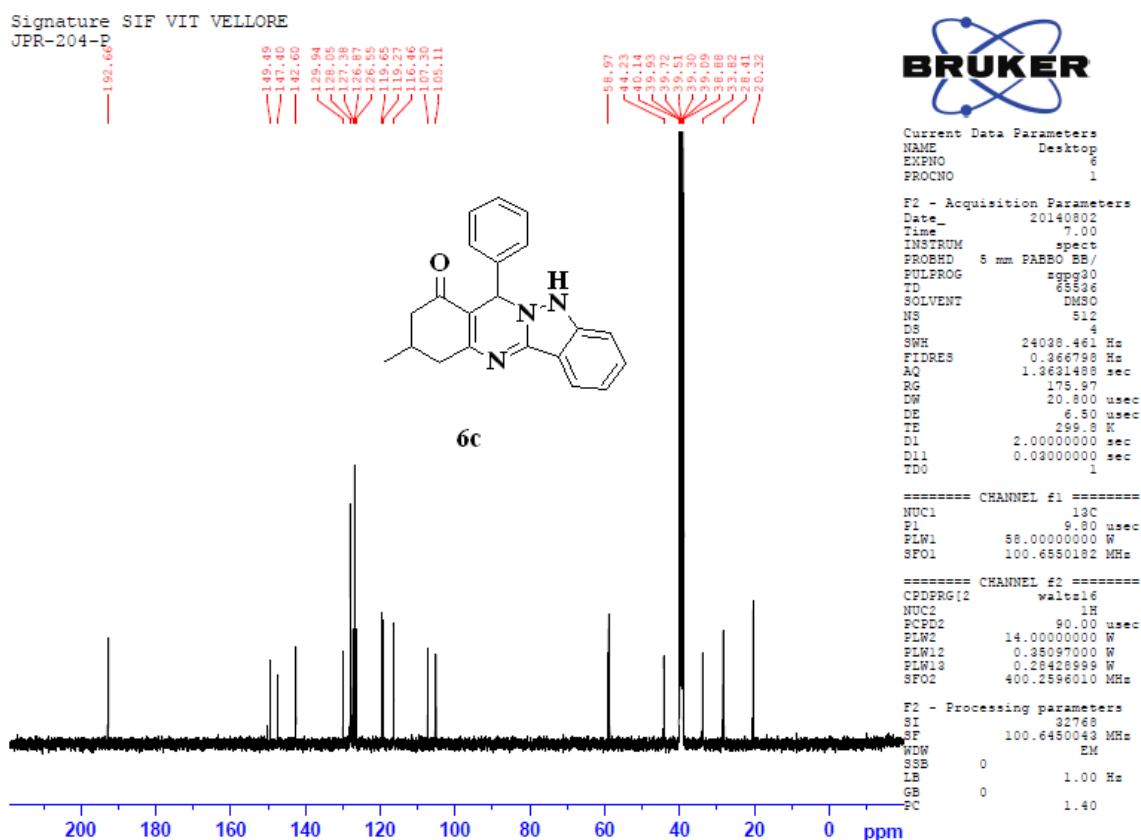
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.25 usec  
LM1 14.00000000 W  
FOL1 400.2604718 MHz

2 - Processing parameters  
SI 65536  
DF 400.2580000 MHz  
WDW EM  
SS 0  
B 0.20 Hz  
S 0  
F 1.00

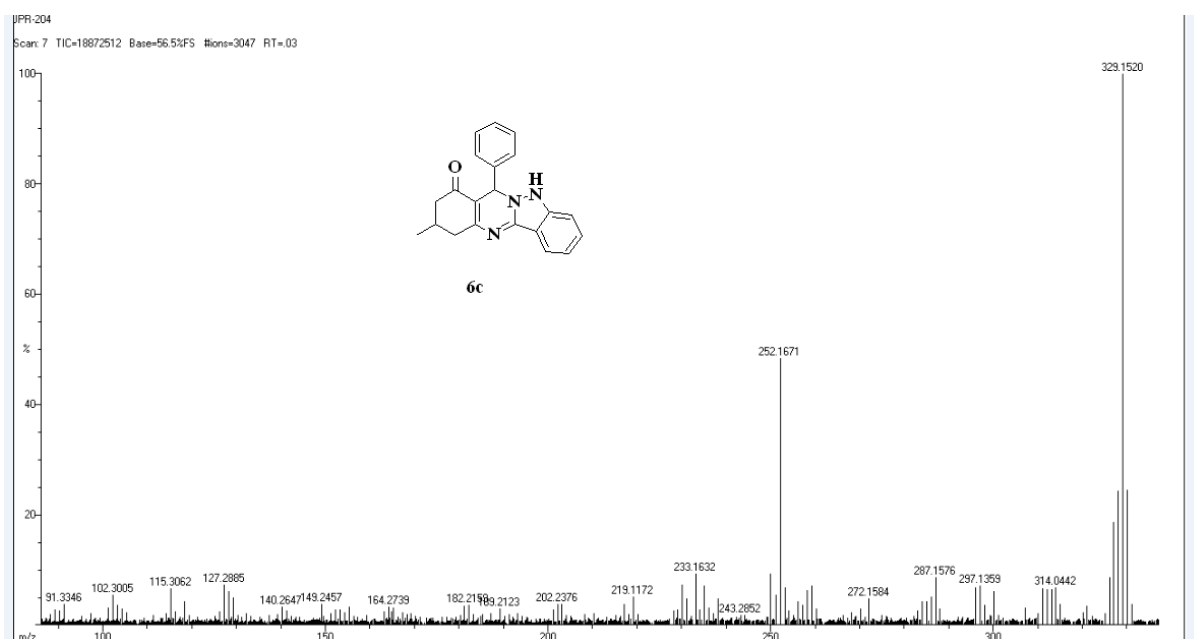




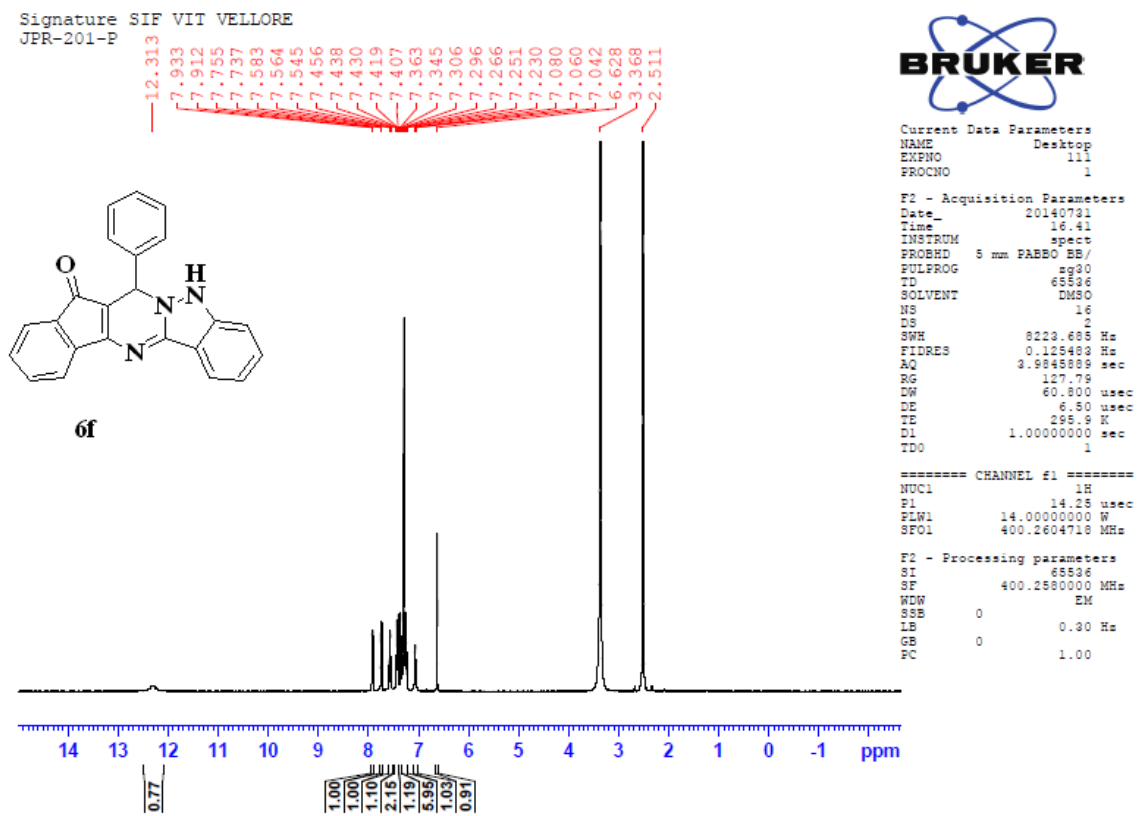
### <sup>13</sup>C NMR spectrum of compound (6c):



### HRMS spectrum of compound (6c):

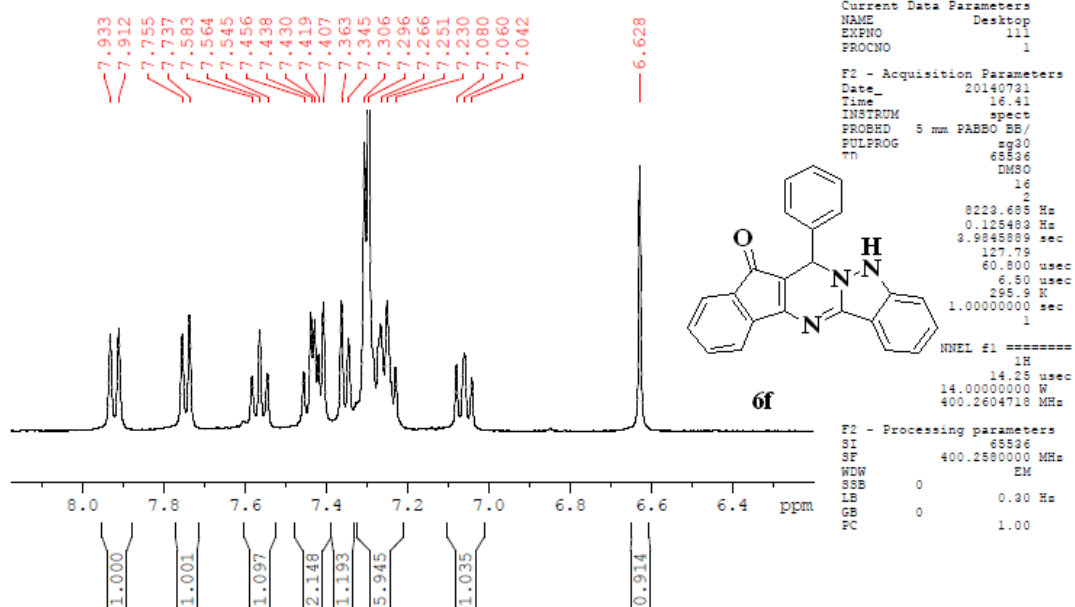


**<sup>1</sup>H NMR spectrum of compound (6f):**



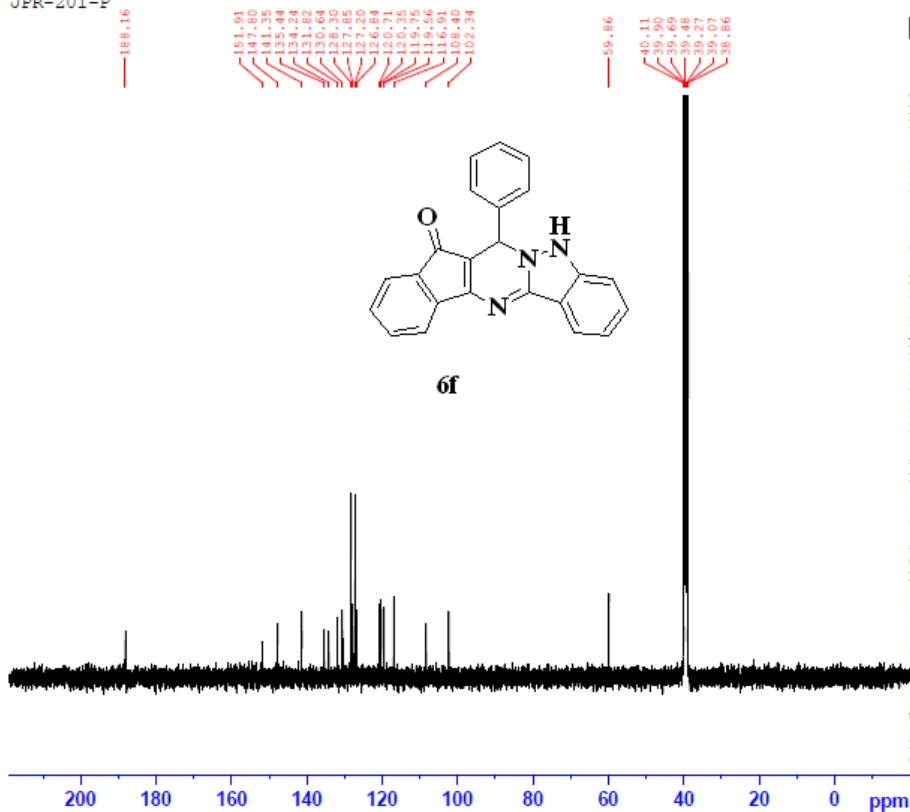
## Expanded <sup>1</sup>H NMR spectrum of compound (6f):

Signature SIF VIT VELLORE  
JPR-201-P



### <sup>13</sup>C NMR spectrum of compound (6f):

Signature SIF VII VELLORE  
JPR-201-P



Current Data Parameters  
NAME Desktop  
EXPNO 114  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140801  
Time 1.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 186.91  
DM 20.800 usec  
DE 6.50 usec  
TE 297.1 K  
DL 2.0000000 sec  
Dl1 0.0300000 sec  
TDO 1

==== CHANNEL #1 =====  
NUC1 13C  
P1 9.80 usec  
PLW1 58.0000000 W  
SFO1 100.6250182 MHz

==== CHANNEL #2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PLW2 14.0000000 W  
PLW3 0.2842899 W  
SFO2 400.2596010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6250043 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

### HRMS spectrum of compound (6f):

