

Supporting Information

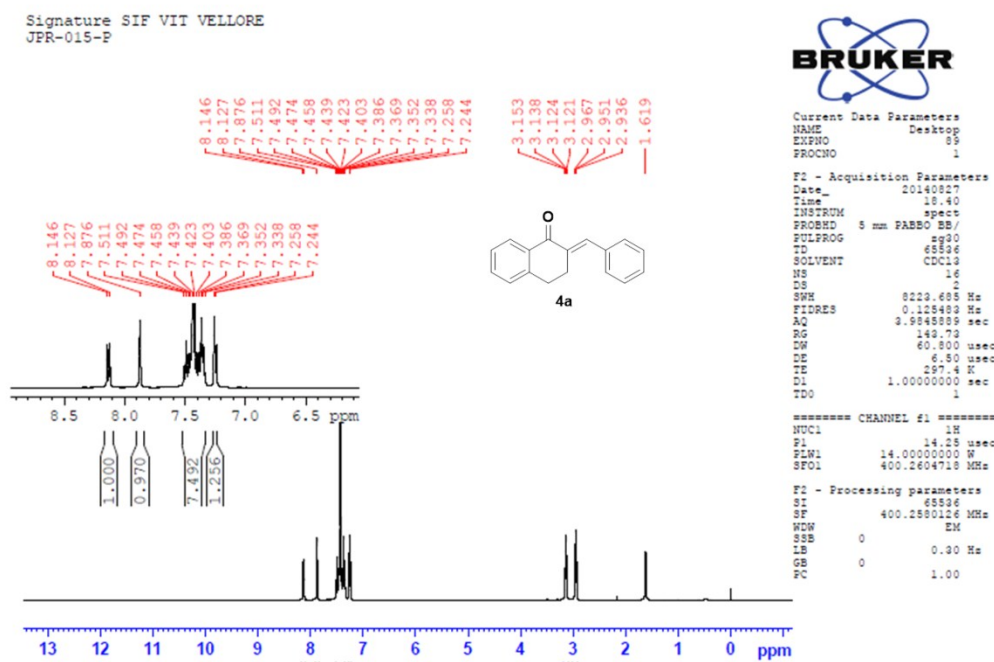
UV-Light induced Domino type reactions: Synthesis and photo physical properties of unreported nitrogen ring junction triazoloquinazolines

Jeyakannu Palaniraja and Selvaraj Mohana Roopan*

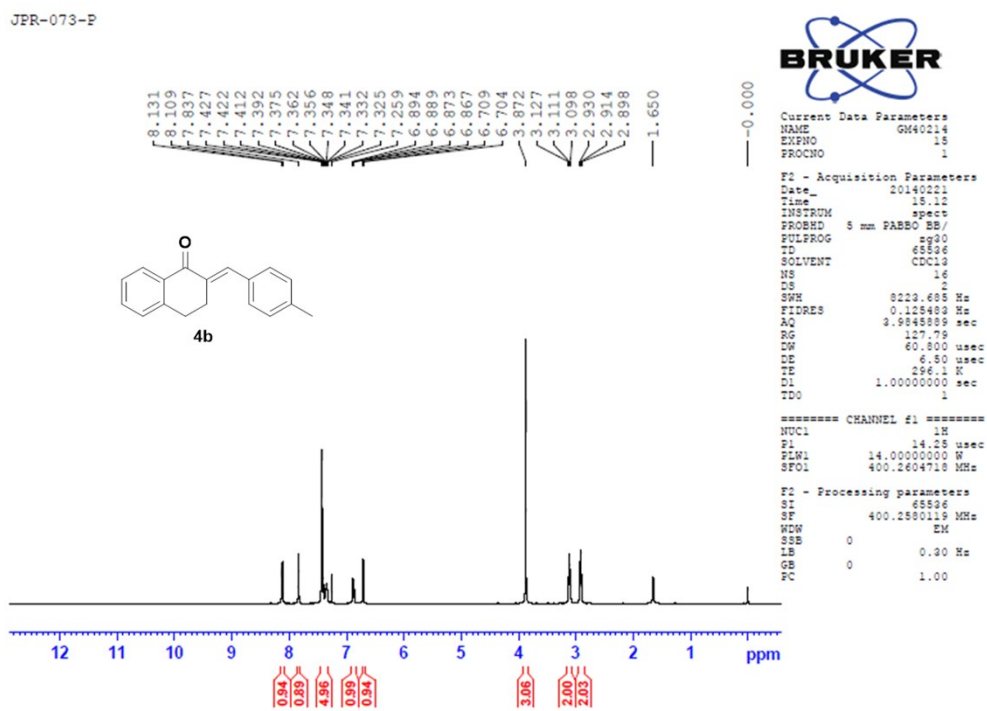
Chemistry Research Laboratory, Organic Chemistry Division, School of Advanced Sciences,
VIT University, Vellore, Tamil Nadu-632014, India. Email: mohanaroopan.s@gmail.com;
Fax: +91-416-224-3092; Tel: +0416-220-2352.

Copies of ^1H NMR of 3(a-v)

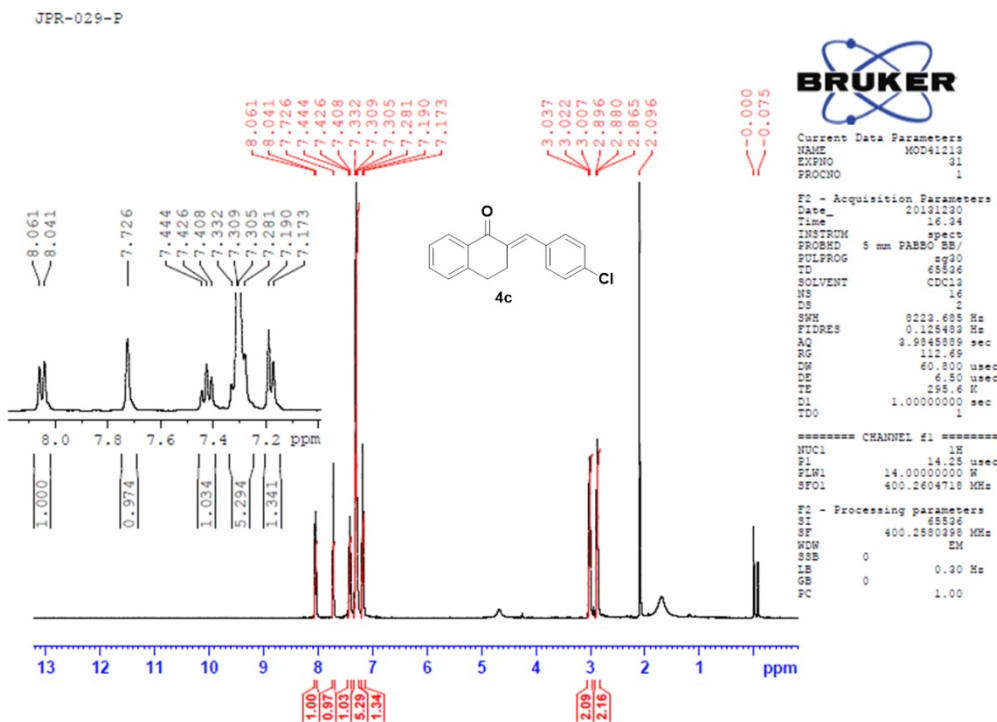
^1H NMR spectrum of compound (3a):



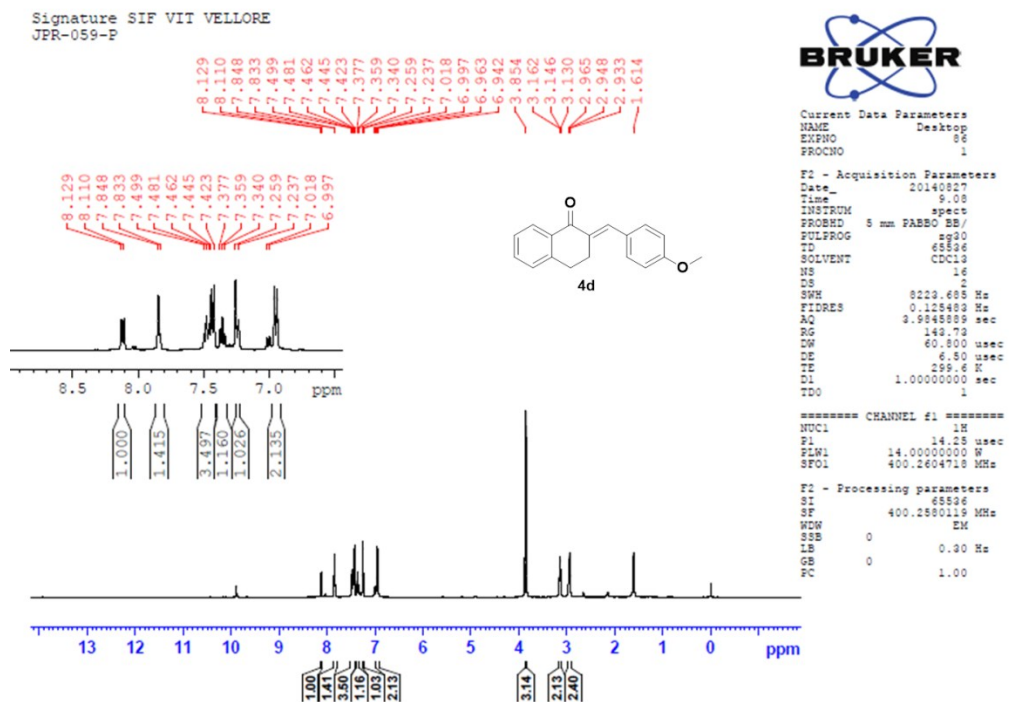
^1H NMR spectrum of compound (3b):



¹H NMR spectrum of compound (3c):

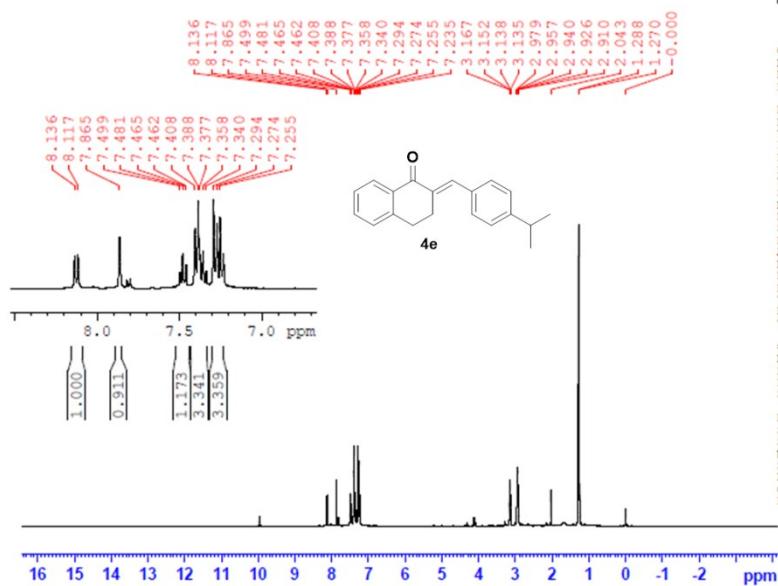


¹H NMR spectrum of compound (3d):



¹H NMR spectrum of compound (3e):

Signature SIF VIT VELLORE
JPR-101-P



Current Data Parameters
NAME Desktop
EXPNO 47
PROCNO 1

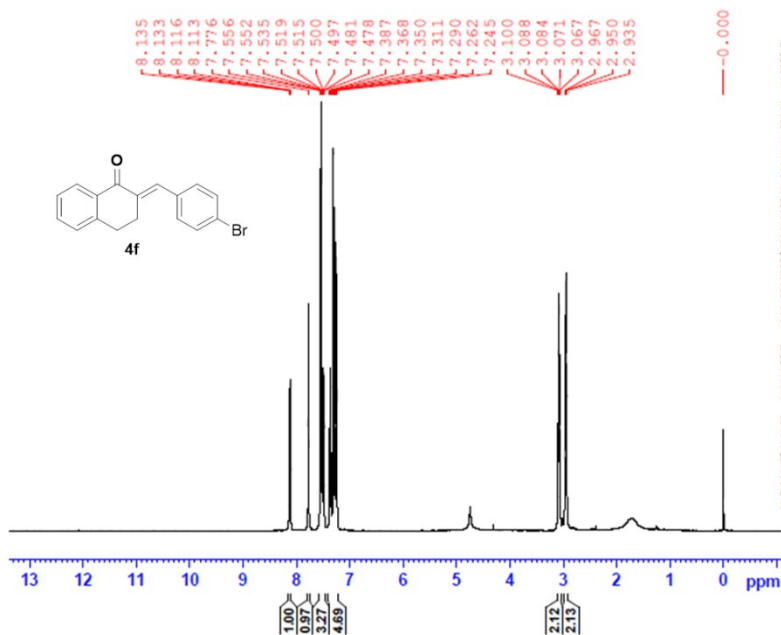
F2 - Acquisition Parameters
Date_ 20140819
Time 12.46
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125489 Hz
AQ 3.9545889 sec
RG 96.88
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
DL 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SF01 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

¹H NMR spectrum of compound (3f):

Signature SIF VIT VELLORE
JPR-126-P



Current Data Parameters
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EXPNO 9
PROCNO 1

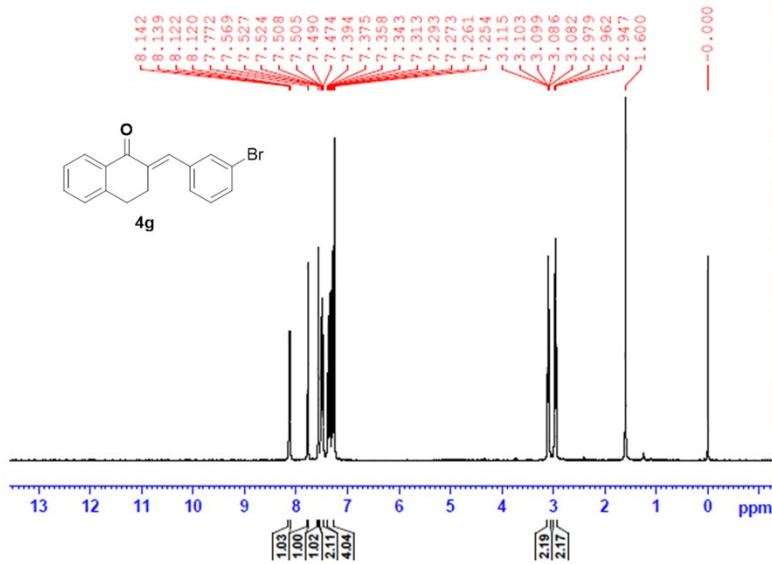
F2 - Acquisition Parameters
Date_ 20140610
Time 14.57
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125489 Hz
AQ 3.9545889 sec
RG 96.88
DW 60.800 usec
DE 6.50 usec
TE 296.1 K
DL 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SF01 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

¹H NMR spectrum of compound (3g):

Signature SIF VIT VELLORE
JPR-122-P



Current Data Parameters
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EXPNO 3
PROCNO 1

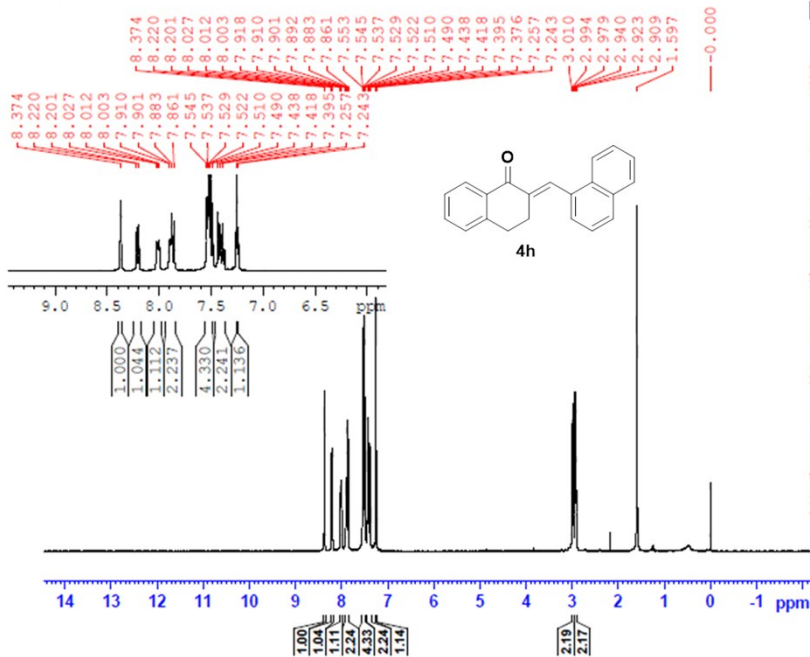
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Time 17.34
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.655 Hz
FIDRES 0.125493 Hz
AQ 2.984889 sec
RG 156.91
DW 60.800 usec
DE 6.30 usec
TE 295.8 K
DL 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.260110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of compound (3h):

Signature SIF VIT VELLORE
JPR-133-P



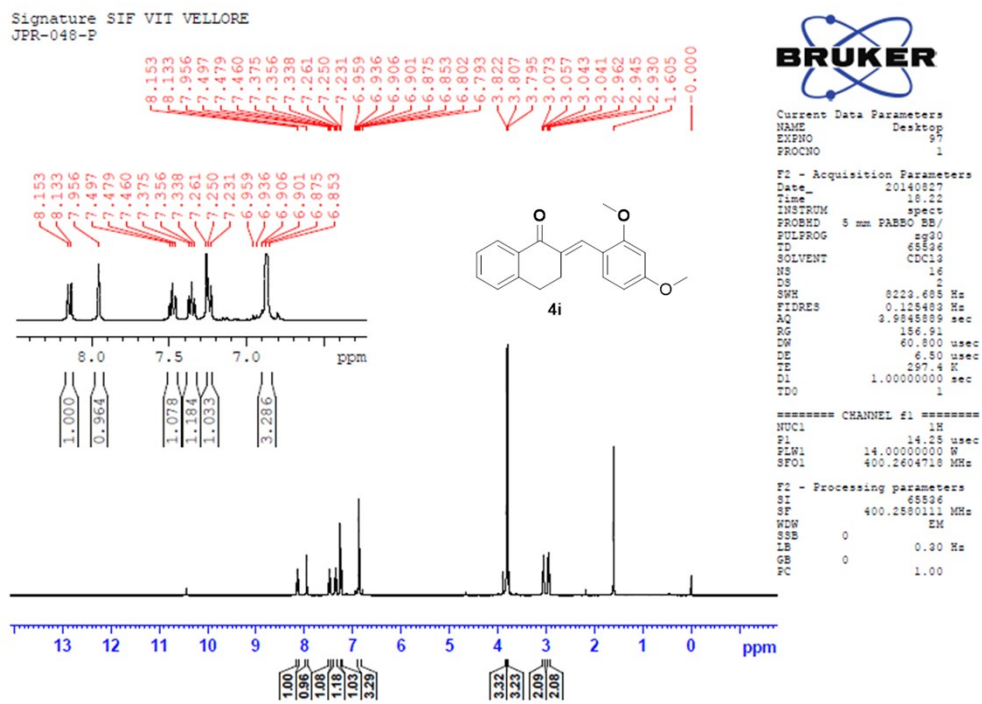
Current Data Parameters
NAME Destrop
EXPNO 98
PROCNO 1

F2 - Acquisition Parameters
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Time 18.26
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PROBHD 5 mm FAPBBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.655 Hz
FIDRES 0.125493 Hz
AQ 2.984889 sec
RG 156.91
DW 60.800 usec
DE 6.30 usec
TE 297.8 K
DL 1.0000000 sec
TDO 1

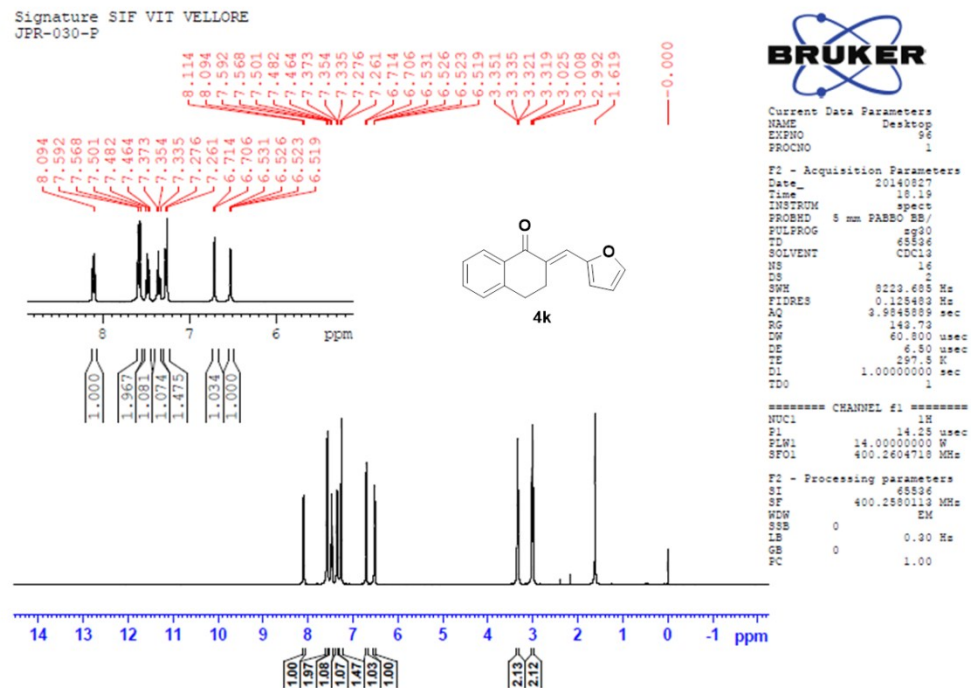
===== CHANNEL f1 =====
NUC1 1H
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PLW1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
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SF 400.260110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

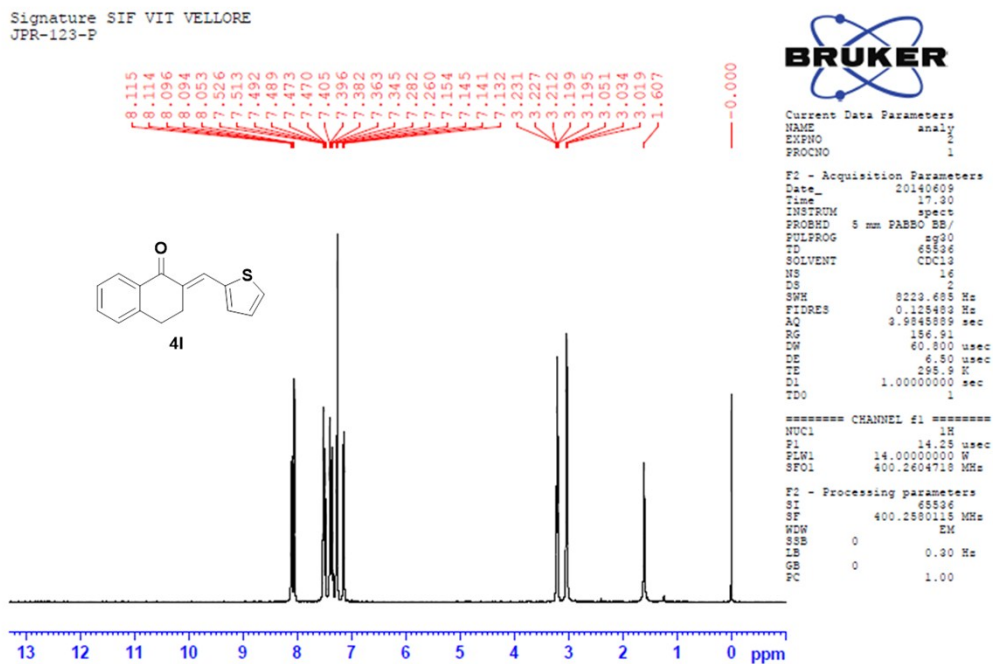
¹H NMR spectrum of compound (3i):



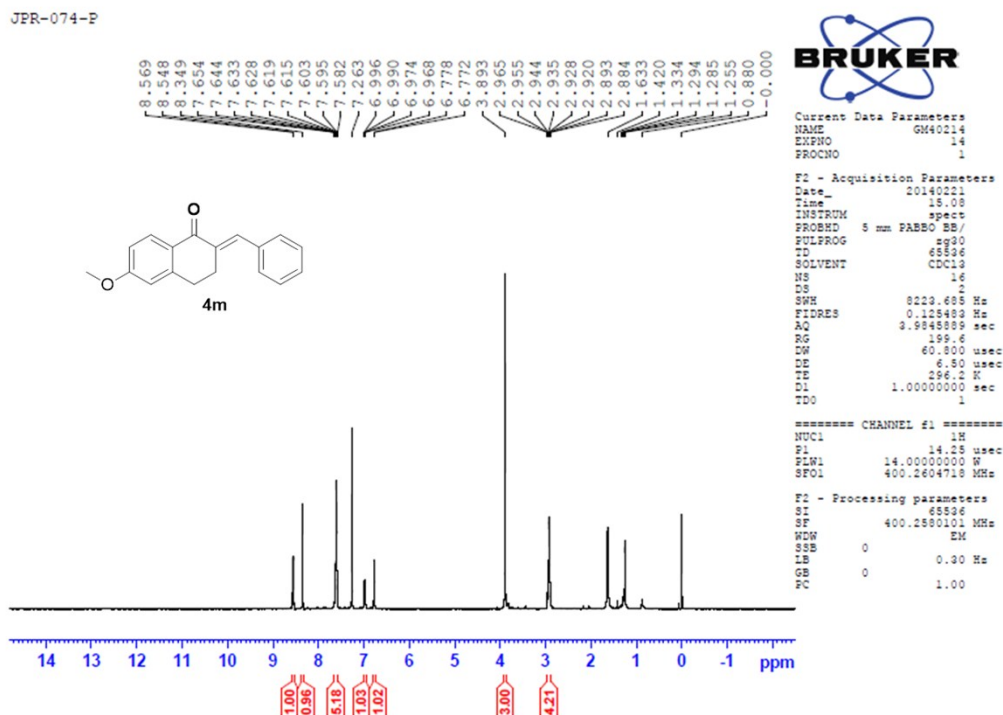
¹H NMR spectrum of compound (3k):



¹H NMR spectrum of compound (3l):

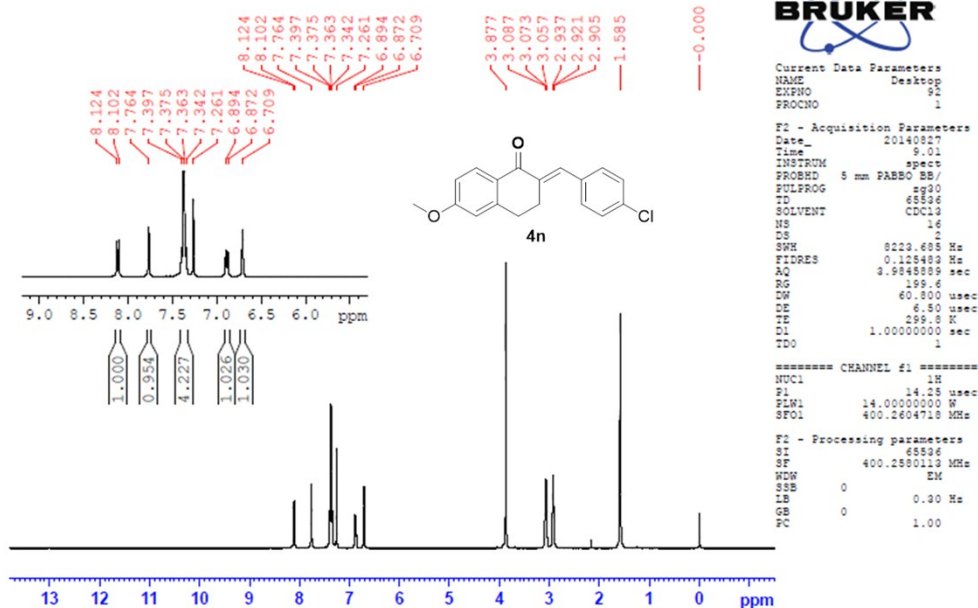


¹H NMR spectrum of compound (3m):



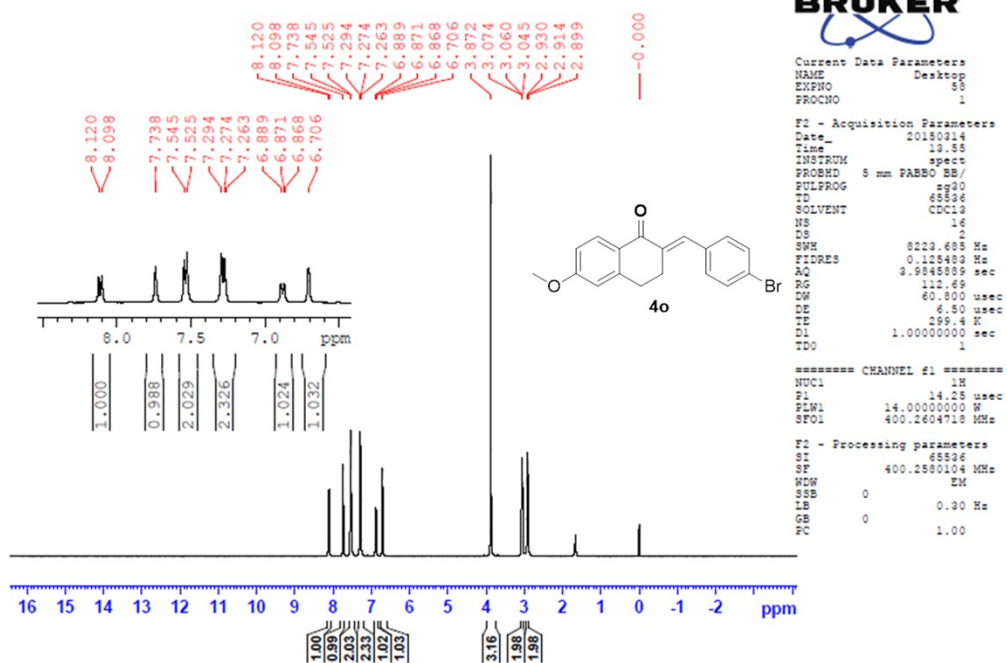
¹H NMR spectrum of compound (3n):

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JPR-086-P

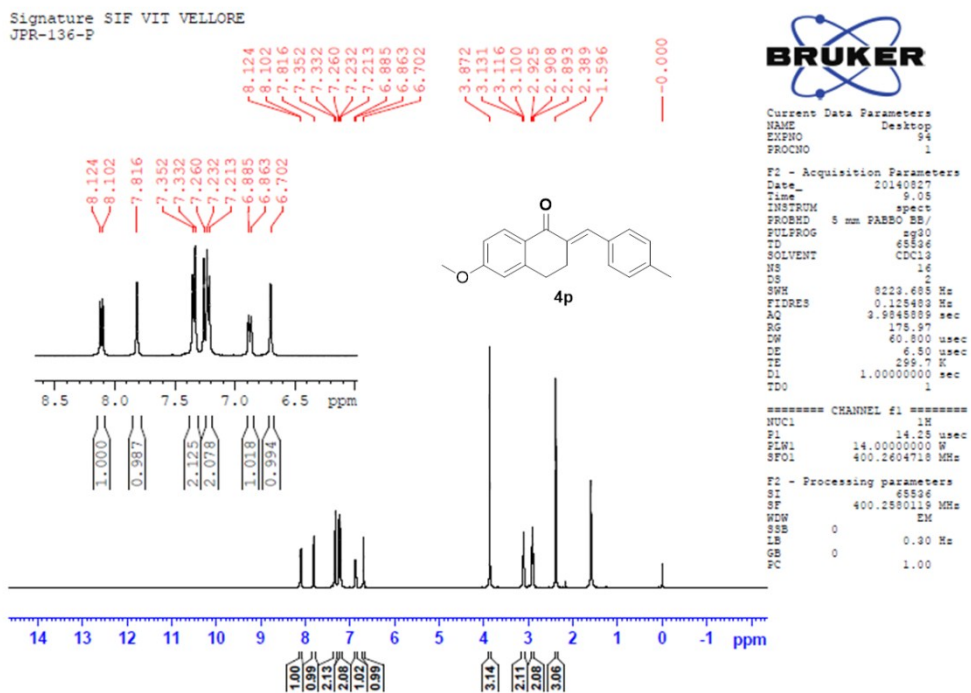


¹H NMR spectrum of compound (3o):

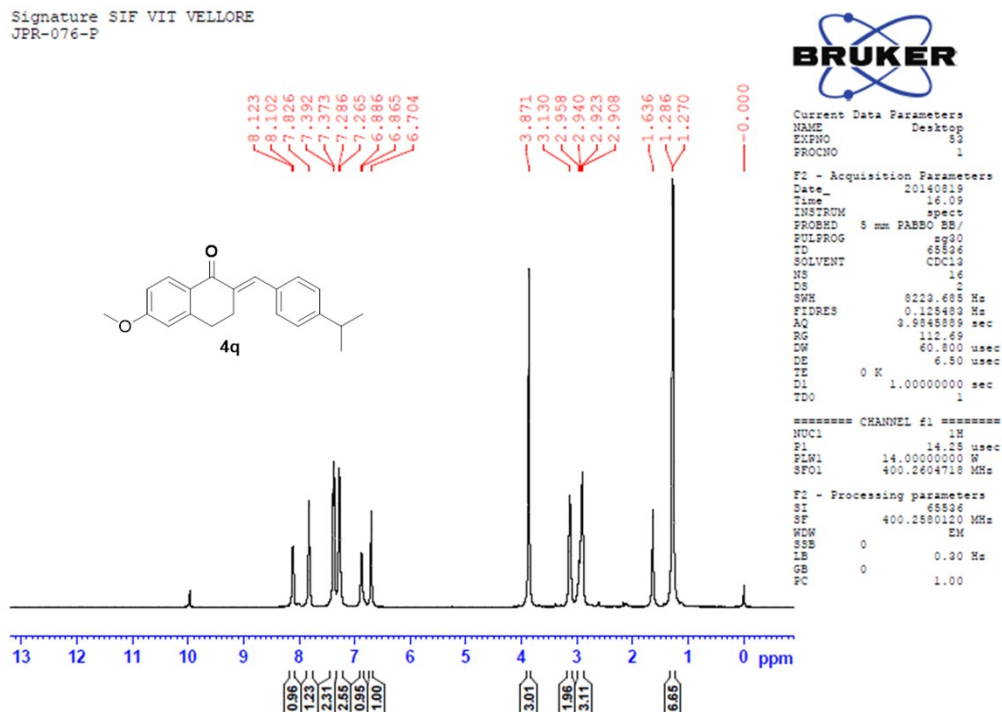
Signature SIF VIT VELLORE
JPR-135-P



¹H NMR spectrum of compound (3p):

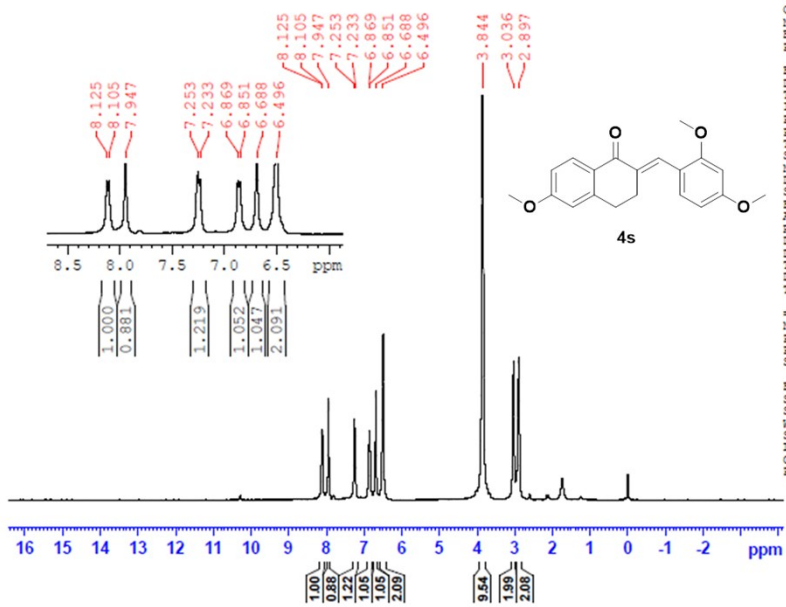


¹H NMR spectrum of compound (3q):



¹H NMR spectrum of compound (3s):

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JPR-136-P



Current Data Parameters
NAME Desktop
EXPNO 56
PROCNO 1

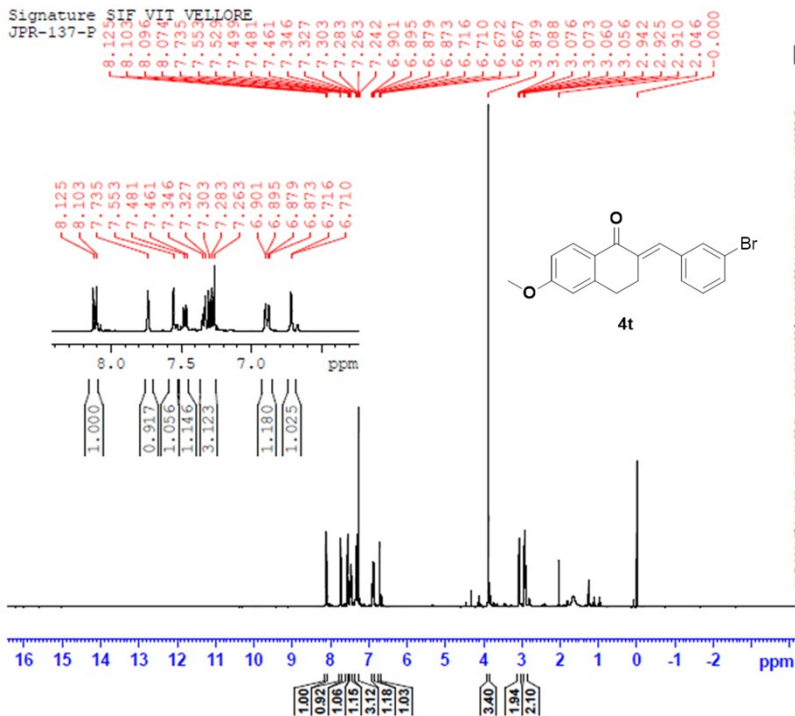
F2 - Acquisition Parameters
Date_ 20150314
Time 13.48
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125498 Hz
AQ 3.9845889 sec
RG 77.73
DW 60.800 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.260103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of compound (3t):

Signature SIF VIT VELLORE
JPR-137-P



Current Data Parameters
NAME Desktop
EXPNO 57
PROCNO 1

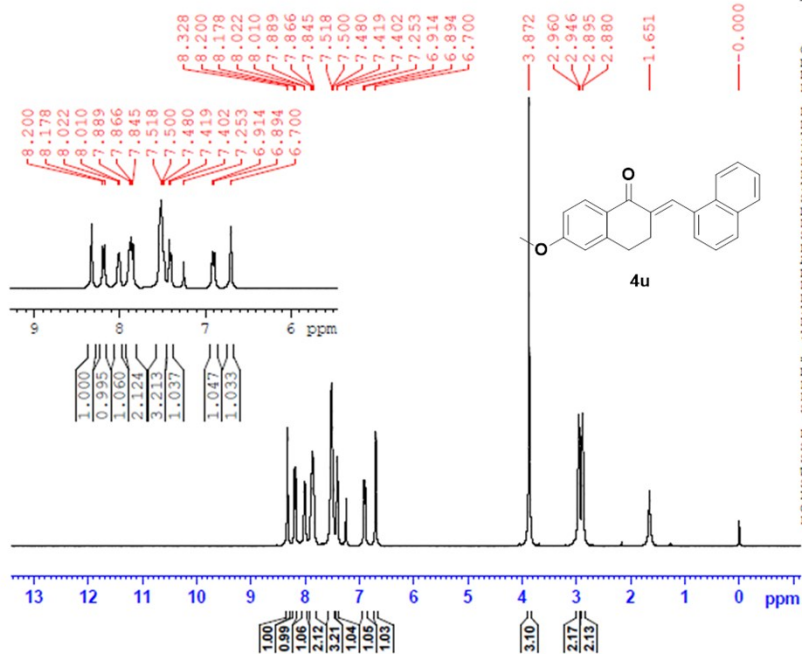
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Time 13.52
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125498 Hz
AQ 3.9845889 sec
RG 143.73
DW 60.800 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.260103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of compound (3u):

Signature SIF VIT VELLORE
JPR-13P-P



Current Data Parameters
NAME Desktop
EXPNO 48
PROCNO 1

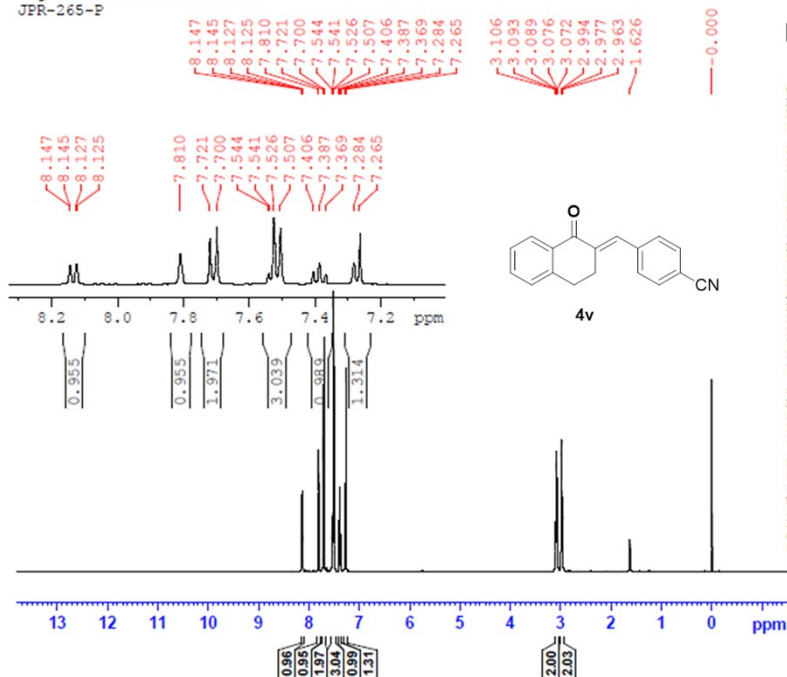
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Date_ 20140813
Time 12.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125493 Hz
AQ 3.984889 sec
RG 127.79
DW 60.800 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.2580147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of compound (3v):

Signature SIF VIT VELLORE
JPR-265-P



Current Data Parameters
NAME desktop
EXPNO 10
PROCNO 1

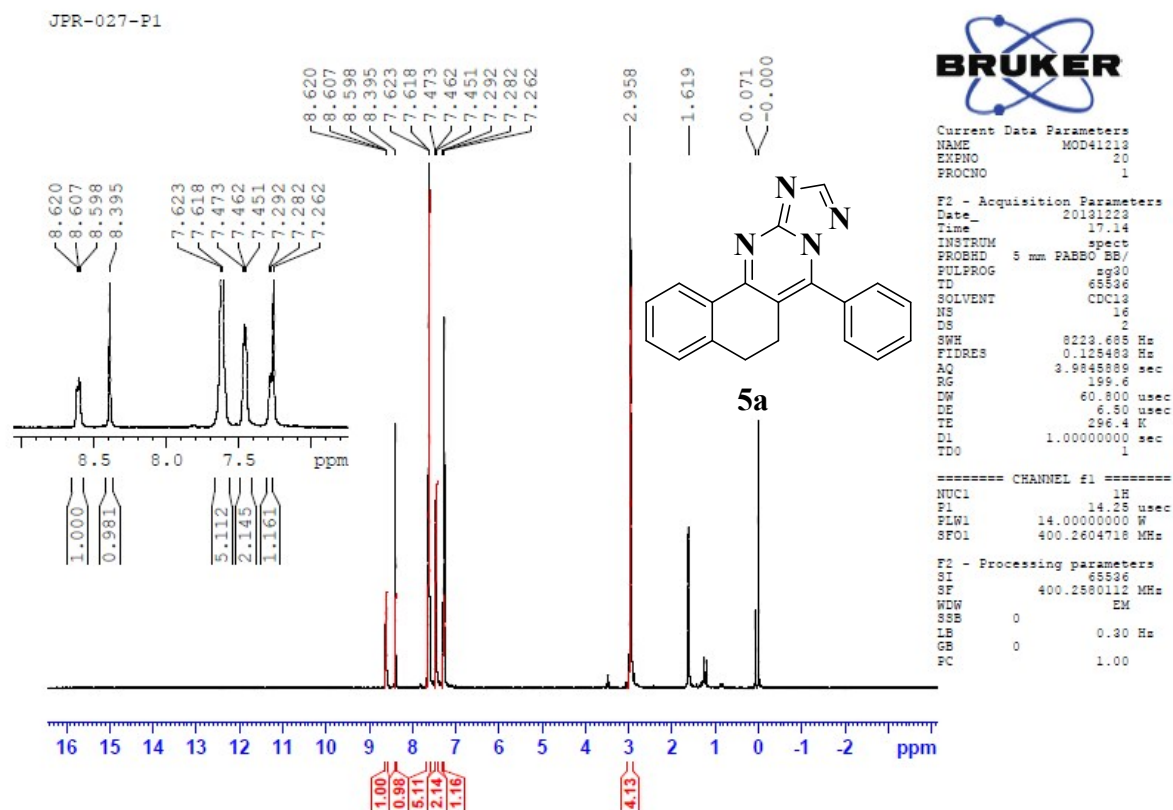
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Time 16.39
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125493 Hz
AQ 3.984889 sec
RG 127.79
DW 60.800 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TDO 1

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

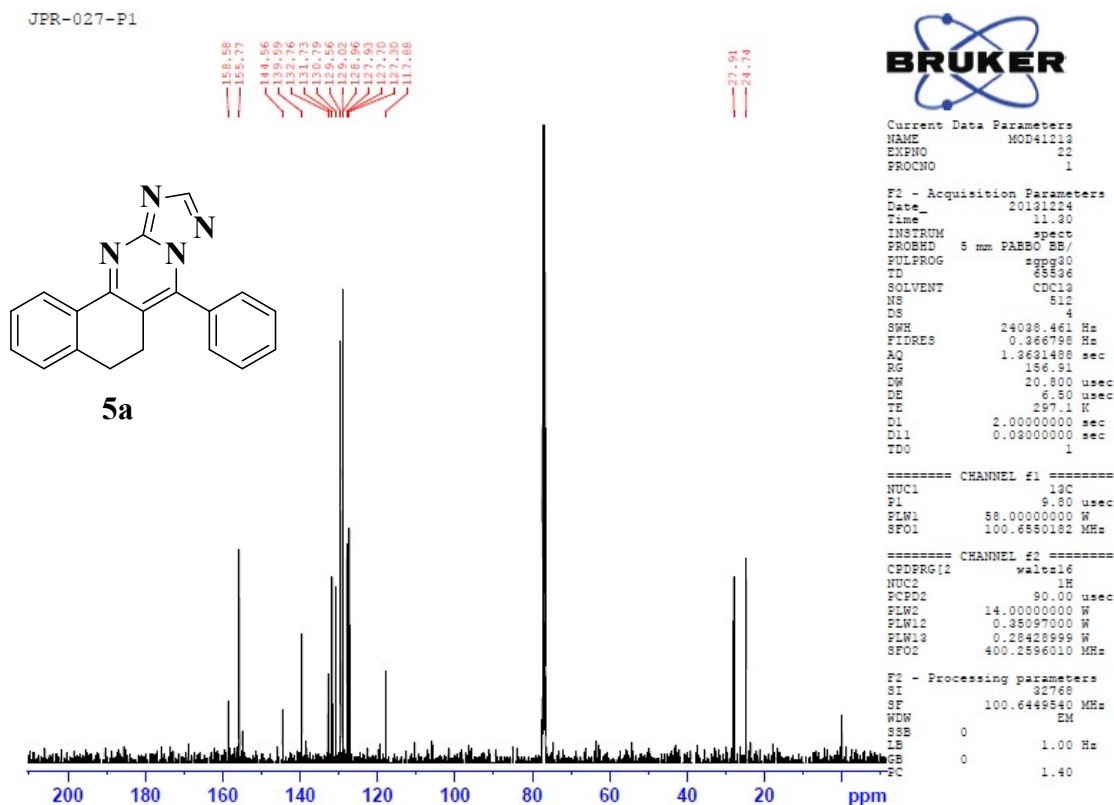
F2 - Processing parameters
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SF 400.2580096 MHz
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LB 0.30 Hz
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PC 1.00

Copies of ¹H NMR, ¹³C NMR and HRMS of [5(a-u) & 6(a-f)]

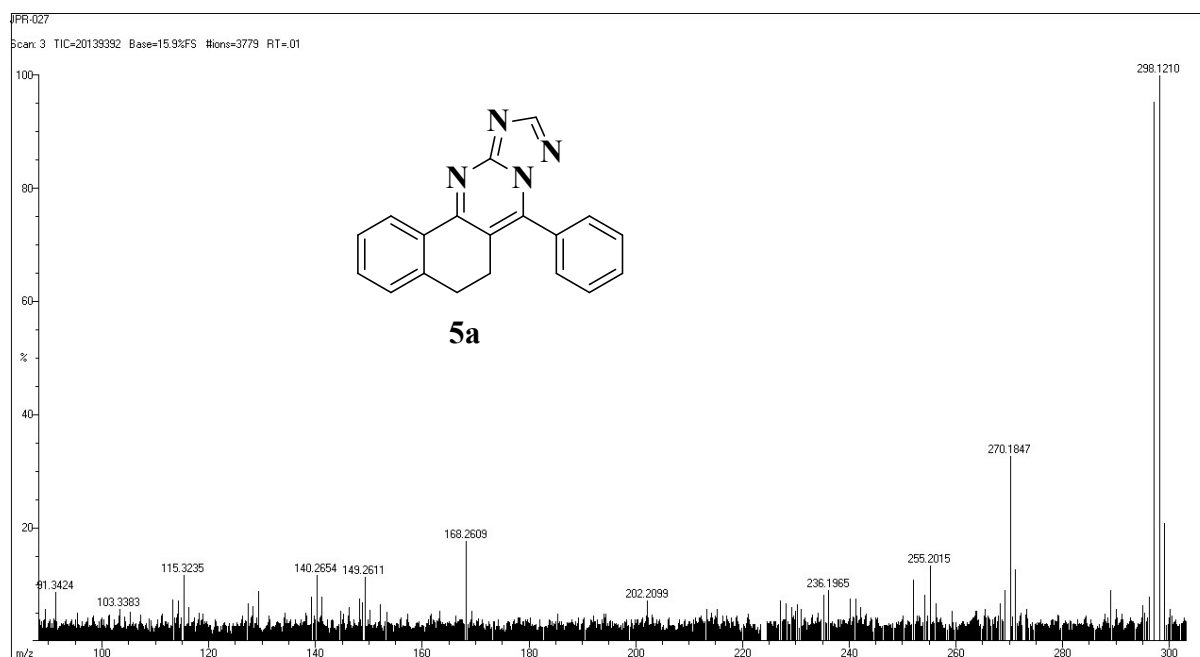
¹H NMR spectrum of compound (5a):



¹³C NMR spectrum of compound (5a):

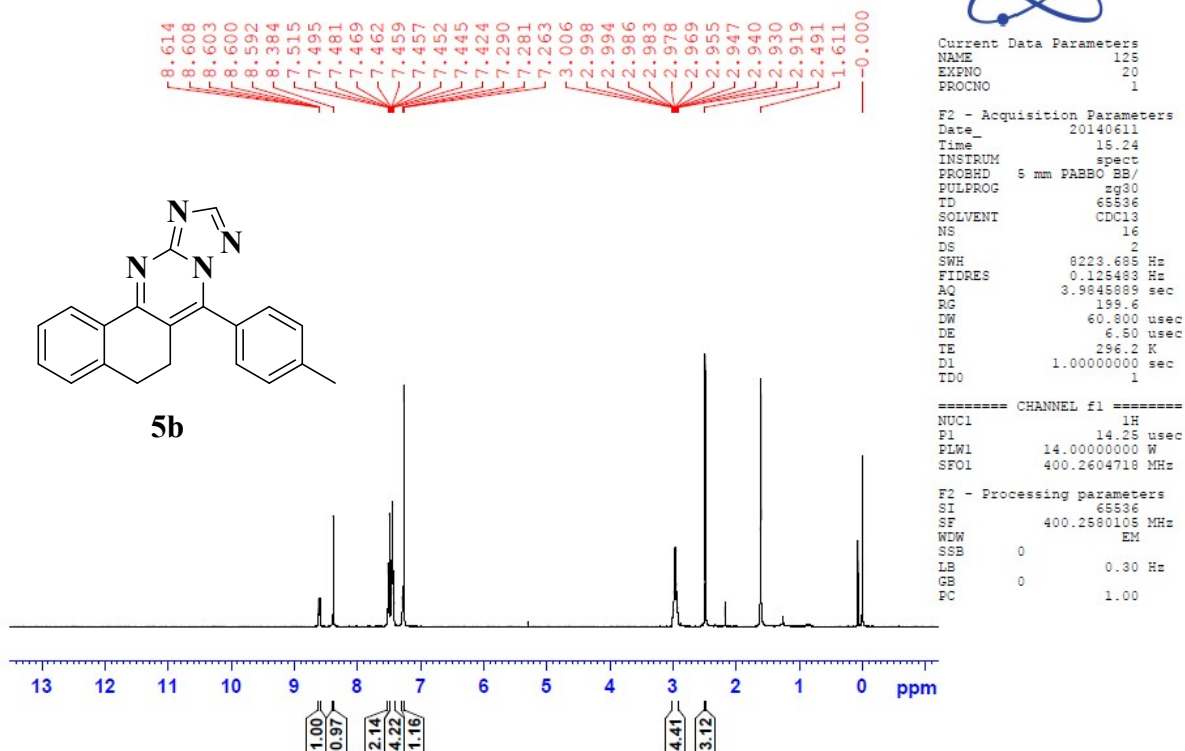


HRMS spectrum of compound (5a):



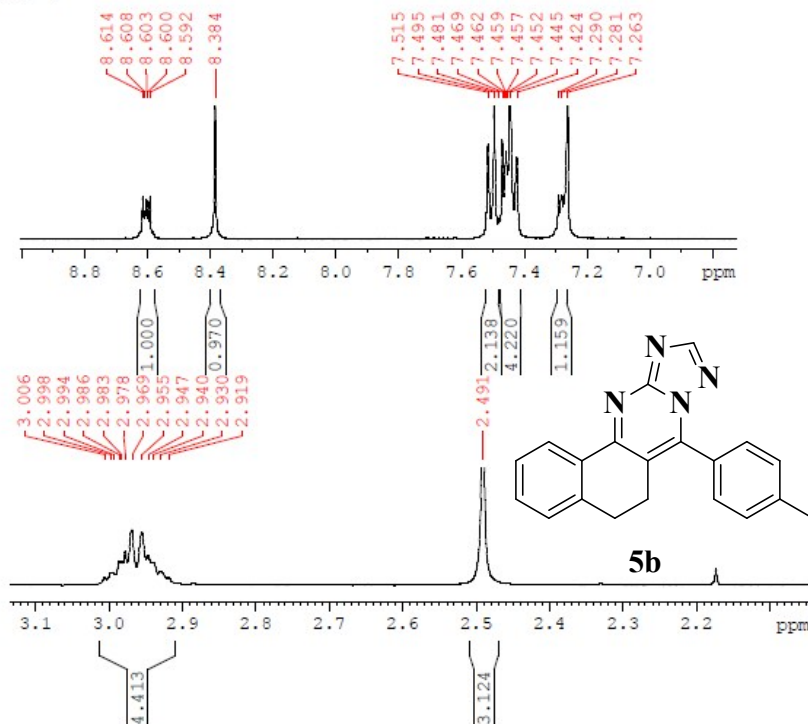
¹H NMR spectrum of compound (5b):

Signature SIF VIT VELLORE
JPR-129-P



Expanded ¹H NMR spectrum of compound (5b):

Signature SIF VIT VELLORE
JPR-129-P



Current Data Parameters
NAME 125
EXPNO 20
PROCNO 1

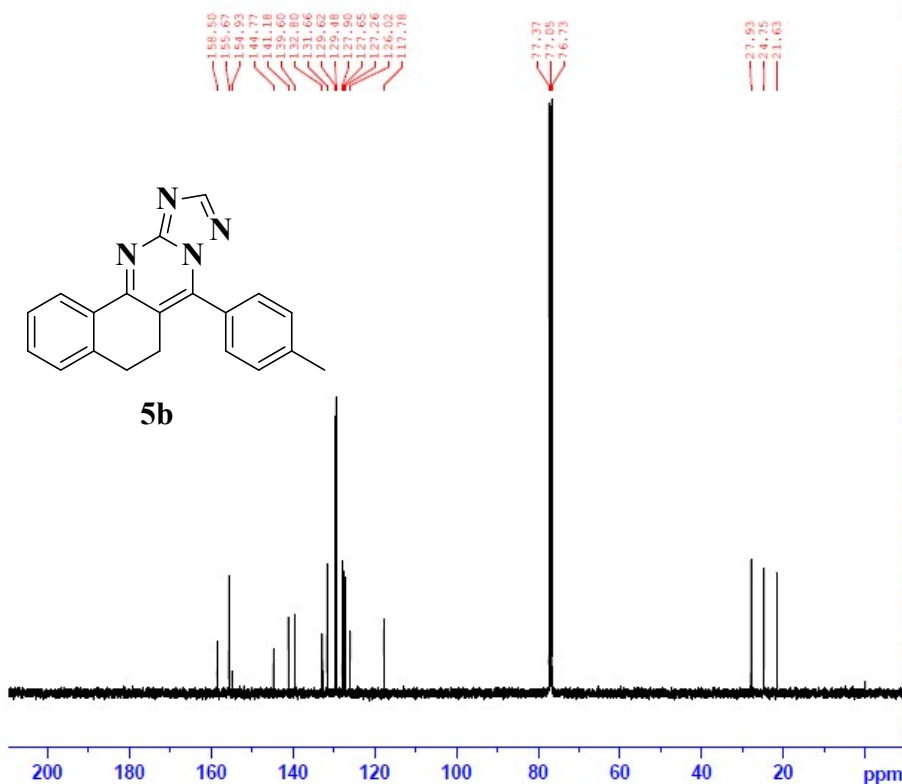
F2 - Acquisition Parameters
Date_ 20140611
Time 15.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.688 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 199.6
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580105 MHz
WDW EM
SSE 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound (5b):

Signature SIF VIT VELLORE
JPR-129-P



Current Data Parameters
NAME 125
EXPNO 8
PROCNO 1

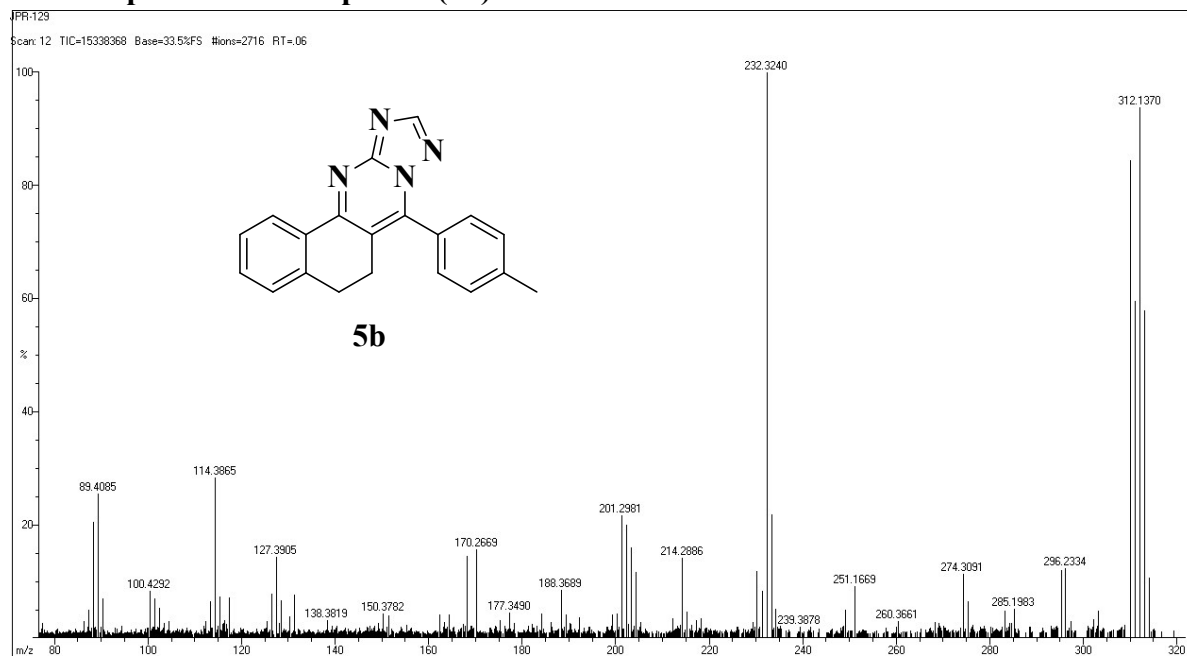
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Time 14.53
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 127.79
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
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PLW1 58.0000000 W
SFO1 100.6250182 MHz

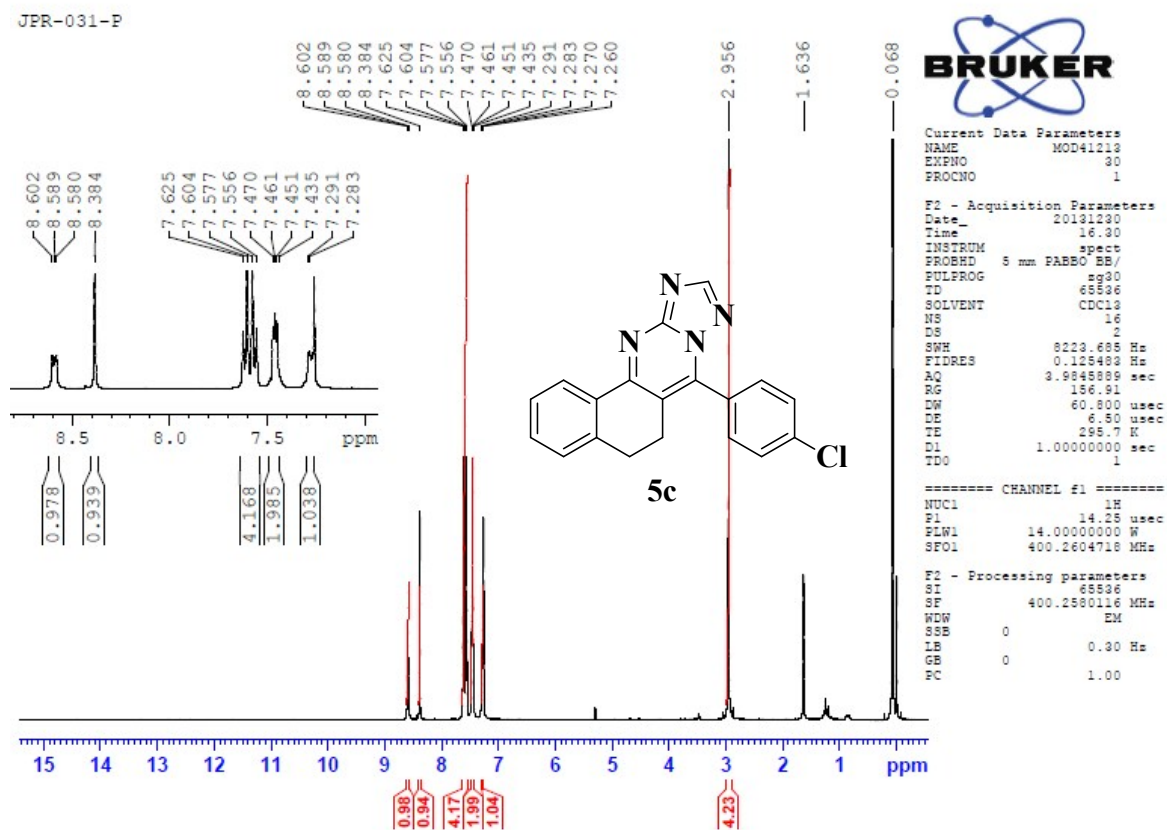
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PCPD2 80.00 usec
PLW2 14.0000000 W
PLW12 0.35807000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSE 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectrum of compound (5b):

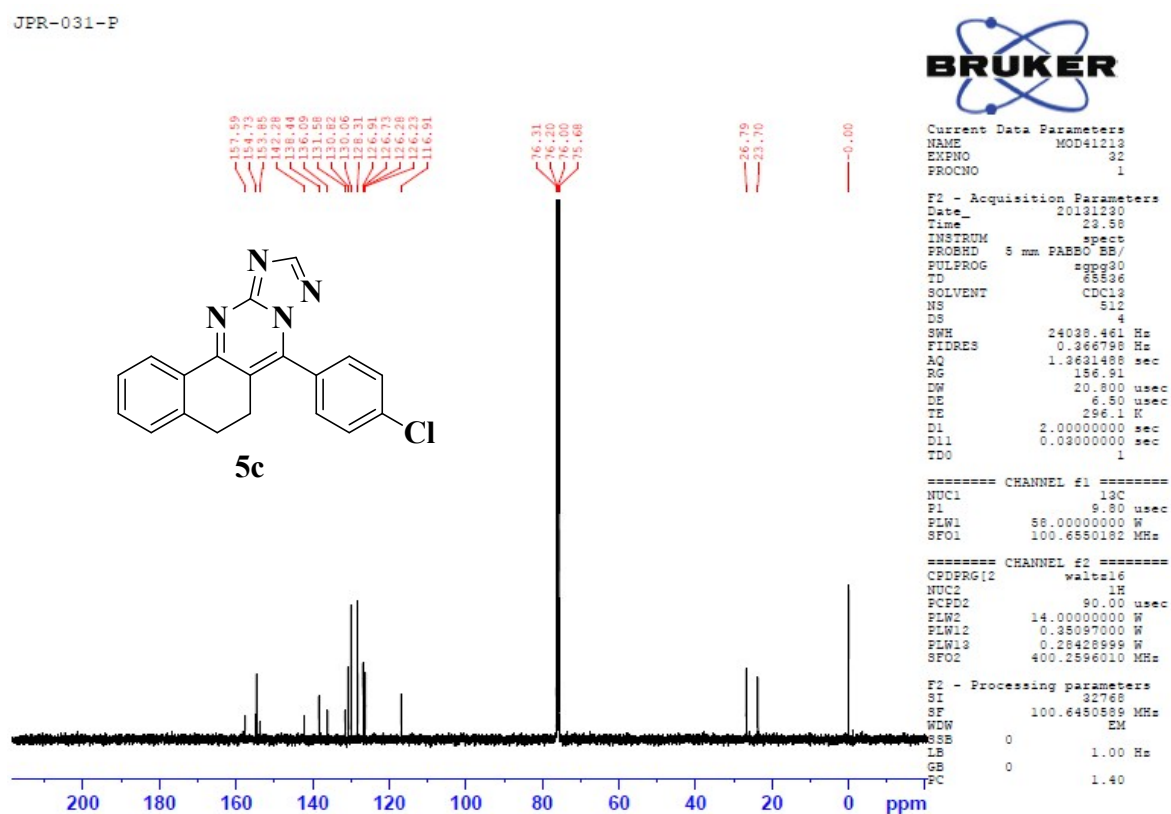


¹H NMR spectrum of compound (5c):

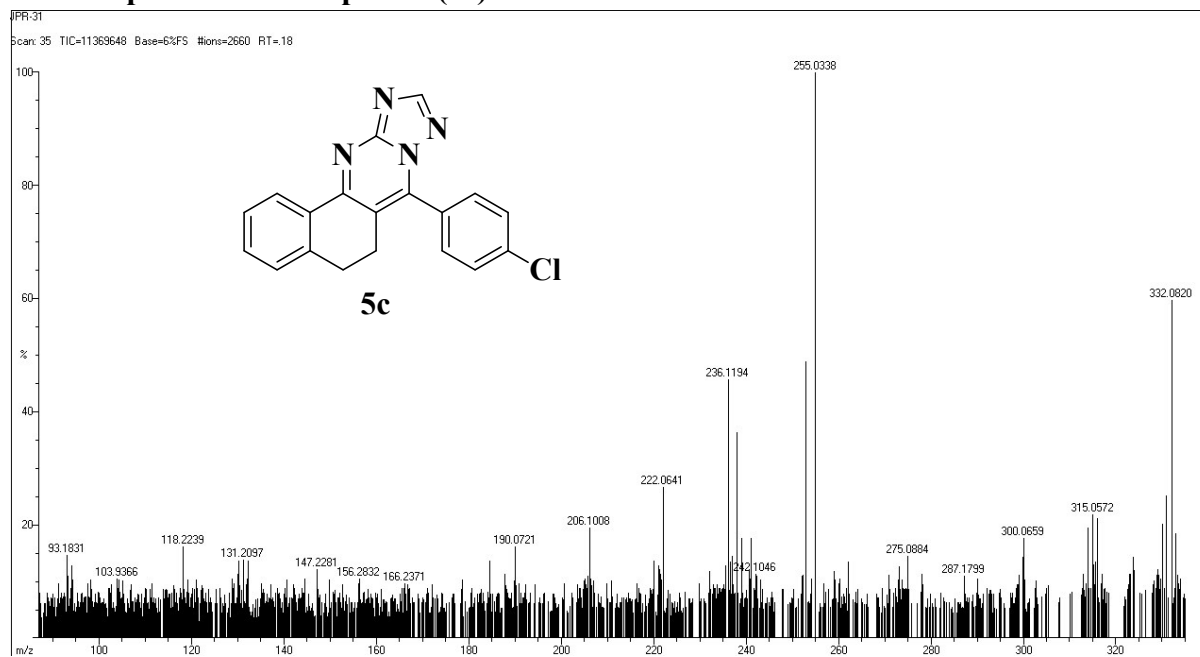


¹³C NMR spectrum of compound (5c):

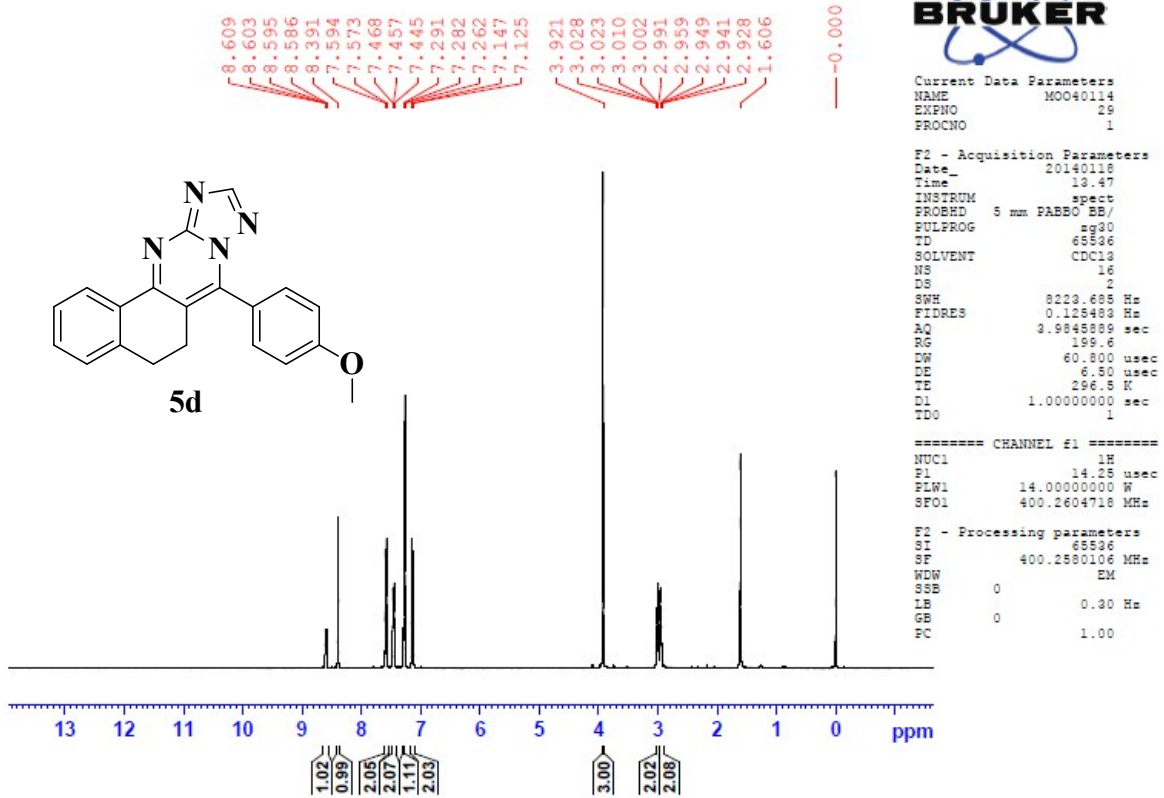
JPR-031-P



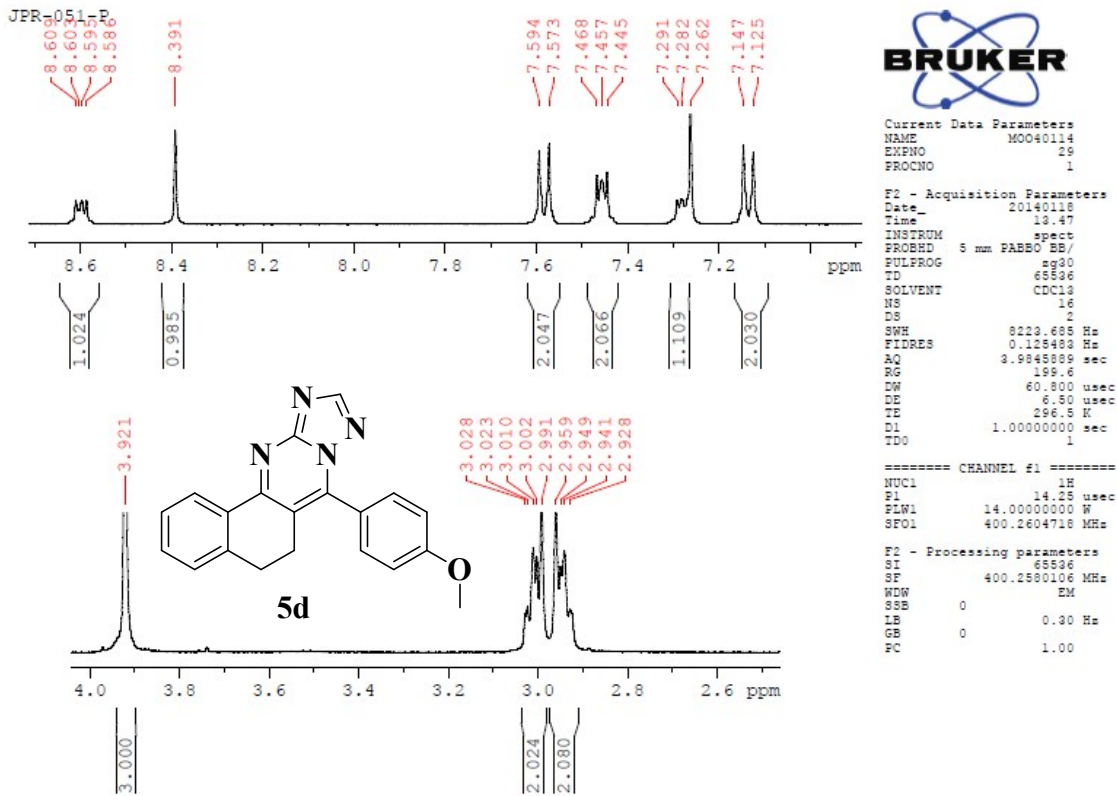
HRMS spectrum of compound (5c):



¹H NMR spectrum of compound (5d):

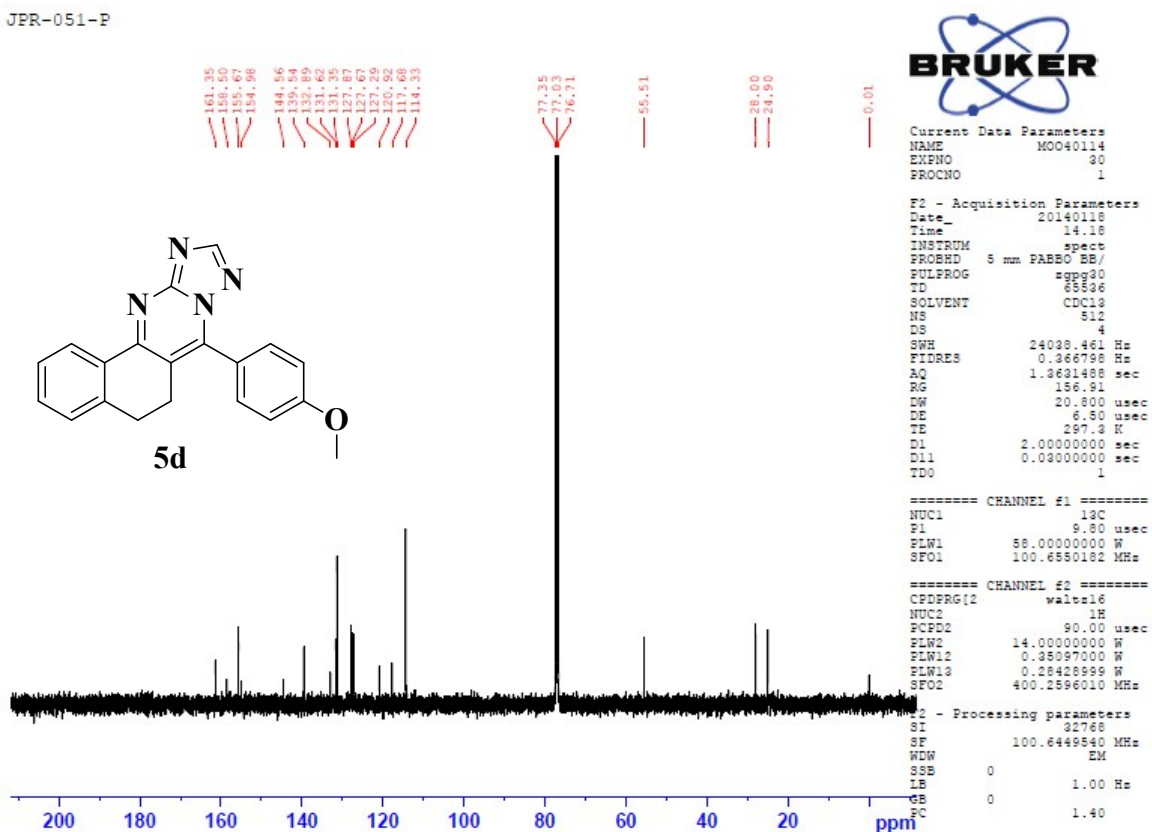


Expanded ¹H NMR spectrum of compound (5d):

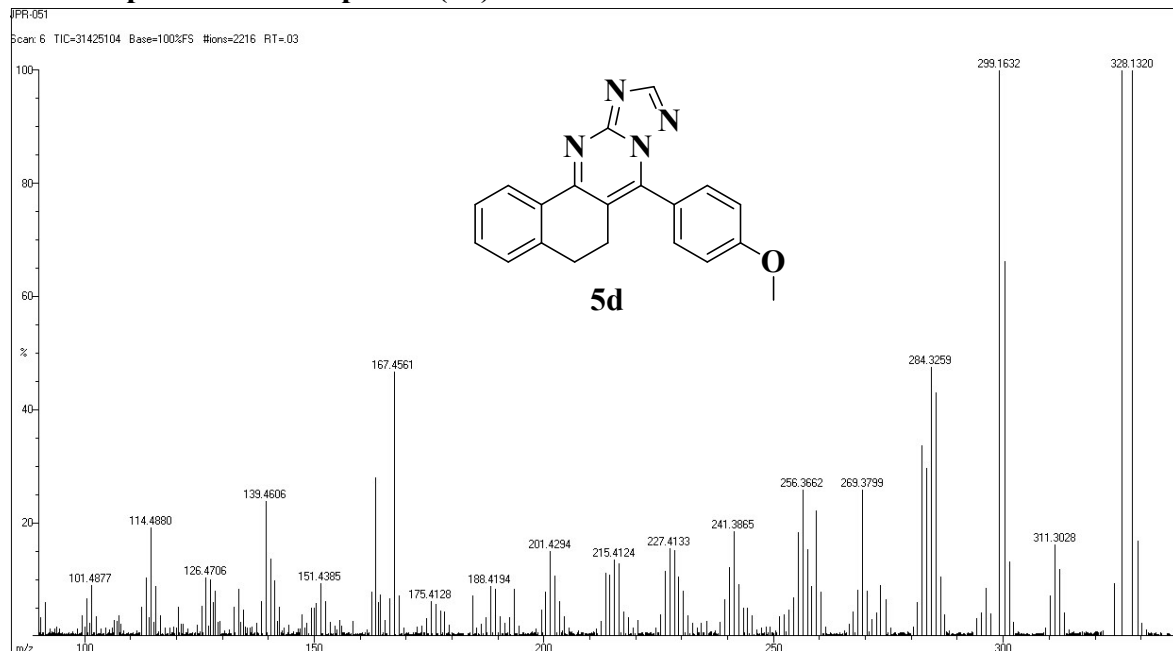


¹³C NMR spectrum of compound (5d):

JPR-051-P

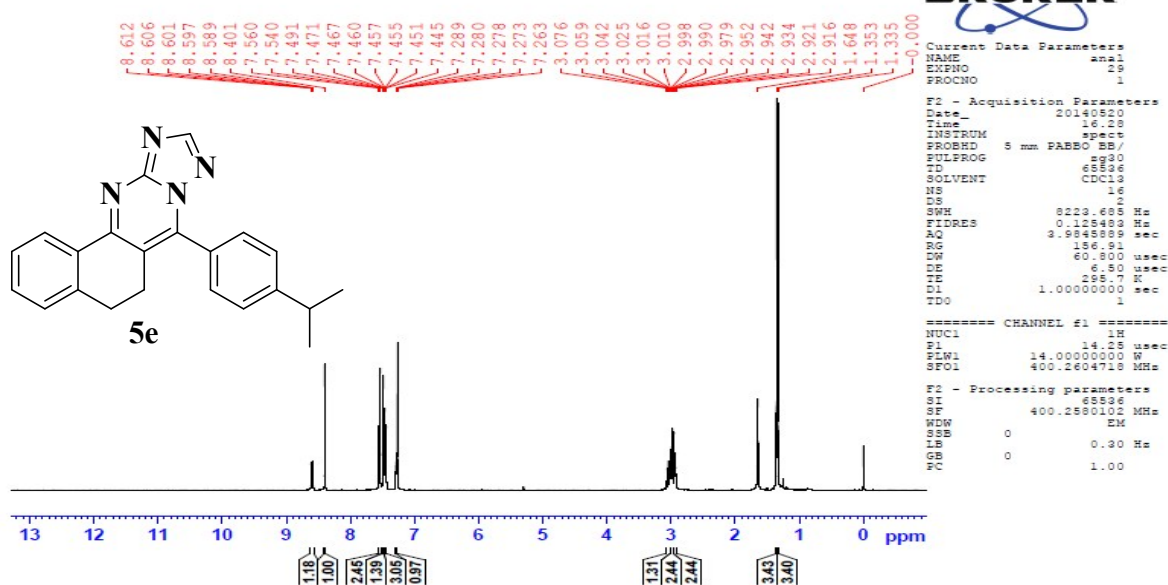


HRMS spectrum of compound (5d):



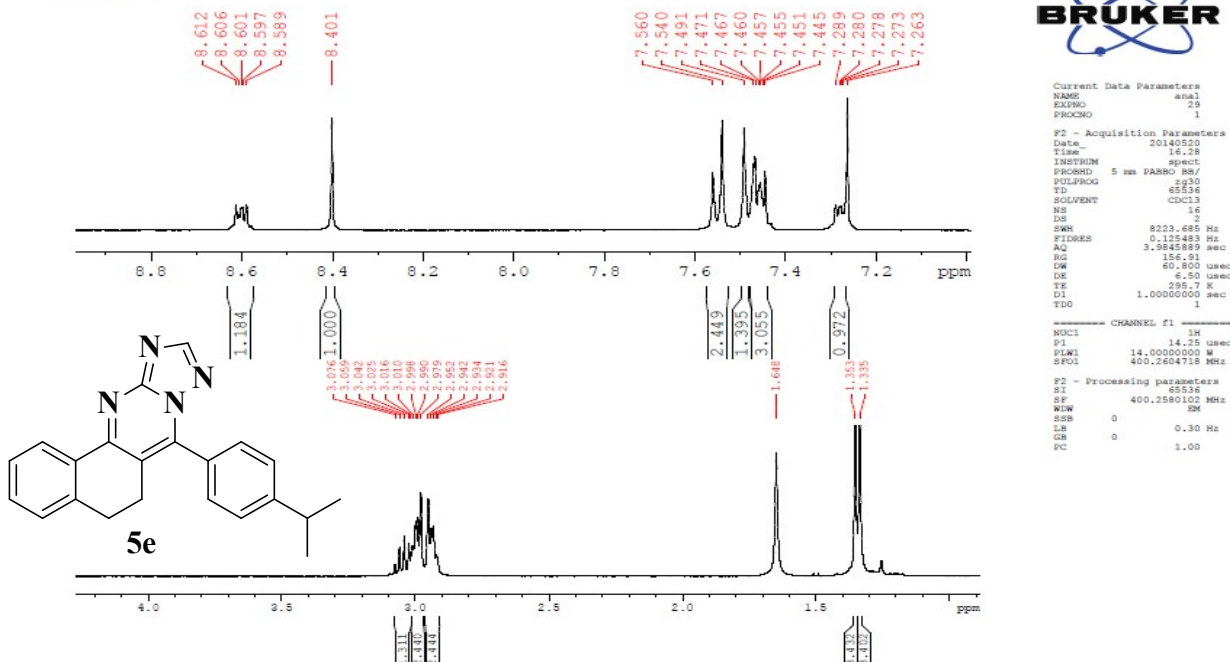
¹H NMR spectrum of compound (5e):

Signature SIF VIT VELLORE
JPR-103P



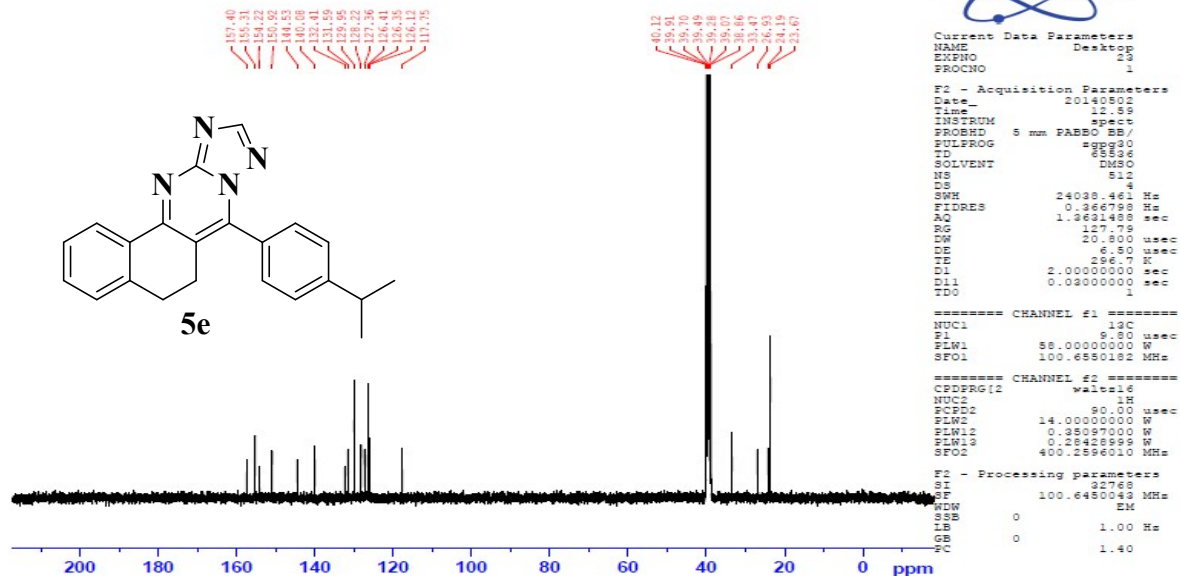
Expanded ¹H NMR spectrum of compound (5e):

Signature SIF VIT VELLORE
JPR-103P

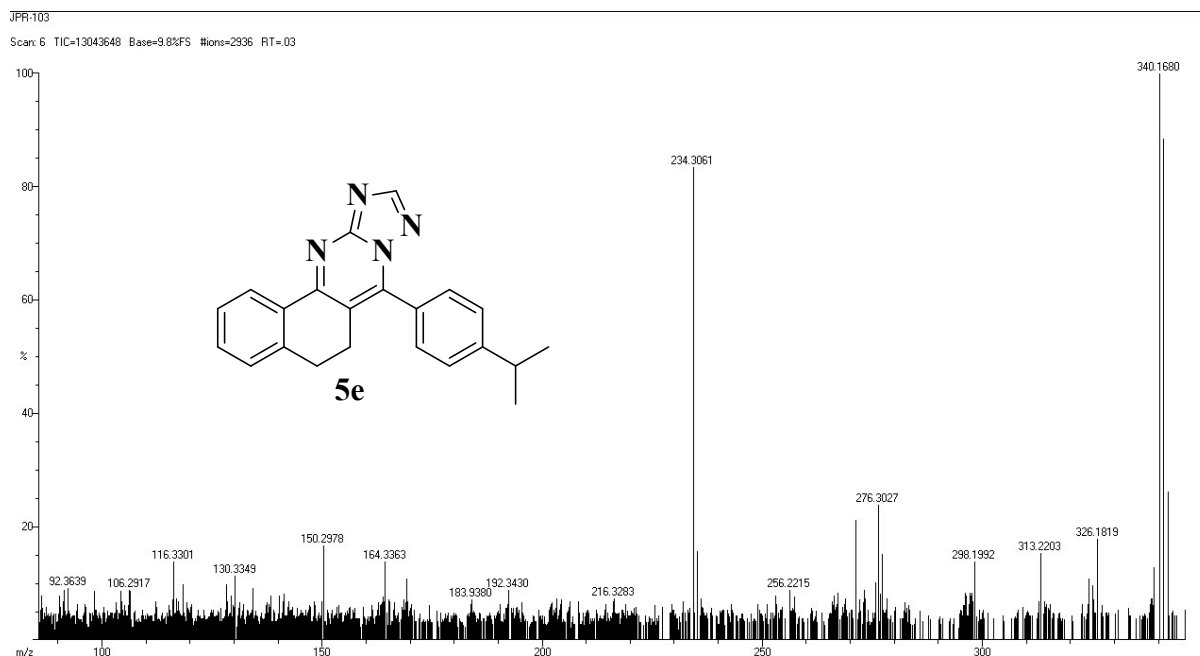


¹³C NMR spectrum of compound (5e):

Signature SIF VIT VELLORE
JPR-103-P

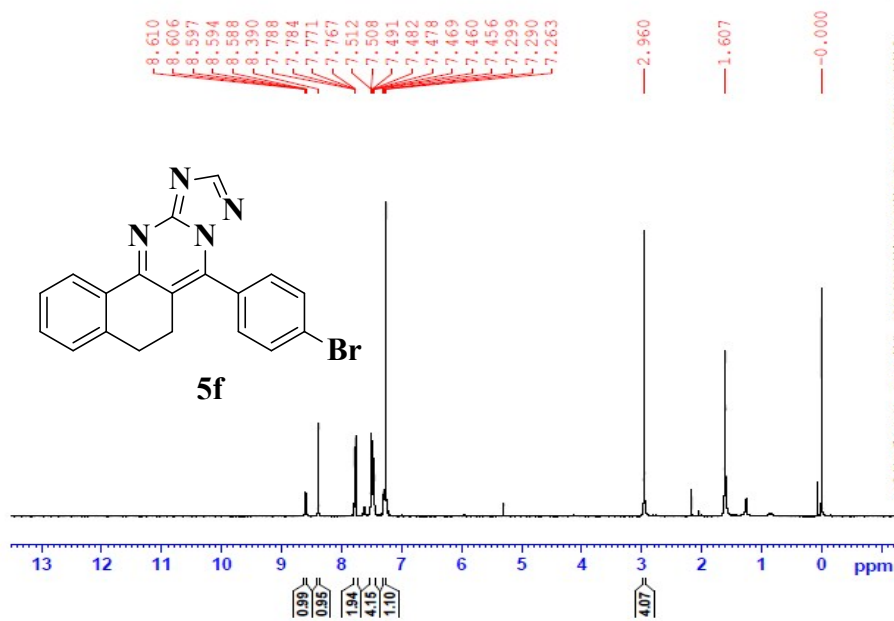


HRMS spectrum of compound (5e):



¹H NMR spectrum of compound (5f):

Signature SIF VIT VELLORE
JPR-130-P



```
Current Data Parameters
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EXPNO    19
PROCNO   1

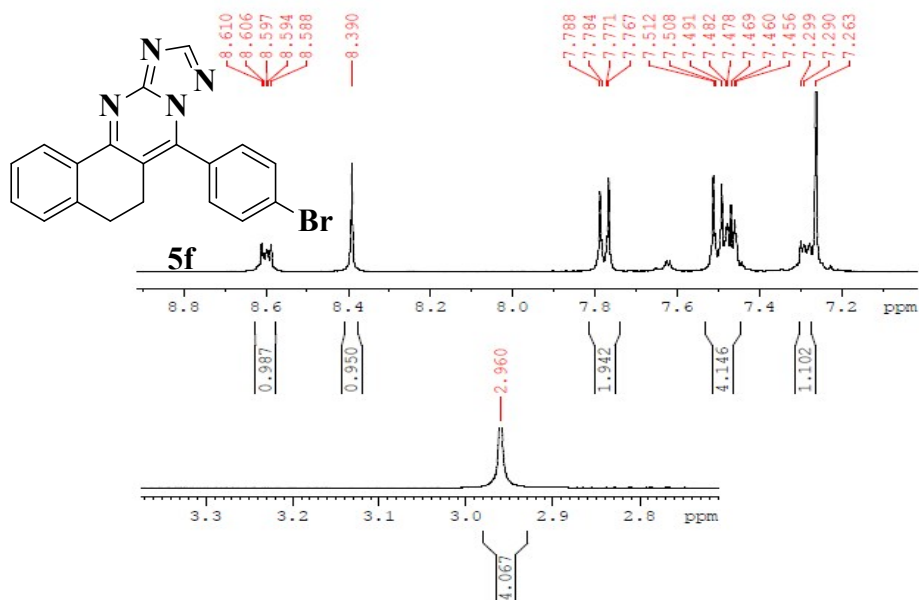
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PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       8223.636 Hz
FIDRES   0.128483 Hz
AQ       3.9845899 sec
RG       199.6
SM       60.800 usec
DE       6.50 usec
TE       296.1 K
D1       1.00000000 sec
TD0      1

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

F2 - Processing parameters
SI       65536
SF       400.2580105 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
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Expanded ¹H NMR spectrum of compound (5f):

Signature SIF VIT VELLORE
JPR-130-P



```
Current Data Parameters
NAME      126
EXPNO    19
PROCNO   1

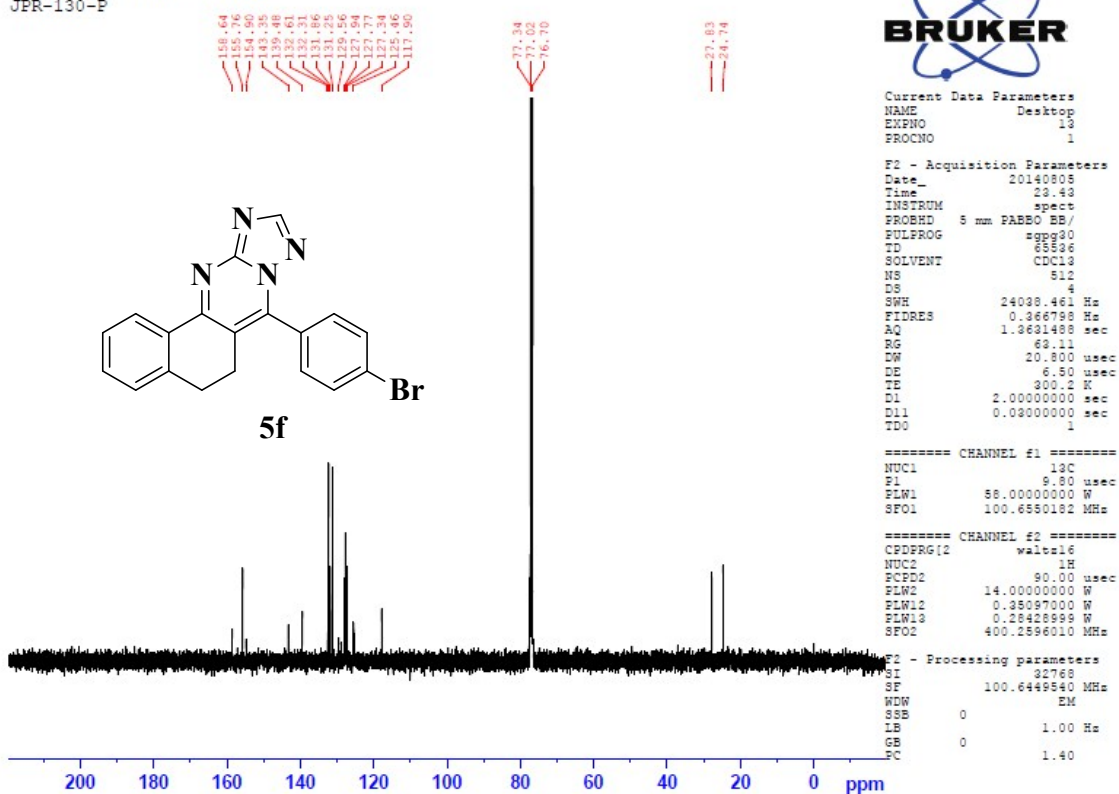
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Date_    20140611
Time     15.20
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       8223.636 Hz
FIDRES   0.128483 Hz
AQ       3.9845899 sec
RG       199.6
SM       60.800 usec
DE       6.50 usec
TE       296.1 K
D1       1.00000000 sec
TD0      1

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

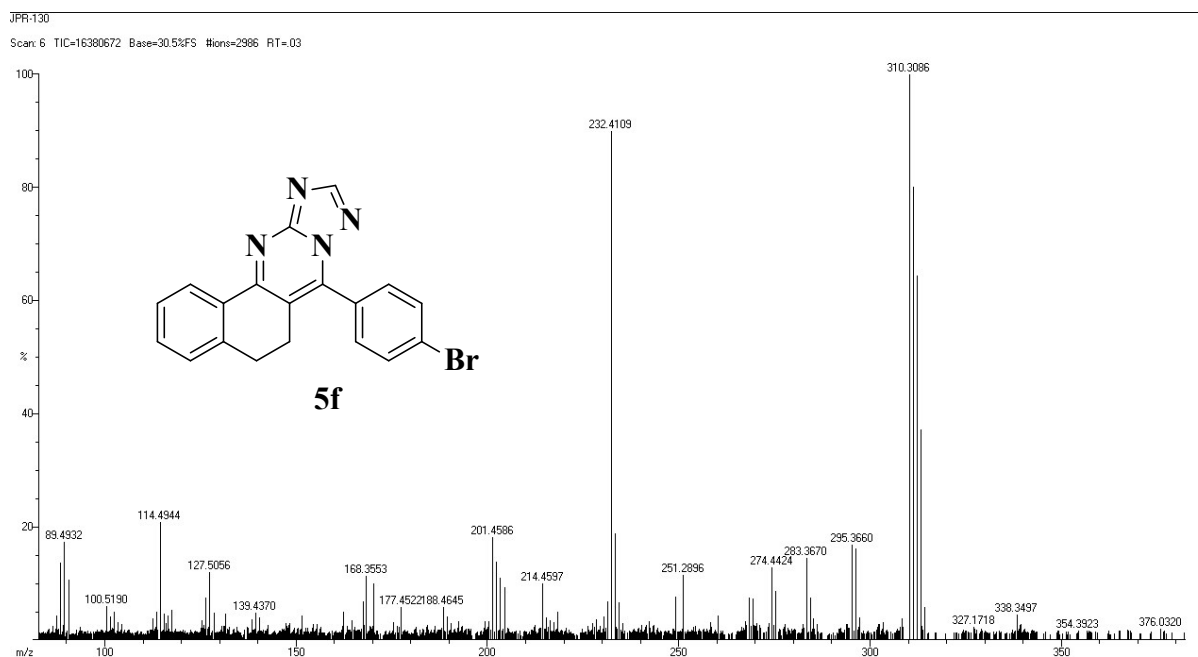
F2 - Processing parameters
SI       65536
SF       400.2580105 MHz
WDW      EM
SSB      0
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GB       0
PC       1.00
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¹³C NMR spectrum of compound (5f):

Signature SIF VIT VELLORE
JPR-130-P

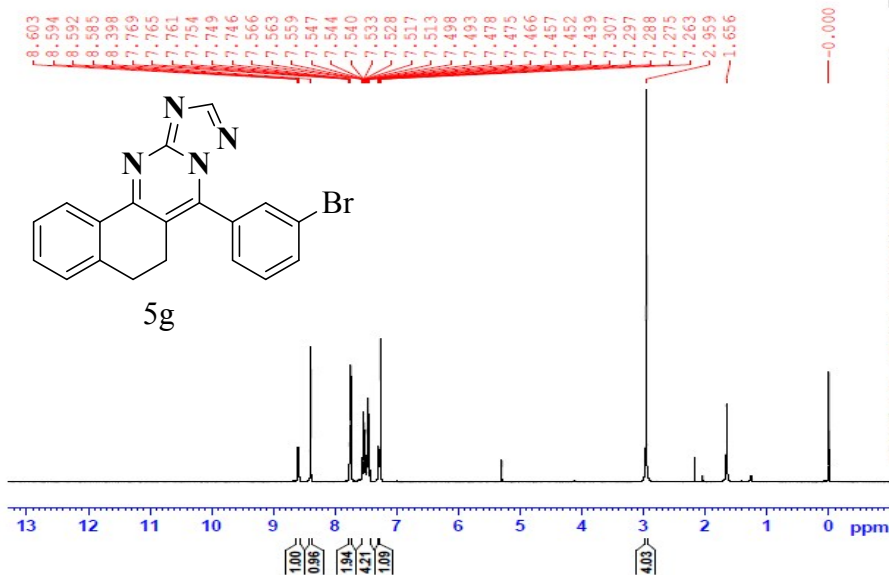


HRMS spectrum of compound (5f):



¹H NMR spectrum of compound (5g):

Signature SIF VIT VELLORE
JPR-131-P



Current Data Parameters
NAME Desktop
EXPNO 5
PROCNO 1

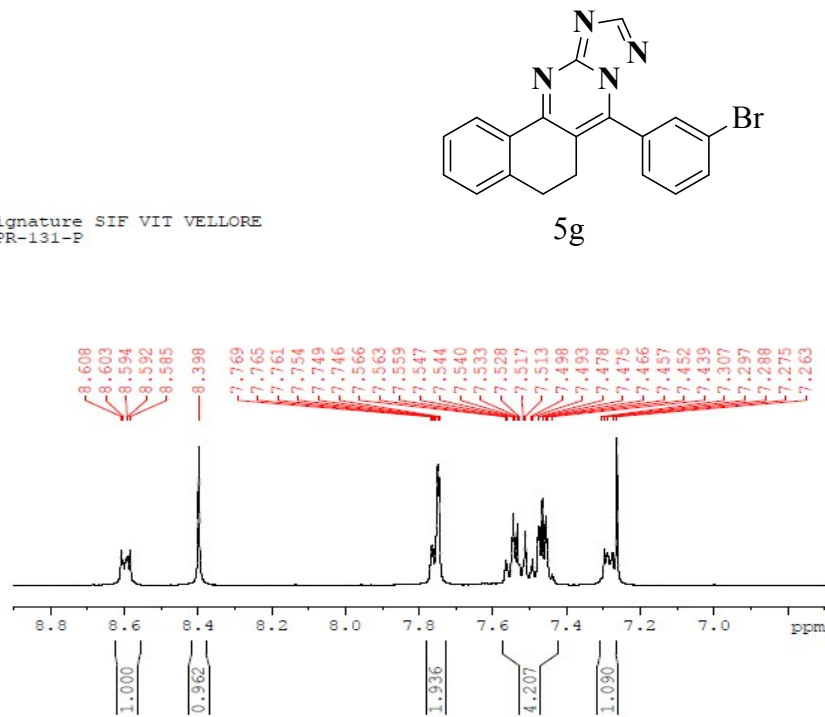
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Time 23.24
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.655 Hz
FIDRES 0.103453 Hz
AQ 3.984583 sec
RG 178.97
DW 178.97 usec
DE 60.800 usec
TE 296.4 K
D1 1.00000000 sec
TDO 1

===== CHANNEL #1 =====
NUC1 1H
P1 14.25 usec
PL1 14.0000000 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 ¹H NMR spectrum of compound (5g):

Signature SIF VIT VELLORE
JPR-131-P



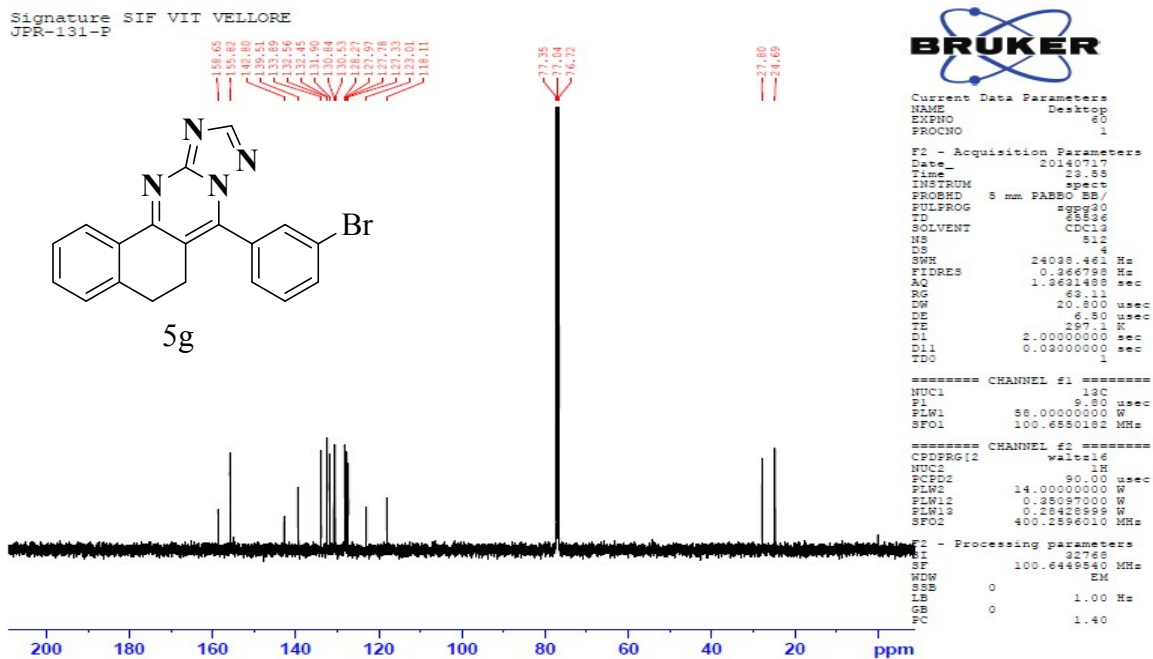
Current Data Parameters
NAME Desktop
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140717
Time 23.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.655 Hz
FIDRES 0.103453 Hz
AQ 3.984583 sec
RG 178.97
DW 178.97 usec
DE 60.800 usec
TE 296.4 K
D1 1.00000000 sec
TDO 1

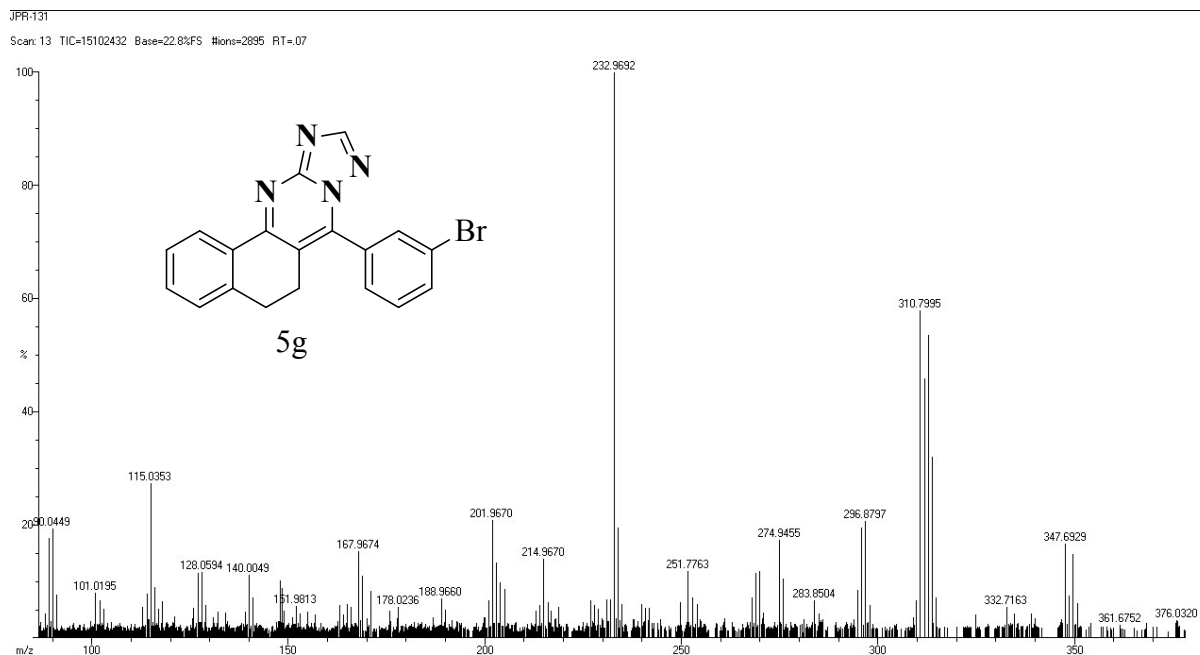
===== CHANNEL #1 =====
NUC1 1H
P1 14.25 usec
PL1 14.0000000 W
SFO1 400.2604718 MHz

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

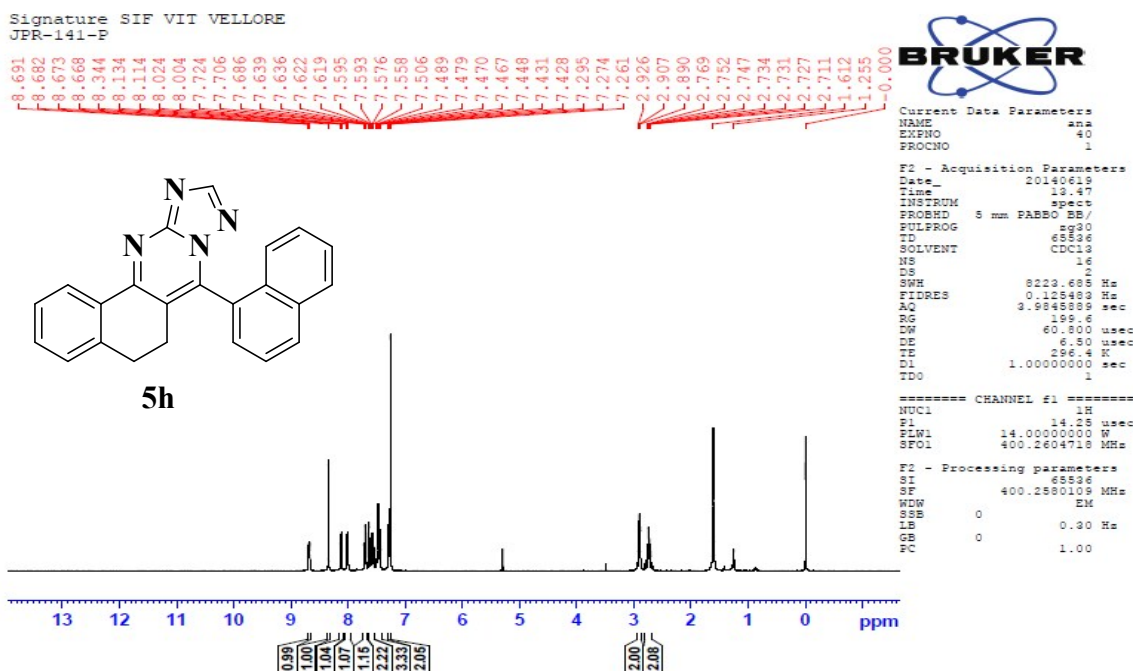
¹³C NMR spectrum of compound (5g):



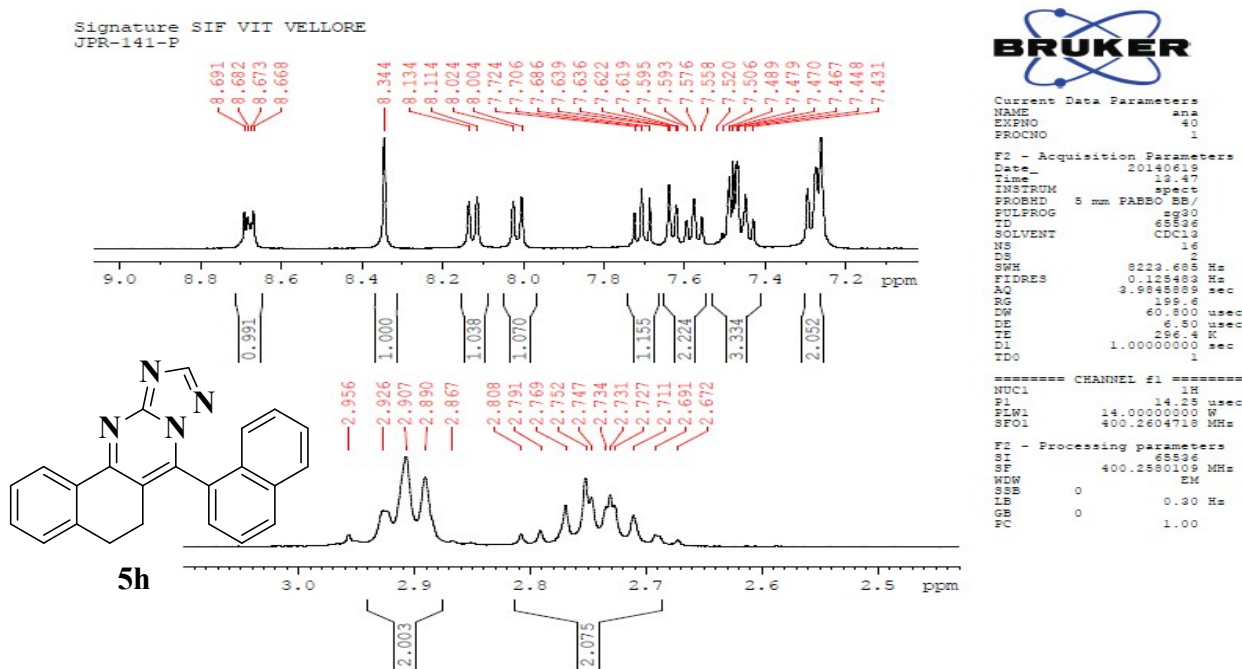
HRMS spectrum of compound (5g):



¹H NMR spectrum of compound (5h):

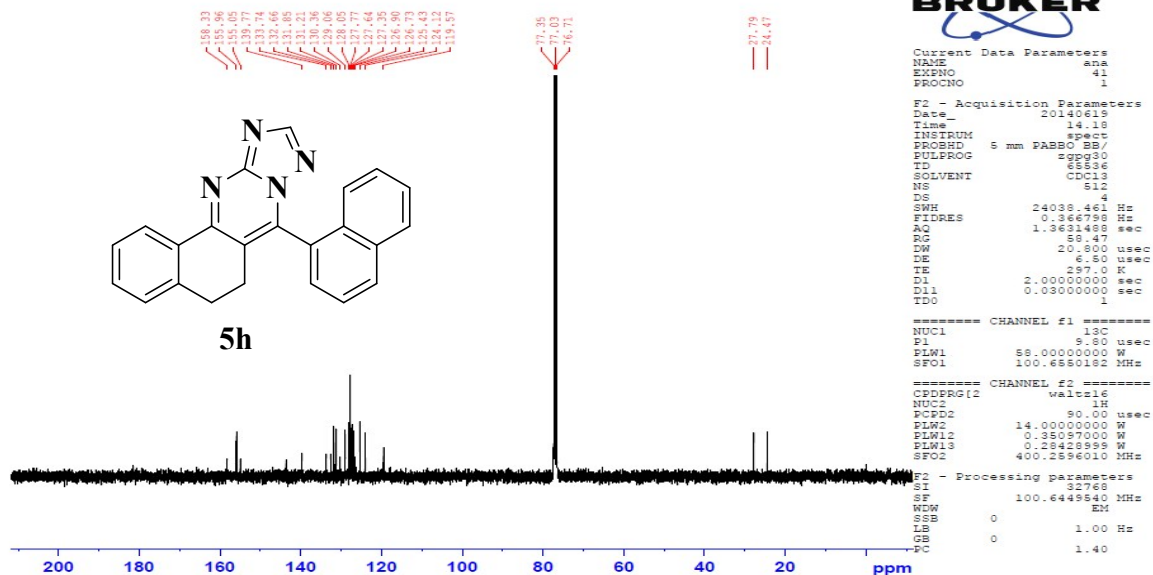


Expanded ¹H NMR spectrum of compound (5h):

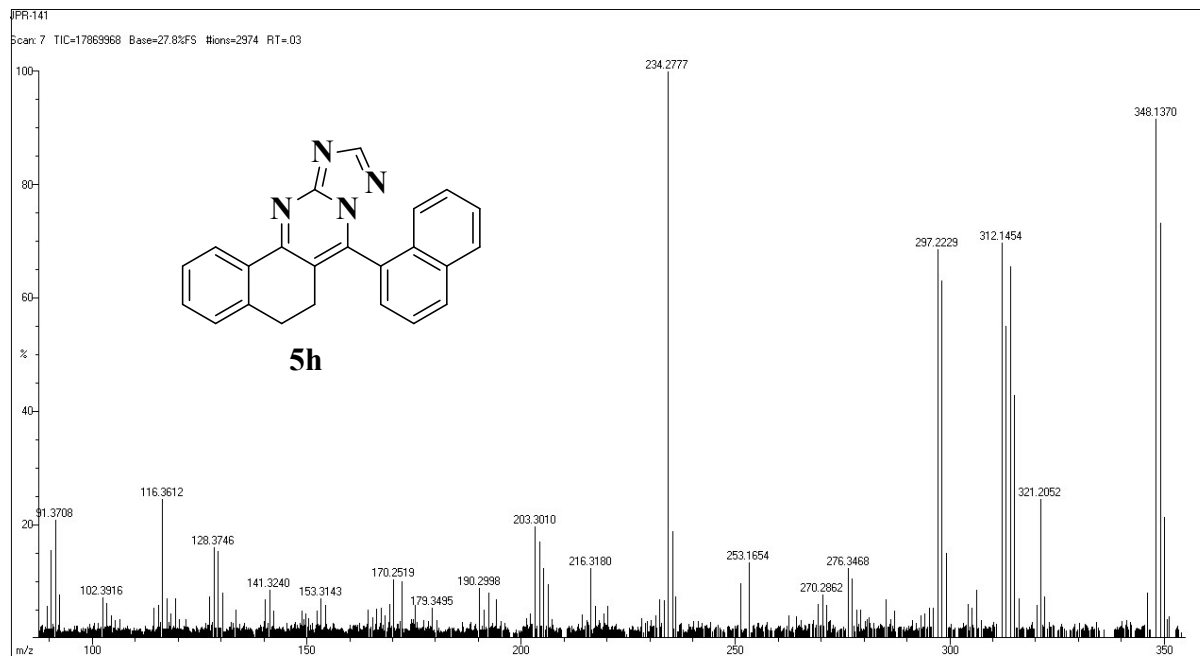


¹³C NMR spectrum of compound (5h):

Signature SIF VIT VELLORE
JPR-141-P

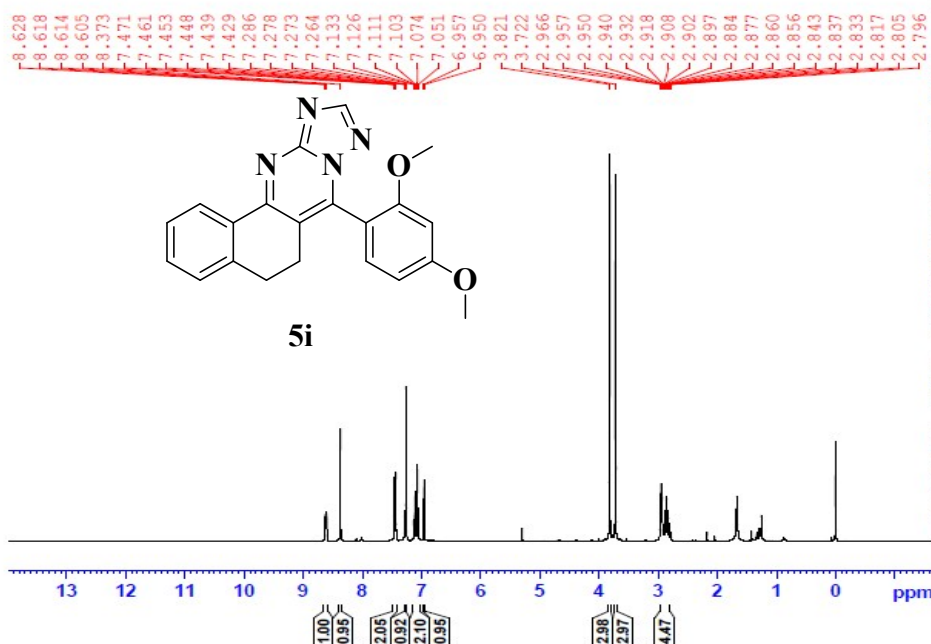


HRMS spectrum of compound (5h):



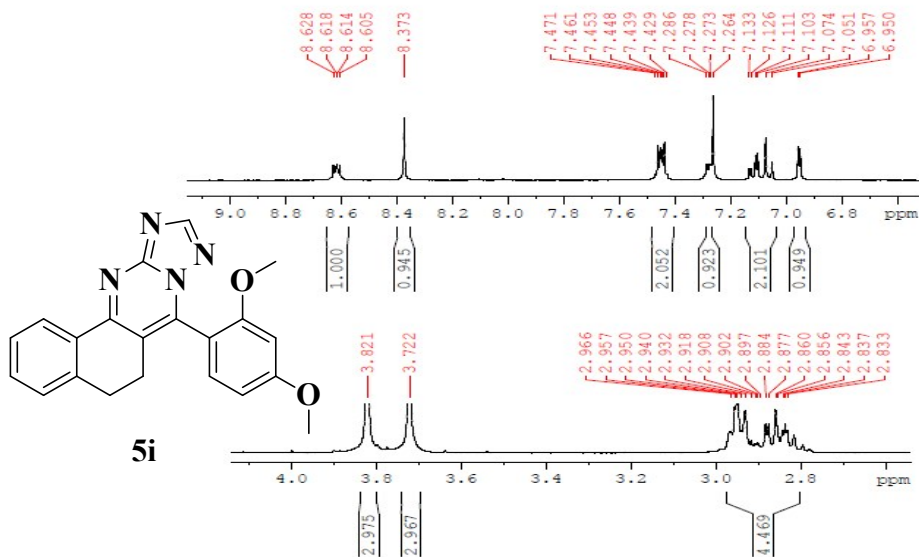
¹H NMR spectrum of compound (5i):

Signature SIF VIT VELLORE
JPR-088-P

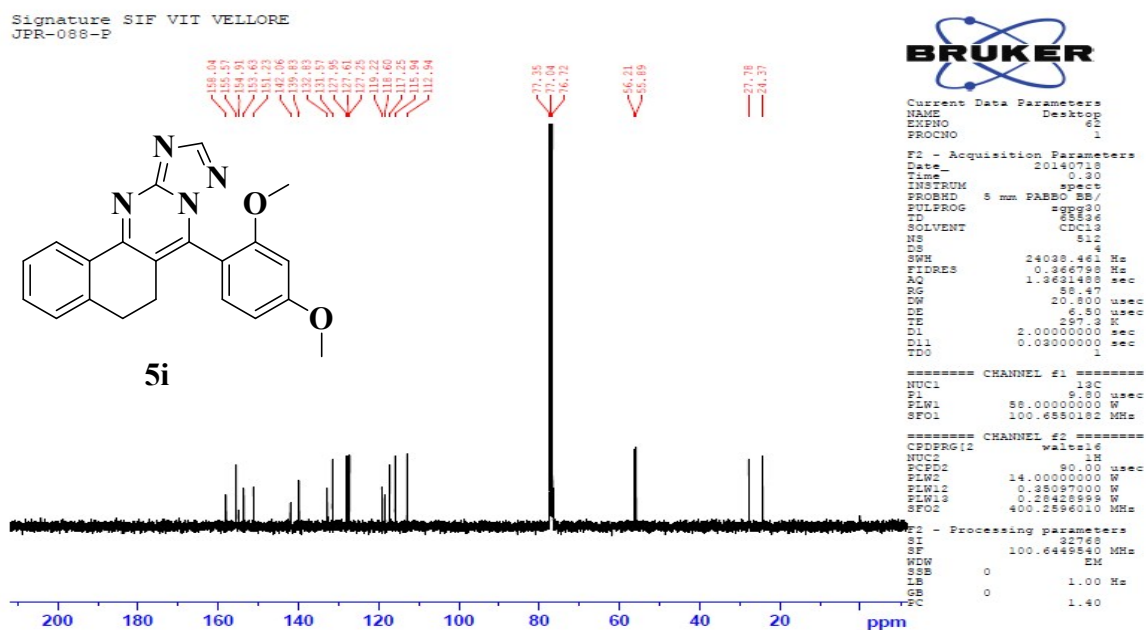


Expanded ¹H NMR spectrum of compound (5i):

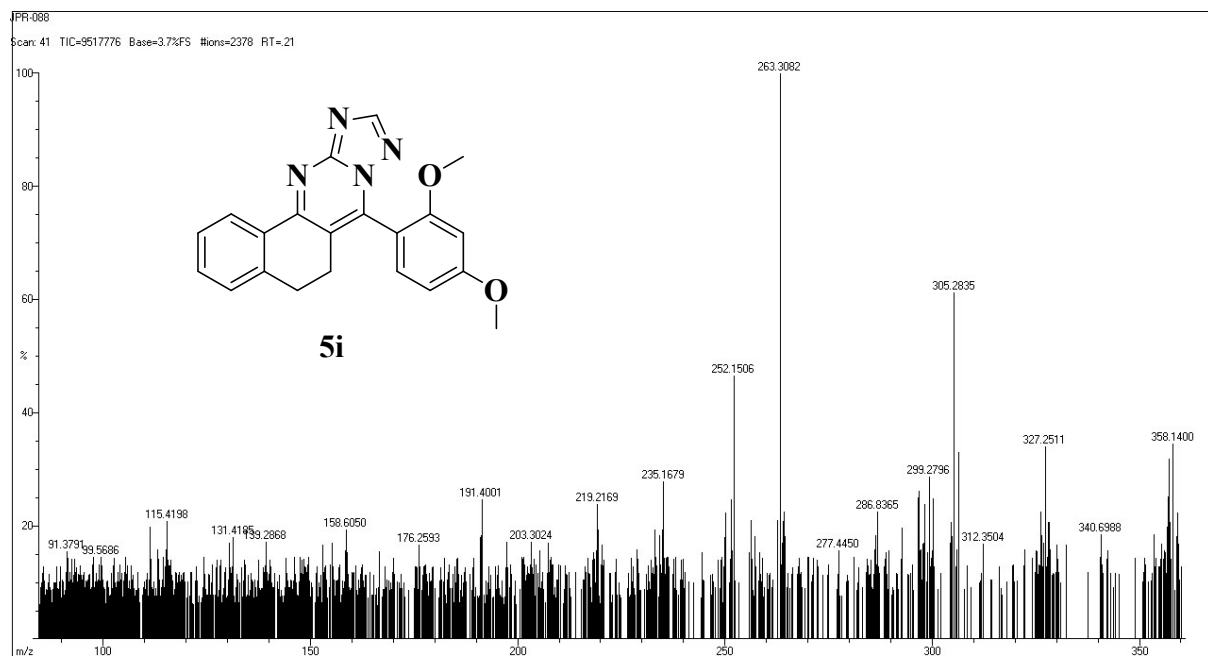
Signature SIF VIT VELLORE
JPR-088-P



¹³C NMR spectrum of compound (5i):

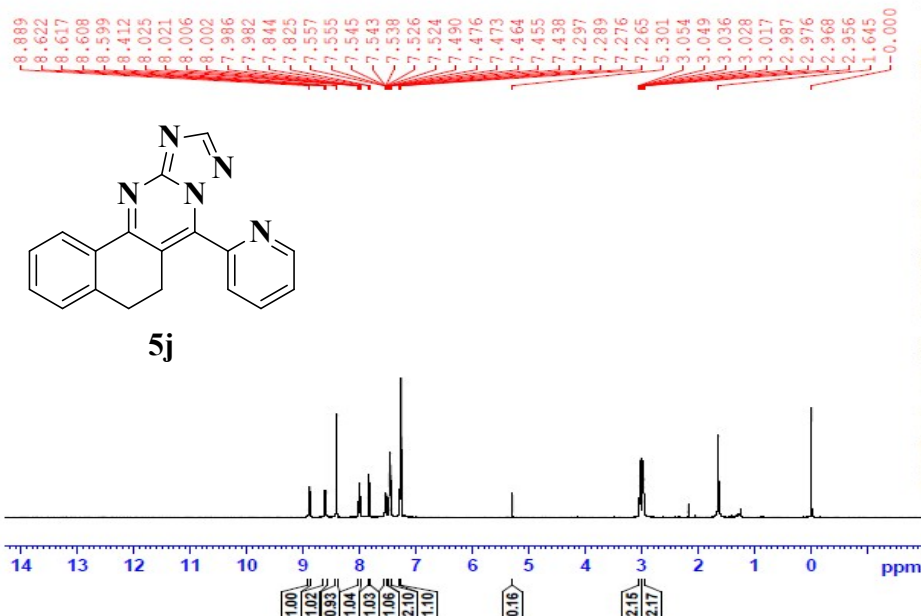


HRMS spectrum of compound (5i):



¹H NMR spectrum of compound (5j):

Signature SIF VIT VELLORE
JPR-089-P



Current Data Parameters
NAME Desktop
EXPNO 65
PROCNO 1

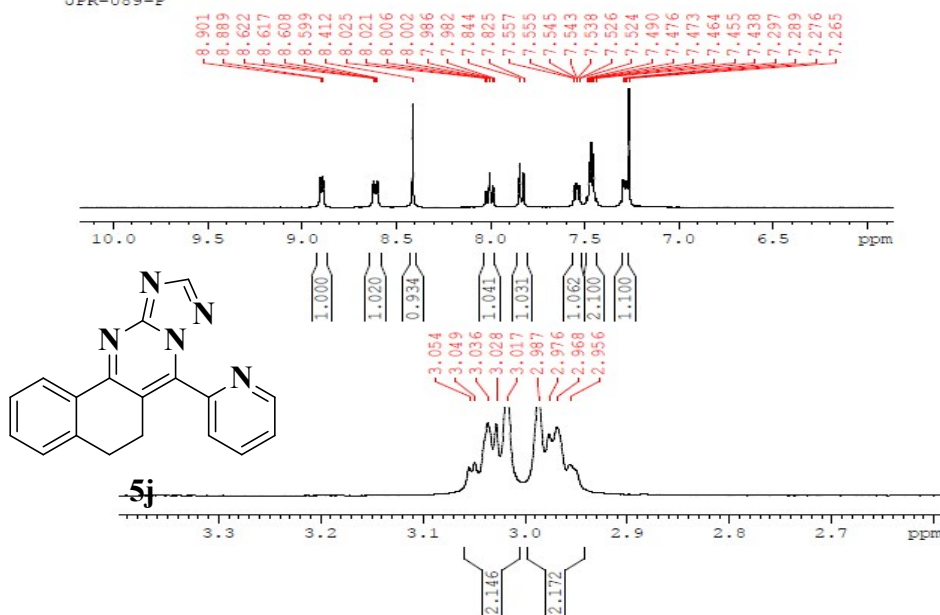
F2 - Acquisition Parameters
Date_ 20140718
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 16
DE 1
SWH 823.688 Hz
FIDRES 0.1125488 Hz
AQ 3.984888 sec
RG 199.6
DM 60.800 usec
HB 6.50 usec
HT 228.8 Hz
DI 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.23 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580096 MHz
WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

Expanded ¹H NMR spectrum of compound (5j):

Signature SIF VIT VELLORE
JPR-089-P



Current Data Parameters
NAME Desktop
EXPNO 65
PROCNO 1

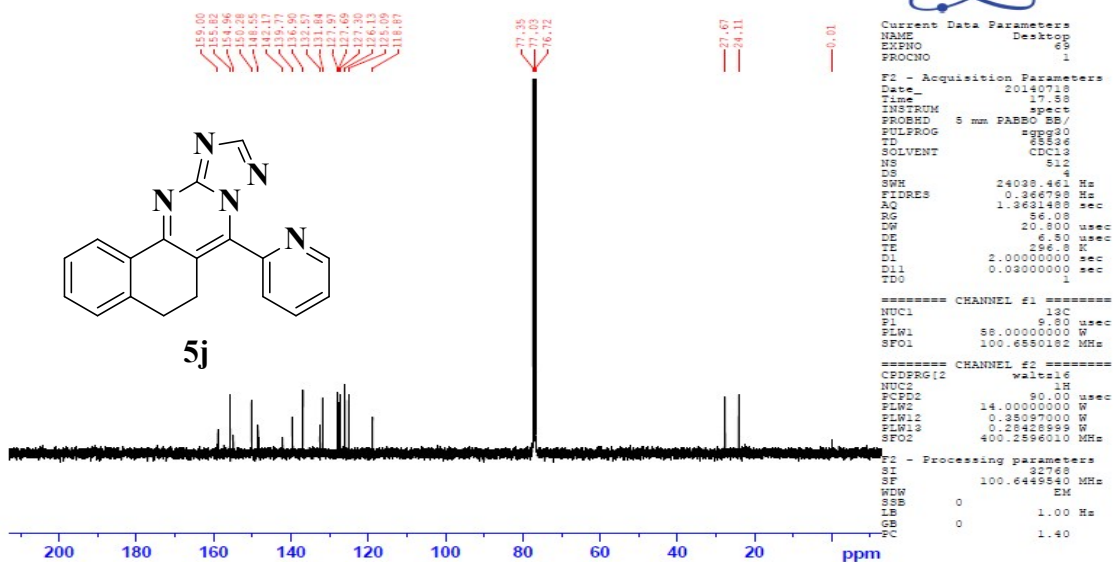
F2 - Acquisition Parameters
Date_ 20140718
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 16
DE 1
SWH 823.688 Hz
FIDRES 0.1125488 Hz
AQ 3.984888 sec
RG 199.6
DM 60.800 usec
HB 6.50 usec
HT 228.8 Hz
DI 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.23 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580096 MHz
WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound (5j):

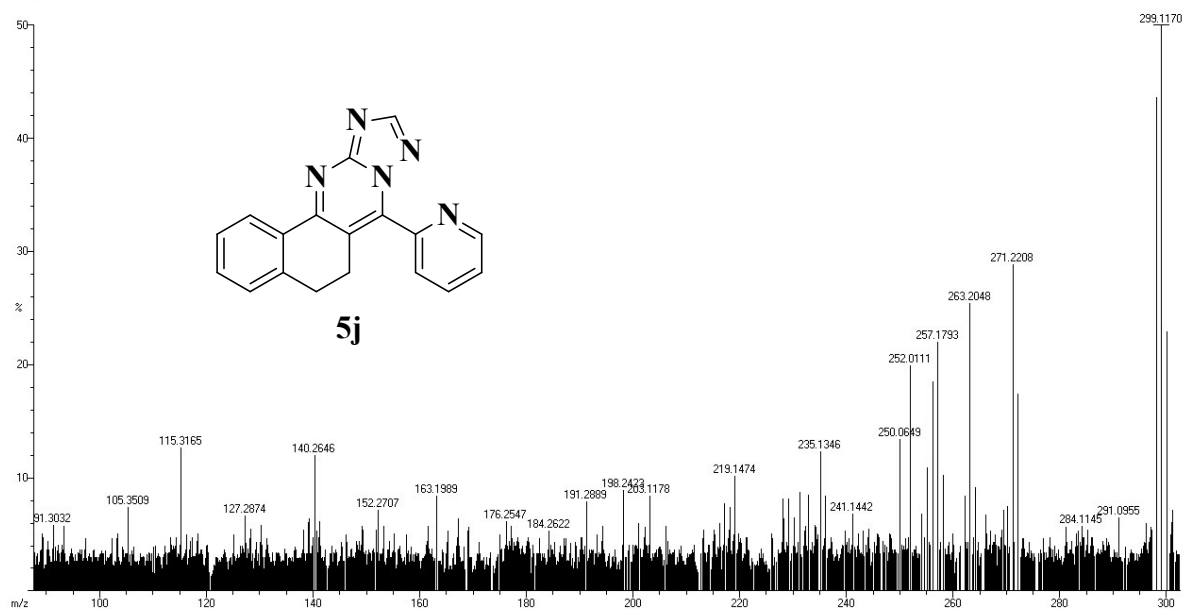
Signature SIF VIT VELLORE
JPR-089-P



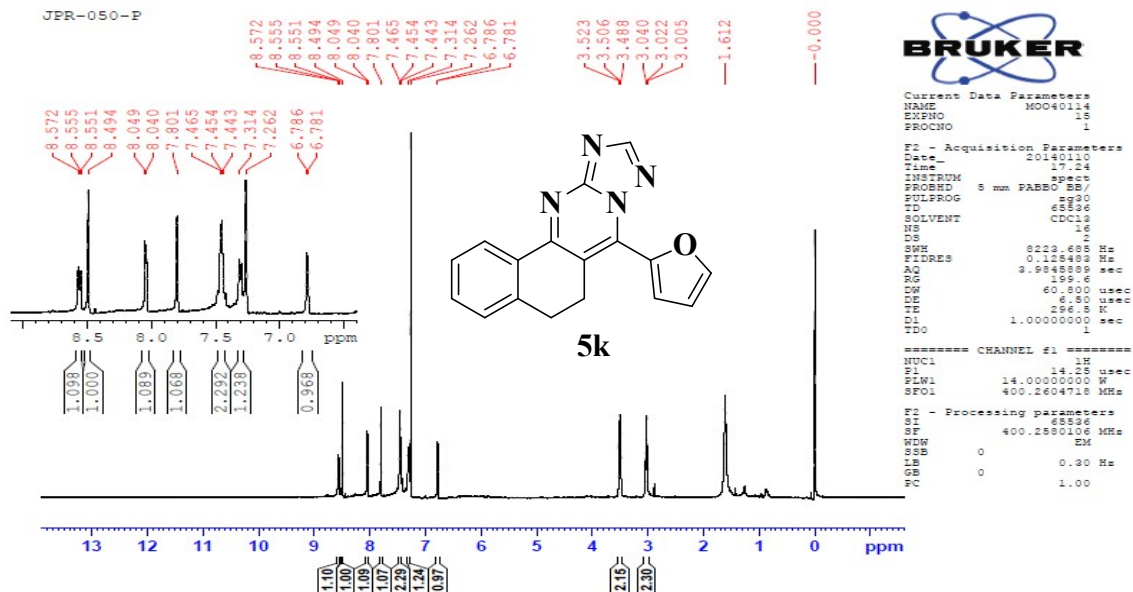
HRMS spectrum of compound (5j):

JPR-089

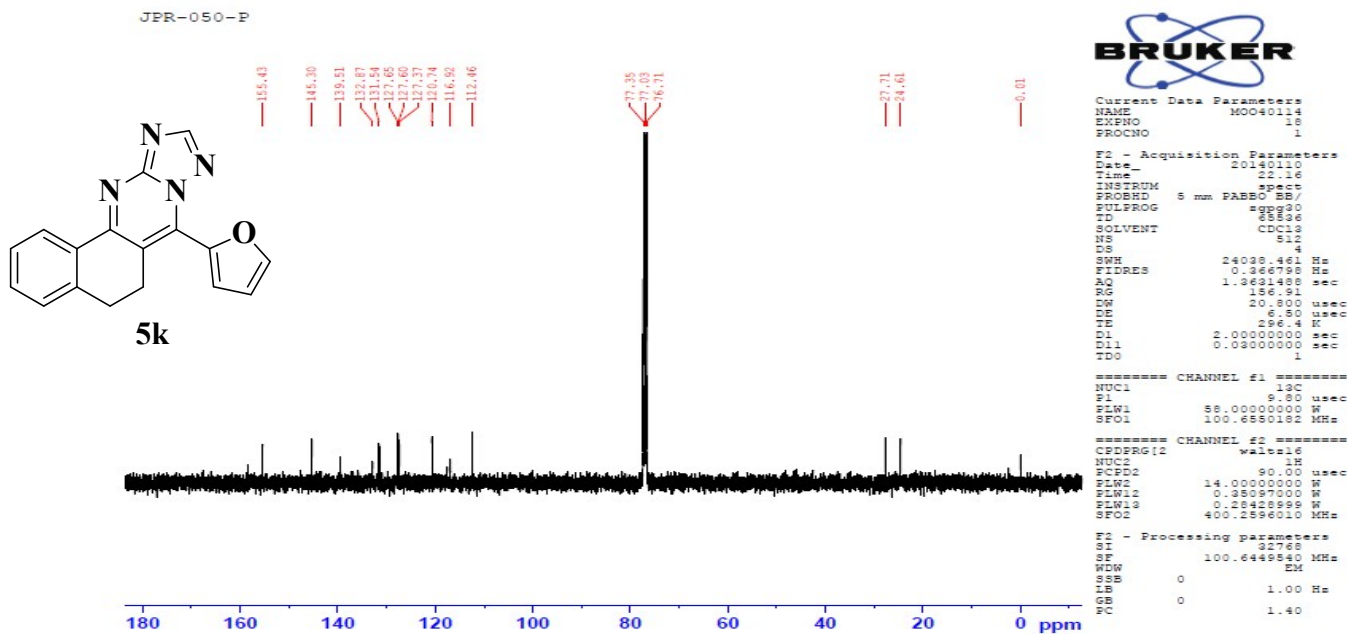
Scan: 3 TIC=18187440 Base=14.13FS #Ions=3586 RT=01



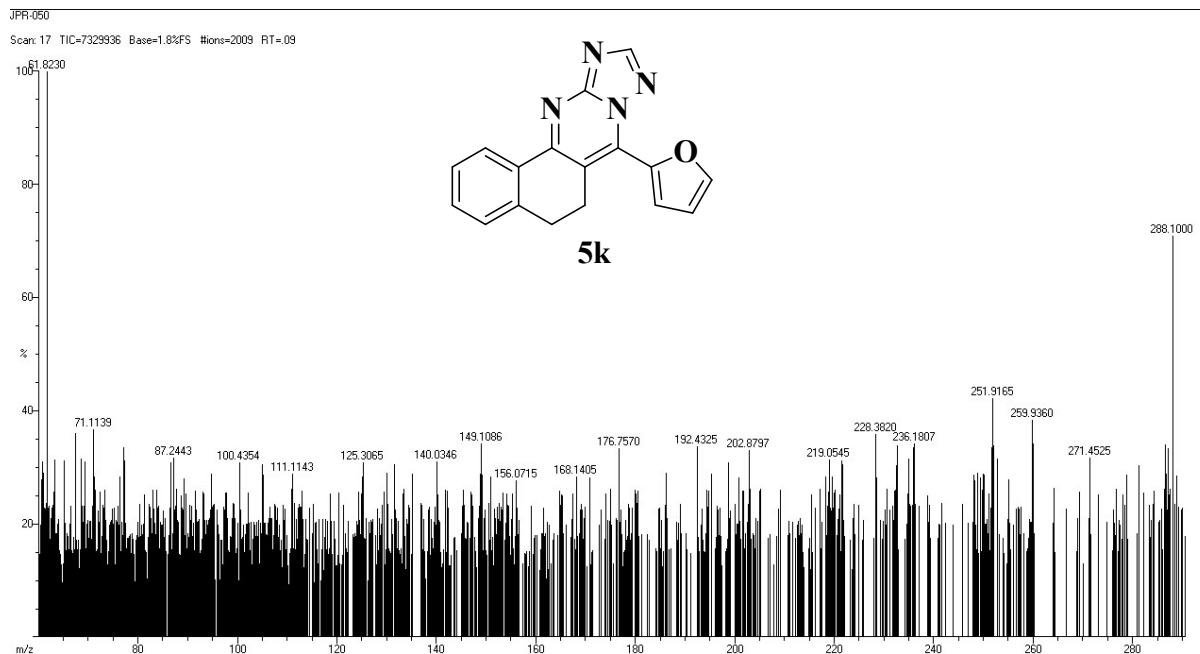
¹H NMR spectrum of compound (5k):



¹³C NMR spectrum of compound (5k):

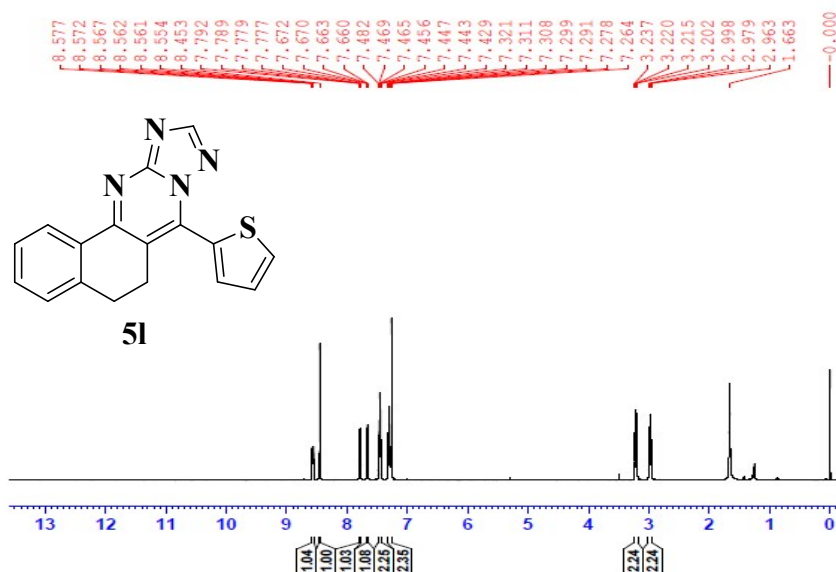


HRMS spectrum of compound (5k):



¹H NMR spectrum of compound (5l):

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JPR-124-P



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```

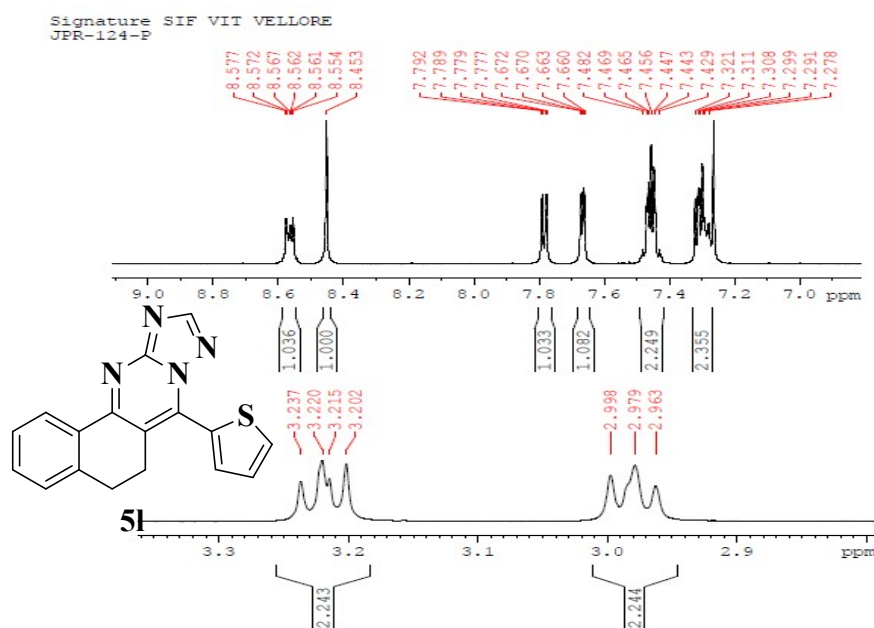
Current Data Parameters
NAME          analy
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20140609
Time          17.26
INSTRUM       spect
PROBHD        5 mm F4BBO BB/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            1638
DS            4
SWH           8220.685 Hz
FIDRES        0.128863 Hz
AQ            9.984888 sec
RG            199.6
DWM           60.800 usec
DE            6.50 usec
TE            299.9 K
TD0           1.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          13C
P1            14.235 usec
PCW1          14.00000000 W
SFO1          400.2604718 MHz

F2 - Processing parameters
SI            65536
SF            400.2600098 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```


Expanded ¹H NMR spectrum of compound (51):



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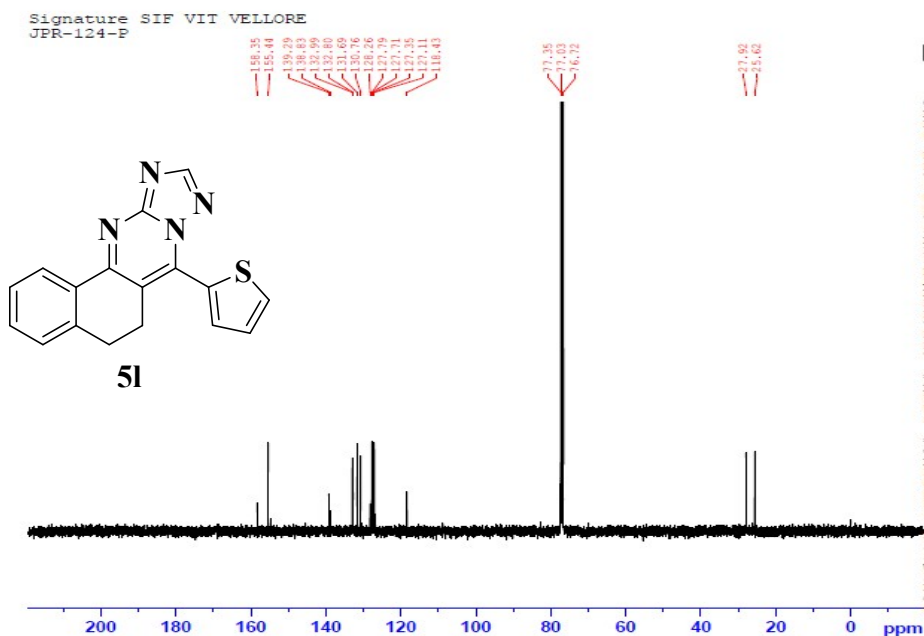
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Current Data Parameters
NAME analy
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140609
Time 17.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 8223.65558 Hz
AQ 0.2484433 sec
FIDRES 199.06
AQRES 6.800 usec
SFO1 400.2580052 MHz
TDO 1.000000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 14.00000000 usec
PL1 0.00000000 W
SFO1 400.2580052 MHz

F - Processing parameters
SFO 400.2580052 MHz
WDW EM
SSB 0
GB 0.20 Hz
CB 0
PC 1.00
```

¹³C NMR spectrum of compound (51):



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```
Current Data Parameters
NAME analy
EXPNO 1
PROCNO 1

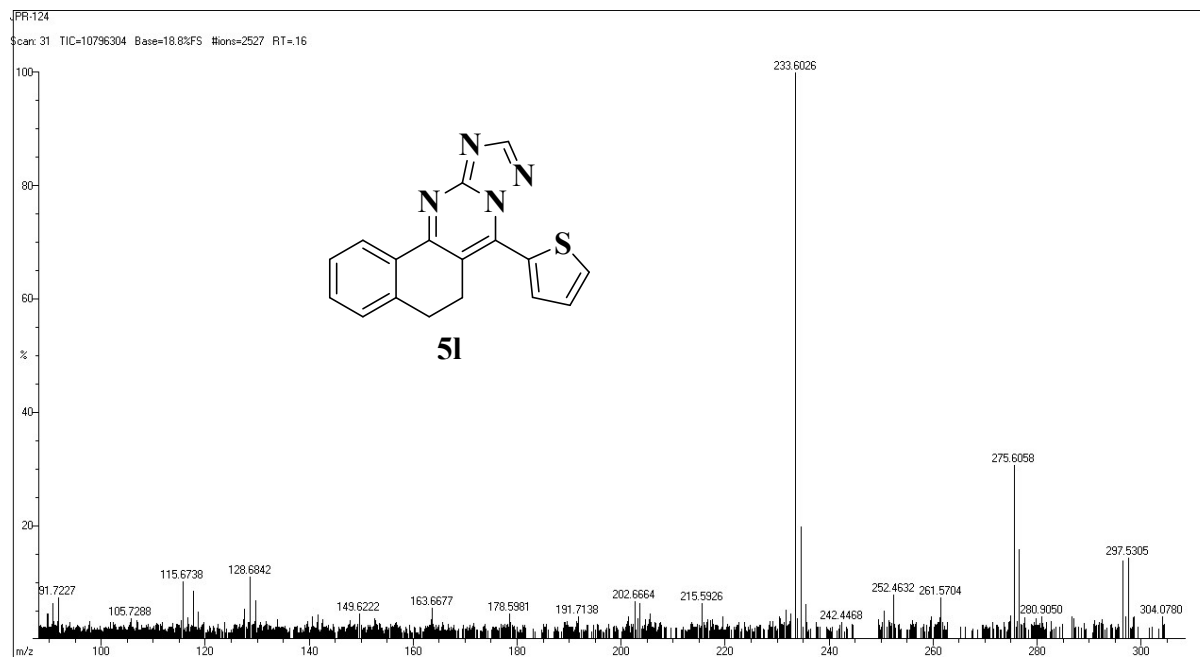
F2 - Acquisition Parameters
Date_ 20140609
Time 22.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 24038.461 Hz
AQ 0.36679 Hz
FIDRES 1.3631458 sec
SFO1 100.6281192 MHz

===== CHANNEL f1 =====
CPDPRG12 waltz16
NUC1 13C
P1 90.00 usec
PL1 0.00000000 W
SFO1 100.6281192 MHz

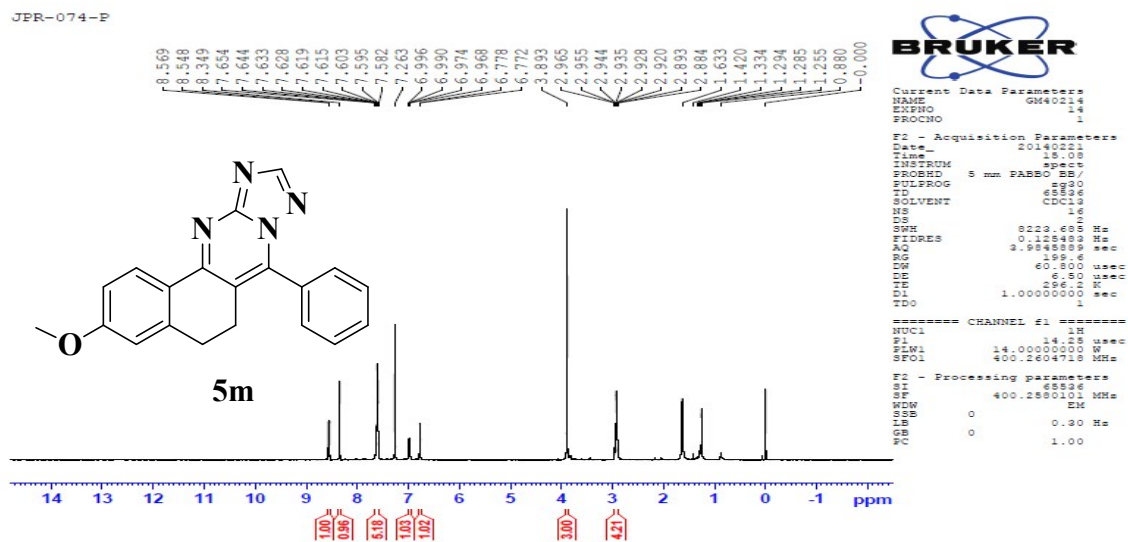
===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
P2 90.00 usec
PL2 0.00000000 W
SFO2 400.2580052 MHz
TDO 0.030000000 sec
TD0 1
```

```
- Processing parameters
SFO 100.6281192 MHz
WDW EM
SSB 0
GB 1.00 Hz
CB 0
PC 1.40
```

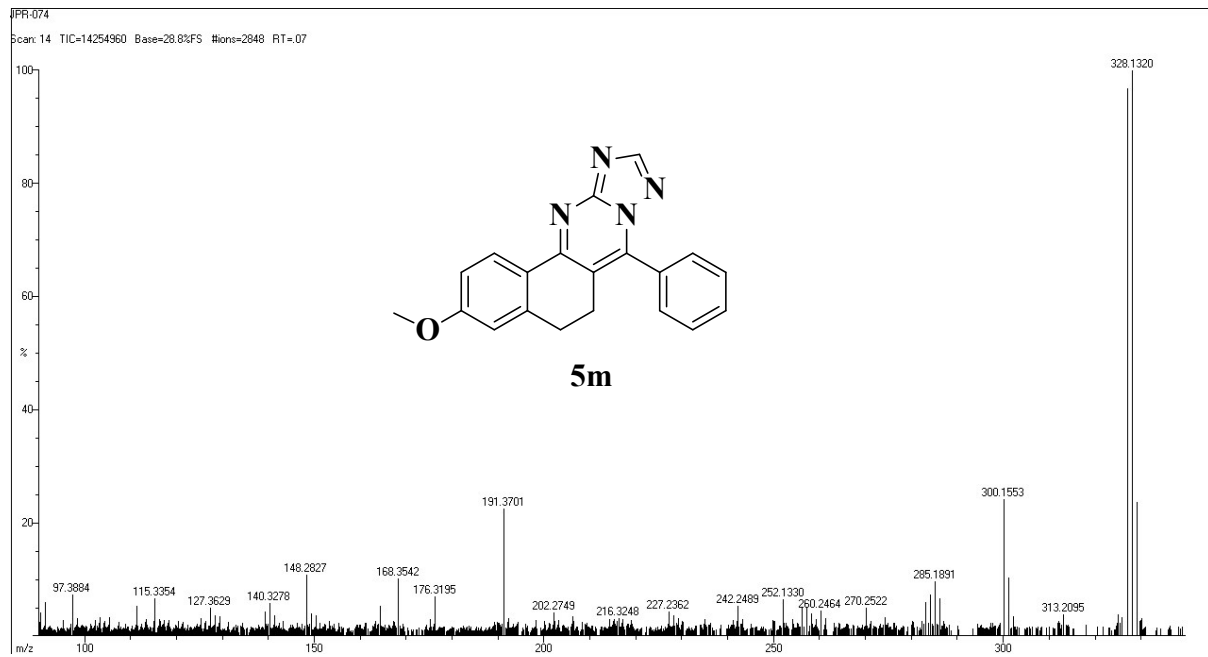
HRMS spectrum of compound (5l):



¹H NMR spectrum of compound (5m):

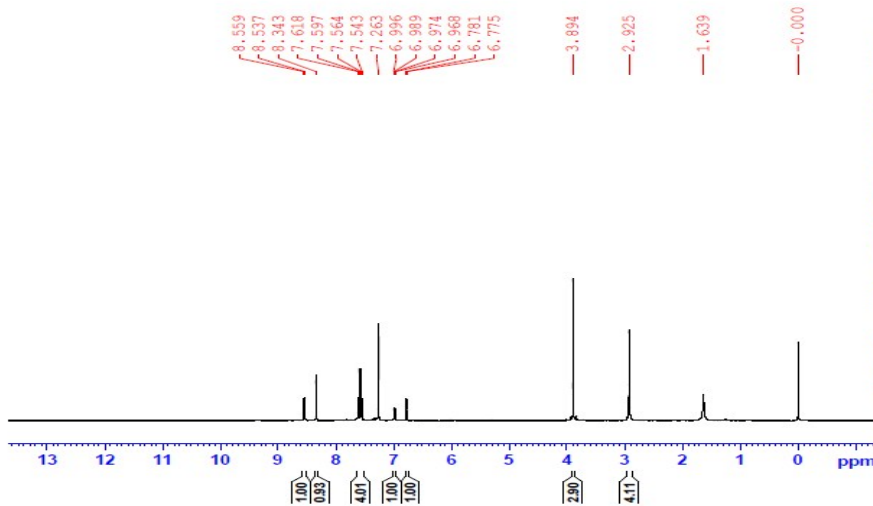


HRMS spectrum of compound (5m):



¹H NMR spectrum of compound (5m):

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JPR-093-P



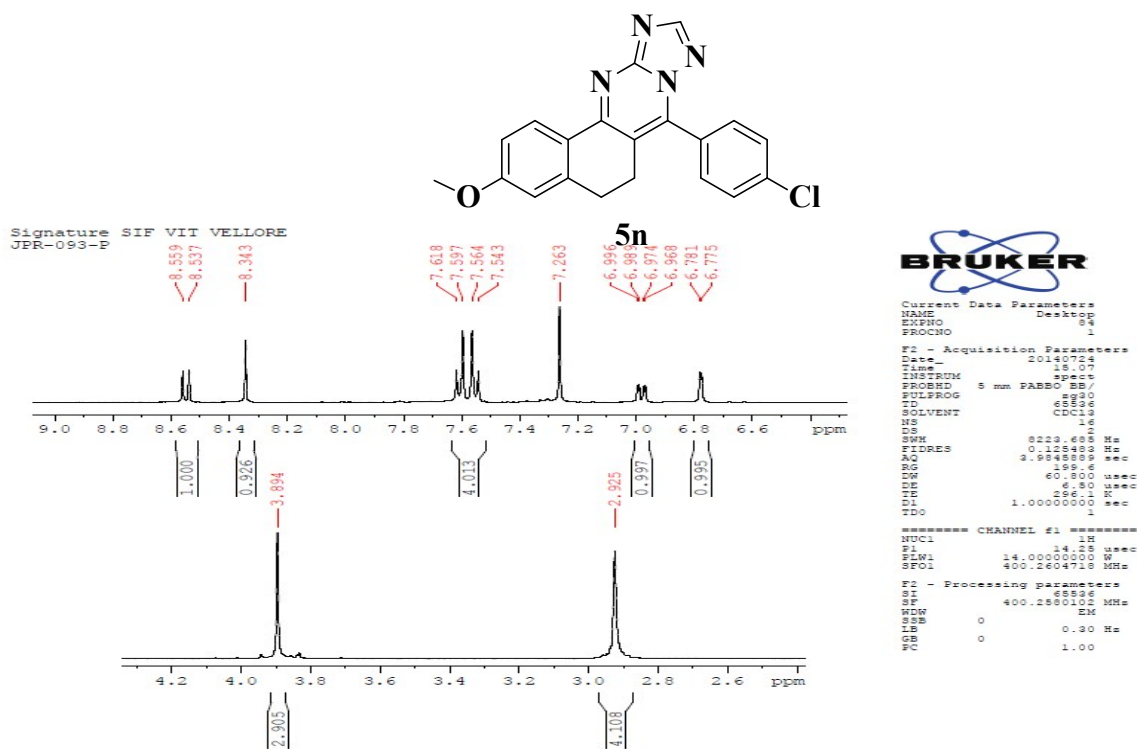
Current Data Parameters
NAME Desktop
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140704
Time 15:09
INSTRUM spect
PROBHD 5 mm F4BBO
PULPROG zgpg30
FILTROG CM30
SOLVENT CDCl3
NS 640
DS 4
SWH 8223.6 MHz
FIDRES 0.1024003 MHz
AQ 0.9888000 sec
RG 655
PC 1.99 sec
LUMS 60.8000 usec
SFO1 400.1464000 MHz
NUC1 13C
NUC2 13C
P1 1.0000000 sec
P2 0.0000000 sec
P3 0.0000000 sec

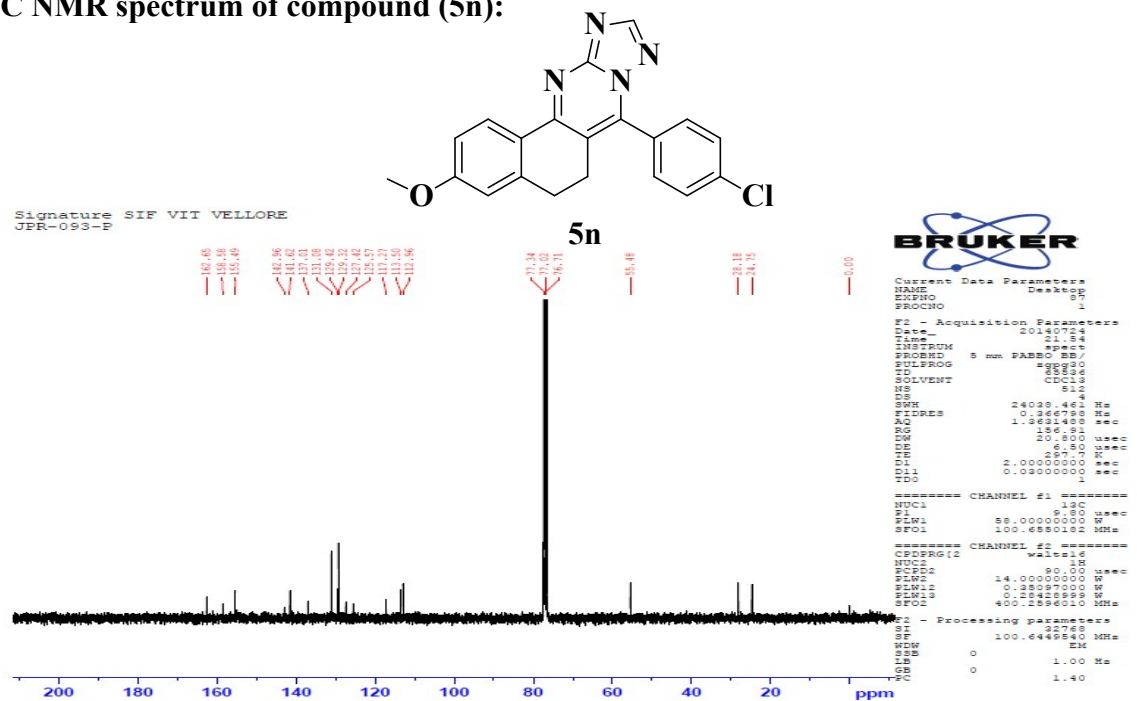
===== CHANNEL f1 =====
NUC1 13C
P1 1.0000000 sec
SFO1 101.6261260 MHz
SFO2 400.2604718 MHz

F2 - Processing parameters
WDWEM 64
SSB 0
GB 0
PC 1.99 sec
SFO1 400.2604718 MHz
EM 0
WDW 0
SSB 0
GB 0
PC 1.99 sec
SFO1 400.2604718 MHz
EM 0
WDW 0
SSB 0
GB 0
PC 1.99 sec
SFO1 400.2604718 MHz
EM 0

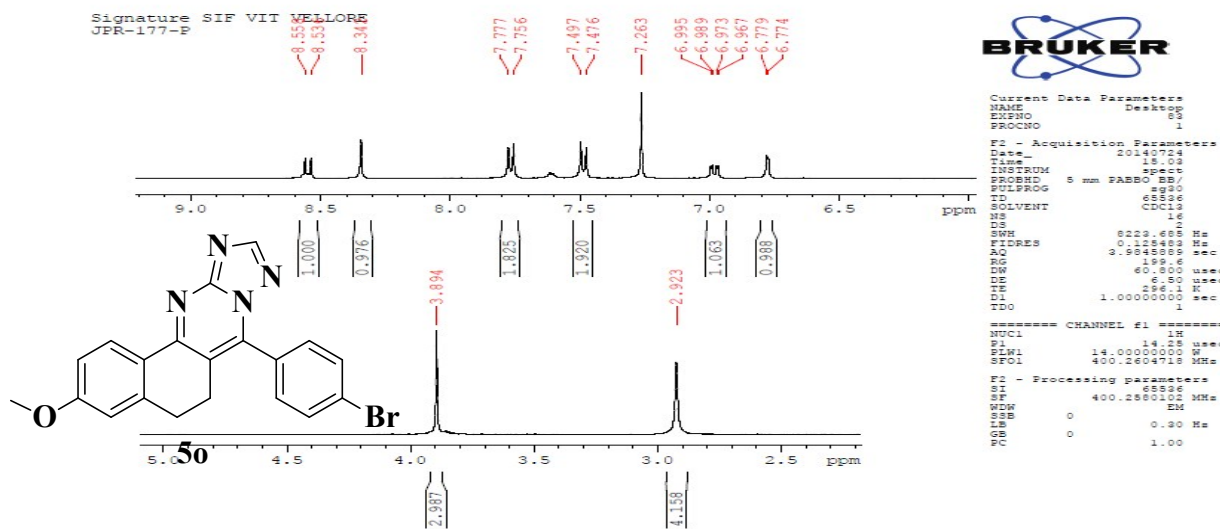
Expanded ¹H NMR spectrum of compound (5n):



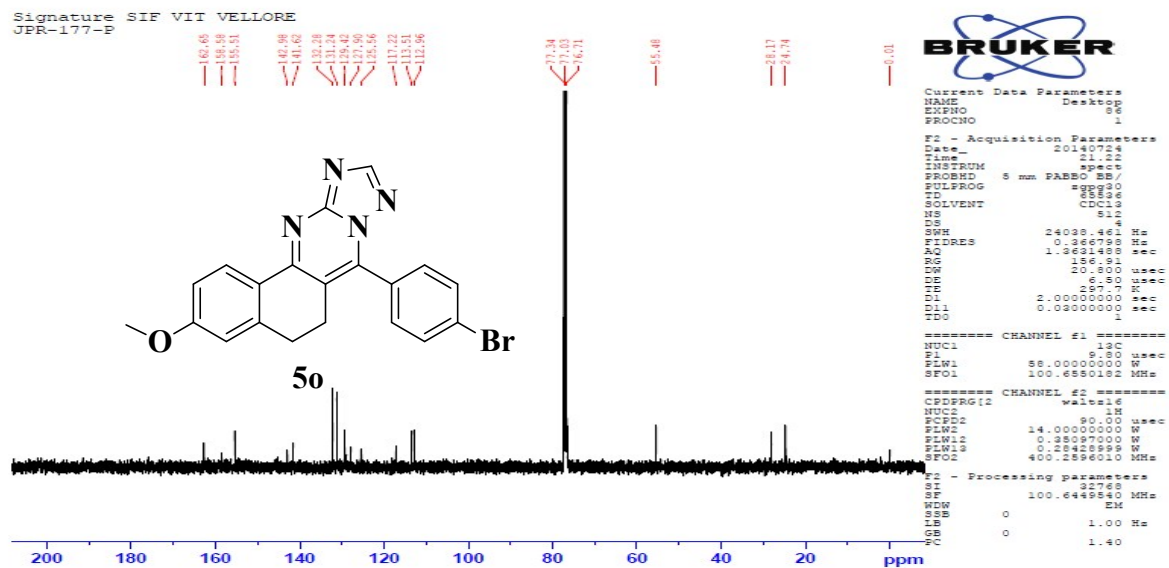
¹³C NMR spectrum of compound (5n):



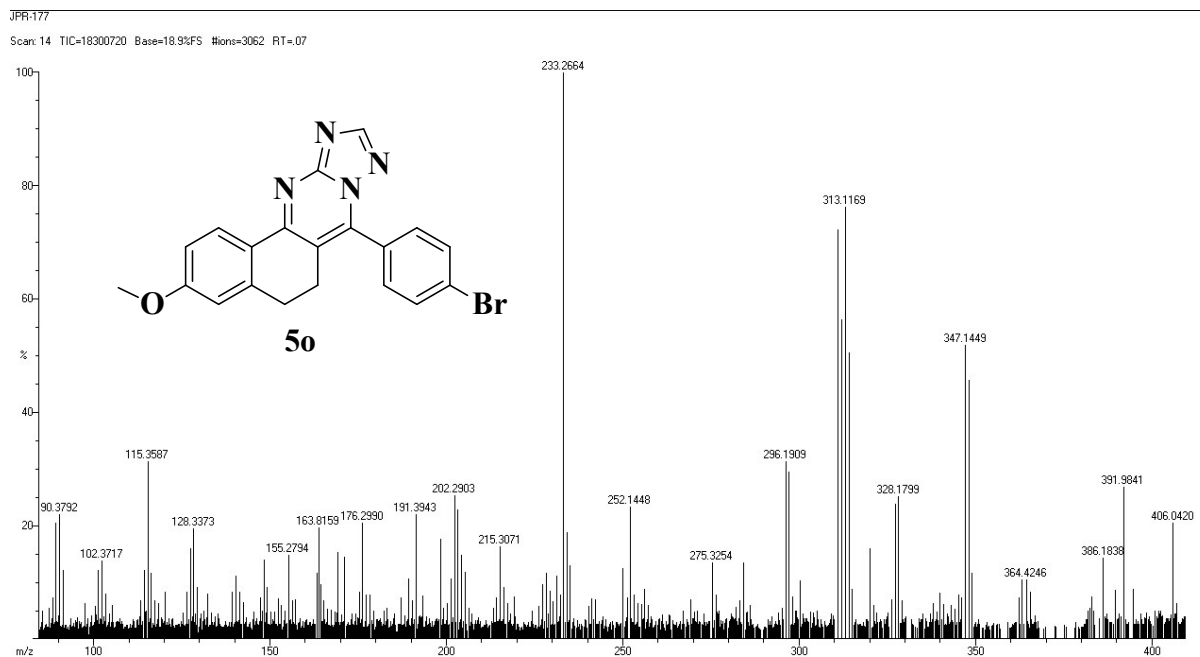
Expanded ¹H NMR spectrum of compound (50):



¹³C NMR spectrum of compound (50):

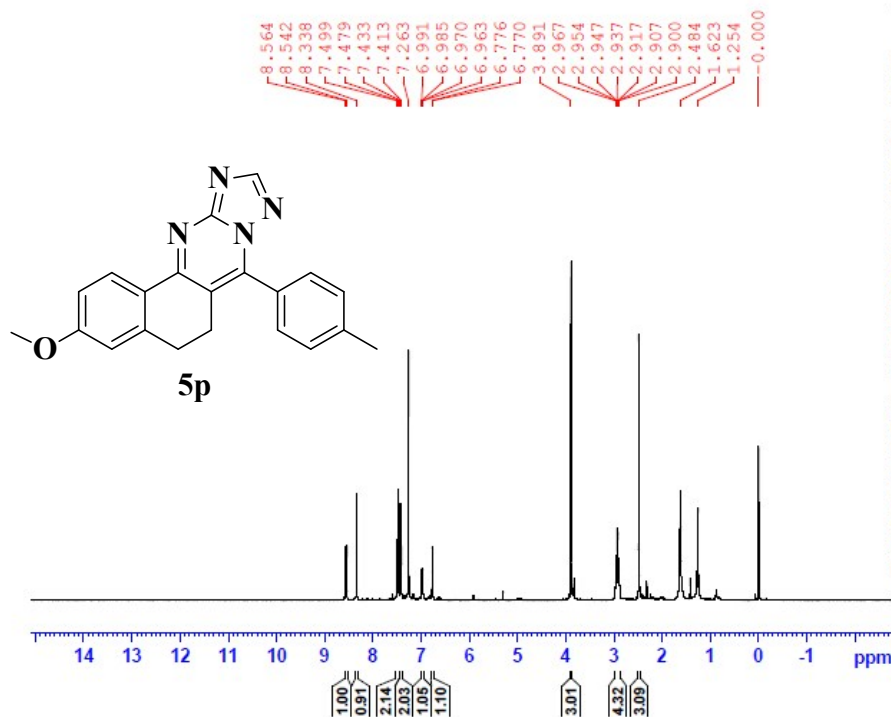


HRMS spectrum of compound (5o):



¹H NMR spectrum of compound (5p):

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JPR-180-P



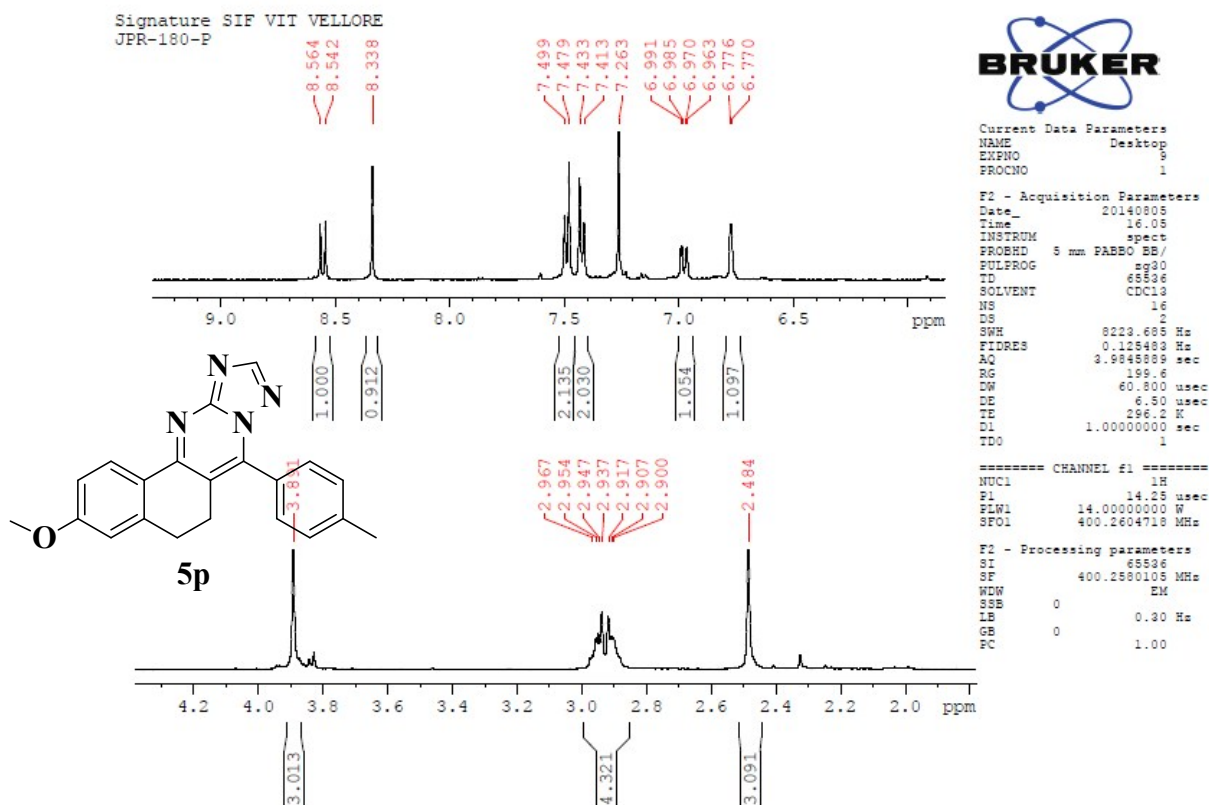
Current Data Parameters
NAME Desktop
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140808
Time_ 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.688 Hz
FIDRES 0.125488 Hz
AQ 3.9849389 sec
RG 199.6
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

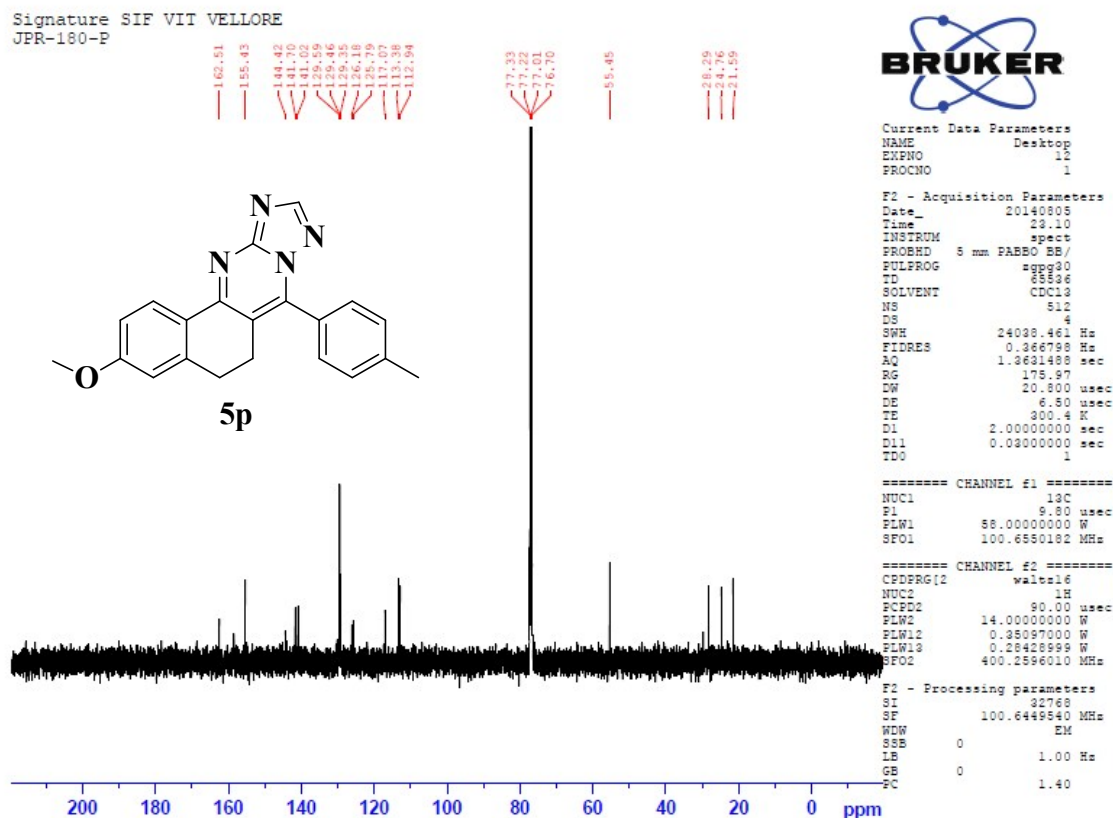
===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

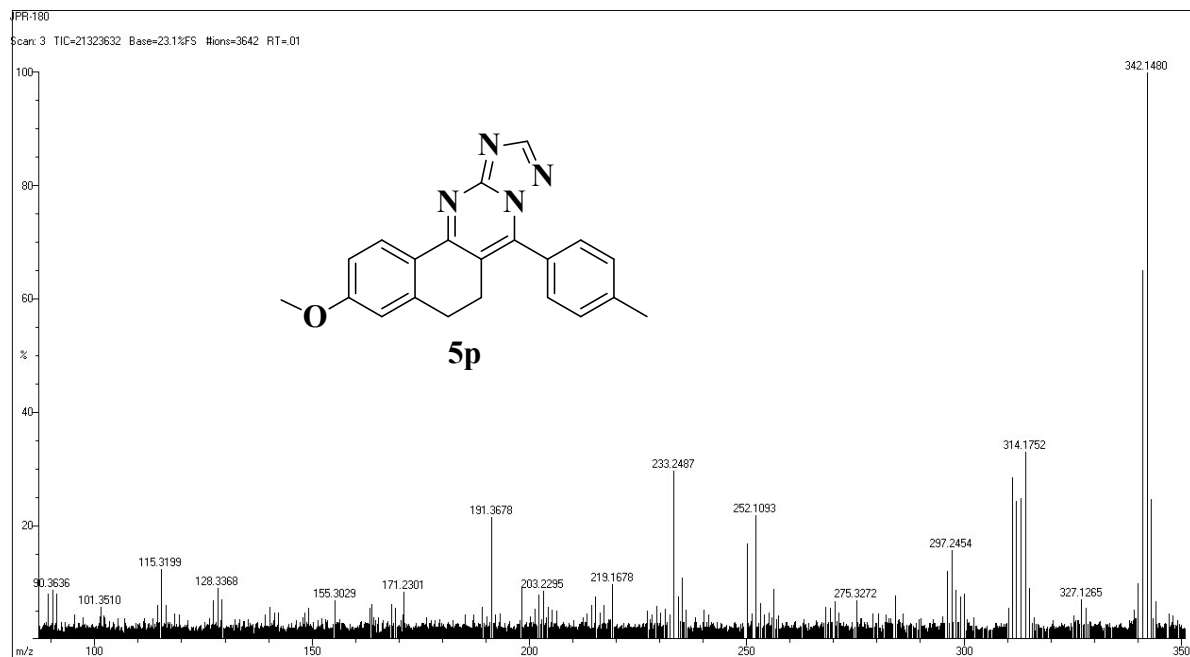
Expanded ¹H NMR spectrum of compound (5p):



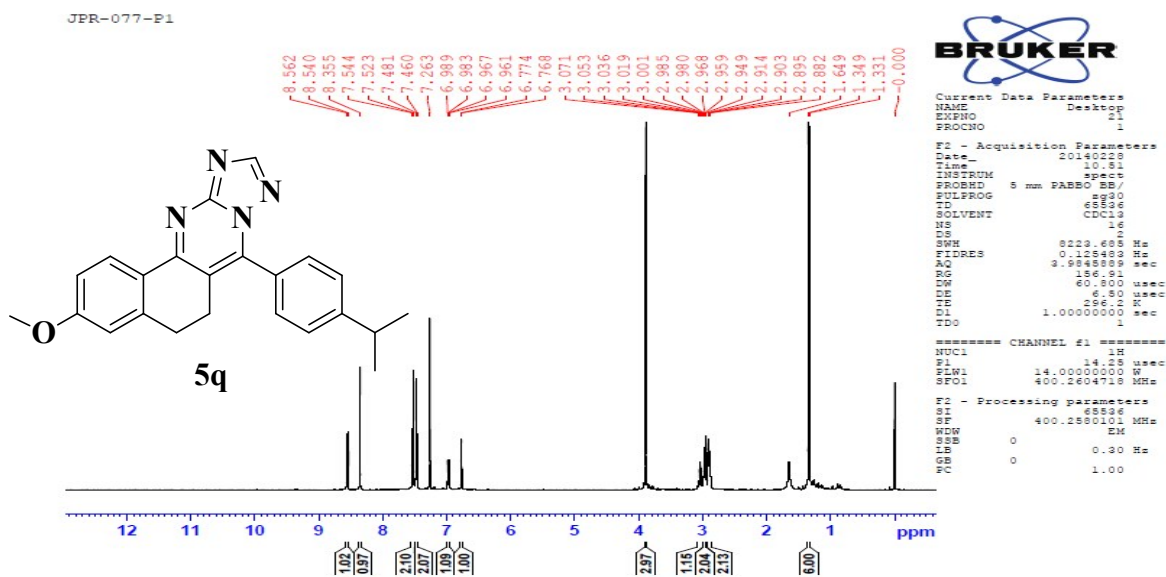
¹³C NMR spectrum of compound (5p):



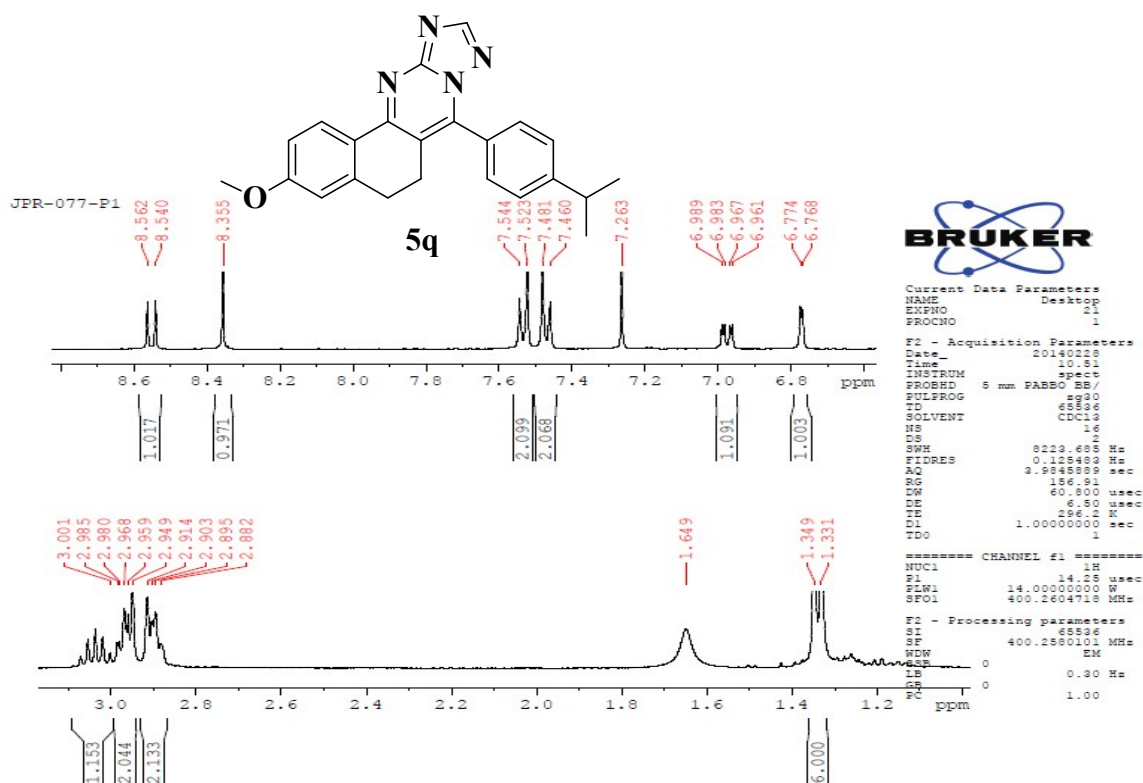
HRMS spectrum of compound (5p):



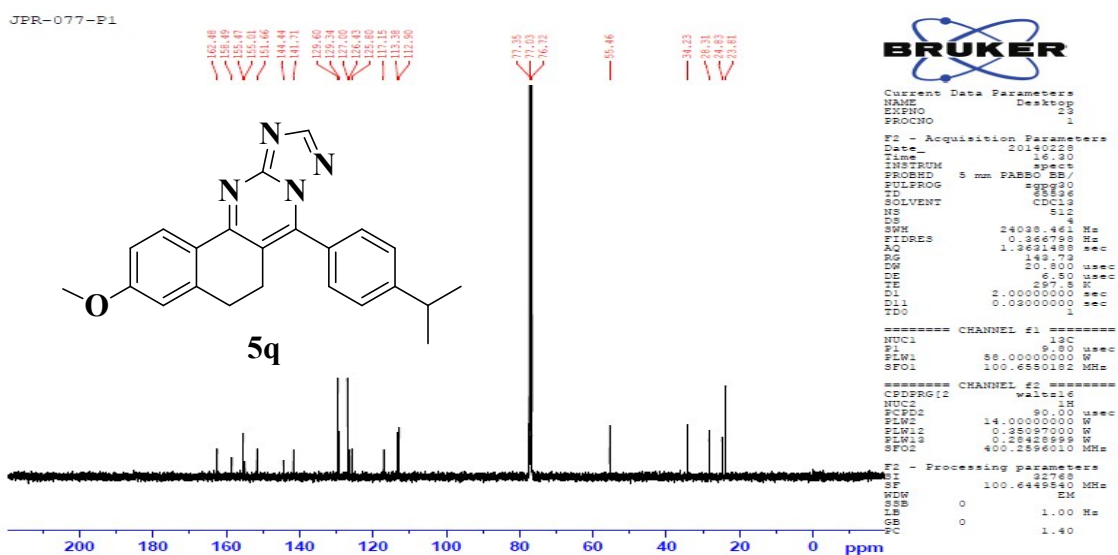
¹H NMR spectrum of compound (5q):



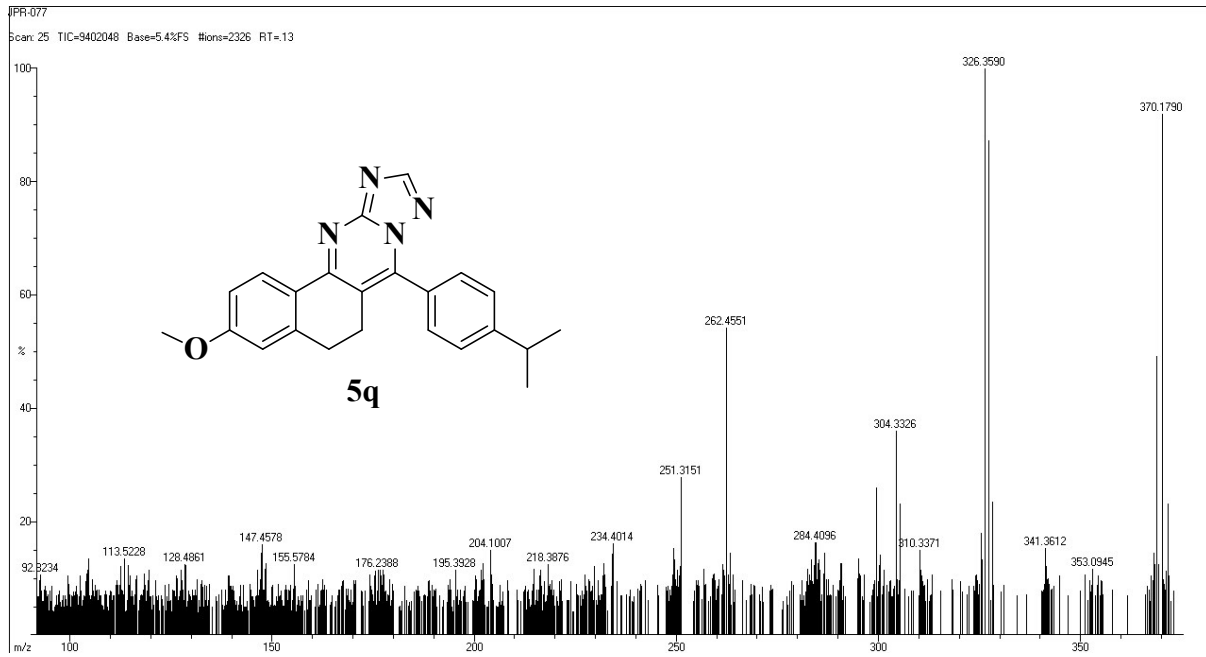
Expanded ¹H NMR spectrum of compound (5q):



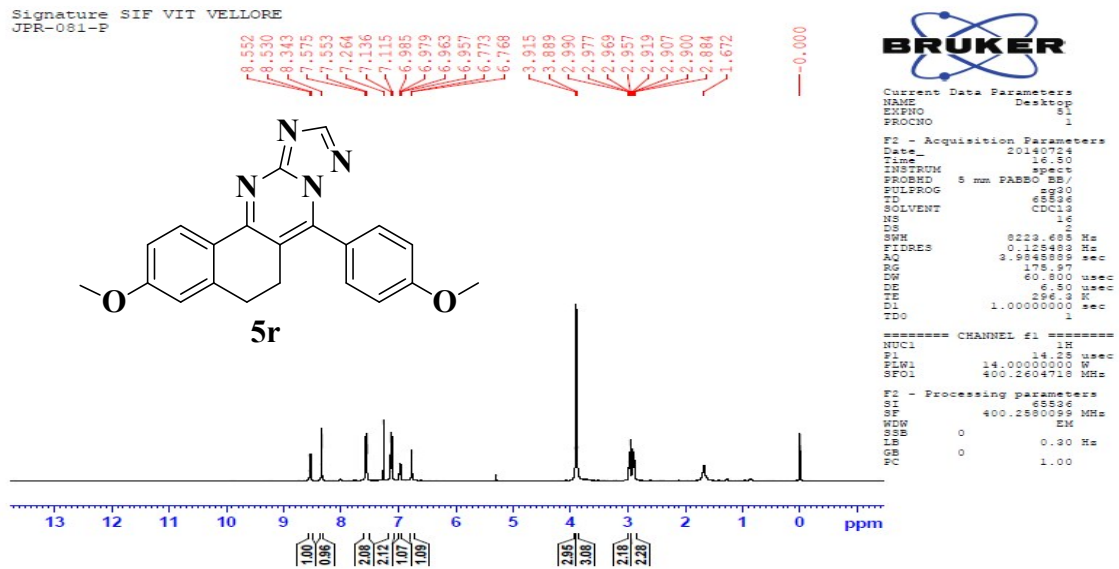
¹³C NMR spectrum of compound (5q):



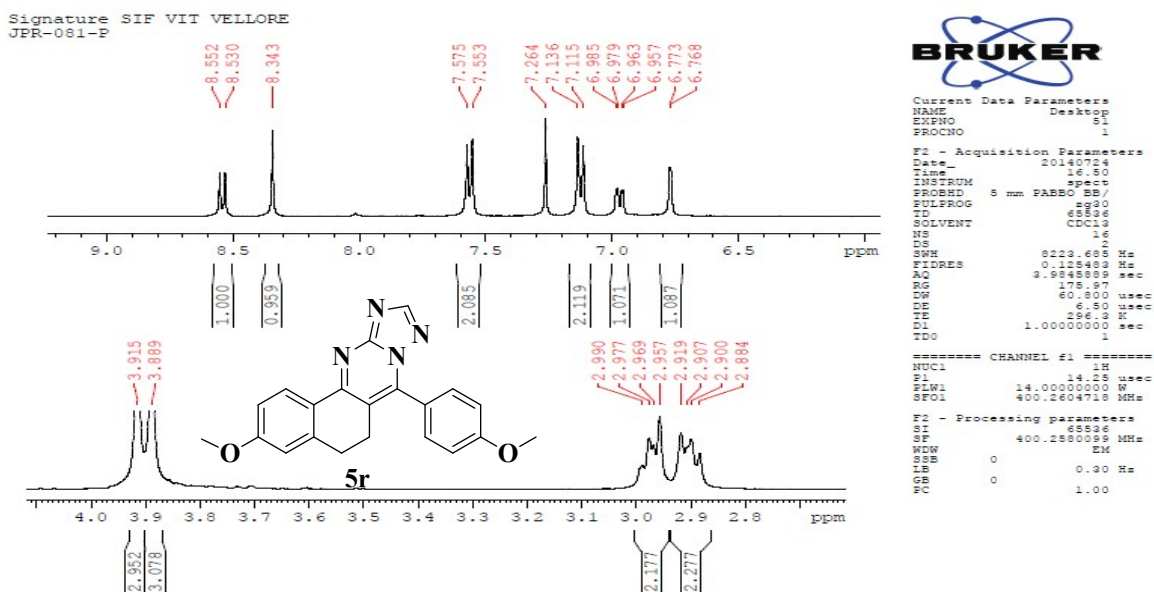
HRMS spectrum of compound (5q):



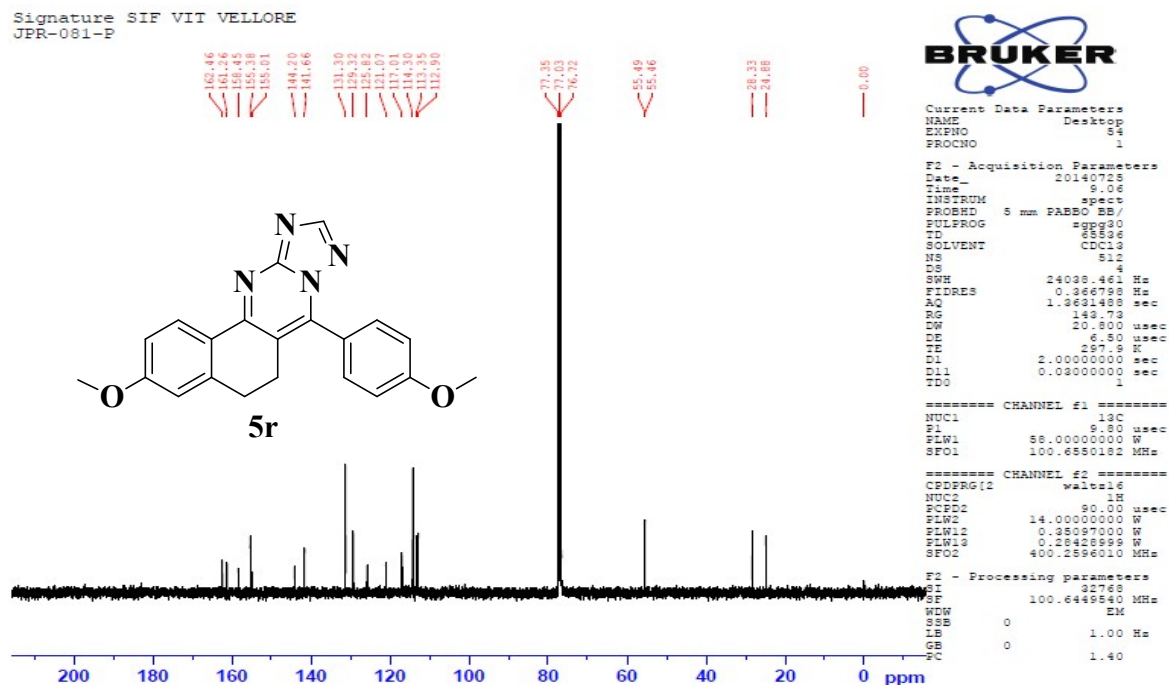
¹H NMR spectrum of compound (5r):



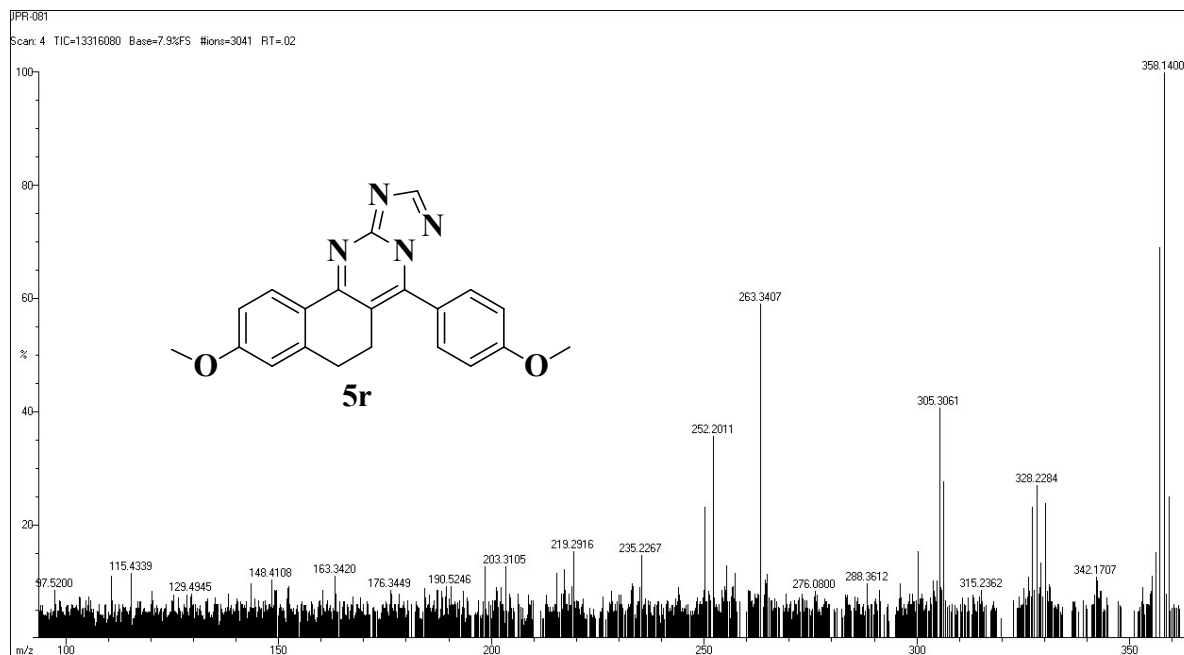
Expanded ¹H NMR spectrum of compound (5r):



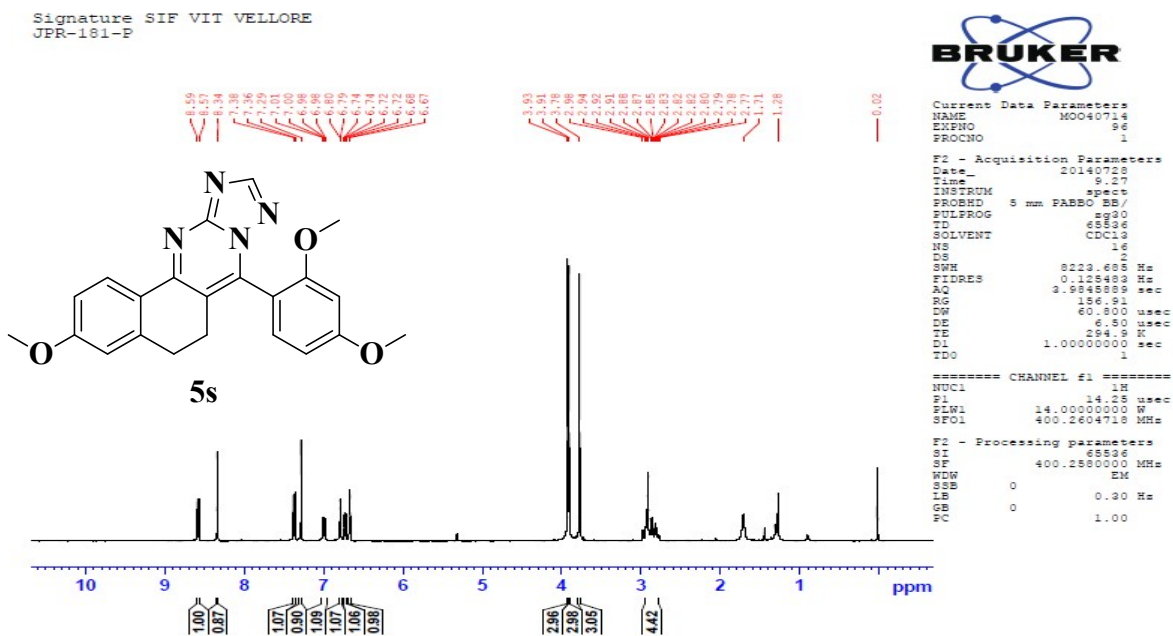
¹³C NMR spectrum of compound (5r):



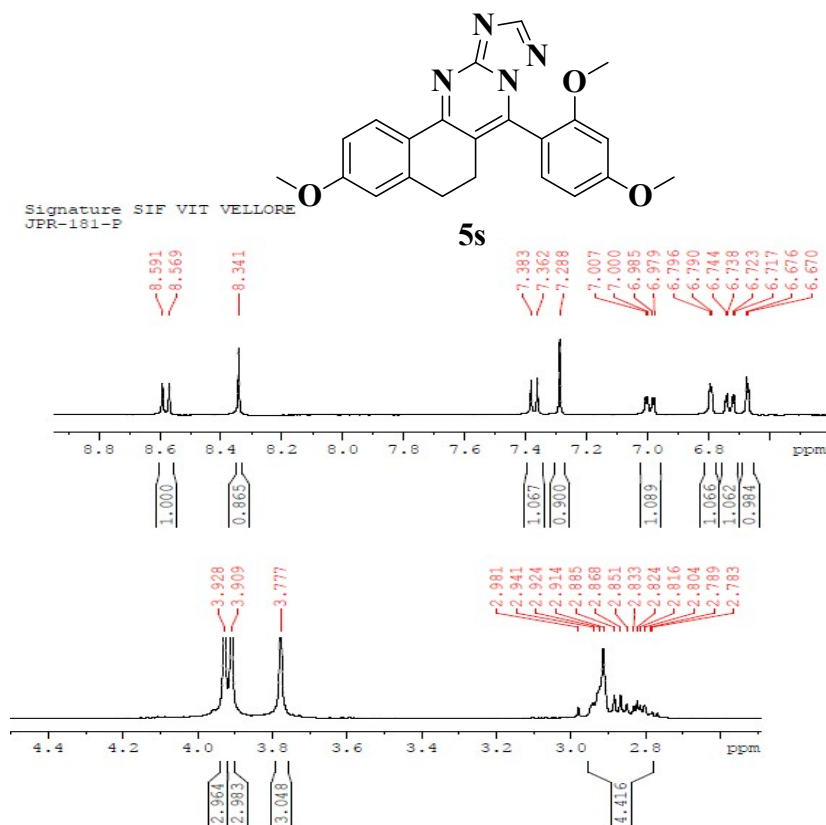
HRMS spectrum of compound (5r):



¹H NMR spectrum of compound (5s):



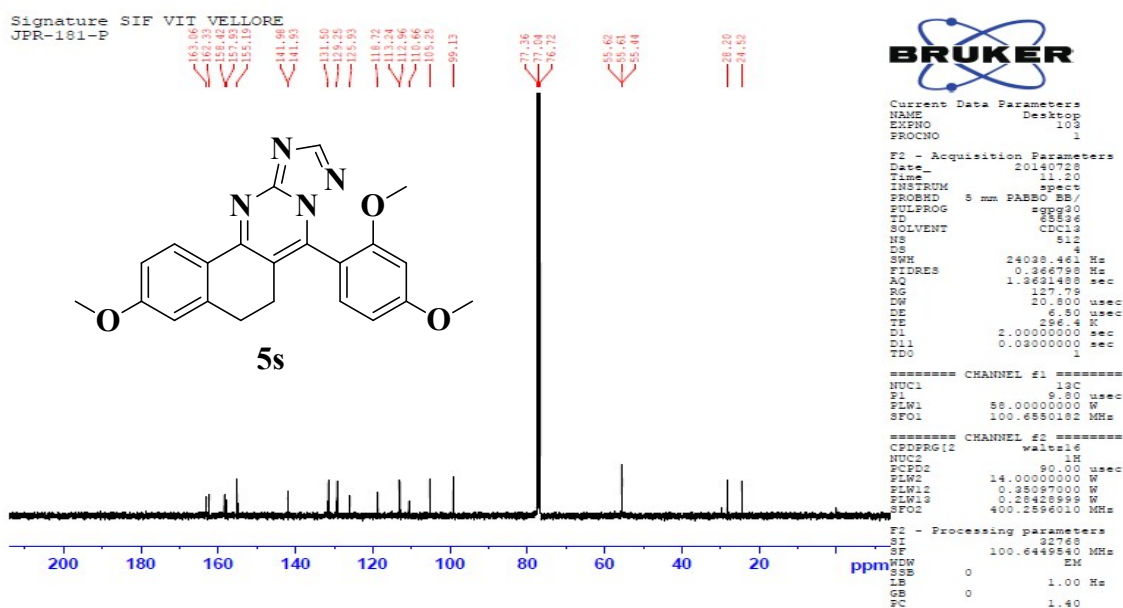
Expanded ¹H NMR spectrum of compound (5s):



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Current Data Parameters
NAME      M0040714
EXPNO    26
PROCNO   1

F2 - Acquisition Parameters
Date_    20140723
Time     9.27
INSTRUM spect
PROBHD   5 mm PABBO BB
PULPROG zgpg30
AQ       6.583333
SOLVENT  CDCl3
NS       512
DS       4
SWH      3229.6 Hz
FIDRES   0.333333 Hz
AQRES    0.9345238 sec
SFO1     156.991 MHz
WDW       EM
SSB       0
GB        0
PC        1.00000000
===== CHANNEL f1 =====
NUC1      1H
P1        14.000000 usec
PL1       0.000000 dB
SFO1     400.1460000 MHz
===== CHANNEL f2 =====
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
F2 - Processing parameters
Date_    20140723
Time     9.27
INSTRUM spect
PROBHD   5 mm PABBO BB
PULPROG zgpg30
AQ       6.583333
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.463 Hz
FIDRES   0.333333 Hz
AQRES    0.9345238 sec
SFO1     156.991 MHz
WDW       EM
SSB       0
GB        0
PC        1.00000000
===== CHANNEL f1 =====
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
===== CHANNEL f2 =====
CDPRG12  waltz16
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
===== CHANNEL f2 =====
F2 - Processing parameters
Date_    20140723
Time     9.27
INSTRUM spect
PROBHD   5 mm PABBO BB
PULPROG zgpg30
AQ       6.583333
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.463 Hz
FIDRES   0.333333 Hz
AQRES    0.9345238 sec
SFO1     156.991 MHz
WDW       EM
SSB       0
GB        0
PC        1.00000000
===== CHANNEL f1 =====
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
===== CHANNEL f2 =====
CDPRG12  waltz16
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
```

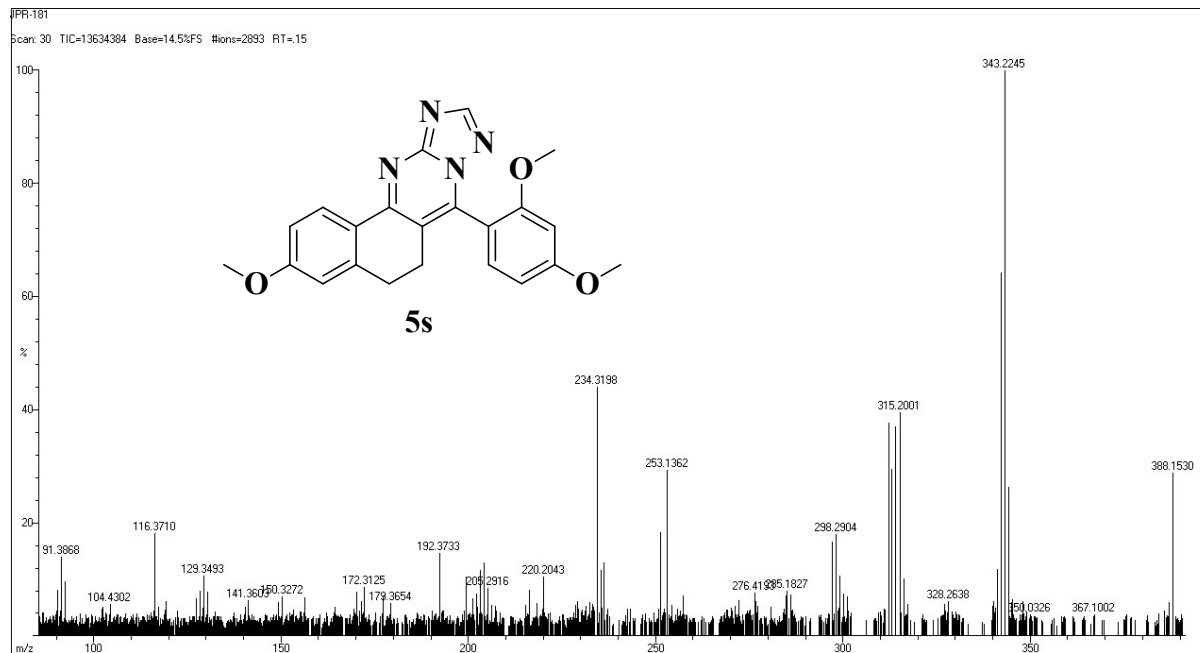
¹³C NMR spectrum of compound (5s):



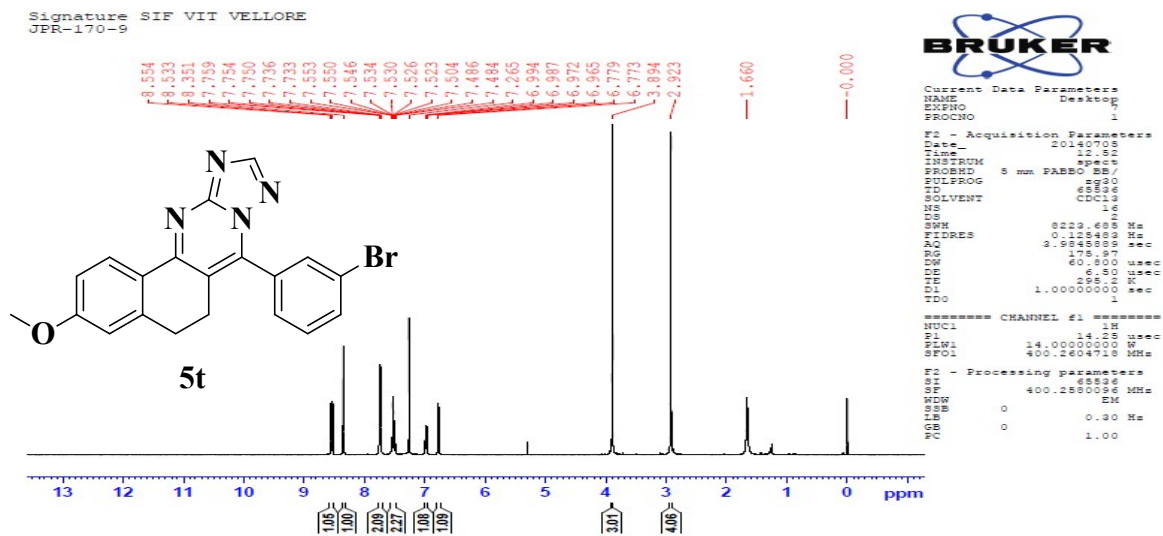
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Current Data Parameters
NAME      Desktop
EXPNO    103
PROCNO   1

F2 - Acquisition Parameters
Date_    20140723
Time     11.00
INSTRUM spect
PROBHD   5 mm PABBO BB
PULPROG zgpg30
AQ       6.583333
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.463 Hz
FIDRES   0.333333 Hz
AQRES    0.9345238 sec
SFO1     156.991 MHz
WDW       EM
SSB       0
GB        0
PC        1.00000000
===== CHANNEL f1 =====
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
===== CHANNEL f2 =====
CDPRG12  waltz16
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
===== CHANNEL f2 =====
F2 - Processing parameters
Date_    20140723
Time     11.00
INSTRUM spect
PROBHD   5 mm PABBO BB
PULPROG zgpg30
AQ       6.583333
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.463 Hz
FIDRES   0.333333 Hz
AQRES    0.9345238 sec
SFO1     156.991 MHz
WDW       EM
SSB       0
GB        0
PC        1.00000000
===== CHANNEL f1 =====
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
===== CHANNEL f2 =====
CDPRG12  waltz16
NUC1      13C
P1        9.000000 usec
PL1       0.000000 dB
SFO1     100.626182 MHz
```

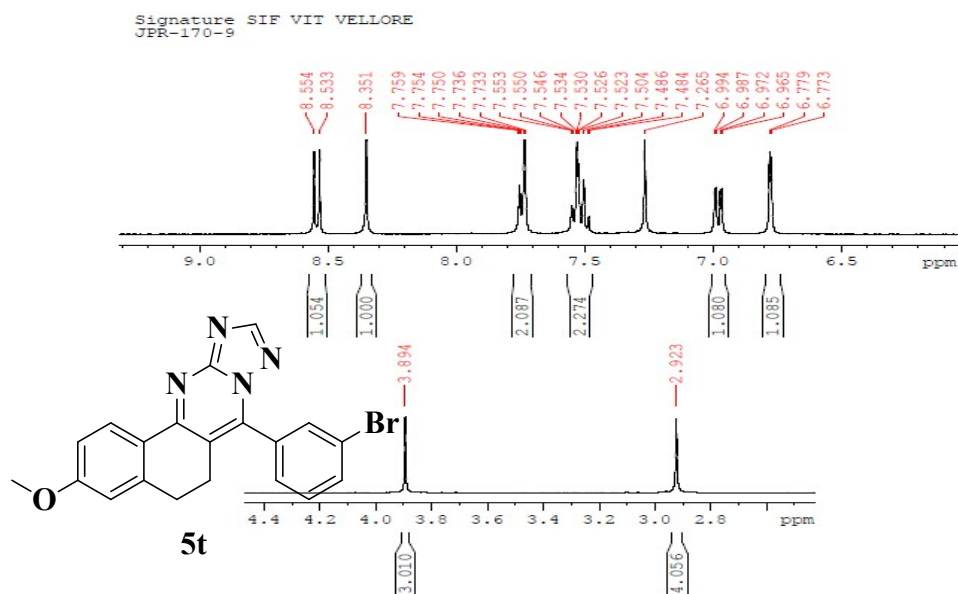
HRMS spectrum of compound (5s):



¹H NMR spectrum of compound (5t):



Expanded ¹H NMR spectrum of compound (5t):



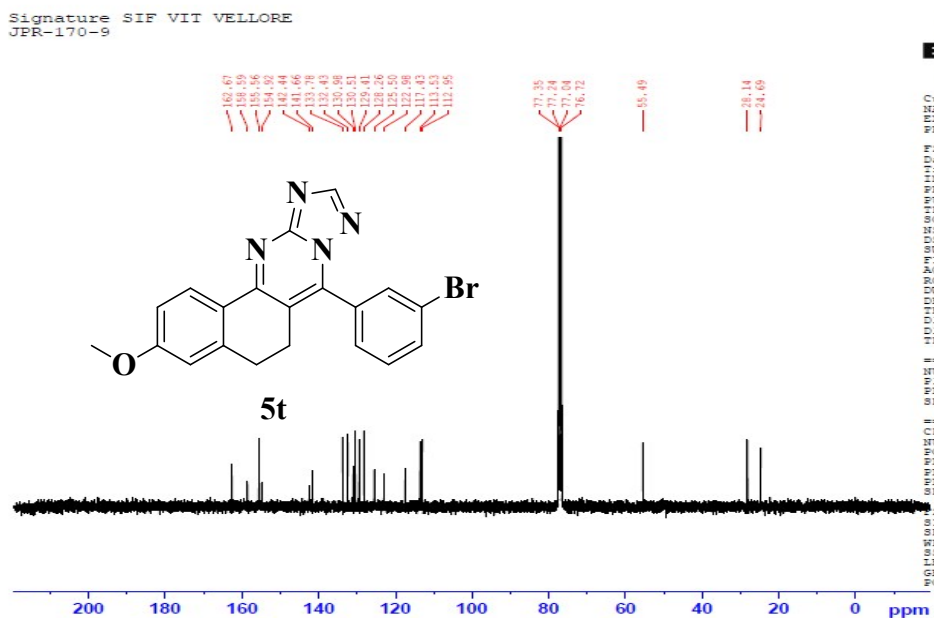
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Current Data Parameters
NAME      Desktop
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20140708
Time     12:24
INSTRUM  spect
PROBHD   5 mm PABBO BB
PULPROG  zgpg30
ID       0
SOLVENT  CDCl3
NS       512
DSH      4
AQ       0.12500000 sec
RG       655.36000000
FIDRES   0.10000000 Hz
AQRES    3.904000000 Hz
SFO1     400.1460000 MHz
NUC1      13C
P1        12.00000000 sec
PL1       0.00000000 dB
SFO2     101.2530000 MHz
NUC2      1H
P2        0.00000000 sec
PL2       0.00000000 dB
SFO3     400.1460000 MHz
NUC3      1H
P3        0.00000000 sec
PL3       0.00000000 dB
SFO4     0.00000000 MHz
NUC4      13C
P4        0.00000000 sec
PL4       0.00000000 dB
===== CHANNEL f1 =====
NUC1      1H
P1        14.00000000 sec
PL1       0.00000000 dB
SFO1     400.1460000 MHz
===== Processing parameters =====
RG       655.36000000
SFO1     400.1460000 MHz
EM       EM
GB1      0
GB2      0
GB3      0
GB4      0
NUC1      1H
NUC2      13C
===== CHANNEL f2 =====
NUC1      13C
P1        12.00000000 sec
PL1       0.00000000 dB
SFO1     101.2530000 MHz
===== CHANNEL f3 =====
NUC1      1H
P1        12.00000000 sec
PL1       0.00000000 dB
SFO1     400.1460000 MHz
===== Processing parameters =====
RG       655.36000000
SFO1     400.1460000 MHz
EM       EM
GB1      0
GB2      0
GB3      0
GB4      0
NUC1      1H
NUC2      13C
===== CHANNEL f4 =====
NUC1      13C
P1        12.00000000 sec
PL1       0.00000000 dB
SFO1     101.2530000 MHz
===== Processing parameters =====
RG       655.36000000
SFO1     400.1460000 MHz
EM       EM
GB1      0
GB2      0
GB3      0
GB4      0

```

¹³C NMR spectrum of compound (5t):



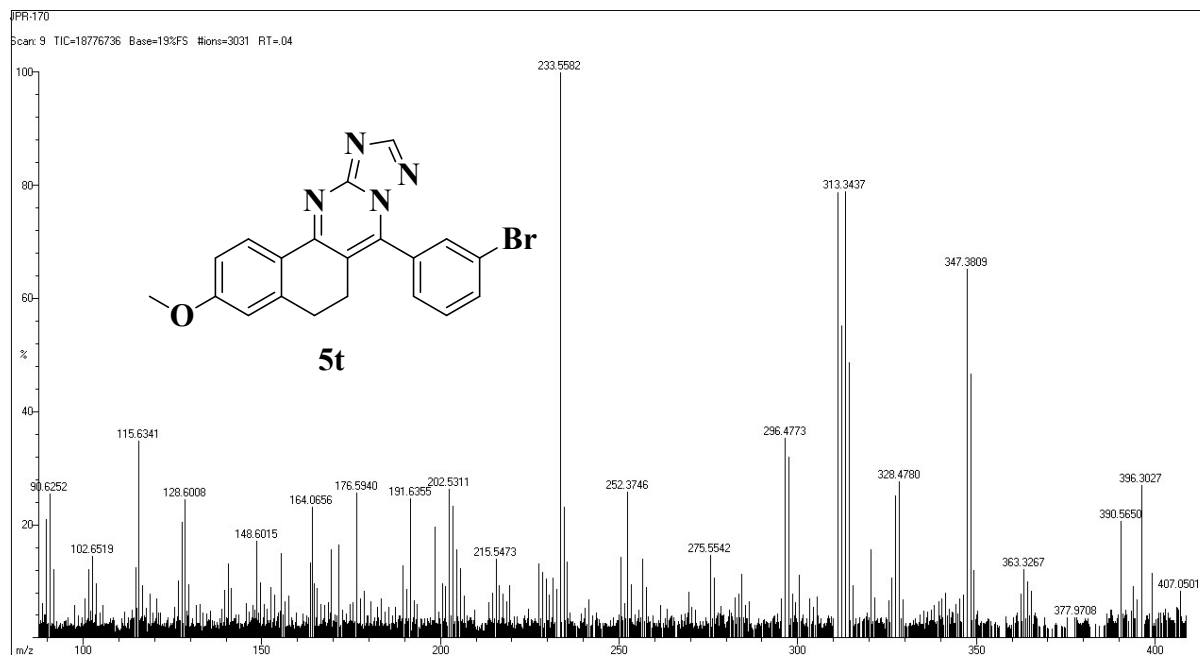
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Current Data Parameters
NAME      Desktop
EXPNO    1
PROCNO   1

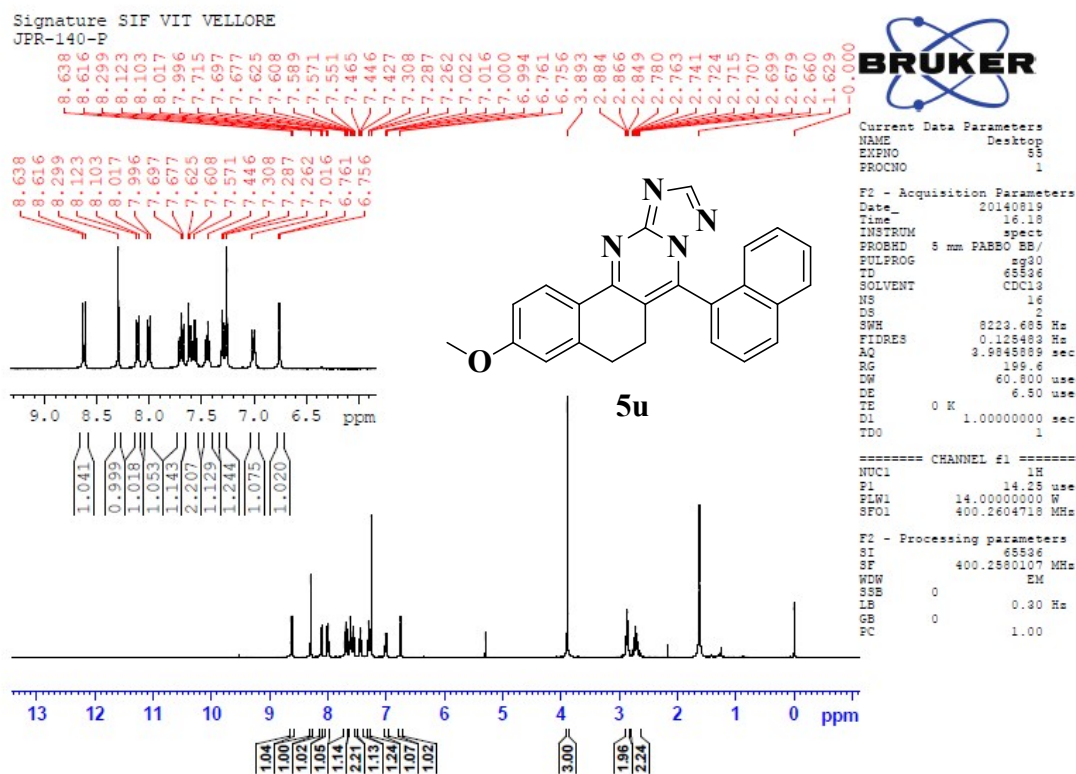
F2 - Acquisition Parameters
Date_    20140708
Time     12:24
INSTRUM  spect
PROBHD   5 mm PABBO BB
PULPROG  zgpg30
ID       0
SOLVENT  CDCl3
NS       512
DSH      4
AQ       0.12500000 sec
RG       655.36000000
FIDRES   0.10000000 Hz
AQRES    3.904000000 Hz
SFO1     400.1460000 MHz
NUC1      13C
P1        12.00000000 sec
PL1       0.00000000 dB
SFO2     101.2530000 MHz
NUC2      1H
P2        0.00000000 sec
PL2       0.00000000 dB
SFO3     400.1460000 MHz
NUC3      1H
P3        0.00000000 sec
PL3       0.00000000 dB
SFO4     0.00000000 MHz
NUC4      13C
P4        0.00000000 sec
PL4       0.00000000 dB
===== CHANNEL f1 =====
NUC1      13C
P1        12.00000000 sec
PL1       0.00000000 dB
SFO1     101.2530000 MHz
===== CHANNEL f2 =====
NUC1      1H
P1        12.00000000 sec
PL1       0.00000000 dB
SFO1     400.1460000 MHz
===== Processing parameters =====
RG       655.36000000
SFO1     400.1460000 MHz
EM       EM
GB1      0
GB2      0
GB3      0
GB4      0
NUC1      1H
NUC2      13C
===== CHANNEL f3 =====
NUC1      13C
P1        12.00000000 sec
PL1       0.00000000 dB
SFO1     101.2530000 MHz
===== Processing parameters =====
RG       655.36000000
SFO1     400.1460000 MHz
EM       EM
GB1      0
GB2      0
GB3      0
GB4      0

```

HRMS spectrum of compound (5t):

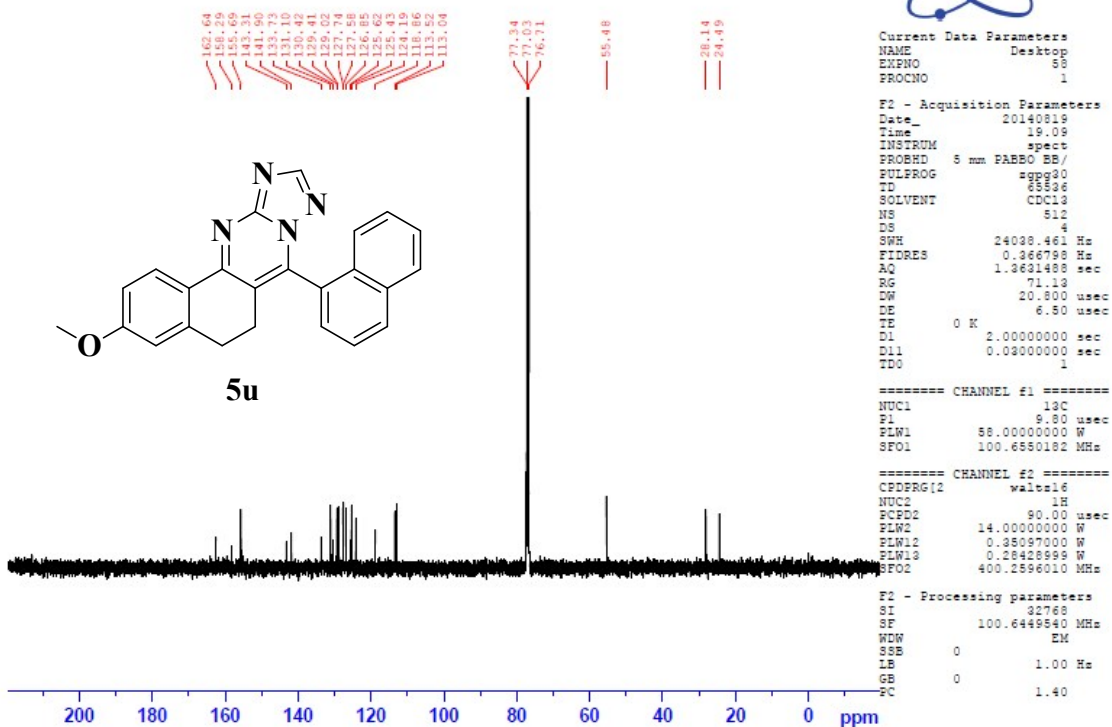


¹H NMR spectrum of compound (5u):

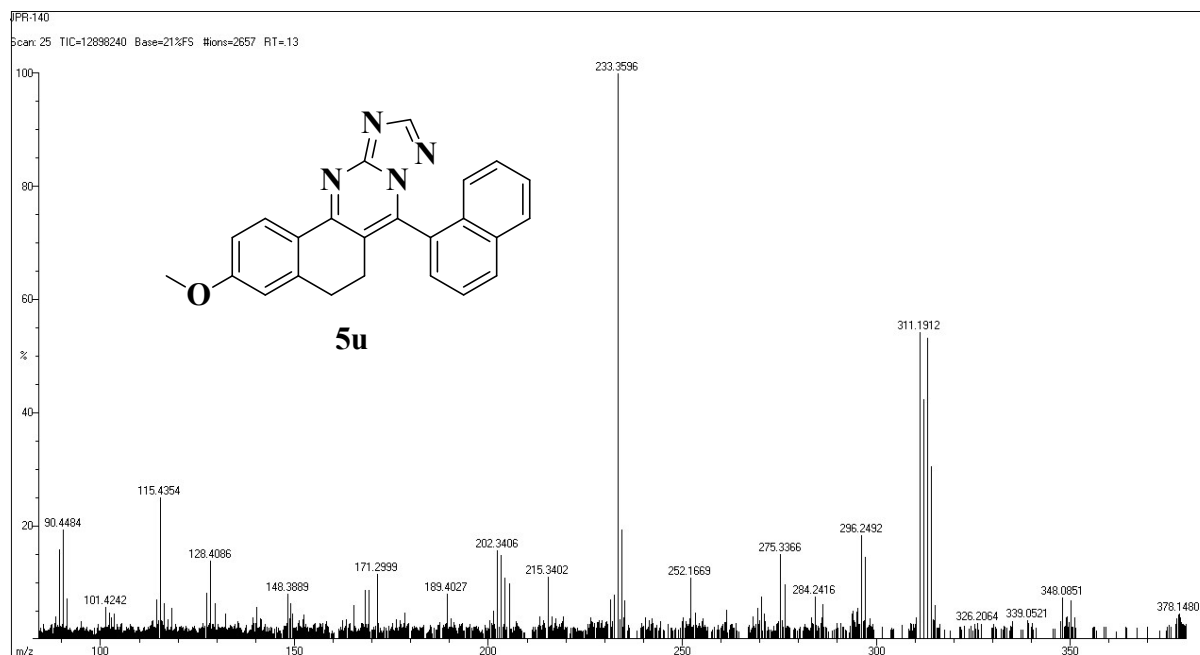


¹³C NMR spectrum of compound (5u):

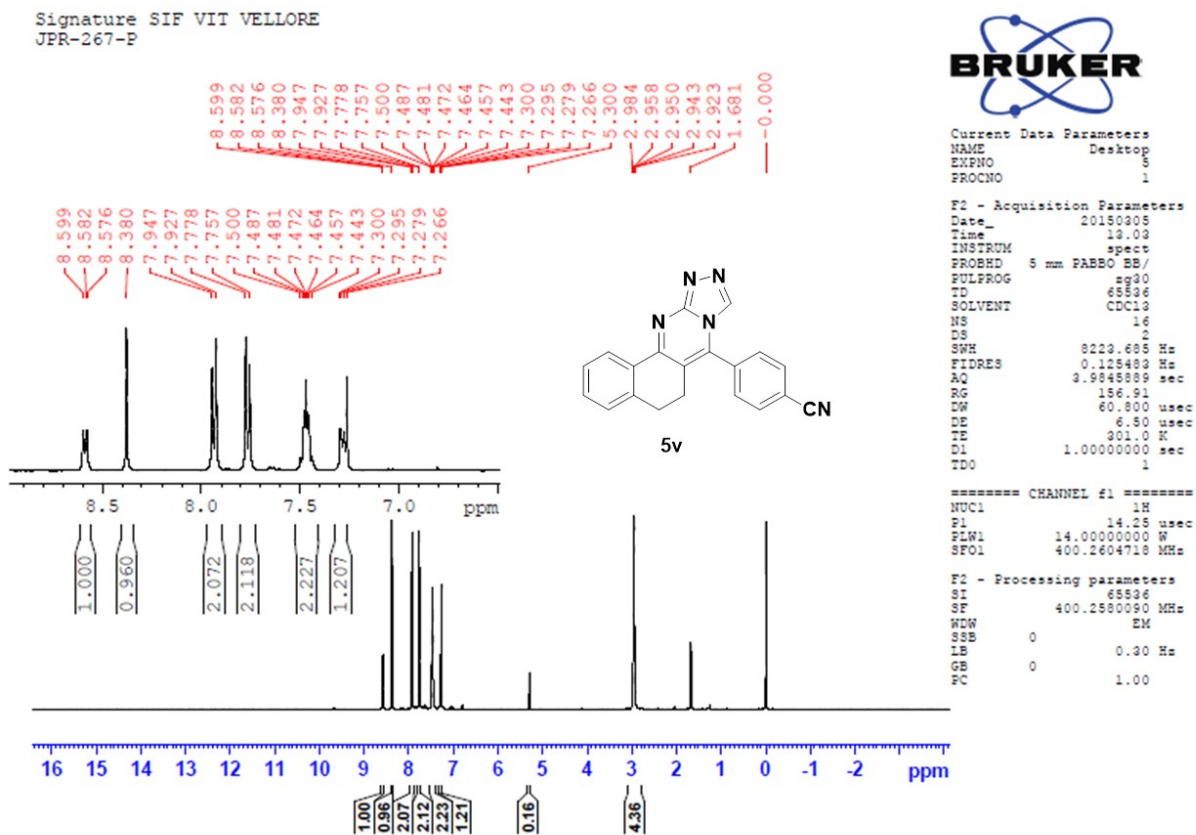
Signature SIF VIT VELLORE
JPR-140-P



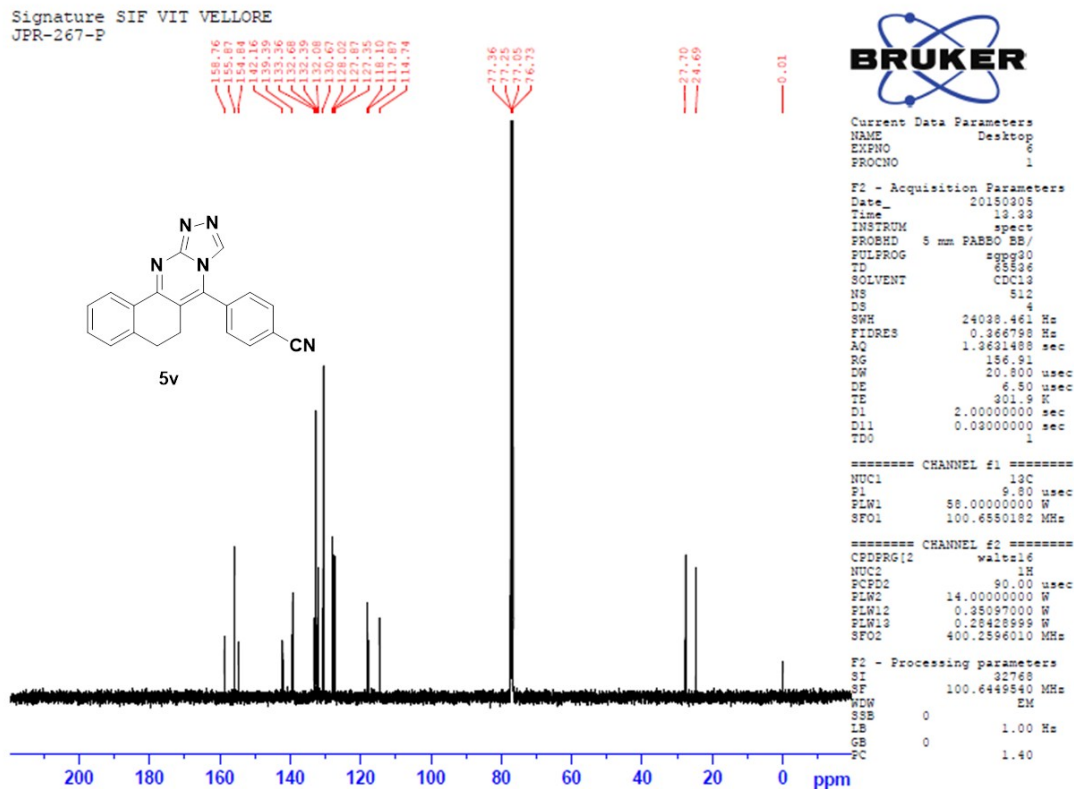
HRMS spectrum of compound (5u):



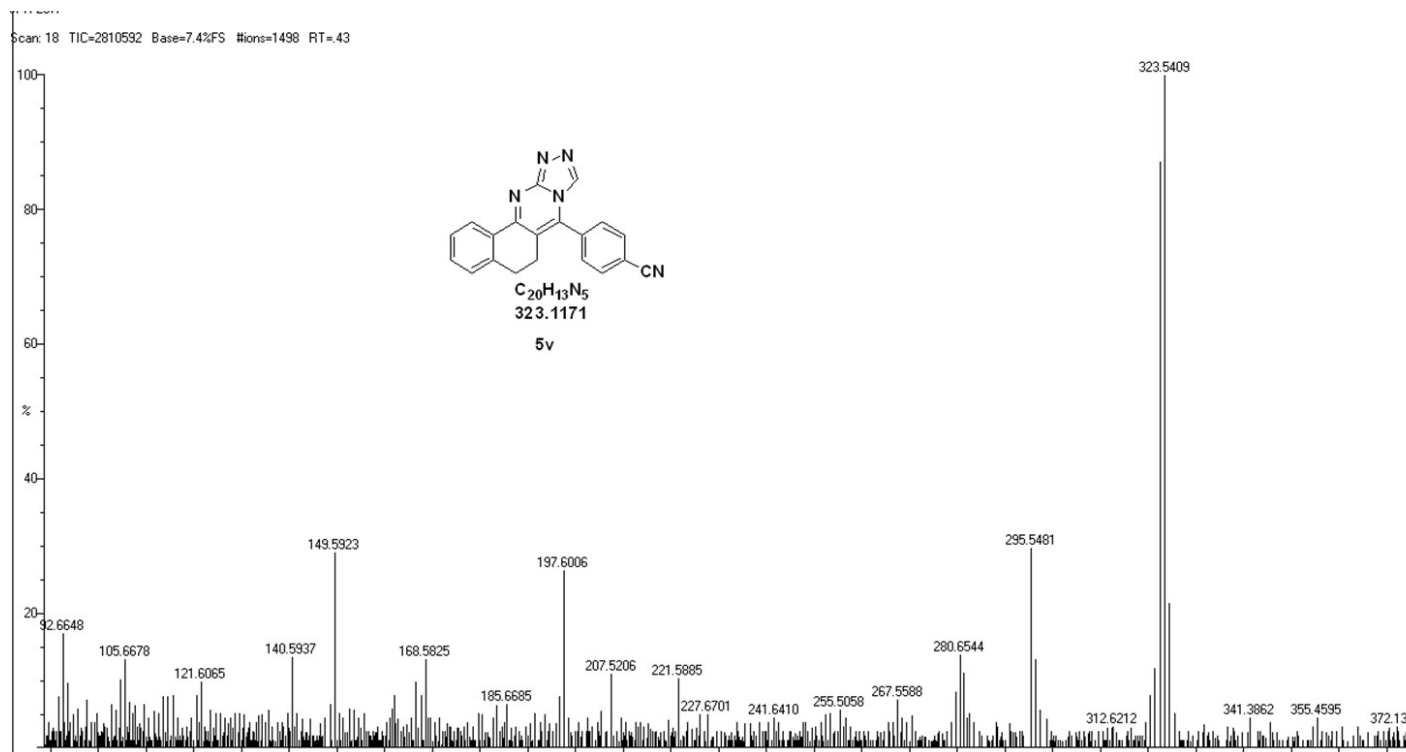
¹H NMR spectrum of compound (5v):



¹³C NMR spectrum of compound (5u):

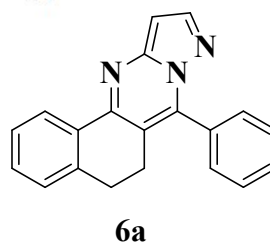
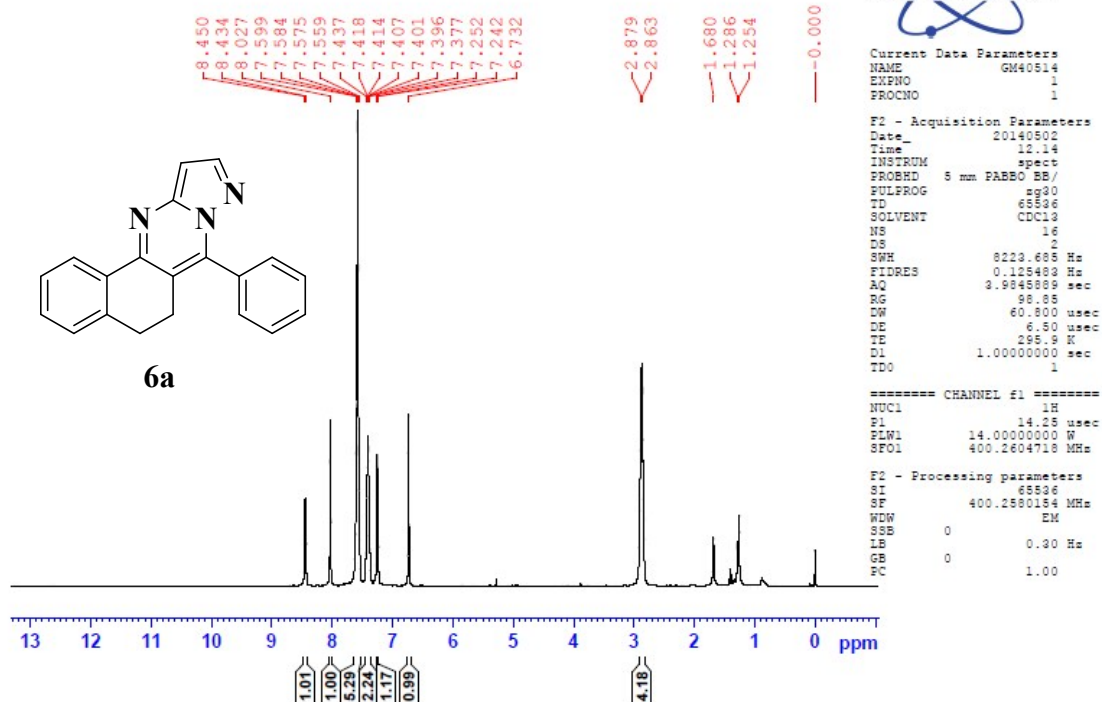


HRMS spectrum of compound (5v):



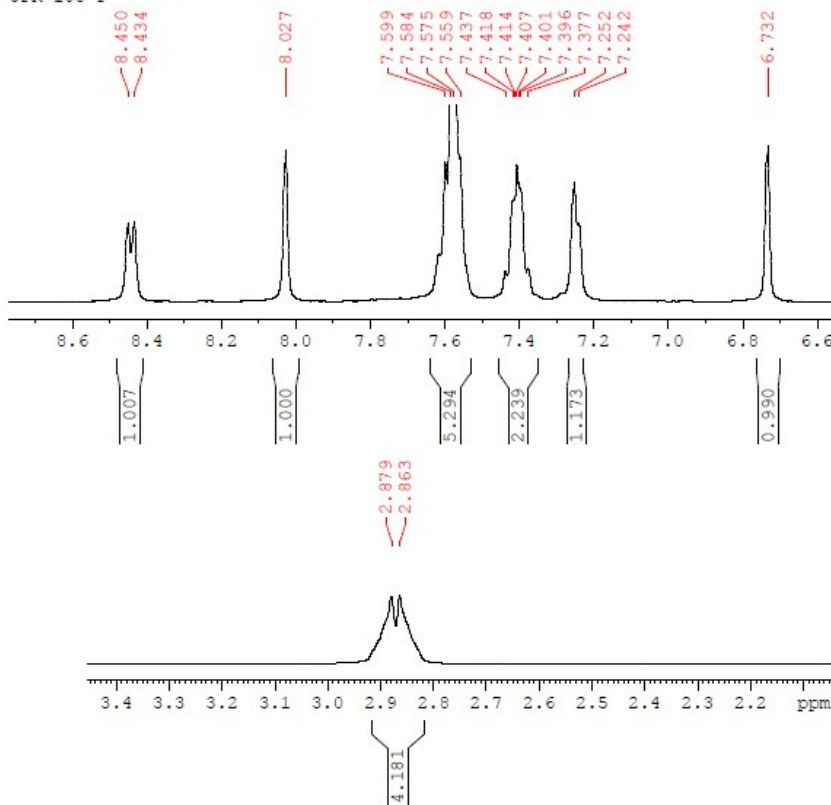
¹H NMR spectrum of compound (6a):

Signature SIF VIT VELLORE
 JPR-108-P



Expanded ¹H NMR spectrum of compound (6a):

Signature SIF VIT VELLORE
JPR-108-P



Current Data Parameters
NAME GM40514
EXNO 1
PROCNO 1

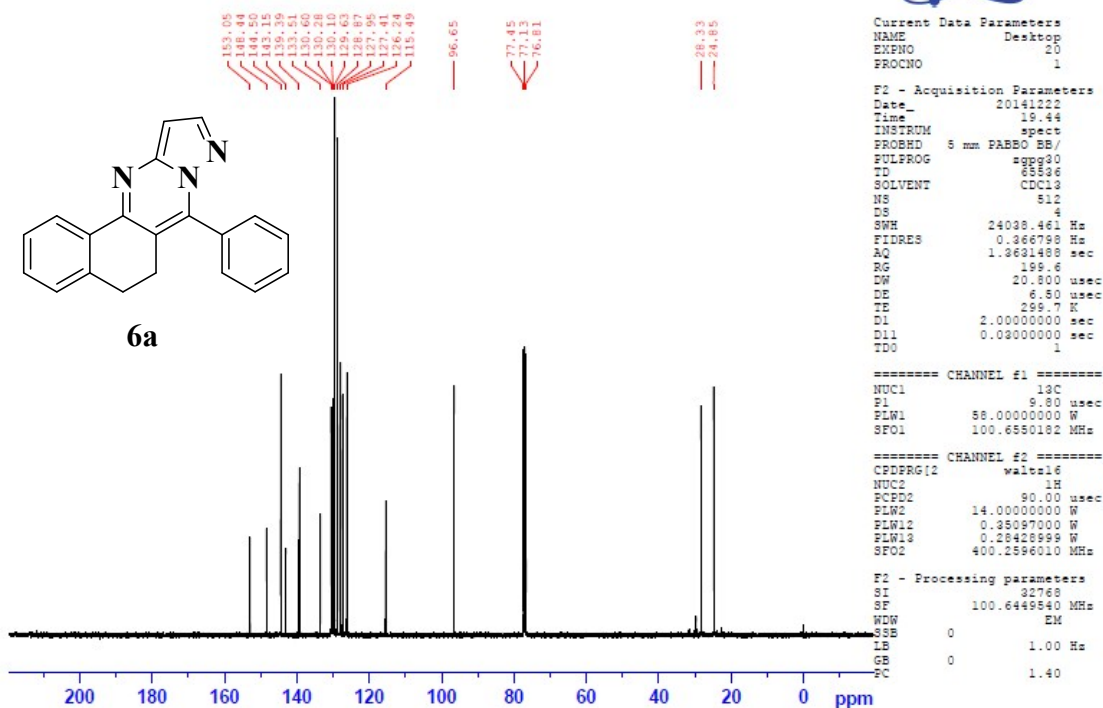
F2 - Acquisition Parameters
Date_ 20140502
Time 12.14
INSTRUM spect
PROBHD 5 mm PABBO ES/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.605 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 88.85
DQ 60.800 usec
DE 6.80 usec
TE 298.9 K
DL 1.00000000 sec
TDO 1

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

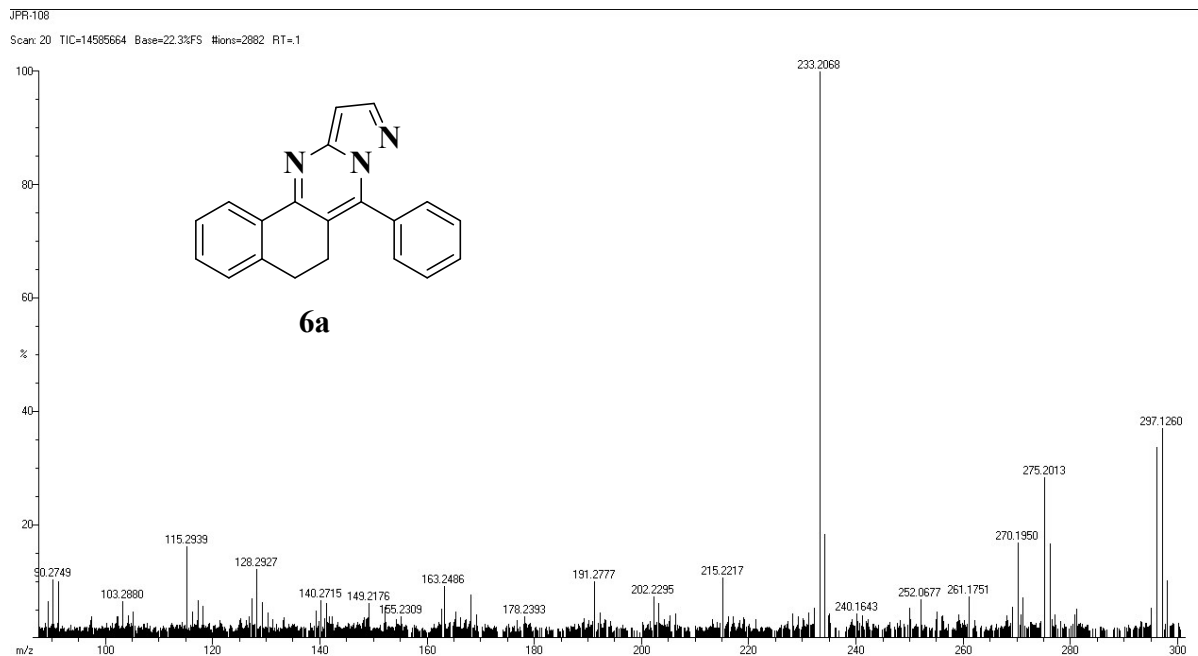
F2 - Processing parameters
SI 65536
SF 400.2880154 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound (6a):

Signature SIF VIT VELLORE
JPR-108-P

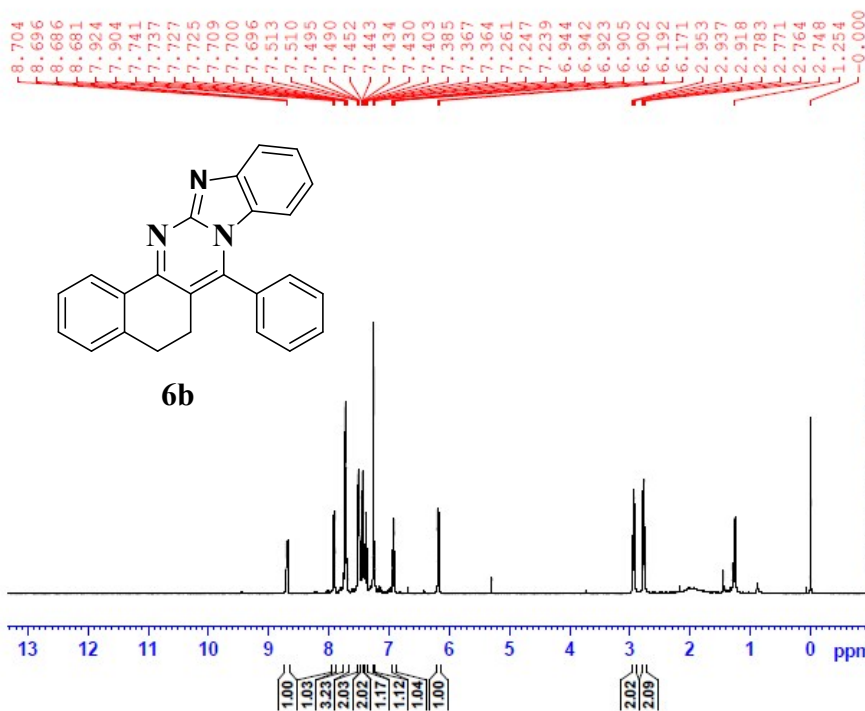


HRMS spectrum of compound (6a):



¹H NMR spectrum of compound (6b):

Signature SIF VIT VELLORE
JPR-095-P



Current Data Parameters
NAME Desktop
EXPNO 77
PROCNO 1

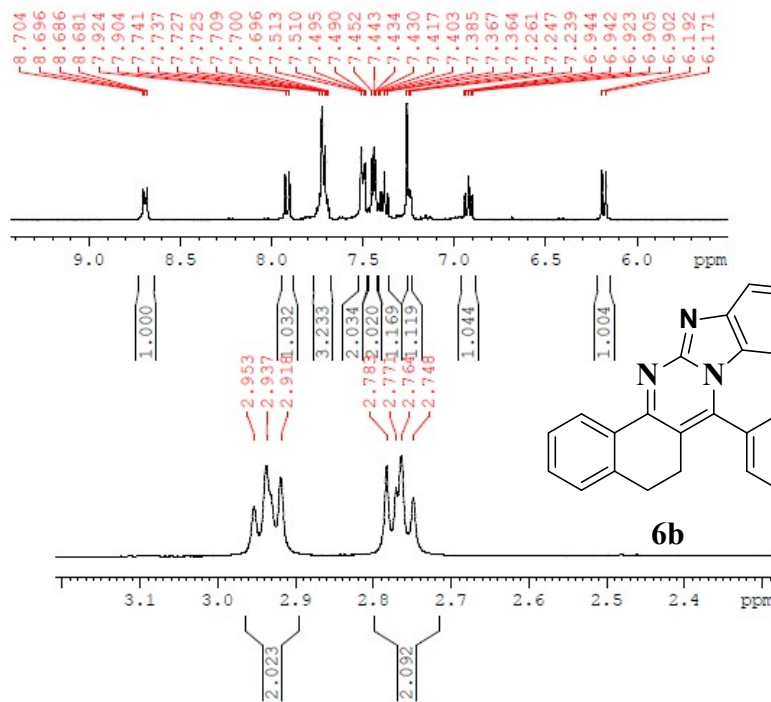
F2 - Acquisition Parameters
Date_ 20140723
Time 10.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 156.91
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.2580110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

Expanded ¹H NMR spectrum of compound (6b):

Signature SIF VIT VELLORE
JPR-095-P



Current Data Parameters
NAME Desktop
EXPNO 77
PROCNO 1

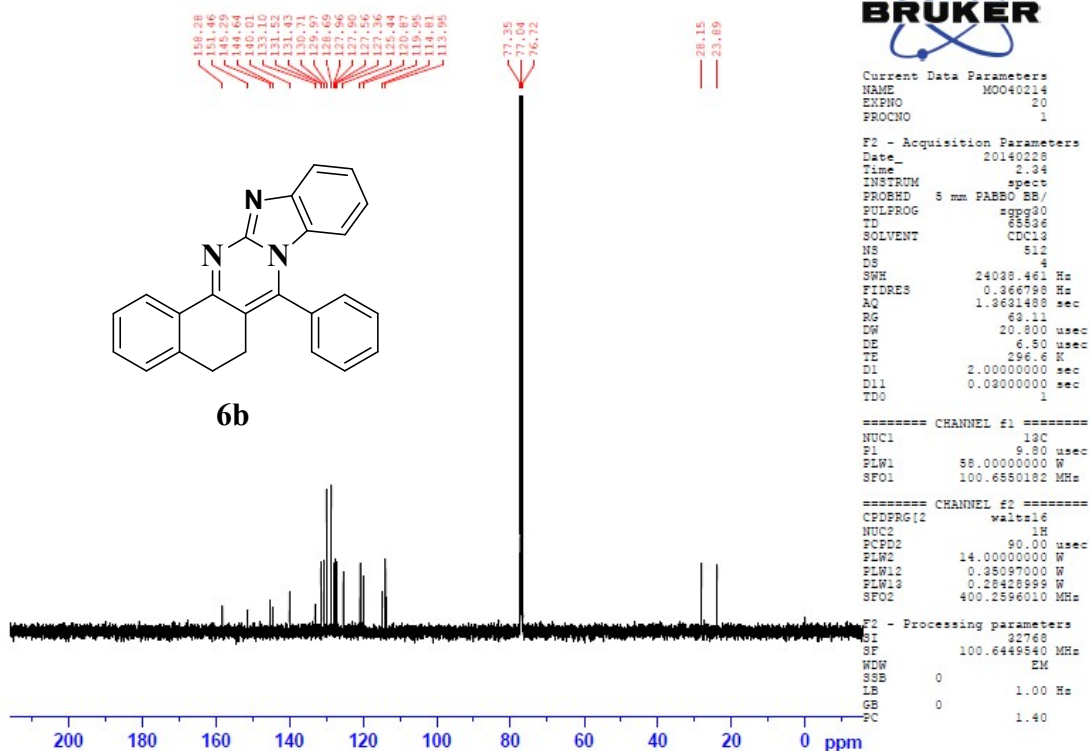
F2 - Acquisition Parameters
Date_ 20140723
Time 10.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 156.91
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.2580110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

¹³C NMR spectrum of compound (6b):

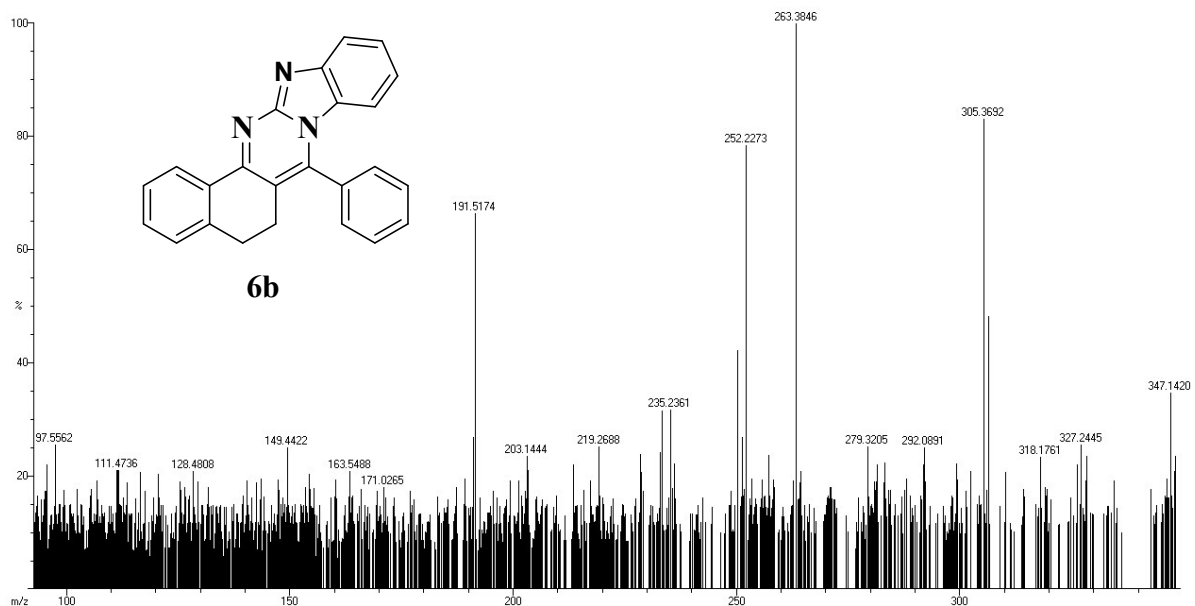
JPR-095-P



HRMS spectrum of compound (6b):

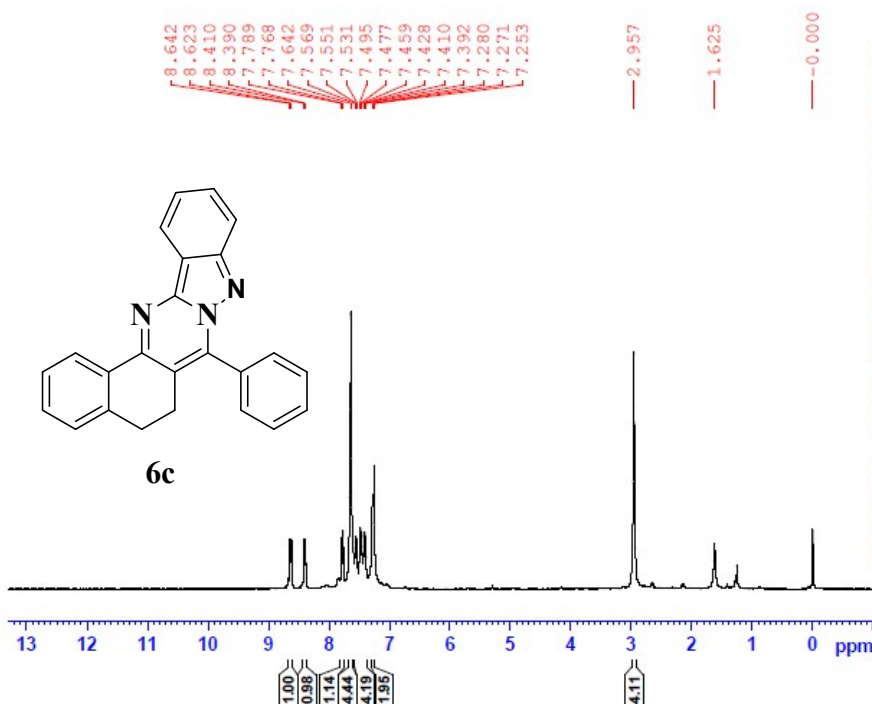
JPR-095

Scan: 8 TIC=10947472 Base=3.2%FS #Ions=2647 RT=.04



¹H NMR spectrum of compound (6c):

Signature SIF VIT VELLORE
JPR-107-P



Current Data Parameters
NAME Desktop
EXPNO 78
PROCNO 1

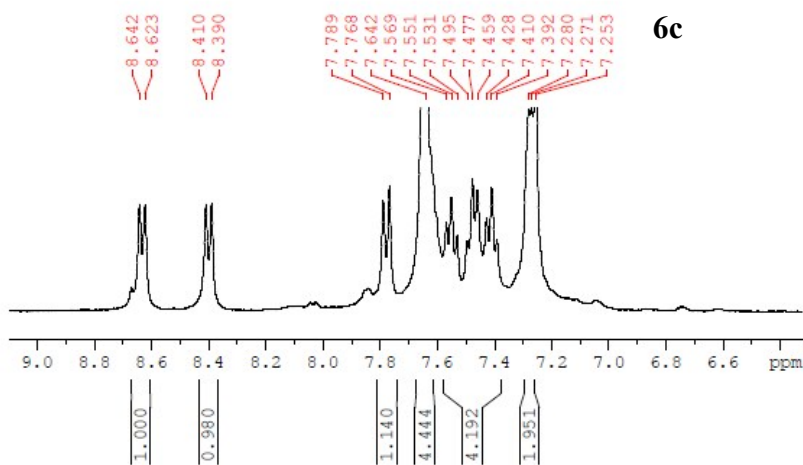
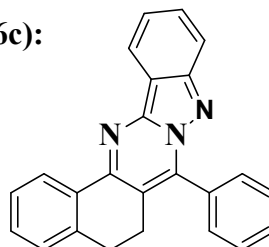
F2 - Acquisition Parameters
Date_ 20140723
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 143.73
DM 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.2580143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

Expanded ¹H NMR spectrum of compound (6c):

Signature SIF VIT VELLORE
JPR-107-P



Current Data Parameters
NAME Desktop
EXPNO 78
PROCNO 1

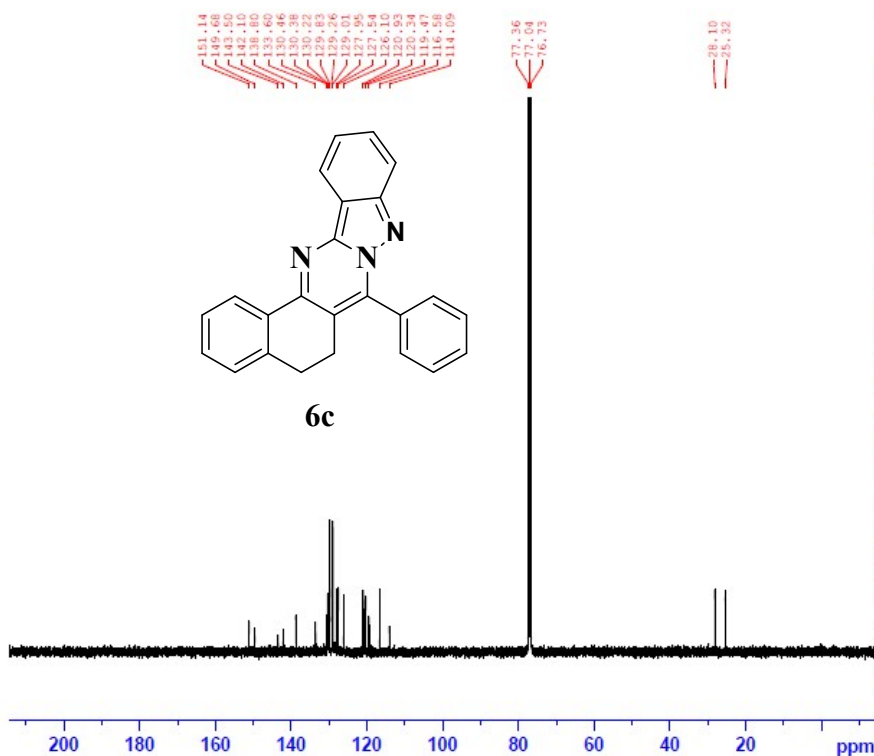
F2 - Acquisition Parameters
Date_ 20140723
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 143.73
DM 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 65536
SF 400.2580143 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

¹³C NMR spectrum of compound (6c):

Signature SIF VIT VELLORE
JPR-107-P



Current Data Parameters
NAME Desktop
EXPNO 79
PROCNO 1

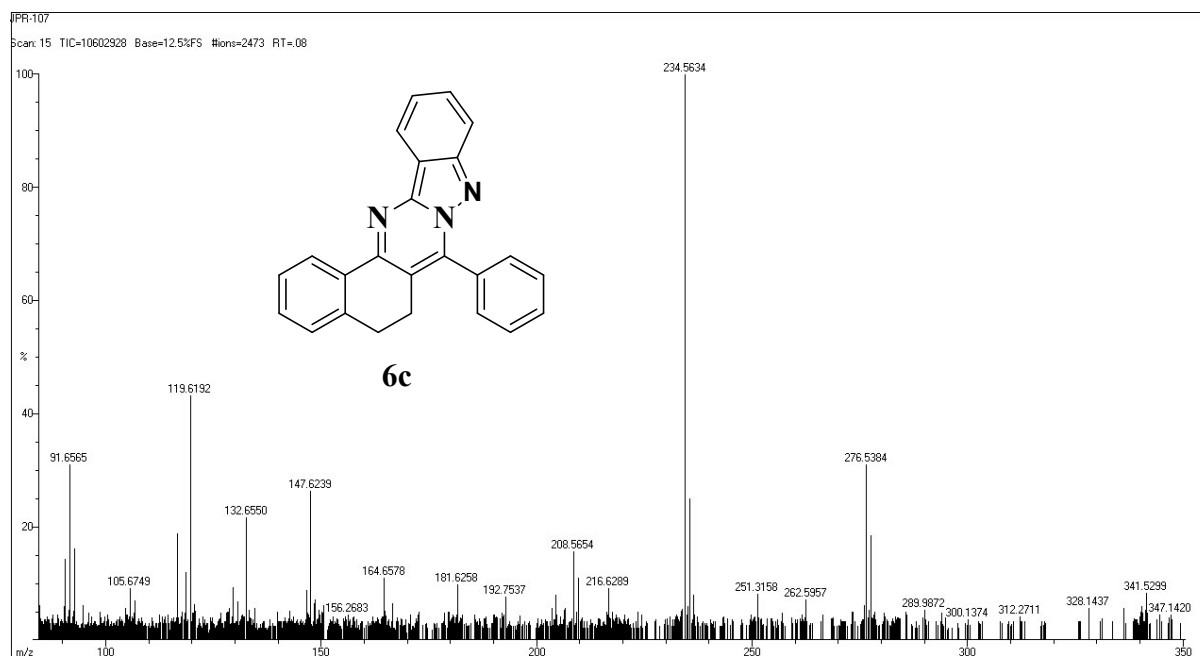
F2 - Acquisition Parameters
Date_ 20140722
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 127.79
SW 20.800 usec
DE 6.50 usec
TE 297.2 K
DL 2.00000000 sec
Dl1 0.03000000 sec
TDO 1

==== CHANNEL #1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6250182 MHz

==== CHANNEL #2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
FLW2 0.35097000 W
PLW3 0.28428999 W
SFO2 400.2596010 MHz

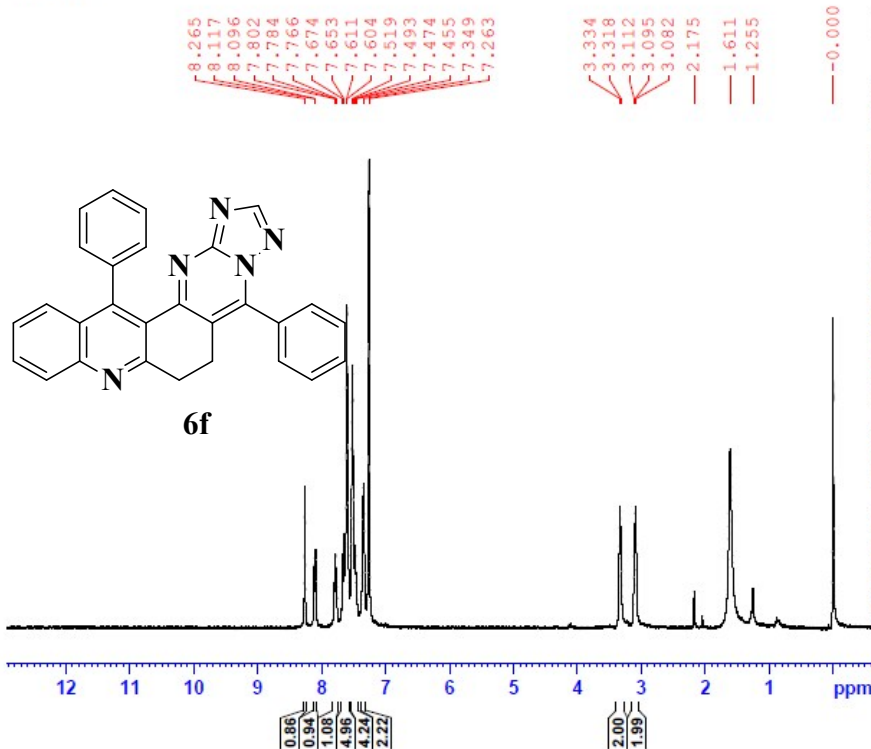
F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectrum of compound (6c):



¹H NMR spectrum of compound (6f):

JPR-064-P



Current Data Parameters
 NAME MOD40114
 EXPNO 13
 PROCNO 1

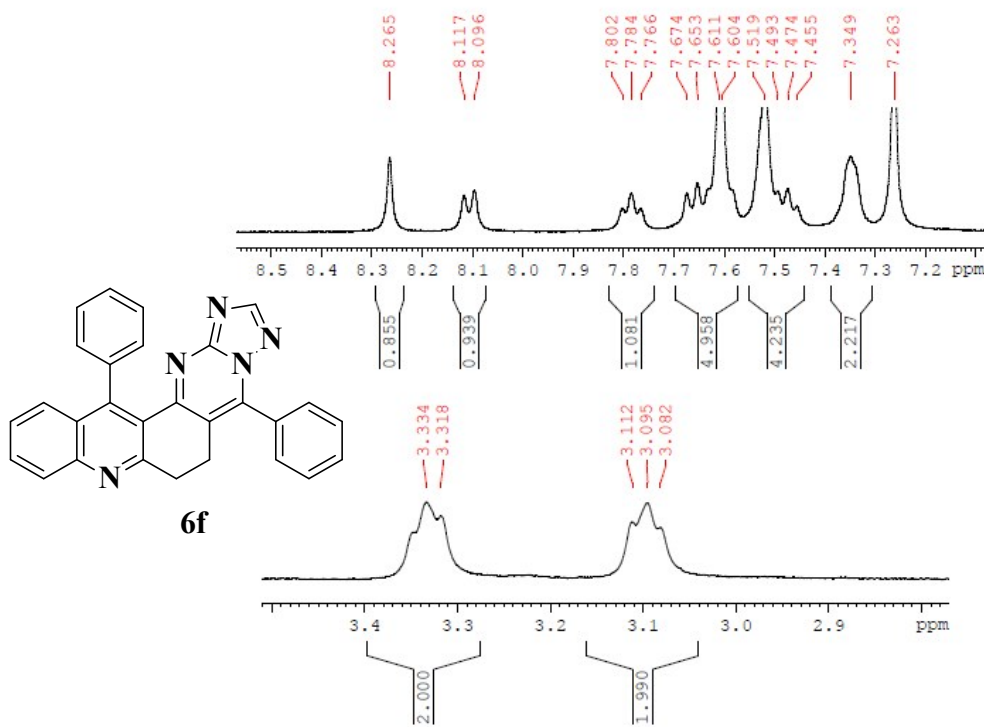
F2 - Acquisition Parameters
 Date_ 20140127
 Time 18.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125493 Hz
 AQ 3.9945889 sec
 RG 199.6
 DW 60.800 usec
 DE 6.50 usec
 TE 295.9 K
 DL 1.00000000 sec
 TDO 1

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

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

Expanded ¹H NMR spectrum of compound (6f):

JPR-064-P



Current Data Parameters
 NAME MOD40114
 EXPNO 13
 PROCNO 1

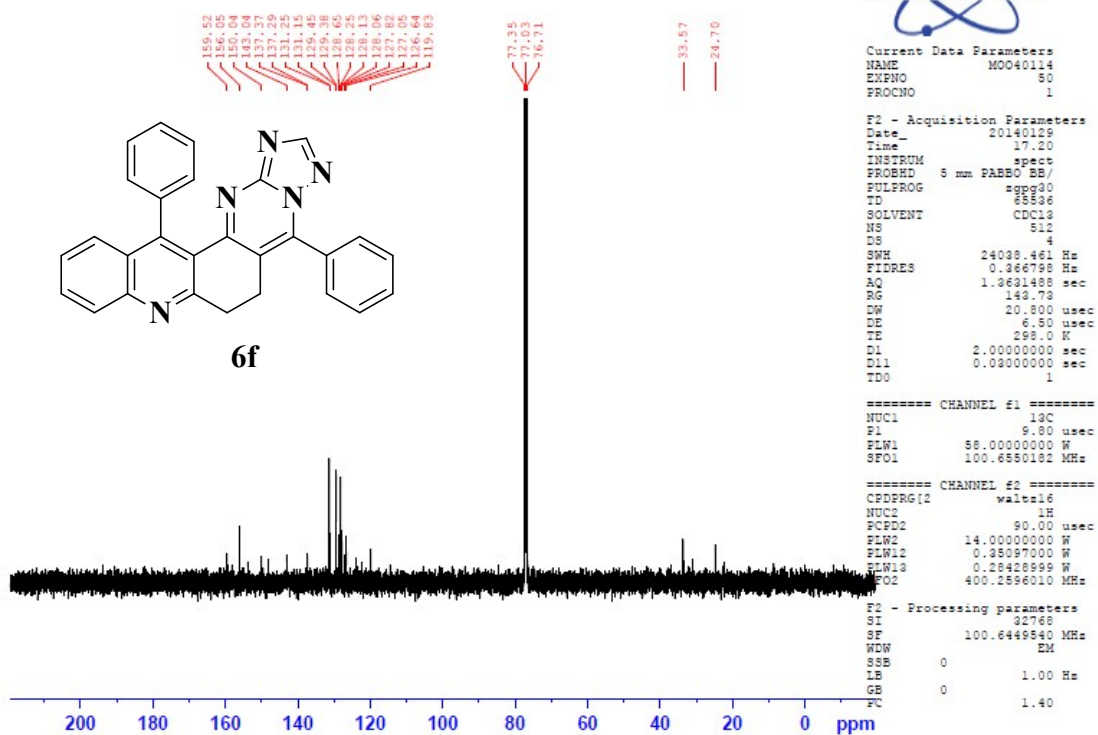
F2 - Acquisition Parameters
 Date_ 20140127
 Time 18.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125493 Hz
 AQ 3.9945889 sec
 RG 199.6
 DW 60.800 usec
 DE 6.50 usec
 TE 295.9 K
 DL 1.00000000 sec
 TDO 1

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

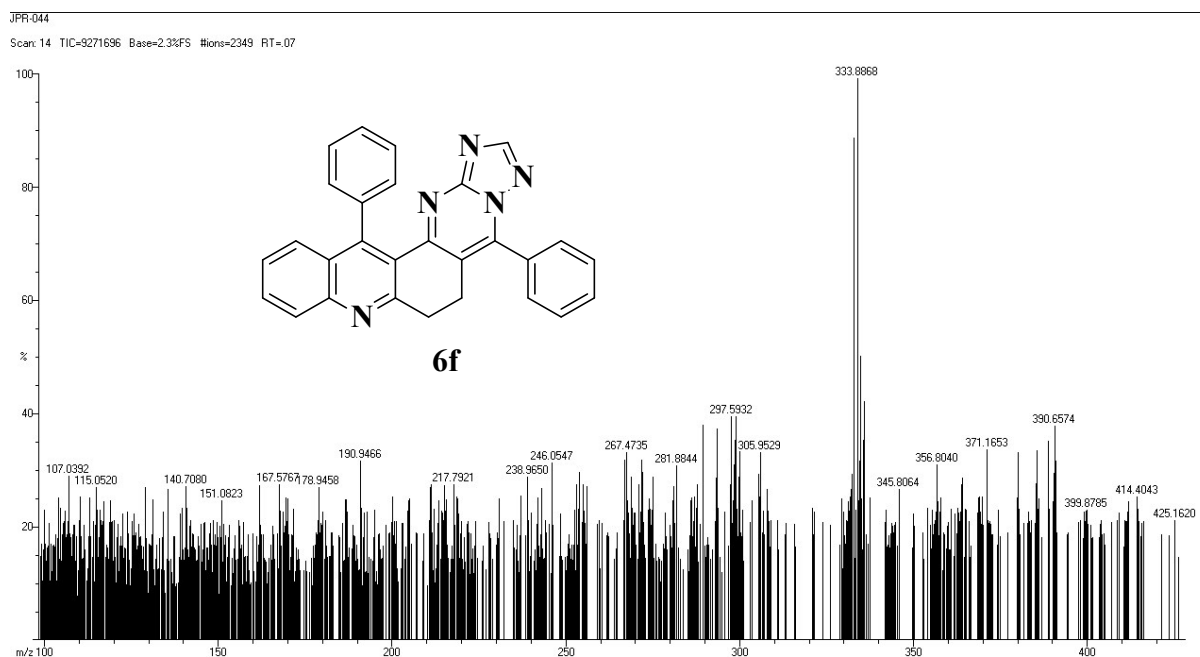
F2 - Processing parameters
 SI 65536
 SF 400.2604718 MHz
 WDW EM
 SSB 0
 GB 0 0.30 Hz
 PC 1.00

¹³C NMR spectrum of compound (6f):

JPR-064-p

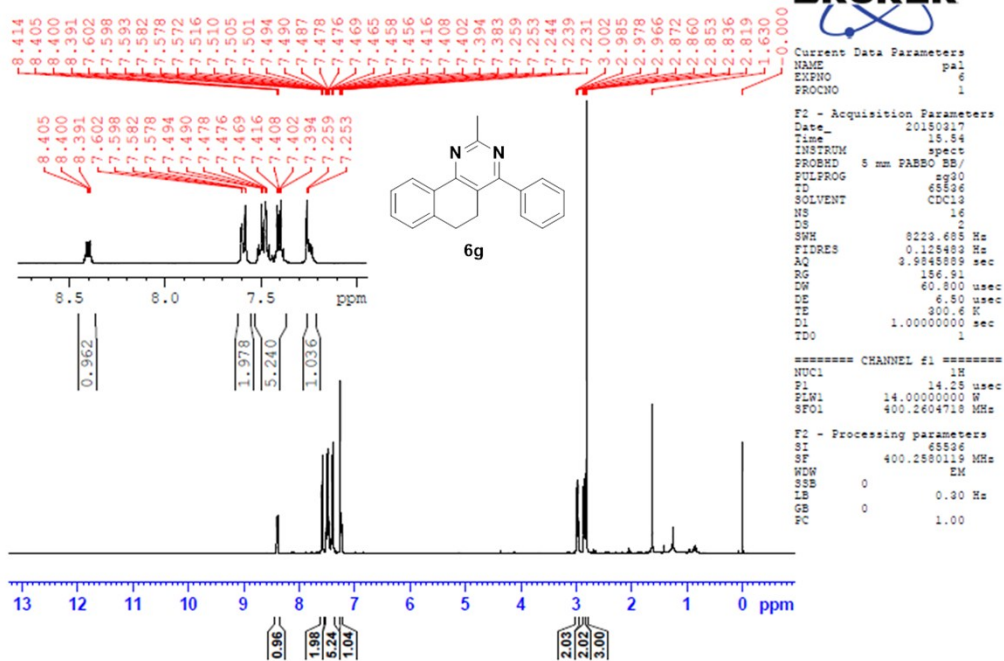


HRMS spectrum of compound (6f):



¹H NMR spectrum of compound (6g):

Signature SIF VIT VELLORE
JPR-271-P



¹³C NMR spectrum of compound (6g):

Signature SIF VIT VELLORE
JPR-271-P

