

Supporting information

Synthesis of 1, 2-Dihydro-1-oxophthalazin-4-yl trifluoromethanesulfonate and its application in the Synthesis of 4-(aryl/heteroaryl/alkynyl)phthalazin-1(2*H*)-one

Ganesh Raosaheb Dhage, Santosh Rangnath Deshmukh and Shankar Ramchandra Thopate*

¹H and ¹³C NMR spectra

Entry	Compound	Code	Page No.
1	1,2-dihydro-1-oxophthalazin-4-yl trifluoromethanesulfonate	3a	S3
2	4-Phenylphthalazin-1(2H)-one	5a	S5
3	4-(4-Methoxyphenyl)phthalazin-1(2H)-one	5b	S7
4	4-(3-Methoxyphenyl)phthalazin-1(2H)-one	5c	S9
5	4-(2-Methoxyphenyl)phthalazin-1(2H)-one	5d	S11
6	4-(1,2-Dihydro-1-oxophthalazin-4-yl)benzaldehyde	5e	S13
7	3-(1,2-Dihydro-1-oxophthalazin-4-yl)benzaldehyde	5f	S15
8	4-(3-(Trifluoromethyl)phenyl)phthalazin-1(2H)-one	5g	S17
9	4-(2-(Trifluoromethyl)phenyl)phthalazin-1(2H)-one	5h	S19
10	4-(3-Hydroxyphenyl)phthalazin-1(2H)-one	5i	S21
11	4-(4-Chlorophenyl)phthalazin-1(2H)-one	5j	S23
12	4-(3-Chlorophenyl)phthalazin-1(2H)-one	5k	S25
13	4-(Pyridin-3-yl)phthalazin-1(2H)-one	5l	S26
14	4-(Thiophen-3-yl)phthalazin-1(2H)-one	5m	S28
15	4-(Benzo[b]thiophen-2-yl)phthalazin-1(2H)-one	5n	S30
16	4-(Naphthalen-3-yl)phthalazin-1(2H)-one	5o	S32
17	4-(2-Phenylethynyl)phthalazin-1(2H)-one	6a	S34
18	4-(2-m-Tolyethynyl)phthalazin-1(2H)-one	6b	S36
19	4-(2-(3-Aminophenyl)ethynyl)phthalazin-1(2H)-one	6c	S38
20	4-(Hept-1-ynyl)phthalazin-1(2H)-one	6d	S40
21	4-(Oct-1-ynyl)phthalazin-1(2H)-one	6e	S42
22	1-Chloro-4-phenylphthalazine	7a	S44
23	1-Chloro-4-(naphthalen-3-yl)phthalazine	7b	S46
24	1-Morpholino-4-phenylphthalazine	8a	S48
25	1-(3-Methoxyphenyl)-4-phenylphthalazine	9a	S50
26	1-Phenyl-4-(2-m-tolyethynyl)phthalazine	10a	S52

RD164

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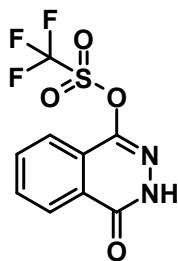
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5.5824

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1.2051



3a

Molecular Weight =294.21
Molecular Formula =C9H5F3N2O4S

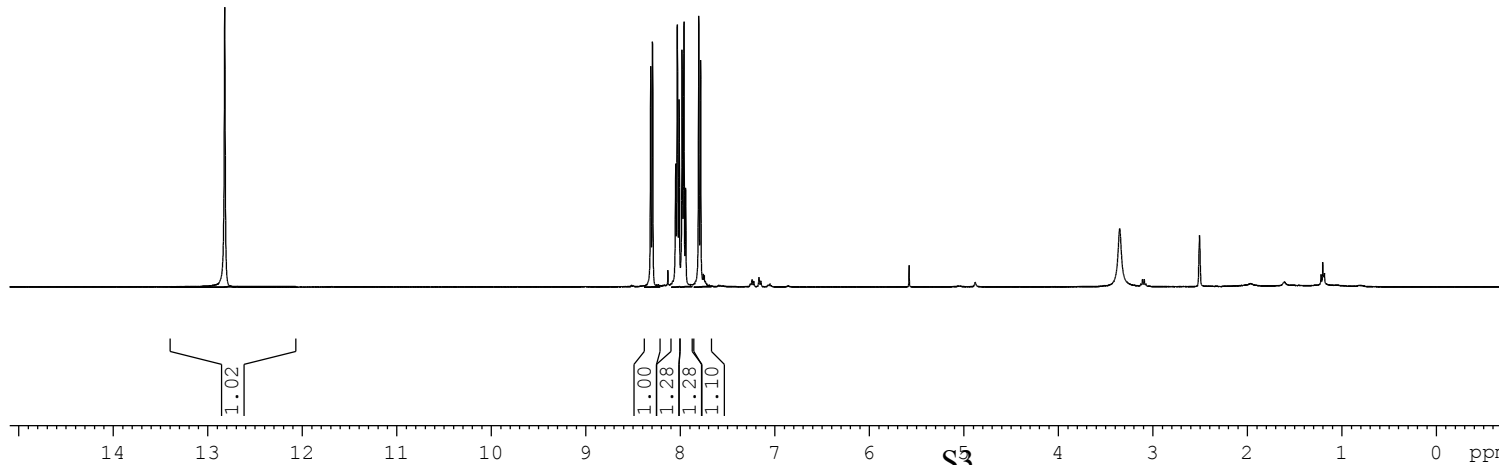
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

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EXPNO 250
PROCNO 1

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TD 65536
SOLVENT DMSO
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FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
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DE 6.00 usec
TE 295.9 K
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TD0 1

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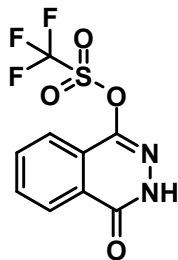
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RD164

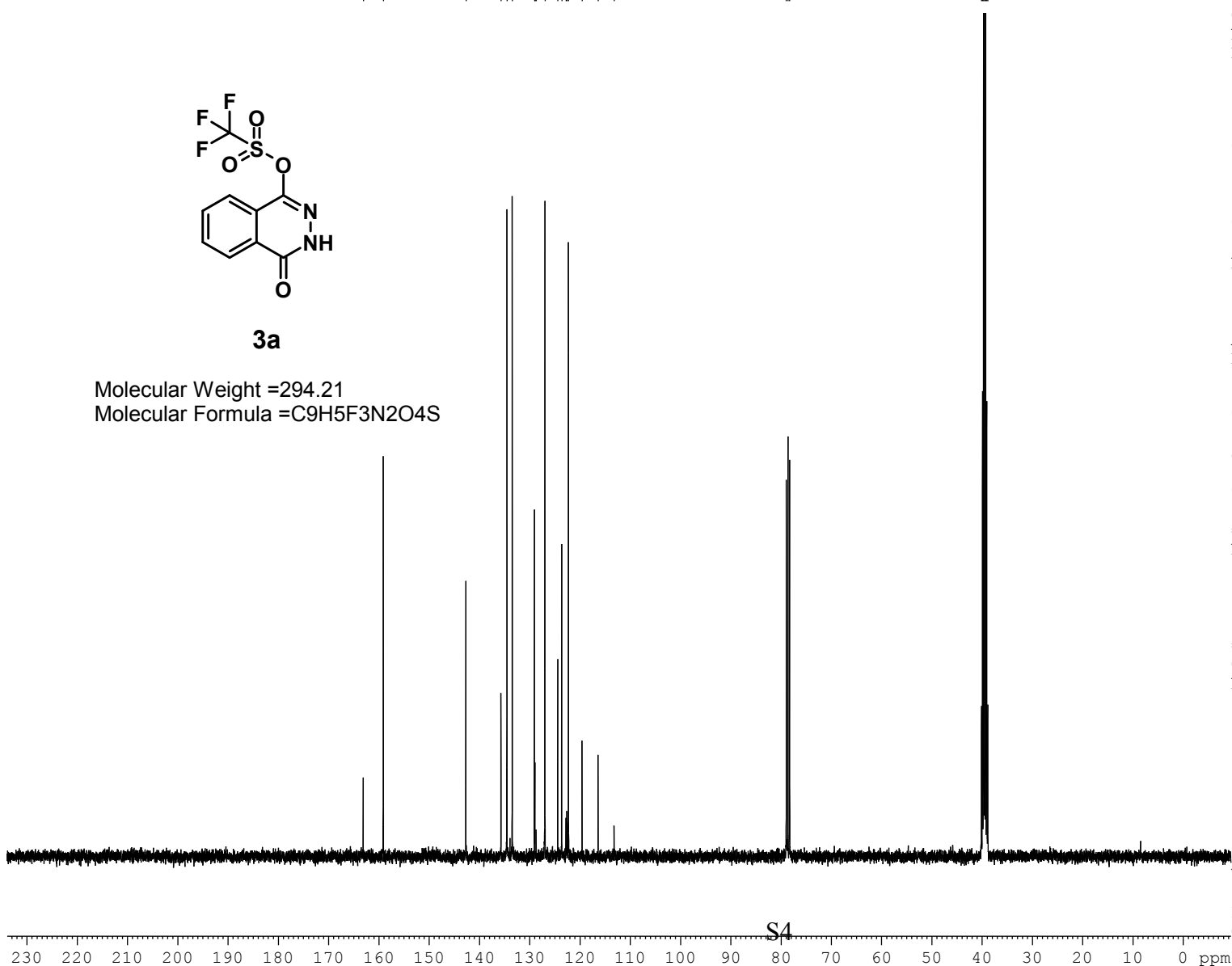
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Chandigarh

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133.44
129.03
128.93
128.71
126.95
124.39
123.60
122.75
122.58
122.26
119.56
116.37
113.19
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78.32
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39.31
39.11
38.90



3a

Molecular Weight =294.21
Molecular Formula =C9H5F3N2O4S



Current Data Parameters
NAME Aug07-2014
EXPNO 251
PROCNO 1

F2 - Acquisition Parameters
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TD 65536
SOLVENT DMSO
NS 512
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SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 724
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DE 6.00 usec
TE 296.4 K
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d11 0.0300000 sec
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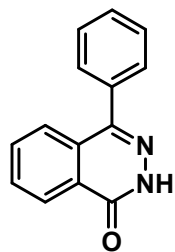
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PL1 -2.00 dB
SFO1 100.6228298 MHz

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

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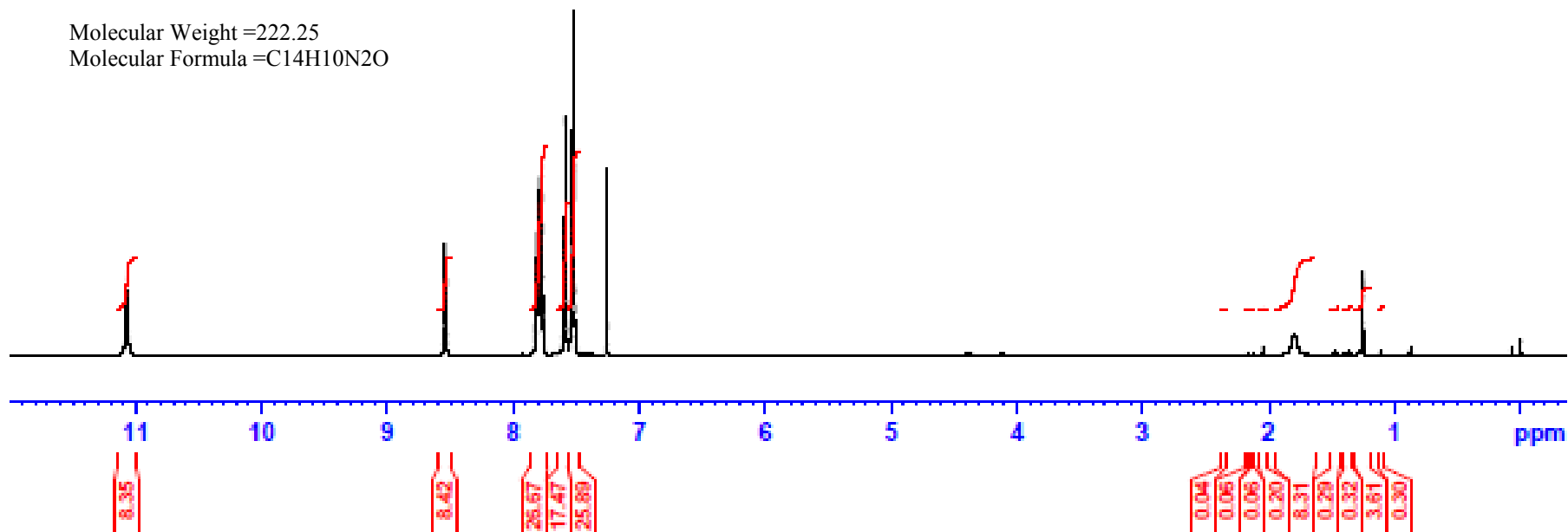
SRD-A
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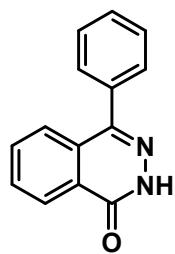


5a

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 Molecular Formula = C₁₄H₁₀N₂O

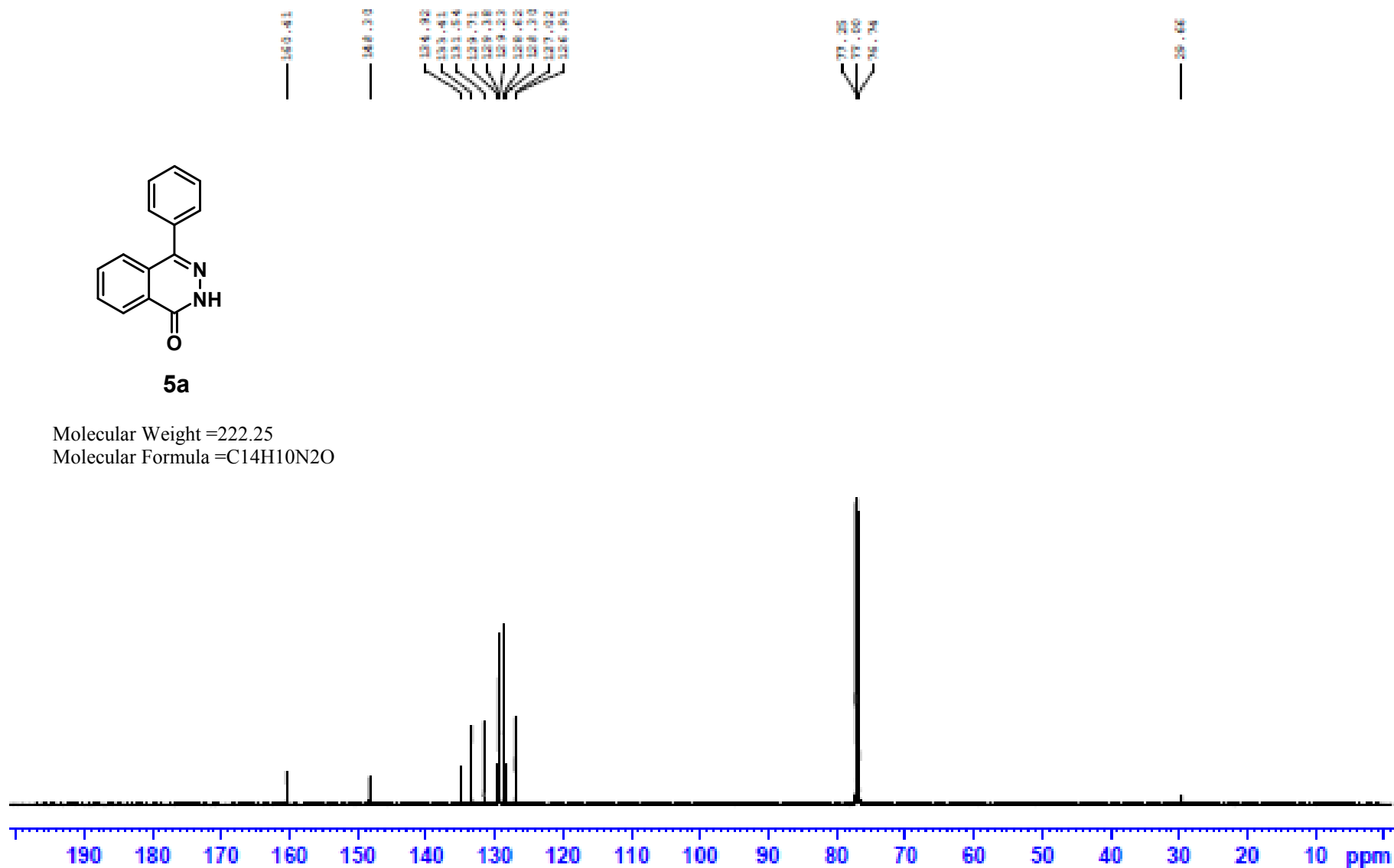


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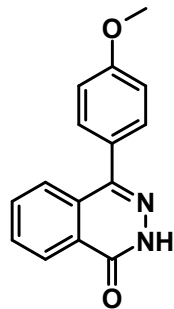


5a

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Molecular Formula =C14H10N2O

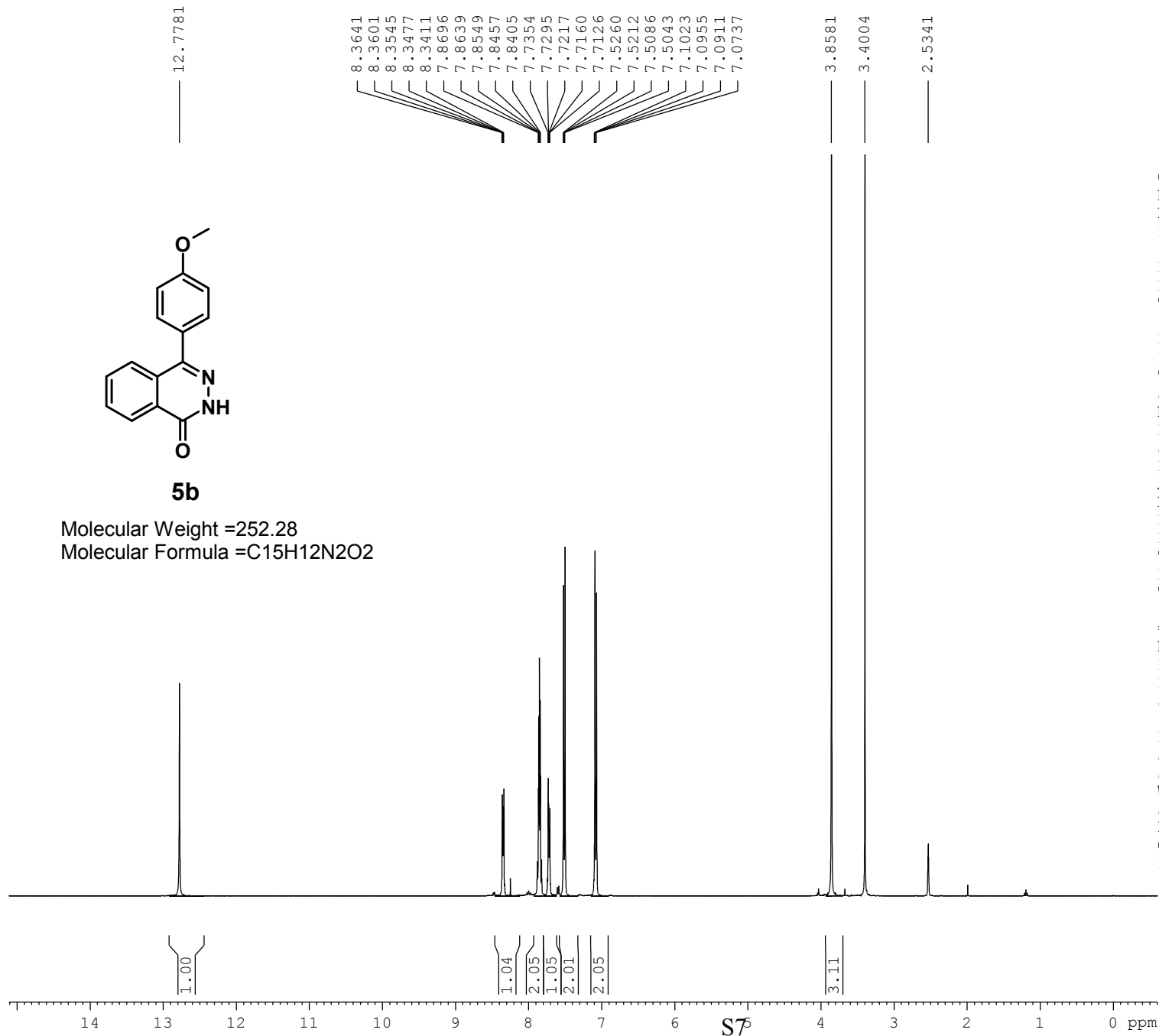


SRD-N



5b

Molecular Weight =252.28
Molecular Formula =C₁₅H₁₂N₂O₂



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Current Data Parameters
NAME Jan01-2015
EXPNO 40
PROCNO 1

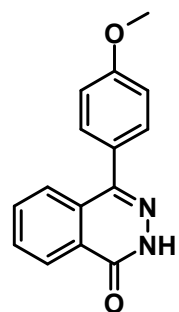
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SOLVENT DMSO
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DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 181
DW 41.600 usec
DE 6.00 usec
TE 292.9 K
D1 1.0000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1299899 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

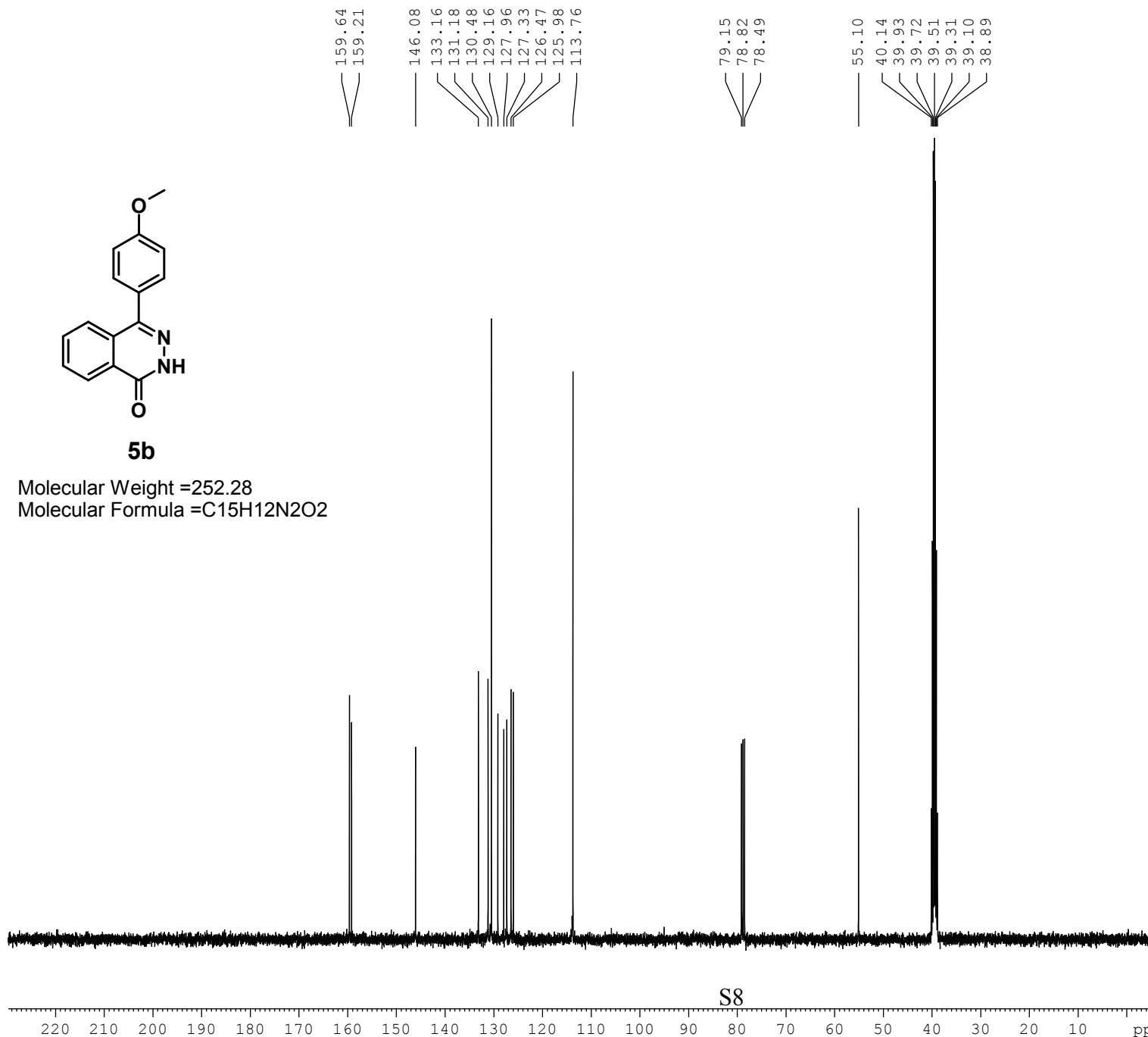
SRD-N

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5b

Molecular Weight =252.28
Molecular Formula =C₁₅H₁₂N₂O₂



Current Data Parameters
NAME Jan01-2015
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 12.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 248
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
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SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SRD-L

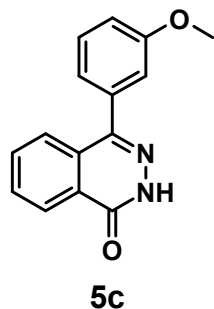
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Current Data Parameters
NAME Jan01-2015
EXPNO 20
PROCNO 1

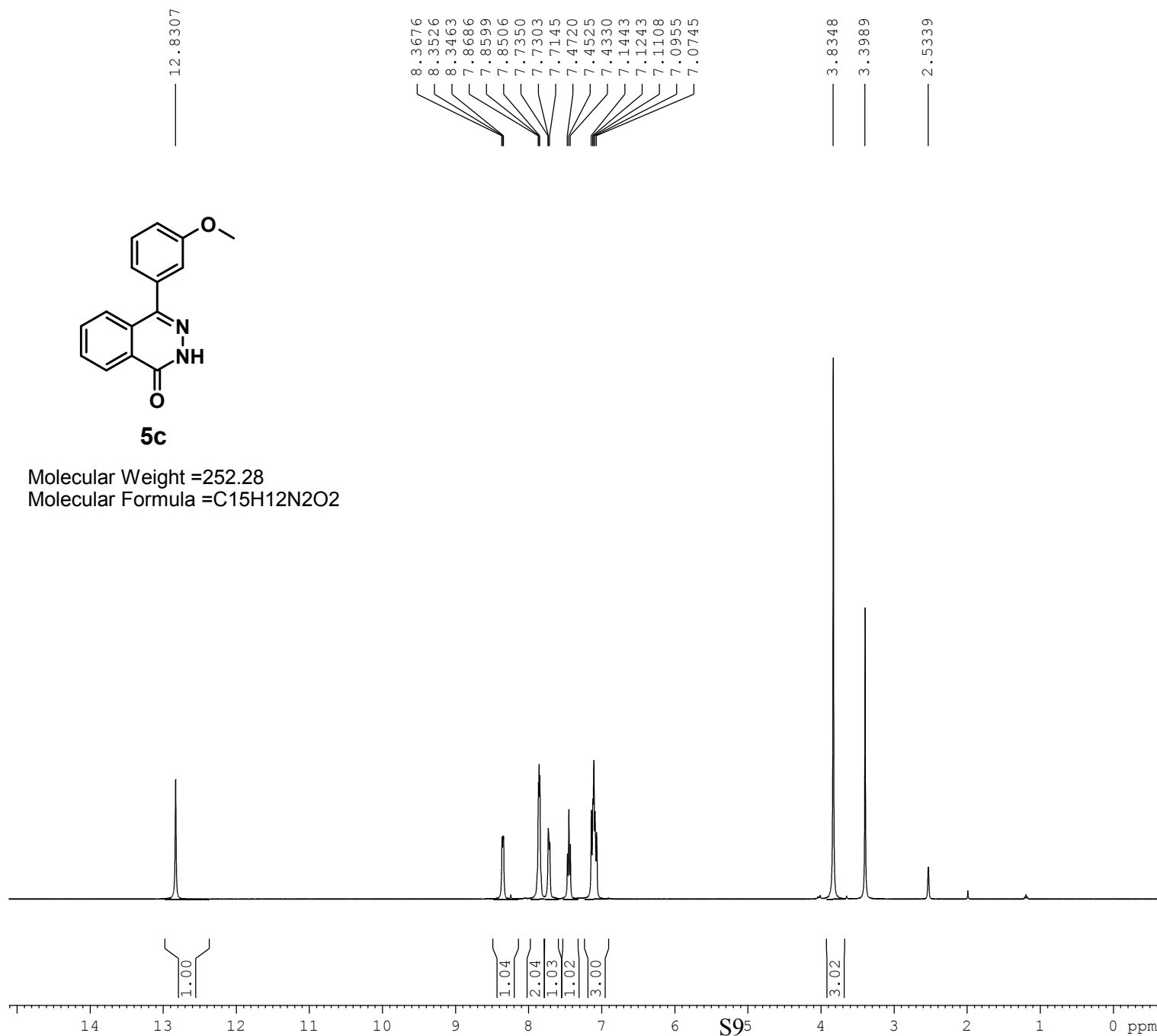
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Time 11.42
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 181
DW 41.600 usec
DE 6.00 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

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

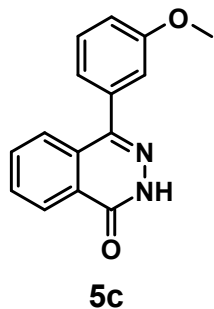
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LB 0.30 Hz
GB 0
PC 1.00



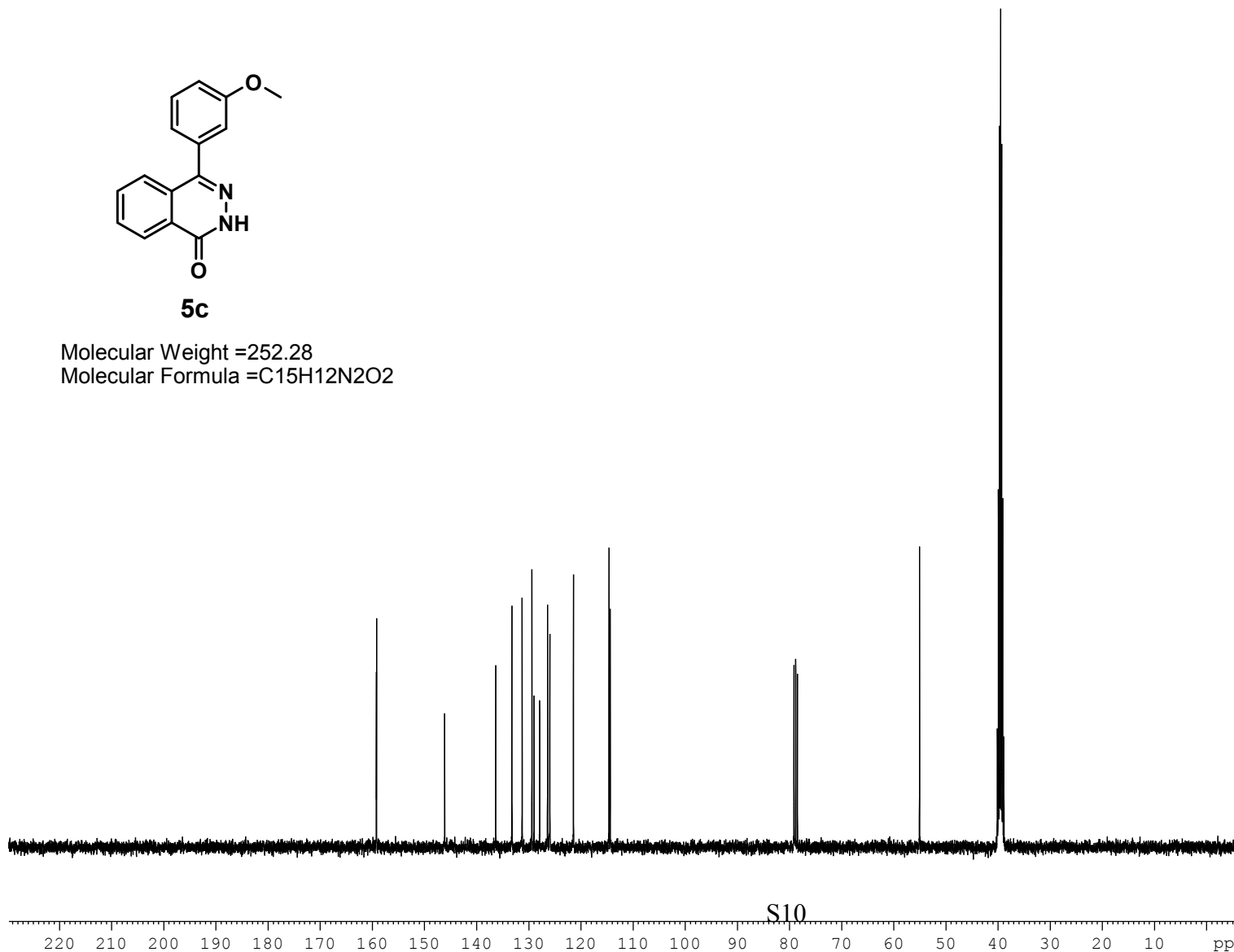
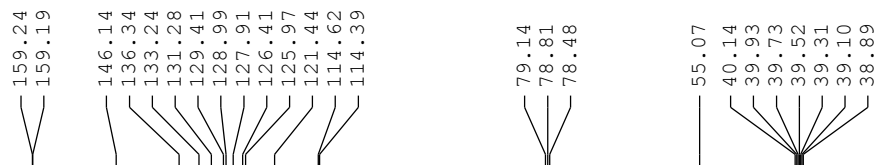
Molecular Weight =252.28
Molecular Formula =C₁₅H₁₂N₂O₂



SRD-L



Molecular Weight =252.28
Molecular Formula =C₁₅H₁₂N₂O₂



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Current Data Parameters
NAME Jan01-2015
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 11.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 240
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
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DE 6.00 usec
TE 293.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.899999998 sec
TD0 1

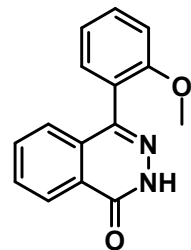
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NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

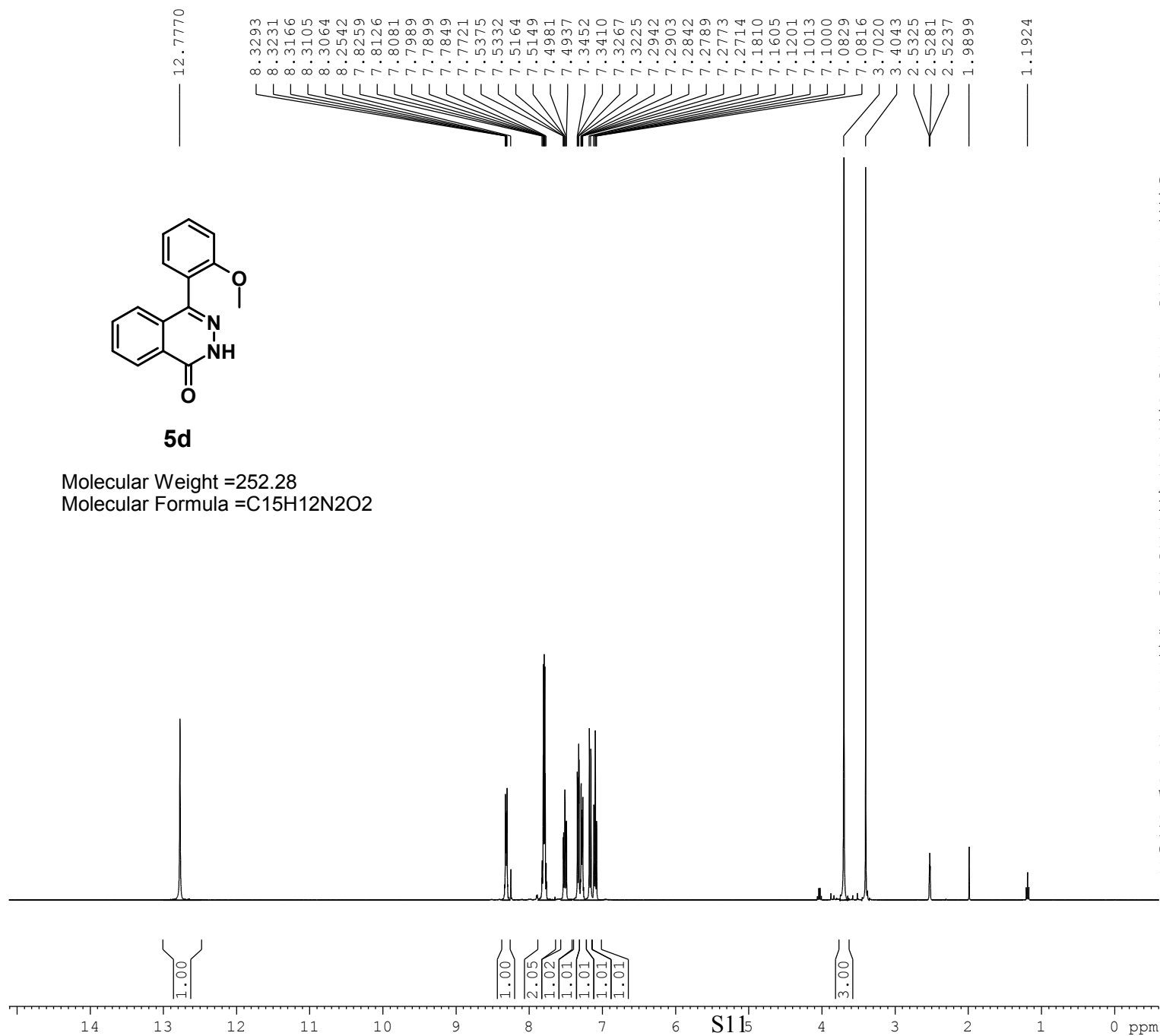
avtar_saifpu@yahoo.co.in

SRD-M



5d

Molecular Weight =252.28
Molecular Formula =C₁₅H₁₂N₂O₂



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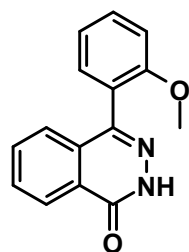
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EXPNO 30
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 292.7 K
D1 1.0000000 sec
TD0 1

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

F2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

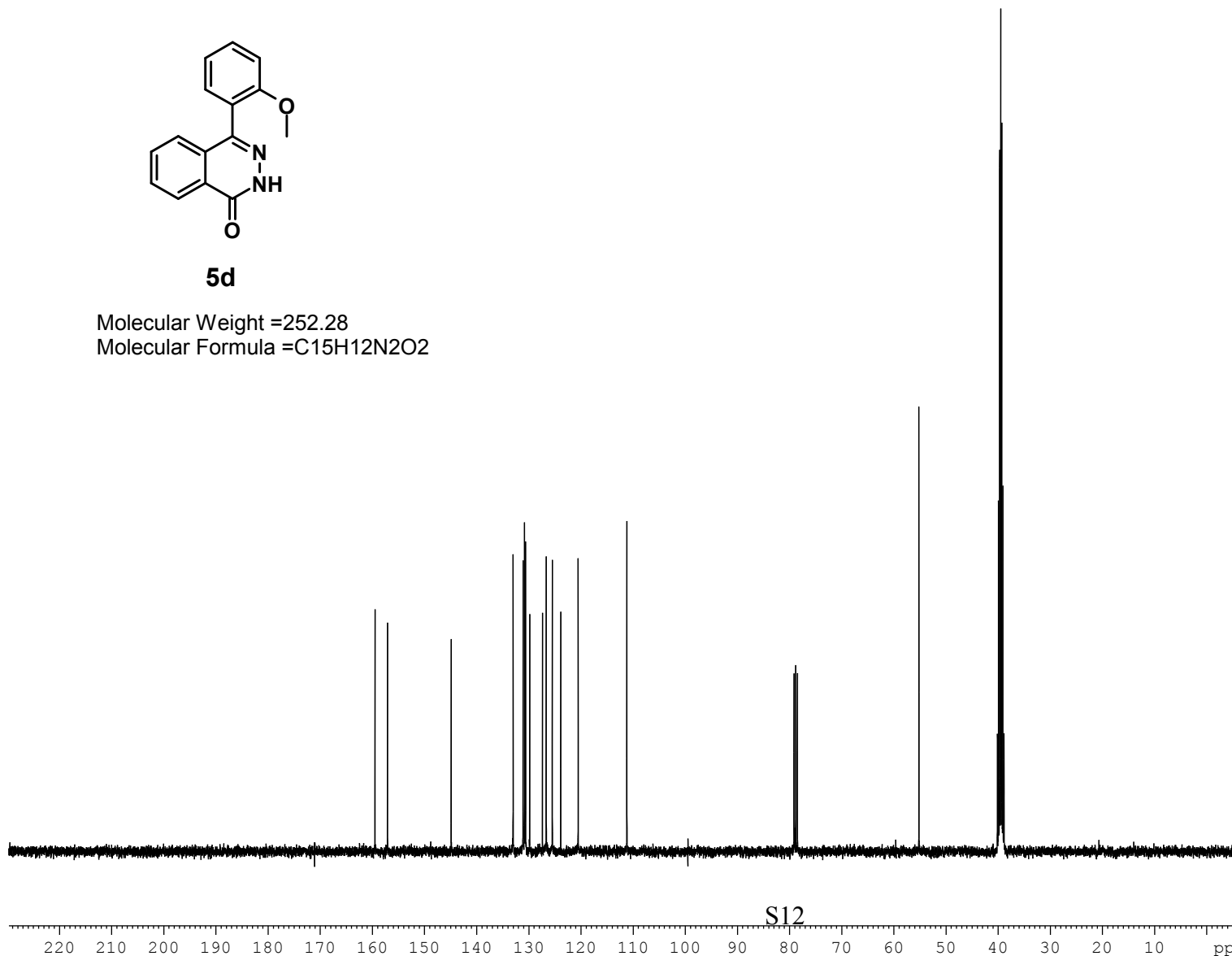
SRD-M



5d

Molecular Weight =252.28
Molecular Formula =C₁₅H₁₂N₂O₂

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130.63
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127.38
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125.51
123.89
120.54
111.20
79.16
78.83
78.50
55.20
40.14
39.93
39.72
39.51
39.30
39.09
38.89



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Current Data Parameters
NAME Jan01-2015
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date 20150101
Time 12.23
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PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 373
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FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 32
DW 16.800 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SRD-T

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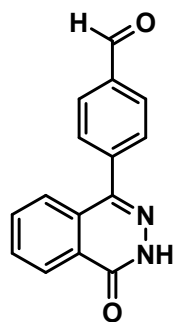
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PROCNO 1

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TD 65536
SOLVENT DMSO
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DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 287
DW 41.600 usec
DE 6.00 usec
TE 293.4 K
D1 1.0000000 sec
TD0 1

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

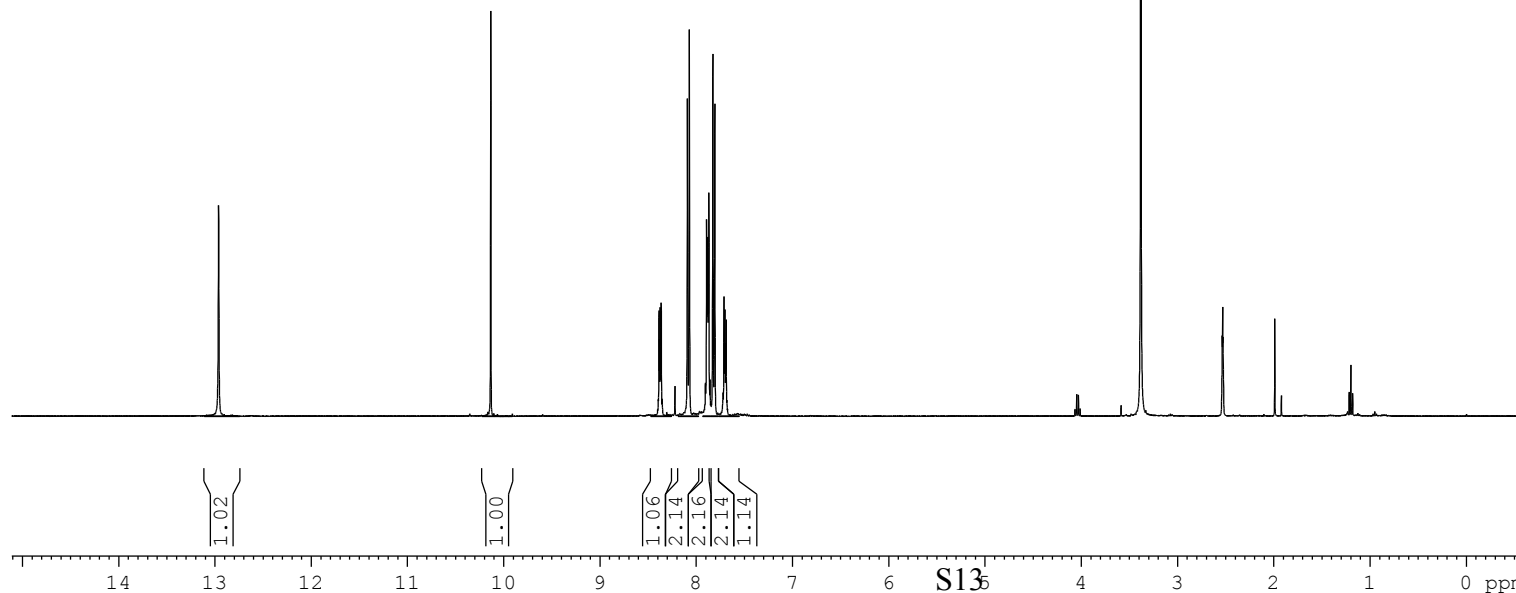
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LB 0.30 Hz
GB 0
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8.3670
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7.8902
7.8849
7.8833
7.8778
7.8725
7.8311
7.8108
7.7153
7.7080
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2.5335
2.5291
1.9924
1.2013



5e

Molecular Weight =250.26
Molecular Formula =C15H10N2O2



SRD-T

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192.28

159.22

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133.39
131.49
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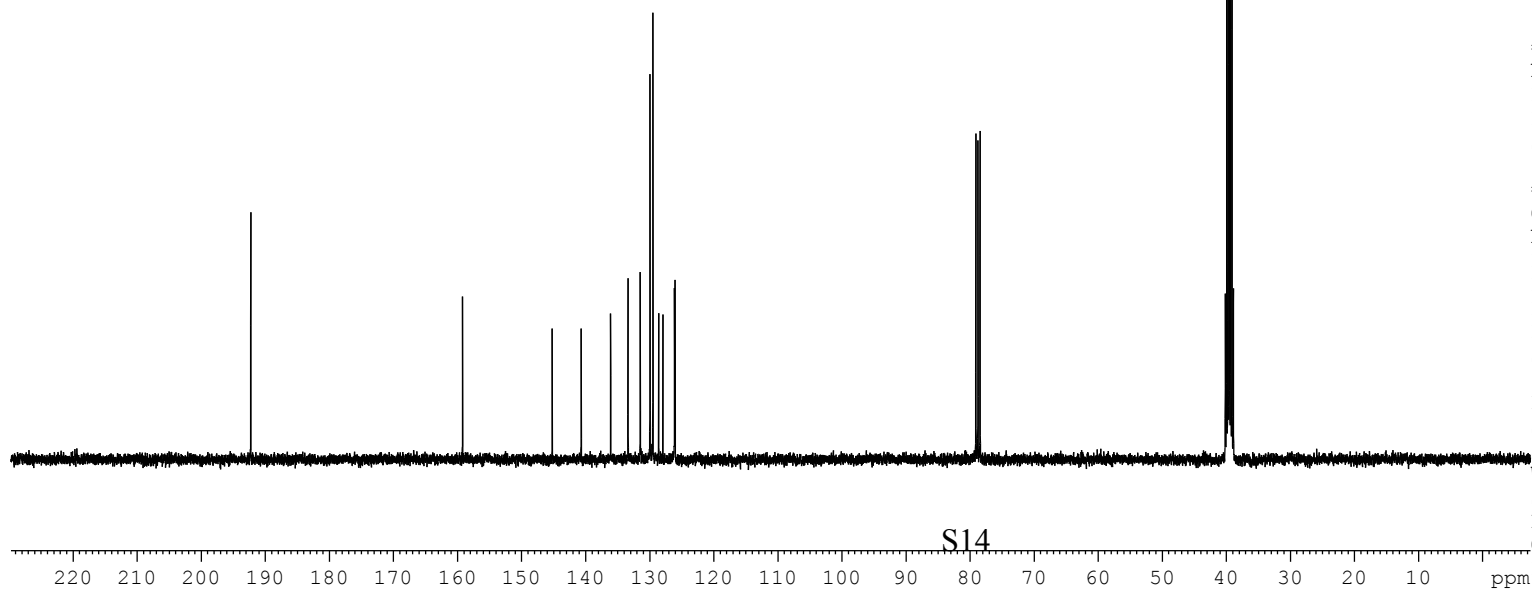
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5e

Molecular Weight =250.26
Molecular Formula =C15H10N2O2



Current Data Parameters
NAME Jan01-2015
EXPNO 101
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 16.00
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PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 293.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

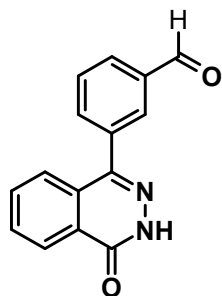
==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

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

F2 - Processing parameters
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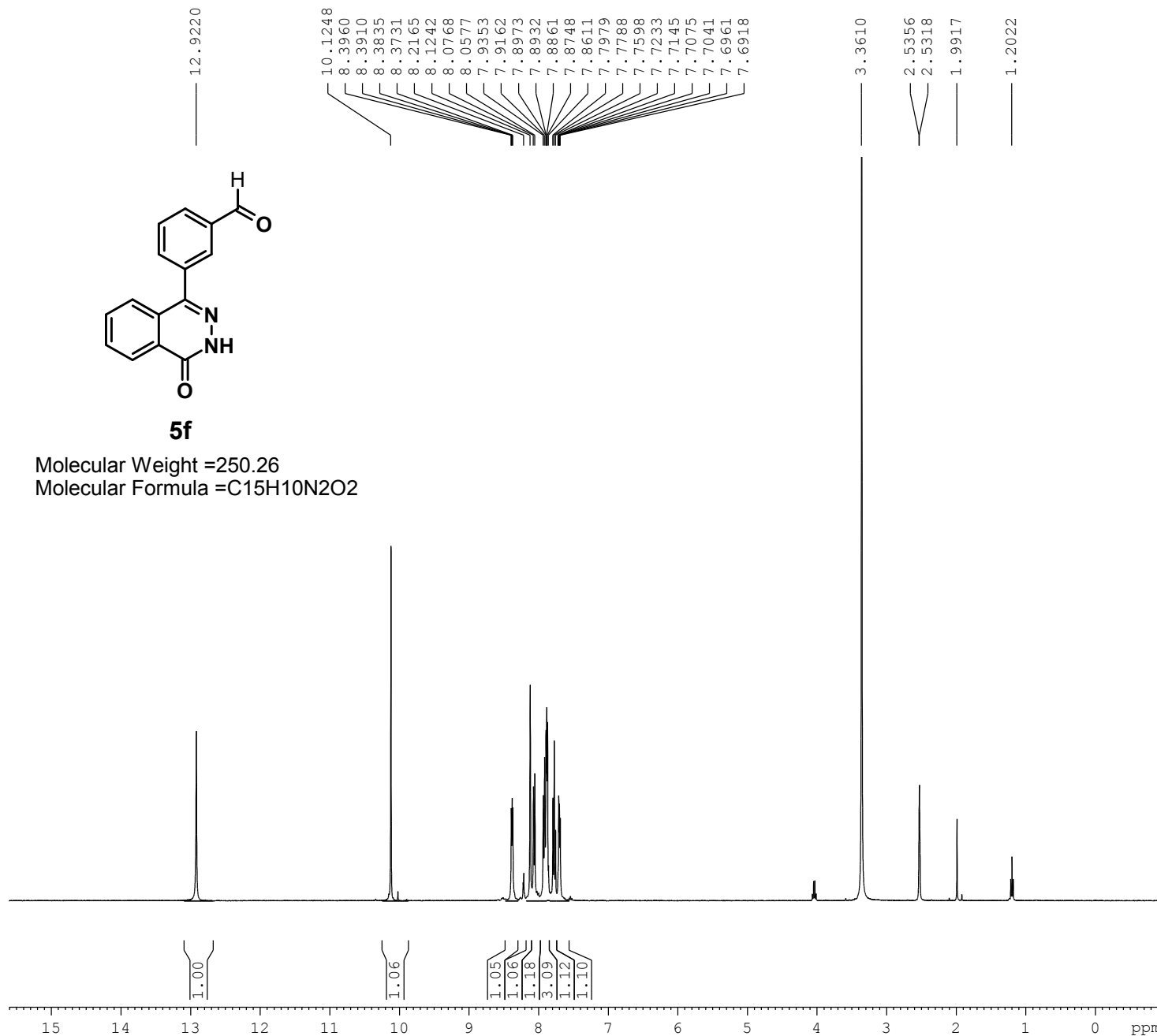
avtar_saifpu@yahoo.co.in

GRD-10



5f

Molecular Weight =250.26
Molecular Formula =C15H10N2O2



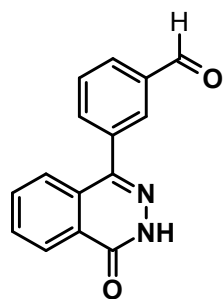
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Current Data Parameters
NAME Nov29-2014
EXPNO 240
PROCNO 1

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Date_ 20141130
Time_ 3.44
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 322
DW 41.600 usec
DE 6.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

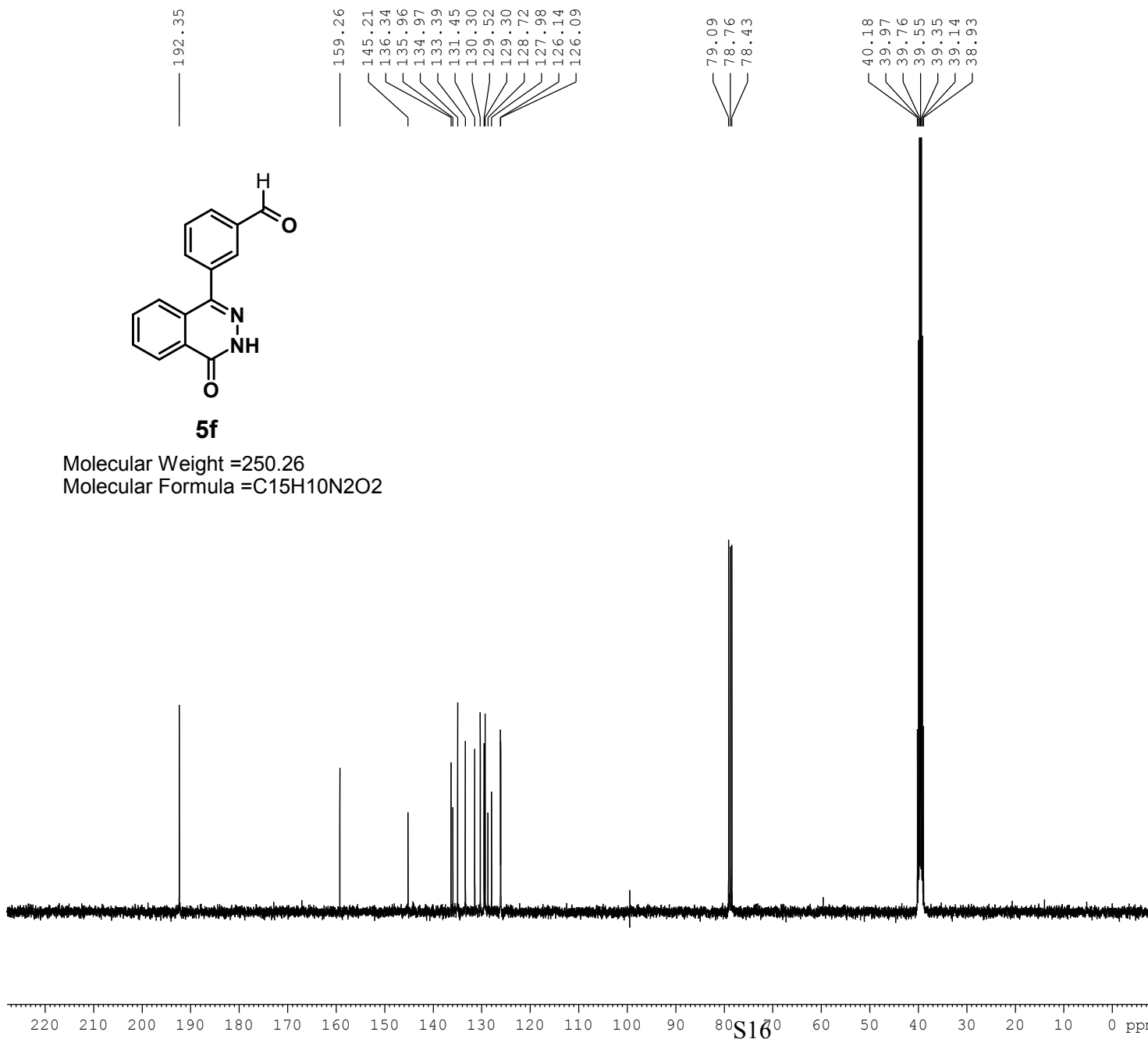
==== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299909 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



5f

Molecular Weight =250.26
Molecular Formula =C15H10N2O2



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```

Current Data Parameters
NAME          Nov29-2014
EXPNO         241
PROCNO        1

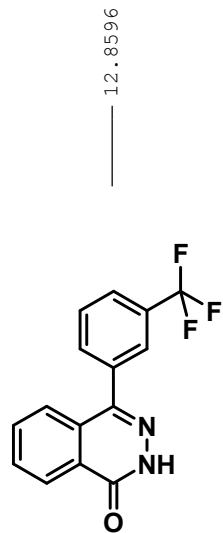
F2 - Acquisition Parameters
Date_         20141130
Time          4.40
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            1024
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            36
DW            16.800 usec
DE            6.00 usec
TE            296.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

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

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

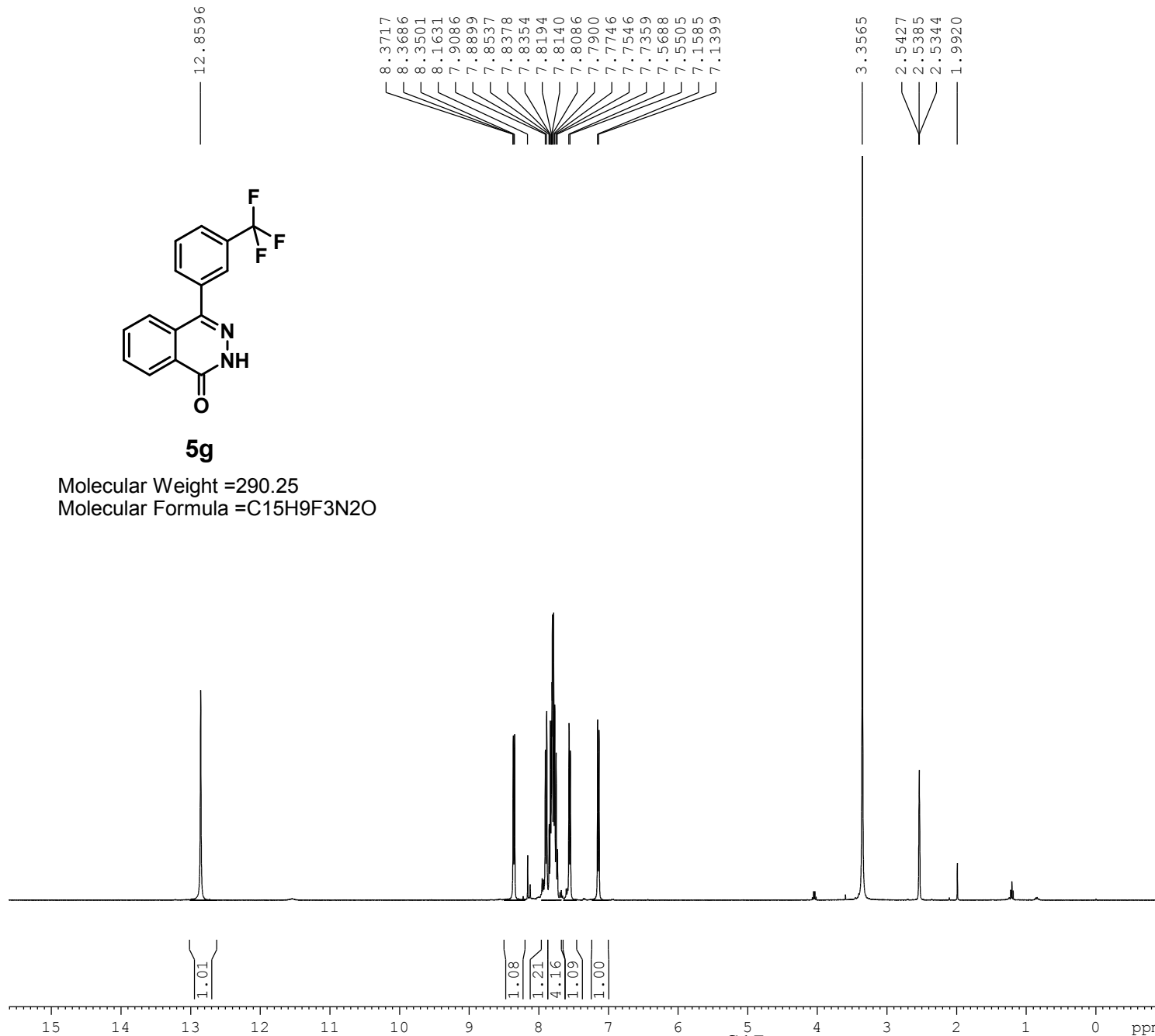
F2 - Processing parameters
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```


GRD-11



5g

Molecular Weight =290.25
Molecular Formula =C15H9F3N2O



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Current Data Parameters
NAME Nov29-2014
EXPNO 250
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141130
Time_ 4.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 362
DW 41.600 usec
DE 6.00 usec
TE 296.0 K
D1 1.0000000 sec
TD0 1

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

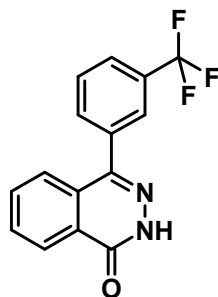
F2 - Processing parameters
SI 32768
SF 400.1299884 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S17

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GRD-11

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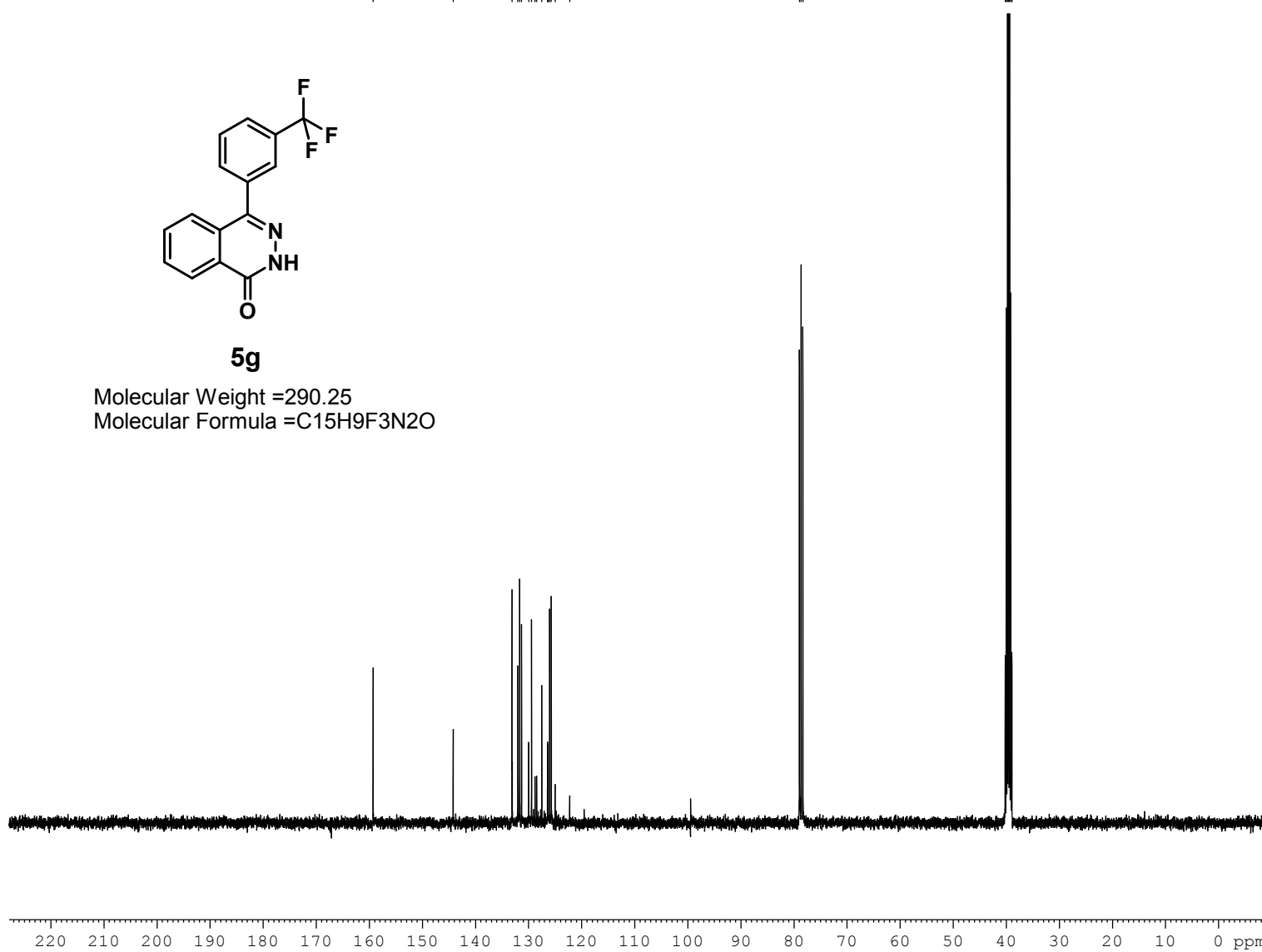
5g

Molecular Weight =290.25
Molecular Formula =C15H9F3N2O

159.30
144.21
133.14
132.04
131.70
131.33
129.99
129.46
128.80
128.50
127.52
126.40
126.35
126.31
126.04
125.73
124.99
122.27

78.98
78.65
78.32

40.20
39.99
39.78
39.57
39.36
39.16
38.95



Current Data Parameters
NAME Nov29-2014
EXPNO 251
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141130
Time_ 5.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 296.3 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

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

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

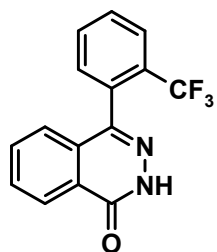
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S18

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SRD-V

12.8873



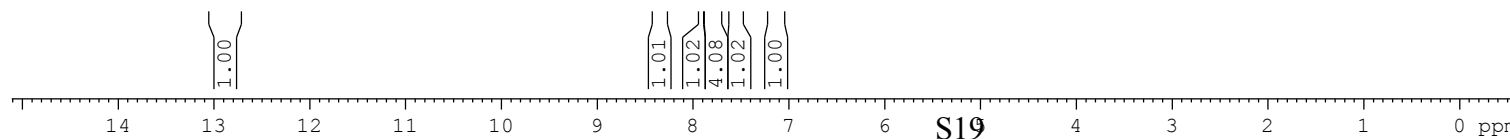
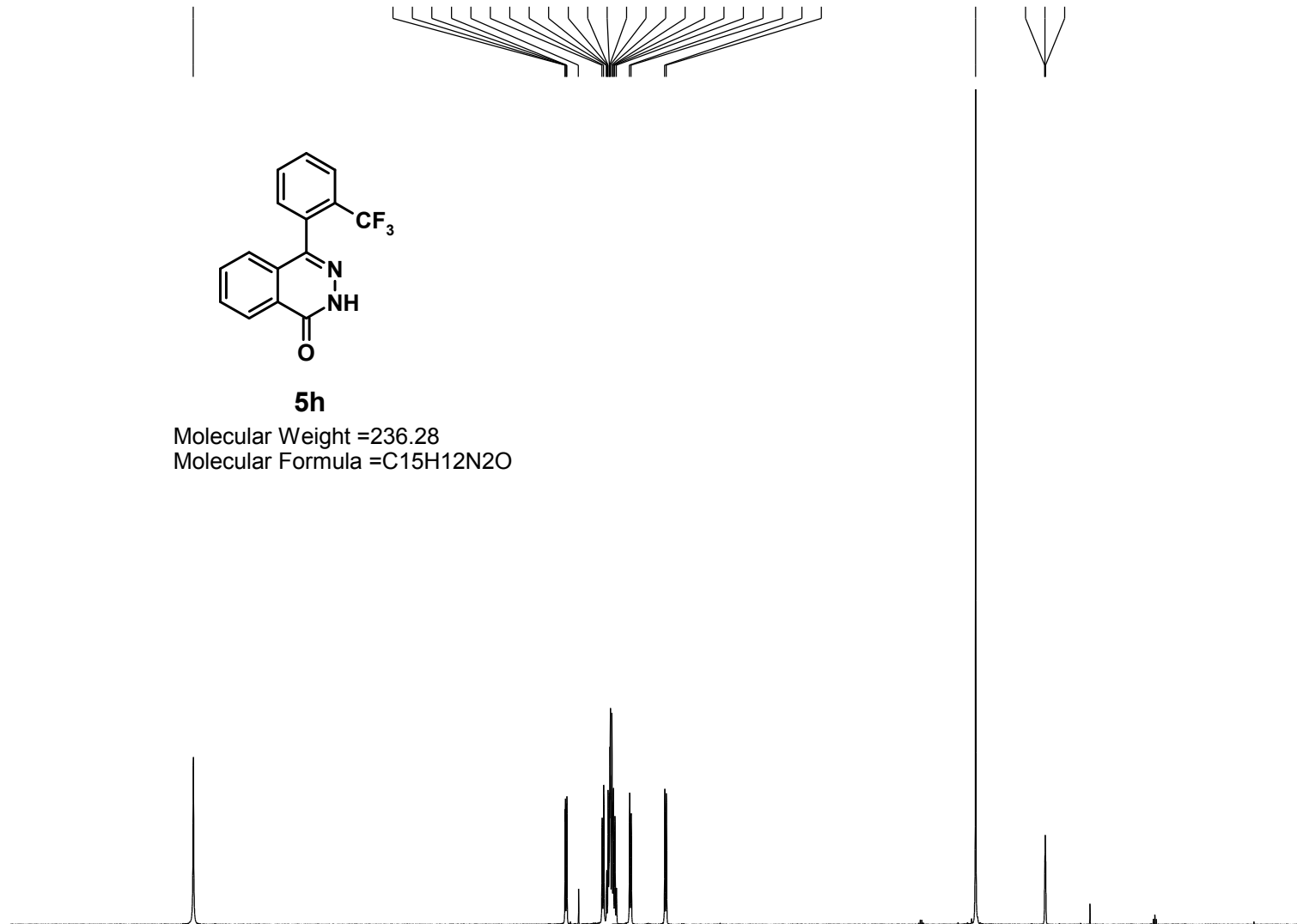
5h

Molecular Weight =236.28
Molecular Formula =C₁₅H₁₂N₂O

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8.3496
8.3473
8.2059
7.9198
7.9012
7.8666
7.8641
7.8485
7.8458
7.8301
7.8254
7.8199
7.8012
7.7859
7.7833
7.7649
7.7462
7.5851
7.5666
7.1588
7.1400

3.3806

2.5399
2.5355
2.5313



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Current Data Parameters
NAME Jan01-2015
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time 16.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 724
DW 41.600 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

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

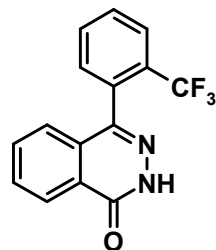
F2 - Processing parameters
SI 32768
SF 400.1299893 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S19

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SRD-V

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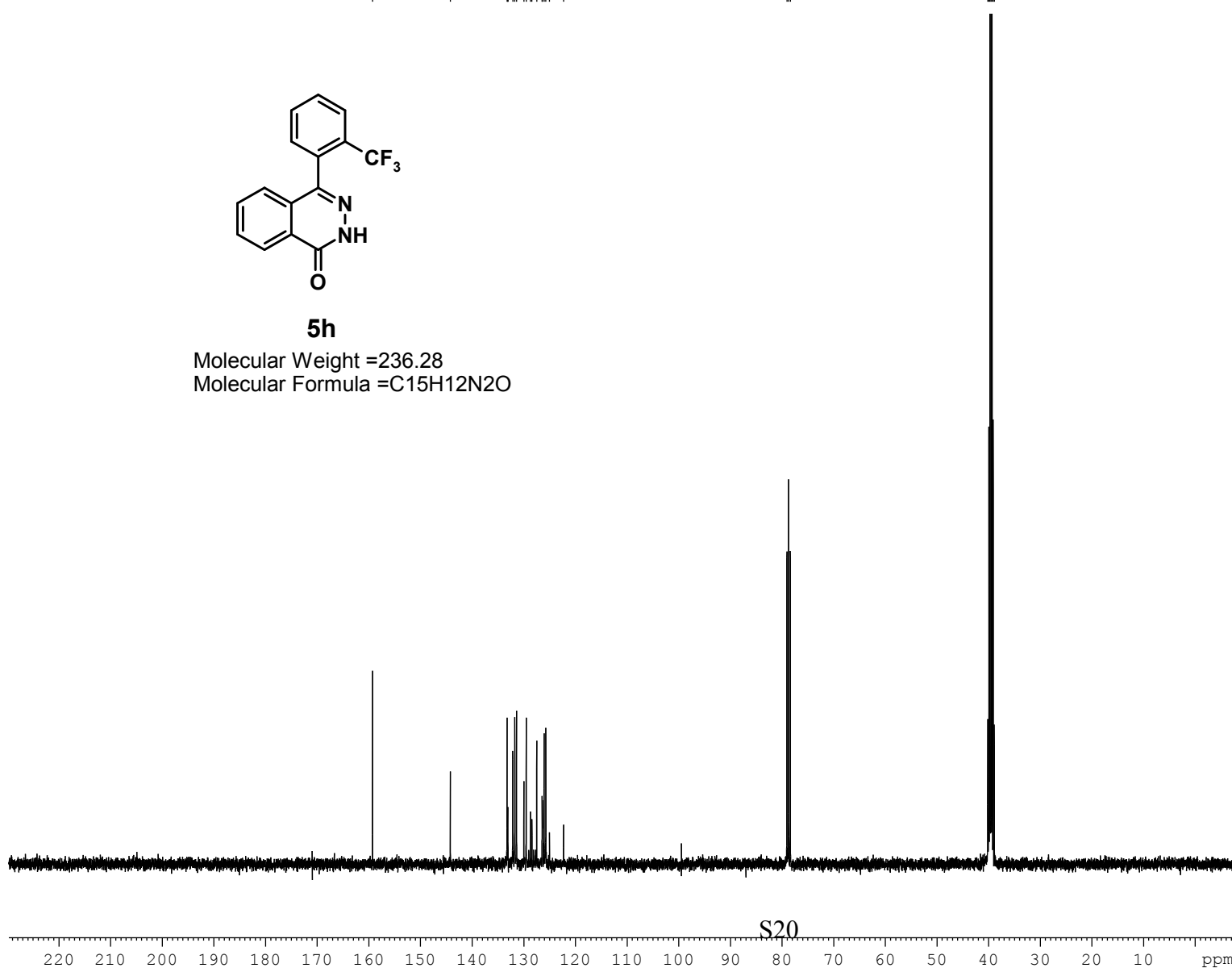
5h

Molecular Weight =236.28
Molecular Formula =C₁₅H₁₂N₂O

159.29
144.22
133.23
133.10
133.08
132.14
131.75
131.42
129.99
129.54
128.73
128.43
127.50
126.44
126.39
126.07
125.75
125.03
122.31

79.06
78.73
78.40

40.16
39.96
39.75
39.54
39.33
39.12
38.91



Current Data Parameters
NAME Jan01-2015
EXPNO 111
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 32
DW 16.800 usec
DE 6.00 usec
TE 293.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.899999998 sec
TD0 1

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

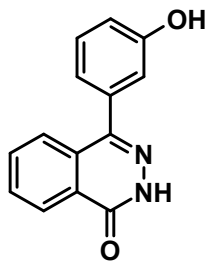
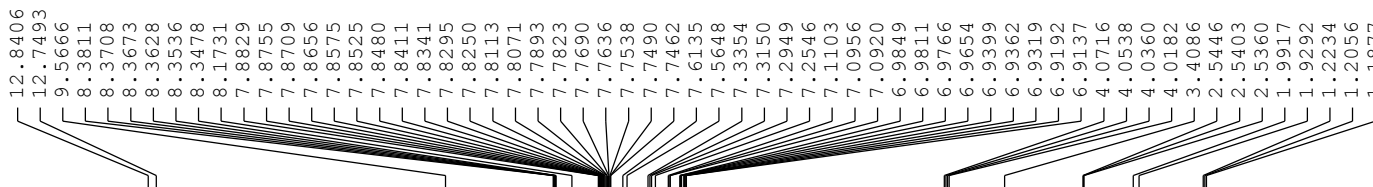
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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GRD-06

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5i

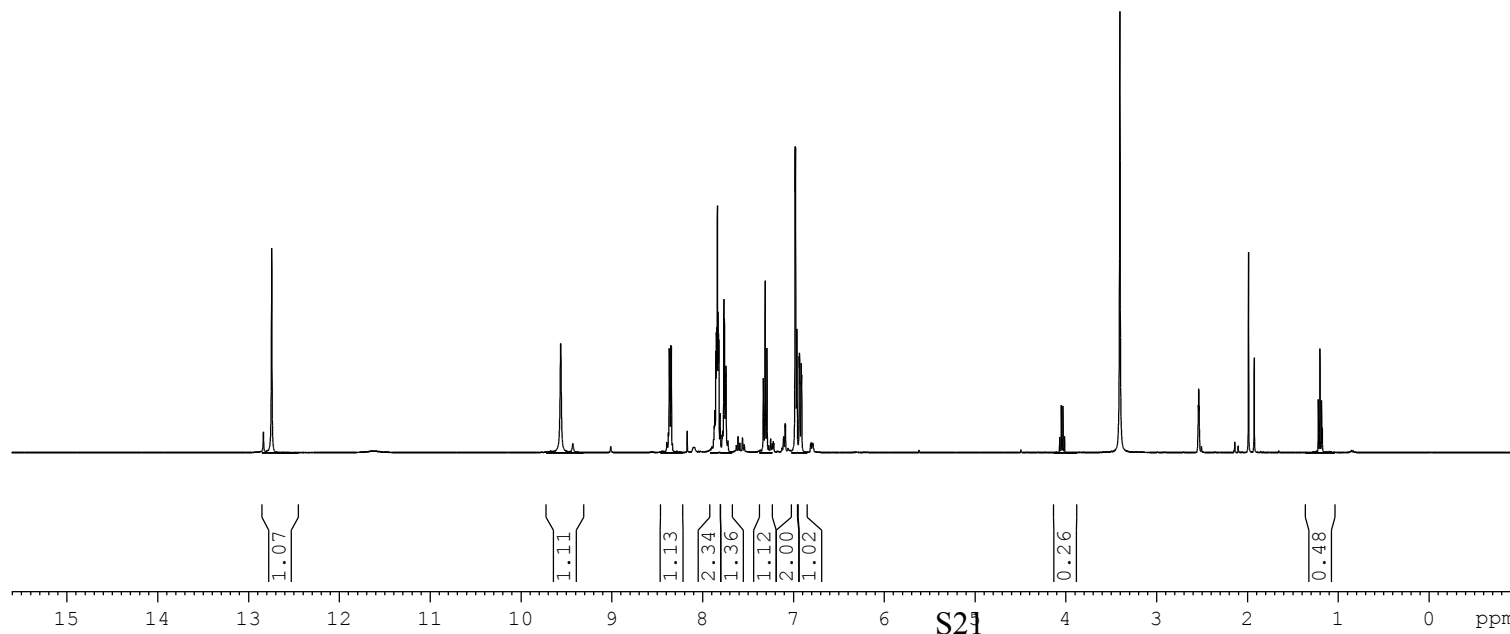
Molecular Weight =238.25
Molecular Formula =C₁₄H₁₀N₂O₂

Current Data Parameters
NAME Nov29-2014
EXPNO 210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141130
Time 0.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
DW 41.600 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

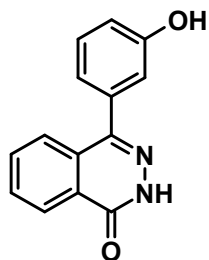
==== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299876 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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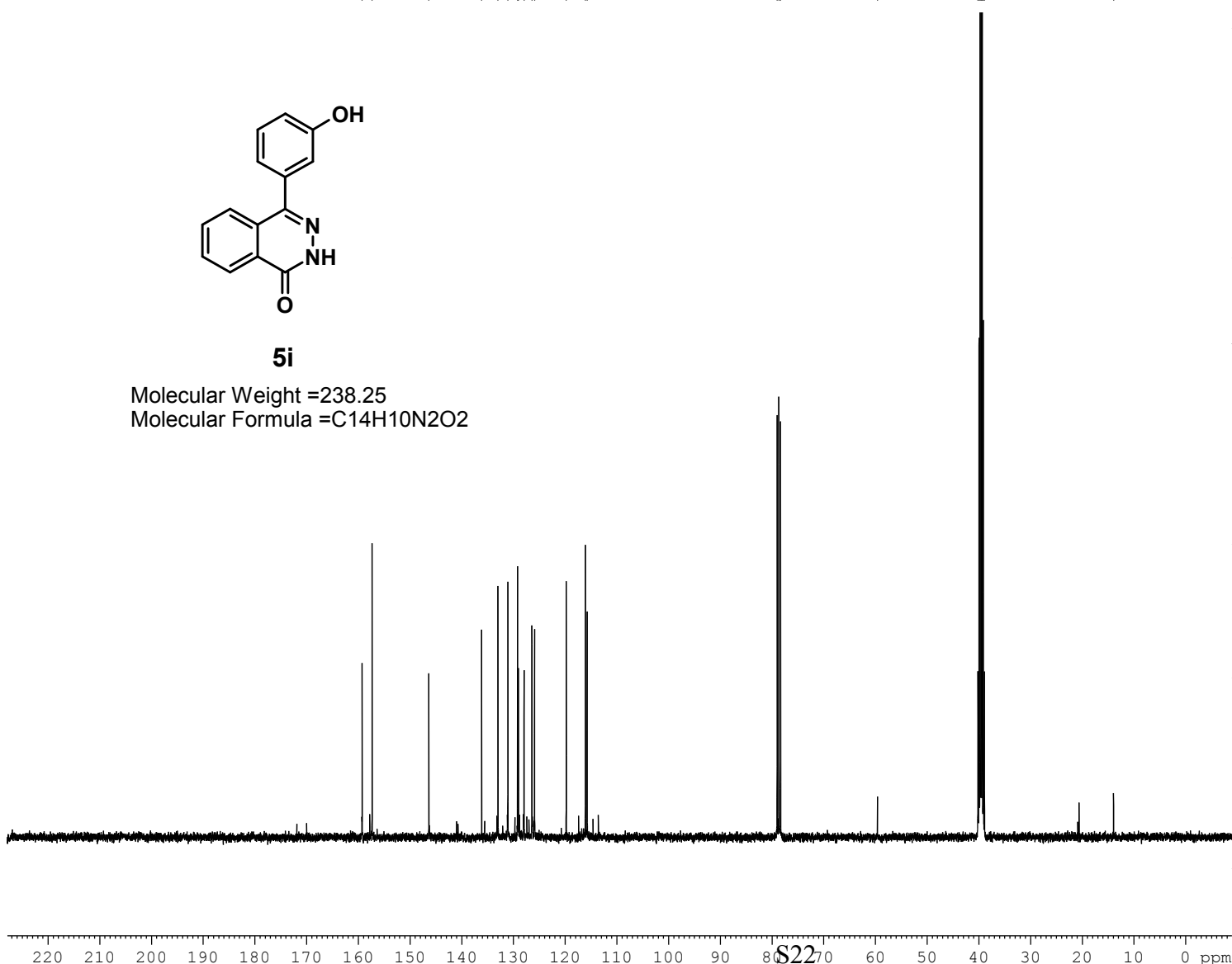
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5i

Molecular Weight =238.25
Molecular Formula =C14H10N2O2

159.28
157.35
146.37
136.16
133.01
131.08
129.21
129.04
127.96
126.44
125.92
119.80
116.10
115.76
79.00
78.68
78.35
59.60
40.17
39.96
39.76
39.55
39.34
39.13
38.92
13.95



Current Data Parameters
NAME Nov29-2014
EXPNO 211
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141130
Time 1.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

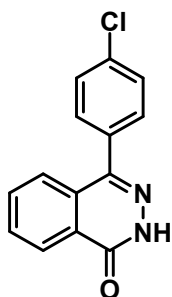
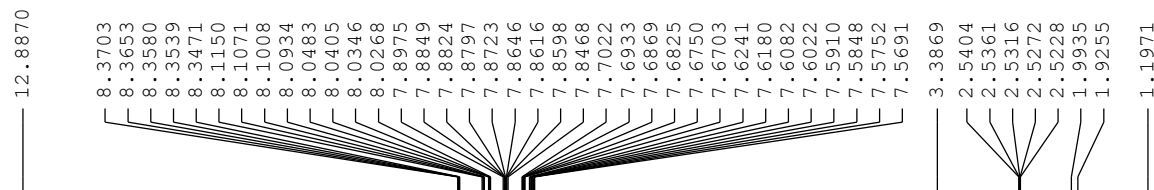
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Current Data Parameters
 NAME Jan01-2015
 EXPNO 140
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150101
 Time_ 19.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 256
 DW 41.600 usec
 DE 6.00 usec
 TE 293.2 K
 D1 1.0000000 sec
 TD0 1

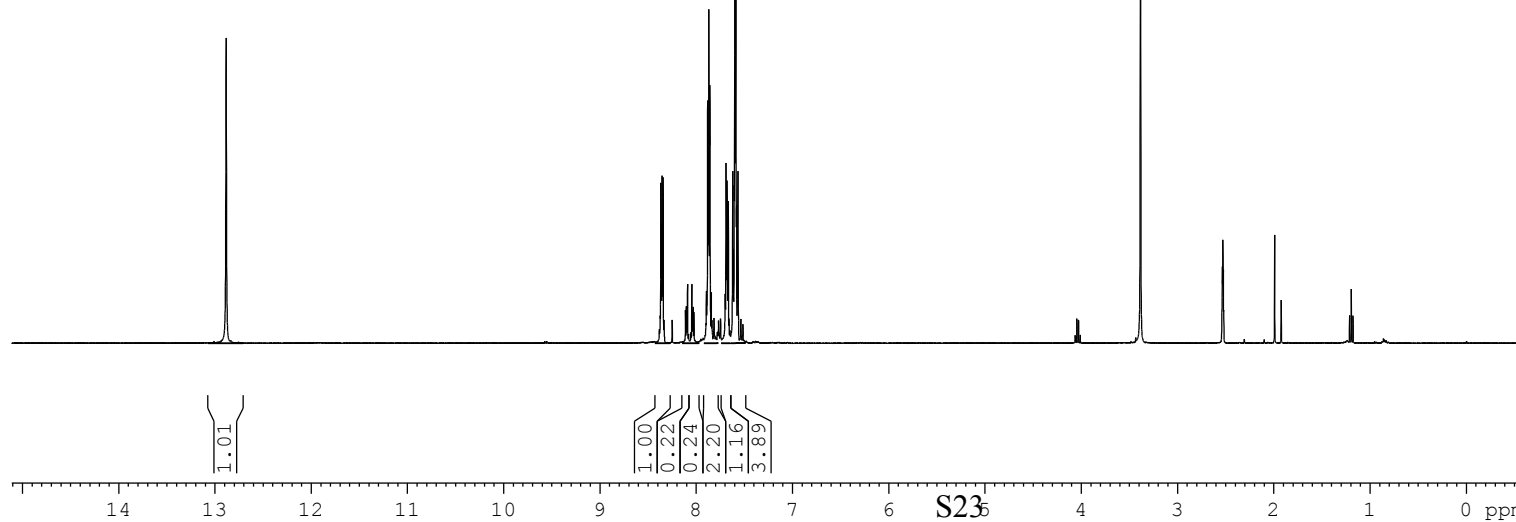
===== CHANNEL f1 =====
 NUC1 1H
 P1 10.90 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1299908 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

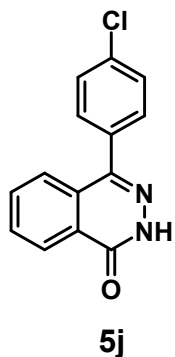


5j

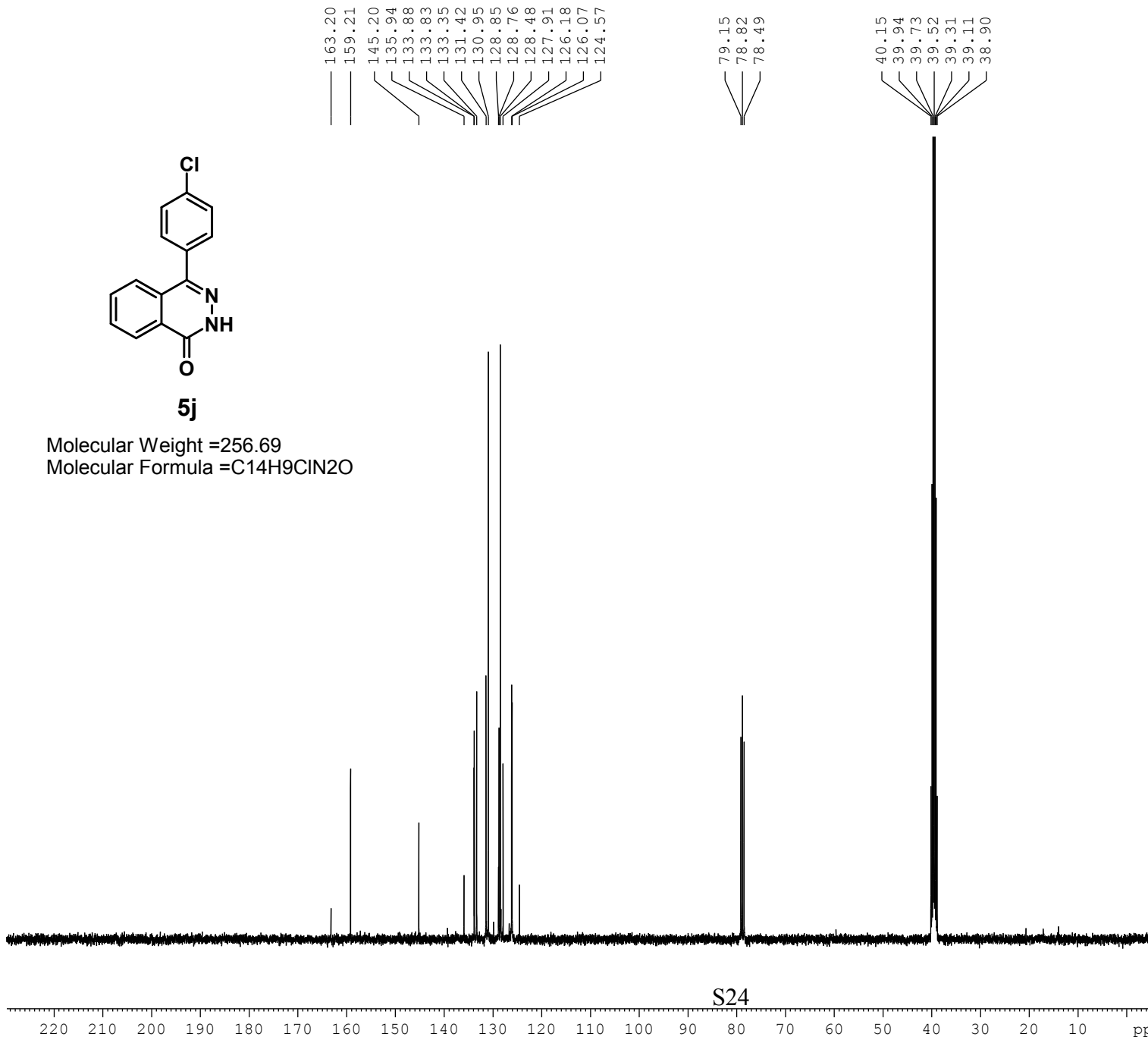
Molecular Weight =256.69
 Molecular Formula =C₁₄H₉ClN₂O



GRD-04



Molecular Weight =256.69
Molecular Formula =C₁₄H₉ClN₂O



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Current Data Parameters
NAME Jan01-2015
EXPNO 141
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 19.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1150
DW 16.800 usec
DE 6.00 usec
TE 293.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

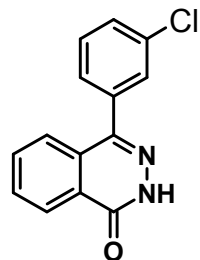
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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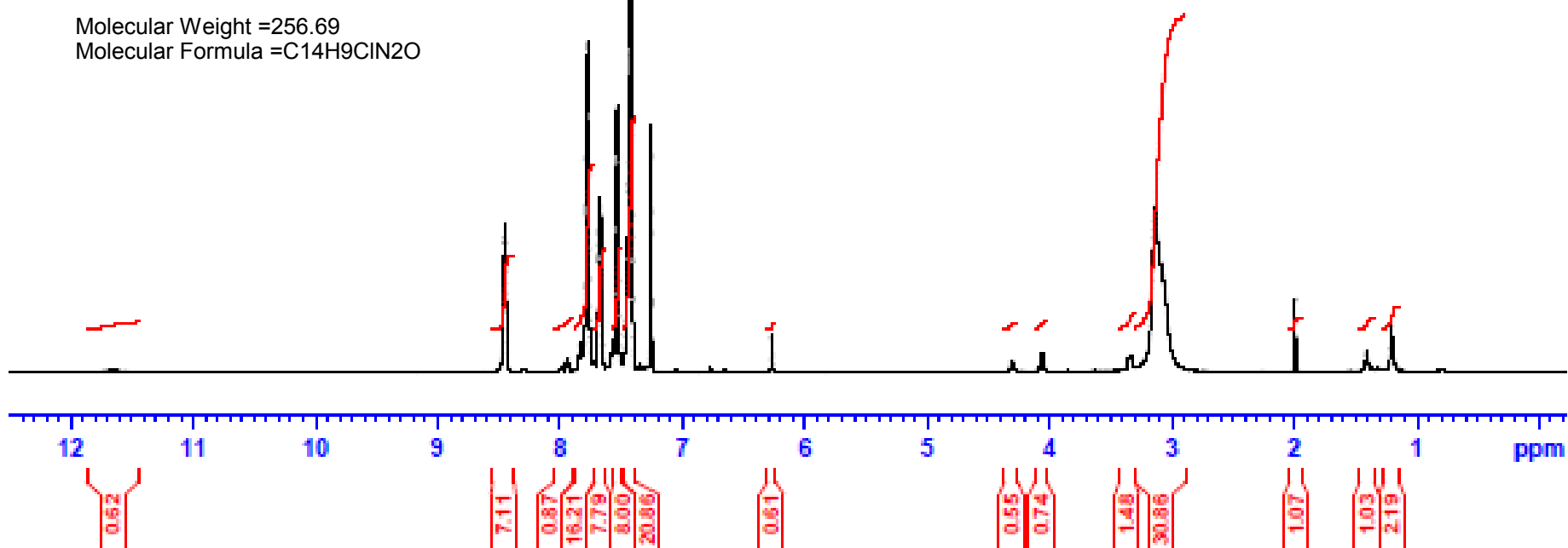
SRD-B
 PROTON_DephtChem CDC13 {D:\AHMEDNAGAR} root 20

11.648
 8.466
 8.457
 8.448
 7.851
 7.836
 7.829
 7.818
 7.804
 7.790
 7.784
 7.776
 7.686
 7.683
 7.677
 7.668
 7.582
 7.567
 7.560
 7.534
 7.464
 7.451
 7.445
 7.442
 7.427
 7.418
 7.260
 7.097
 6.782
 6.778
 6.760
 6.669
 6.273
 6.266
 4.319
 4.310
 4.305
 4.296
 4.291
 4.087
 4.073
 4.064
 4.059
 4.050
 4.045
 3.337
 3.144
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 1.987
 1.431
 1.417
 1.408
 1.403
 1.394
 1.220
 1.206

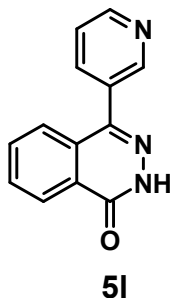


5k

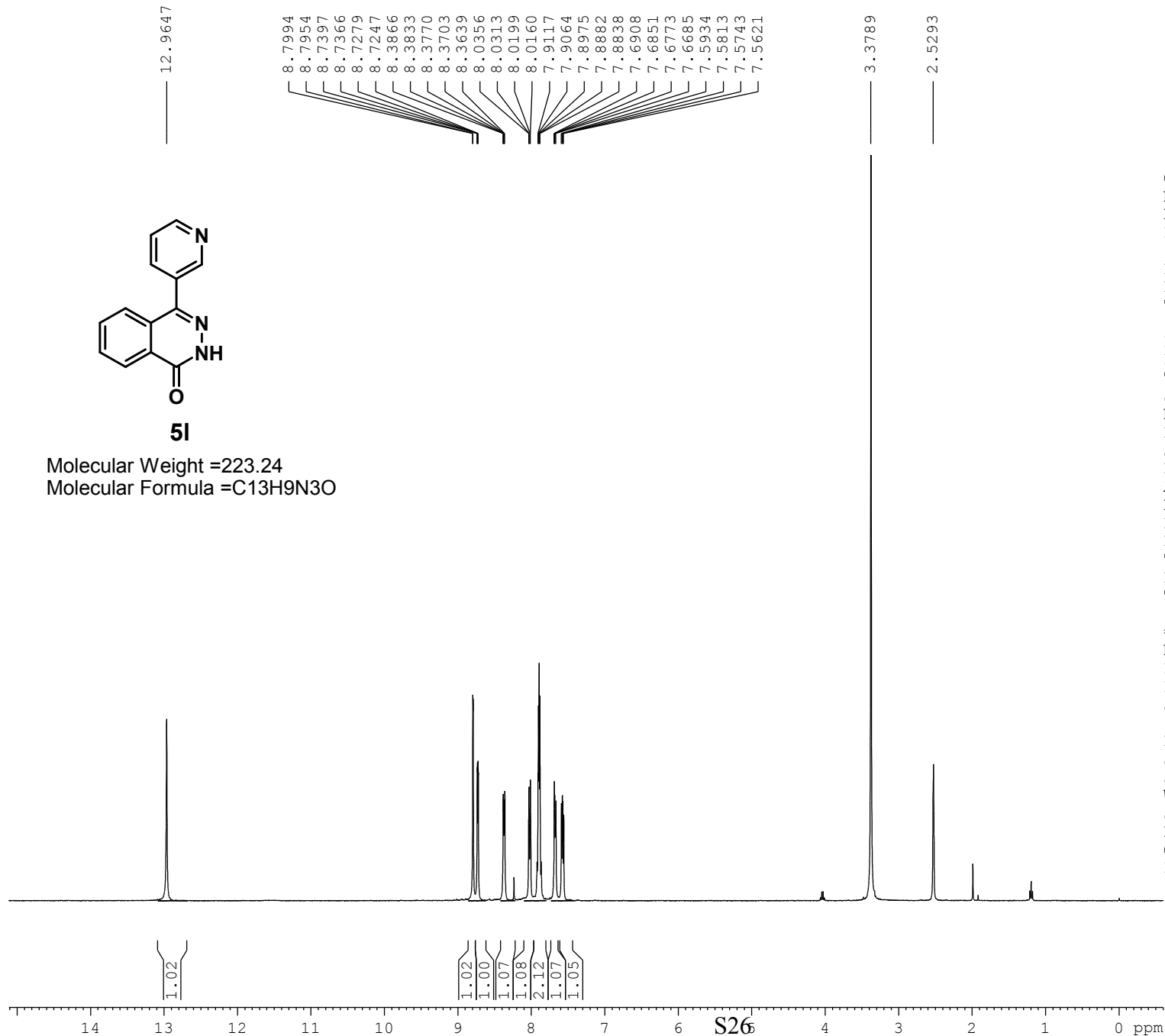
Molecular Weight = 256.69
 Molecular Formula = C₁₄H₉ClN₂O



GRD-08



Molecular Weight =223.24
Molecular Formula =C₁₃H₉N₃O



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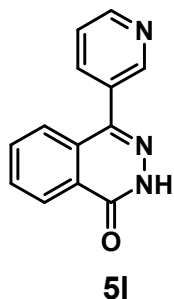
Current Data Parameters
NAME Jan01-2015
EXPNO 160
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 512
DW 41.600 usec
DE 6.00 usec
TE 293.3 K
D1 1.0000000 sec
TD0 1

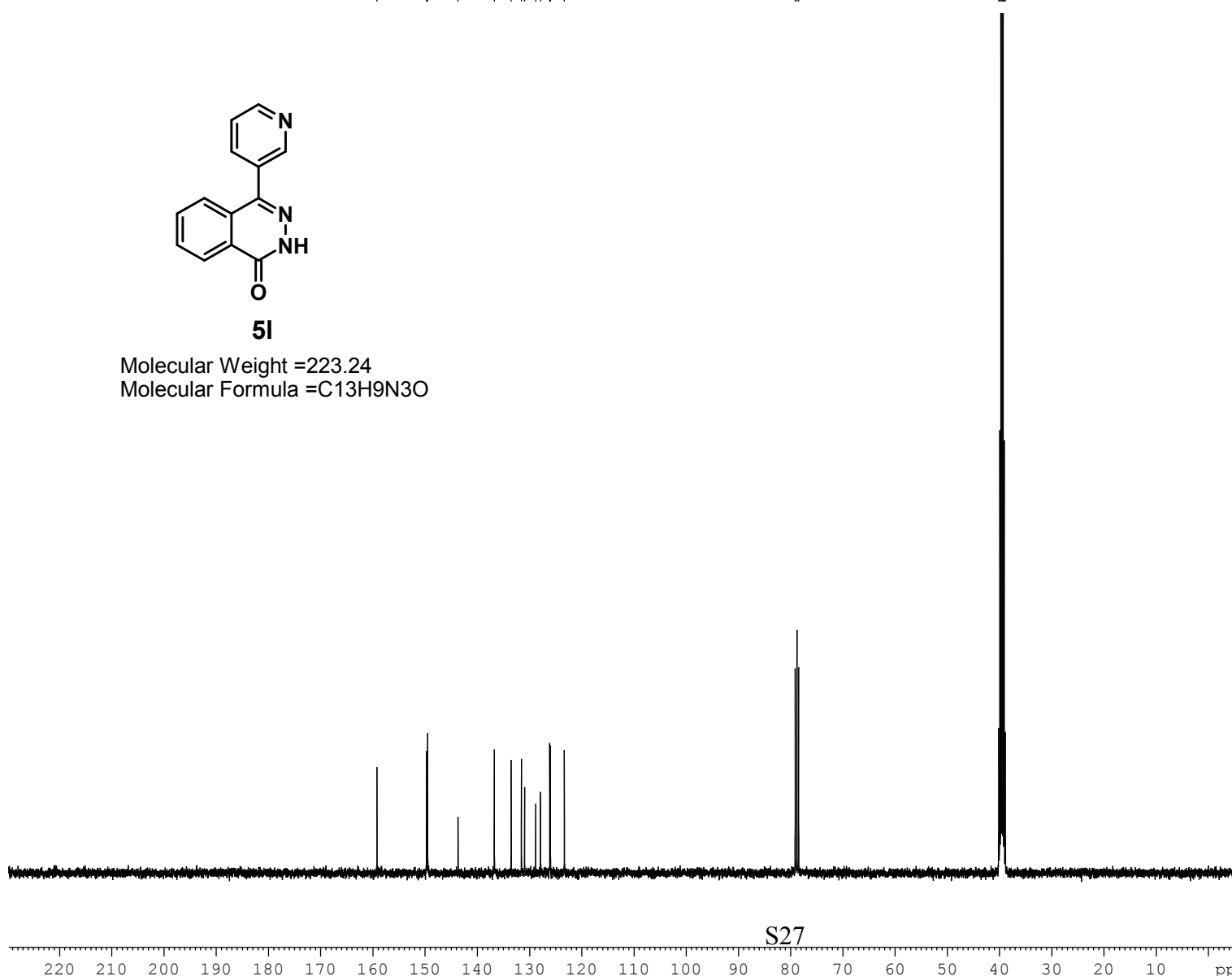
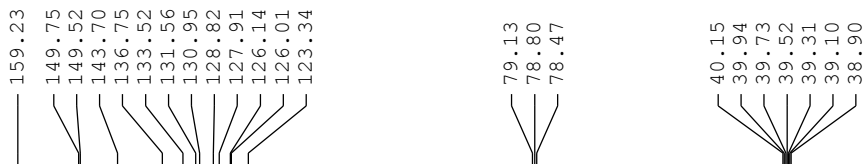
==== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299918 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Molecular Weight =223.24
 Molecular Formula =C₁₃H₉N₃O



Current Data Parameters
 NAME Jan01-2015
 EXPNO 161
 PROCNO 1

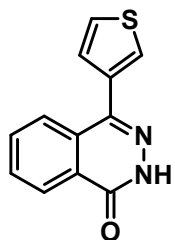
F2 - Acquisition Parameters
 Date_ 20150101
 Time_ 20.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 1030
 DW 16.800 usec
 DE 6.00 usec
 TE 293.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

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

F2 - Processing parameters
 SI 32768
 SF 100.6128193 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

GRD-07



5m

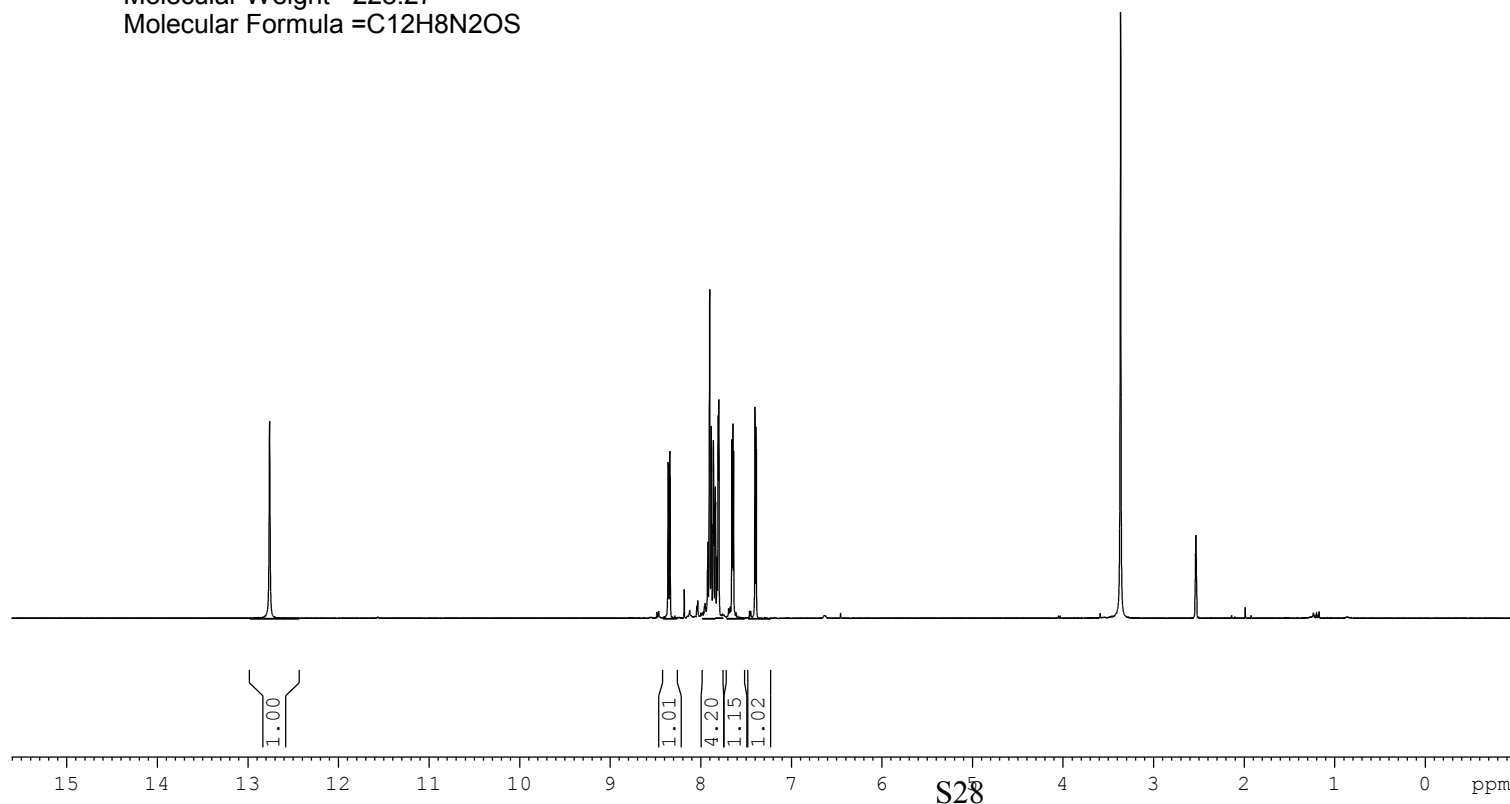
Molecular Weight =228.27
Molecular Formula =C12H8N2OS

12.7611

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8.3427
8.1860
7.9284
7.9244
7.9047
7.8879
7.8844
7.8683
7.8635
7.8579
7.8438
7.8398
7.8271
7.8225
7.8128
7.8102
7.8055
7.8030
7.7608
7.6534
7.6486
7.6412
7.4058
7.4033
7.3937
7.3907

3.3681

2.5402
2.5360
2.5317



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Current Data Parameters
NAME Nov29-2014
EXPNO 220
PROCNO 1

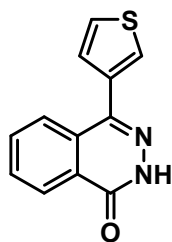
F2 - Acquisition Parameters
Date_ 20141130
Time 1.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 287
DW 41.600 usec
DE 6.00 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1299893 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

avtar_saifpu@yahoo.co.in

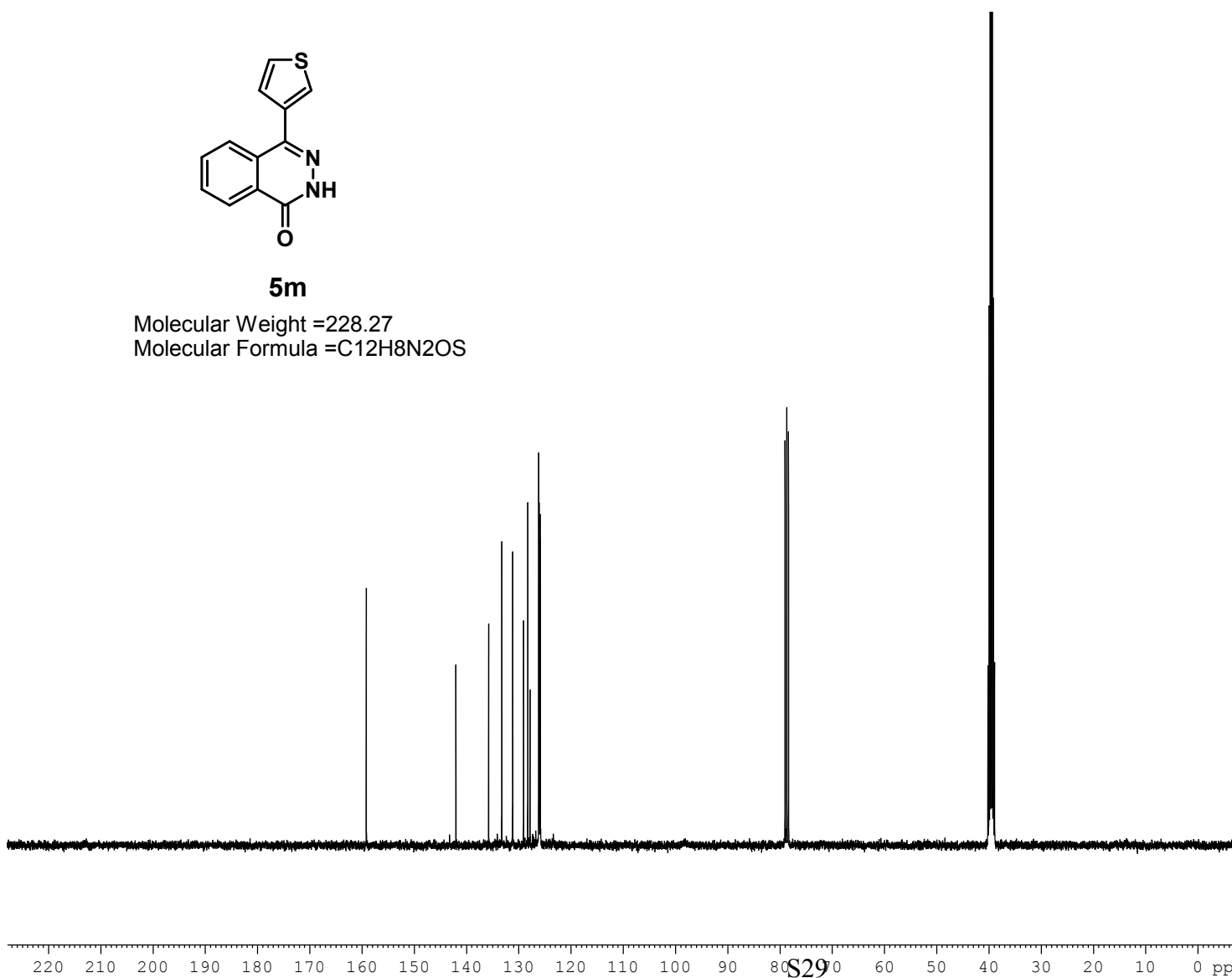
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh



5m

Molecular Weight =228.27
Molecular Formula =C12H8N2OS

159.19
142.04
135.77
133.26
131.18
129.10
128.29
127.84
126.21
126.13
125.96
125.89
79.04
78.71
78.38
40.19
39.98
39.78
39.57
39.36
39.15
38.94



Current Data Parameters
NAME Nov29-2014
EXPNO 221
PROCNO 1

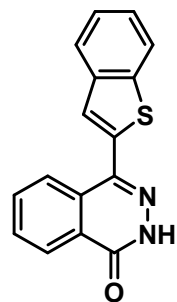
F2 - Acquisition Parameters
Date_ 20141130
Time 2.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

GRD-05



5n

Molecular Weight =278.33
Molecular Formula =C16H10N2OS

12.9996

8.4015
8.3821
8.3272
8.3071
8.0736
8.0283
7.9941
7.9766
7.9582
7.9478
7.9387
7.9331
7.9192
7.9033
7.8846
7.4520
7.4420
7.4336
7.4272
7.4192
7.4087

3.3796

2.5333

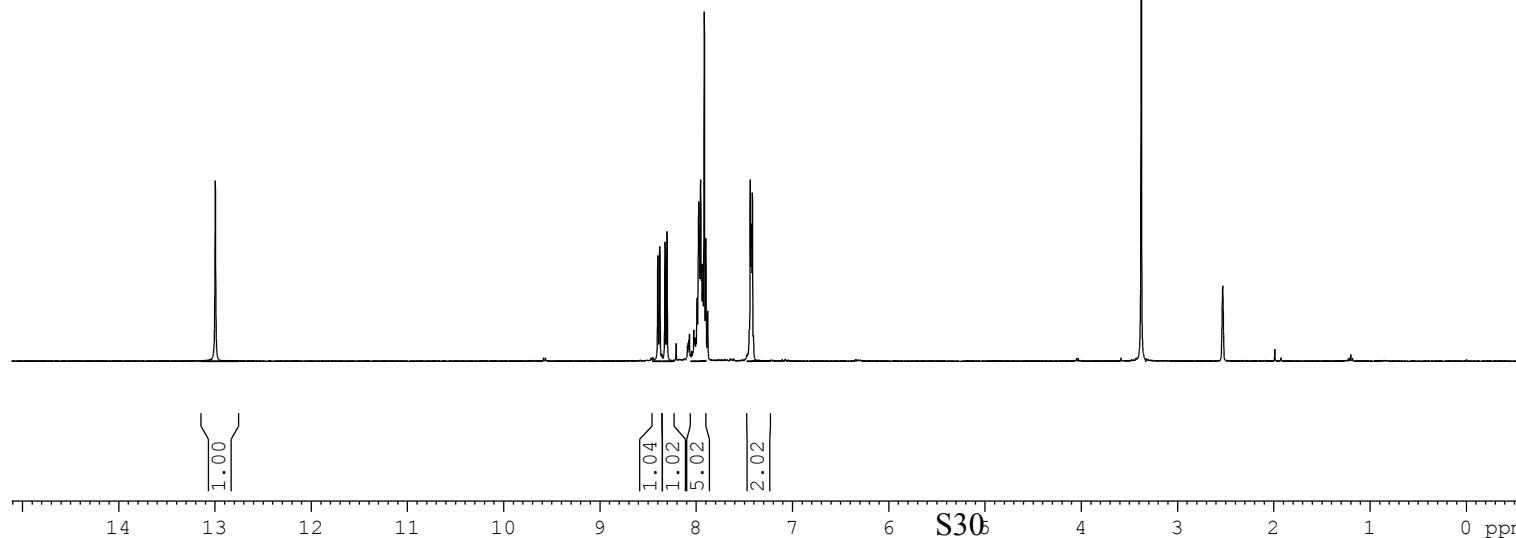
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Current Data Parameters
NAME Jan01-2015
EXPNO 150
PROCNO 1

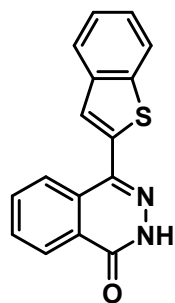
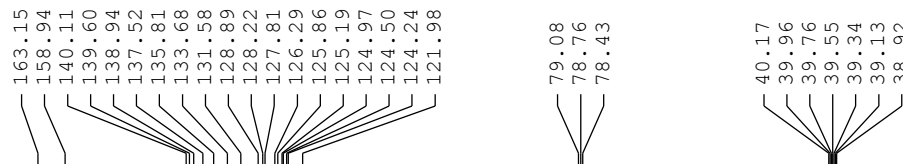
F2 - Acquisition Parameters
Date 20150101
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 456
DW 41.600 usec
DE 6.00 usec
TE 293.3 K
D1 1.0000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1299904 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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5n

Molecular Weight =278.33
 Molecular Formula =C16H10N2OS

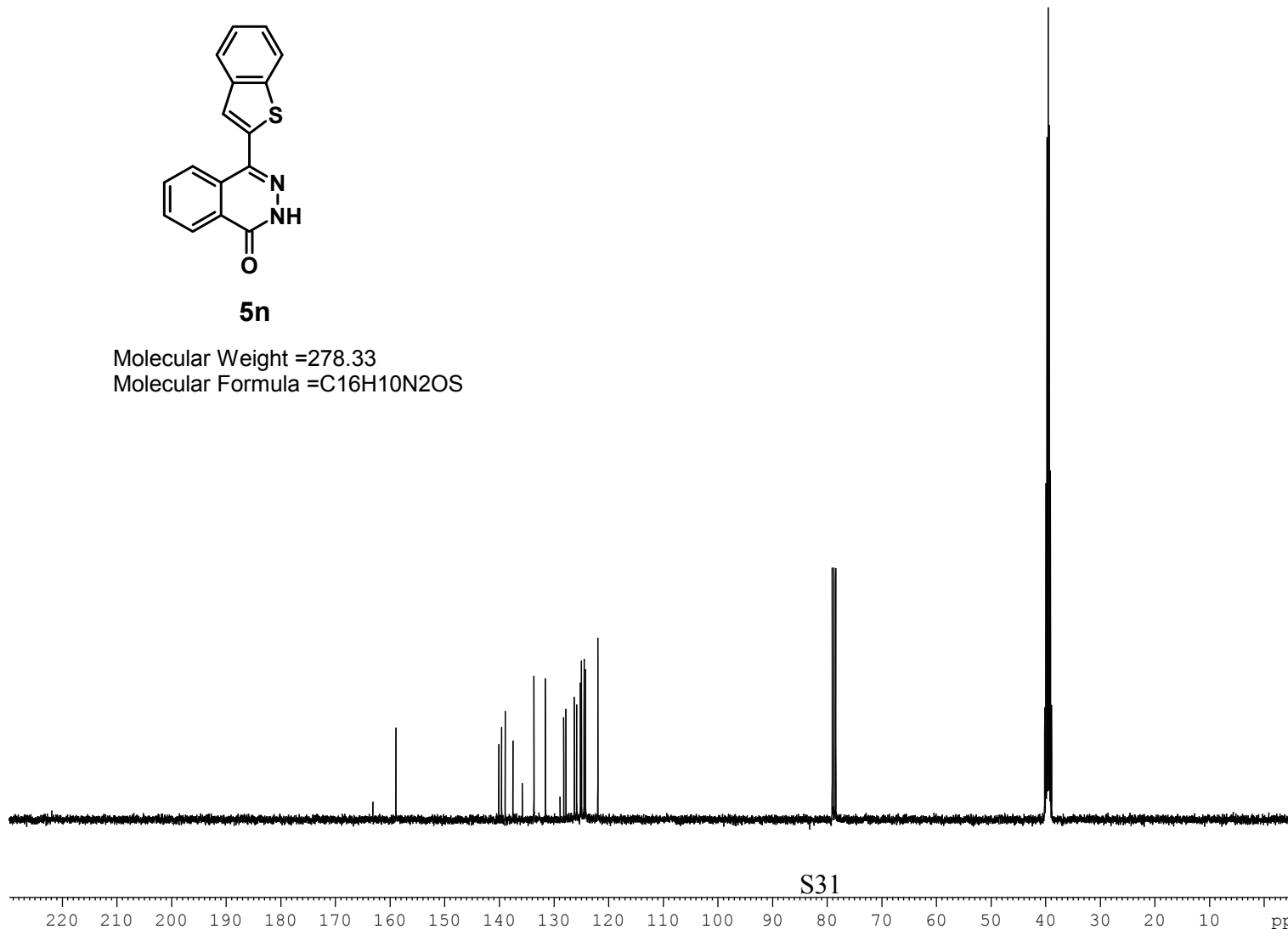
Current Data Parameters
 NAME Jan01-2015
 EXPNO 151
 PROCNO 1

F2 - Acquisition Parameters
 Date 20150101
 Time 20.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 912
 DW 16.800 usec
 DE 6.00 usec
 TE 293.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

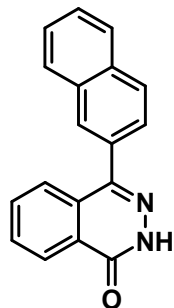
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

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

F2 - Processing parameters
 SI 32768
 SF 100.6128193 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

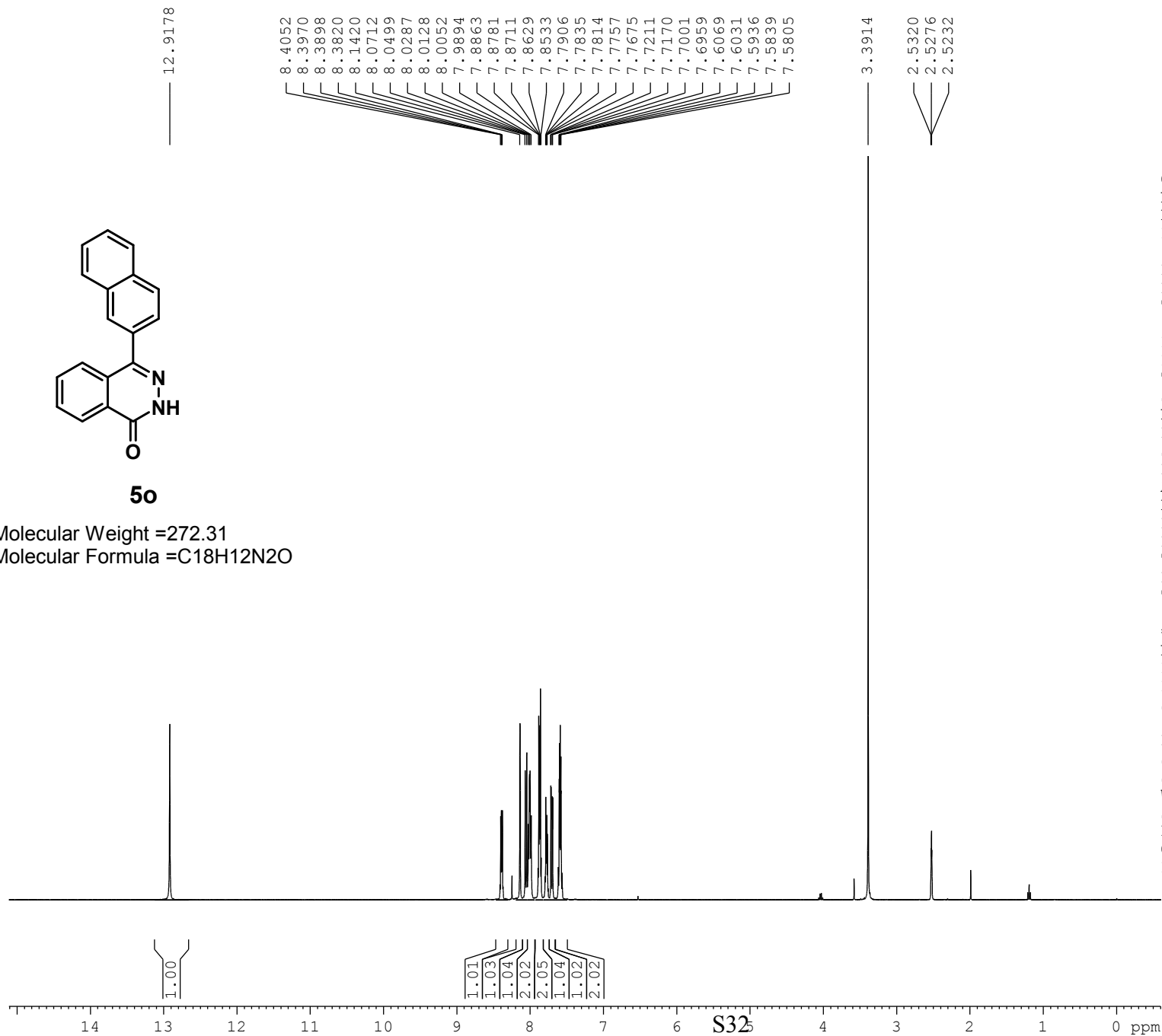


SRD-O



50

Molecular Weight =272.31
 Molecular Formula =C₁₈H₁₂N₂O



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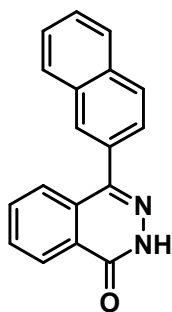
Current Data Parameters
 NAME Jan01-2015
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date 20150101
 Time 12.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 228
 DW 41.600 usec
 DE 6.00 usec
 TE 293.0 K
 D1 1.0000000 sec
 TD0 1

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

F2 - Processing parameters
 SI 32768
 SF 400.1299925 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

SRD-O



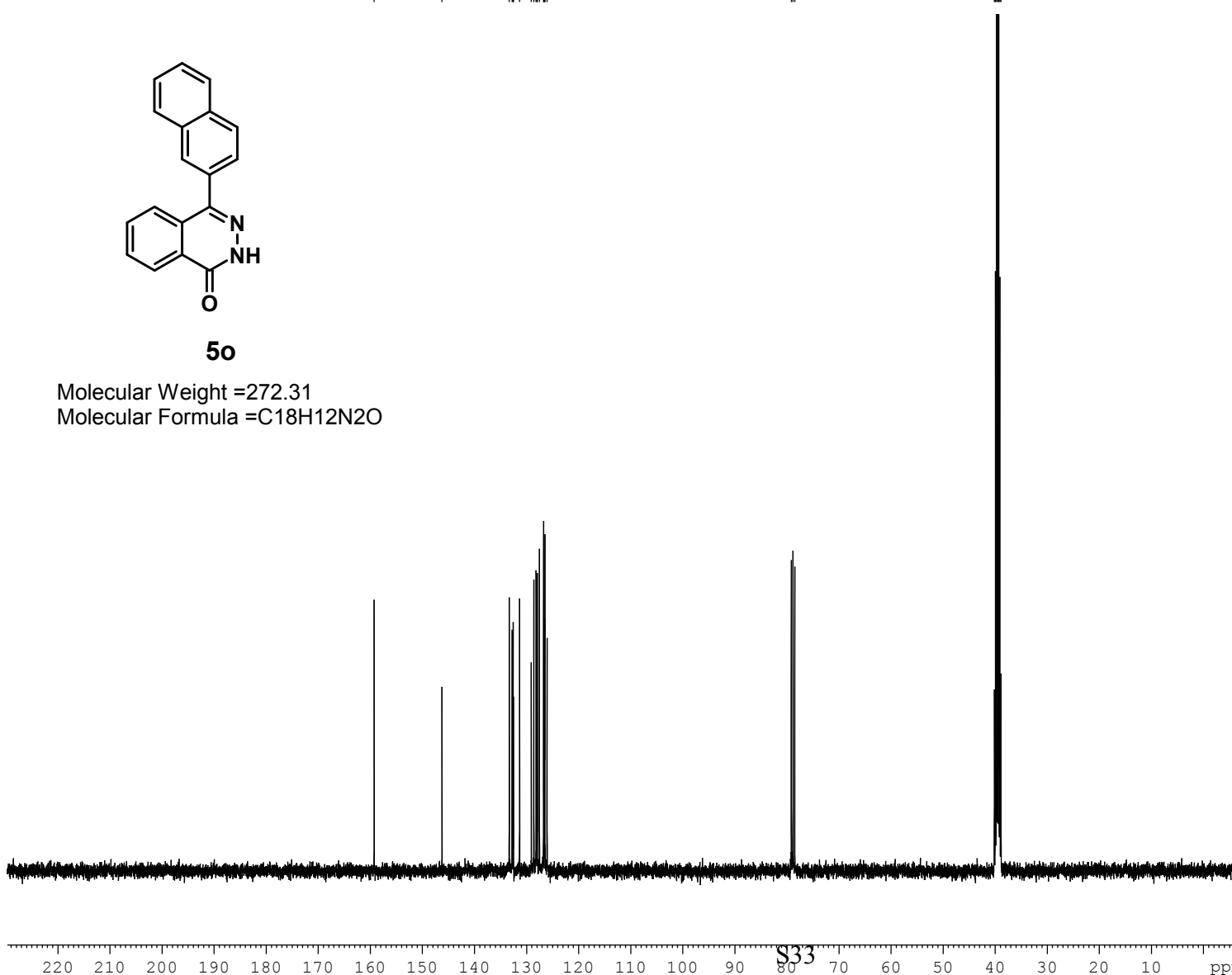
5o

Molecular Weight =272.31
Molecular Formula =C18H12N2O

159.28
146.25
133.33
132.78
132.58
132.51
131.34
129.10
128.60
128.17
127.99
127.93
127.54
126.74
126.71
126.52
126.48
126.06

79.16
78.83
78.50

40.15
39.94
39.74
39.53
39.32
39.11
38.90



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Current Data Parameters
NAME Jan01-2015
EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 13.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 400
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 912
DW 16.800 usec
DE 6.00 usec
TE 293.5 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TDO 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

avtar_saifpu@yahoo.co.in

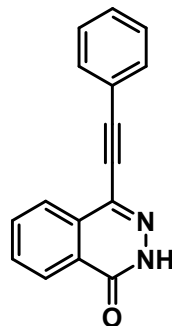
BRUKER
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 Spectrometer
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Current Data Parameters
 NAME Jan01-2015
 EXPNO 60
 PROCNO 1

F2 - Acquisition Parameters
 Date 20150101
 Time 14.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 512
 DW 41.600 usec
 DE 6.00 usec
 TE 293.2 K
 D1 1.0000000 sec
 TD0 1

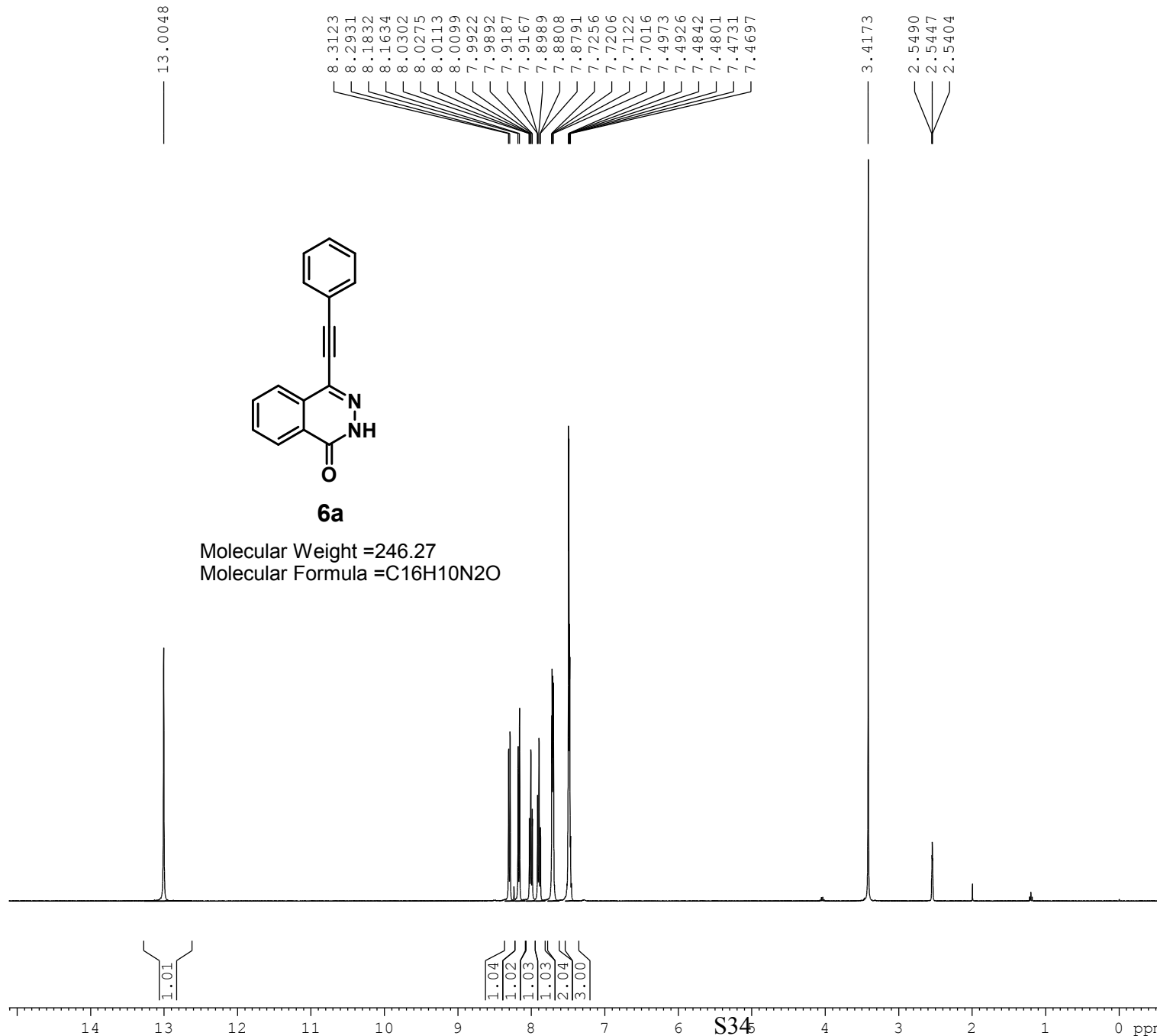
==== CHANNEL f1 =====
 NUC1 1H
 P1 10.90 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1299856 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

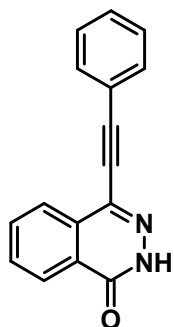


6a

Molecular Weight =246.27
 Molecular Formula =C16H10N2O

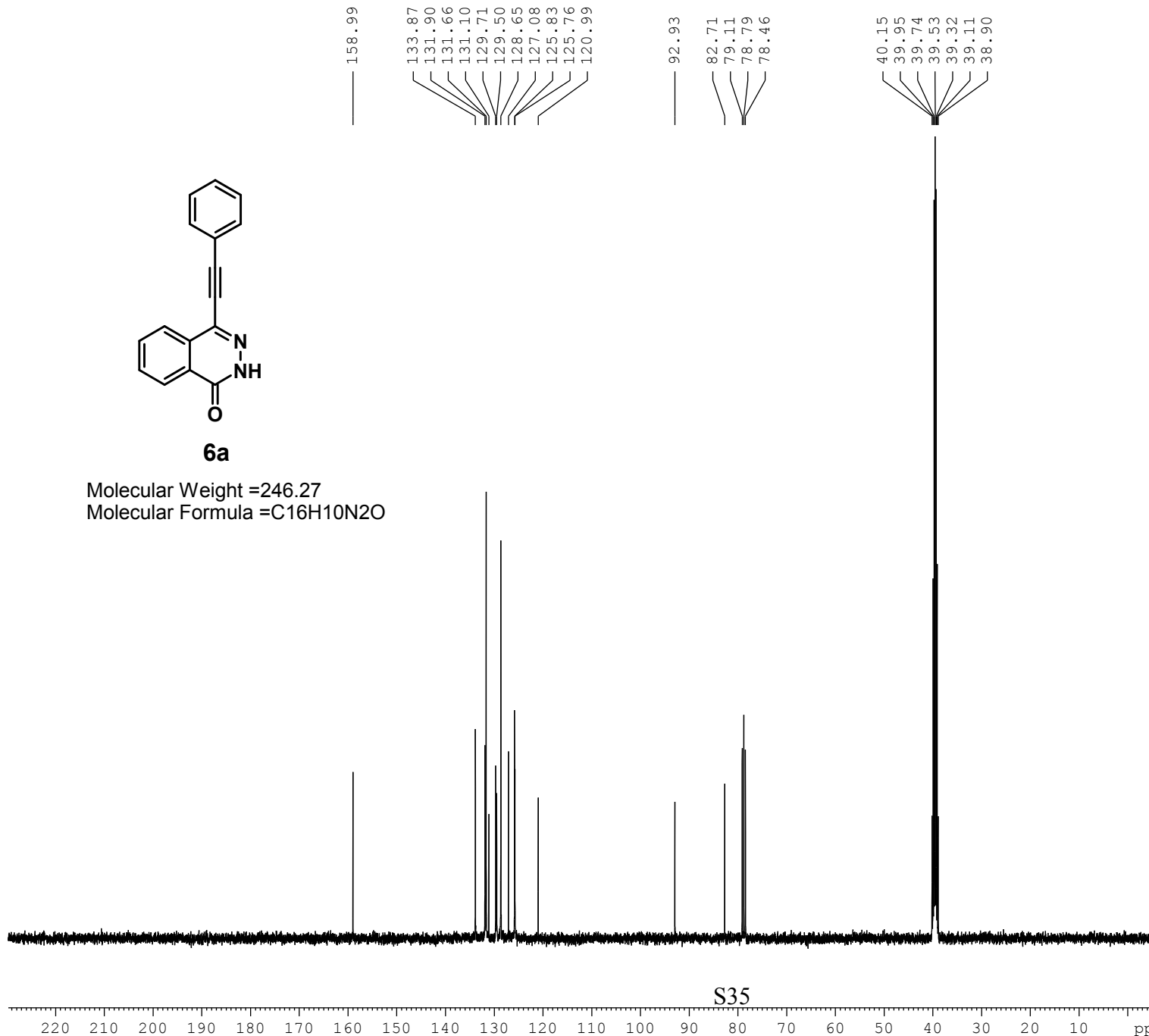


SRD-P



6a

Molecular Weight = 246.27
Molecular Formula = C₁₆H₁₀N₂O



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Current Data Parameters
NAME Jan01-2015
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 14.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 244
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 912
DW 16.800 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

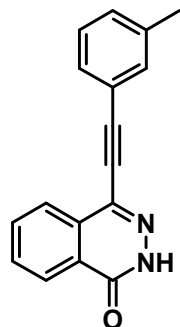
==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

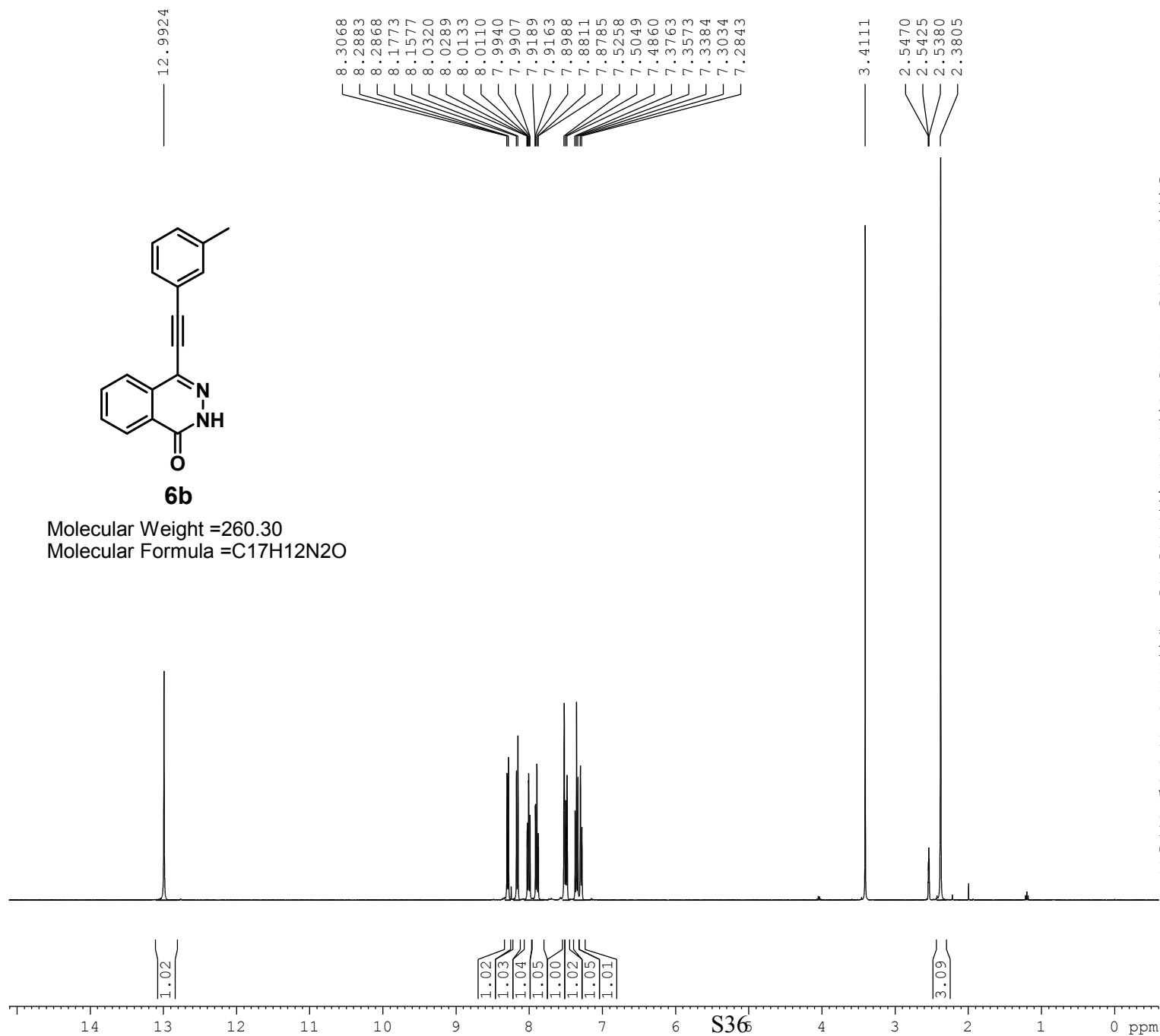
avtar_saifpu@yahoo.co.in

SRD-W



6b

Molecular Weight =260.30
Molecular Formula =C17H12N2O



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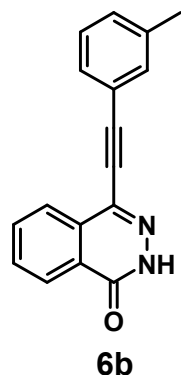
Current Data Parameters
NAME Jan01-2015
EXPNO 130
PROCNO 1

F2 - Acquisition Parameters
Date 20150101
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 406
DW 41.600 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

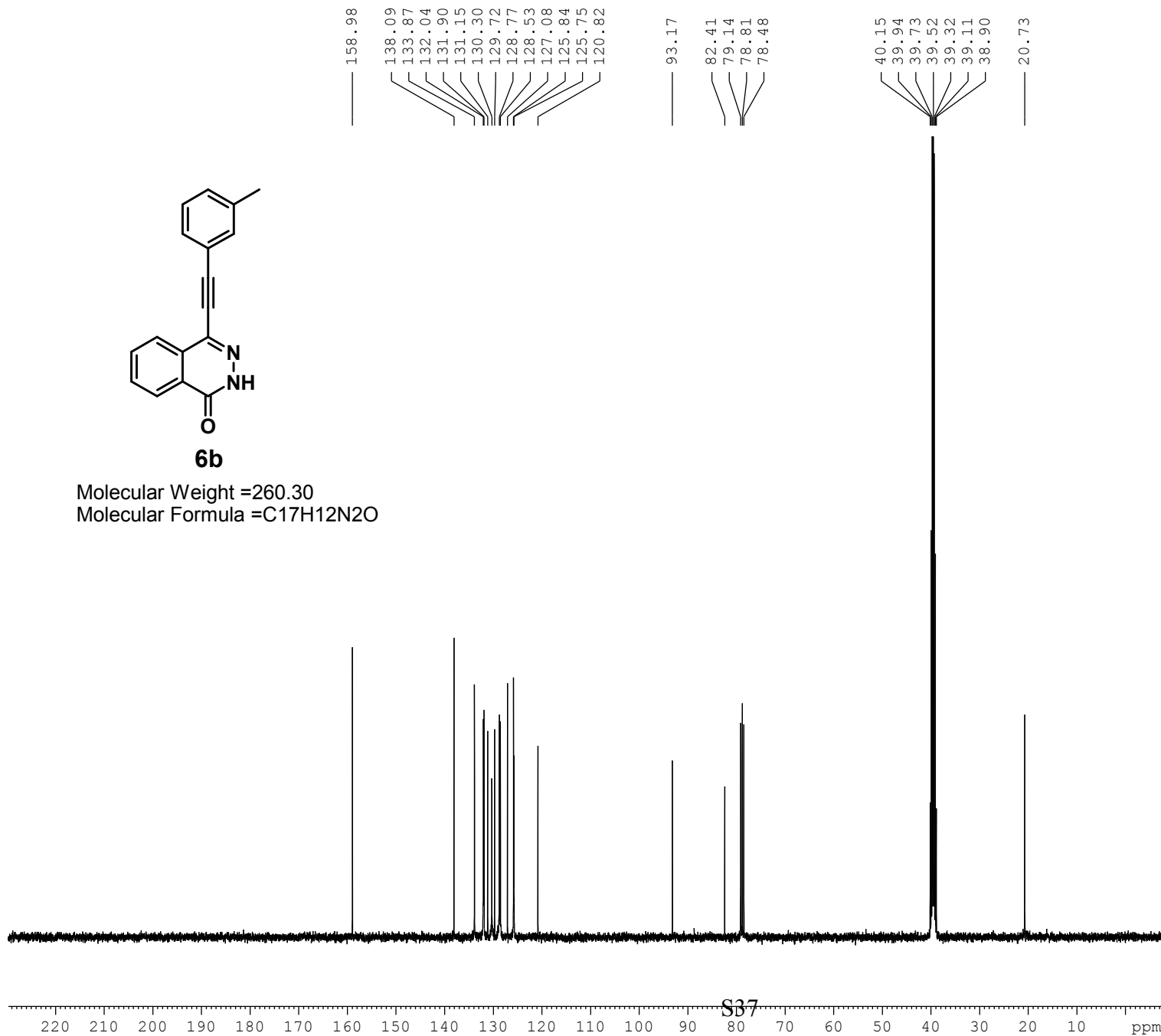
==== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299864 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

SRD-W



Molecular Weight =260.30
Molecular Formula =C₁₇H₁₂N₂O



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Current Data Parameters
NAME Jan01-2015
EXPNO 131
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 293.6 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

avtar_saifpu@yahoo.co.in

SRD-X

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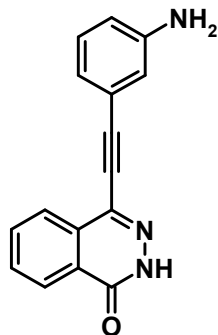
Current Data Parameters
NAME Jan01-2015
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150101
Time_ 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 575
DW 41.600 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

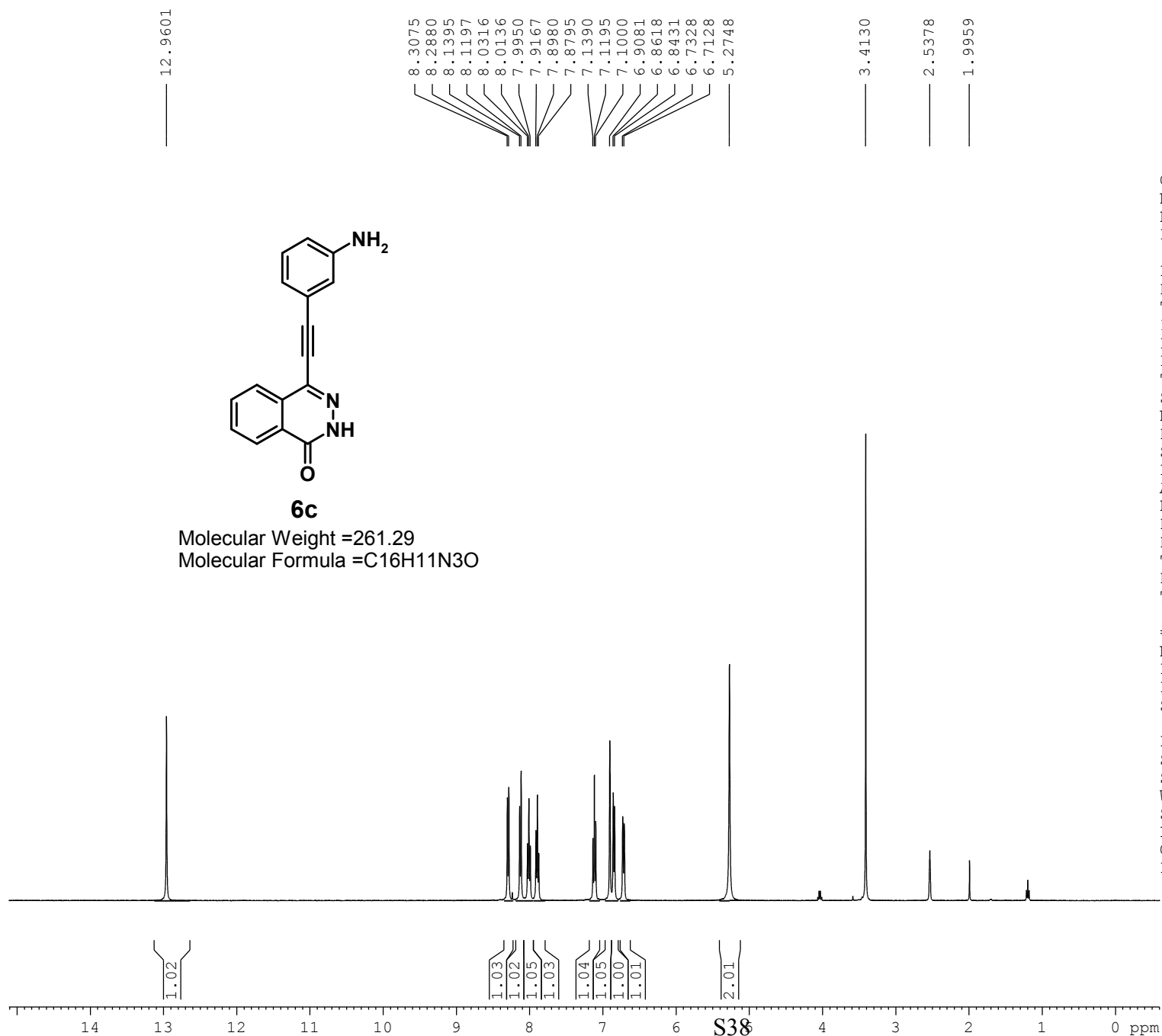
==== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

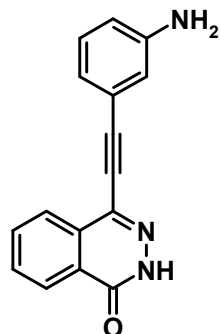


6c

Molecular Weight =261.29
Molecular Formula =C₁₆H₁₁N₃O

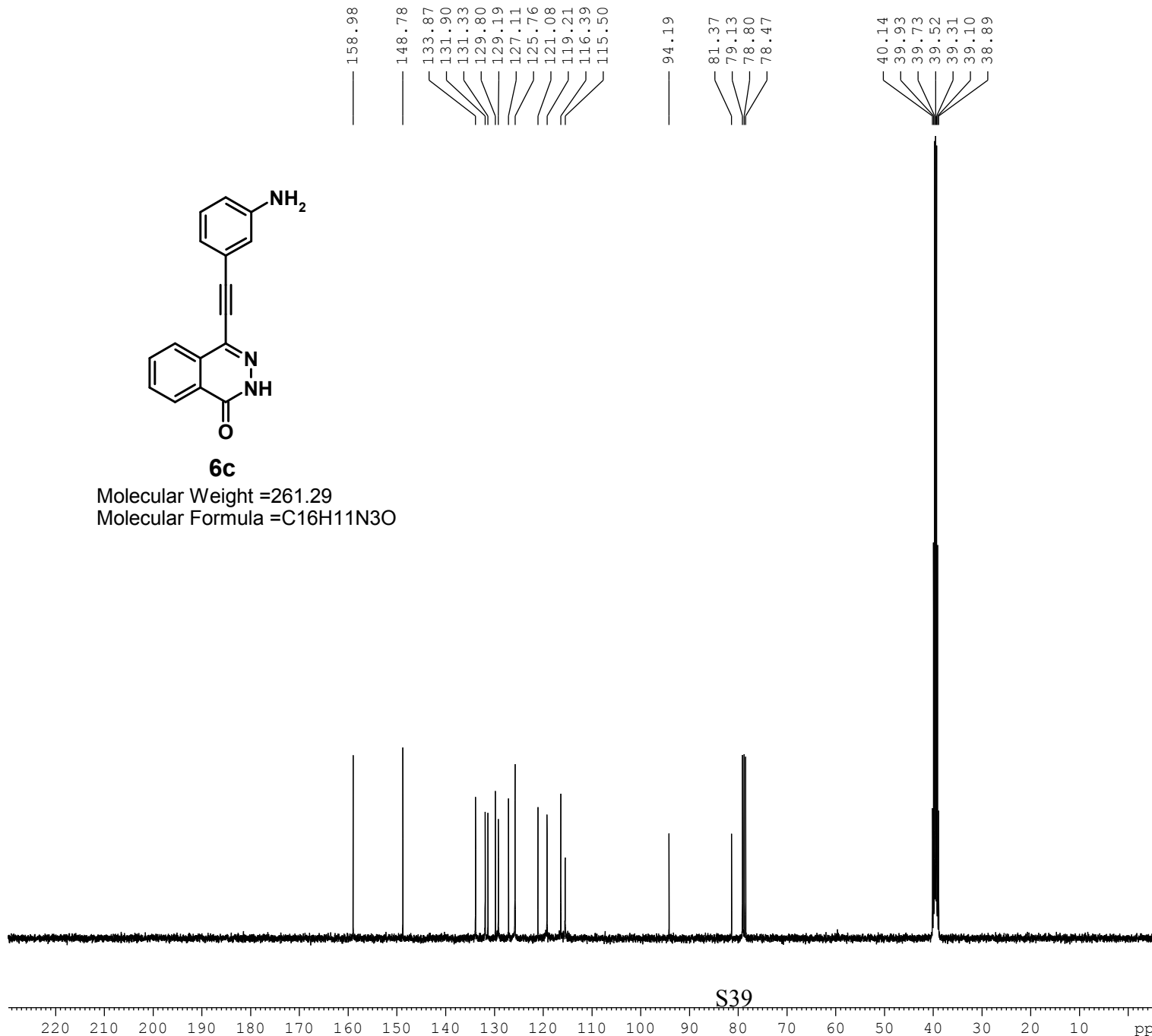


SRD-X



6c

Molecular Weight =261.29
Molecular Formula =C16H11N3O



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Current Data Parameters
NAME Jan01-2015
EXPNO 121
PROCNO 1

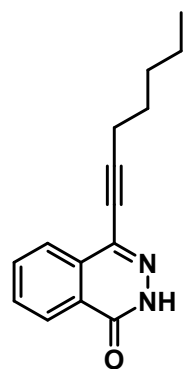
F2 - Acquisition Parameters
Date 20150101
Time 17.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 912
DW 16.800 usec
DE 6.00 usec
TE 293.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SRD-S



6d

Molecular Weight =240.31
Molecular Formula =C₁₅H₁₆N₂O

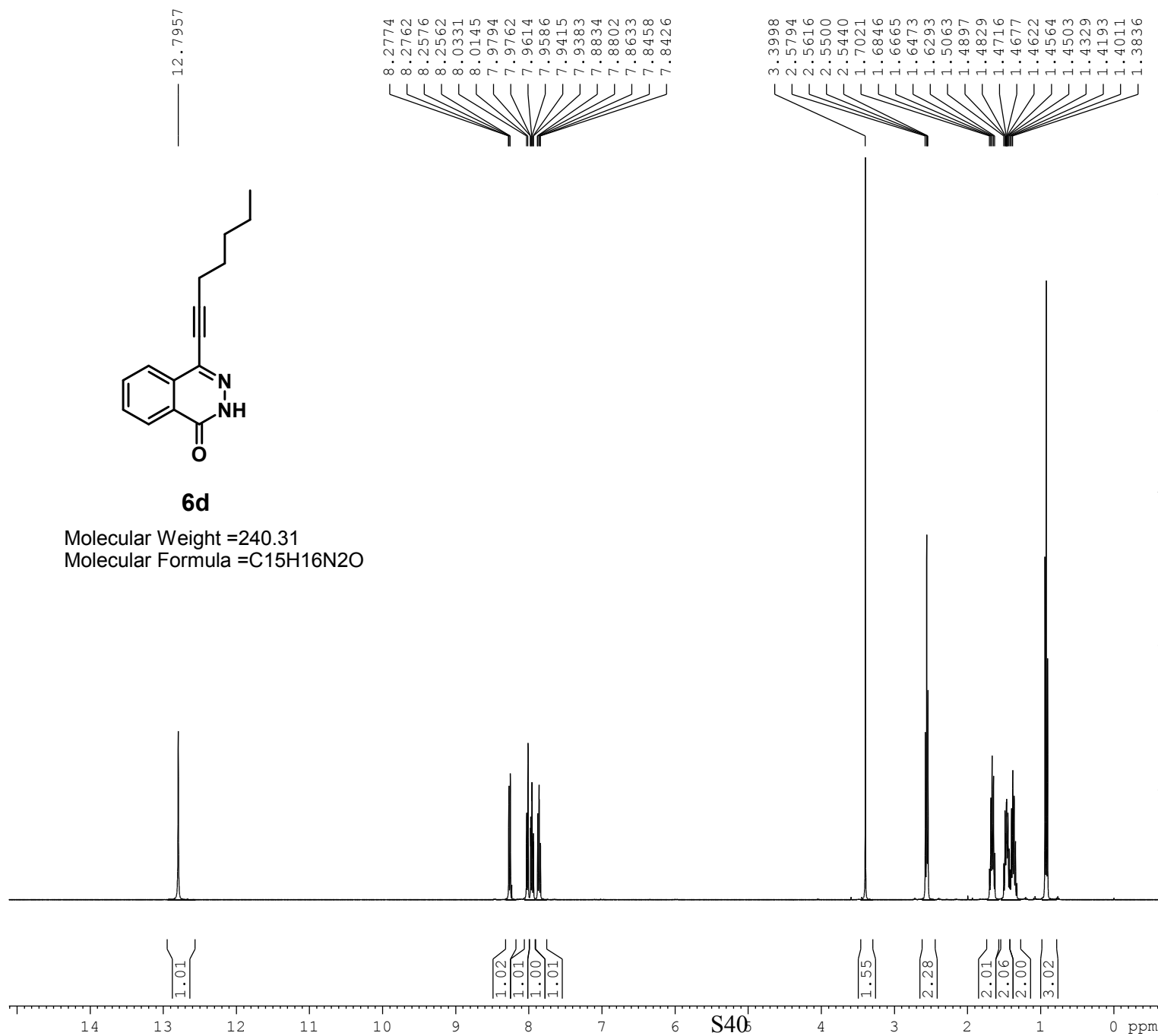
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Current Data Parameters
NAME Jan01-2015
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 15.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 362
DW 41.600 usec
DE 6.00 usec
TE 293.4 K
D1 1.0000000 sec
TD0 1

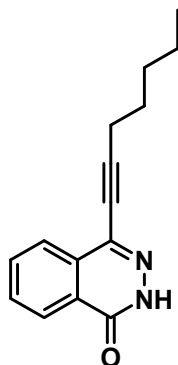
==== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299851 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



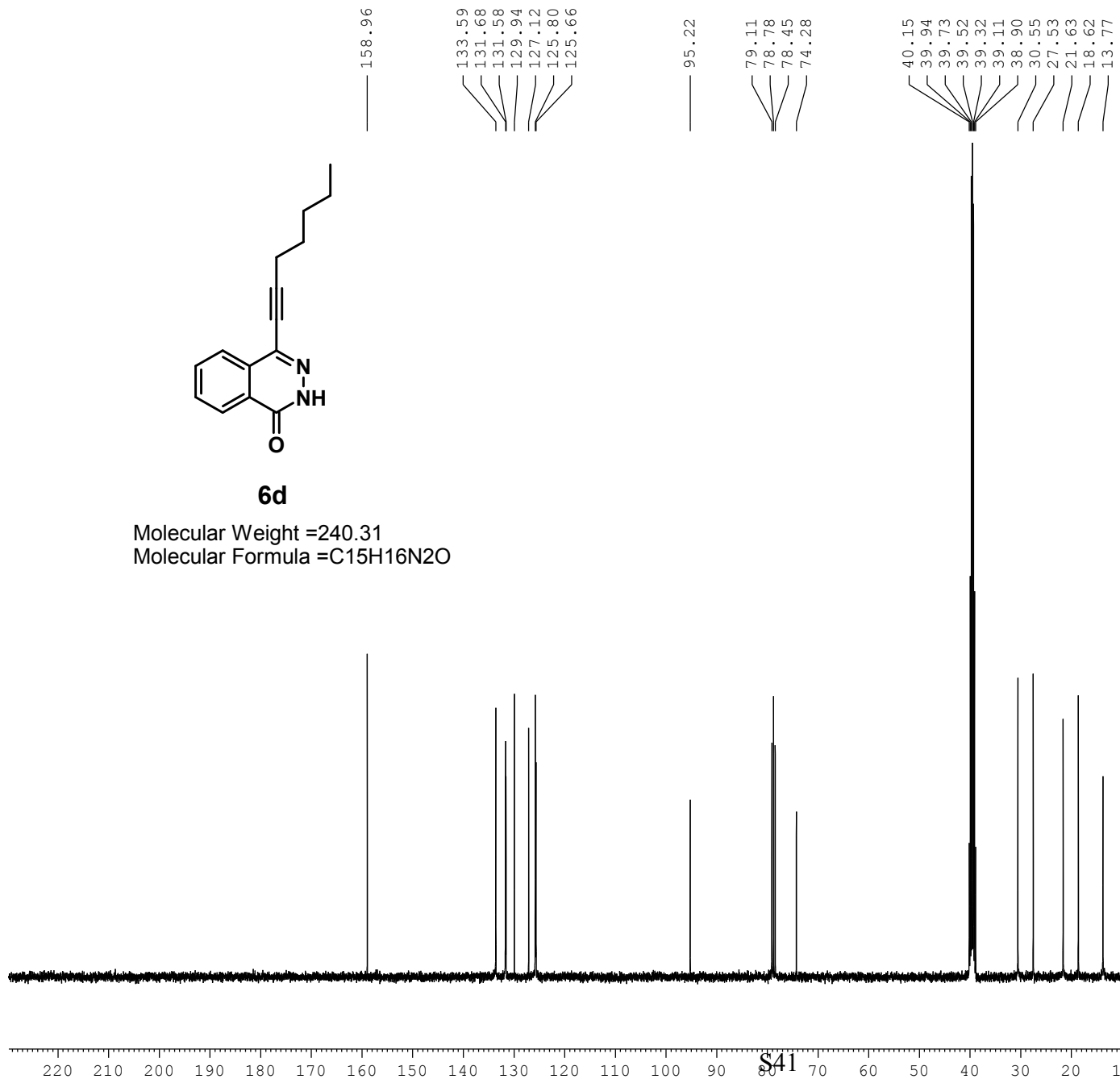
SRD-S

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6d

Molecular Weight =240.31
Molecular Formula =C₁₅H₁₆N₂O



Current Data Parameters
NAME Jan01-2015
EXPNO 91
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 293.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

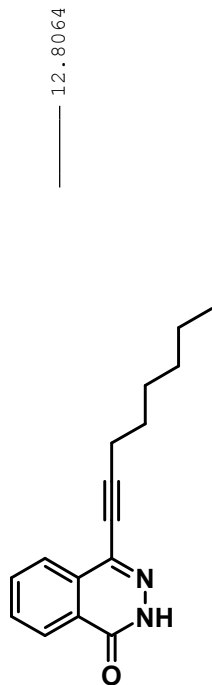
==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

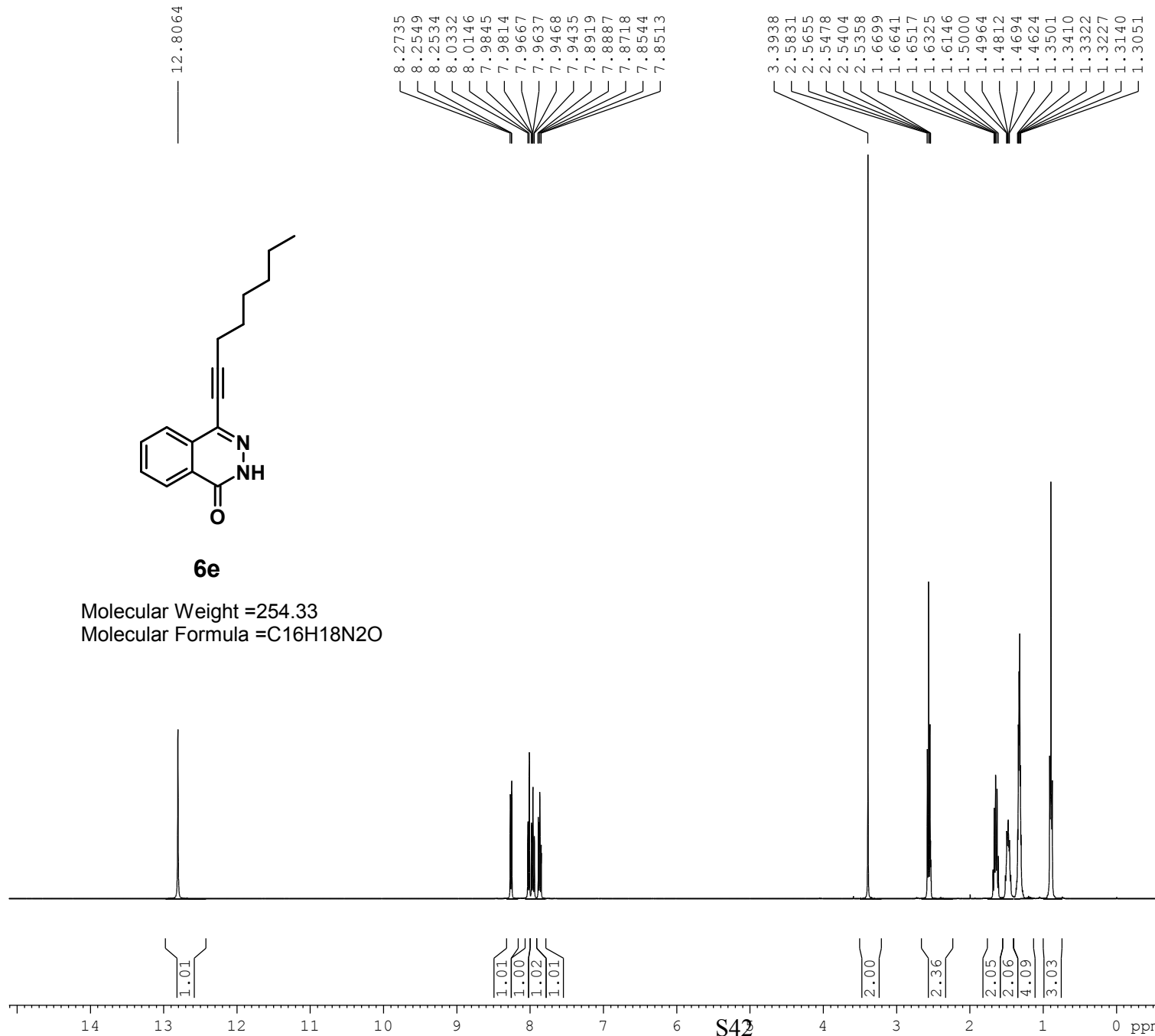
avtar_saifpu@yahoo.co.in

SRD-R



6e

Molecular Weight =254.33
Molecular Formula =C₁₆H₁₈N₂O



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Current Data Parameters
NAME Jan01-2015
EXPNO 80
PROCNO 1

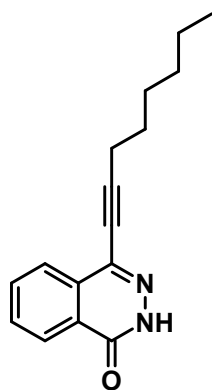
F2 - Acquisition Parameters
Date_ 20150101
Time_ 14.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 144
DW 41.600 usec
DE 6.00 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1299874 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

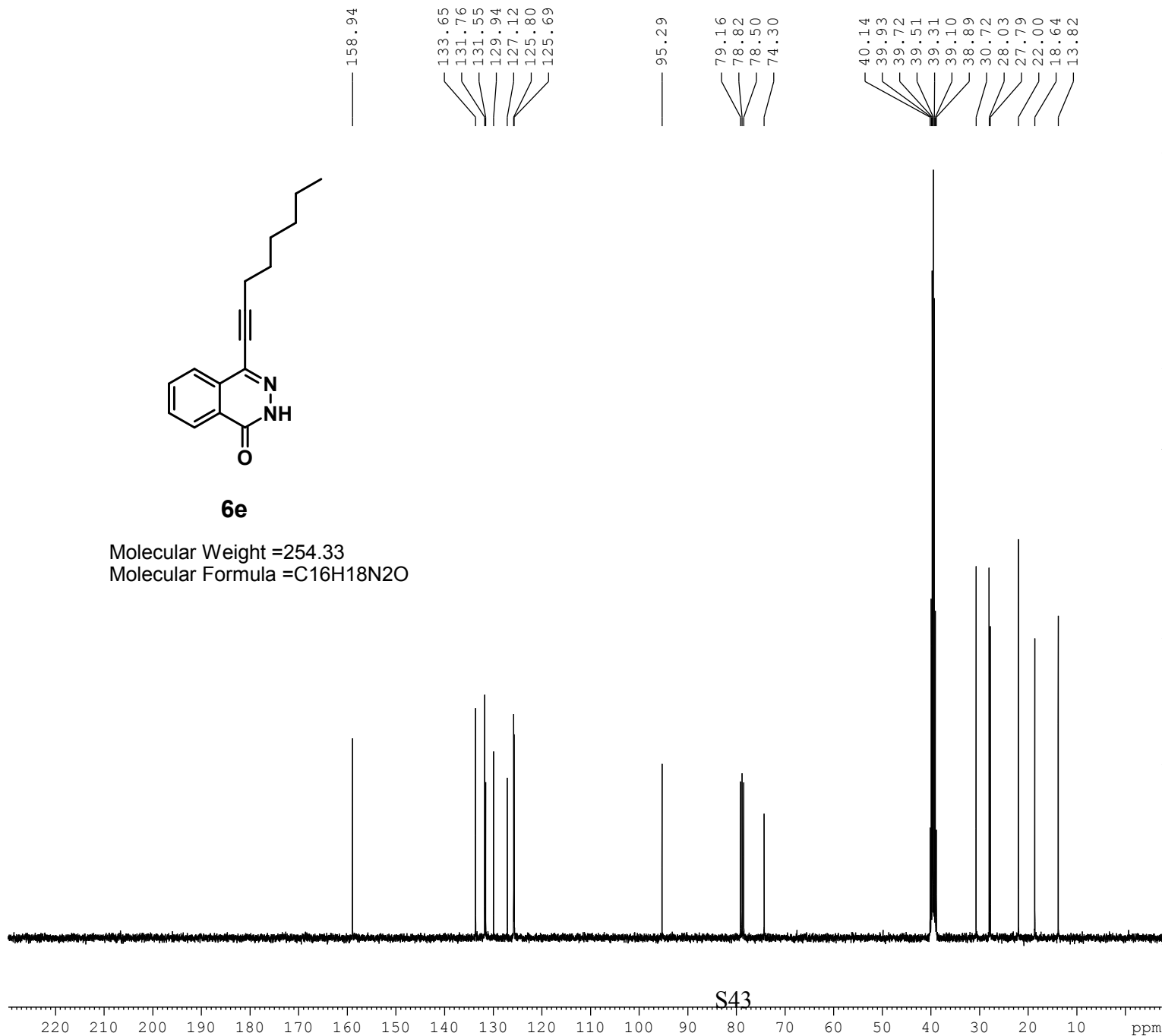
SRD-R

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6e

Molecular Weight =254.33
Molecular Formula =C16H18N2O



Current Data Parameters
NAME Jan01-2015
EXPNO 81
PROCNO 1

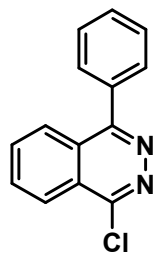
F2 - Acquisition Parameters
Date_ 20150101
Time_ 15.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 418
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 293.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

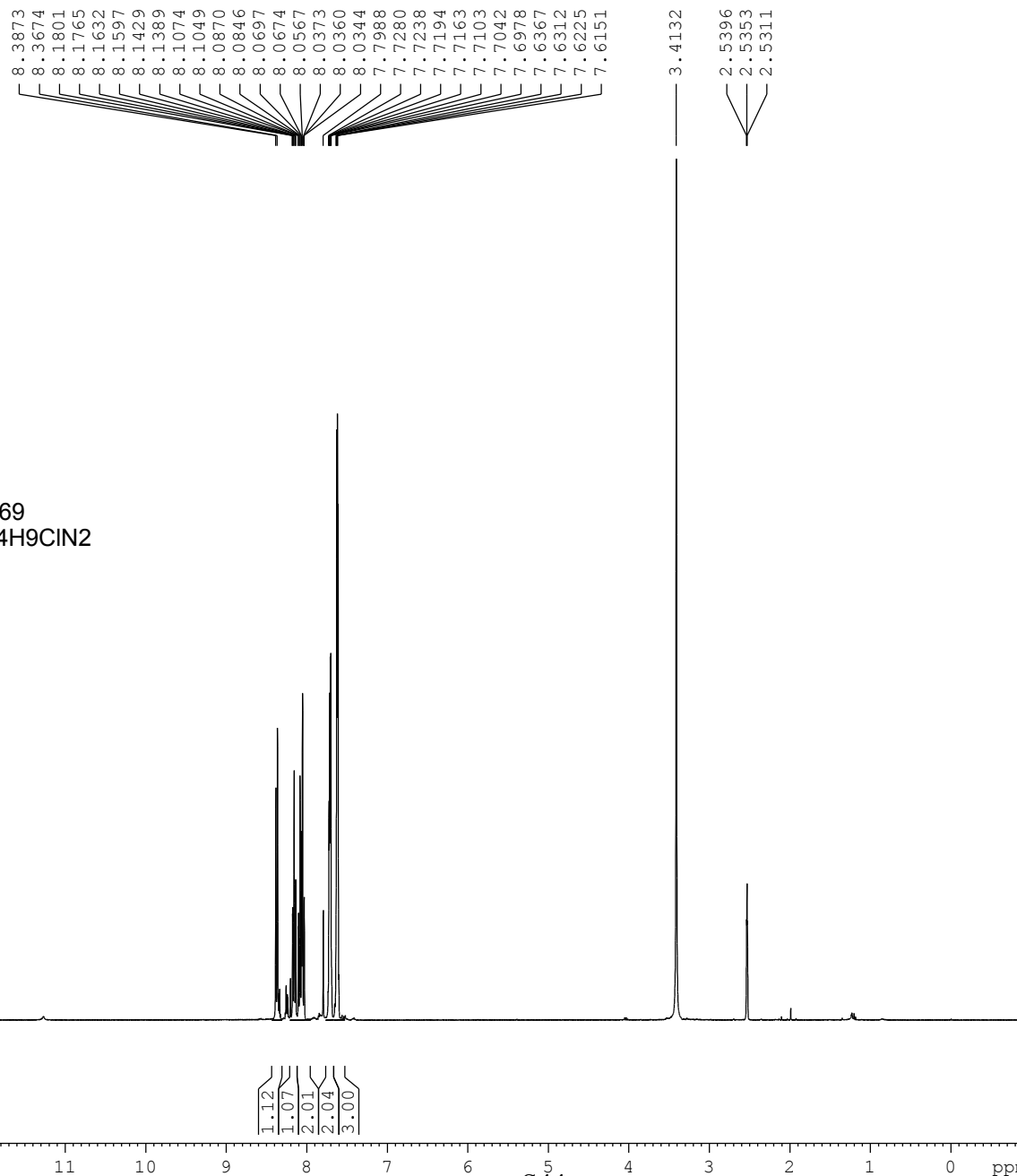
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

avtar_saifpu@yahoo.co.in



7a

Molecular Weight =240.69
 Molecular Formula =C₁₄H₉ClN₂



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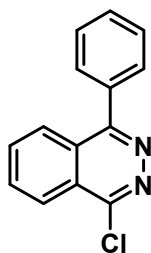
Current Data Parameters
 NAME Nov29-2014
 EXPNO 260
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141130
 Time_ 5.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 456
 DW 41.600 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

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

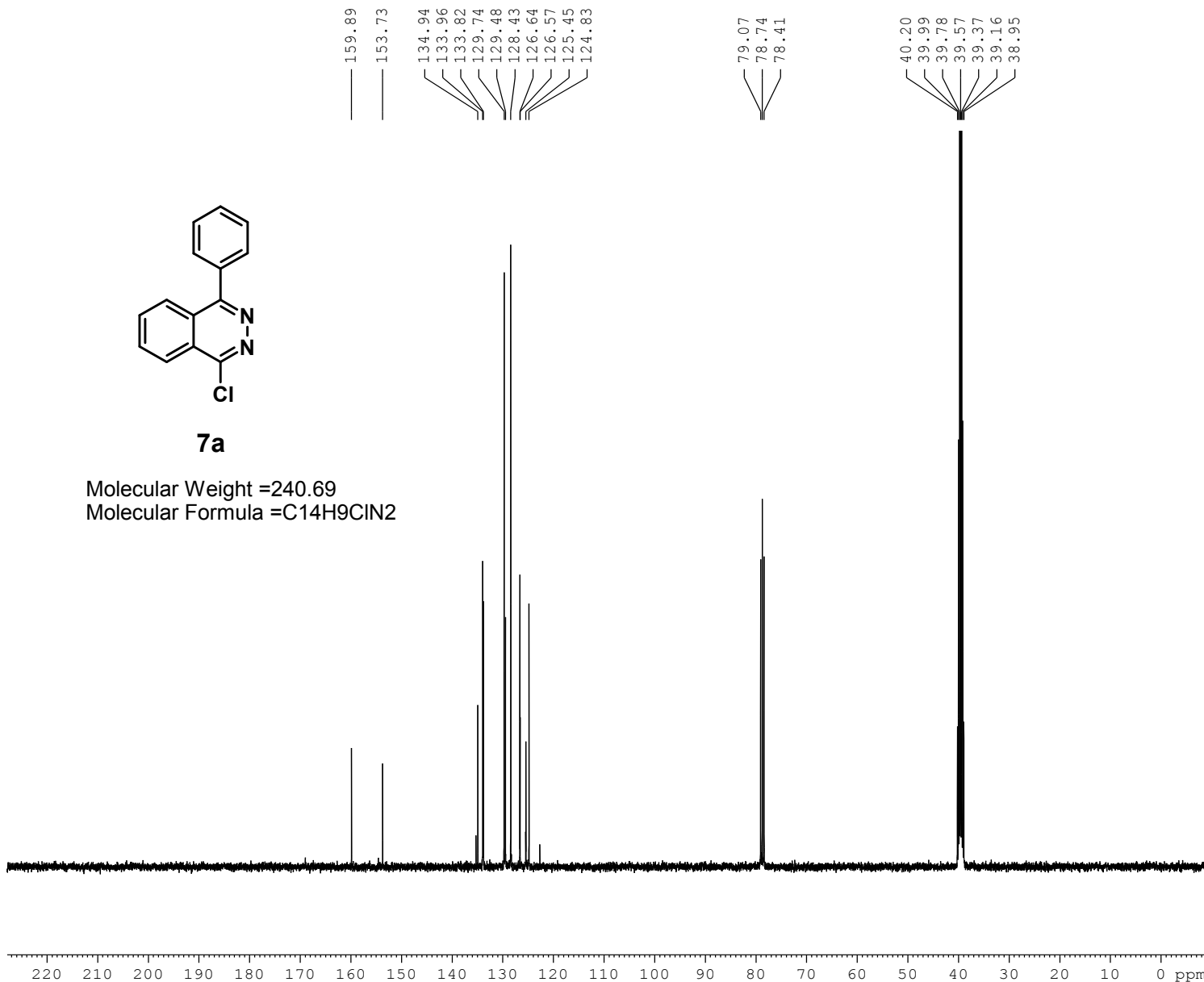
F2 - Processing parameters
 SI 32768
 SF 400.1299896 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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7a

Molecular Weight =240.69
Molecular Formula =C14H9ClN2



Current Data Parameters
NAME Nov29-2014
EXPNO 261
PROCNO 1

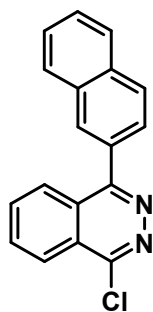
F2 - Acquisition Parameters
Date_ 20141130
Time 6.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

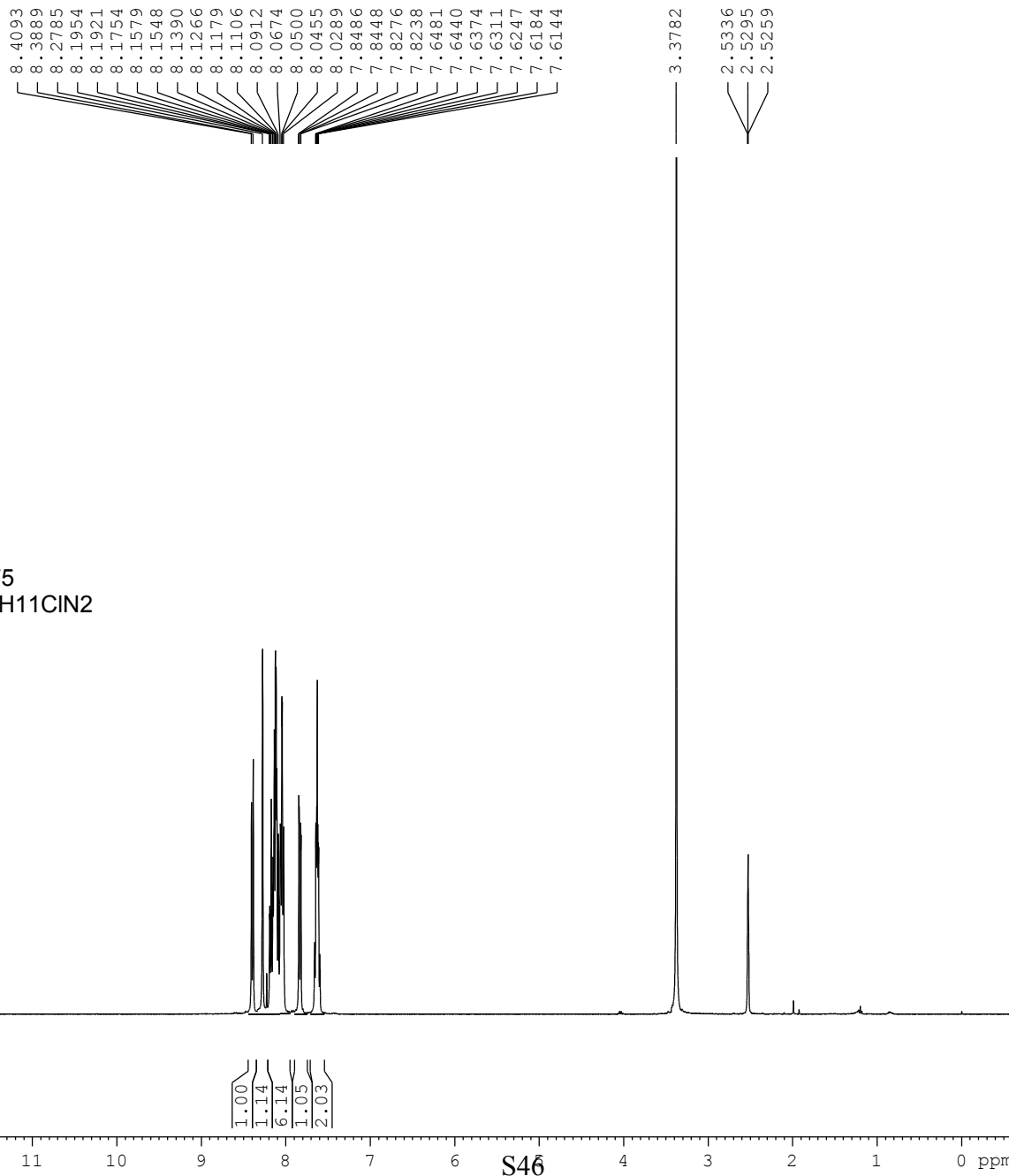
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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7b

Molecular Weight =290.75
 Molecular Formula =C18H11ClN2



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Current Data Parameters
 NAME Jan01-2015
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150101
 Time 14.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 287
 DW 41.600 usec
 DE 6.00 usec
 TE 293.2 K
 D1 1.00000000 sec
 TD0 1

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

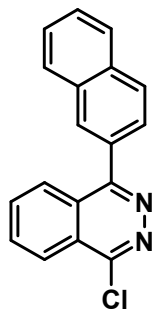
F2 - Processing parameters
 SI 32768
 SF 400.1299917 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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159.89
153.75
134.10
133.90
133.11
132.45
132.38
129.65
128.38
128.08
127.58
127.13
126.94
126.81
126.69
126.65
125.47
124.88

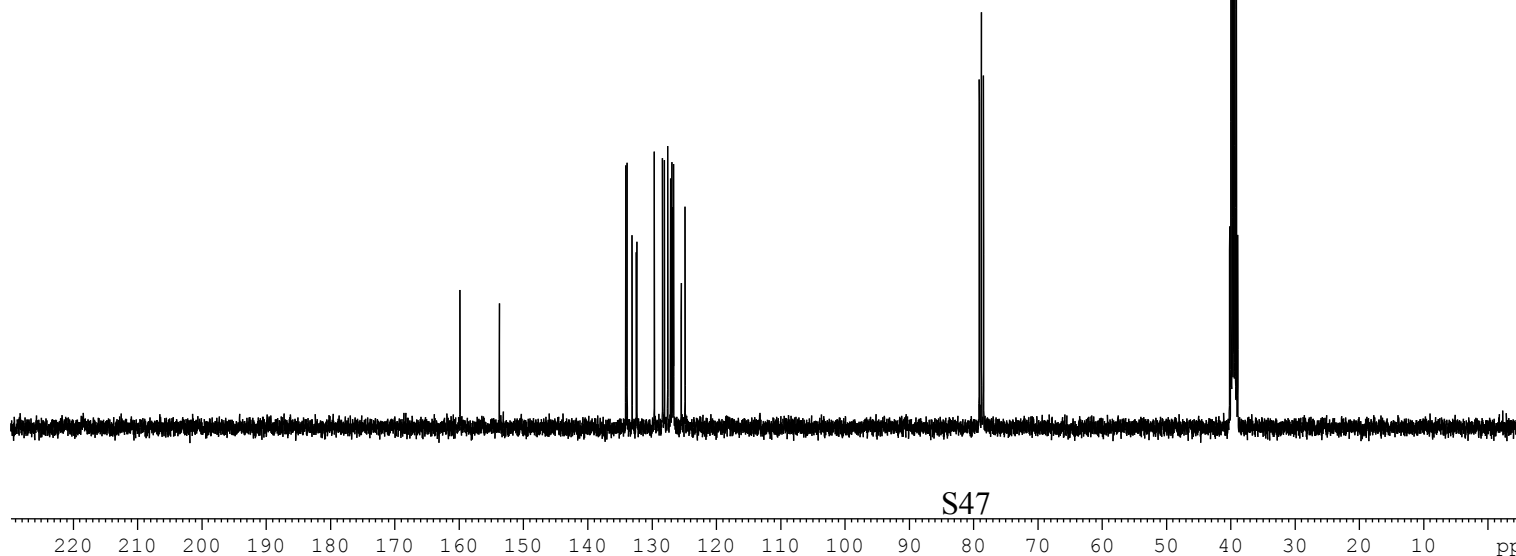
79.12
78.79
78.46

40.18
39.97
39.76
39.55
39.34
39.13
38.93



7b

Molecular Weight =290.75
Molecular Formula =C18H11ClN2



Current Data Parameters
NAME Jan01-2015
EXPNO 71
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time_ 14.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 308
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 293.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

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

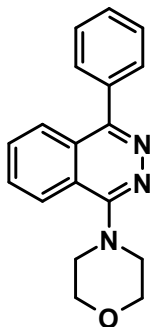
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SRD-K

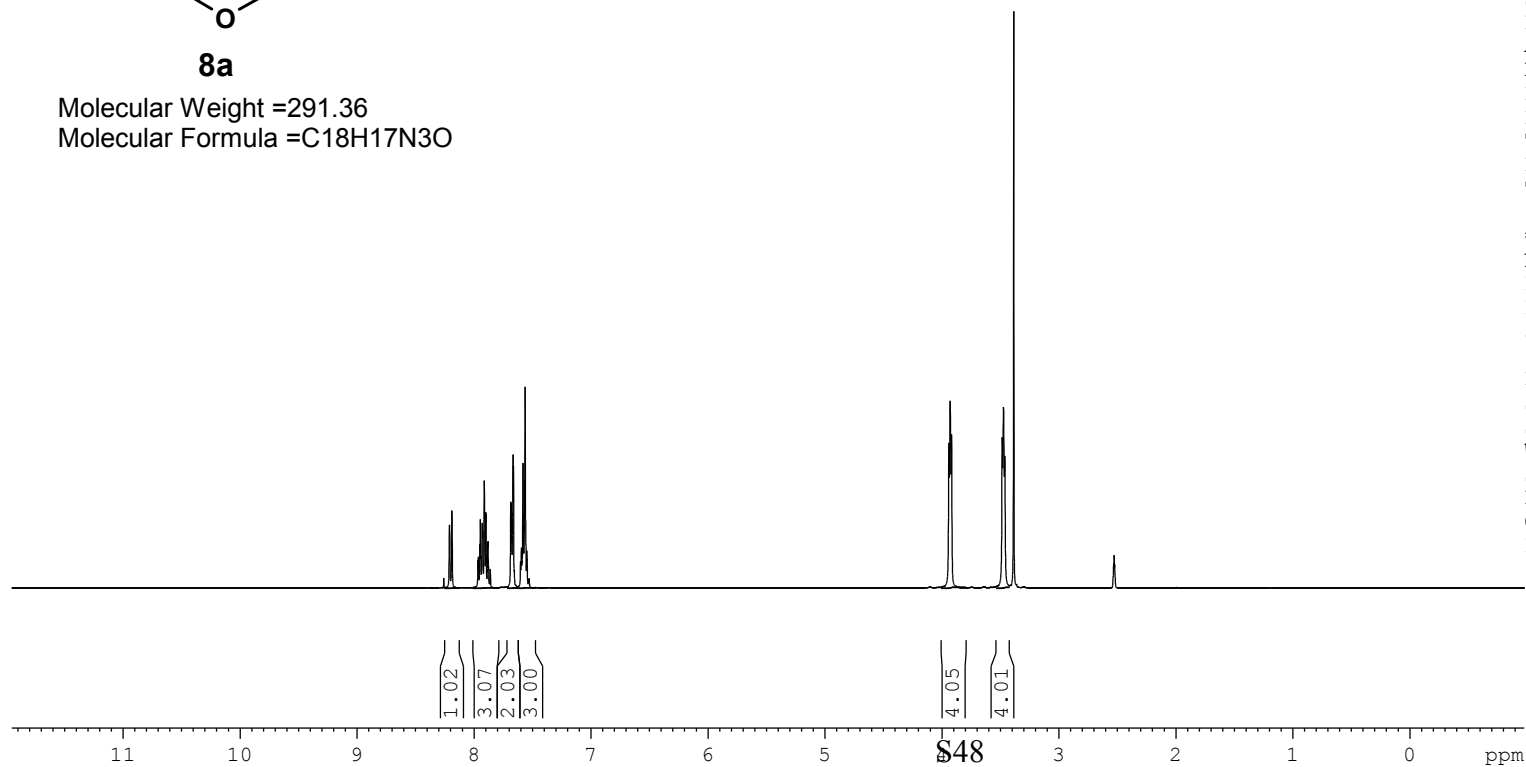
8.2117
8.1914
7.9689
7.9646
7.9525
7.9485
7.9443
7.9323
7.9283
7.9150
7.9019
7.8992
7.8856
7.8827
7.8784
7.6882
7.6837
7.6684
7.6647
7.6053
7.6008
7.5976
7.5931
7.5834
7.5698
7.5653
7.5515
7.5487

3.9428
3.9320
3.9201
3.4866
3.4752
3.4641
3.3885
2.5336
2.5292
2.5247



8a

Molecular Weight =291.36
Molecular Formula =C₁₈H₁₇N₃O



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Current Data Parameters
NAME Jan01-2015
EXPNO 10
PROCNO 1

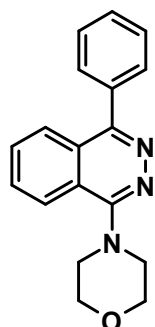
F2 - Acquisition Parameters
Date_ 20150101
Time_ 11.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 292.5 K
D1 1.0000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1299918 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

SRD-K

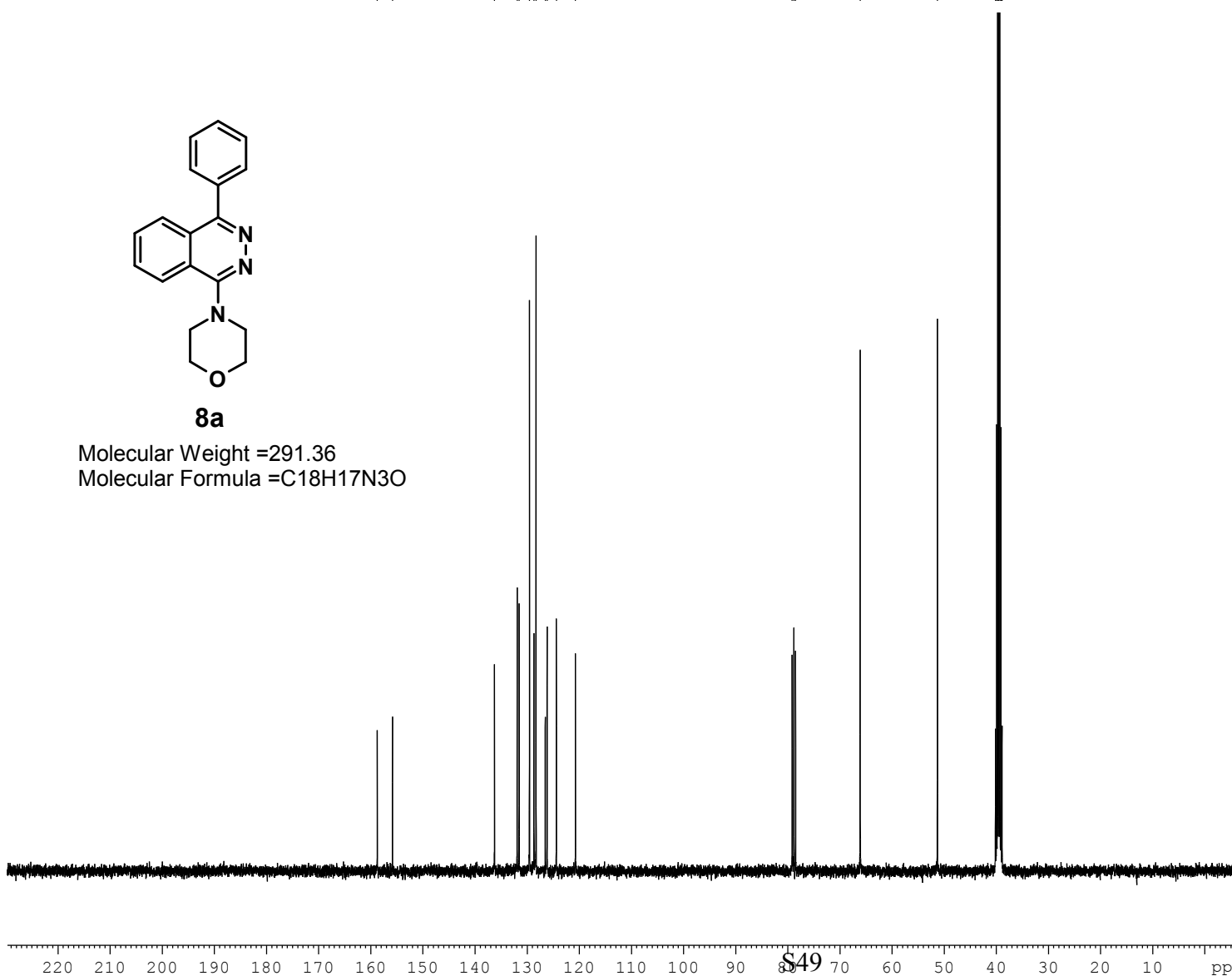
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8a

Molecular Weight =291.36
Molecular Formula =C18H17N3O

158.76	136.27	79.17	66.12	51.30
155.84	131.92	78.84		40.16
	131.55	78.51		39.95
	129.56			39.74
	128.70			39.53
	128.30			39.32
	126.54			39.11
	126.18			38.90
	124.40			
	120.75			



```

Current Data Parameters
NAME          Jan01-2015
EXPNO         11
PROCNO        1

F2 - Acquisition Parameters
Date_         20150101
Time          11.37
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            348
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            724
DW            16.800 usec
DE            6.00 usec
TE            293.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

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

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

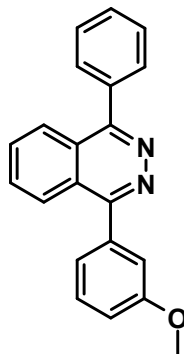
F2 - Processing parameters
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

SRD-Y
 PROTON_DepttChem DMSO {D:\AHMEDNAGAR} root 28

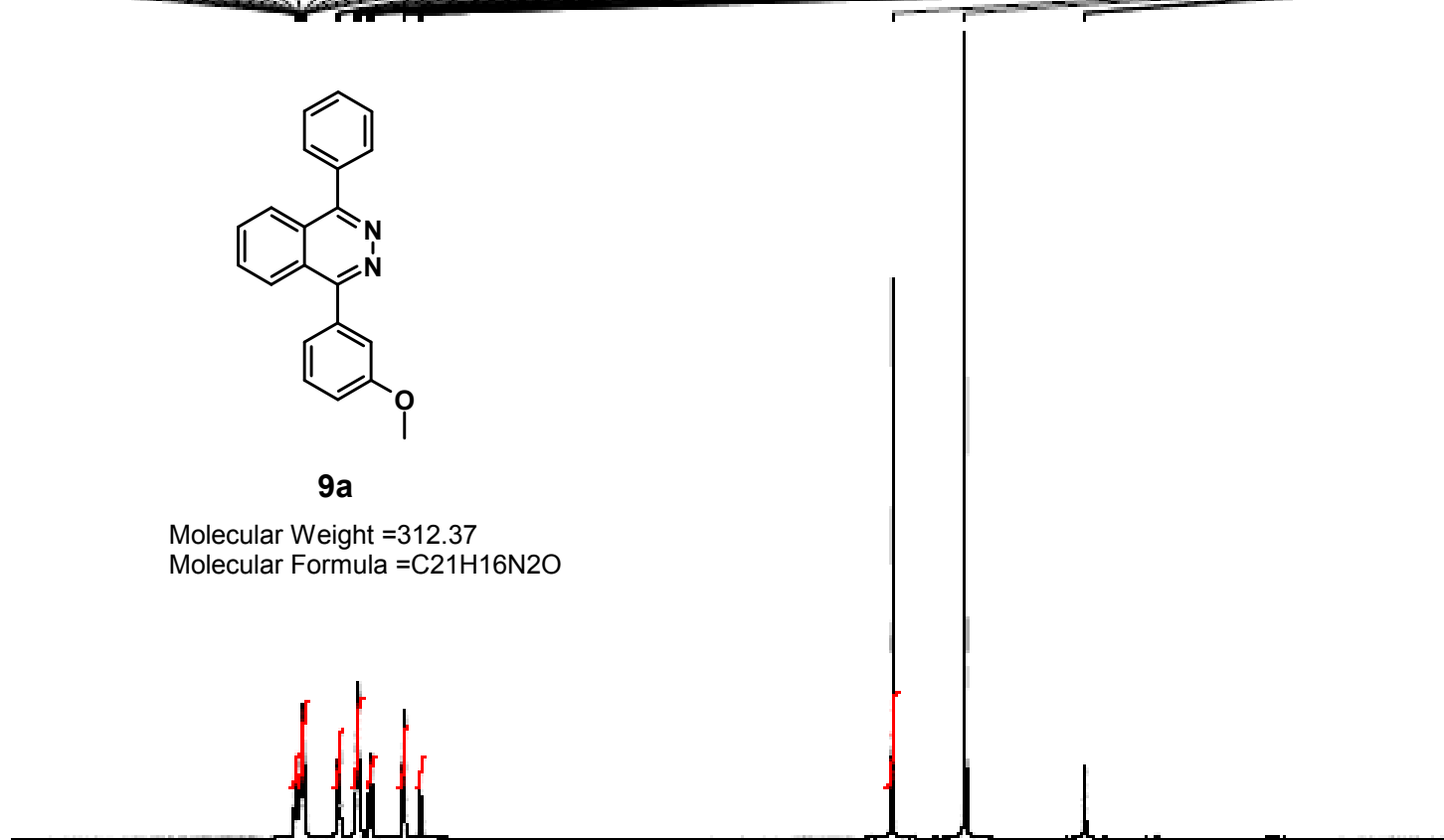


8.090
 8.084
 8.081
 8.076
 8.072
 8.064
 8.058
 8.055
 8.051
 8.045
 8.038
 8.033
 8.026
 8.021
 8.014
 7.787
 7.782
 7.771
 7.768
 7.668
 7.665
 7.661
 7.657
 7.650
 7.638
 7.636
 7.629
 7.625
 7.589
 7.581
 7.553
 7.537
 7.327
 7.326
 7.323
 7.319
 7.318
 7.315
 7.204
 7.200
 7.189
 7.187
 7.184
 3.859
 3.345
 2.503
 2.500
 2.496



9a

Molecular Weight = 312.37
 Molecular Formula = C₂₁H₁₆N₂O



1.17
 2.76
 1.88
 2.86
 1.02
 1.96
 0.98

3.00

Current Data Parameters
 NAME Dec31-2014
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141231
 Time_ 18.53
 INSTRUM spect
 PROBNM 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 96
 DW 50.000 usec
 DE 6.50 usec
 TR 296.4 K
 D1 1.00000000 sec
 TDD 1

----- CHANNEL f1 -----
 SFO1 500.1320885 MHz
 NUQ1 1H
 P1 9.22 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300035 MHz
 MDW RM
 SGB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

SRD-Y
 C13CPD DMSO {D:\AHMEDNAGAR} root 2B



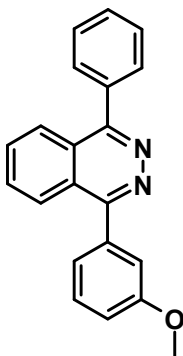
Current Data Parameters
 NAME Dec31-2014
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141231
 Time 17.03
 INSTRUM spect
 PROBRD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 800
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 189.76
 DW 16.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDD 1

===== CHANNEL F1 =====
 SFO1 125.7703637 MHz
 NUQ1 13C
 P1 9.25 usec
 PLW1 100.00000000 W

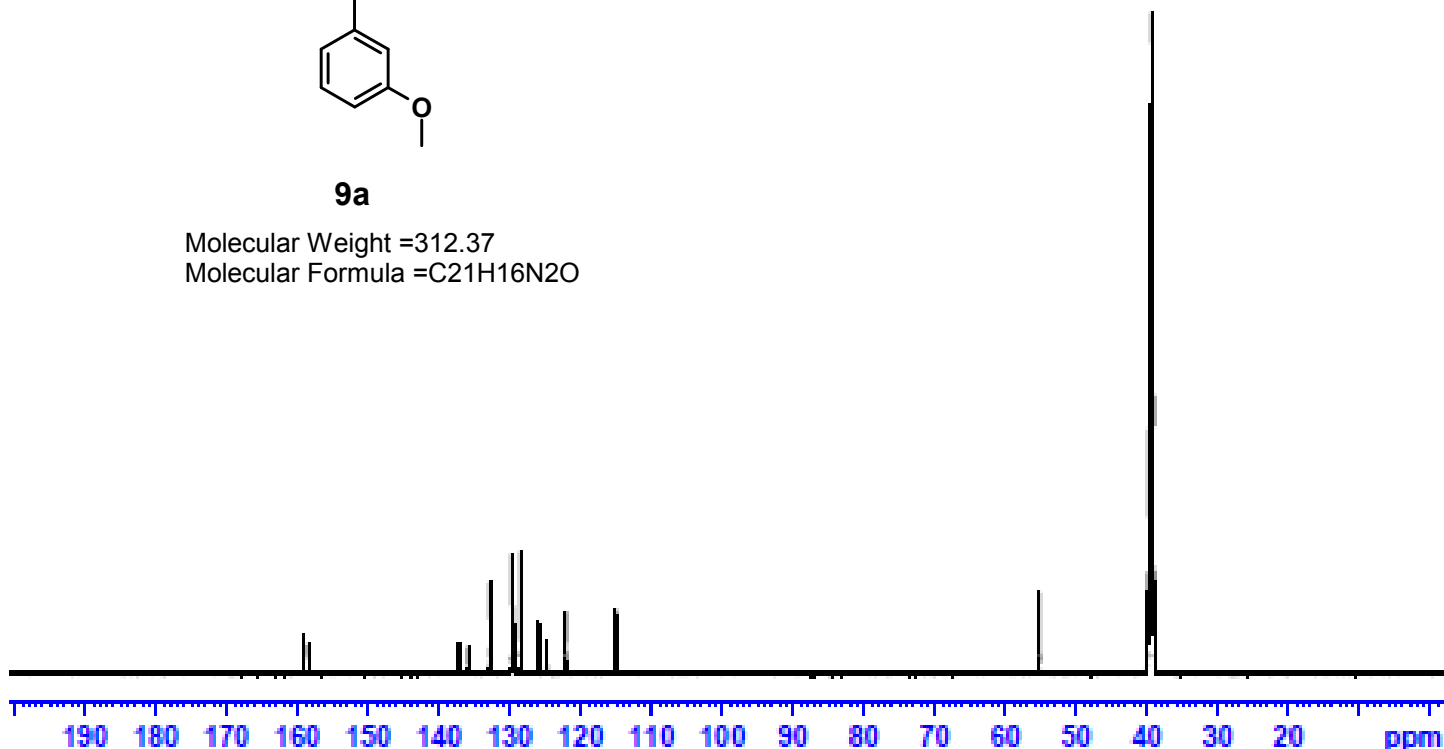
===== CHANNEL F2 =====
 SFO2 500.1320005 MHz
 NUQ2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 22.00000000 W
 PLW12 0.29222000 W
 PLW13 0.18702000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578569 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



9a

Molecular Weight =312.37
 Molecular Formula =C21H16N2O



SRD-AA
 PROTON_DepttChem DMSO {D:\AHMEDNAGAR} root 27

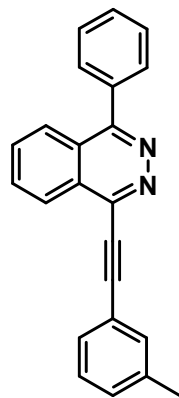
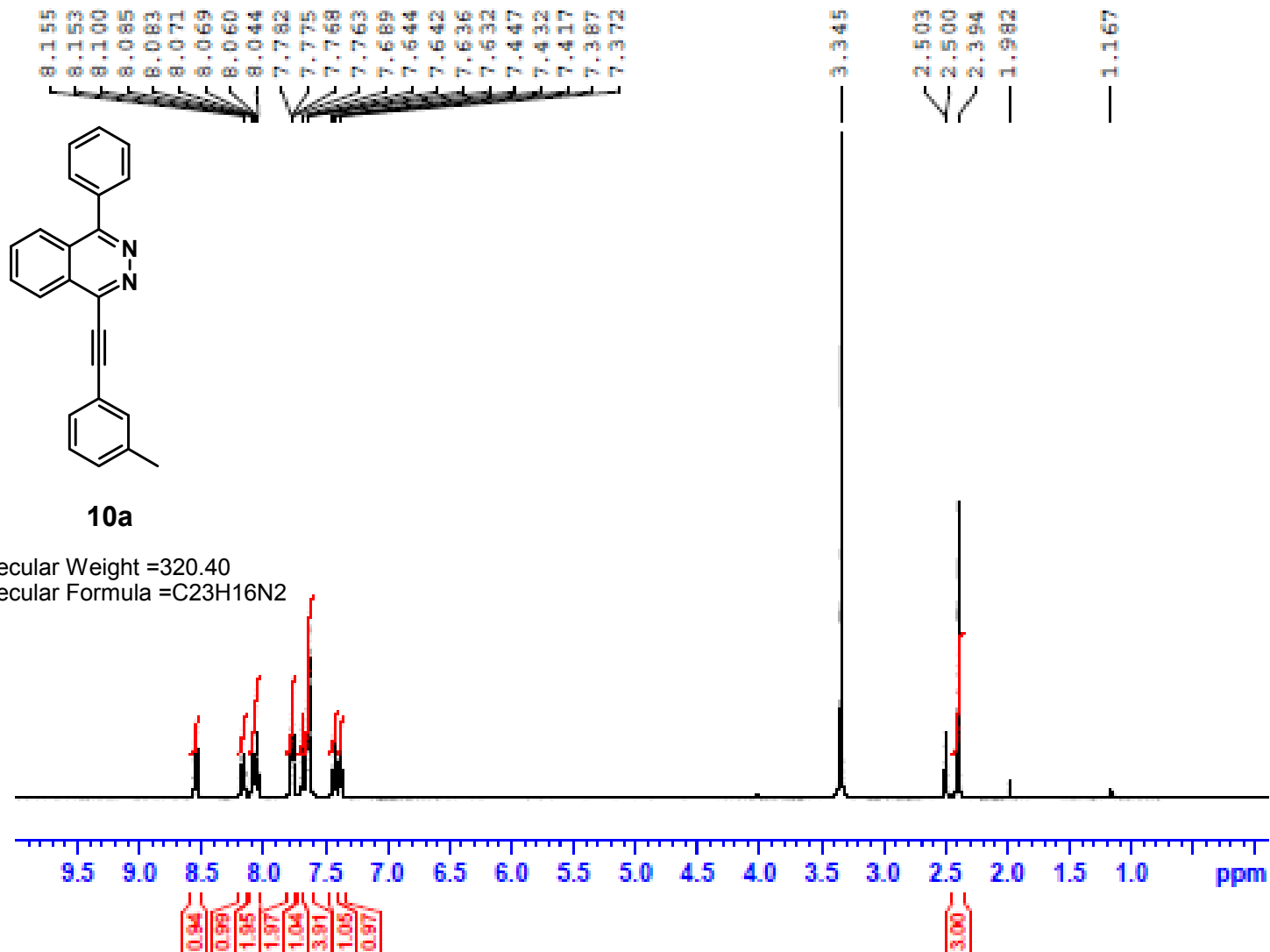


Current Data Parameters
 NAME Dec31-2014
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141231
 Time 18.48
 INSTRUM spect
 PROBP1 5 mm PABBO QNP/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 1.2787999 sec
 RG 96
 DW 50.000 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL F1 =====
 SFO1 500.1320885 MHz
 NUC1 1H
 P1 9.22 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300015 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



10a

Molecular Weight =320.40
 Molecular Formula =C23H16N2

SRD-AA
 C13CPD DMSO {D:\AHMEDNAGAR} root 27

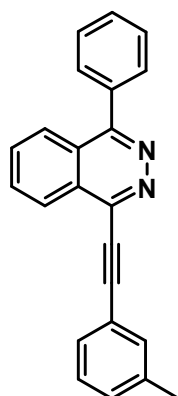
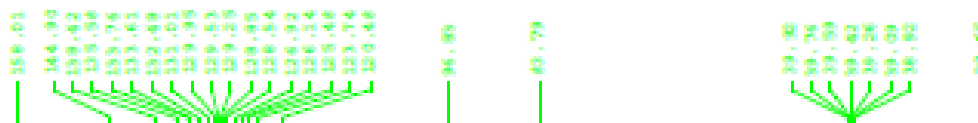


Current Data Parameters
 NAME Dec11-2014
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141231
 Time_ 16.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 800
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 189.76
 DW 16.800 usec
 DE 6.50 usec
 TE 297.7 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 100.00000000 W
 ----- CHANNEL f2 -----
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG(2) waltz16
 PCPD2 80.00 usec
 PLW2 22.00000000 W
 PLW12 0.29222000 W
 PLW13 0.18702000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578570 MHz
 WDW EM
 SSR 0
 LB 1.00 Hz
 GB 0
 PC 1.40



10a

Molecular Weight =320.40
 Molecular Formula =C23H16N2

