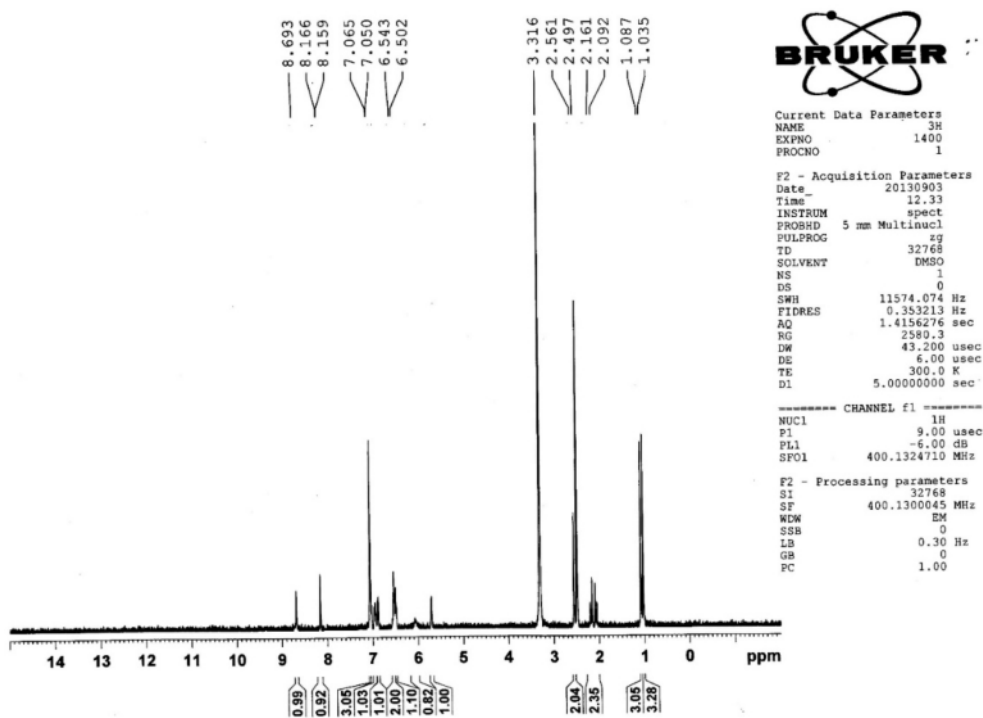
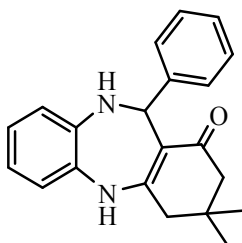


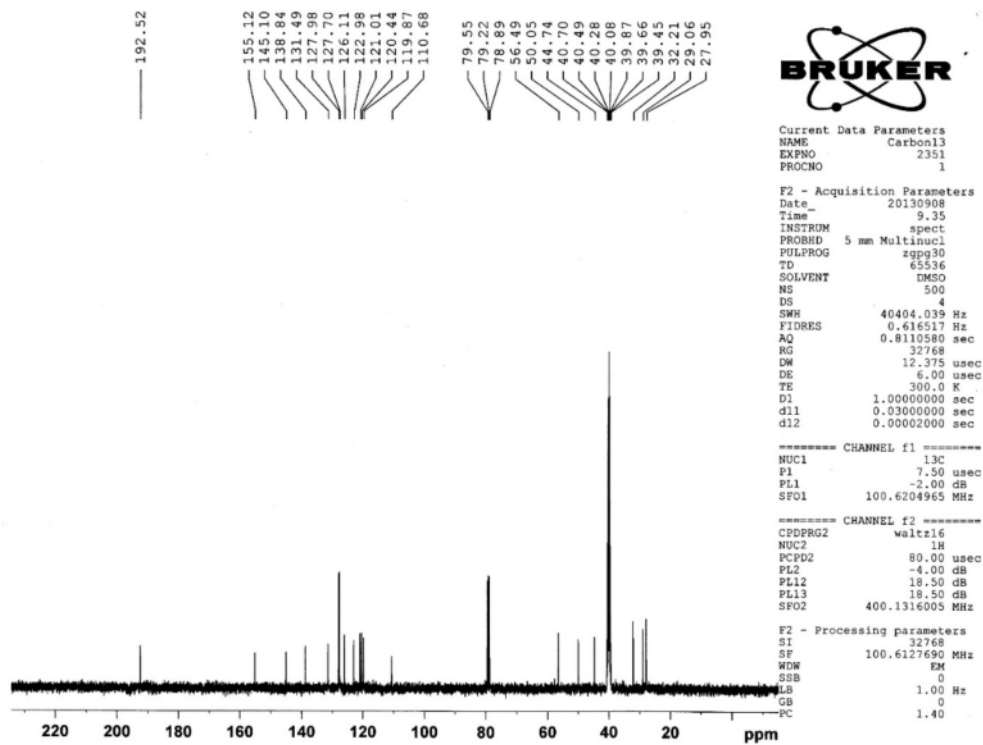
Supplementary Data:

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3a**):

Pale green solid



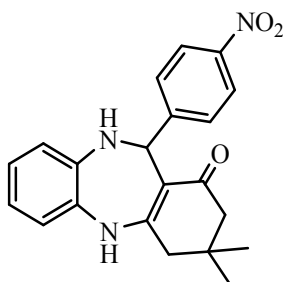
¹H NMR Spectrum

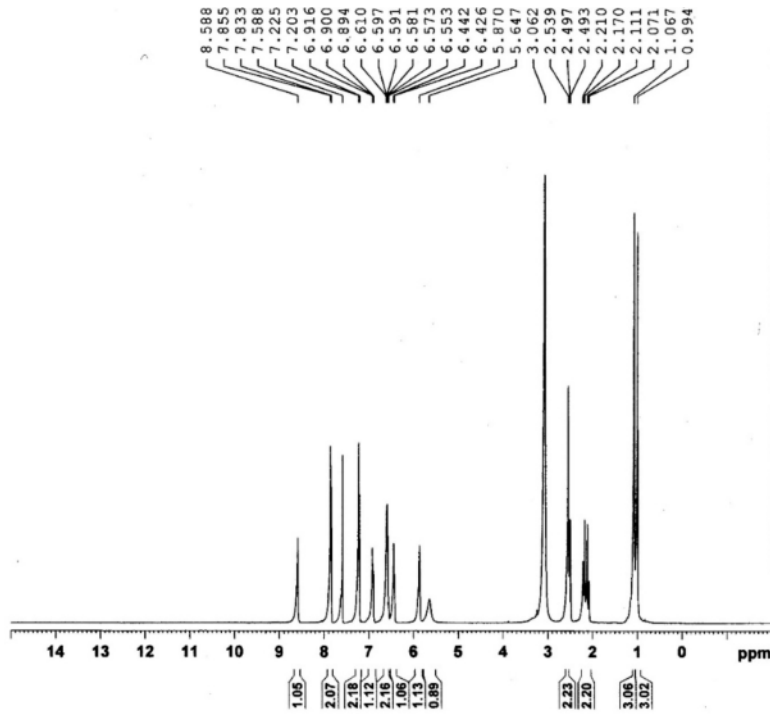


¹³C NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(4-nitro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3b**):

Yellow solid





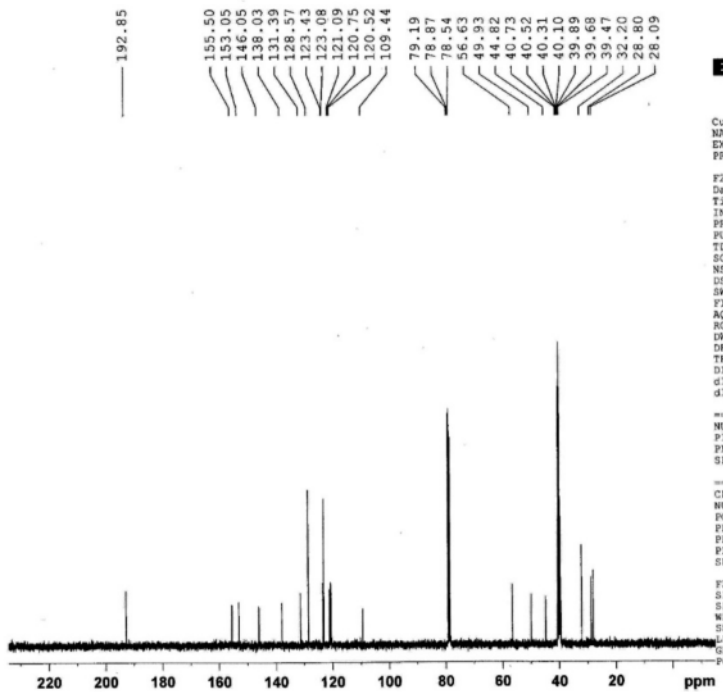
Current Data Parameters
 NAME 3H
 EXPNO 1214
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130731
 Time 10.18
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 11574.074 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 256
 DW 43.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 5.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 9.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300045 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR Spectrum



Current Data Parameters
 NAME Carbon13
 EXPNO 2292
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130731
 Time 12.39
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 500
 DS 4
 SWH 40404.039 Hz
 FIDRES 0.616517 Hz
 AQ 0.8110580 sec
 RG 32768
 DW 12.375 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 7.50 usec
 PL1 -2.00 dB
 SFO1 100.6204965 MHz

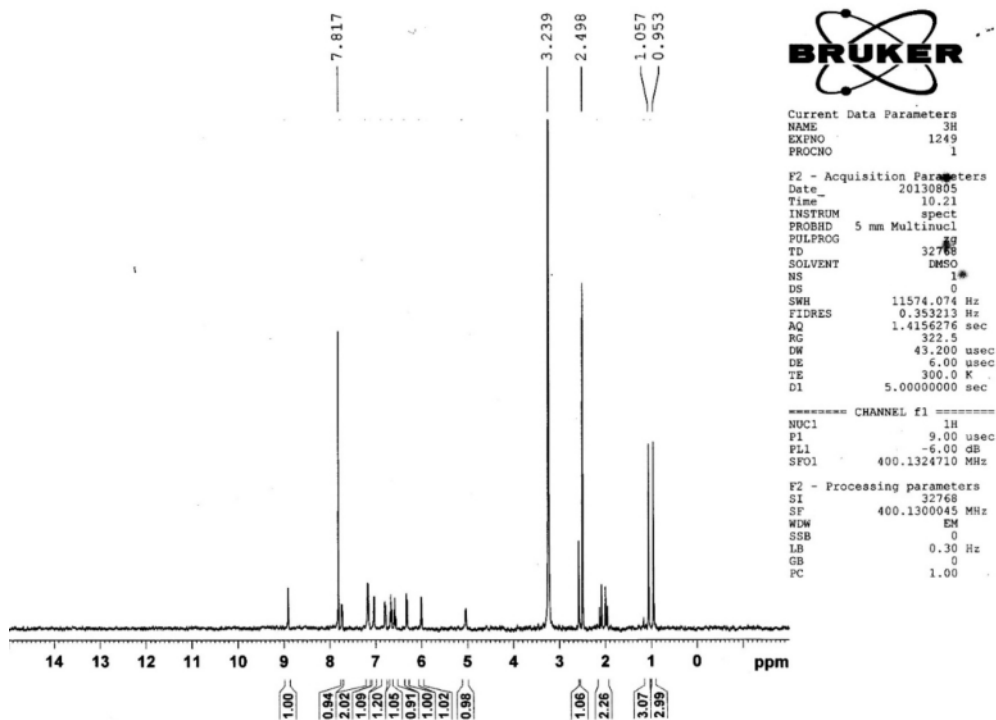
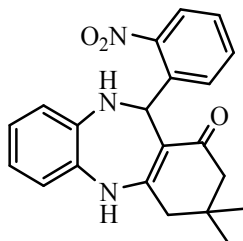
----- CHANNEL f2 -----
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 18.50 dB
 PL13 18.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(2-nitro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(3c):

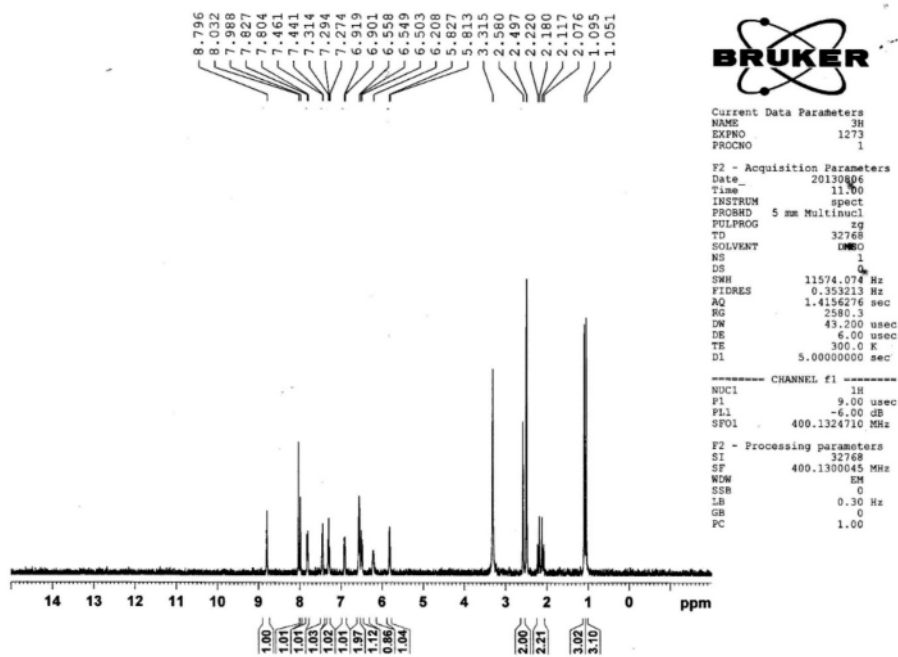
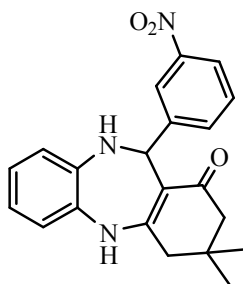
Orange solid



¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(3-nitro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(3d):

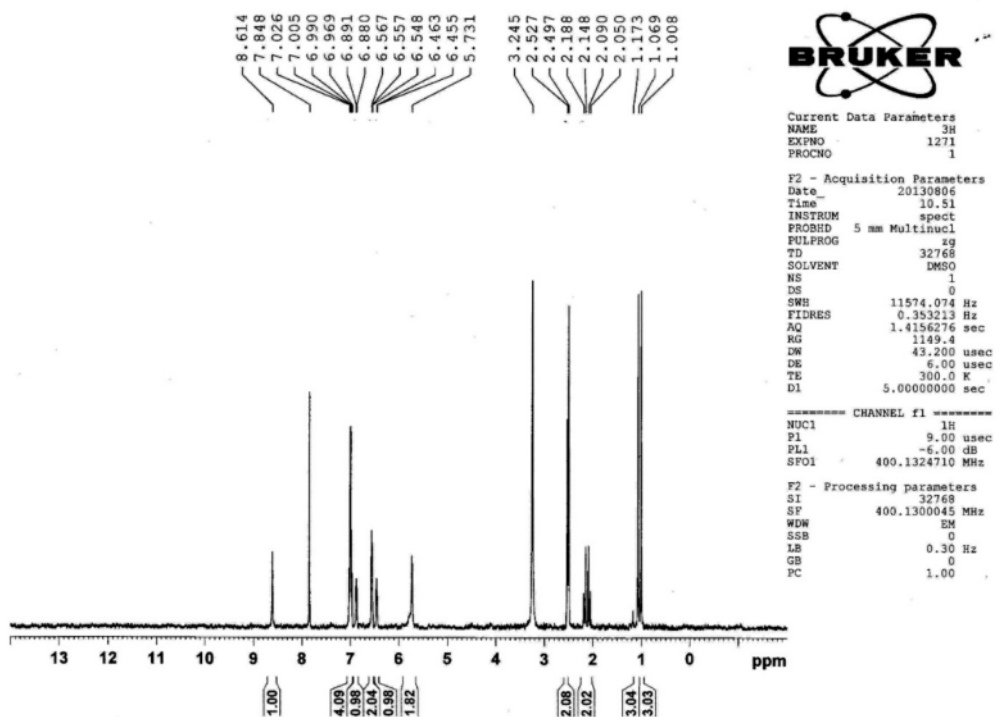
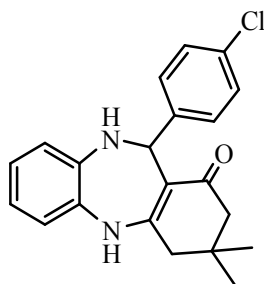
Pale yellow solid



¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(4-chloro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3e**):

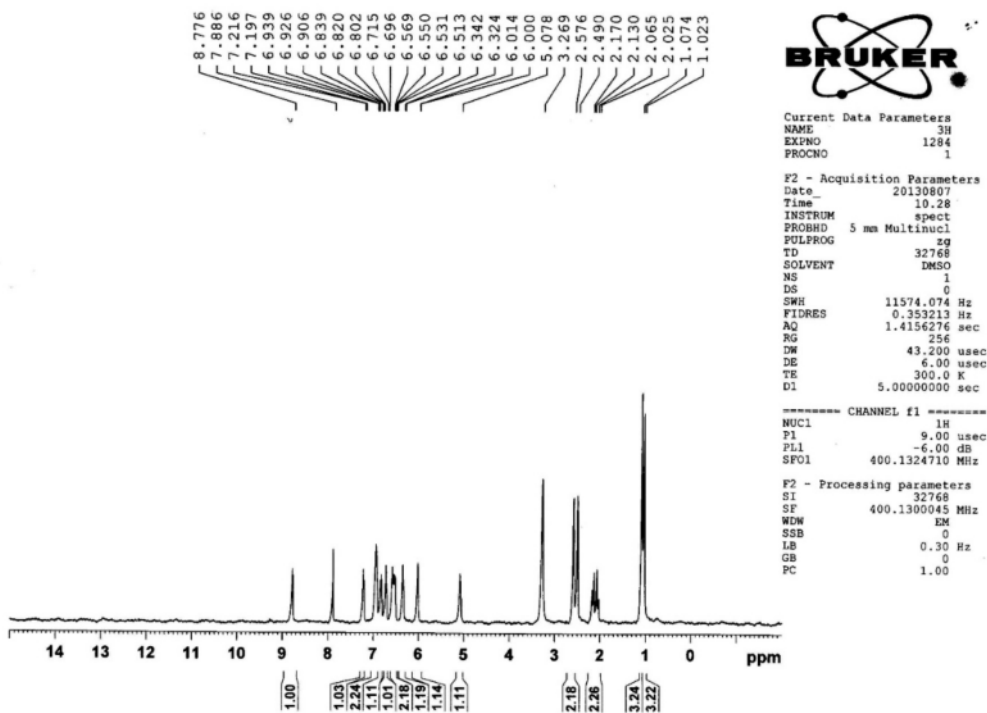
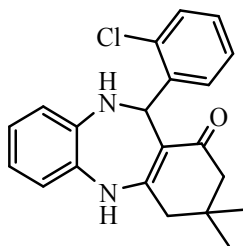
Pale green solid



¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(2-chloro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3f**):

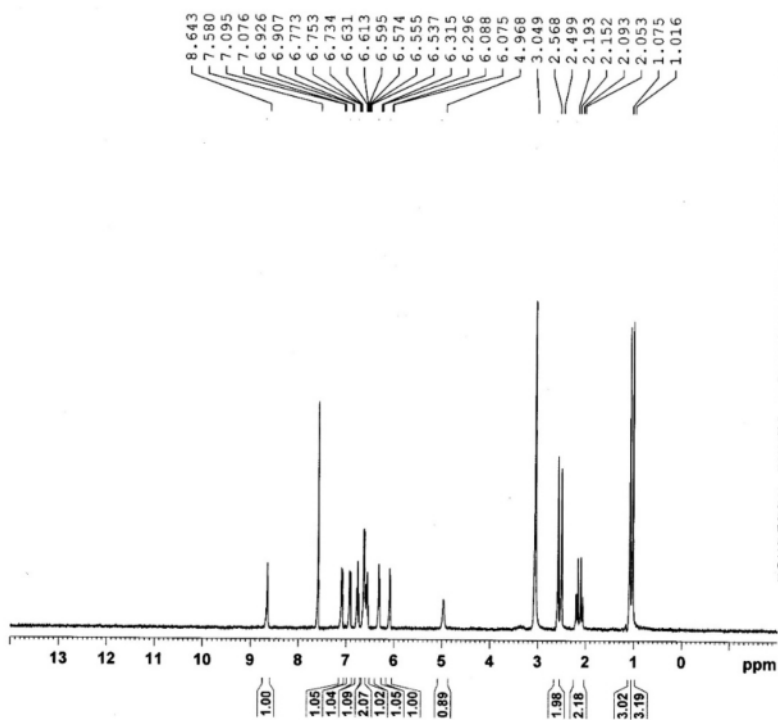
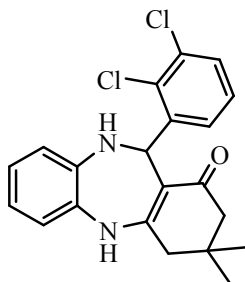
White solid



¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(2,3-dichloro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3g**):

Pale green solid



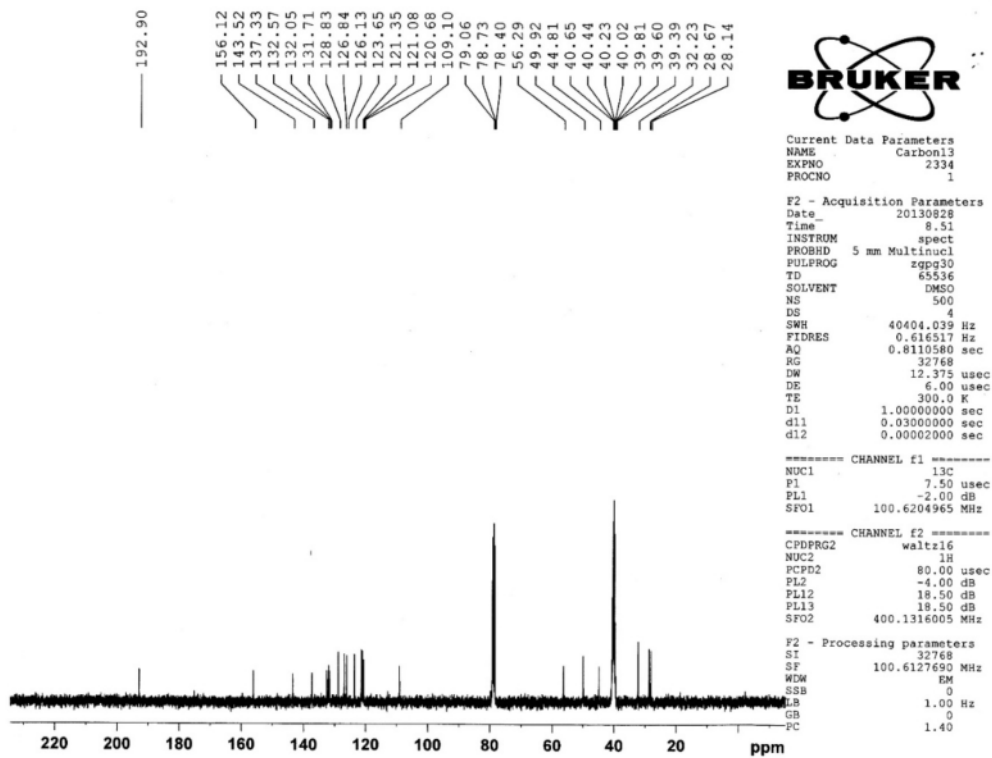
Current Data Parameters
 NAME 3H
 EXPNO 1244
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130803
 Time 12.27
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 11574.074 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 456.1
 DW 43.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 5.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 9.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

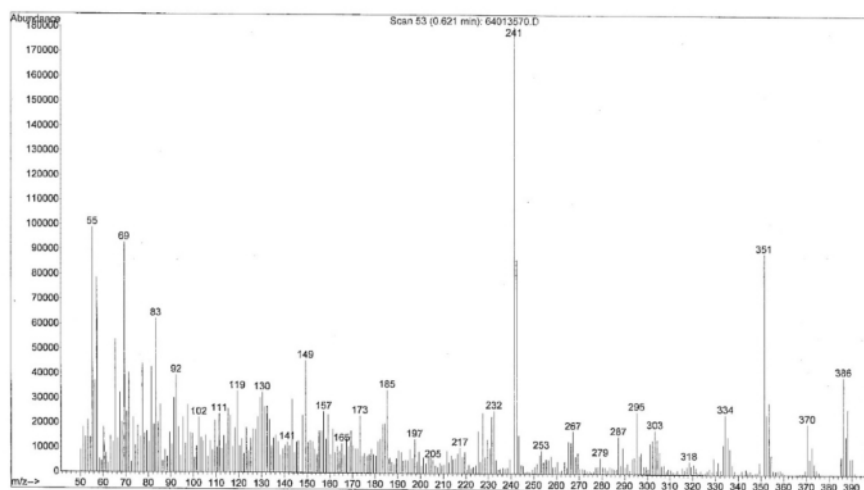
F2 - Processing parameters
 SI 32768
 SF 400.1300045 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR Spectrum



¹³C NMR Spectrum

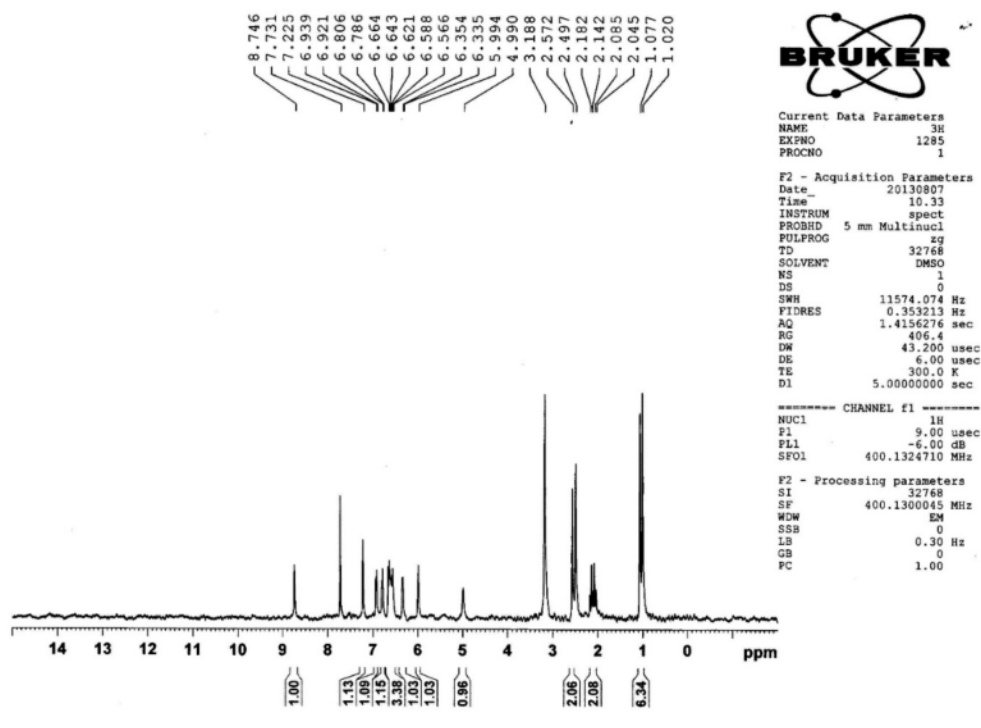
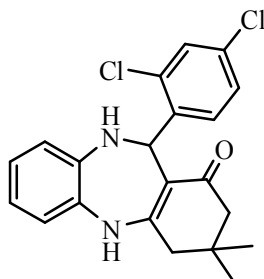
File : C:\MSDCHEM\4\DATA\64013570.D
 Operator :
 Acquired : 4 Jan 1980 1:57 using AcqMethod TEST ARI
 Instrument : Instrumen
 Sample Name: M8
 Misc Info :
 Vial Number: 1



EI-MASS Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(2,4-dichloro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3h**):

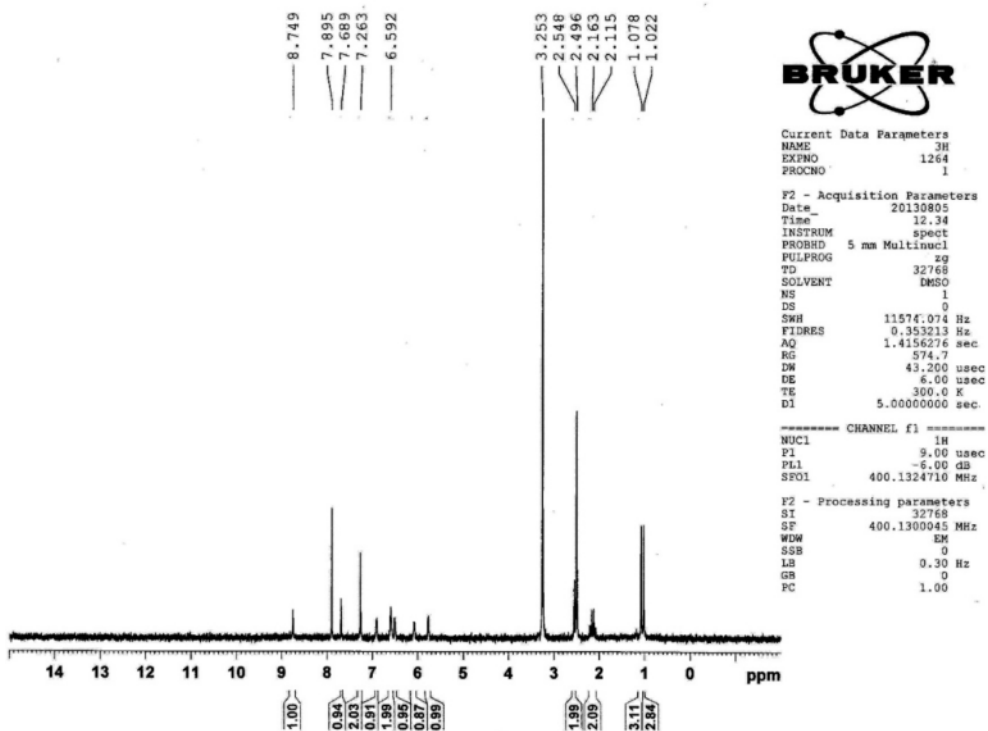
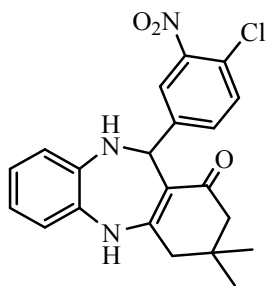
Pale green solid



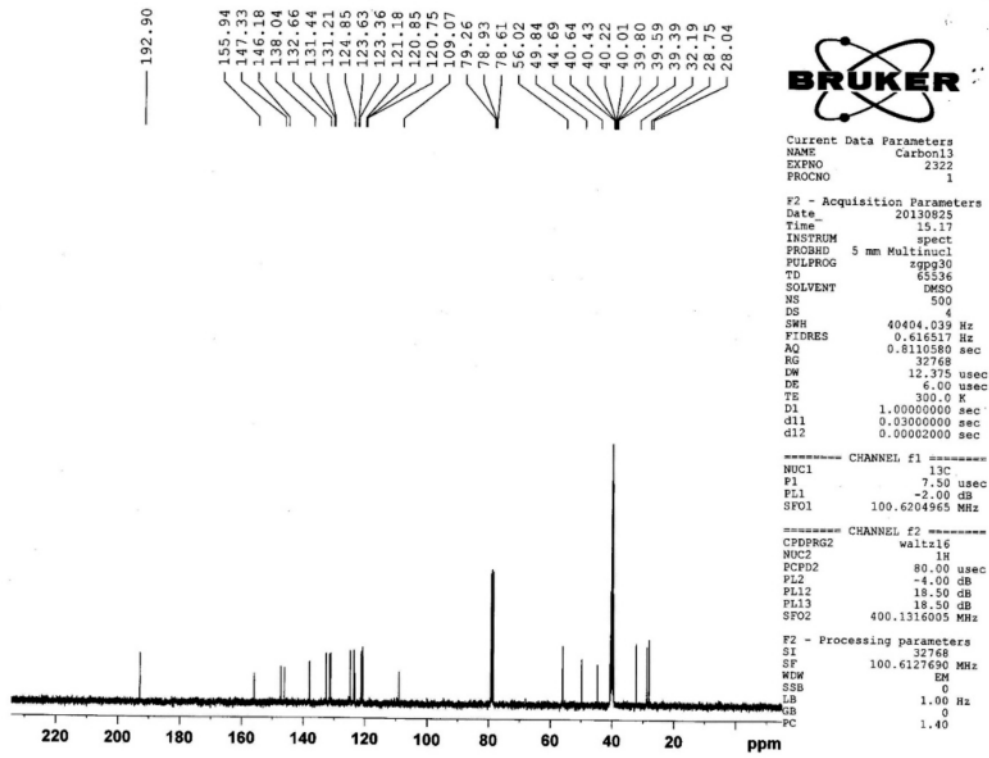
¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(4-chloro-3-nitro)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3i**):

Pale yellow solid

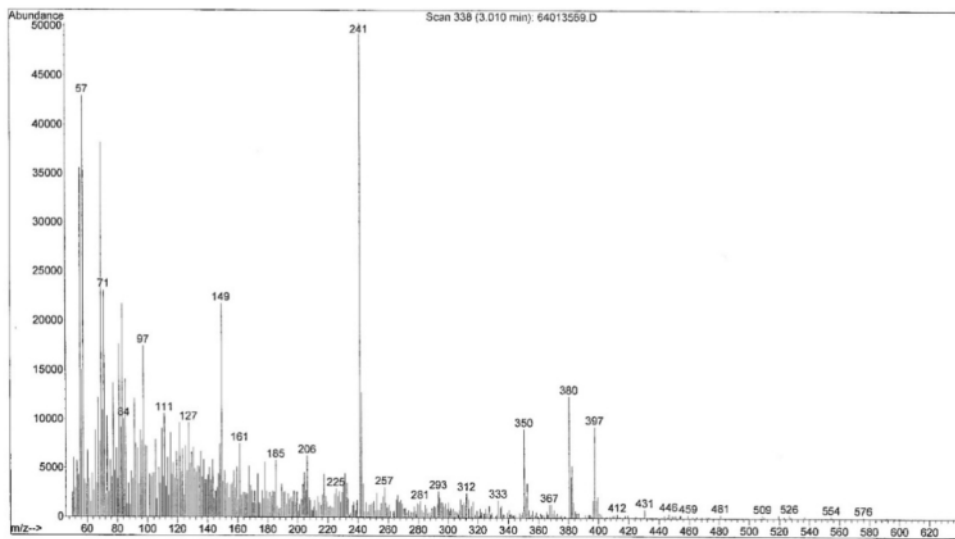


¹H NMR Spectrum



¹³CNMR Spectrum

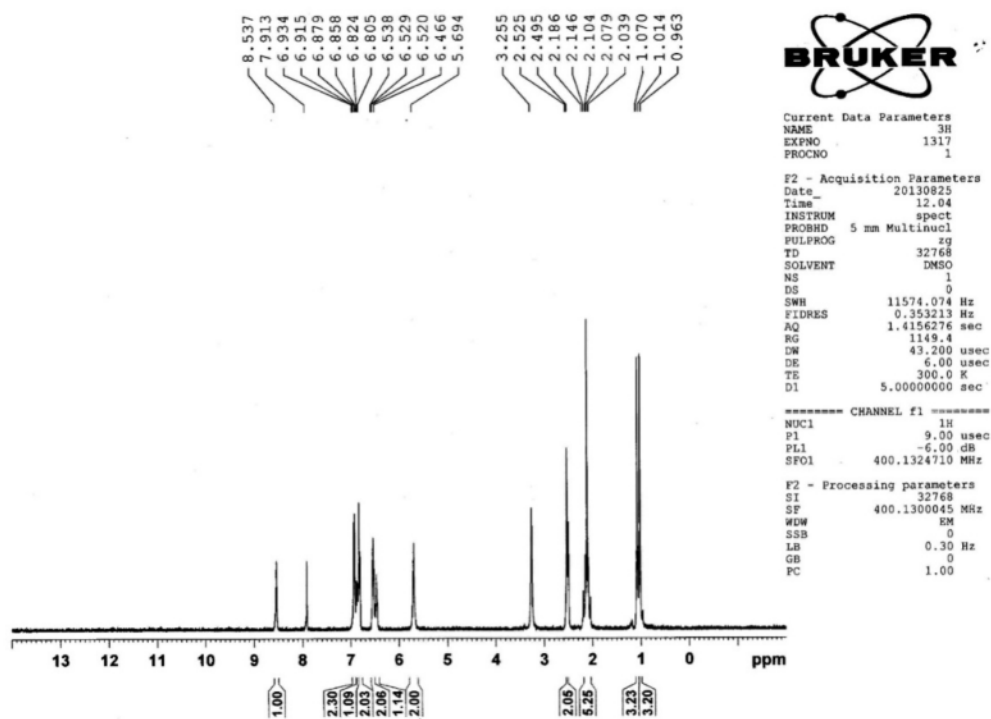
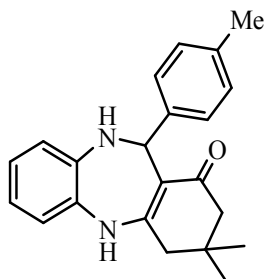
File : C:\MSDCHEM\4\DATA\64013569.D
 Operator :
 Acquired : 4 Jan 1980 1:53 using AcqMethod TEST ARI
 Instrument : Instrumen
 Sample Name: M5
 Misc Info :
 Vial Number: 1



EI-MASS Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(4-methyl)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3j**):

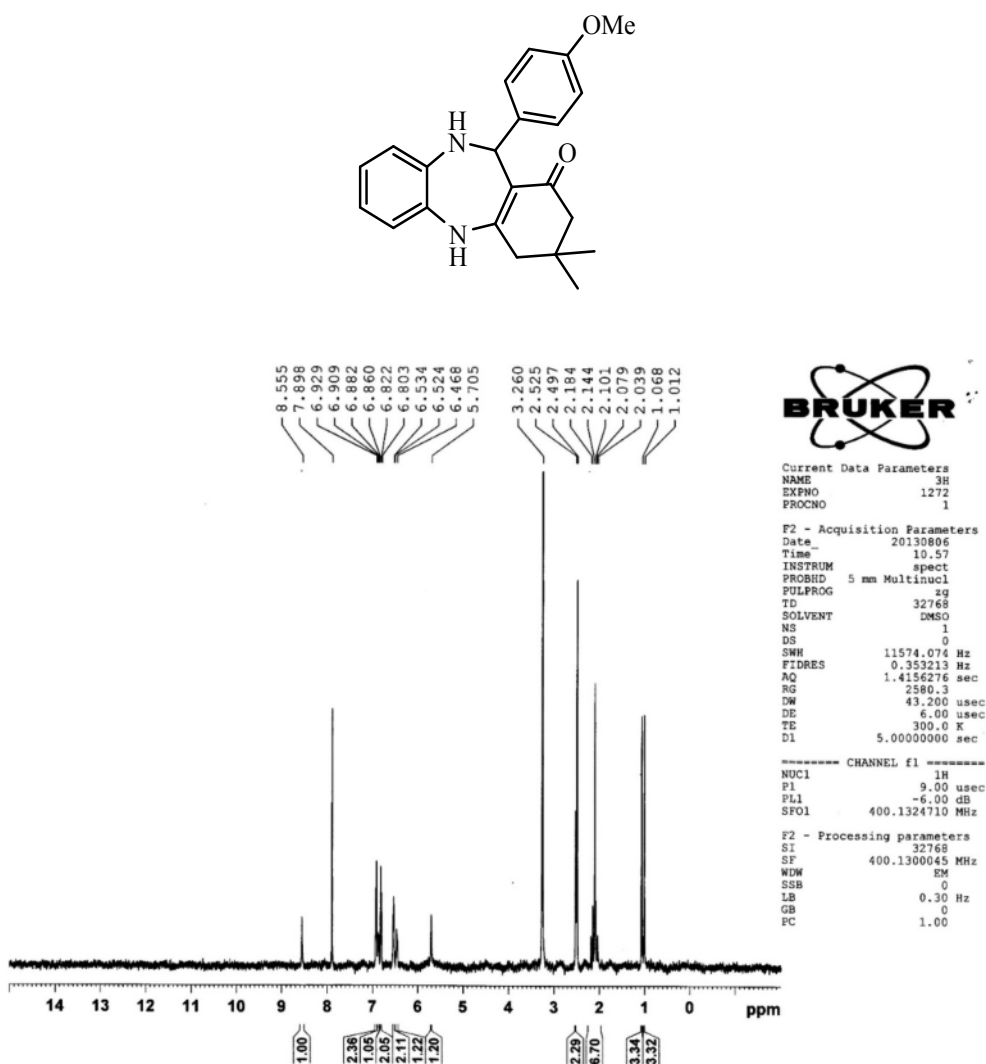
Pale green solid



¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(4-methoxy)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**3k**):

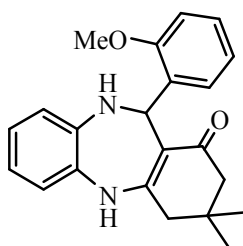
Pale cream solid

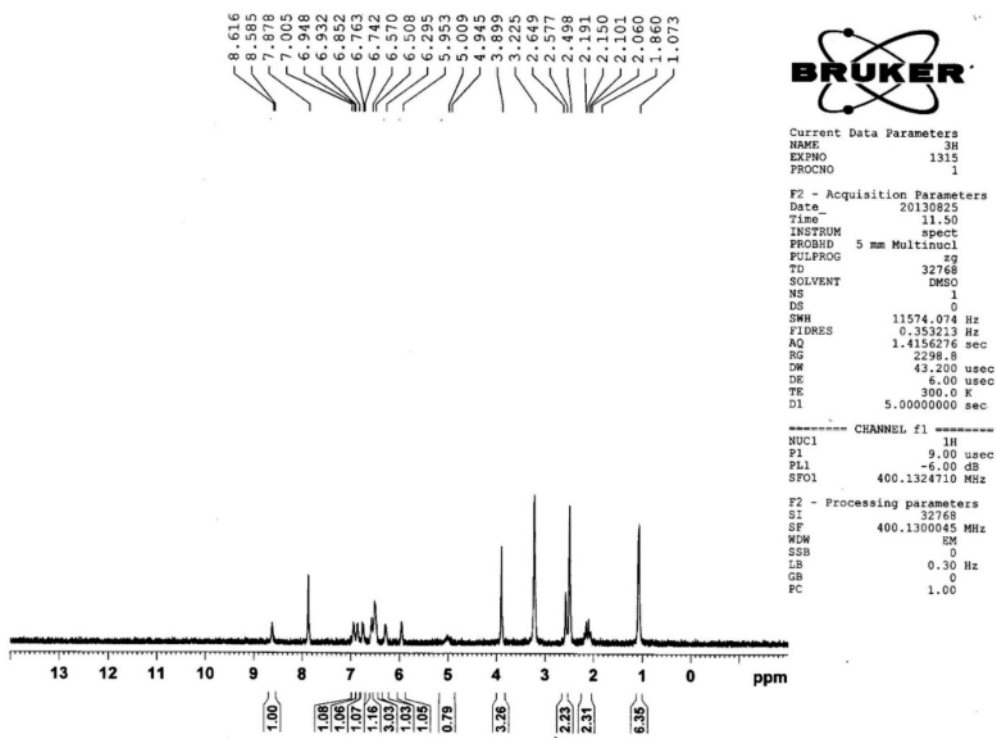


¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(2-methoxy)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one (**31**):

Pale cream solid

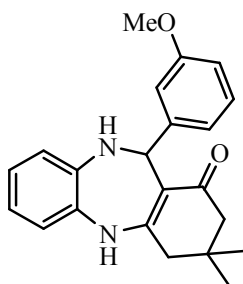


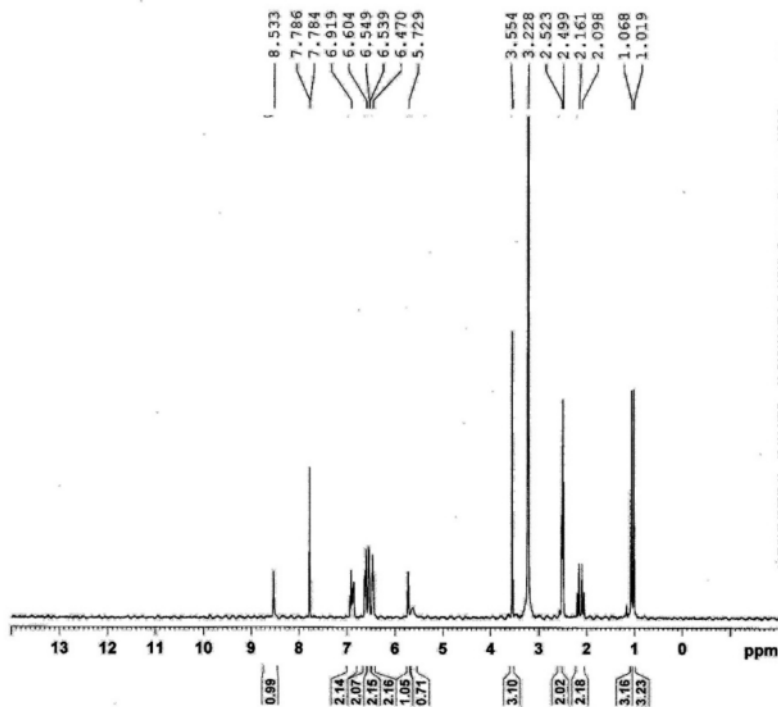


¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(3-methoxy)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one (**3m**):

Pale green solid





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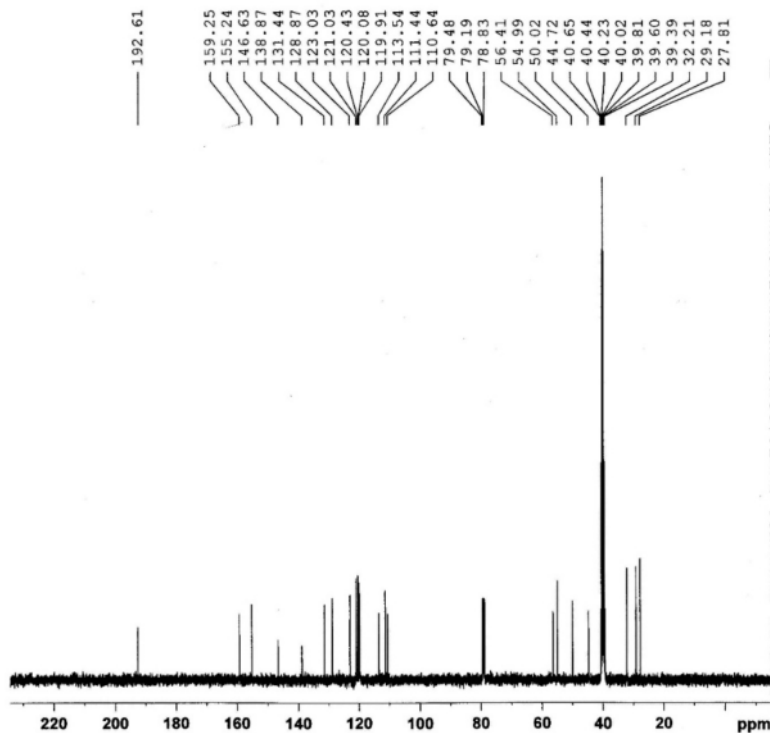
Current Data Parameters
NAME      3H
EXPNO    1248
PROCNO    1

F2 - Acquisition Parameters
Date_    20130805
Time     10.05
INSTRUM  spect
PROBHD   5 mm Multinucl
PULPROG  zg
TD        32768
SOLVENT  DMSO
NS        1
DS        0
SWH      11574.074 Hz
FIDRES   0.353213 Hz
AQ        1.4156276 sec
RG        322.5
DW        43.200 usec
DE        6.00 usec
TE        300.0 K
D1        5.0000000 sec

----- CHANNEL f1 -----
NUC1      1H
P1        9.00 usec
PL1       -6.00 dB
SFO1      400.1324710 MHz

F2 - Processing parameters
SI        32768
SF        400.1300045 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

¹H NMR Spectrum



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Current Data Parameters
NAME      Carbon13
EXPNO    2333
PROCNO    1

F2 - Acquisition Parameters
Date_    20130828
Time     8.26
INSTRUM  spect
PROBHD   5 mm Multinucl
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4
DS        4
SWH      40404.039 Hz
FIDRES   0.616517 Hz
AQ        0.8110580 sec
RG        32768
DW        12.373 usec
DE        6.00 usec
TE        300.0 K
D1        1.0000000 sec
d11       0.0300000 sec
d12       0.0000200 sec

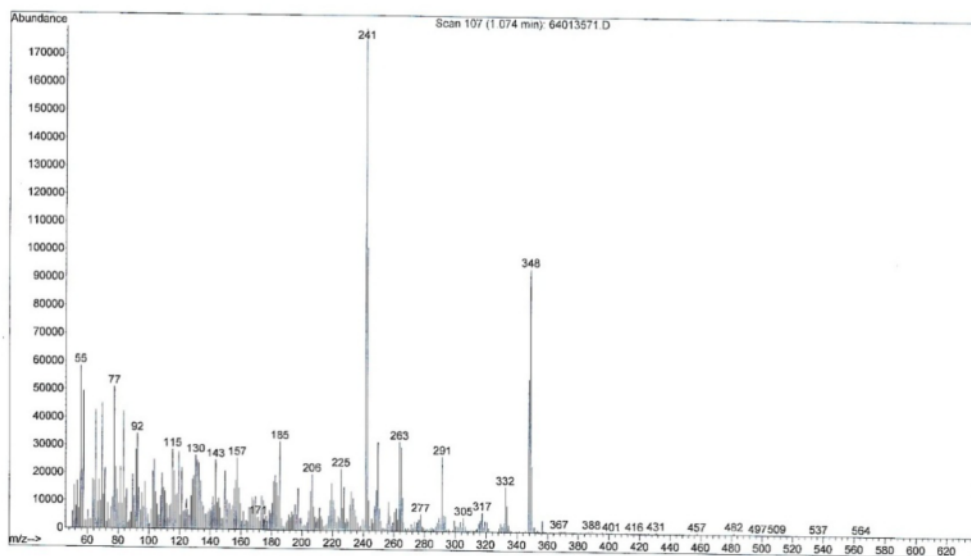
----- CHANNEL f1 -----
NUC1      13C
P1        7.50 usec
PL1       -2.00 dB
SFO1      100.6204965 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -4.00 dB
PL12     18.50 dB
PL13     18.50 dB
SFO2      400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

¹³C NMR Spectrum

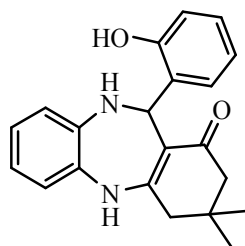
File : C:\MSDCHEM\4\DATA\64013571.D
Operator :
Acquired : 4 Jan 1980 1:58 using AcqMethod TEST ARI
Instrument : Instrumen
Sample Name: M13
Misc Info :
Vial Number: 1

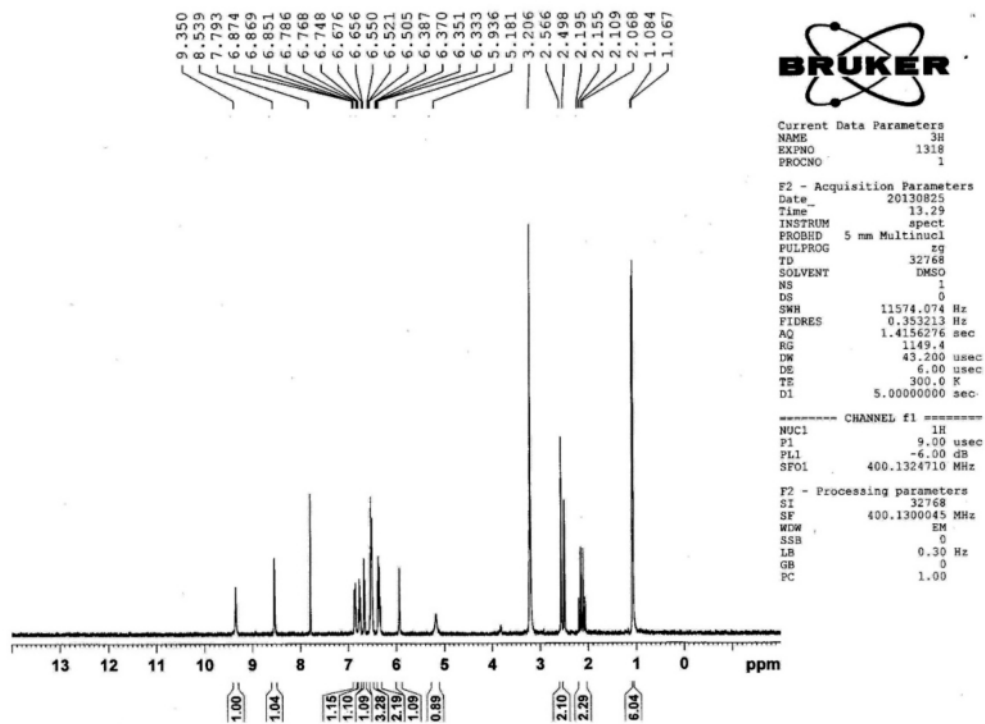


EI-MASS Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(2-hydroxy)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(3n):

Pale cream solid

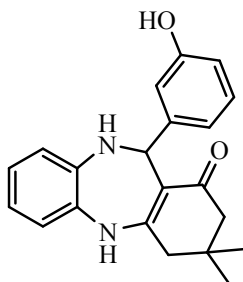


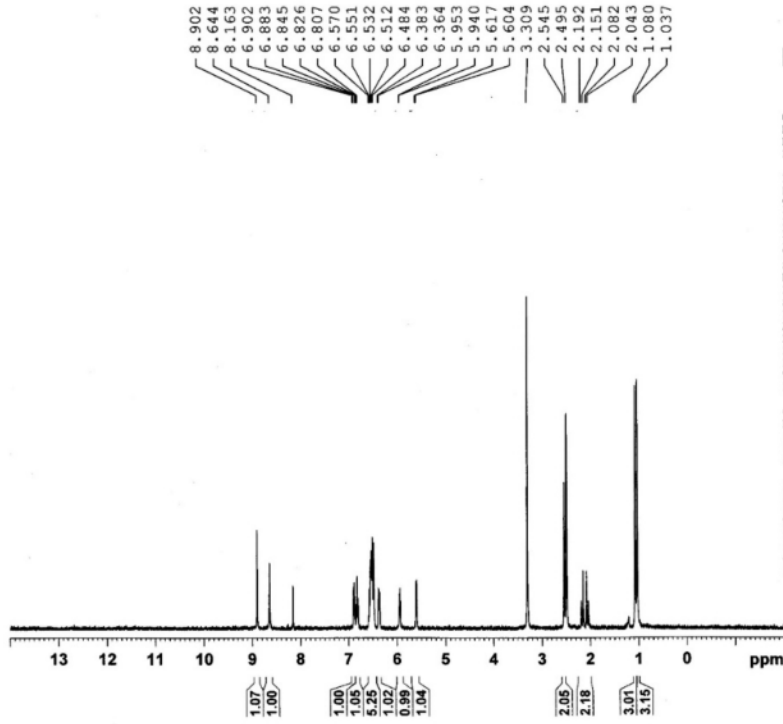


¹H NMR Spectrum

3,3-dimethyl-2,3,4,5,10,11-hexahydro-11-[(3-hydroxy)phenyl]-1H-dibenzo[b,e][1,4]diazepin-1-one(**30**):

Pale green solid





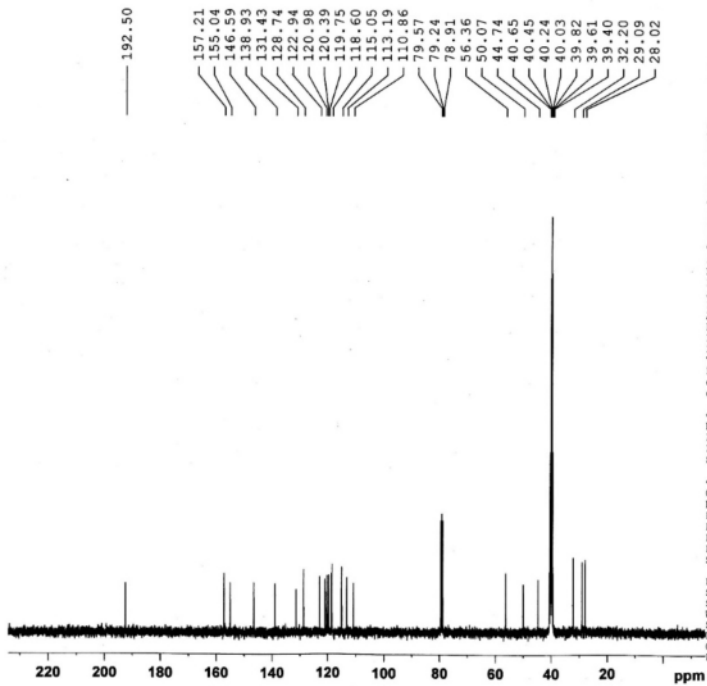
Current Data Parameters
 NAME 3H
 EXPNO 1319
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130825
 Time 13.33
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 11574.074 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1149.4
 DW 43.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 5.0000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300045 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR Spectrum



Current Data Parameters
 NAME Carbon13
 EXPNO 2375
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130917
 Time 11.06
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 500
 DS 4
 SWH 40404.039 Hz
 FIDRES 0.616517 Hz
 AQ 0.811580 sec
 RG 32768
 DW 12.375 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 d11 0.0300000 sec
 d12 0.0002000 sec

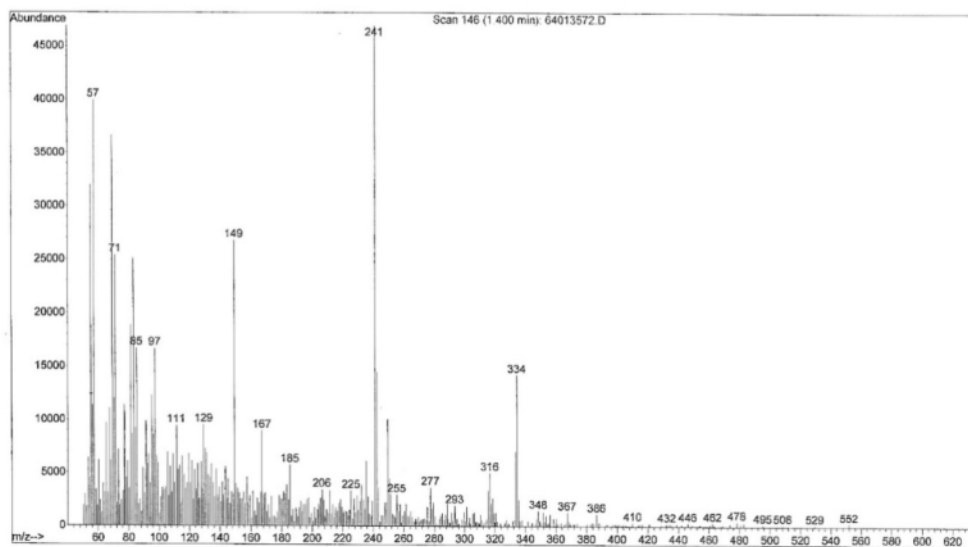
==== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 -2.00 dB
 SFO1 100.6204965 MHz

==== CHANNEL f2 =====
 CDPFRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 18.50 dB
 PL13 18.50 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR Spectrum

File : C:\MSDCHEM\4\DATA\64013572.D
Operator :
Acquired : 4 Jan 1980 2:00 using AcqMethod TEST ARI
Instrument : Instrumen
Sample Name: M15
Misc Info :
Vial Number: 1



EI-MASS Spectrum