

Supporting Information (Part-B)

Novel Syntheses of Tetrahydrobenzodiazepines and Dihydropyrazines via Isocyanide-based Multicomponent Reactions of Diamines

Ahmad Shaabani,^{*,a} Ali Maleki,^a Fatemeh Hajishaabanha,^a Hamid Mofakham,^a

Mozhdeh Seyyedhamzeh,^a Mojtaba Mahyari,^a and Seik Weng Ng^b

^aDepartment of Chemistry, Shahid Beheshti University, 19396-4716, Tehran, Iran

a-shaabani@cc.sbu.ac.ir

^bDepartment of Chemistry, University of Malaya, 50603, Kuala Lumpur, Malaysia

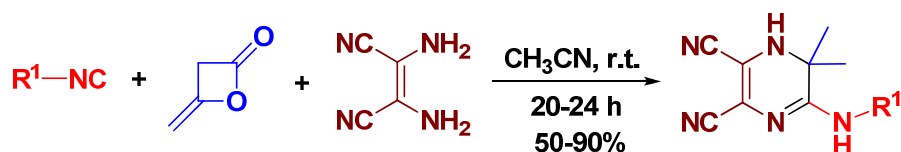
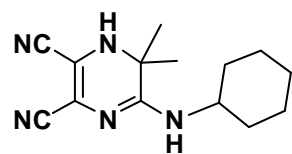


Table 2. Detailed list of CONTENTS of the supporting information **6a-e** and **8d-h**

List of contents	Page	List of contents	Page
Title, authors' name, address and tables	S1	Mass of 6c	S16
Compounds Characterization Data	S2-S4	IR of 6d	S17
IR of 6a	S5	¹ H NMR of 6d	S18
¹ H NMR of 6a	S6	¹³ C NMR of 6d	S19
¹³ C NMR of 6a	S7	Mass of 6d	S20
Mass of 6a	S8	IR of 6e	S21
IR of 6b	S9	¹ H NMR of 6e	S22
¹ H NMR of 6b	S10	¹³ C NMR of 6e	S23
¹³ C NMR of 6b	S11	Mass of 6e	S24
Mass of 6b	S12	IR of 8d-h	S25
IR of 6c	S13	¹ H NMR of 8d-h	S26
¹ H NMR of 6c	S14	¹³ C NMR of 8d-h	S27
¹³ C NMR of 6c	S15	Mass of 8d-h	S28

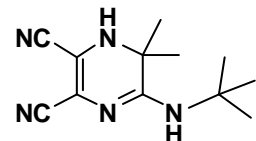
Compounds Characterization Data

5-(Cyclohexylamino)-1,6-dihydro-6,6-dimethylpyrazine-2,3-dicarbonitrile (6a).



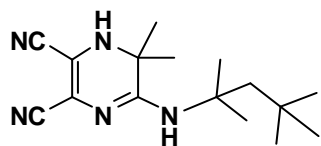
Colorless crystals; mp 252–254°C. IR (KBr) cm^{-1} : 3343, 3081, 2931, 2852, 2217, 1579, 1539, 1451, 1391. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$) δ : 1.00–2.10 (16H, m, 5CH_2 of cyclohexyl and 2CH_3), 3.69 (1H, m, CH of cyclohexyl), 6.86 (1H, d, $J = 7.6$ Hz, NH), 7.12 (1H, br s, NH). ^{13}C NMR (75.47 MHz, $\text{DMSO-}d_6$) δ : 24.3, 25.2, 25.7, 31.9, 49.6, 50.0, 110.2, 110.8, 114.9, 118.4, 155.8. MS m/z : 257 (M^+ , 20), 242 (25), 175 (25), 160 (100), 133 (22), 57 (45), 41 (75). Anal. Calcd for $\text{C}_{14}\text{H}_{19}\text{N}_5$: C, 65.34; H, 7.44; N, 27.22; found C, 65.28; H, 7.33; N, 27.20.

5-(*tert*-Butylamino)-1,6-dihydro-6,6-dimethylpyrazine-2,3-dicarbonitrile (6b).



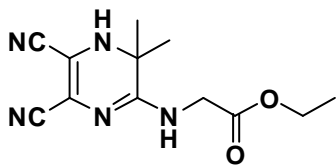
Light yellow crystals; mp 225–228°C. IR (KBr) cm^{-1} : 3457, 3362, 3303, 3183, 2931, 2852, 2214, 1661, 1622, 1526, 1467, 1428, 1380. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$) δ : 1.18 (6H, br s, 2CH_3), 1.32 (9H, br s, 3CH_3), 6.18 (1H, br s, NH), 7.14 (1H, br s, NH). ^{13}C NMR (75.47 MHz, $\text{DMSO-}d_6$) δ : 24.0, 28.5, 49.3, 52.5, 110.2, 110.2, 115.0, 118.4, 154.8. MS m/z : 232 (M^+ , 20), 160 (100), 133 (26), 57 (50), 41 (75). Anal. Calcd for $\text{C}_{12}\text{H}_{17}\text{N}_5$: C, 62.31; H, 7.41; N, 30.28; found C, 62.21; H, 7.32; N, 30.18.

5-(2,4,4-Trimethylpentan-2-ylamino)-1,6-dihydro-6,6-dimethylpyrazine-2,3-dicarbonitrile (6c).



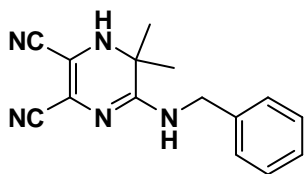
White powder; mp 150–151°C. IR (KBr) cm^{-1} : 3424, 3342, 2951, 2852, 2214, 1573, 1548, 1447, 1350, 1312. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$) δ : 0.93 (9H, br s, 3 CH_3), 1.17 (6H, br s, 2 CH_3), 1.36 (6H, br s, 2 CH_3), 1.83 (2H, br s, CH_2), 6.06 (1H, br s, NH), 7.14 (1H, br s, NH). ^{13}C NMR (75.47 MHz, $\text{DMSO-}d_6$) δ : 23.9, 29.3, 31.7, 31.8, 49.3, 49.8, 56.5, 109.8, 110.1, 115.0, 118.4, 154.1. MS m/z : 287 (M^+ , 17), 176 (48), 160 (100), 133 (15), 97 (17), 57 (60), 41 (63). Anal. Calcd for $\text{C}_{16}\text{H}_{25}\text{N}_5$: C, 66.86; H, 8.77; N, 24.37; found C, 66.76; H, 8.70; N, 24.27.

Ethyl 2-(5,6-dicyano-3,4-dihydro-3,3-dimethylpyrazin-2-ylamino)acetate (6d).



Colorless crystals; mp 189–191°C. IR (KBr) cm^{-1} : 3379, 3286, 3004, 2968, 2932, 2216, 1743, 1578, 1504, 1461, 1405, 1322. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$) δ : 1.00-1.00-1.35 (9H, m, 3 CH_3), 3.89 (2H, d, $J = 5.8$, CH_2), 4.09 (2H, q, $J = 7.1$, CH_2), 7.37 (1H, br s, NH), 7.78 (1H, t, $J = 5.8$, NH). ^{13}C NMR (75.47 MHz, $\text{DMSO-}d_6$) δ : 14.5, 24.4, 43.0, 50.0, 60.8, 109.5, 111.7, 114.5, 118.2, 156.6, 169.8. MS m/z : 262 ($\text{M}^+ + 1$, 50), 246 (45), 172 (100), 133 (25), 42 (27). Anal. Calcd for $\text{C}_{12}\text{H}_{15}\text{N}_5\text{O}_2$: C, 55.16; H, 5.79; N, 26.80; found C, 55.10; H, 5.69; N, 26.70.

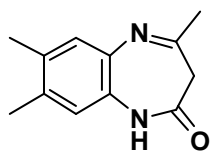
5-(Benzylamino)-1,6-dihydro-6,6-dimethylpyrazine-2,3-dicarbonitrile (6e).



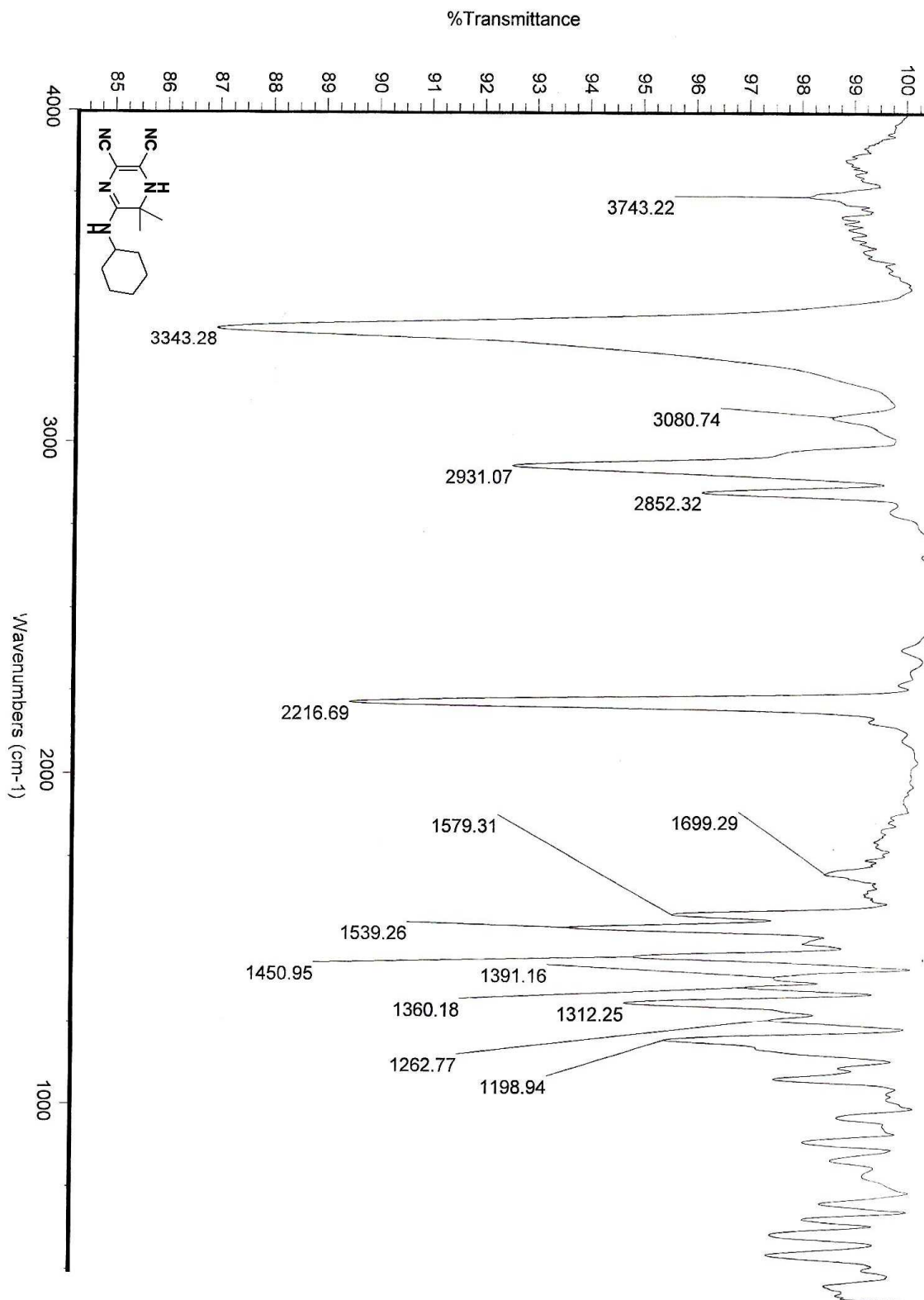
Brown powder; mp 152–154°C. IR (KBr) cm^{-1} : 3461, 3310, 3245, 3173, 3034, 2921, 2202, 1704, 1631, 1531, 1376. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$) δ : 2.17 (6H, br s, 2 CH_3), 3.46 (2H, br s, CH_2), 7.24 (6H, m, H-Ar and NH), 9.32 (1H, br s, NH). ^{13}C NMR (75.47 MHz,

DMSO-*d*₆) δ : 24.4, 30.6, 51.2, 89.2, 114.1, 117.1, 127.2, 127.4, 127.5, 128.8, 139.3
165.9. MS *m/z*: 266 ($M^{+}+1$, 3), 250 (4), 193 (6), 174 (9), 132 (22), 108 (45), 43 (100).
Anal. Calcd for C₁₅H₁₅N₅: C, 67.90; H, 5.70; N, 26.40; found C, 67.80; H, 5.62; N, 26.30.

4,7,8-Trimethyl-1*H*-benzo[*b*][1,4]diazepin-2(3*H*)-one (8d-h).

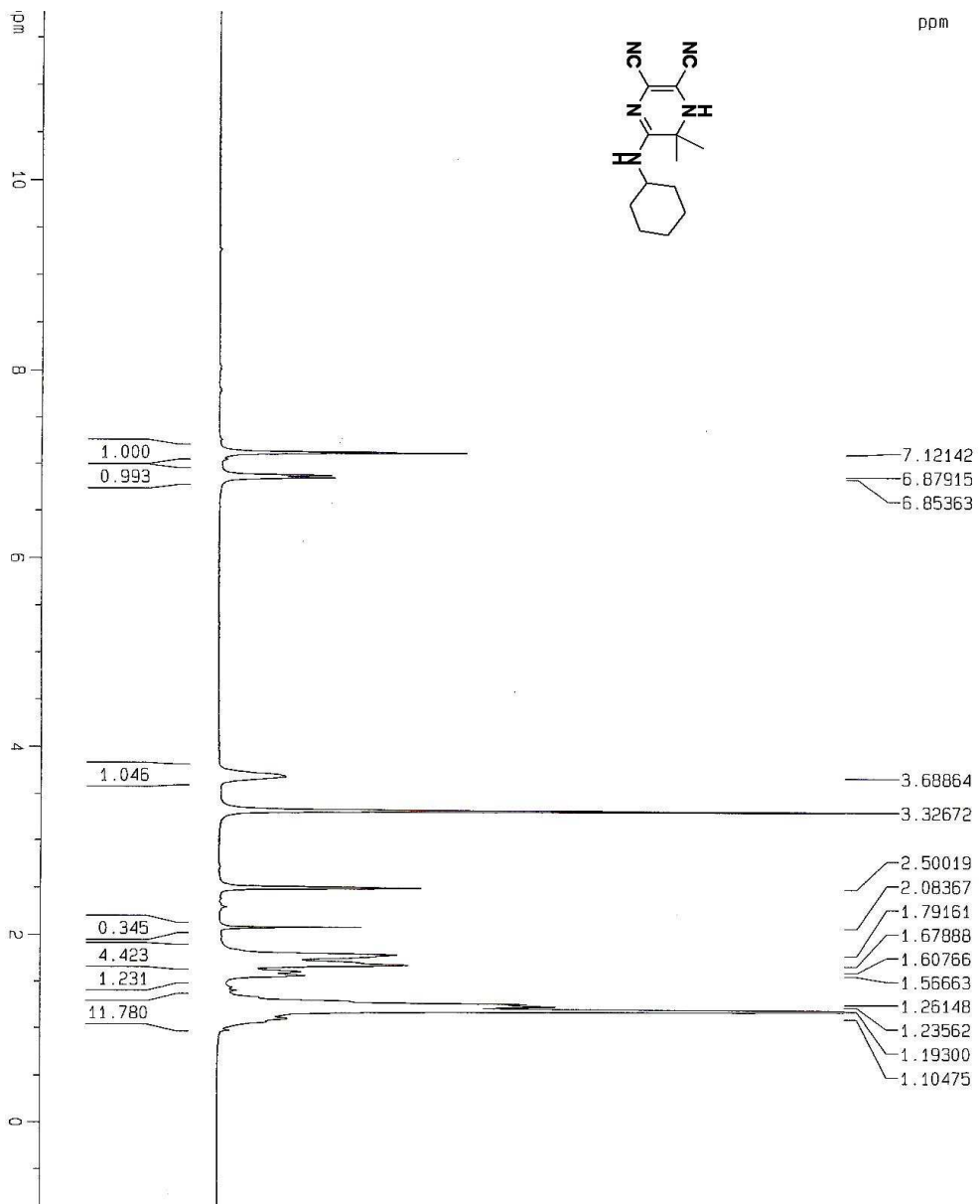
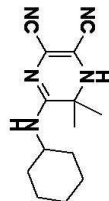


Colorless crystals; mp 191–192°C. IR (KBr) cm^{-1} : 3204, 3091, 2932,
2850, 1674, 1645, 1555, 1448, 1494, 1422, 1380. ¹H NMR (300.13
MHz, DMSO-*d*₆) δ : 2.18 (6H, br s, 2CH₃), 2.22 (3H, br s, CH₃), 2.97
(2H, br s, CH₂), 6.86 (1H, br s, H-Ar), 6.99 (1H, br s, H-Ar), 10.20 (1H, br s, NH-CO).
¹³C NMR (75.47 MHz, DMSO-*d*₆) δ : 19.2, 19.4, 27.8, 44.2, 122.7, 127.9, 128.1, 132.4,
134.3, 137.7, 162.2, 166.1. MS *m/z*: 202 (M^{+} , 25), 160 (100), 145 (75), 91 (20), 39 (45).
Anal. Calcd for C₁₂H₁₄N₂O: C, 71.26; H, 6.98; N, 13.85; found C, 71.16; H, 6.95; N,
13.94.



IR of 6a

¹H NMR

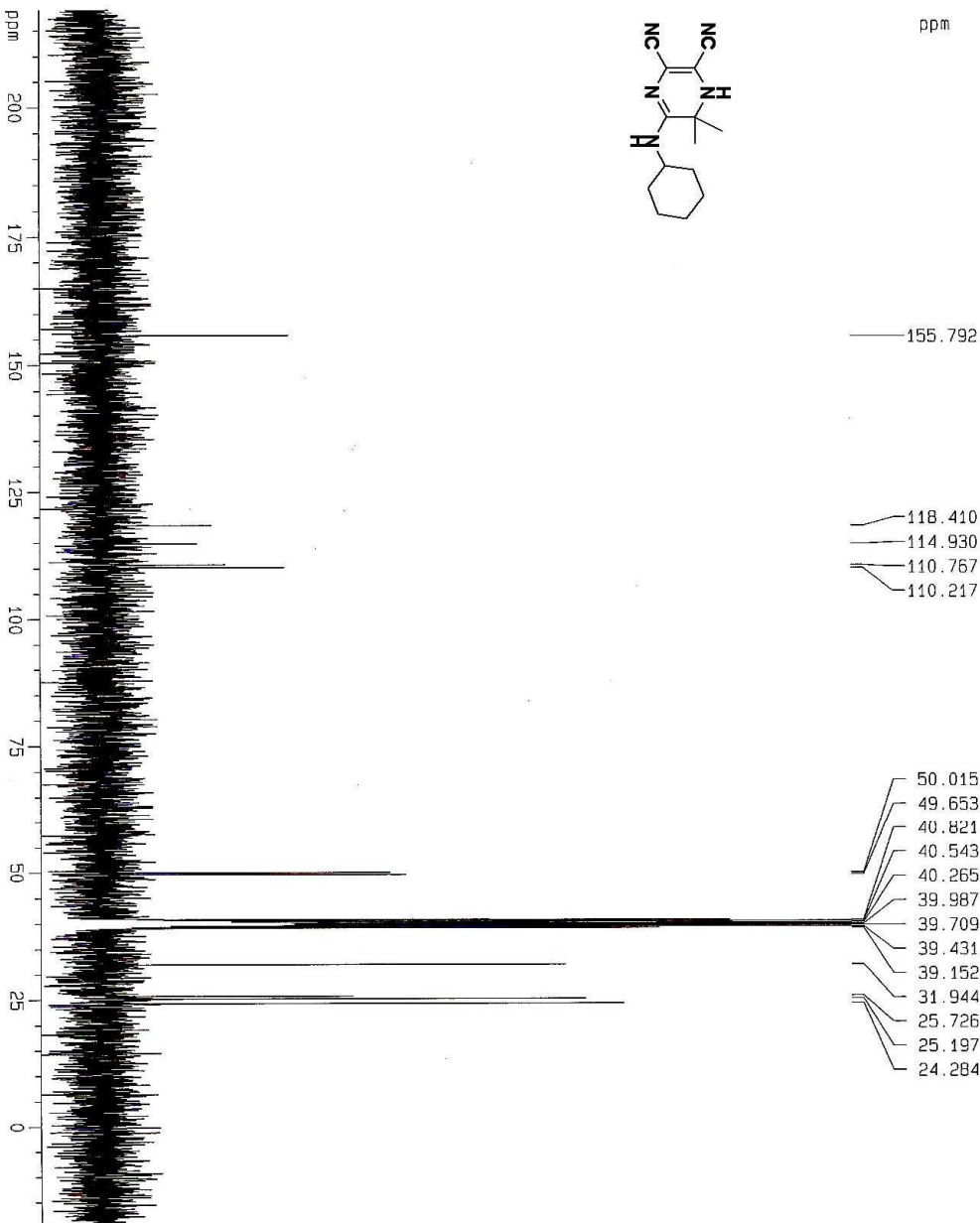
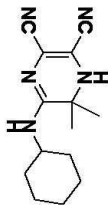


¹H NMR of 6a

```

Current Data Parameters
NAME      Maleki-PhD
EXPNO    389
PROCNO   1
----- Acquisition Parameters
Date_    20090310
Time     12.34
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zg30
TD        32768
SOLVENT  DMSO
NS        10
DS        1
SMH       7812.500 Hz
FIDRES   0.238419 Hz
AQ        2.0972021 sec
RG        228.1
DM        64.000 usec
DE        6.00 usec
TE        380.0 K
D1        2.00000000 sec
----- CHANNEL f1 -----
NUC1      1H
P1        15.50 usec
PL1       -2.00 dB
SFO1      300.1323986 MHz
F2 - Processing parameters
SI         65536
SF         300.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
ID NMR plot parameters
CX         20.00 cm
CY         32.80 cm
FLP        11.850 DDM
F1         3536.39 Hz
F2         -0.897 ppm
PPM1CH    0.63734 ppm/cm
HZCM      191.28345 Hz/cm
  
```

¹³C {1H} NMR



¹³C NMR of 6a

```

Current Data Parameters
NAME      Matkxi-PhD
EXNO     570
PROCNO   1

F2 - Acquisition Parameters
Date_    20090310
Time     12.40
INSTRUM spect
PROBHD   5 mm BBO BB-1H
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       278
DS       2
SH       17995.611 Hz
AQ       0.274439 Hz
RG       1.8219508 sec
DM       2048
DE       27.800 usec
TE       300.0 K
D1       0.03000000 sec
d11      0.03000000 sec
d12      0.00002000 sec

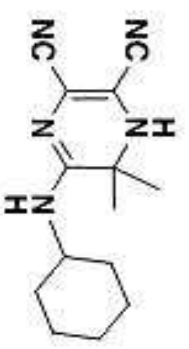
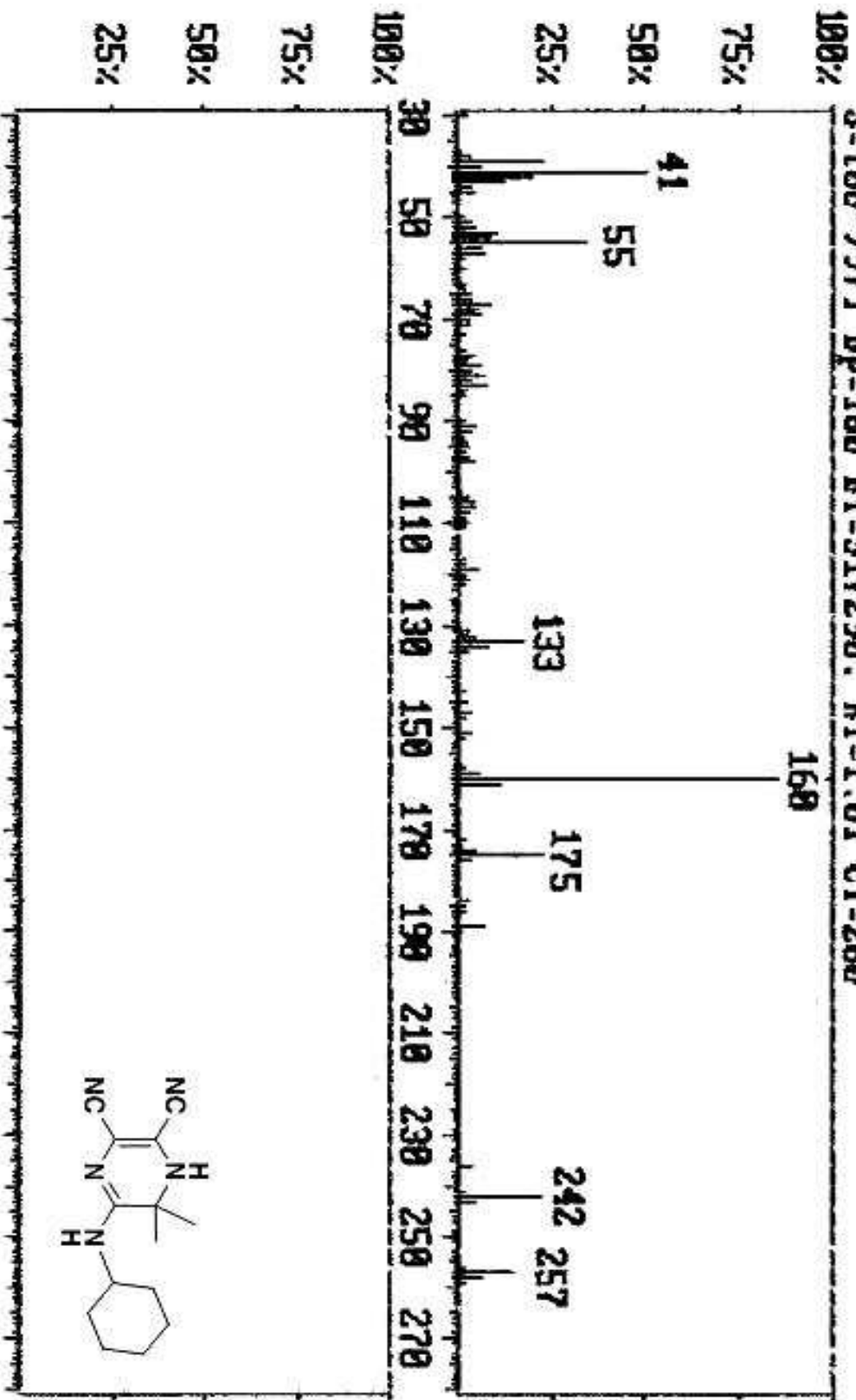
===== CHANNEL f1 =====
NUC1     13C
P1       8.75 usec
PL1      -2.00 dB
SFO1     75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    87.00 usec
PL2      2.00 dB
PL12     12.00 dB
PL13     18.00 dB
SFO2     300.1312005 MHz

F2 - Processing parameters
SI       65536
SF       75.4677490 MHz
MDM      EN
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
CY       70.01 cm
F1P      219.195 ppm
F1       16539.10 Hz
F2P      -19.187 ppm
F2       -1446.51 Hz
PRPMCK   11.91609 ppm/cm
HZCN     899.28058 Hz/cm
    
```

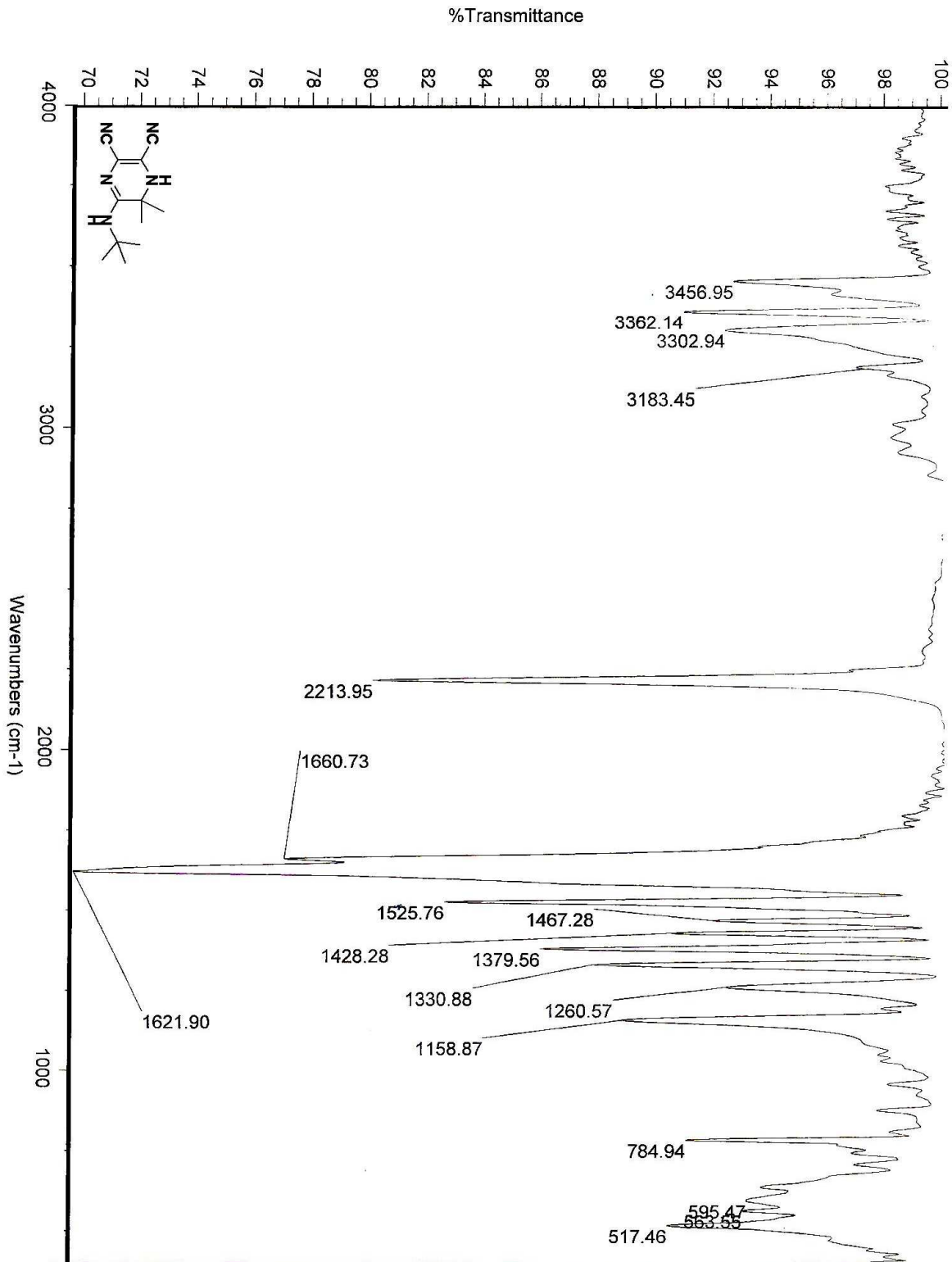
File : D1_49.X51 Date 8/ 3/10 Time 14:46:29
 S=[188->971] Bp=160 R1=317290. RT=1.61 CT=260



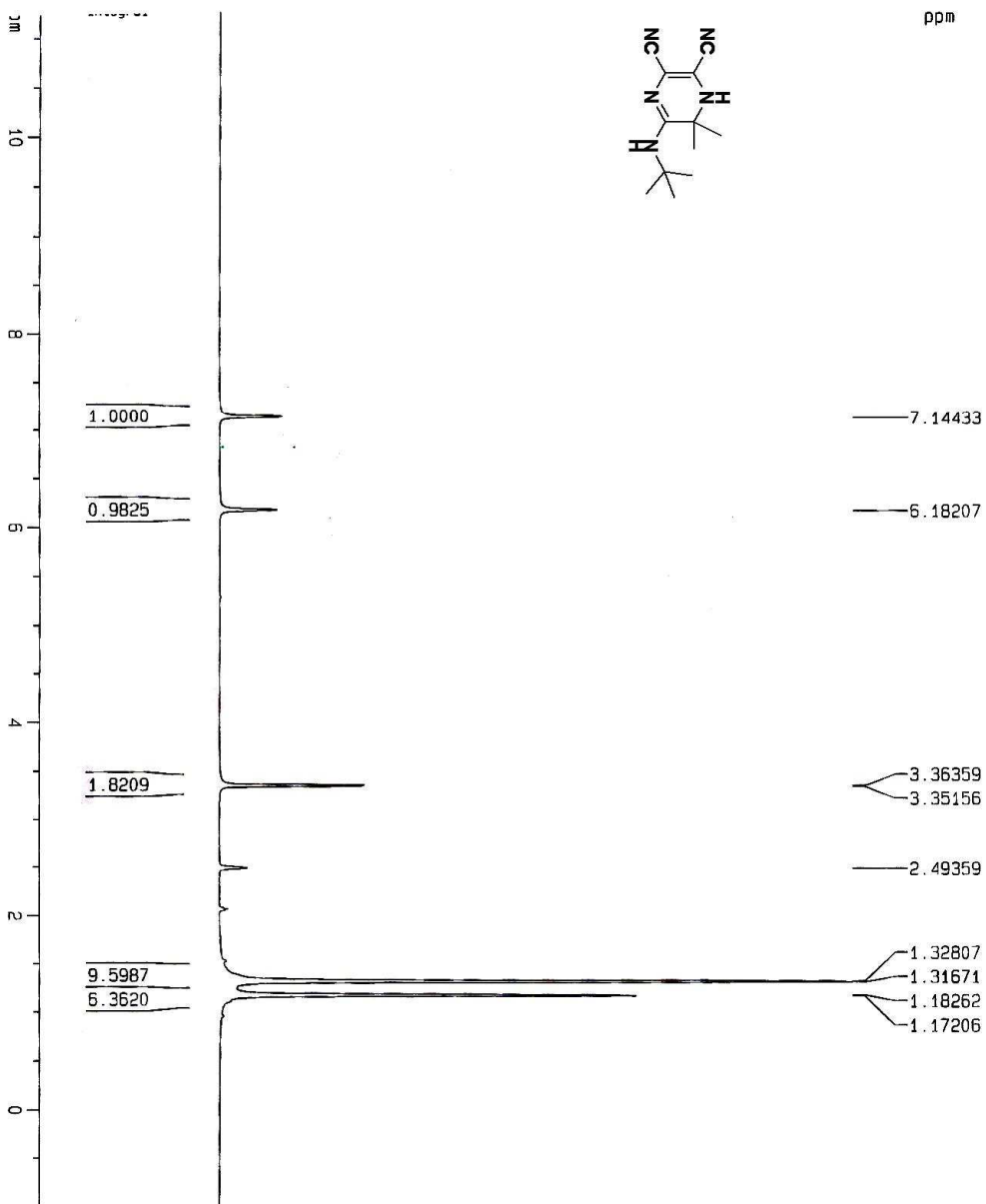
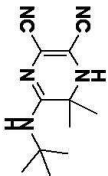
280 300 320 340 360 380 400 420 440 460 480 500 520
 SB=30 SE=510 DB=30 DE=510 N=0 Z=2 T=0.0 Fact1 -> 1 *1
 S List > S=[188->971] B=0 Pos=6 Tot=6

Mass of 6a

IR of 6b



¹H NMR



¹H NMR of 6b

```

Current Data Parameters
NAME      Maleki-1PHD
EXPNO    386
PROCNO   1

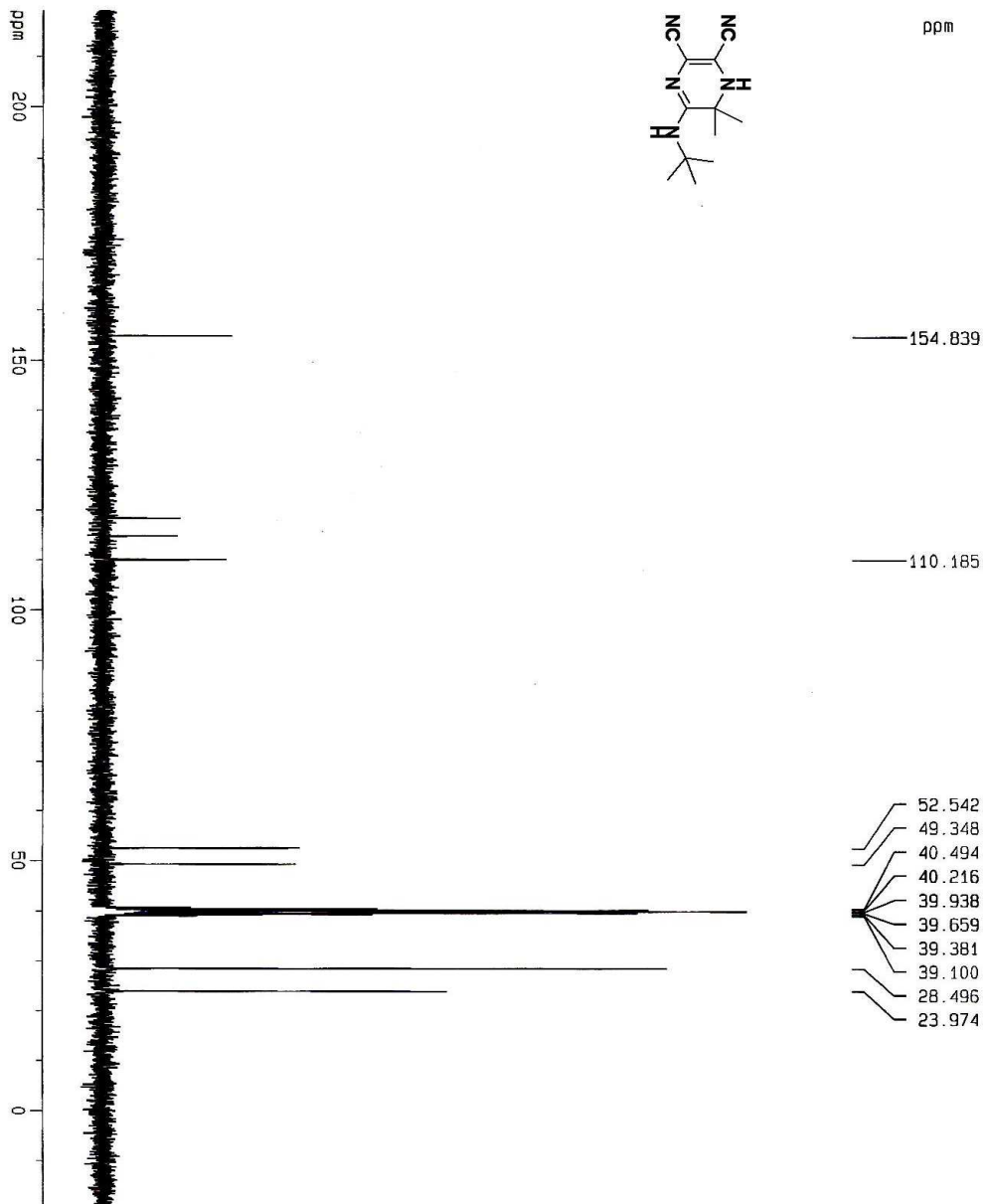
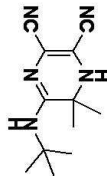
F2 - Acquisition Parameters
Date_    20090510
Time     20.50
INSTRUM spect
PROBHD   5 mm BBO BB-1H
PULPROG zg30
TD       32768
SOLVENT  DMSO
NS       10
DS       1
SMH      7812.500 Hz
FIDRES   0.238419 Hz
AQ       2.0972021 sec
RG       229.1
DM       64.000 usec
DE       5.00 usec
TE       380.0 K
D1       2.00000000 sec

***** CHANNEL f1 *****
NUC1     1H
P1       15.50 usec
PL1      -2.00 dB
SFO1     300.1323986 MHz

F2 - Processing parameters
SI       65536
SF       300.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

ID NMR plot parameters
CX       20.00 cm
CY       10.68 cm
F1P      11.380 ppm
F1       3415.45 Hz
F2P      -1.032 ppm
F2       -309.59 Hz
PPMCM    0.62057 ppm/c
HZCM     186.25162 Hz/c
  
```

¹³C (1H) NMR



¹³C NMR of 6b

```

Current Data Parameters
NAME      Molek1-PHD
EXPNO     387
PROCNO    1

F2 - Acquisition Parameters
Date_     20090510
Time      20.54
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         70
DS         2
SWH        17965.611 Hz
FIDRES     0.274439 Hz
AQ         1.8219508 sec
RG         3248
DE         27.800 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

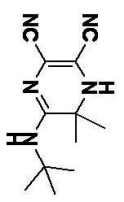
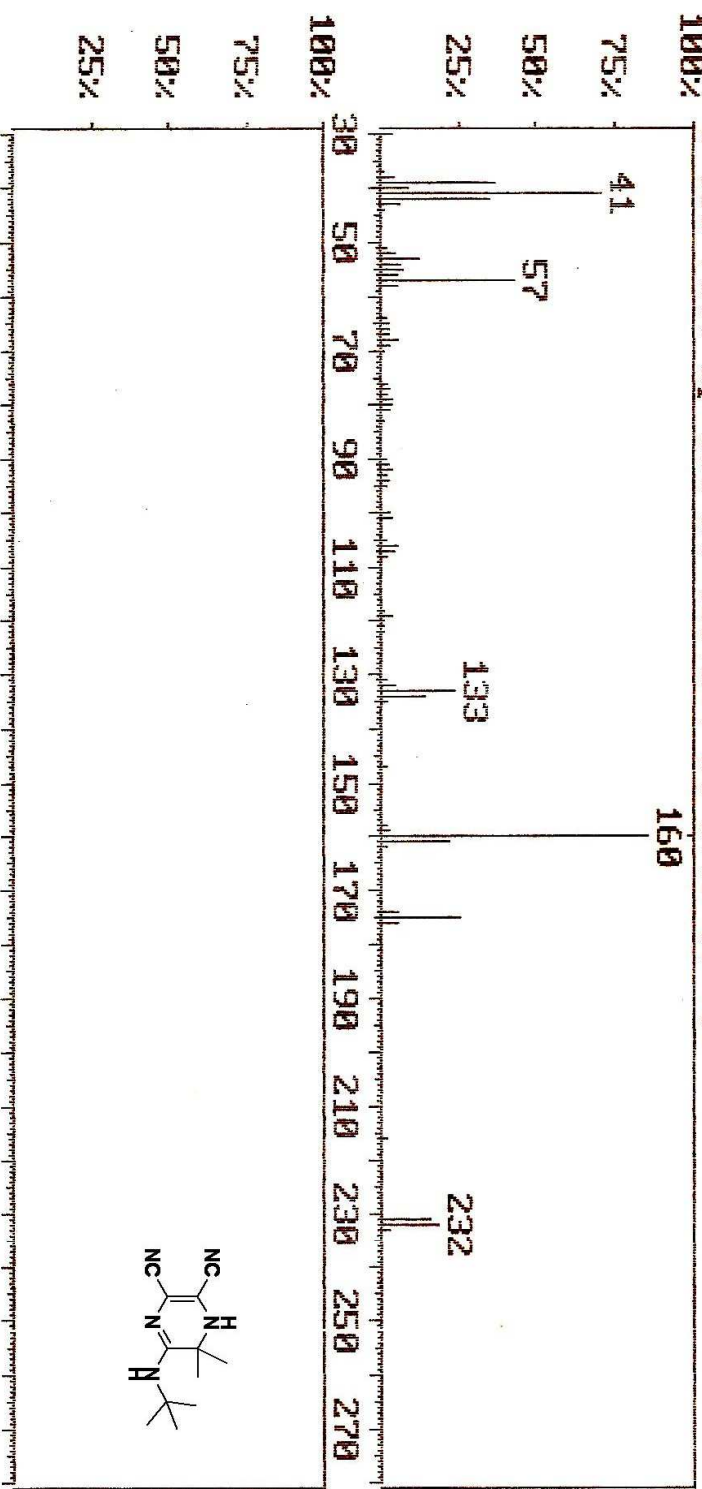
----- CHANNEL f1 -----
NUC1       13C
P1         8.75 usec
PL1        -2.00 dB
SFO1       75.4752983 MHz

----- CHANNEL f2 -----
CHOPRG2    waltz16
NUC2        1H
PCPD2      87.00 usec
PL2        -2.00 dB
PL13       12.00 dB
PL13       18.00 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         65536
SF         75.4677490 MHz
MOM        EN
SSB        0
L8         1.00 Hz
BB         0
PC         1.40

10 NMR plot parameters
CX         20.00 cm
CY         10.77 cm
F1P        219.155 ppm
F1         16539.10 Hz
F2P        -1446.51 Hz
F2         -19.167 ppm
PRWCM      11.91609 ppm/cm
HZCM       899.28058 Hz/cm
    
```

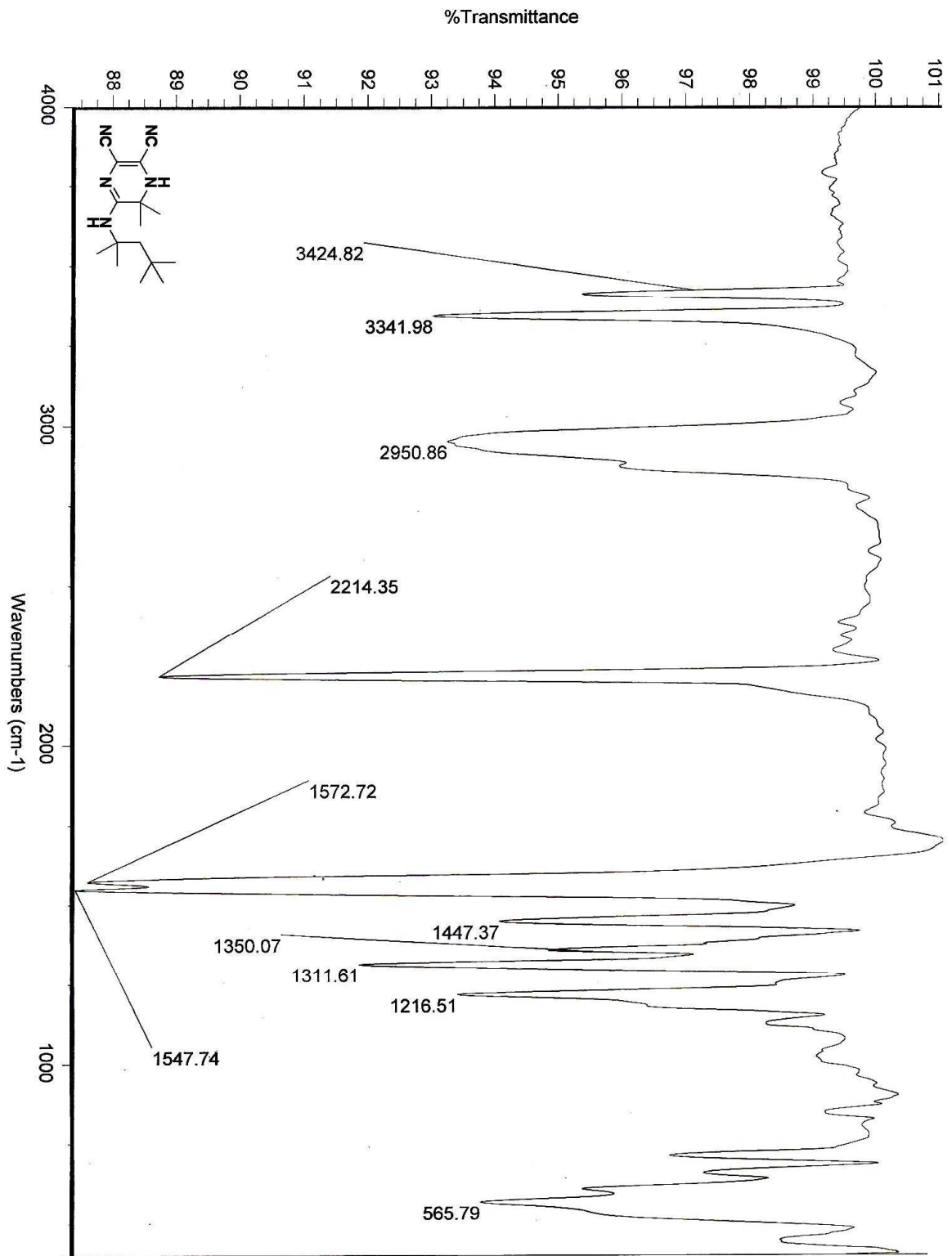
DI/MALEKI-N1/88.03.03
 File : DI_70.X63 Date 8/29/10 Time 15:28:04
 S=[56->68] Bp=160 Bi=403750. RT=1.12 CT=198

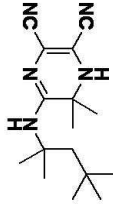


280 300 320 340 360 380 400 420 440 460 480 500 520
 SB=30 SE=530 DB=30 DE=530 N=0 Z=2 T=0.0 Fact1 -> 1 *1
 S List > S=[56->68] B=0 Pos=2 Tot=

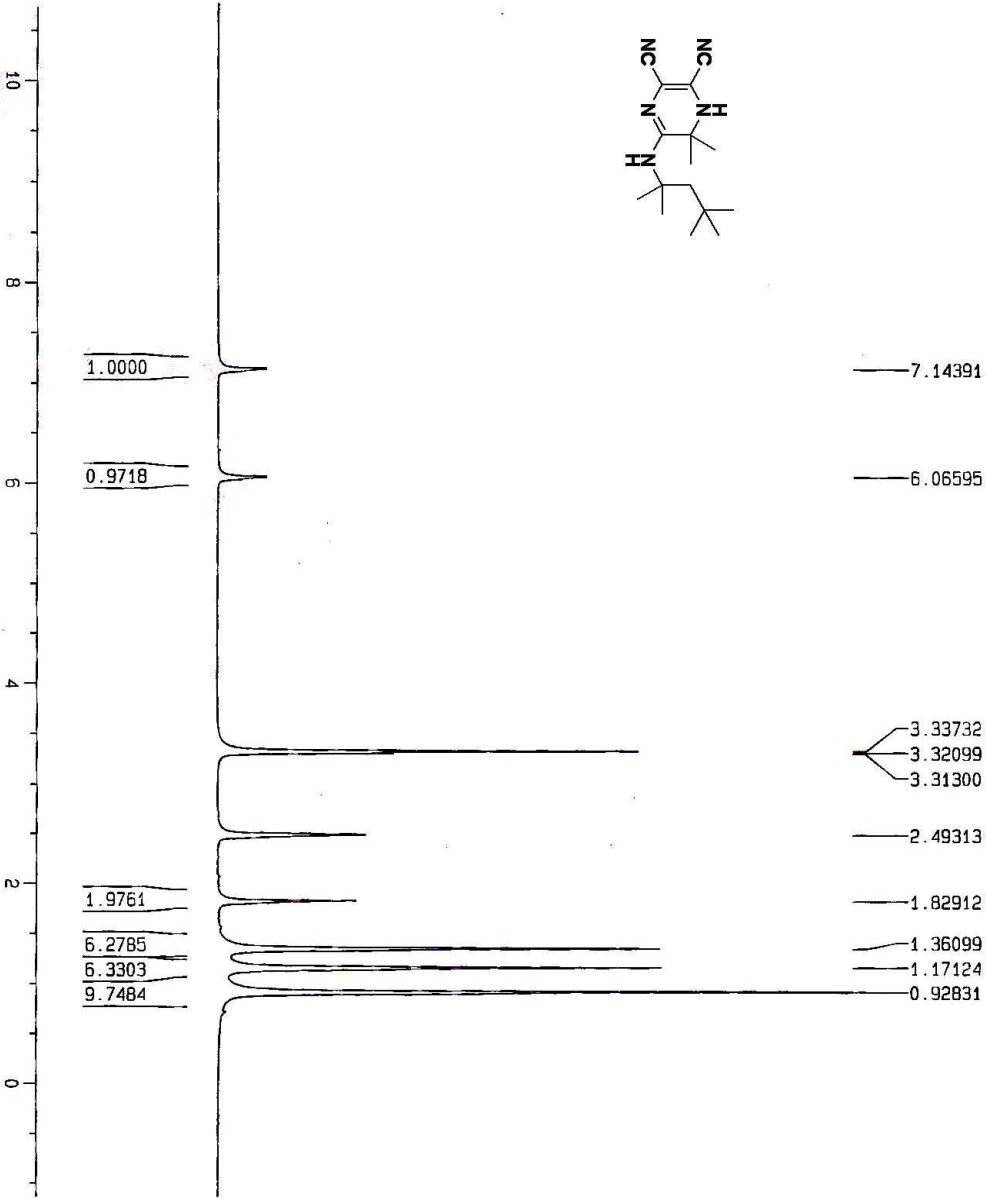
Mass of 6b

IR of 6c





¹H NMR



Current Data Parameters
 NAME Maleki-PHD
 EXNO 378
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090510
 Time 19.30

INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 10

DS 1
 SMH 7812.500 Hz
 FIDRES 0.238419 Hz
 AQ 2.0972021 sec

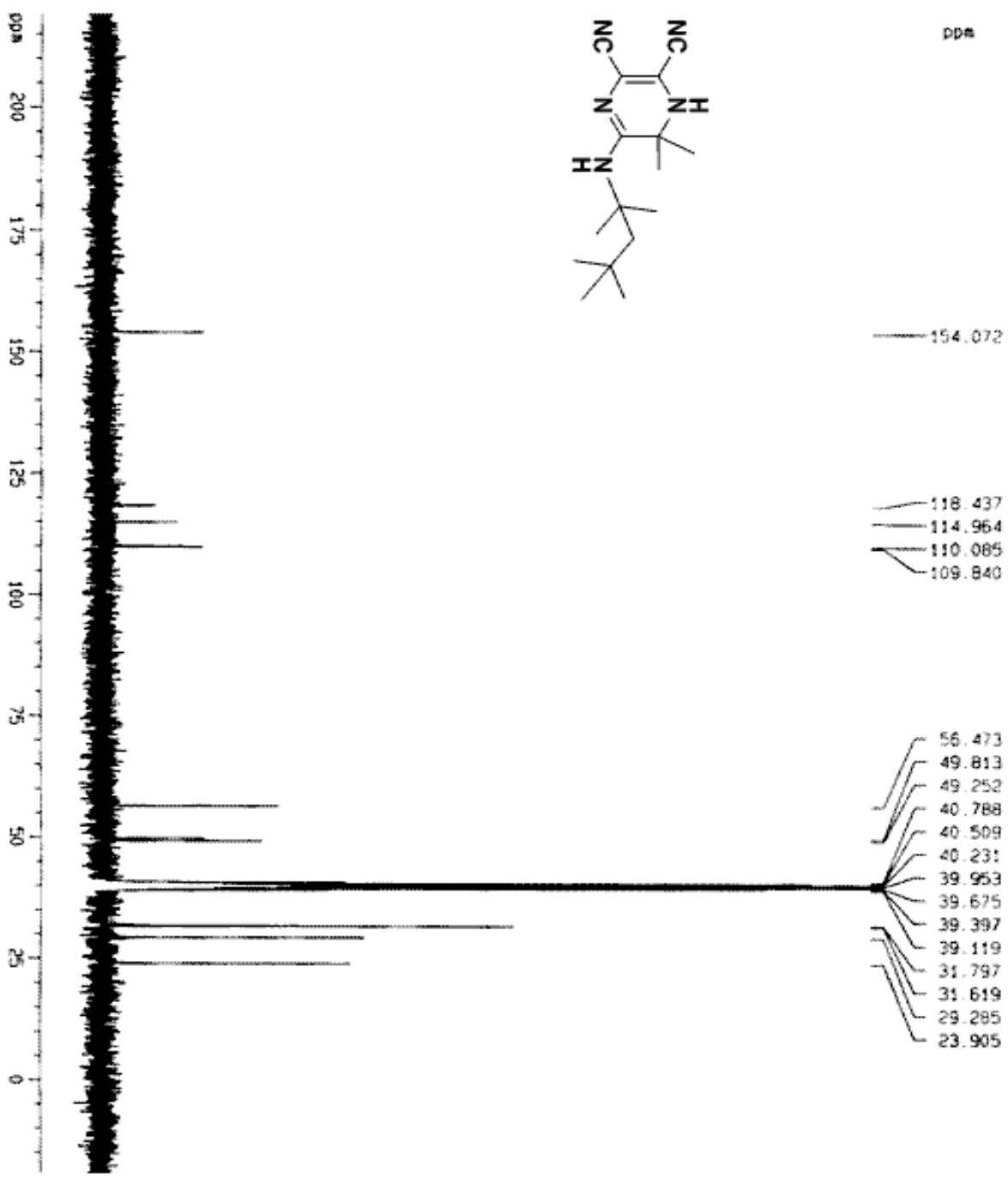
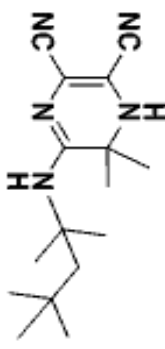
RG 228.1
 DM 64.000 usec
 DE 6.00 usec
 TE 380.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.50 usec
 PL1 -2.00 dB
 SF01 300.1323986 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300000 MHz
 MDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 11.37 cm
 F1P 11.246 ppm
 F1 3375.18 Hz
 F2P -1.132 ppm
 F2 -339.79 Hz
 PPMCM 0.61889 ppm/cm
 HZCM 185.74823 Hz/cm

¹H NMR of 6c

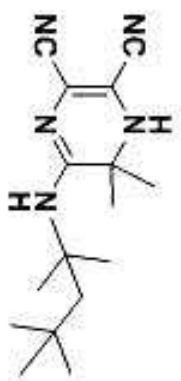
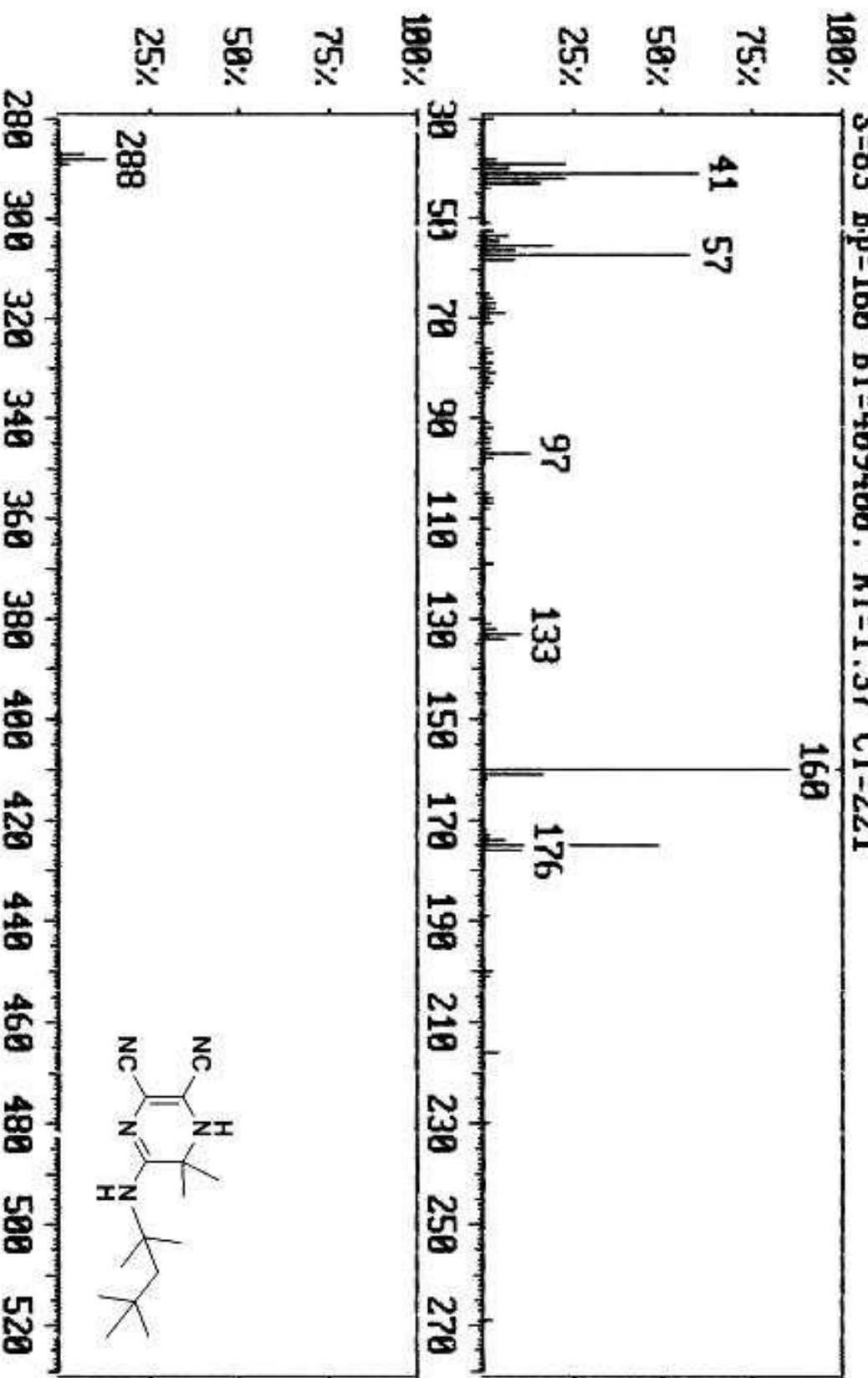


^{13}C NMR of 6c

```

Current Data Parameters
NAME:          height1
EXPNO:        124
PROCNO:       1
----- Acquisition Parameters
Date_         20070109
Time         14.25
INSTRUM:      spect
PROBHD:       5 mm BBO BB-1H
PULPROG:     zgpg30
RG:           655.56
SOLVENT:      DMSO
NS:           257
DS:           2
SWH:          17395.611 Hz
FIDRES:       0.274429 Hz
AQ:           1.8219568 sec
RG:           2048
DM:           27.800 uSec
DE:           6.00 uSec
TE:           300.0 K
O1:           2.00000000 SFC
O11:          0.03000000 SFC
O12:          0.00000000 SFC
----- CHANNEL f1 -----
NUC1:         13C
P1:           8.75 uSec
PC1:          -2.00 dB
SFO1:         75.4752933 MHz
----- CHANNEL f2 -----
CPDPRG2:      waltz16
NUC2:         1H
PCPD2:        87.00 uSec
PC2:          -2.00 dB
PC12:         12.00 dB
PC13:         18.00 dB
SFO2:         300.1312005 MHz
----- Processing parameters
SI:           65536
SF:           75.4677493 MHz
WDW:          EM
SSB:          0
LB:           1.00 Hz
GB:           0
PC:           1.40
----- 1D NMR 0101 parameters
CA:           20.00 cm
CF:           25.63 cm
F2P:         219.155 ppm
F1:          16039.11 Hz
F2:          -15.167 ppm
PITCH:       11.91699 deg/cm
WDW:         899.29029 Hz/cm
  
```

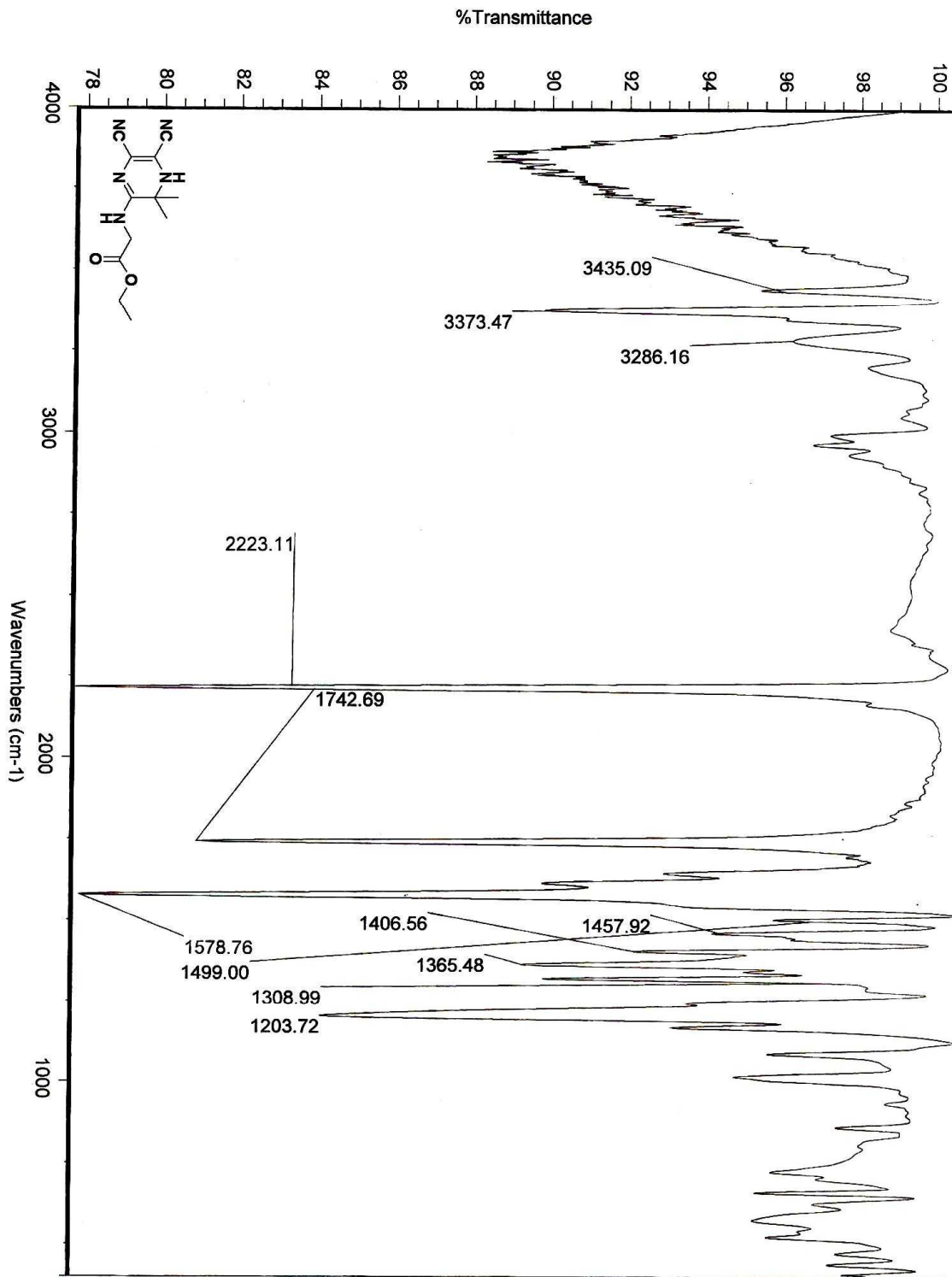
File : DI_50.X04 Date 8/ 4/10 Time 03: 8:01
 S=83 Bp=160 Bi=409400. RT=1.37 CI=221



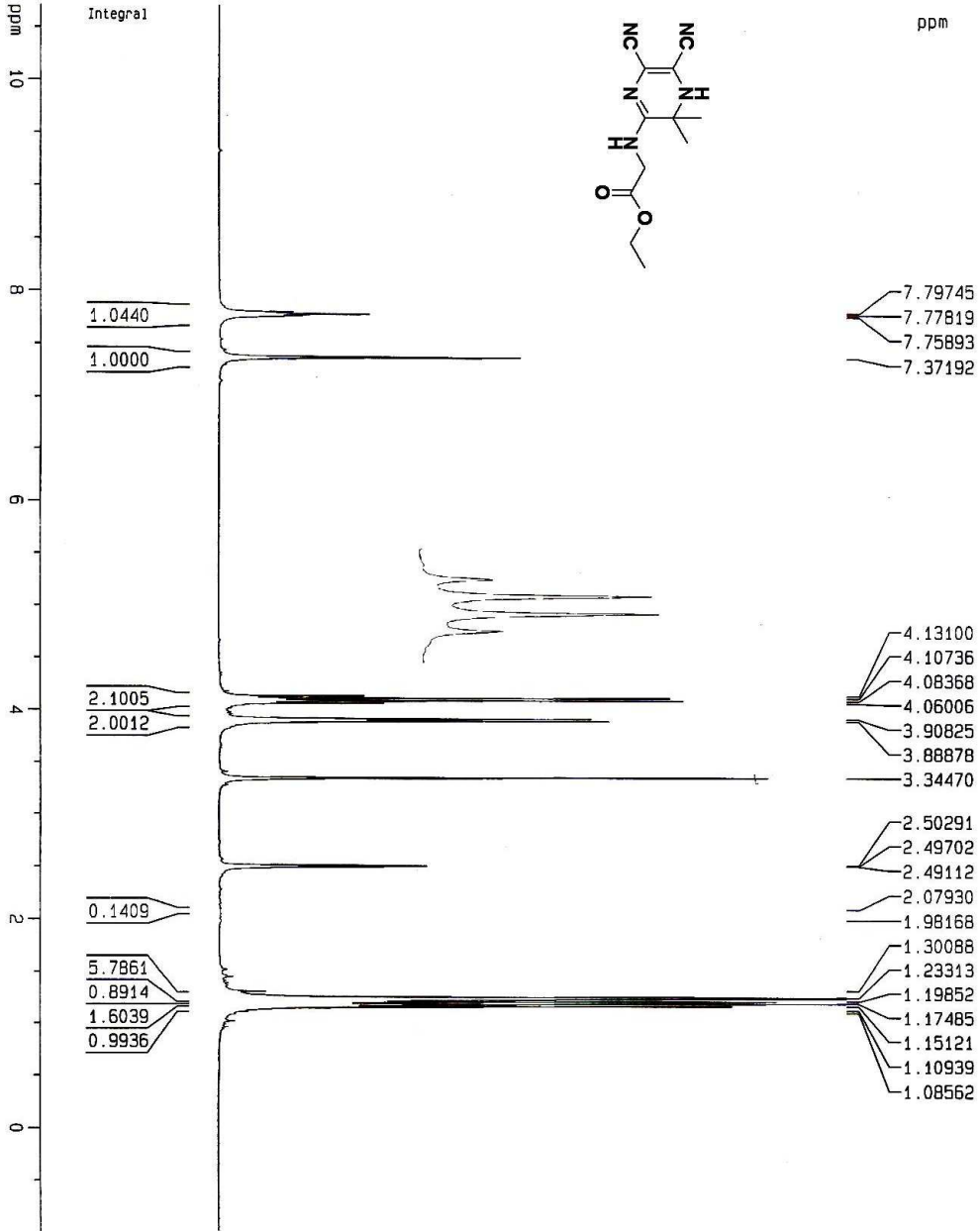
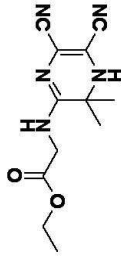
SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 FacIL -> 1 *1
 S List > S=83 B=0 Pos=5 Tot=5

Mass of 6c

IR of 6d



¹H NMR



¹H NMR of 6d

```

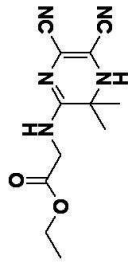
Current Data Parameters
NAME:          Set1d hamze
EXPNO:         148
PROCNO:        1

F2 - Acquisition Parameters
Date_:         20090505
Time:          23.09
INSTRUM:       spect
PROBHD:        5 mm BBO BB-1H
PULPROG:       zg30
TD:            32768
SOLVENT:       DMSO
NS:            10
DS:            1
SWH:           7812.500 Hz
FIDRES:        0.238419 Hz
AQ:            2.0972021 sec
RG:            228.1
DM:            64.000 usec
DE:            6.00 usec
TE:            380.0 K
D1:            2.00000000 sec

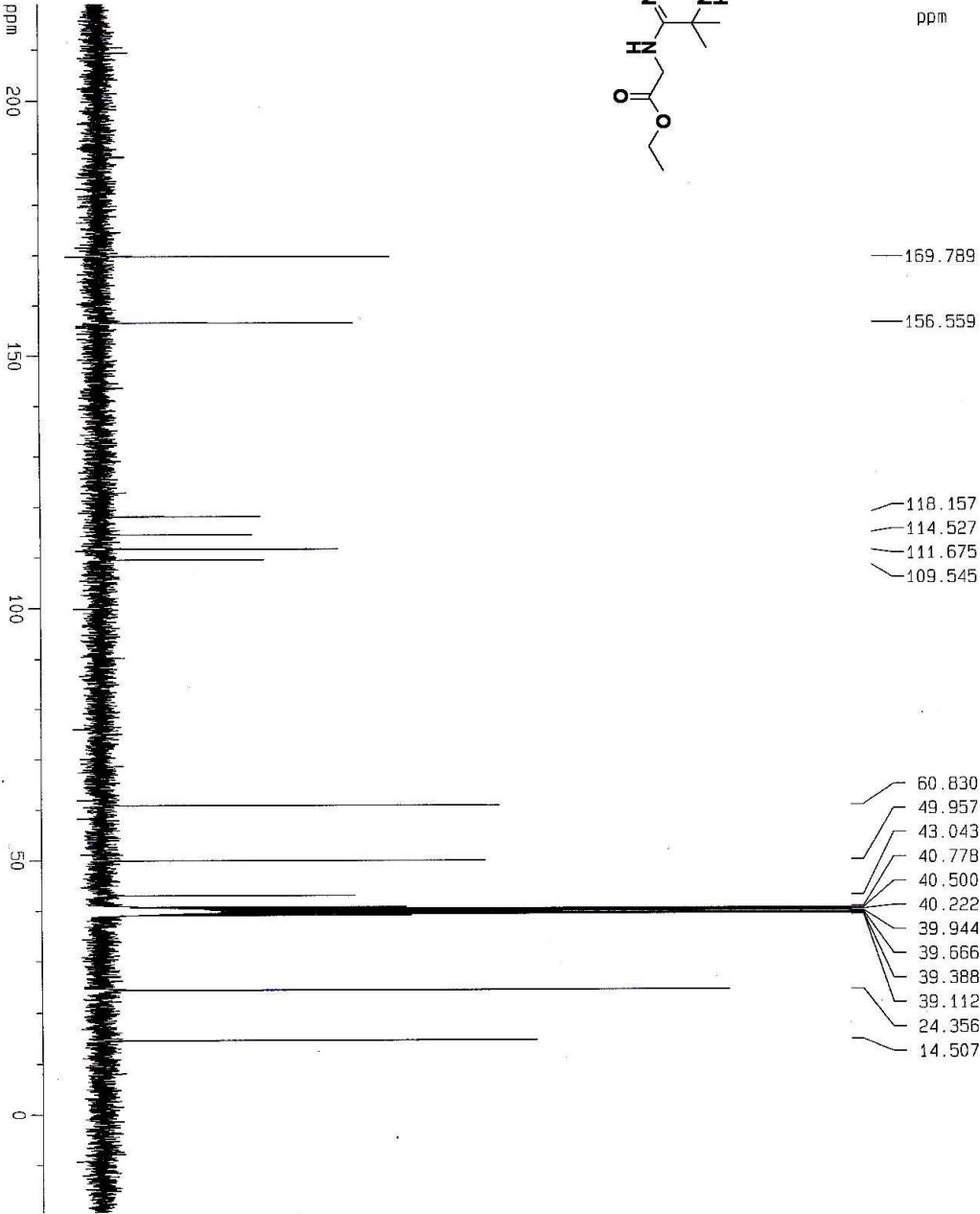
===== CHANNEL f1 =====
NUC1:           1H
P1:            15.50 usec
PL1:           -2.00 dB
SFO1:          300.1323986 MHz

F2 - Processing parameters
SI:            65536
SF:            300.1300000 MHz
WDW:           EM
SSB:           0
LB:            0.30 Hz
GB:            0
PC:            1.00

1D NMR plot parameters
CX:            20.00 cm
CY:            39.62 cm
F1P:           10.709 ppm
F1:            3214.09 Hz
F2P:           -0.998 ppm
F2:            -299.52 Hz
PPMCM:         0.58535 ppm/cm
HZCM:         175.68059 Hz/cm
    
```



¹³C {1H} NMR



Current Data Parameters
 NAME Setid hamze
 EXPNO 147
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090505
 Time 22:26

INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 348
 DS 2

SMH 17995.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2048
 DM 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 d12 0.00002000 sec

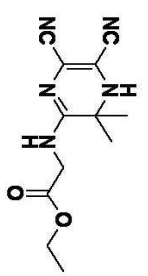
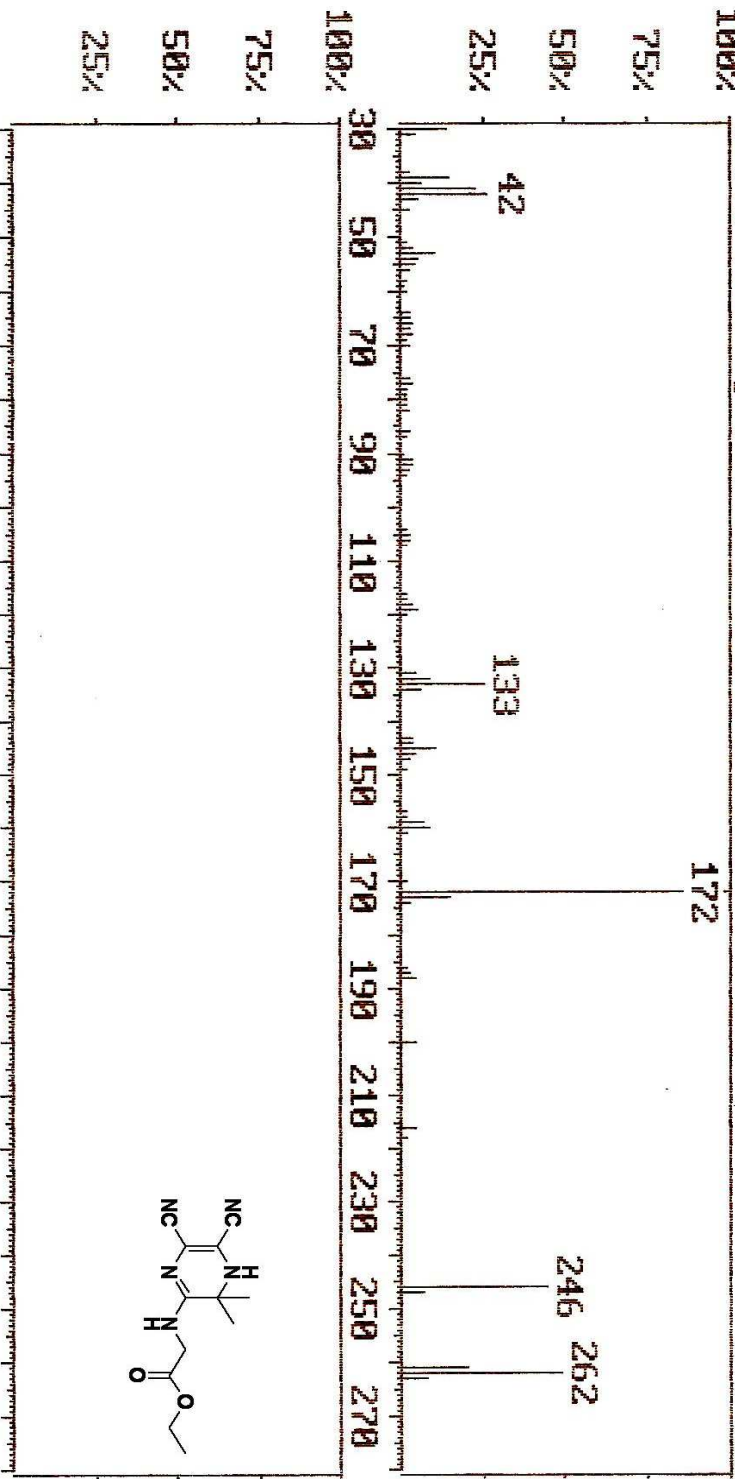
***** CHANNEL f1 *****
 NUC1 13C
 P1 8.75 usec
 PL1 -2.00 dB
 SF01 75.4752953 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 87.00 usec
 PL2 -2.00 dB
 PL12 12.00 dB
 PL13 18.00 dB
 SF02 300.1312009 MHz

F2 - Processing parameters
 SI 65536
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 36.44 cm
 F1P 219.155 ppm
 F1 16559.10 Hz
 F2P -19.167 ppm
 F2 -146.51 Hz
 PPM/CX 11.91609 ppm/cm
 HZ/CX 899.28058 Hz/cm

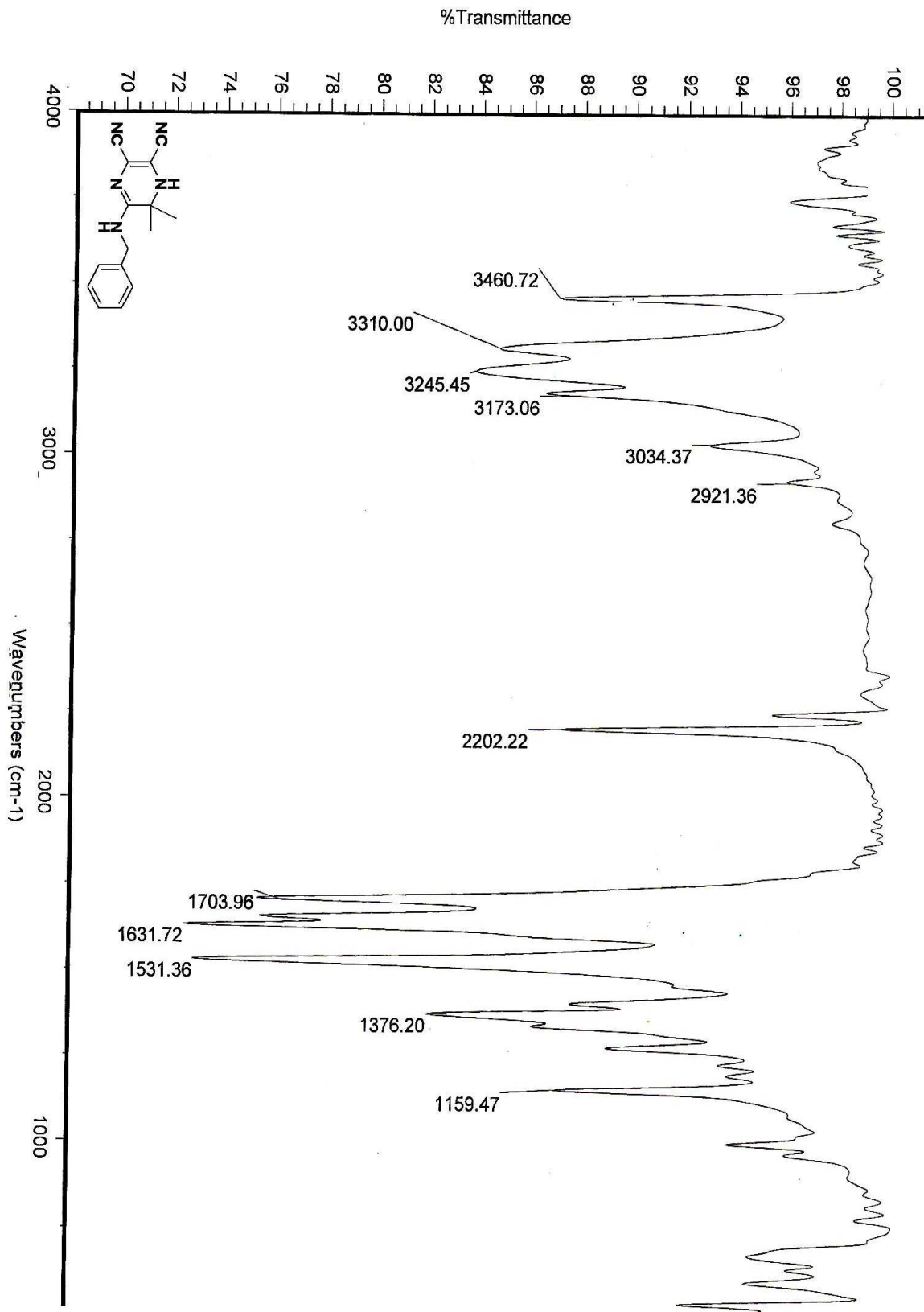
DI/MALEKI-5/88.03.03
 File : D1_70.X65 Date 8/29/10 Time 15:42:22
 S=173->841 Bp=172 Bi=375700. RT=1.39 CI=226



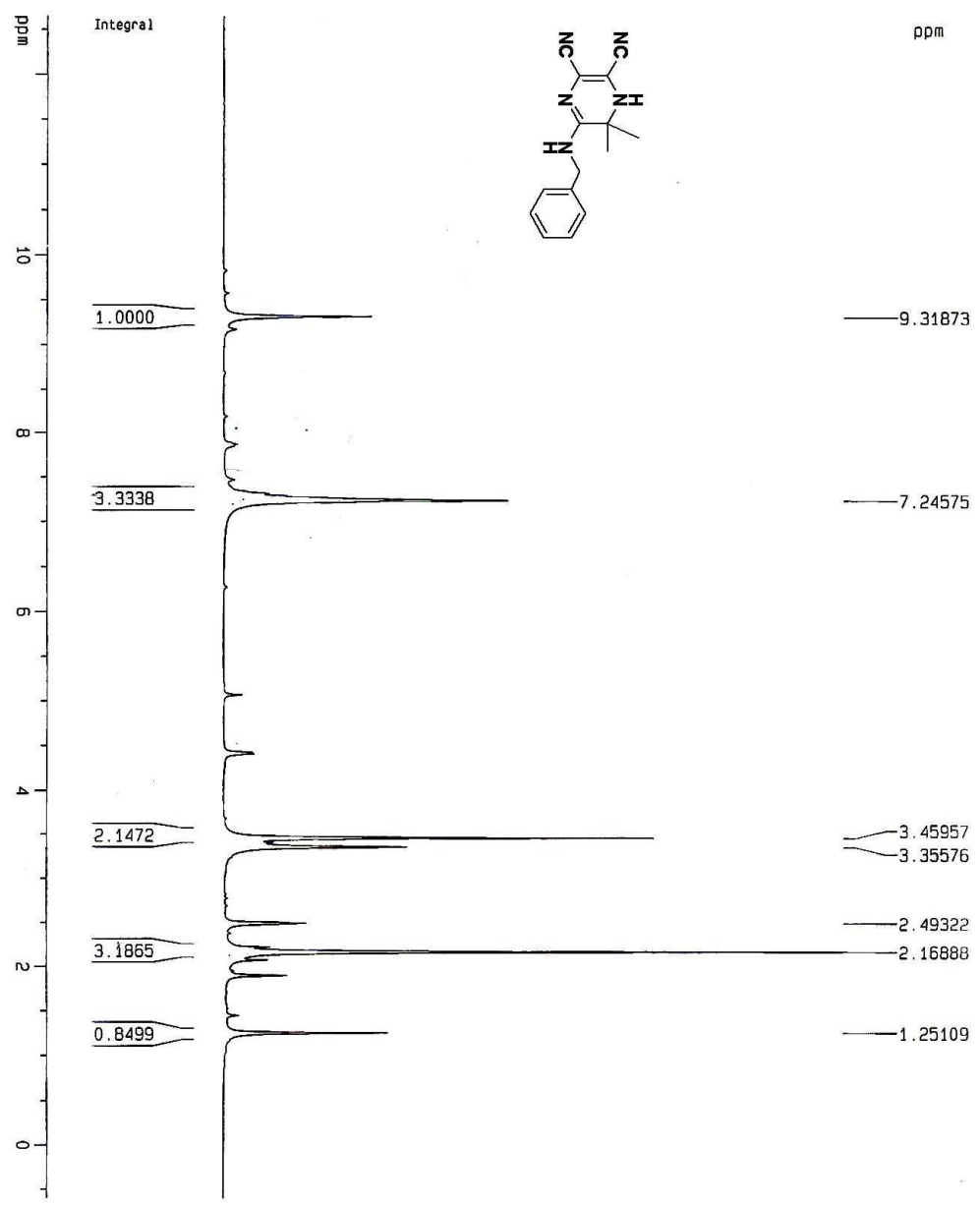
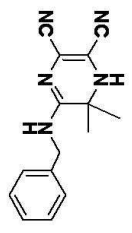
SB=30 SE=288 DB=30 DE=510 N=0 Z=2 T=0.0 FactL -> 1 *1
 S List > S=173->841 B=0 Pos=4 Tot=4

Mass of 6d

IR of 6e



1H NMR



1H NMR of 6e

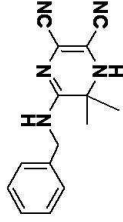
Current Data Parameters
 NAME: Nalaki-PHD
 EXPNO: 402
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20090518
 Time: 17.50
 INSTRUM: spect
 PROBHD: 5 mm BBO BB-1H
 PULPROG: zg30
 TD: 32768
 SOLVENT: DMSO
 NS: 10
 DS: 1
 SMH: 7812.500 Hz
 FIDRES: 0.238419 Hz
 AQ: 2.0972021 sec
 RG: 228.1
 DW: 64.000 usec
 DE: 6.00 usec
 TE: 380.0 K
 D1: 2.00000000 sec

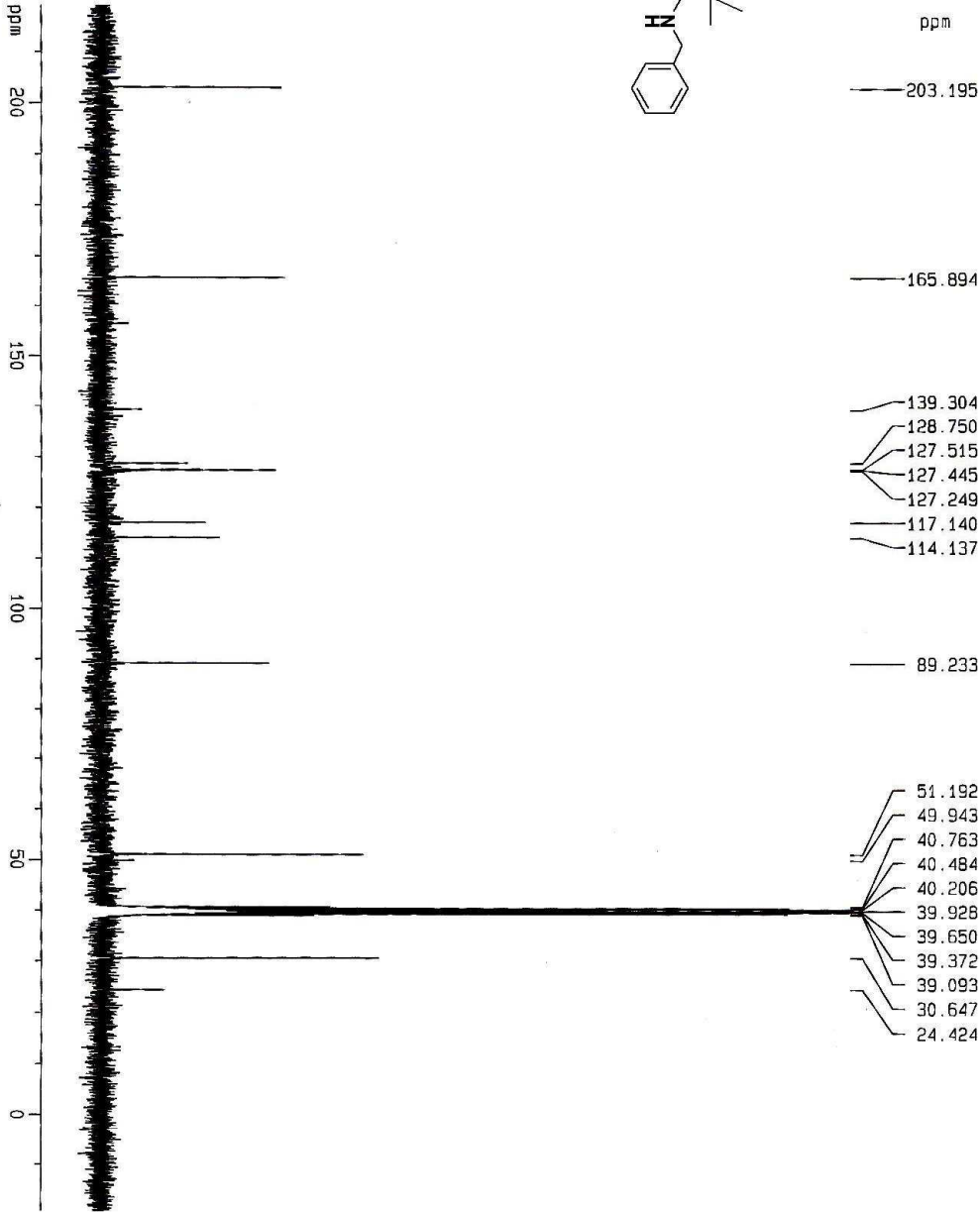
===== CHANNEL f1 =====
 NUC1: 1H
 P1: 15.50 usec
 PL1: -2.00 dB
 SFO1: 300.1323986 MHz

F2 - Processing parameters
 SI: 65536
 SF: 300.1300000 MHz
 MDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 CY: 11.97 cm
 F1P: 12.655 ppm
 F1: 3798.02 Hz
 F2P: -0.595 ppm
 F2: -178.71 Hz
 PPM1CH: 0.66250 ppm/cm
 HZ1CH: 198.83617 Hz/cm



¹³C (1H) NMR



¹³C NMR of 6e

```

Current Data Parameters
NAME           Maleki-PHD
EXPNO          403
PROCNO         1

F2 - Acquisition Parameters
Date_          20090518
Time           18.00
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        zgpg30
TD             65536
SOLVENT        DMSO
NS             358
DS             2
SMH            17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG             2048
OH             27.800 usec
DE             6.00 usec
TE             300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
d12            0.00020000 sec

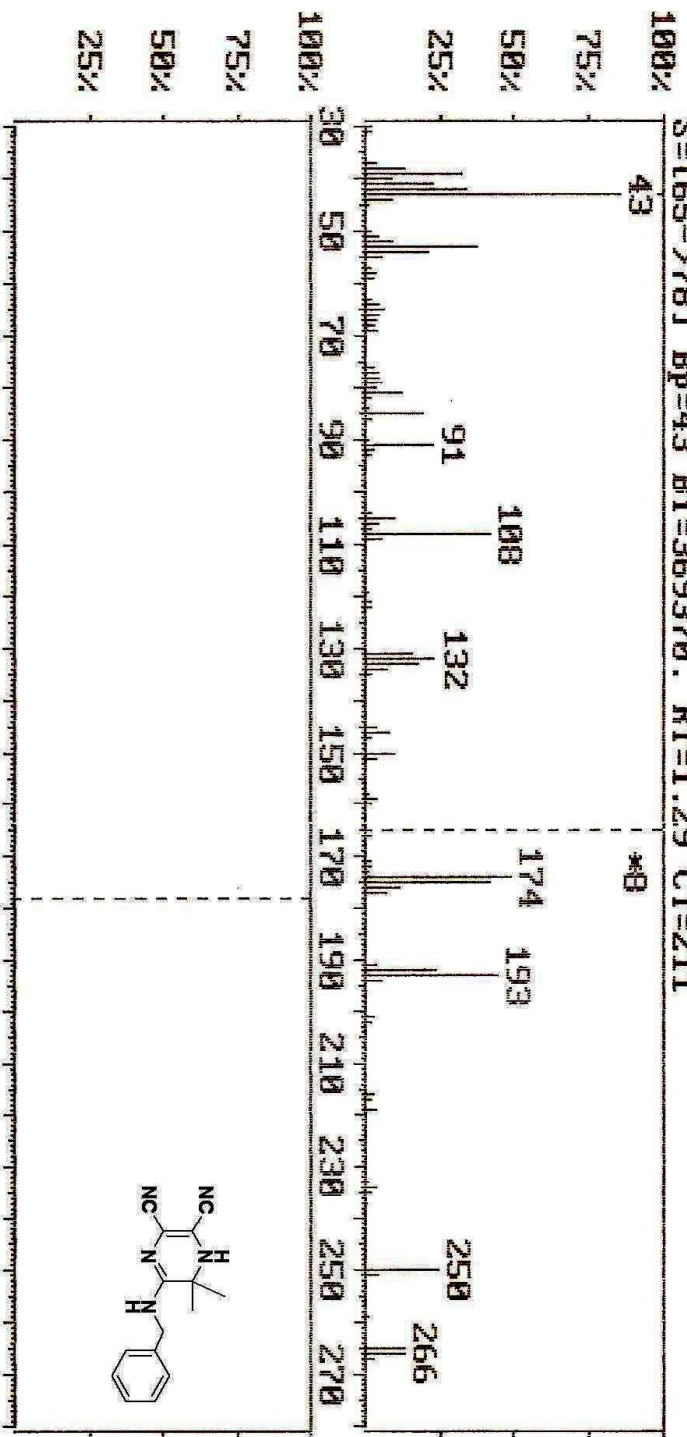
===== CHANNEL f1 =====
NUC1           13C
P1             8.75 usec
PL1            -2.00 dB
SFO1           75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2        mltz16
NUC2           1H
PCPD2          87.00 usec
PL2            -2.00 dB
PL12           12.00 dB
PL13           18.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI             65536
SF             75.4677490 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40

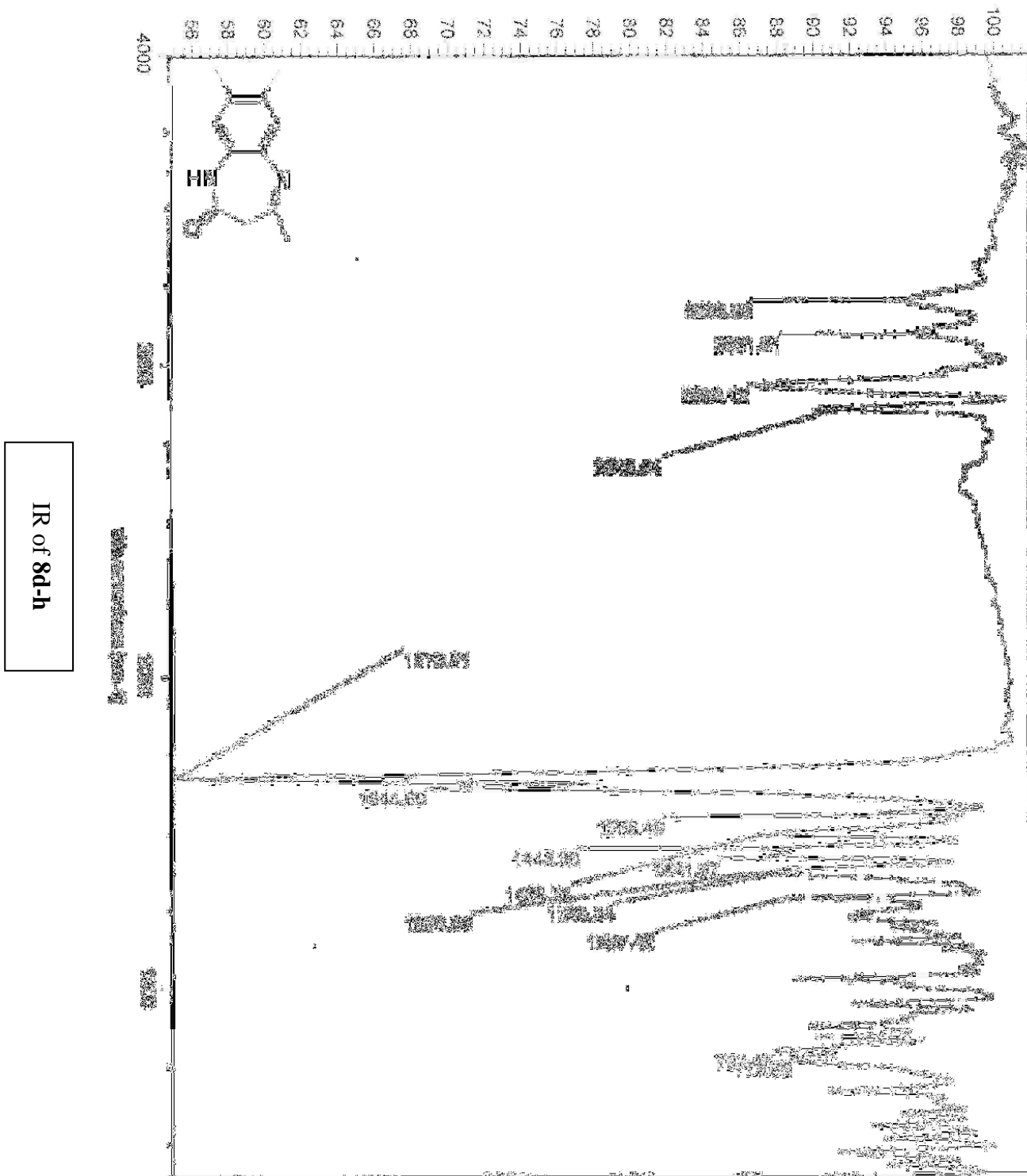
10 NMR plot parameters
CX             20.00 cm
CY             26.55 cm
F1P           219.155 ppm
F1            16539.10 Hz
F2P           -19.167 ppm
F2            -1466.51 Hz
PPHCK         11.91609 ppm/cm
HZCK          899.28058 Hz/cm
  
```

DI/MALEKI-M4/88.03.03
 File : DI_70.X64 Date 8/29/10 Time 15:34:24
 S=165->781 Bp=43 Bi=369370. RT=1.29 CT=211



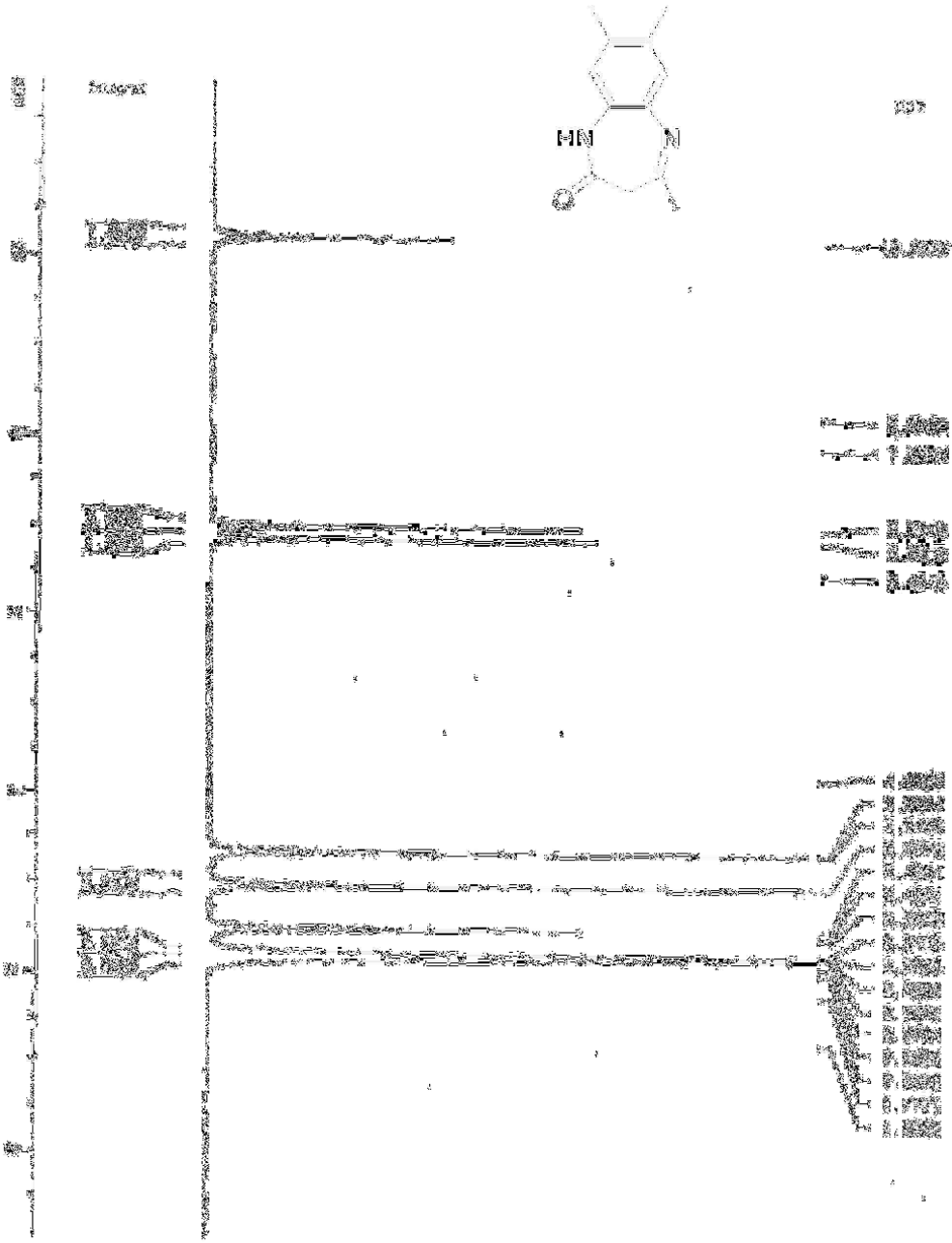
SB=30 SE=530 DB=30 DE=530 N=0 Z=2 T=0.0 Fact1165->4281 *8
 S List > S=165->781 B=0 Pos=4 Tot=4

Mass of 6e

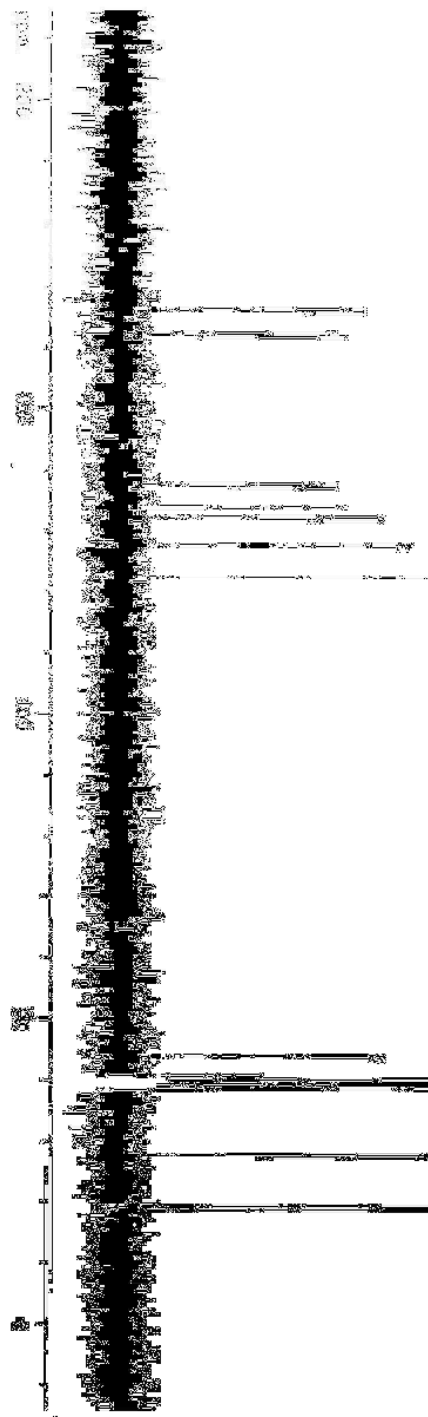
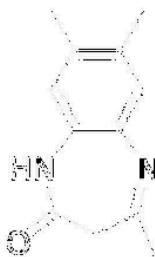


IR of 8d-h

¹H NMR of 8d-h



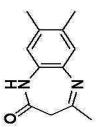
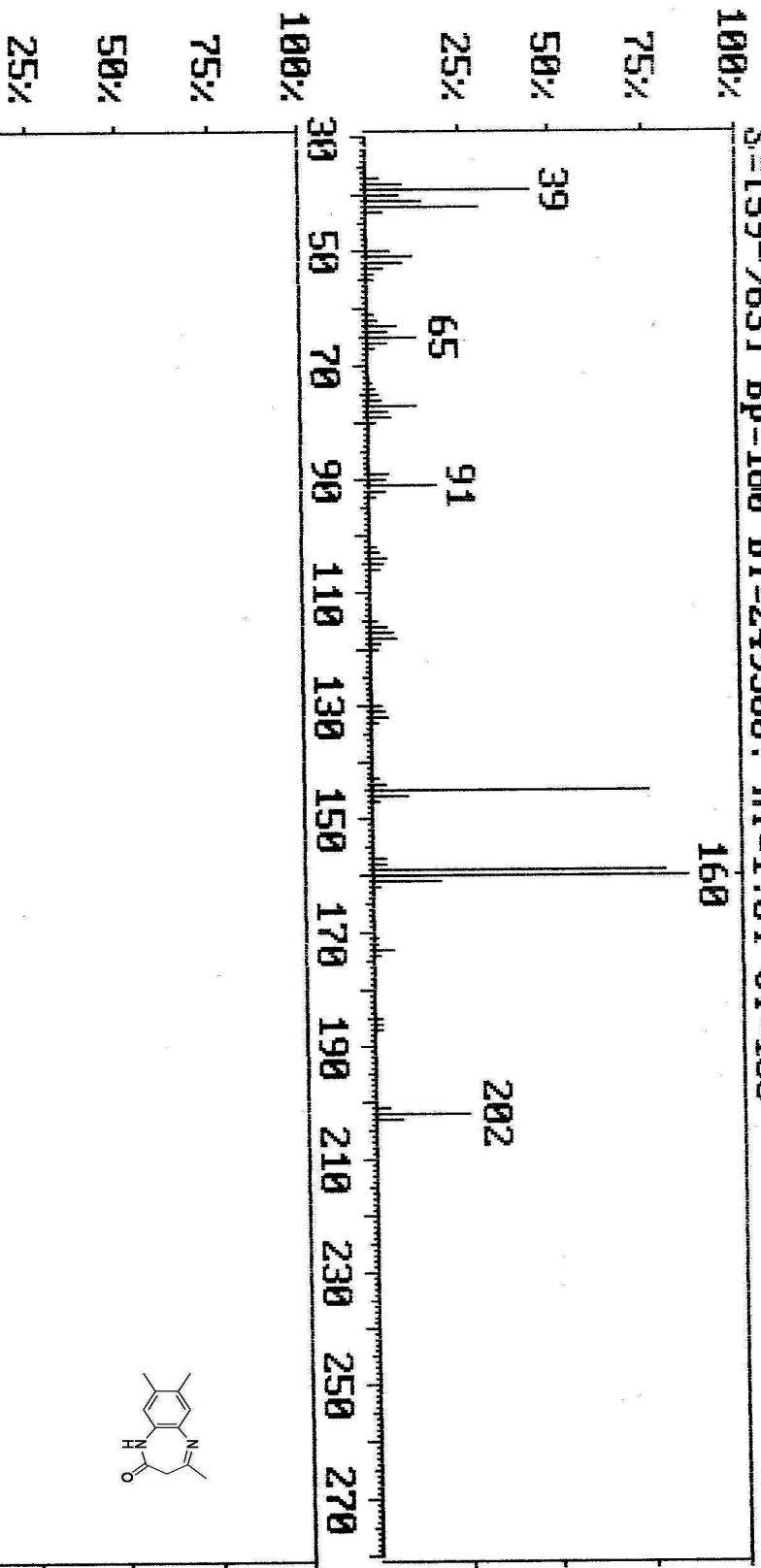
¹H NMR spectrum of 8d-h in CDCl₃. The spectrum shows a complex pattern of peaks, including a multiplet at approximately 7.5 ppm, a multiplet at approximately 7.2 ppm, a multiplet at approximately 6.8 ppm, a multiplet at approximately 6.5 ppm, a multiplet at approximately 6.2 ppm, a multiplet at approximately 5.8 ppm, a multiplet at approximately 5.5 ppm, a multiplet at approximately 5.2 ppm, a multiplet at approximately 4.8 ppm, a multiplet at approximately 4.5 ppm, a multiplet at approximately 4.2 ppm, a multiplet at approximately 3.8 ppm, a multiplet at approximately 3.5 ppm, a multiplet at approximately 3.2 ppm, a multiplet at approximately 2.8 ppm, a multiplet at approximately 2.5 ppm, a multiplet at approximately 2.2 ppm, a multiplet at approximately 1.8 ppm, a multiplet at approximately 1.5 ppm, a multiplet at approximately 1.2 ppm, a multiplet at approximately 0.8 ppm, and a multiplet at approximately 0.5 ppm.



¹³C NMR of 8d-h

13C NMR (400 MHz, DMSO-d6) δ: 198.2 (s, 1C), 159.8 (s, 1C), 158.5 (s, 1C), 157.2 (s, 1C), 155.8 (s, 1C), 154.5 (s, 1C), 153.2 (s, 1C), 151.8 (s, 1C), 150.5 (s, 1C), 149.2 (s, 1C), 147.8 (s, 1C), 146.5 (s, 1C), 145.2 (s, 1C), 143.8 (s, 1C), 142.5 (s, 1C), 141.2 (s, 1C), 139.8 (s, 1C), 138.5 (s, 1C), 137.2 (s, 1C), 135.8 (s, 1C), 134.5 (s, 1C), 133.2 (s, 1C), 131.8 (s, 1C), 130.5 (s, 1C), 129.2 (s, 1C), 127.8 (s, 1C), 126.5 (s, 1C), 125.2 (s, 1C), 123.8 (s, 1C), 122.5 (s, 1C), 121.2 (s, 1C), 119.8 (s, 1C), 118.5 (s, 1C), 117.2 (s, 1C), 115.8 (s, 1C), 114.5 (s, 1C), 113.2 (s, 1C), 111.8 (s, 1C), 110.5 (s, 1C), 109.2 (s, 1C), 107.8 (s, 1C), 106.5 (s, 1C), 105.2 (s, 1C), 103.8 (s, 1C), 102.5 (s, 1C), 101.2 (s, 1C), 99.8 (s, 1C), 98.5 (s, 1C), 97.2 (s, 1C), 95.8 (s, 1C), 94.5 (s, 1C), 93.2 (s, 1C), 91.8 (s, 1C), 90.5 (s, 1C), 89.2 (s, 1C), 87.8 (s, 1C), 86.5 (s, 1C), 85.2 (s, 1C), 83.8 (s, 1C), 82.5 (s, 1C), 81.2 (s, 1C), 79.8 (s, 1C), 78.5 (s, 1C), 77.2 (s, 1C), 75.8 (s, 1C), 74.5 (s, 1C), 73.2 (s, 1C), 71.8 (s, 1C), 70.5 (s, 1C), 69.2 (s, 1C), 67.8 (s, 1C), 66.5 (s, 1C), 65.2 (s, 1C), 63.8 (s, 1C), 62.5 (s, 1C), 61.2 (s, 1C), 59.8 (s, 1C), 58.5 (s, 1C), 57.2 (s, 1C), 55.8 (s, 1C), 54.5 (s, 1C), 53.2 (s, 1C), 51.8 (s, 1C), 50.5 (s, 1C), 49.2 (s, 1C), 47.8 (s, 1C), 46.5 (s, 1C), 45.2 (s, 1C), 43.8 (s, 1C), 42.5 (s, 1C), 41.2 (s, 1C), 39.8 (s, 1C), 38.5 (s, 1C), 37.2 (s, 1C), 35.8 (s, 1C), 34.5 (s, 1C), 33.2 (s, 1C), 31.8 (s, 1C), 30.5 (s, 1C), 29.2 (s, 1C), 27.8 (s, 1C), 26.5 (s, 1C), 25.2 (s, 1C), 23.8 (s, 1C), 22.5 (s, 1C), 21.2 (s, 1C), 19.8 (s, 1C), 18.5 (s, 1C), 17.2 (s, 1C), 15.8 (s, 1C), 14.5 (s, 1C), 13.2 (s, 1C), 11.8 (s, 1C), 10.5 (s, 1C), 9.2 (s, 1C), 7.8 (s, 1C), 6.5 (s, 1C), 5.2 (s, 1C), 3.8 (s, 1C), 2.5 (s, 1C), 1.2 (s, 1C), 0.0 (s, 1C).

DI/MALEKI-13/88.03.23
 File : DI_71.X14 Date 8/30/10 Time 04:26:34
 S=[159->631 Bp=160 Bi=249300. RT=1.04 CT=185



280 300 320 340 360 380 400 420 440 460 480 500 520
 SB=30 SE=204 DB=30 DE=510 N=0 Z=2 T=0.0 Fact1 -> 1 *1
 S List > S=[159->631 B=0 Pos=1 Tot=1

Mass of 8d-h