

Supporting Information

Heteropoly Acid Promoted Highly Efficient 1,4-Additions of Indoles and Pyrrole to Enones and Nitroalkene in Water

Mohammad R. Saidi* Fezzeh Arynasab and Najmodin Azizi

Department of Chemistry, Sharif University of Technology, P. O.

Box 11465-9516 Tehran 11365, Iran

Email saidi@sharif.edu

Table of content

| Contents: | Page number |
|---|-------------|
| Experimental Section | S2 |
| ¹ H and ¹³ C NMR spectra for products | S4-S27 |

Experimental Section

General. All chemicals were purchased and used without any further purification. NMR spectra were recorded at 500 MHz for proton and at 125.7 MHz for carbon nuclei in ($\text{CDCl}_3/\text{CCl}_4$) or ($\text{DMSO-d}_6/\text{CDCl}_3$). The products were purified by column chromatography carried out on silica gel by using ethyl acetate/ petroleum ether mixtures. Reactions were carried out room temperature, all the indole derivatives and Michael acceptors were employed, are commercially available. All products obtained are known compound. $\text{H}_3\text{PMO}_{12}\text{O}_{40}$ and $\text{H}_3\text{PW}_{12}\text{O}_{40}$ and other catalyst used without further purification. Water distilled before used.

General procedure for the Catalytic Michael addition of indole:

In the test tube equipped with magnet were introduces $\text{H}_3\text{PMO}_{12}\text{O}_{40}$ (10 mg, 0.0055 mmol) or $\text{H}_3\text{PW}_{12}\text{O}_{40}$ (10 mg, 0.0035 mmol), indole (1 mmol) and 2 ml of water. The Michael acceptor (1mmol) was added in one portion and the test tube was kept at room temperature under vigorous stirring for 1 -18. After the reaction was completed, water (2 ml) was added and the aqueous mixture was extracted with 10 ml of diethyl ether or ethyl acetate and dried over anhydrous Na_2SO_4 , and solvent was removed under reduce pressure to give the Michael addition products. The crude product was analyzed by ^1H and ^{13}C NMR. Further purification was carried out by short column chromatography on silica gel (ethyl acetate/petroleum ether). All compounds were characterized on the basis of their spectroscopic data (IR, NMR) and by comparison with those reported in the literature.¹⁻¹²

General procedure for the Catalytic Michael addition of Pyrrole

In the test tube equipped with magnet were introduced Michael acceptor (1-2.5 mmol, see Table 4), pyrrole (1 mmol) and 2 ml of water. $\text{H}_3\text{PMO}_{12}\text{O}_{40}$ (10 mg, 0.0055 mmol) or $\text{H}_3\text{PW}_{12}\text{O}_{40}$ (10 mg, 0.0035 mmol), was added in one portion and the test tube was kept at room temperature under vigorous stirring for 1-12. After the reaction was completed, water (2 ml) was added and the aqueous mixture was extracted with 10 ml of diethyl ether or ethyl acetate and dried over anhydrous Na_2SO_4 , and solvent was removed under reduced pressure to give the Michael addition products. The crude product was analyzed by ^1H and ^{13}C NMR. Further purification was carried out by short column chromatography on silica gel (ethyl acetate/petroleum ether). All compounds were characterized on the basis of their spectroscopic data (IR, NMR).

T17 1HNMR in CDCl3 at 298 K B4/4/14

Current Data Parameters
 NAME AZ171
 EXPNO 144
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050705
 Time 10.42
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg
 TO 32766
 SOLVENT CDCl3
 NS B
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 35.9
 DM 50.000 usec
 DE 6.50 usec
 TE 369.1 K
 D1 3.0000000 sec
 MCREST 0.0000000 sec
 MCWRRK 0.015000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 32.00 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 XDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 18.00 cm
 CY 16.77 cm
 F1P 10.115 ppm
 F1 5060.49 Hz
 F2P 0.121 ppm
 F2 60.49 Hz
 PPMCM 0.55541 ppm/cm
 HZCM 277.77777 Hz/cm

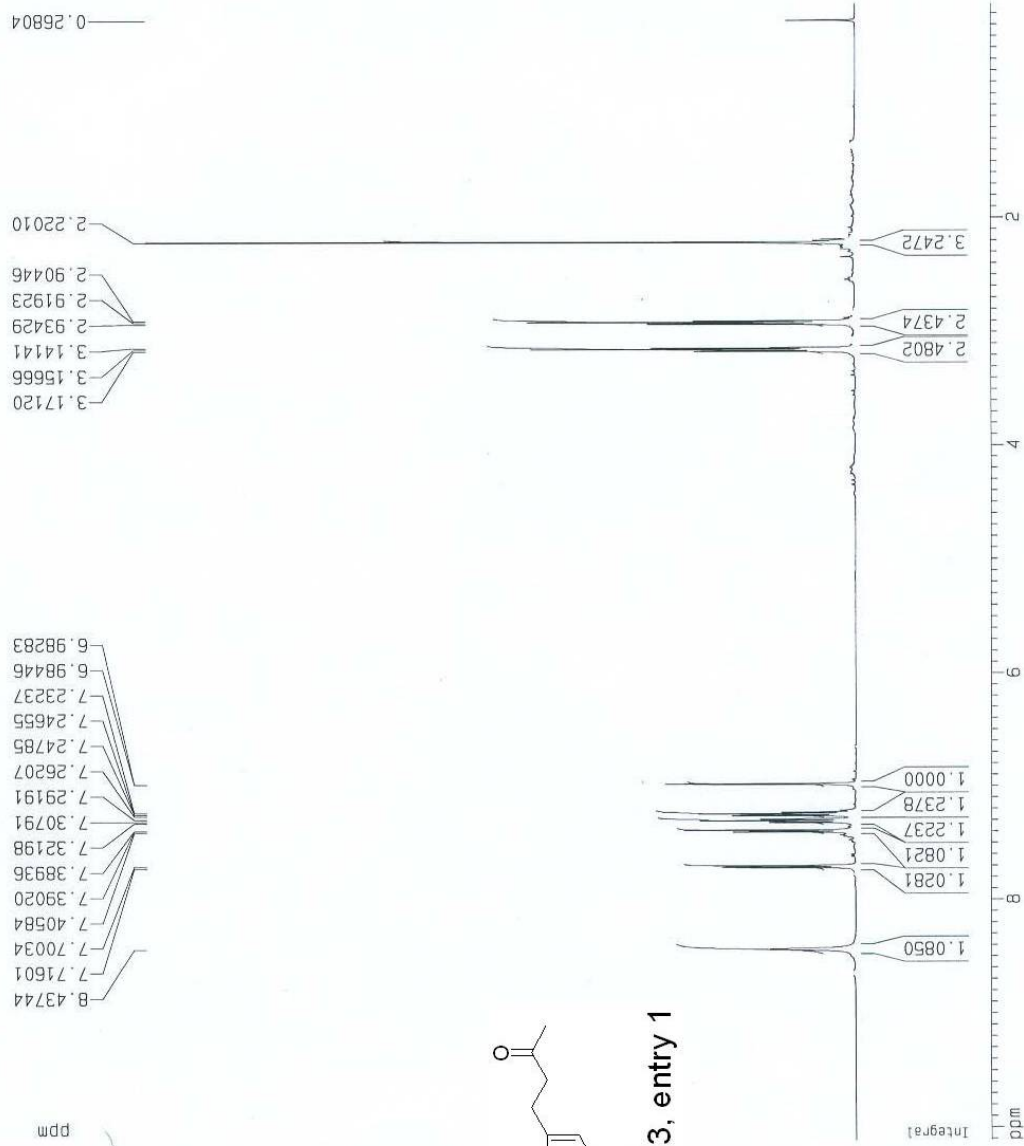


Table 3, entry 1

T17 13CNMR in CDC13 at 298 K 84/4/14

Current Data Parameters
NAME Az121
EXPNO 145
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060705
Time 10.45
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 32768
DK 16.650 usec
DE 6.50 usec
TE 367.7 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8959998 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
SF01 125.7703643 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 67.00 usec
PL2 -6.00 dB
PL12 12.00 dB
PL13 12.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577590 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.41 cm
FIP 218.504 ppm
F1 27478.52 Hz
F2 -3.049 ppm
F2 -383.39 Hz
PRMCK 11.07761 ppm/cm
HZCM 4393.09556 Hz/cm

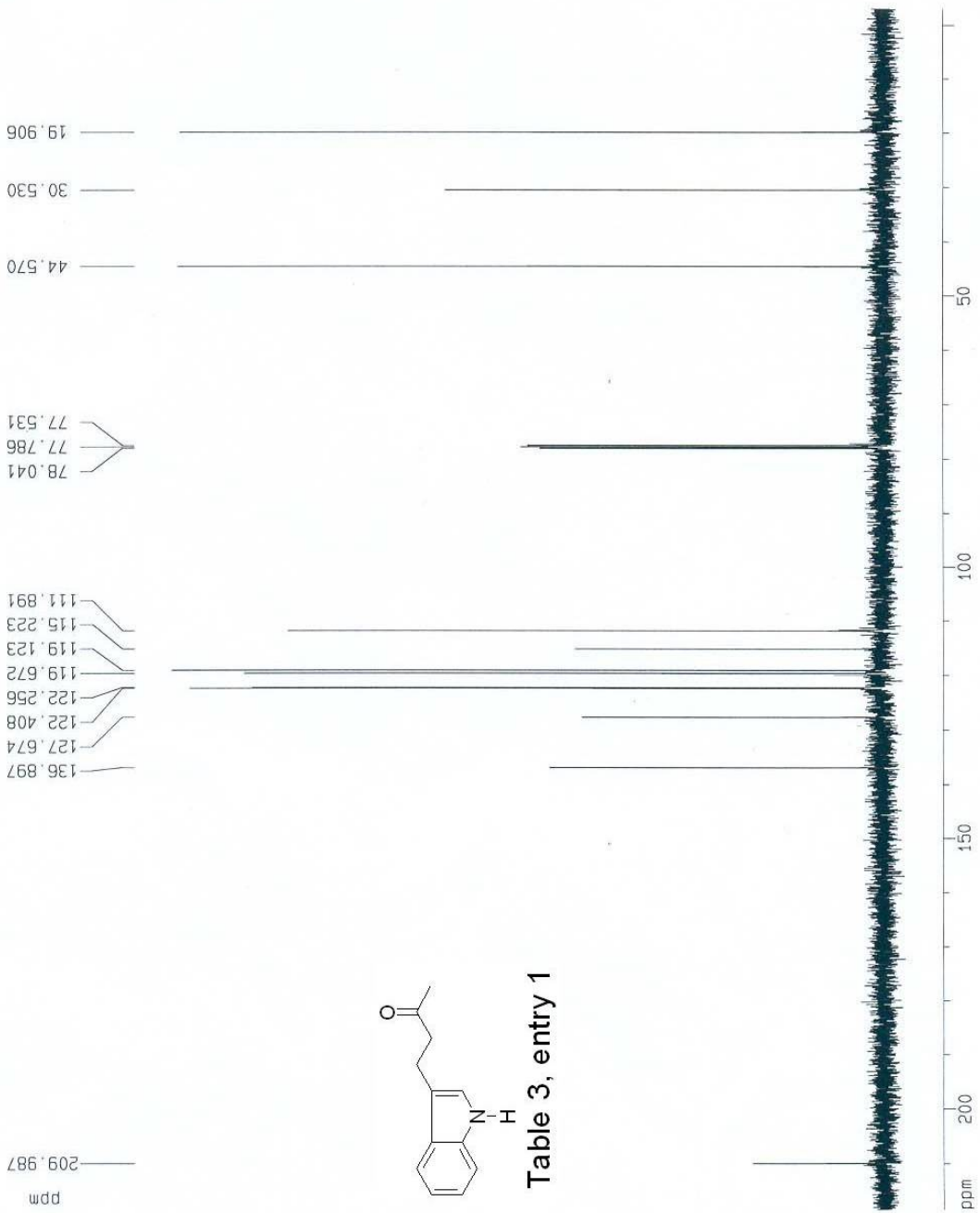


Table 3, entry 1

a-247 1HNMR in CDCl3 at 298 K 84/10/13

```

Current Data Parameters
NAME      Azizi
EXPNO    64
PROCNO   1

F2 - Acquisition Parameters
Date_    20060103
Time     17.27
INSTRUM  spect
PROBHD   5 mm BBI 1H-BB
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       4
DS       0
SMH      10330.578 Hz
FIDRES   0.315264 Hz
AQ       1.5860696 sec
RG       40.3
RW       48.400 usec
DE       6.50 usec
TE       291.4 K
D1       2.00000000 sec
MCREST   0.00000000 sec
MCMRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       10.30 usec
PL1      2.00 dB
SF01     500.1330885 MHz

F2 - Processing parameters
SI       32768
SF       500.1330000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       18.00 cm
CY       23.88 cm
F1P      12.023 ppm
F1       6013.30 Hz
F2P      0.195 ppm
F2       97.49 Hz
PPMCM    0.65714 ppm/cm
HZCM     328.65564 Hz/cm
  
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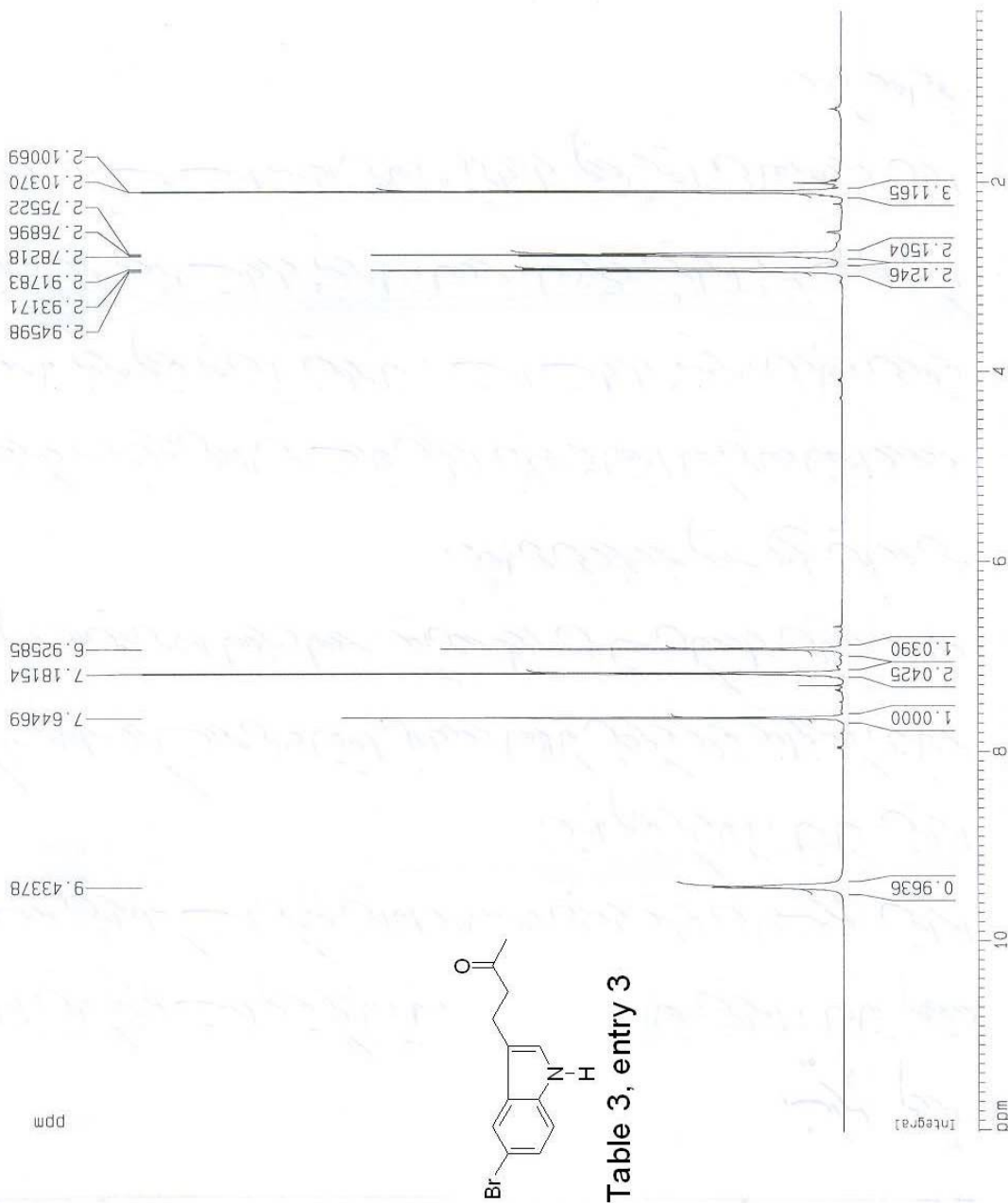


Table 3, entry 3

a-247 13C NMR in CDCl3 at 298 K 84/10/13

Current Data Parameters
 NAME Az121
 EXPNO 65
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050103
 Time 17 29
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 48
 DS 2
 SWH 40000.000 Hz
 FIDRES 0.610352 Hz
 AQ 0.8192625 sec
 RG 2298.8
 DK 12.500 usec
 DE 6.50 usec
 TE 292.1 K
 D1 3.0000000 sec
 d11 0.0300000 sec
 DELTA 2.9000010 sec
 MCFST 0.0000000 sec
 MCWRK 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SFO1 125.7703143 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 87.00 usec
 PL2 -6.00 dB
 PL12 12.00 dB
 PL13 12.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32788
 SF 125.7577350 MHz
 MDW FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.96 cm
 F1P 219.273 ppm
 F1 27575.29 Hz
 F2P -2.250 ppm
 F2 -287.96 Hz
 PRMCM 11.07815 ppm/cm
 HZCM 1383.16248 Hz/cm

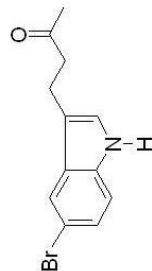
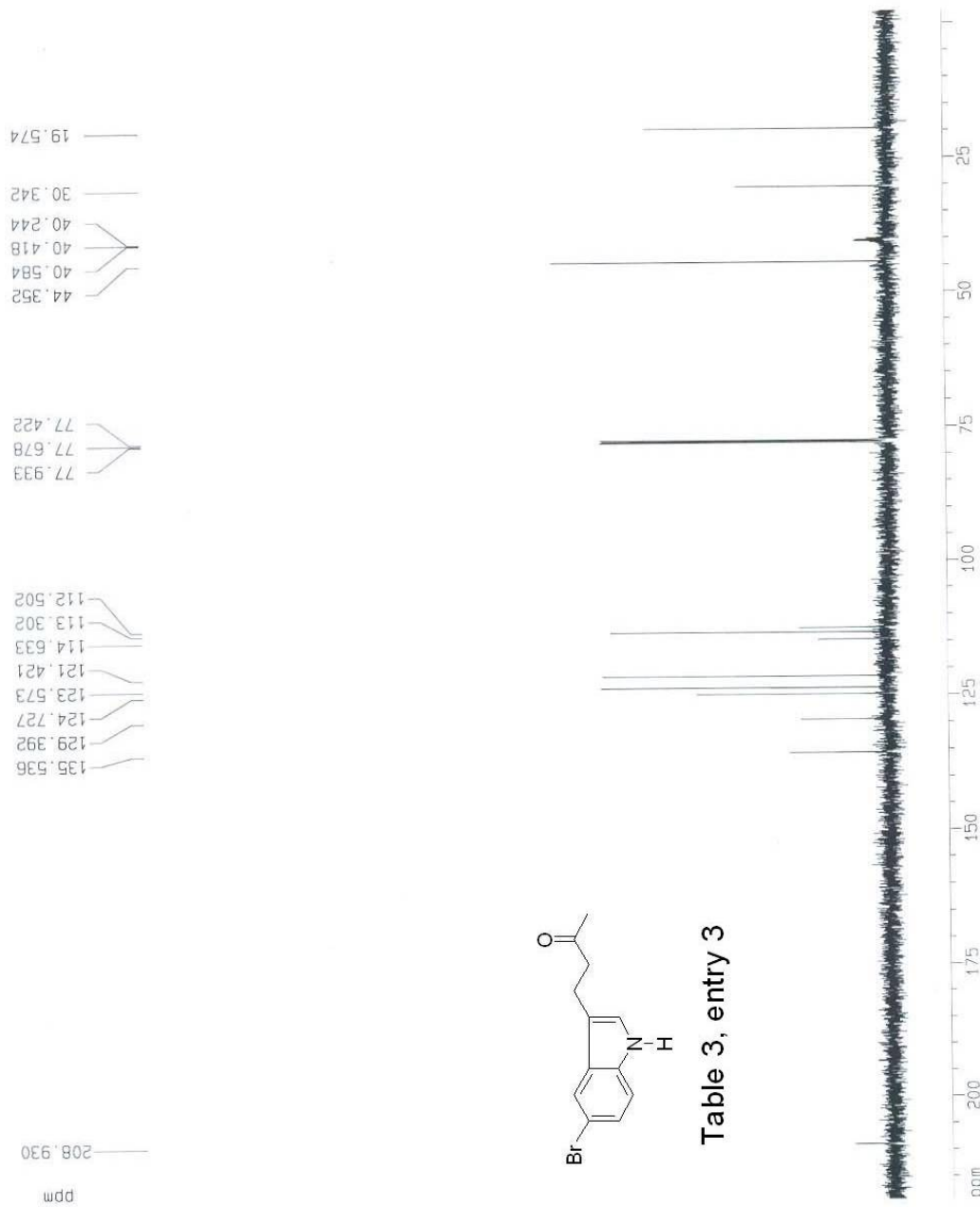


Table 3, entry 3

A34, ¹H NMR in CDCl₃ at 298 K 84/5/22

```

Current Data Parameters
NAME      AZ121
EXPNO    B
PROCNO   1

F2 - Acquisition Parameters
Date_    20050814
Time     9.23
INSTRUM spect
PROBHD   5 mm GNP 1H/13
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        4
DS        2
SWH       10000.000 Hz
FIDRES    0.305175 Hz
AQ        1.6385000 sec
RG        11.3
DW        50.000 usec
DE        6.50 usec
TE        298.0 K
D1        3.0000000 sec
MCREST    0.0000000 sec
MCWRK     0.0150000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        32.00 usec
PL1       2.00 dB
SFO1      500.1350885 MHz

F2 - Processing parameters
SI         32768
SF         500.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         18.0 cm
CY         26.06 cm
F1P        9.471 ppm
F1         4736.74 Hz
F2P        0.004 ppm
F2         2.22 Hz
PPMCM      0.52592 ppm/cm
HZCM       263.07850 Hz/cm
  
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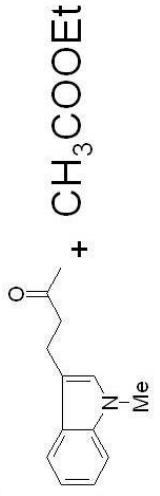
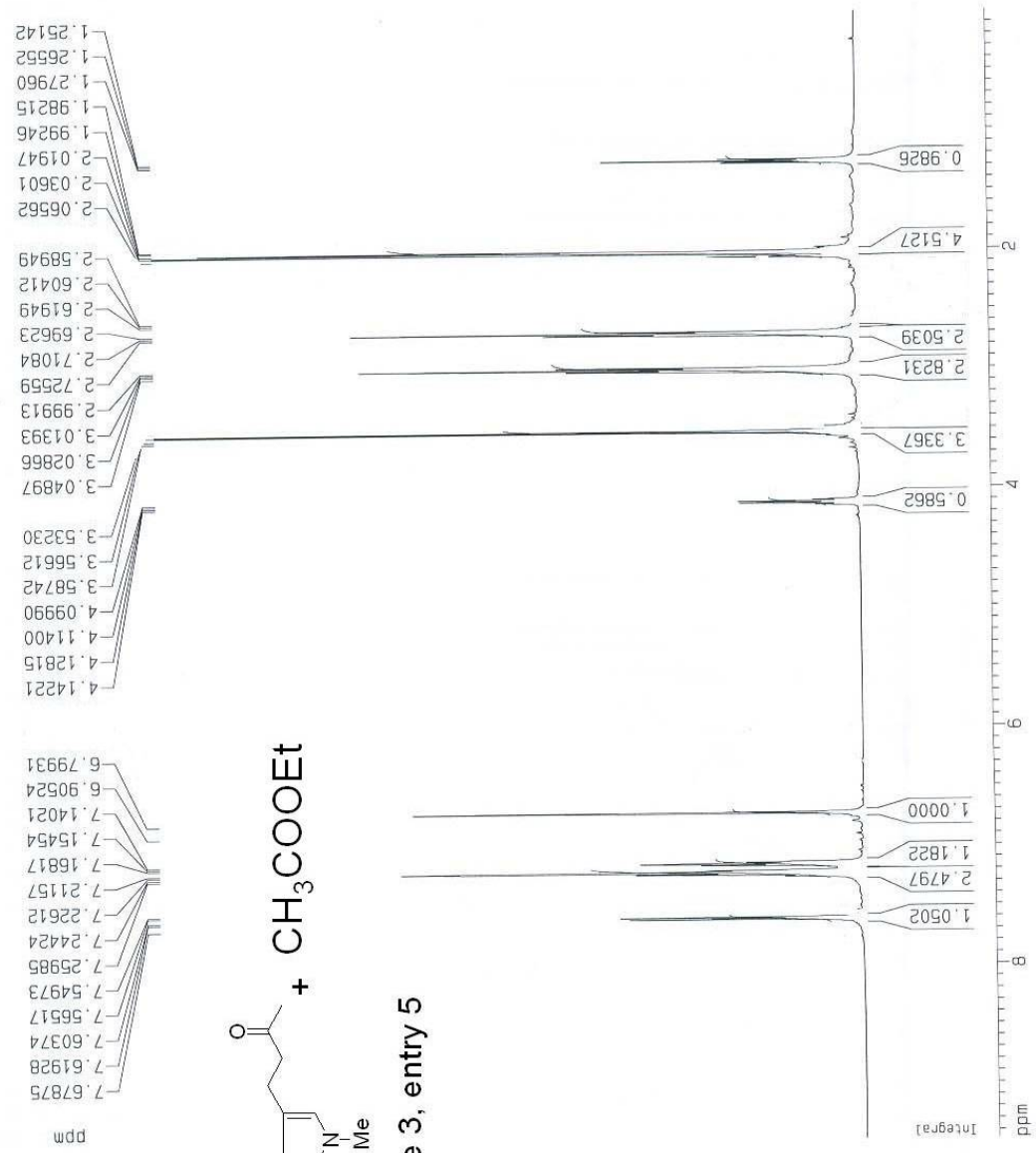
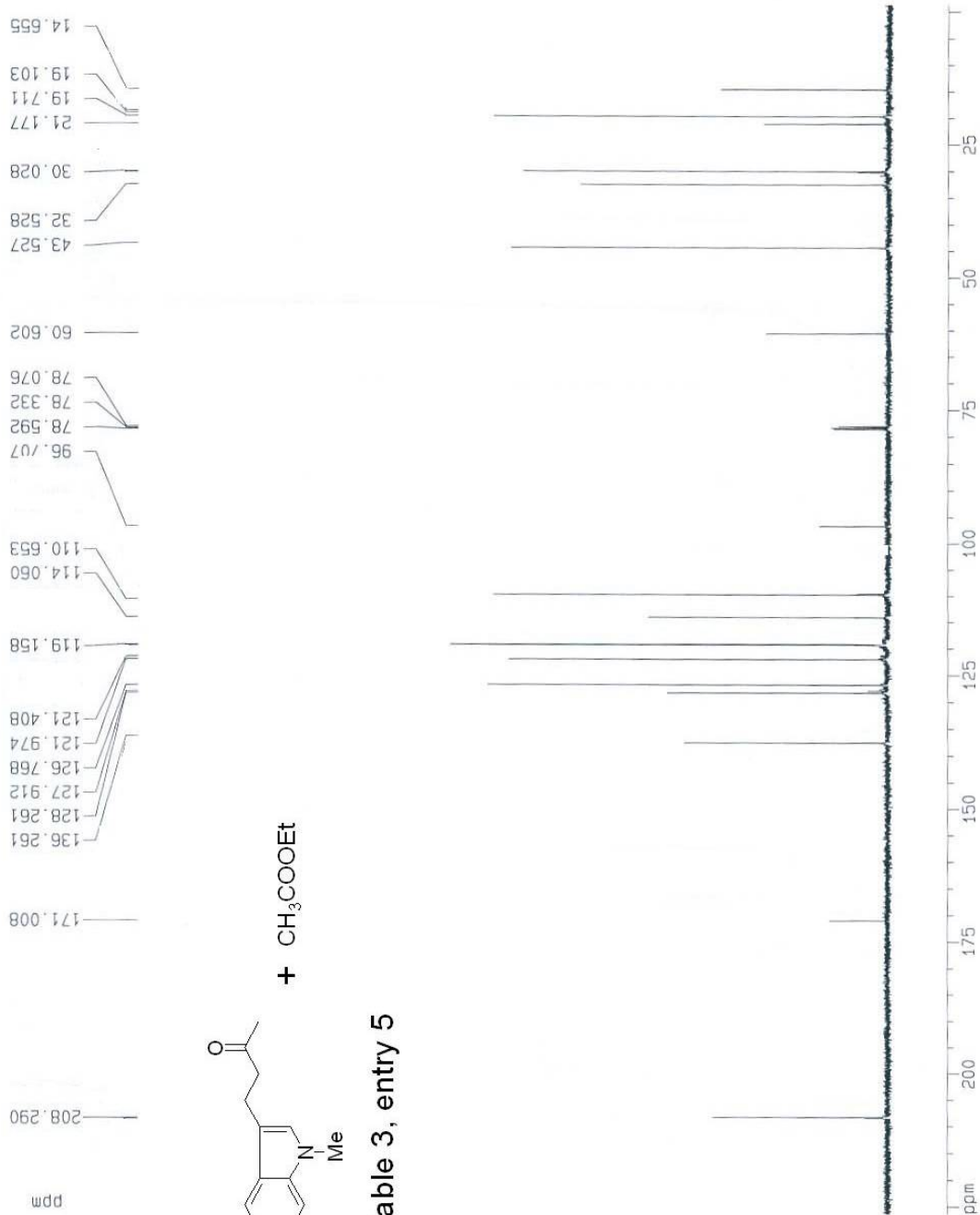


Table 3, entry 5

A-34 ¹³CNMR in CDCl₃ at 298 K 84/5/22



```

Current Data Parameters
NAME Az121
EXPNO 9
PROCNO 1
F2 Acquisition Parameters
Date_ 20050814
Time 9:26
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLV NT CDCl3
NS 51
DS 2
SWH 40000.000 Hz
FIDRES 0.610352 Hz
AQ 0.6191625 s.c.
RG 2560.3
Dw -2.570 u.s.
DE 6.50 u.s.
TE -90.0 K
D1 3.0000000 s.
d11 0.0500000 s.c.
DELTA 2.9000000 s.c.
MGREST 0.0000000 s.
AcqPrk 1.000000 s.

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 u.s.
PL1 3.00 dB
SFO1 125.7703143 MHz

***** CHANNEL f2 *****
C13PRG2 waltz16
NUC2 1H
P2 80.00 u.s.
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7677350 MHz
WDW EM
SS 0
LB 0.00 Hz
GB 0
PC 1.40

.D NMR p.p.t. parameters
CX 20.00 CF
CY 7.30 CF
F1P 226.310 DC.
F1 28460.25 Hz
F2P -1.375 ppm
F2 -188.07 Hz
PPMCM 11.00233 ppm/cm
HZCM 1431.41585 Hz/cm
  
```

a-80 1H NMR in CDCl3 at 300 K 84/6/22

Current Data Parameters
 NAME Aryanasab
 EXPNO 28
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050913
 Time 10.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305175 Hz
 AQ 1.6385000 sec
 RG 362
 DW 50.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWAK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 32.00 usec
 PL1 2.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 18.00 cm
 CY 13.07 cm
 F1P 10.228 ppm
 F1 5115.21 Hz
 F2P -0.401 ppm
 F2 -200.33 Hz
 PPMCM 0.59046 ppm/cm
 HZCM 295.30740 Hz/cm

8.05233
7.98969
7.97529
7.97298
7.49312
7.47750
7.46225
7.41448
7.39965
7.36836
7.35206
7.32226
7.30639
7.29182
7.21182
7.19526
7.06733
7.03444
7.03097
5.14098
5.12655
5.11229
4.20284
4.18858
4.17429
4.16002
3.88092
3.86118
3.84756
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1.31661
1.30236
0.06325

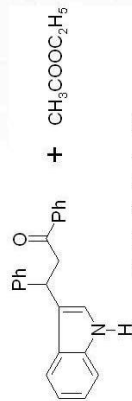
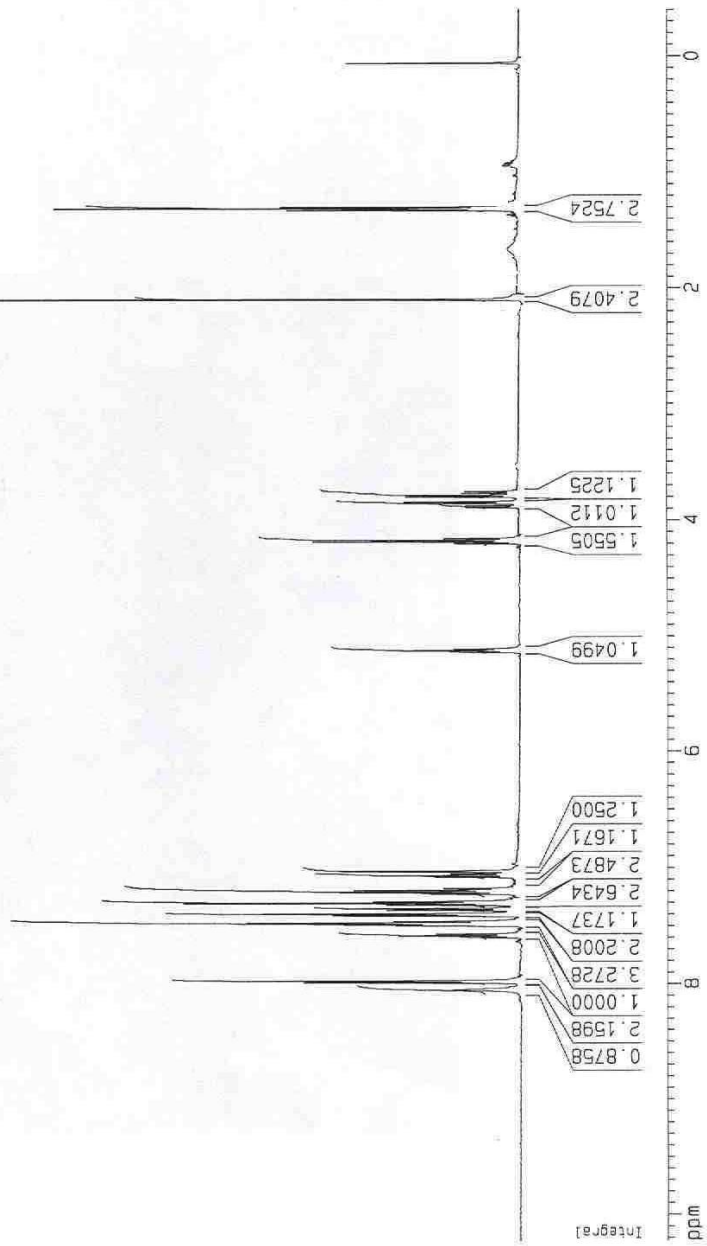


Table 3, Entry 7



a-133 1HNMR in CDCl3 at 298 K 8/7/11

Current Data Parameters
 NAME Aryanasab
 EXPNO 34
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051003
 Time 13.48
 INSTRUM spect
 PROBHD 5 mm BBI 4H-BB
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 2
 SMH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 45.3
 DM 50.000 usec
 DE 6.50 usec
 TE 291.8 K
 D1 3.00000000 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

===== CHANNEL f1 =====
 NUJC1 4H
 F1 32.00 usec
 PL1 2.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 S1 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 18.00 cm
 CY 26.38 cm
 FIP 11.391 ppm
 F1 5697.20 Hz
 F2p -0.171 ppm
 F2 -85.41 Hz
 PPMCM 0.54235 ppm/cm
 HZCM 321.255607 Hz/cm

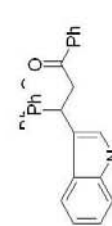
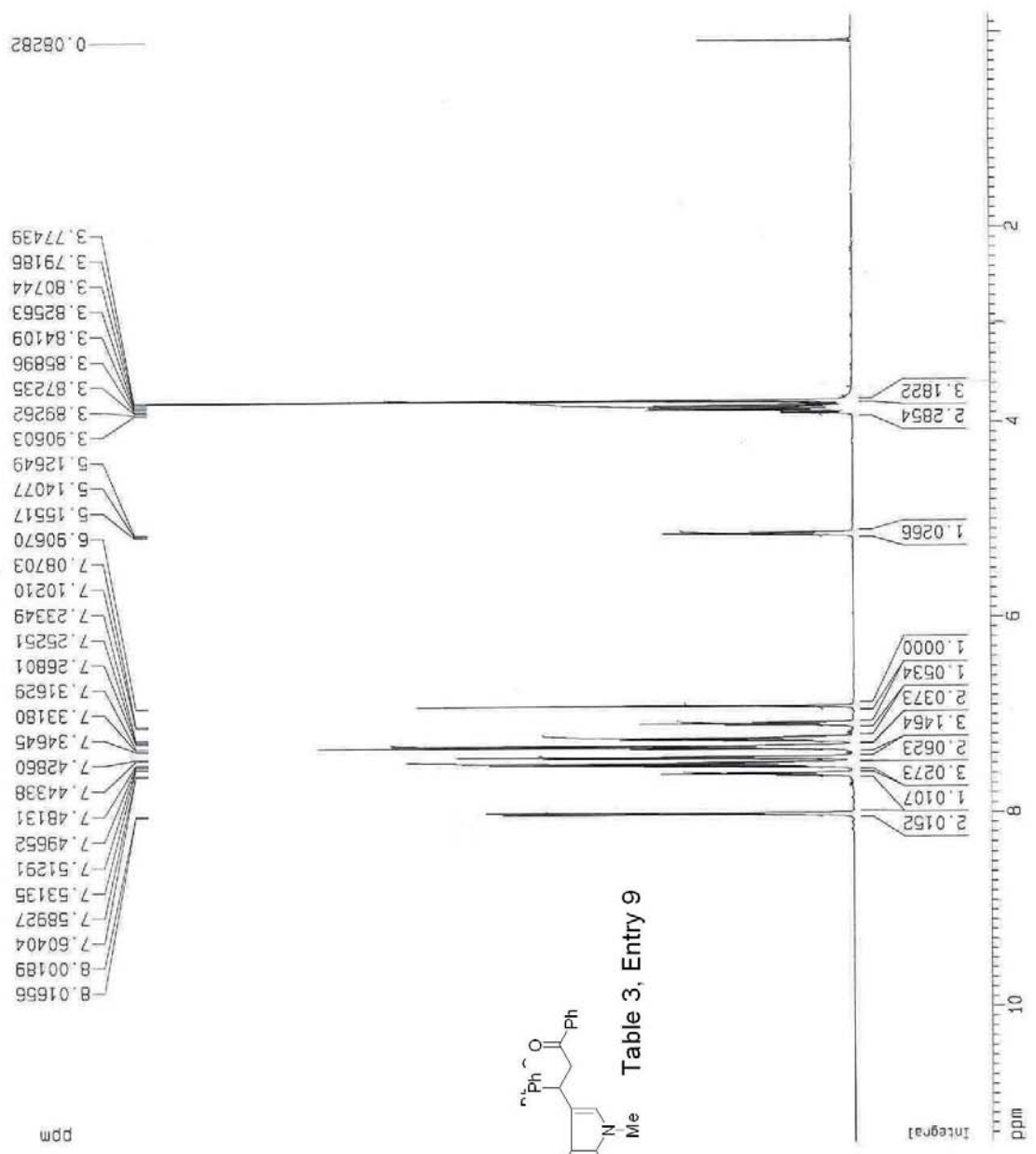


Table 3, Entry 9

a-133 13CNMR in CDCl3 at 298 K 84/7/11

198.934

144.871
137.822
137.662
133.376
128.991
128.865
128.543
128.266
127.484
126.685
122.131
120.059
119.312
118.309
109.633

45.810
38.631
33.097

Current Data Parameters
 NAME Aryanasab
 EXPNO 35
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051003
 Time 13.50
 INSTRUM spect
 PROBH0 5 mm BBI 4H-BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 104
 DS 2
 SWH 40000.000 Hz
 FIDRES 0.610352 Hz
 AQ 0.8192625 sec
 RG 2560.3
 DW 12.500 usec
 DE 6.50 usec
 TE 292.7 K
 D1 3.0000000 sec
 d11 0.0300000 sec
 DELTA 2.9000010 sec
 ACQRES 0.0000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 125.7703143 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 87.00 usec
 PL2 -6.00 dB
 PL12 12.00 dB
 PL13 12.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577390 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 16.28 cm
 F1P 224.459 ppm
 F1 28227.46 Hz
 F2P 2.846 ppm
 F2 357.90 Hz
 PPMCM 11.08066 ppm/cm
 HZCM 1393.47803 Hz/cm

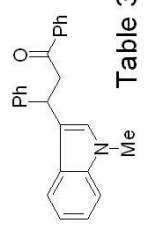
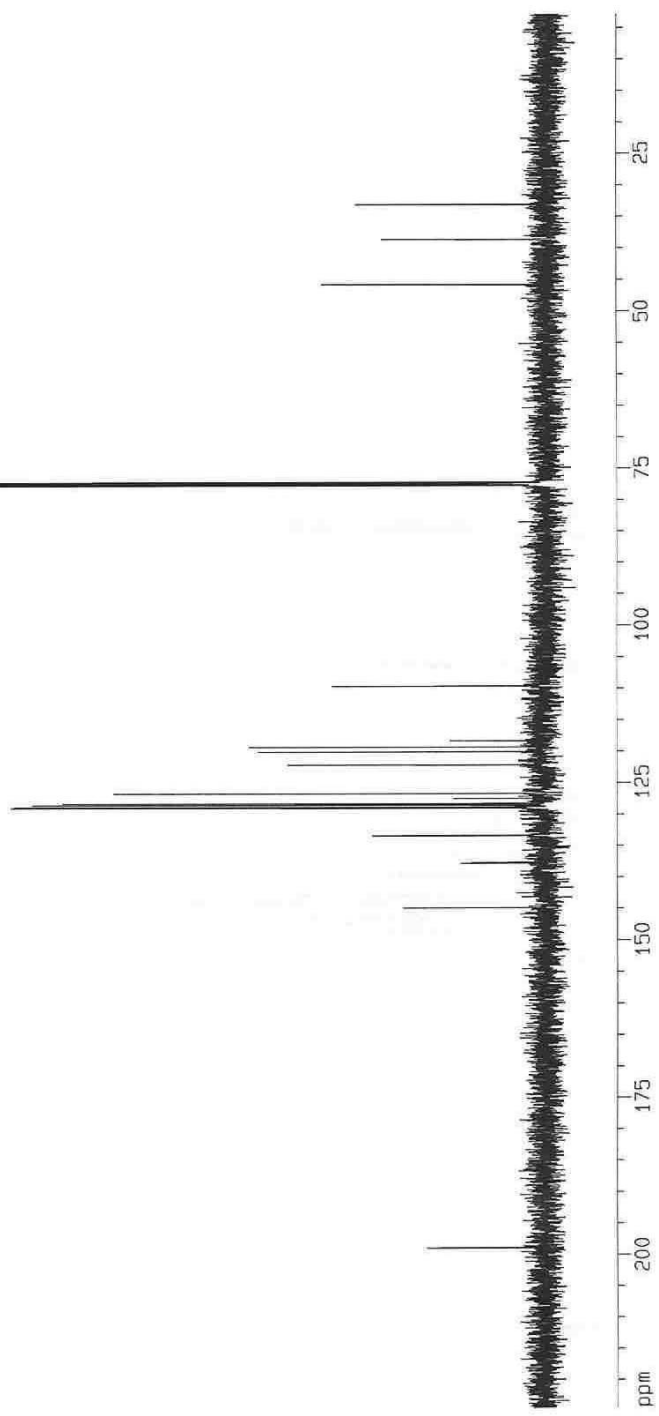


Table 3, Entry 9



a-83 1HNMR in DMSO at 298 K 84/B/2

Current Data Parameters
 NAME Aryanasab
 EXPNO 52
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051024
 Time 11.28
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg
 TO 32768
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 h1 161.3
 DW 50.000 usec
 DE 6.50 usec
 TE 291.5 K
 D1 3.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.30 usec
 PL1 2.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 18.00 cm
 CY 461.12 cm
 F1P 12.478 ppm
 F1 6240.68 Hz
 F2P -0.453 ppm
 F2 -226.71 Hz
 PPMCM 0.71841 ppm/c
 HZCM 359.29953 Hz/cm

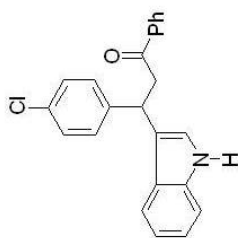
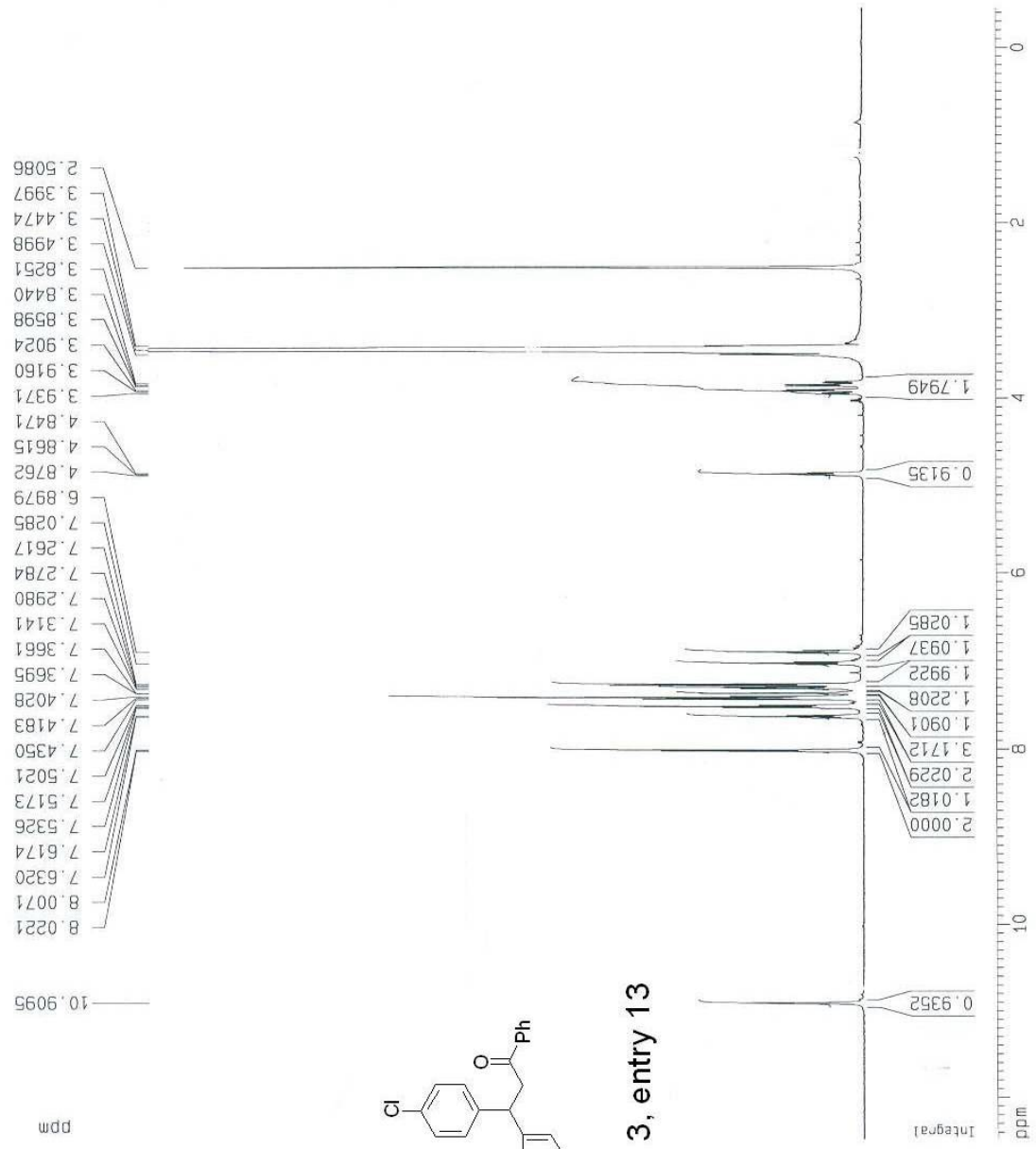
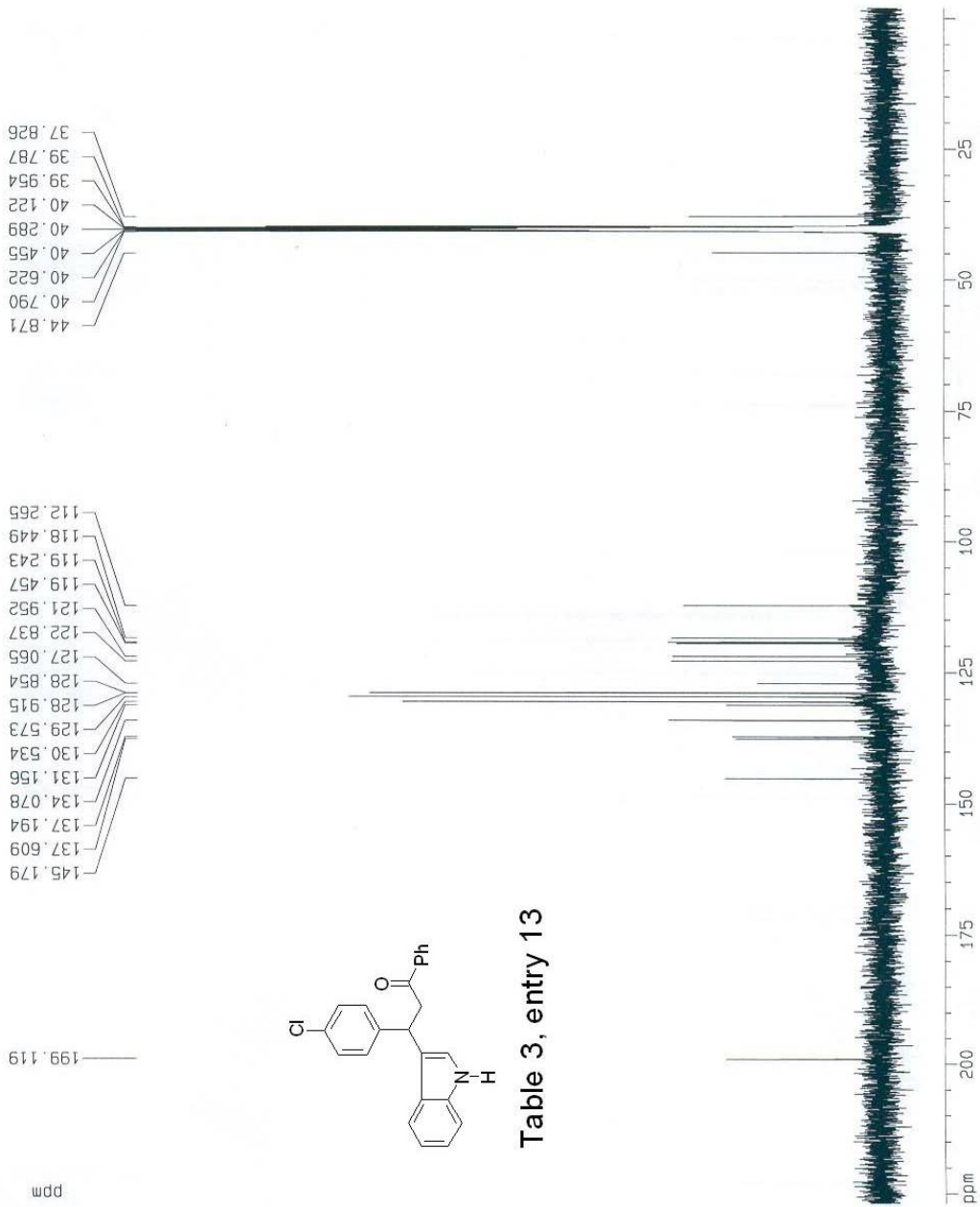


Table 3, entry 13

a-83_13CNMR in DMSO at 298 K 84/B/2



Current Data Parameters
NAME Aryanesab
EXPNO 53
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051024
Time 12.21
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 568
DS 2
SWH 40000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192625 sec
RG 4597.6
DM 12.500 usec
DE 6.50 usec
TE 292.0 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 2.50000010 sec
ACREST 0.00000000 sec
MCWRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
SF01 125.7703143 MHz

***** CHANNEL f2 *****
CPOPRG2 waltz16
NUC2 1H
P2 87.00 usec
PL2 -6.00 dB
PL12 12.00 dB
PL13 12.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
S1 32768
SF 125.7577350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 74.73 cm
F1P 226.679 ppm
F1 28531.82 Hz
F2P -1.954 ppm
F2 -250.79 Hz
PPMCM 11.44367 ppm/cm*
HZCM 1439.13037 Hz/cm

Table 3, entry 13

a-134 1H NMR in CDCl3 at 300 K 84/7/23

```

Current Data Parameters
NAME Arynesab
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051015
Time 9.05
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 10000.000 Hz
FIDRES 0.305175 Hz
AQ 1.6385000 sec
RG 128
DN 50.000 usec
DE 6.50 usec
TE 292.5 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCWRRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 32.00 usec
PL1 2.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 18.00 cm
CY 15.13 cm
F1P 9.999 ppm
F1 5000.90 Hz
F2P -0.255 ppm
F2 -127.31 Hz
PPMCM 0.56965 ppm/cm
HZCM 284.90030 Hz/cm
  
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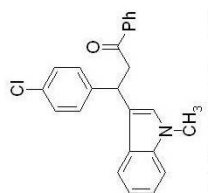
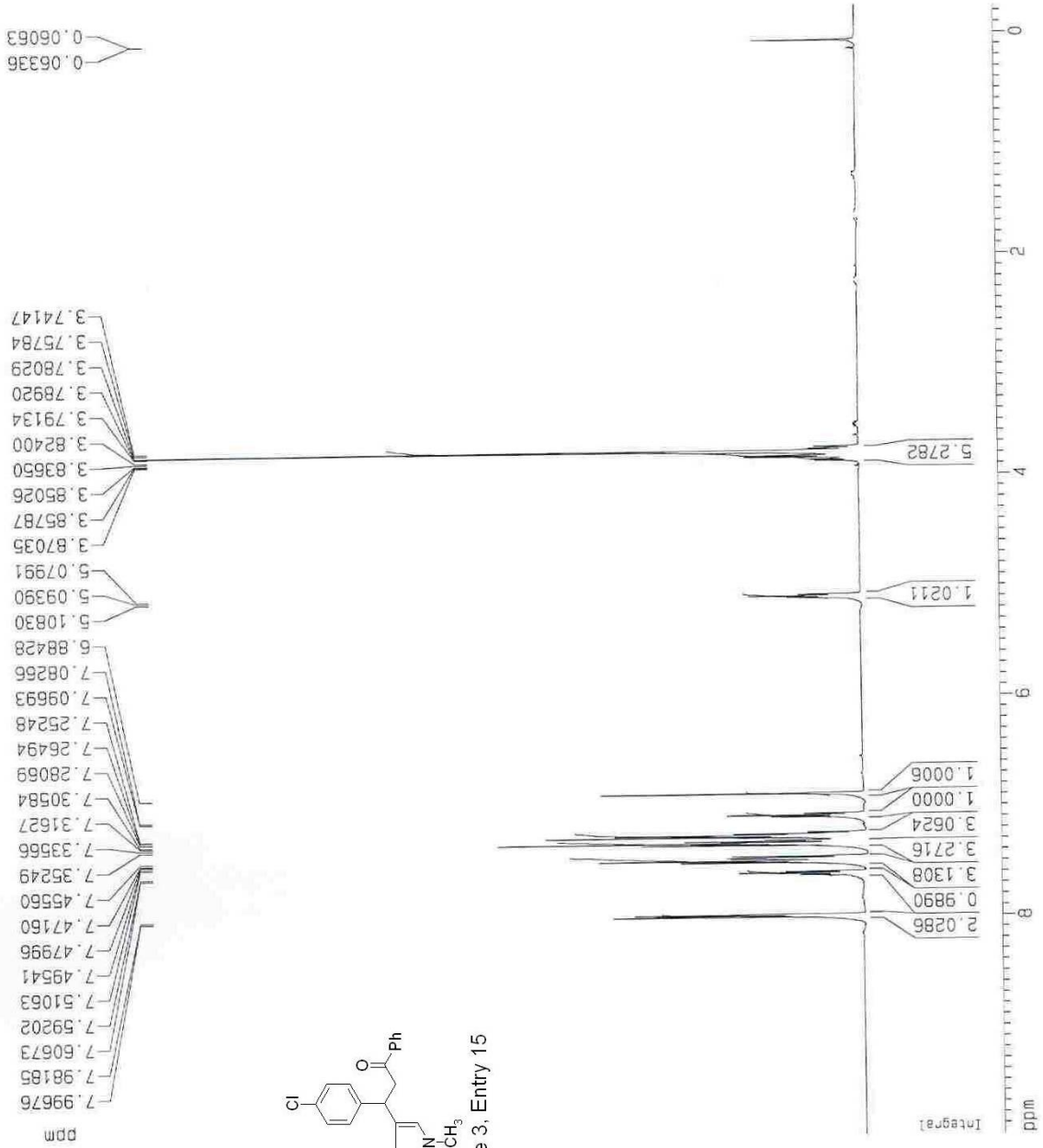
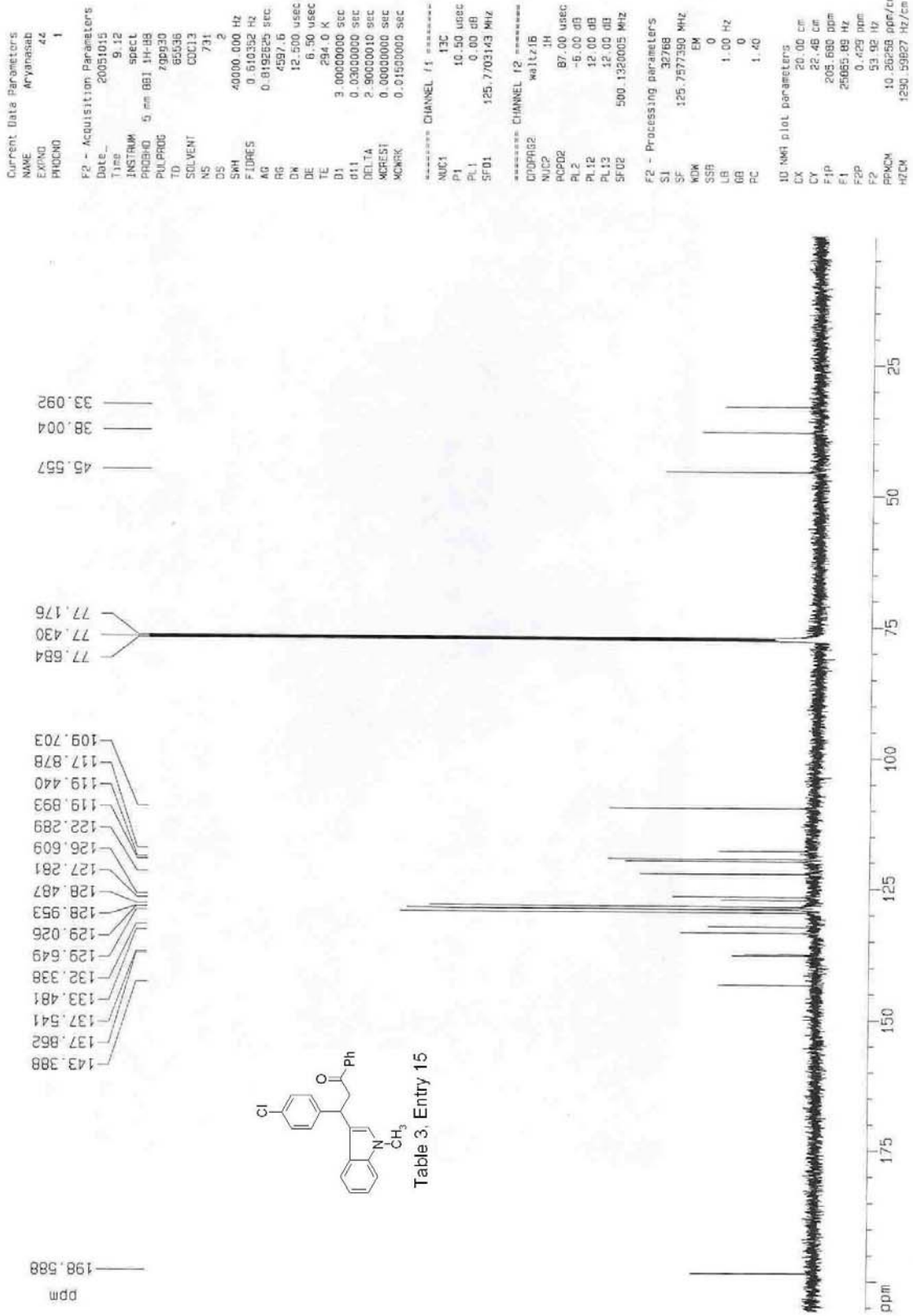
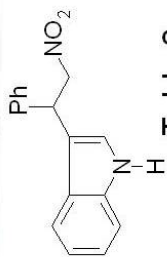


Table 3, Entry 15

α-134 13CNMR in CDCl3 at 300 K B4/7/23

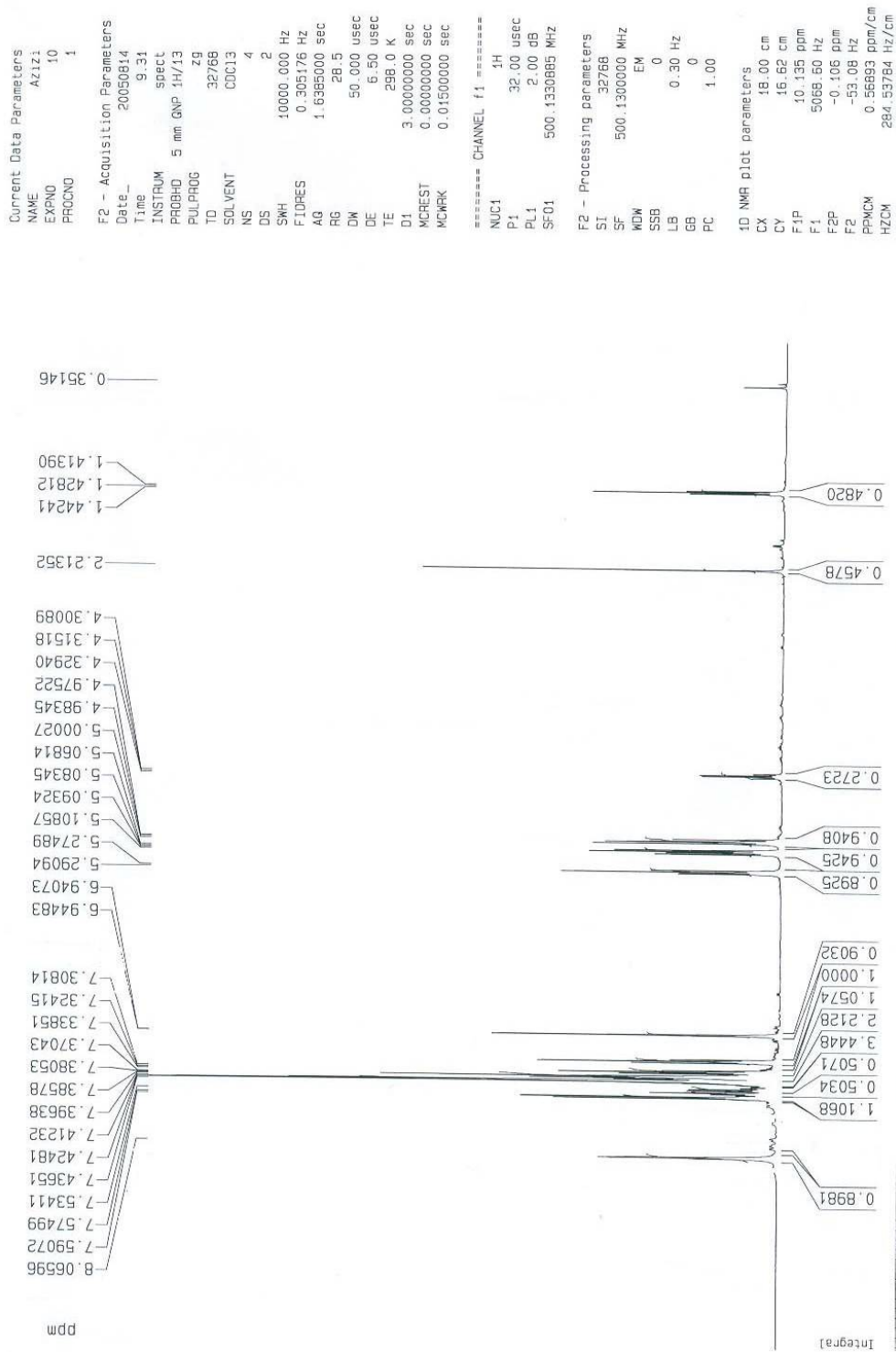




+ CH₃COOEt

-25 1HNMR in CDCl₃ at 298 K 84/5/22

Table 3, entry 17



A-25 ¹³CNMR in CDCl₃ at 298 K 84/5/22

```

Current Data Parameters
NAME Az121
EXPNO 11
PROCNO 1

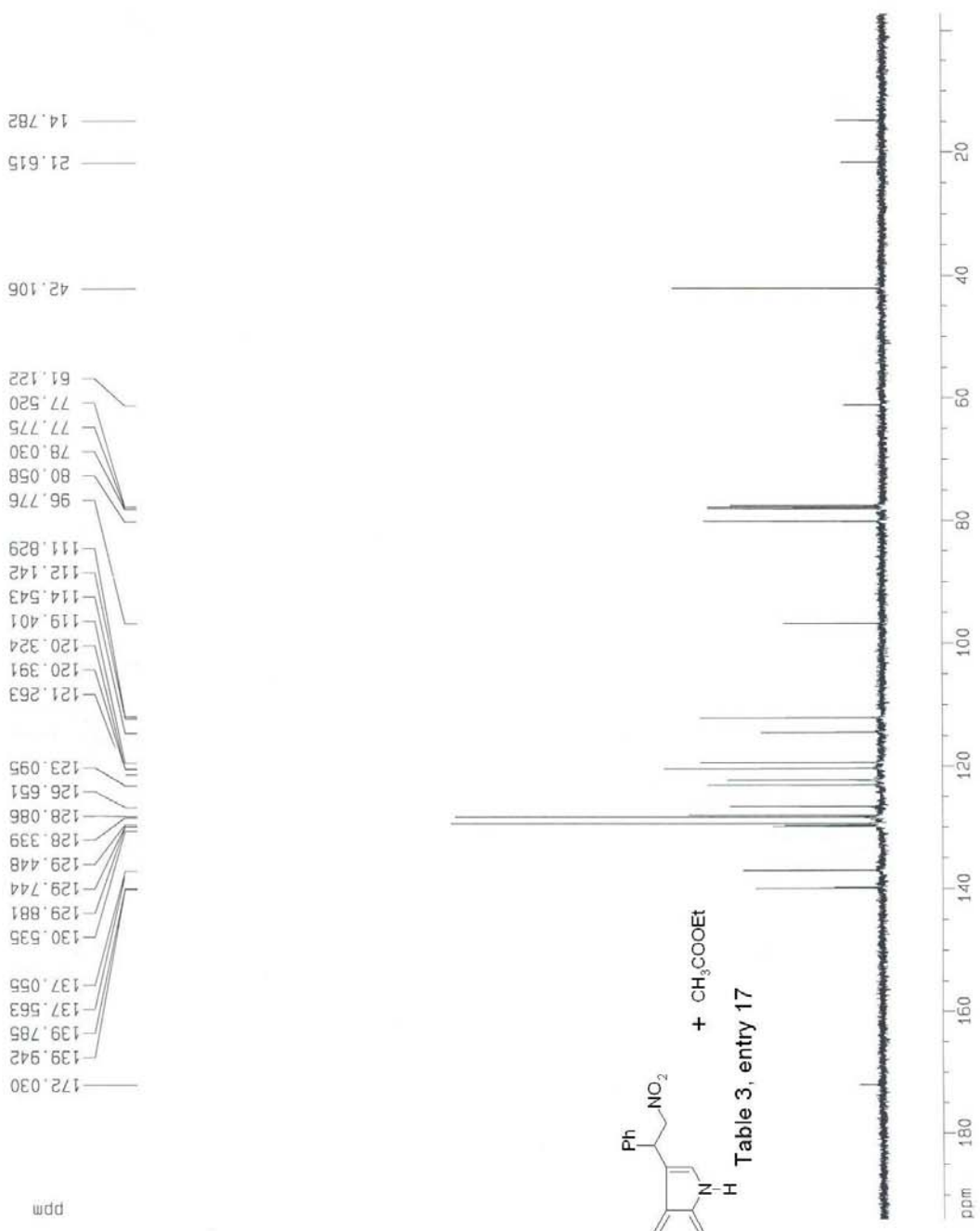
F2 - Acquisition Parameters
Date_ 20050814
Time 9:34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 65
DS 2
SWH 40000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192625 sec
RG 2580.3
DW 12.500 usec
DE 5.50 usec
TE 298.0 K
D1 3.0000000 sec
d11 0.0300000 sec
DELTA 2.9000010 sec
MCREST 0.0000000 sec
MCWRK 0.015500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SF01 125.7703143 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
P2 60.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.30 cm
FJP 193.940 ppm
F1 24389.45 Hz
F2 -2.744 ppm
F3 -345.06 Hz
PRMCM 9.83419 ppm/cm
HZCM 1236.72546 Hz/cm
  
```



a-79 1H NMR in CDCl3 at 300 K 84/6/22

```

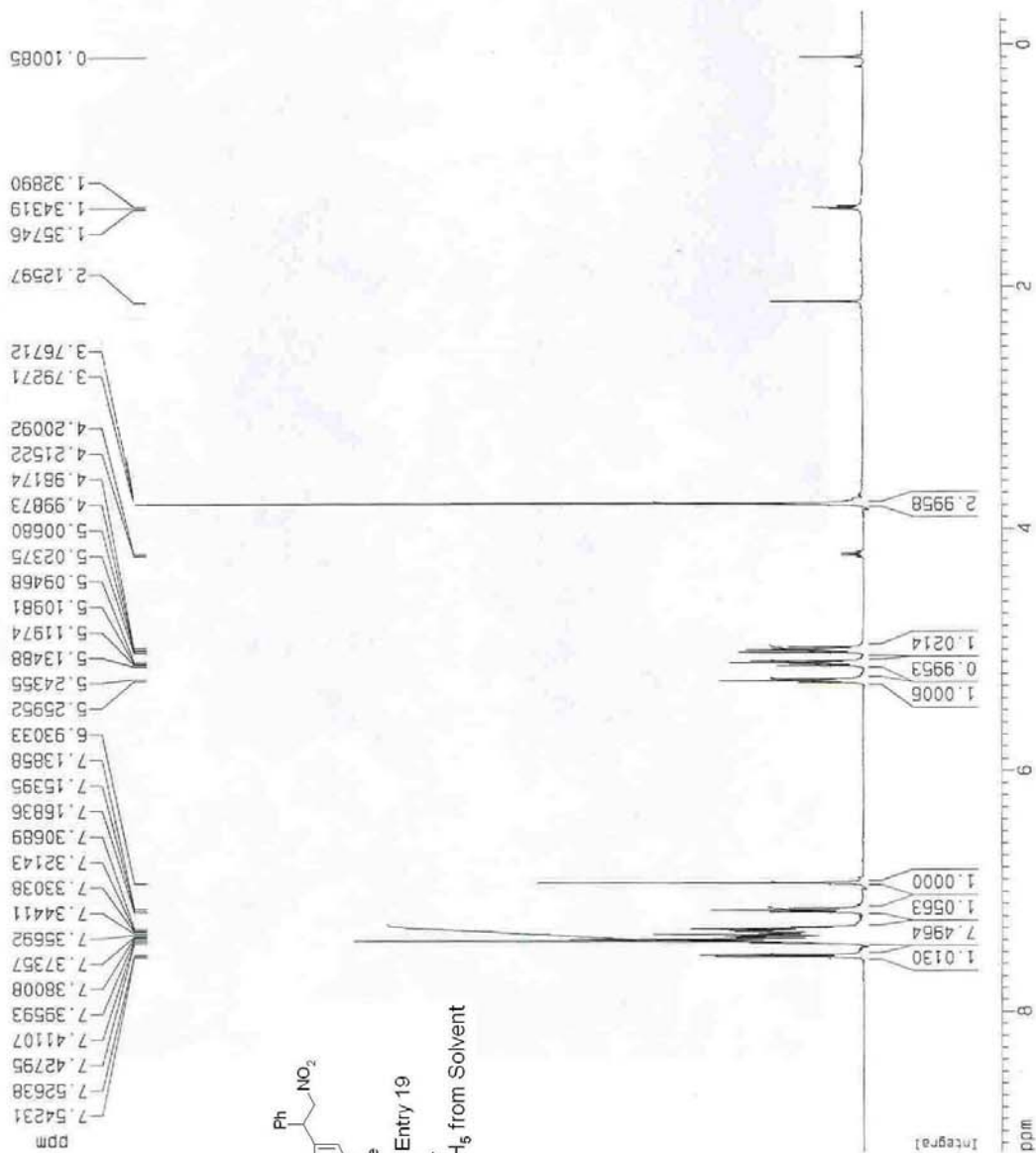
Current Data Parameters
NAME      Aryanassb
EXPNO    22
PROCNO   1

F2 - Acquisition Parameters
Date_    20050913
Time     9.46
INSTRUM  spect
PROBHD   5 mm GNP 1H/13
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        1
DS        0
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        1.6385000 sec
RG        181
DM        50.000 usec
DE        6.50 usec
TE        300.0 K
D1        1.00000000 sec
MCREST    0.00000000 sec
MCWRK    0.01500000 sec

***** CHANNEL f1 *****
NUC1      1H
P1        32.00 usec
PL1       2.00 dB
SF01      500.1330685 MHz

F2 - Processing parameters
SI        32768
SF        500.1300000 MHz
KOH       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        18.00 cm
CY        18.75 cm
F1P       9.179 ppm
F1        4590.70 Hz
F2P       -0.270 ppm
F2        -135.18 Hz
PPMCM     0.52465 ppm/cm
HZCM      262.54874 Hz/cm
  
```



a-79 ¹³CNMR in CDCl₃ at 300K 84/6/22

```

Current Data Parameters
NAME      Aryanasab
EXPNO    23
PROCNO    1

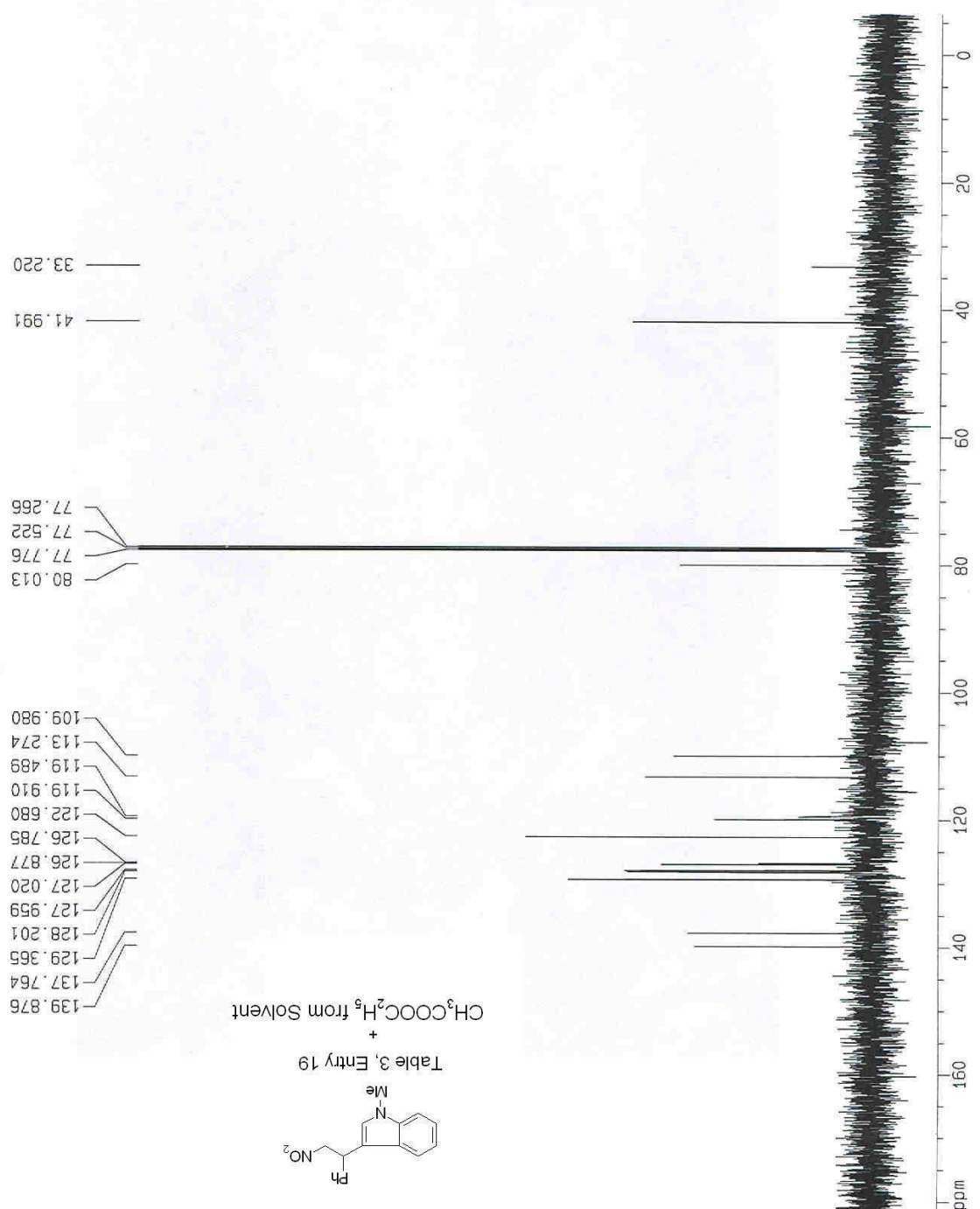
F2 - Acquisition Parameters
Date_     20050913
Time      9.48
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         46
DS         2
SWH        40000.000 Hz
FIDRES     0.610352 Hz
AQ         0.8192625 sec
RG         2580.3
DW         12.500 usec
DE         6.50 usec
TE         300.0 K
D1         3.0000000 sec
d11        0.03000000 sec
DELTA      2.90000010 sec
MCREST    0.00000000 sec
MCWPRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         9.10 usec
PL1        3.00 dB
SFO1       125.7703143 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       60.00 usec
PL2         0.00 dB
PL12        15.50 dB
PL13        15.50 dB
SFO2        500.1320005 MHz

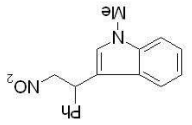
F2 - Processing parameters
SI          32768
SF          125.7577350 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

1D NMR plot parameters
CX          20.00 cm
CY          21.75 cm
F1P         181.258 ppm
F1          22794.59 Hz
F2P         -6.377 ppm
F2          -801.90 Hz
PPMCM       9.38173 ppm/cm
HZCM        1179.82458 Hz/cm
  
```



CH₃COOC₂H₅ from Solvent

Table 3, Entry 19



a-190 1H-NMR in CDCl3 at 298 K 84/B/11

Current Data Parameters
 NAME Aryanasab
 EXPNO 60
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051102
 Time 10.39
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 2
 SNH 10000.000 Hz
 FIDRES 0.305175 Hz
 AQ 1.6385000 sec
 RG 32
 DM 50.000 usec
 DE 6.50 usec
 TE 292.5 K
 D1 3.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.30 usec
 PL1 2.00 dB
 SFO1 500.1330865 MHz

F2 - Processing parameters
 SI 32768
 SF 100.1300000 MHz
 N IM EM
 SS 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 18.00 cm
 CY 12.58 cm
 FIP 10.739 ppm
 F1 5371.12 Hz
 F2 -0.171 ppm
 F2 -85.41 Hz
 PPMCM 0.60612 ppm/cm
 HZCM 303.14014 Hz/cm

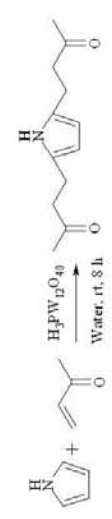
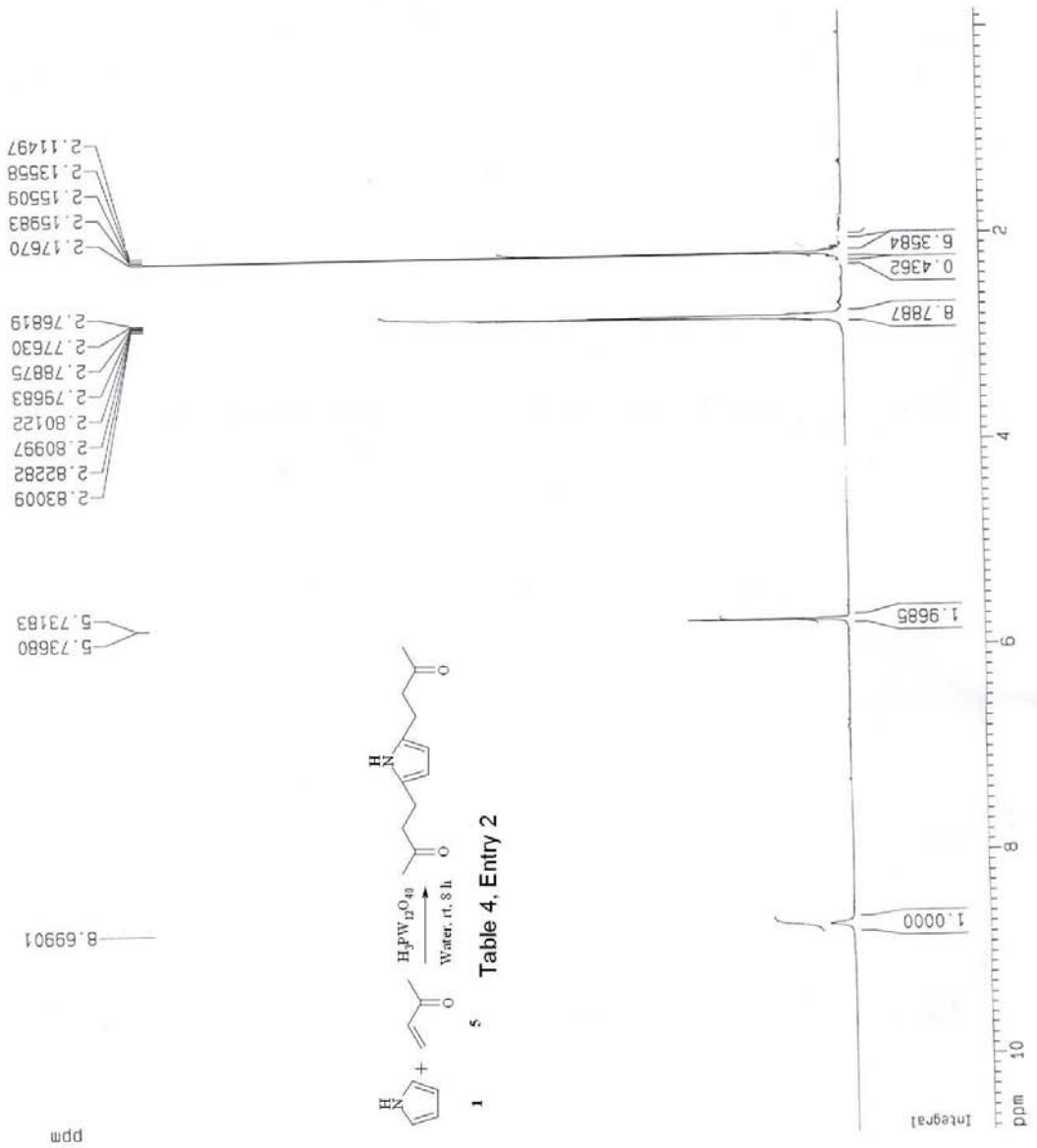


Table 4, Entry 2

a-190 1H NMR in CDCl3 at 298 K 84/8/11

Current Data Parameters
 NAME Aryanasab
 EXPNO 61
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051102
 Time 10.40
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 33
 DS 2
 SWH 40000.000 Hz
 FIDRES 0.151362 Hz
 AQ 0.6192525 sec
 RG 4597.6
 DW 12.500 usec
 DE 6.50 usec
 TE 292.5 K
 D1 3.0000000 sec
 d11 0.0300000 sec
 DELTA 2.90000010 sec
 MCREST 0.0000000 sec
 MCWK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0.00 dB
 SF01 125.7703143 MHz

===== CHANNEL f2 =====
 CPROGR2 waltz16
 NUC2 1H
 P2 87.00 usec
 PL2 -6.00 dB
 PL12 12.00 dB
 PL13 12.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577393 MHz
 MDW FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR p1.c. parameters
 CX 20.00 cm
 CY 10.10 cm
 F1 292.730 ppm
 F1 26010.07 Hz
 F2 7.180 ppm
 F2 -902.57 Hz
 PPMCK 11.45953 ppm/cm
 HZCM 1445.65210 Hz/cm

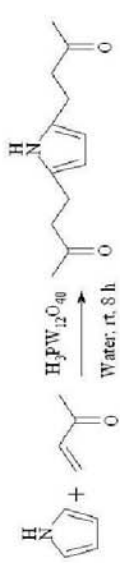
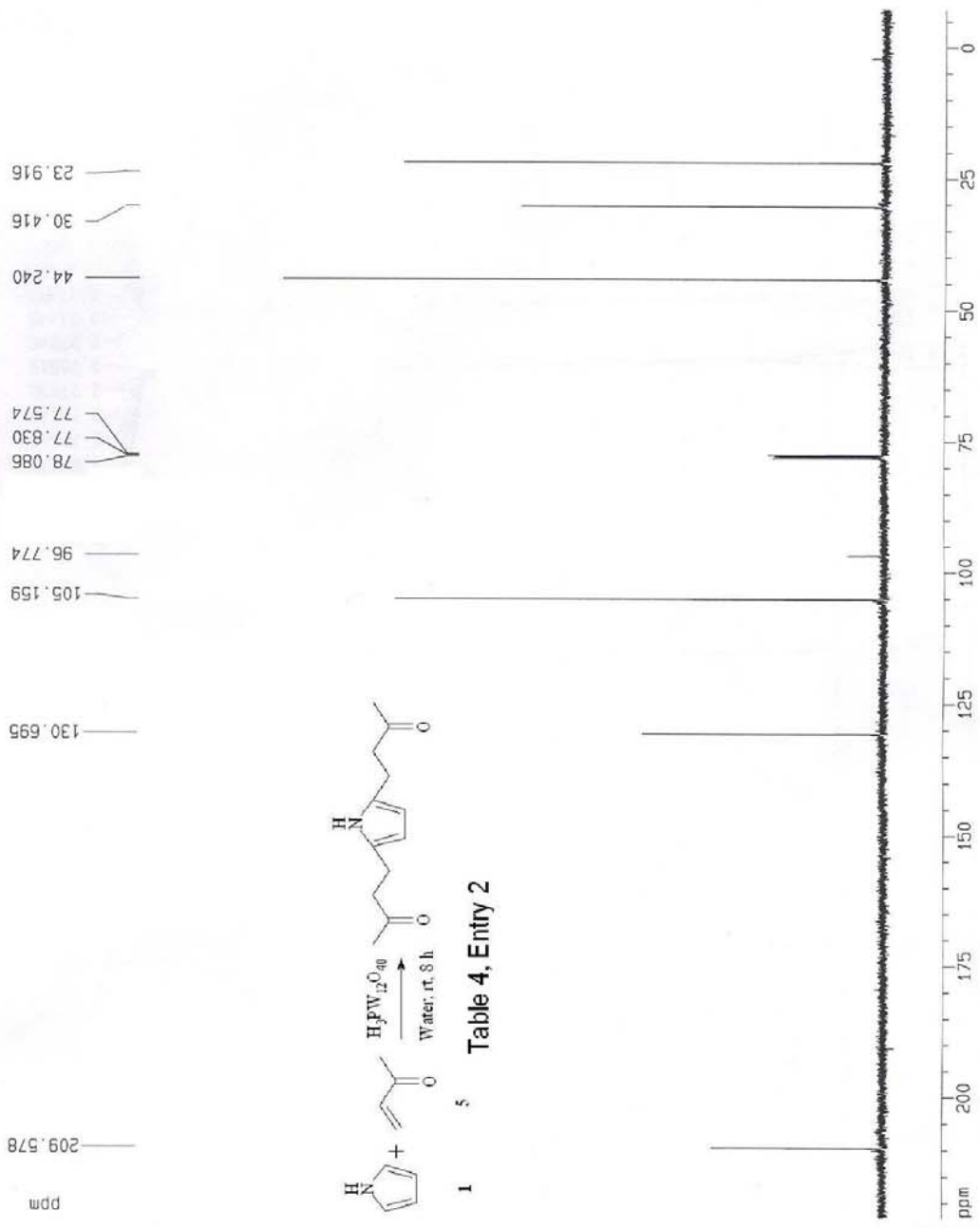
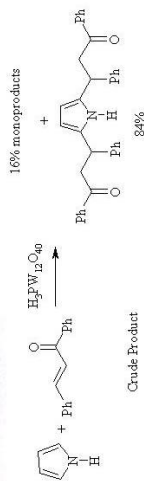


Table 4, Entry 2



a-92 1HNMR in CDCl3 at 300 K 84/6/26

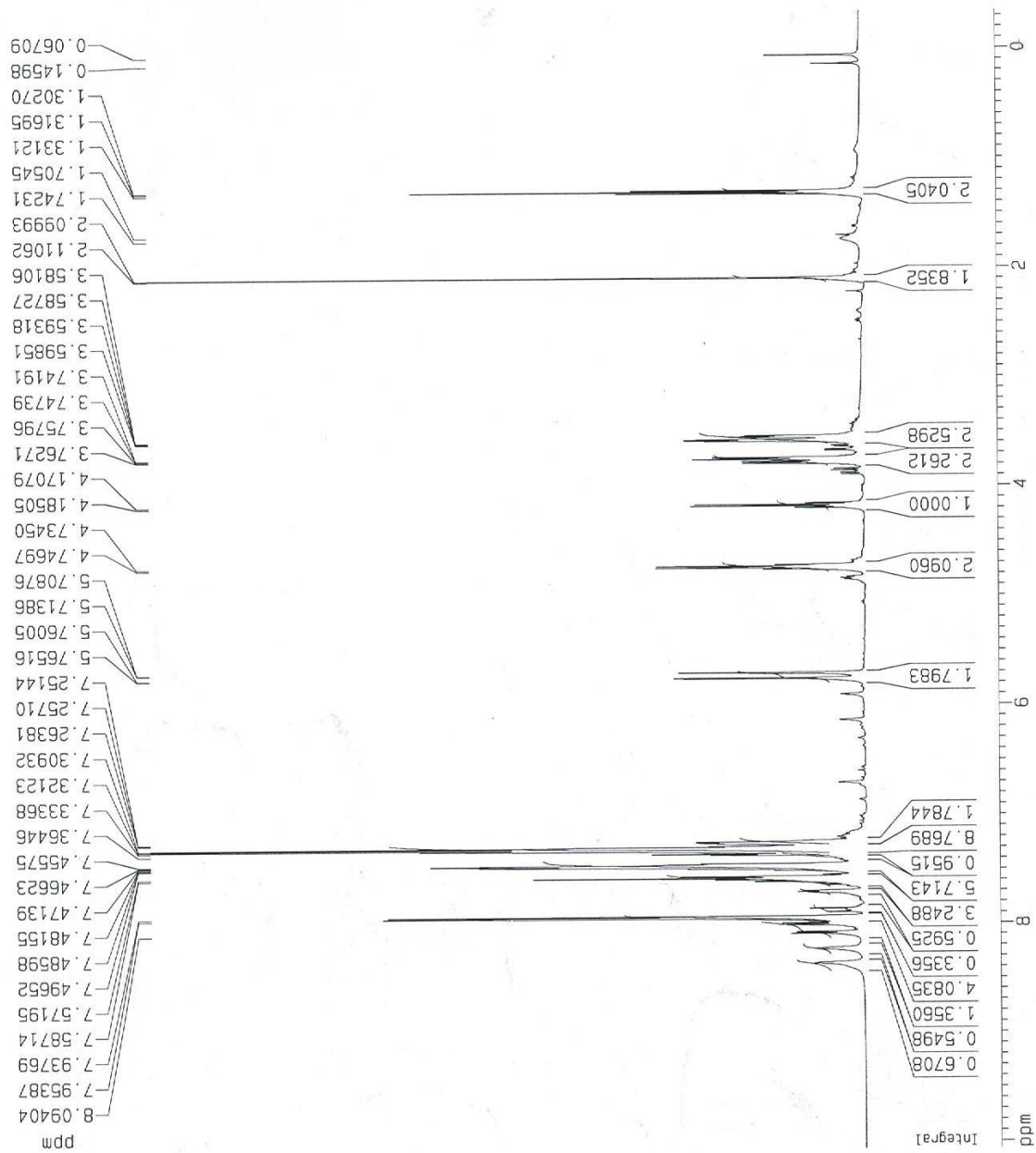
Current Data Parameters
 NAME Aryanasab
 EXPNO 32
 PROCNO 1

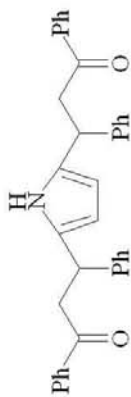
F2 - Acquisition Parameters
 Date_ 20050917
 Time 11.15
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 161.3
 DW 50.000 usec
 DE 6.50 usec
 TE 293.7 K
 D1 3.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 32.00 usec
 PL1 2.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

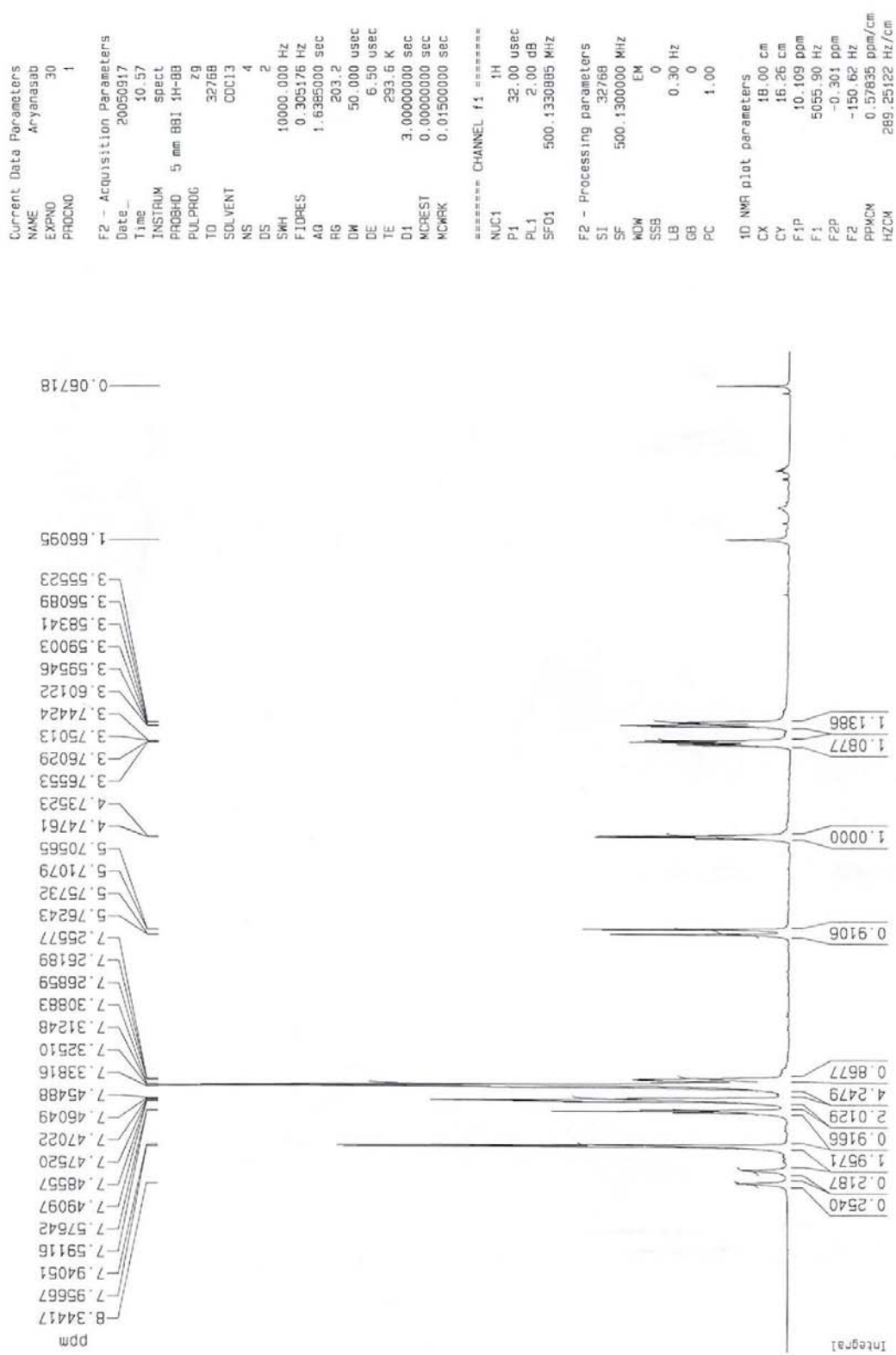
1D NMR plot parameters
 CX 18.00 cm
 CY 16.15 cm
 F1P 10.066 ppm
 F1 5034.16 Hz
 F2P -0.343 ppm
 F2 -172.36 Hz
 PPMCM 0.57835 ppm/cm
 HZCM 289.25122 Hz/cm





a-91-A ¹H NMR in CDCl₃ at 300 K 84/6/22

Table 4, Entry 3



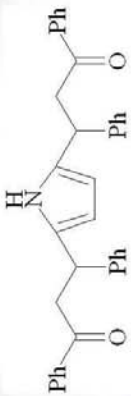
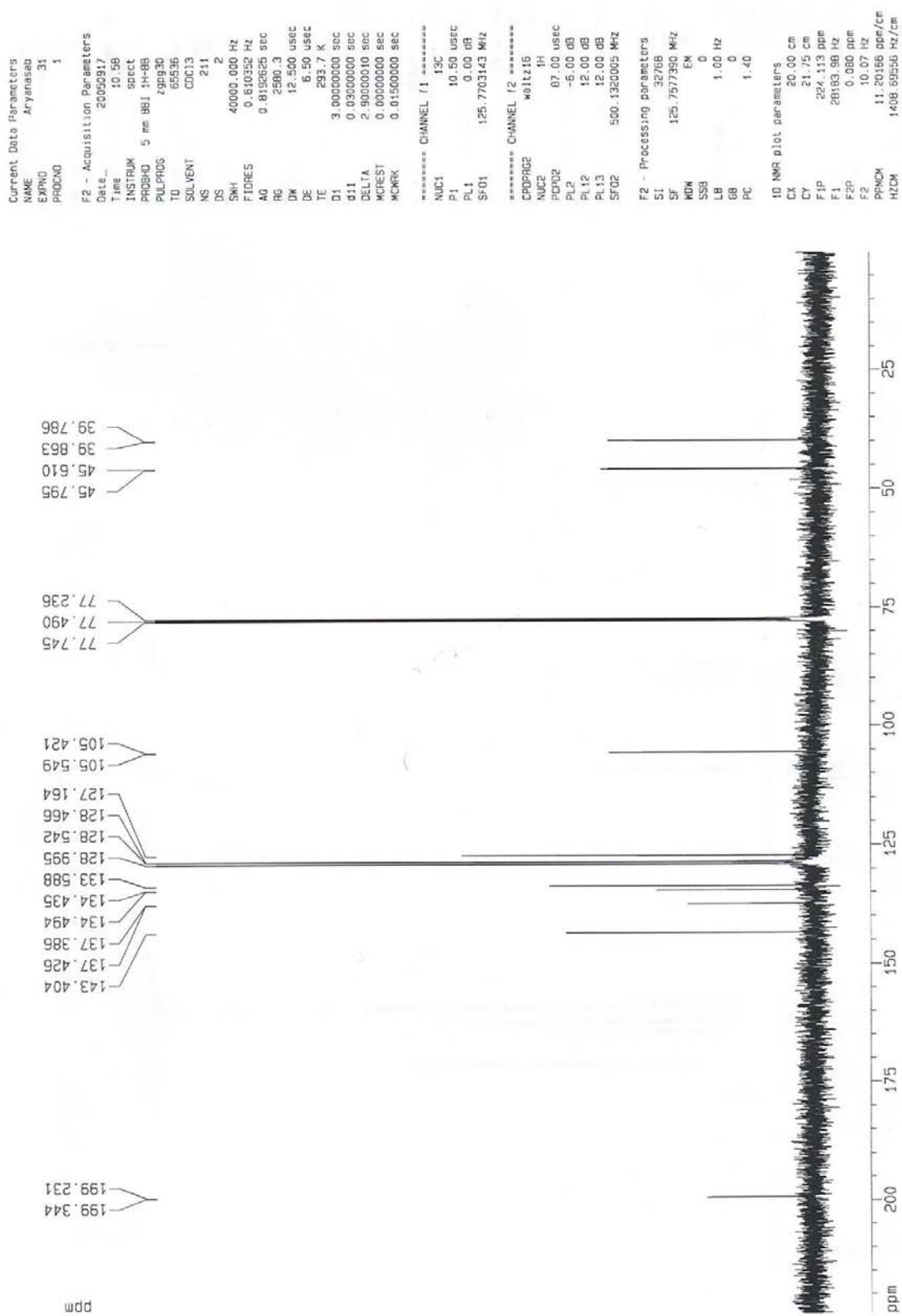
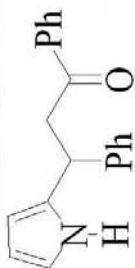


Table 4, Entry 3

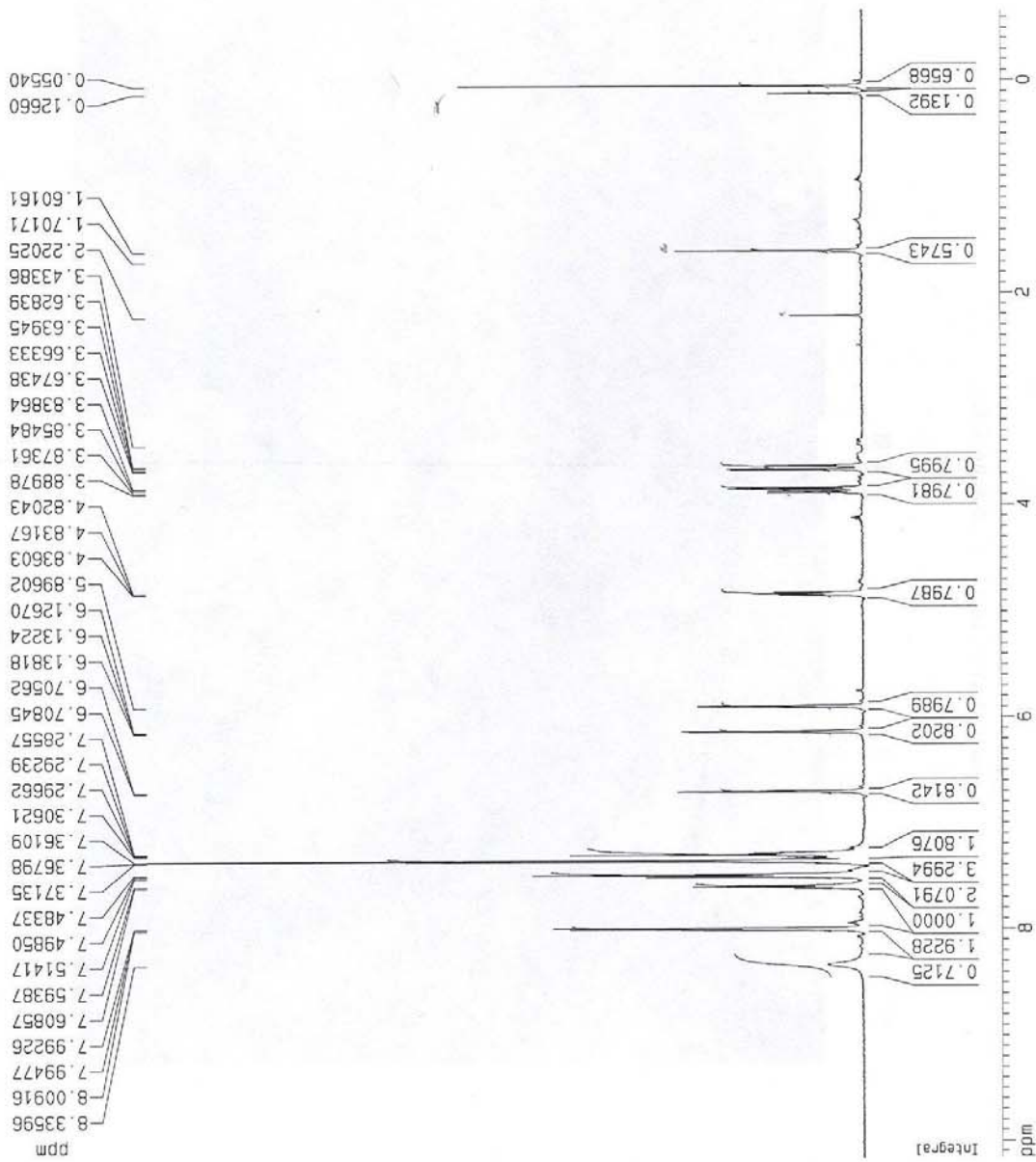
α-91A ¹³CNMR in CDCl₃ at 300 K 84/5/26





a-91B 1H NMR in CDCl3 at 300 K 84/6/22

Table 4, Entry 3



Current Data Parameters
 NAME Aryanasab
 EXPNO 24
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050913
 Time 9.53
 INSTRUM spect
 PROCNO 5 mm GNP 1H/13
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SMH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6385000 sec
 RG 574.7
 DW 50.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCKR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 32.00 usec
 PL1 2.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 18.00 cm
 CY 17.48 cm
 F1P 10.166 ppm
 F1 5084.12 Hz
 F2P -0.665 ppm
 F2 -332.55 Hz
 PRMCM 0.60170 ppm/cm
 HZCM 300.92583 Hz/cm

References

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