

Supporting Information

Reagent for safe and efficient diazo-transfer to primary amines:

2-azido-1,3-dimethylimidazolium hexafluorophosphate

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S-2 ¹H and ¹³C NMR charts of compound **5b**, **10a-t**, **12**, **14a-b**, **16**, **18**, **22**, **23**

S-31 Table S1. Cartesian Coordinates of Computational Data for ADMP **5b**
(B3LYP/6-31G**)

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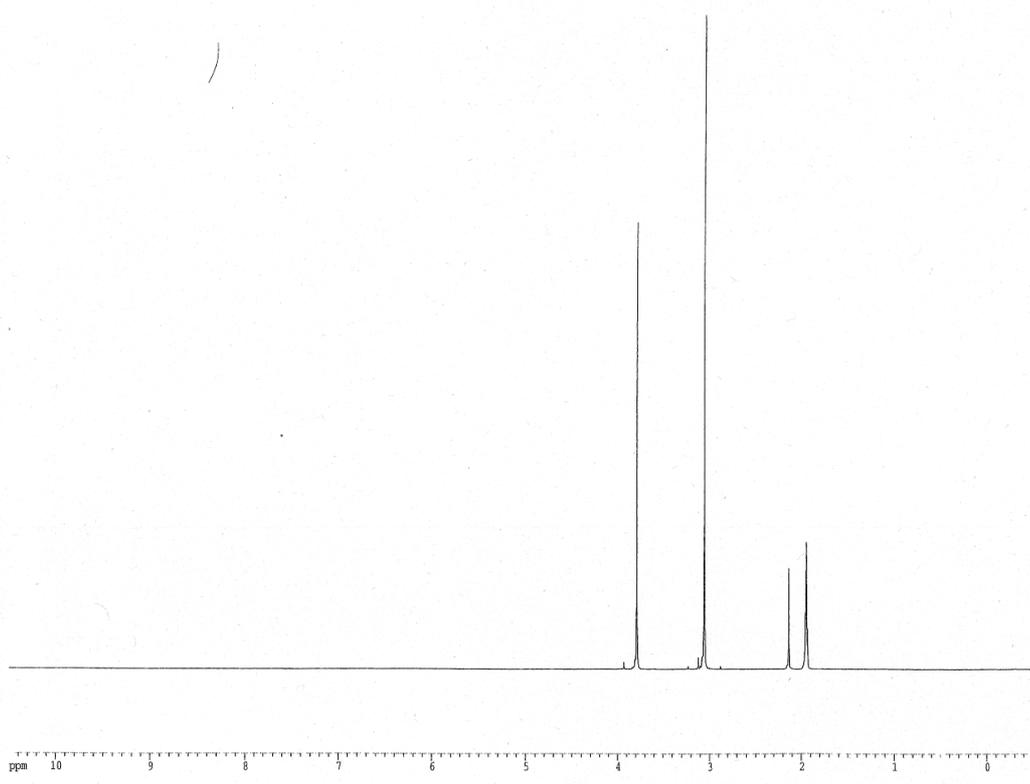
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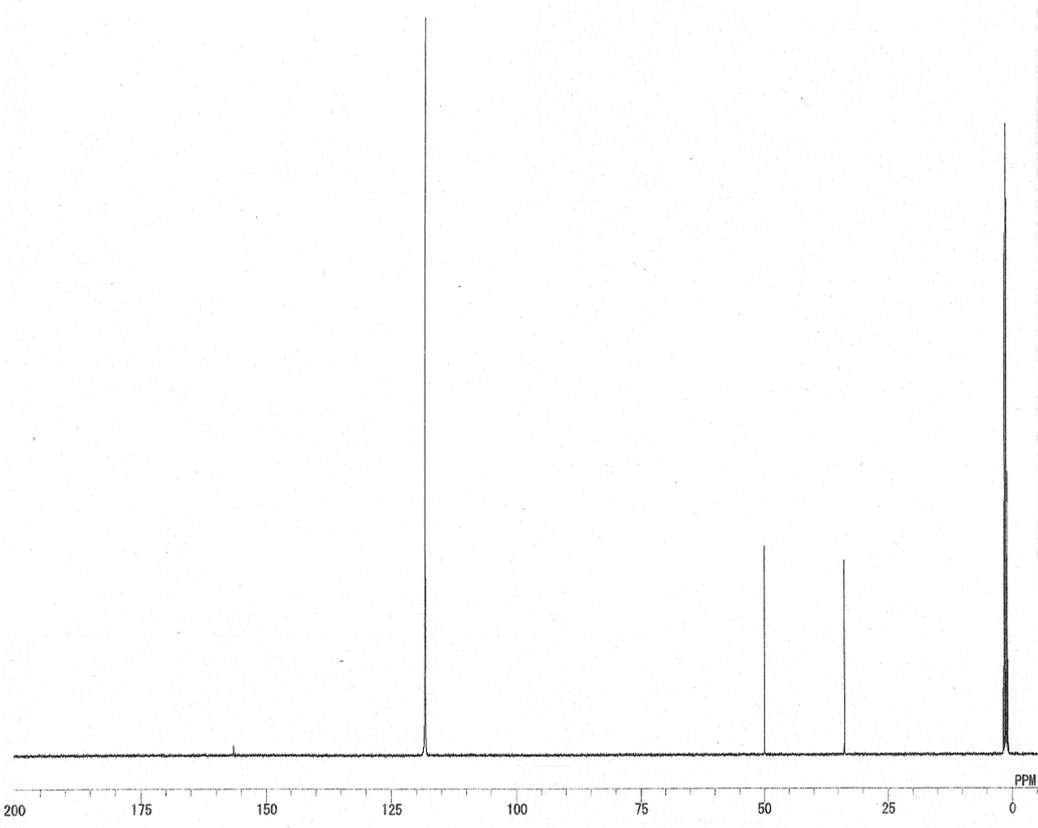
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F2         -4.500 ppm
F3         -200.07 Hz
PPMCM      0.36667 ppm/cm
RDCM       146.71434 Hz/cm

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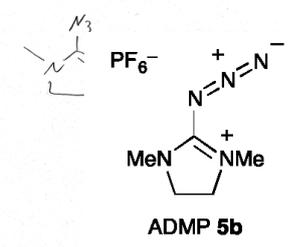
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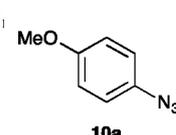
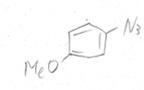
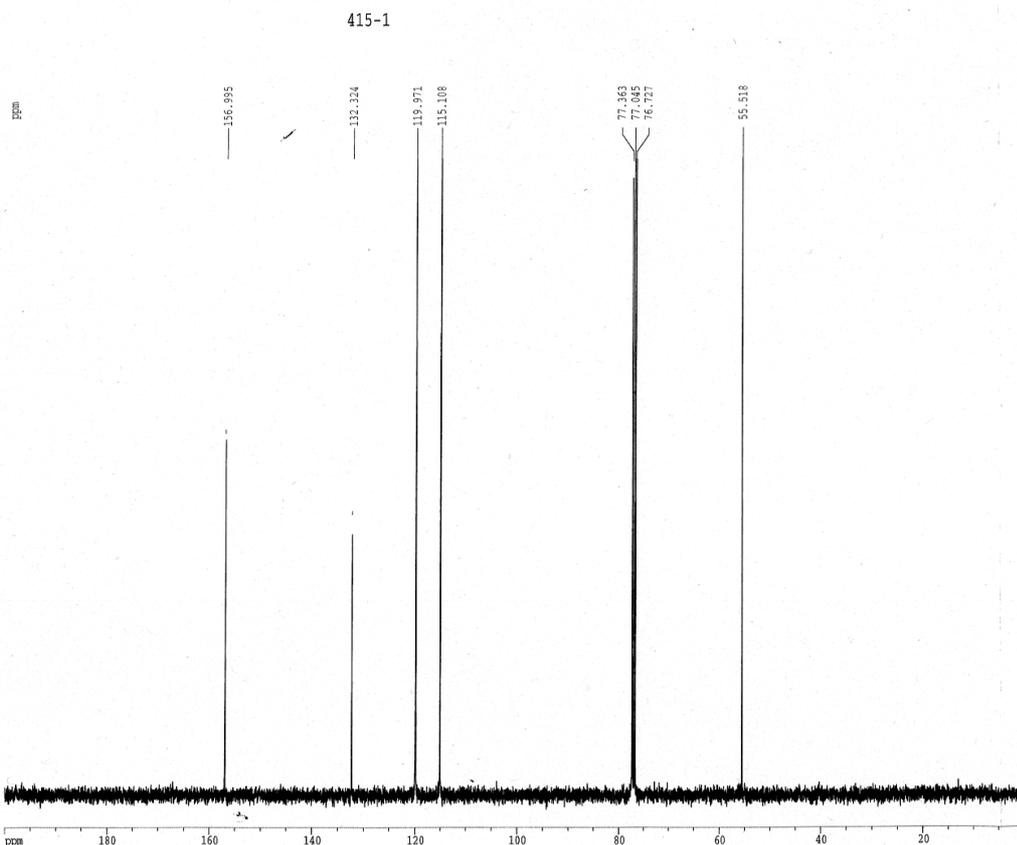
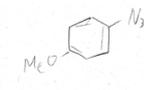
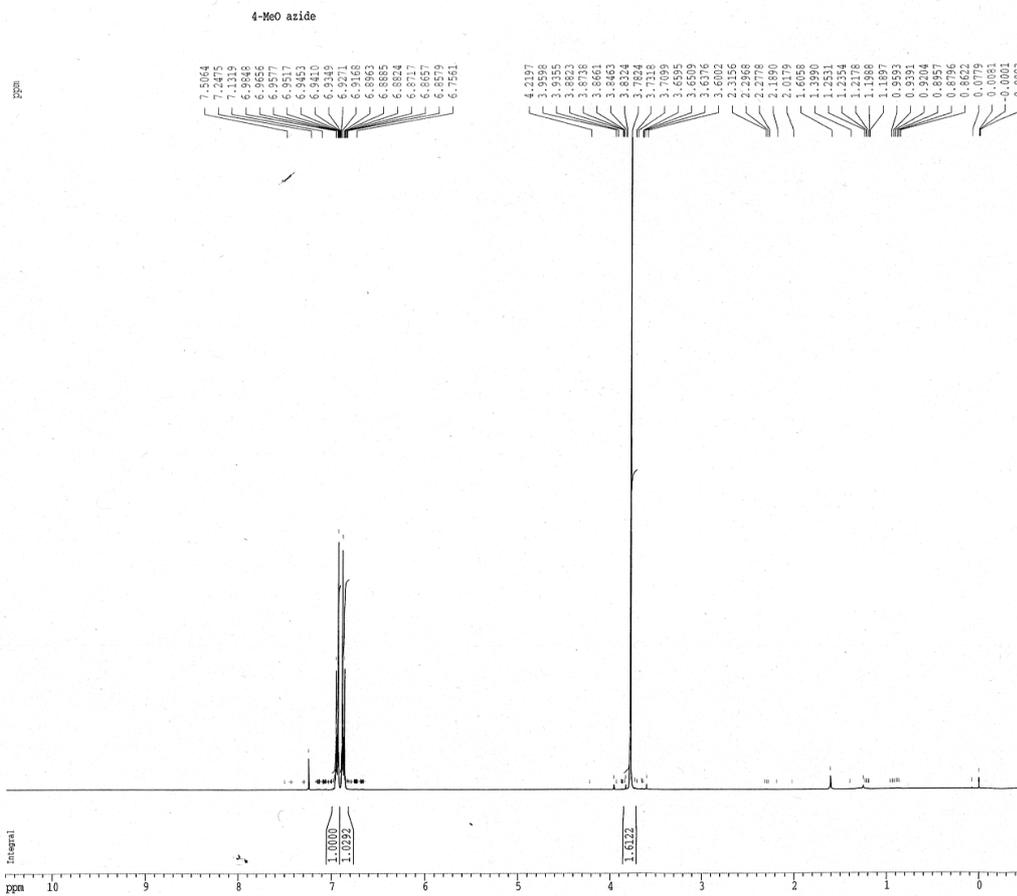


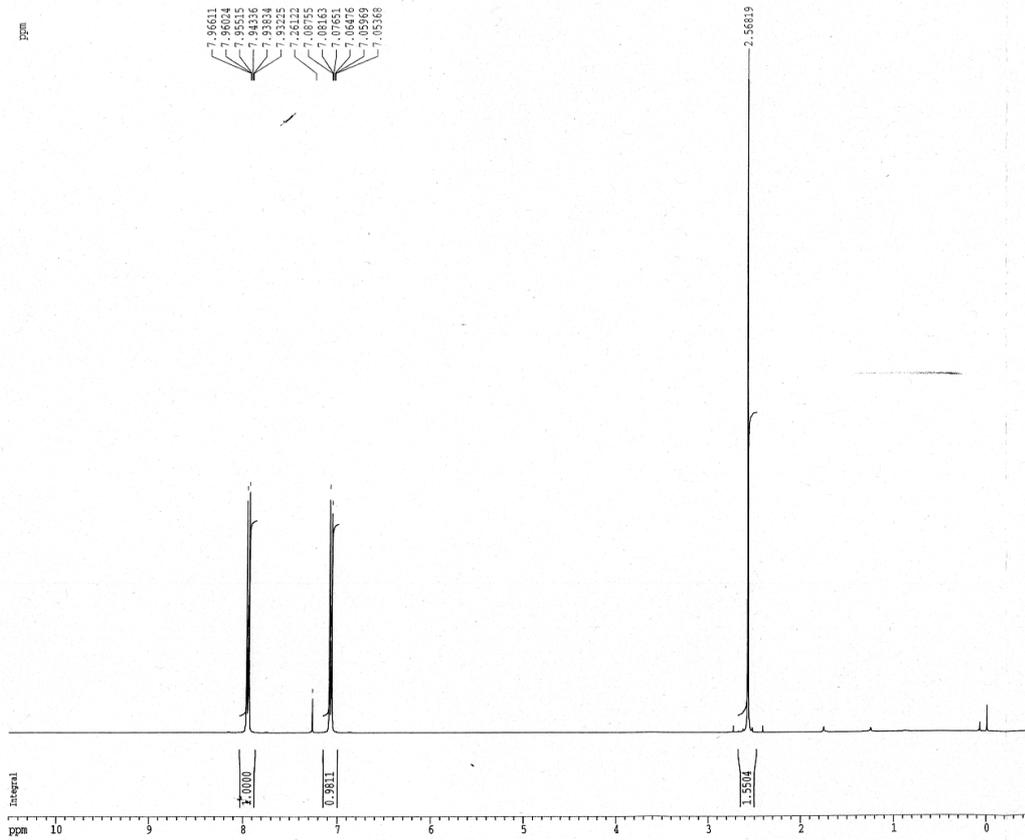
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T2 0.00
T3 90.00
T4 100.00
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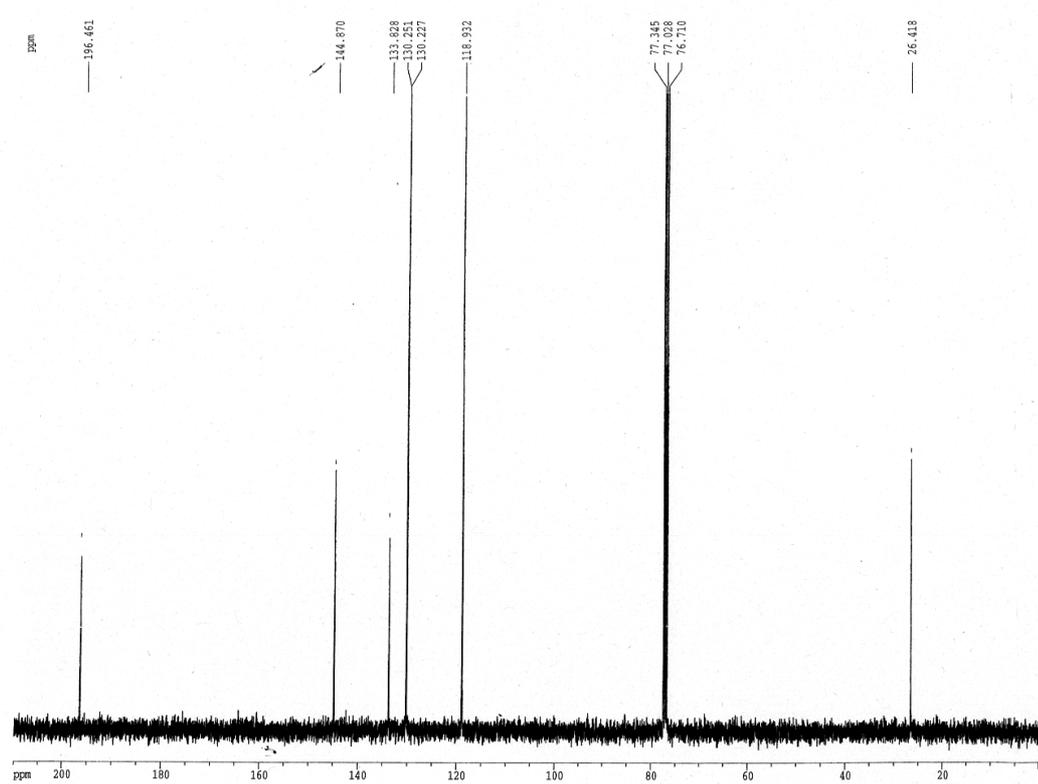
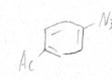
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 F2P -0.500 ppm
 F2 -200.07 Hz
 FWHM 0.36667 ppm/cm
 HZCM 146.71434 Hz/cm



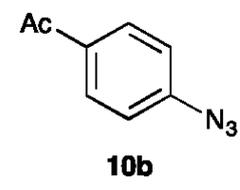
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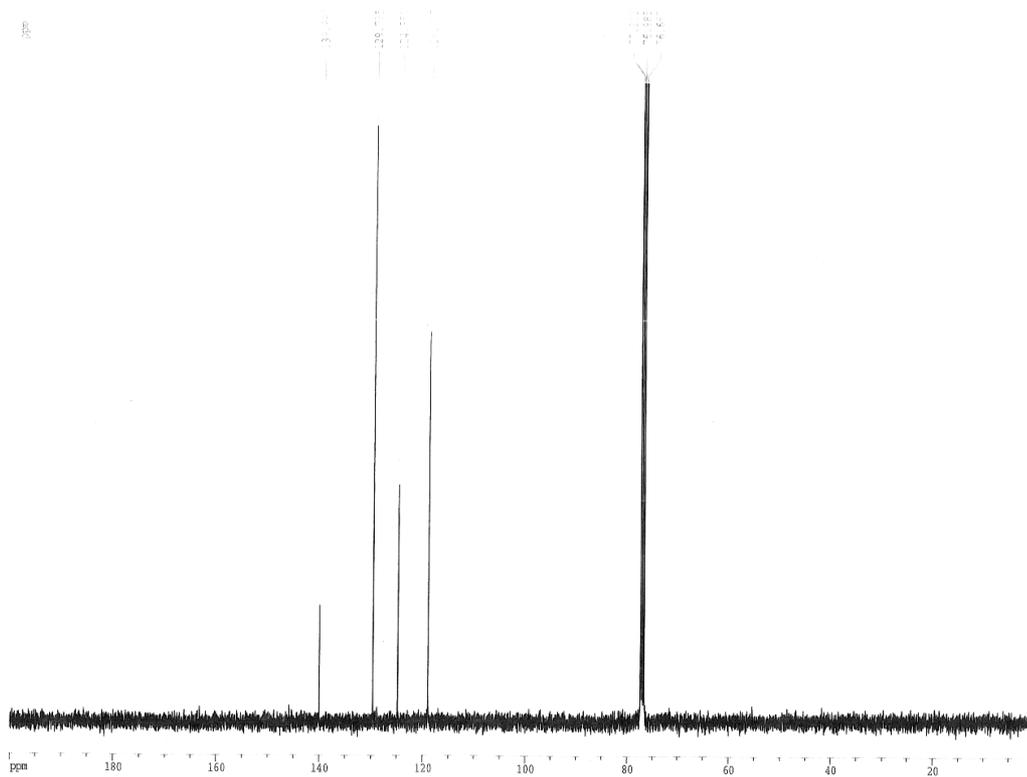
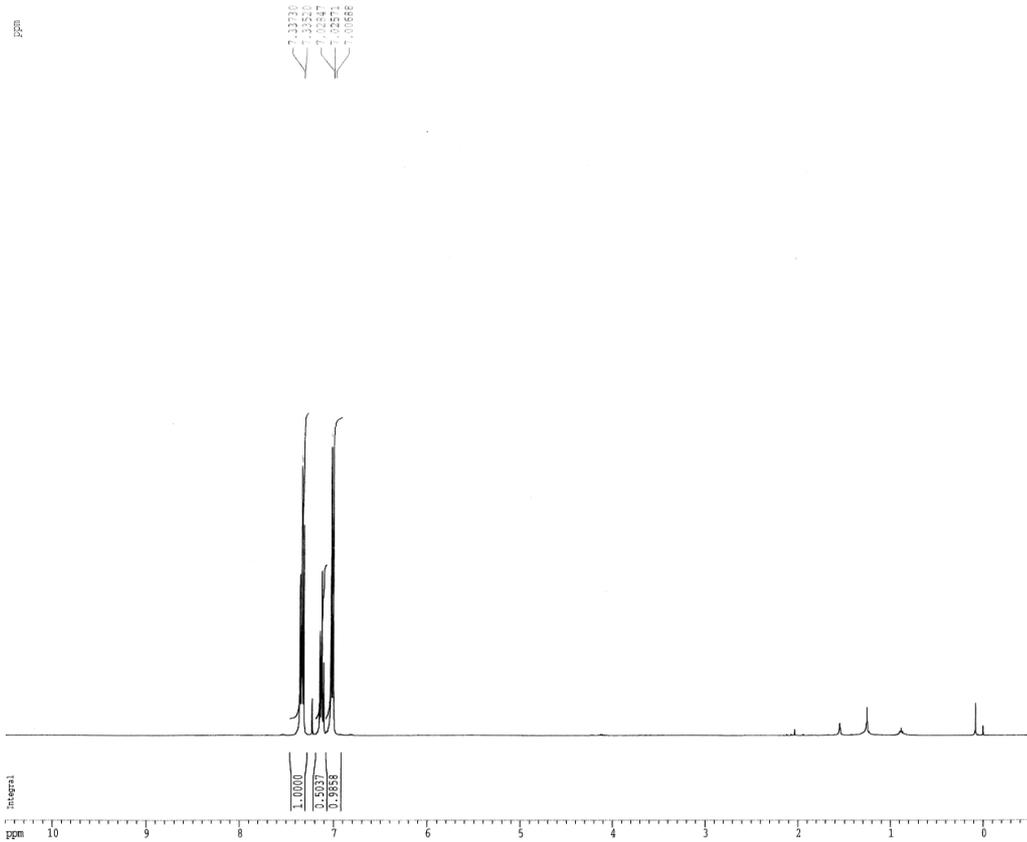
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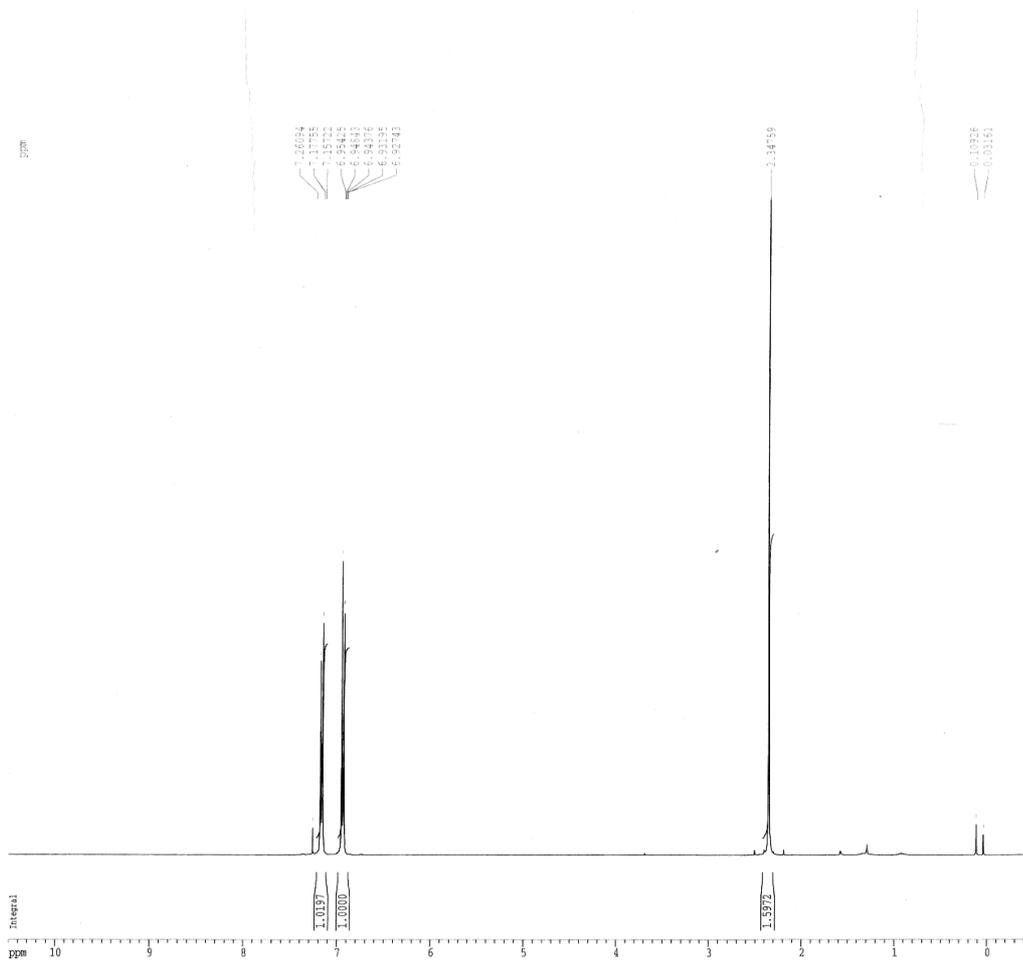
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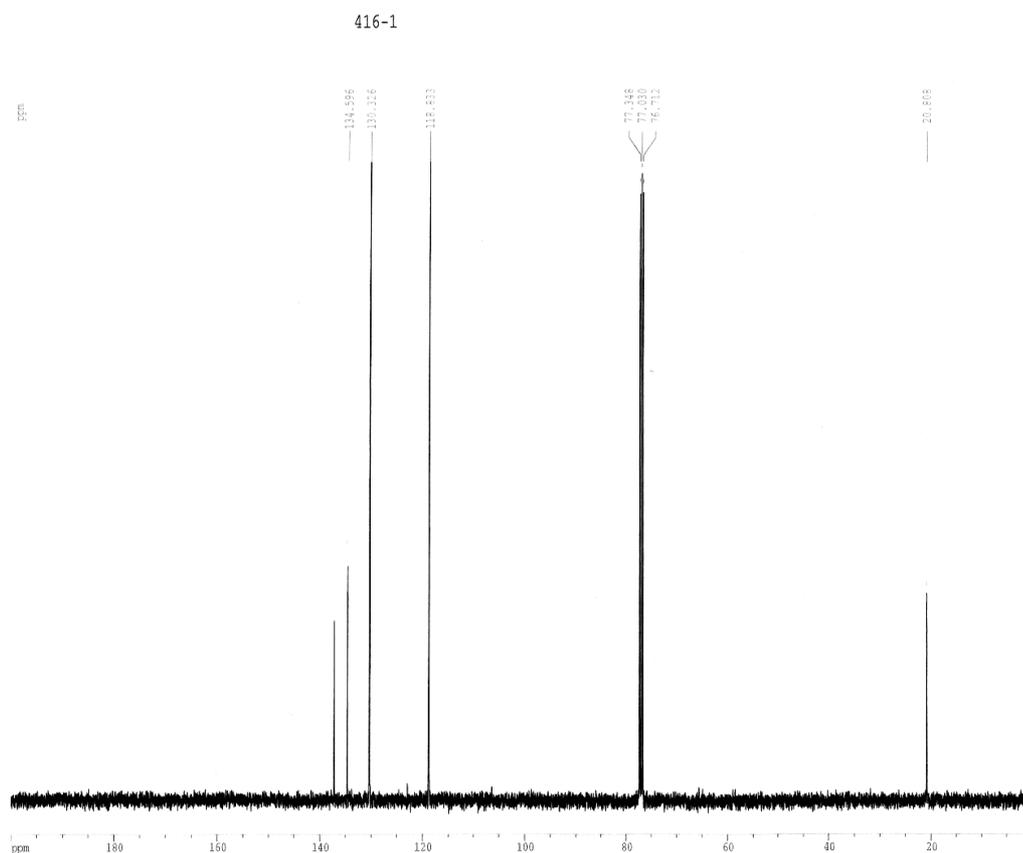


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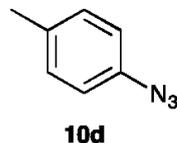
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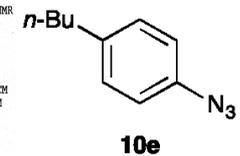
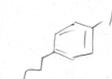
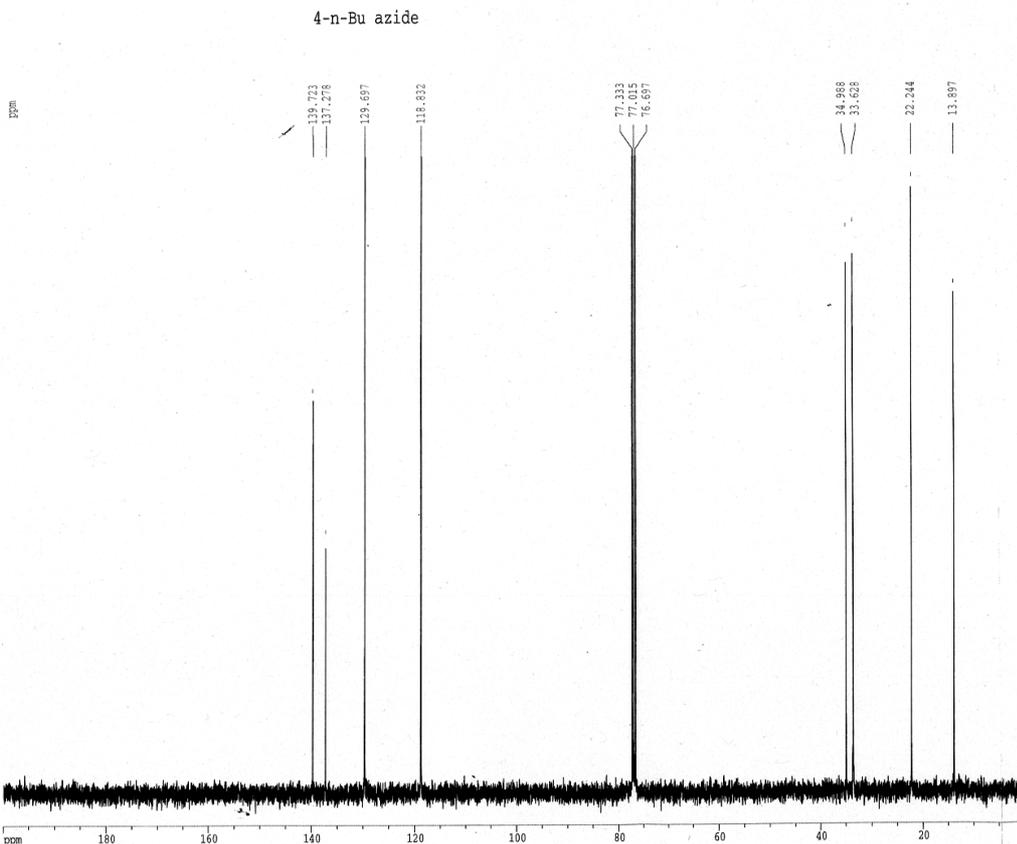
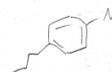
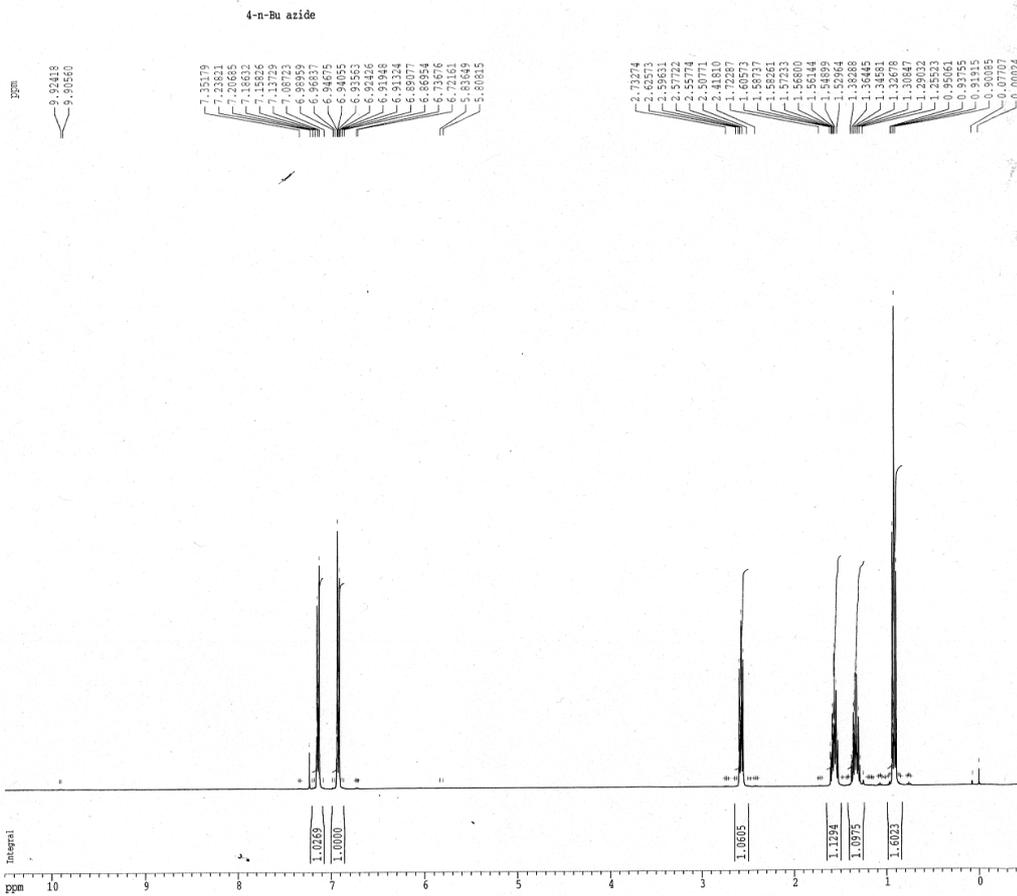
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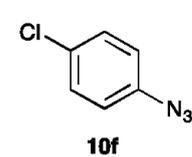
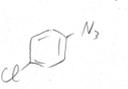
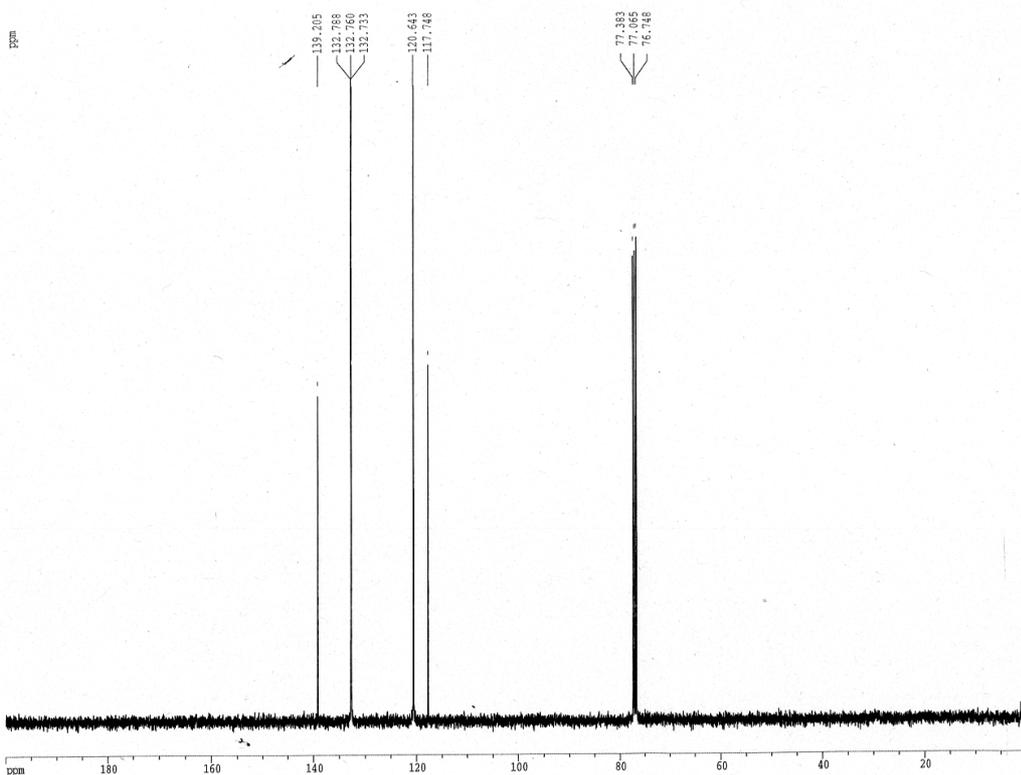
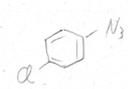
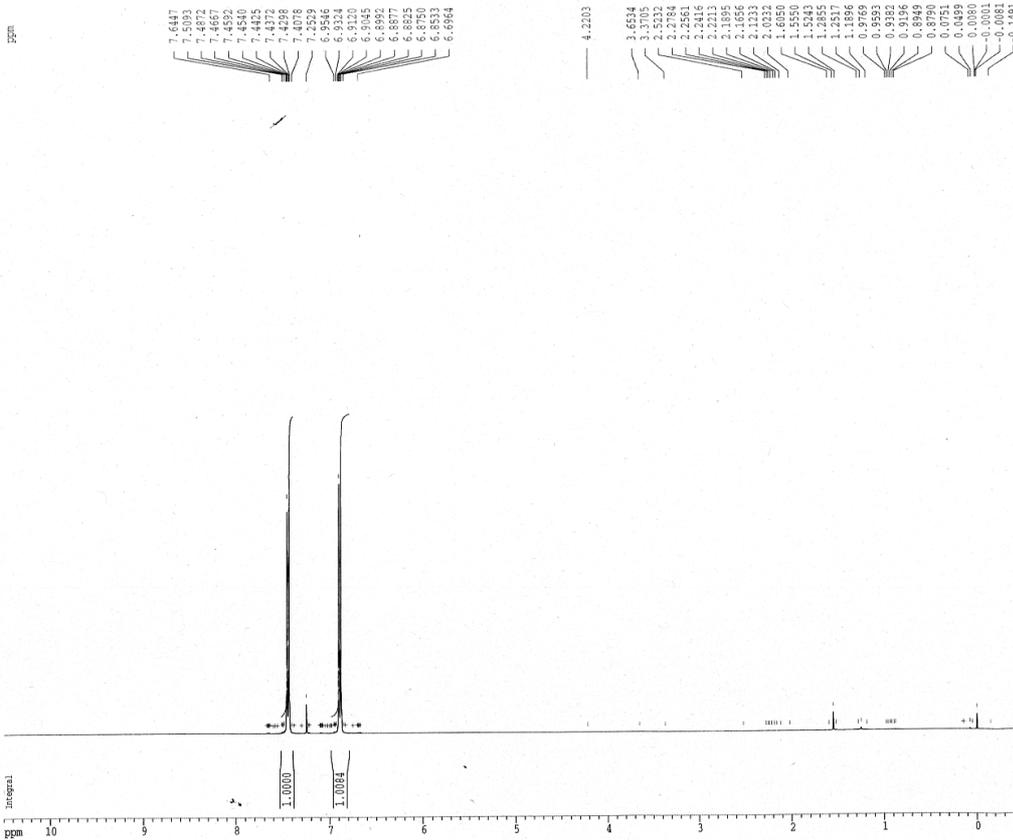
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 LB
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1D NMR |
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 PIP
 F1
 F2P
 F2
 FWHM
 HZCM

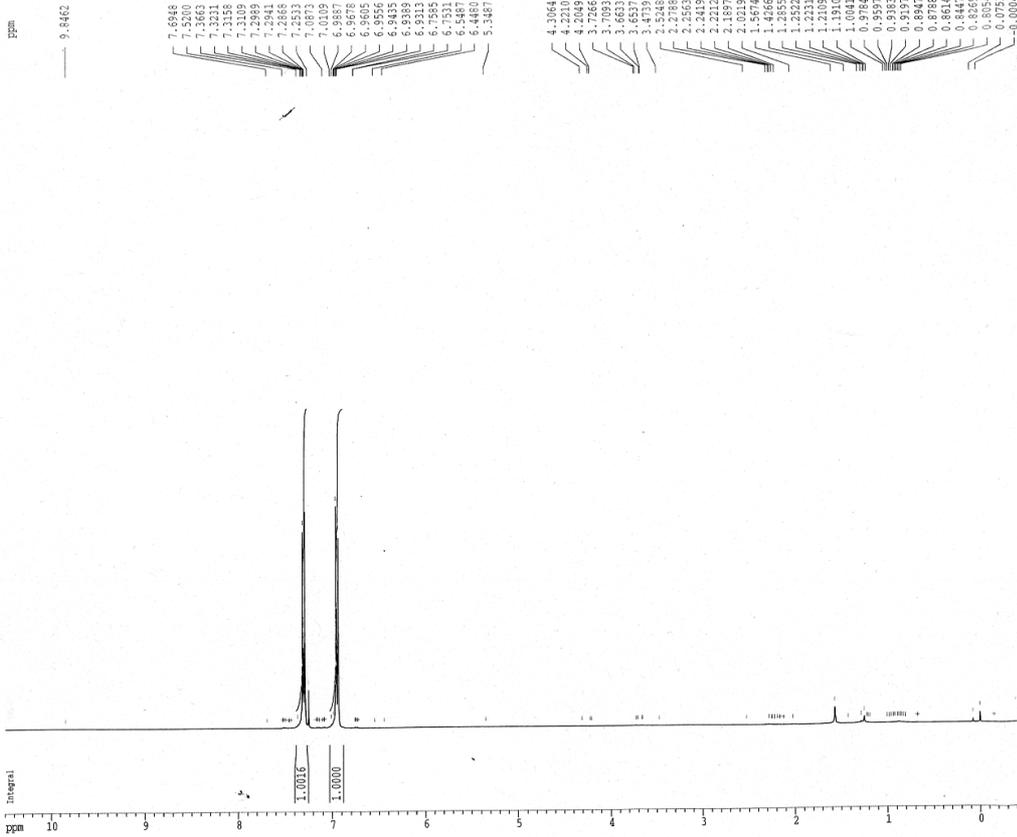




4-Cl azide



4-Br azide



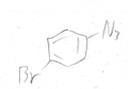
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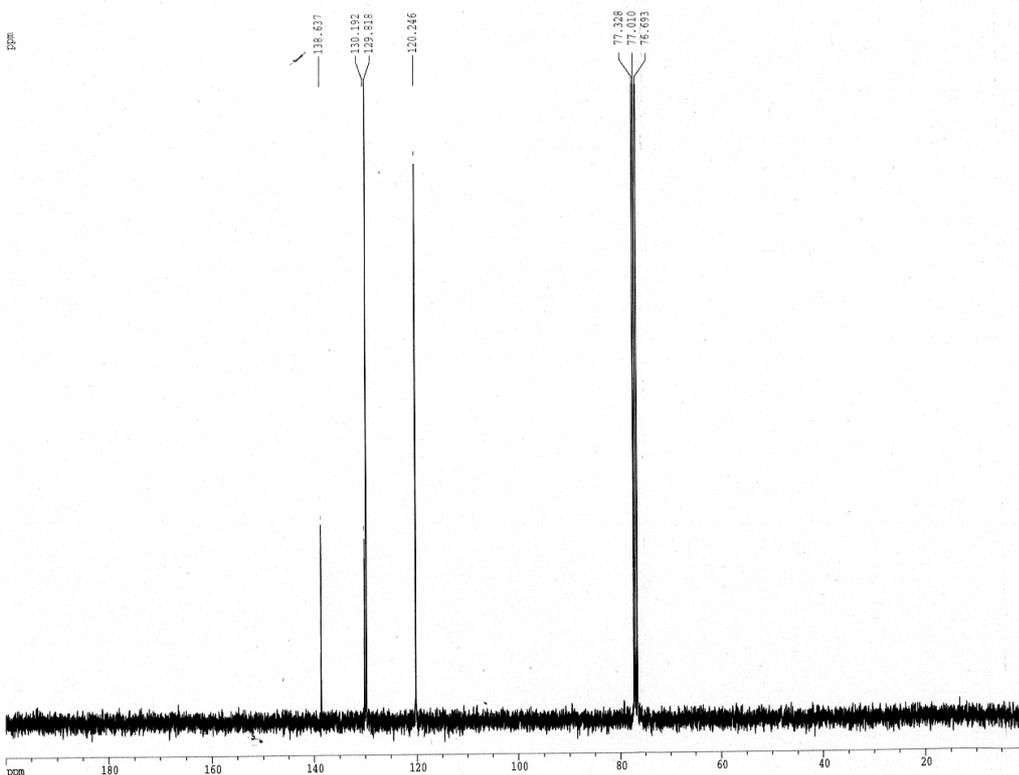
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1D NMR plot parameters
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 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCN 0.36667 ppm/cm
 HZCN 146.71434 Hz/cm



4-Br azide



Current Data Parameters
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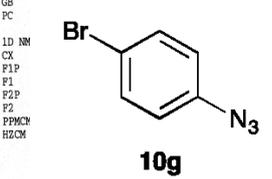
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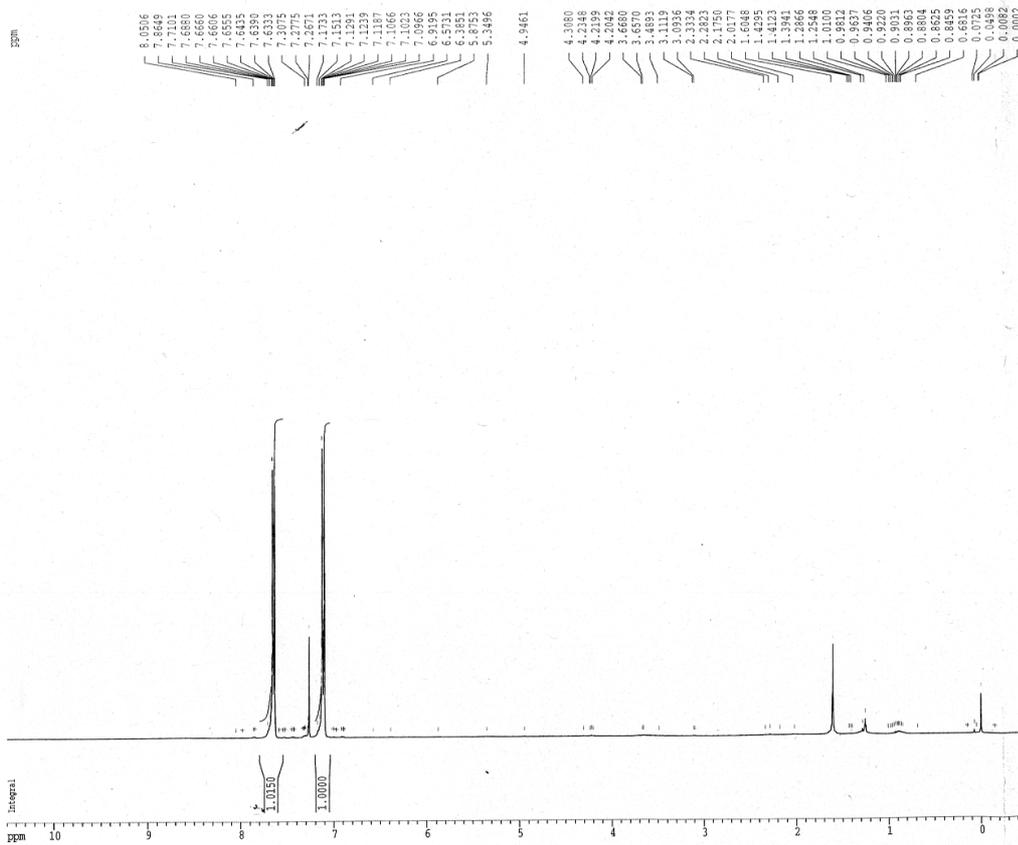
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1D NMR
 CX
 F1P
 F1
 F2P
 F2
 PPMCN
 HZCN



4-CN azide



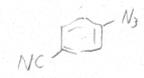
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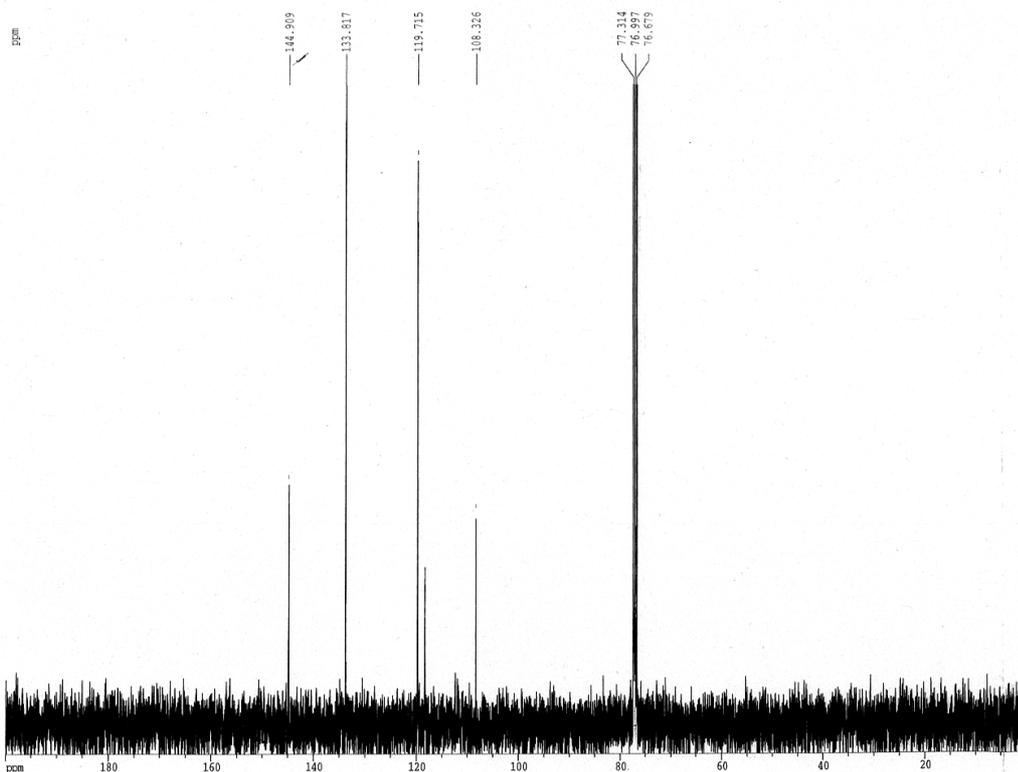
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1D NMR plot parameters
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 FIP 10.500 ppm
 F1 4201.37 Hz
 F2 -0.500 ppm
 F2 200.07 Hz
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 HECM 146.71434 Hz/cm



4-CN azide



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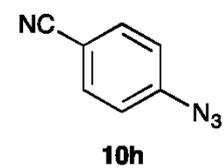
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 AQ 1.3074932 sec
 RG 14596.5
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
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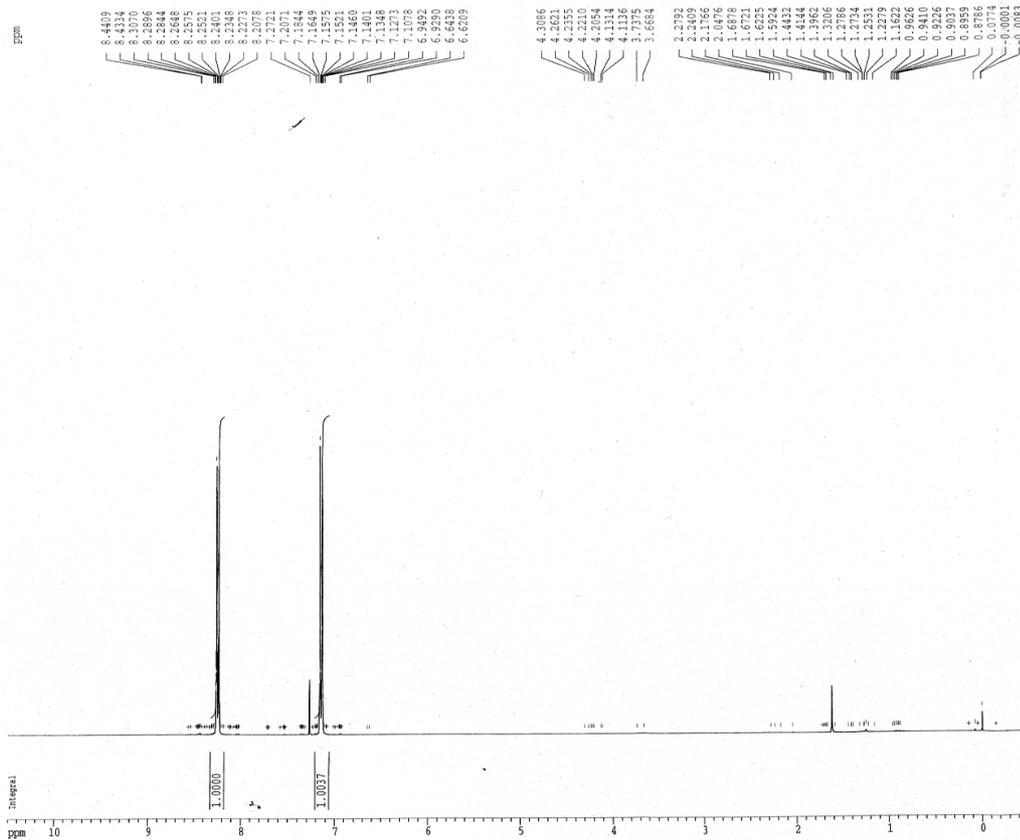
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1D N
 CX
 FIP
 F1
 F2
 F2
 FWHM
 HECM



4-NO2 azide



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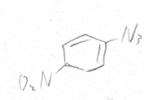
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NS         16
DS         2
SWH        8250.825 Hz
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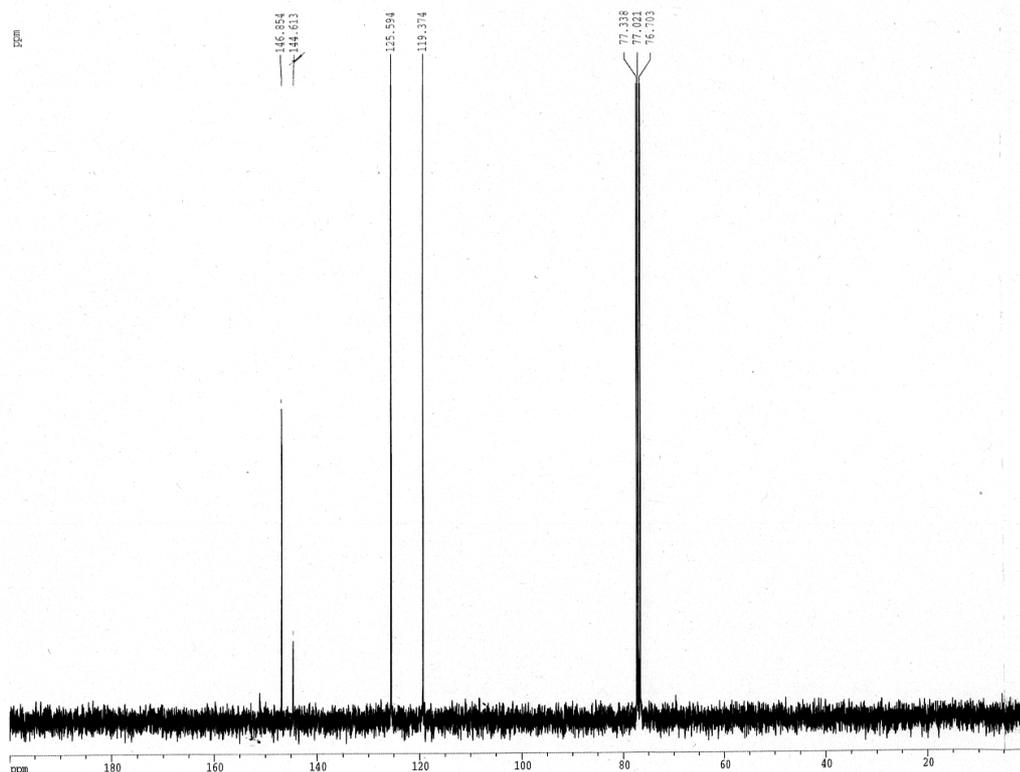
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SSB         0
LB          0.30 Hz
GB          0
PC          1.00

1D NMR plot parameters
CX          30.00 cm
F1P         10.500 ppm
F1          4203.37 Hz
F2P         -2.500 ppm
F2          -200.07 Hz
PFMCM       0.36667 ppm/cm
HECM        146.71434 Hz/cm
    
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4-NO2 azide



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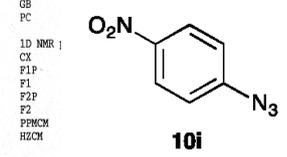
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DS         2
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FIDRES     0.382426 Hz
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RG         14596.5
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DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
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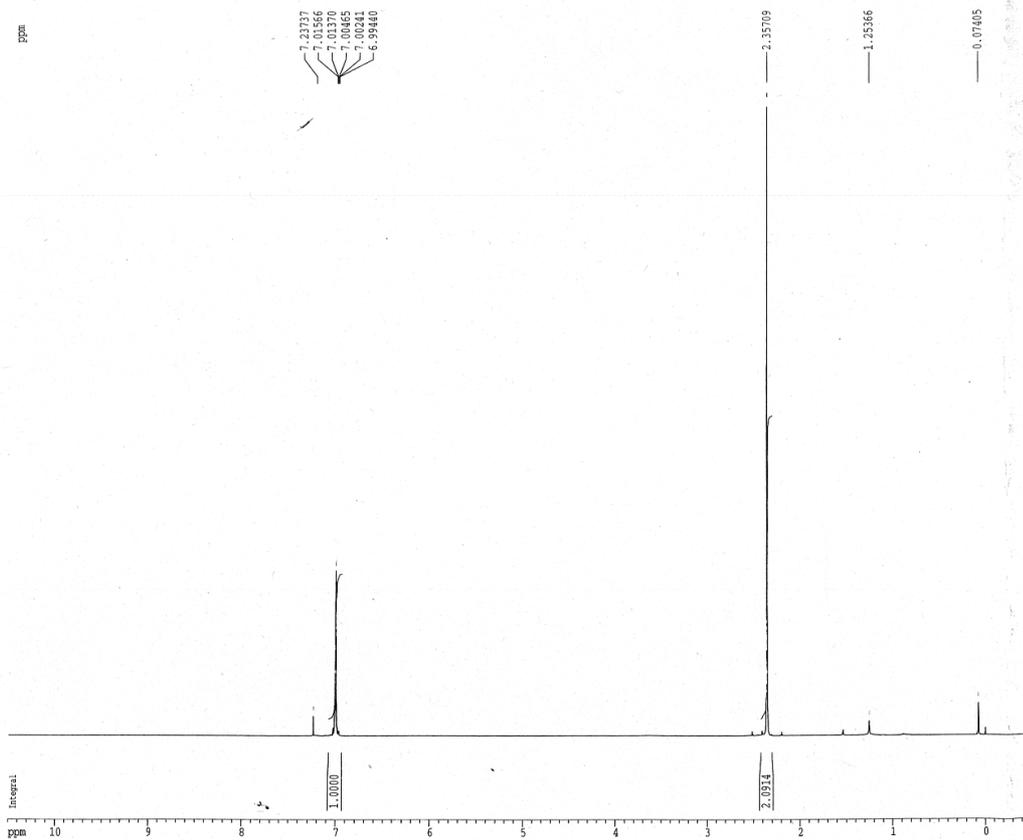
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CX          30.00 cm
F1P         10.500 ppm
F1          4203.37 Hz
F2P         -2.500 ppm
F2          -200.07 Hz
PFMCM       0.36667 ppm/cm
HECM        146.71434 Hz/cm
    
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421-1 678



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 DS 2
 SWH 8150.825 Hz
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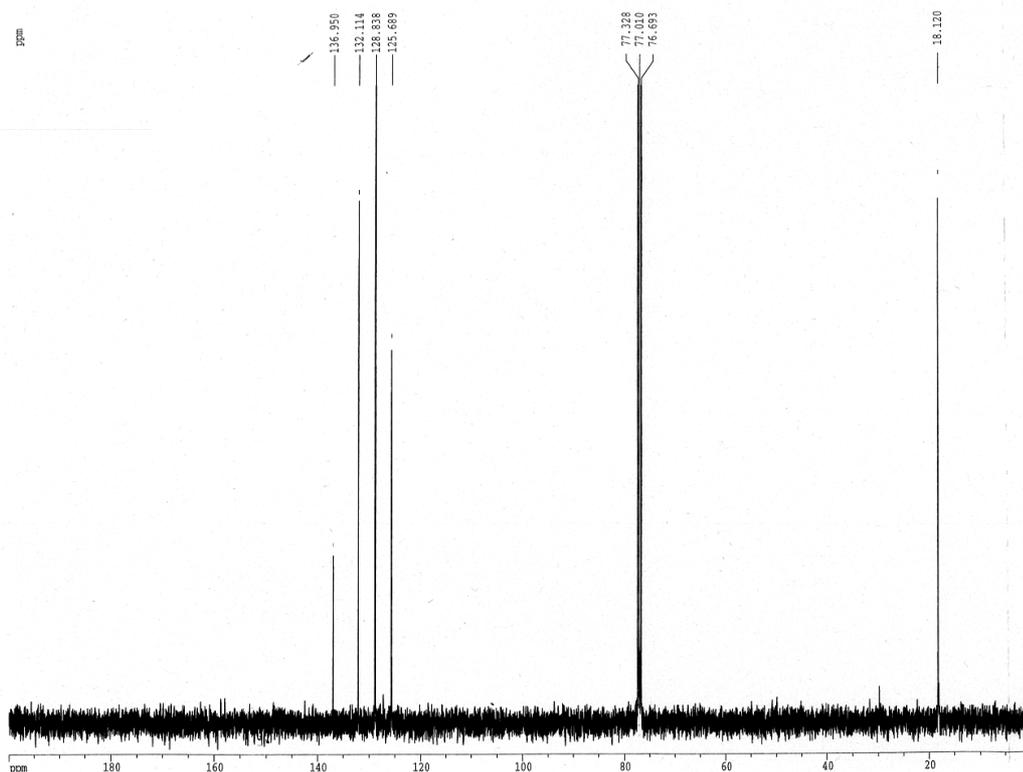
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 SFO1 400.1324710 MHz

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1D NMR plot parameters
 CX 30.00 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 FPCMC 0.36667 ppm/cm
 HZCM 146.71434 Hz/cm



421-1



Current Data Parameters
 NAME 09yano
 EXPNO 1117
 PROCNO 1

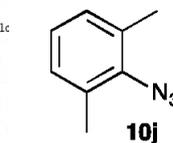
F2 - Acquisition Parameters
 Date_ 20100516
 Time 2.45
 INSTRUM dpx400
 PROBHID 5 mm BBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 13004
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -3.90 dB
 SFO1 100.6237959 MHz

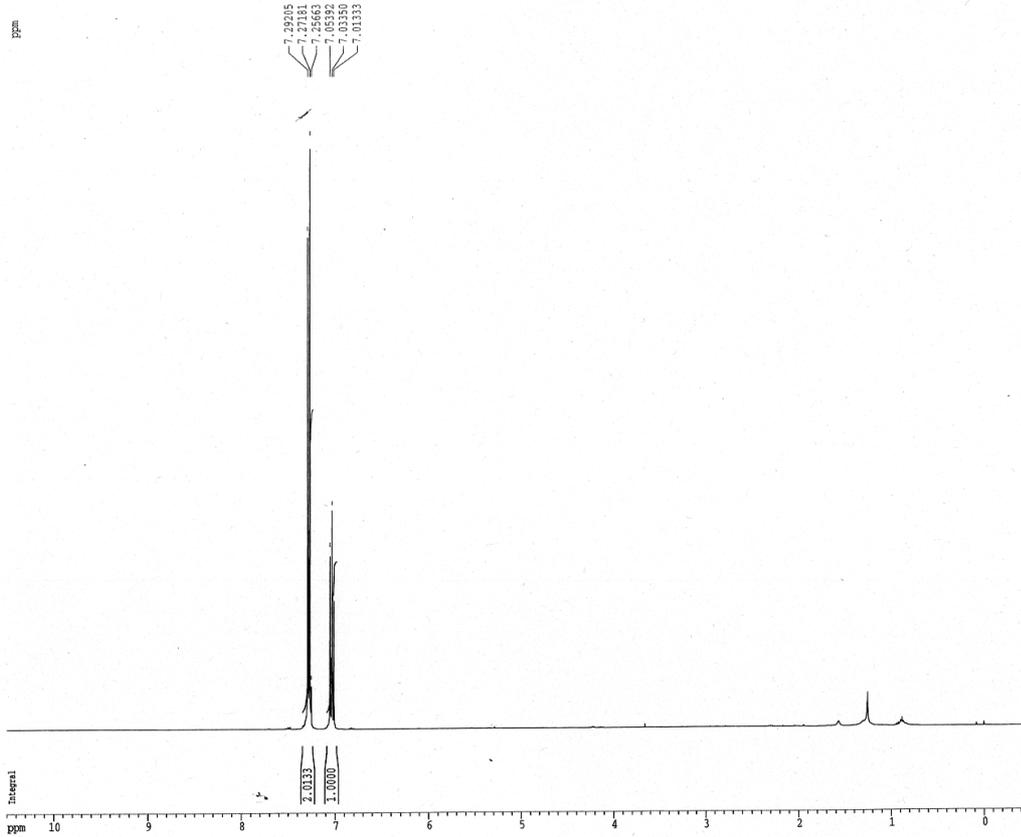
===== CHANNEL f2 =====
 CFCPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 9.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127721 MHz
 WDW EM
 SSB 0
 LB ...
 GB
 FC

1D NMR plot
 CX
 FIP
 F1
 F2P
 F2
 FPCMC
 HZCM



2,6-dichloro azide



```

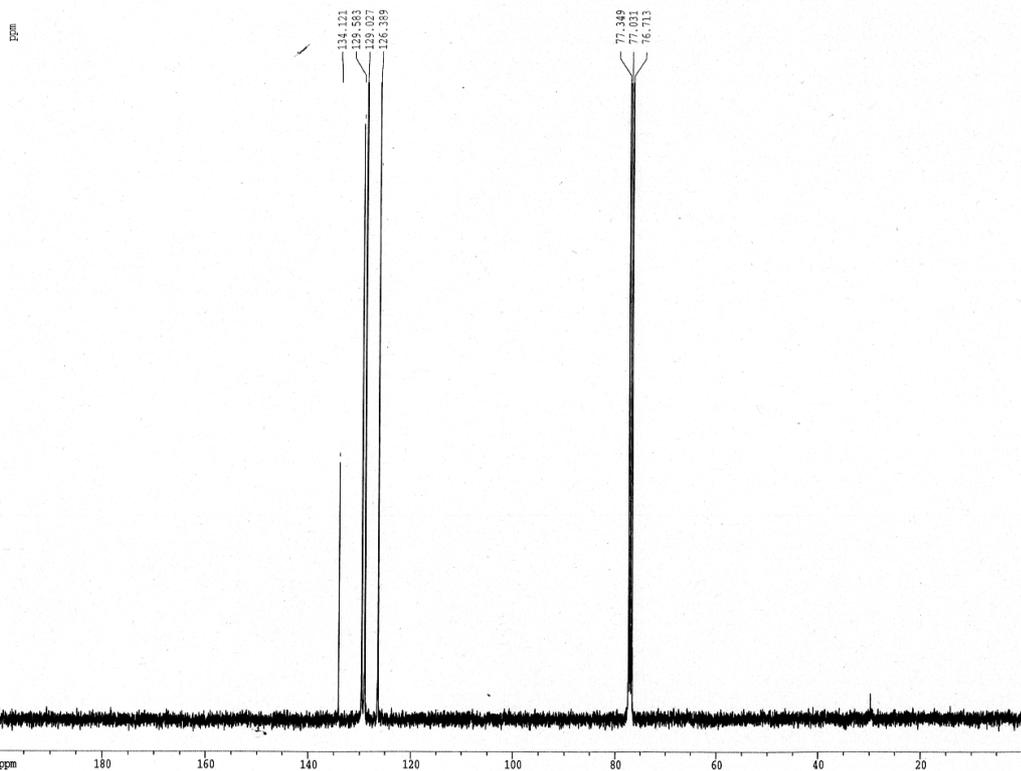
Current Data Parameters
NAME      09yano
EXPNO    1199
PROCNO   1

F2 - Acquisition Parameters
Date_    20100827
Time     18.24
INSTRUM  dpx400
PROBHD   5 mm BBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8250.825 Hz
FIDRES   0.125888 Hz
AQ       3.9715316 sec
RG       128
DW       60.000 usec
DE       6.00 usec
TE       300.0 K
D1       1.00000000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       12.00 usec
PL1      -6.00 dB
SFO1    400.1324710 MHz

F2 - Processing parameters
SI       32768
SF       400.1300112 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       30.00 cm
F1P      10.200 ppm
F1       4201.37 Hz
F2P      -3.500 ppm
F2       -300.07 Hz
PPMCM    0.35667 ppm/cm
HZCM     146.71434 Hz/cm
    
```



```

Current Data Parameters
NAME      09yano
EXPNO    1201
PROCNO   1

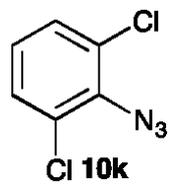
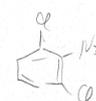
F2 - Acquisition Parameters
Date_    20100829
Time     14.26
INSTRUM  dpx400
PROBHD   5 mm BBO BB-
PULPROG  zgdc30
TD       65536
SOLVENT  CDCl3
NS       911
DS       2
SWH      25062.656 Hz
FIDRES   0.382426 Hz
AQ       1.3074932 sec
RG       14596.5
DW       19.950 usec
DE       6.00 usec
TE       300.0 K
D1       2.00000000 sec
d11      0.03000000 sec

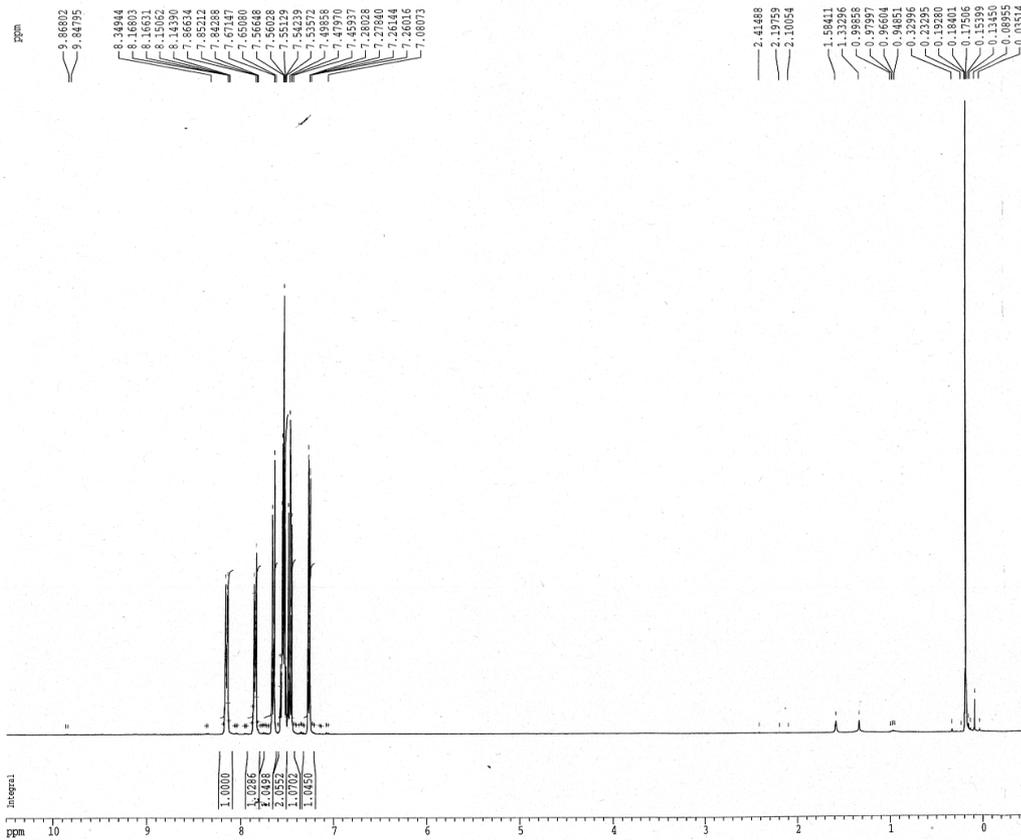
===== CHANNEL f1 =====
NUC1     13C
P1       10.00 usec
PL1      -3.90 dB
SFO1    100.6237959 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -6.00 dB
PL12     9.00 dB
SFO2    400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127721 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00

1D NMR
CX
F1P
F1
F2P
F2
PPMCM
HZCM
    
```





Current Data Parameters
 NAME 09yano
 EXPNO 809
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091028
 Time 19.25
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.122898 Hz
 AQ 3.9715316 sec
 RG 64
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

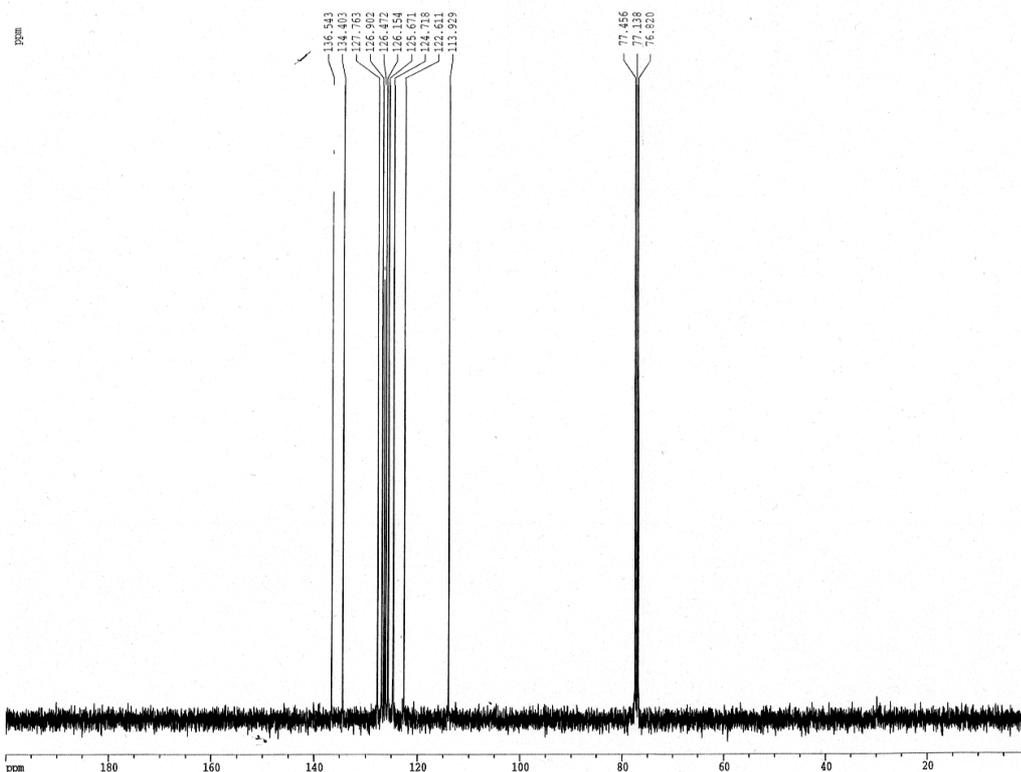
===== CHANNEL f1 =====
 NUCL1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFOL 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300034 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 FIP 10.800 ppm
 F1 4201.37 Hz
 F2 -0.500 ppm
 F2 -200.07 Hz
 FPMCM 0.36667 ppm/cm
 HZCM 146.71434 Hz/cm



449--1



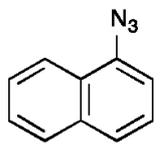
Current Data Parameters
 NAME 09yano
 EXPNO 1186
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100821
 Time 17.52
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 14596.5
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

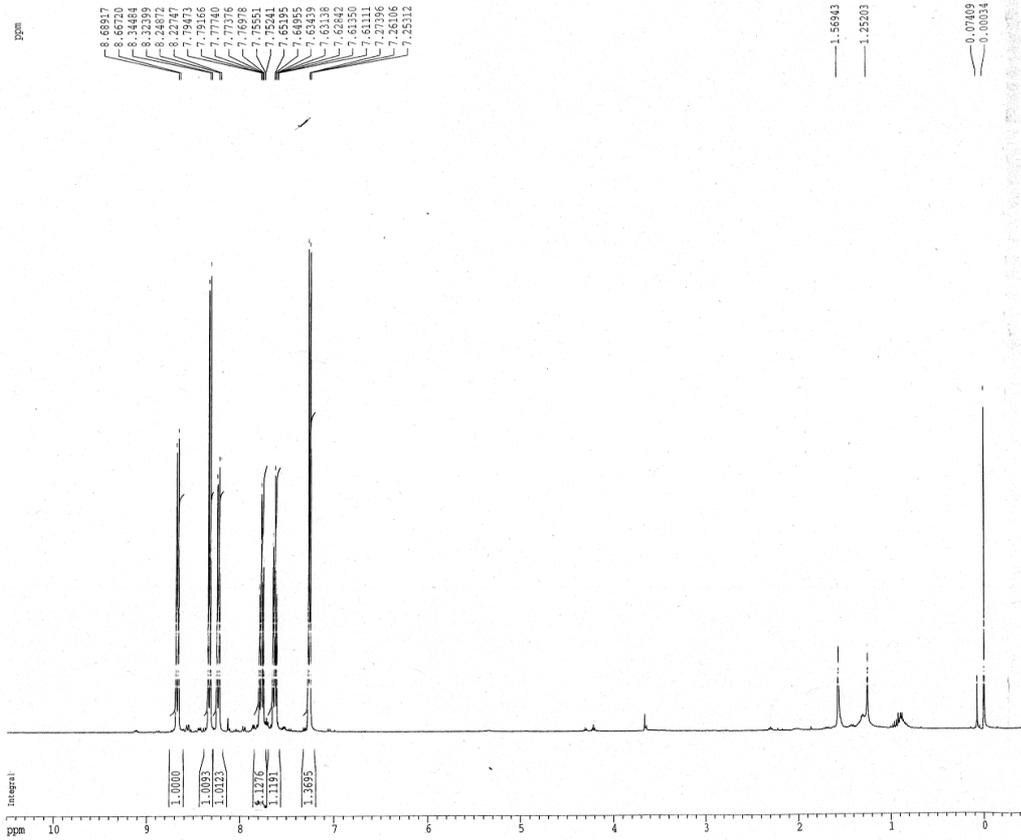
===== CHANNEL f1 =====
 NUCL1 13C
 P1 10.00 usec
 PL1 -3.90 dB
 SFOL 100.6237959 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCL2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 9.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127721 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC



101



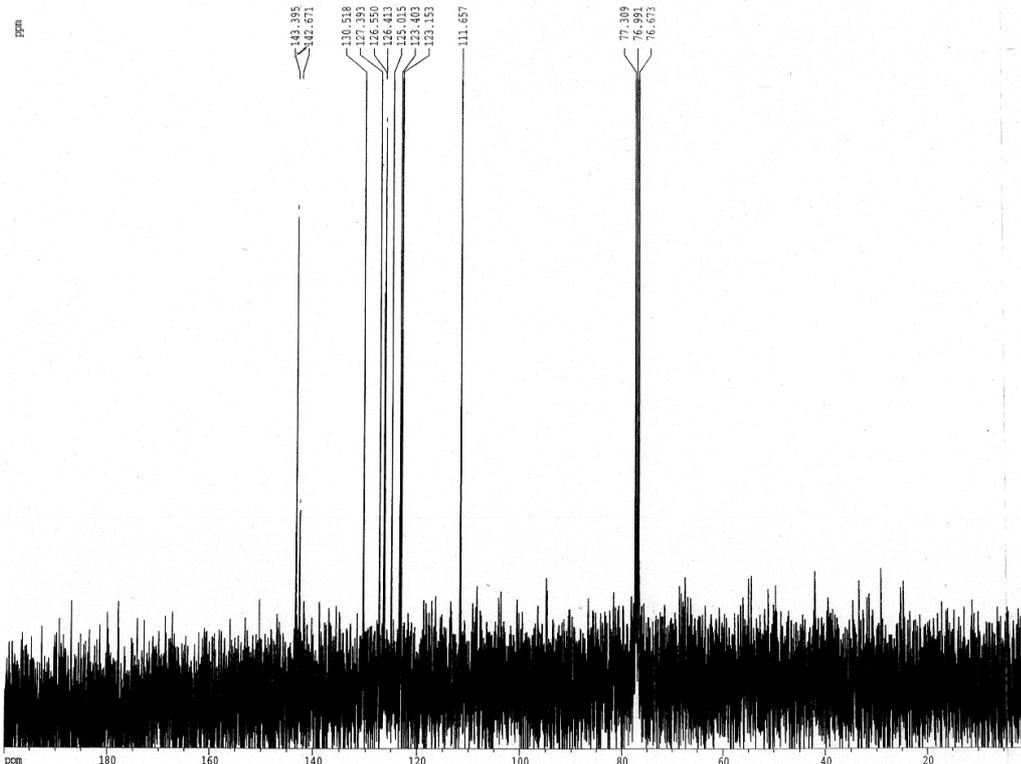
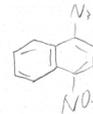
Current Data Parameters
 NAME 09yano
 EXPNO 1109
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100511
 Time 0.38
 INSTRUM dpx400
 PROBHD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.856 Hz
 FIDRES 0.126888 Hz
 AQ 3.9715316 sec
 RG 256
 DW 60.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324719 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2 -0.500 ppm
 F2 -200.07 Hz
 FWHM 0.36667 ppm/cm
 HZCM 166.71434 Hz/cm



Current Data Parameters
 NAME 09yano
 EXPNO 934
 PROCNO 1

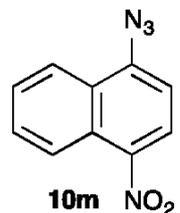
F2 - Acquisition Parameters
 Date_ 20091222
 Time 23.38
 INSTRUM dpx400
 PROBHD 5 mm BBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 2896.3
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

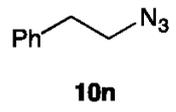
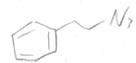
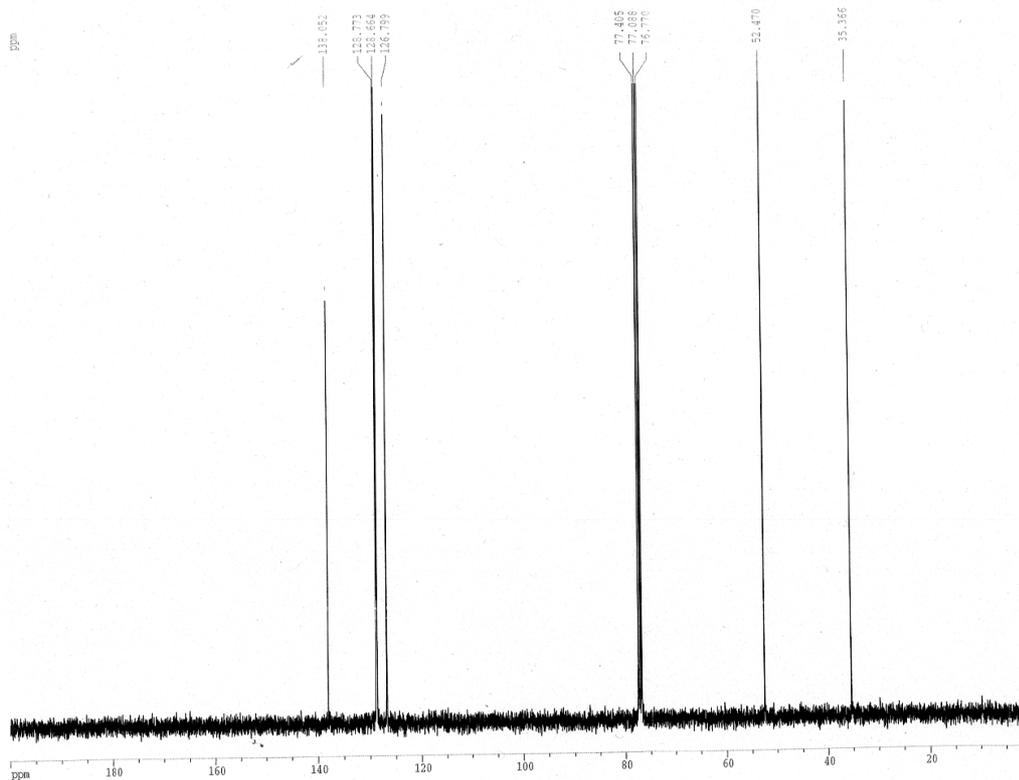
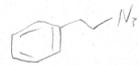
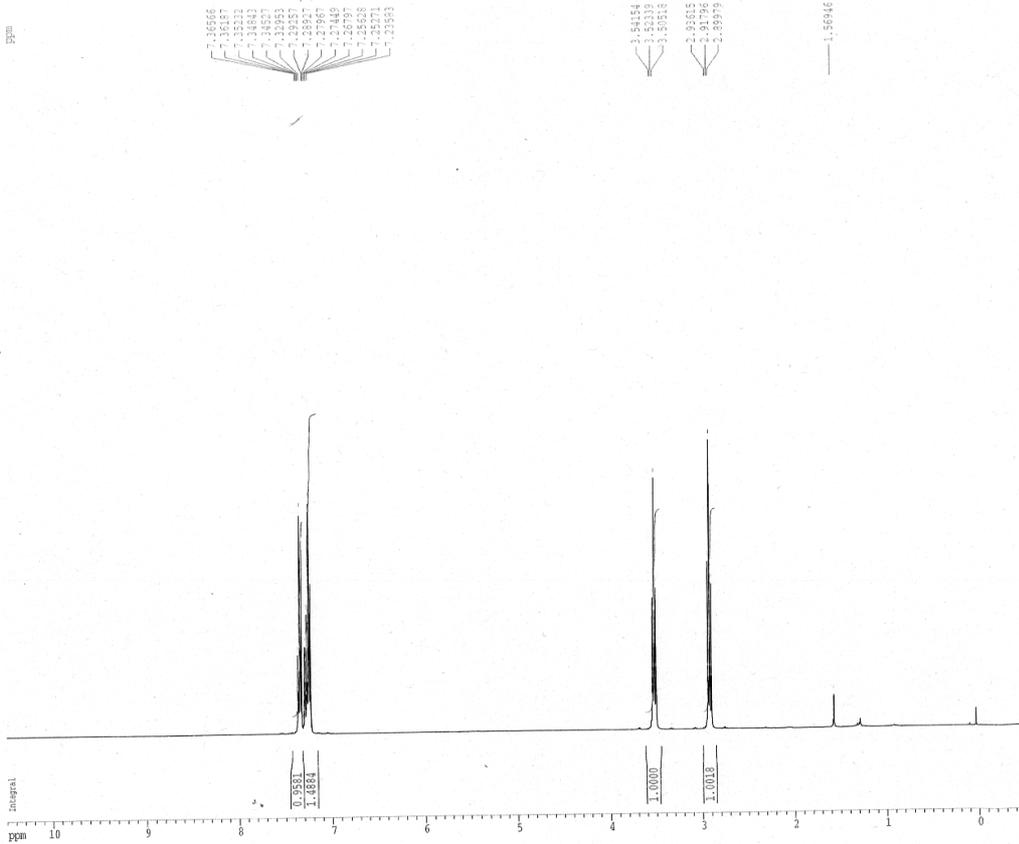
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -3.90 dB
 SFO1 100.6237959 MHz

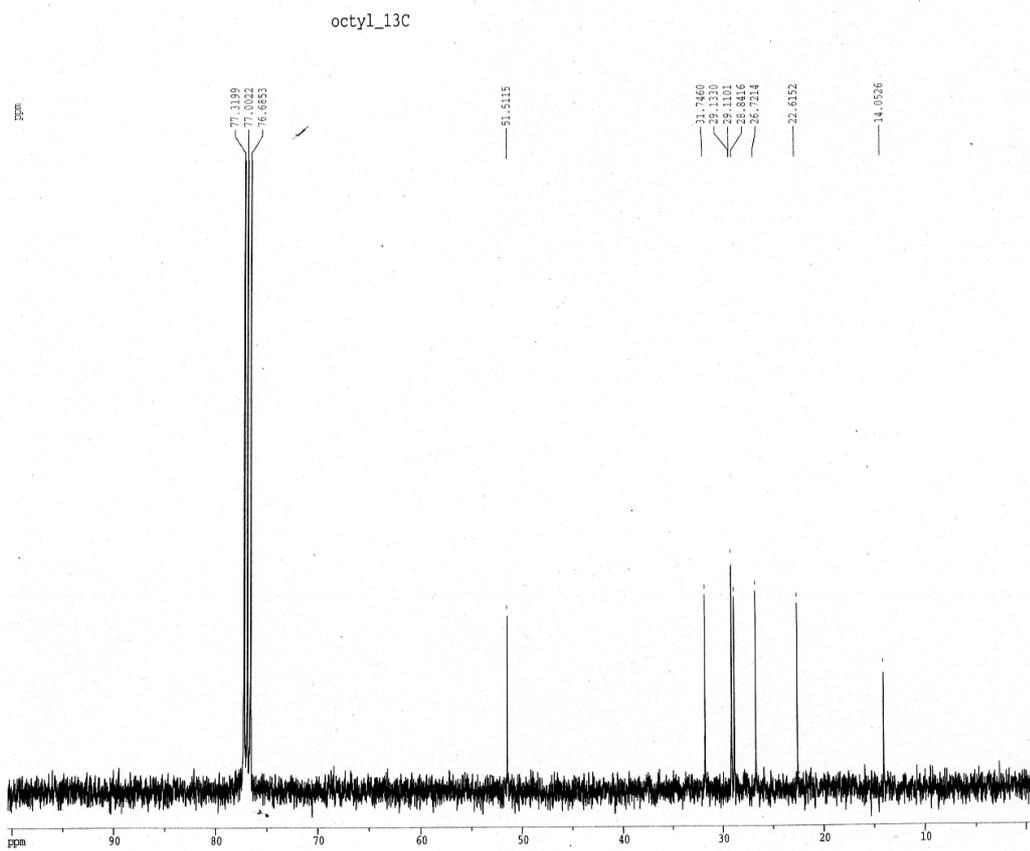
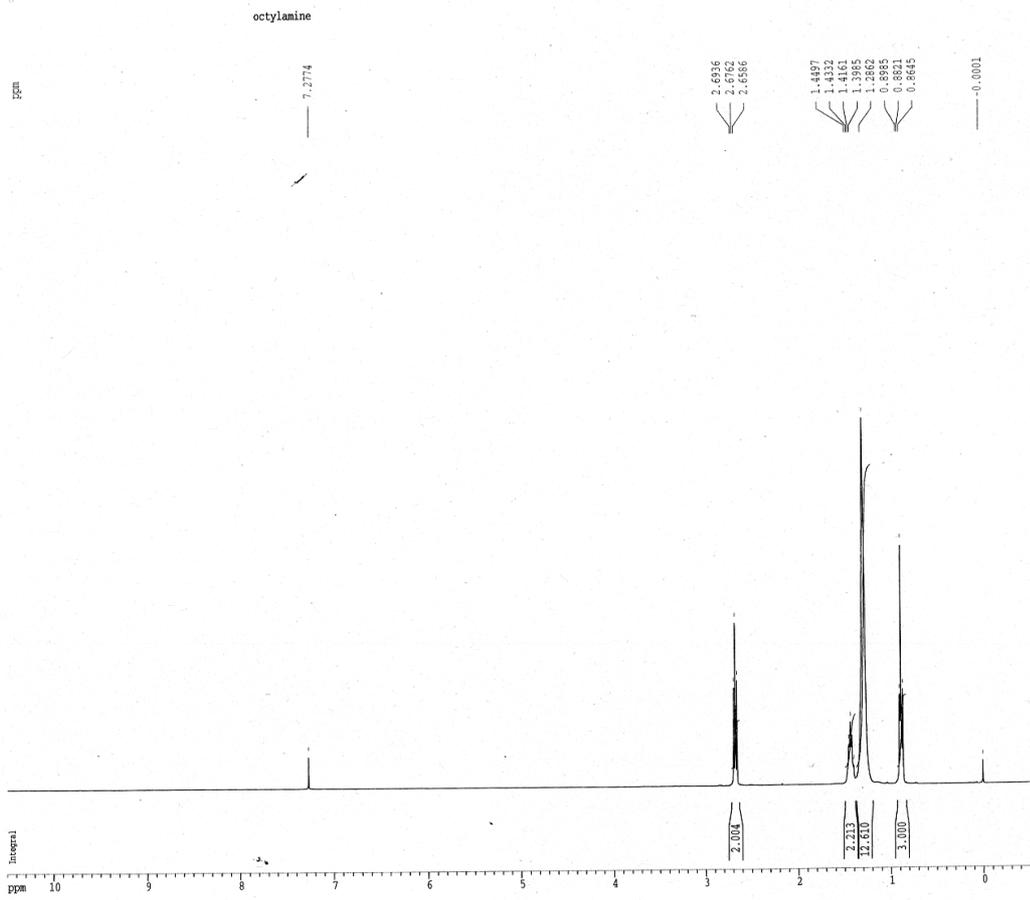
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 9.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127721 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1

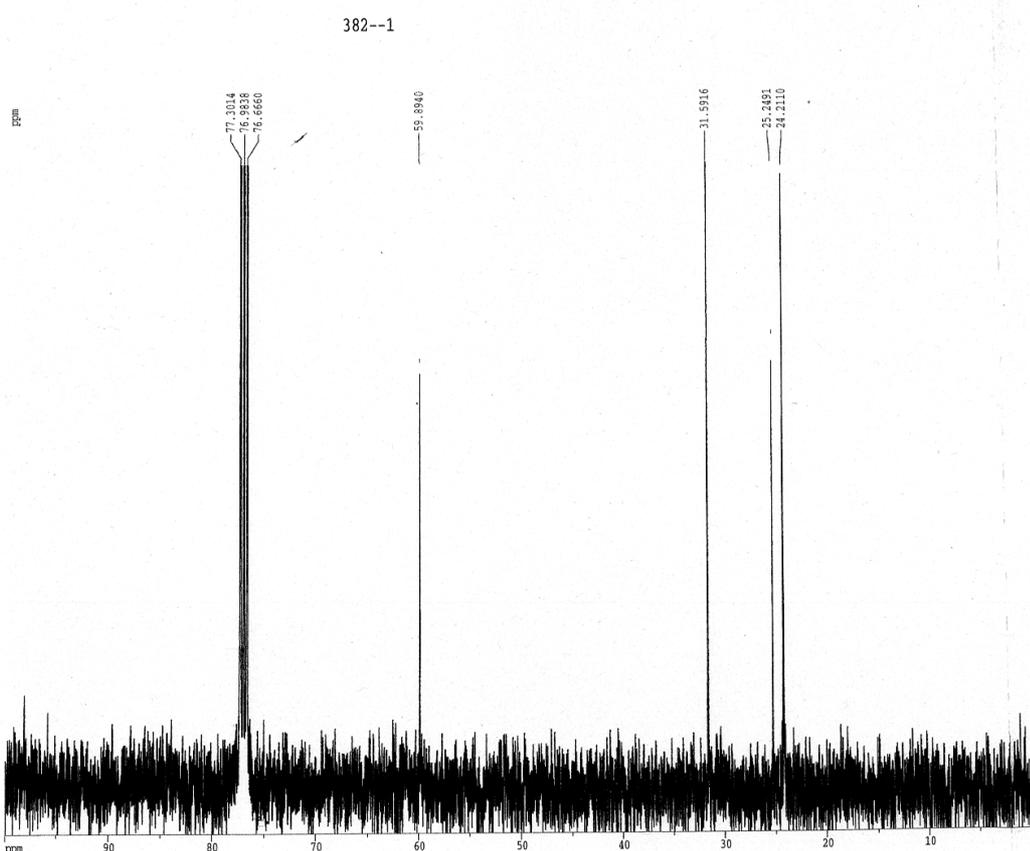
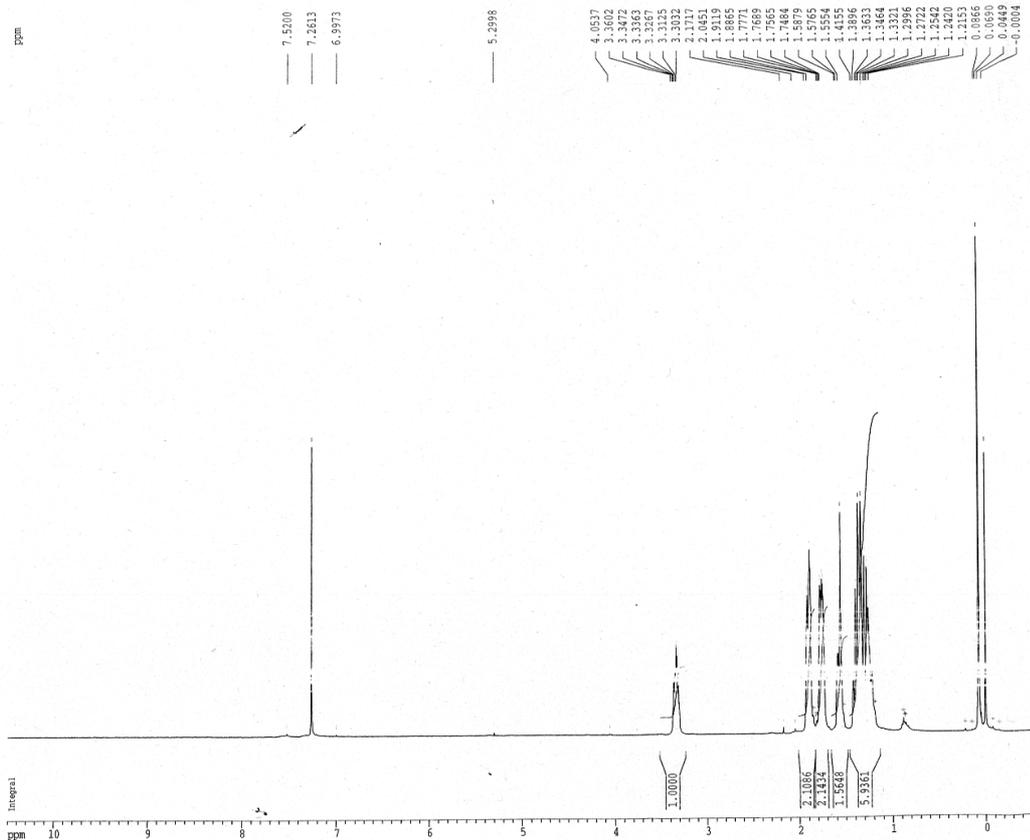
1D
 CX
 F11
 F1
 F21
 F2
 PP
 HZ







n-Oct-N₃
100



ppm

7.4071
7.4329
7.4301
7.4301
7.4329
7.4273
7.4157
7.4097
7.3940
7.3671
7.3523
7.3498
7.3468
7.3362
7.3332
7.3291
7.2607
6.8966

4.8246
4.8075
4.7979
4.6654
4.6484
4.6313
4.6142
4.4677
4.4505

2.1858
2.1709
2.1709
1.7108
1.6194
1.6023
1.5694
1.5593
1.5195
1.4972
1.3902
1.3048
1.2651
0.2700
0.1174
0.1174
0.1131
0.1242
0.1152
0.0980
0.0742
0.0429
-0.0247

Current Data Parameters
NAME 09yano
EXNO 946
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100206
Time 23.06
INSTRUM apx400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 9250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715316 sec
RG 64
RW 60.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SFO1 400.1324110 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPHM 0.36667 ppm/cm
HSCM 146.71434 Hz/cm

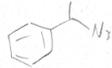
Integral

ppm

2.0175
3.0239

1.0000

1.1277



ppm

347---1

140.878

128.769
128.124
126.350

77.374
77.056
76.739

61.095

21.561

Current Data Parameters
NAME 09yano
EXNO 951
PROCNO 1

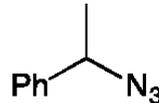
F2 - Acquisition Parameters
Date_ 20091119
Time 20.21
INSTRUM apx400
PROBHD 5 mm BBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3074932 sec
RG 5792.6
RW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -3.90 dB
SFO1 100.6237959 MHz

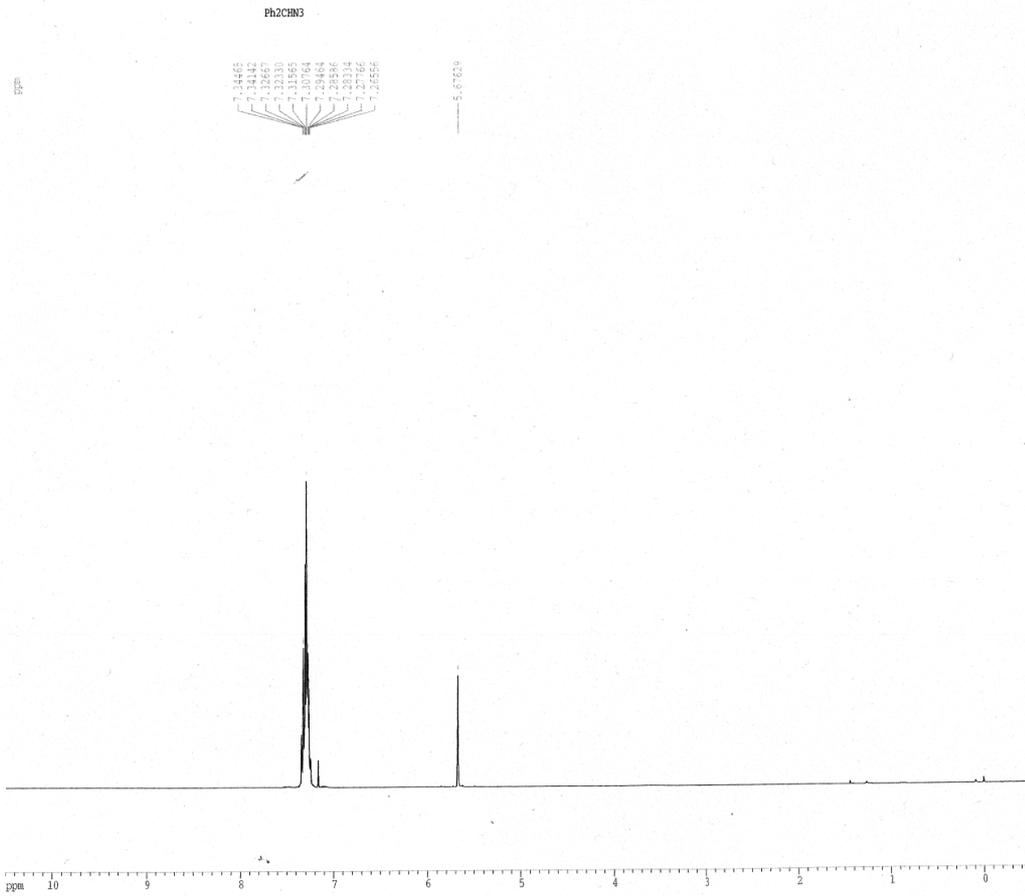
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR
CX
F1P
F1
F2P
F2
PPHM
HSCM



10q



```

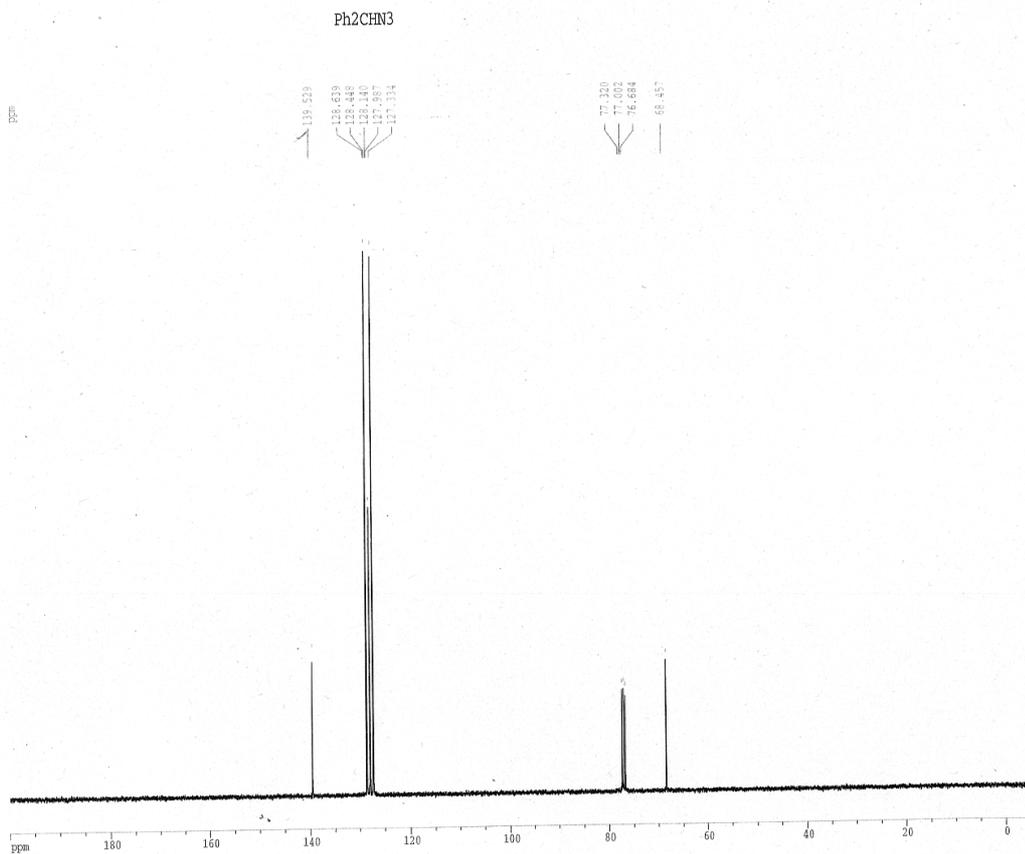
Current Data Parameters
NAME      09kato
EXPNO    395
PROCNO   1

F2 - Acquisition Parameters
Date_    20131122
Time     21.18
INSTRUM  dxp400
PROBHD   5 mm BBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8250.825 Hz
FIDRES   0.125898 Hz
AQ        3.3715116 sec
RG        32
DM        66.600 usec
DE        6.00 usec
TE        300.0 K
D1        1.00000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        12.00 usec
PL1       -6.00 dB
SFO1     400.1324710 MHz

F2 - Processing parameters
SI        32768
SF        400.1300474 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        36.00 cm
F1P       10.500 ppm
F1        4201.37 Hz
F2P       -0.500 ppm
F2        -200.07 Hz
PPHMC    0.36667 ppm/cm
HZCM     146.71434 Hz/cm
  
```



```

Current Data Parameters
NAME      09kato
EXPNO    396
PROCNO   1

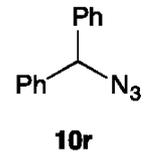
F2 - Acquisition Parameters
Date_    20131122
Time     21.23
INSTRUM  dxp400
PROBHD   5 mm BBO BB-
PULPROG  zgdc30
TD        65536
SOLVENT  CDCl3
NS        84
DS        2
SWH       25062.656 Hz
FIDRES   0.382426 Hz
AQ        1.3074932 sec
RG        4597.6
DM        19.950 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d11      0.03000000 sec

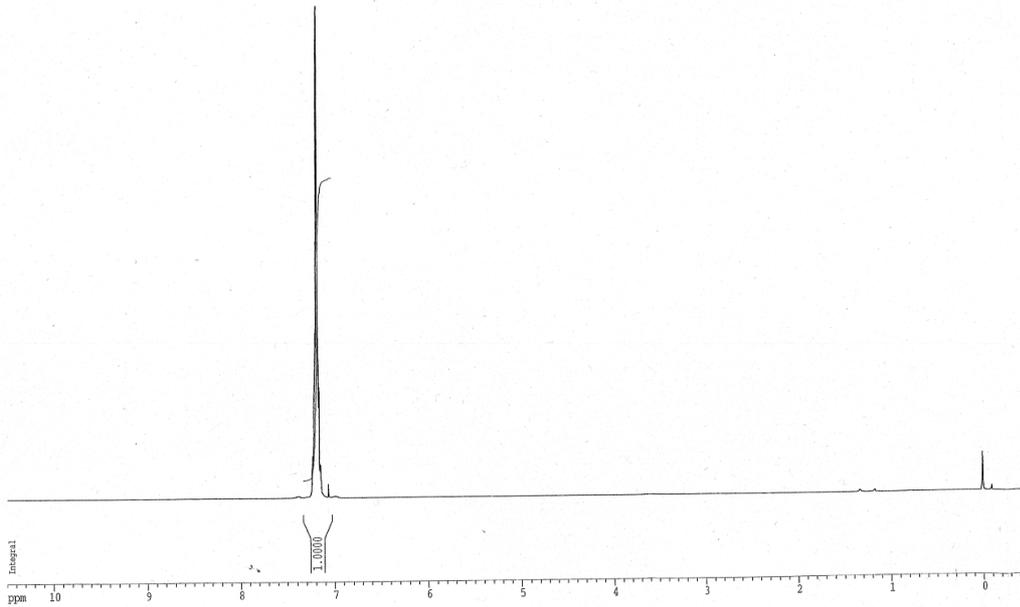
===== CHANNEL f1 =====
NUC1      13C
P1        12.00 usec
PL1       -6.00 dB
SFO1     100.6237959 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -6.00 dB
PL12     11.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6127843 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00

1D NMR |
CX        36.00 cm
F1P       10.500 ppm
F1        4201.37 Hz
F2P       -0.500 ppm
F2        -200.07 Hz
PPHMC    0.36667 ppm/cm
HZCM     146.71434 Hz/cm
  
```





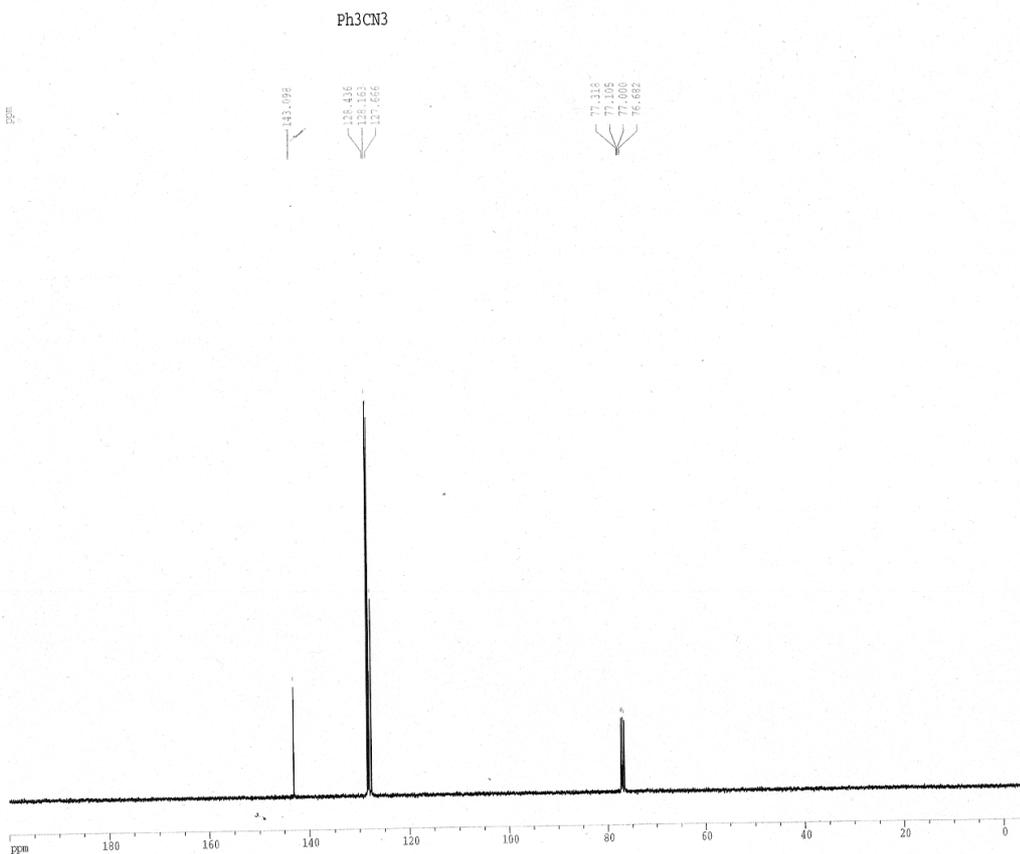
Current Data Parameters
 NAME 09kato
 EXPNO 866
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091124
 Time 16.25
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 1.9715316 sec
 RG 32
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130863 MHz
 WMW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 F1P 18.500 ppm
 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.00 Hz
 PPMCH 0.36667 ppm/cm
 HZCH 166.71437 Hz/cm



Current Data Parameters
 NAME 09kato
 EXPNO 398
 PROCNO 1

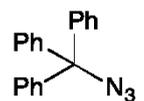
F2 - Acquisition Parameters
 Date_ 20131122
 Time 21.33
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT CDCl3
 NS 57
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 9195.2
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 100.6237959 MHz

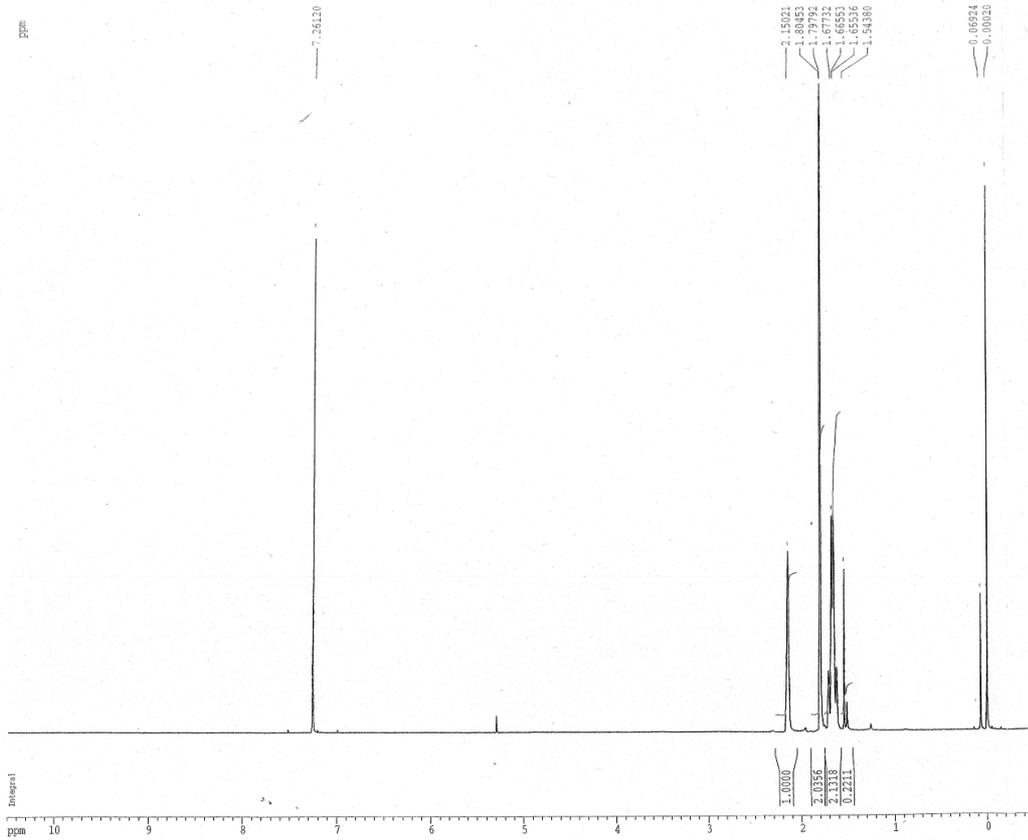
===== CHANNEL f2 =====
 CHDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 11.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127813 MHz
 WMW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot
 CX
 F1P
 F1
 F2P
 F2
 PPMCH
 HZCH



358-1



Current Data Parameters
 NAME 09yano
 EXPRO 302
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091209
 Time 23.04
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT cnc13
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.9715316 sec
 RG 256
 DM 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

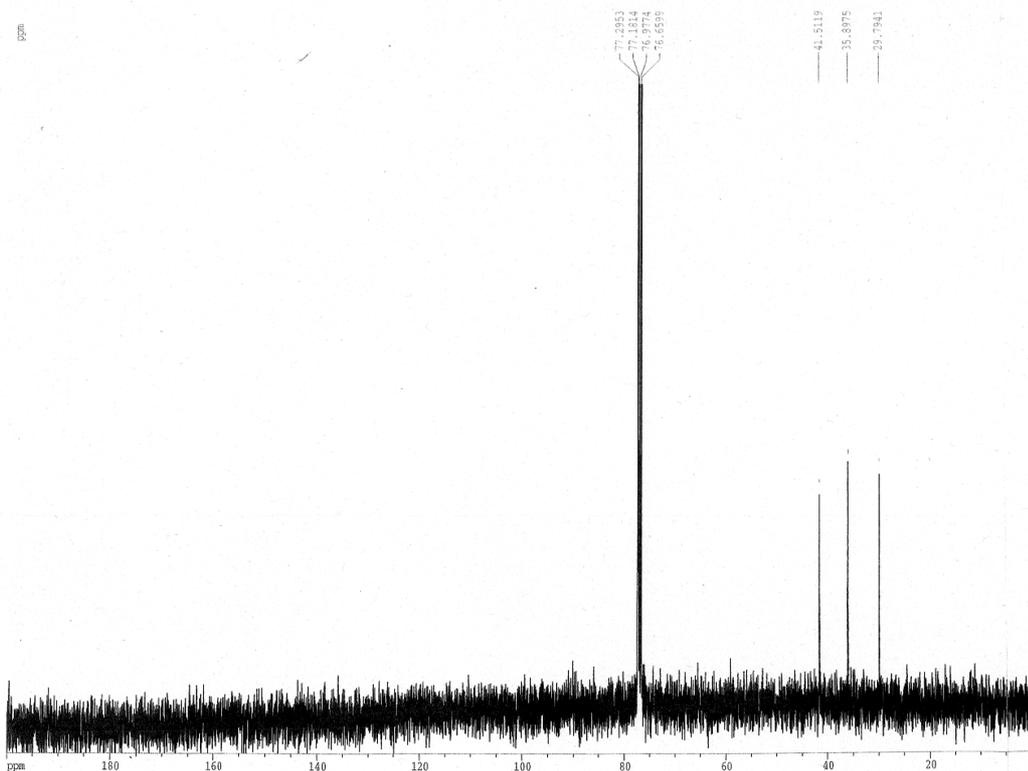
===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1306094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.97 Hz
 PPRCM 0.3667 ppm/cm
 HZCM 146.71434 Hz/cm



354-1 adamantane



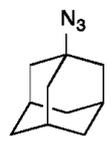
Current Data Parameters
 NAME 09yano
 EXPRO 887
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091204
 Time 11.57
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT cnc13
 NS 256
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 5792.6
 DM 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -3.90 dB
 SFO1 100.6237959 MHz

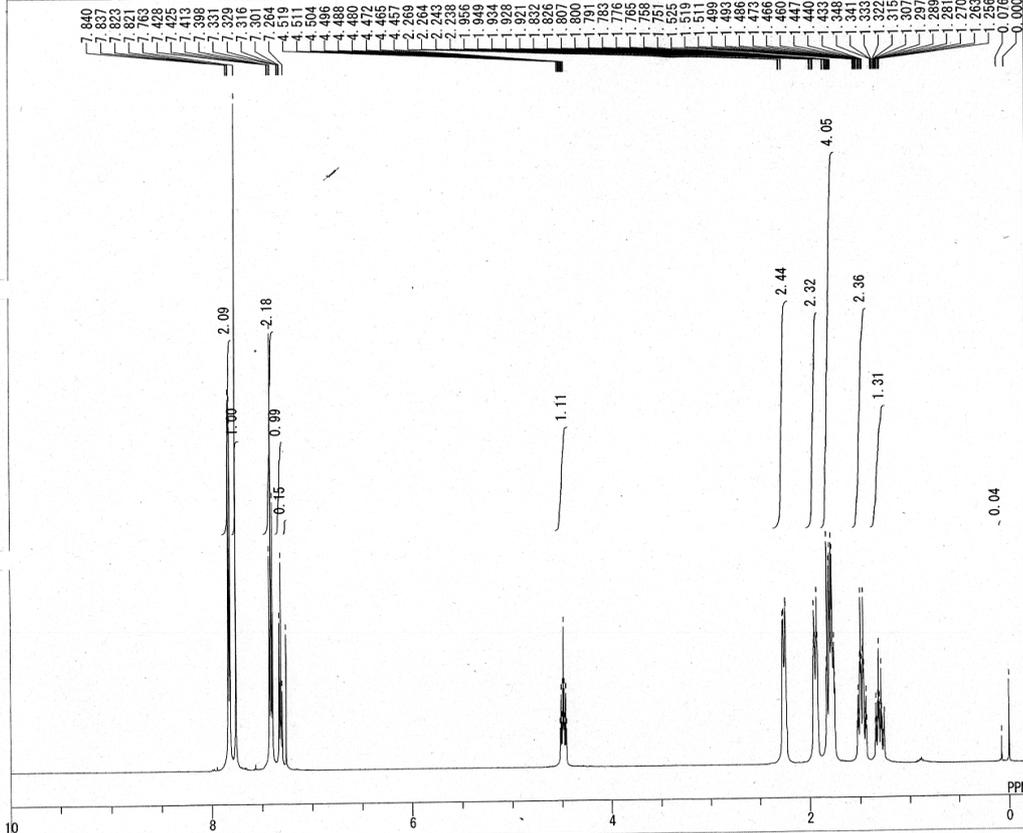
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 9.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127721 MHz
 WDW EM
 SSB 0

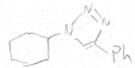


10t

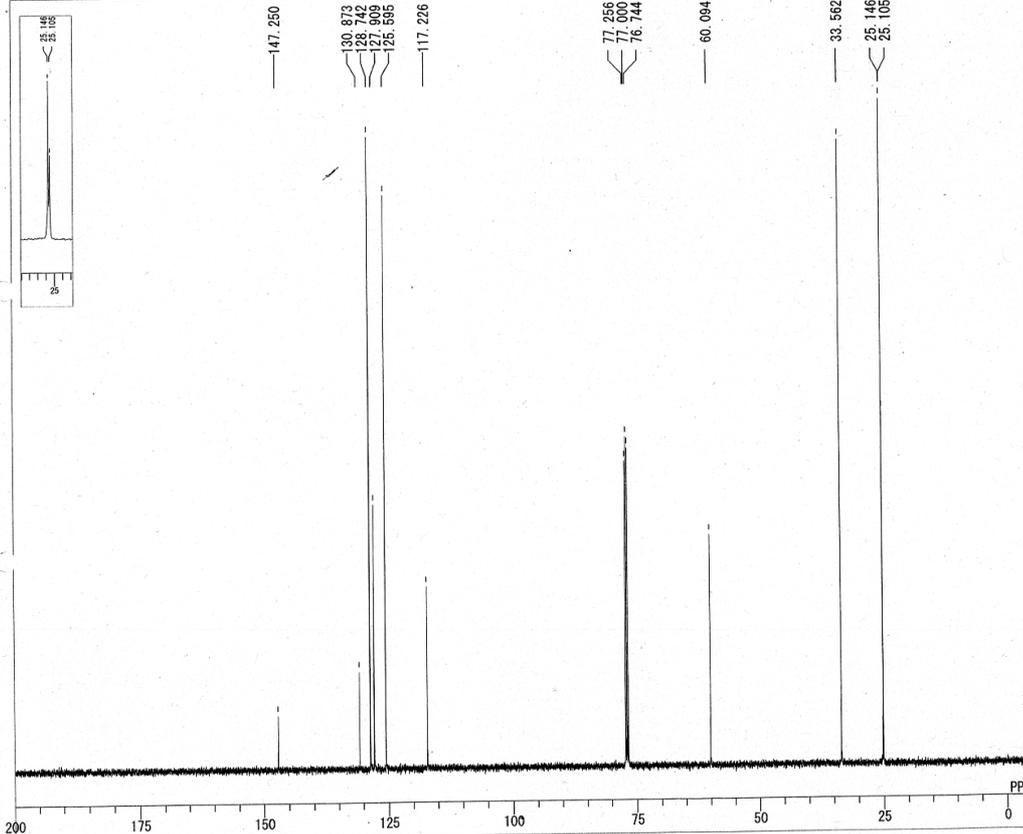
C:\NMRdata\00kunisue\9katoH-triazole_H2ft.als
9katoH-triazole_H



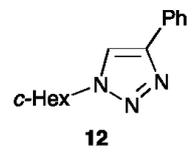
MENUI SINGL 1H
 OBNUC 1H
 OBFRO 500.00 MHz
 OBFIN 162410.00 Hz
 PW1 6.50 usec
 DEADT 56.75 usec
 PREDL 0.20000 msec
 INIWT 10.0000 msec
 POINT 32768
 SAMPO 32768
 TIMES 8
 DUMMY 1
 FREQU 10000.00 Hz
 FILTR 5000 Hz
 DELAY 40.00 usec
 ACOTM 3.2768 sec
 PD 2.0000 sec
 ADBIT 16
 RGAIN 15
 BF 0.15 Hz
 T1 0.00
 T2 0.00
 T3 90.00
 T4 100.00
 EXMOD SINGL
 EXPCM Single pulse
 IRNUC 1H
 IRFRQ 500.00 MHz
 IRFIN 162410.00 Hz
 IRRPW 50 usec
 IRATN 511
 DF FILE C:\NMRdata\00kunisue\9katoH-triazole_H2ft.
 SHMFL TH5AT_4cm29katoH-triazole_H
 CTEMP 25.0 c
 LKF IN 70334.0 Hz
 LKLEV 200
 LGAIN 22
 LKPHS 135
 LKSIG 967
 CSPED 14 Hz
 FILDC
 FILDF



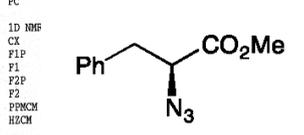
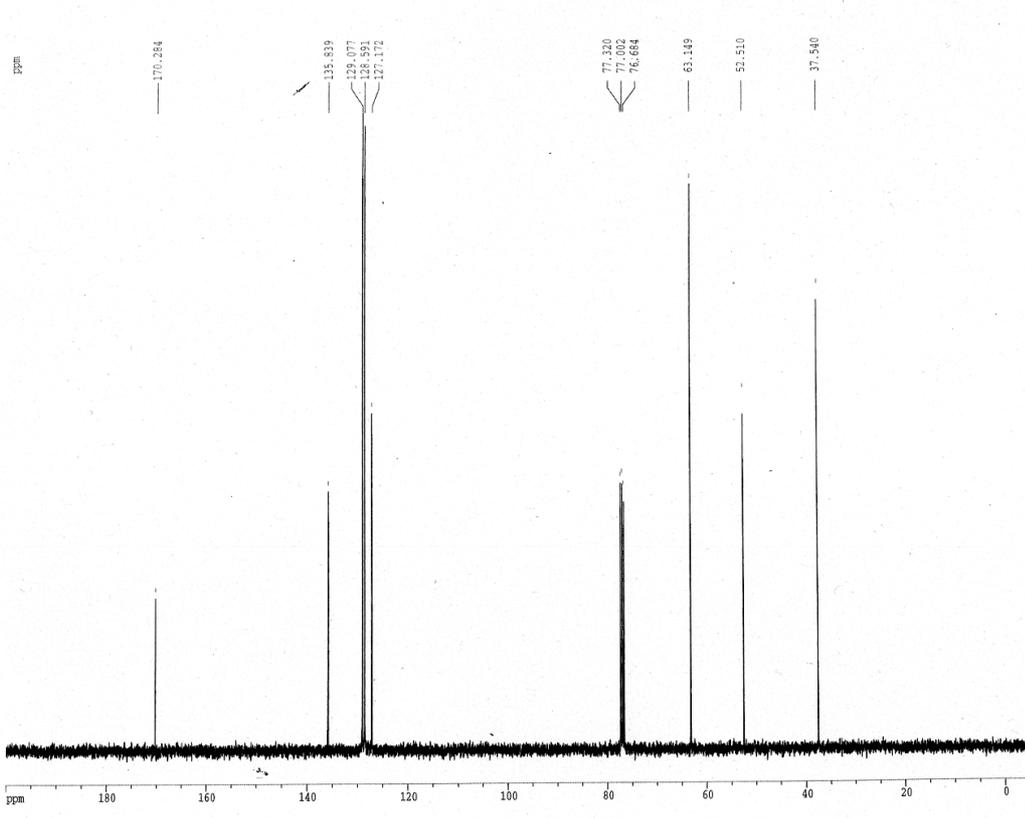
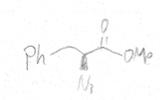
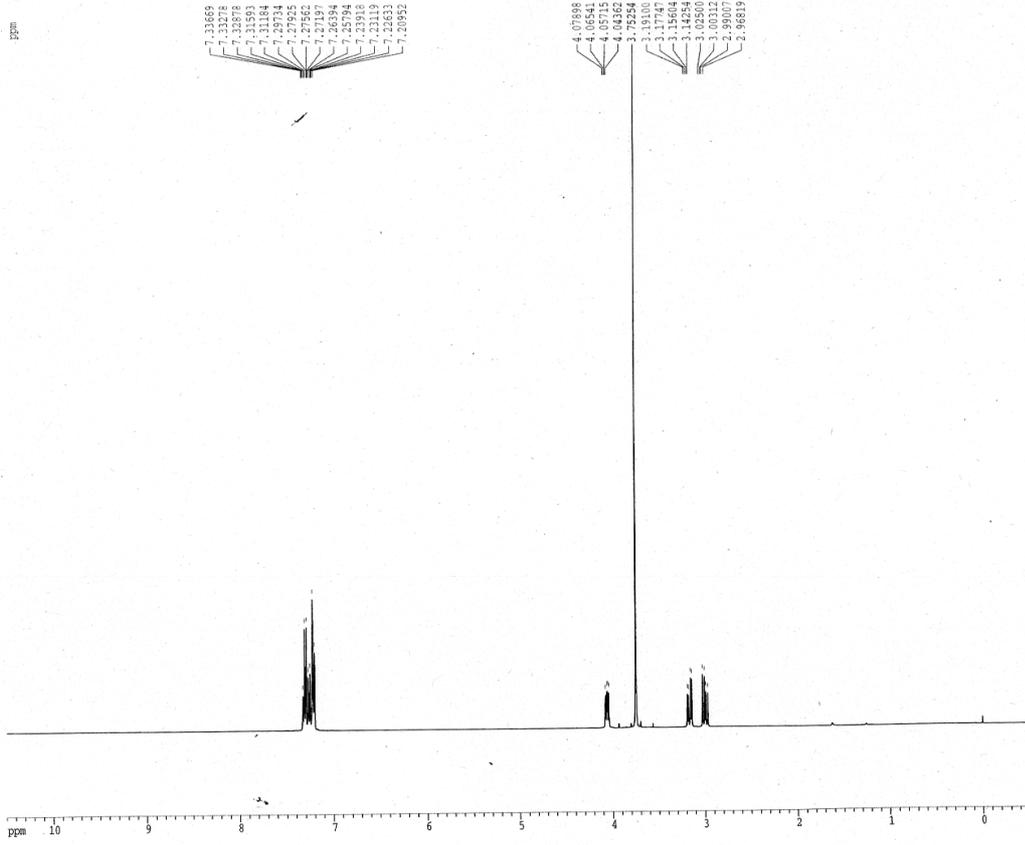
C:\NMRdata\00kunisue\9katoH-triazole_C.als
9katoH-triazole_C



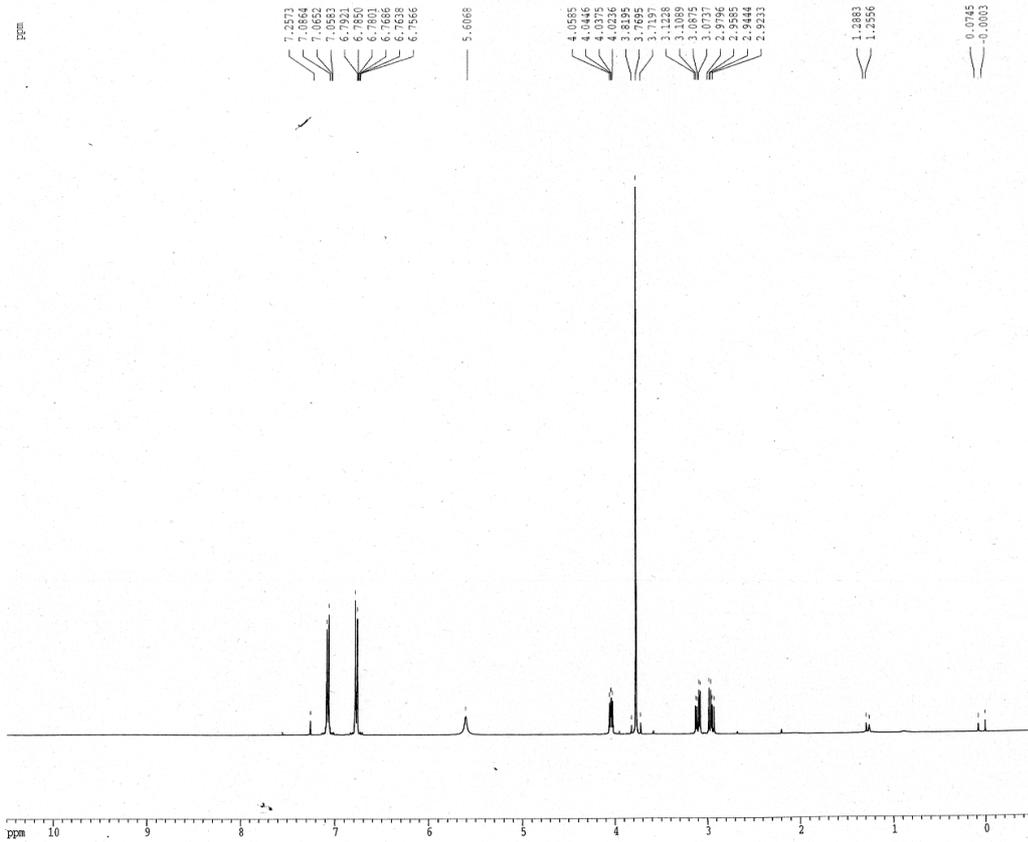
MENUI SINGL 13C
 OBNUC 13C
 OBFRO 125.65 MHz
 OBFIN 127958.00 Hz
 PW1 4.50 usec
 DEADT 15.93 usec
 PREDL 0.20000 msec
 INIWT 10.0000 msec
 POINT 32768
 SAMPO 32768
 TIMES 512
 DUMMY 1
 FREQU 33003.30 Hz
 FILTR 16500 Hz
 DELAY 12.12 usec
 ACOTM 0.9929 sec
 PD 2.0000 sec
 ADBIT 16
 RGAIN 32
 BF 1.00 Hz
 T1 0.00
 T2 0.00
 T3 90.00
 T4 100.00
 EXMOD SINGL
 EXPCM Single pulse
 IRNUC 13C
 IRFRQ 125.65 MHz
 IRFIN 127958.00 Hz
 IRRPW 50 usec
 IRATN 511
 DF FILE C:\NMRdata\00kunisue\9katoH-triazole_C.als
 SHMFL TH5AT_4cm29katoH-triazole_C
 CTEMP 25.7 c
 LKF IN 70334.0 Hz
 LKLEV 200
 LGAIN 22
 LKPHS 135
 LKSIG 967
 CSPED 14 Hz
 FILDC
 FILDF



12



14a



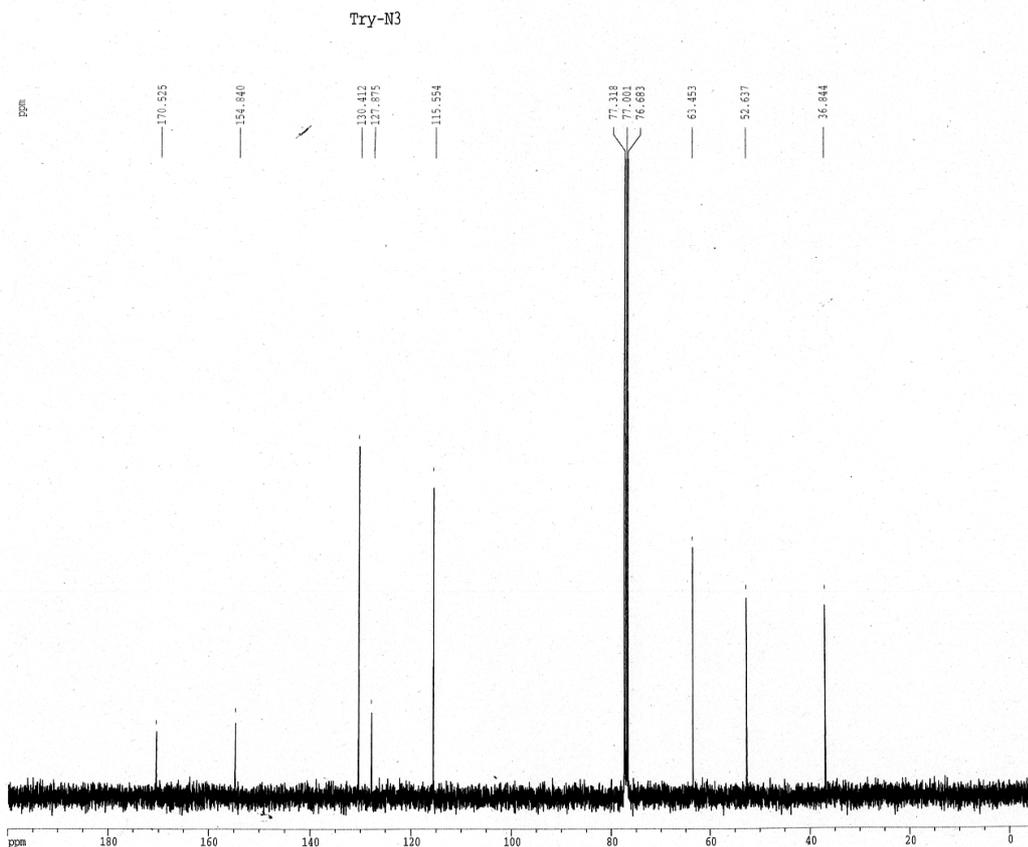
Current Data Parameters
 NAME 09kato
 EXPNO 404
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131203
 Time 17.10
 INSTRUM dpx400
 PROBHID 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.971516 sec
 RG 64
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300109 MHz
 WMW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 F1P 10.500 ppm
 F1 400.17 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 FREQM 0.36667 ppm/cm
 HZCM 146.71434 Hz/cm



Try-N3

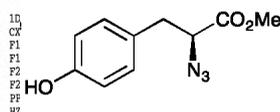
Current Data Parameters
 NAME 09kato
 EXPNO 391
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131121
 Time 11.35
 INSTRUM dpx400
 PROBHID 5 mm BBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 170
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 3649.1
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 100.6237959 MHz

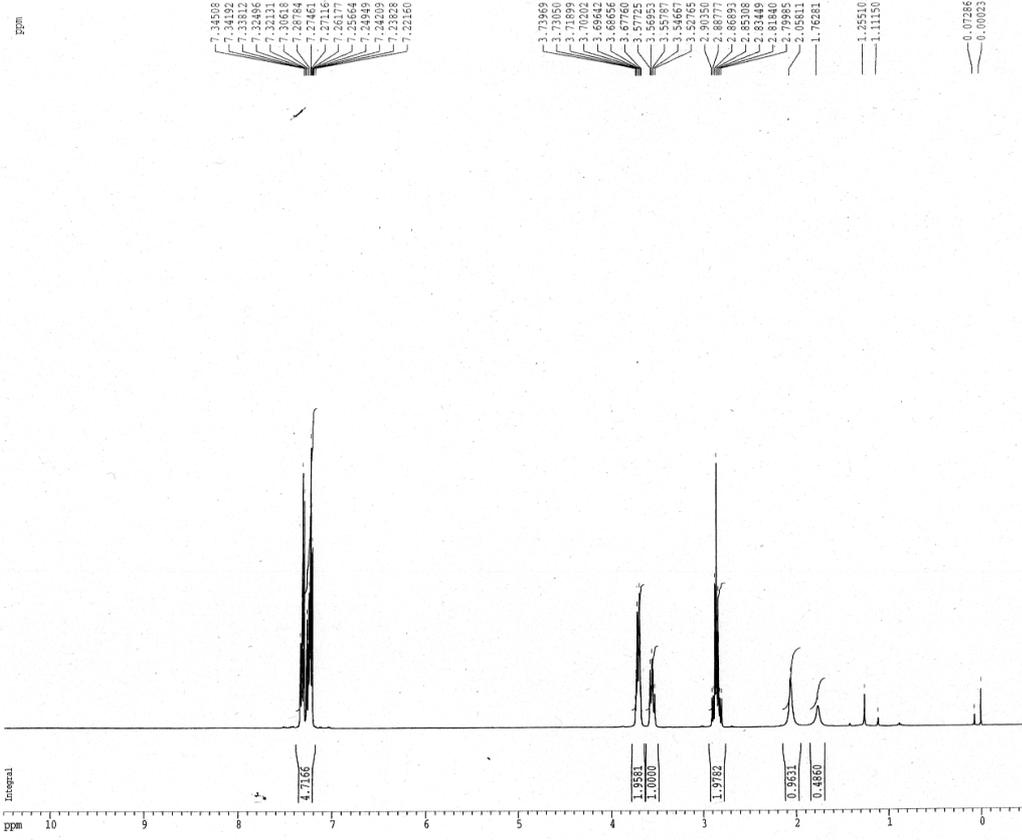
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FPCP2 80.00 usec
 PL2 -6.00 dB
 PL12 11.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 127168
 SF 100.6127721 MHz
 WMW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

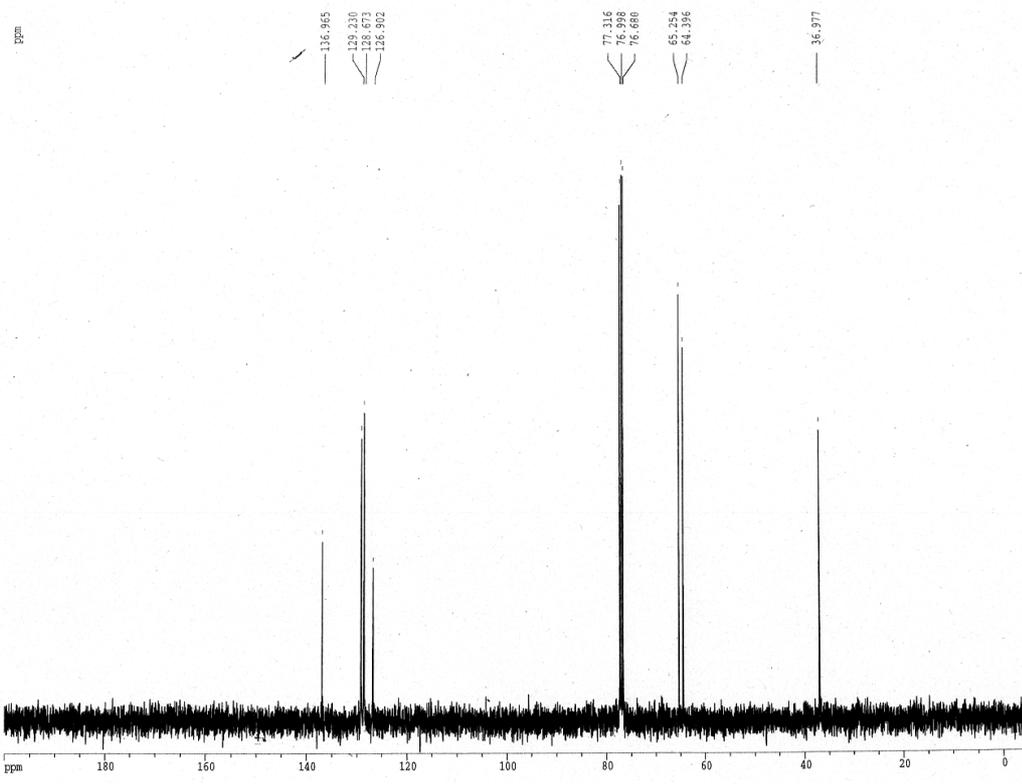


14b

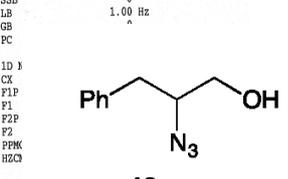
exp259_P



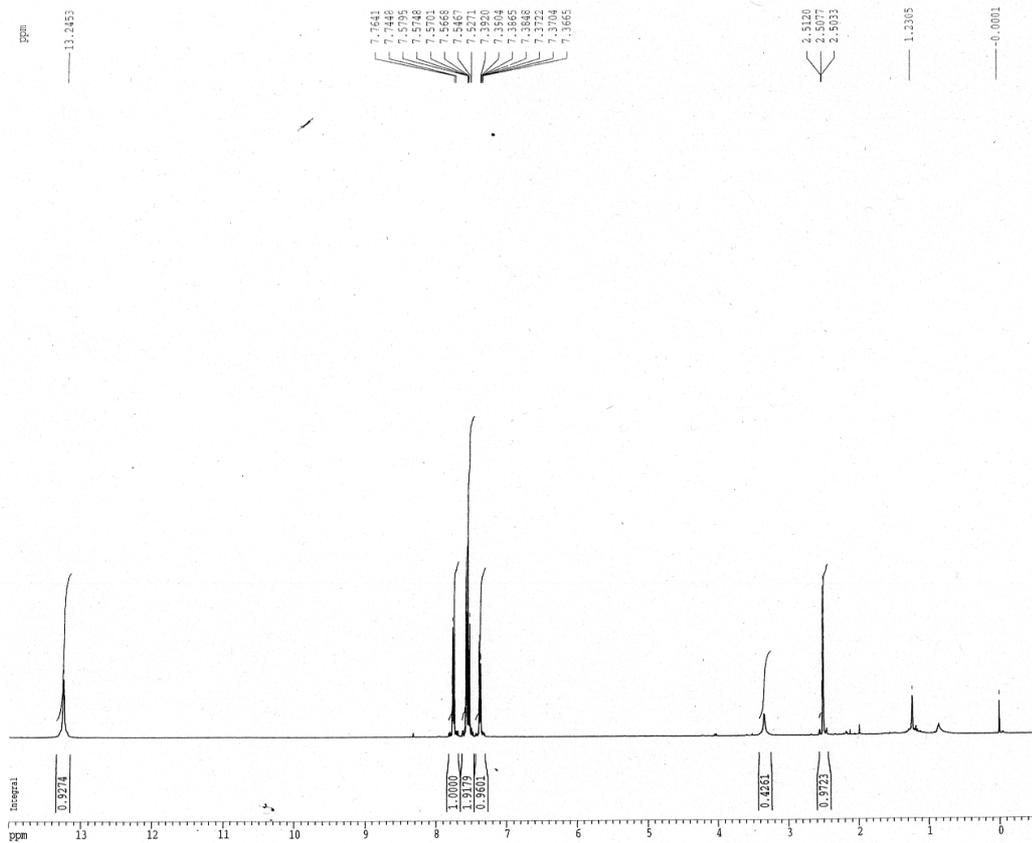
Current Data Parameters
 NAME 09kato
 EXPNO 375
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131006
 Time 18.51
 INSTRUM dpx400
 PROBHD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT ccd13
 NS 16
 DS 2
 SWH 8150.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.915316 sec
 RG 64
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300140 MHz
 MW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 30.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.36667 ppm/cm
 HZCM 146.71834 Hz/cm



Current Data Parameters
 NAME 09kato
 EXPNO 374
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131006
 Time 0.51
 INSTRUM dpx400
 PROBHD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT ccd13
 NS 100
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 13004
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.50000000 sec
 d11 0.03000000 sec
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 23.00 usec
 PL1 -3.90 dB
 SFO1 100.6237959 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -6.00 dB
 PL12 9.00 dB
 SFO2 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127736 MHz
 MW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

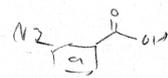


azide-acid

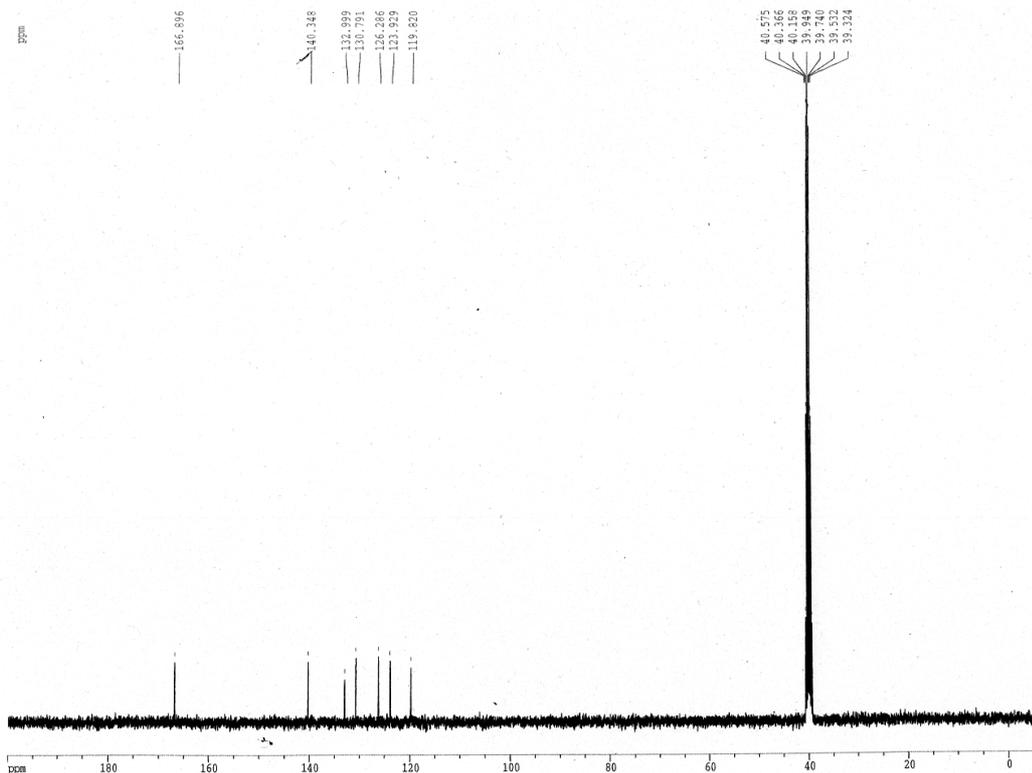


Current Data Parameters
 NAME 09kato
 EXPNO 430
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140122
 Time 1.33
 INSTRUM dpx400
 PROBHD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.5715216 sec
 RG 256
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.130014 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 30.00 cm
 F1P 14.000 ppm
 F1 5801.80 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 FREQM 0.48133 ppm/cm
 HZCM 193.39618 Hz/cm



azide-acid

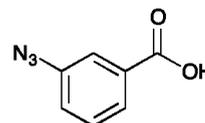


Current Data Parameters
 NAME 09kato
 EXPNO 431
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140122
 Time 1.42
 INSTRUM dpx400
 PROBHD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT DMSO
 NS 143
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 11585.2
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 100.6237959 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 11.00 dB
 SFO2 400.1316005 MHz

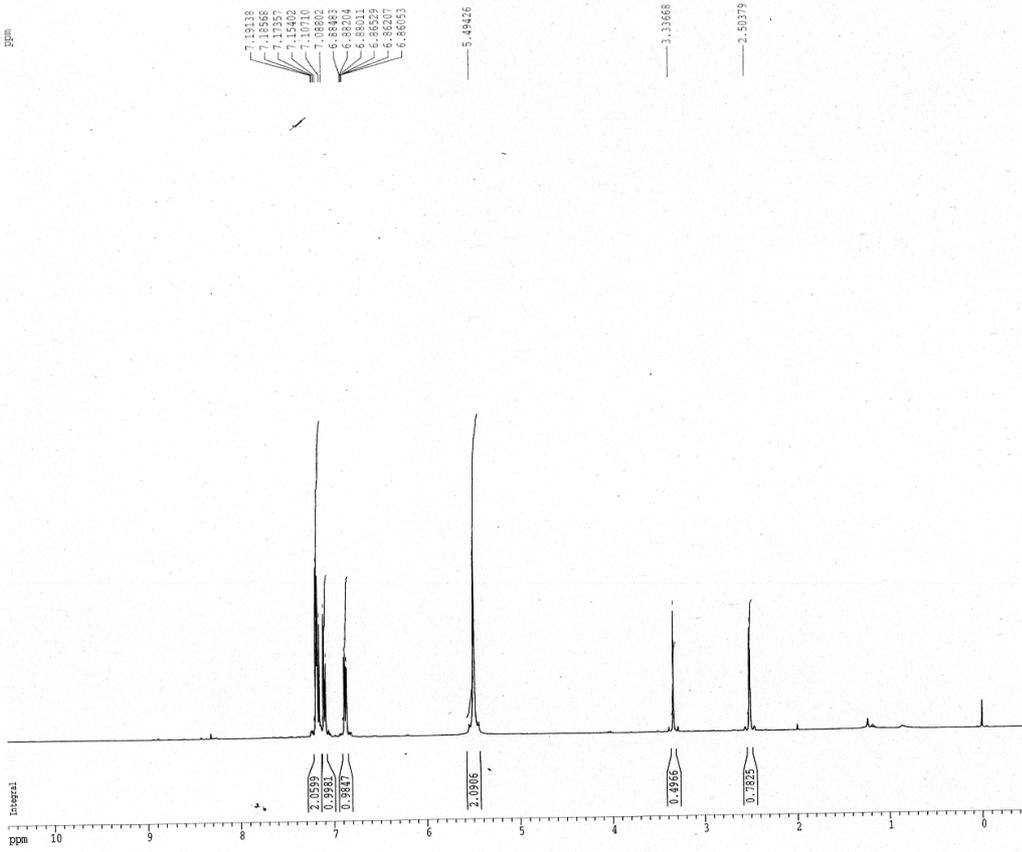
F2 - Processing parameters
 SI 32768
 SF 100.6127272 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR
 CX
 F1P
 F1
 F2P
 F2
 FREQM
 HZCM



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amine_acid_azide



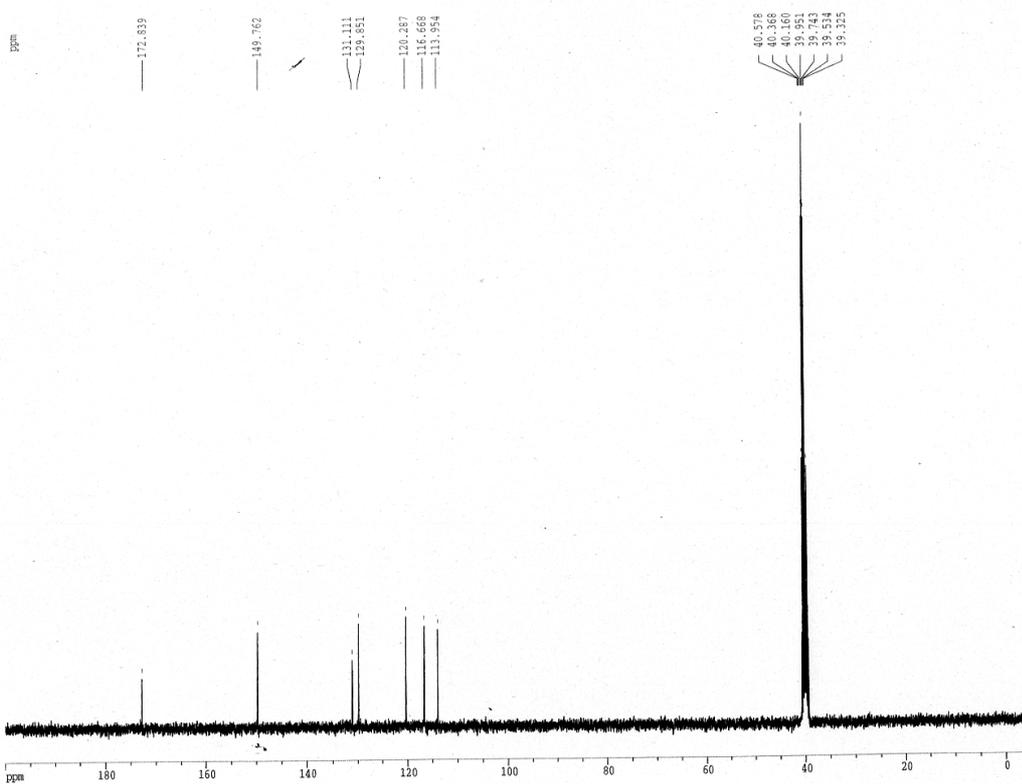
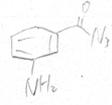
Current Data Parameters
 NAME 09kato
 EXPNO 429
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140122
 Time 1.24
 INSTRUM dpx400
 PROBRD 5 mm BBO WB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.9715316 sec
 RG 256
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NU1 18
 P1 12.00 usec
 PL1 -4.00 dB
 SFO1 400.134710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300031 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.16667 ppm/cm
 HZCM 146.71434 Hz/cm



Current Data Parameters
 NAME 09kato
 EXPNO 422
 PROCNO 1

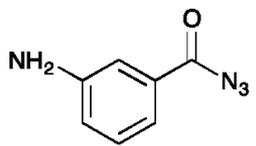
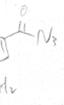
F2 - Acquisition Parameters
 Date_ 20140109
 Time 20.34
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 150
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 9195.2
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NU1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 100.6237959 MHz

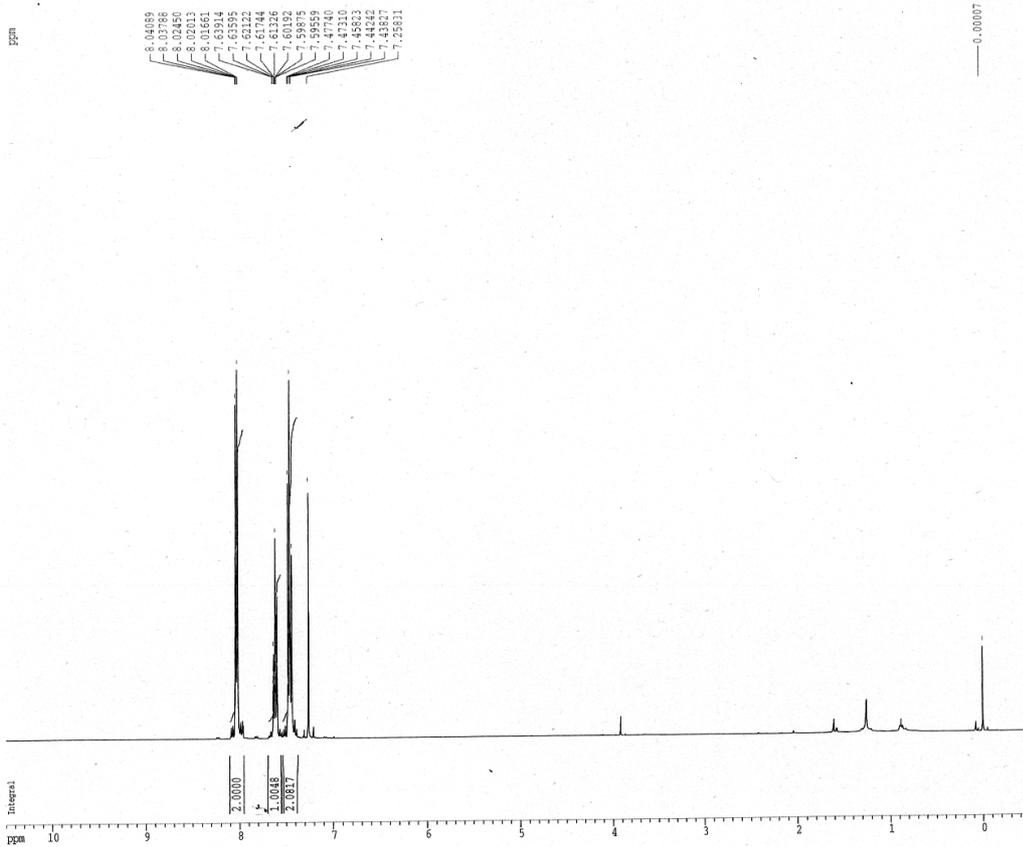
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NU2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 11.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127742 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR
 CX
 FIP
 F1
 F2P
 F2
 PPMCM
 HZCM



benzoic azido

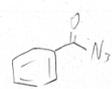


Current Data Parameters
 NAME 09kato
 EXPNO 432
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140123
 Time 19.15
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.123898 Hz
 AQ 3.9715316 sec
 RG 128
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

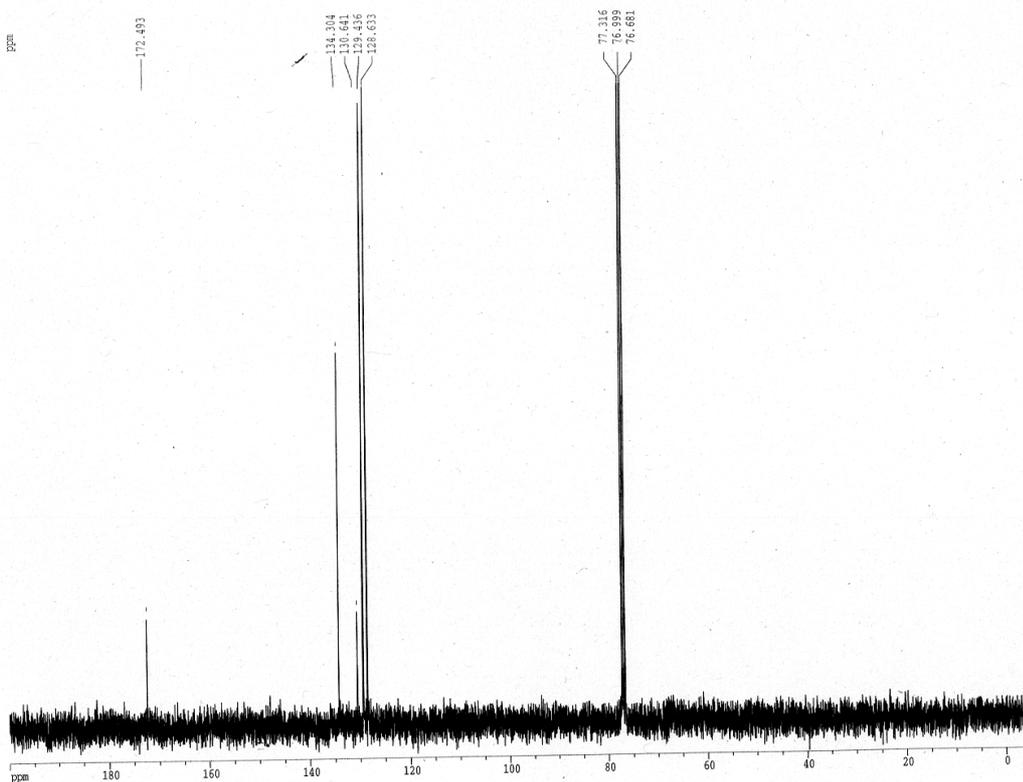
===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300114 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 F1P 10.500 ppm
 F1 4201.37 Hz
 F2P -8.500 ppm
 F2 -209.07 Hz
 PRNCM 0.36667 ppm/cm
 HZCM 146.71434 Hz/cm



benzoic azido



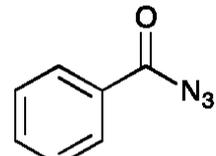
Current Data Parameters
 NAME 09kato
 EXPNO 433
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140123
 Time 19.20
 INSTRUM dpx400
 PROBRD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT CDCl3
 NS 67
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 9195.2
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

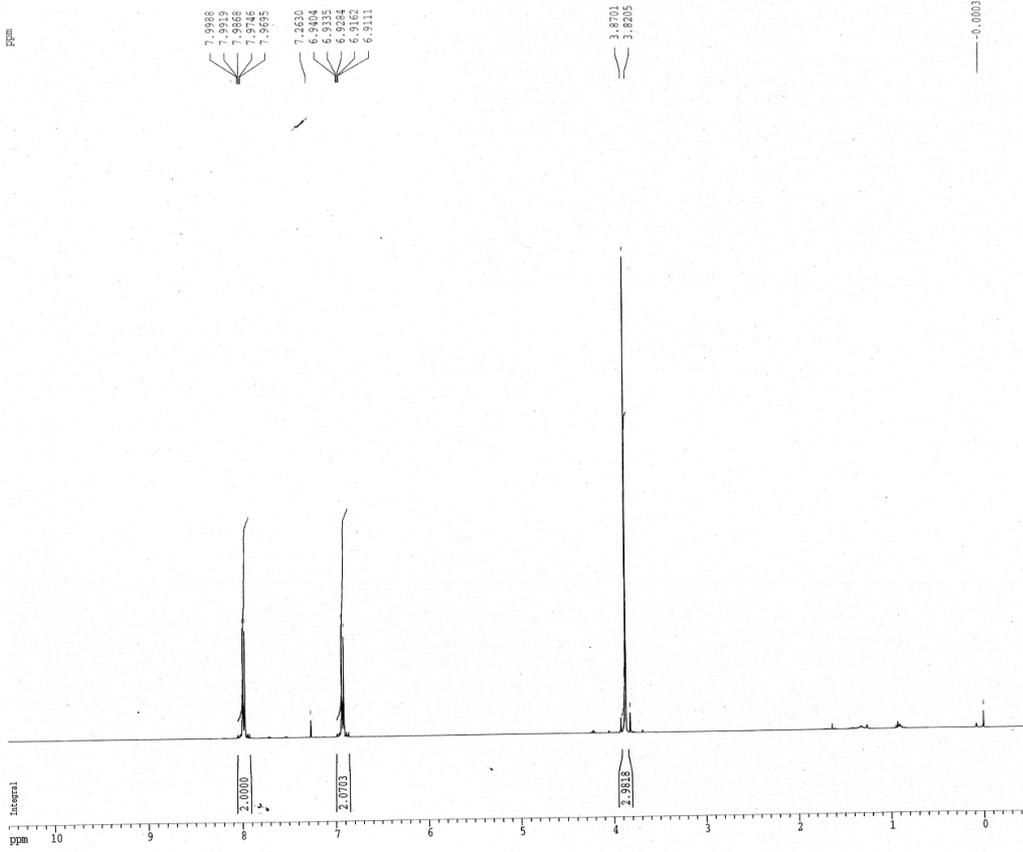
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SF01 100.6237959 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 11.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127736 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



4-Meobenzoic azido



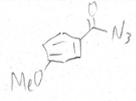
Current Data Parameters
 NAME 09kato
 EXPNO 434
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140123
 Time 19.26
 INSPRM dpx400
 PROBD 5 mm BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.815 Hz
 FIDRES 0.122898 Hz
 AQ 3.9115316 sec
 RG 128
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

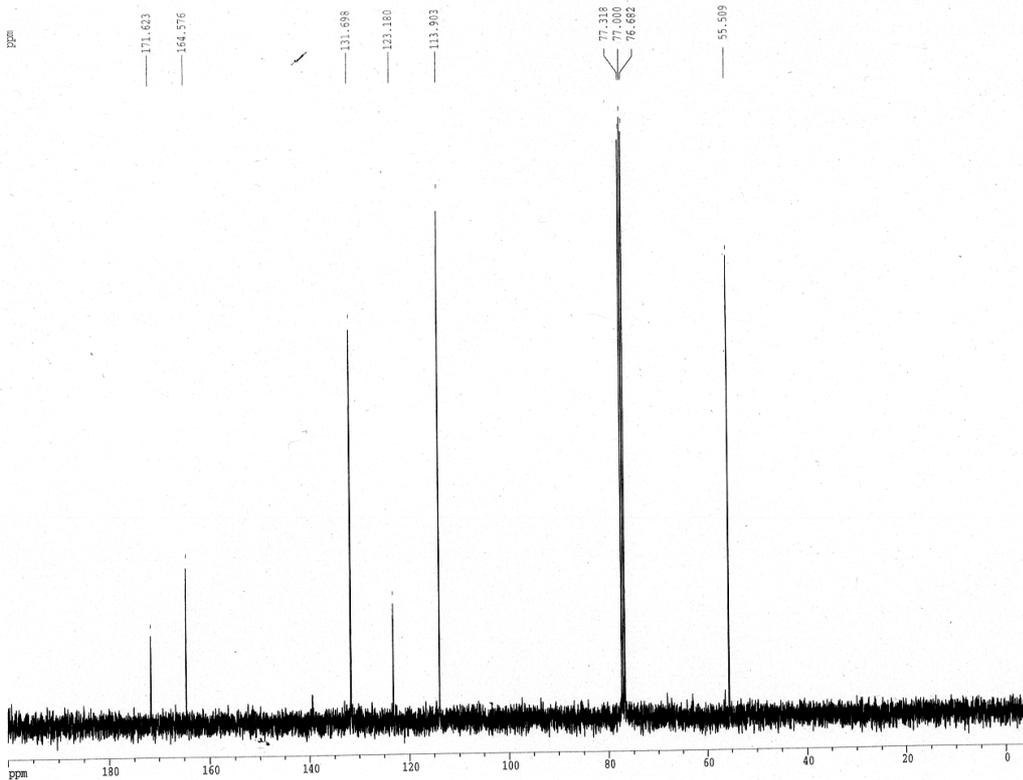
===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2 -0.500 ppm
 FZ -200.07 Hz
 PPMCM 0.36667 ppm/cm
 HZCM 146.71434 Hz/cm



4-Meobenzoic azido



Current Data Parameters
 NAME 09kato
 EXPNO 435
 PROCNO 1

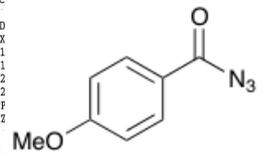
F2 - Acquisition Parameters
 Date_ 20140123
 Time 19.31
 INSPRM dpx400
 PROBD 5 mm BBO BB-
 PULPROG zgdc30
 TD 65536
 SOLVENT CDCl3
 NS 77
 DS 2
 SWH 25062.656 Hz
 FIDRES 0.382426 Hz
 AQ 1.3074932 sec
 RG 4597.6
 DW 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 100.6237959 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -6.00 dB
 PL12 11.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127736 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D
 CX
 F1
 F2
 PF
 HZ



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Table S1. Cartesian Coordinates of Computational Data for ADMP **5b** (Angstroms)

Atom	X	Y	Z
1 P	1.883522	-0.005654	-0.029555
2 F	0.895879	1.257640	-0.478923
3 F	2.281248	-0.232310	-1.577563
4 F	0.566349	-1.016833	-0.234613
5 F	1.370359	0.226411	1.530771
6 F	3.102148	1.019981	0.203379
7 F	2.761224	-1.270986	0.446393
8 N	-1.743941	0.095334	1.194041
9 N	-1.967093	1.225642	-0.705736
10 N	-2.213404	-1.072808	-0.895027
11 N	-1.681500	-2.180551	-0.657991
12 N	-1.317367	-3.248484	-0.617067
13 C	-1.917347	0.029231	-0.124447
14 C	-1.397585	1.480584	1.574674
15 C	-1.671119	2.277314	0.280089
16 C	-1.455055	-1.003780	2.106664
17 C	-1.822233	1.470190	-2.134316
18 H	-0.344590	1.509550	1.859561
19 H	-2.030139	1.796359	2.408792
20 H	-2.525997	2.956142	0.365063
21 H	-0.786977	2.829648	-0.040521
22 H	-0.377758	-1.184878	2.130968
23 H	-1.991664	-1.902665	1.803571
24 H	-1.812150	-0.722645	3.100034
25 H	-2.460455	2.308781	-2.424018
26 H	-2.127368	0.581459	-2.684997
27 H	-0.774440	1.697460	-2.352938