

## Supporting Information

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

2-azido-1,3-dimethylimidazolium hexafluorophosphate

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## Contents

S-2 <sup>1</sup>H and <sup>13</sup>C 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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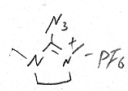
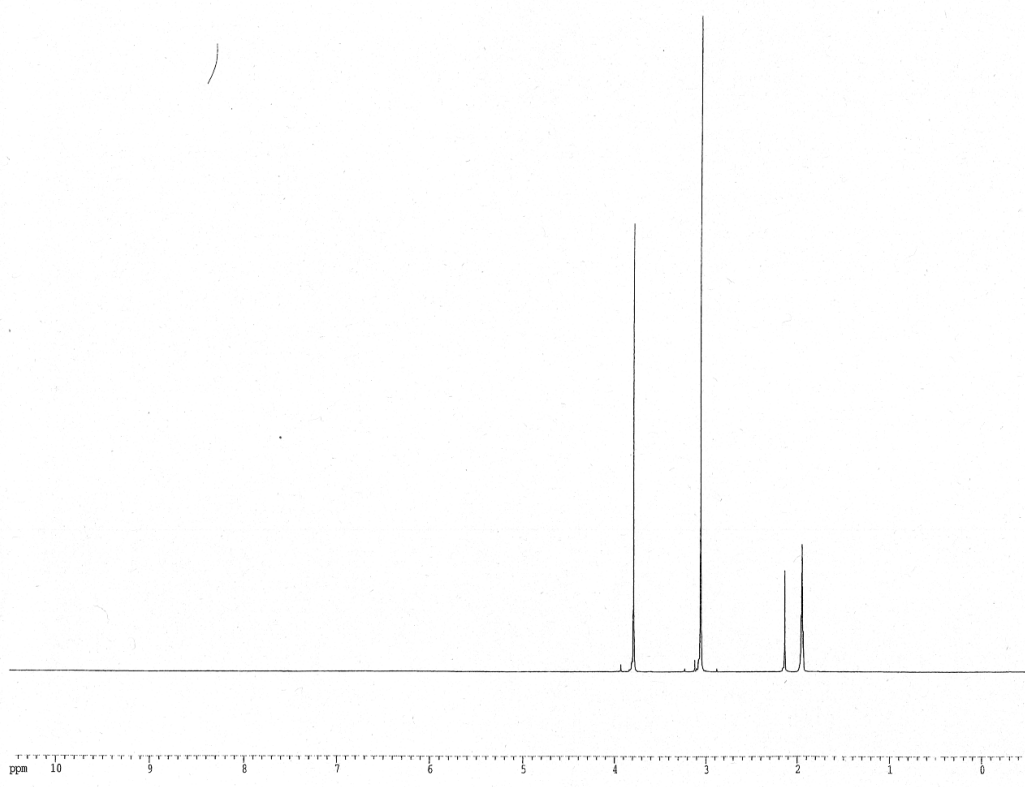
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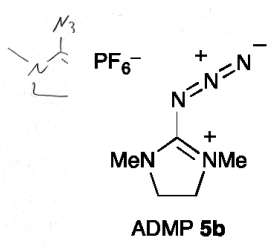
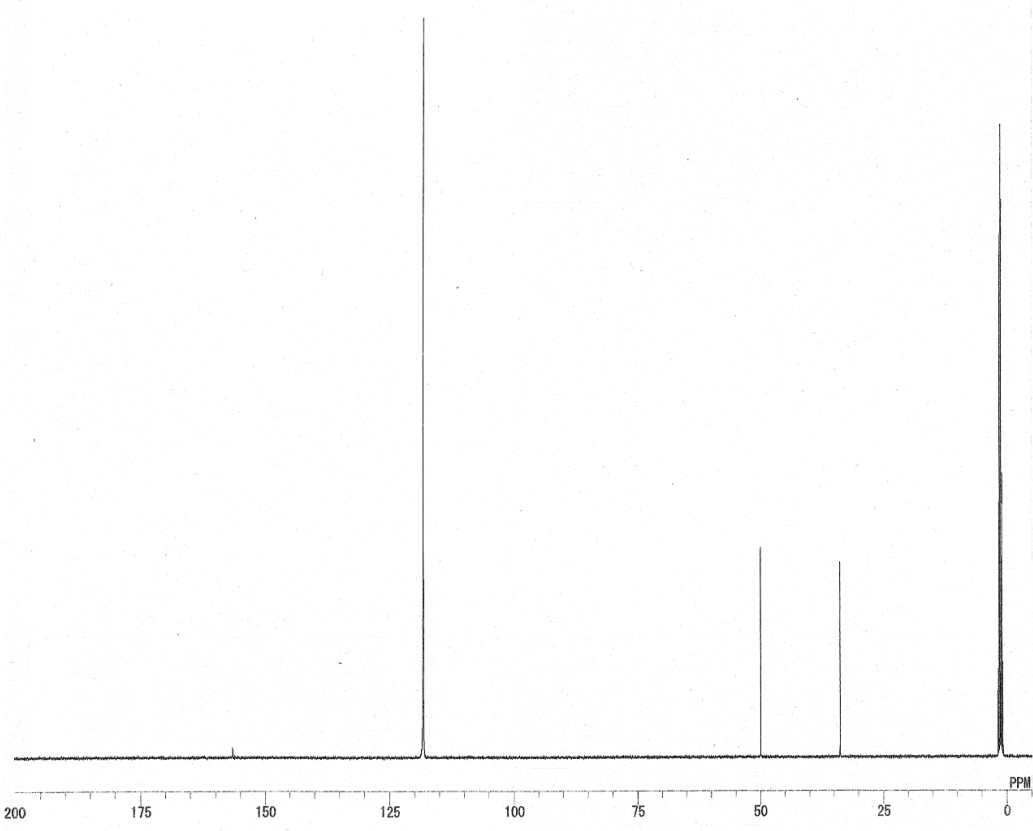


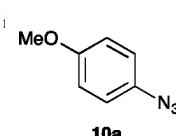
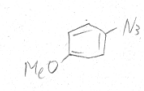
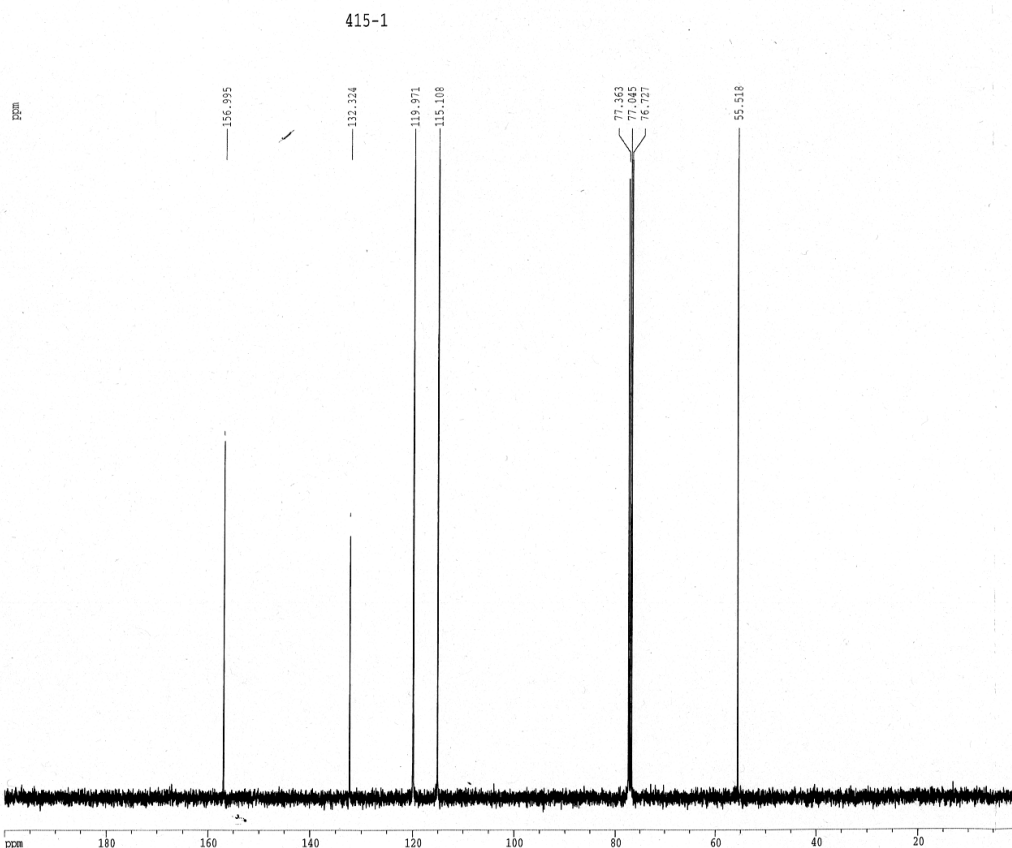
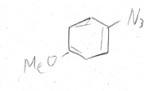
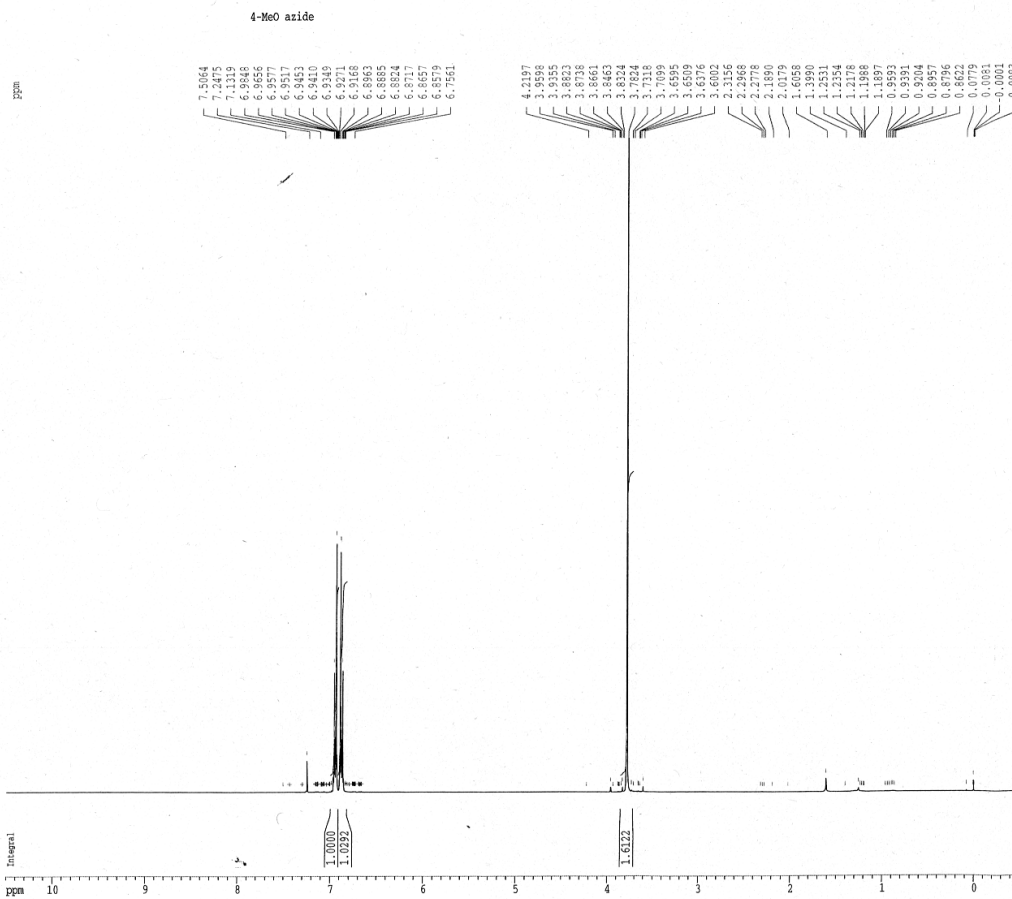
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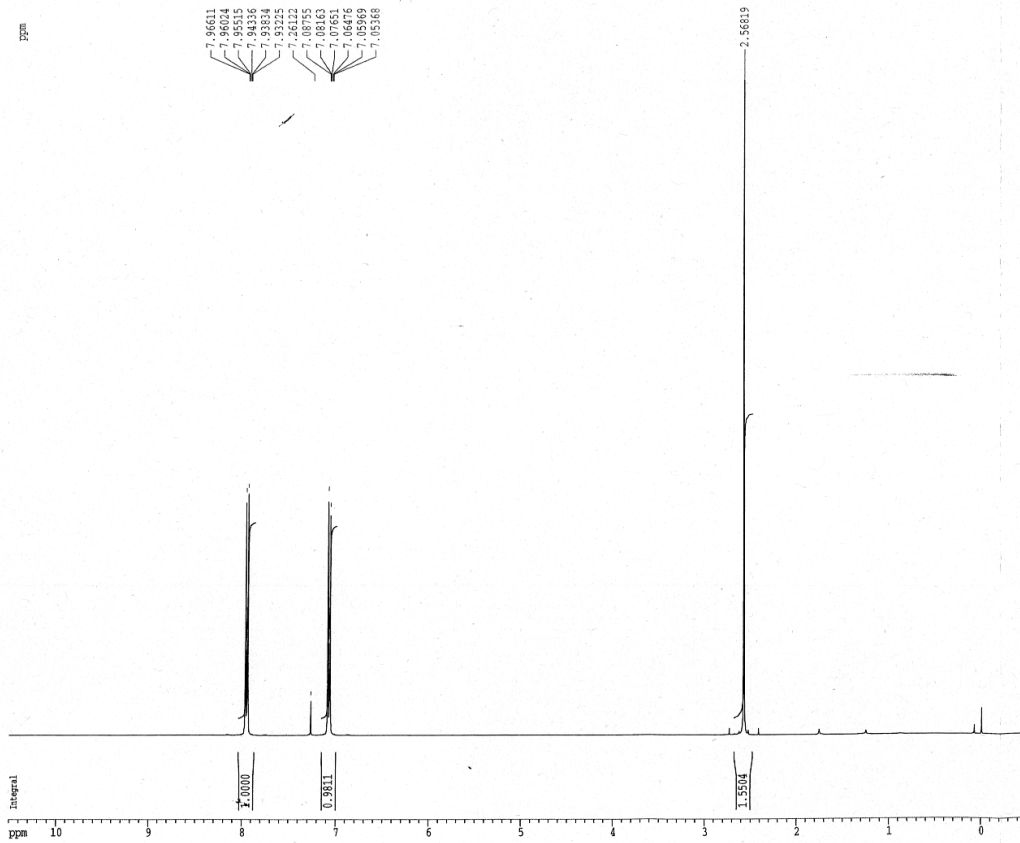
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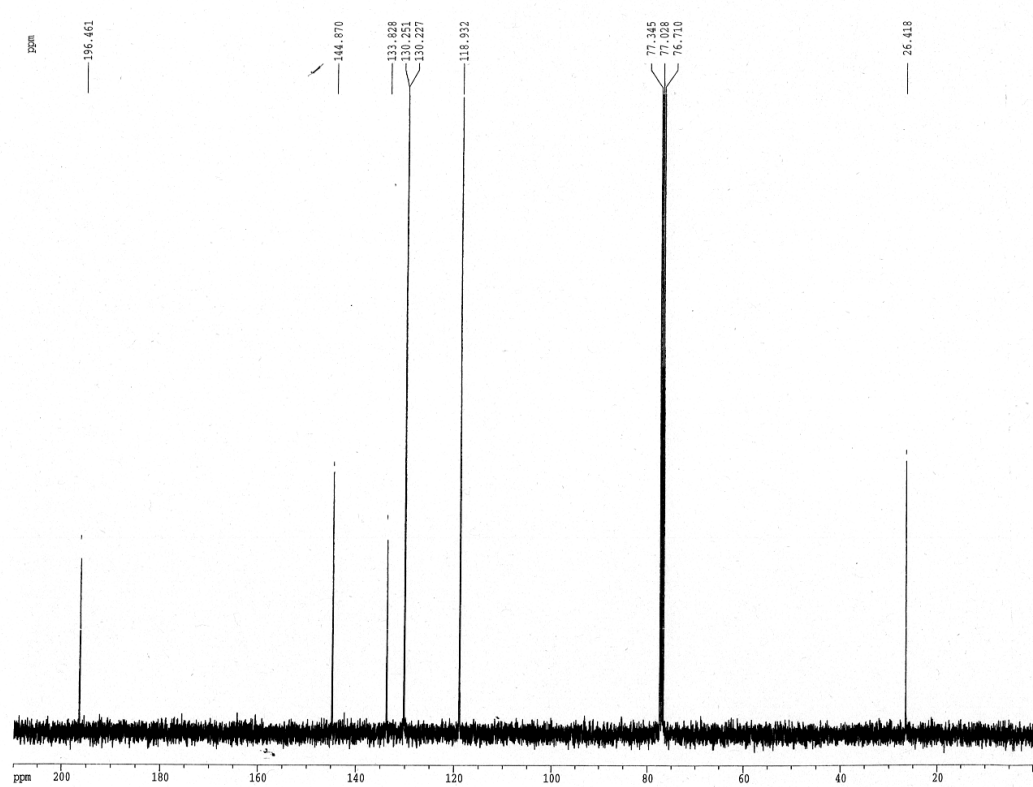
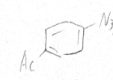
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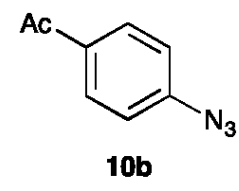
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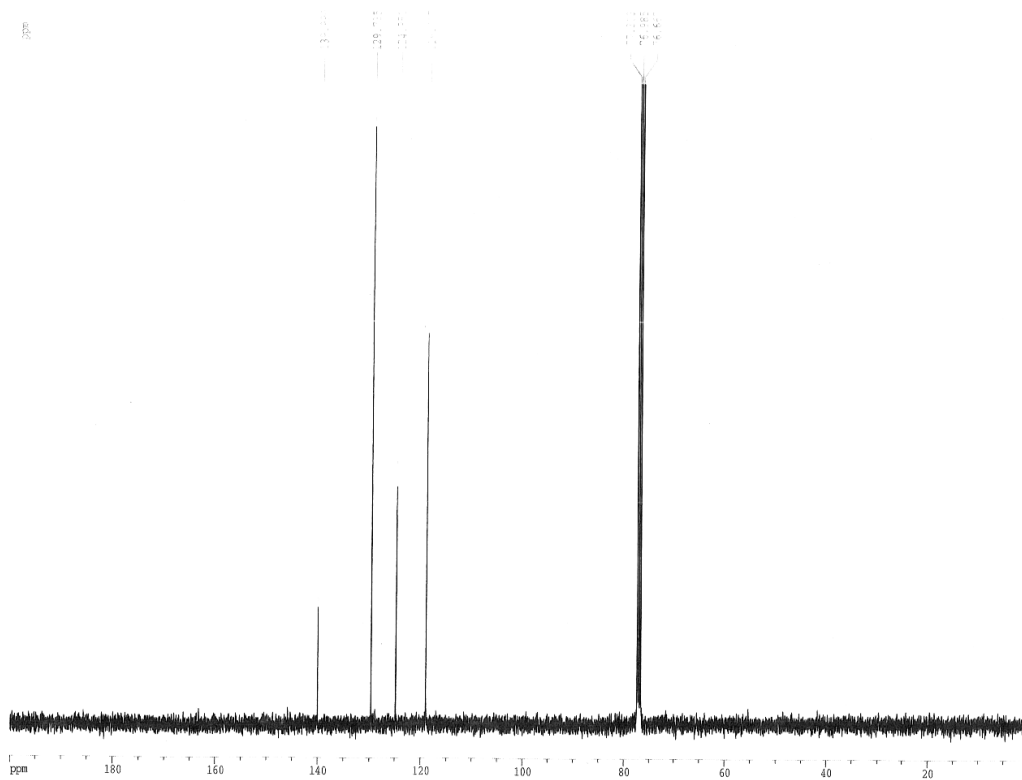
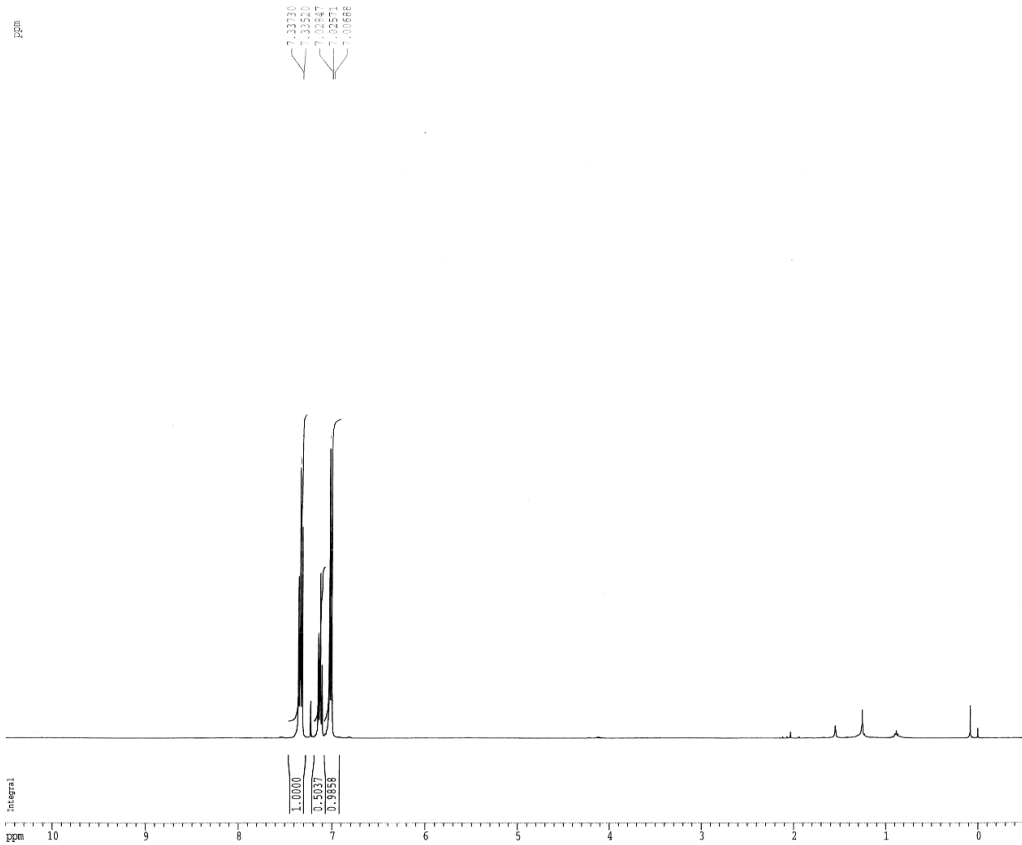
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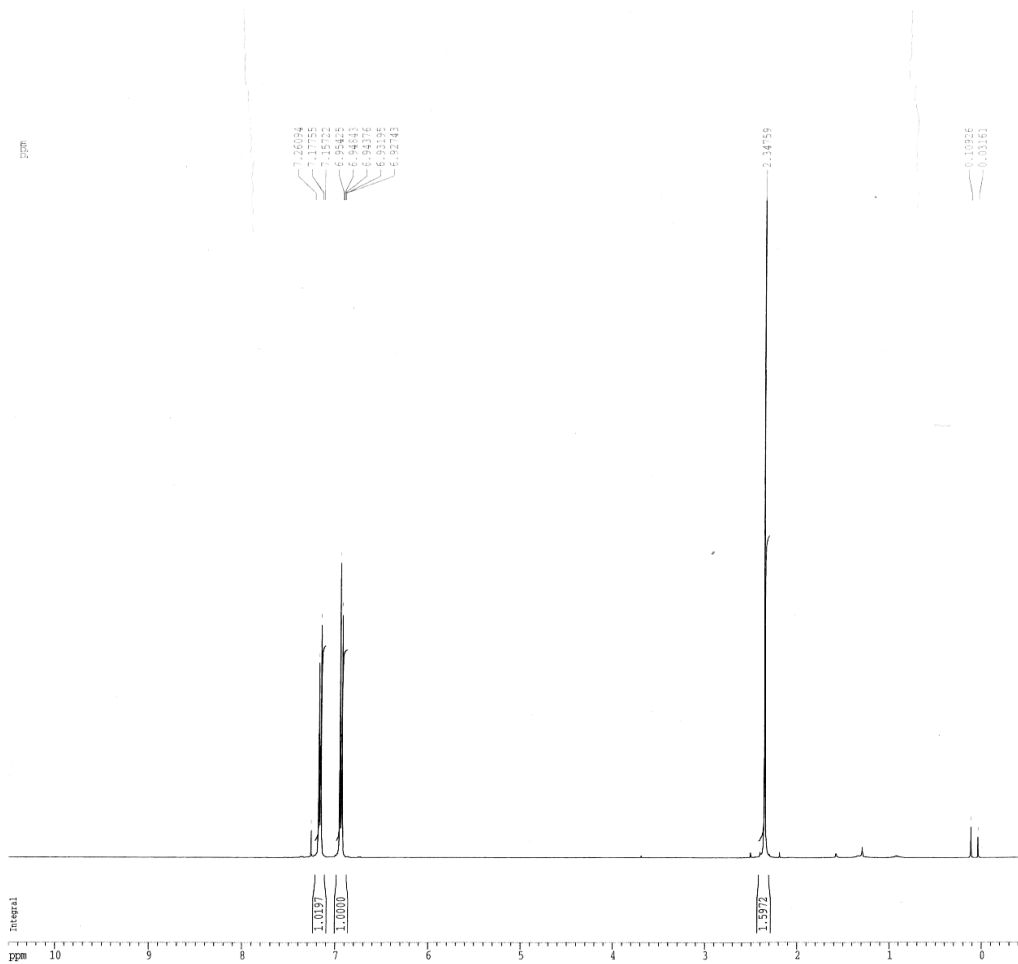
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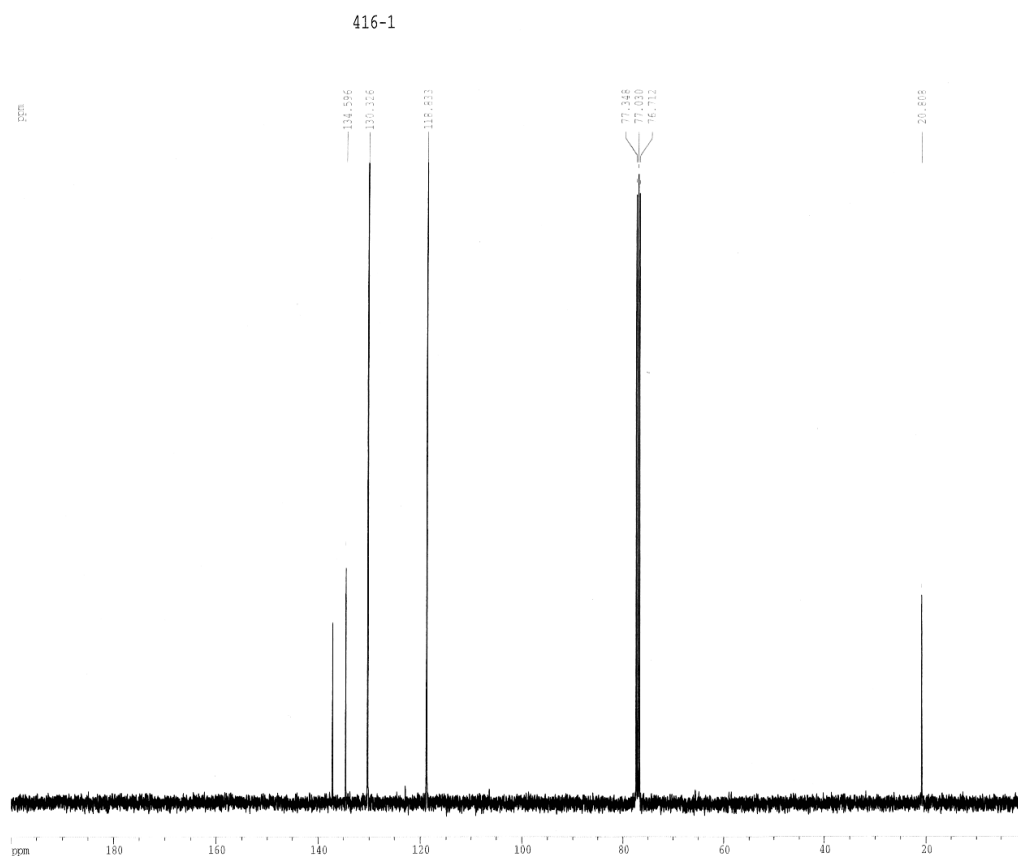
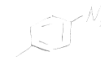


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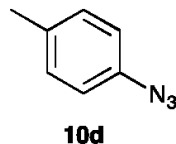


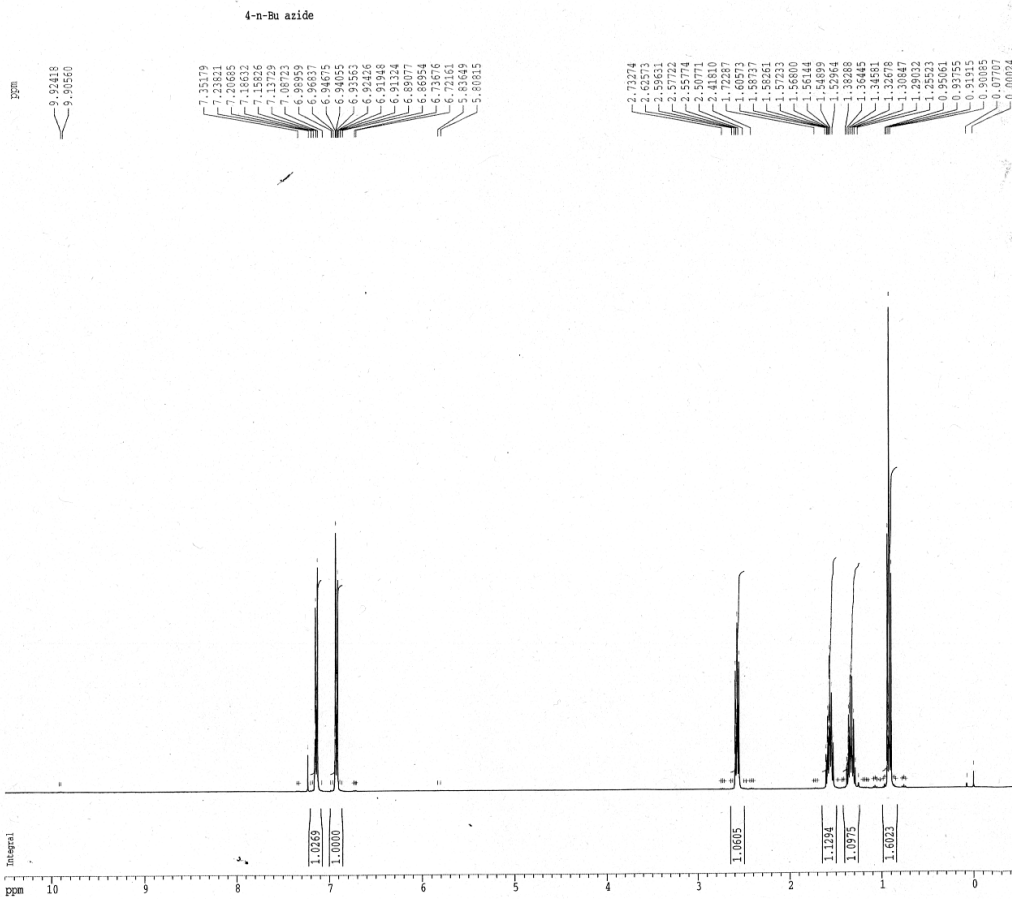
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1D NMR |  
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 PIP  
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 F2P  
 F2  
 FWHM  
 HZCM





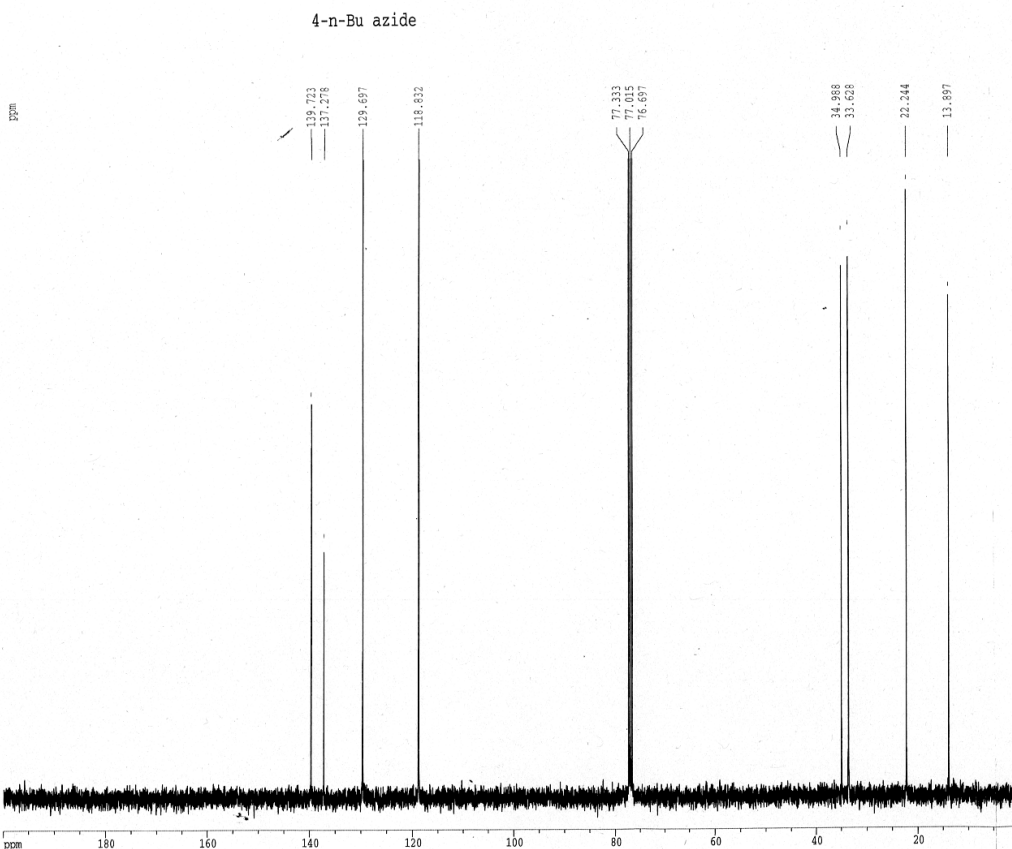
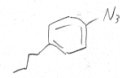
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1D NMR plot parameters  
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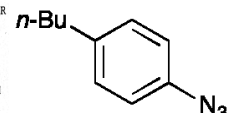
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 DW 19.950 usec  
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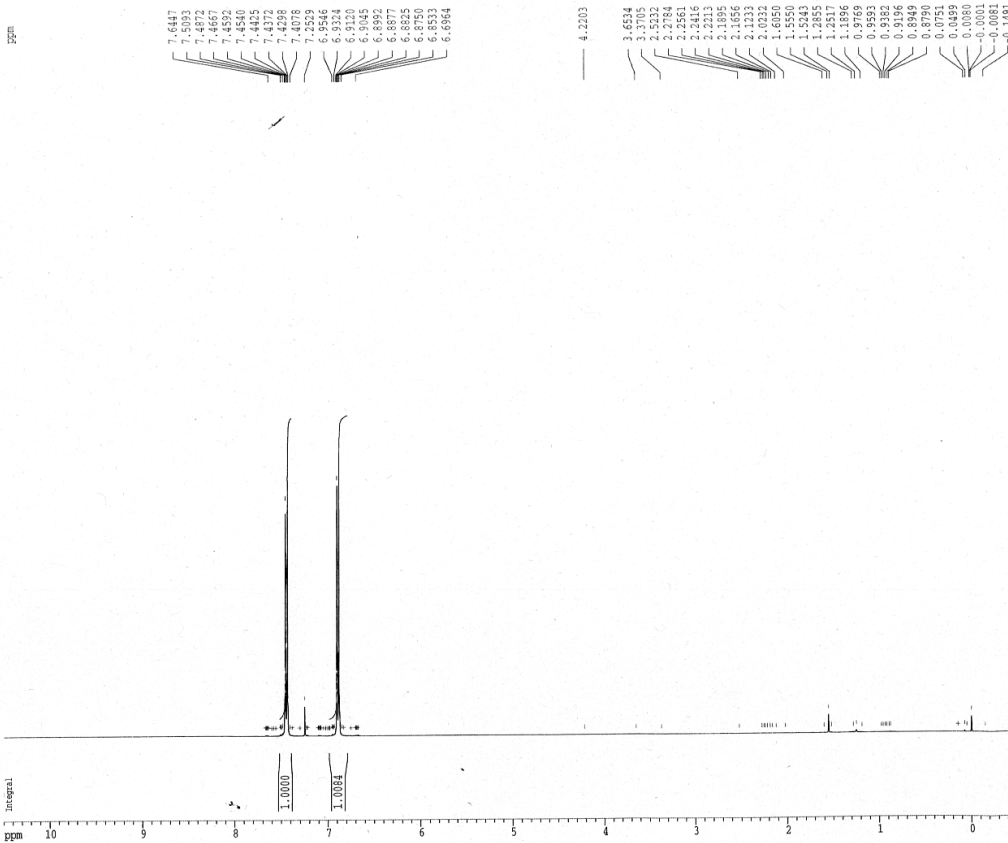
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1D NMR  
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 F1  
 F2P  
 F2  
 PPMCM  
 HzCM



10e

4-Cl azide



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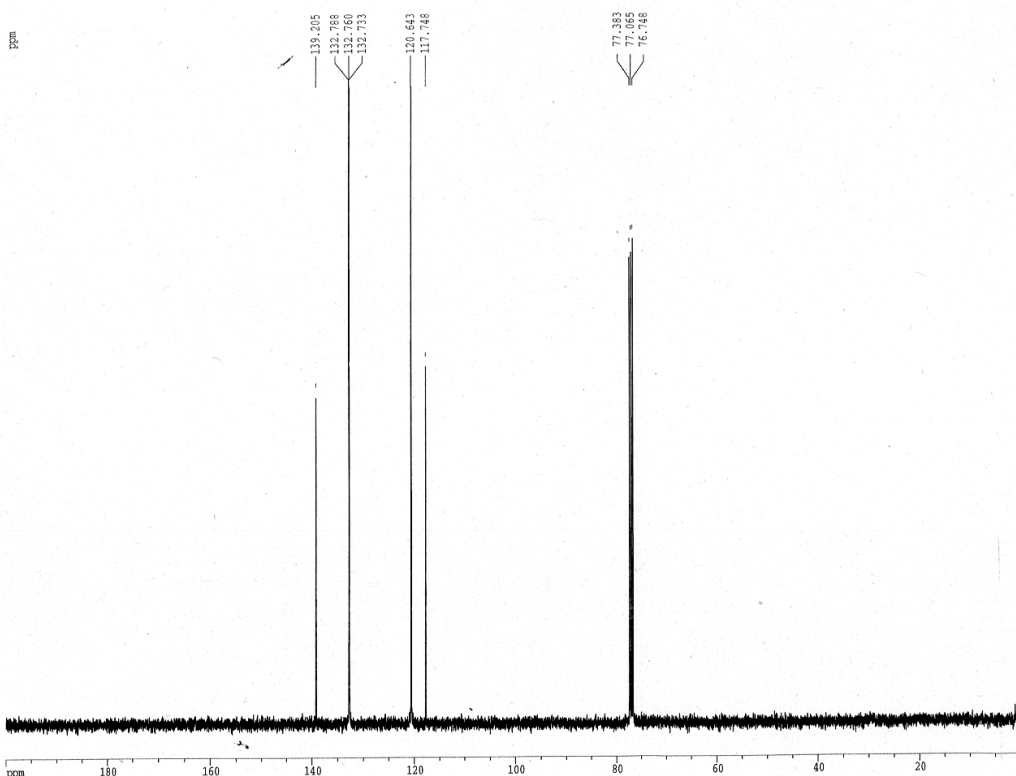
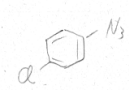
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1D NMR plot parameters
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F1         4201.37 Hz
F2P        -0.500 ppm
F2         -200.07 Hz
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H2CM       166.7134 Hz/cm
    
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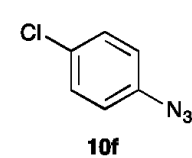
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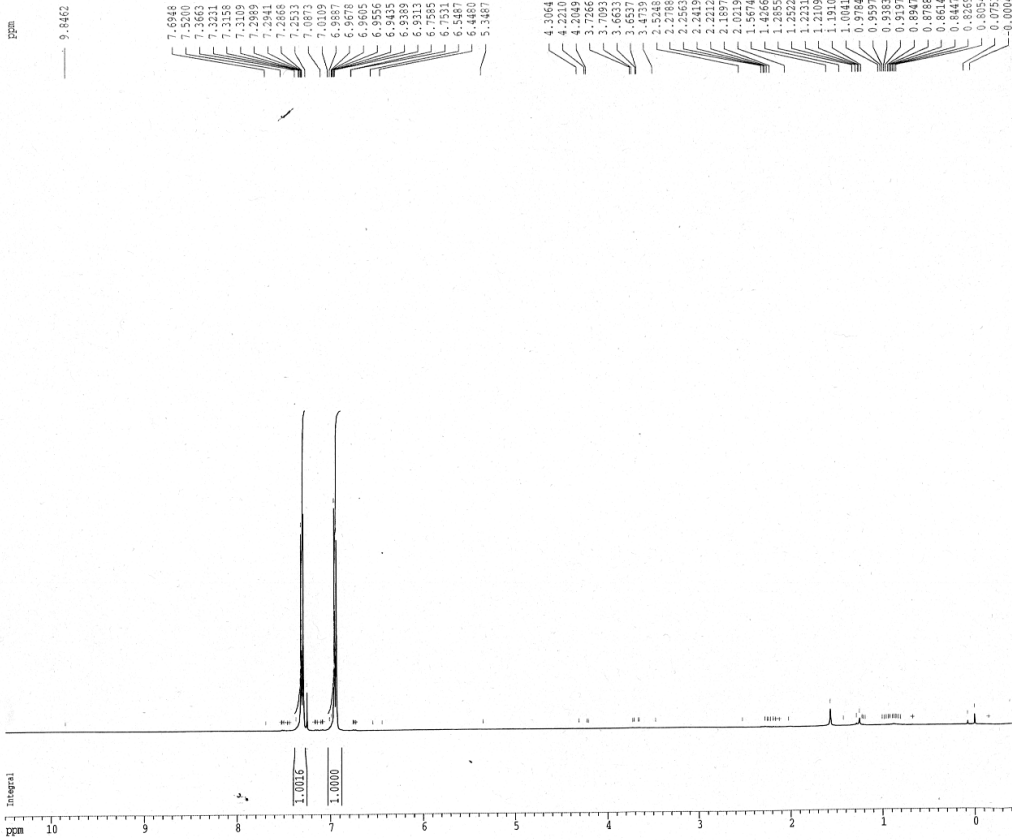
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1D
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F1         4201.37 Hz
F2P        -0.500 ppm
F2         -200.07 Hz
P1MCM      0.36667 ppm/cm
H2CM       166.7134 Hz/cm
    
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4-Br azide



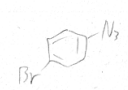
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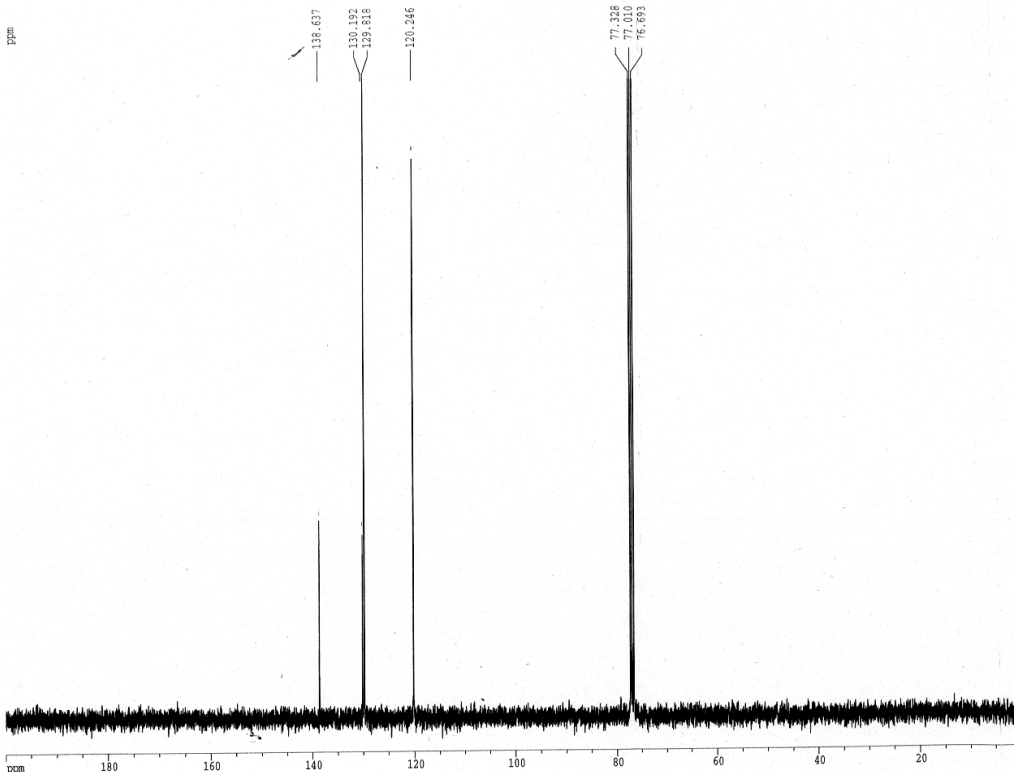
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1D NMR plot parameters  
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 F1 4201.37 Hz  
 F2P -0.500 ppm  
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4-Br azide



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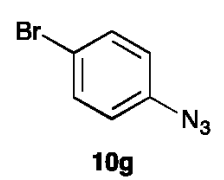
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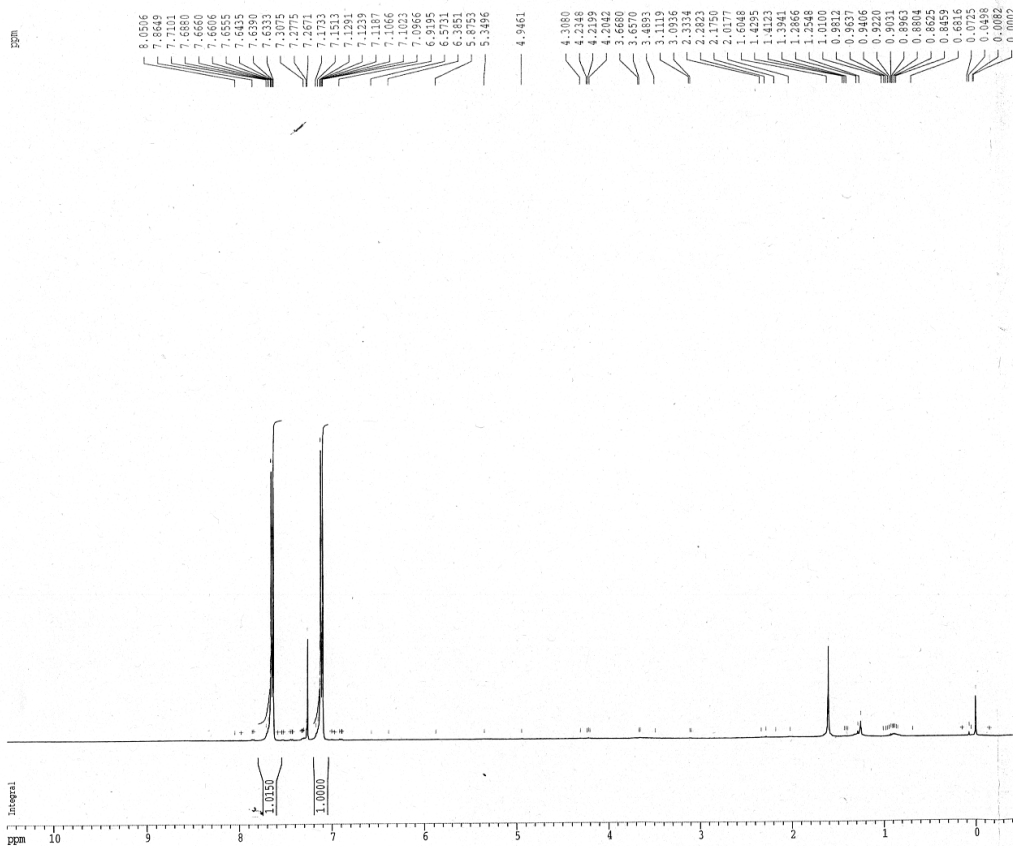
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1D NMR  
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 F1  
 F2P  
 F2  
 PPMCN  
 HZCN



4-CN azide



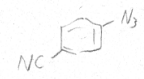
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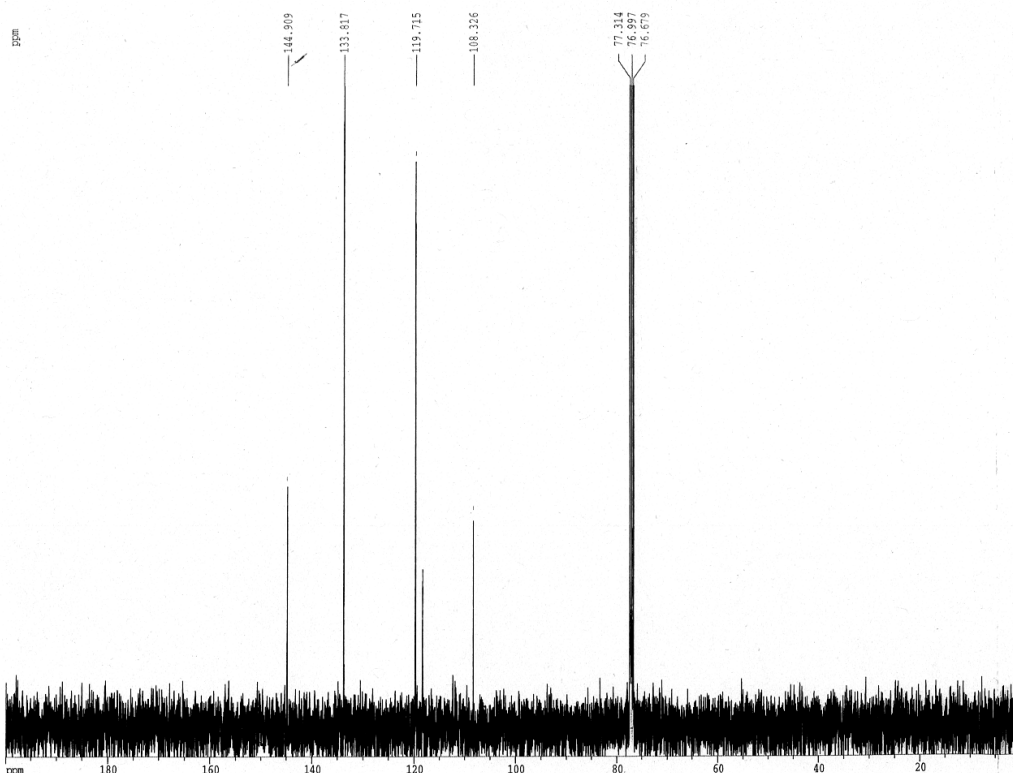
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1D NMR plot parameters  
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 F1 4201.37 Hz  
 F2 -0.500 ppm  
 F2 200.07 Hz  
 FWHM 0.36667 ppm/cm  
 HECM 146.71434 Hz/cm



4-CN azide



Current Data Parameters  
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 EXPNO 1089  
 PROCNO 1

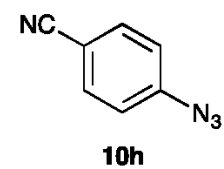
F2 - Acquisition Parameters  
 Date\_ 20100503  
 Time 22.13  
 INSTRUM dpx400  
 PROBDH 5 mm BBO BB-  
 PULPROG zgdc30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 14596.5  
 DW 19.950 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec

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

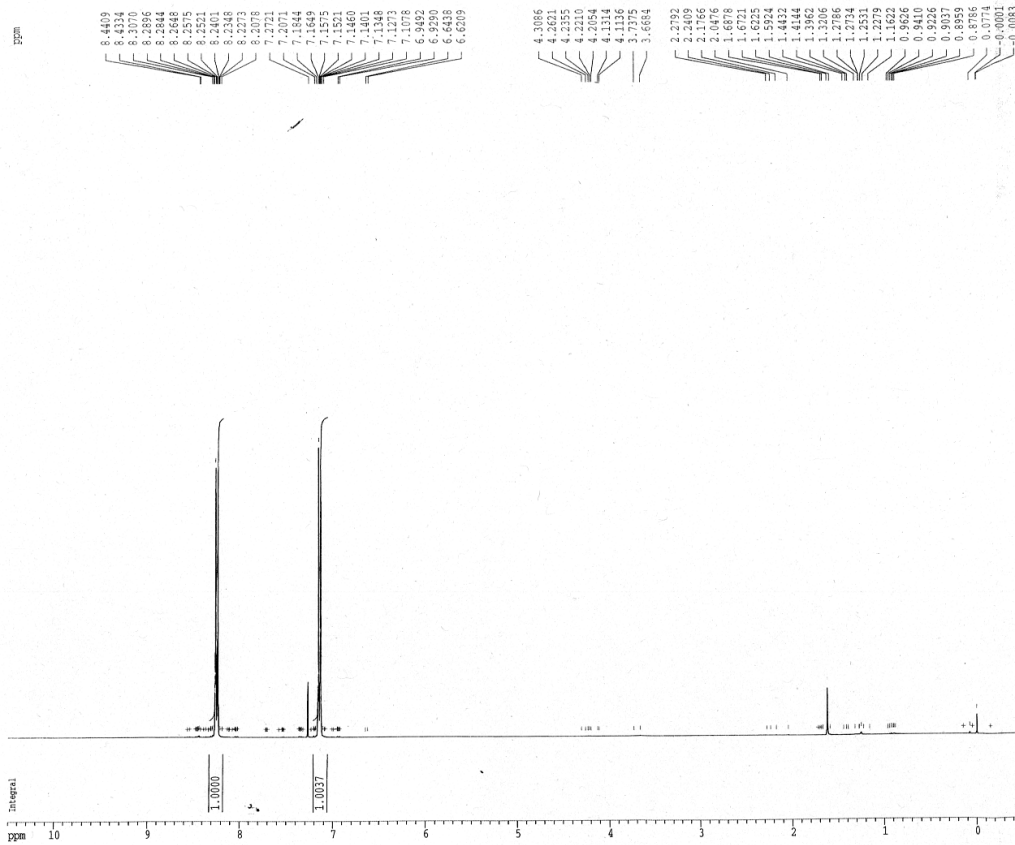
===== CHANNEL f2 =====  
 CPDPR2 waltz16  
 NUC2 1H  
 FCPD2 80.00 usec  
 PL2 -6.00 dB  
 PL12 9.00 dB  
 SFO2 400.1316005 MHz

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

1D N  
 CX  
 FIP  
 F1  
 F2  
 F2  
 FWHM  
 HECM



4-NO2 azide



```

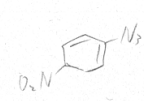
Current Data Parameters
NAME      09yano
EXPNO     1092
PROCNO    1

F2 - Acquisition Parameters
Date_     20100504
Time      21.08
INSTRUM   gp400
PROBHD    5 mm BBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8250.825 Hz
FIDRES     0.155898 Hz
AQ         3.9715316 sec
RG         128
DW         60.600 usec
DE         6.00 usec
TE         300.0 K
D1         1.00000000 sec

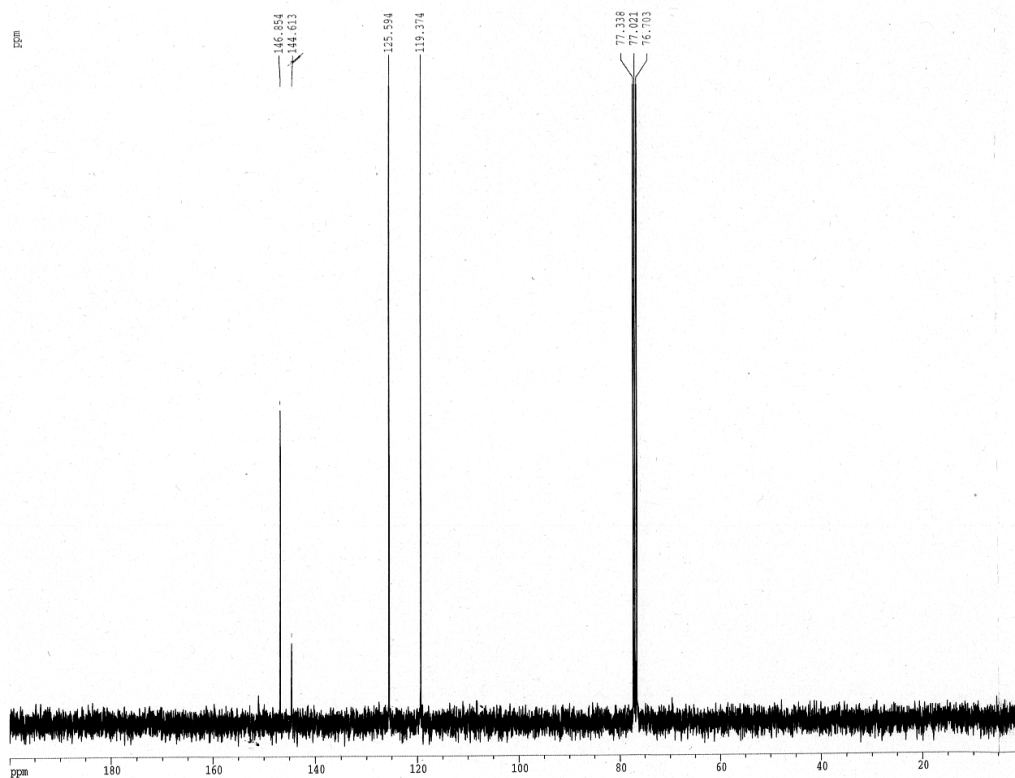
===== CHANNEL f1 =====
NUC1       1H
P1         12.00 usec
PL1        -6.00 dB
SFO1       400.1324716 MHz

F2 - Processing parameters
SI         32768
SF         400.1300049 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         4203.37 Hz
F2P        -2.500 ppm
F2         -200.07 Hz
PFMCM      0.36667 ppm/cm
HECM       146.71434 Hz/cm
    
```



4-NO2 azide



```

Current Data Parameters
NAME      09yano
EXPNO     1093
PROCNO    1

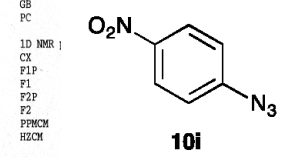
F2 - Acquisition Parameters
Date_     20100504
Time      21.25
INSTRUM   gp400
PROBHD    5 mm BBO BB-
PULPROG   zgdc30
TD         65536
SOLVENT   CDCl3
NS         256
DS         2
SWH        25062.656 Hz
FIDRES     0.382426 Hz
AQ         1.3074932 sec
RG         14596.5
DW         19.950 usec
DE         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

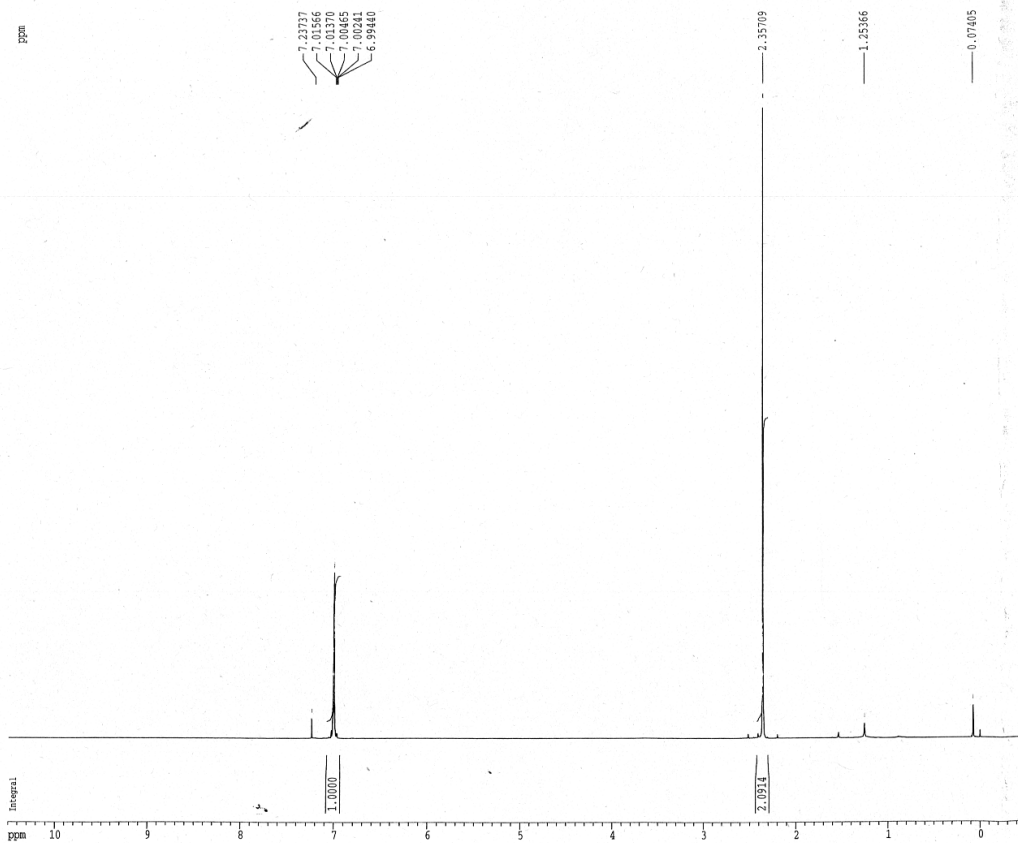
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -6.00 dB
PL12       9.00 dB
SFO2       400.1316005 MHz

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

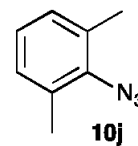
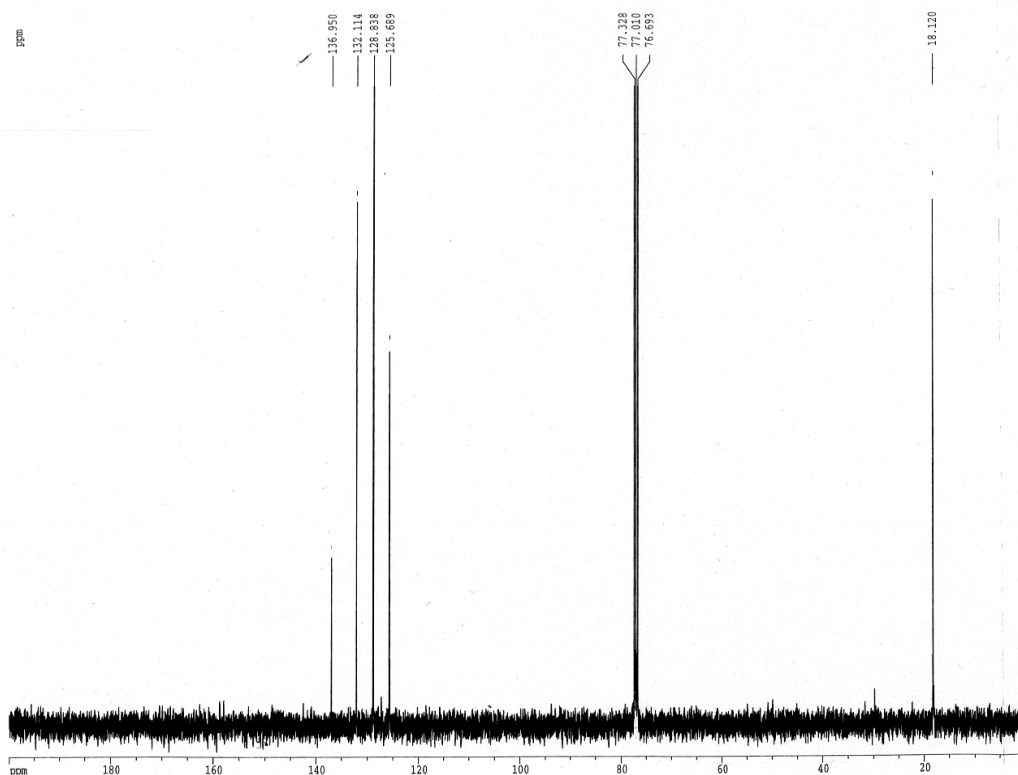
1D NMR 1
CX         30.00 cm
F1P        10.500 ppm
F1         4203.37 Hz
F2P        -2.500 ppm
F2         -200.07 Hz
PFMCM      0.36667 ppm/cm
HECM       146.71434 Hz/cm
    
```



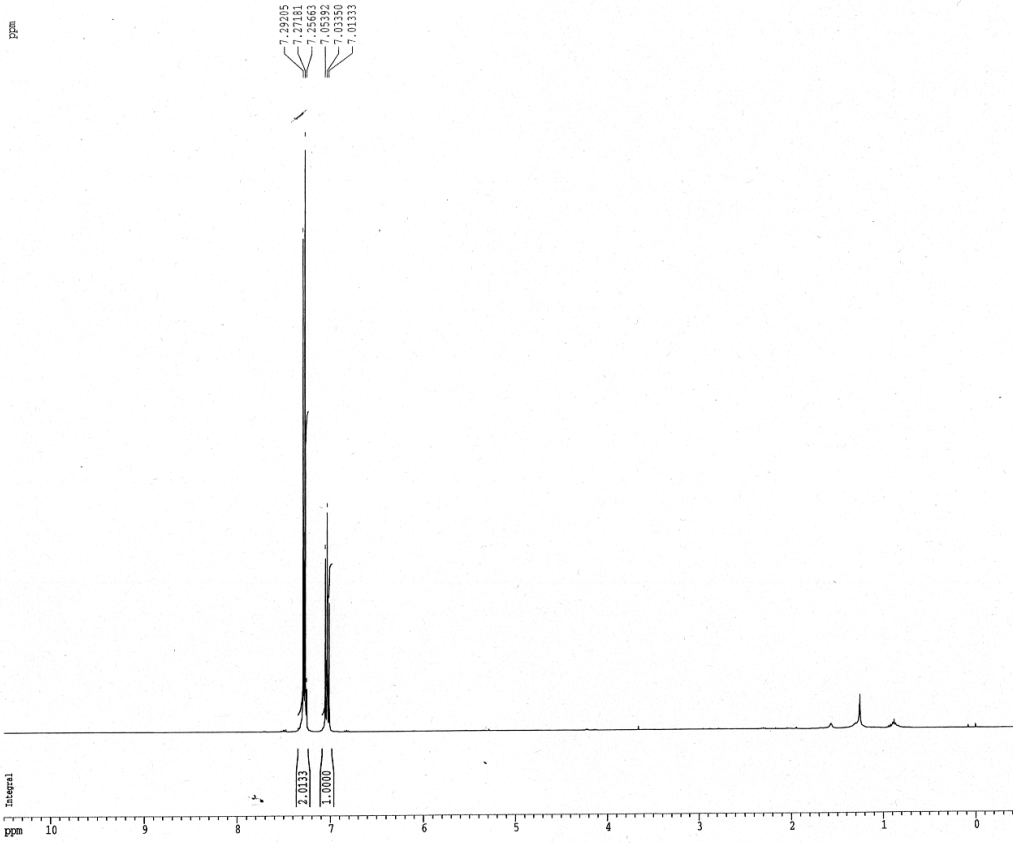
421-1 678



421-1



2,6-dichloro azide



```

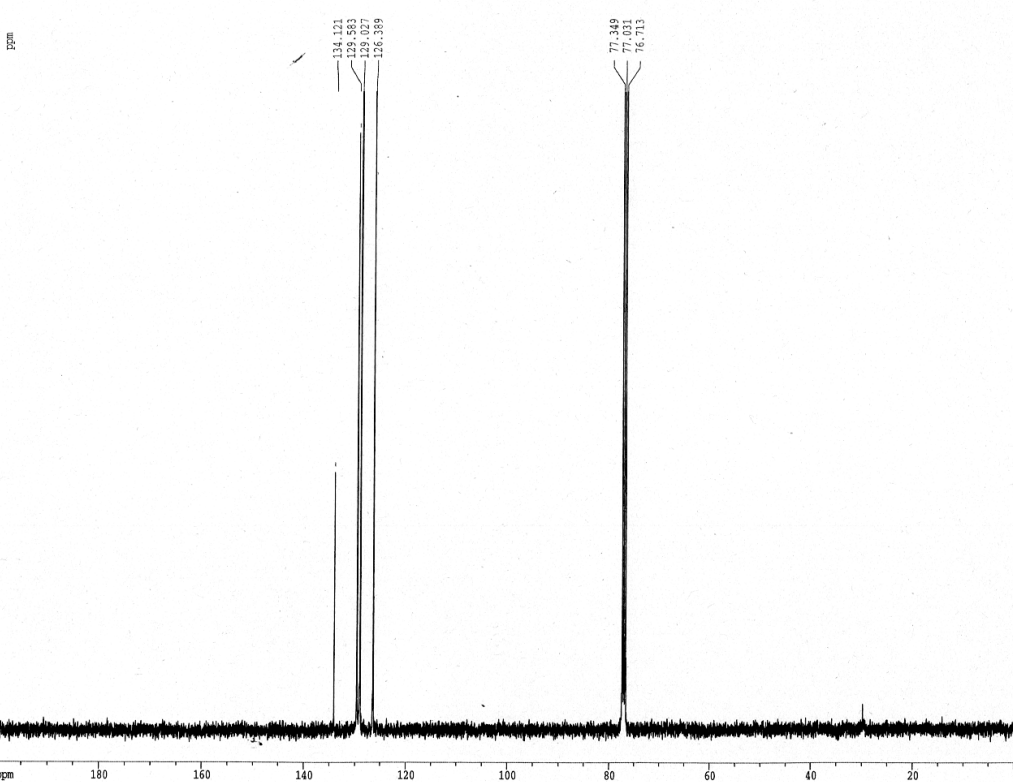
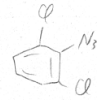
Current Data Parameters
NAME      09yano
EXPNO    1199
PROCNO   1

F2 - Acquisition Parameters
Date_    20100827
Time     18.24
INSTRUM  dpx400
PROBHD   5 mm BBO BB-
PULPROG  zg10
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8250.825 Hz
FIDRES   0.125888 Hz
AQ       3.9715316 sec
RG       128
DW       60.400 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

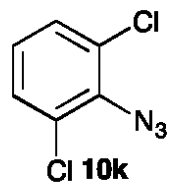
F2 - Acquisition Parameters
Date_    20100829
Time     14.26
INSTRUM  dpx400
PROBHD   5 mm BBO BB-
PULPROG  zgdc30
TD       65536
SOLVENT  CDCl3
NS       911
DS       2
SWH      25062.656 Hz
FIDRES   0.382426 Hz
AQ       1.3074932 sec
RG       14596.5
DW       19.950 usec
DE       6.00 usec
TE      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

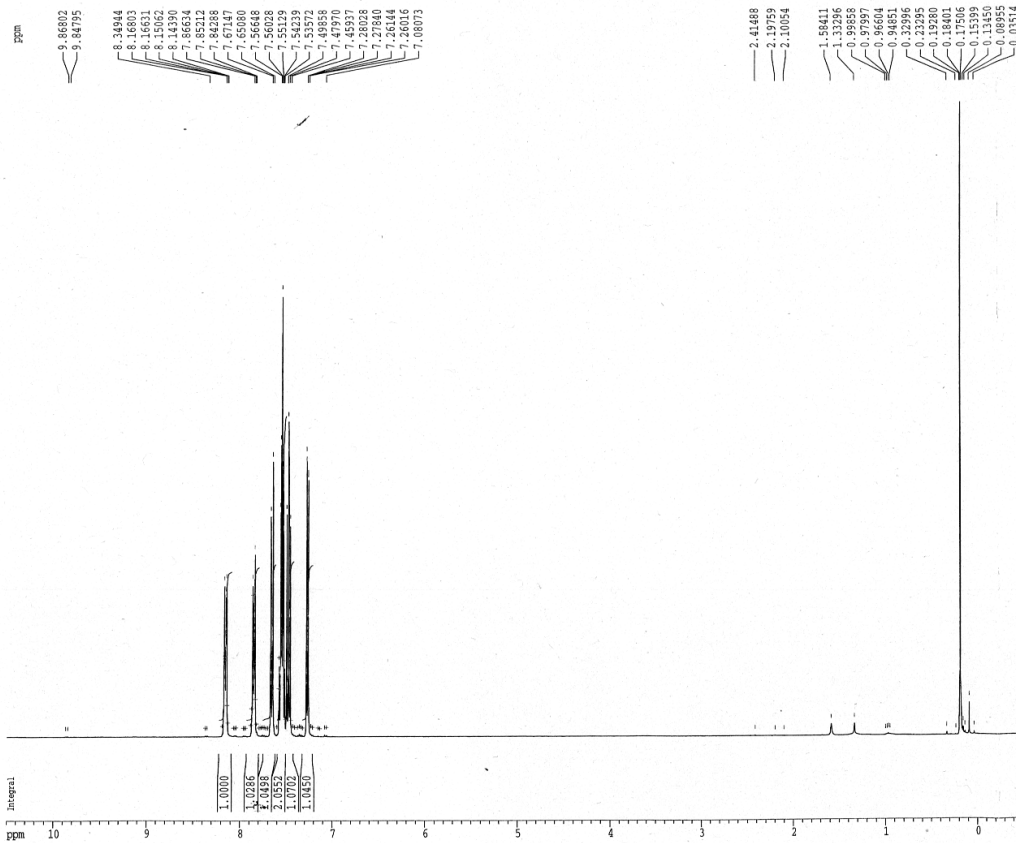
===== CHANNEL f1 =====
NUC1     13C
P1       10.00 usec
PL1      -3.90 dB
SFO1    100.6237959 MHz

===== 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  
 PROBHD 5 mm BBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8250.825 Hz  
 FIDRES 0.125898 Hz  
 AQ 3.9715316 sec  
 RG 64  
 DW 60.600 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec

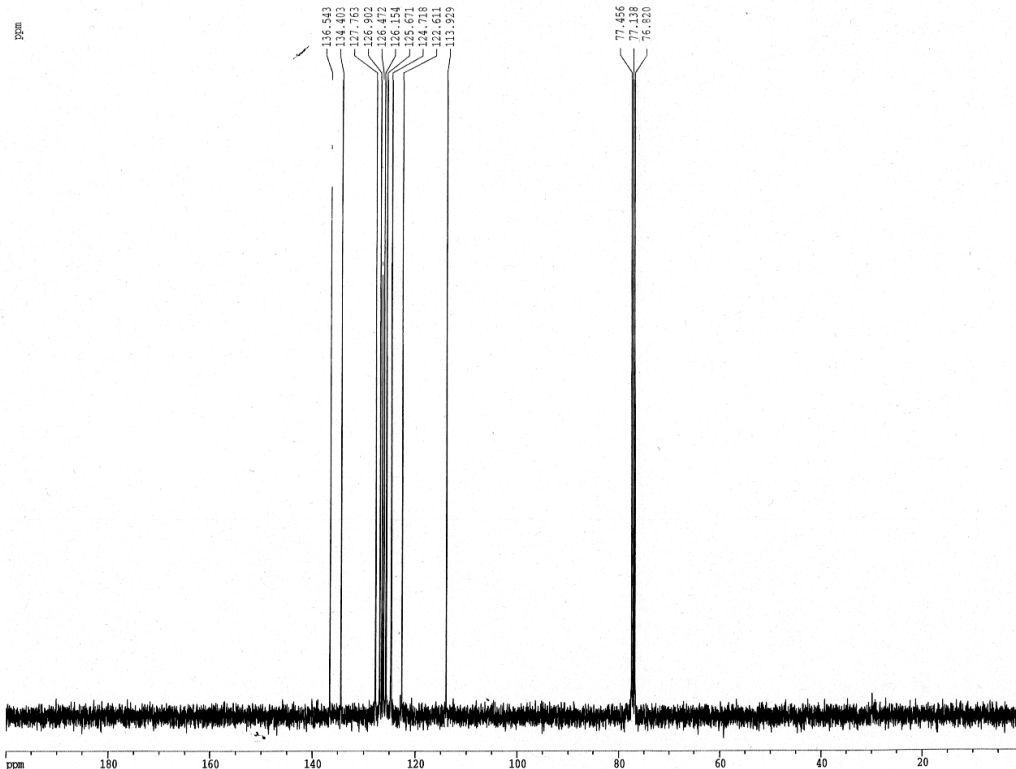
===== CHANNEL f1 =====  
 NUCL1 1H  
 P1 12.00 usec  
 PL1 -6.00 dB  
 SF01 400.1324710 MHz

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  
 PPMCM 0.36667 ppm/cm  
 HZCM 146.71434 Hz/cm



449--1



Current Data Parameters  
 NAME 09yano  
 EXPNO 1186  
 PROCNO 1

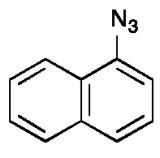
F2 - Acquisition Parameters  
 Date\_ 20100821  
 Time 17.52  
 INSTRUM dpx400  
 PROBHD 5 mm BBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 14596.5  
 DW 19.950 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec

===== CHANNEL f1 =====  
 NUCL1 13C  
 P1 10.00 usec  
 PL1 -3.90 dB  
 SF01 100.6237959 MHz

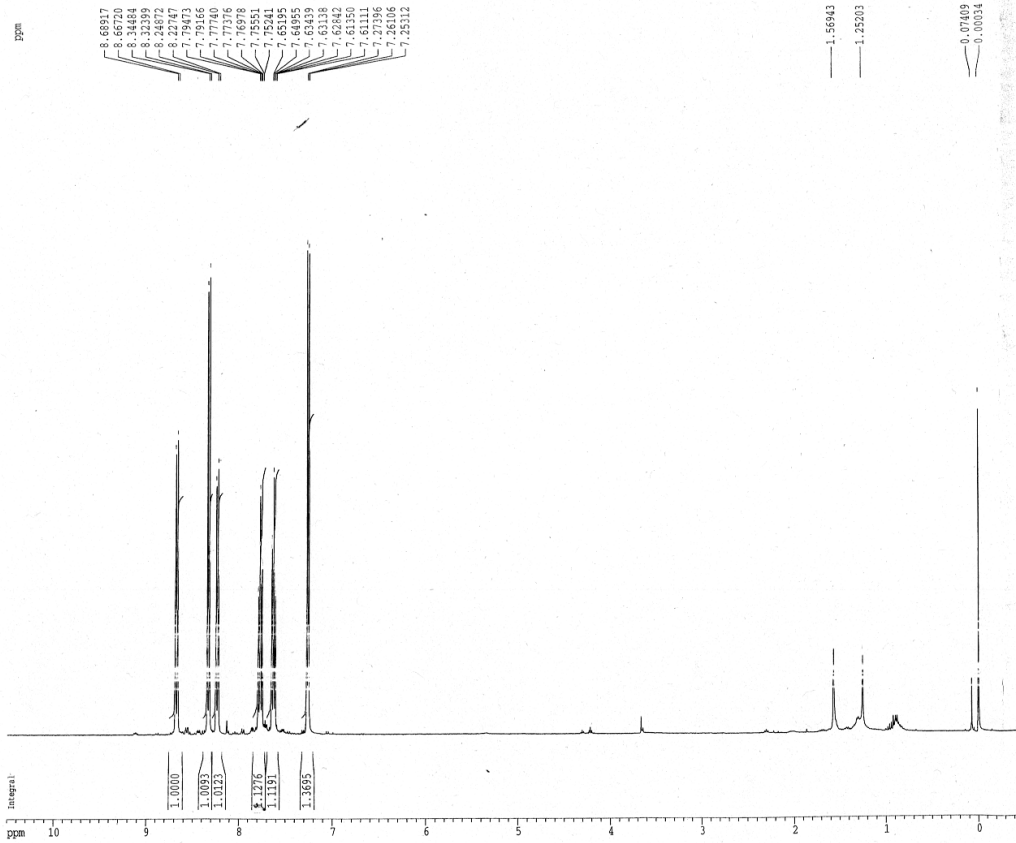
===== CHANNEL f2 =====  
 CQPRG2 waltz16  
 NUCL2 1H  
 PCPD2 80.00 usec  
 PL2 -6.00 dB  
 PL12 9.00 dB  
 SF02 400.1316005 MHz

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

1D NMR  
 CX  
 FIP  
 F1  
 F2P  
 F2  
 PPMCM  
 HZCM



101



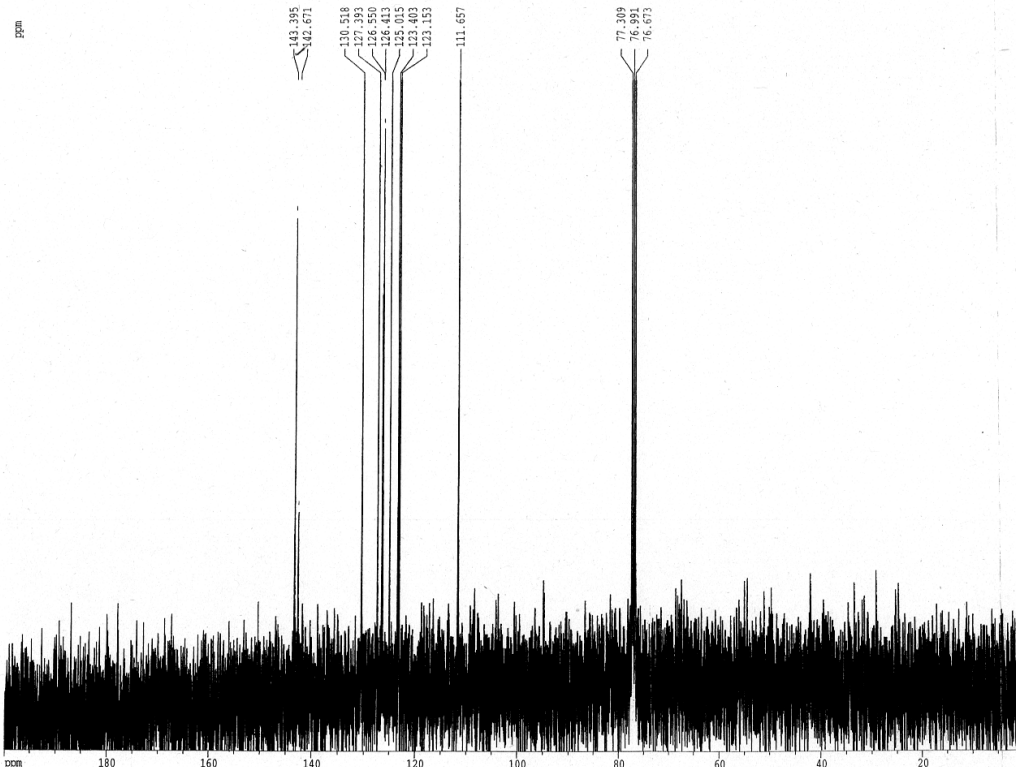
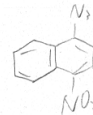
Current Data Parameters  
 NAME 09yano  
 EXPNO 1109  
 PROCNO 1

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

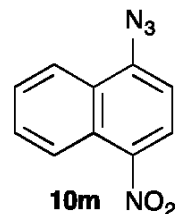
F2 - Acquisition Parameters  
 Date\_ 20091222  
 Time 23.38  
 INSTRUM dpx400  
 PROBHD 5 mm BBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 2896.3  
 DW 19.950 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000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

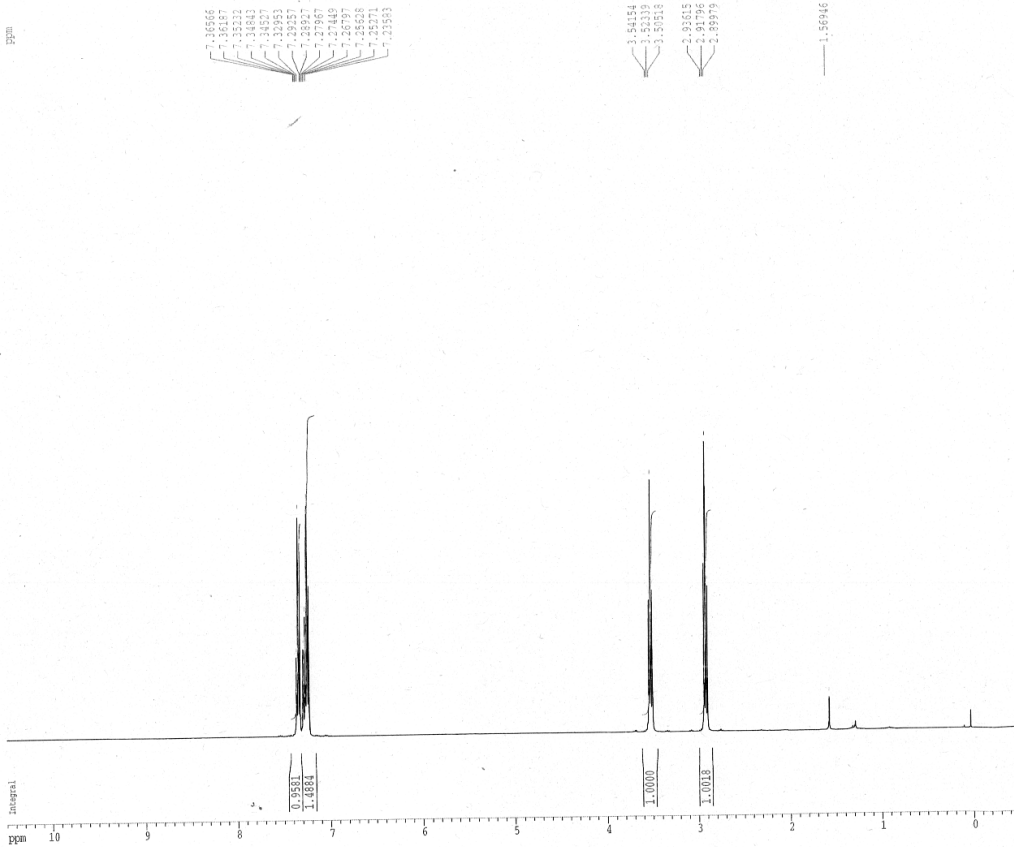
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PL1 -3.90 dB  
 SFO1 100.6237959 MHz

===== 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





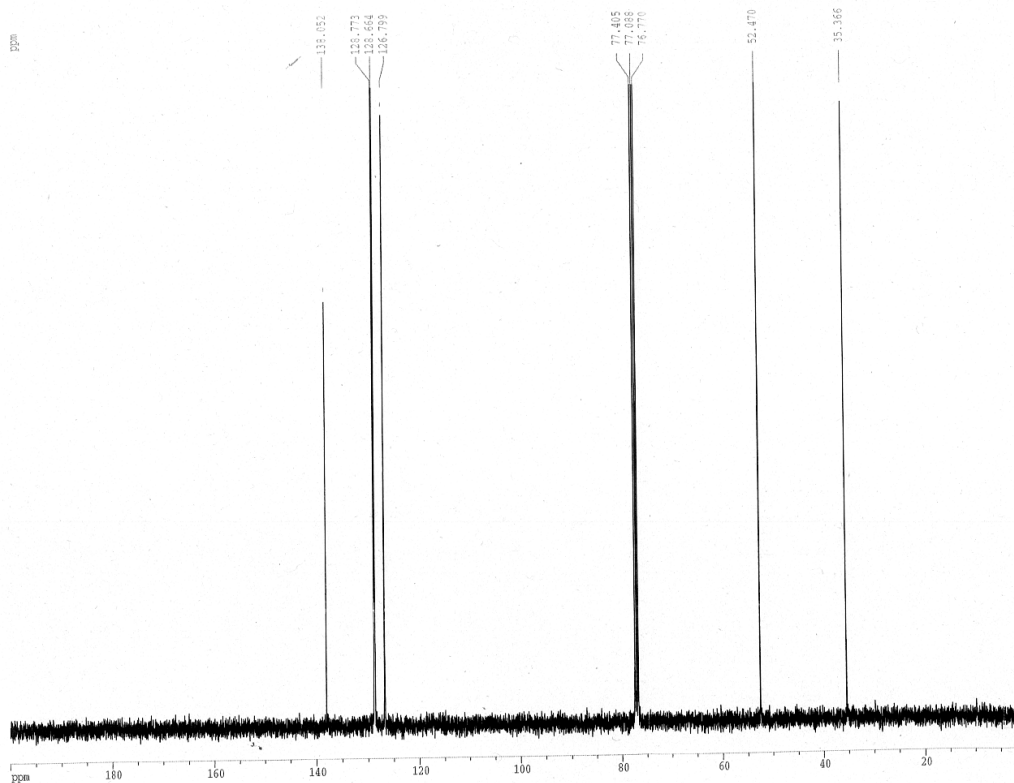
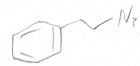
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Current Data Parameters
NAME      09yano
EXPNO     1101
PROCNO    1

F2 - Acquisition Parameters
Date_     20100505
Time      19.13
INSTRUM   gp4000
PROBHD    5 mm BBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8259.815 Hz
FIDRES     0.123898 Hz
AQ         1.9713316 sec
RG         64
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         400.1300094 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

```
ID NMR plot parameters
CX         30.00 cm
F1P        10.500 ppm
F1         4201.37 Hz
F2P        -0.500 ppm
F2         -200.07 Hz
FREQM      0.36667 ppm/cm
HZCM       146.71444 Hz/cm
```



```
Current Data Parameters
NAME      09yano
EXPNO     1081
PROCNO    1
```

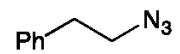
```
F2 - Acquisition Parameters
Date_     20100502
Time      22.04
INSTRUM   gp4000
PROBHD    5 mm BBO BB-
PULPROG   zgdc30
TD         65536
SOLVENT   CDCl3
NS         256
DS         2
SWH        25062.656 Hz
FIDRES     0.382426 Hz
AQ         1.3074932 sec
RG         14596.5
DM         19.950 usec
DE         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
```

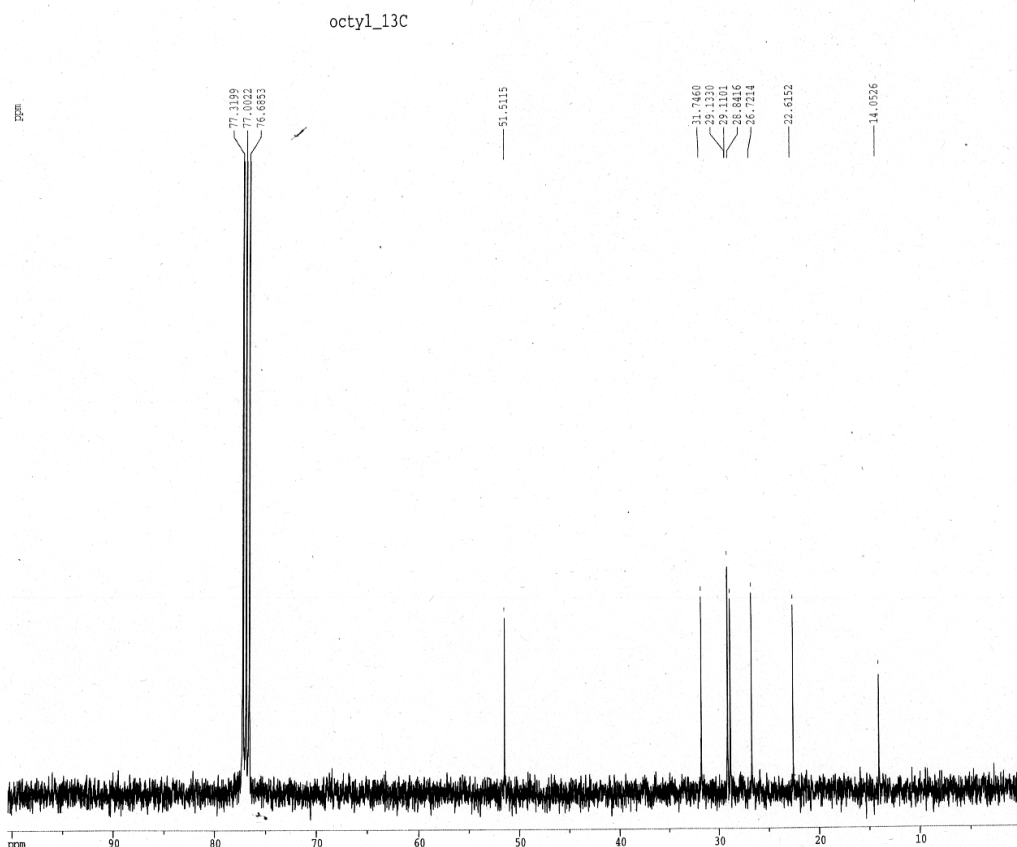
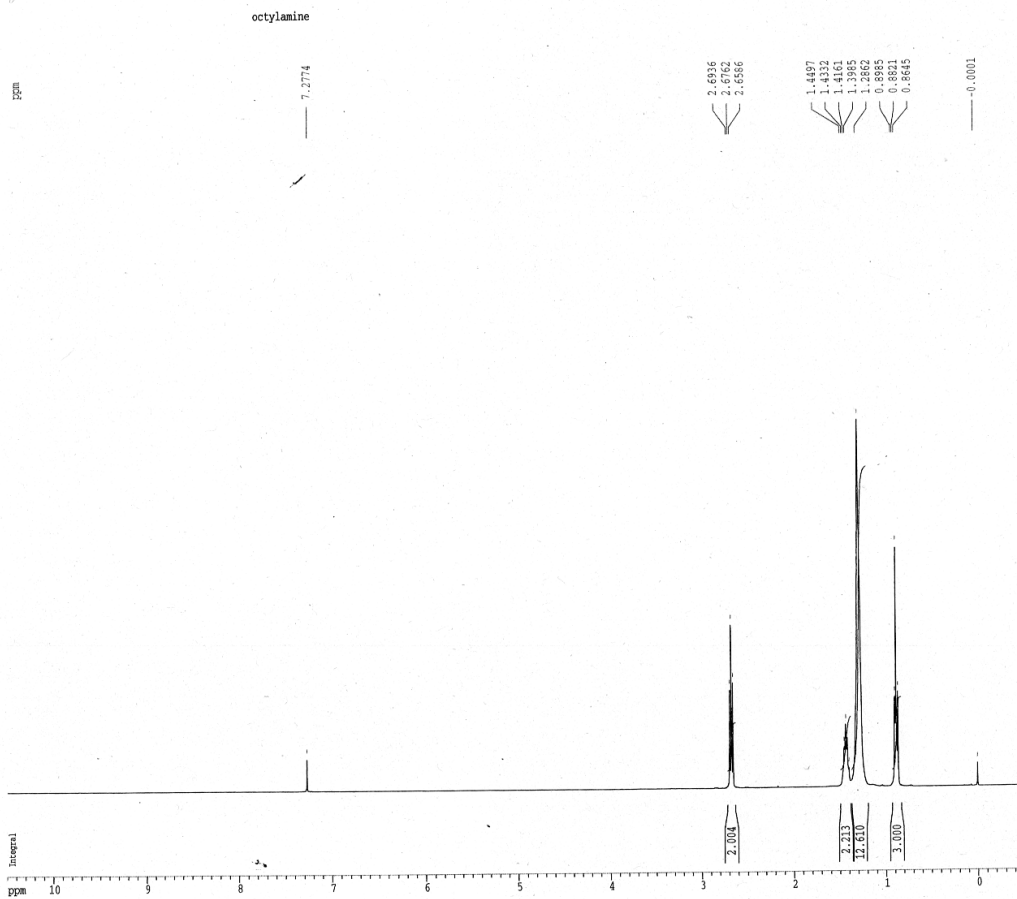
```
F2 - Processing parameters
SI         32768
SF         100.6127721 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         ^
PC         1.00
```

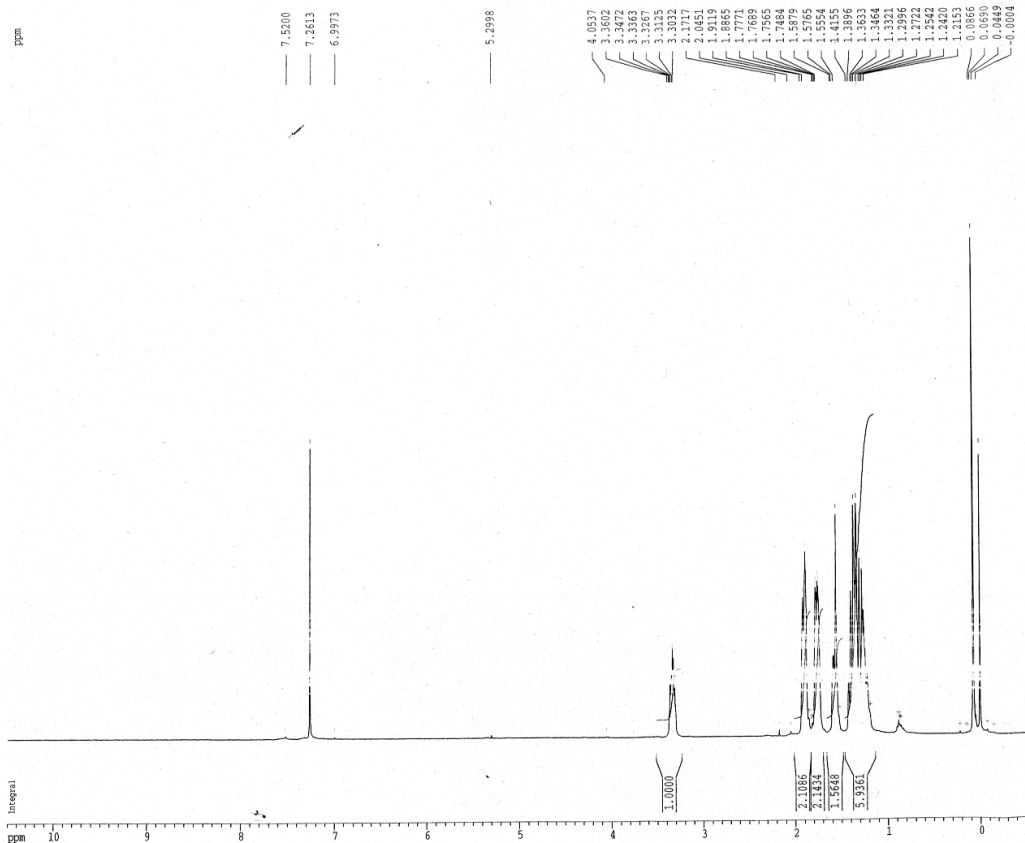
```
ID 1
CX
F1P
F1
F2P
F2
FPM
HZC
```



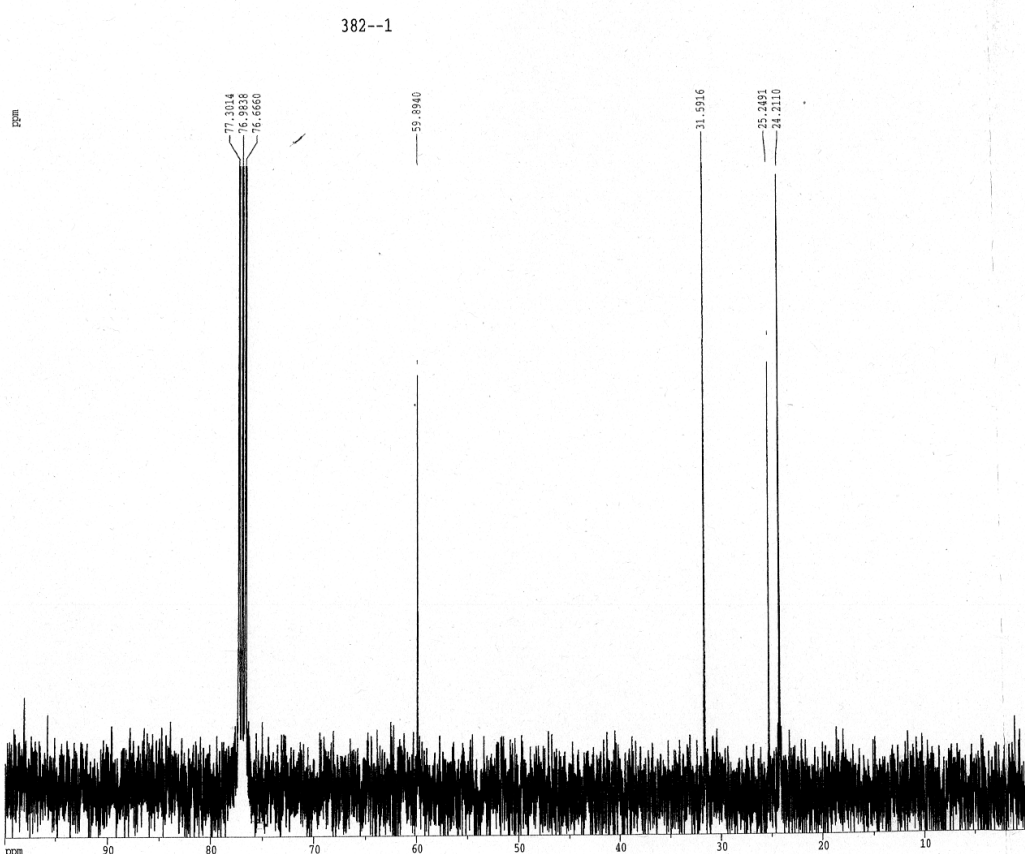
10n



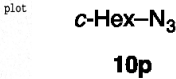




Current Data Parameters  
 NAME 09yano  
 EXPRD 967  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20100119  
 Time 19.25  
 INSTRUM dpx400  
 PROBHD 5 mm BBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8250.825 Hz  
 FIDRES 0.125898 Hz  
 AQ 3.9715316 sec  
 RG 256  
 DW 60.600 usec  
 DE 8.00 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 400.1300094 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00  
 1D NMR plot parameters  
 CX 30.00 cm  
 F1P 10.300 ppm  
 F1 4201.37 Hz  
 F2P -0.500 ppm  
 F2 -200.06 Hz  
 FWHM 0.16667 ppm/cm  
 HZCN 146.71434 Hz/cm



Current Data Parameters  
 NAME 09yano  
 EXPRD 968  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20100119  
 Time 19.42  
 INSTRUM dpx400  
 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 9195.2  
 DW 19.950 usec  
 DE 8.00 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 plot  
 CX 30.00 cm  
 F1P 10.300 ppm  
 F1 4201.37 Hz  
 F2P -0.500 ppm  
 F2 -200.06 Hz  
 FWHM 0.16667 ppm/cm  
 HZCN 335.37589 Hz/cm



ppm

7.4071  
7.4329  
7.4301  
7.4301  
7.4329  
7.4273  
7.4117  
7.4097  
7.3940  
7.3671  
7.3523  
7.3498  
7.3498  
7.3362  
7.3332  
7.3291  
7.2607  
6.9966

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

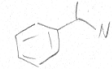
Integral

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

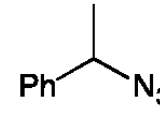
F2 - Acquisition Parameters  
Date\_ 20091119  
Time 20.21  
INSTRUM apx400  
PROBHD 5 mm BBO BB-  
PULPROG zgdc30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 2  
SWH 25062.656 Hz  
FIDRES 0.382426 Hz  
AQ 1.3074932 sec  
RG 5792.6  
RW 19.950 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000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

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

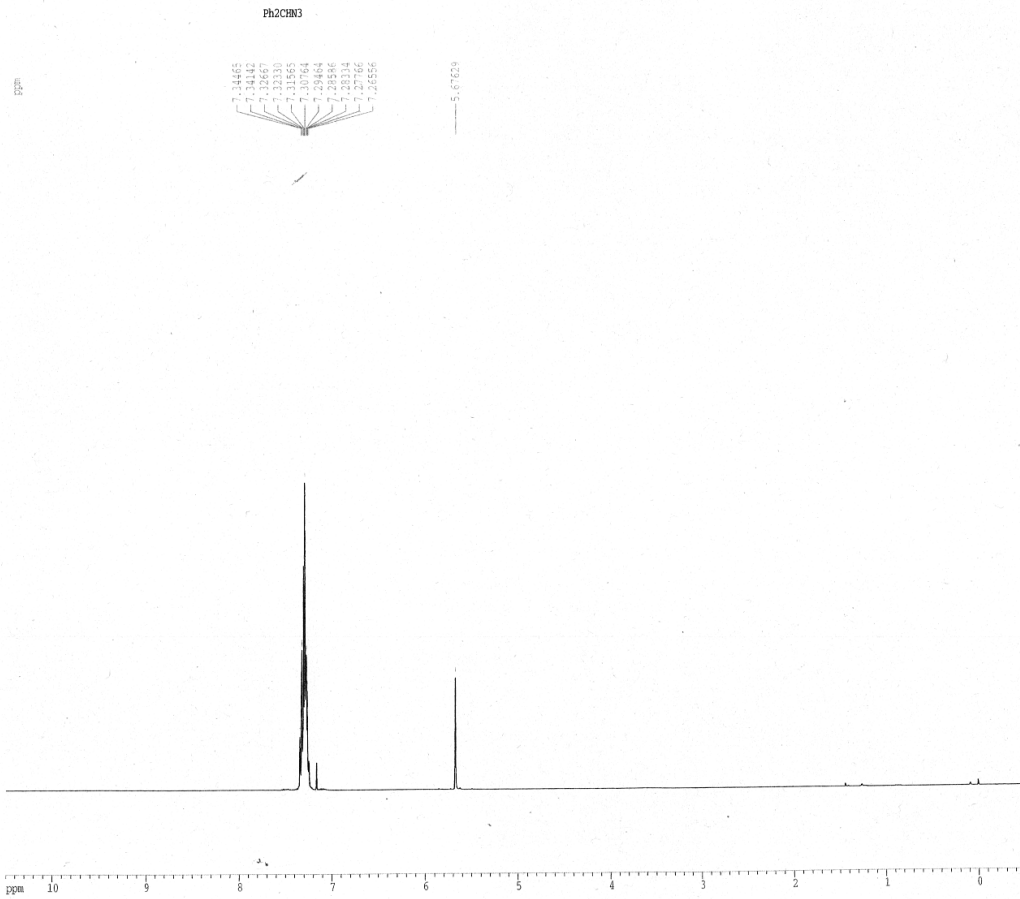
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 9.00 dB  
SFO2 400.1316005 MHz

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



```

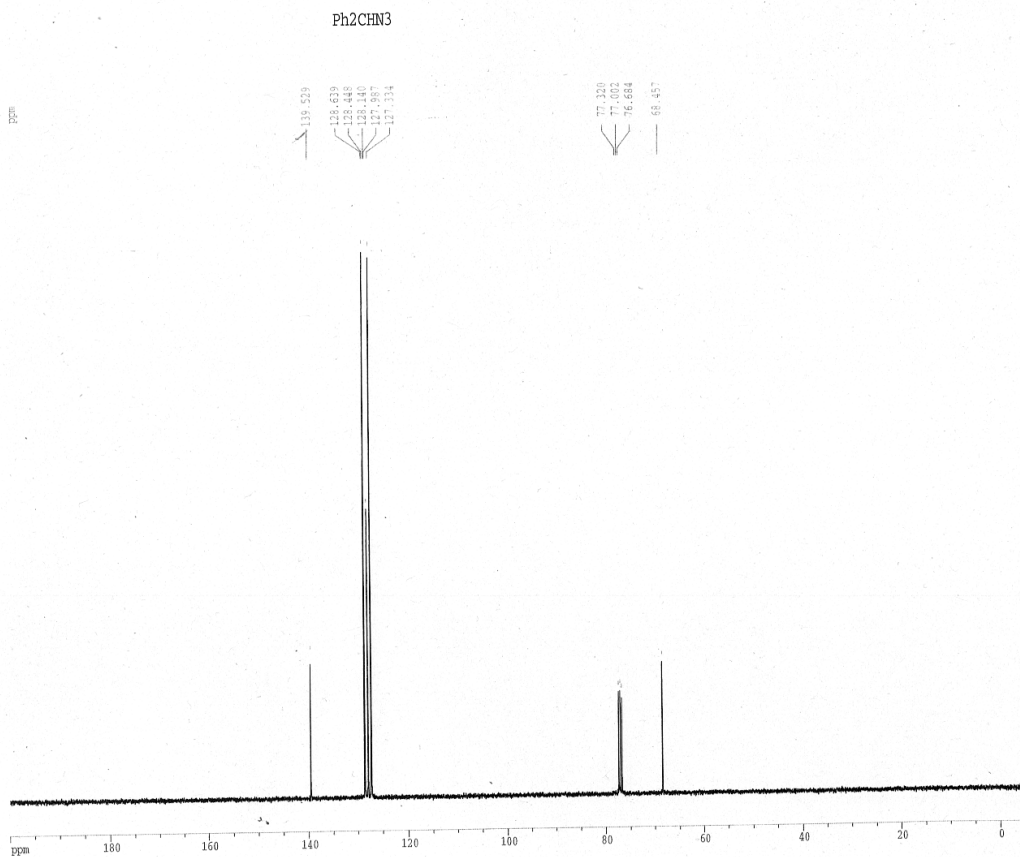
Current Data Parameters
NAME      09kato
EXPNO    395
PROCNO   1

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        3.9715116 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        -300.07 Hz
PPHMCN   0.36667 ppm/cm
HZCM      146.71434 Hz/cm
  
```



```

Current Data Parameters
NAME      09kato
EXPNO    396
PROCNO   1

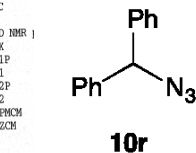
F2 - Acquisition Parameters
Date_    20131122
Time     21.23
INSTRUM  dxp400
PROBHD   5 mm BBO BB-
PULPROG  zgdc30
TD        65536
SOLVENT  CDCl3
NS        84
DS        2
SWH       25062.656 Hz
FIDRES   0.382426 Hz
AQ        1.3074932 sec
RG        4597.6
DM        19.950 usec
DE        6.00 usec
TE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

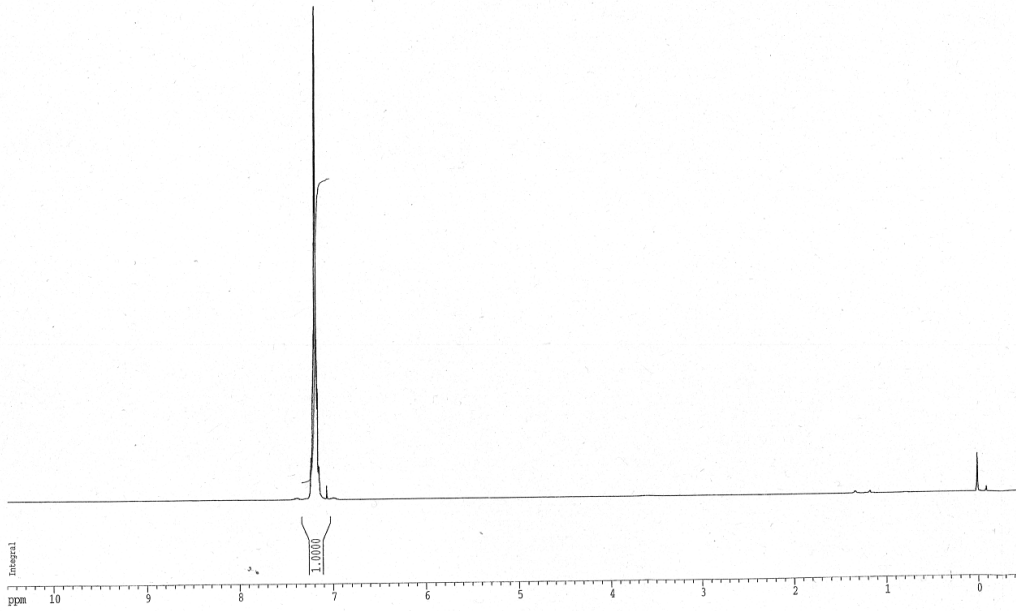
===== CHANNEL f1 =====
NUC1      13C
P1        12.00 usec
PL1       -6.00 dB
SFO1     100.6237959 MHz

===== 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        -300.07 Hz
PPHMCN   0.36667 ppm/cm
HZCM      146.71434 Hz/cm
  
```





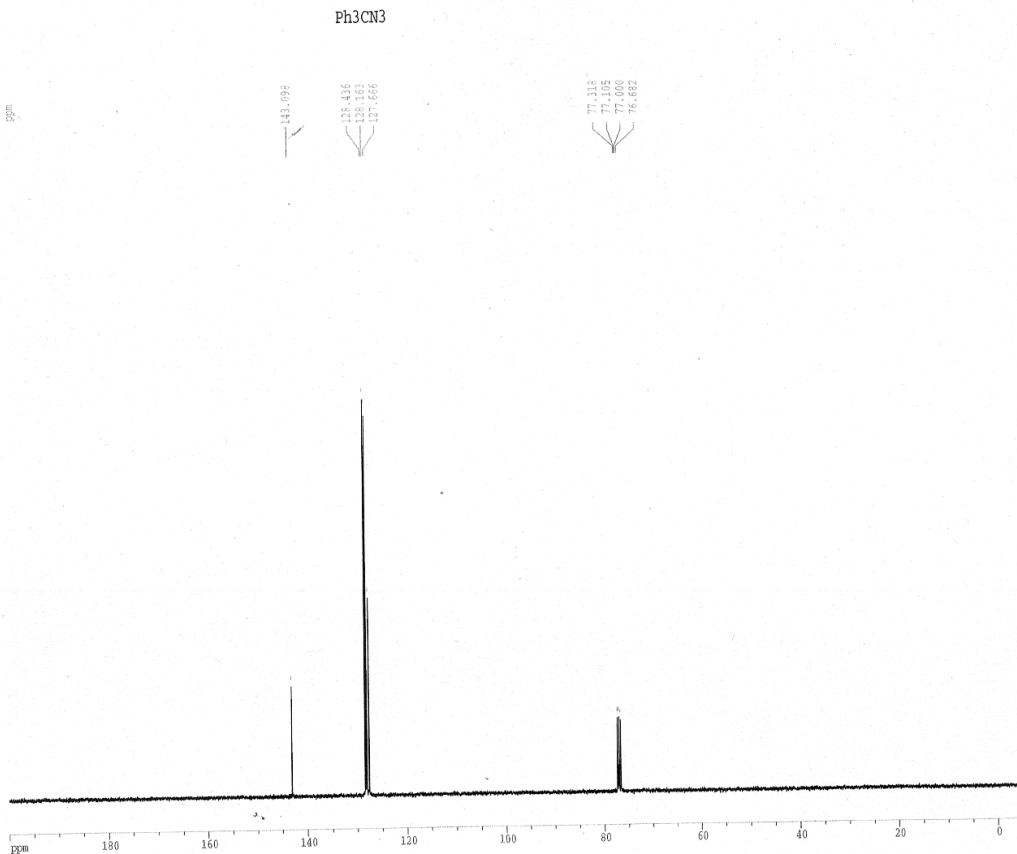
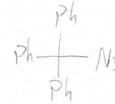
Current Data Parameters  
 NAME 09kato  
 EXPNO 866  
 PROCNO 1

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 8150.825 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  
 WDW EM  
 SSB 0  
 LB 0.10 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 -200.00 Hz  
 FWHM 0.36667 ppm/cm  
 HZCM 166.71437 Hz/cm



Current Data Parameters  
 NAME 09kato  
 EXPNO 398  
 PROCNO 1

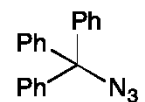
F2 - Acquisition Parameters  
 Date\_ 20131122  
 Time 21.33  
 INSTRUM dpx400  
 PROBRD 5 mm BBO BB-  
 PULPROG zgdc30  
 TD 65536  
 SOLVENT CDCl3  
 NS 57  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 9195.2  
 DW 19.950 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.0000000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

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

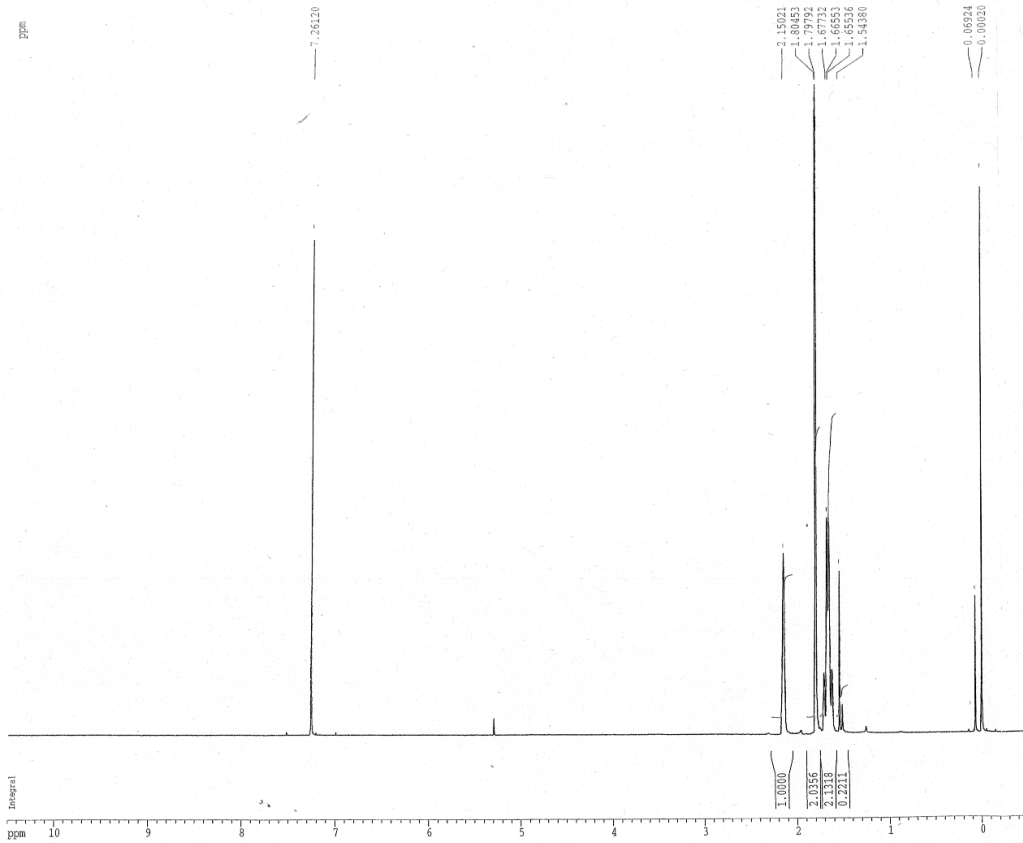
===== CHANNEL f2 =====  
 CHDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -6.00 dB  
 PL12 11.00 dB  
 SFO2 400.1316005 MHz

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

1D NMR plot  
 CX  
 F1P  
 F1  
 F2P  
 F2  
 FWHM  
 HZCM



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

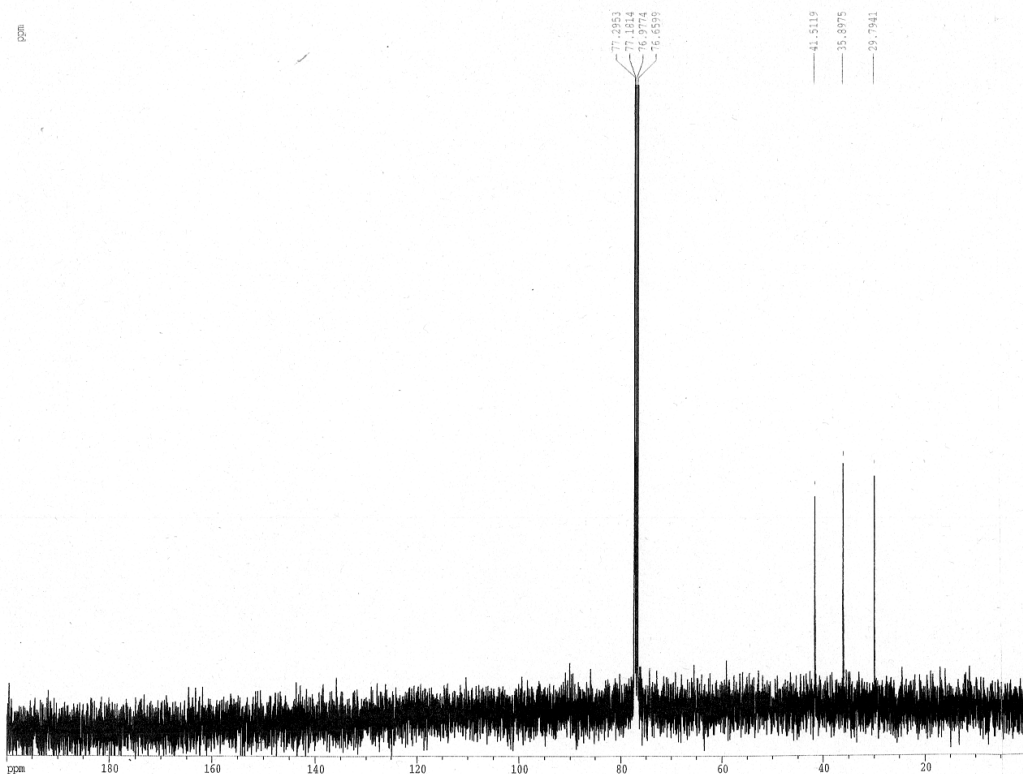
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -6.00 dB  
 SFO1 400.1324710 MHz

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 0.36657 ppm/cm  
 HZCM 146.71434 Hz/cm



354-1 adamantane



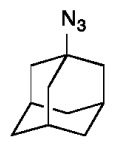
Current Data Parameters  
 NAME 09yano  
 EXPRO 887  
 PROCNO 1

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

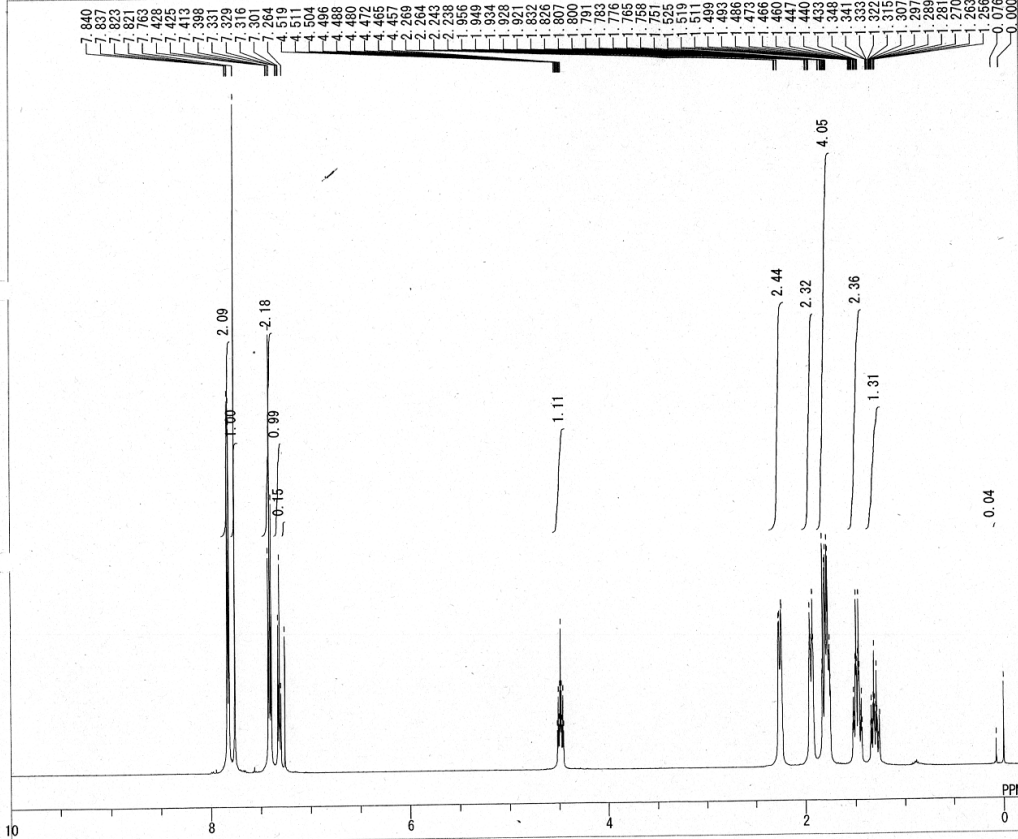
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -6.00 dB  
 PL12 9.00 dB  
 SFO2 400.1316005 MHz

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

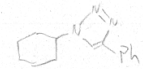


10t

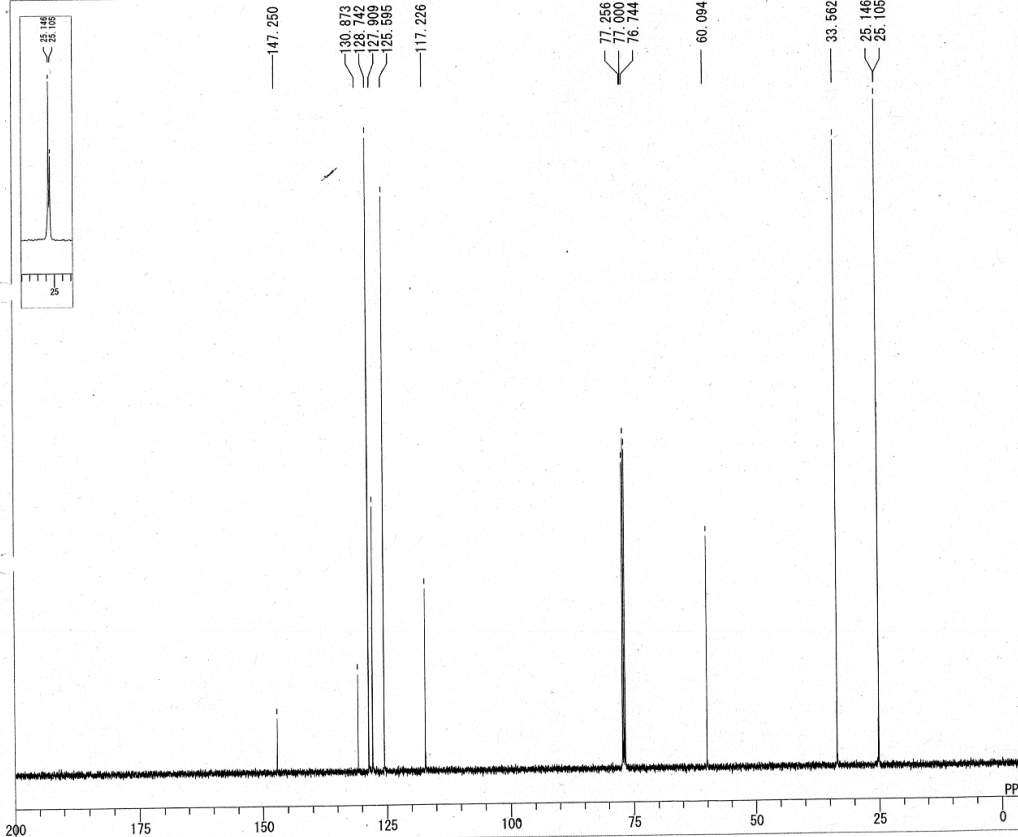
C:\NMRdata\00kunisue\9katoH-triazole\_H2ft.als  
9katoH-triazole\_H



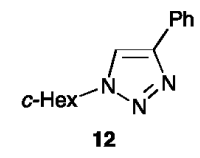
|       |                                            |
|-------|--------------------------------------------|
| MENUP | SINGL 1H                                   |
| OBNUC | 1H                                         |
| OBFRQ | 500.00 MHz                                 |
| OBFIN | 162410.00 Hz                               |
| PW1   | 6.50 usec                                  |
| DEADT | 56.75 usec                                 |
| PREDL | 0.20000 msec                               |
| INWIT | 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                                        |
| DFILE | C:\NMRdata\00kunisue\9katoH-triazole_H2ft. |
| SHMFL | TH5AT_4cm29katoH-triazole_H                |
| CTEMP | 25.0 c                                     |
| LKFIN | 70334.0 Hz                                 |
| LKLEV | 200                                        |
| LGAIN | 22                                         |
| LKPHS | 135                                        |
| LKSIG | 967                                        |
| CSPED | 14 Hz                                      |
| FILDC |                                            |
| FILDF |                                            |



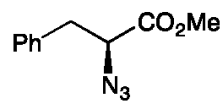
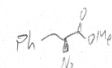
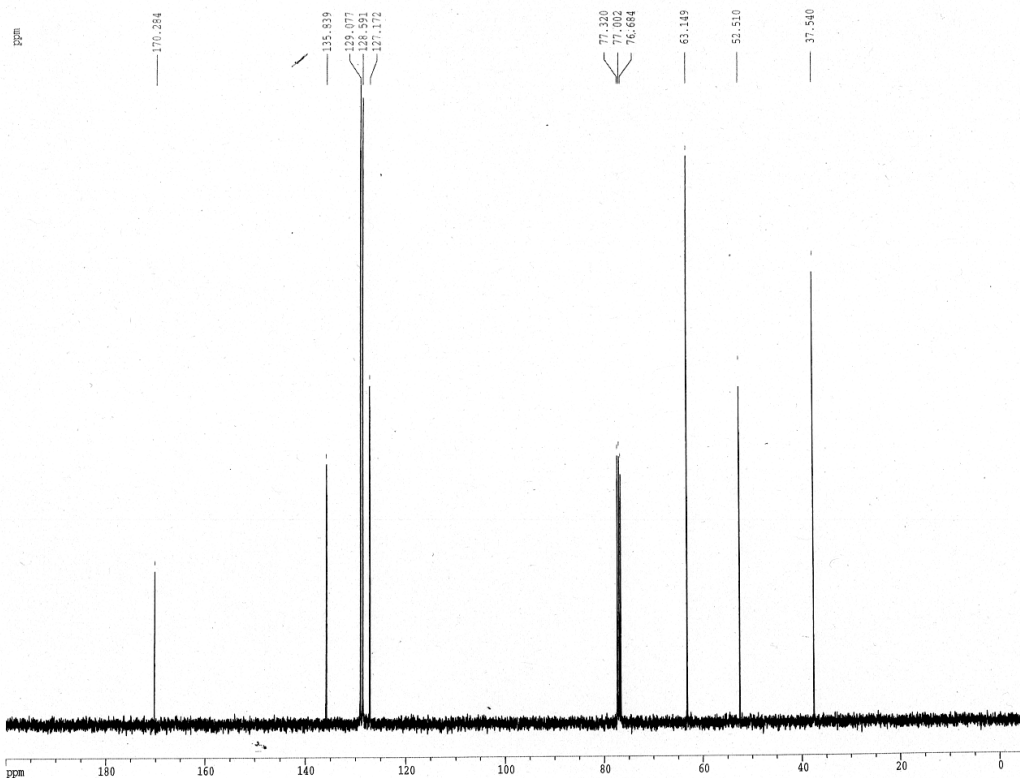
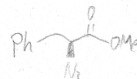
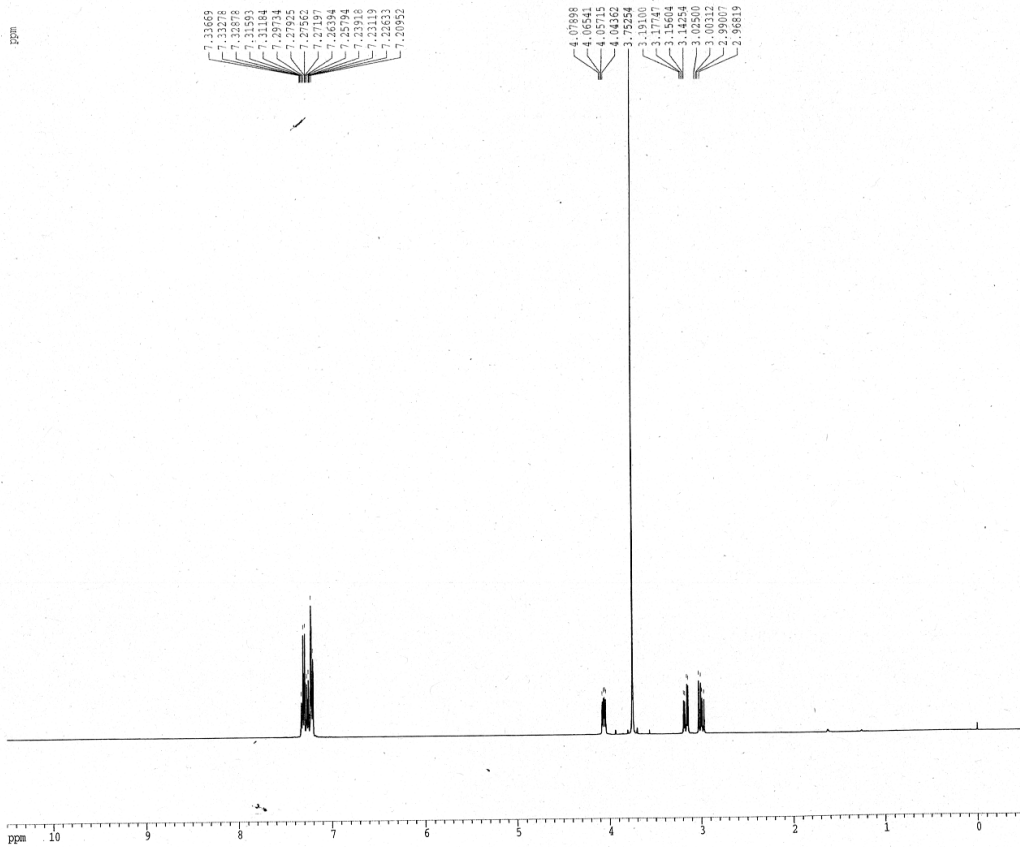
C:\NMRdata\00kunisue\9katoH-triazole\_C.als  
9katoH-triazole\_C



|       |                                            |
|-------|--------------------------------------------|
| MENUP | SINGL 13C                                  |
| OBNUC | 13C                                        |
| OBFRQ | 125.65 MHz                                 |
| OBFIN | 127958.00 Hz                               |
| PW1   | 4.50 usec                                  |
| DEADT | 15.93 usec                                 |
| PREDL | 0.20000 msec                               |
| INWIT | 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 | 500.00 MHz                                 |
| IRFIN | 162410.00 Hz                               |
| IRRPW | 50 usec                                    |
| IRATN | 511                                        |
| DFILE | C:\NMRdata\00kunisue\9katoH-triazole_C.als |
| SHMFL | TH5AT_4cm29katoH-triazole_C                |
| CTEMP | 25.7 c                                     |
| LKFIN | 70334.0 Hz                                 |
| LKLEV | 200                                        |
| LGAIN | 22                                         |
| LKPHS | 135                                        |
| LKSIG | 967                                        |
| CSPED | 14 Hz                                      |
| FILDC |                                            |
| FILDF |                                            |

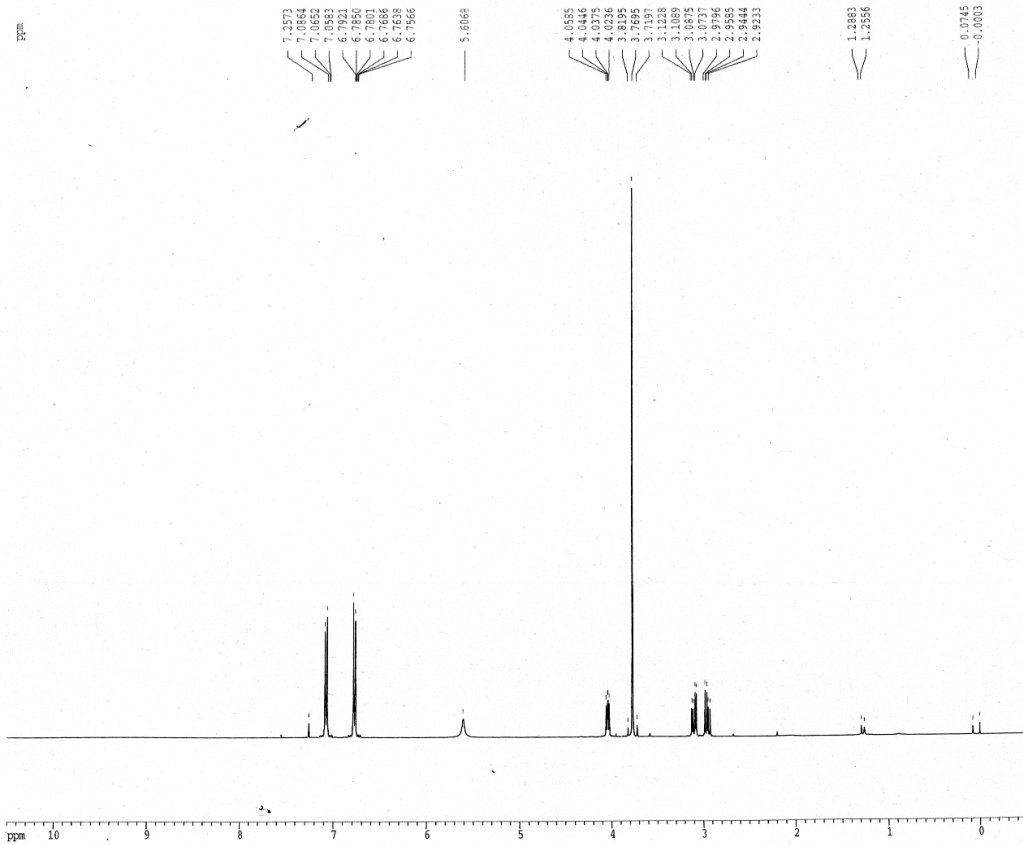


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14a





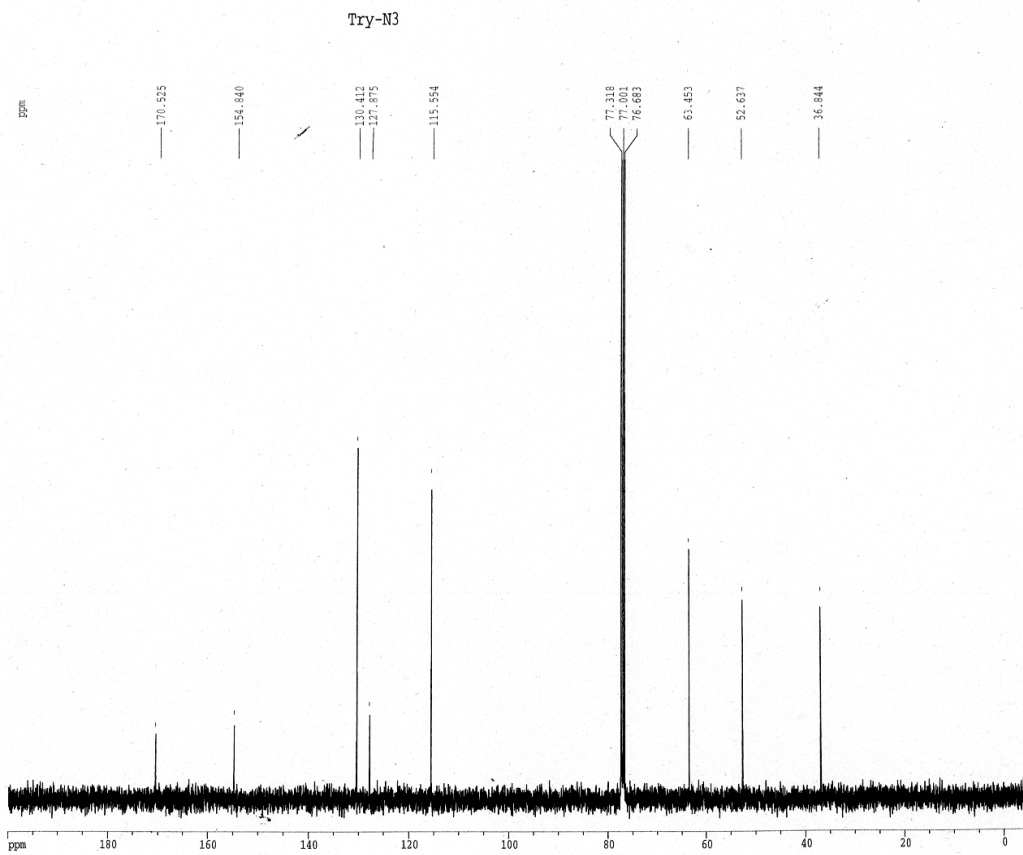
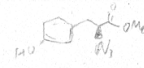
Current Data Parameters  
 NAME 09kato  
 EXPNO 404  
 PROCNO 1

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



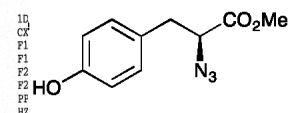
Current Data Parameters  
 NAME 09kato  
 EXPNO 391  
 PROCNO 1

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 0.0300000 sec

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

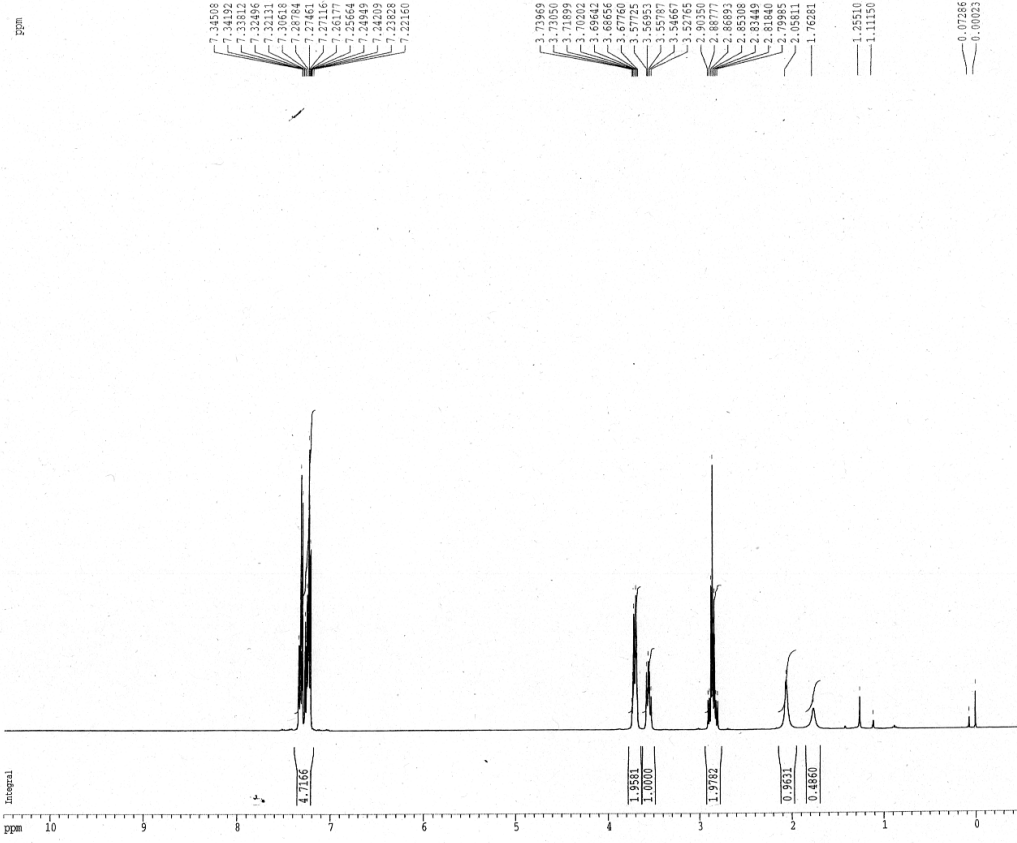
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 FREQ2 80.00 usec  
 PL2 -6.00 dB  
 PL12 11.00 dB  
 SFO2 400.1316005 MHz

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

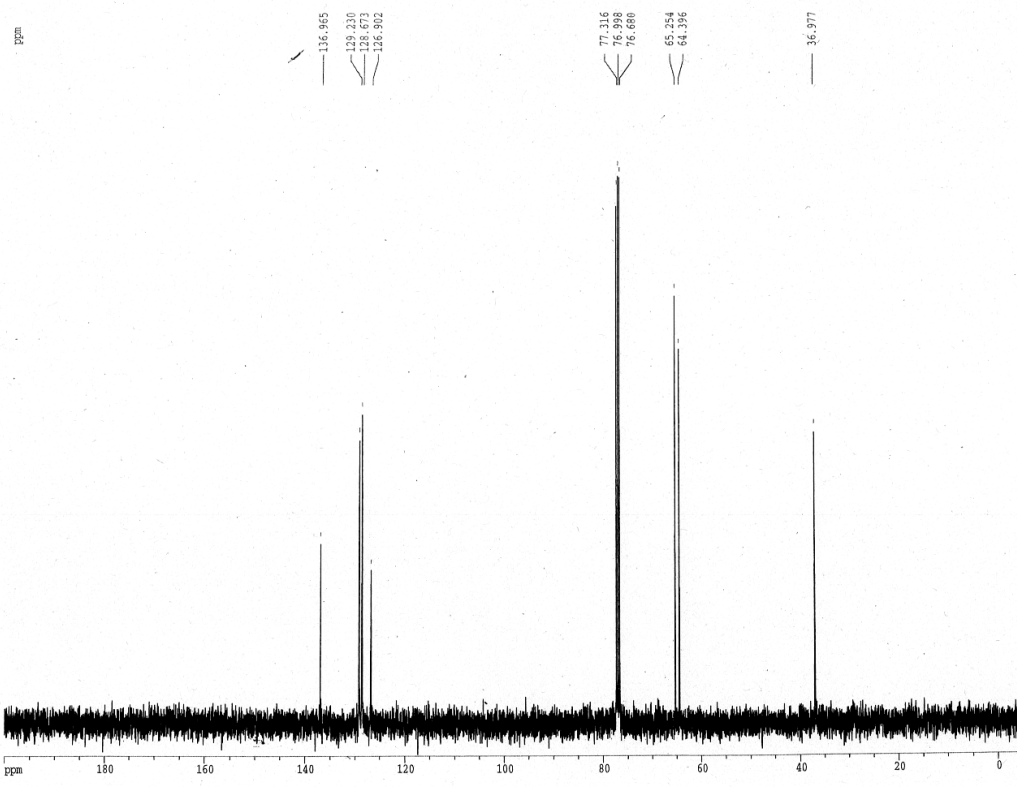
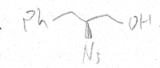


14b

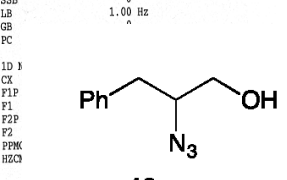
exp259\_P



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 3.9151316 sec  
 RG 64  
 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 400.1300140 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

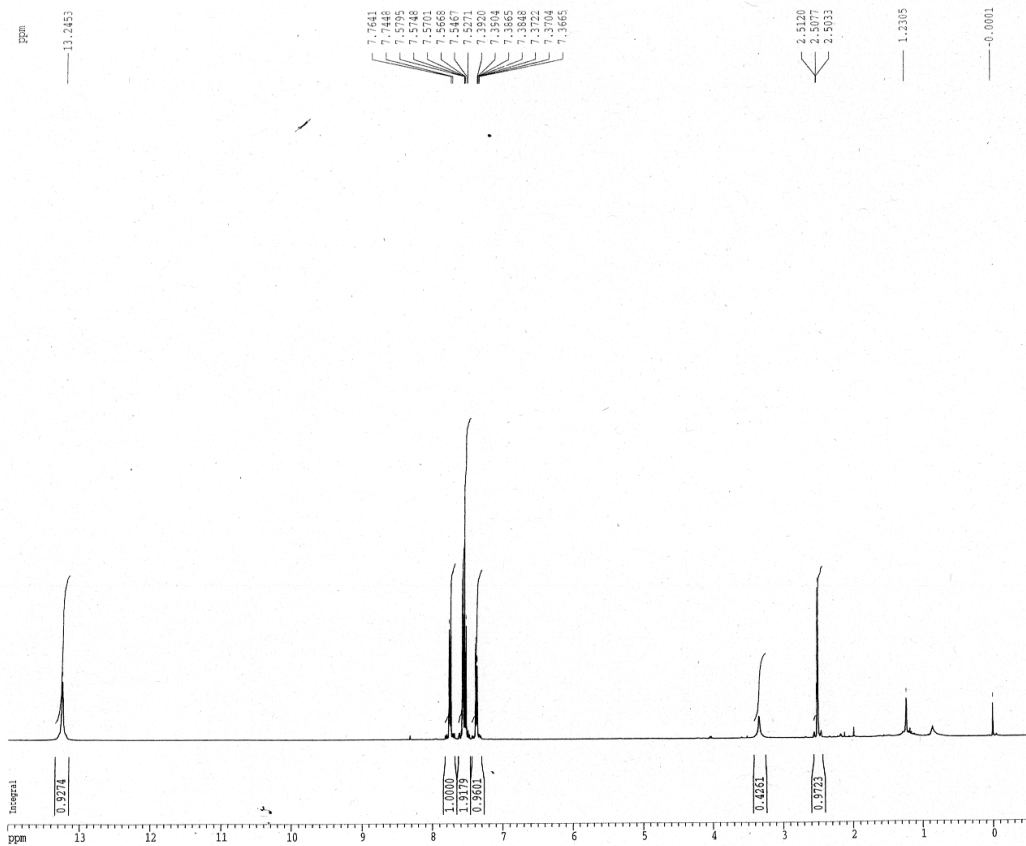


Current Data Parameters  
 NAME 09kato  
 EXPNO 374  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20131006  
 Time 0.51  
 INSTRUM dpx400  
 PROBHD 5 mm BBO BB-  
 PULPROG zgdc30  
 TD 65536  
 SOLVENT ccd13  
 NS 100  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 13004  
 DM 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



16

azide-acid

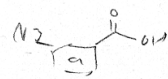


Current Data Parameters  
 NAME 09kato  
 EXPNO 430  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20140122  
 Time 1.33  
 INSTRUM dpx400  
 PROBHD 5 mm BBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8250.825 Hz  
 FIDRES 0.125898 Hz  
 AQ 3.5715216 sec  
 RG 256 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

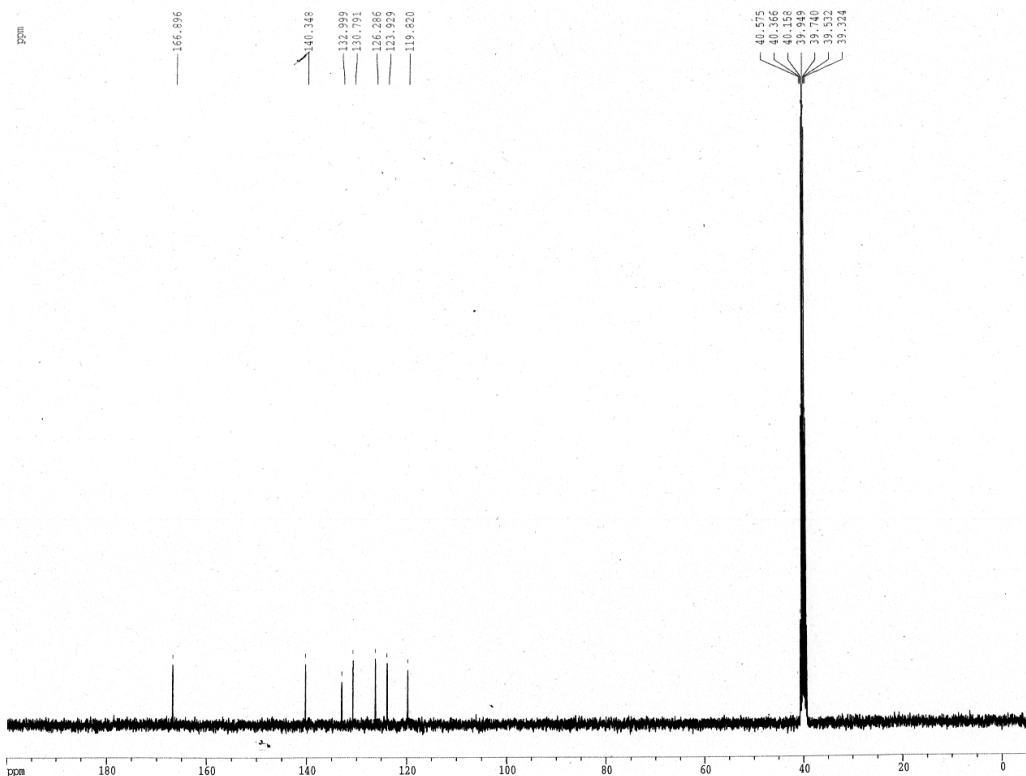
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 P1 12.00 usec  
 PL1 -6.00 dB  
 SFO1 400.1324710 MHz

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 5601.80 Hz  
 F2P -0.500 ppm  
 F2 -200.07 Hz  
 FREQM 0.48133 ppm/cm  
 HZCM 193.39618 Hz/cm



azide-acid



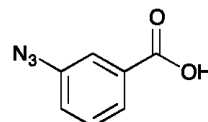
Current Data Parameters  
 NAME 09kato  
 EXPNO 431  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20140122  
 Time 1.42  
 INSTRUM dpx400  
 PROBHD 5 mm BBO BB-  
 PULPROG zgdc30  
 TD 65536  
 SOLVENT DMSO  
 NS 143  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 11585.2  
 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

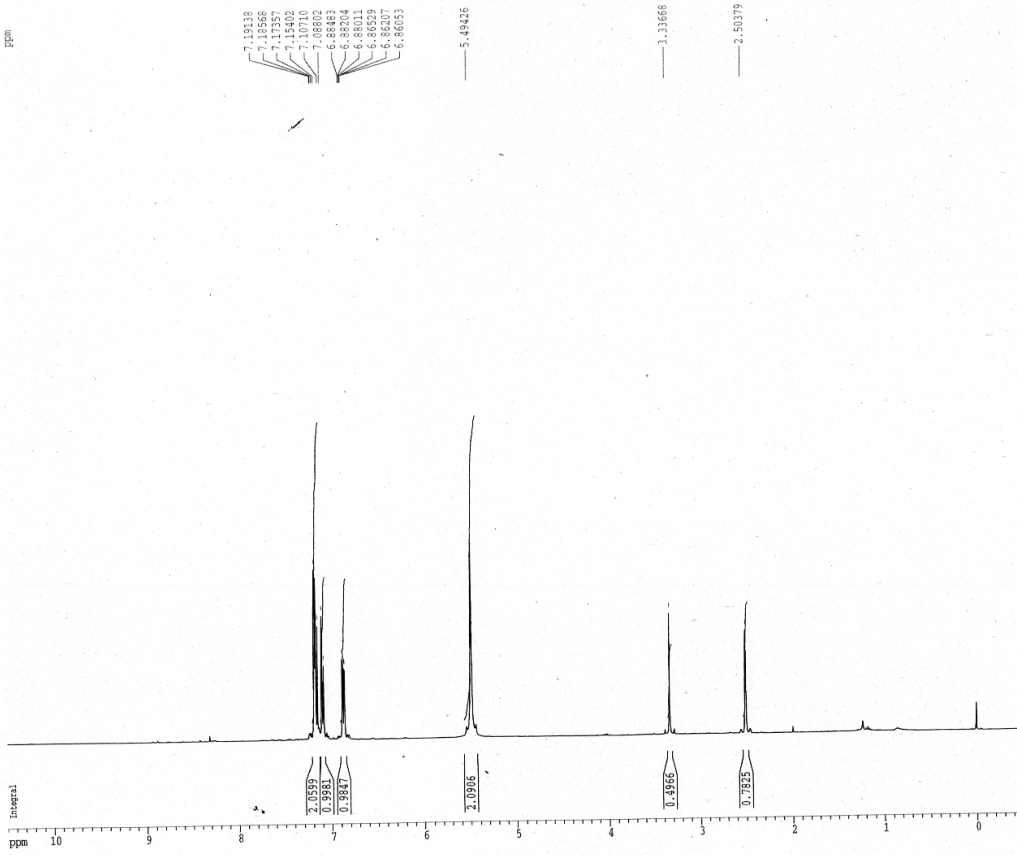
F2 - Processing parameters  
 SI 32768  
 SF 100.6127272 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

1D NMR  
 CX  
 F1P  
 F1  
 F2P  
 F2  
 FREQM  
 HZCM



18

amine\_acid\_azide



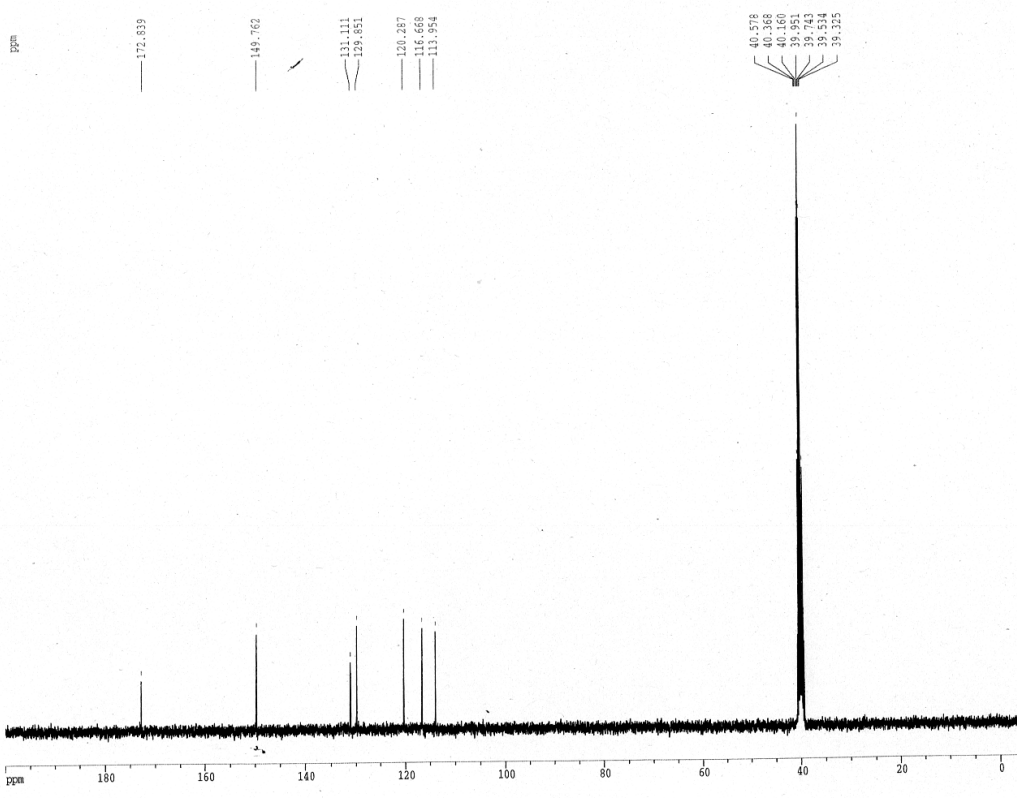
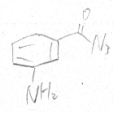
Current Data Parameters  
 NAME 09kato  
 EXPNO 429  
 PROCNO 1

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 16  
 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

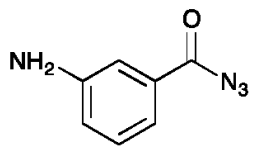
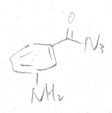
F2 - Acquisition Parameters  
 Date\_ 20140109  
 Time 20.34  
 INSTRUM dpx400  
 PROBRD 5 mm BBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 150  
 DS 2  
 SWH 25062.656 Hz  
 FIDRES 0.382426 Hz  
 AQ 1.3074932 sec  
 RG 9195.2  
 DW 19.950 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000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

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

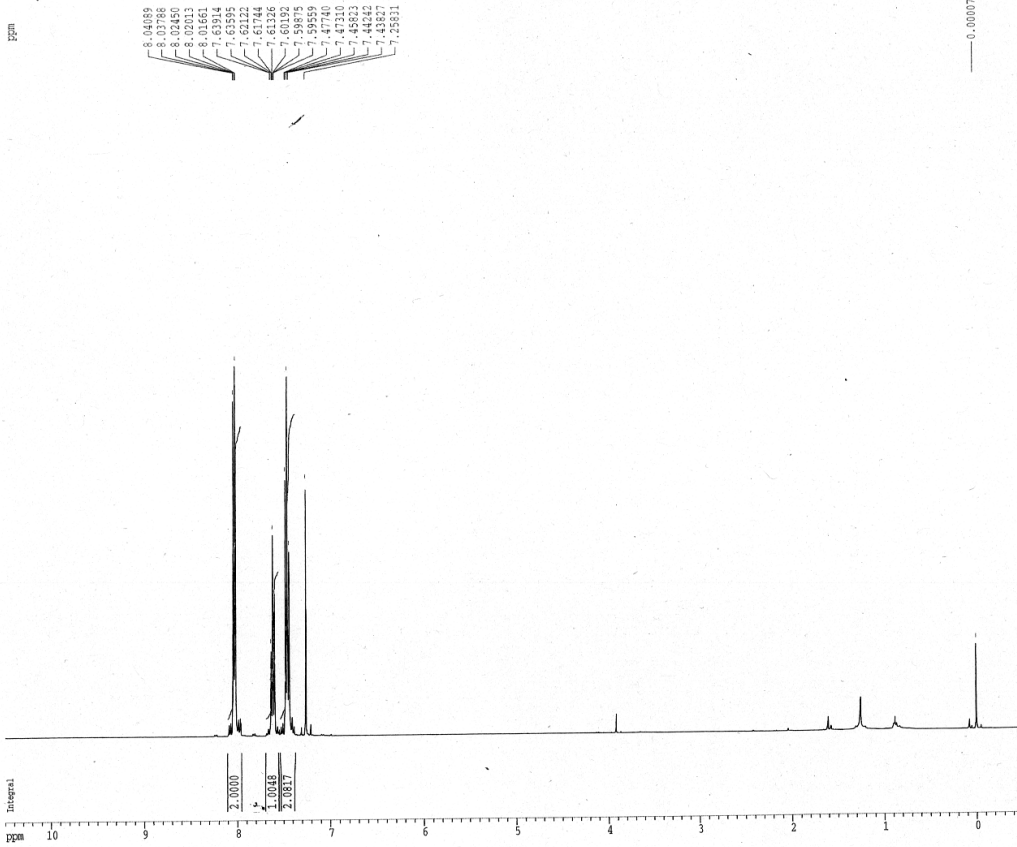
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NU2 1H  
 PCPD2 80.00 usec  
 PL2 -6.00 dB  
 PL12 11.00 dB  
 SFO2 400.1316005 MHz

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

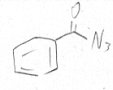


Current Data Parameters  
 NAME 09kato  
 EXPNO 432  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20140123  
 Time 19.15  
 INSTRUM dpx400  
 PROBRD 5 mm BBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8250.825 Hz  
 FIDRES 0.123898 Hz  
 AQ 3.9715316 sec  
 RG 128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

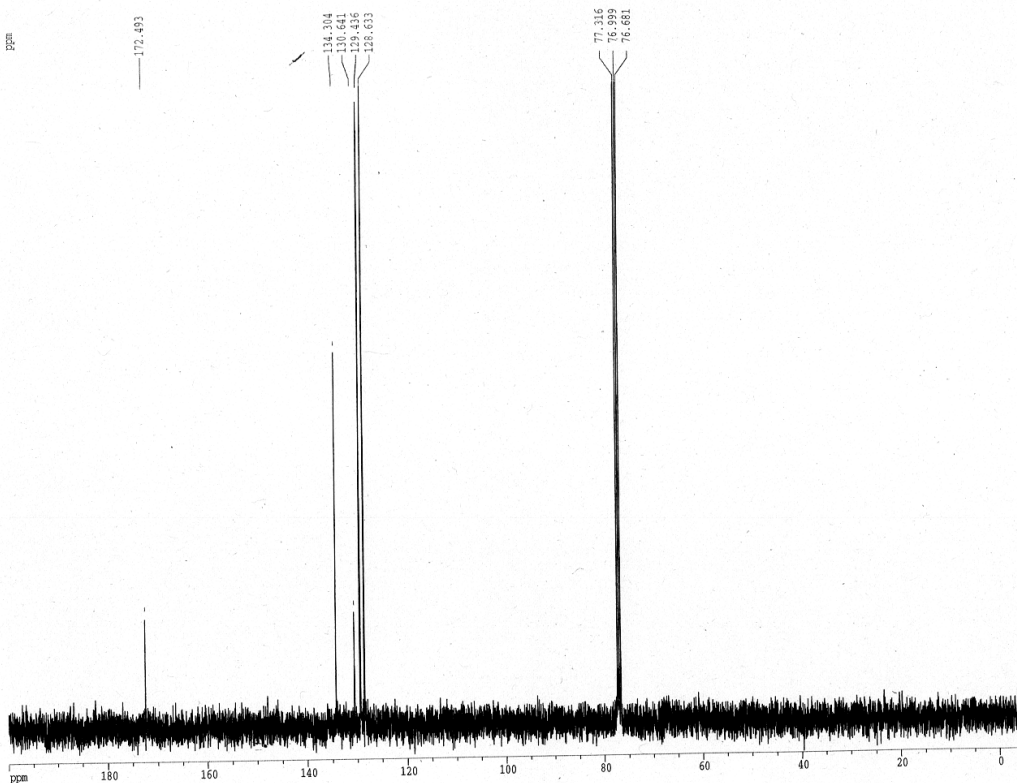
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -6.00 dB  
 SFO1 400.1324710 MHz

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  
 FIP 10.500 ppm  
 F1 4201.37 Hz  
 F2 -8.500 ppm  
 P2 -200.07 Hz  
 PRMCM 0.36667 ppm/cm  
 RZCM 146.71434 Hz/cm



benzoic azido



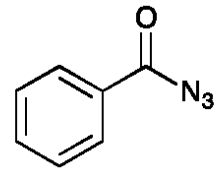
Current Data Parameters  
 NAME 09kato  
 EXPNO 433  
 PROCNO 1

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

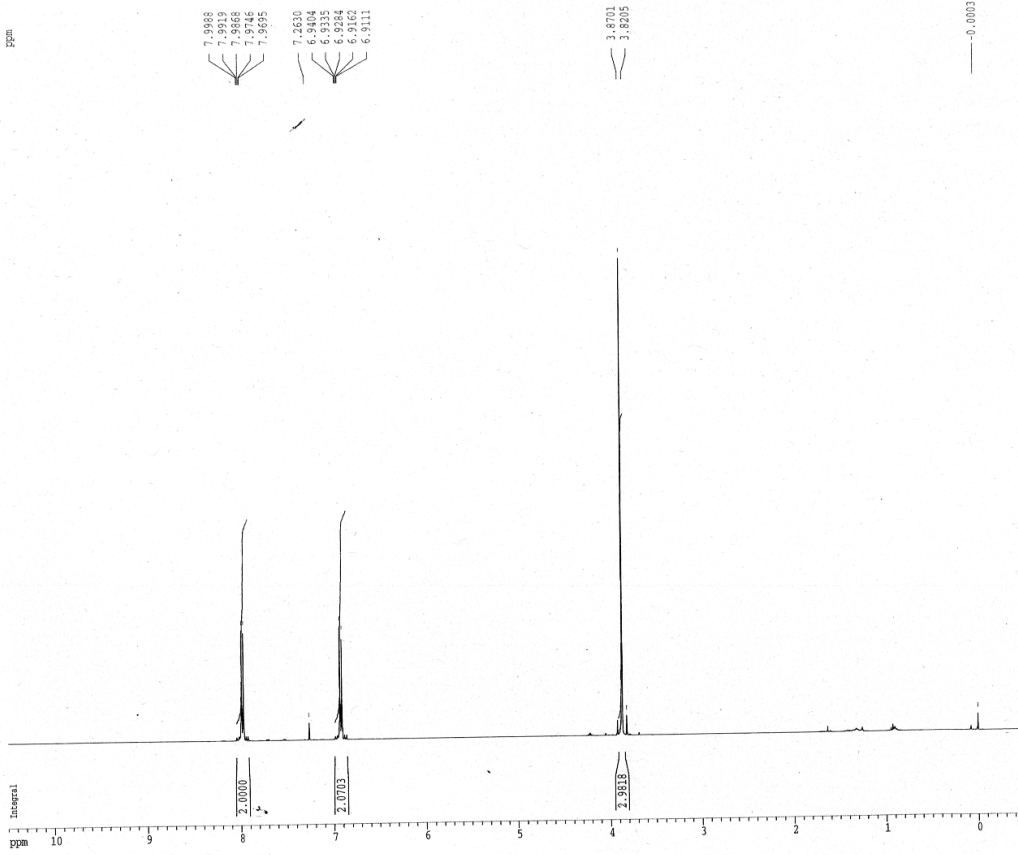
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.00 usec  
 PL1 -6.00 dB  
 SFO1 100.6237959 MHz

===== 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 1.40



4-Meobenzoic azido



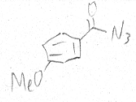
Current Data Parameters  
 NAME 09kato  
 EXPNO 434  
 PROCNO 1

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

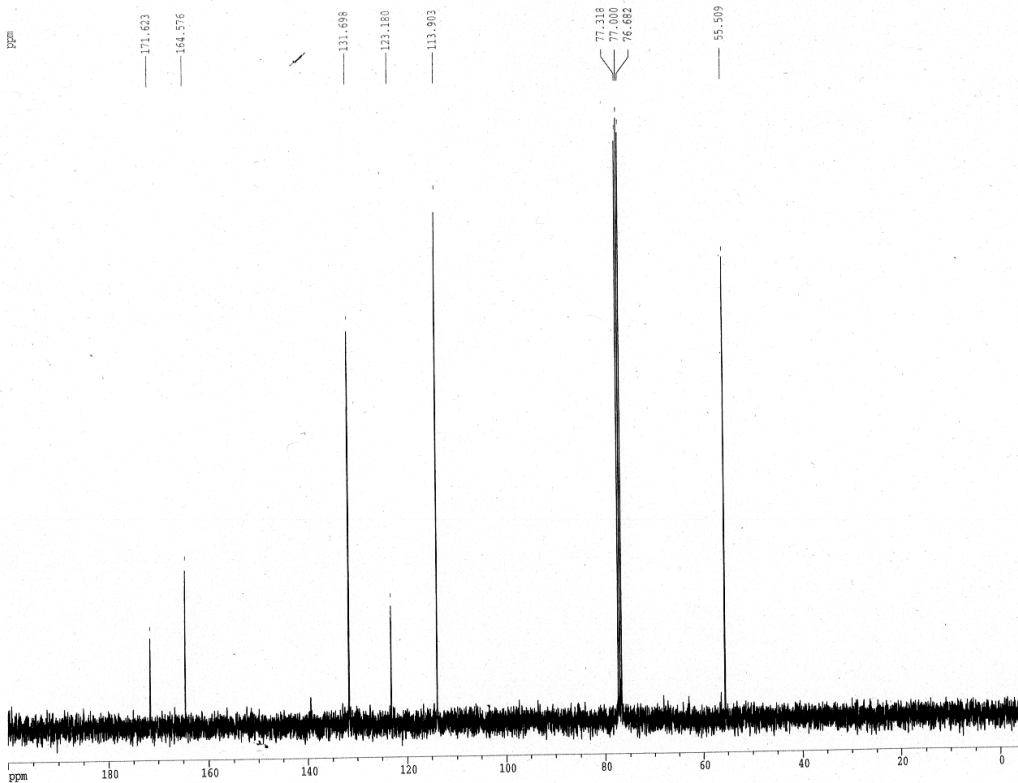
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -6.00 dB  
 SFO1 400.1324710 MHz

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 -6.500 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

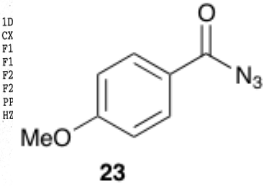


Table S1. Cartesian Coordinates of Computational Data for ADMP **5b** (Angstroms)

| 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 |