

# Supporting Information

## Lewis Acid Mediated Intramolecular C-C Bond Formation of Alkyne-Epoxide Leading to Six Membered Nitrogen and Oxygen Heterocycles

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Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039, India

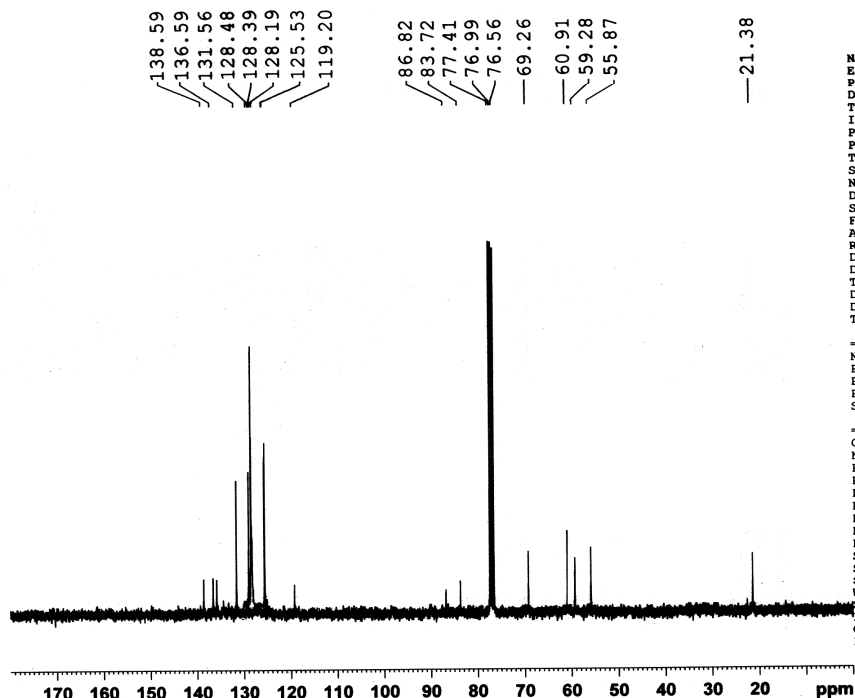
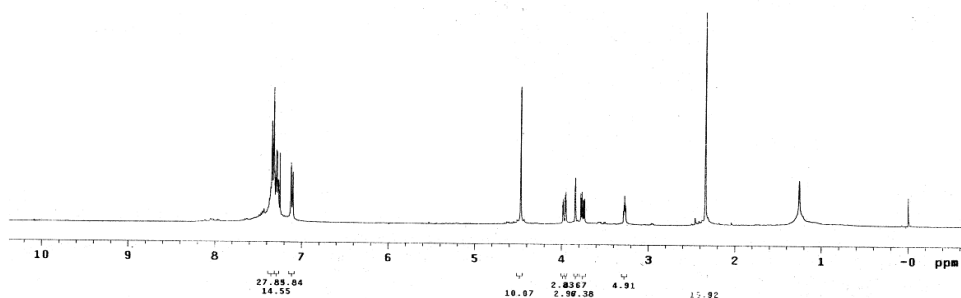
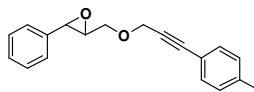
### Contents:

1.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1b-g**, **1i-q**, **2a-d**, **2f-g**, **2j-m**, **2o-q**, COSY and DEPT spectra of **2a-2b**, COSY, DEPT and HMQC of **2c**, DEPT and HMQC of **2d** **S2-S34**
2. Crystal parameters and ORTEP diagram of **2a** **S35-S36**

# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1b**

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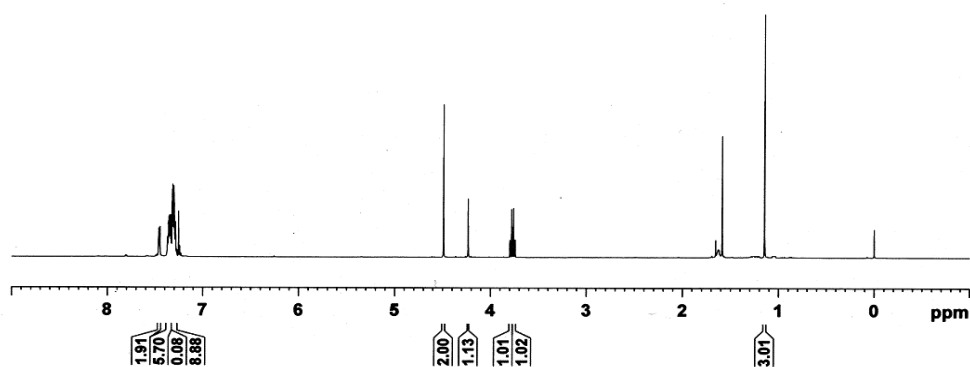
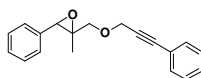
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SSB ( )  
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# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1c

aks-GP-111-26-1



**BRUKER**

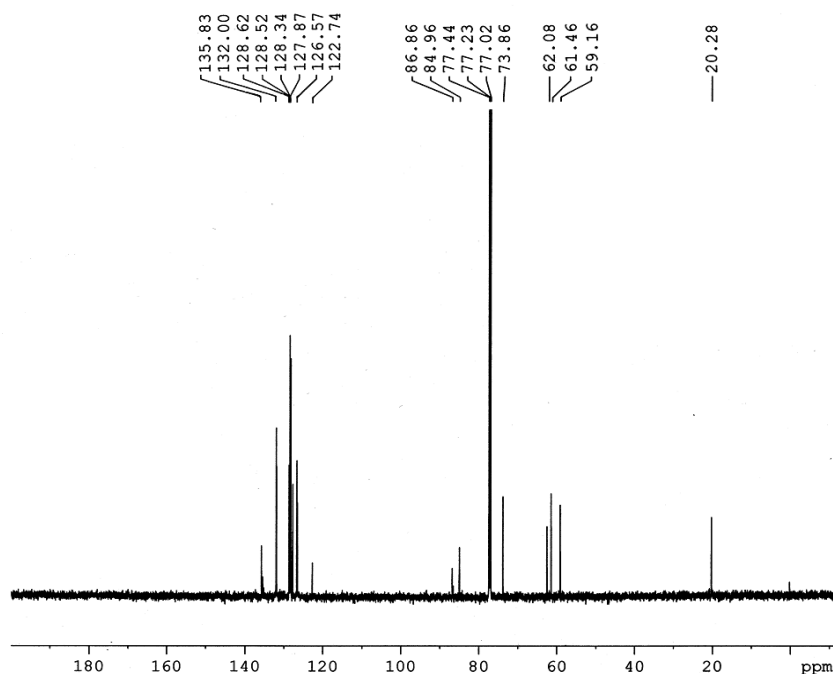
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aks-gp-111-26-13C



**BRUKER**

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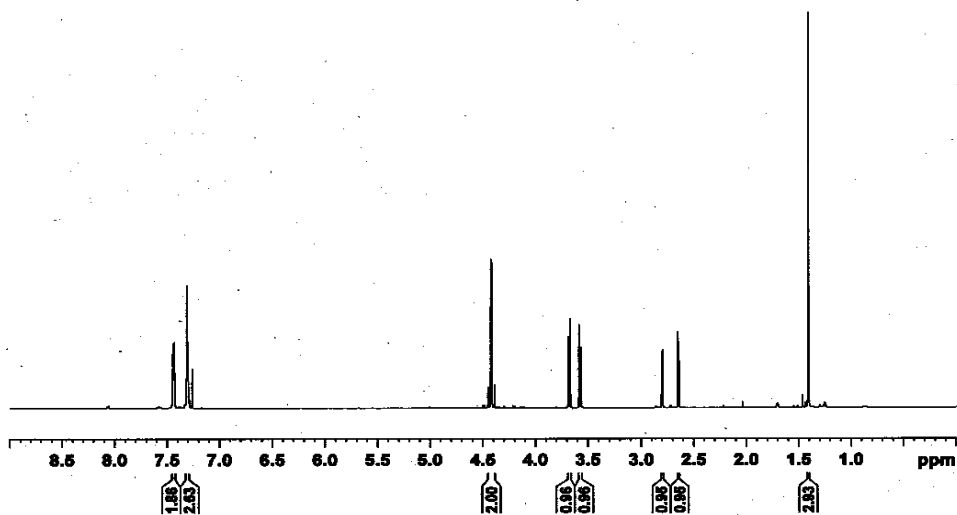
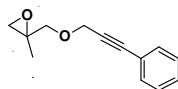
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# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1d

GP-111\_1H

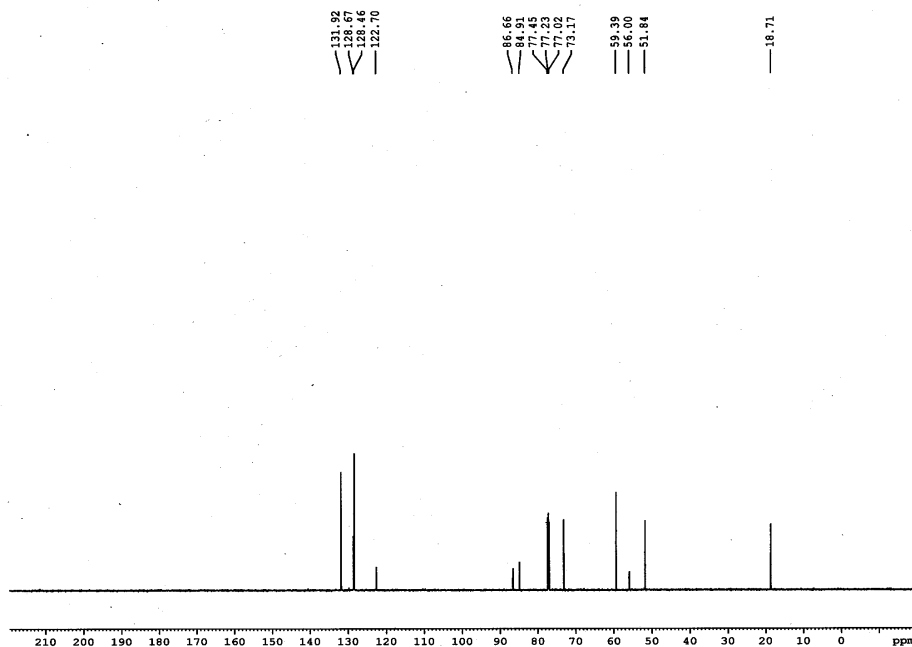


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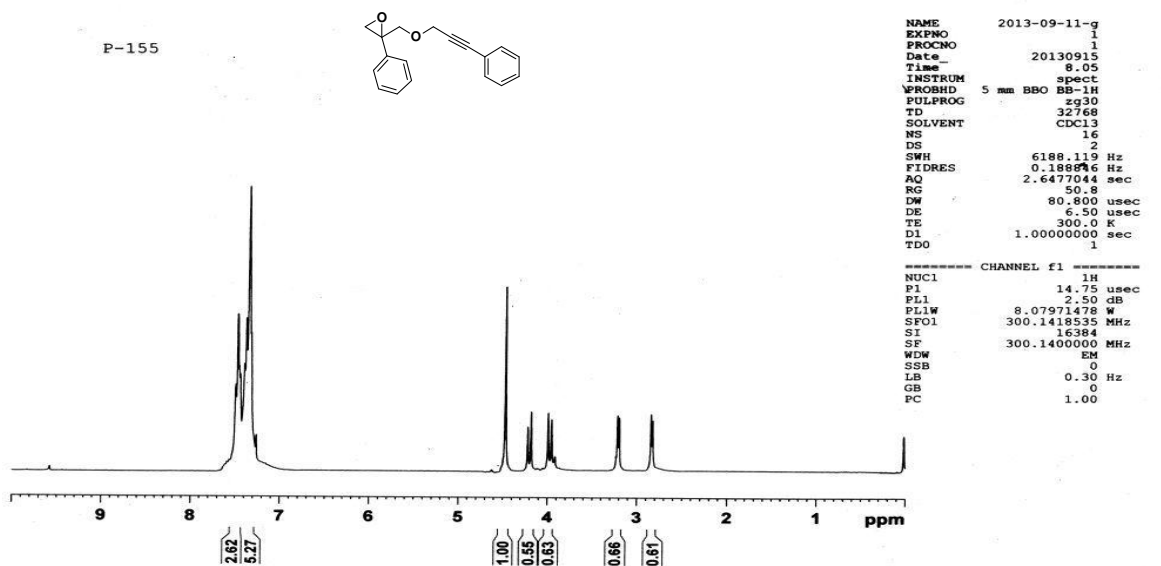
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AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
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TE 298.0 K  
D1 2.00000000 sec  
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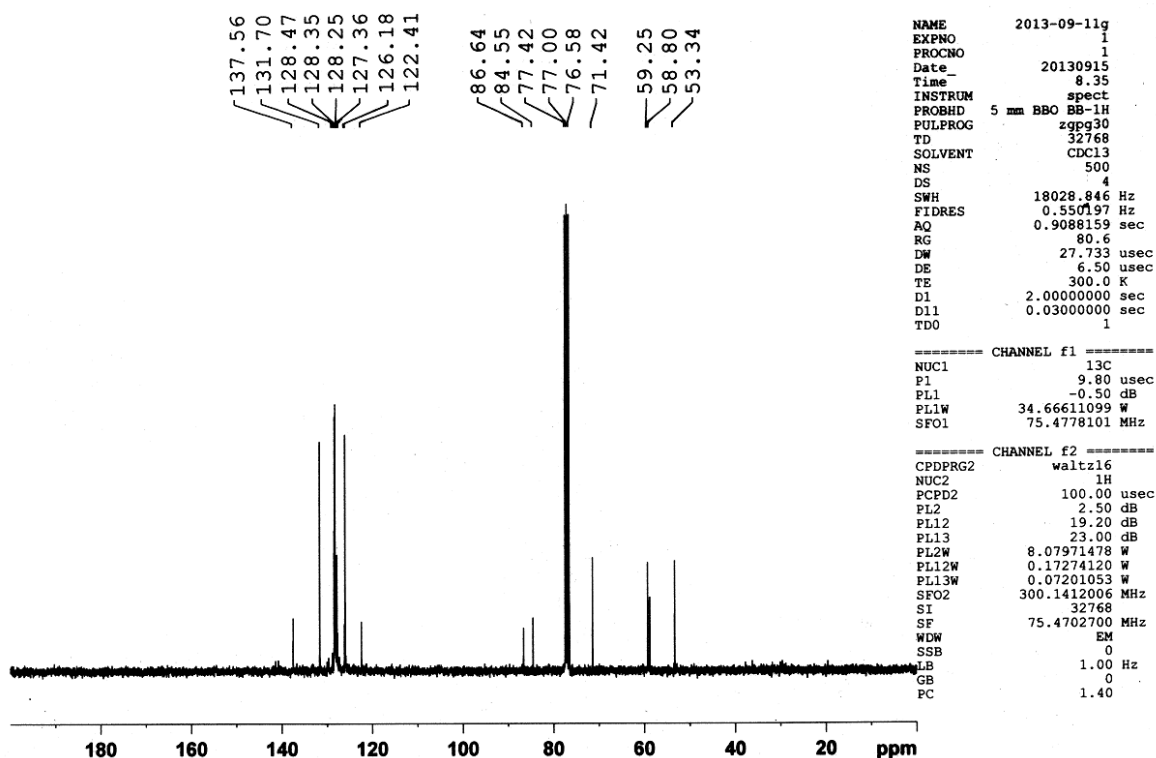
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PLW13 0.30239999 W

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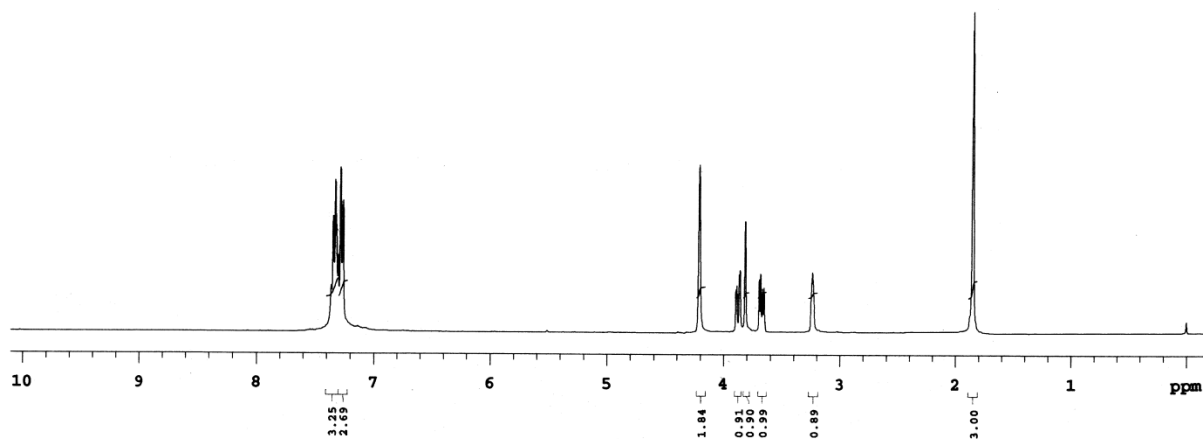
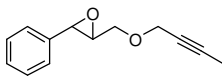
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **1e**



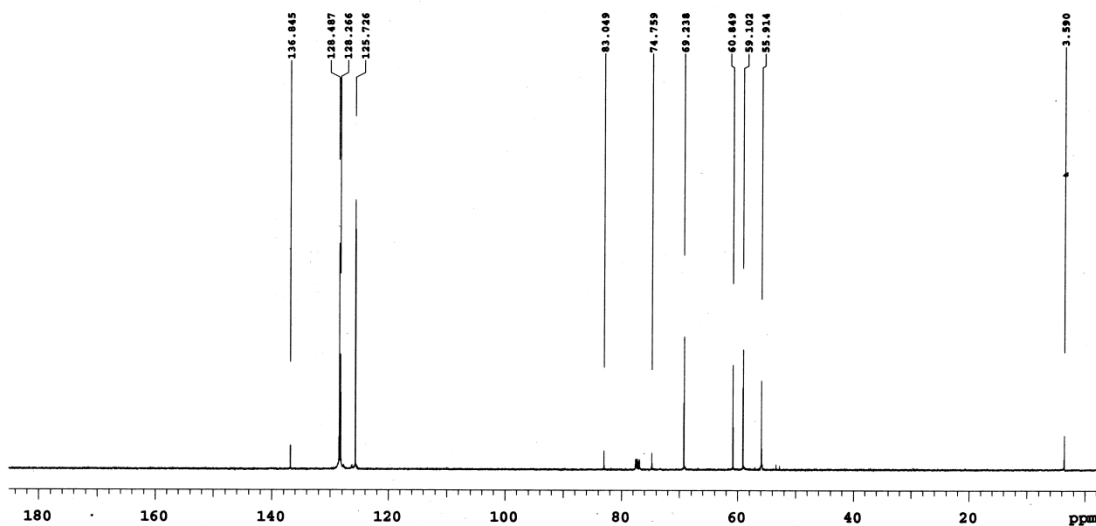
p-155



# <sup>1</sup>H and <sup>13</sup>C Spectra of compound **1f**

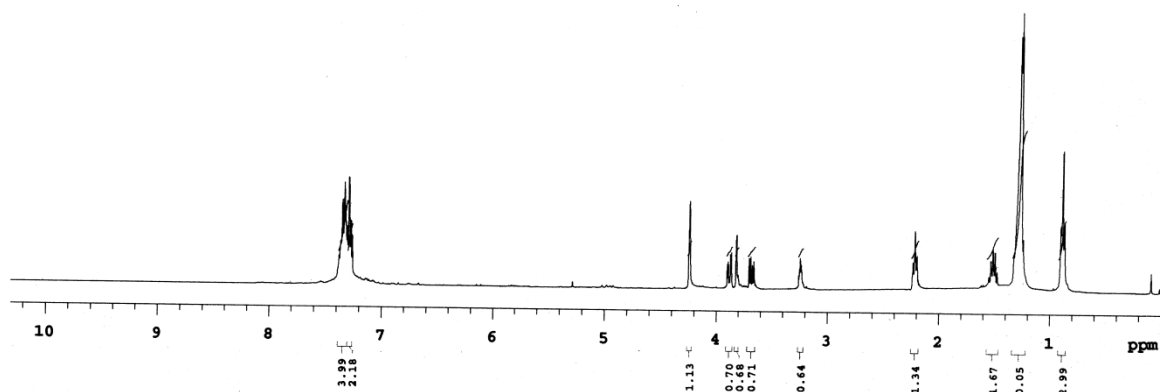
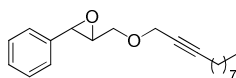


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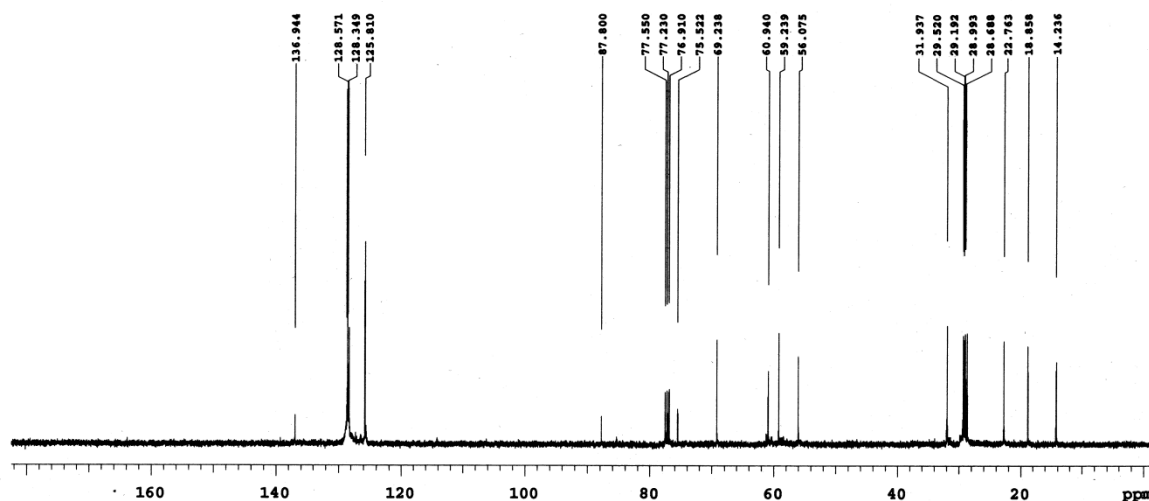


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 160 repetitions	<b>OBSERVE</b> C13, 100.5426062 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 6 minutes	<b>GP-AKS_Me_ipo_13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: GP-AKS_Me_ipo_13C Mercury-400 "IITG-INMR"
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$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **1g**



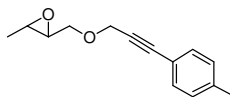
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# $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of compound **1i**

aks-gp-85-1H

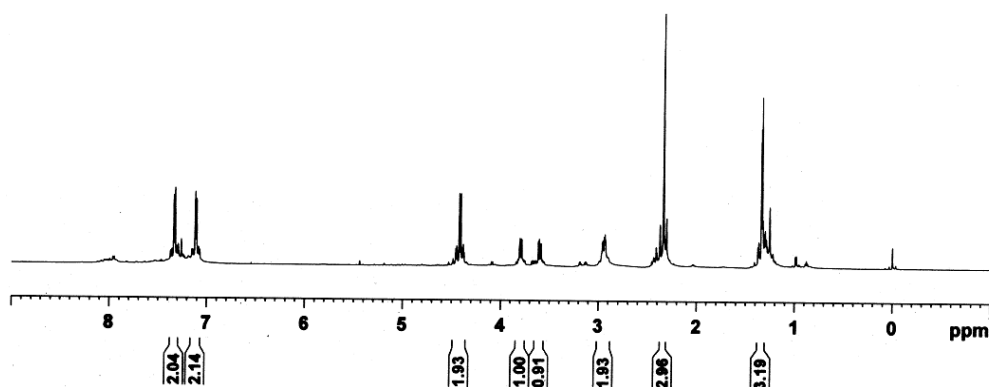


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RG 39.59  
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D1 1.00000000 sec  
TDO 1

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aks-gp-85-13C

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131.68  
128.06  
119.42  
86.75  
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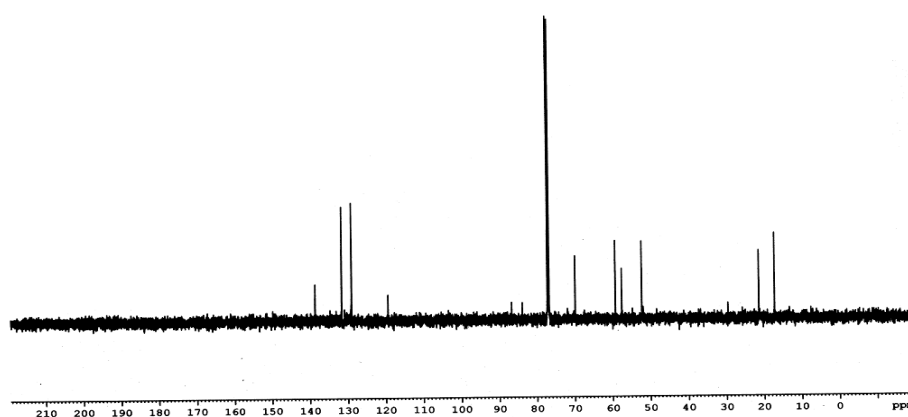
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RG 200.18  
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DE 6.50 usec  
TE 298.9 K  
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D11 0.03000000 sec  
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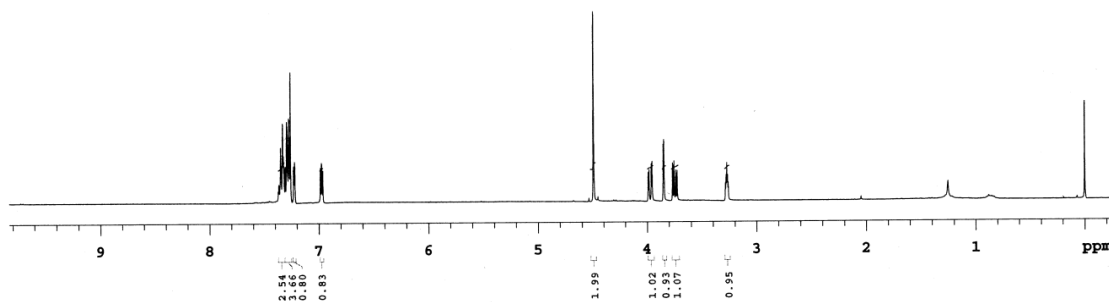
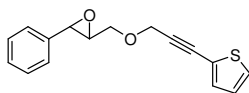
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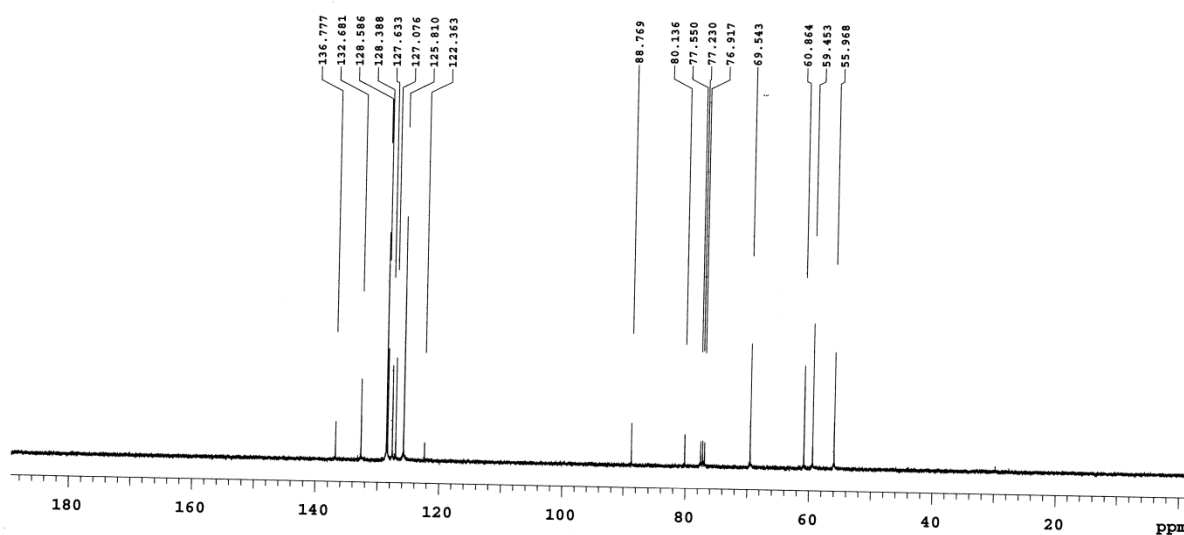




# <sup>1</sup>H and <sup>13</sup>C NMR Spectra of **1j**

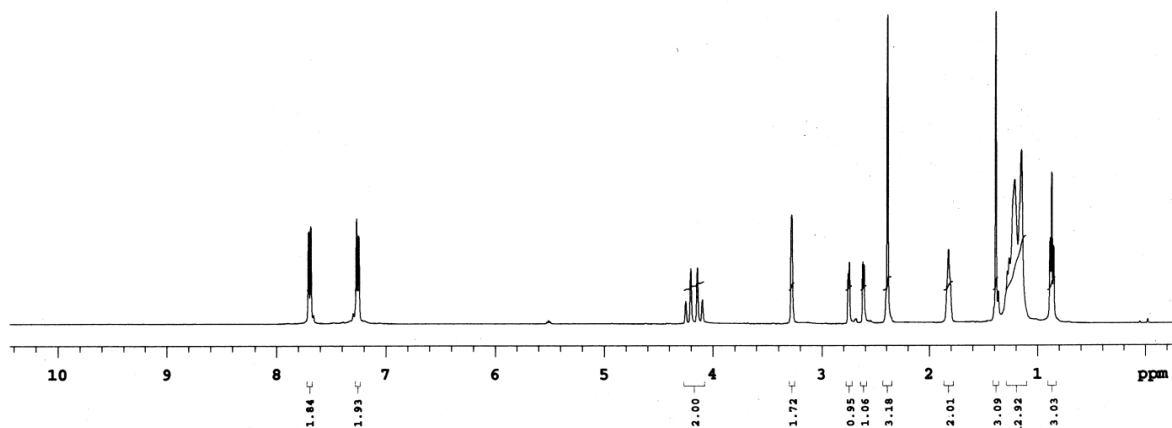
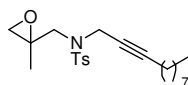


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-Th-EPO</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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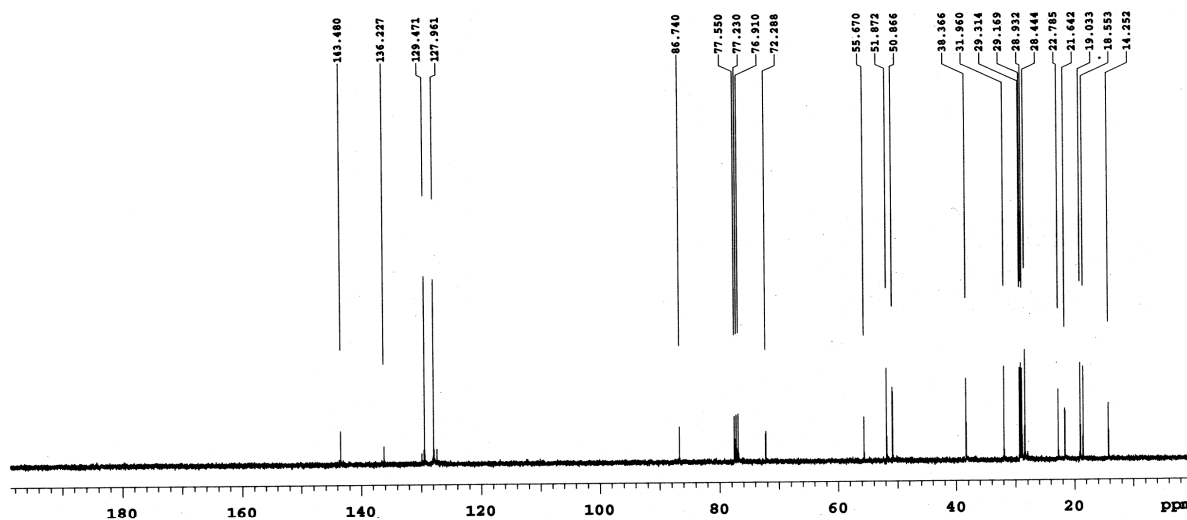


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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 1k



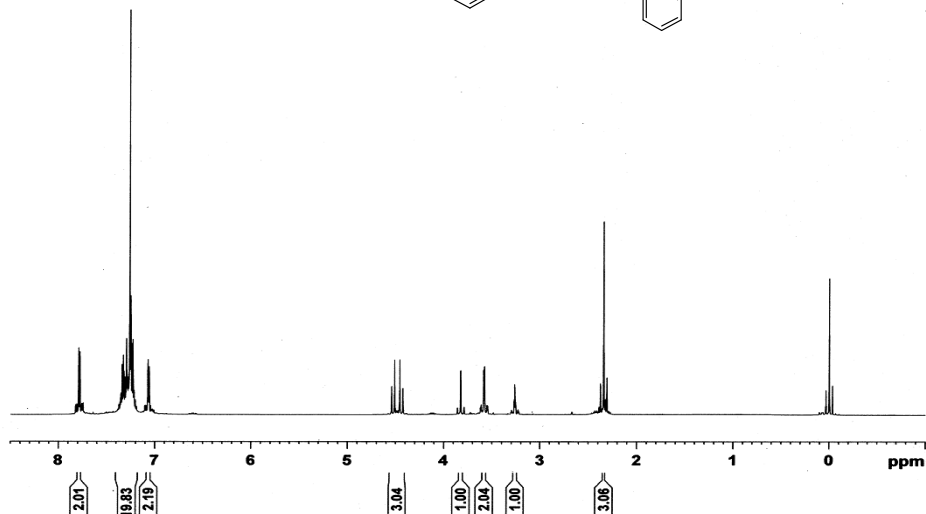
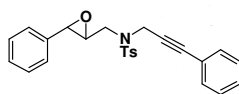
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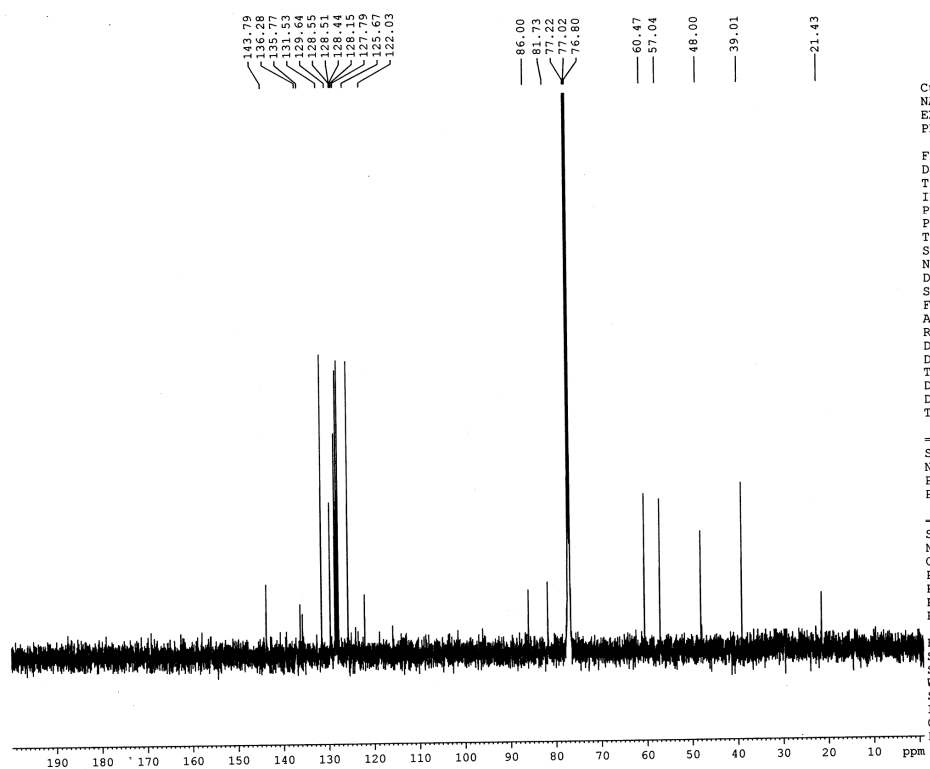
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aks-gp-173



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SOLVENT CDCl3  
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DS 15  
SWH 12019.230 Hz  
FIDRES 0.366788 Hz  
AQ 1.363188 sec  
RG 89.67  
DW 41.600 usec  
DE 6.50 usec  
TE 297.4 K  
D1 1.00000000 sec  
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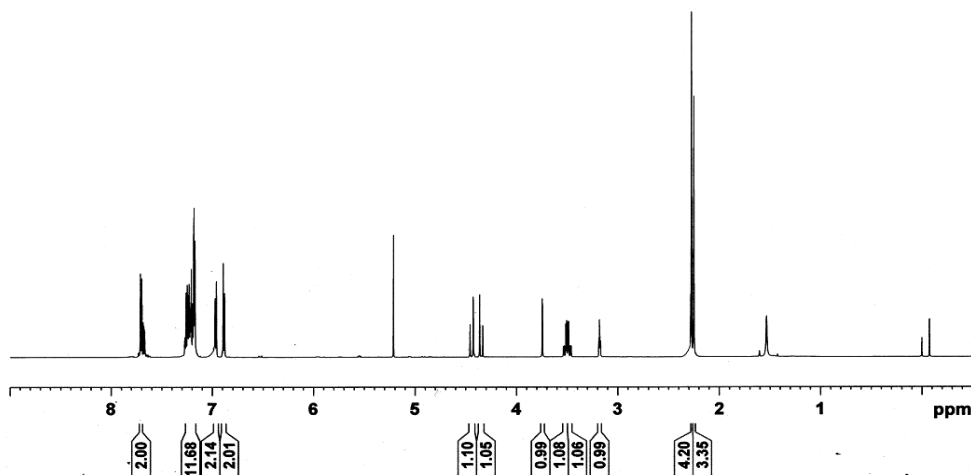
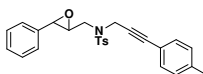
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AQ 0.4543829 sec  
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PLW13 0.30239999 W

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# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1m**

aks-gp-177--26-1H



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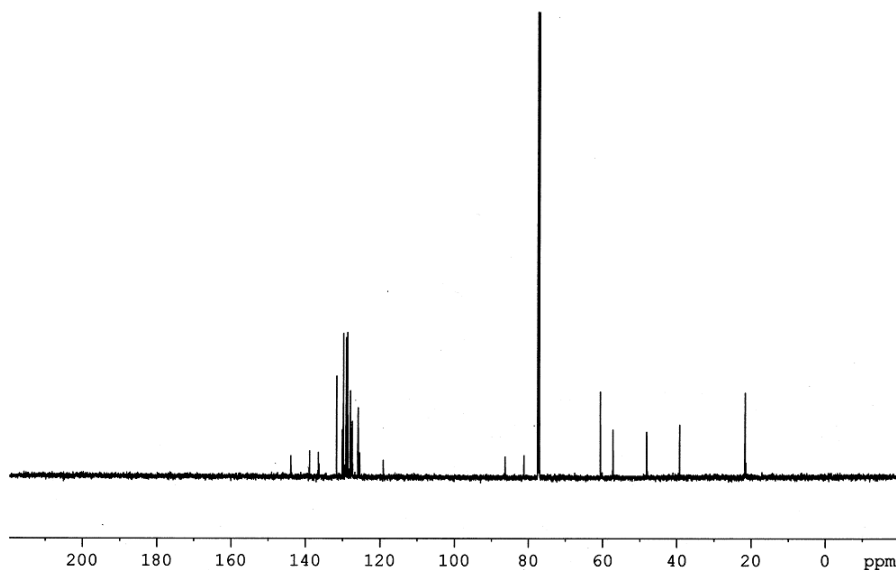
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DW 41.600 usec  
DE 6.50 usec  
TE 299.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700629 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

AKS-GP-177-26-13C

143.92  
138.87  
136.52  
131.63  
129.82  
129.09  
128.74  
128.66  
127.60  
127.48  
125.82  
119.15  
86.34  
81.20  
77.43  
77.23  
77.01  
60.63  
57.27  
48.16  
39.24  
21.71



Current Data Parameters  
NAME AKS-GP-177-26-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131026  
Time 20.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 213  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

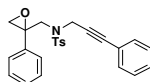
===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128392 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **1n**

GP-180-1H

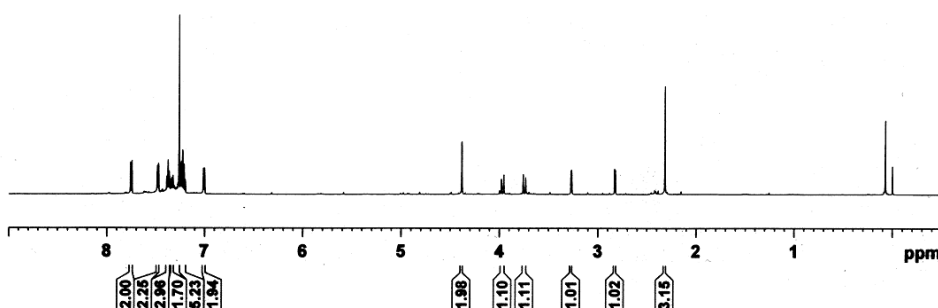


Current Data Parameters  
NAME GP-180-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20131105  
Time 13.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 65.24  
DW 41.600 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700148 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



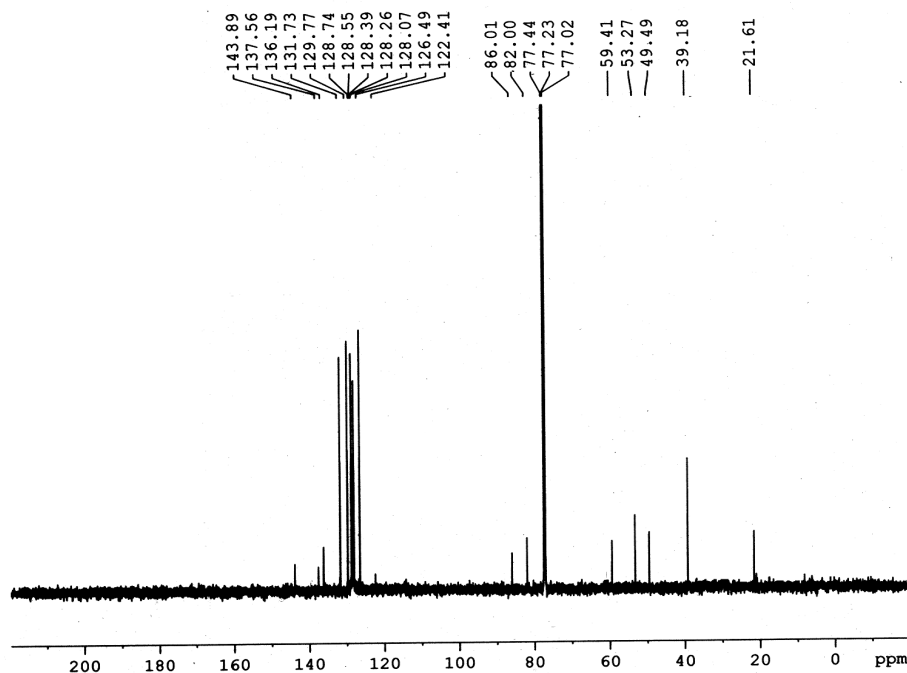
Current Data Parameters  
NAME aks-gp-180-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20131106  
Time 18.39  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 550  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 301.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

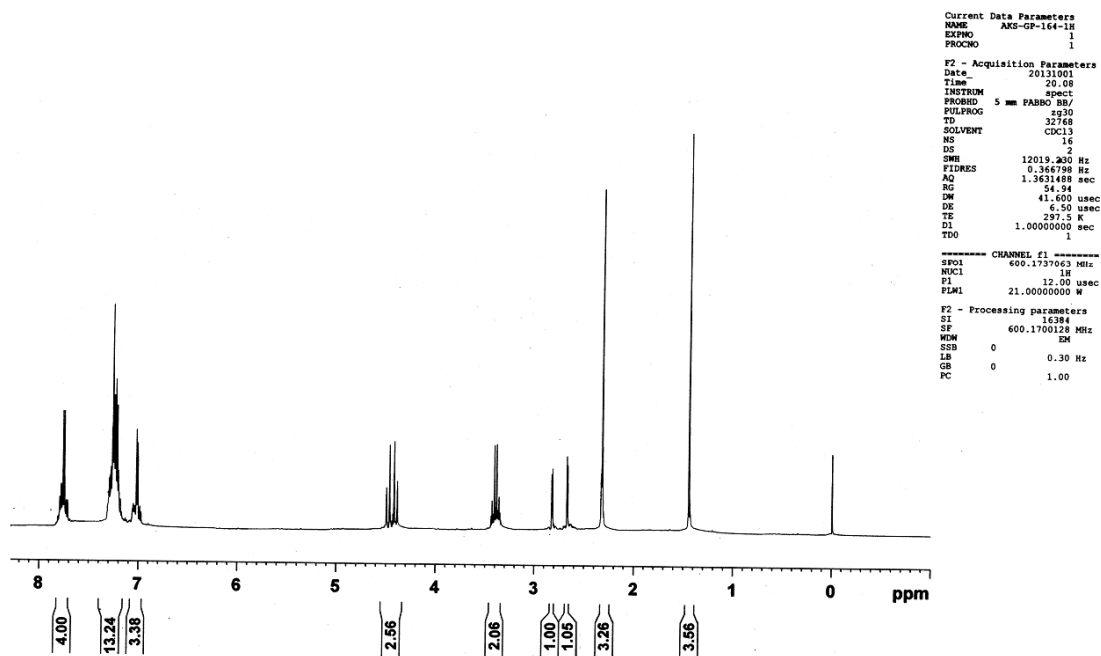
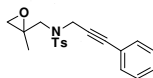
===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128348 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

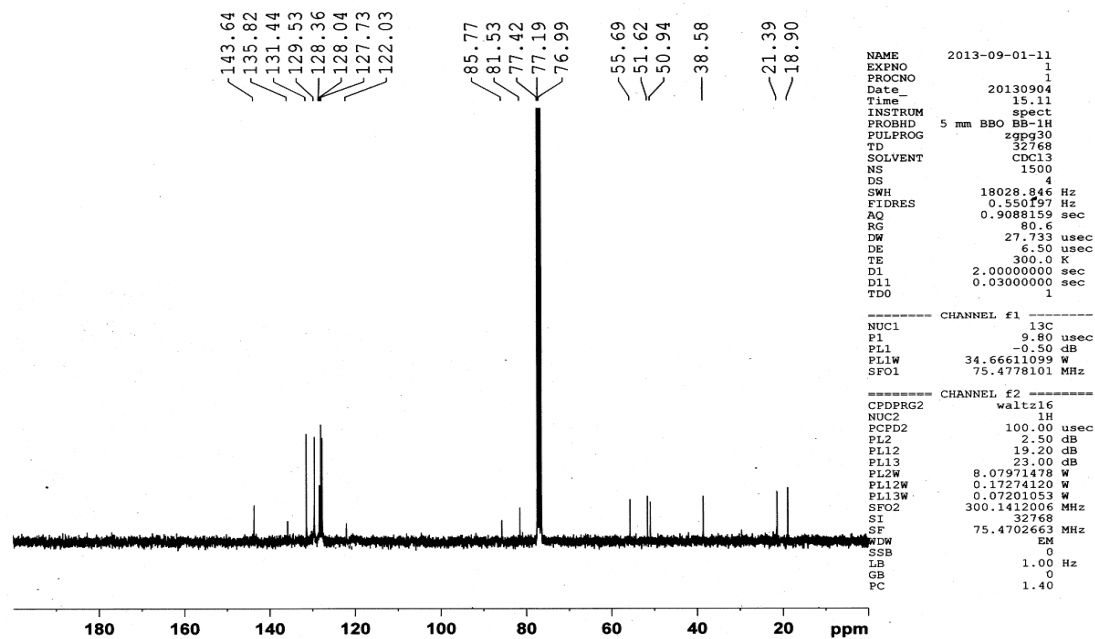


# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1o

aks-gp-164

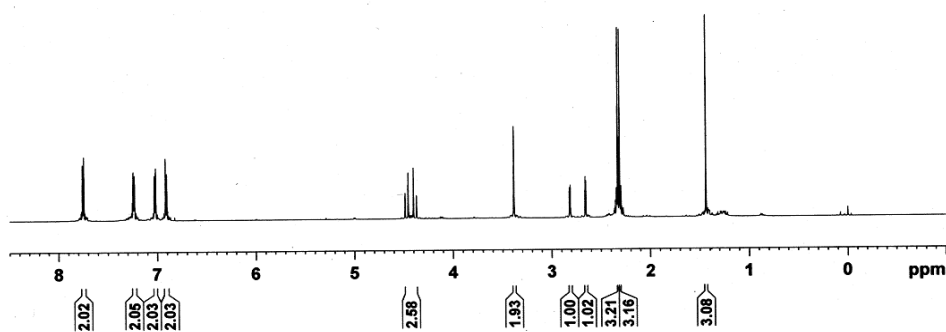
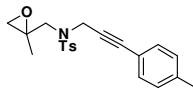


GP-164



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1p

aks-gp-171



Current Data Parameters  
NAME aks-gp-171-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131002  
Time 11.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.166798 Hz  
AQ 1.363146 sec  
RG 31.5  
DM 41.600 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700142 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

aks-gp-171-13C

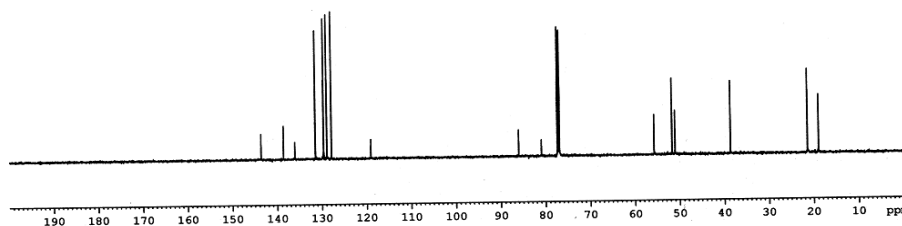
143.61  
138.56  
135.98  
131.40  
129.56  
127.78  
119.03

85.97  
80.90  
77.28  
77.07  
76.86

55.67  
51.71  
51.02

38.68

21.43  
18.95



Current Data Parameters  
NAME aks-gp-171-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131002  
Time 11.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 113  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 200.18  
DM 13.867 usec  
DE 6.50 usec  
TE 298.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

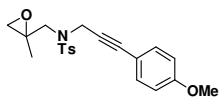
===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9126670 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 1q

aks-gp-170-1H

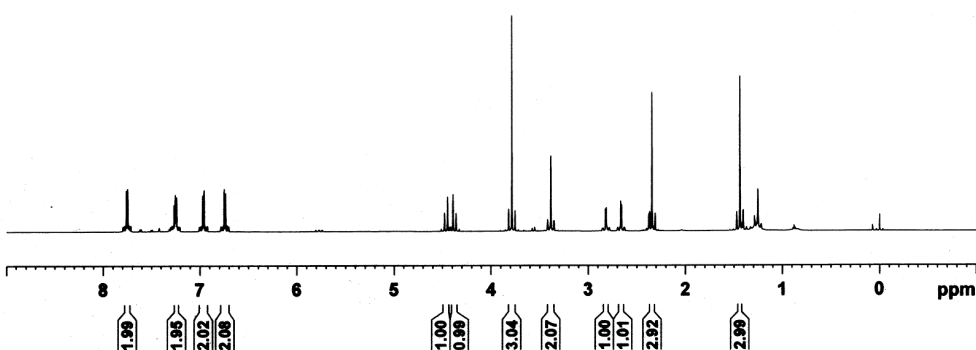


Current Data Parameters  
NAME aks-gp-170-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131001  
Time 20.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 49.39  
DW 41.600 usec  
DE 6.50 usec  
TE 297.4 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700123 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



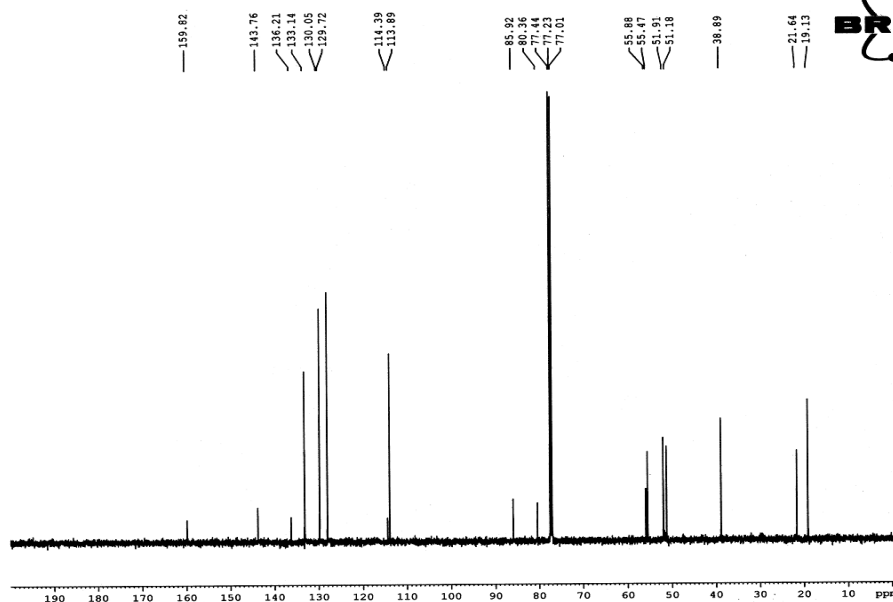
Current Data Parameters  
NAME aks-gp-170-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131001  
Time 19.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 218  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100383 Hz  
AQ 0.4543829 sec  
RG 200.18  
DW 13.867 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

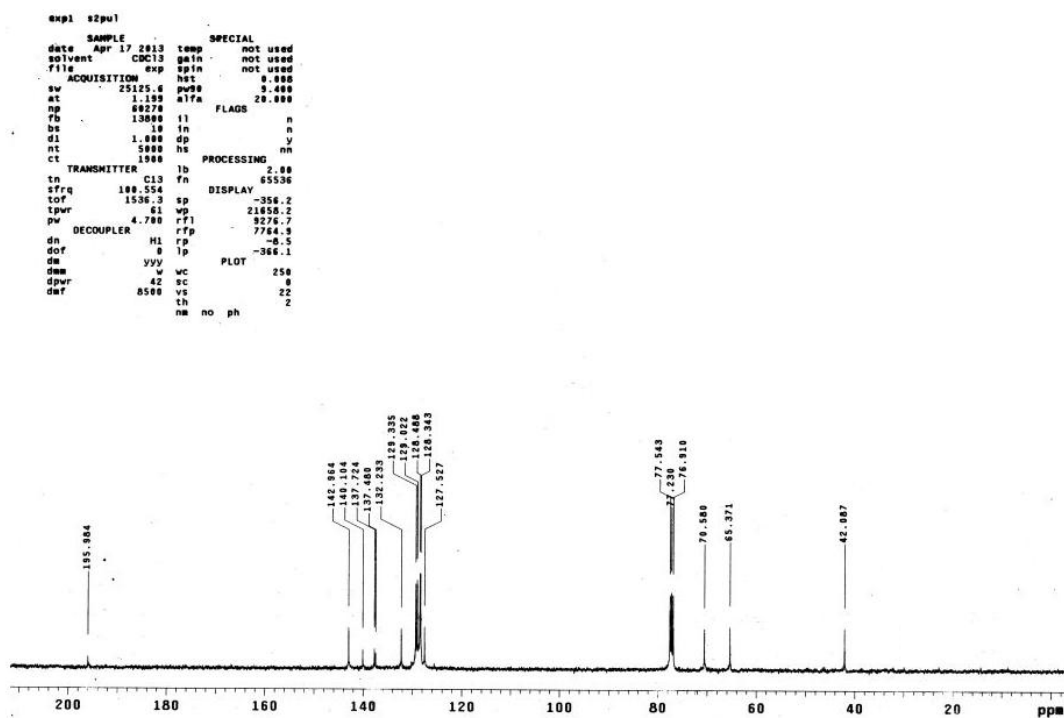
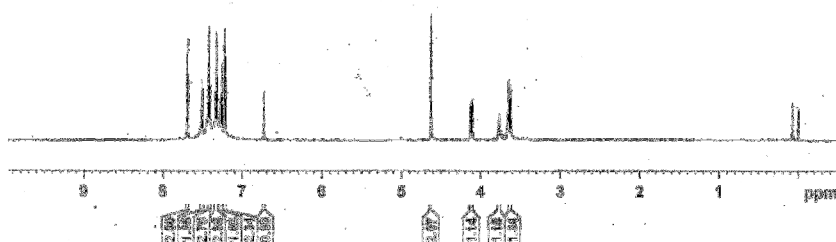
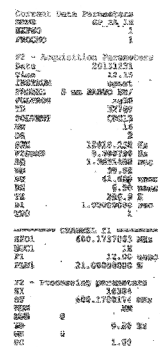
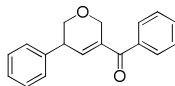
===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128390 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

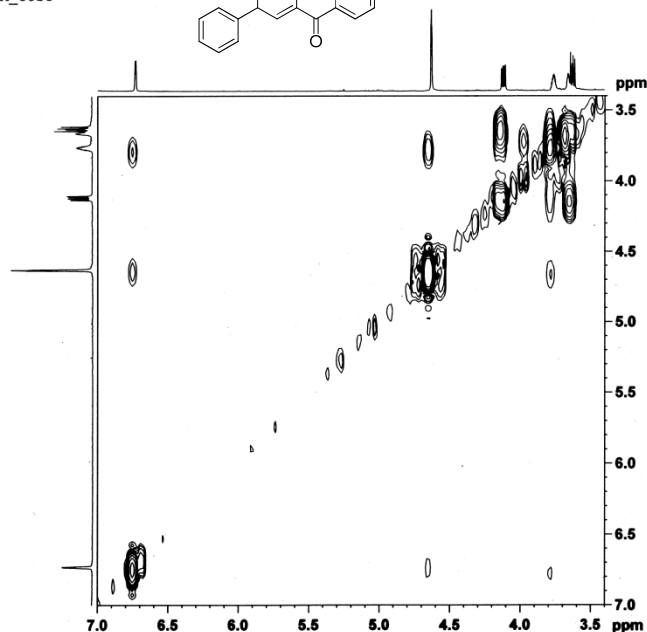
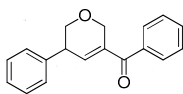




<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **2a**

## COSY Spectra of 2a

GP\_2A\_COSY



Current Data Parameters  
NAME GP\_2A\_COSY  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131231  
Time 12.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG cosypprog  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 16  
SWH 13019.330 Hz  
FIDRES 5.868765 Hz  
AQ 0.0811968 sec  
RG 39.39  
DW 41.600 usec  
DE 6.50 usec  
TE 296.2 K  
DO 0.0000330 sec  
D1 2.0000000 sec  
D11 0.0300000 sec  
D12 0.0002000 sec  
D13 0.0000400 sec  
D14 0.0002000 sec  
IMP 0.0000320 sec

===== CHANNEL f1 =====  
SFO1 600.137963 MHz  
NUC1 1H  
P1 12.00 usec  
P11 12.00 usec  
P12 2500.00 usec  
PLW1 21.0000000 W  
PLW2 4.4734012 W

===== GRADIENT CHANNEL =====  
GPMW[1] SMOG10.100  
GCE1 10.00 t  
P16 1000.00 usec

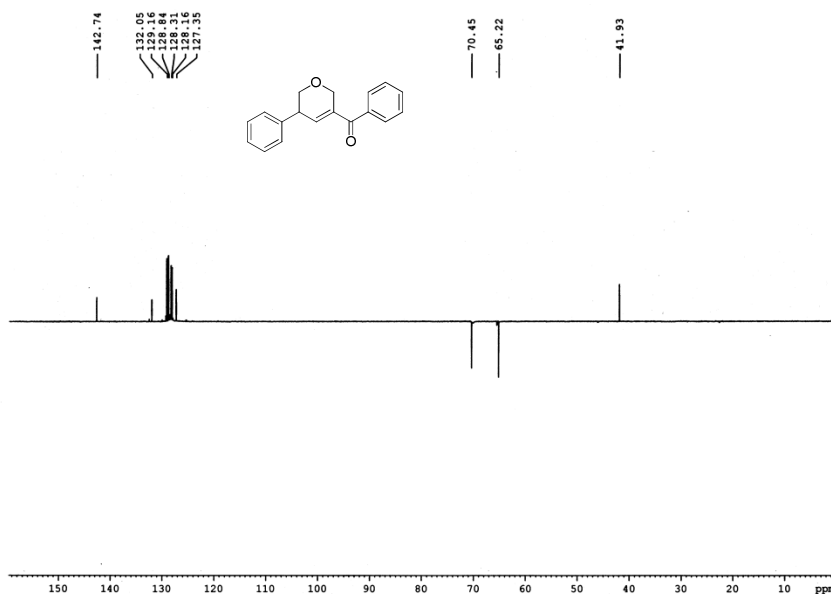
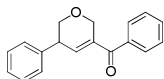
F1 - Acquisition Parameters  
Date\_ 20131231  
Time 12.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptap135  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 16  
SWH 13019.330 Hz  
FIDRES 5.868765 Hz  
AQ 0.0811968 sec  
RG 39.39  
DW 41.600 usec  
DE 6.50 usec  
TE 296.2 K  
DO 0.0000330 sec  
D1 2.0000000 sec  
D11 0.0300000 sec  
D12 0.0002000 sec  
D13 0.0000400 sec  
D14 0.0002000 sec  
IMP 0.0000320 sec

F2 - Processing parameters  
SI 16384  
SF 600.1700000 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 16384  
SF 600.1700000 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

## DEPT Spectra of 2a

GP-2a\_DEPT135



Current Data Parameters  
NAME GP-2a\_DEPT135  
EXPNO 1  
PROCNO 1

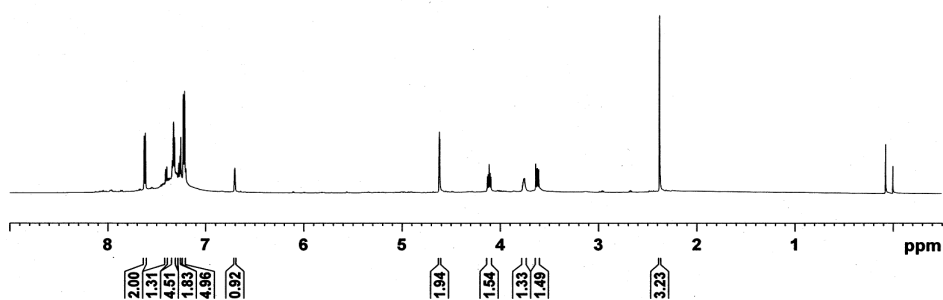
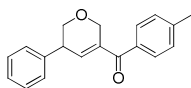
F2 - Acquisition Parameters  
Date\_ 20140103  
Time 11.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptap135  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 16  
SWH 24038.464 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 200.18  
DW 20.800 usec  
DE 6.50 usec  
TE 296.2 K  
CNST2 145.0000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.0002000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9249385 MHz  
NUC1 13C  
P1 10.50 usec  
P11 10.50 usec  
P12 2000.00 usec  
PLW0 0 W  
PLW1 95.0000000 W  
SPNAM[5] Crp60comp.4  
SFOAL5 0 Hz  
SPORT5 0 Hz  
SPW5 16.00300026 W

===== CHANNEL f2 =====  
SFO2 600.1719194 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
F3 12.00 usec  
F4 24.00 usec  
PCPD2 70.00 usec  
PLW2 21.0000000 W  
PLW12 0.61714000 W

F2 - Processing parameters  
SI 16384  
SF 150.9128723 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **2b**

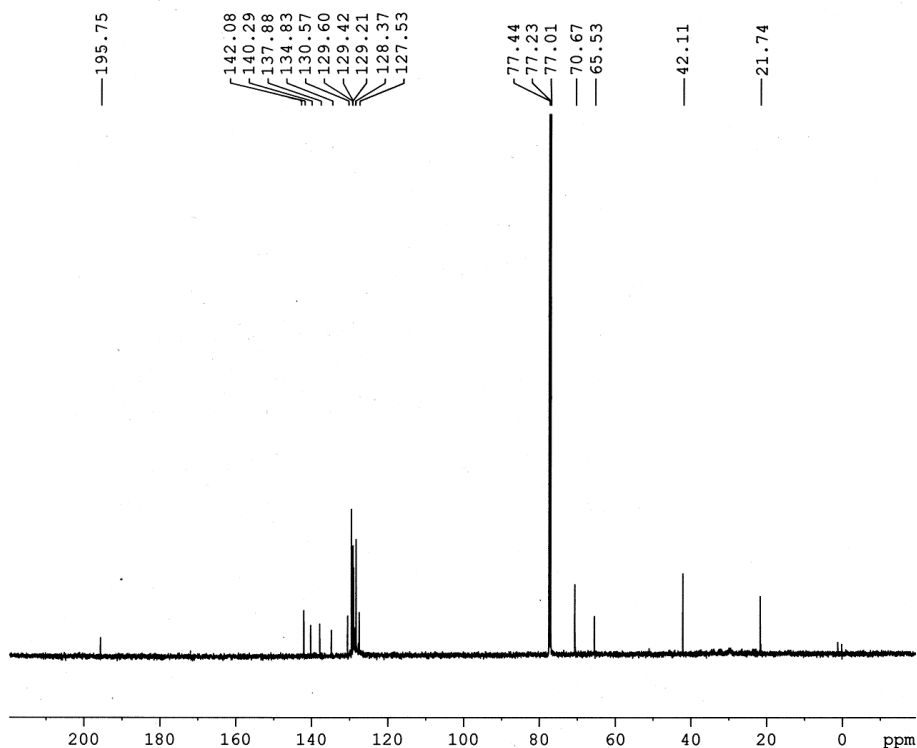


Current Data Parameters  
NAME GE\_2b\_1h  
EXFO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20131231  
Time 13.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 39.79  
DM 41.600 usec  
DE 6.50 usec  
TE 296.7 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700189 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME aks-GE-106-13C  
EXFO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20131027  
Time 15.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 510  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DM 13.867 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

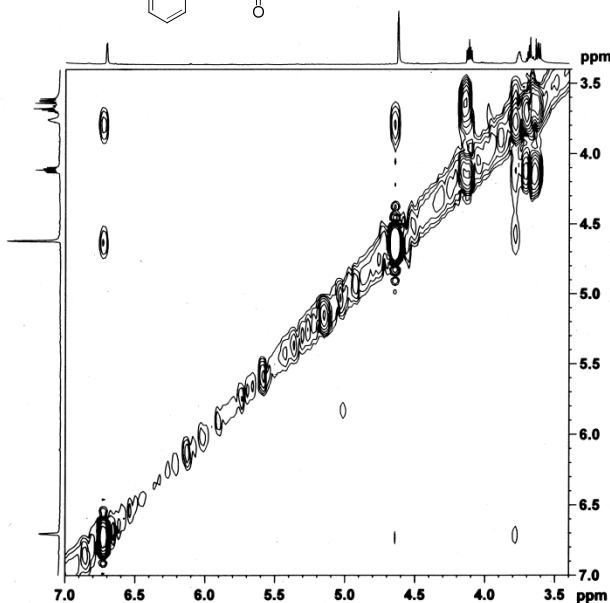
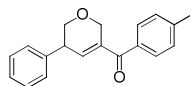
===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128370 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# COSY Spectra of 2b

GP\_2B\_COSY



```
Current Data Parameters
NAME      GP_2B_COSY
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20131231
Time      13.27
INSTRUM   spect
PROBHD    5 mm F400 BB/
PULPROG   zgpg30
TD         65536
SOLVENT    CDCl3
NS         4
DS         16
SWH        12019.230 Hz
FIDRES     0.0667455 Hz
AQ         0.0851998 sec
RG         39.59
RW         41.000 usec
DE         6.50 usec
TE         296.2 K
DQ         0.0000300 sec
DL         2.0000000 sec
D11        0.0300000 sec
D12        0.0000200 sec
D13        0.0000400 sec
D16        0.0000000 sec
D18        0.0000320 sec

===== CHANNEL f1 =====
SFO1      600.137003 MHz
NUC1       1H
P1         12.00 usec
P17        2500.00 usec
PLW1       21.0000000 W
PLW10      4.47340012 W

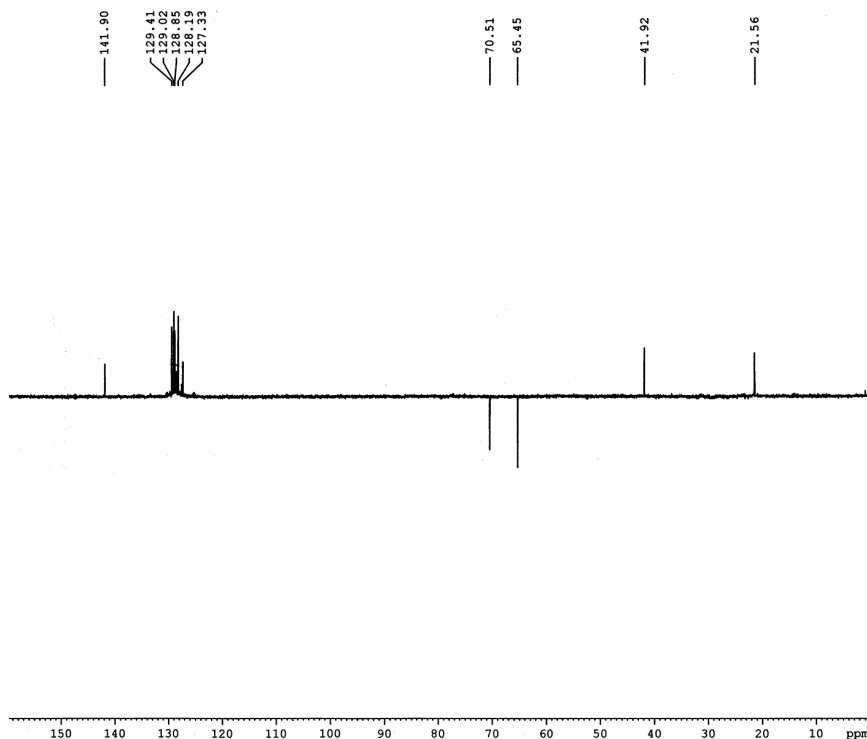
===== GRADIENT CHANNEL =====
GNAME[1]   SFO1:130
GPR1       100.00 usec
P14        1000.00 usec

F1 - Acquisition parameters
TD         130
SFO1      600.13717 MHz
FIDRES     80.128204 Hz
AQ         20.026 usec
RG         0
PC         1.00

F1 - Processing parameters
SI         1024
SF         600.1700000 MHz
WDW         EM
SSB         0
LB          0 Hz
GB          0
PC          1.00

F1 - Processing parameters
SI         1024
SF         600.1700000 MHz
WDW         EM
SSB         0
LB          0 Hz
GB          0
PC          1.00
```

GP-2b 30jan DEPT135



```
Current Data Parameters
NAME      GP-2b_30jan_DEPT135
EXPNO     1
PROCNO    1

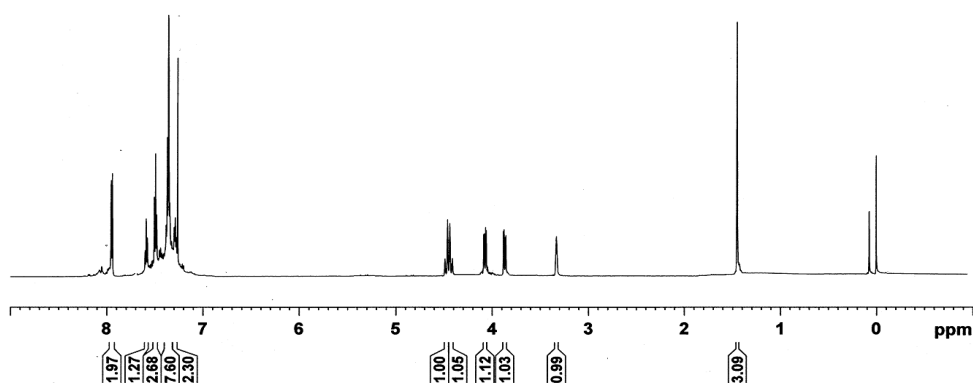
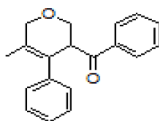
F2 - Acquisition Parameters
Date_     20140130
Time      13.15
INSTRUM   spect
PROBHD    5 mm F400 BB/
PULPROG   zgpg30
TD         32768
SOLVENT    CDCl3
NS         4
DS         16
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         200.18
RW         20.800 usec
DE         6.50 usec
TE         296.2 K
DQ         0.0000000 sec
DL         2.0000000 sec
D1         0.00344828 sec
D12        0.0000200 sec
D13        0.0000000 sec
D16        0.0000000 sec
D18        0.0000000 sec
D19        0.0000000 sec
D20        0.0000000 sec

===== CHANNEL f1 =====
SFO1      150.9249389 MHz
NUC1       13C
P1         10.50 usec
P13        2000.00 usec
PLW1       0 W
PLW10      95.00000000 W
SPNAM[5]   Crp60comp.4
SFO15      0 Hz
SPOFFS5    0 Hz
SPW5       16.00300026 W

===== CHANNEL f2 =====
SFO2      600.1719194 MHz
NUC2       1H
CPDPRG2    waltz16
P3         12.00 usec
P4         24.00 usec
PCPD2      70.00 usec
PLW2       21.00000000 W
PLW12      0.61714000 W

F2 - Processing parameters
SI         16384
SF         150.9128670 MHz
WDW         EM
SSB         0
LB          0 Hz
GB          0
PC          1.40
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$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **2c**



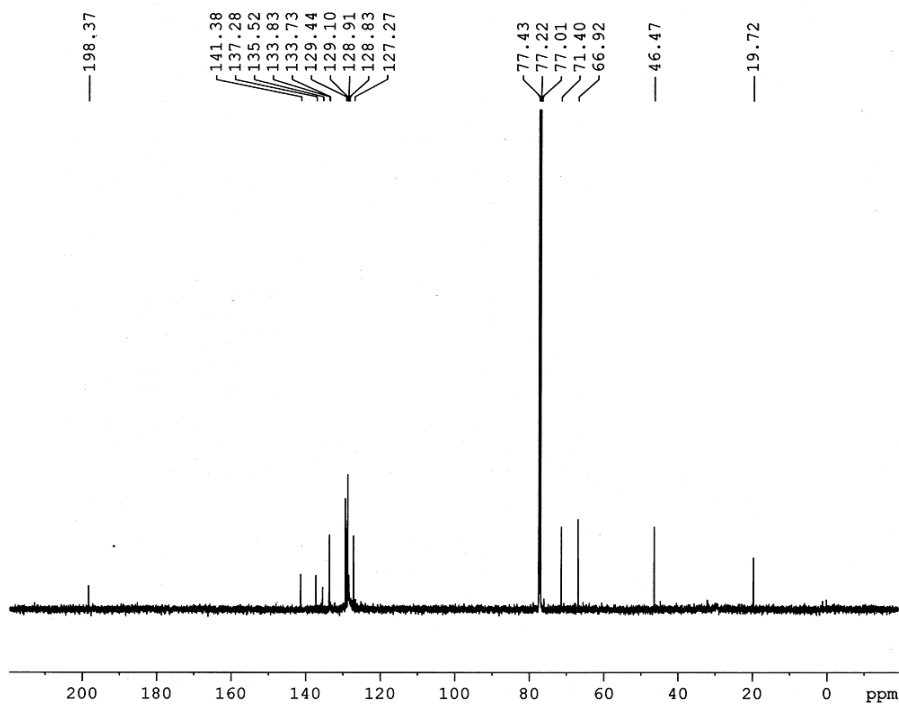
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NAME aks-GP-112-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20131027  
Time 17.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.363488 sec  
RG 34.34  
DW 41.600 usec  
DE 6.50 usec  
TE 298.5 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1737043 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700146 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

aks-Gp-112-13C



Current Data Parameters  
NAME aks-Gp-112-13C  
EXPNO 1  
PROCNO 1

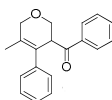
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INSTRUM spect  
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PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 558  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 299.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

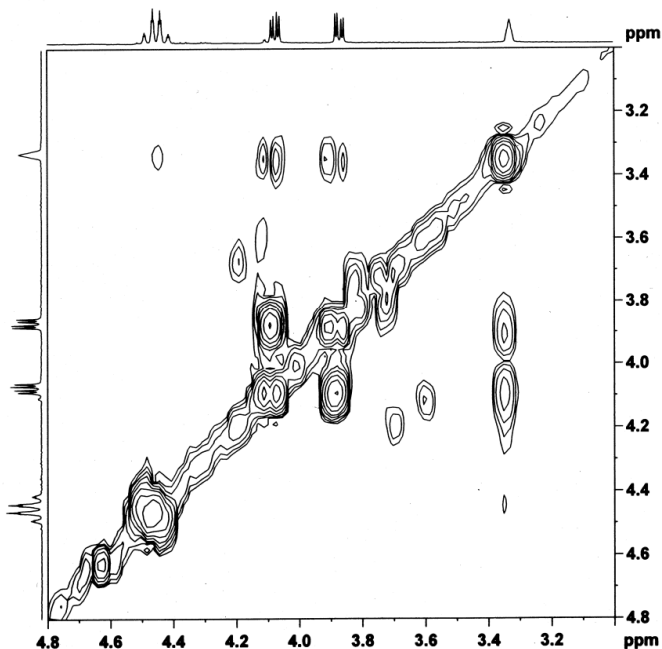
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SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
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PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128370 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# COSY Spectra of 2c



GP-2c\_COSY



```

Current Data Parameters
NAME      GP-2c_COSY
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140101
Time      19.23
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   cosypppgq
TD         2568
SOLVENT   CDCl3
NS         4
DS         8
SWH        12019.230 Hz
FIDRES     5.868765 Hz
AQ         0.0851968 sec
RG         54.94
DW         41.600 usec
DE         6.50 usec
TE         296.9 K
D0         0.00000000 sec
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00020000 sec
D13        0.00000400 sec
D15        0.00020000 sec
LNO        0.0006320 sec

===== CHANNEL f1 =====
NUC1       600.1737063 MHz
P0         1H
P1         12.00 usec
P17        2500.00 usec
PLW1       21.00000000 W
PLW10      4.47340012 W

===== GRADIENT CHANNEL =====
GPMRG[1]   JMOD10.100
GP11        10.00 %
P16         1000.00 usec

F1 - Acquisition parameters
SI         256
SF01       600.1737 MHz
FIDRES     46.950119 Hz
SW         20.026 ppm
FNUCIDE    QF

F2 - Processing parameters
SI         1024
SF         600.1700000 MHz
WDW        Q5INE
SSB         0
LB          0 Hz
GB          0
PC          1.00

F1 - Processing parameters
SI         1024
MC2         QF
SF         600.1700000 MHz
WDW        Q5INE
SSB         0
LB          0 Hz
GB          0
PC          1.40
    
```

# DEPT Spectra of 2c

GP-2C\_DEPT135



135.25

129.25

128.91

128.72

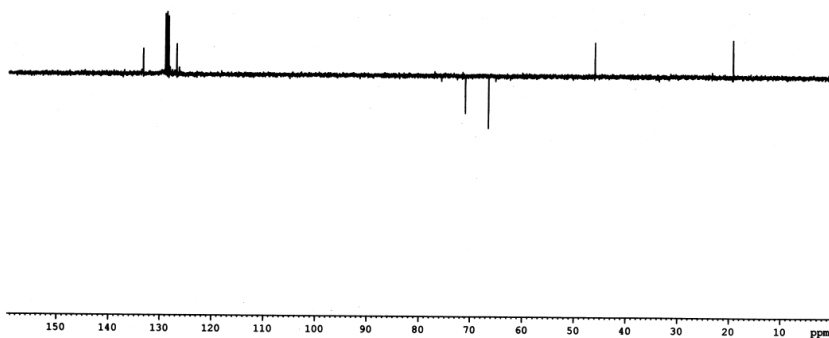
127.07

71.26

66.83

46.26

19.55



```

Current Data Parameters
NAME      GP-2C_DEPT135
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140103
Time      11.56
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   deptpl35
TD         32768
SOLVENT   CDCl3
NS         256
DS         4
SWH        24038.461 Hz
FIDRES     0.733556 Hz
AQ         0.6815744 sec
RG         250.14
DW         20.800 usec
DE         6.50 usec
TE         297.0 K
CRST2     145.0000000
D1         2.00000000 sec
D2         0.00348828 sec
D12        0.00002000 sec
TDO        1

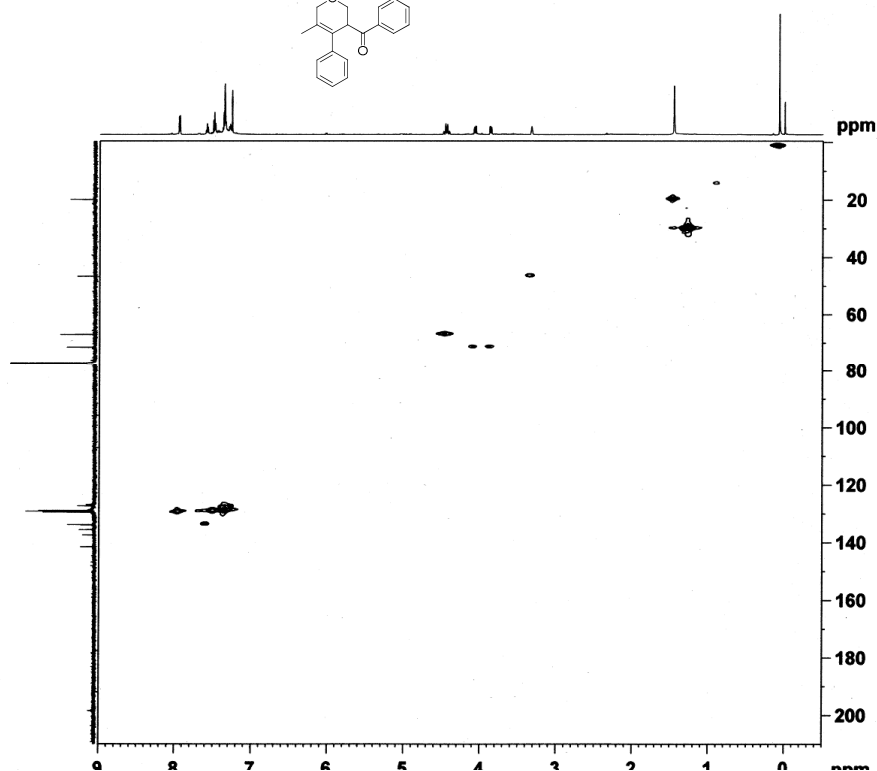
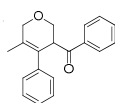
===== CHANNEL f1 =====
SF01       150.9249389 MHz
NUC1       13C
P1         10.50 usec
P13        2000.00 usec
PLW0       0 W
PLW1       95.00000000 W
SPNAM[5]   Crp60comp.4
SFOALS     0 Hz
SPOFFS5    0 Hz
SPOFFS5    16.00300026 W

===== CHANNEL f2 =====
SF02       600.1719154 MHz
NUC2       1H
CROPRG[2]   waltz16
P3         12.00 usec
P4         24.00 usec
PCPD2      70.00 usec
PDM2       21.00000000 W
PLW12      0.41714000 W

F2 - Processing parameters
SI         16384
SF         150.9128670 MHz
WDW        EM
SSB         0
LB          0 Hz
GB          0
PC          1.40
    
```

# HMQC Spectra of 2c

GP-2C\_HMQC



```

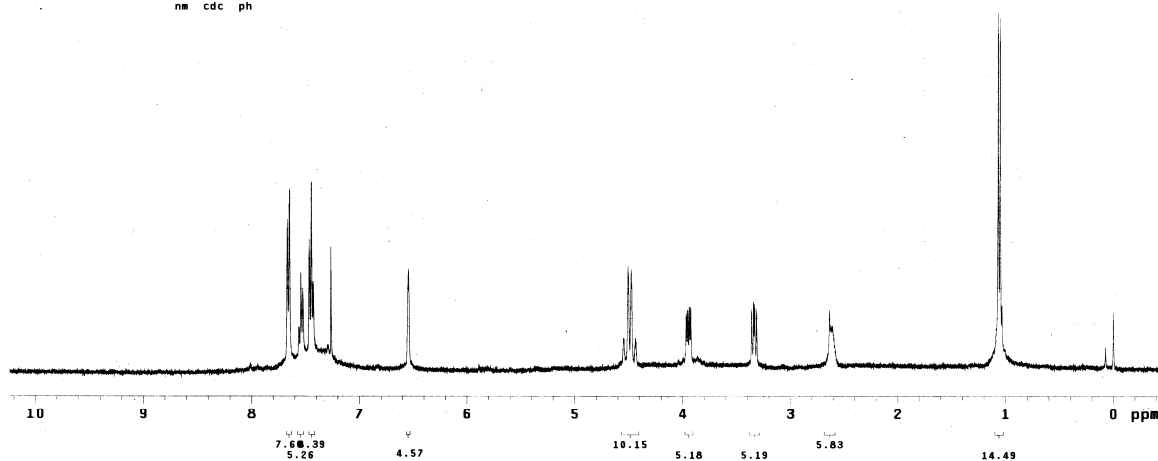
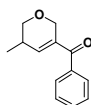
Current Data Parameters
NAME GP-2C_HMQC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140315
Time 15:37
INSTRUM spect
PROBHD 5 mm PABBO RF
PULPROG hmqcpgpg
TD 124
SOLVENT CDCl3
NS 8
DS 16
FIDRES 12019.1300 Hz
AQ 0.0425984 sec
RG 87.22
DW 41.600 usec
DE 350.1 K
TE 300.2 K
CMPT2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00144828 sec
D3 0.00000000 sec
D13 0.00000400 sec
D16 0.00000000 sec
ZNO 0.00011390 sec
===== CHANNEL f1 =====
SFO1 600.137063 MHz
NUC1 13C
P1 12.00 usec
F1 24.00 usec
FID1 21.00000000 W
===== CHANNEL f2 =====
SFO2 150.924843 MHz
NUC2 13C
CROSSP2 13C
P2 10.50 usec
PCPD2 60.00 usec
F2 95.00000000 W
FID2 2.00000000 W
===== GRADIENT CHANNEL =====
GPMAN[1] SHGQ10.100
GPMAN[2] SHGQ10.100
GPMAN[3] SHGQ10.100
GP21 50.00 %
GP22 30.00 %
GP23 40.10 %
F16 1000.00 usec
F1 - Acquisition parameters
TD 256
SFO1 150.9248 MHz
FIDRES 140.512589 Hz
RG 238.160
PULPROG QF
F2 - Processing parameters
SI 1024
SF 600.1708000 MHz
WDW QFHM
GB 0
PC 1.00
F1 - Processing parameters
SI 1024
SF 150.912870 MHz
WDW QFHM
GB 0

```

# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **2d**

OP\_AKS\_152\_M  
expt1 s2pu1

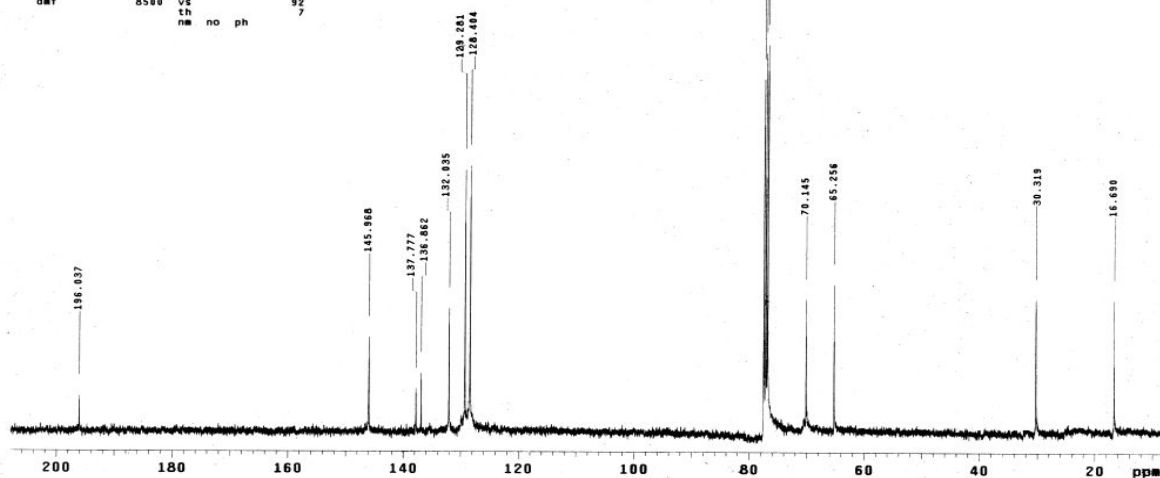
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date	Jul 23 2013	temp	not used
solvent	CDCl <sub>3</sub>	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.000
sw	6389.8	pwd	15.100
at	1.998	alfa	20.000
np	25526	FLAGS	
td	not used	il	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nn
ct	TRANSMITTER	32	hs
tn	H1	fn	0.10
sfrq	399.853	fn	65536
tof	362.8	sp	188.6
tpwr	59	wp	4282.1
pw	7.550	rfl	793.1
DECOUPLER		rp	162.9
dn	C13	lp	-104.3
dof	0	PLOT	
dm	nnn	wc	250
dmm	c	sc	0
dpr	44	vs	105
daf	17100	th	6
	nm	cdc	ph



OP\_AKS\_152\_13C

expt1 s2pu1

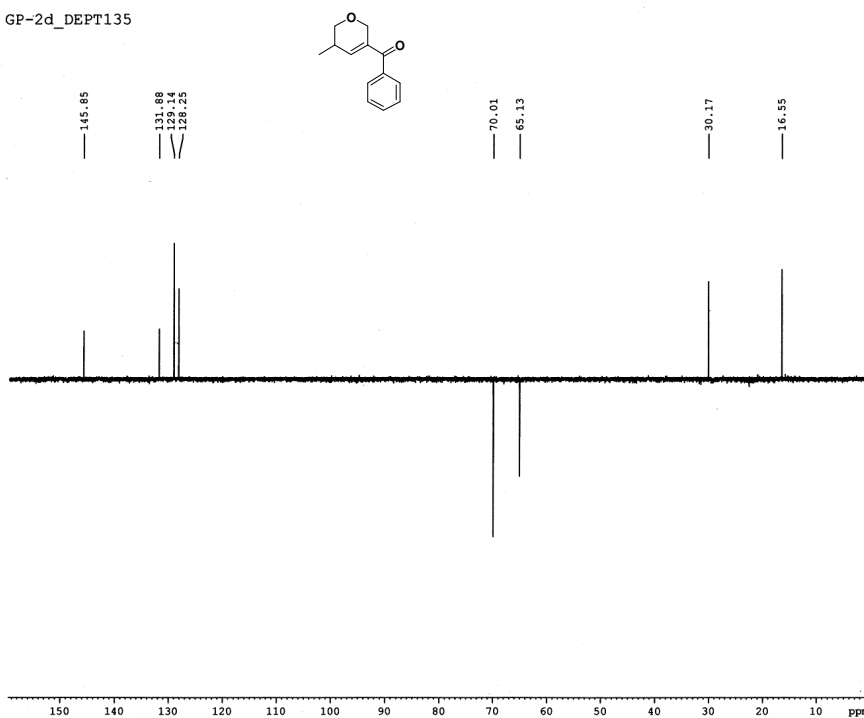
SAMPLE		SPECIAL	
date	Jul 28 2013	temp	not used
solvent	CDCl <sub>3</sub>	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.000
sw	25125.6	pwd	9.400
at	1.199	alfa	20.000
np	68270	FLAGS	
td	13000	il	n
bs	16	in	n
d1	1.000	dp	y
nt	10000	hs	nn
ct	TRANSMITTER	10000	hs
tn	C13	fn	2.00
sfrq	100.625	fn	65536
tof	1536.3	sp	769.4
tpwr	61	wp	28139.9
pw	4.700	rfl	9272.3
DECOUPLER		rp	7764.9
dn	H1	lp	-88.6
dof	0	PLOT	
dm	yyy	wc	250
dmm	42	sc	0
dpr	8500	vs	92
daf		th	7
	nm	no	ph





# DEPT and HMQC spectra of compound 2d

GP-2d\_DEPT135



Current Data Parameters  
NAME GP-2d\_DEPT135  
EXPNO 1  
PROCNO 1

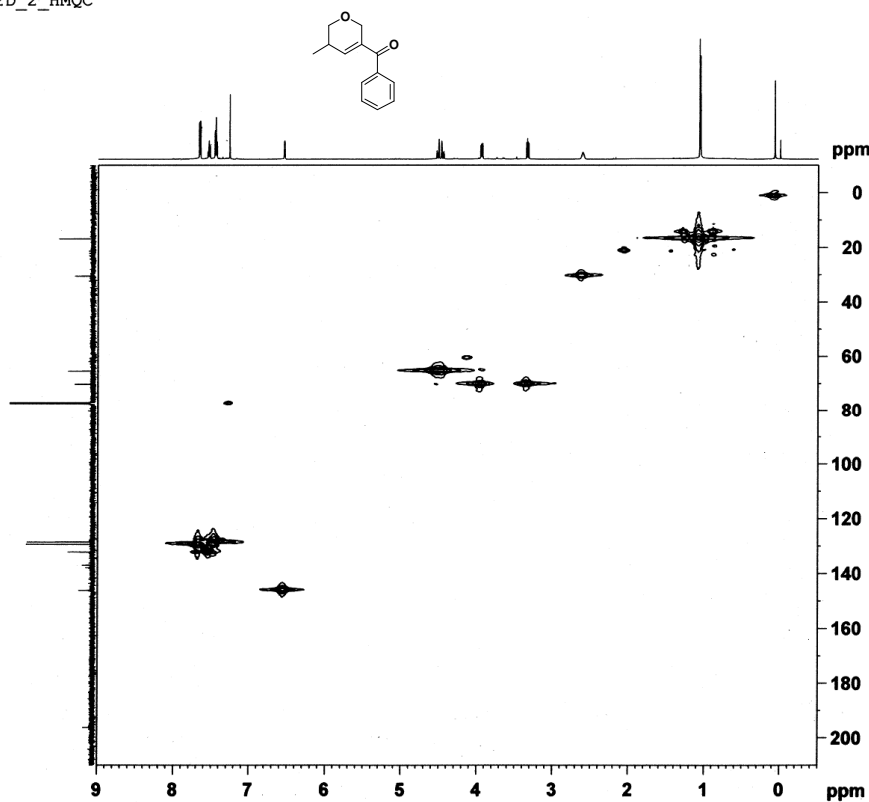
F2 - Acquisition Parameters  
Date\_ 20140322  
Time 11.50  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptap135  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 200.18  
RW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
CHST2 145.0000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.0002000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9249389 MHz  
NUC1 13C  
P1 10.50 usec  
PL1 0 W  
PL12 2000.00 usec  
PL13 95.0000000 W  
SENAM(5) Ccp600cnc4  
SFOALS 0.500  
SFOFSS 0 Hz  
SPW5 16.0030026 W

===== CHANNEL f2 =====  
SFO2 600.1719194 MHz  
NUC2 1H  
CPDPRG2 waltz16  
F3 12.00 usec  
F4 24.00 usec  
PCPD2 70.00 usec  
PL12 21.0000000 W  
PLW12 0.61714000 W

F2 - Processing parameters  
SI 16384  
SF 150.9128670 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

GP-2D\_2\_HMQC



Current Data Parameters  
NAME GP-2D\_2\_HMQC  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140325  
Time 20.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG hmqc  
TD 1024  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 12019.230 Hz  
FIDRES 11.727530 Hz  
AQ 0.642394 sec  
RG 60.22  
RW 41.600 usec  
DE 6.50 usec  
TE 300.0 K  
CHST2 145.0000000  
D0 0.00000000 sec  
D1 1.00000000 sec  
D2 0.00344828 sec  
D12 0.00000000 sec  
D13 0.00000000 sec  
D16 0.00000000 sec  
IND 0.0001390 sec

===== CHANNEL f1 =====  
SFO1 600.1727063 MHz  
NUC1 1H  
P1 12.00 usec  
PL1 0 W  
PLW1 21.0000000 W

===== CHANNEL f2 =====  
SFO2 150.9241843 MHz  
NUC2 13C  
CPDPRG2 sg2  
F3 10.50 usec  
F4 24.00 usec  
PCPD2 95.0000000 W  
PLW12 2.90939995 W

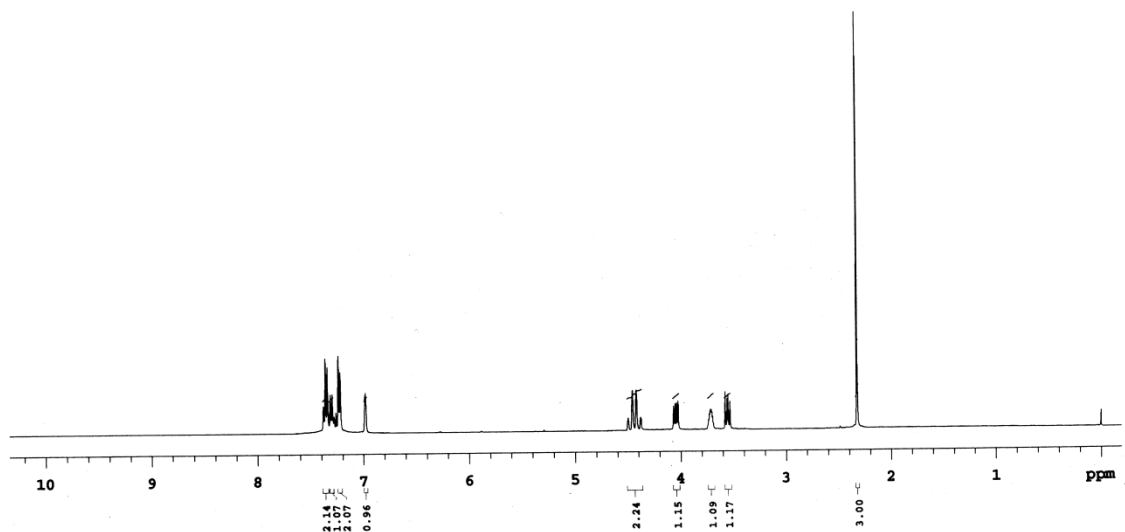
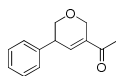
===== GRADIENT CHANNEL =====  
GRNM(1) SNG10.100  
GRNM(2) SNG10.100  
GRNM(3) SNG10.100  
GF1 50.00 %  
GF2 30.00 %  
GF3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 150.9242 MHz  
FIDRES 140.512389 Hz  
SW 238.340 ppm  
FNUCSE CD

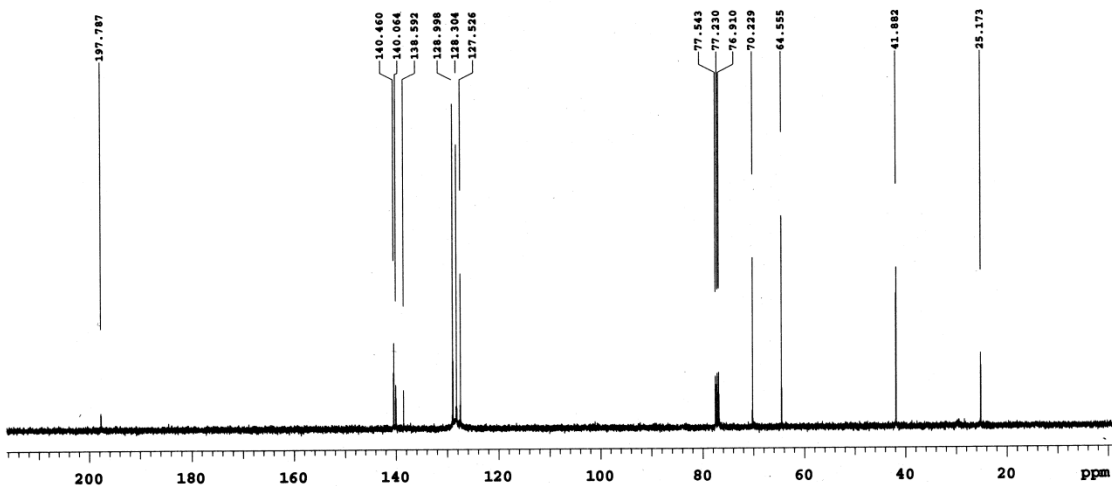
F2 - Processing parameters  
SI 1024  
SF 600.1700000 MHz  
WDW QDMC  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 CD  
SF 150.9128670 MHz  
WDW QDMC  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 2f

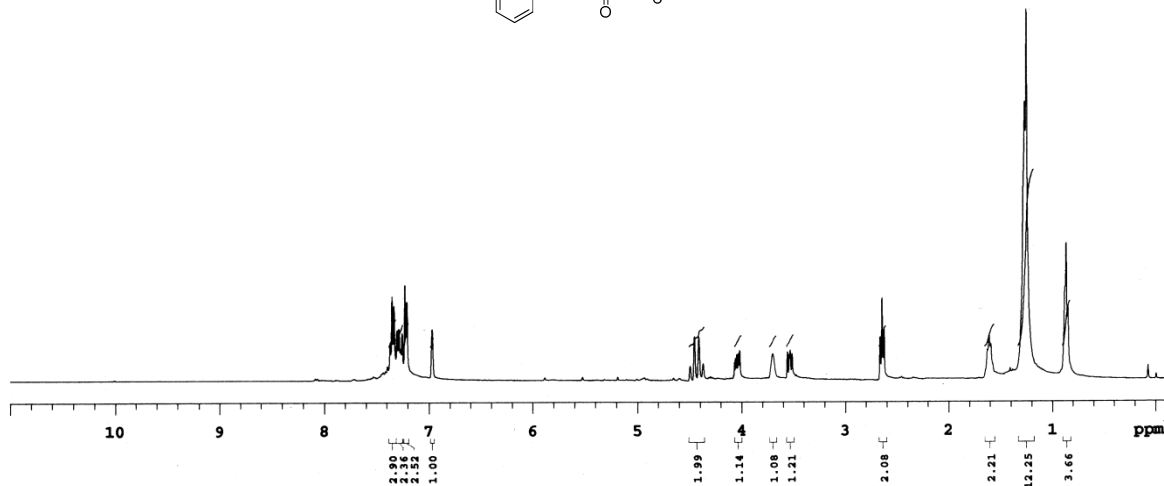
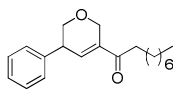


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509629	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>GP_AKS_Ma_pro_1H</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: GP_AKS_Ma_pro_1H Mercury-400 "IITG-NMR"
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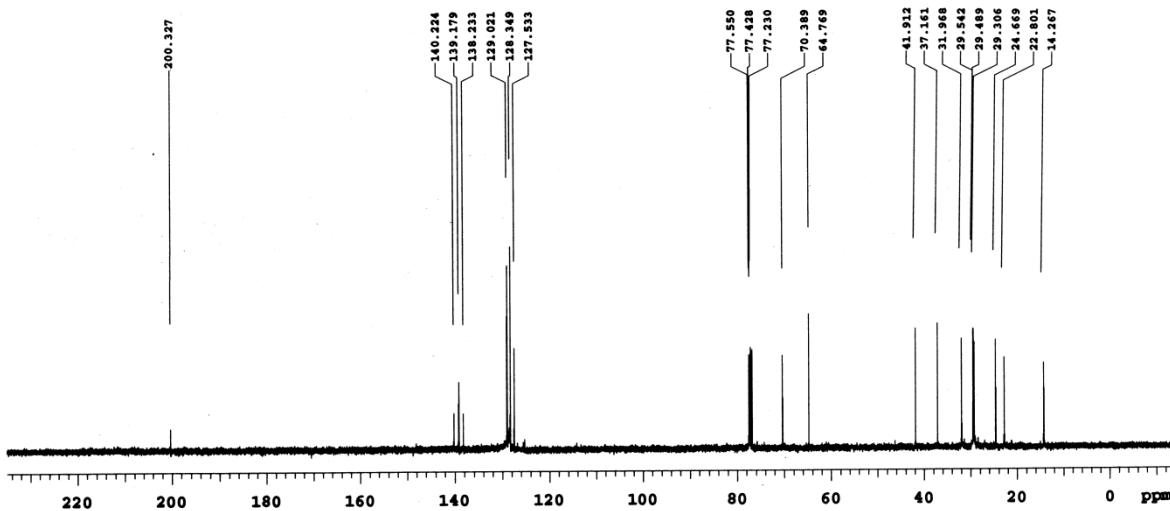


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 160 repetitions	<b>OBSERVE</b> C13, 100.5425947 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 6 minutes	<b>GP_AKS_Ma_pro_13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: GP_AKS_Ma_pro_13C Mercury-400 "IITG-NMR"
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### <sup>1</sup>H and <sup>13</sup>C Spectra of compound **2g**

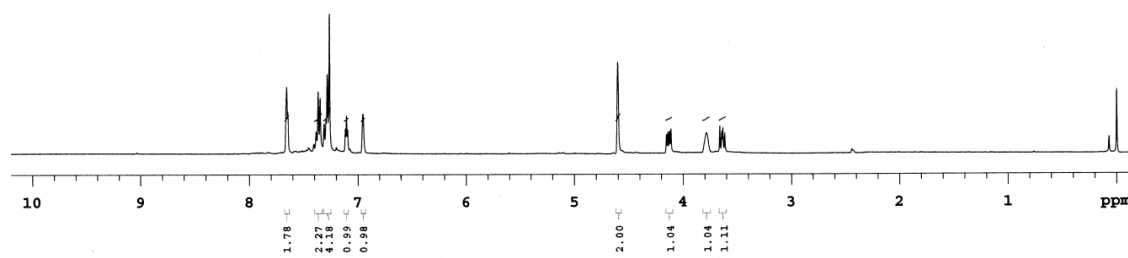
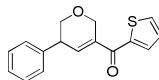


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>GP_AKS_p_dec</b>  Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chm File: GP_AKS_p_dec Mercury-400 "1H7G-NMR"
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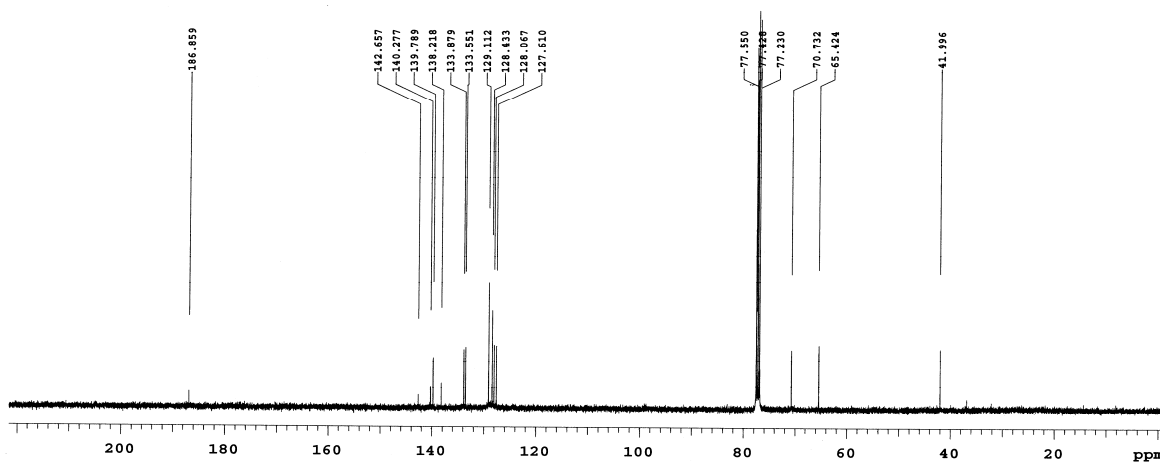


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 260 repetitions	OBSERVE C13, 100.5425893 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 9 minutes	_2_13C Solvent: cdc13 Temp. 25.0 C / 298.1 K Operator: cham File: GP-1-DMC-C13 Mercury-400 "1170-MMR"
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# <sup>1</sup>H and <sup>13</sup>C NMR Spectra of **2j**

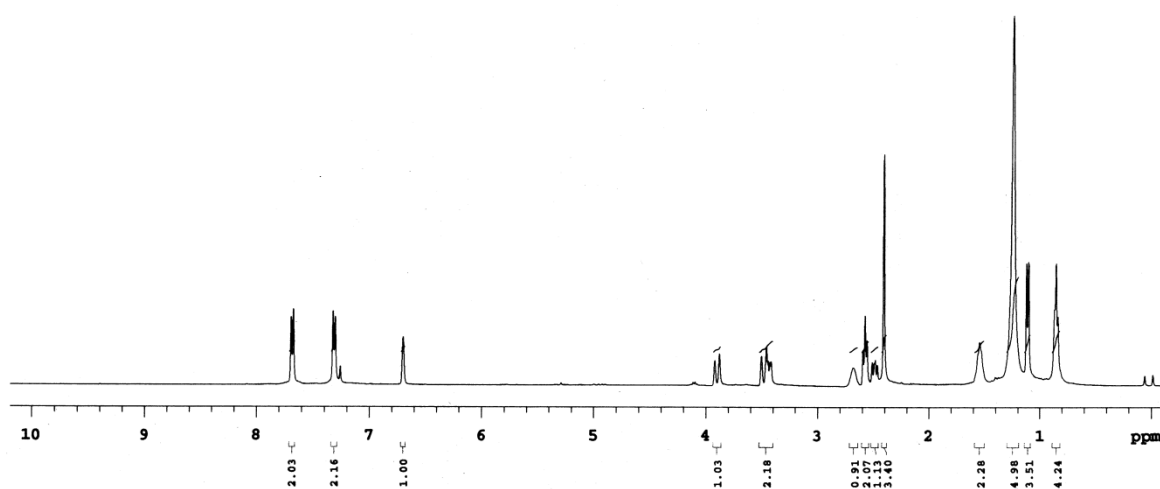
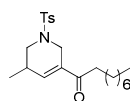


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 100 Repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 5 minutes	<b>IK-Th-Pro</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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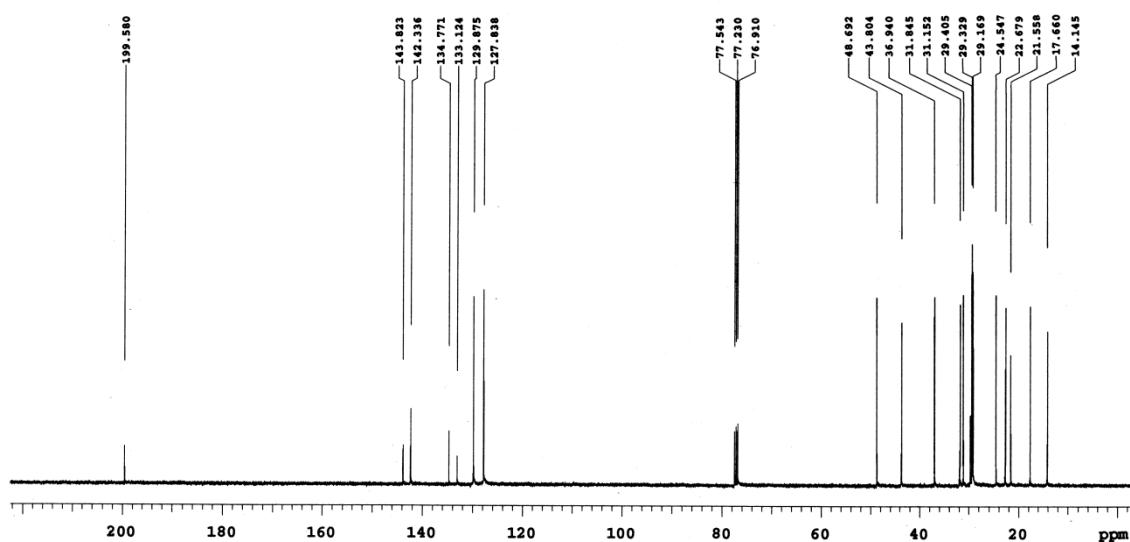


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 1216.6 Hz 5120 repetitions	<b>OBSERVE</b> C13, 100.6425832 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ 16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 3.3 hours	<b>IK-TH-Pro-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: IK-TH-Pro-13C Mercury-400 *IITG-NMR*
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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound **2k**



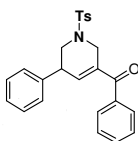
<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509650	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>GP-aks-1_DEC_NTs_1H</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: GP-aks-1_DEC_NTs_1H Mercury-400 "IITG-MMR"
---	--------------------------------	---	---



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 630 repetitions	<b>OBSERVE</b> C13, 100.5425901 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 24 minutes	<b>GP-AKS-1-DEC-NTs-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: GP-AKS-1-DEC-NTs-13C Mercury-400 "IITG-MMR"
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# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 21

AKS-GP-176-31-1H

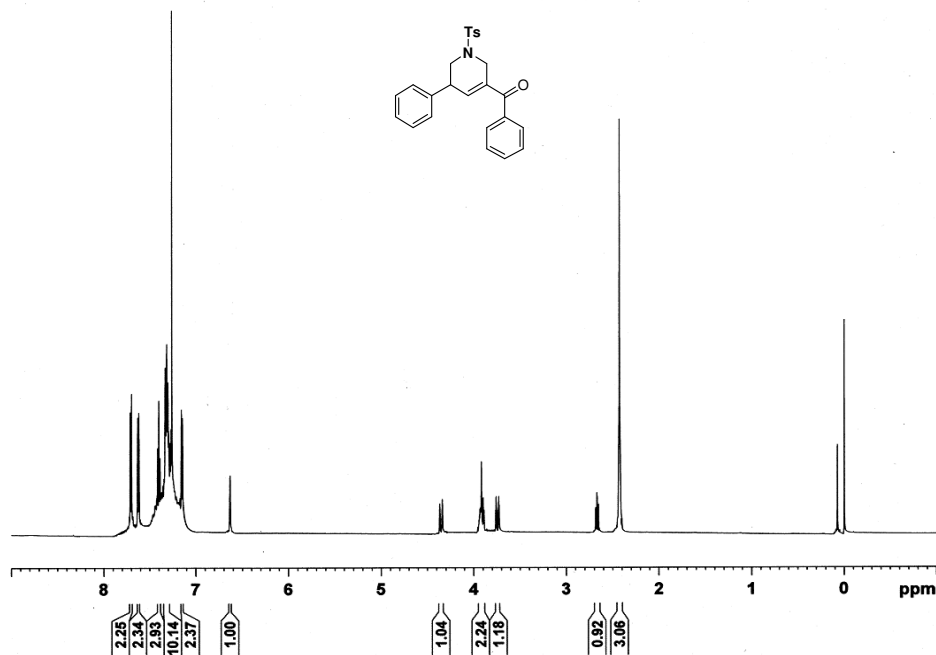


Current Data Parameters  
NAME AKS-GP-176-31-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131031  
Time 20.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 2  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.166798 Hz  
AQ 1.3631488 sec  
RG 54.94  
DW 41.600 usec  
DE 6.50 usec  
TE 297.5 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700148 MHz  
WDW DM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



aks-GP-176-31-13C



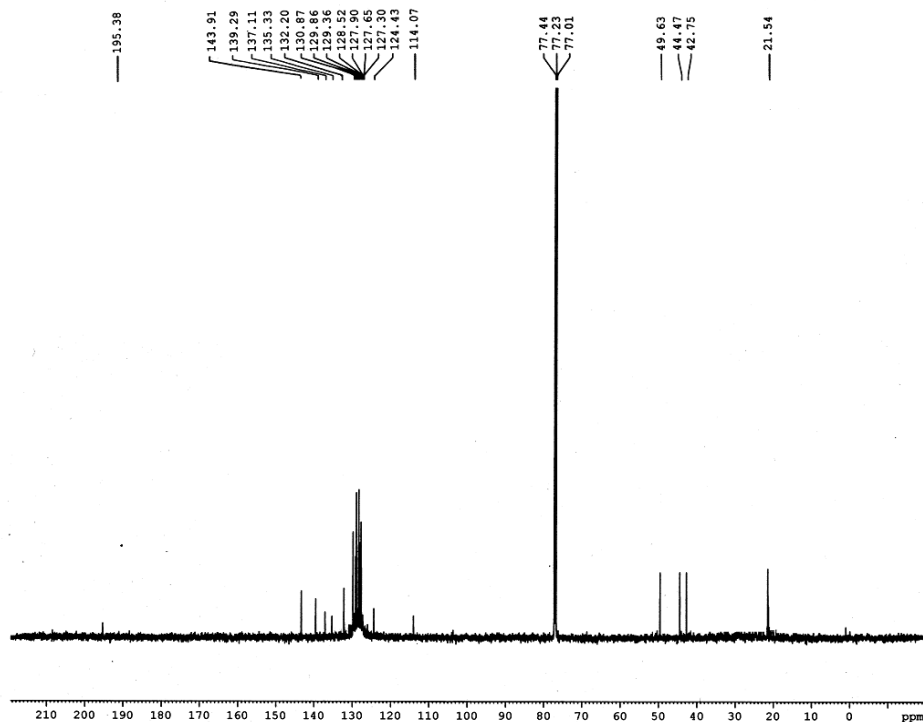
Current Data Parameters  
NAME aks-GP-176-31-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131031  
Time 23.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 2048  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

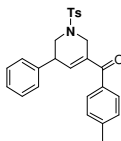
===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128670 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 2m

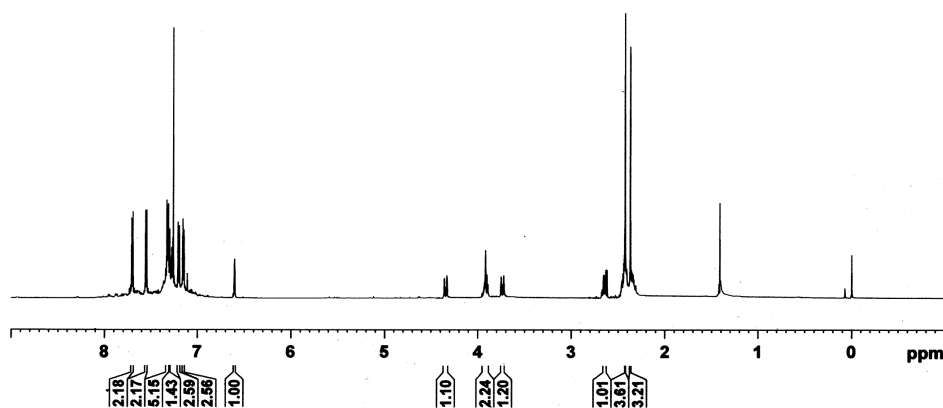


Current Data Parameters  
NAME GP-178-U\_1h  
EXFNO 1  
PROCNO 1

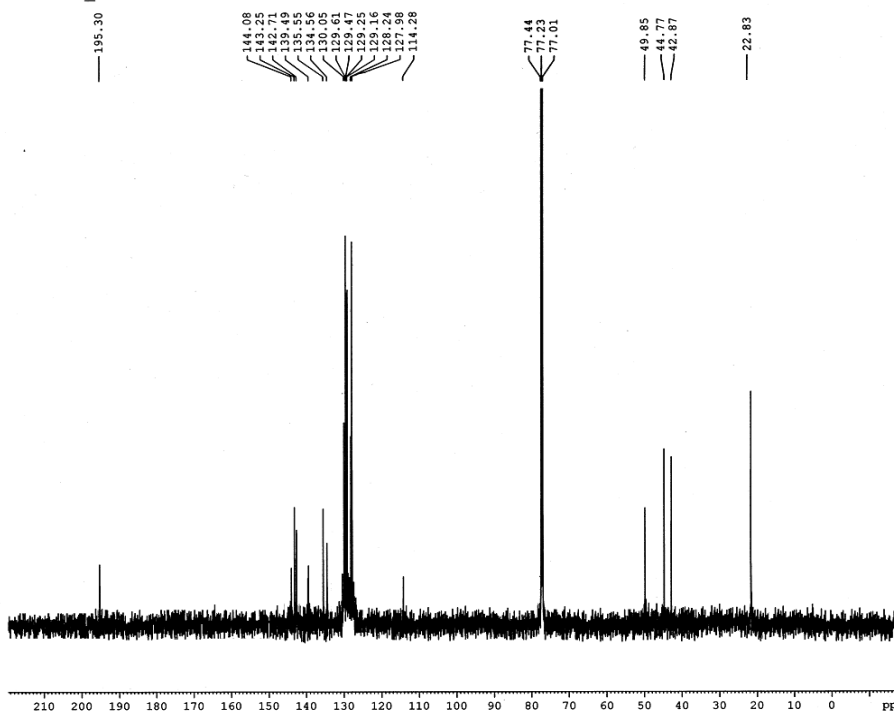
F2 - Acquisition Parameters  
Date 20131030  
Time 12.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.750 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 65.24  
DW 41.600 usec  
DE 6.50 usec  
TE 297.5 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700149 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



GP-178-U\_13C



Current Data Parameters  
NAME GP-178-U\_13C  
EXFNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20131030  
Time 17.39  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 297.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

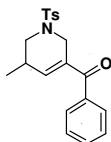
CHANNEL f1  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

CHANNEL f2  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

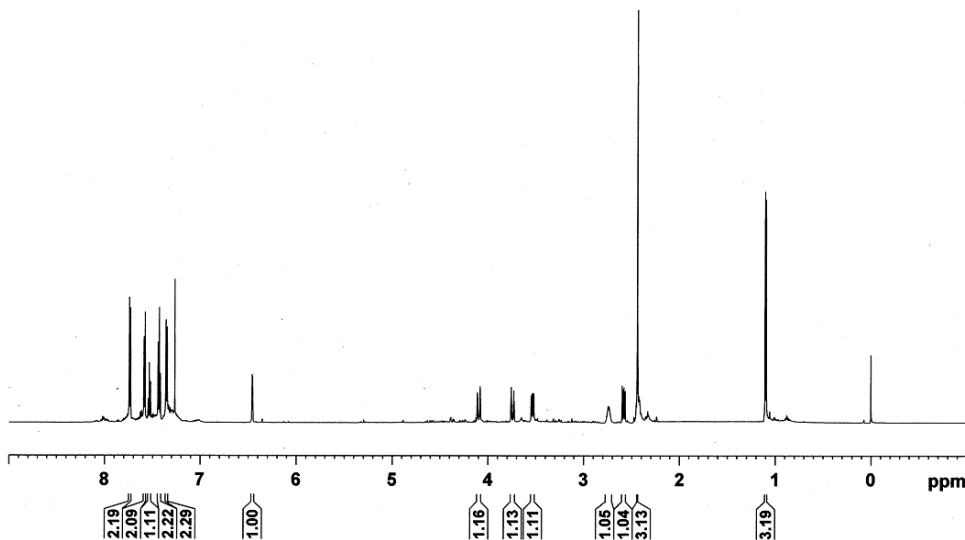
F2 - Processing parameters  
SI 16384  
SF 150.9128369 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 2o

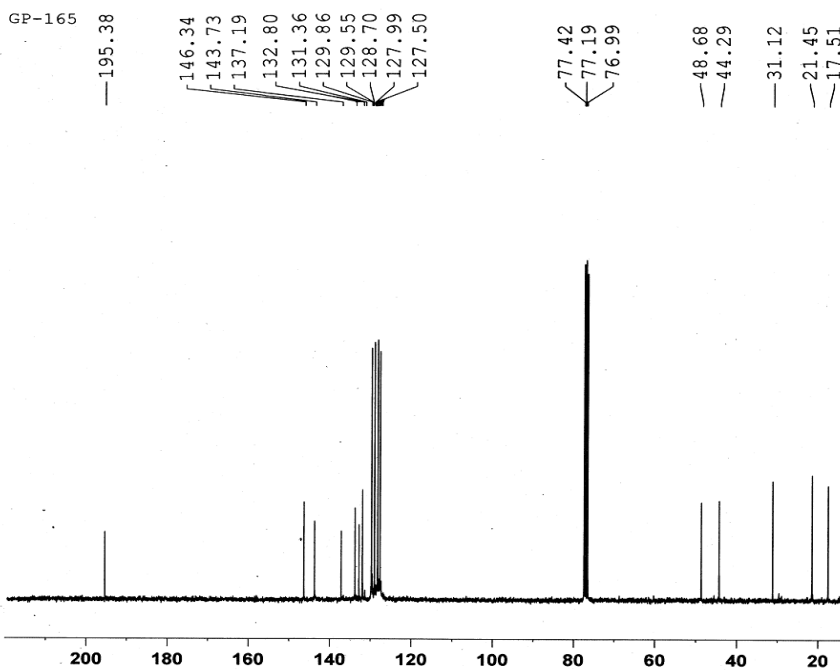
aks-GP-165-1H



Current Data Parameters  
 NAME aks-GP-165-1H  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date 20131027  
 Time 17.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 12019.239 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 54.94  
 DW 41.600 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TDO 1  
 ===== CHANNEL f1 =====  
 SFO1 600.137063 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PL1 21.00000000 W  
 F2 - Processing parameters  
 SI 16384  
 SF 600.1700123 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



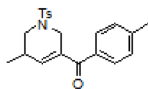
GP-165



NAME 2013-09-01-mm  
 EXPNO 1  
 PROCNO 1  
 Date 20130904  
 Time 16.12  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 1000  
 DS 4  
 SWH 18028.946 Hz  
 FIDRES 0.550197 Hz  
 AQ 0.9088159 sec  
 RG 80.6  
 DW 27.733 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1  
 ===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.80 usec  
 PL1 -0.50 dB  
 PL1W 34.66611099 W  
 SFO1 75.4778101 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 2.50 dB  
 PL12 19.20 dB  
 PL13 23.00 dB  
 PL2W 8.07971478 W  
 PL12W 0.17274120 W  
 PL13W 0.07201053 W  
 SFO2 300.1412006 MHz  
 SI 32768  
 SF 75.4702718 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

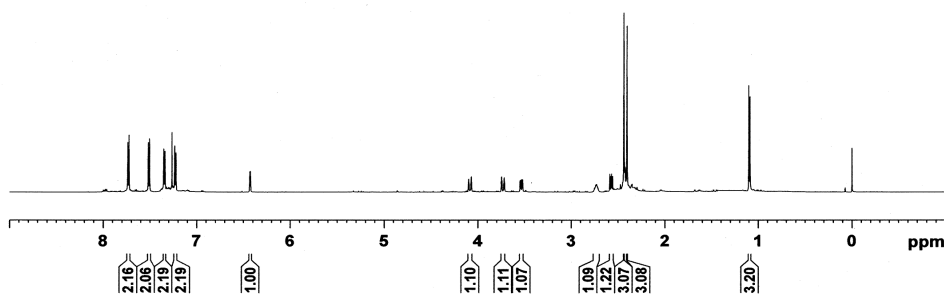


# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 2p



Current Data Parameters  
 NAME aks-gp-174-1h  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date 20131027  
 Time 16.30  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 12019.230 Hz  
 FIDRES 0.266798 Hz  
 AQ 1.3631498 sec  
 RG 49.39  
 DW 41.600 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TDO 1

CHANNEL f1  
 SFO1 600.1737063 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 21.00000000 W  
 F2 - Processing parameters  
 SI 16384  
 SF 600.1700126 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



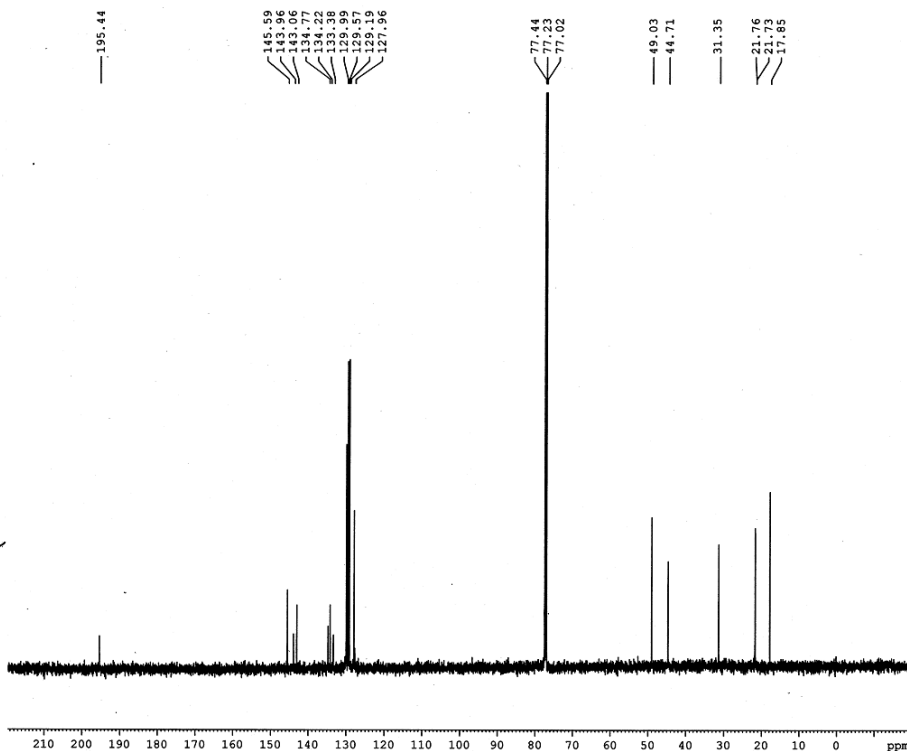
aks-gp-174-13C



Current Data Parameters  
 NAME aks-gp-174-13C  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date 20131027  
 Time 16.40  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 333  
 DS 2  
 SWH 36057.691 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 65.24  
 DW 13.867 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

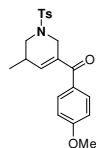
CHANNEL f1  
 SFO1 150.9279571 MHz  
 NUC1 13C  
 P1 10.50 usec  
 PLW1 95.00000000 W  
 CHANNEL f2  
 SFO2 600.1724007 MHz  
 NUC2 1H  
 CPDPRG12 waltz16  
 PCPD2 70.00 usec  
 PLW2 21.00000000 W  
 PLW12 0.61714000 W  
 PLW13 0.30239999 W

F2 - Processing parameters  
 SI 16384  
 SF 150.9128370 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 2q

aks-Gp-175-1H

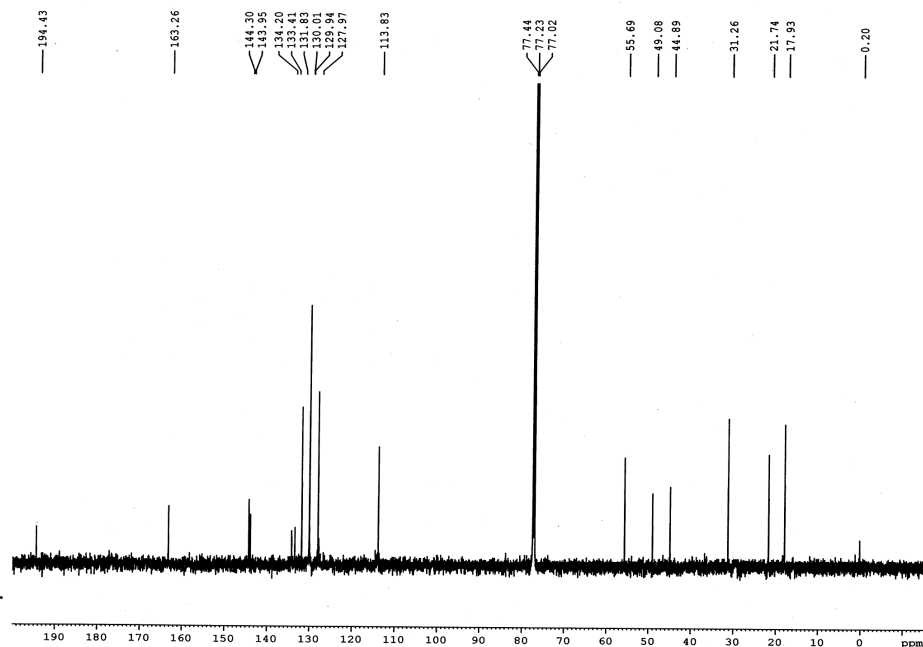
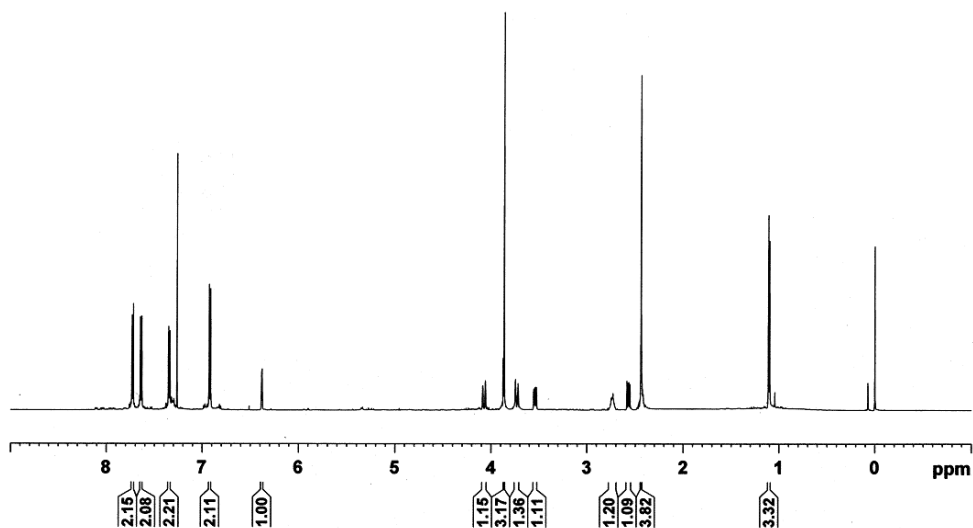


Current Data Parameters  
NAME aks-Gp-175-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131027  
Time 15.00  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 792  
DM 41.600 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700123 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME aks-Gp-175-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131027  
Time 15.14  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 479  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DM 13.867 usec  
DE 6.50 usec  
TE 299.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

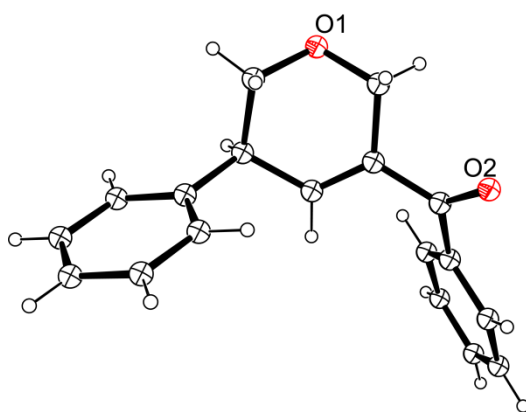
CHANNEL f1  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

CHANNEL f2  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128348 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

The crystal parameters of compound **2a**

	<b>2a- CCDC 979057</b>
Formula	C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>
Formula weight	264.31
<i>T</i> /K	296(2)
Crystal system	Monoclinic
Space group	P 21/c
<i>a</i> /Å	12.3796(15)
<i>b</i> /Å	10.5493(15)
<i>c</i> /Å	11.3168(13)
$\alpha$ /°	90.00
$\beta$ /°	106.991(8)
$\gamma$ /°	90.00
<i>V</i> /Å <sup>3</sup>	1413.4(3)
<i>Z</i>	4
Abs. Coeff./mm <sup>-1</sup>	0.080
Abs. Correction	Multi-scan
GOF on <i>F</i> <sup>2</sup>	1.008
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> 1 = 0.0448 <i>wR</i> 2 = 0.1138
<i>R</i> indices [all data]	<i>R</i> 1 = 0.0752 <i>wR</i> 2 = 0.1295



ORTEP diagram of **2a**: ORTEP diagram is drawn with 30% probability ellipsoid.