

## Supporting Information

### Stereoselective Synthesis of *O*-Tosyl Azabicyclic Derivatives *via* Aza Prins

### Reaction of Endocyclic *N*-Acyliminium Ions: Application to the Total

### Synthesis of (±)-*epi*-Indolizidine 167B and 209D

*KiranIndukuri, Jagadish Das and Anil K. Saikia\**

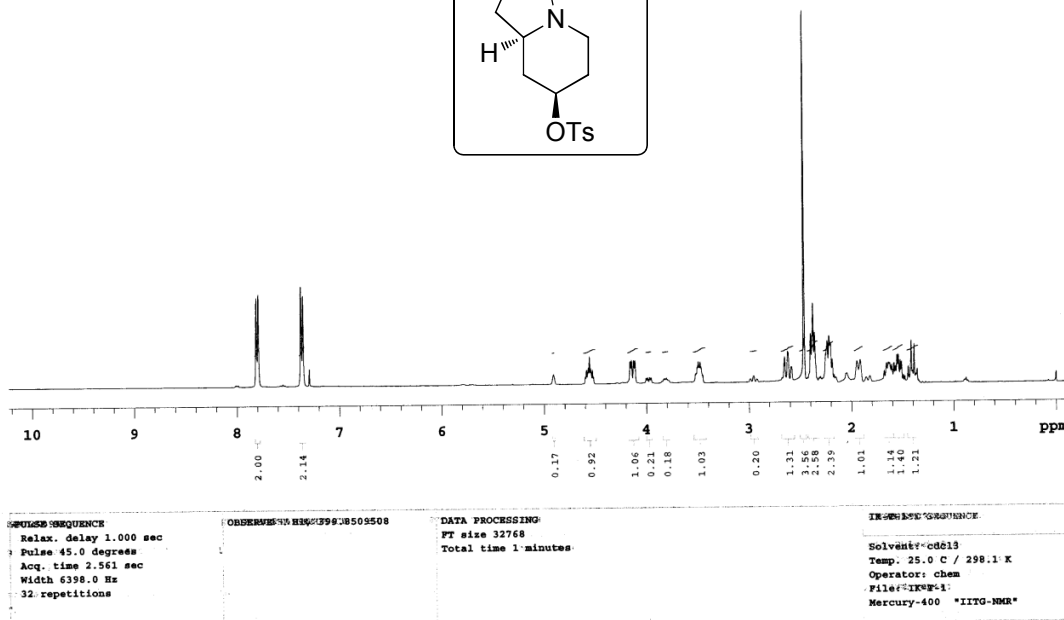
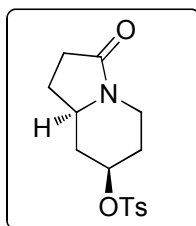
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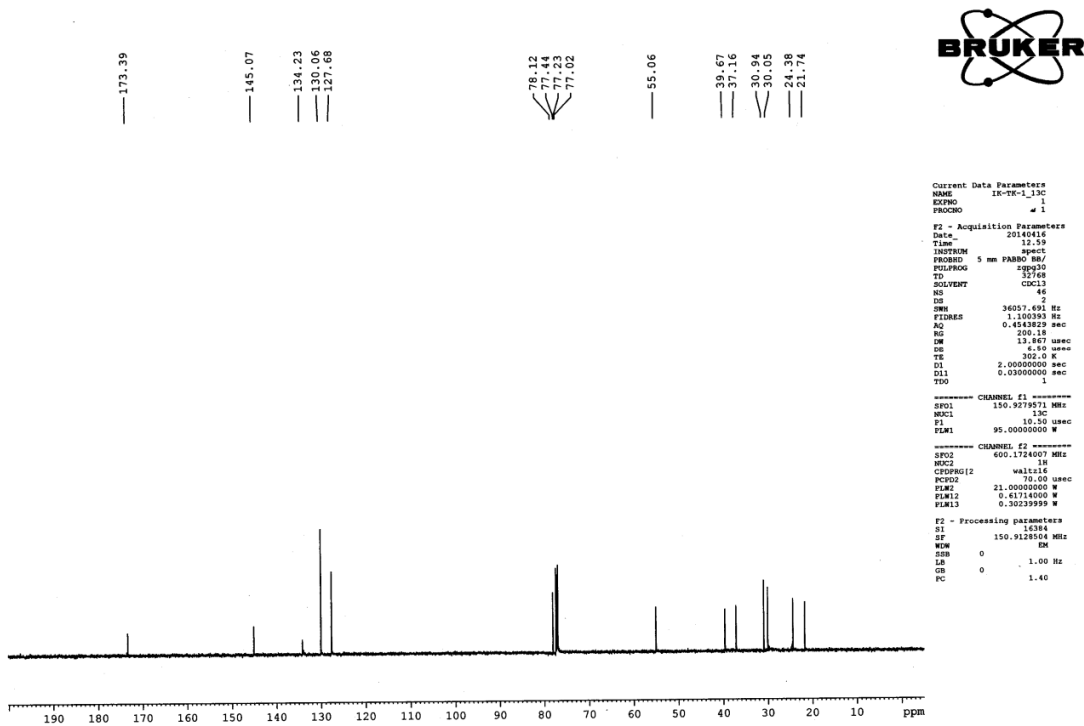
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# $^1\text{H}$ and $^{13}\text{C}$ Spectra of compound **6a**



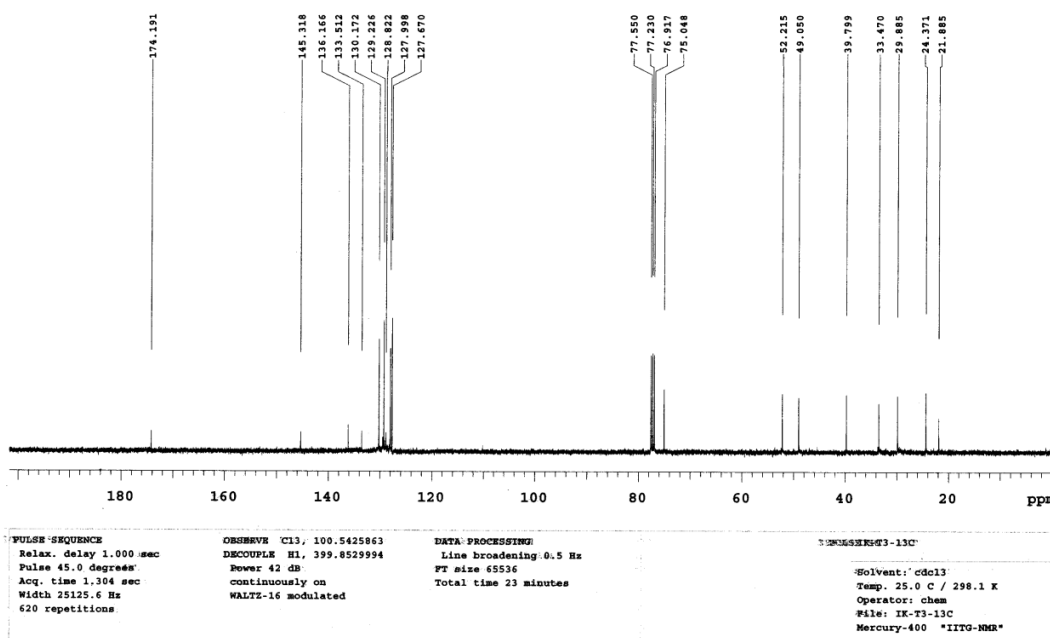
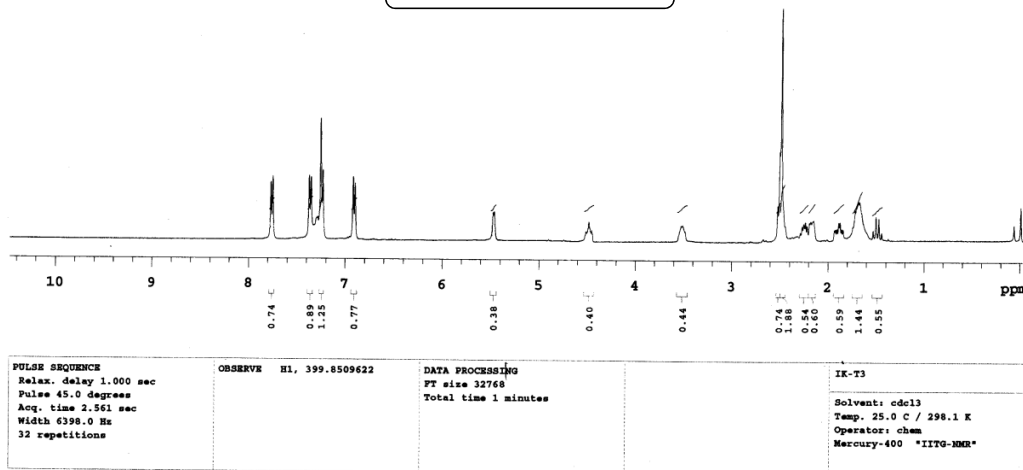
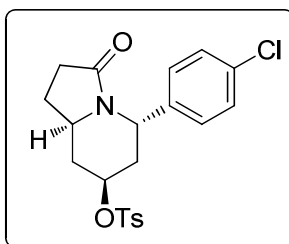
IK-TK-1\_13C



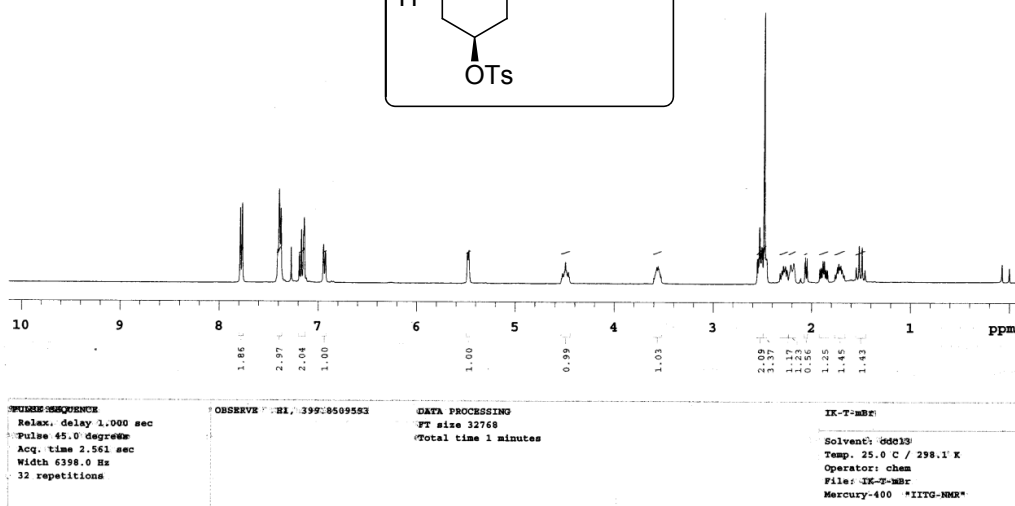
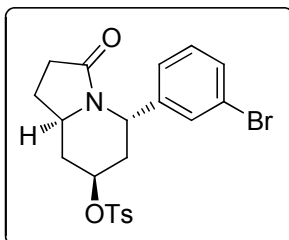
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PROCNO: 1
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PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
AQ: 45
DS: 2
SWH: 3637.493 Hz
FIDRES: 1.100393 Hz
RG: 0.4143029 sec
AQ: 200.18
DE: 13.807 usec
DB: 4.50 usec
TE: 292.0 K
D1: 2.0000000 sec
d11: 0.0300000 sec
TD0: 1
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SFO1 150.9279571 MHz
NUC1 13C
P1 10.00 usec
PLM1 95.0000000 W
===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPOPRG12 waltz16
PCPDZ 70.00 usec
PLM2 21.0000000 W
PLM12 0.41714000 W
PLM13 0.30239999 W
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PC 1.40
    
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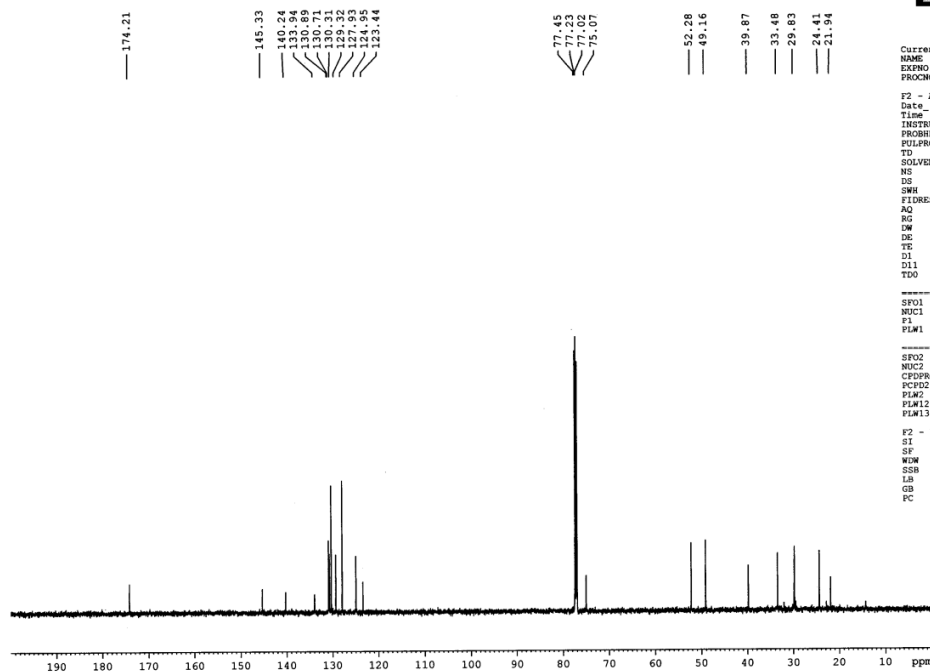
$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6b**



# $^1\text{H}$ and $^{13}\text{C}$ Spectra of compound **6c**



IK\_TMBR\_13C



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 PROCNO 1

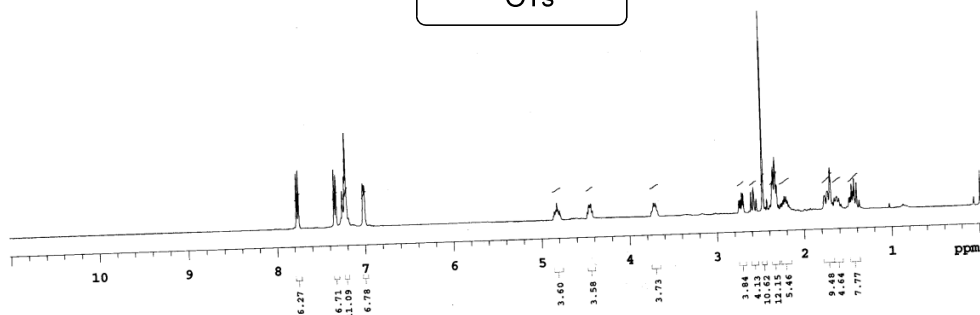
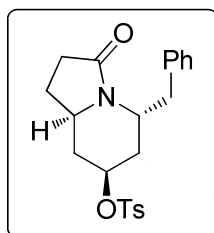
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 TD 32768  
 SOLVENT CDCl3  
 NS 170  
 DS 4  
 SWH 36057.651 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 65.24  
 DW 13.867 usec  
 DE 6.50 usec  
 TE 301.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

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 P1 10.50 usec  
 PLW1 95.00000000 W

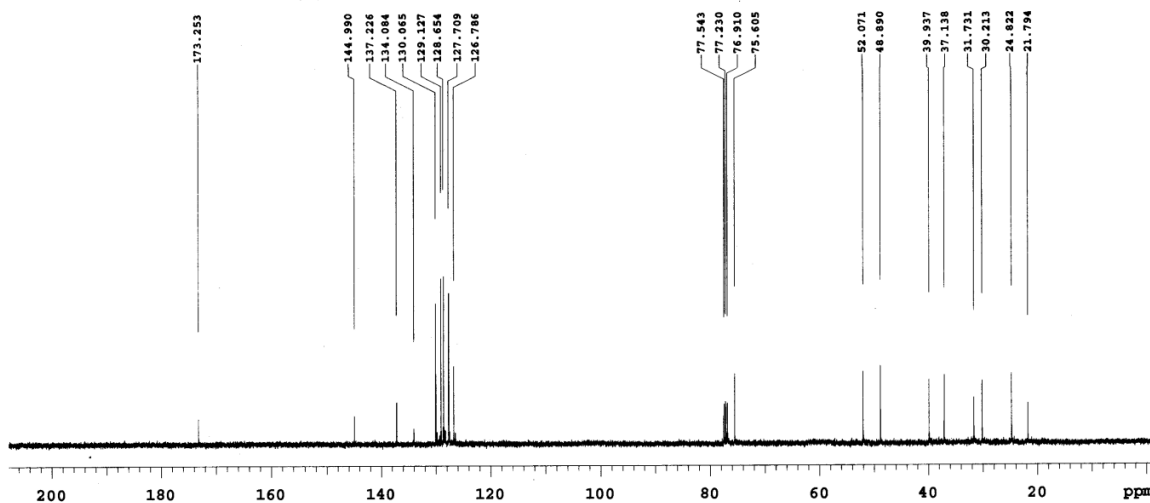
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 PLW2 21.00000000 W  
 PLW12 0.61714000 W  
 PLW13 0.30219999 W

F2 - Processing parameters  
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 SF 150.9126371 MHz  
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 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6d**

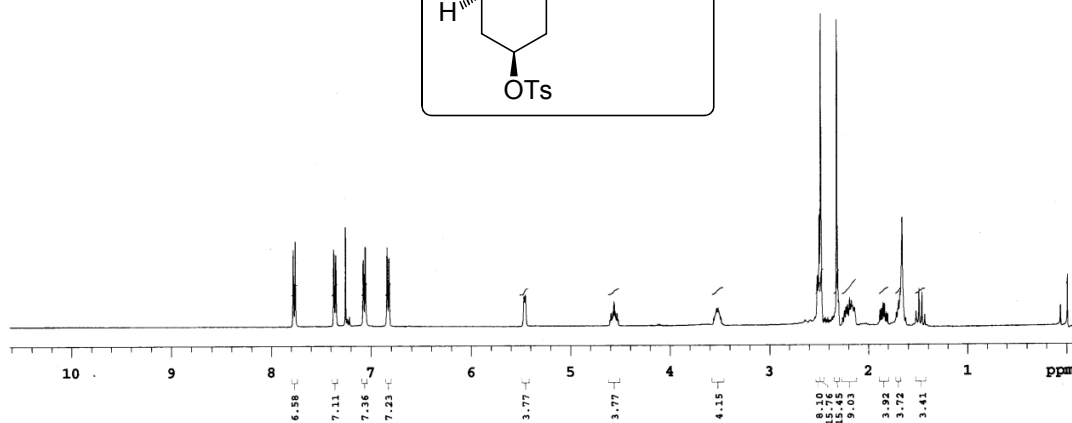
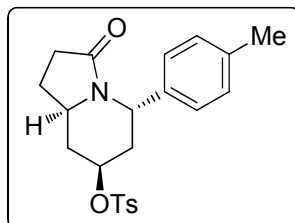


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509634	DATA PROCESSING FT size 32768 Total time 1 minutes	IK-T5
			Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"

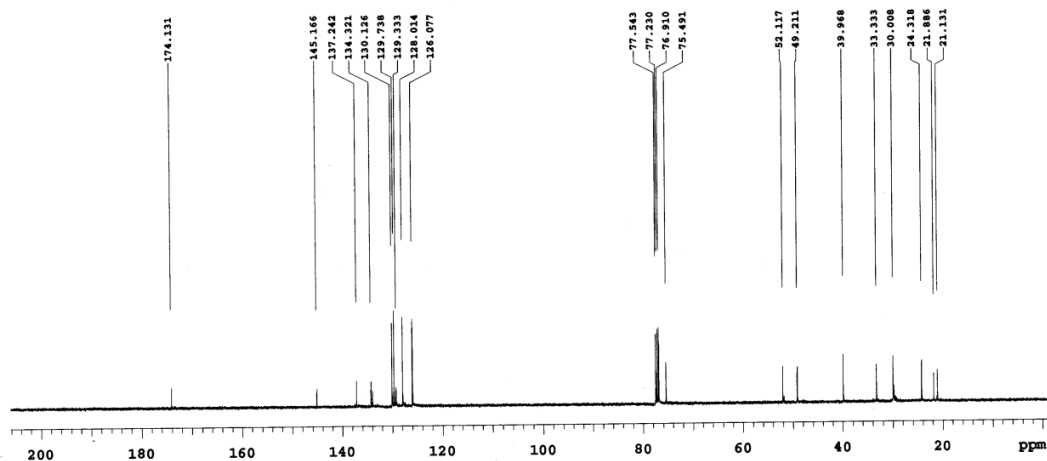


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 100 repetitions	OBSERVE C13, 100.5425970 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 3 minutes	IK-T5-13C
			Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"

$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6e**

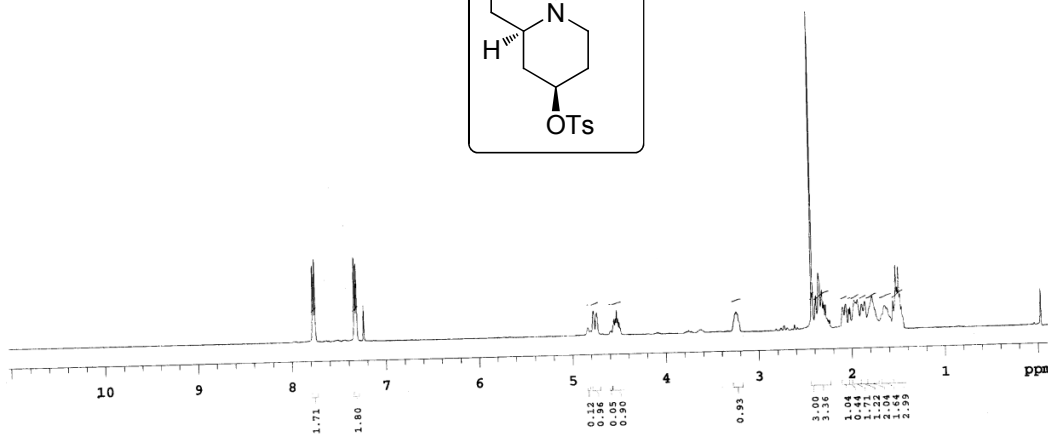
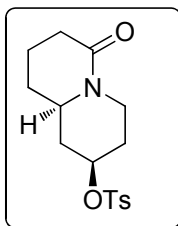


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>EX-T2</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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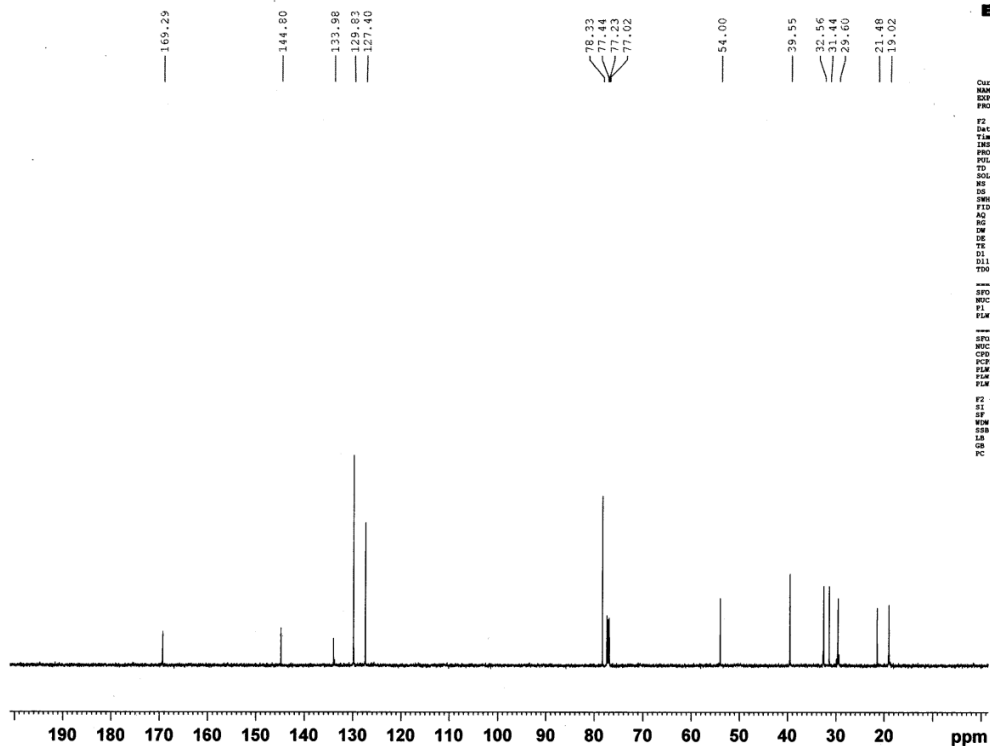
<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1420 repetitions	<b>OBSERVE</b> C13, 100.5425878 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 54 minutes	<b>EX-T-2-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 6g



PULSE SEQUENCE	OBSERVE	DATA PROCESSING	IK-T10
Relax. delay 1.000 sec Pulse 45.0 degree Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	H1, 399.8509722	PT size 32768 Total time 1 minutes	Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *117G-NMR*

IK-T10\_13C



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PROCNO   1

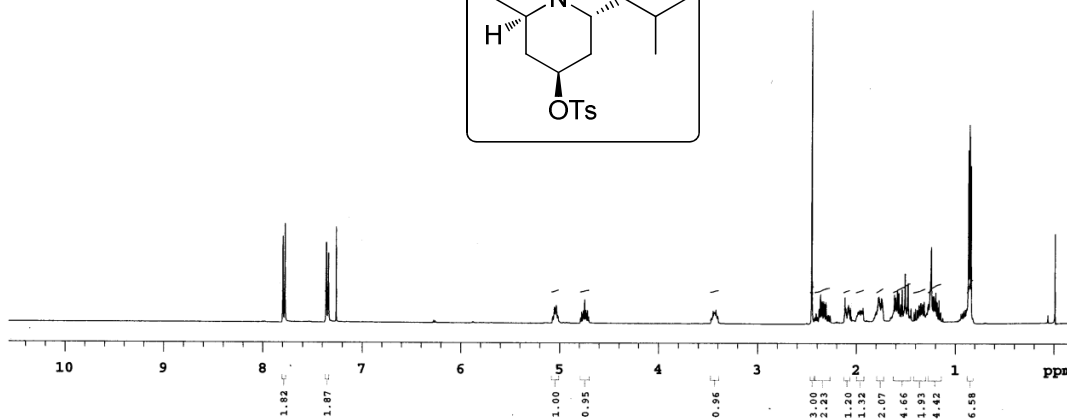
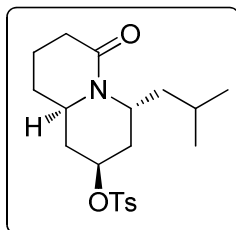
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INSTRUM  spect
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PULPROG  zgpg30
SOLVENT  CDCl3
NS       88
DS       2
SWH      34057.461 Hz
FIDRES   1.100393 Hz
AQ        0.4543829 sec
RG        60.24
DE        15.467 usec
TE        300.2 K
D1        2.0000000 sec
d11       0.03000000 sec
TD        1

===== CHANNEL f1 =====
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P1       19.50 usec
PL1      05.0000000 W

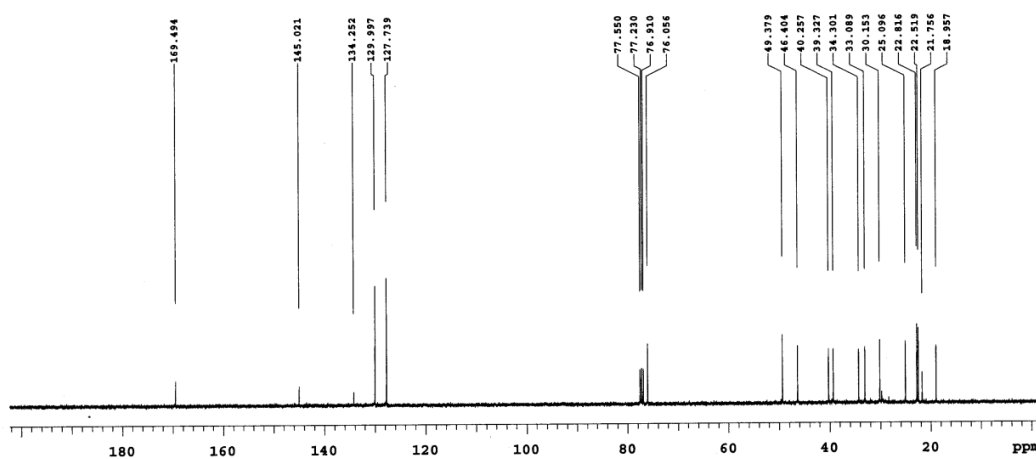
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P2       70.00 usec
PL2      0.43714000 W
PL12     0.30239999 W

F2 - Processing parameters
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SF        150.912774 MHz
WDW       EM
SSB       0
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PC        1.40
    
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$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6h**



<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>IX-T14</b> Solvent: cdCl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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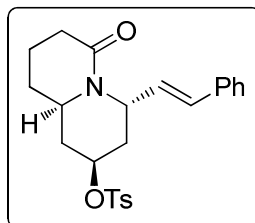


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 190 repetitions	<b>OBSERVE</b> C13, 100.5425924 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 7 minutes	<b>IX-T14-13C</b> Solvent: cdCl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound **6i**

IK-T12\_1H



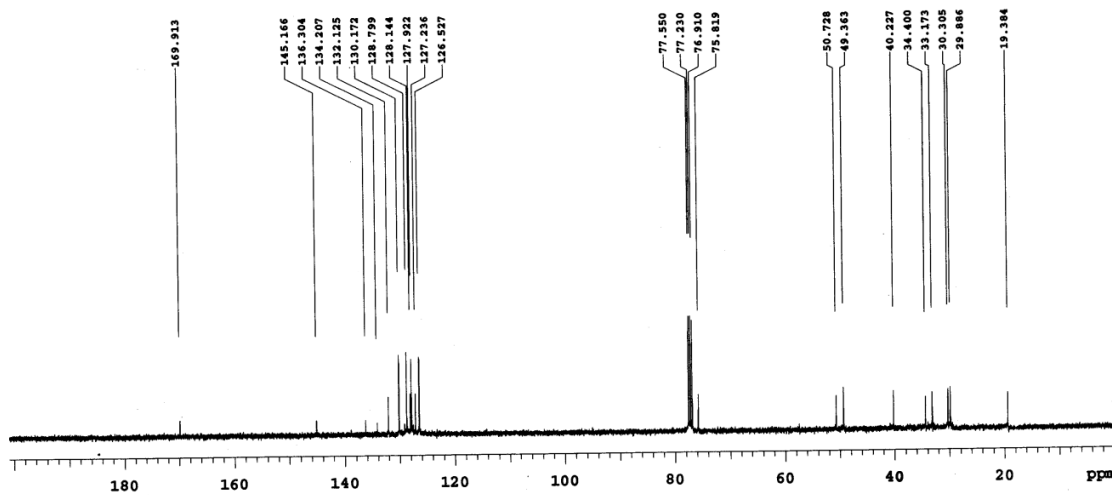
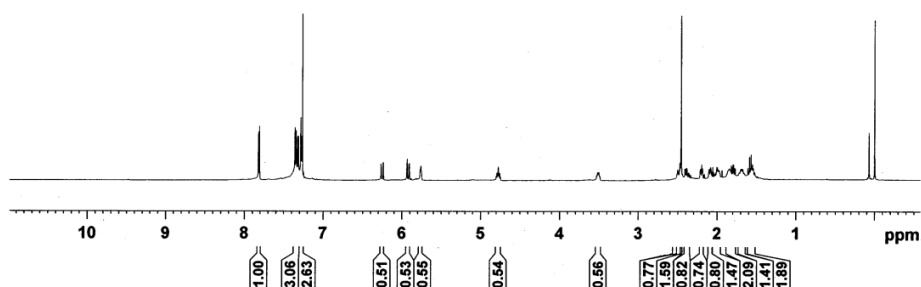
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PROCNO    1

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PULPROG   zgpg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.368798 Hz
AQ         1.3631998 sec
RG         80.22
DM         41.600 usec
DE         1.50 usec
TE         299.1 K
D1         1.00000000 sec
TDO        1

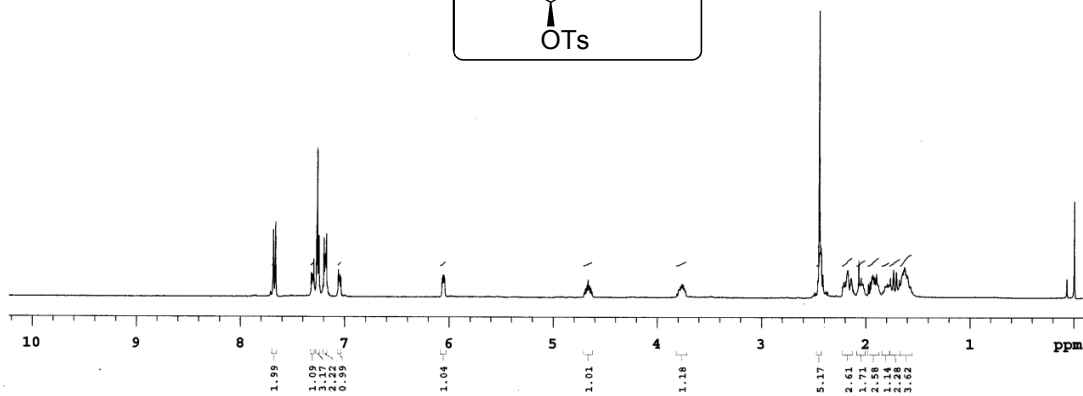
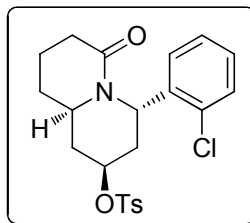
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NUC1       13
P1         12.00 usec
PLM1      21.00000000 W

F2 - Processing parameters
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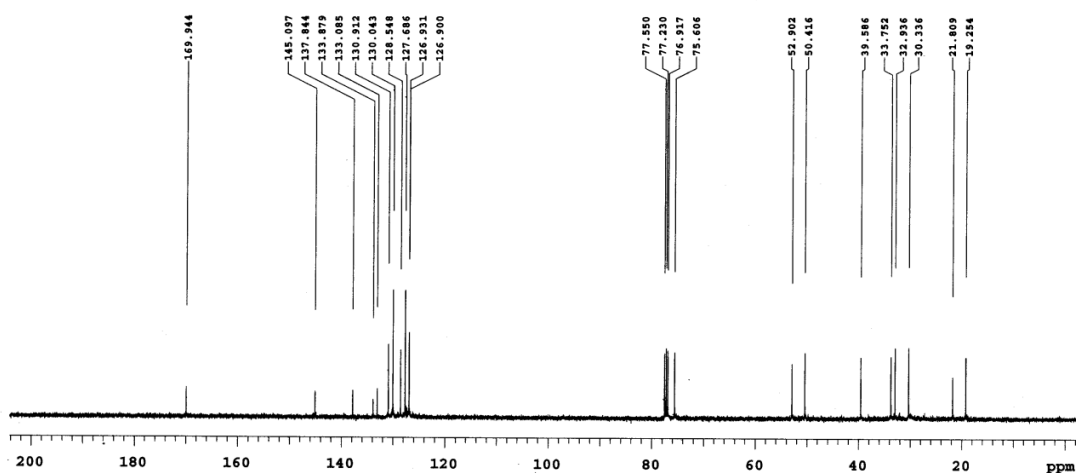


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25325.6 Hz 1710 repetitions	<b>OBSERVE</b> C13, 100.5425855 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 65 minutes	<b>IK-T12-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *11TG-NMR*
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<sup>1</sup>H and <sup>13</sup>C Spectra of compound **6j**

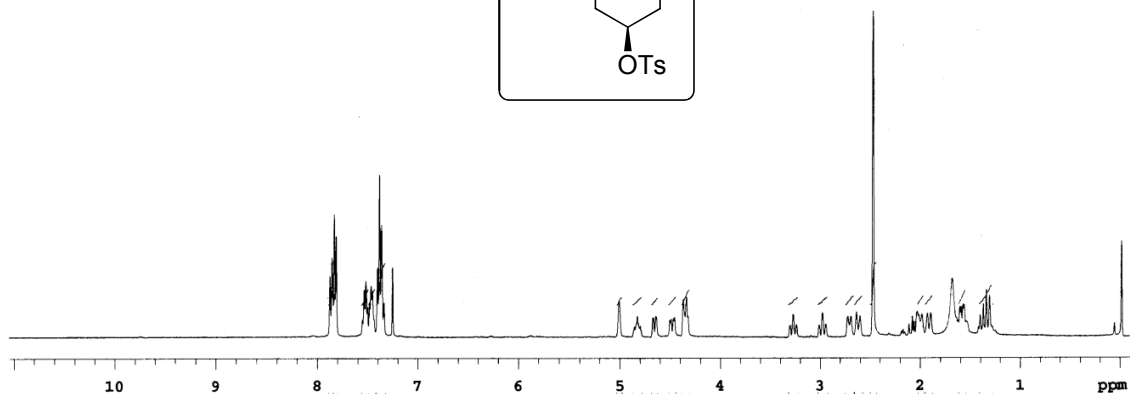
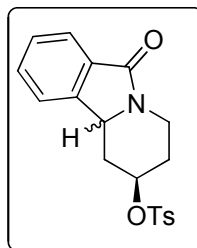


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634 DECOUPLE H1, 399.8509634 Power: 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> IK-T13 FT size 32768 Total time 1 minutes	<b>IK-T13</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: IK-T13 Mercury-400 *IITG-NMR*
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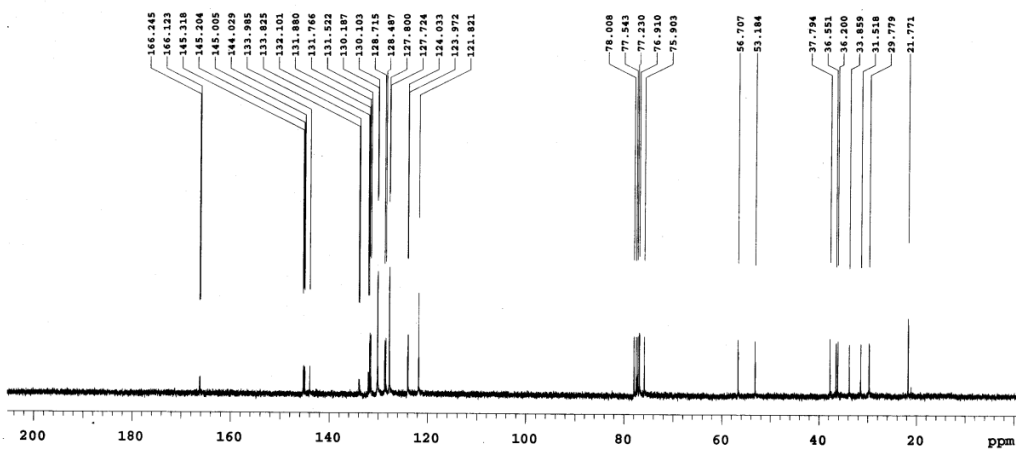


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 620 repetitions	<b>OBSERVE</b> C13, 100.5425909 DECOUPLE H1, 399.8529994 Power: 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> IK-T13-13C Line broadening 0.5 Hz FT size 65536 Total time 23 minutes	<b>IK-T13-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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<sup>1</sup>H and <sup>13</sup>C Spectra of compound **6k**



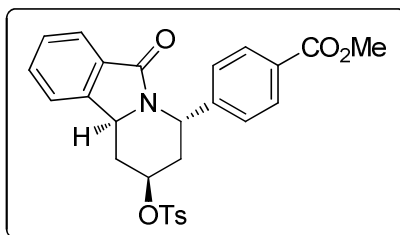
<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-T7</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-MMR*
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<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 350 repetitions	<b>OBSERVE</b> C13, 100.5426361 <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 13 minutes	<b>IK-T7-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-MMR*
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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 6I

IK-T6\_1H



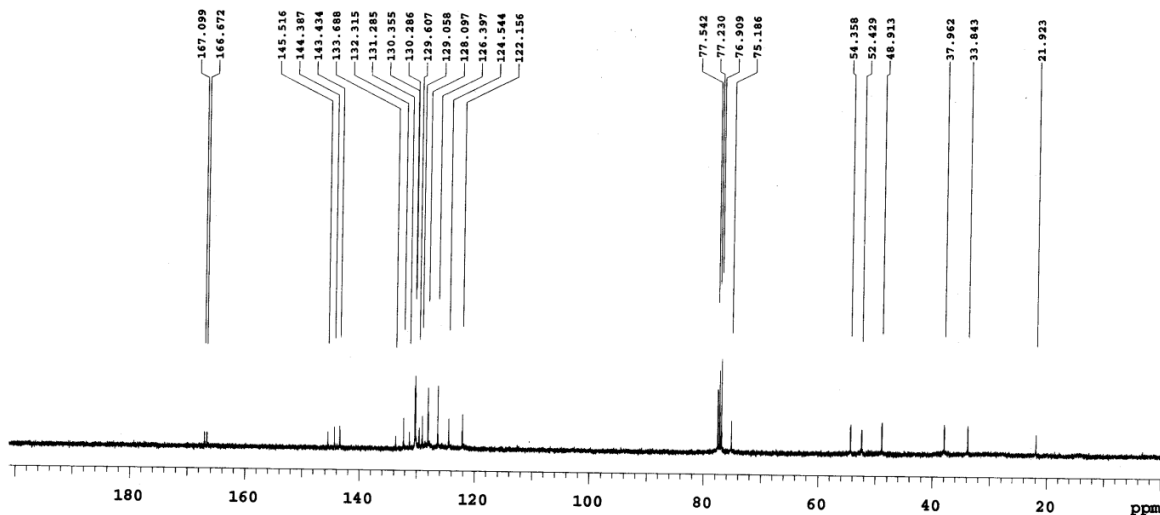
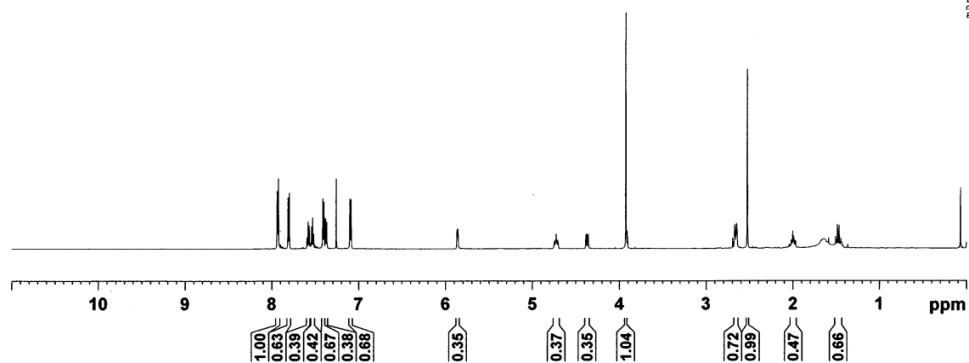
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PROCNO   1

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PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ       1.3611486 sec
RG       80.22
IN       41.600 usec
DE       6.50 usec
TE       299.0 K
D1       1.00000000 sec
TD0      1

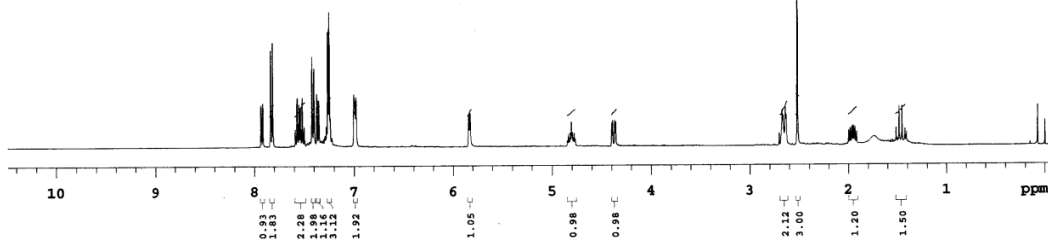
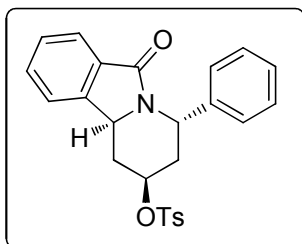
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NUC1     13C
P1       12.00 usec
PLW1     21.00000000 W

F2 - Processing parameters
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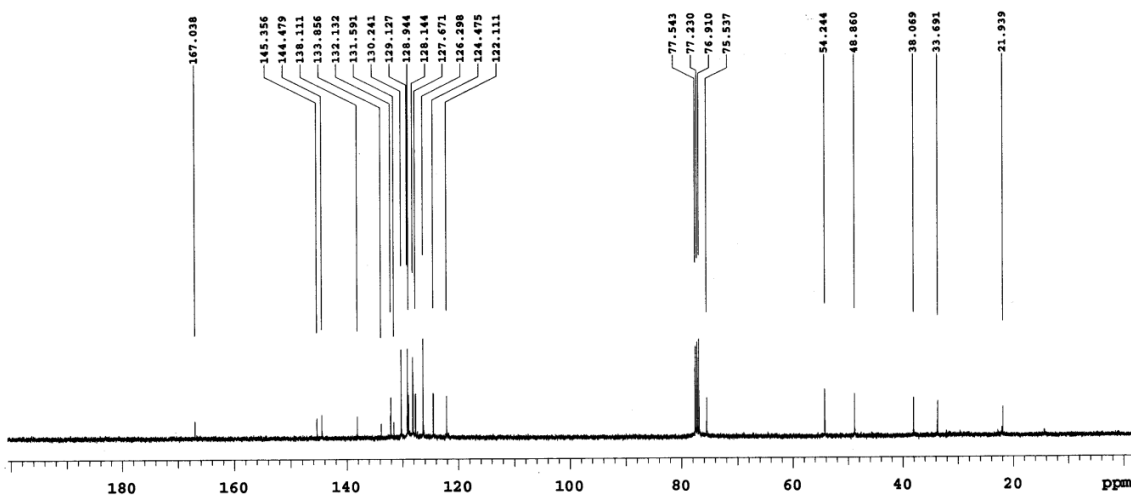


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1970 repetitions	<b>OBSERVE C13, 100.5425610</b> DDCOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 75 minutes	<b>IK-T6</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: cham Mercury-400 *IITG-NMR*
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$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6m**

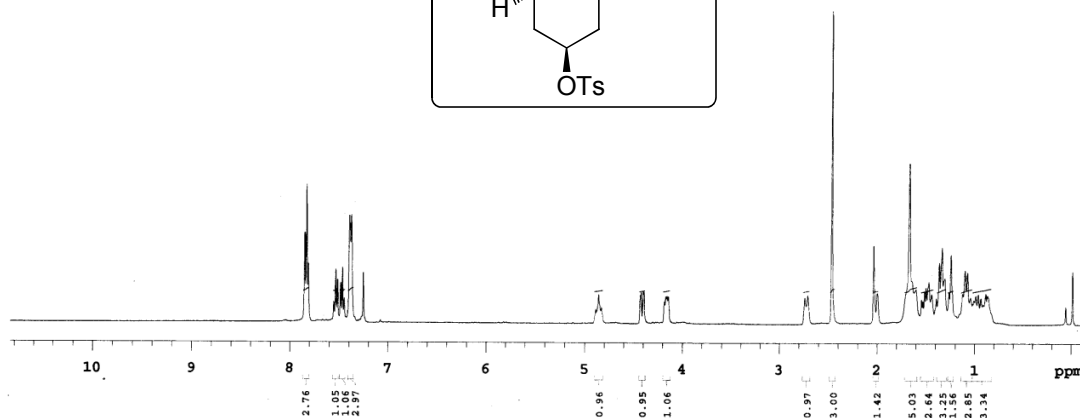
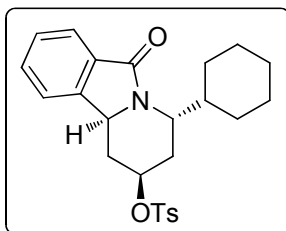


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509621	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-T11</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: IK-T11 Mercury-400 *IITG-RMR*
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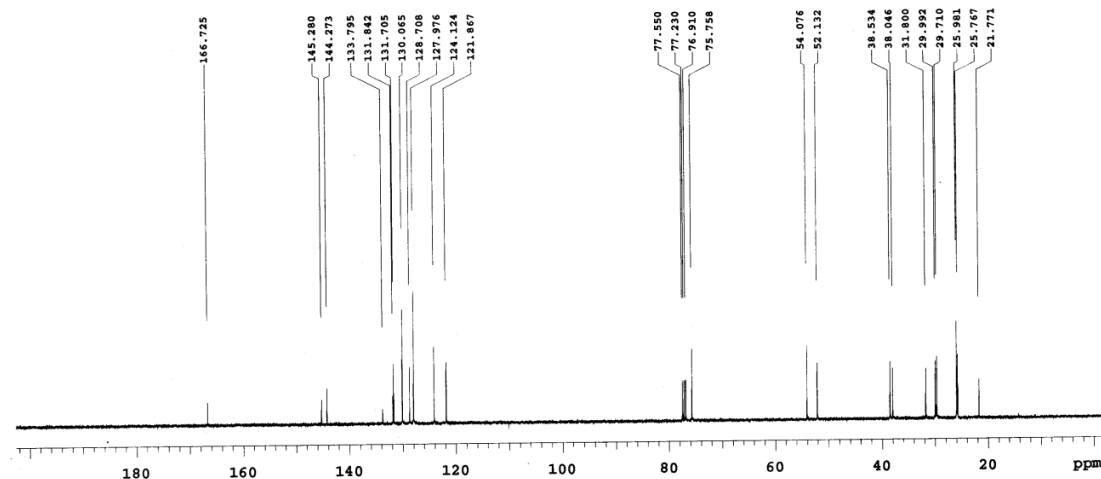


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 2010 repetitions	<b>OBSERVE</b> C13, 100.5425863 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 77 minutes	<b>IK-T11-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: IK-T11-13C Mercury-400 *IITG-RMR*
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$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6n**

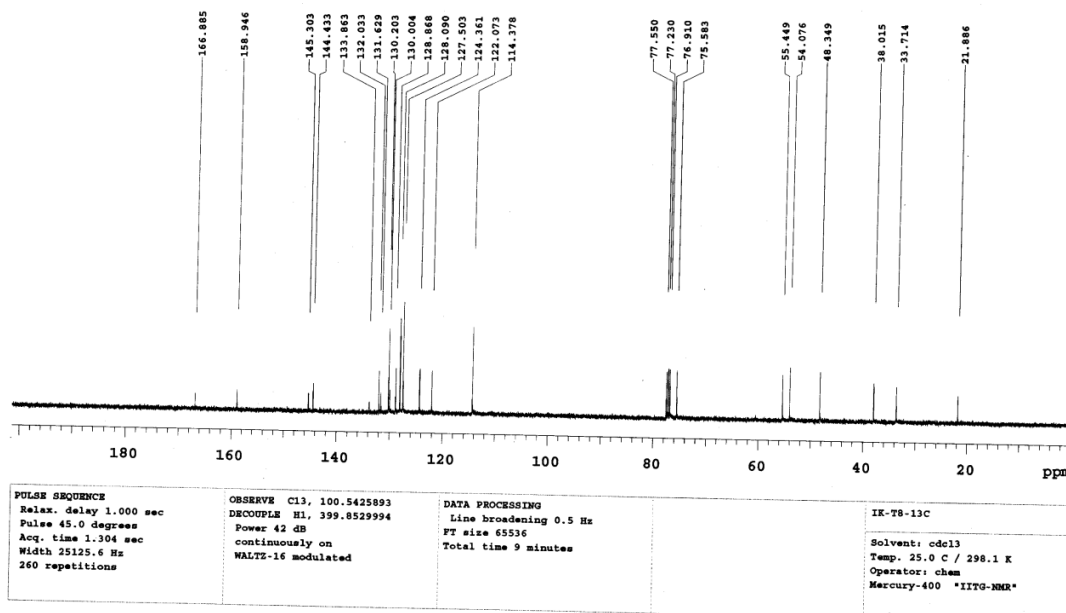
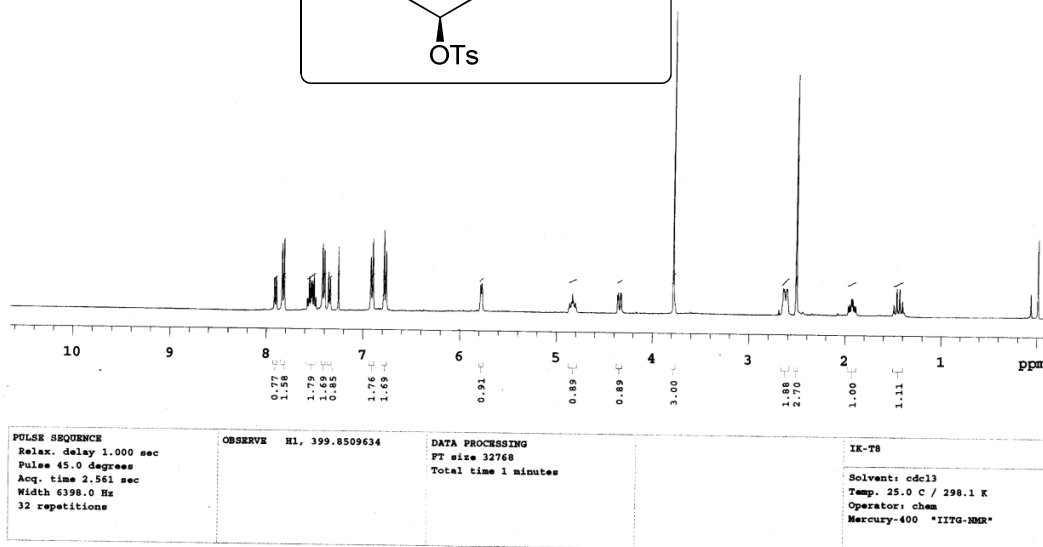
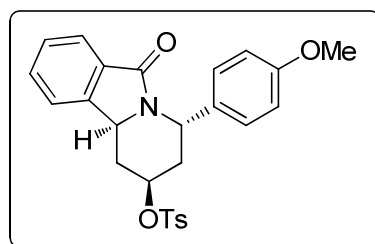


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-T9</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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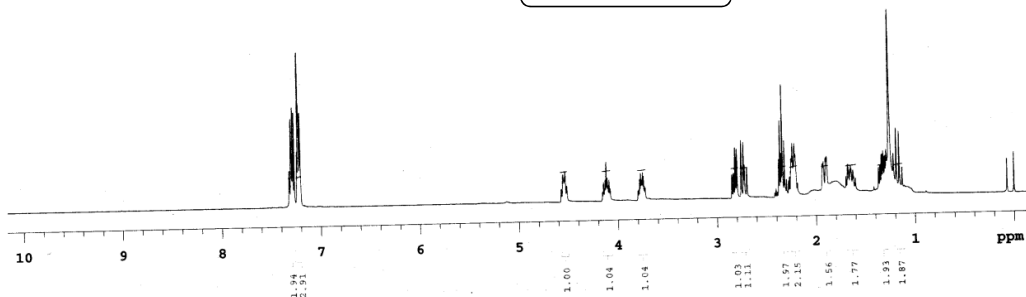
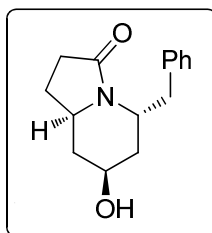


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 230 repetitions	<b>OBSERVE</b> C13, 100.5425932 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 8 minutes	<b>IK-T9-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **60**



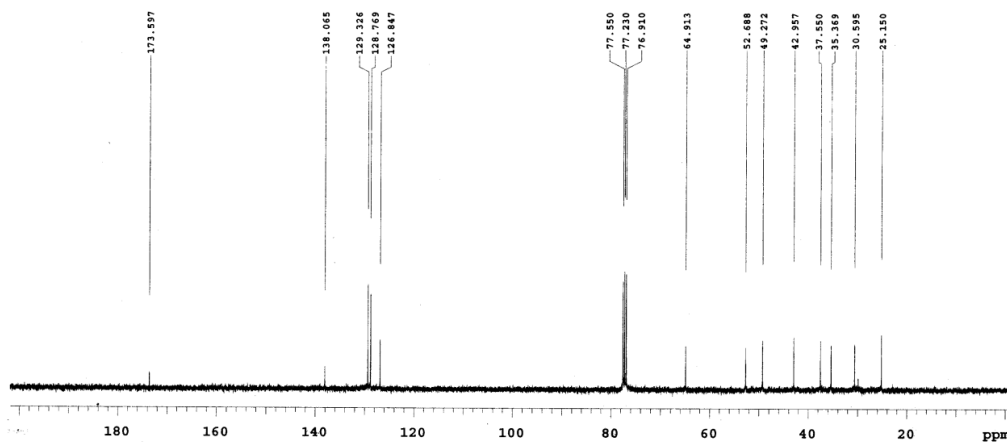
<sup>1</sup>H and <sup>13</sup>C Spectra of compound 6d'



PULSE SEQUENCE: OBSERVE H1, 399.8509613  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.561 sec  
 Width 6398.0 Hz  
 32 repetitions

DATA PROCESSING: FT size 32768  
 Total time 1 minutes

IX-BN-OH  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 \*IITG-NMR\*



PULSE SEQUENCE: OBSERVE H1, 100.5425840  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.304 sec  
 Width 25125.6 Hz  
 1200 repetitions

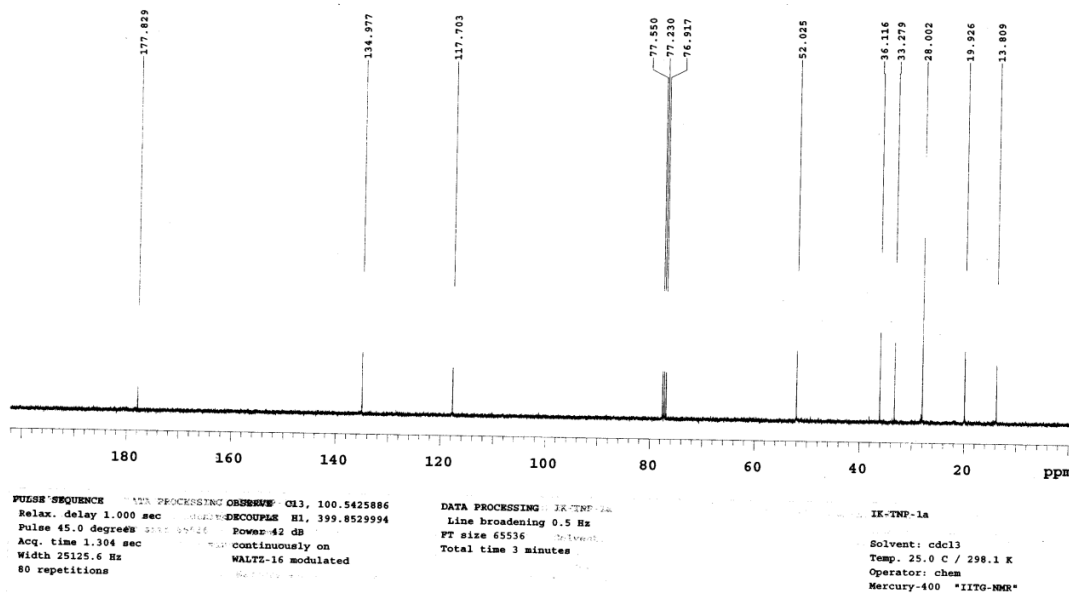
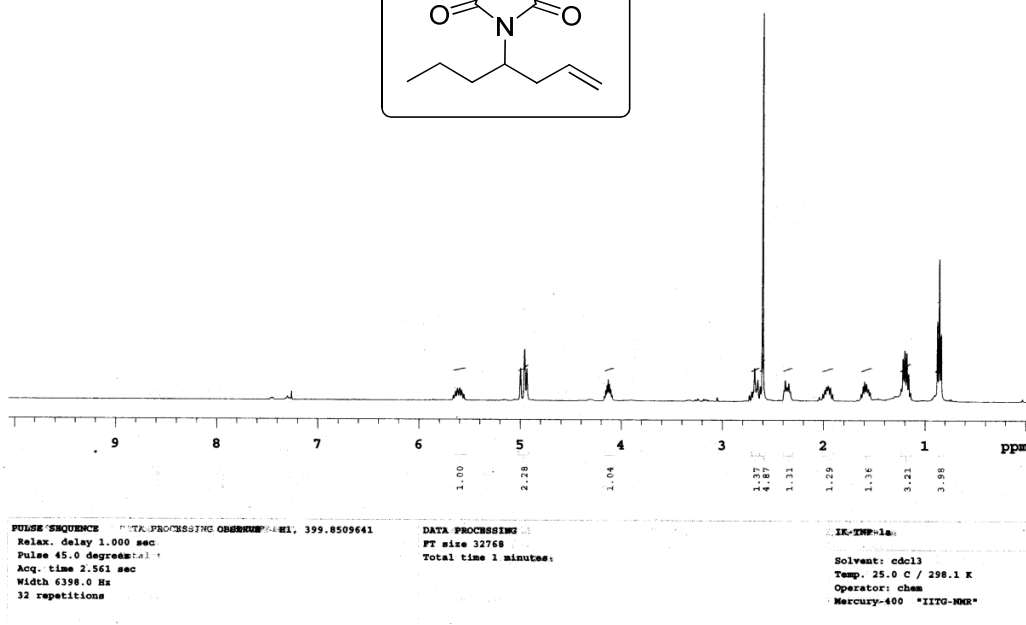
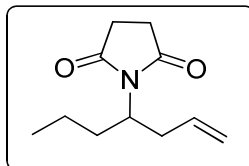
DECOUPLE H1, 399.8529994  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated

DATA PROCESSING: FT size 65536  
 Line broadening 0.5 Hz  
 Total time 46 minutes

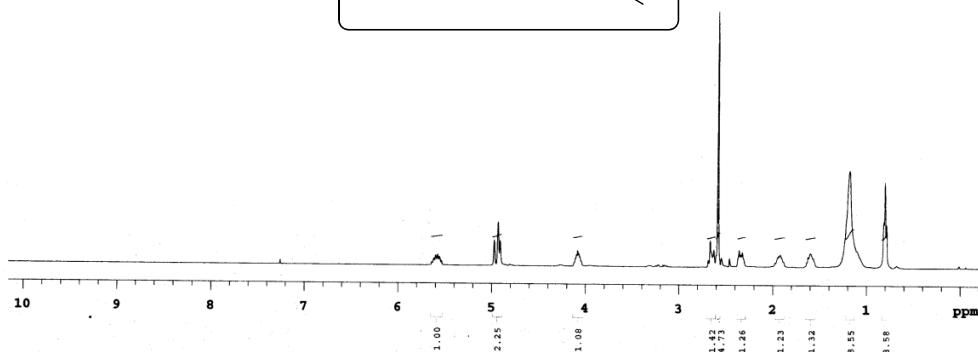
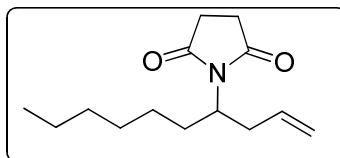
IX-BN-OH-13C  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 \*IITG-NMR\*



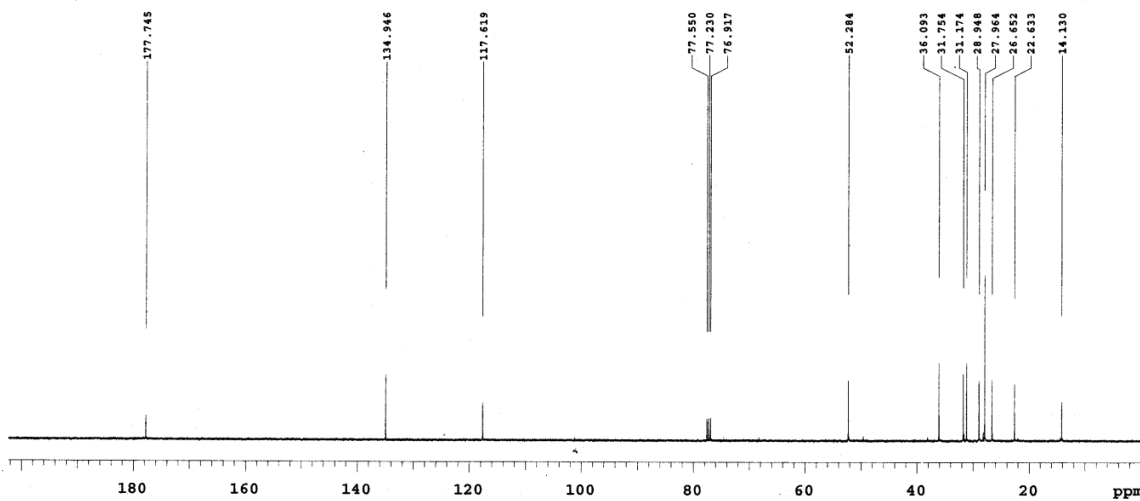
# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 9p



$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **9q**

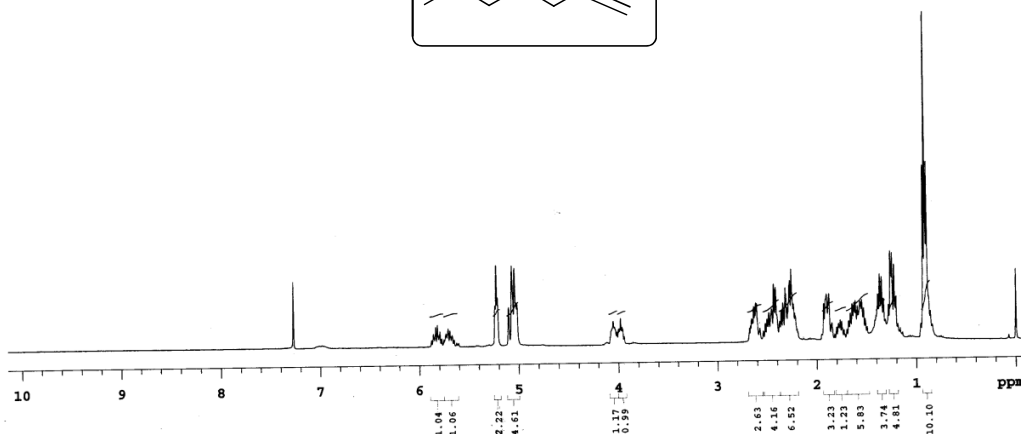
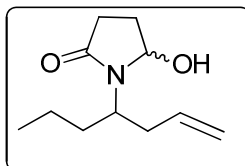


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> $^1\text{H}$ , 399.8509641	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-TMP-2a</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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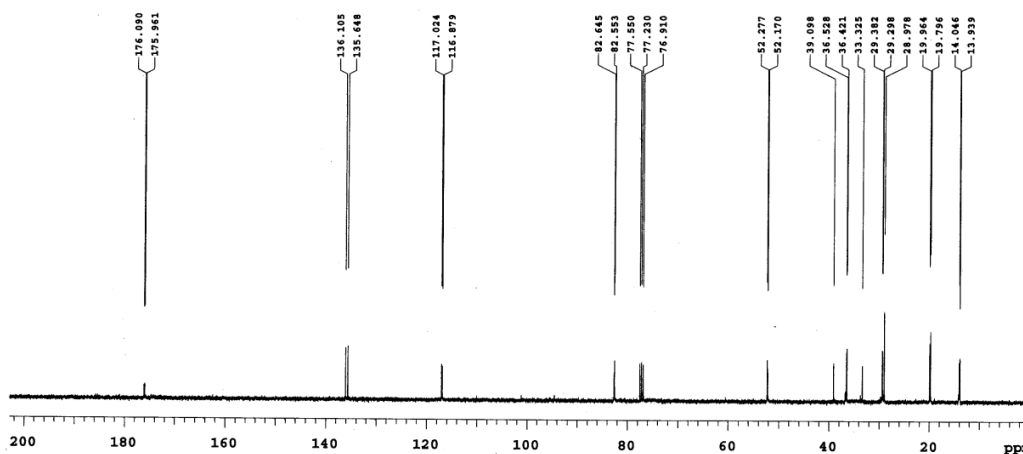


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 110 repetitions	<b>OBSERVE</b> $^{13}\text{C}$ , 100.9425909 <b>DECOUPLE</b> $^1\text{H}$ , 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 4 minutes	<b>IK-TMP-2a-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: IK-TMP-2a-13C Mercury-400 *IITG-NMR*
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<sup>1</sup>H and <sup>13</sup>C Spectra of compound 5p

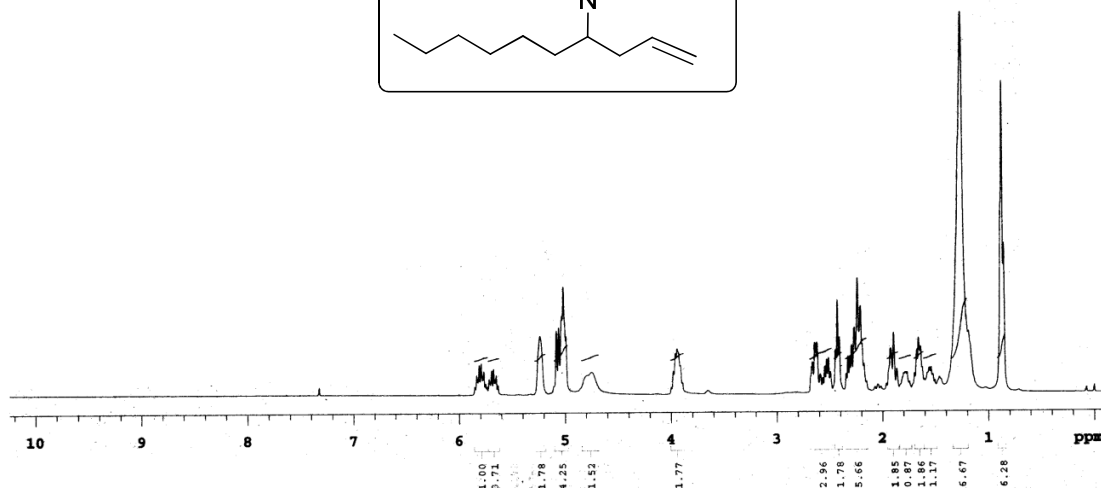
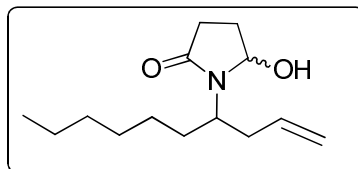


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-TNP-1b</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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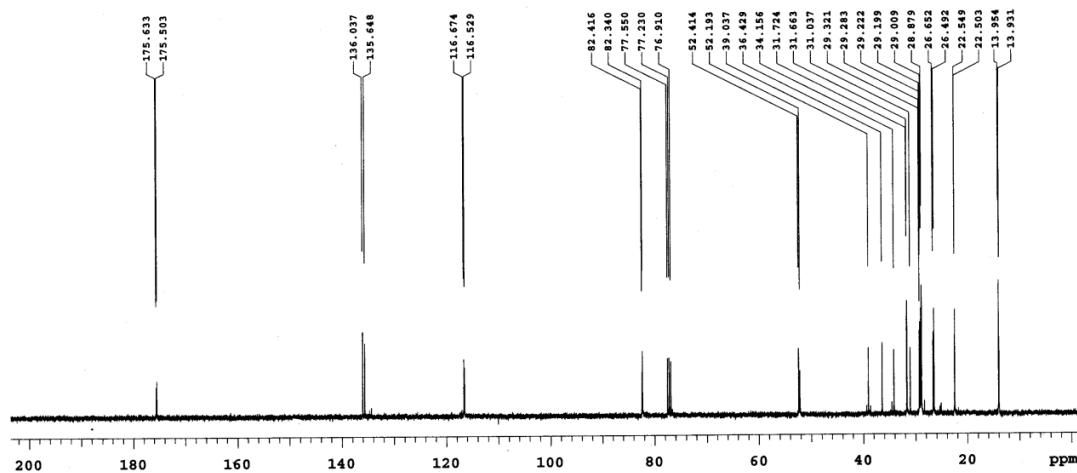


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 90 repetitions	<b>OBSERVE</b> C13, 100.5425955 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 3 minutes	<b>IK-TNP-1b-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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<sup>1</sup>H and <sup>13</sup>C Spectra of compound 5q

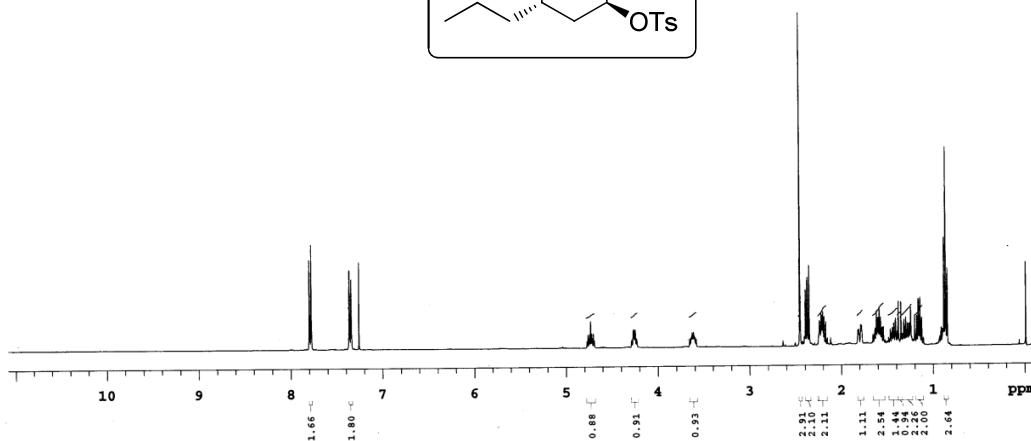
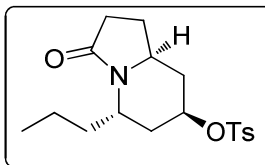


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> <sup>1</sup> H, 399.8509371	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IX-TWP-2b1</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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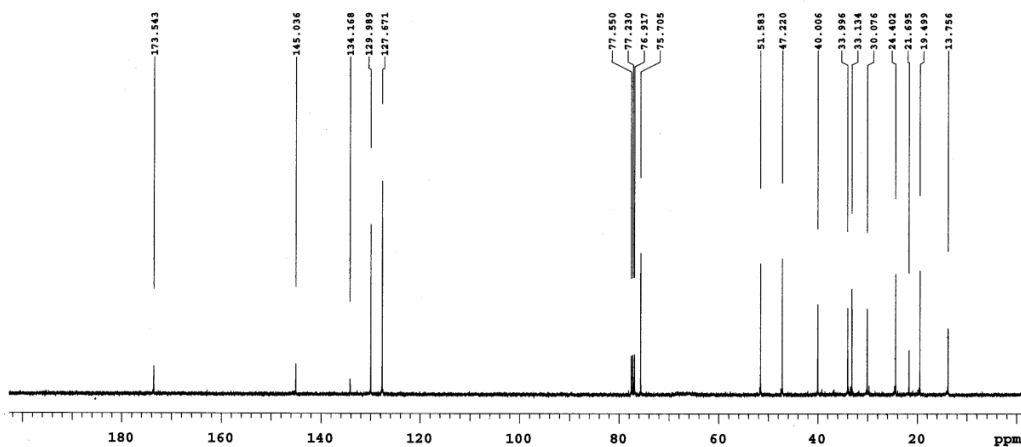


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 120 repetitions	<b>OBSERVE</b> <sup>13</sup> C, 100.5425978 <b>DECOUPLE</b> <sup>1</sup> H, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 4 minutes	<b>IX-TWP-2b-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6p**

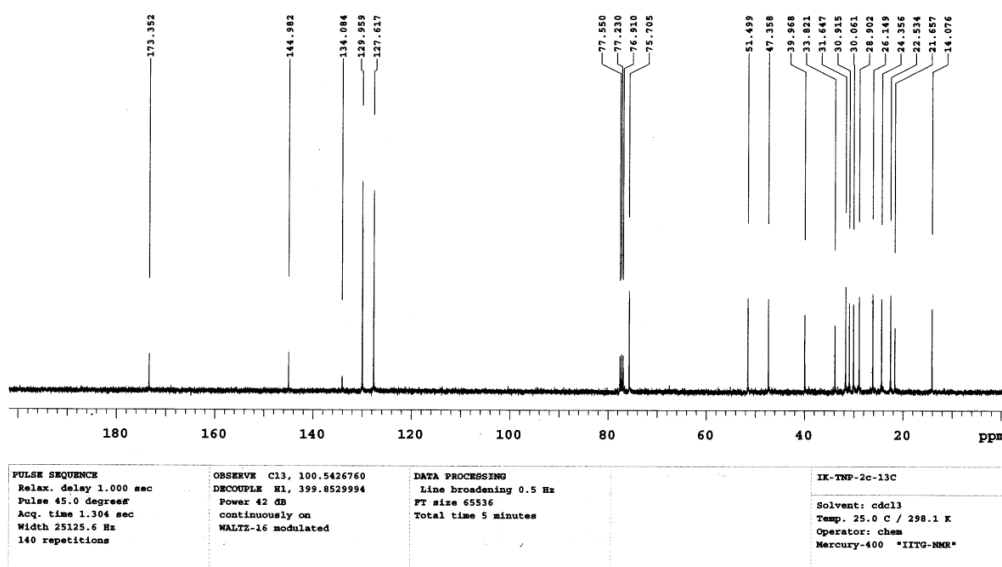
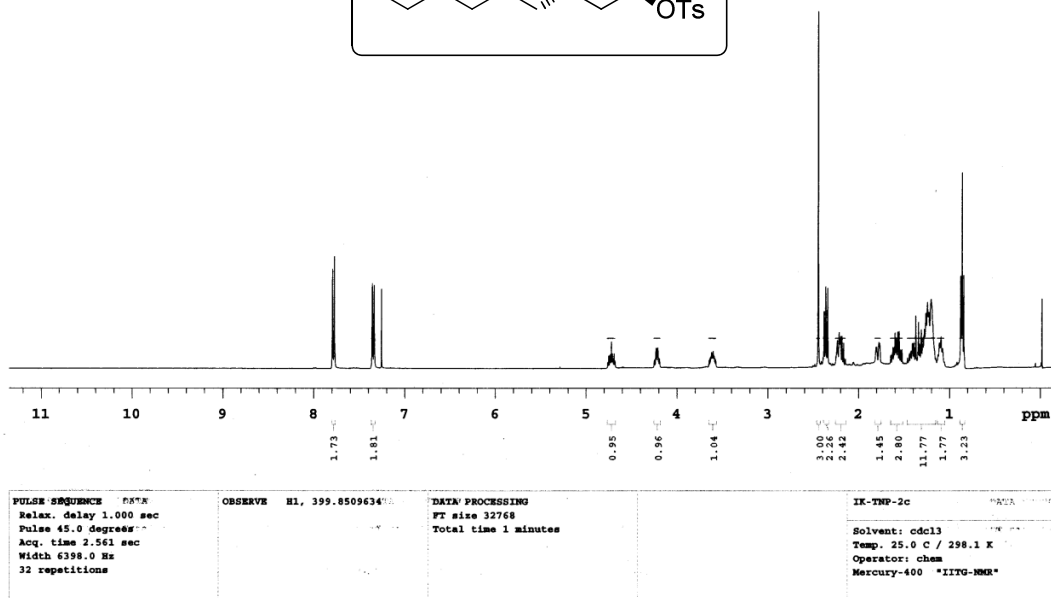
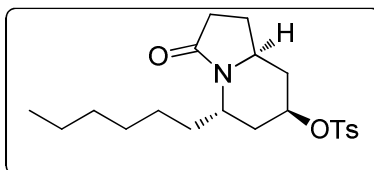


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>IK-TNP-1c</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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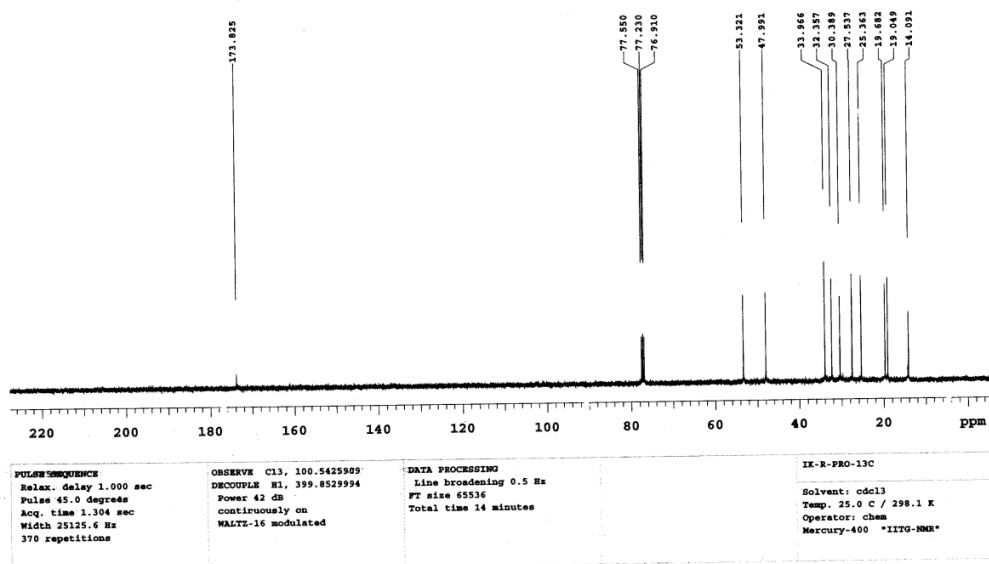
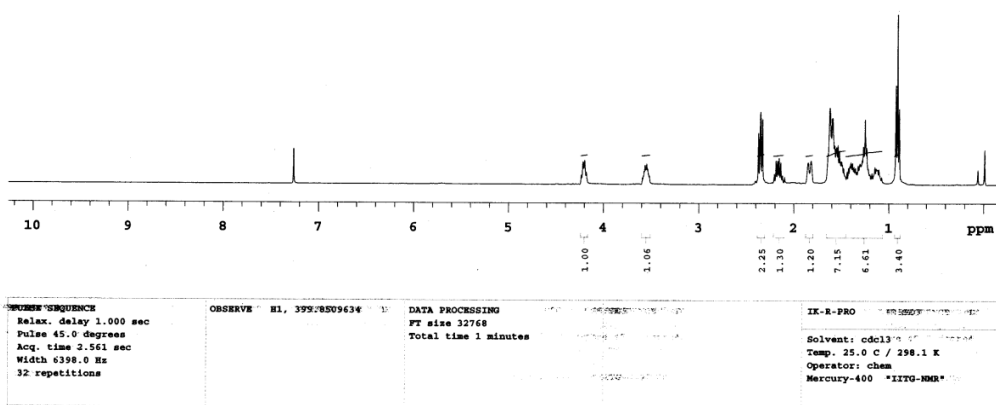
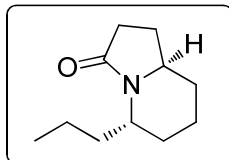


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 250 repetitions	<b>OBSERVE</b> C13, 100.5425955 <b>DECOUPLE</b> H1, 399.8529994 Power 42 db continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 9 minutes	<b>IK-TNP-1c-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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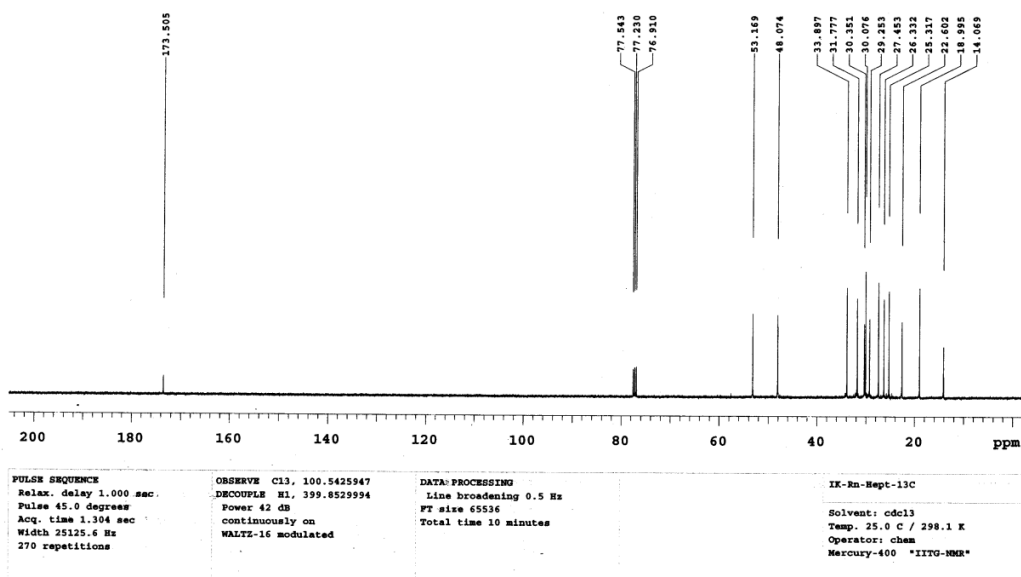
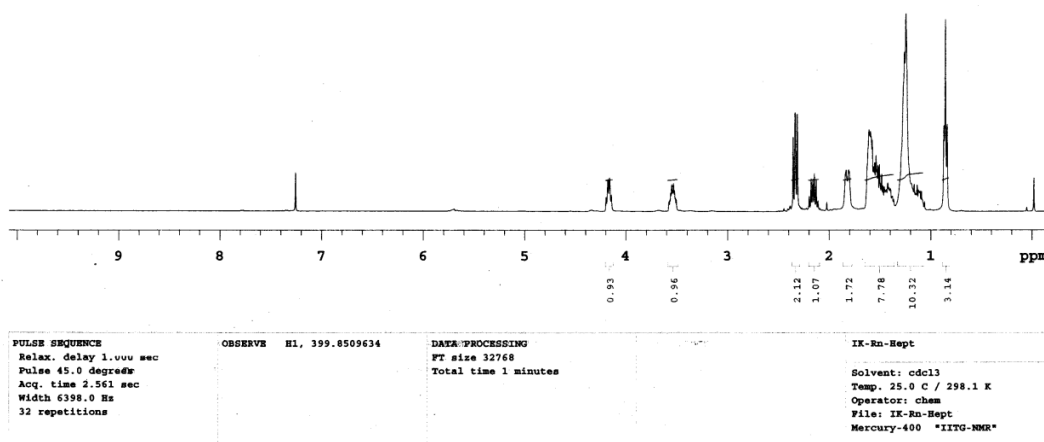
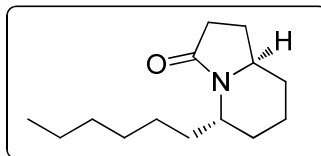
$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound **6q**



$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound 10p

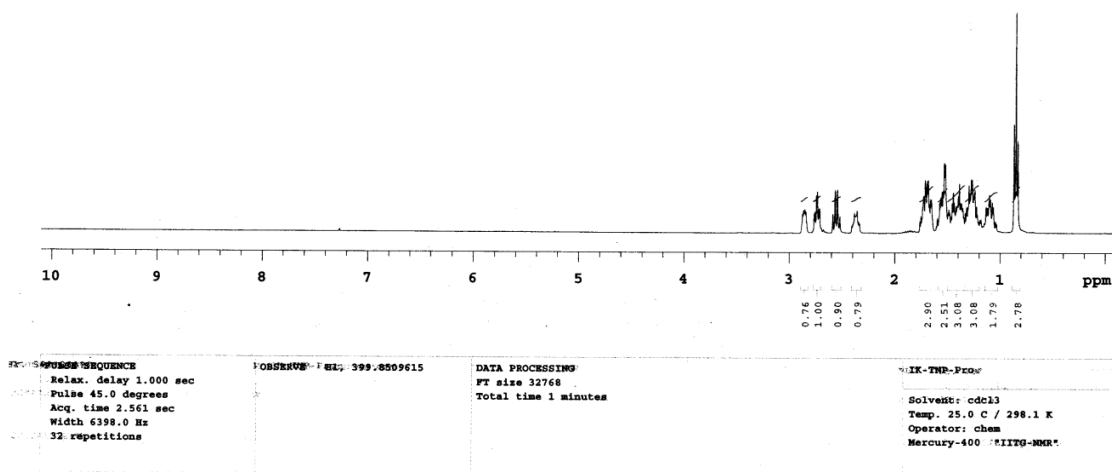
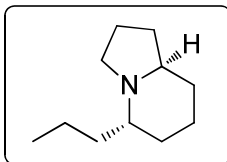


$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound 10q

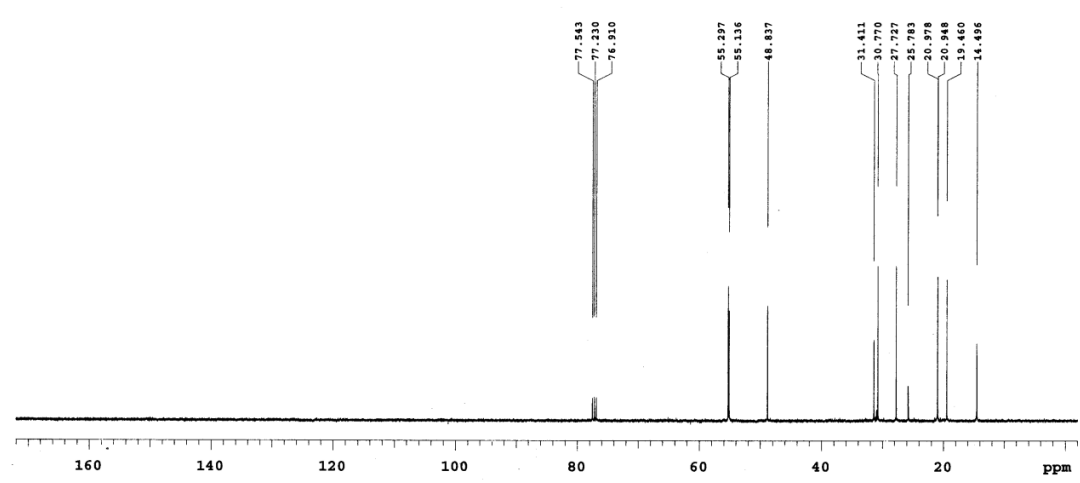




$^1\text{H}$  and  $^{13}\text{C}$  Spectra of compound *epi-3p*



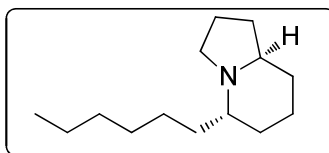
<p>EXPERIMENTAL SEQUENCE</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degrees</p> <p>Acq. time 2.561 sec</p> <p>Width 6398.0 Hz</p> <p>32 repetitions</p>	<p>OBSERVE F1, 399.8509615</p>	<p>DATA PROCESSING</p> <p>FT size 32768</p> <p>Total time 1 minutes</p>	<p>IK-TNP-Pro</p> <p>Solvent: cdcl3</p> <p>Temp. 25.0 C / 298.1 K</p> <p>Operator: chem</p> <p>Mercury-400 "IITG-NMR"</p>
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<p>EXPERIMENTAL SEQUENCE</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degrees</p> <p>Acq. time 1.304 sec</p> <p>Width 25125.6 Hz</p> <p>10 repetitions</p>	<p>OBSERVE C13, 130.5425878</p> <p>DECOUPLE H1, 399.8529994</p> <p>Power 42 dB</p> <p>continuously on</p> <p>WALTZ-16 modulated</p>	<p>DATA PROCESSING IK-TNP-Pro-13C</p> <p>Line broadening 0.5 Hz</p> <p>FT size 65536</p> <p>Total time 1 minute</p>	<p>IK-TNP-Pro-13C</p> <p>Solvent: cdcl3</p> <p>Temp. 25.0 C / 298.1 K</p> <p>Operator: chem</p> <p>Mercury-400 "IITG-NMR"</p>
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# $^1\text{H}$ and $^{13}\text{C}$ Spectra of compound *epi-3q*

IK-HEPT-1H

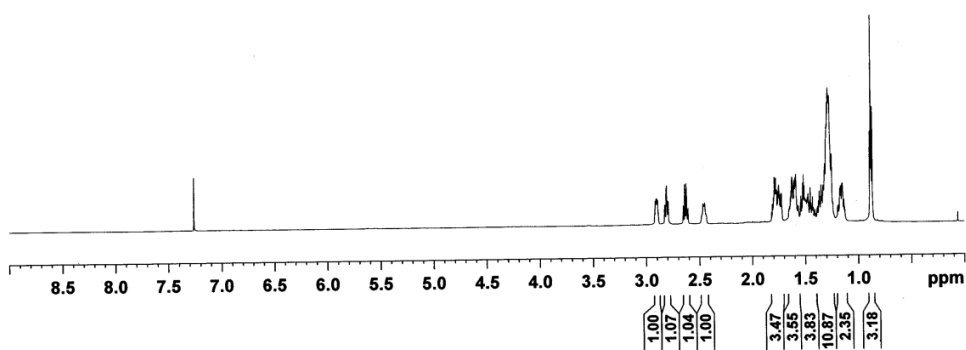


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Current Data Parameters
NAME      IK-HEPT-1H
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20140320
Time     16.05
INSTRUM  spect
PROBHD   5 mm PABBO 301
PULPROG  zg30
TD       2149
SOLVENT  CDCl3
NS       16
DS       2
SWH      10019.250 Hz
FIDRES   0.366798 Hz
AQ       1.2631488 sec
RG       64.94
DW       41.600 usec
DE       6.50 usec
TE       301.3 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
SFO1    600.137063 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
```



IK-HEPT-13C

77.44  
77.23  
77.01

55.32  
55.36

49.02

32.11  
21.43  
30.86  
27.89  
27.82  
23.77  
21.16  
19.58

14.30



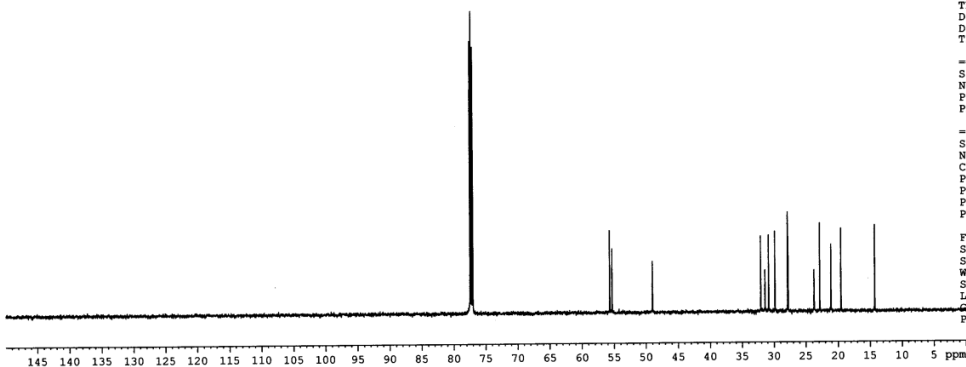
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Current Data Paramet
NAME      IK-HEPT-
EXPNO    1
PROCNO   1

F2 - Acquisition Par
Date_    2014
Time     11
INSTRUM  sf
PROBHD   5 mm PABBO
PULPROG  zg30
TD       32
SOLVENT  CI
NS       16
DS       2
SWH      36057.
FIDRES   1.100
AQ       0.4541
RG       64
DW       13.
DE       6
TE       30
D1       2.00000
D11      0.03000
TDO

===== CHANNEL f1 =====
SFO1    150.9275
NUC1    13C
P1      10
PLW1    95.00000

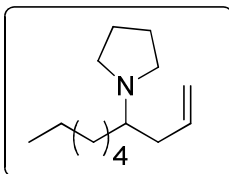
===== CHANNEL f2 =====
SFO2    600.1724
NUC2    13C
CPDPRG2  walt
PCPD2    70
PLW2    21.00000
PLW12   0.61714
PLW13   0.30235

F2 - Processing para
SI      16
SF      150.9126
WDW     EM
SSB     0
LB      0
GB      0
PC      1
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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 11

IK-LAH-L\_1H



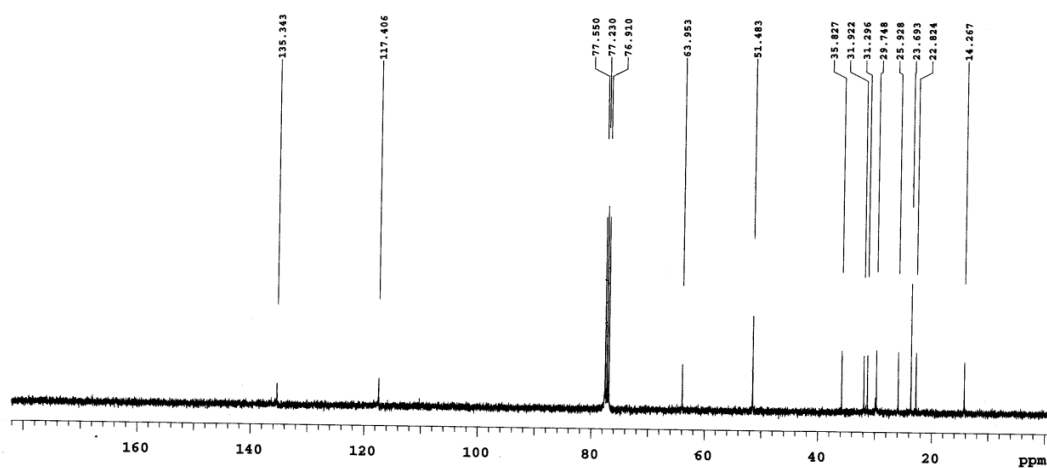
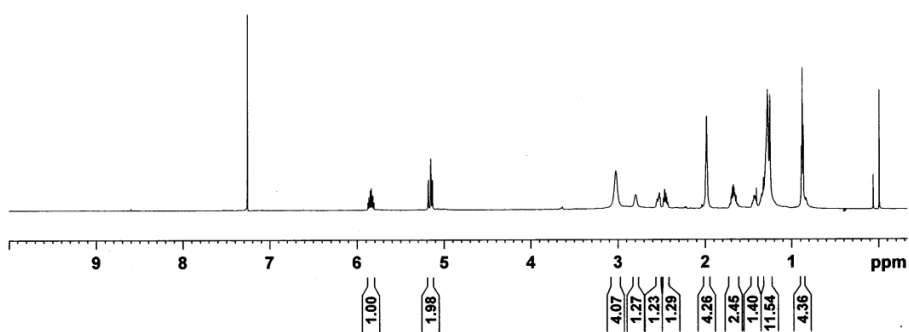
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Current Data Parameters
NAME      IK-LAH-L_1H
EXNO      1
PROCNO    1

F2 - Acquisition Parameters
Date      20140322
Time      12:27
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         4
SFO1      12019.230 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         80.22
DM         41.600 usec
DE         6.50 usec
TE         300.1 K
D1         1.00000000 sec
TD0        1

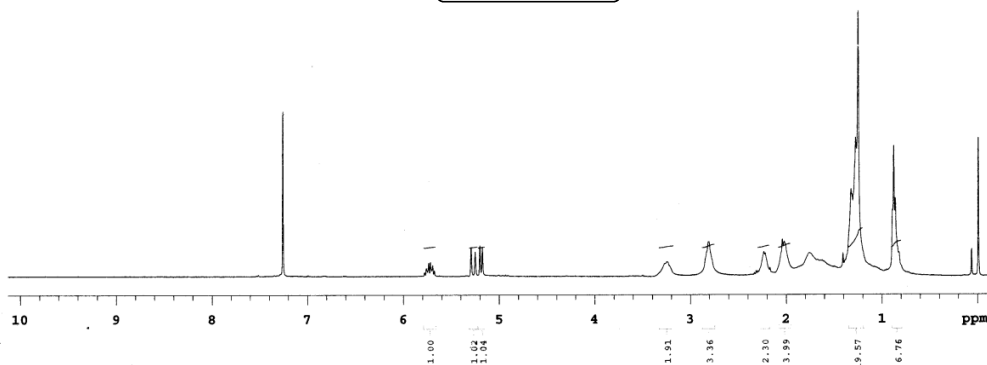
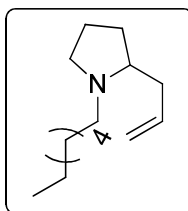
===== CHANNEL f1 =====
SFO1      600.137063 MHz
NUC1       13
P1         12.00 usec
PLM1       21.00000000 W

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

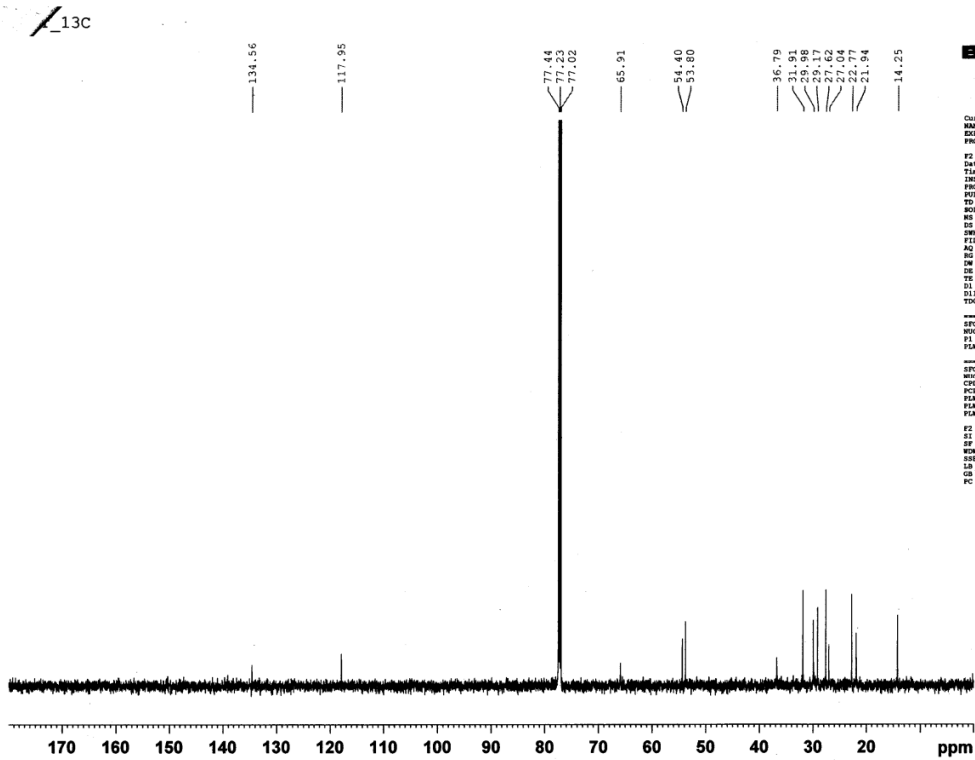


<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 2040 repetitions	<b>OBSERVE</b> CL3, 100754258177 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 78 minutes	IX-18-2-14 Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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# <sup>1</sup>H and <sup>13</sup>C Spectra of compound 12



PARAMETER	VALUE	UNIT
RELAX_DELAY	1.000	sec
PULSE	45.0	deg
ACQ_TIME	2.561	sec
WIDTH	6398.0	Hz
REPS	200	
FT_SIZE	32768	
TOTAL_TIME	11	minutes
SOLVENT	cdcl3	
TEMP	25.0	C / 298.1 K
OPERATOR	chem	
INSTRUM	Mercury-400	<sup>1</sup> H NMR



```

Current Data Parameters
NAME      12C_13C
EXPNO     1
PROCNO    1

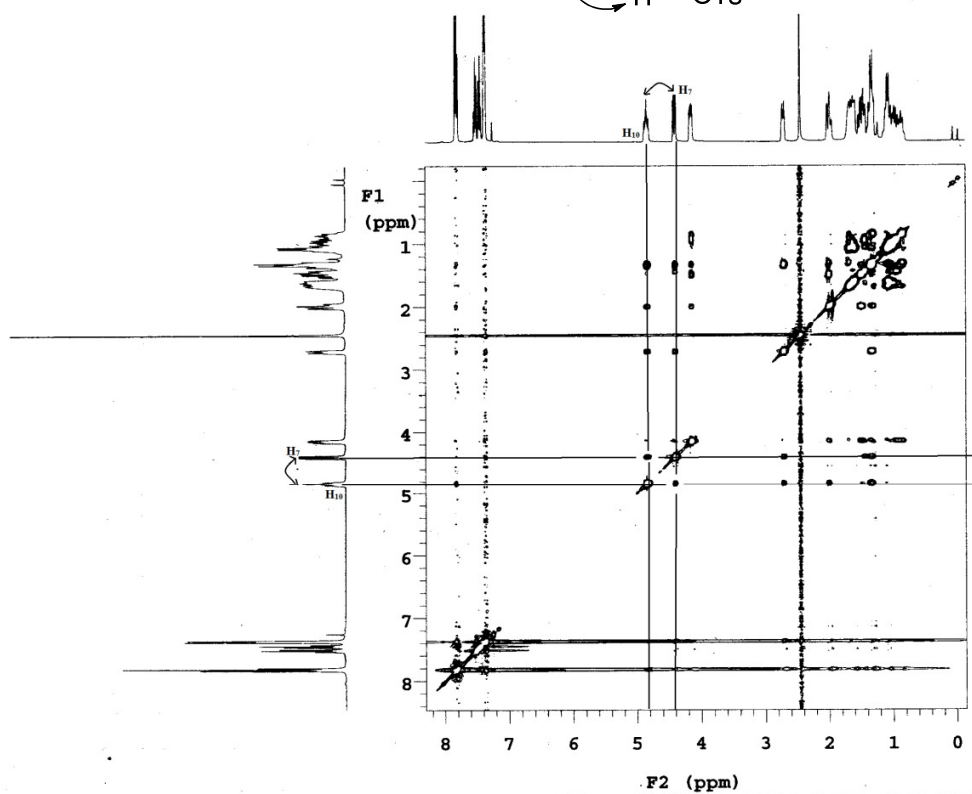
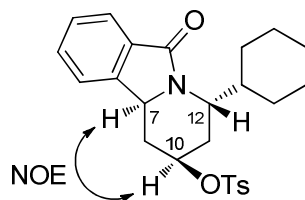
F2 - Acquisition Parameters
Date_     20140217
Time      17.25
INSTRUM   spect
PROBHD    5 mm PABBO 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         2
SWH        36057.491 Hz
FIDRES     1.160393 Hz
AQ          0.4543829 sec
RG          65.74
DM          13.867 usec
DE          6.50 usec
TE          300.9 K
TEPROG    2.00000000 sec
D1         0.03000000 sec
TD1        1

===== CHANNEL f1 =====
SFO1      150.9179211 MHz
NUC1       13C
P1         10.00 usec
PL1        0.00000000 dB

===== CHANNEL f2 =====
SFO2      600.1714007 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     70.00 usec
PL12      0.00000000 dB
PL13      0.61714000 dB
PL14      0.30238999 dB

F2 - Processing parameters
SI         32768
SF         150.9128143 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

# NOE Spectra of compound 6n



PULSE SEQUENCE: NOESY  
 Relax. delay 2.000 sec  
 Acq. time 0.150 sec  
 Width 6398.0 Hz  
 2D Width 6398.0 Hz  
 8 repetitions  
 2 x 400 increments

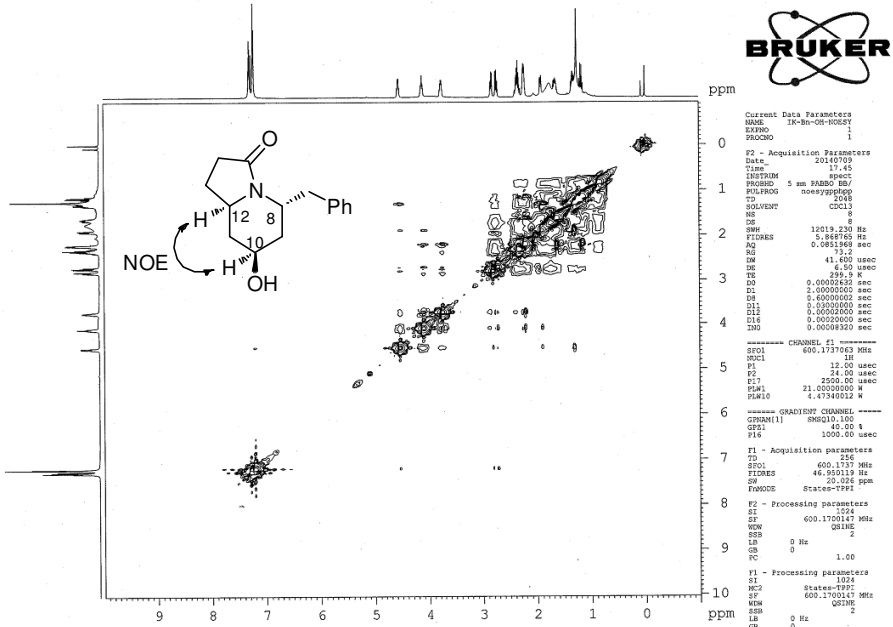
OBSERVE: x H1: 399.3509634

DATA PROCESSING  
 Gauss apodization 0.069 sec  
 F1 DATA PROCESSING  
 Gauss apodization 0.058 sec  
 FT size 4096 x 4096  
 Total time 3.9 hours

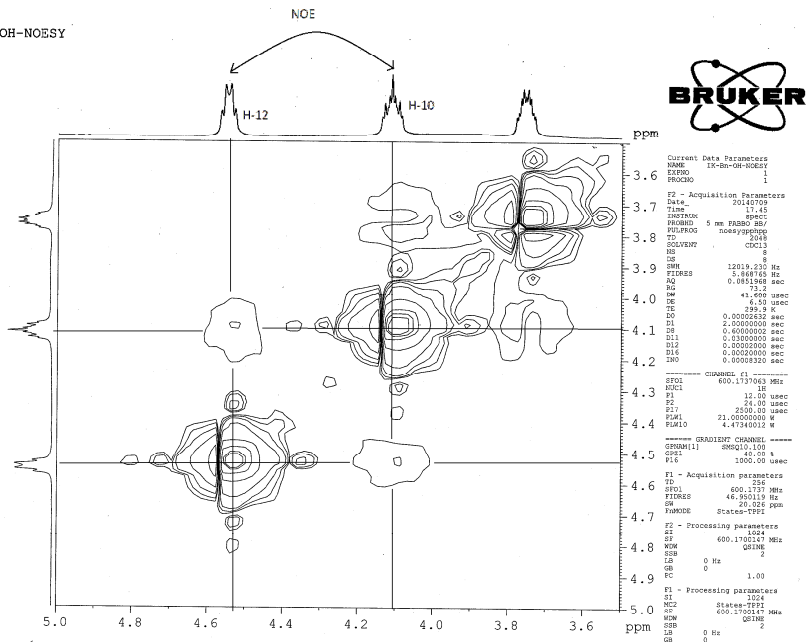
TK-T9-NOESY  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 File: TK-T9-NOESY  
 Mercury 400 "IITG-NMR"

# NOE Spectra of compound 6d'

IK-Bn-OH-NOESY



IK-Bn-OH-NOESY



The crystal parameters of compound **6n**

	CCDC 1000260
Formula	C <sub>25</sub> H <sub>29</sub> N O <sub>4</sub> S
Formula weight	439.56
<i>T</i> /K	296(2)
Crystal system	Monoclinic
Space group	P2(1)/c
<i>a</i> /Å	10.812(3)
<i>b</i> /Å	11.923(3)
<i>c</i> /Å	18.961(5)
<i>α</i> /°	90.00
<i>β</i> /°	93.50
<i>γ</i> /°	90.00
<i>V</i> /Å <sup>3</sup>	2439.7(11)
<i>Z</i>	4
Abs. Coeff./mm <sup>-1</sup>	0.162
Abs. Correction	Multi-scan
GOF on <i>F</i> <sup>2</sup>	0.949
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> 1 = 0.0467 <i>wR</i> 2 = 0.1265
<i>R</i> indices [all data]	<i>R</i> 1 = 0.0674 <i>wR</i> 2 = 0.1433

ORTEP Diagram of **6n**

