

SUPPORTING INFORMATION

PROTON NMR AND SELECTED CARBON NMR SPECTRA

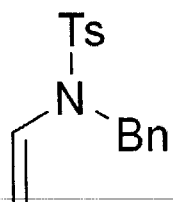
for the
communication
entitled

An Enamide-Benzyne-[2 + 2] Cycloaddition: Stereoselective Tandem [2 + 2]–Intramolecular *N*-Tethered [4 + 2] Cycloadditions.

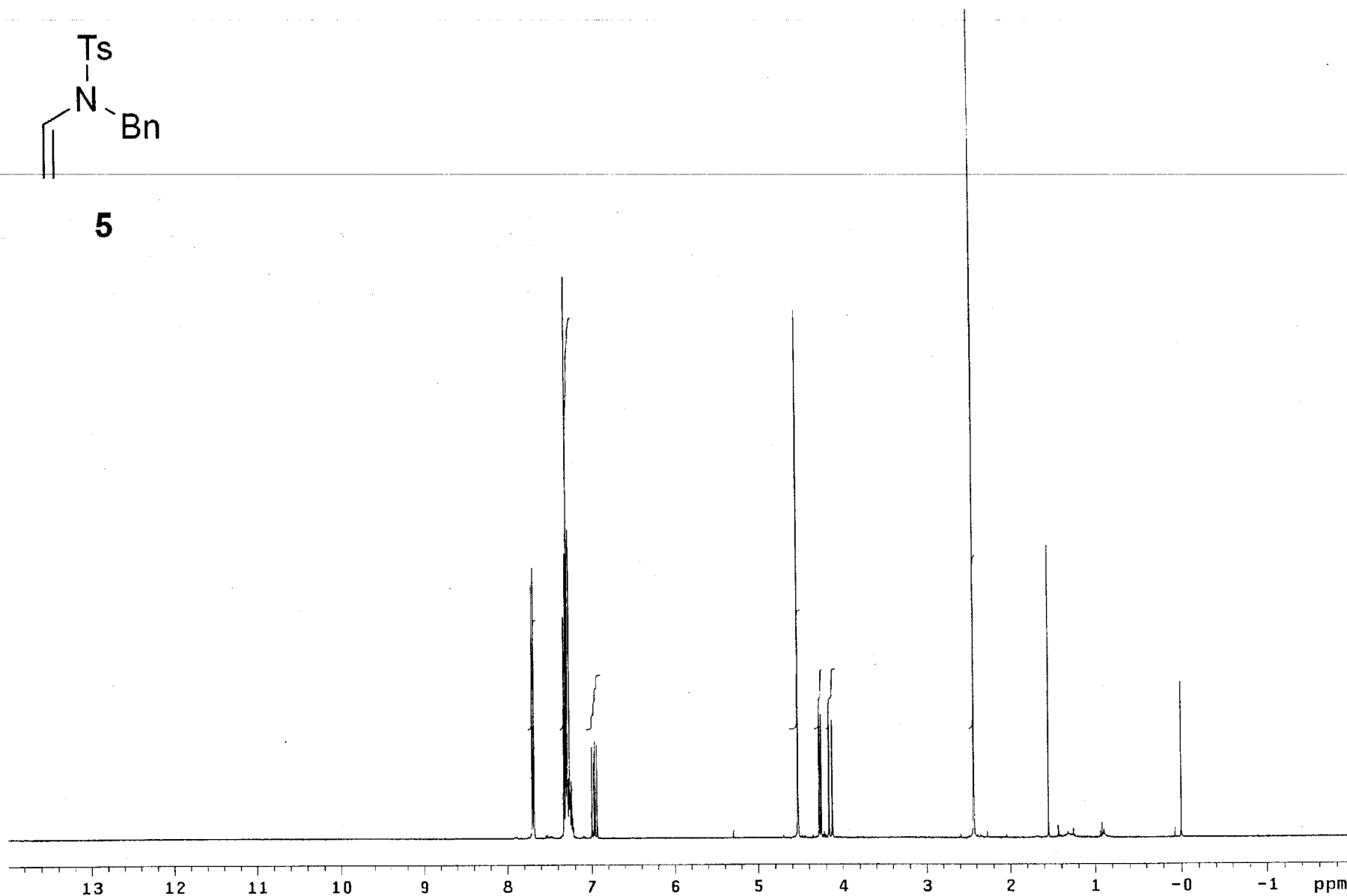
authored by

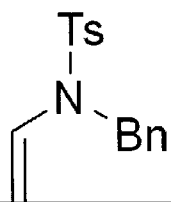
John B. Feltenberger, Ryuji Hayashi, Yu Tang, Eric S. C. Babiash and Richard P. Hsung*

*Division of Pharmaceutical Sciences and Department of Chemistry,
7111 Rennebohm Hall, 777 Highland Avenue
University of Wisconsin at Madison, Madison, WI 53705-2222*

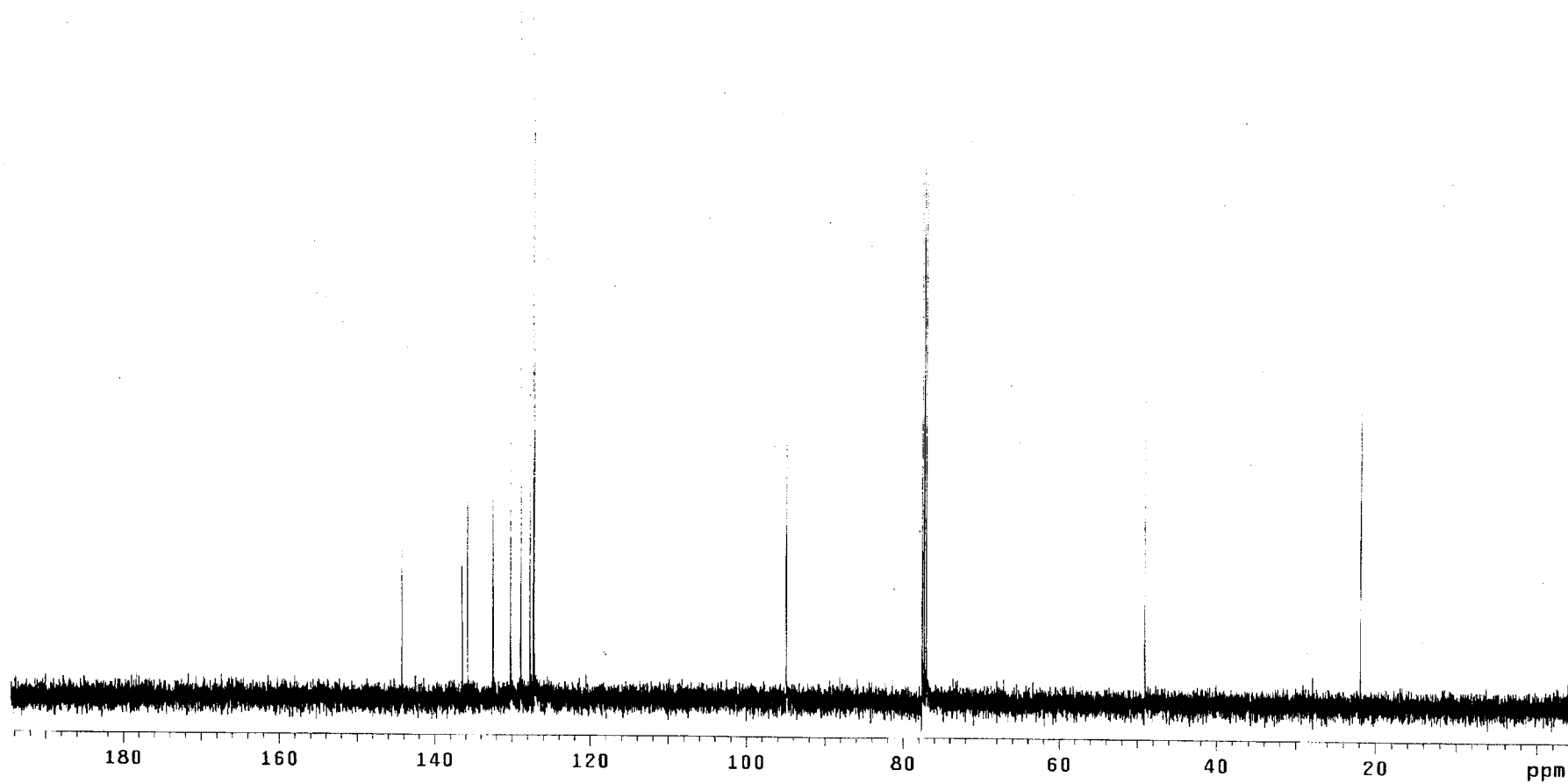


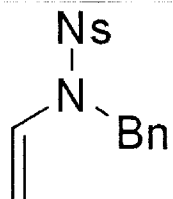
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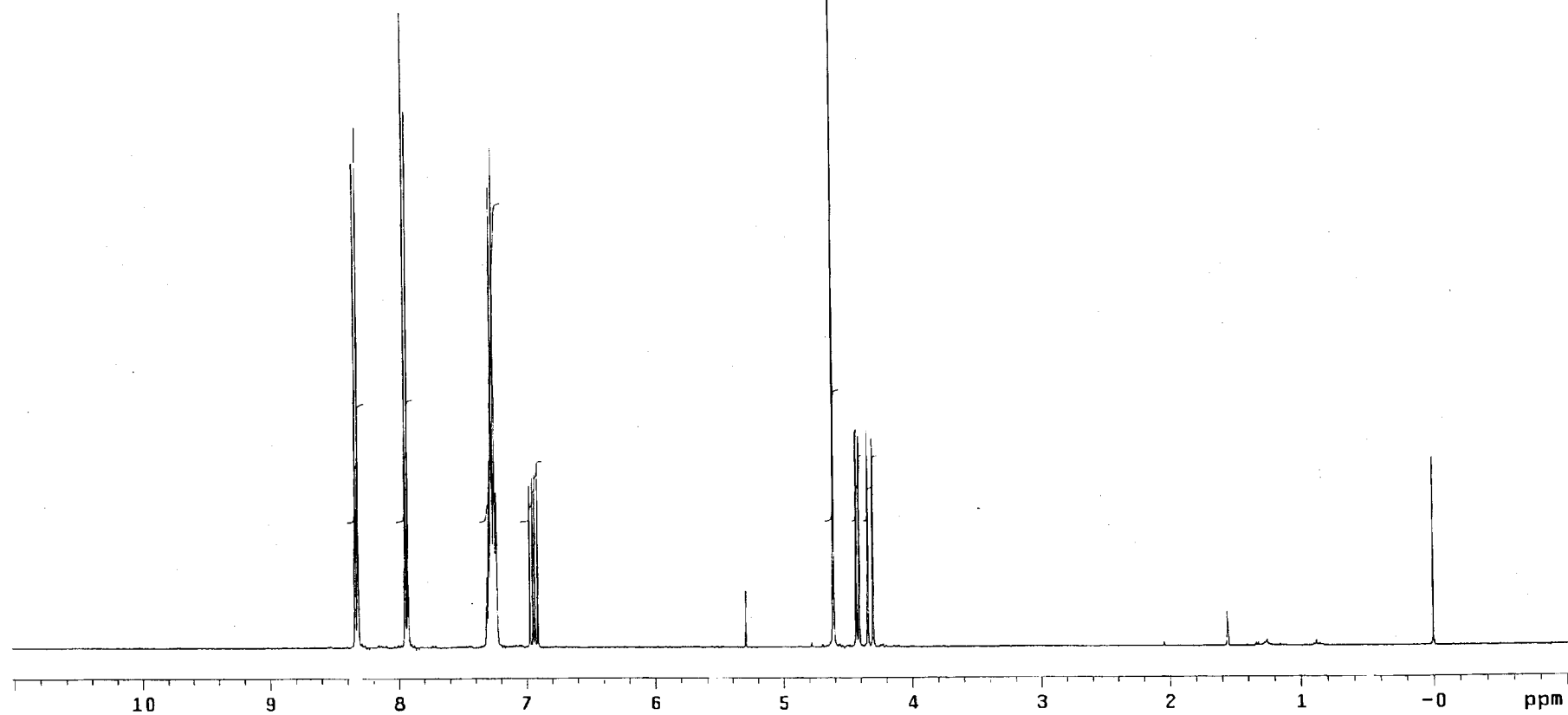


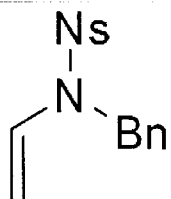
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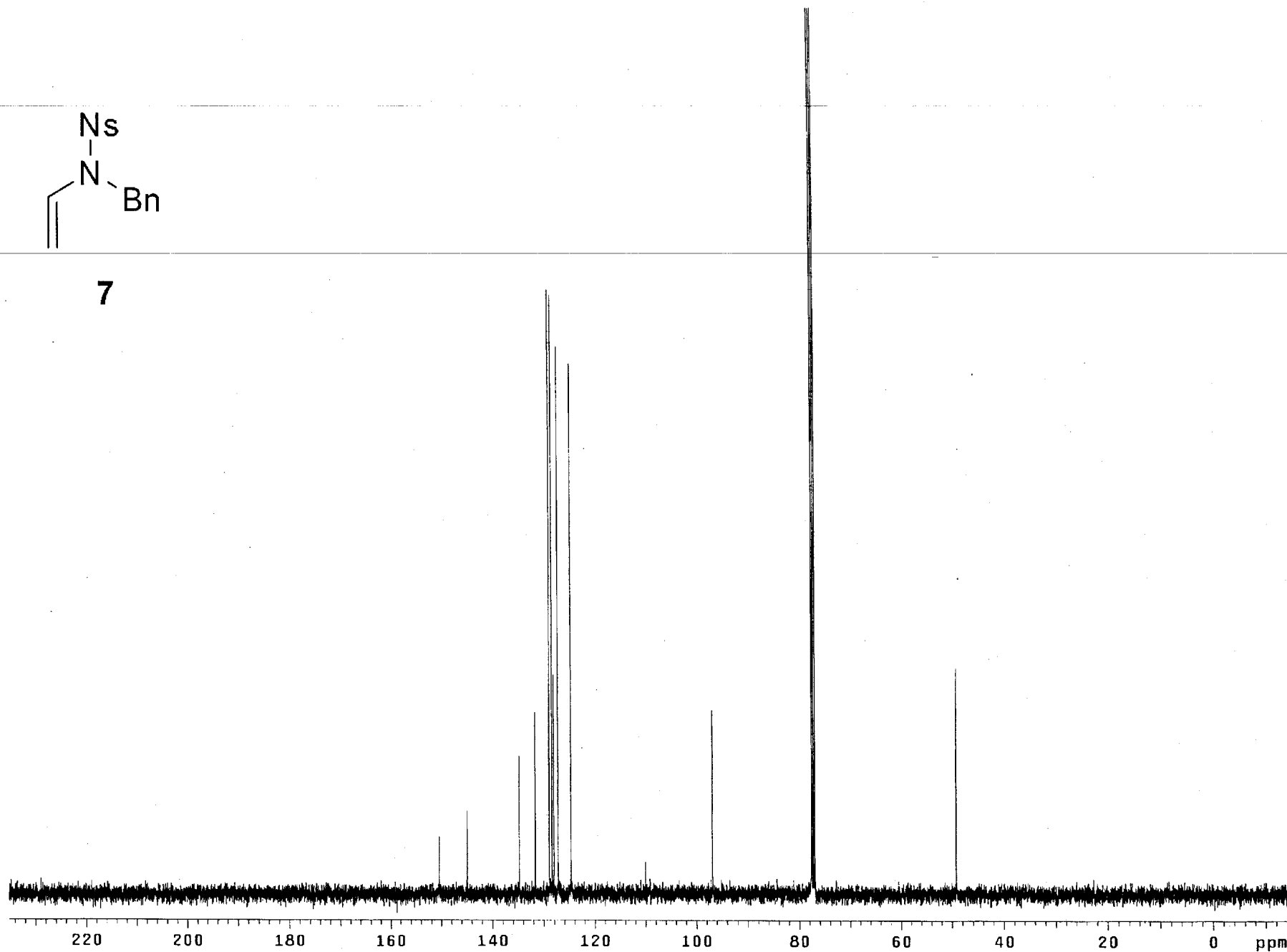


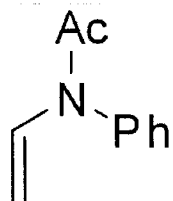
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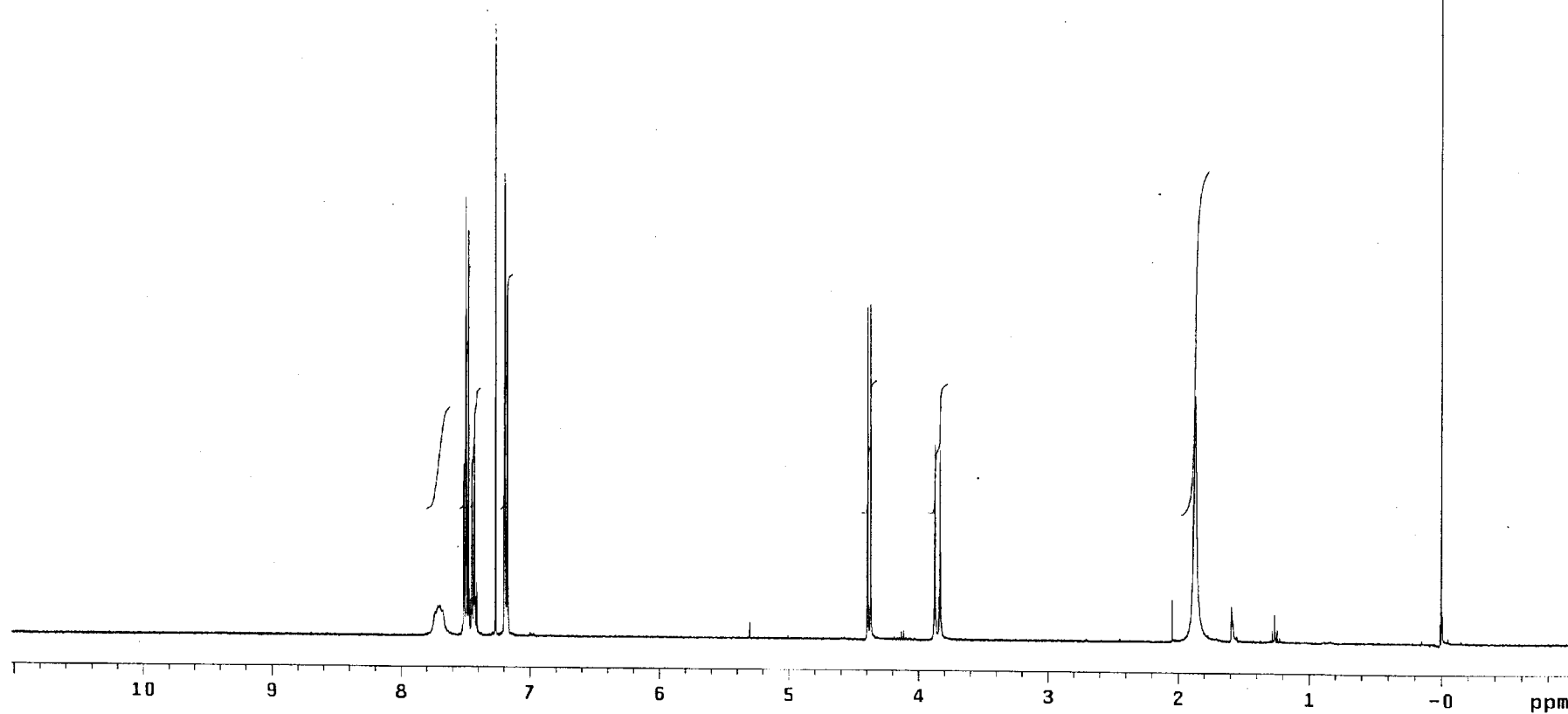


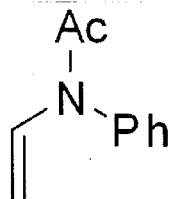
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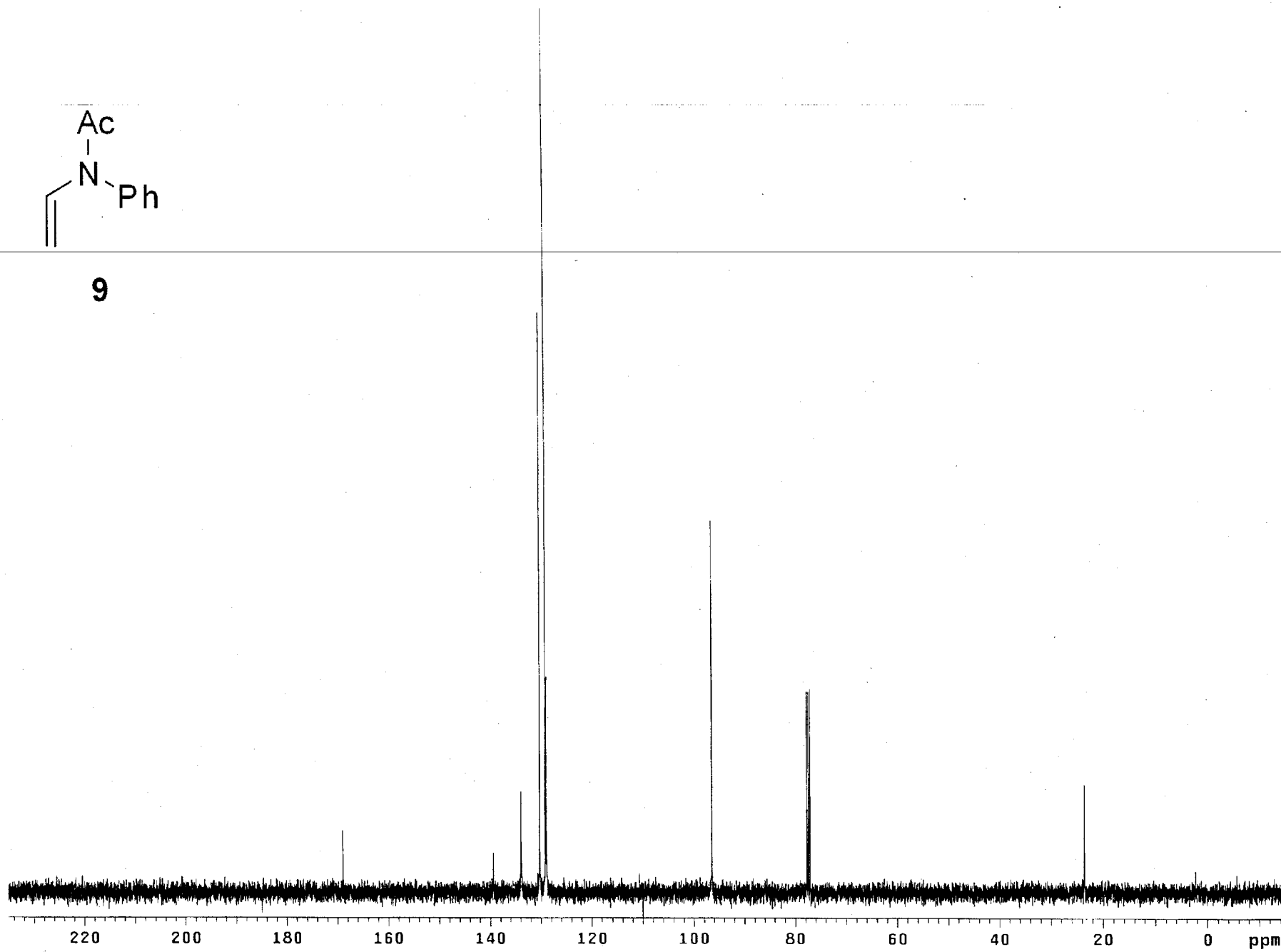


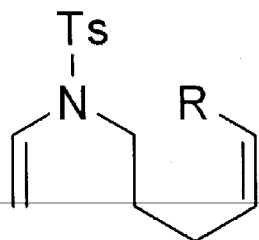
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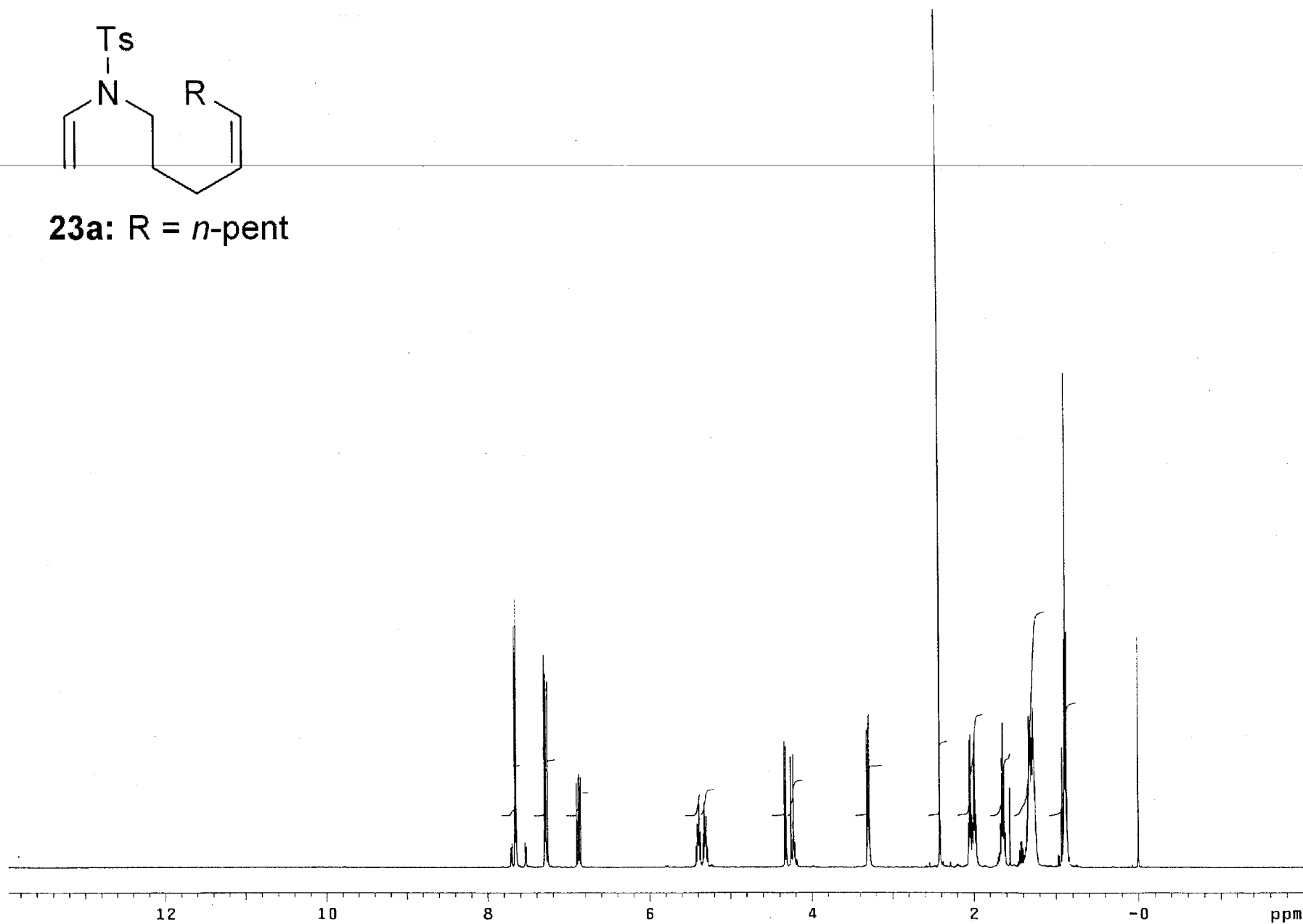


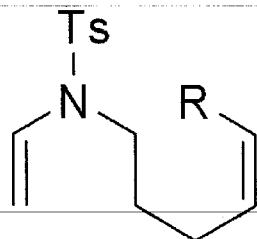
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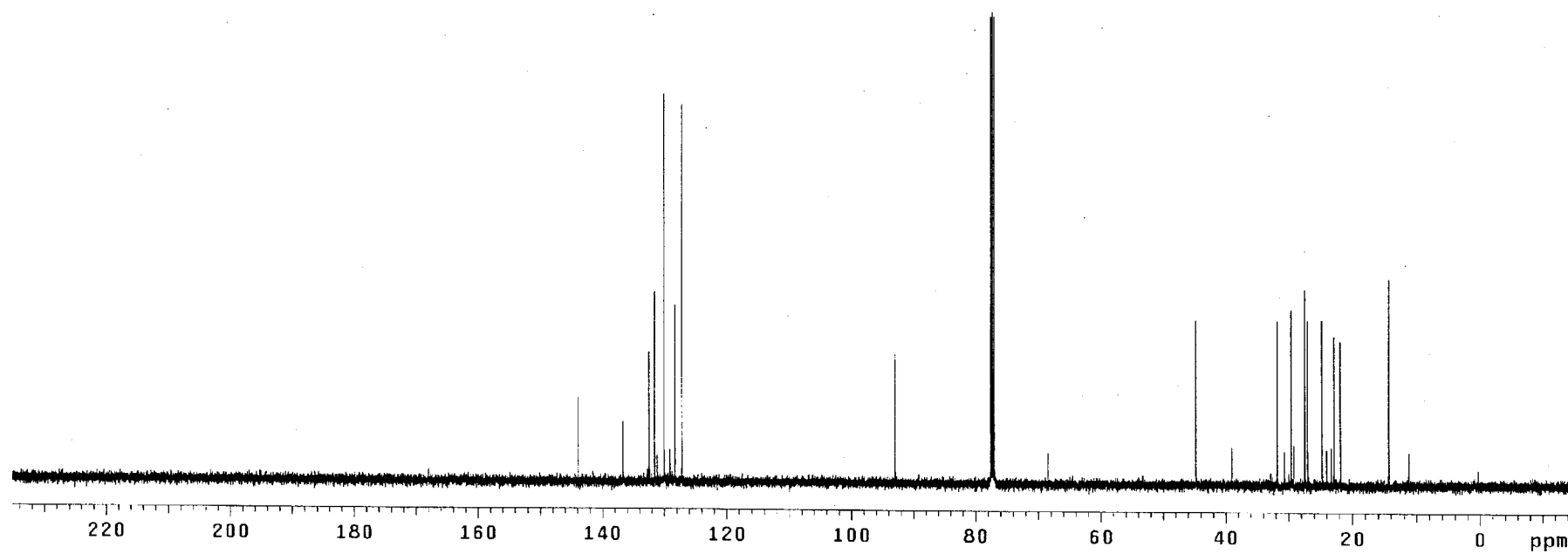


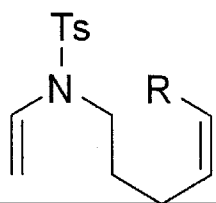
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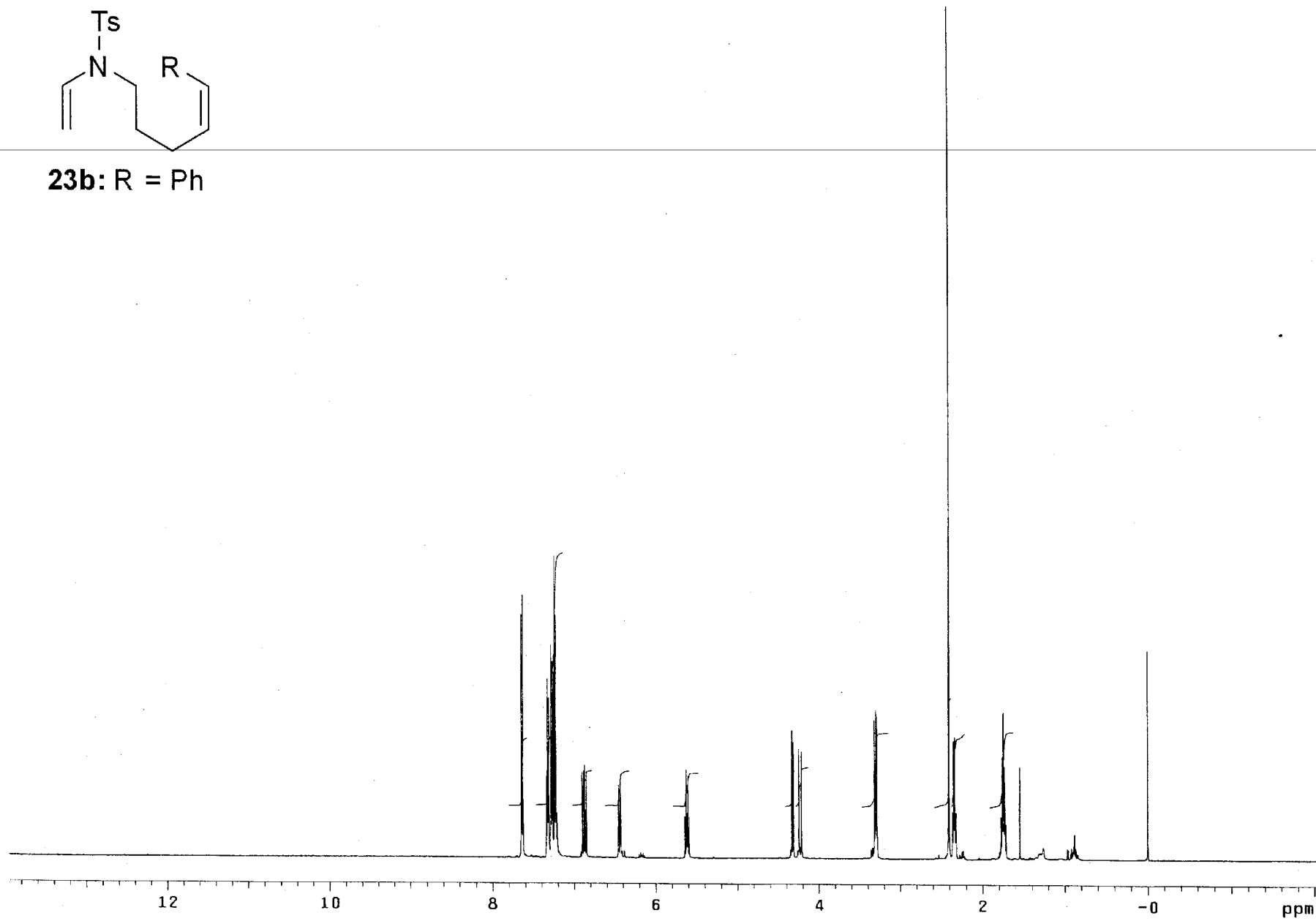


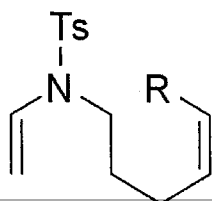
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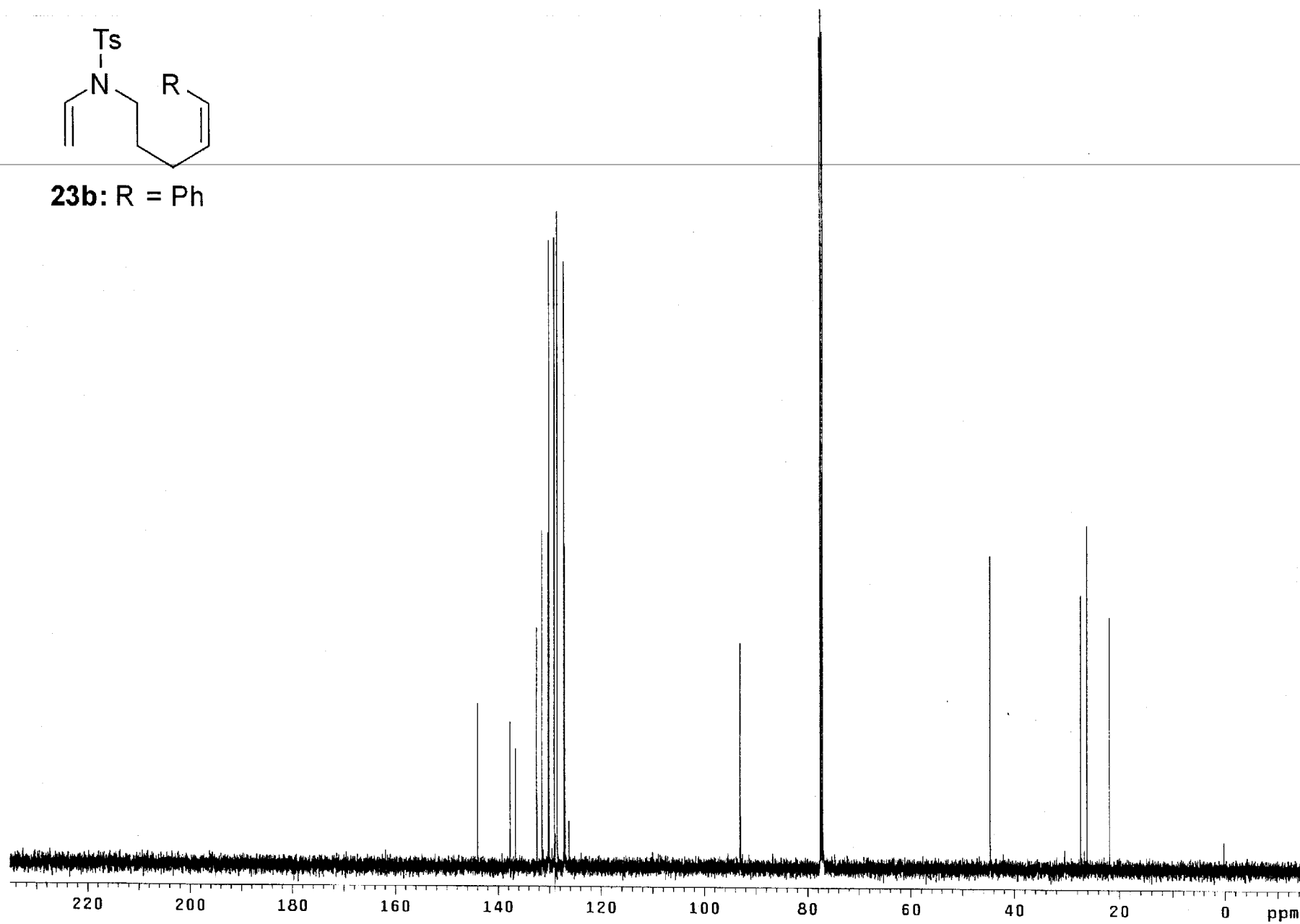


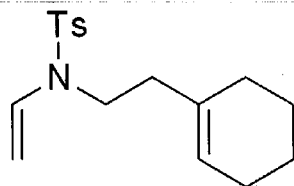
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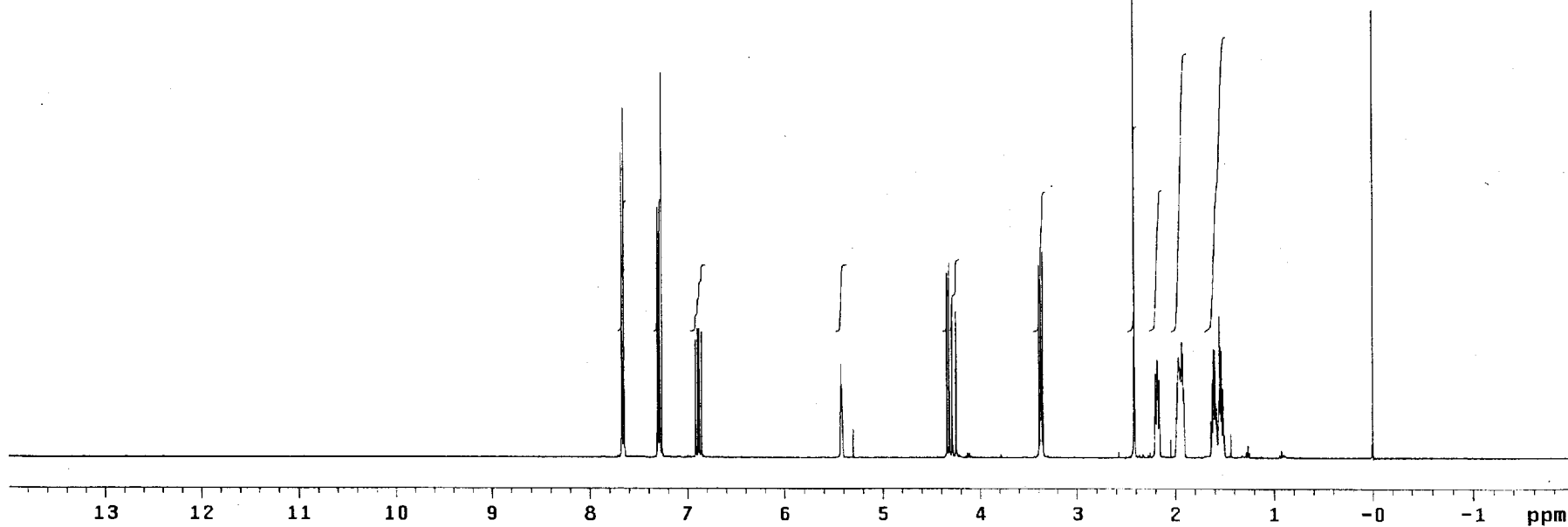


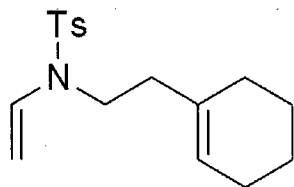
23b: R = Ph



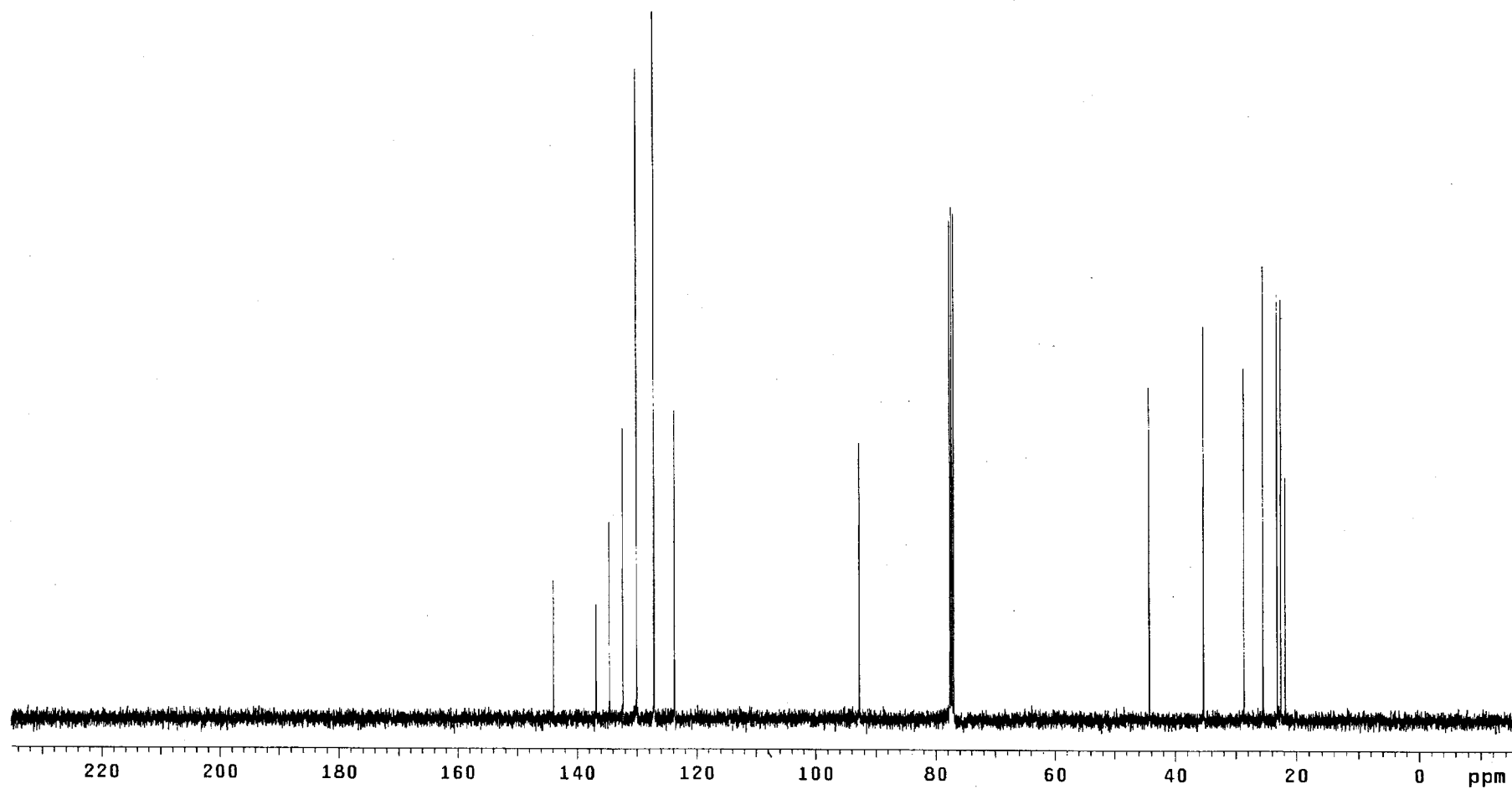


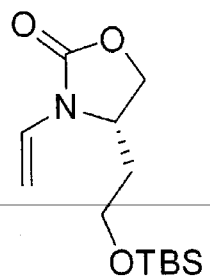
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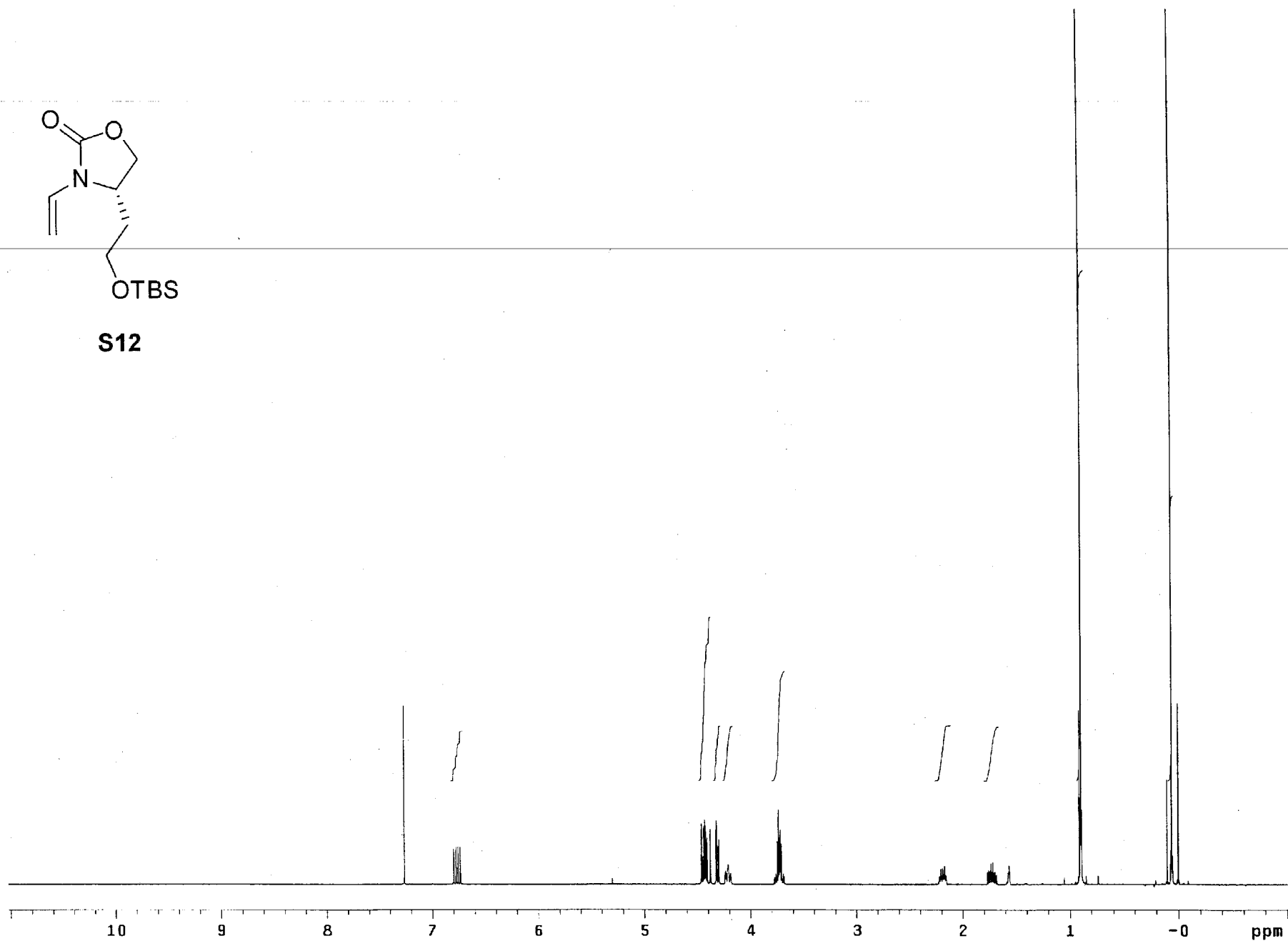


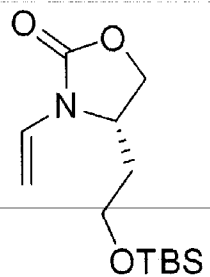
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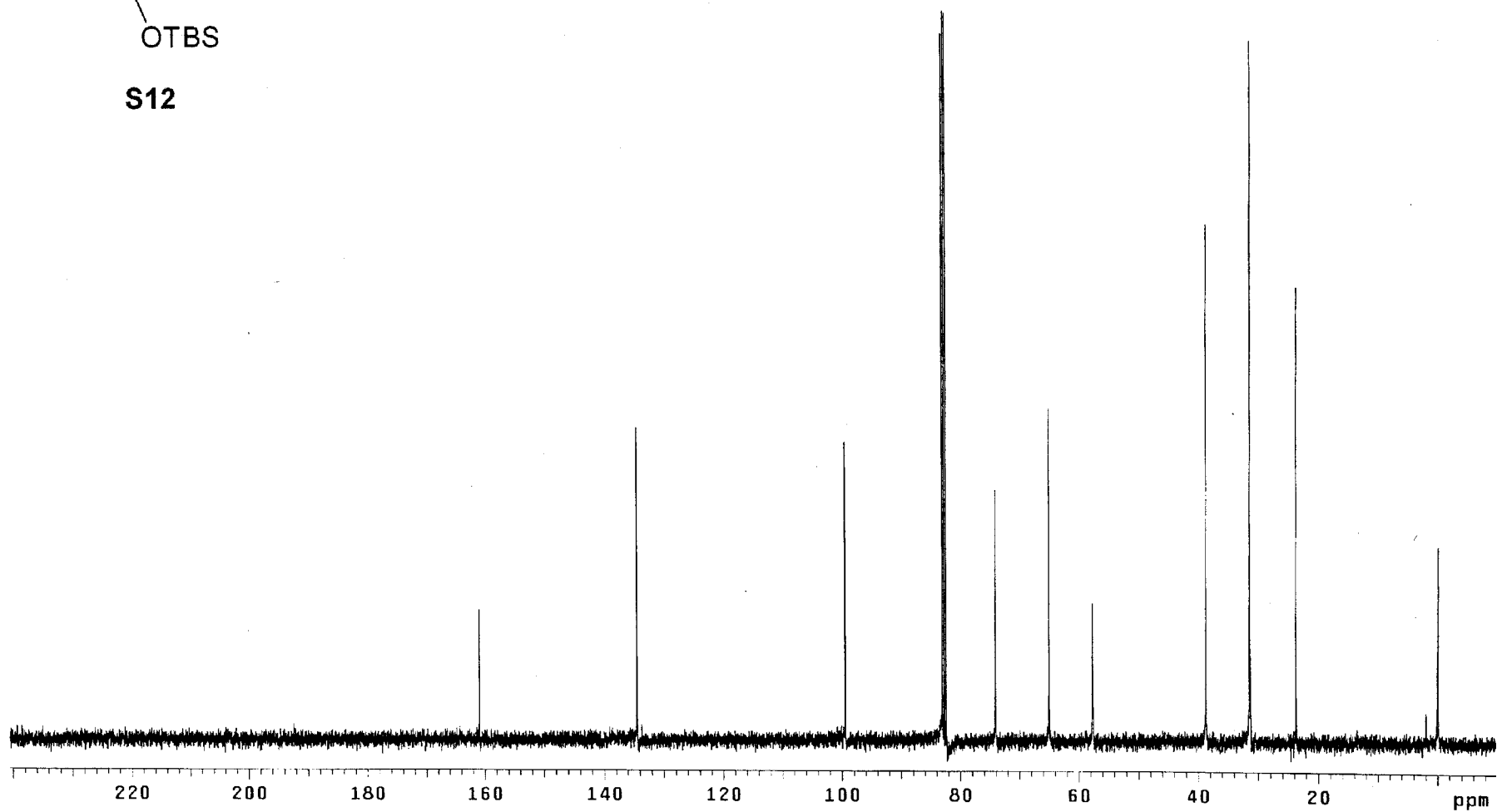


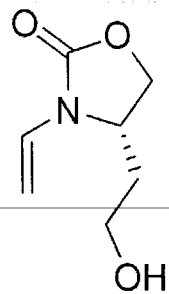
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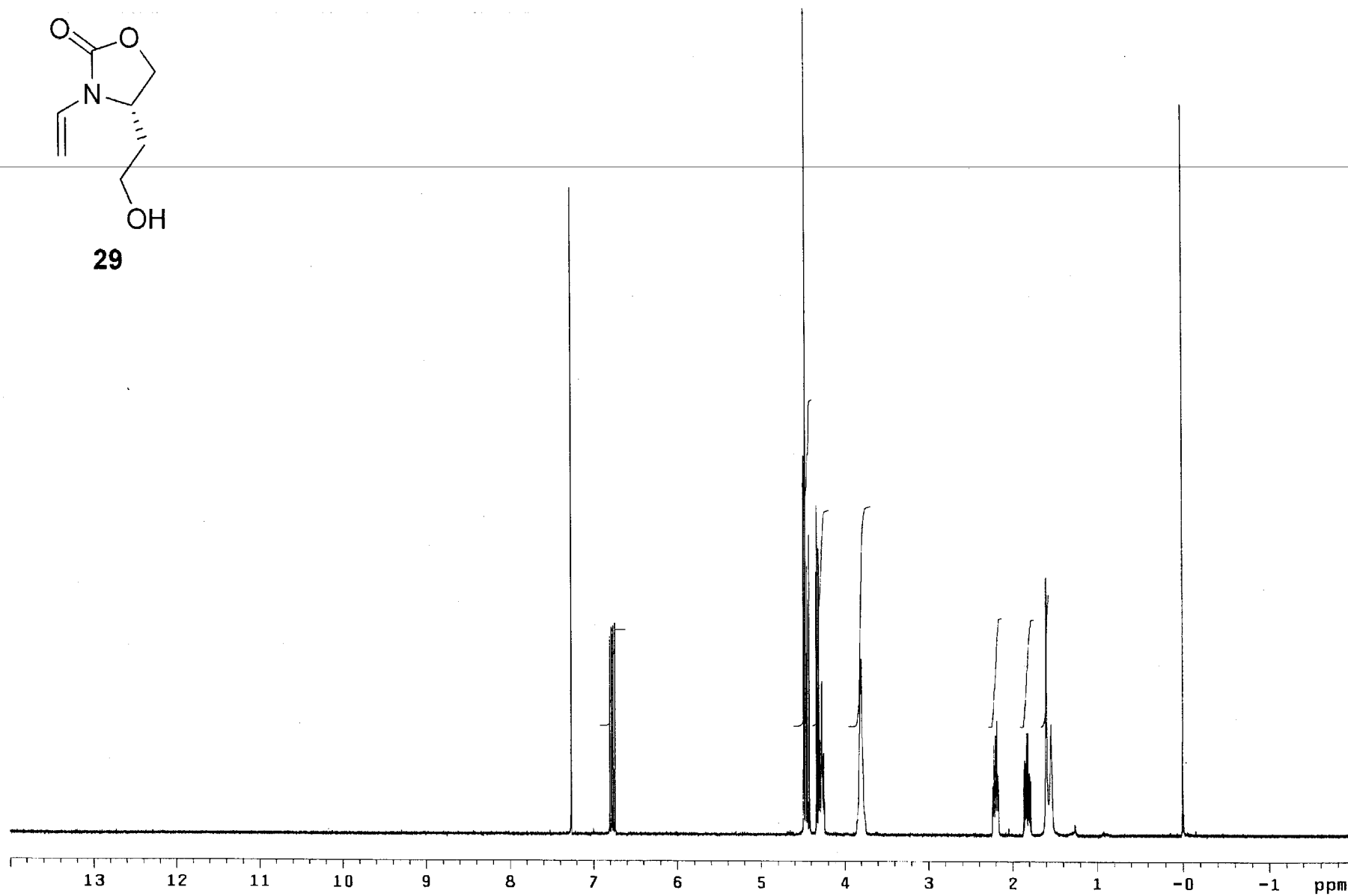


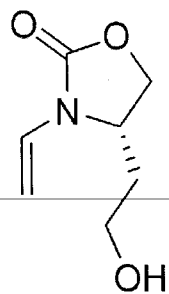
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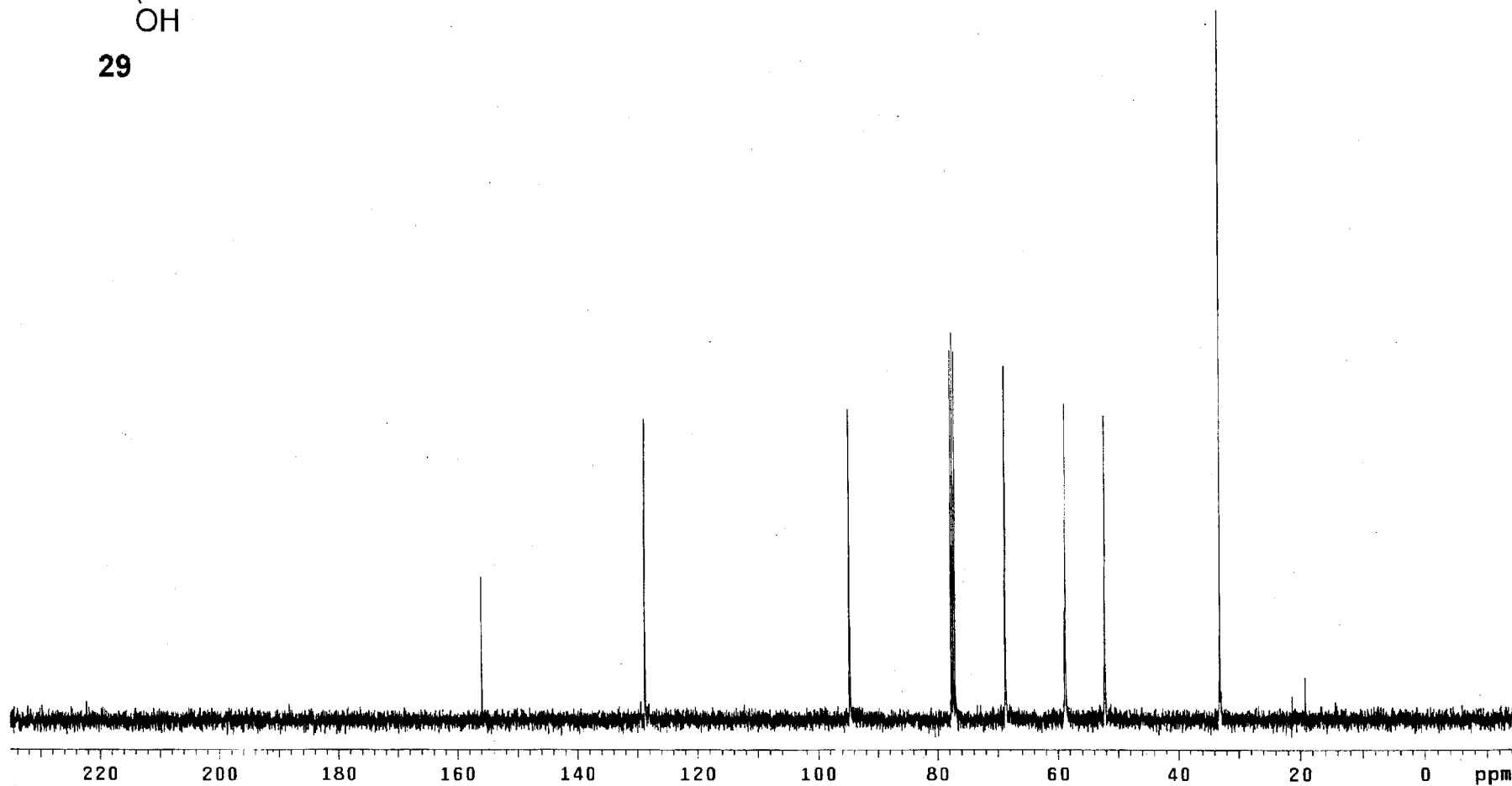


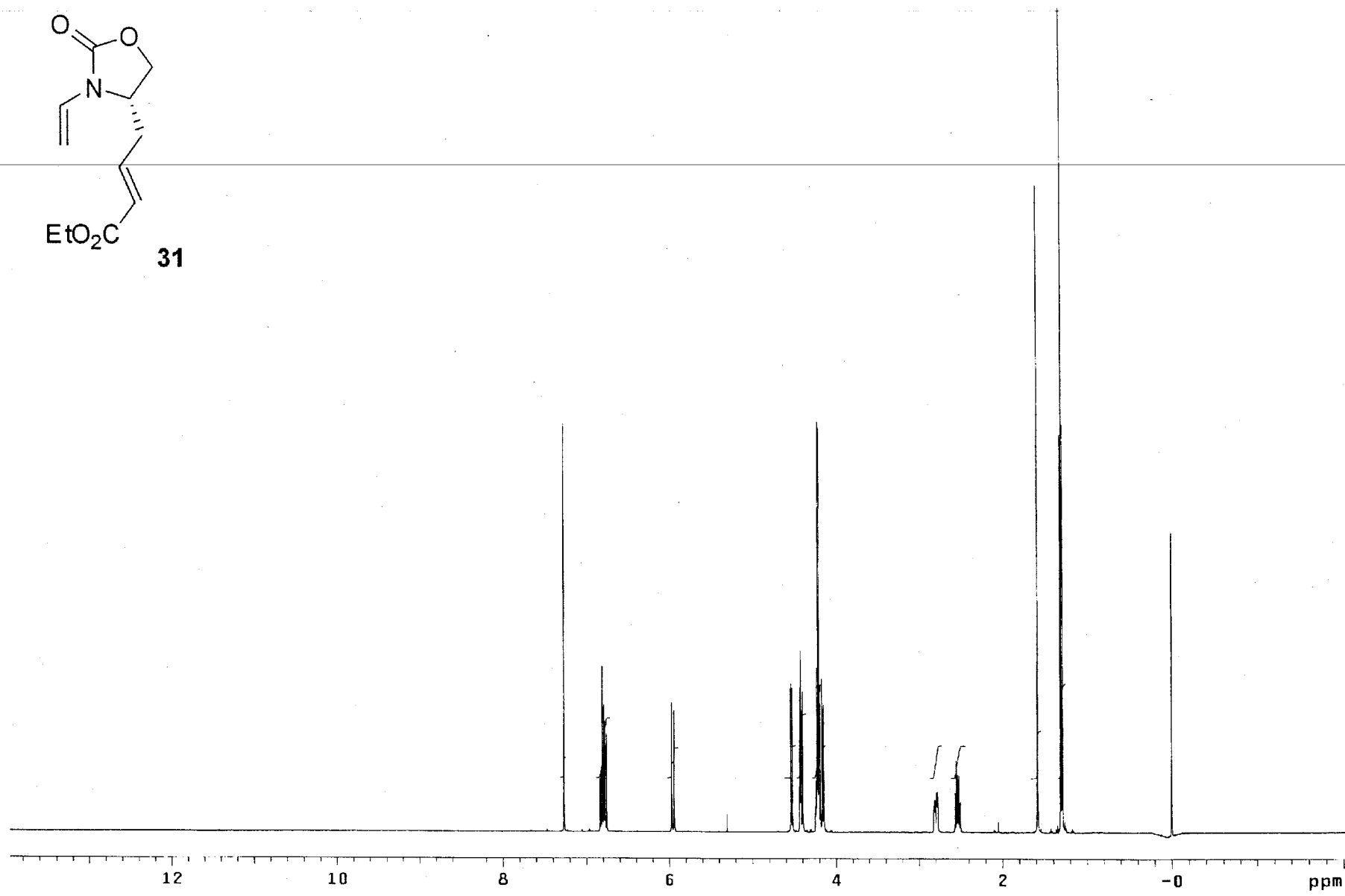
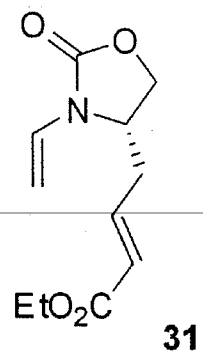
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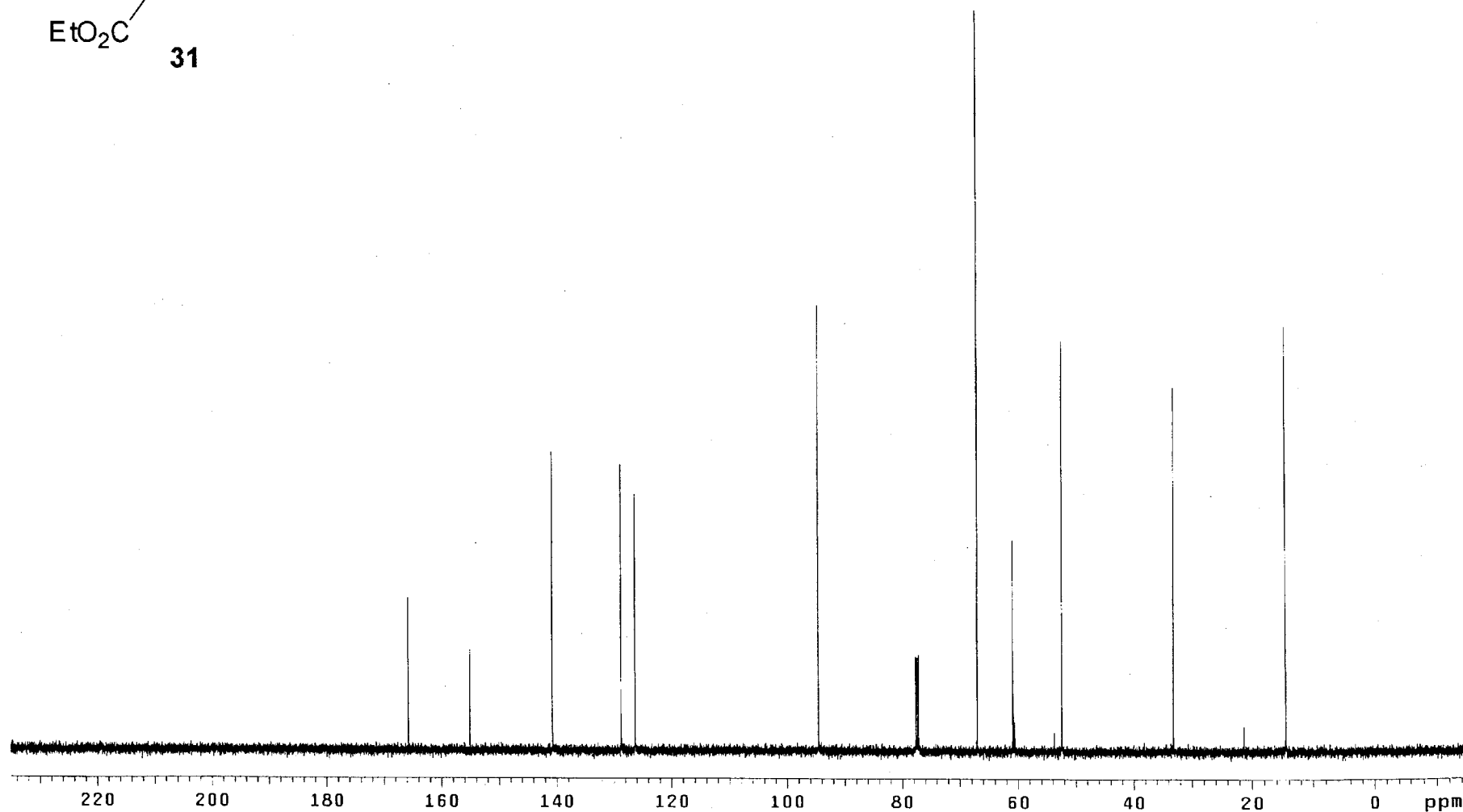
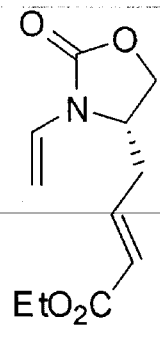


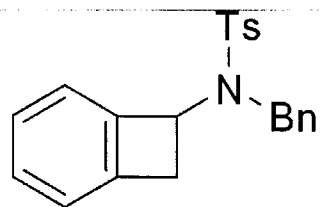


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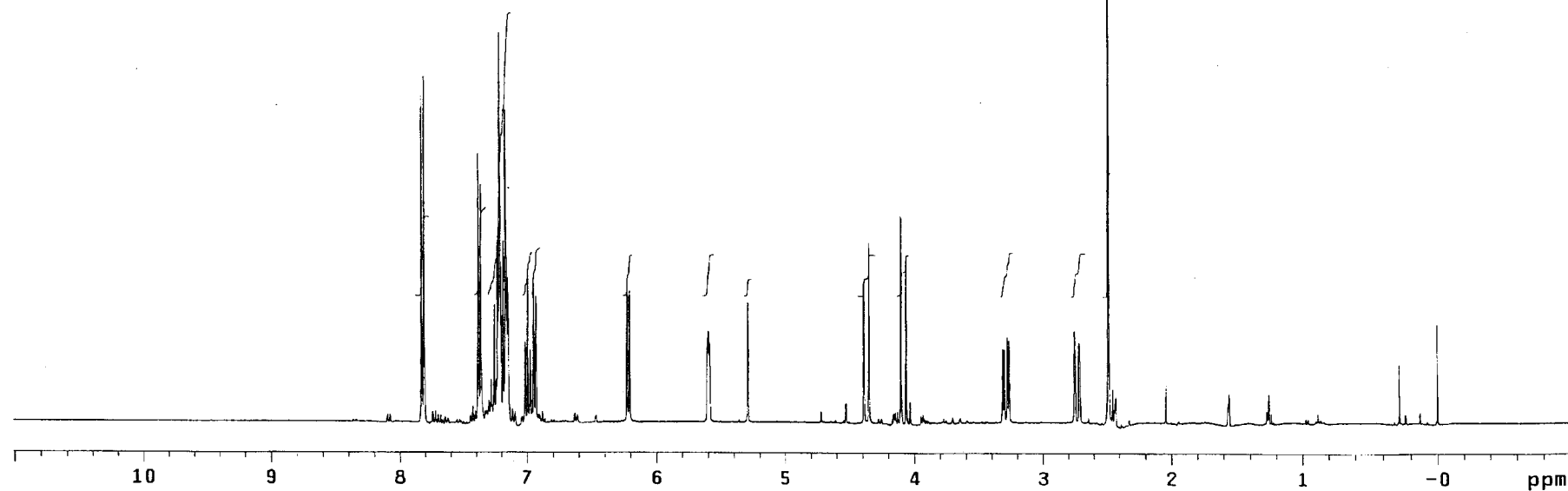


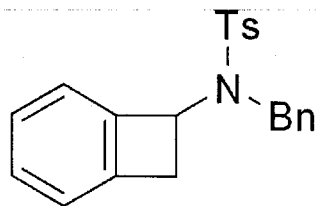




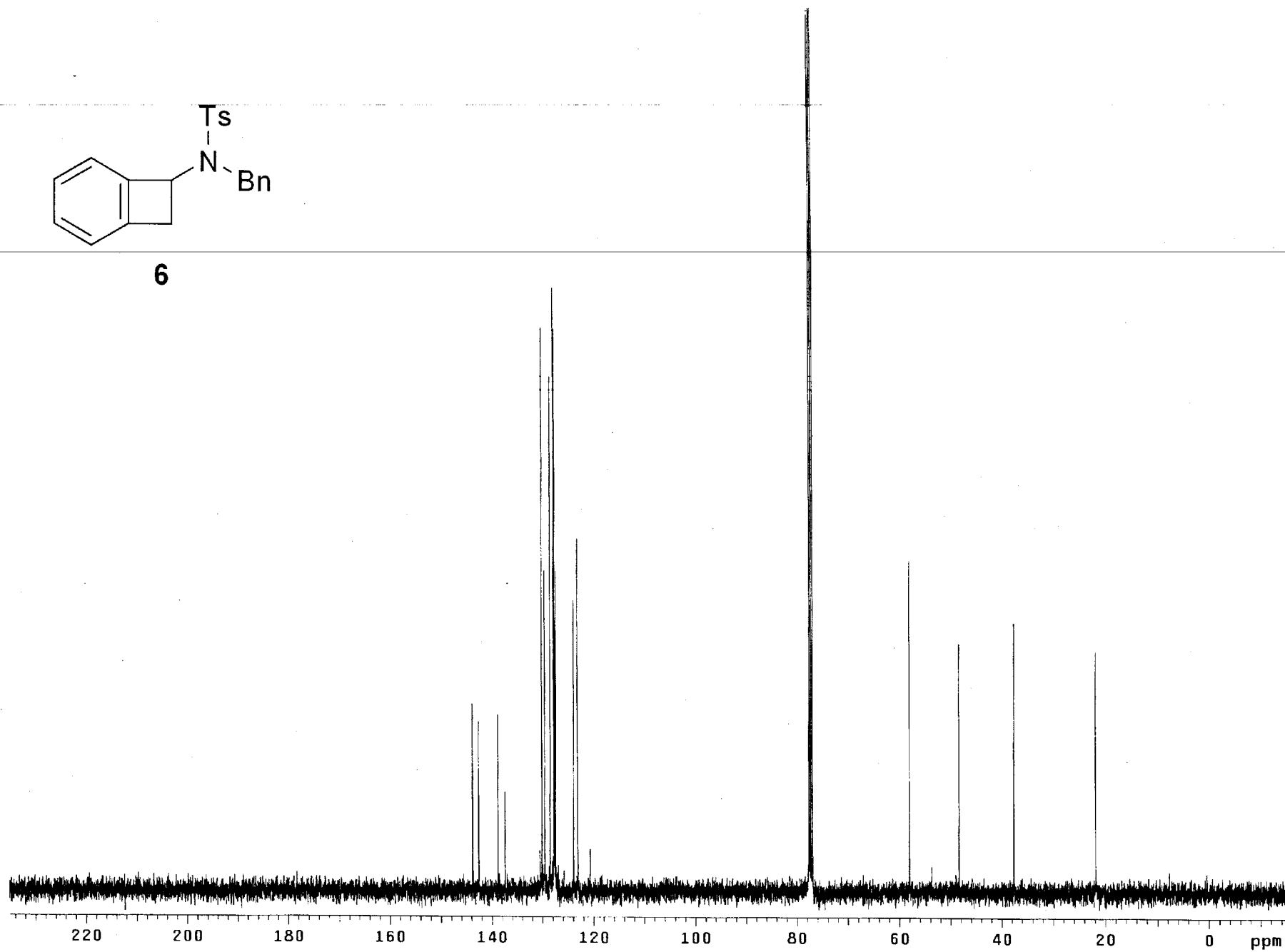


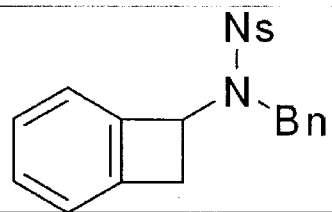
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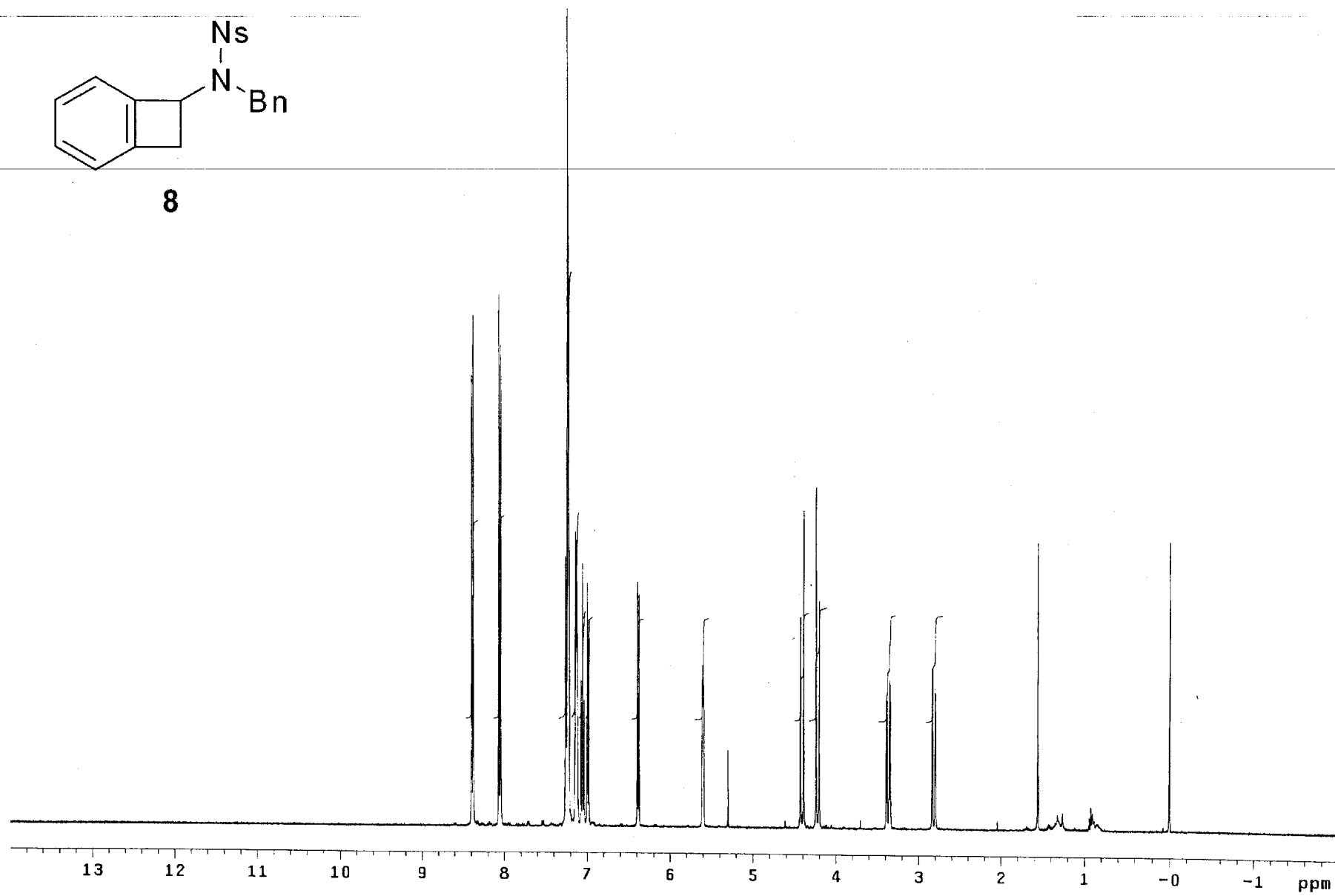


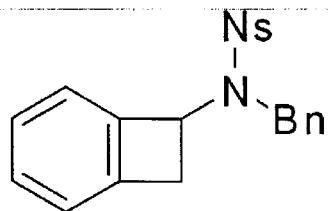
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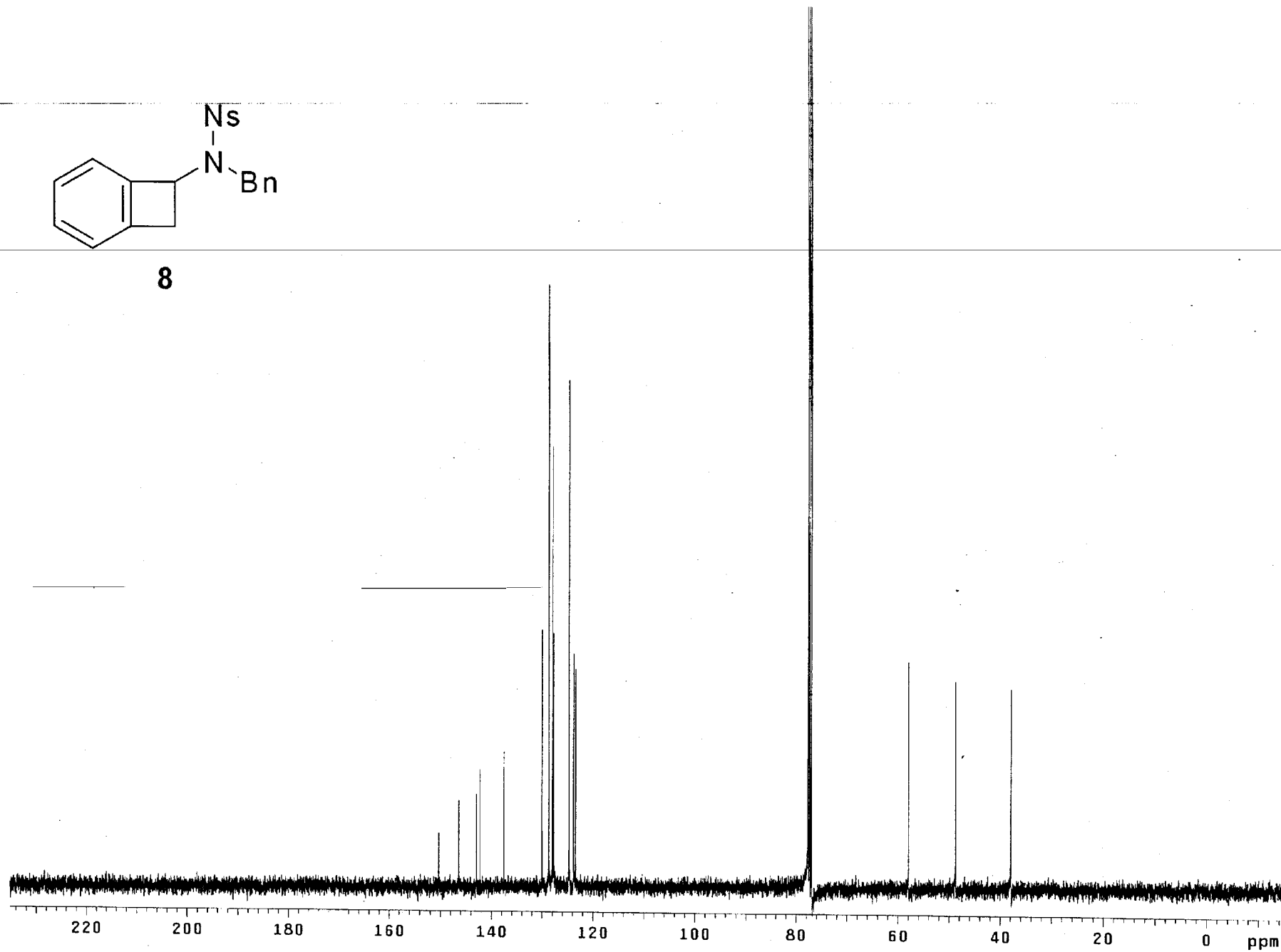


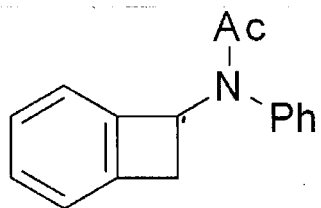
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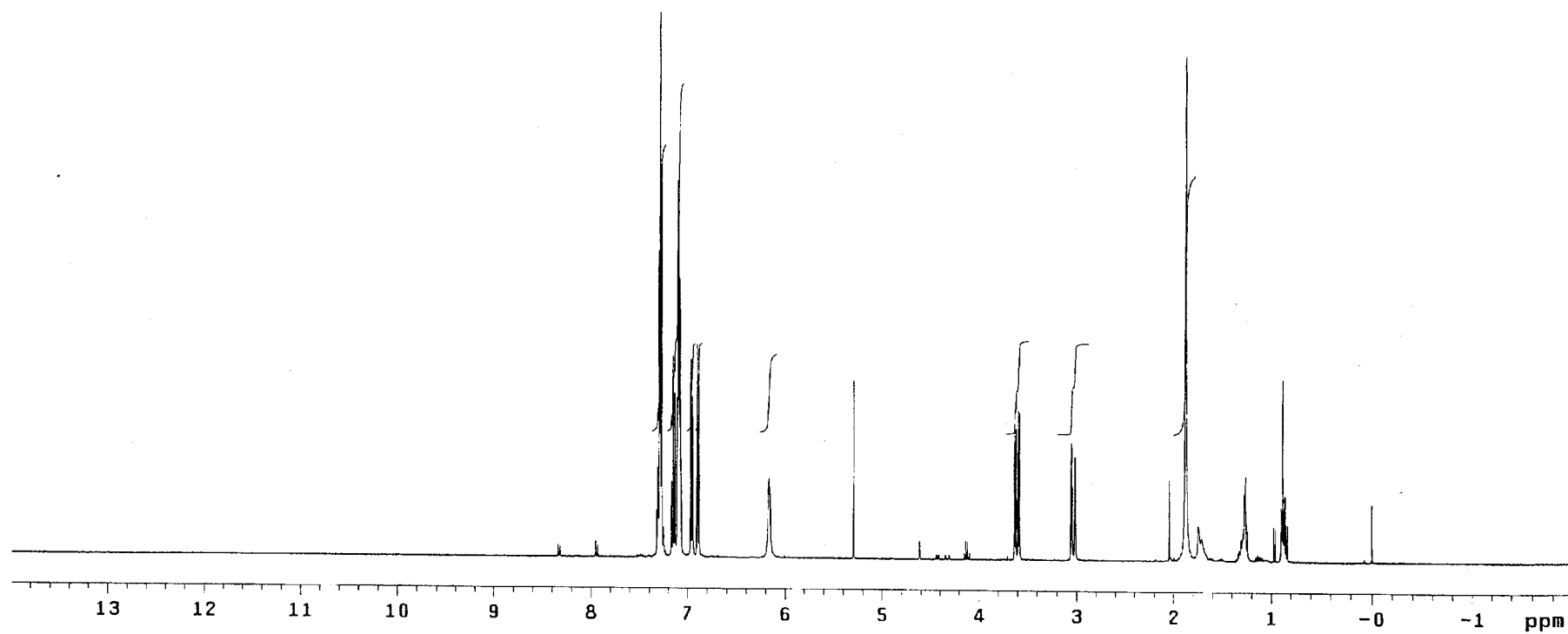


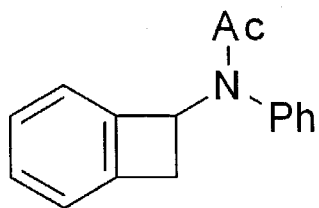
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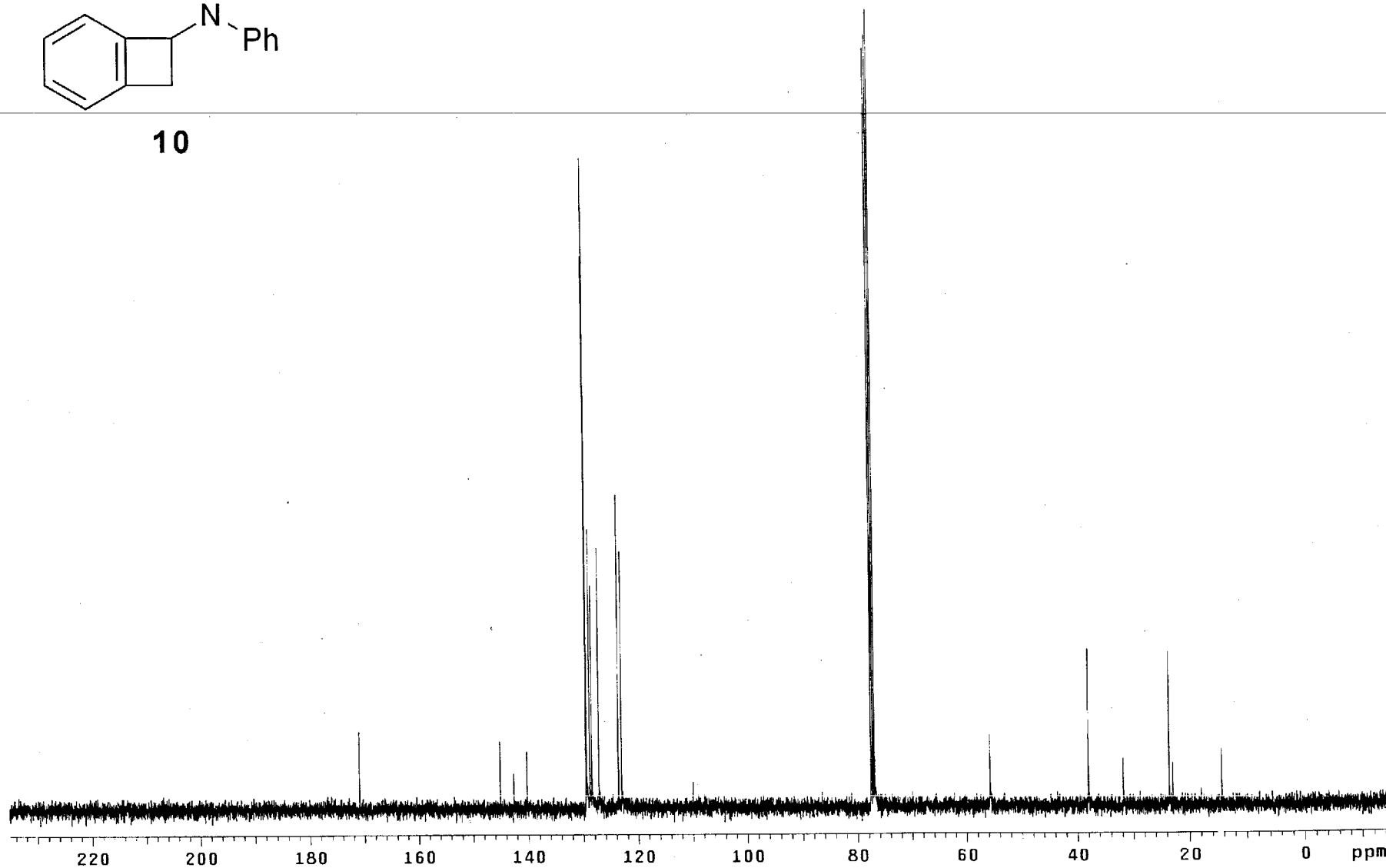


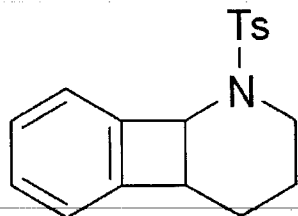
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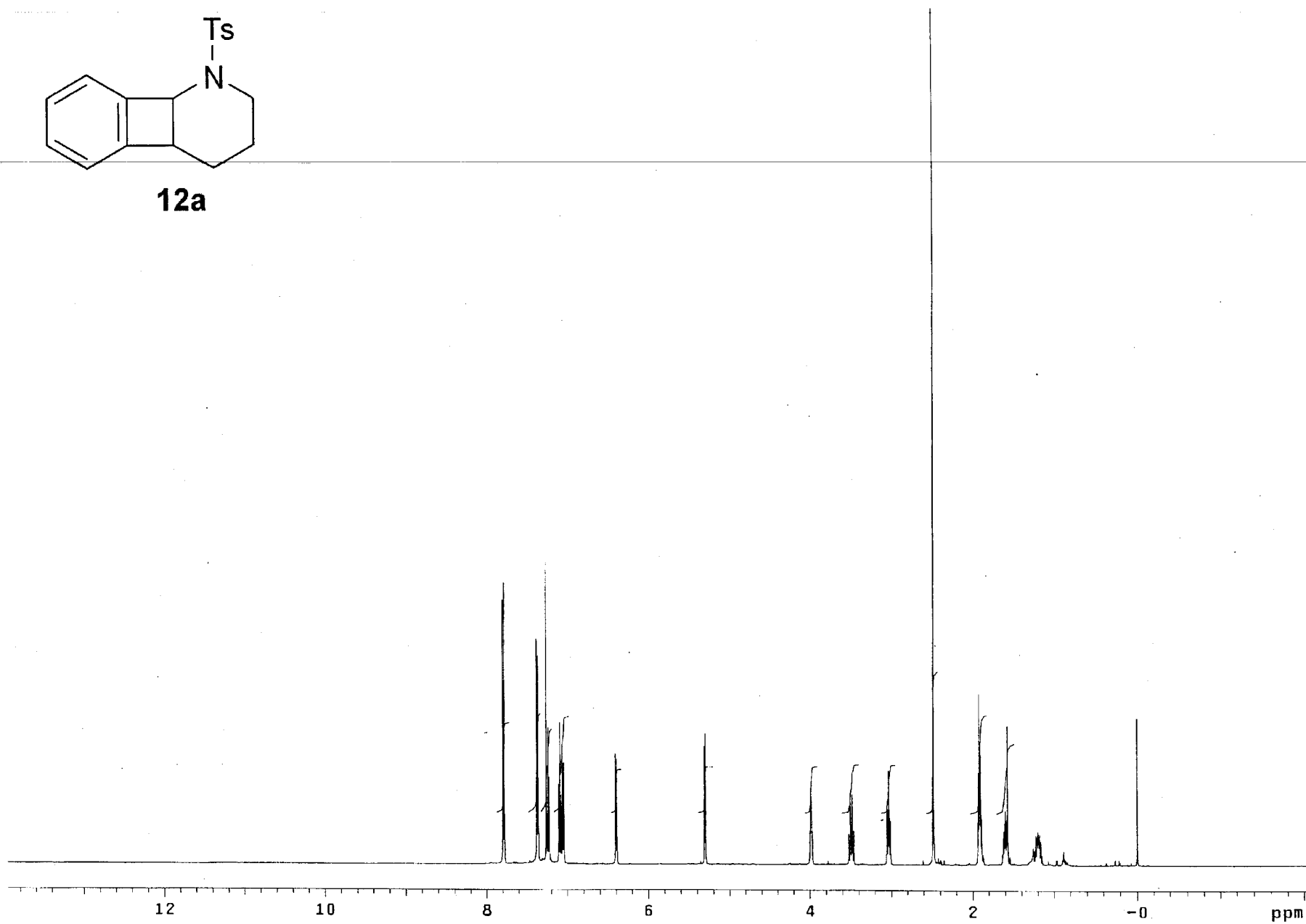


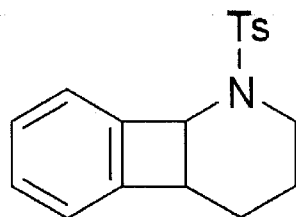
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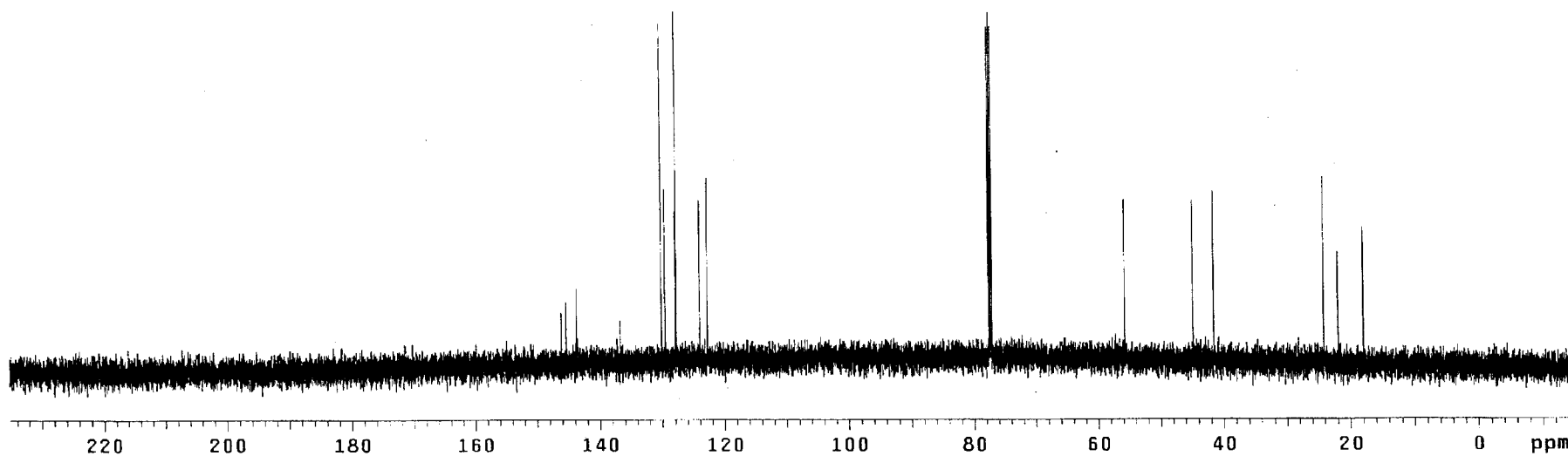


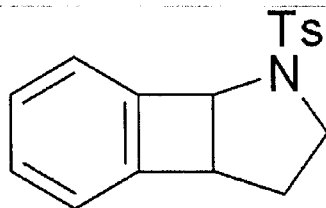
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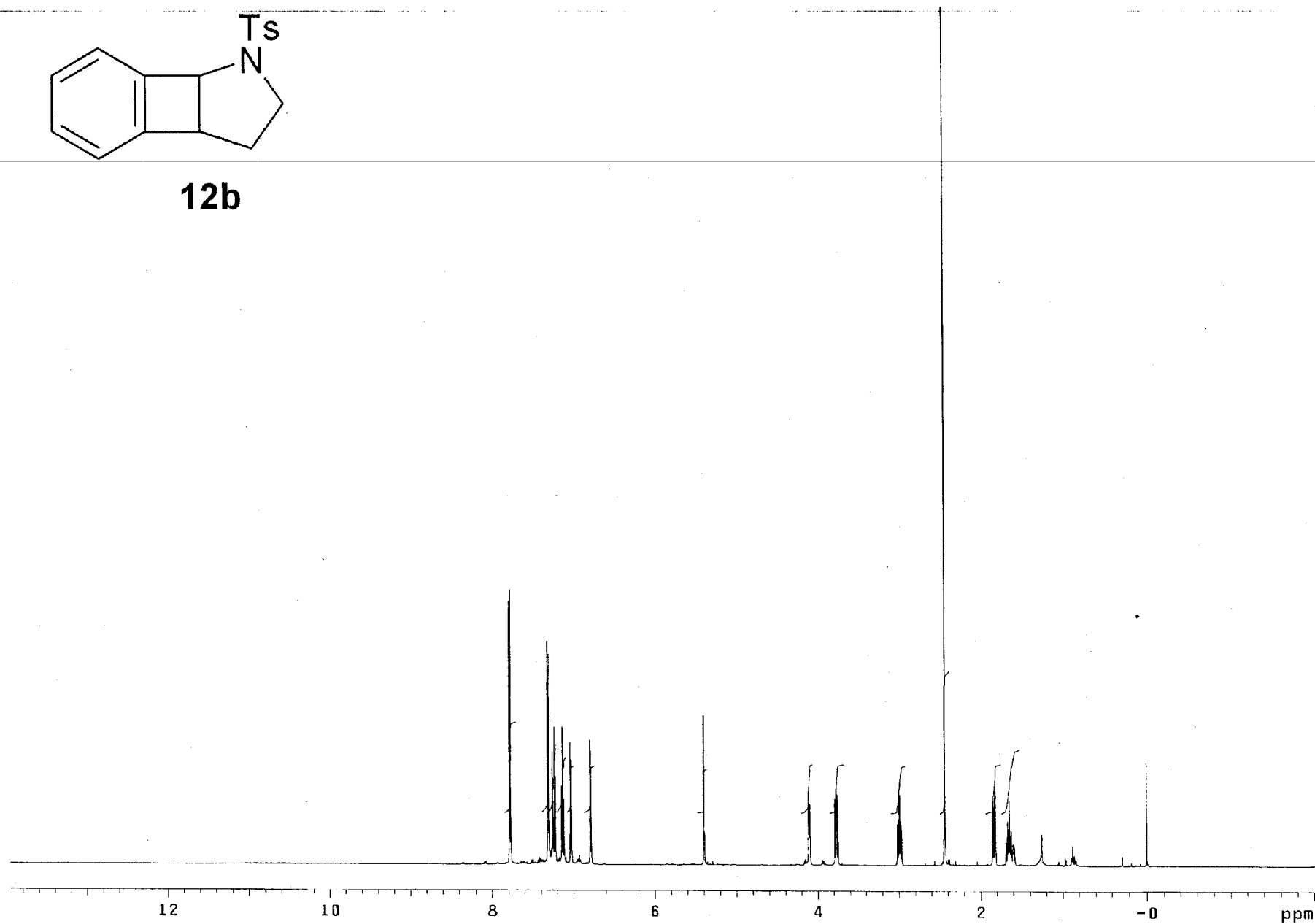


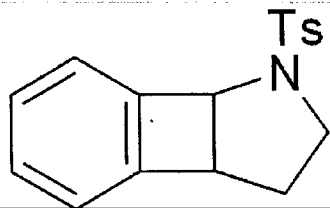
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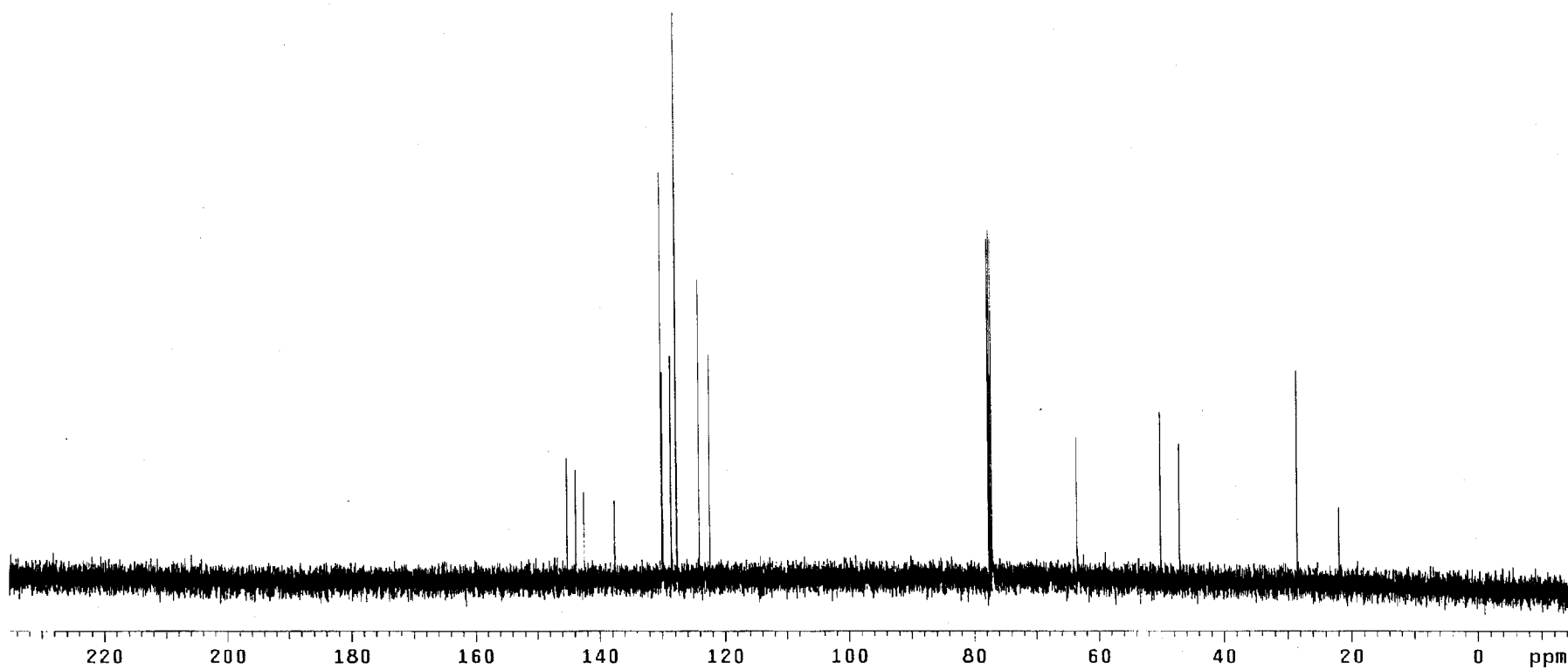


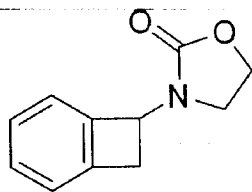
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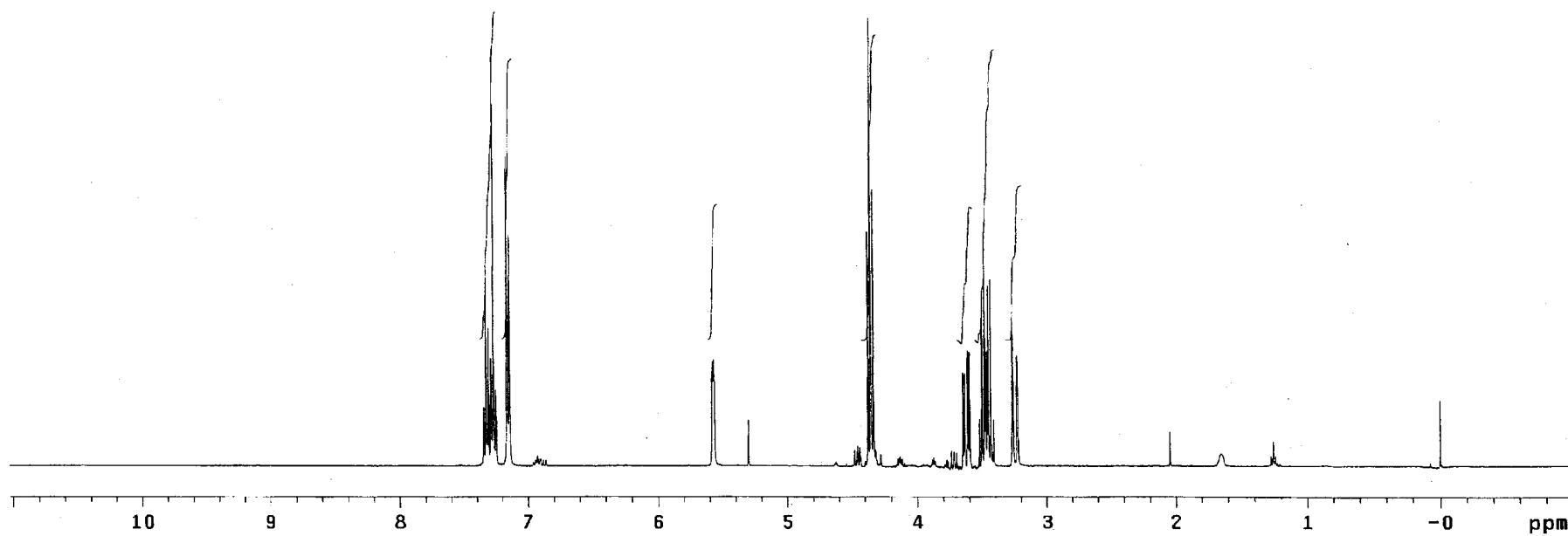


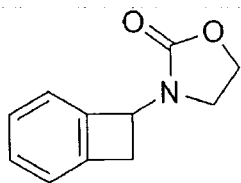
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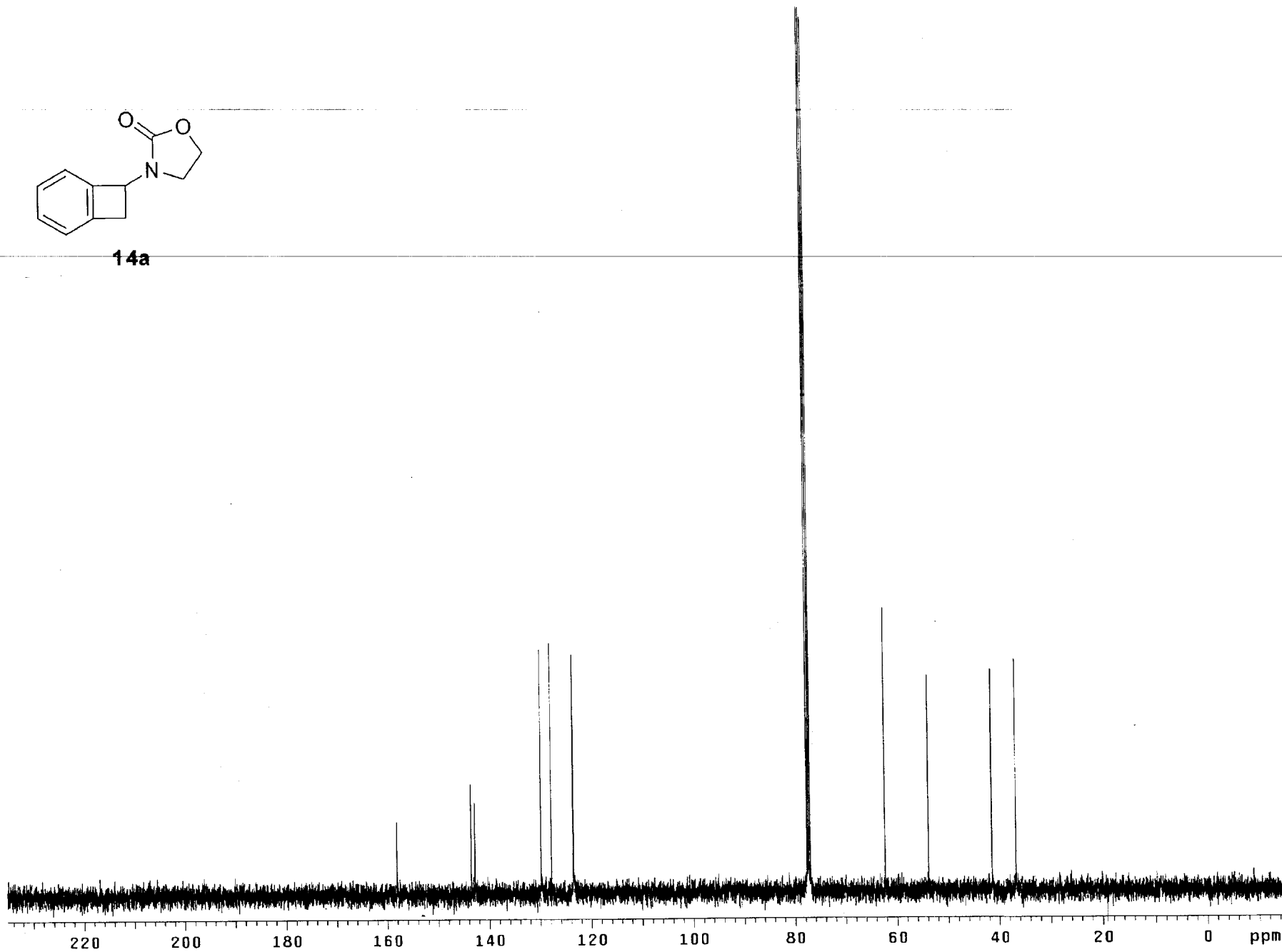


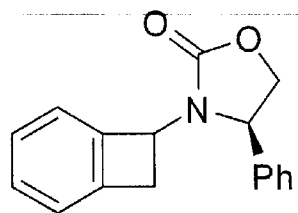
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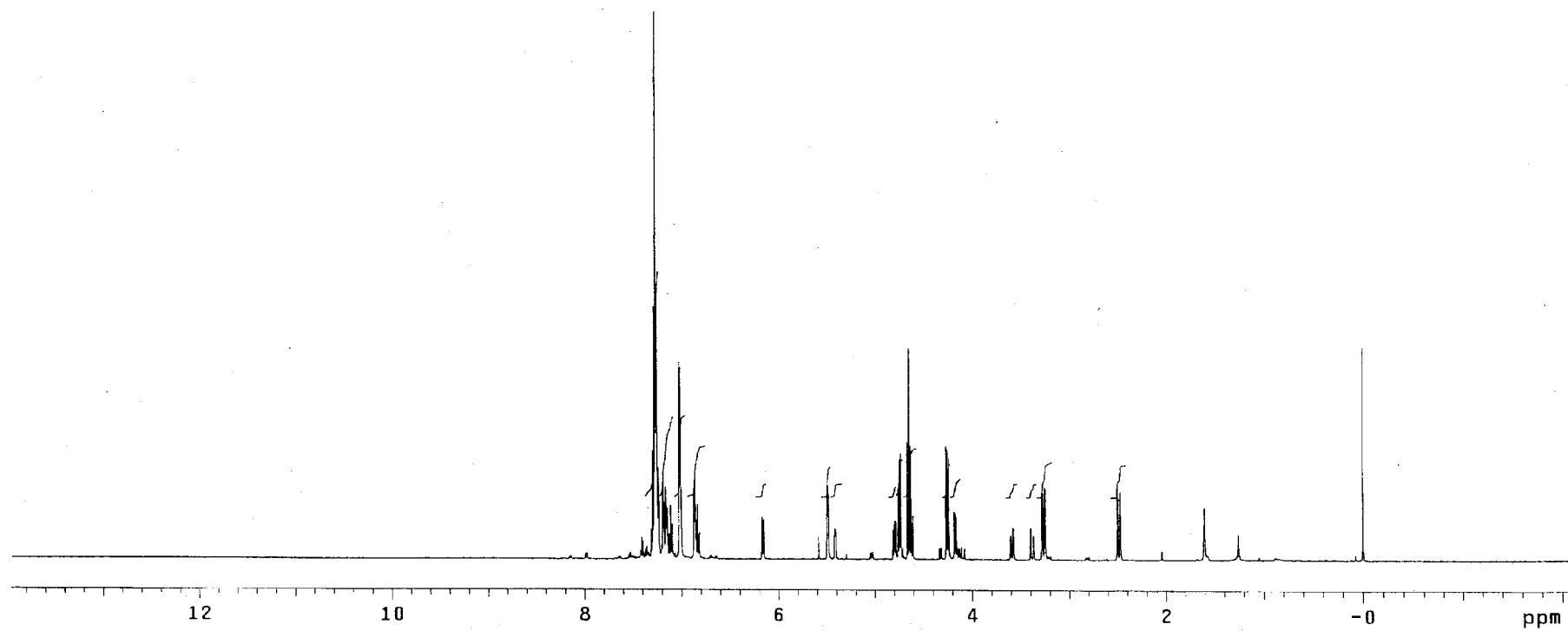


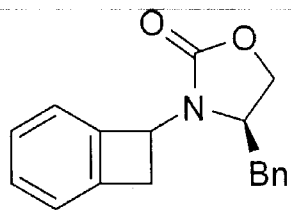
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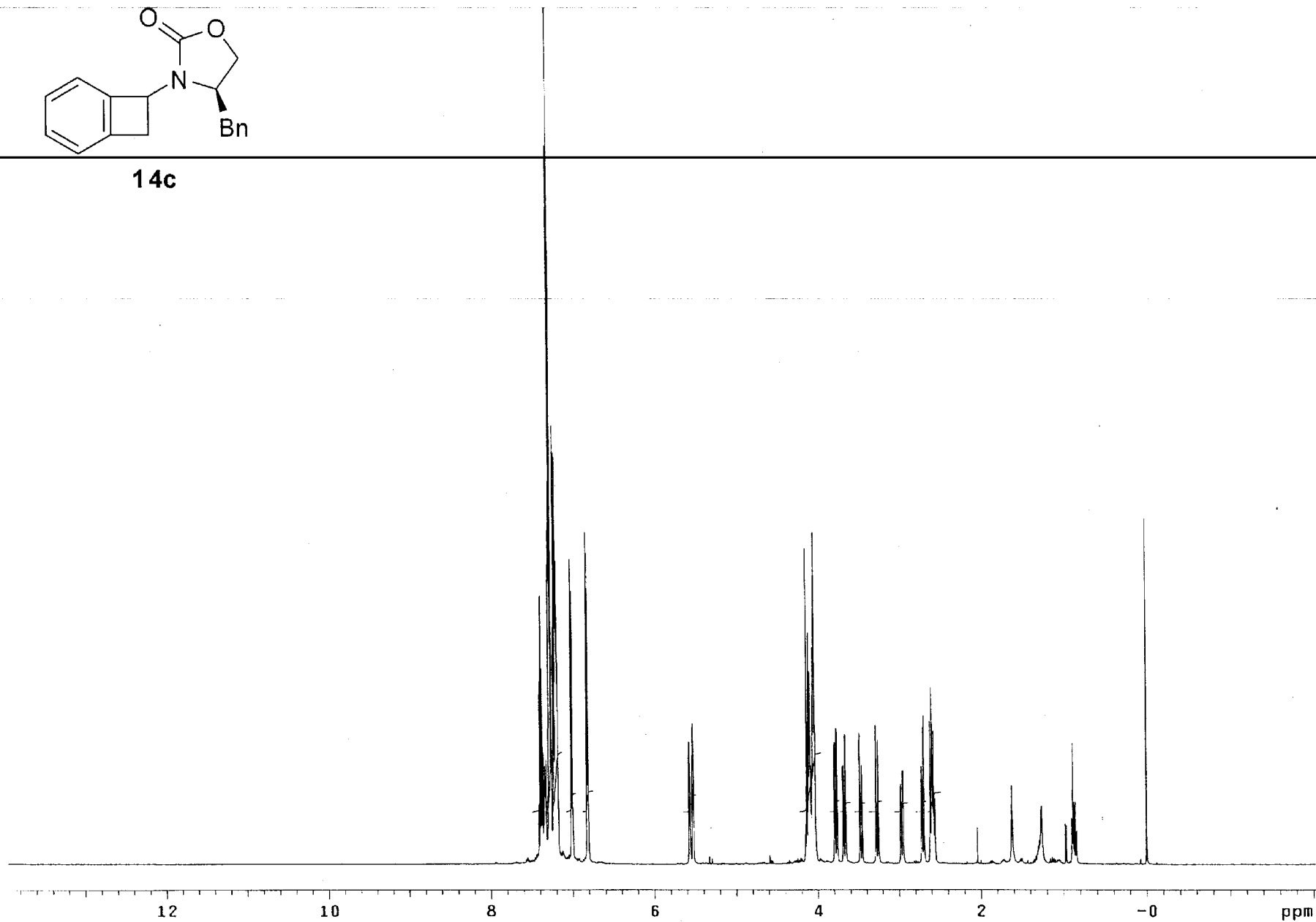


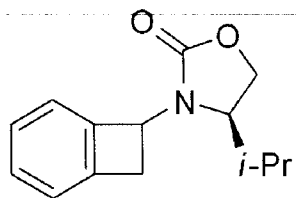
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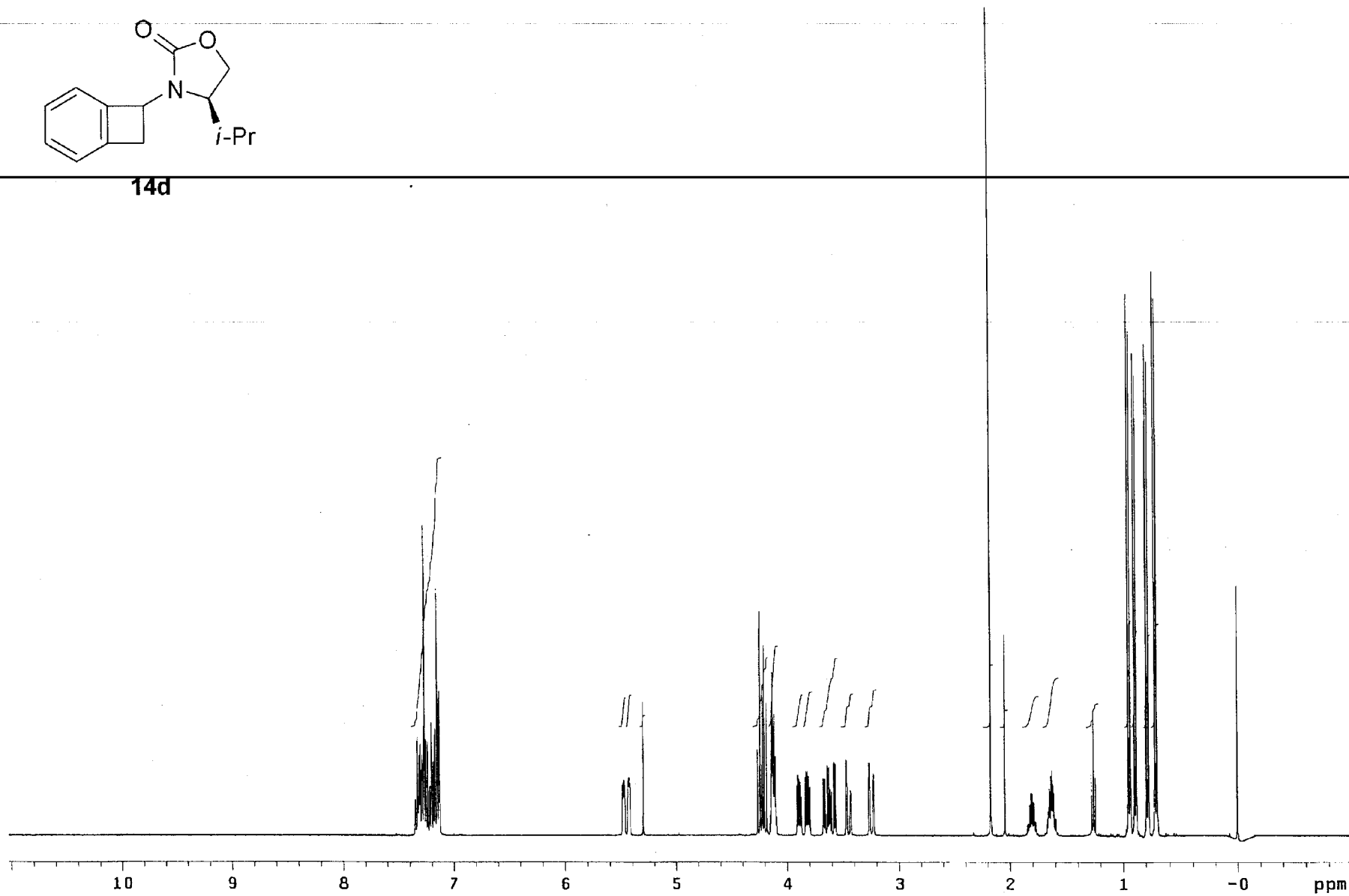


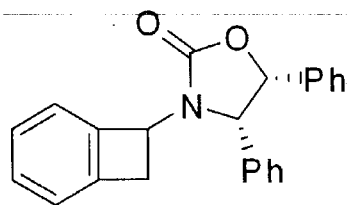
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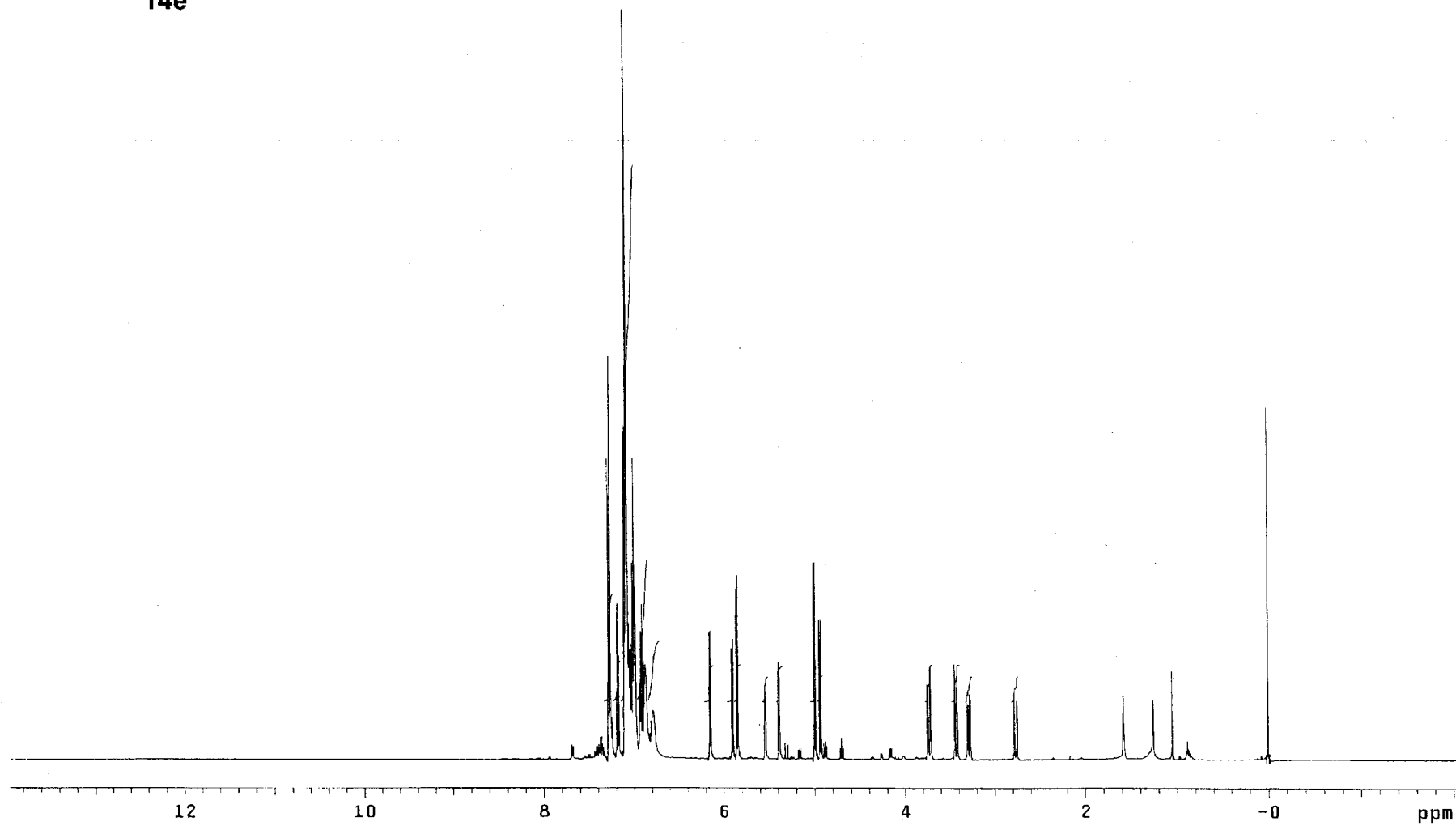


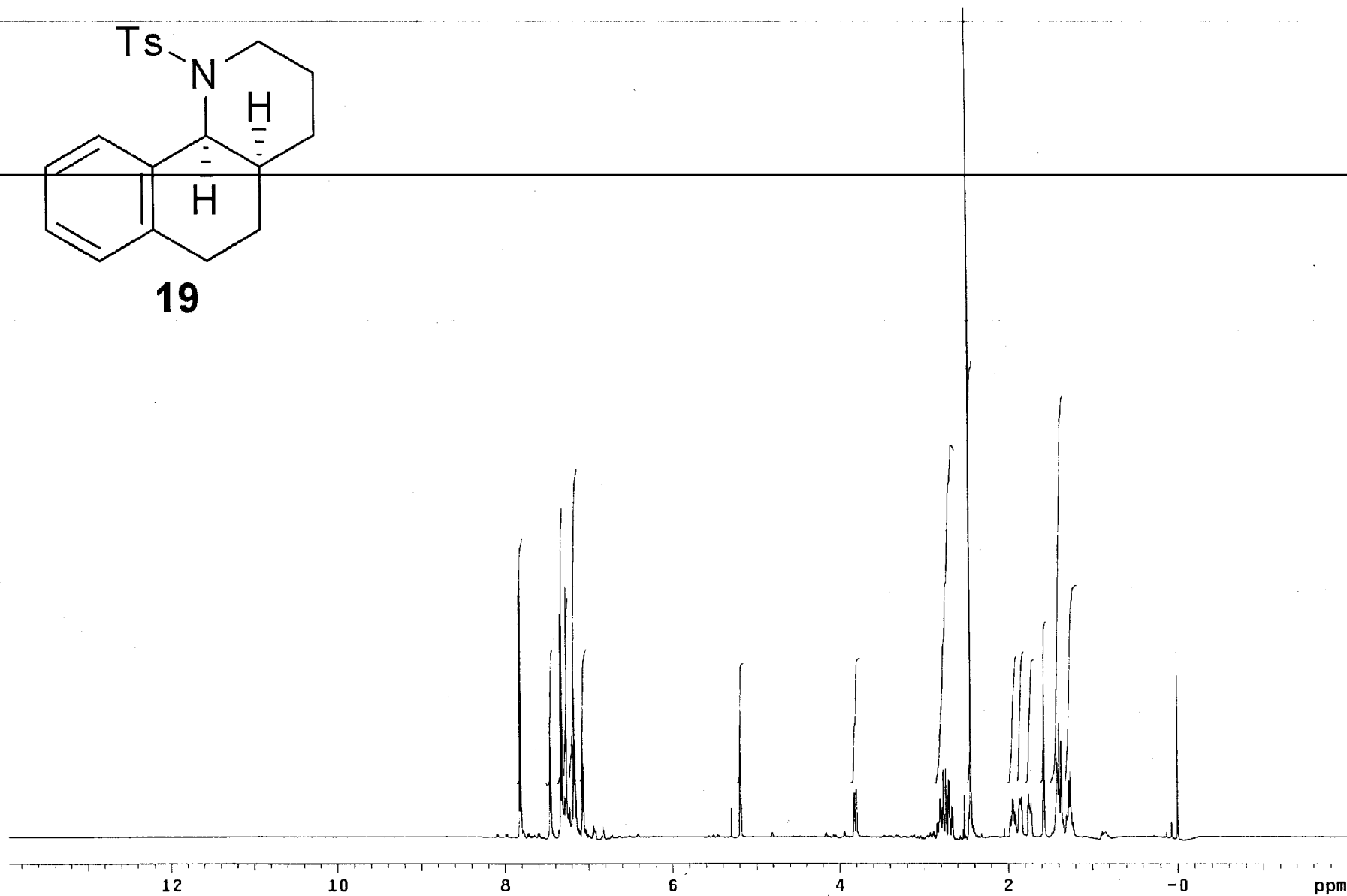
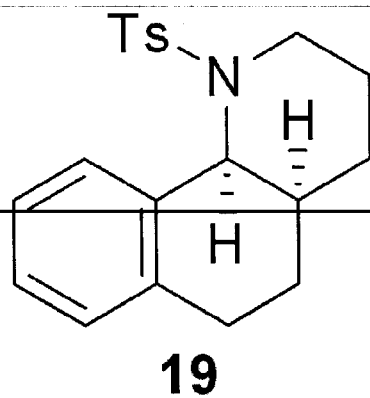
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14e







EB-113-3-Fr.12-16

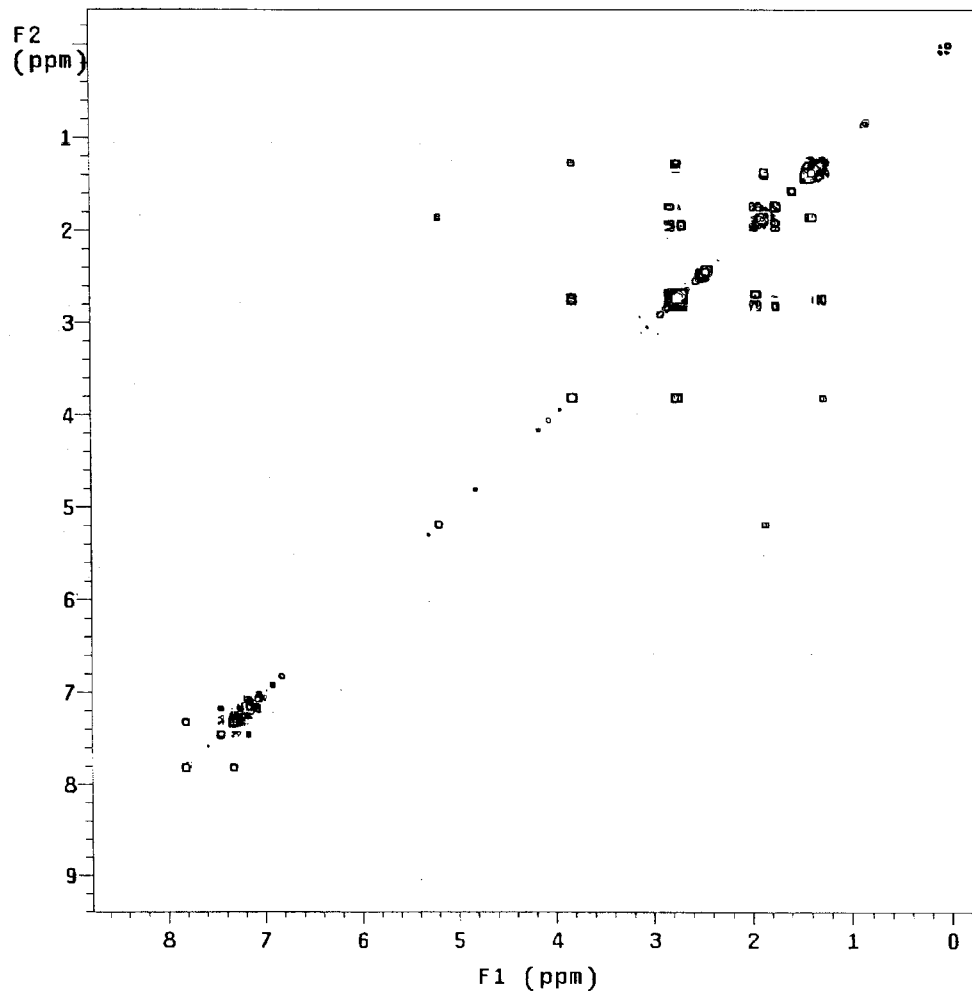
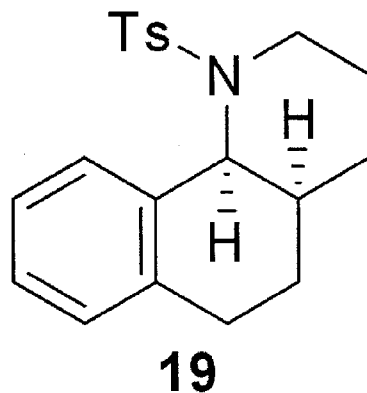
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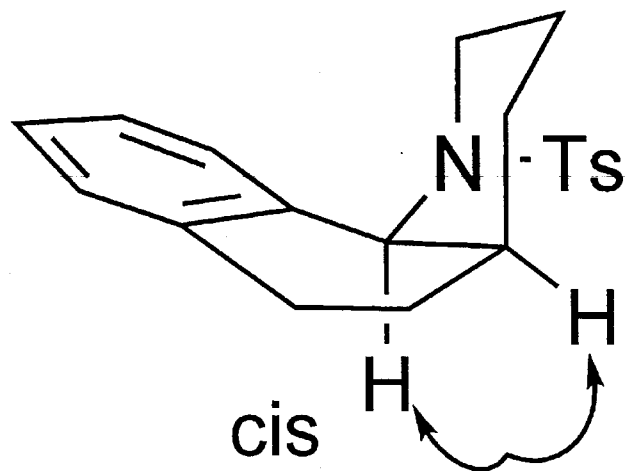
Pulse Sequence: gCOSY

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
Single scan
128 increments

OBSERVE H1, 499.728183 MHz
DATA PROCESSING
Sq. sine bell 0.064 sec
F1 DATA PROCESSING
Sq. sine bell 0.016 sec
FT size 2048 x 2048
Total time 2 min, 45 sec





key nOe of 19

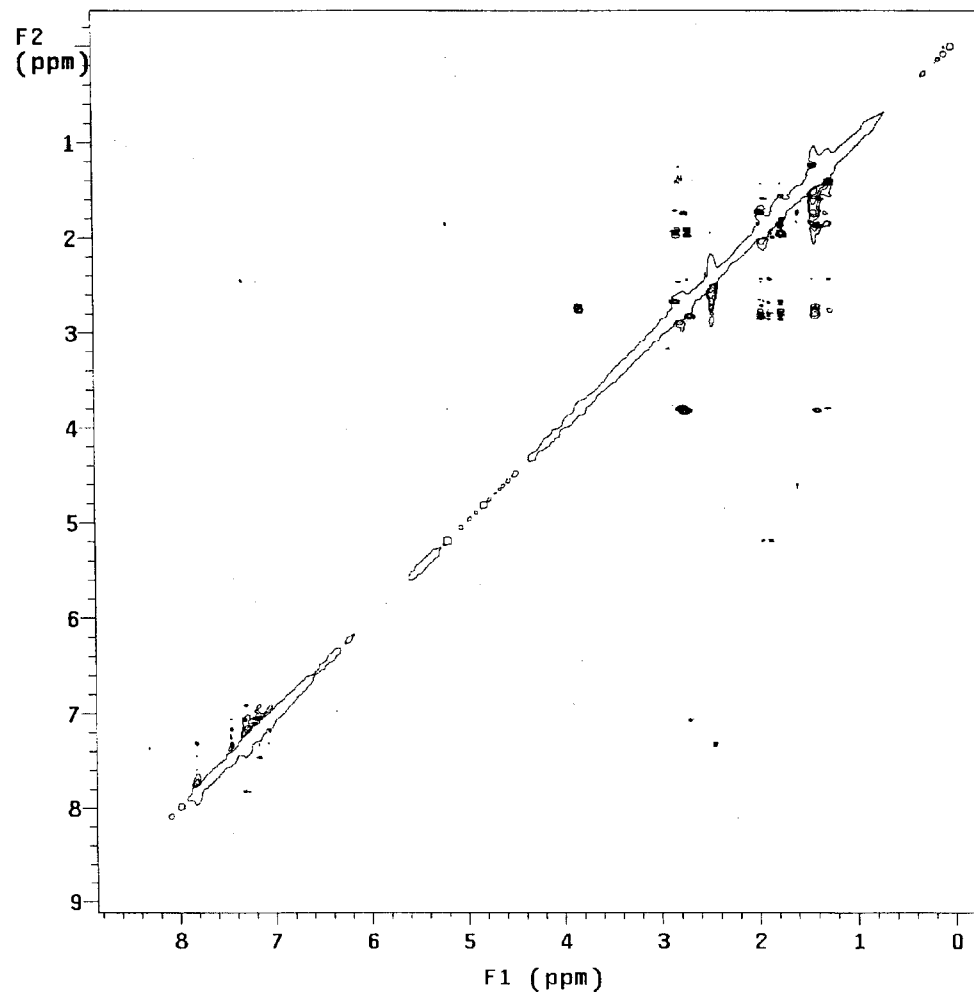
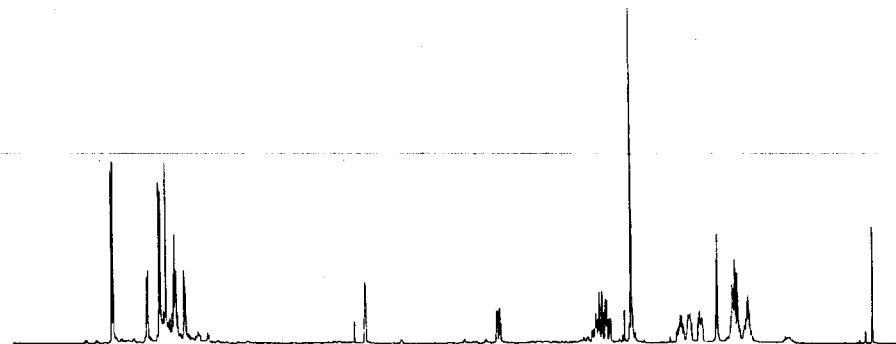
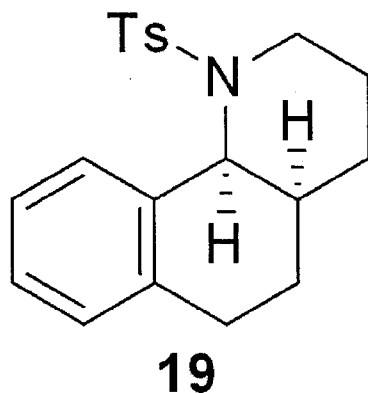
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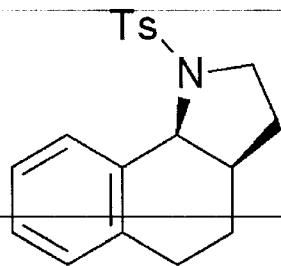
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Pulse Sequence: NOESY

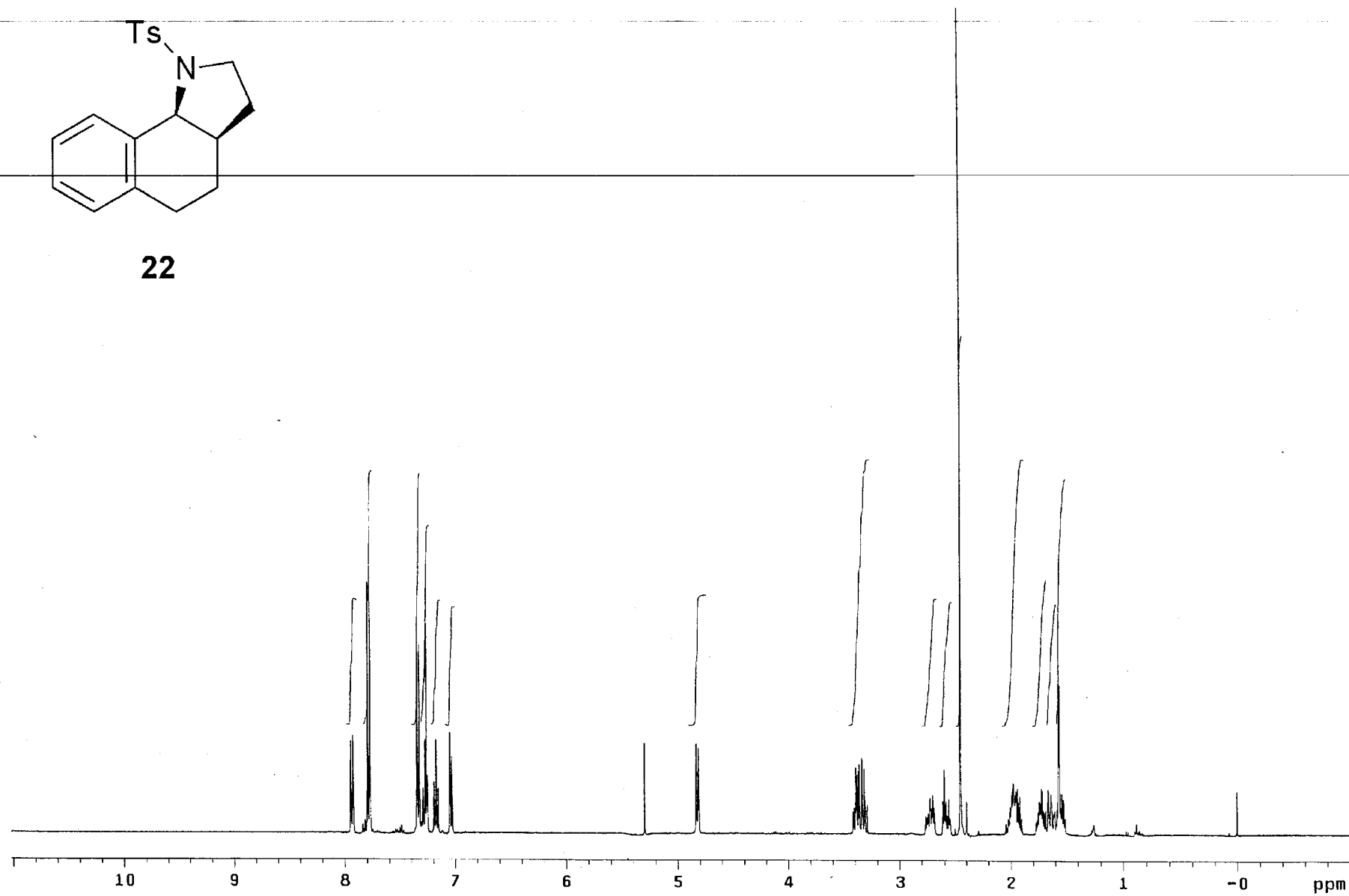
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: NOESY
INOVA-500 "nmr03"

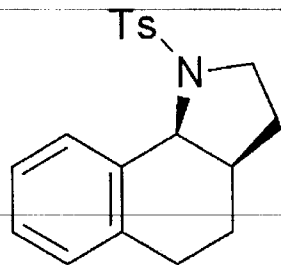
Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 128 increments
OBSERVE H1, 499.7288183 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.015 sec
FT size 2048 x 2048
Total time 1 hr, 32 min, 51 sec



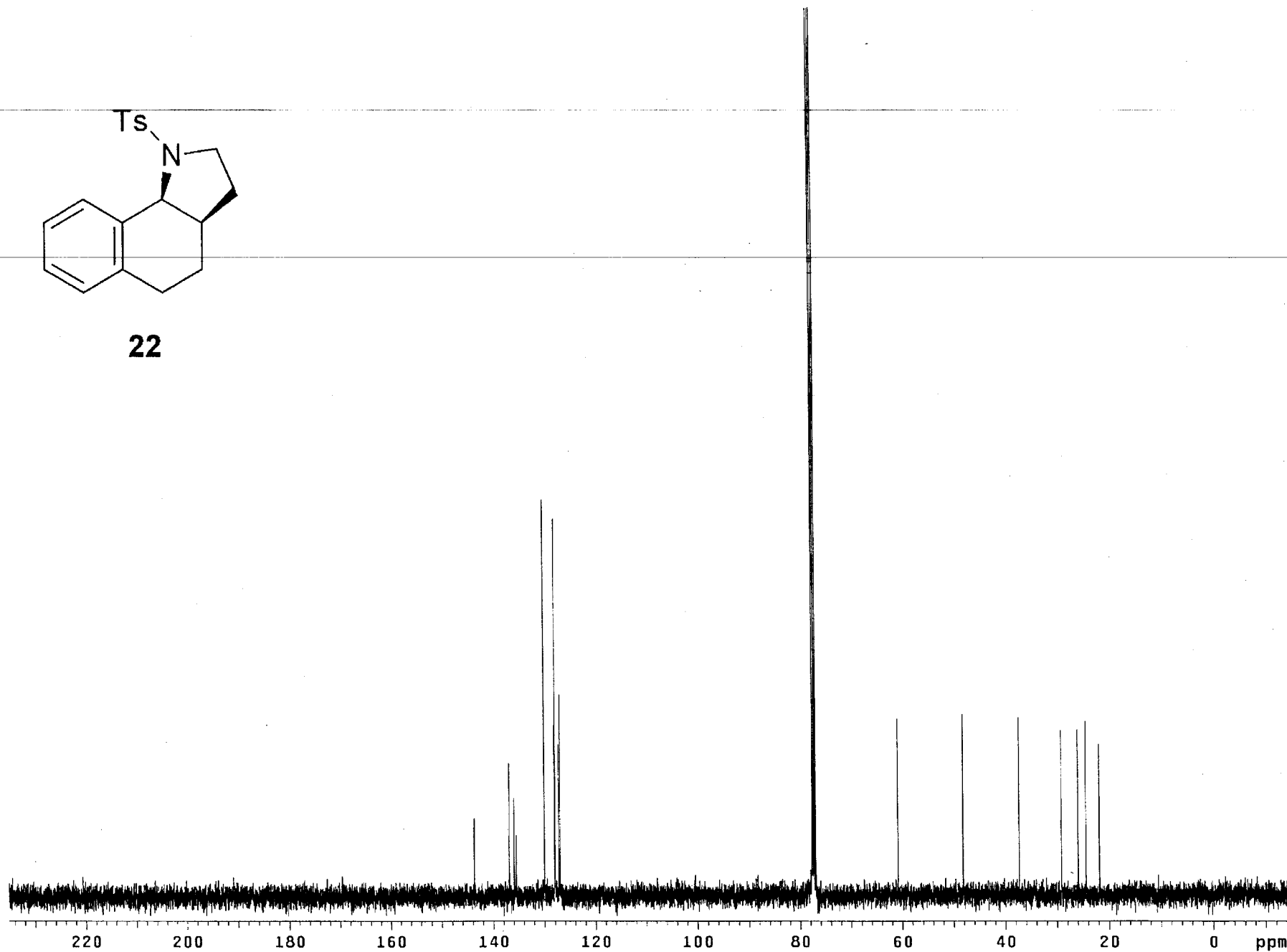


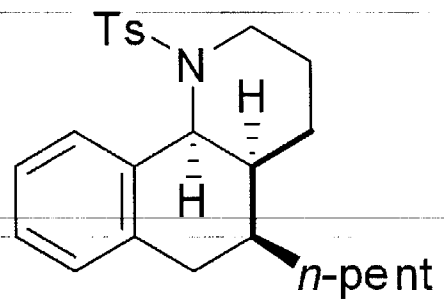
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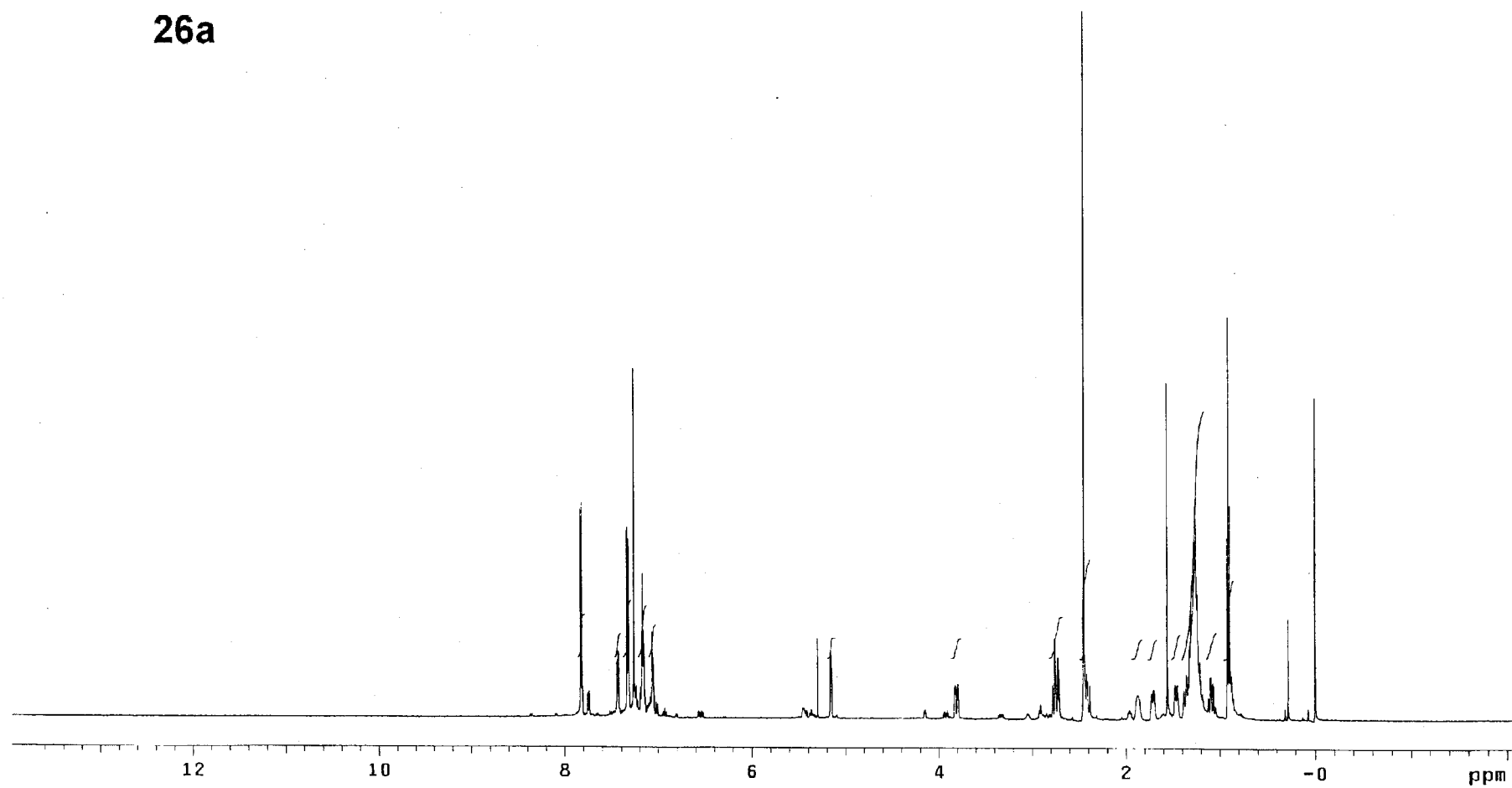


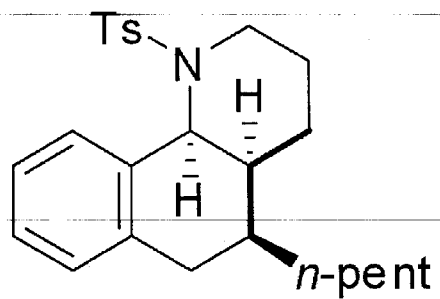
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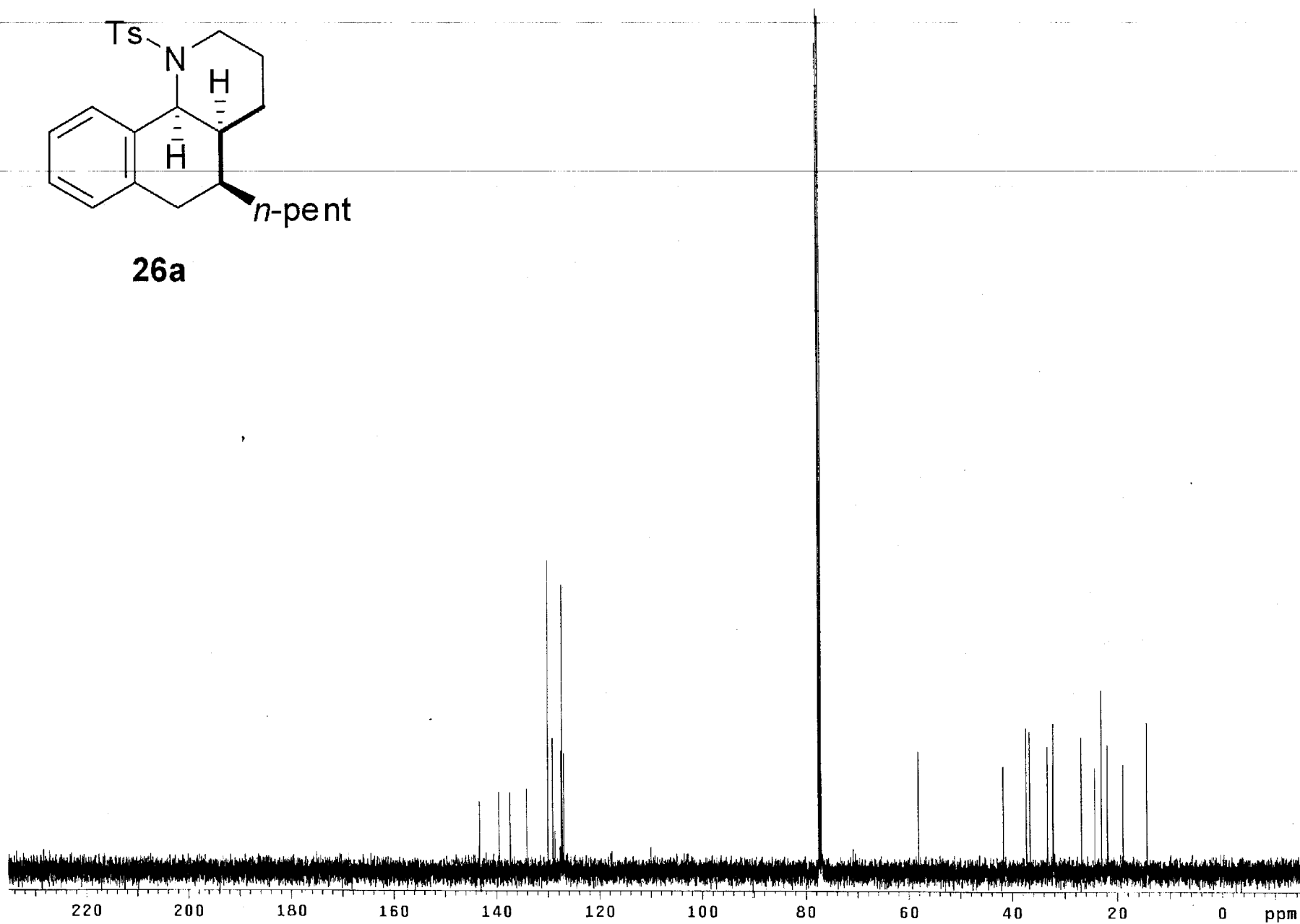


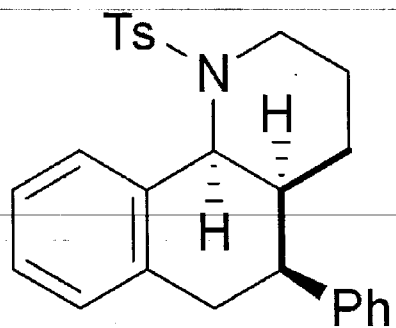
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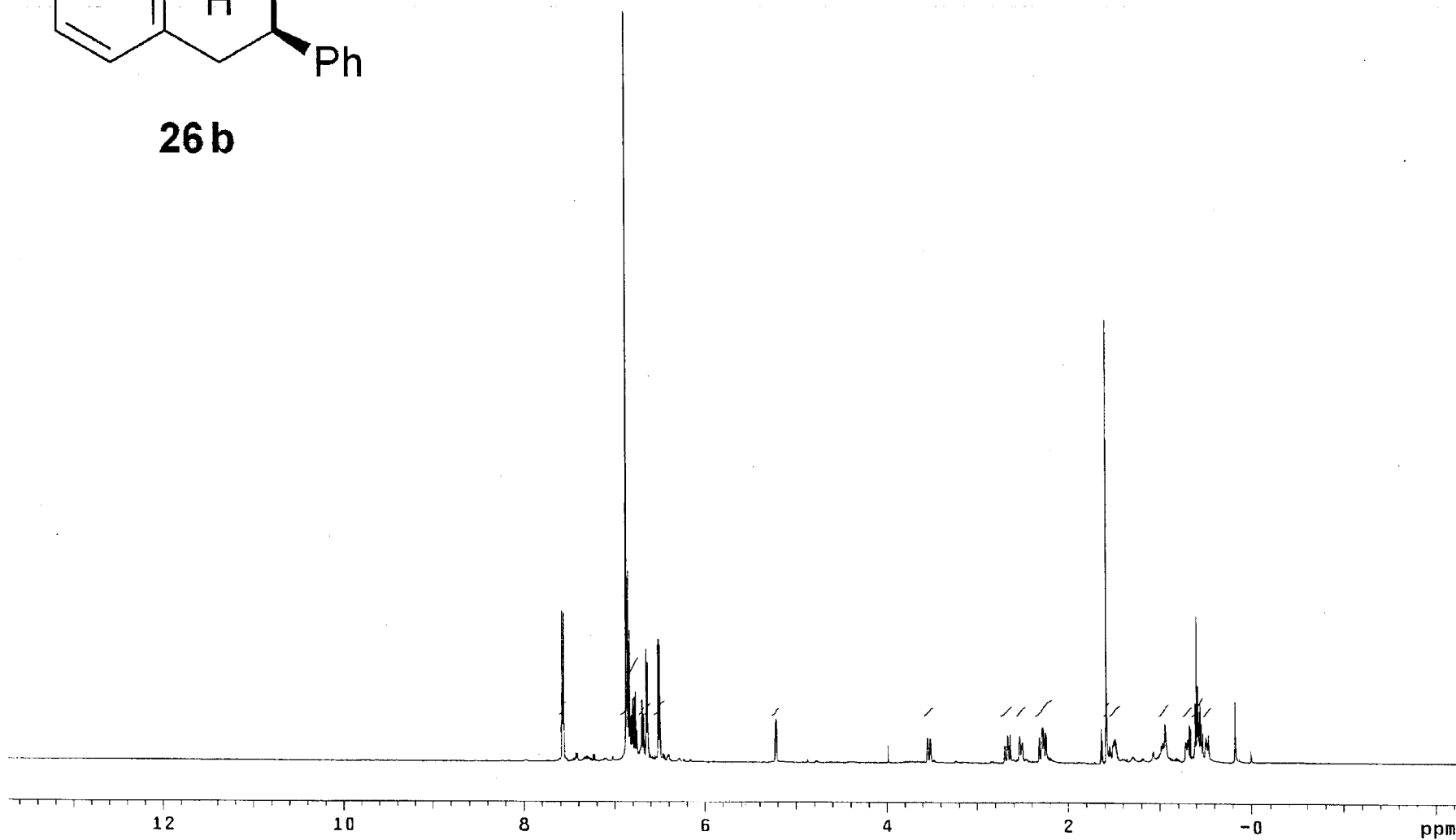


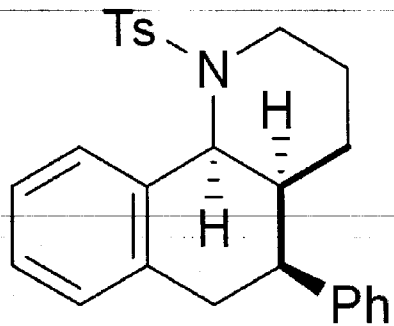
26a



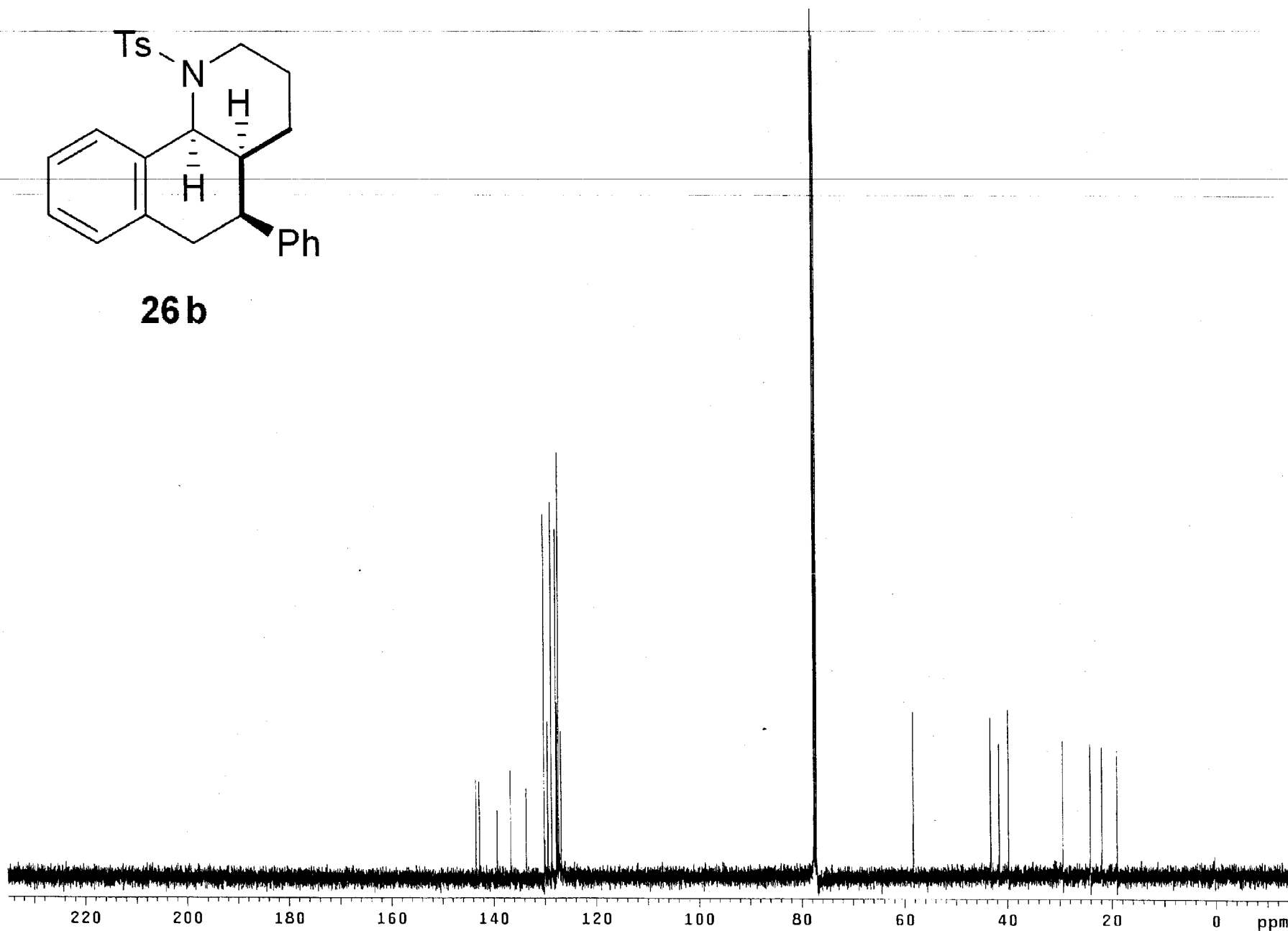


26b





26b



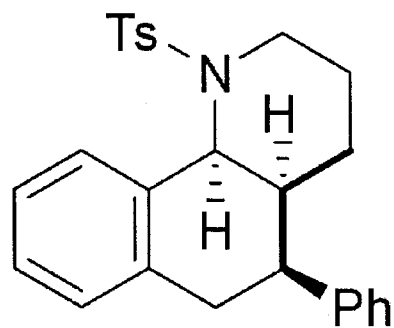
RH-2-281-1COSY-benzene_13Jun2009

Archive directory: /export/home/ryuji/vnmrsys/data
Sample directory: RH-2-281-1COSY-benzene_18Jun2009

Pulse Sequence: gCOSY

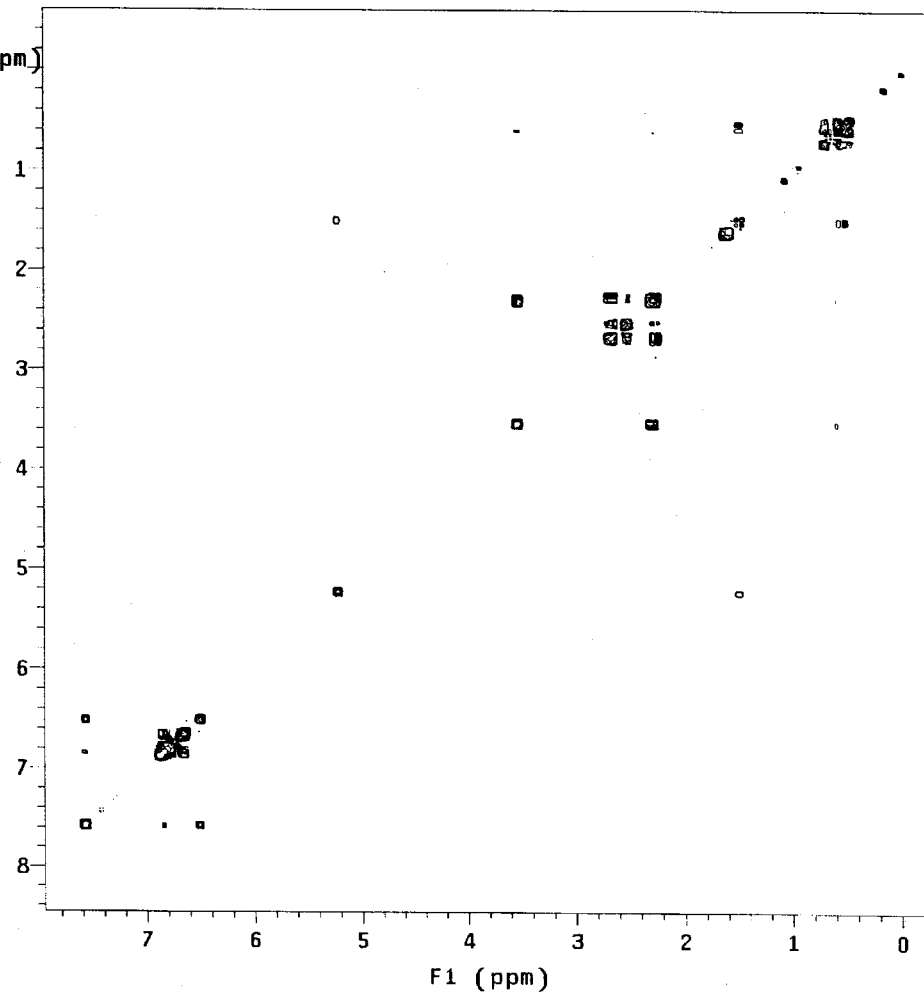
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

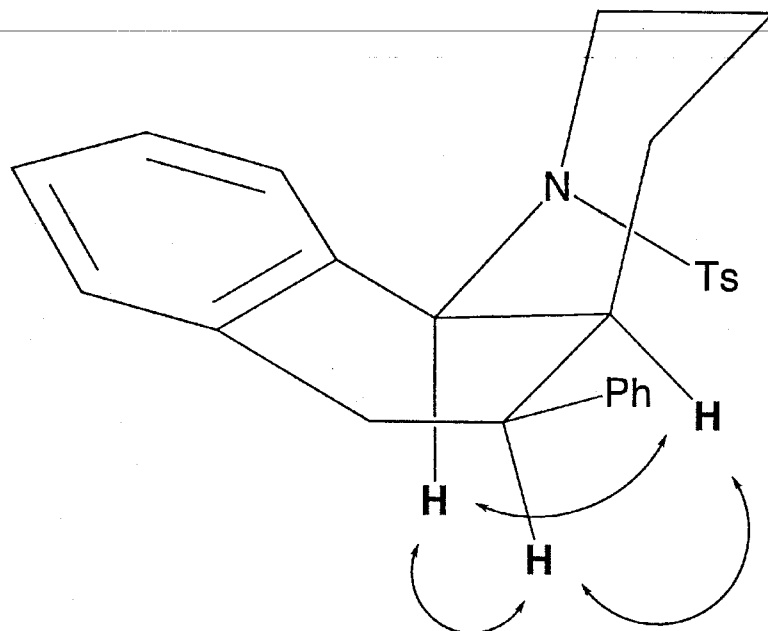
Relax. delay 1.000 sec
Acq. time 0.160 sec
Width 6387.7 Hz
2D Width 6387.7 Hz
Single scan
128 increments
OBSERVE H1, 399.7866651 MHz
DATA PROCESSING
Sq. sine bell 0.080 sec
F1 DATA PROCESSING
Sq. sine bell 0.020 sec
FT size 2048 x 2048
Total time 2 min, 50 sec



26b

F2
(ppm)





Key nOe

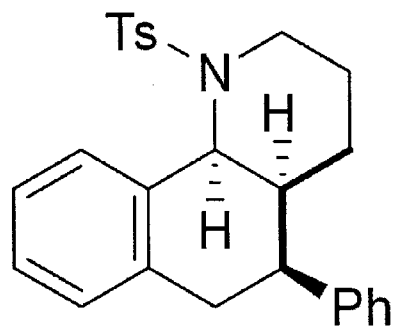
RH-2-281-benzene-NOESY_19Jun2009

Archive directory: /export/home/ryuji/vnmrsys/data
Sample directory: RH-2-281-benzene-NOESY_19Jun2009

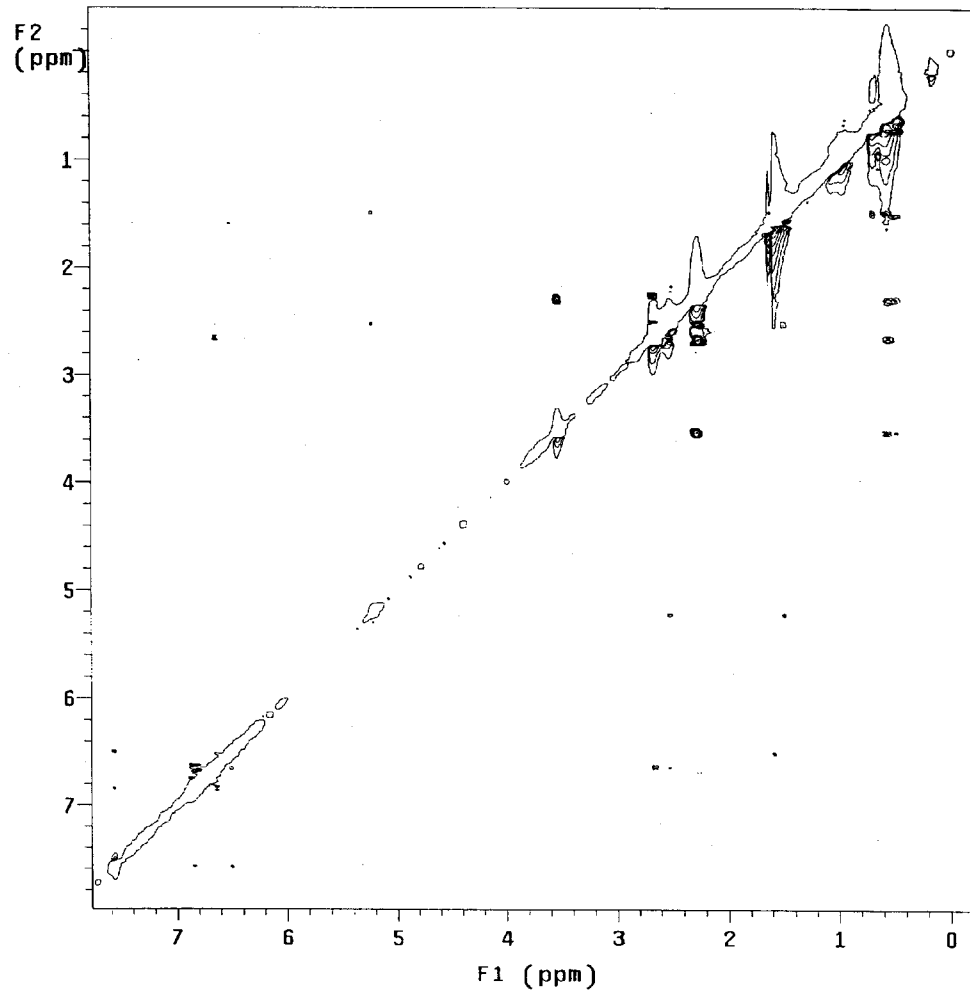
Pulse Sequence: NOESY

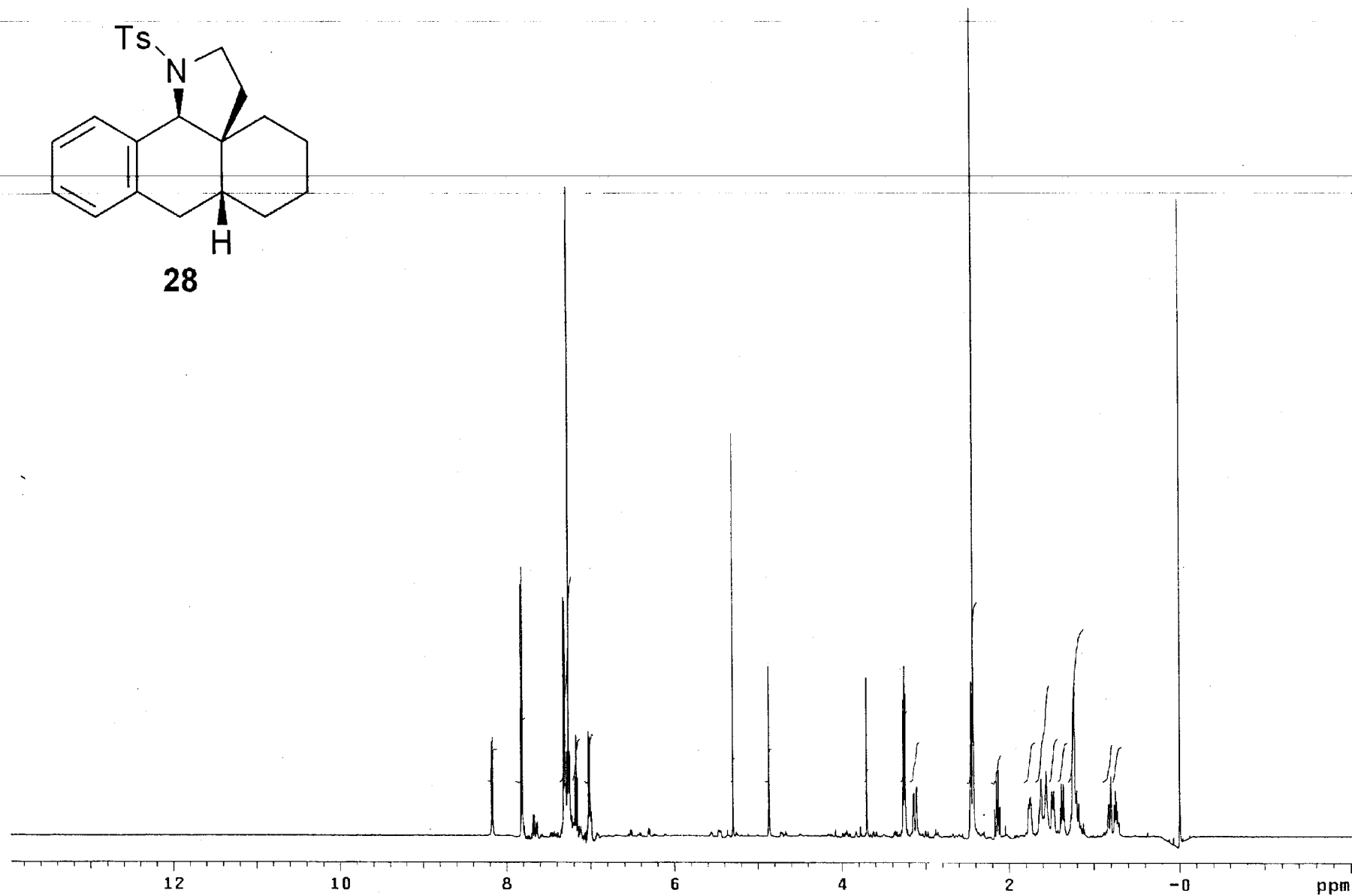
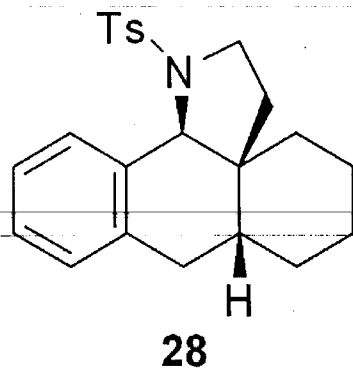
Solvent: C6D6
Temp. 25.0 C / 298.1 K
File: NOESY
INOVA-500 "nmr03"

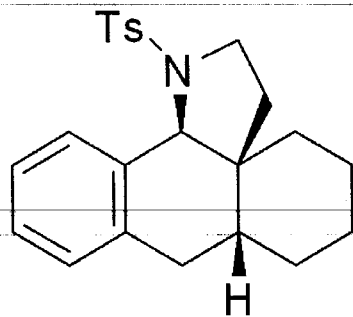
Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 128 increments
OBSERVE H1, 499.7289891 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.015 sec
FT size 2048 x 2048
Total time 1 hr, 32 min, 51 sec



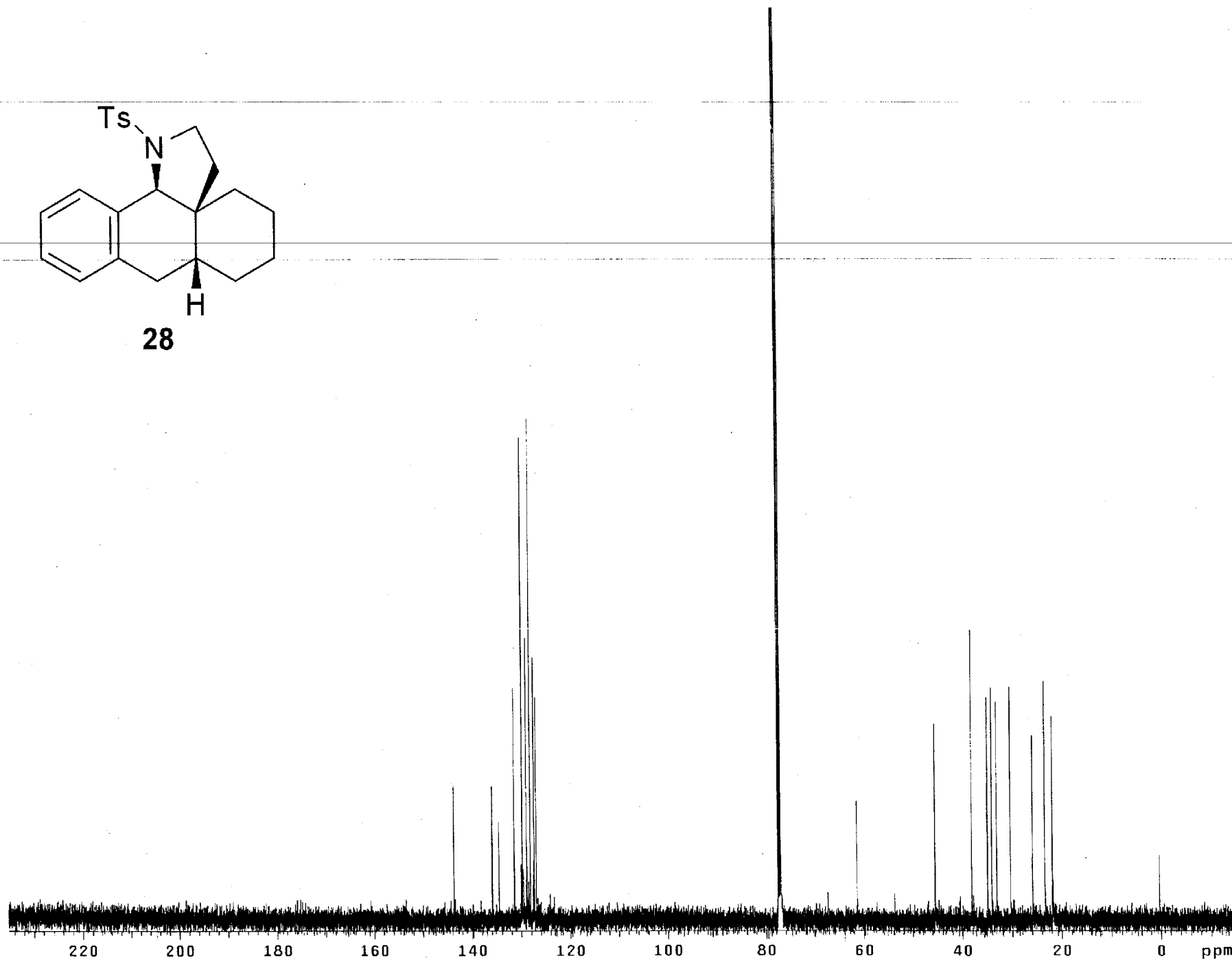
26b

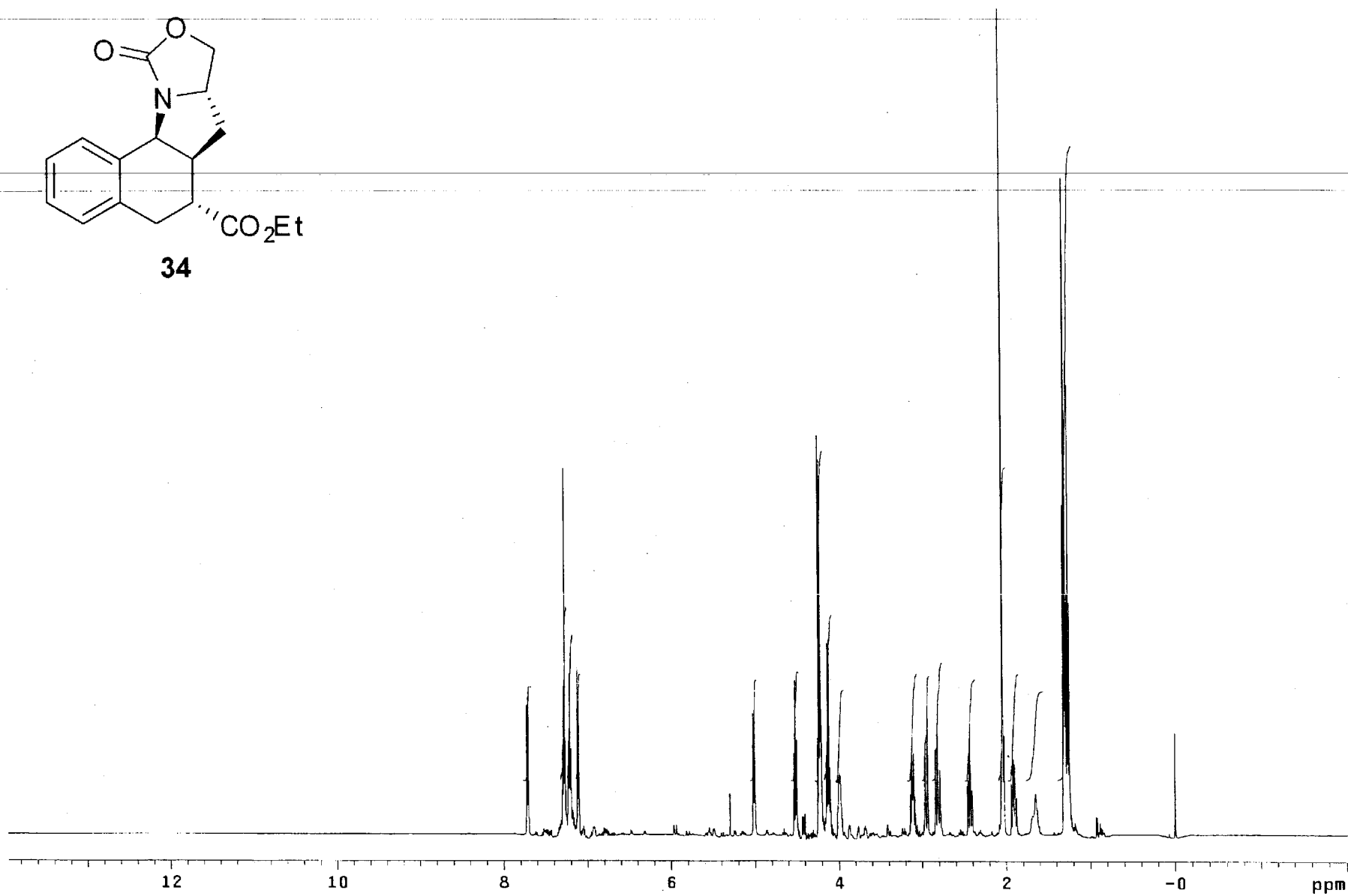
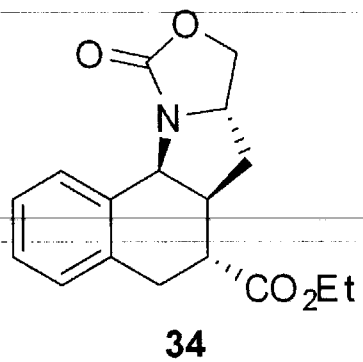


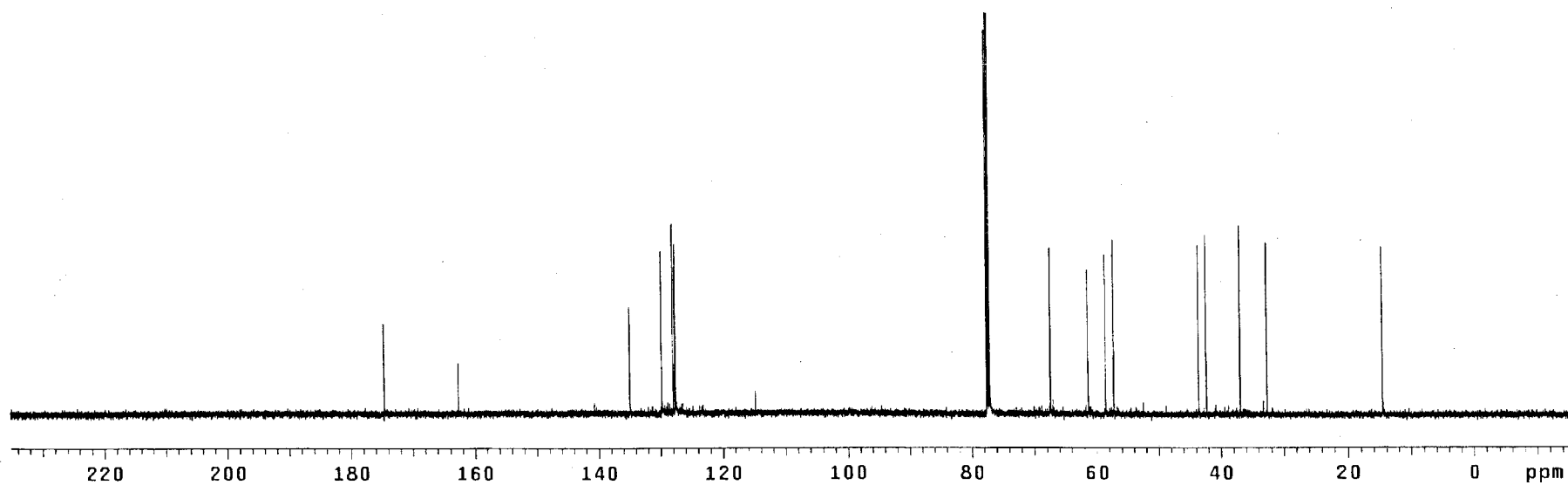
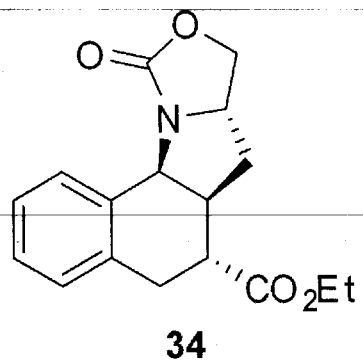




28







JF-III081-3

Archive directory: /export/home/jfelten/vnmrsys/data
Sample directory: JF-III081-3_27May2009

Pulse Sequence: gCOSY

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

File: gCOSY

INOVA-500 "nmr03"

Relax. delay 1.000 sec

Acq. time 0.128 sec

Width 8000.0 Hz

2D Width 8000.0 Hz

Single scan

128 increments

OBSERVE H1, 499.7288151 MHz

DATA PROCESSING

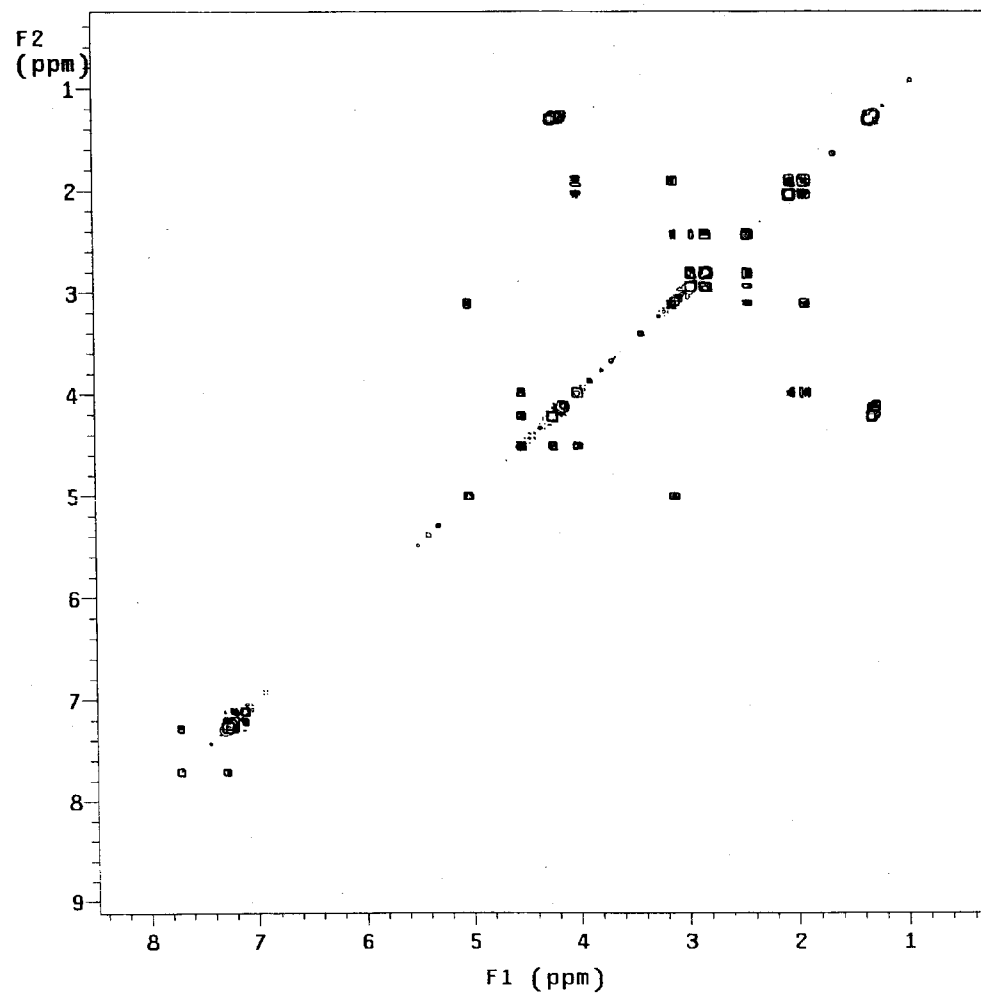
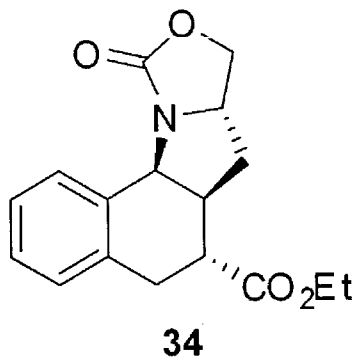
Sq. sine bell 0.064 sec

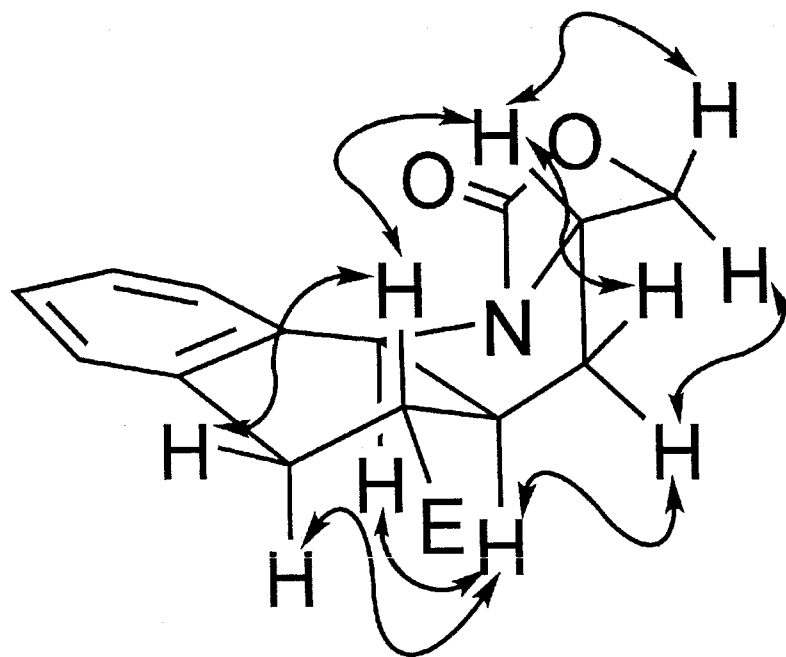
F1 DATA PROCESSING

Sq. sine bell 0.016 sec

FT size 2048 x 2048

Total time 2 min, 45 sec





nOe of 34
E = CO₂Et

JF-III081-3

Archive directory: /export/home/jfelten/vnmrsys/data
Sample directory: JF-III081-3_30May2009-13:31:24

Pulse Sequence: NOESY

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: NOESY
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Mixing 0.500 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
2 x 128 increments
OBSERVE H1, 499.7288156 MHz
DATA PROCESSING
Gauss apodization 0.059 sec
F1 DATA PROCESSING
Gauss apodization 0.015 sec
FT size 2048 x 2048
Total time 1 hr, 53 min, 29 sec

