

SUPPORTING INFORMATION

PROTON NMR AND SELECTED CARBON NMR SPECTRA

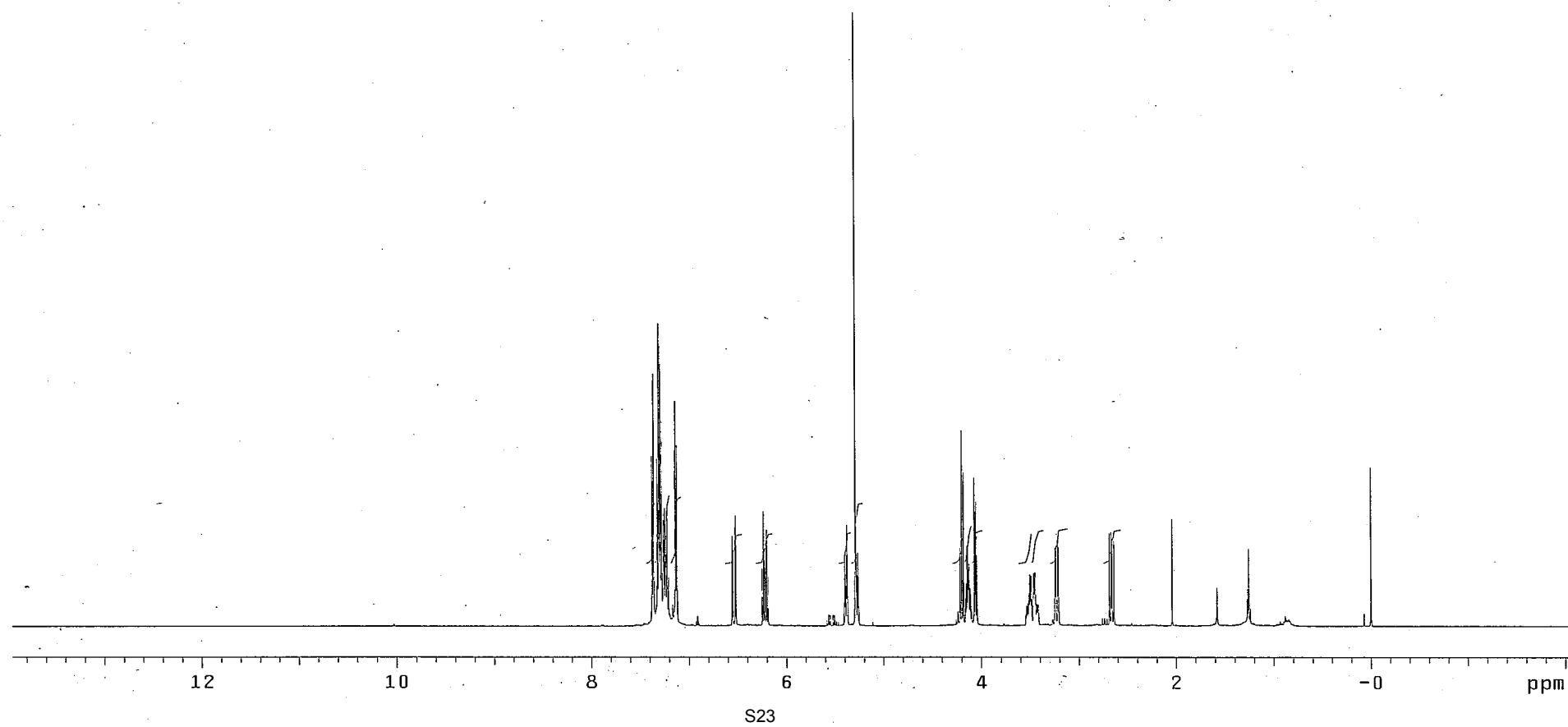
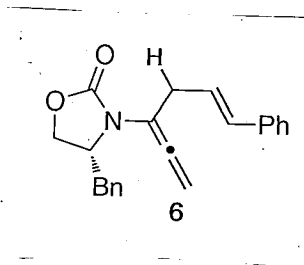
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communication
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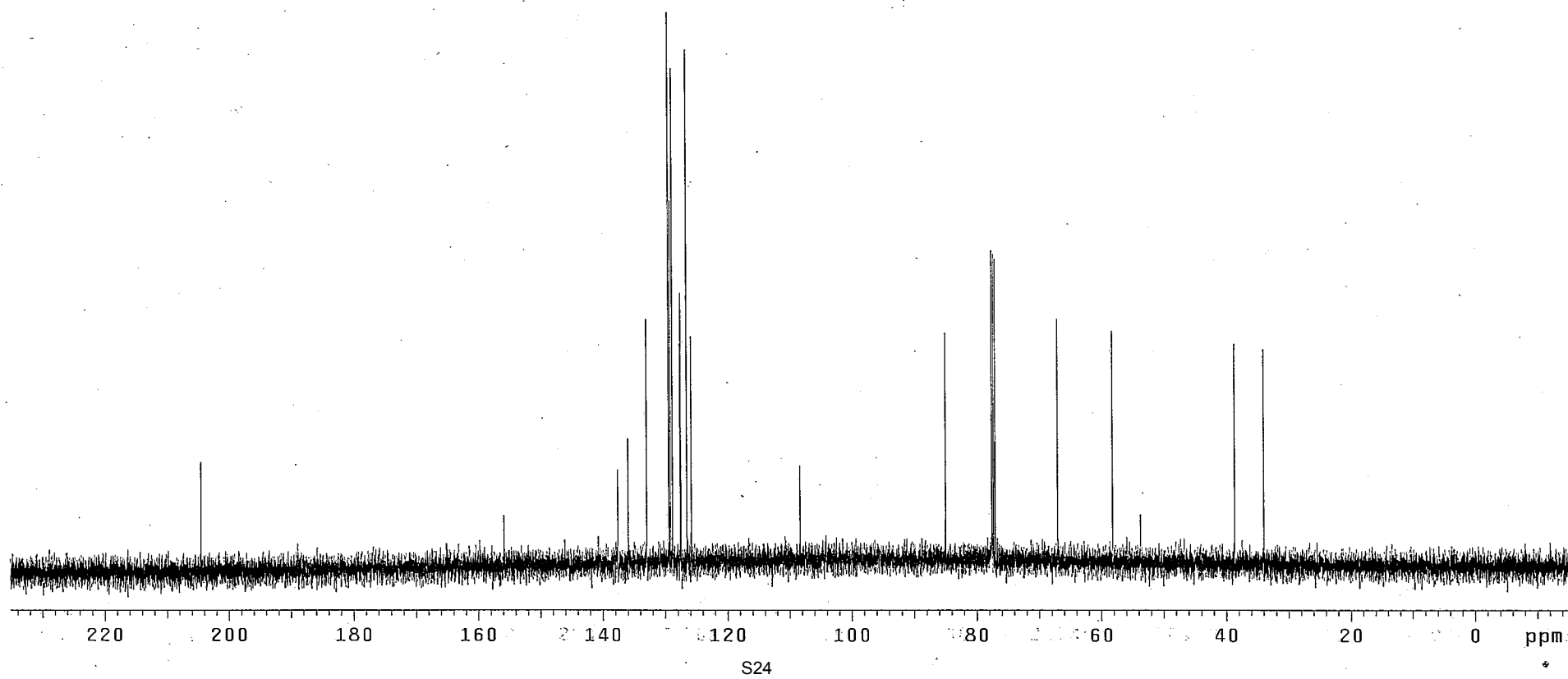
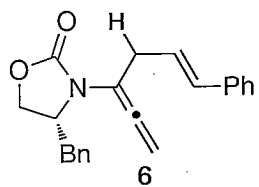
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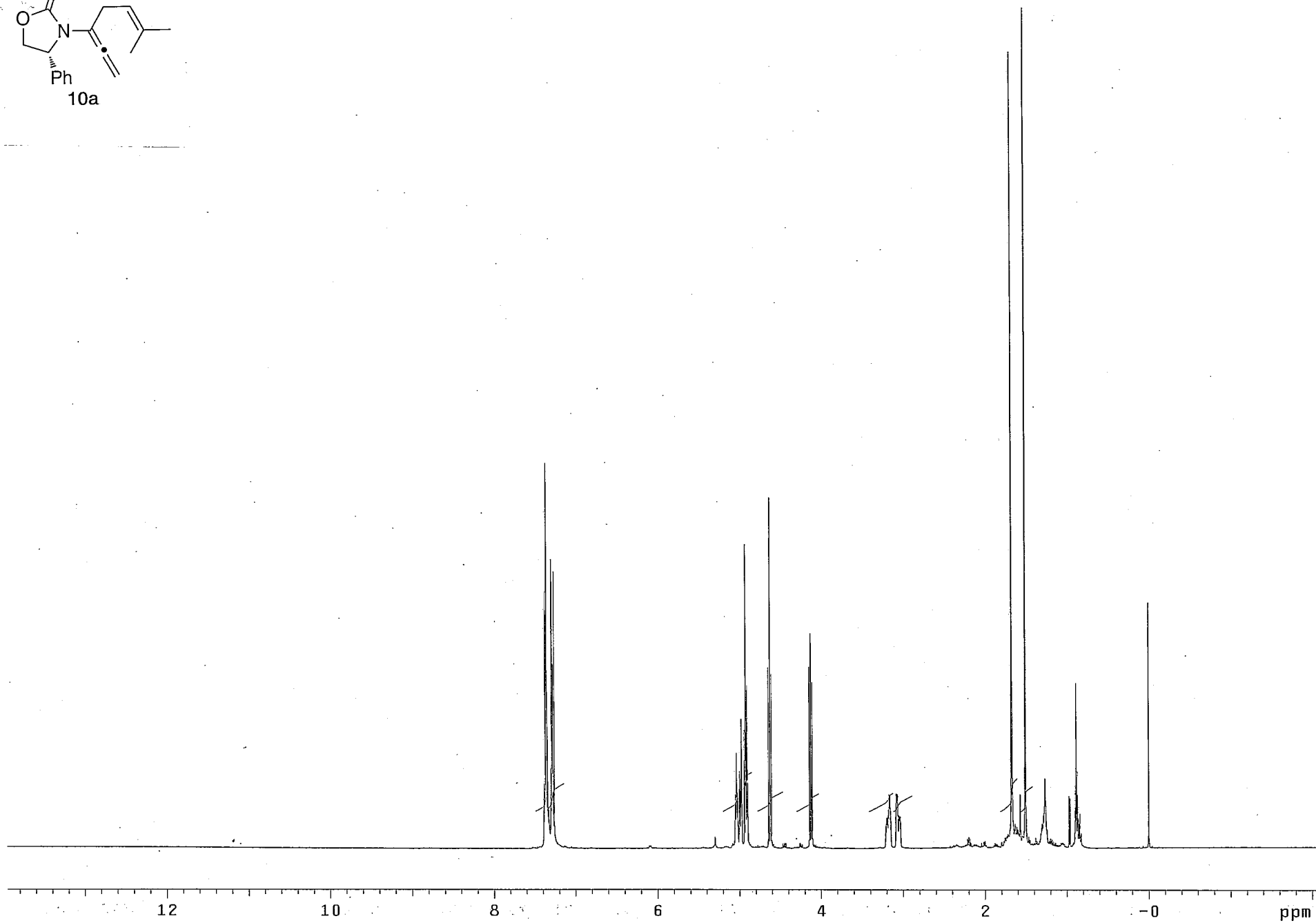
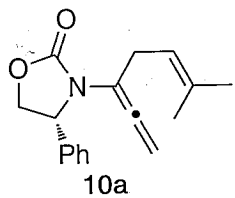
authored by

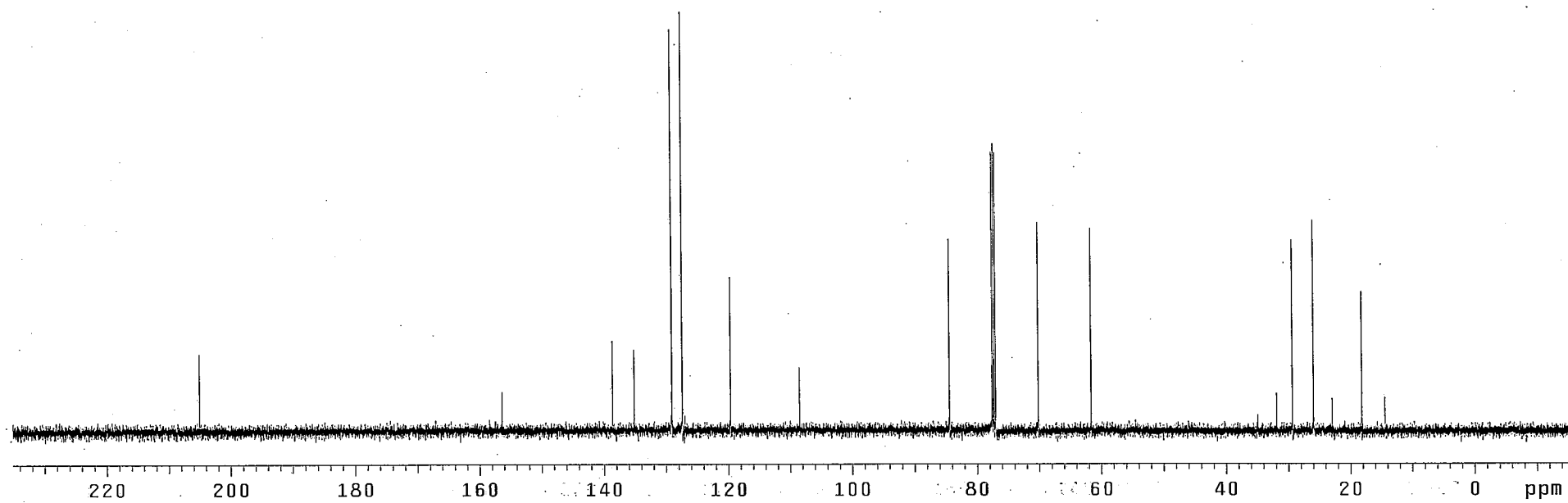
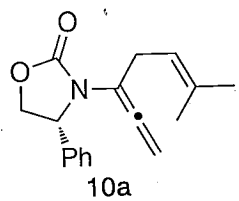
Ryuji Hayashi, John B. Feltenberger, and Richard P. Hsung*

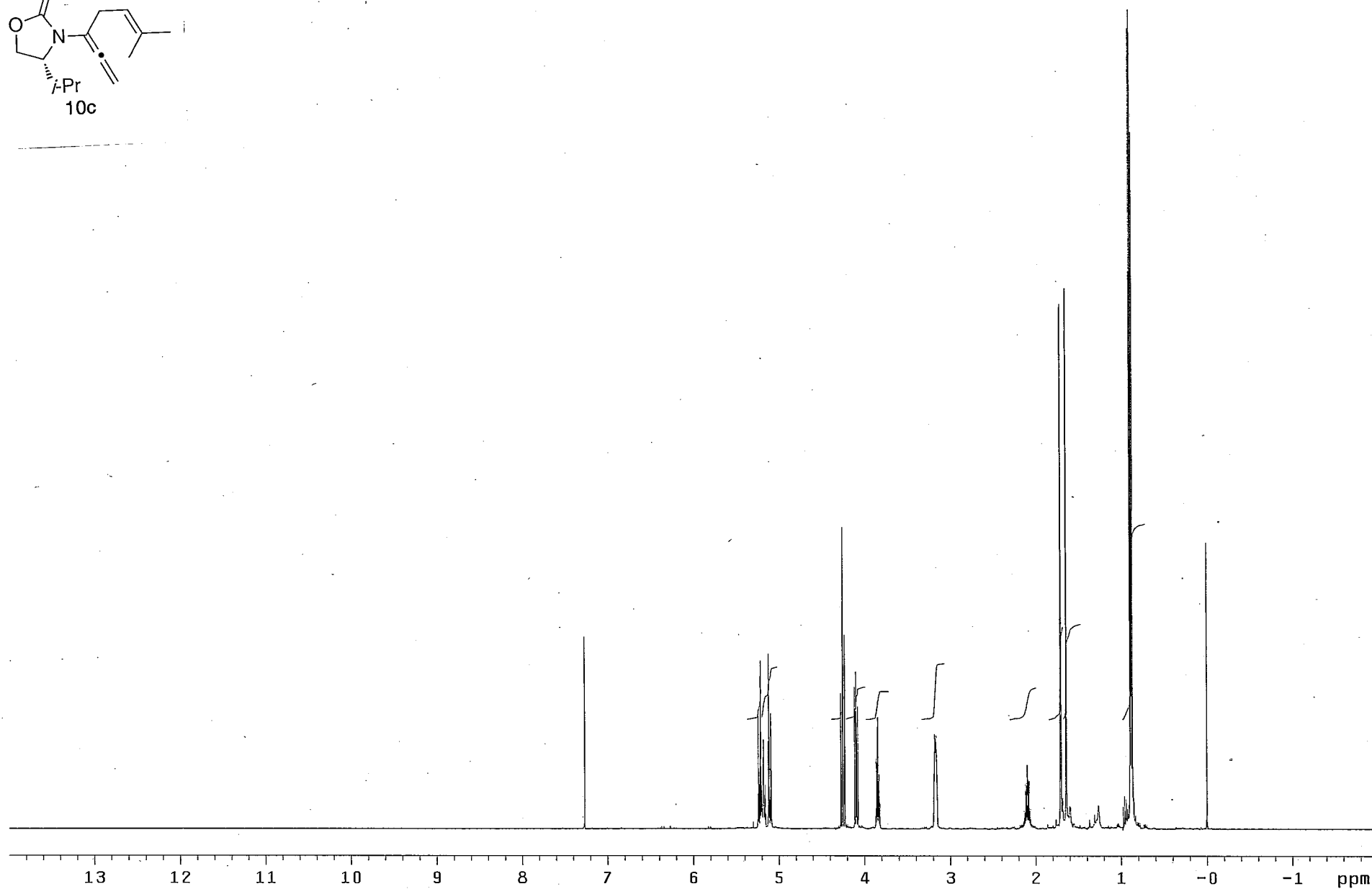
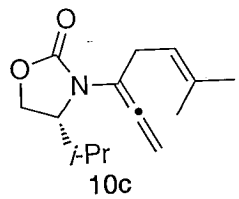
*Department of Chemistry and Division of Pharmaceutical Sciences
7111 Rennebohm Hall, 777 Highland Avenue
University of Wisconsin at Madison, Madison, WI 53705-2222*

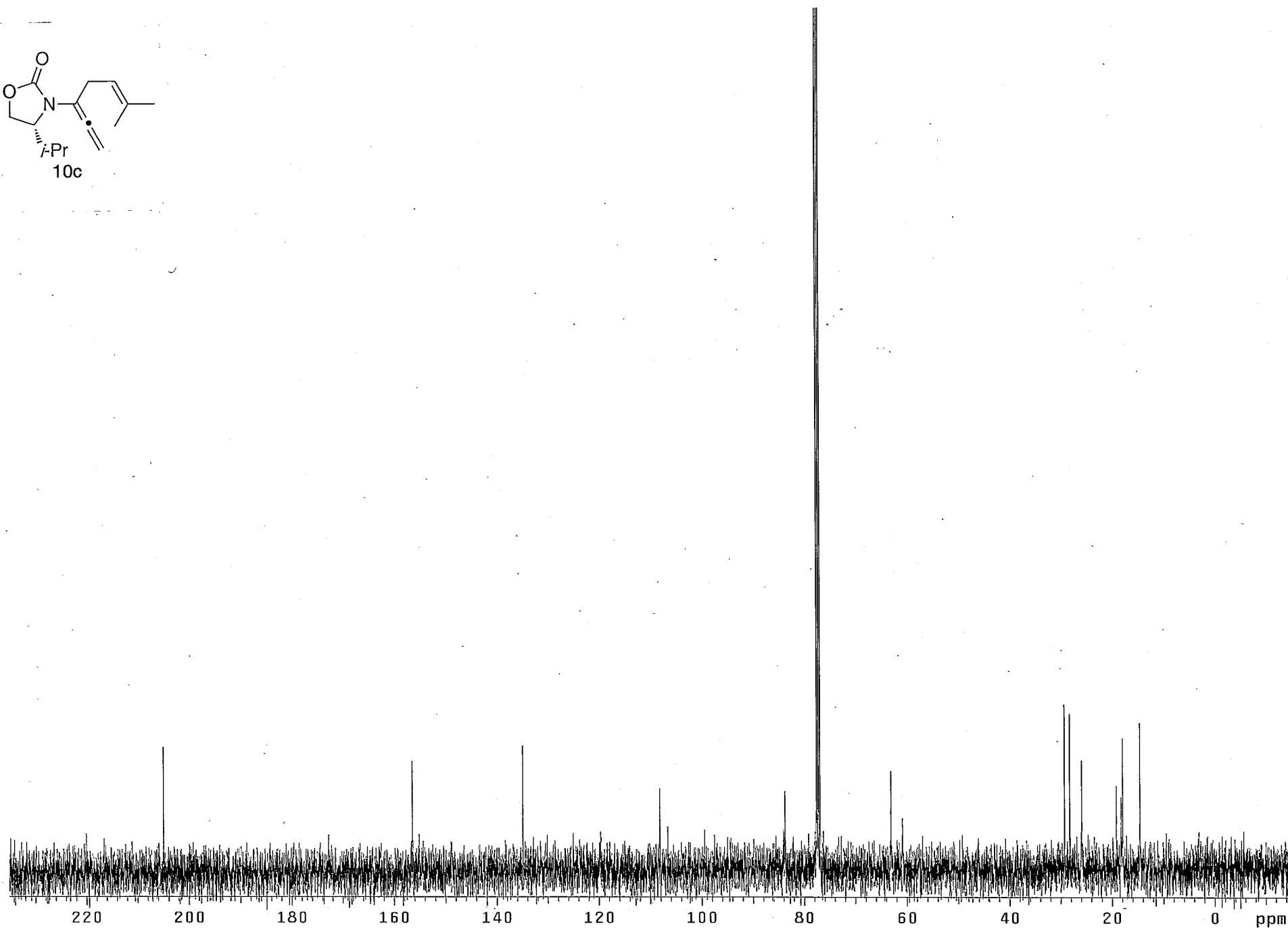
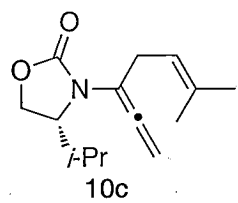


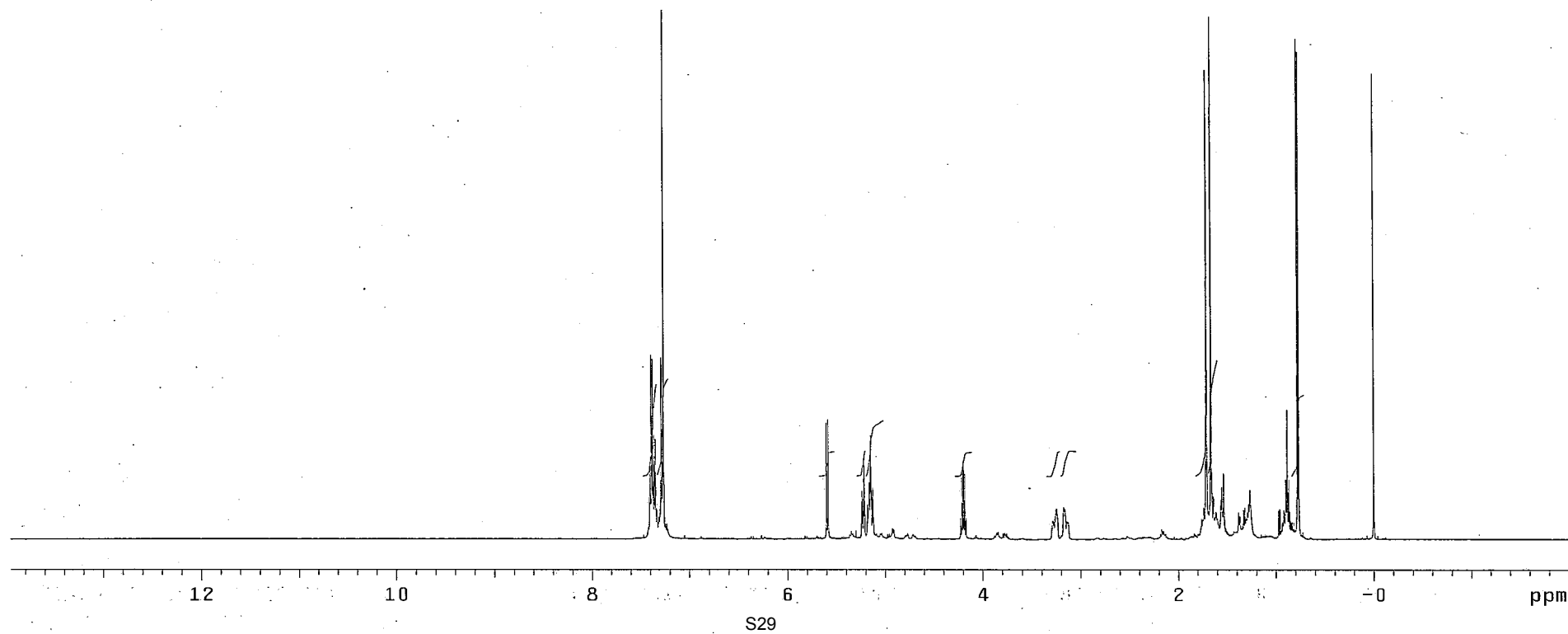
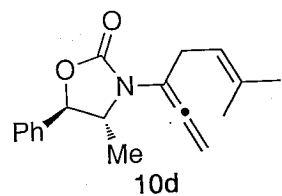


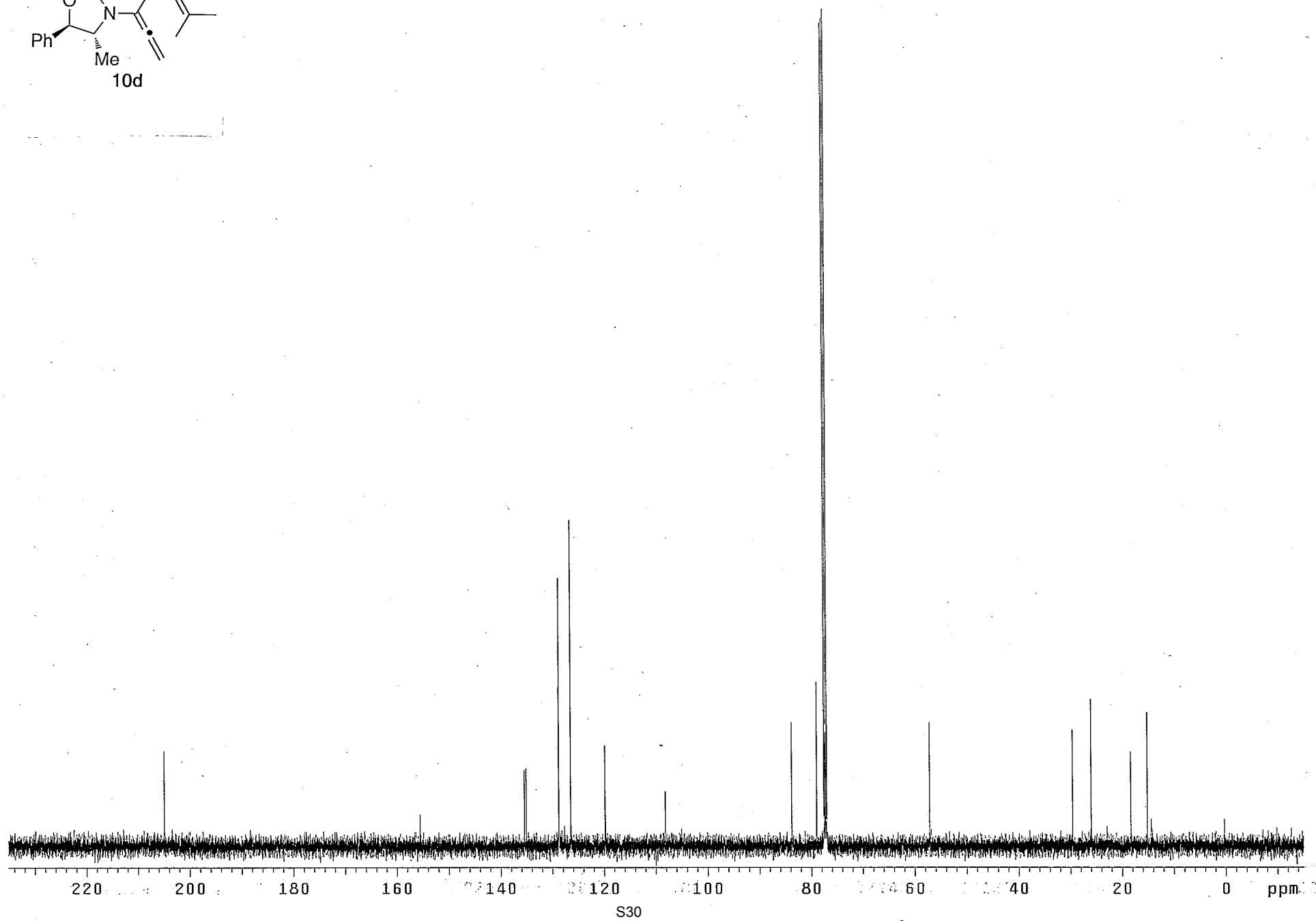
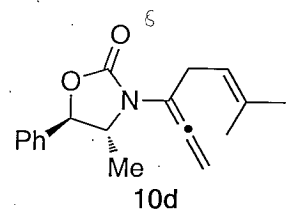


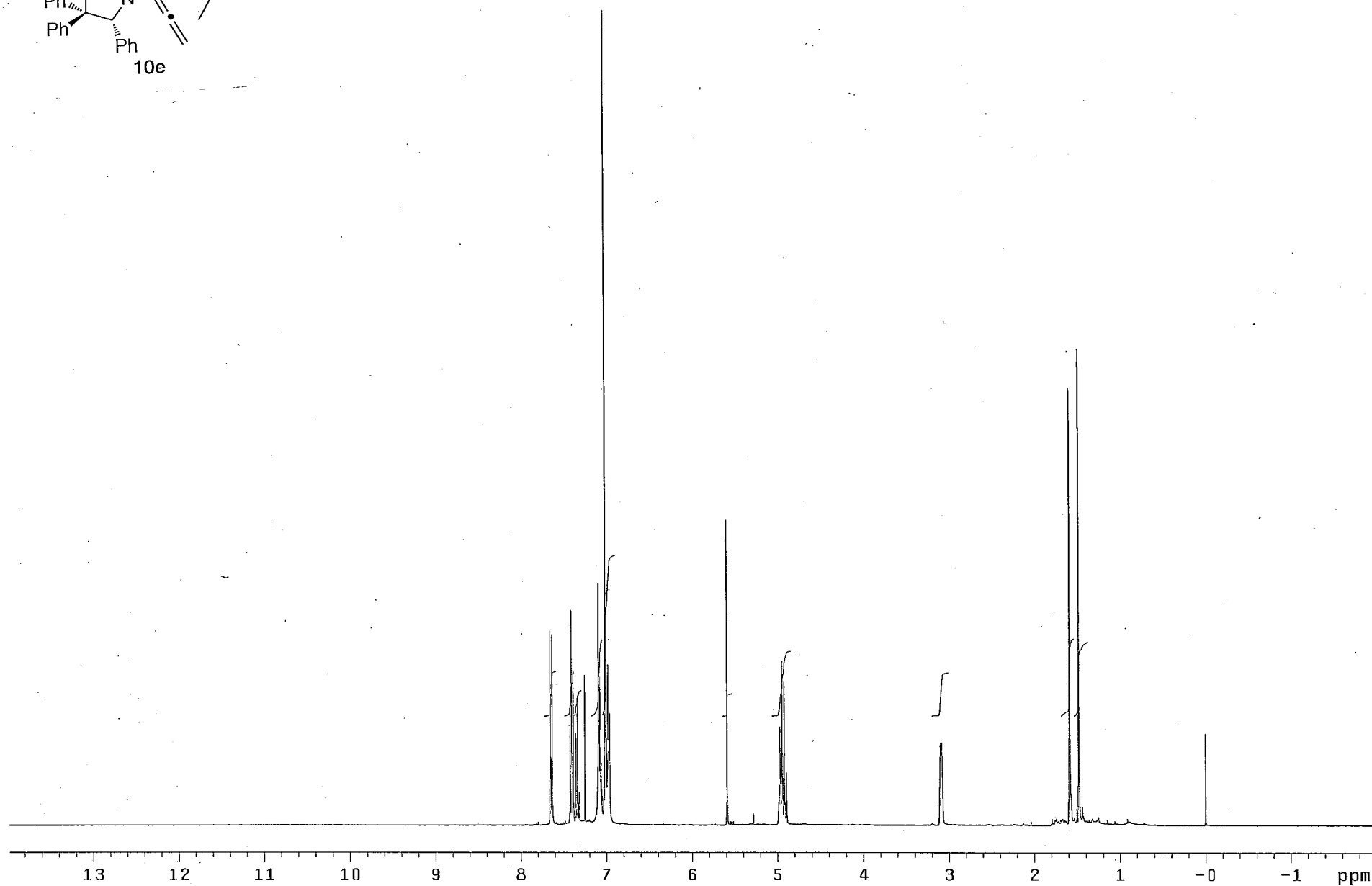
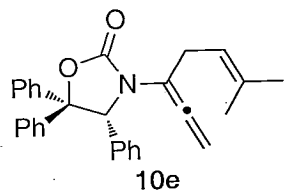


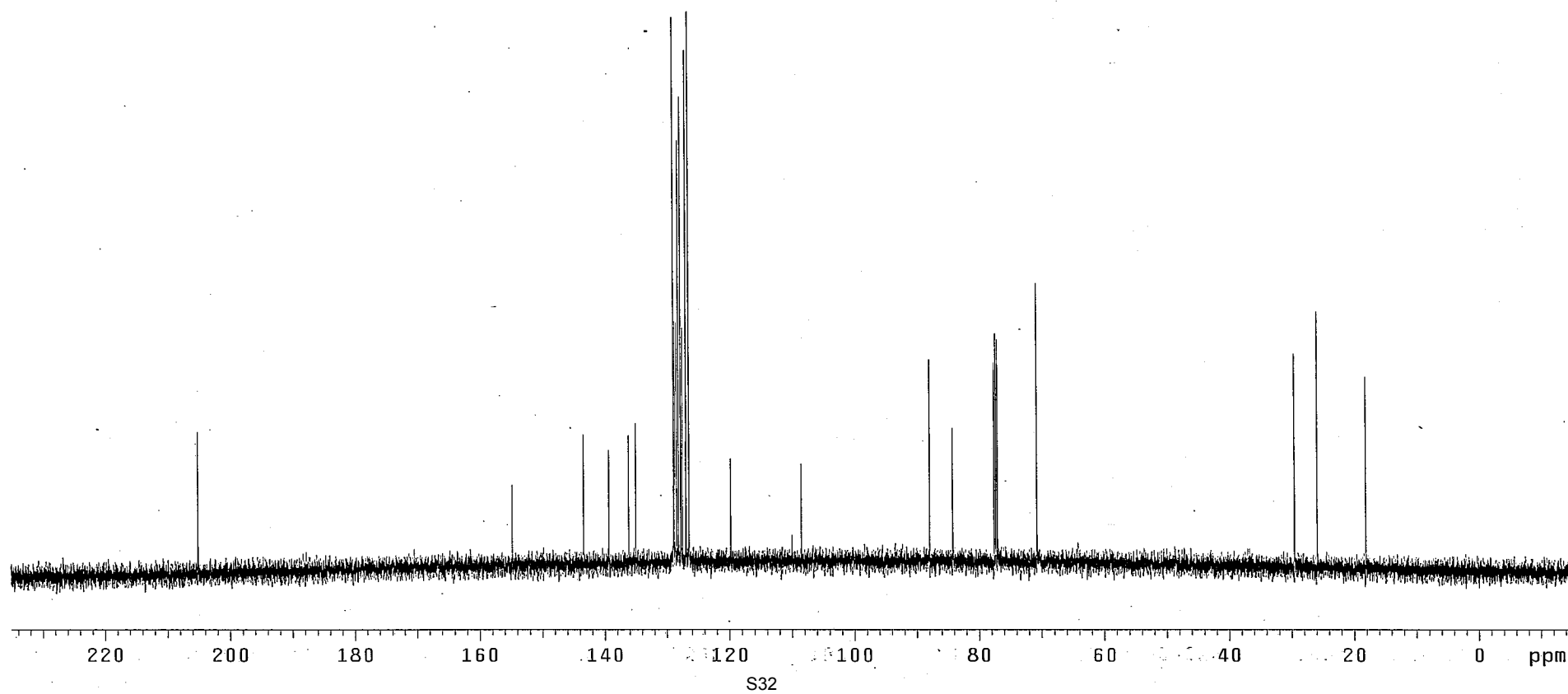
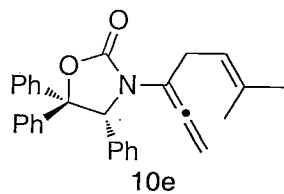


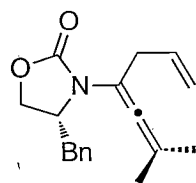




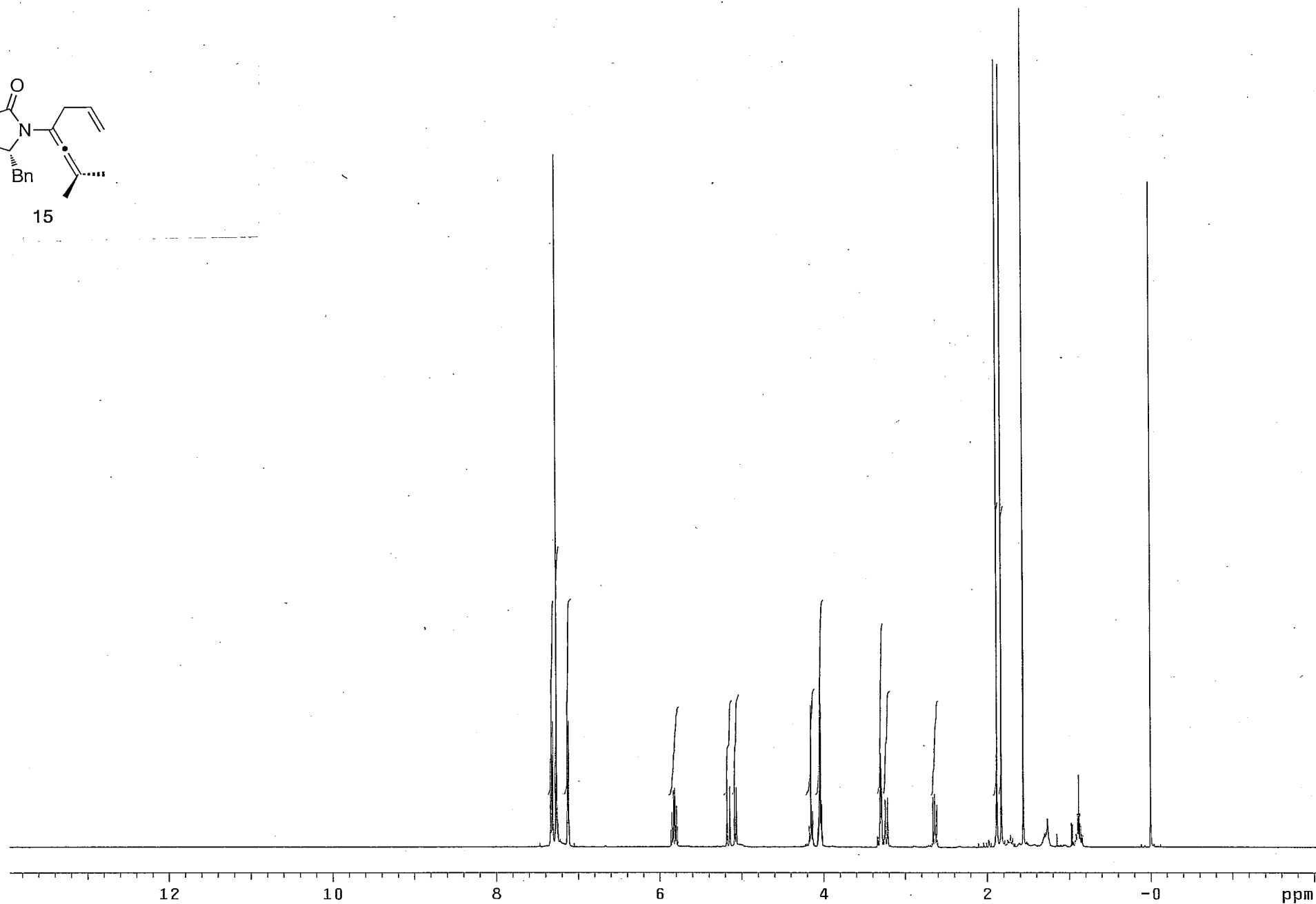


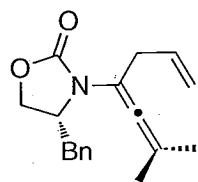




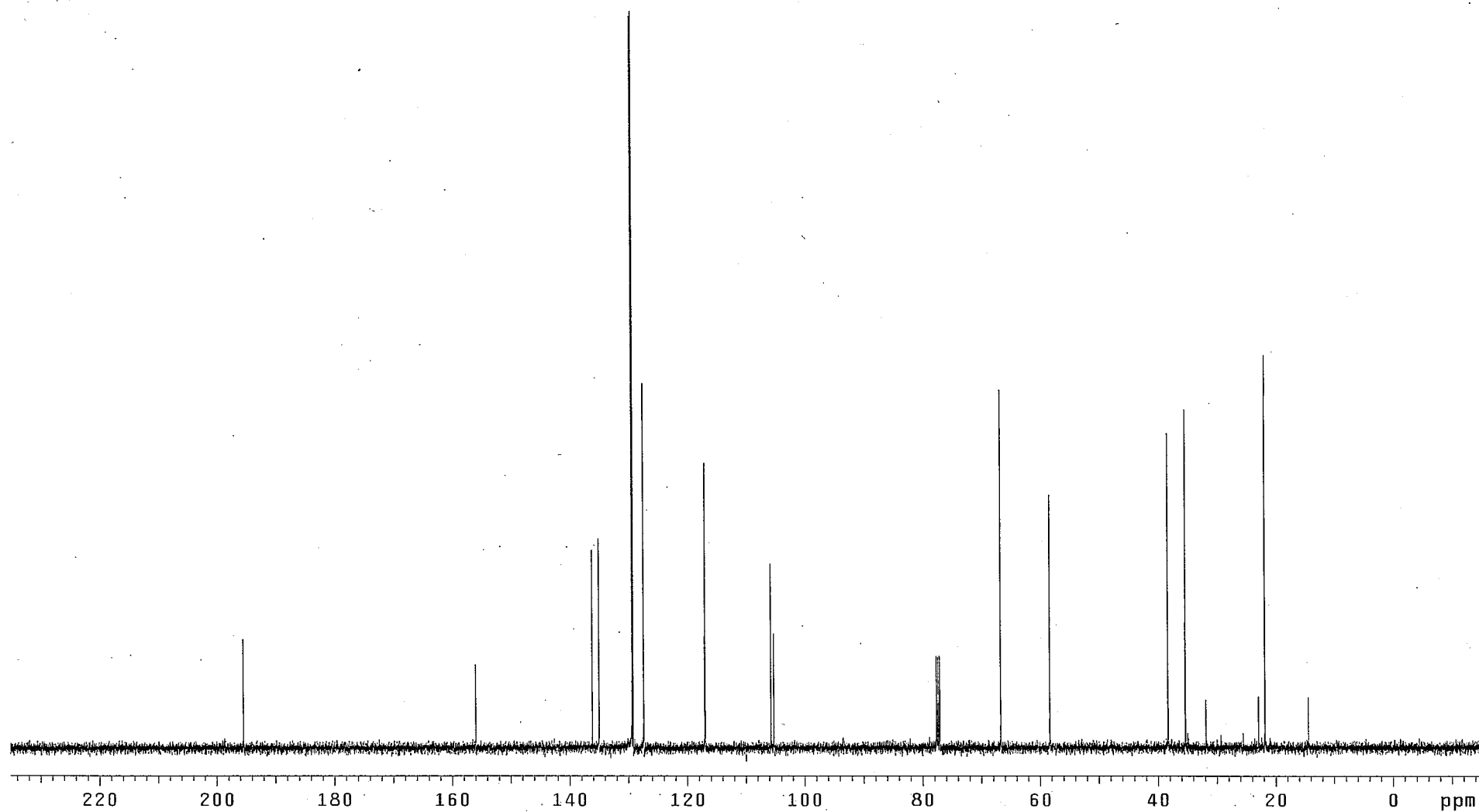


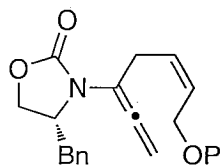
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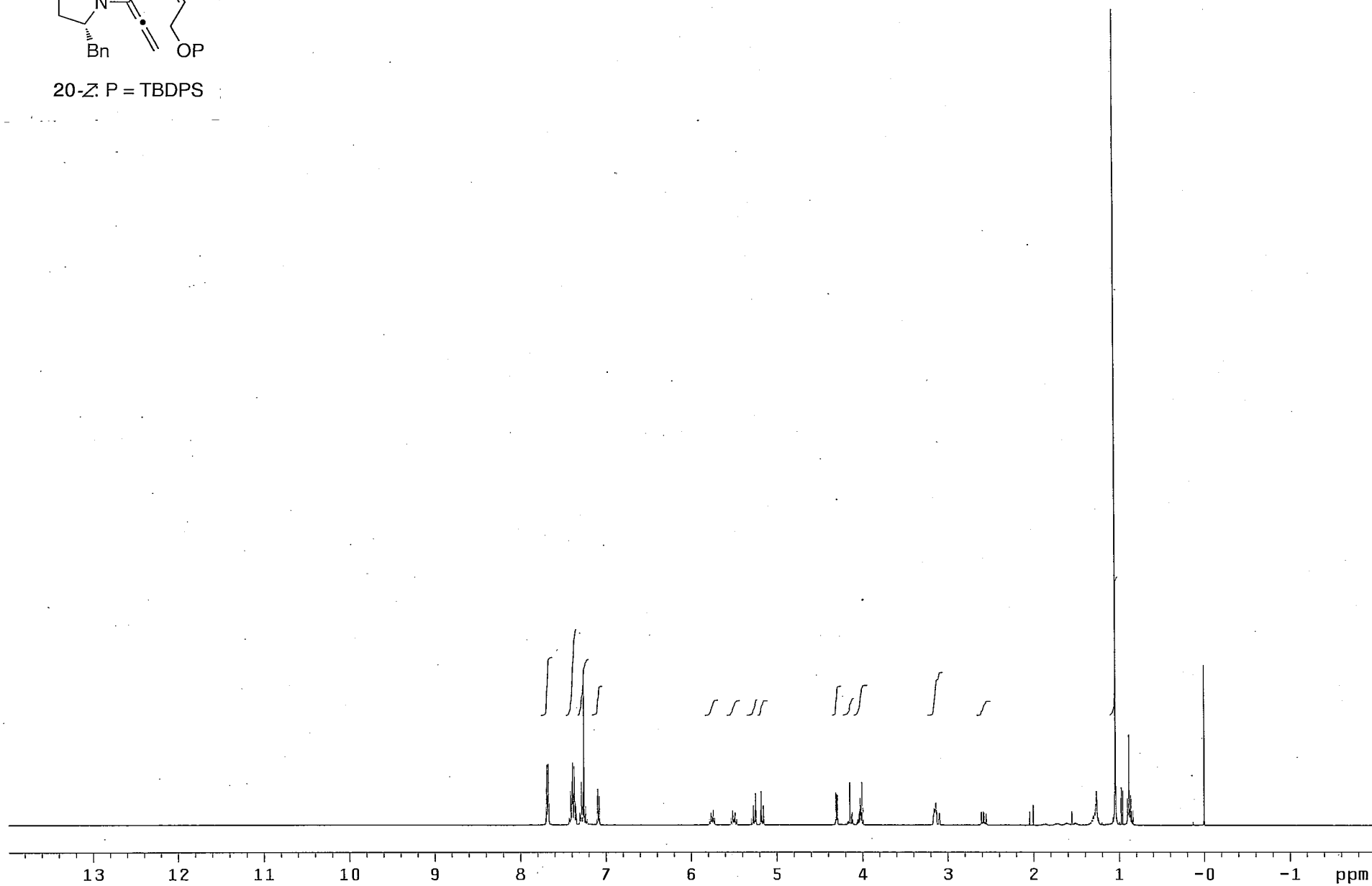


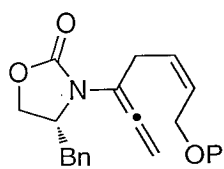
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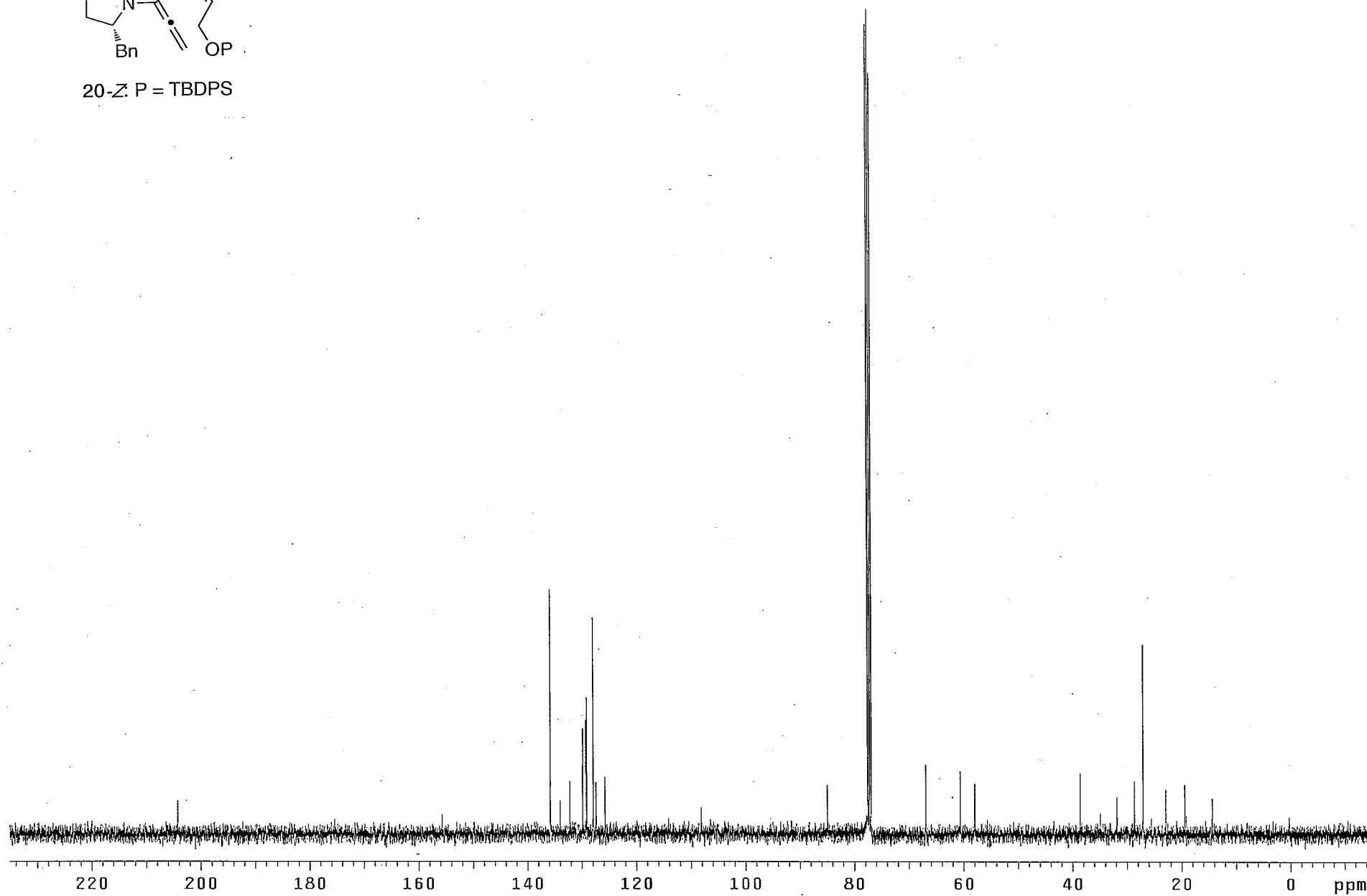


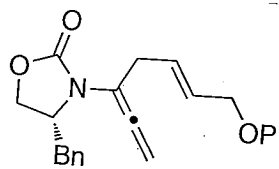
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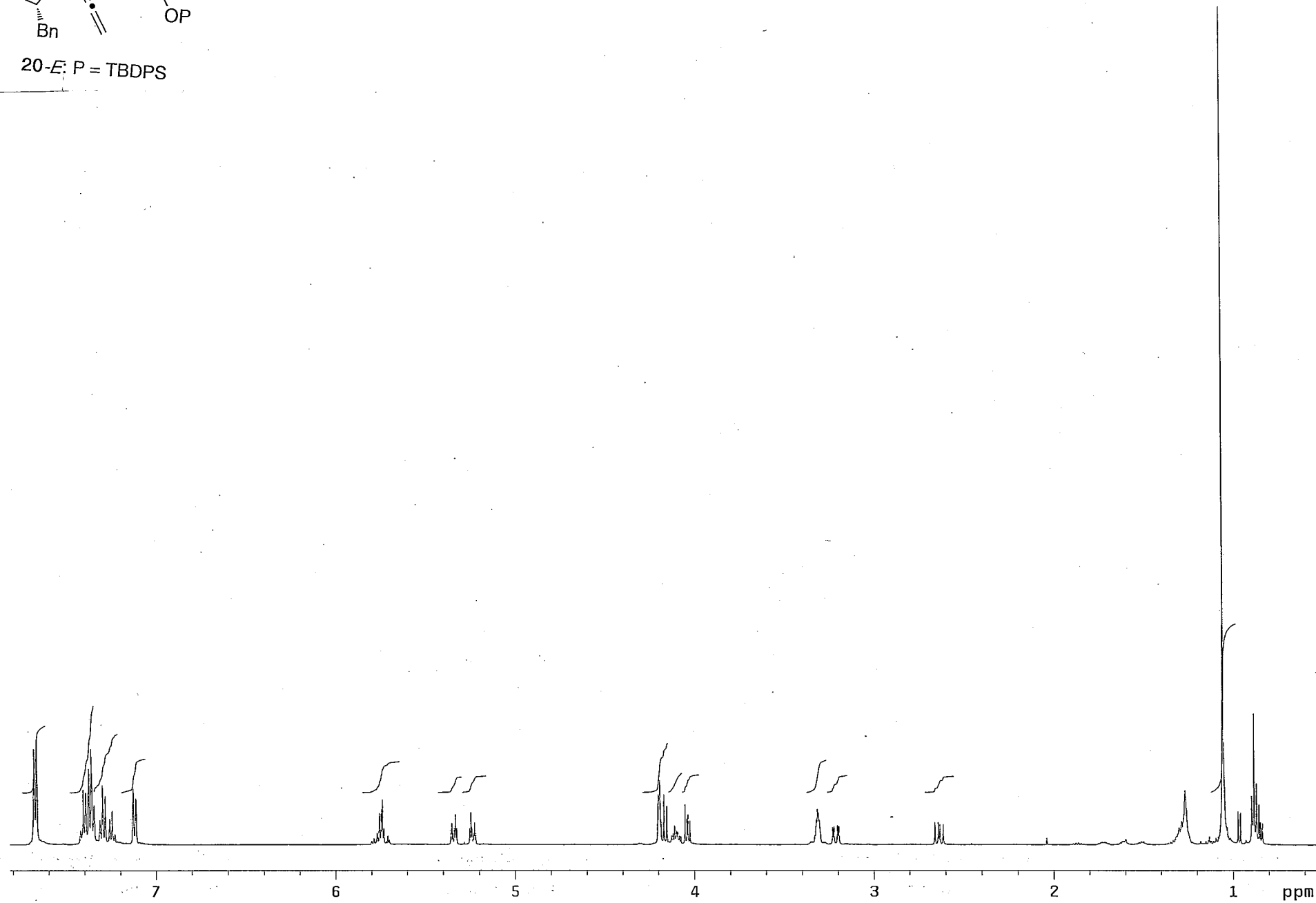


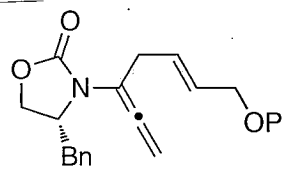
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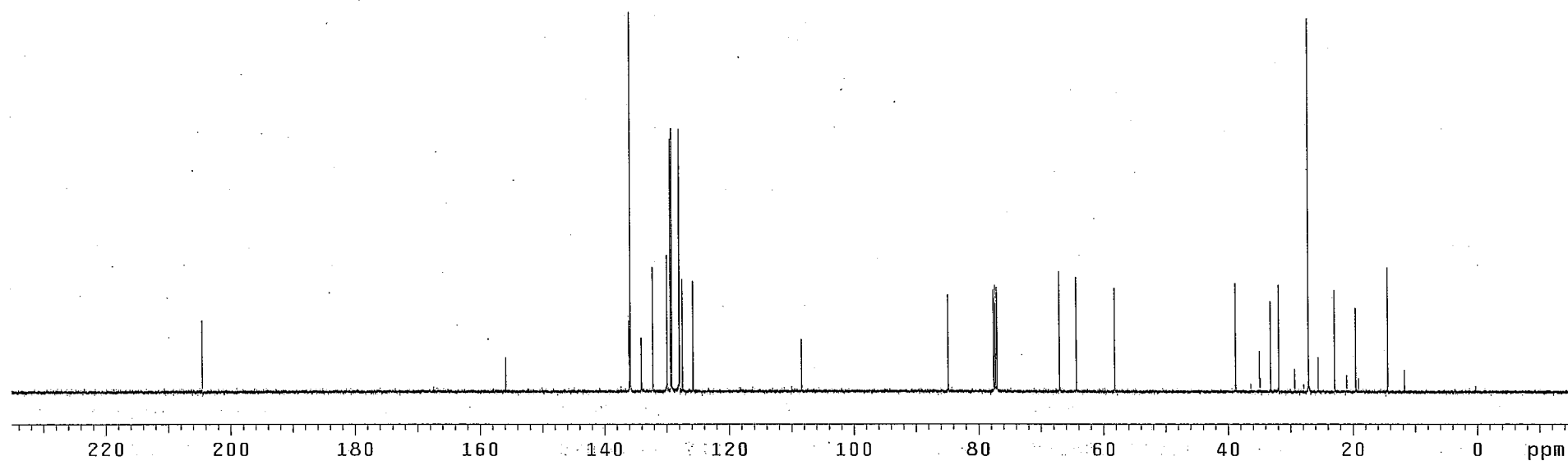


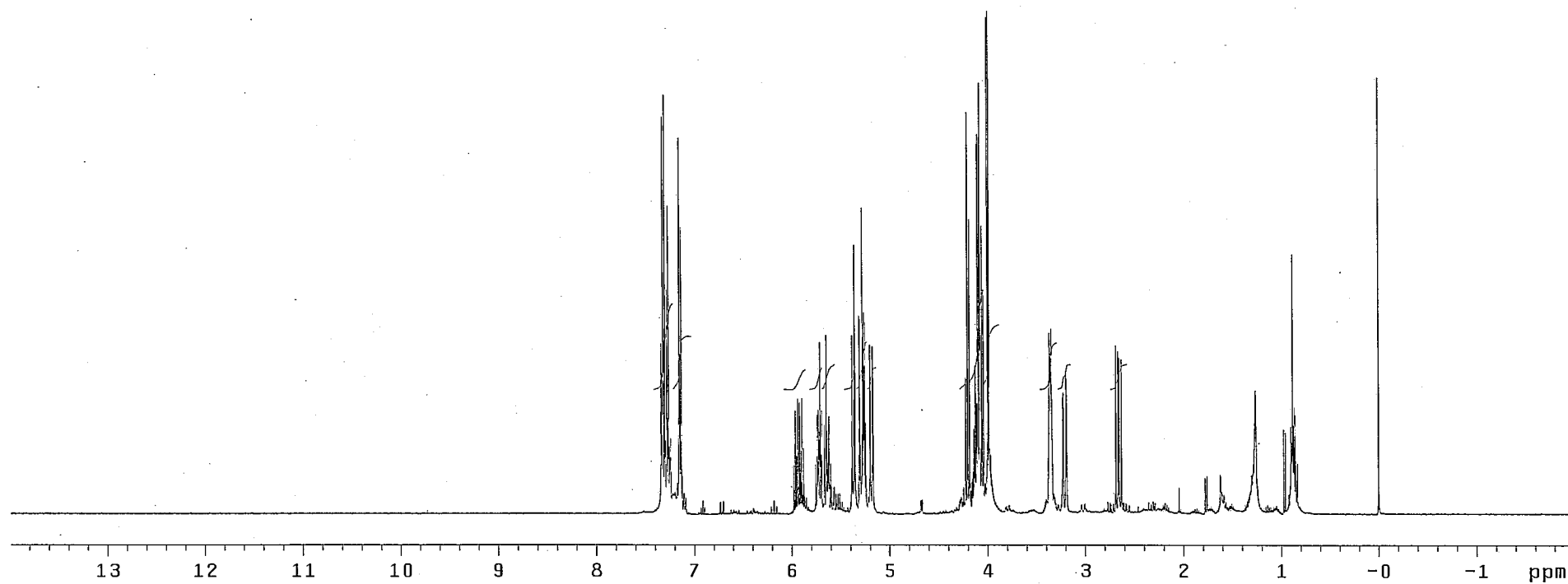
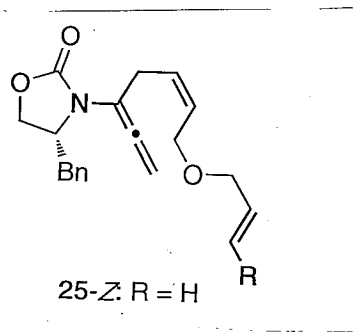
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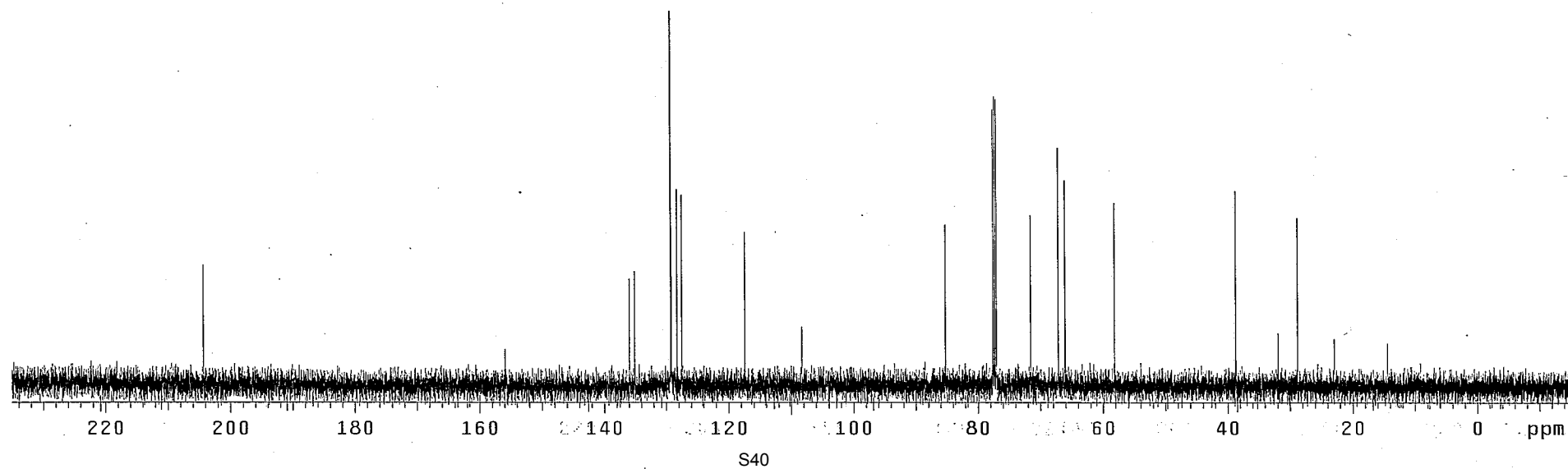
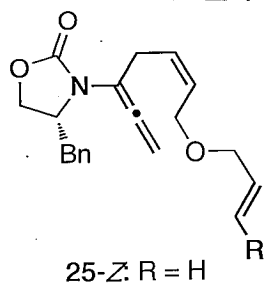


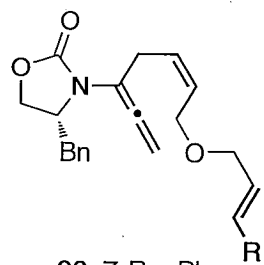


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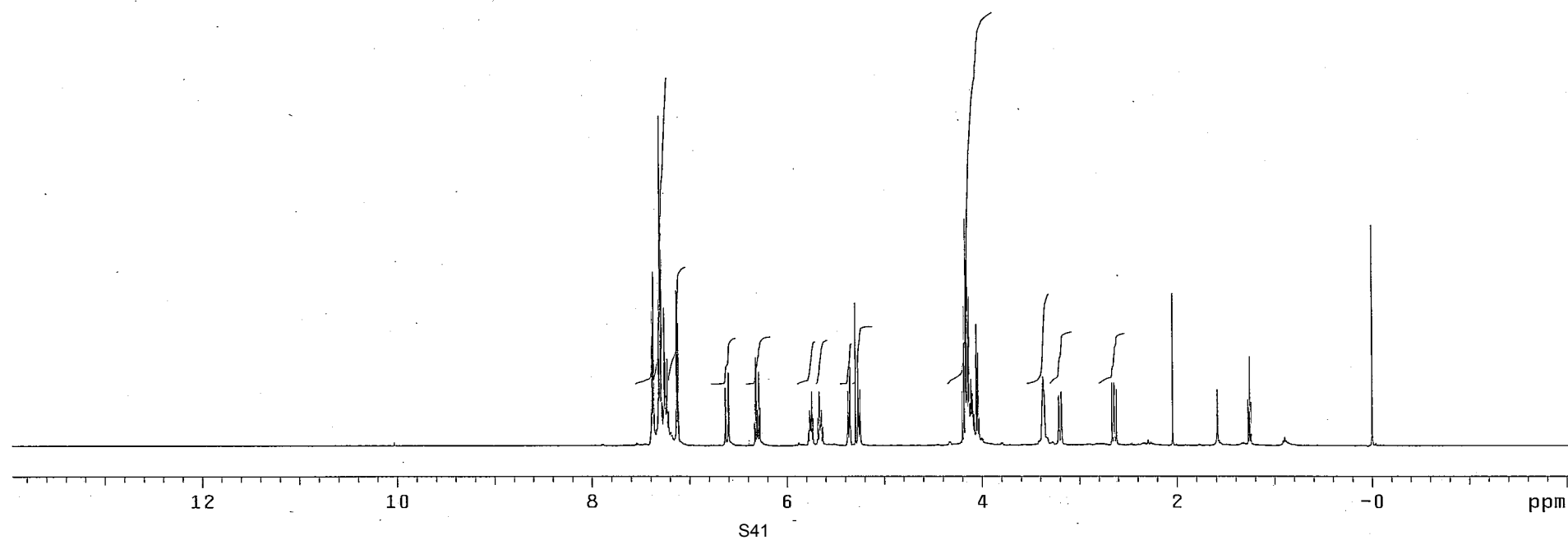


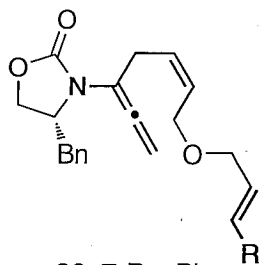




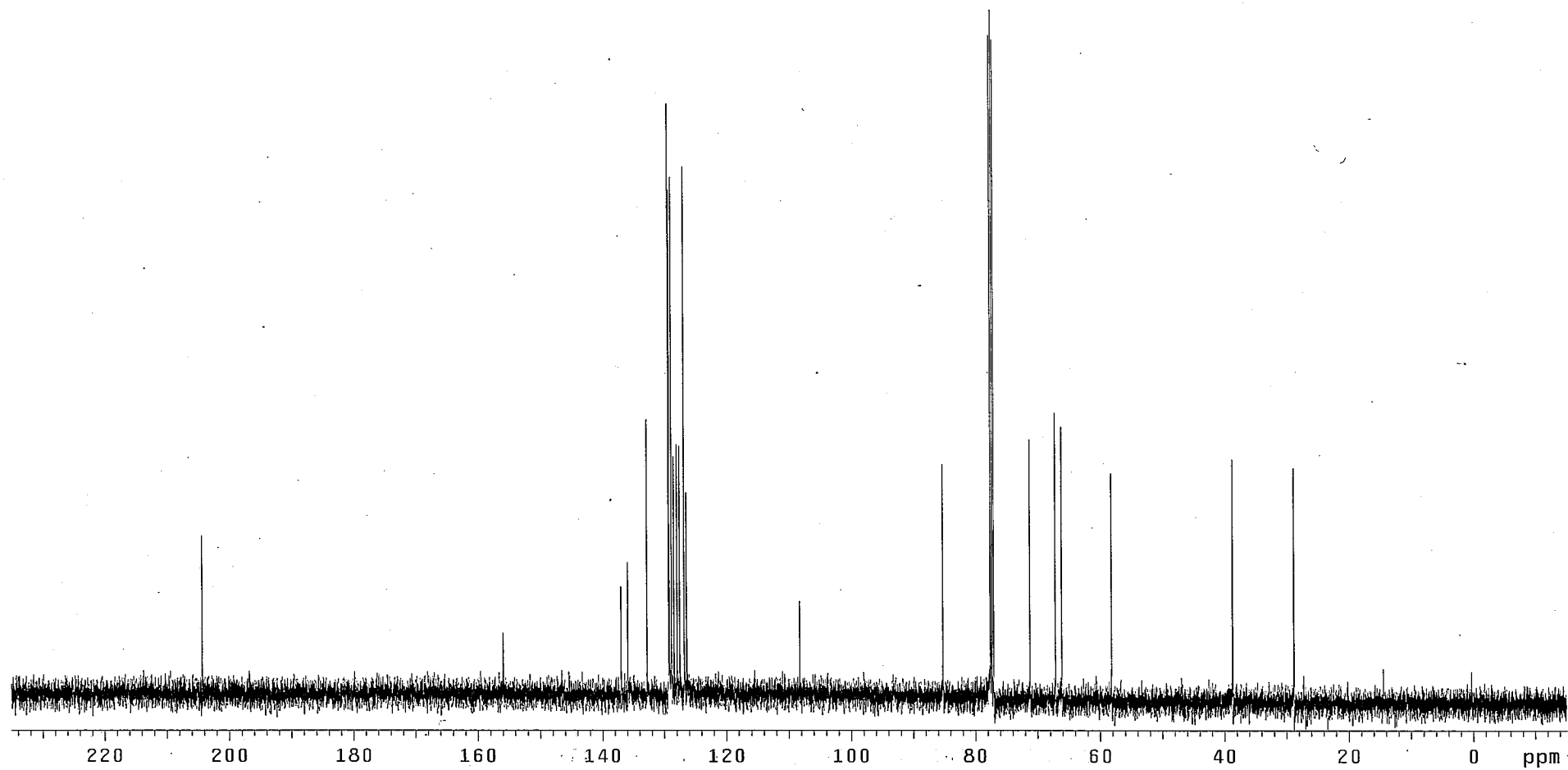


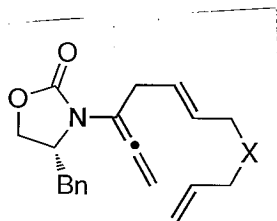
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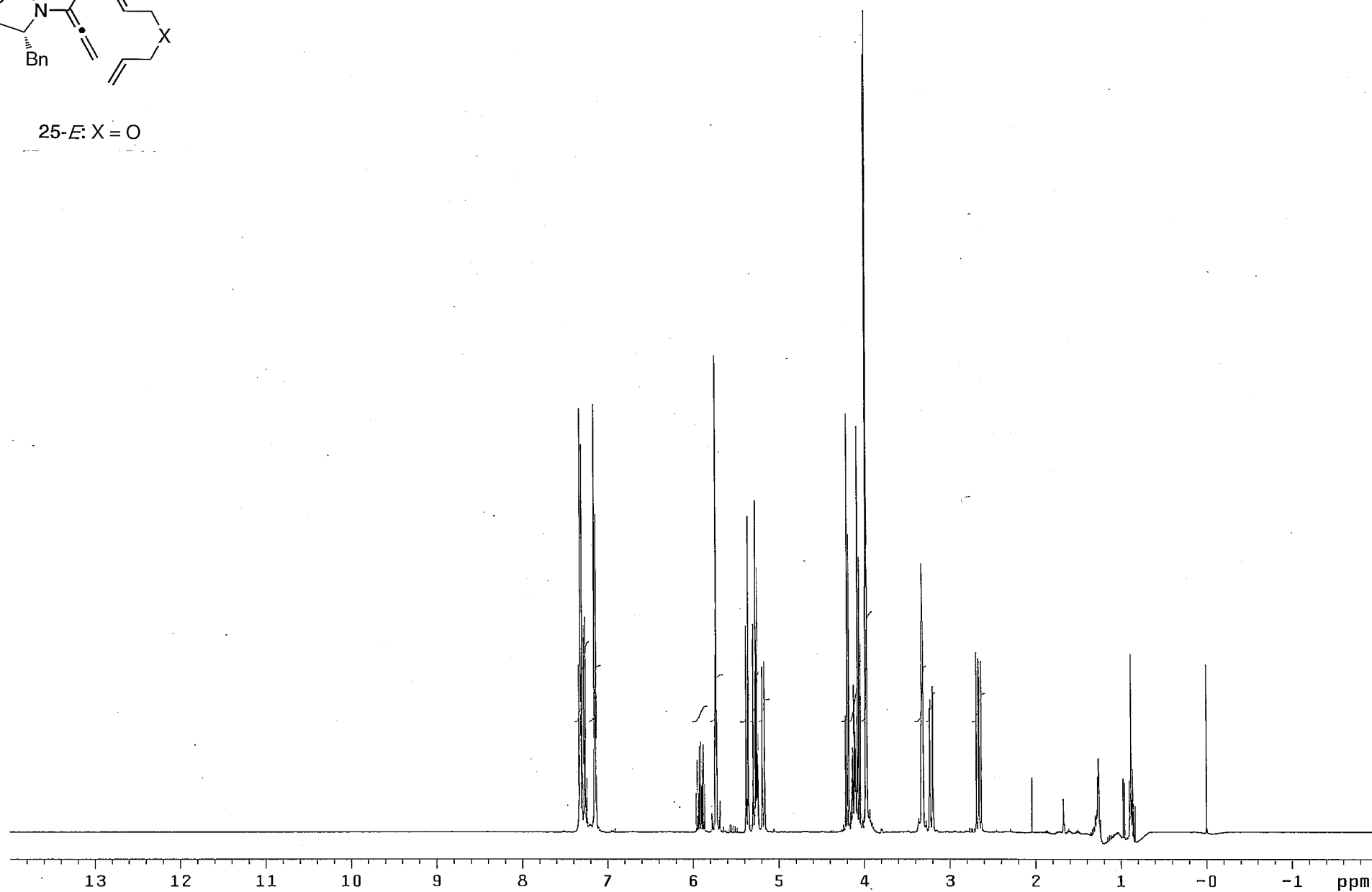


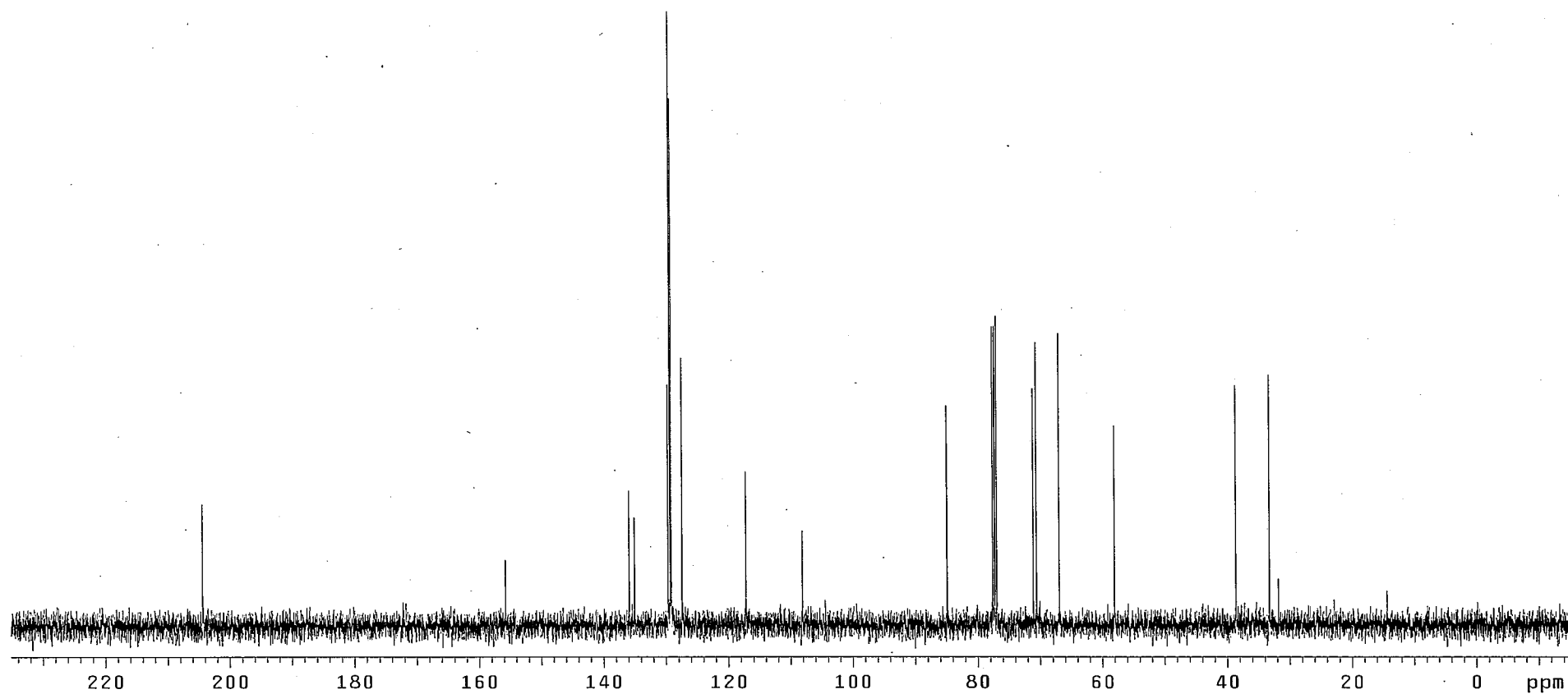
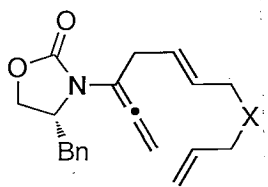
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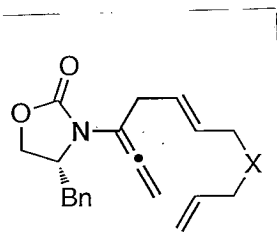




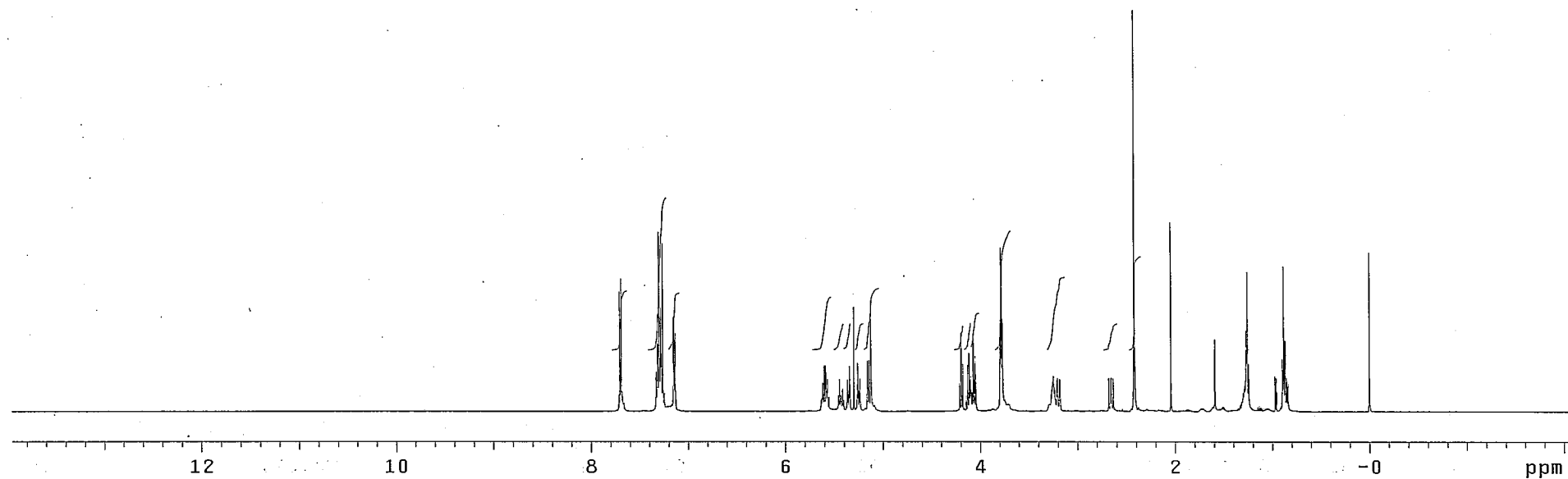
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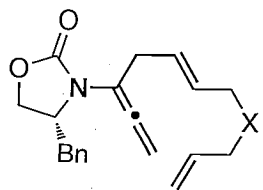




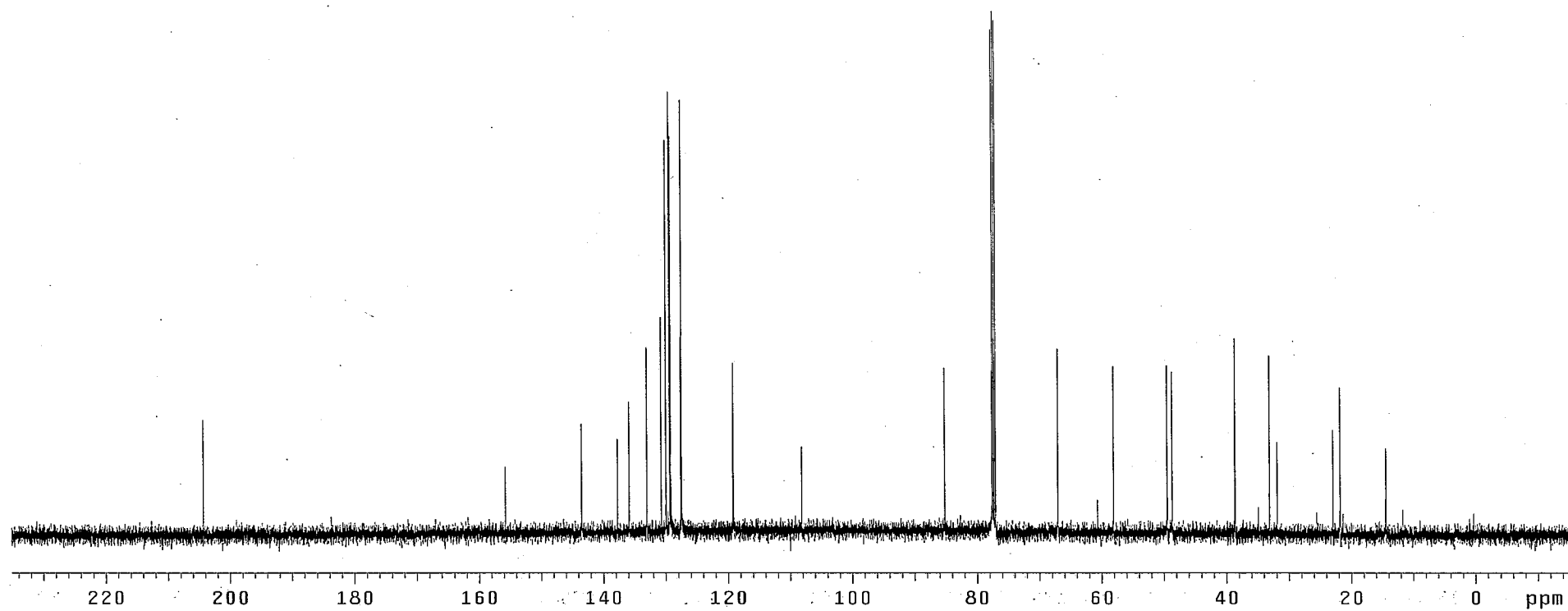


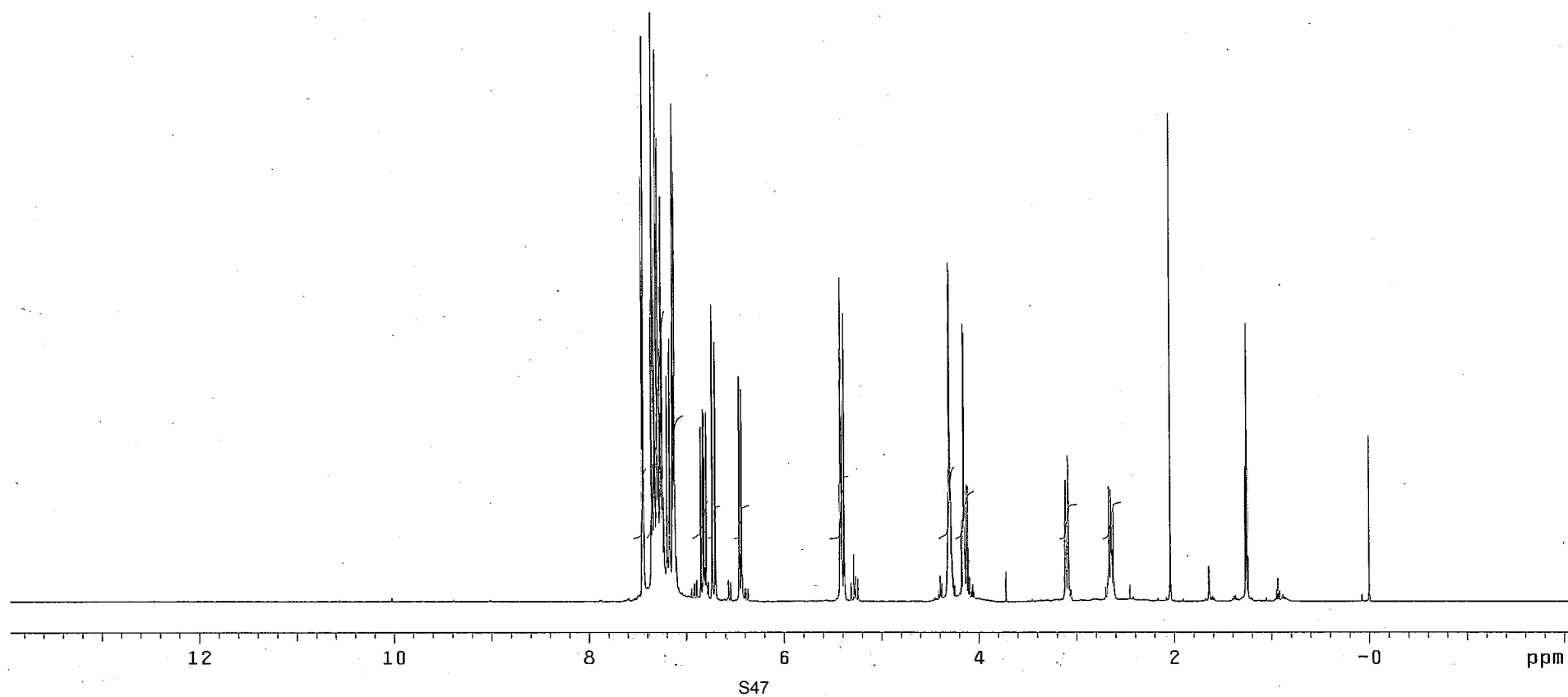
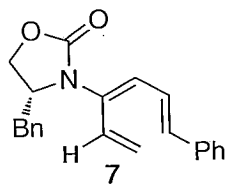
29-E: X = NTs

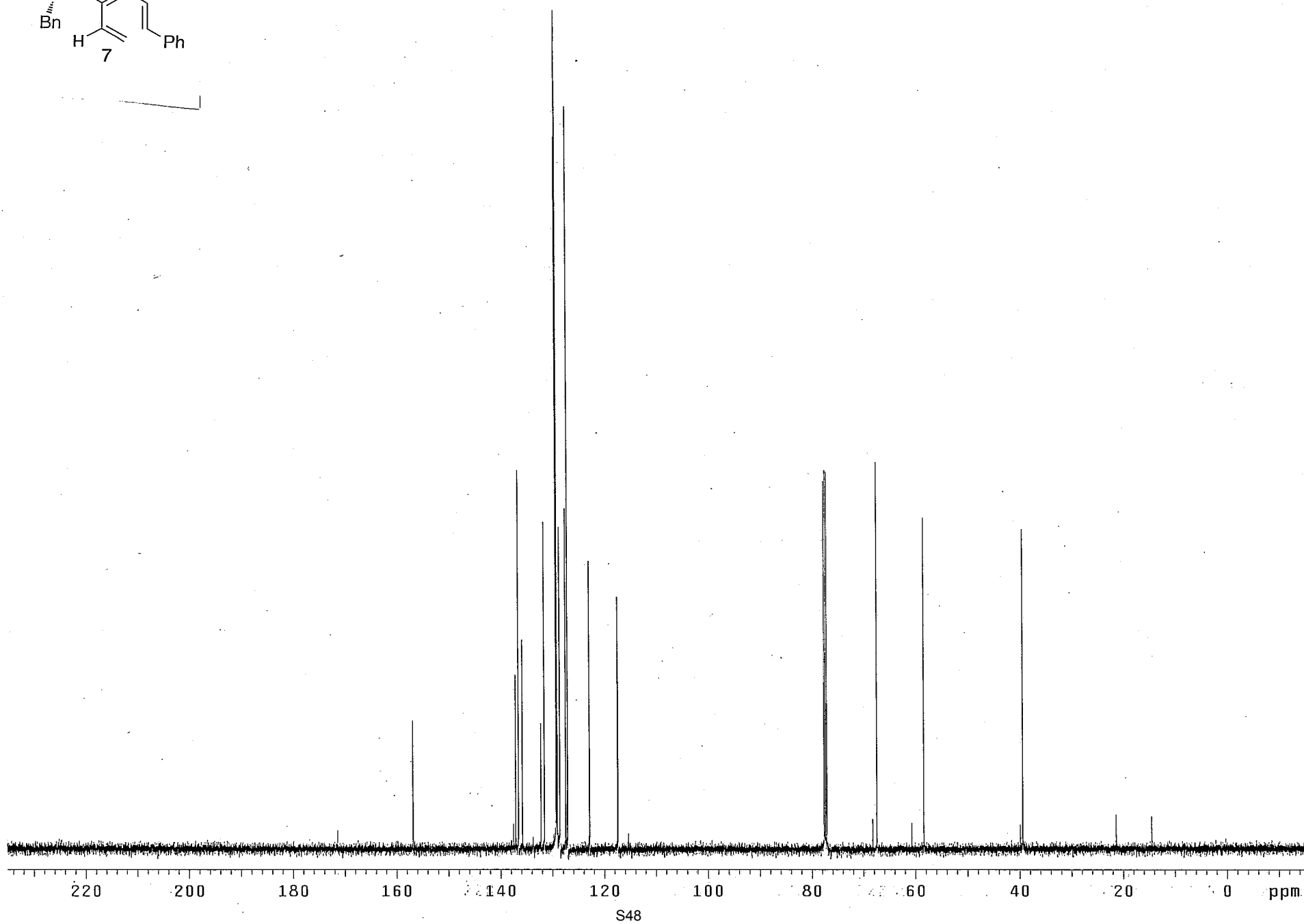
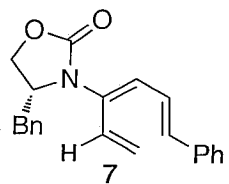


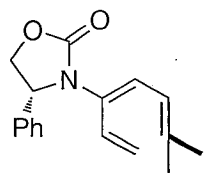


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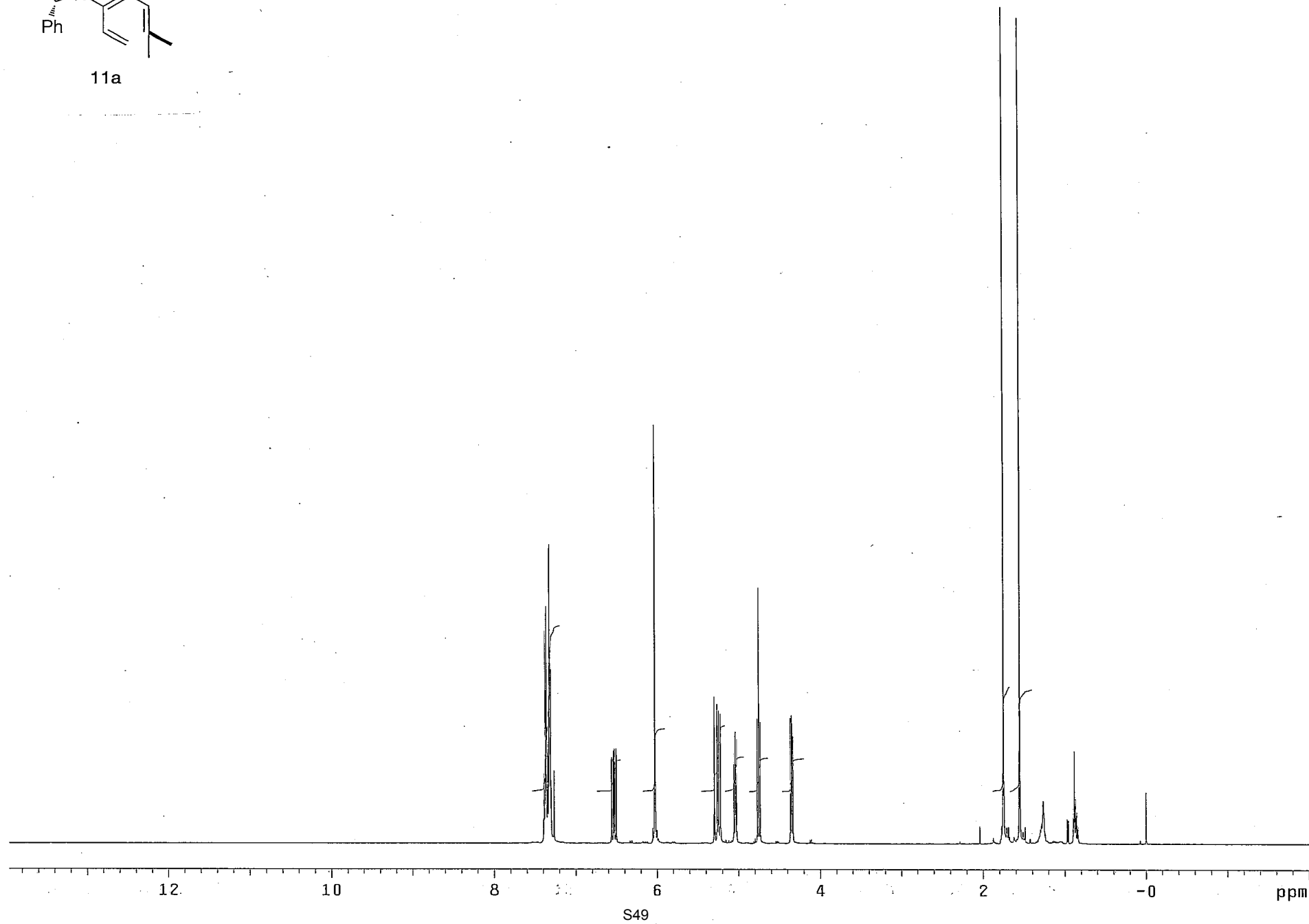


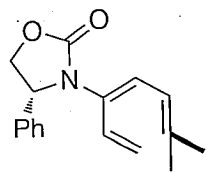




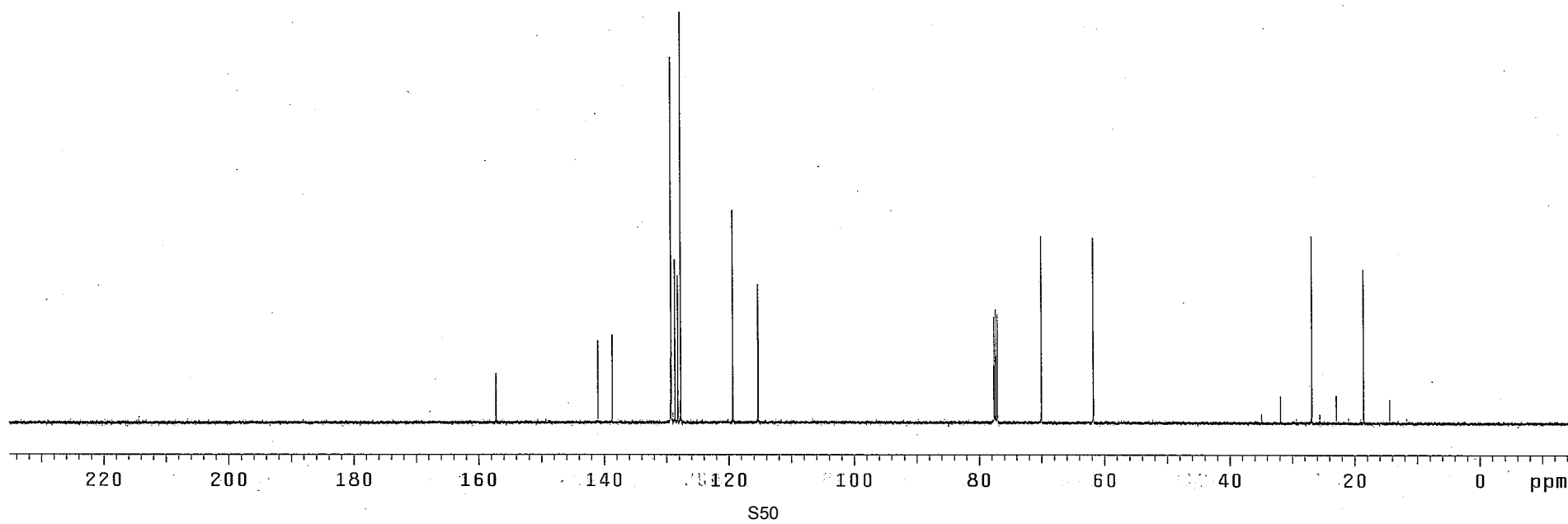


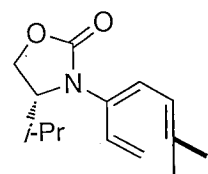
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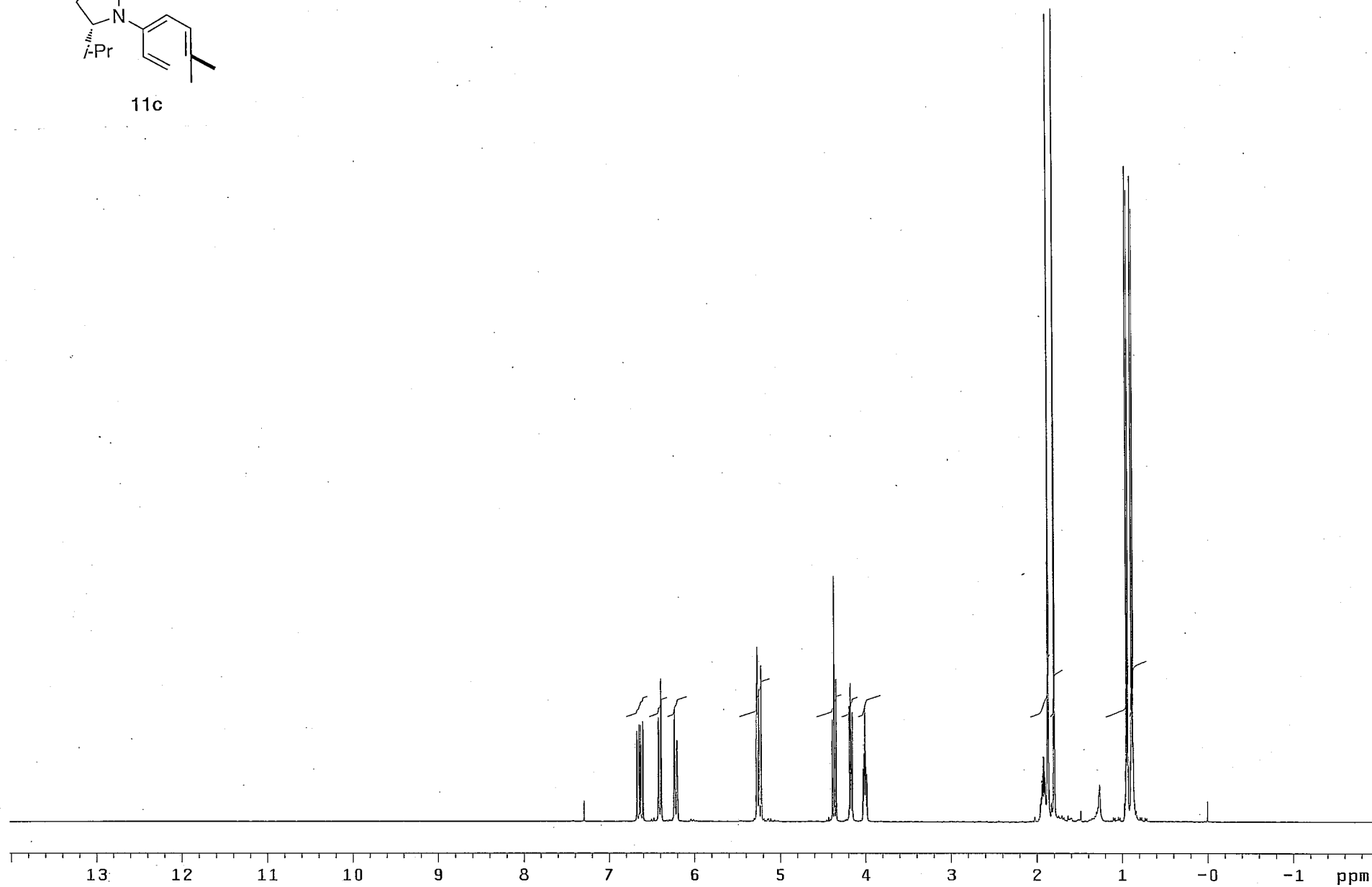


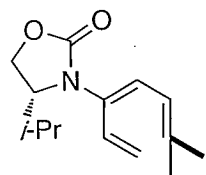
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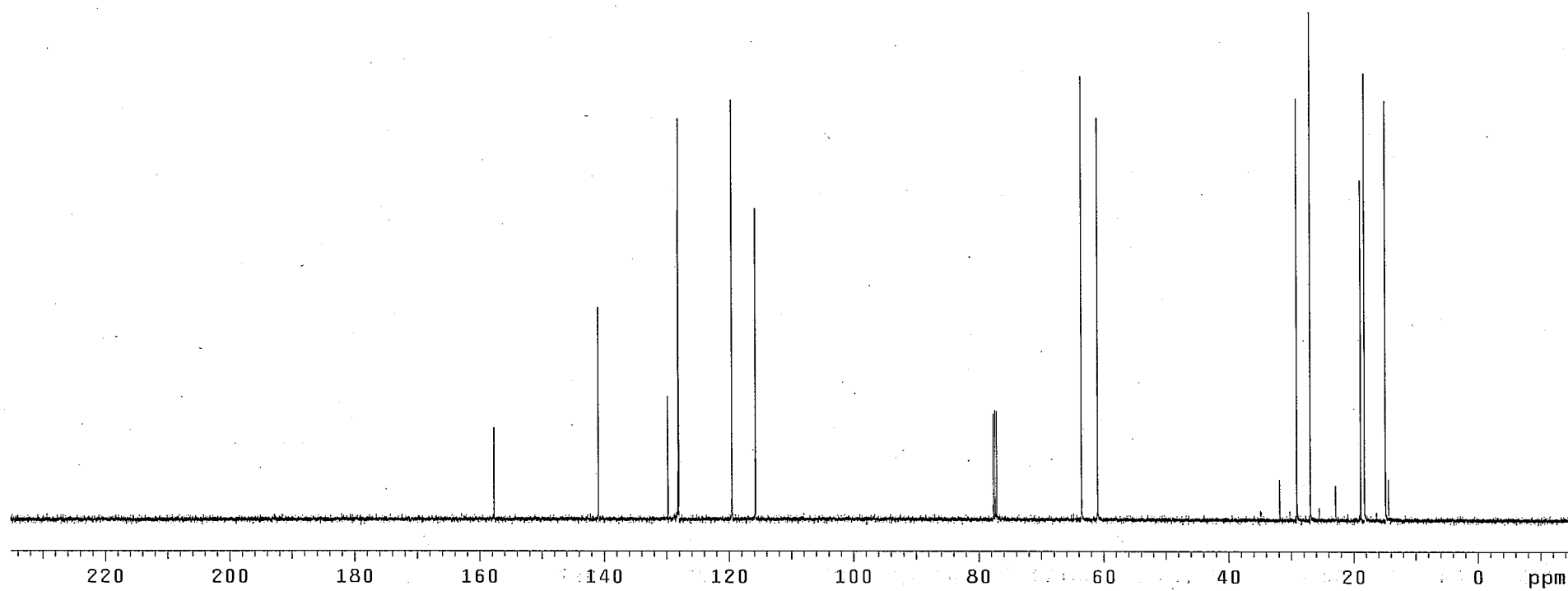


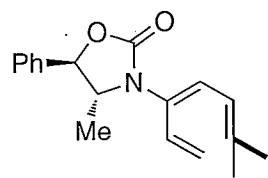
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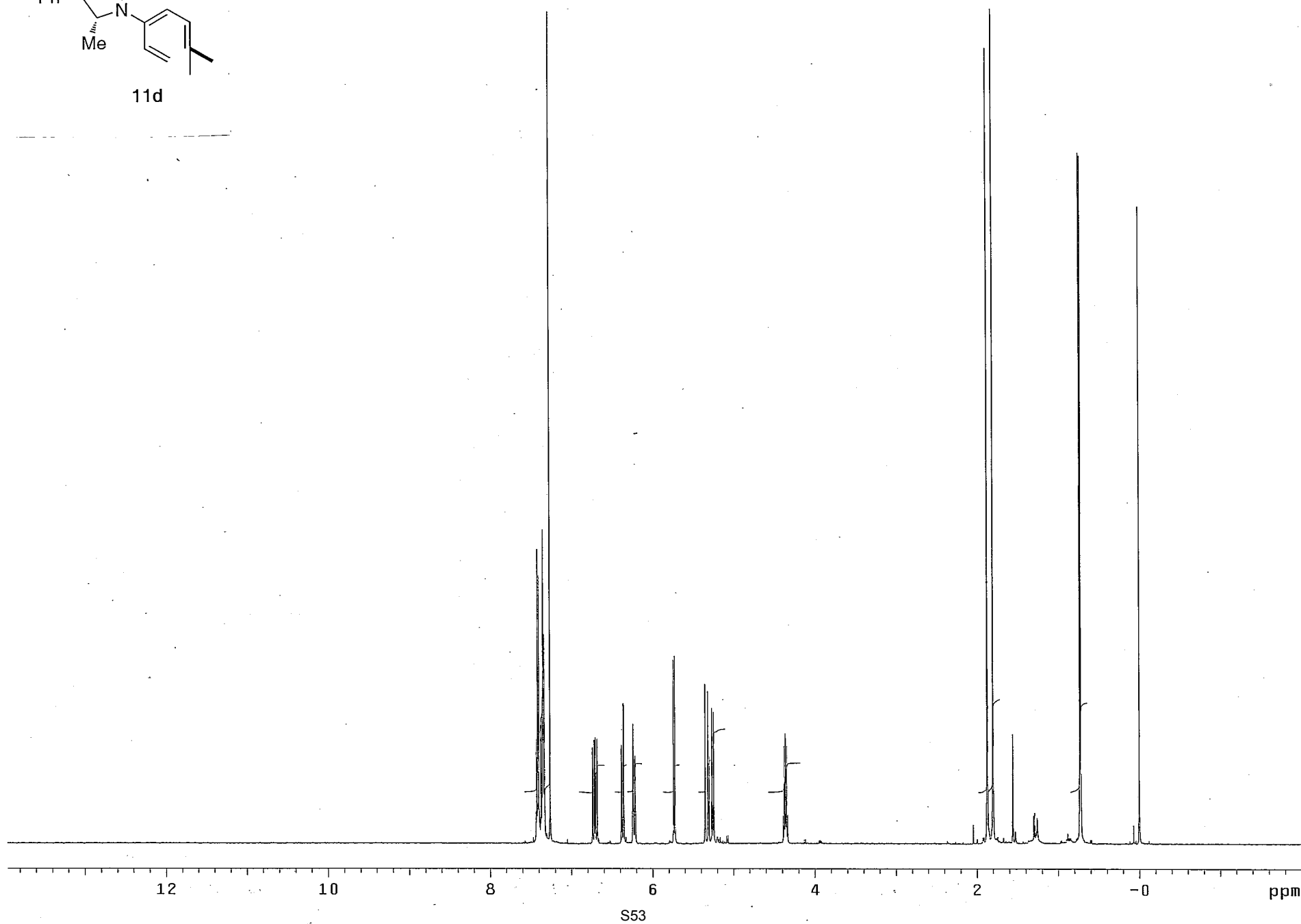


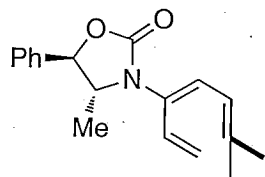
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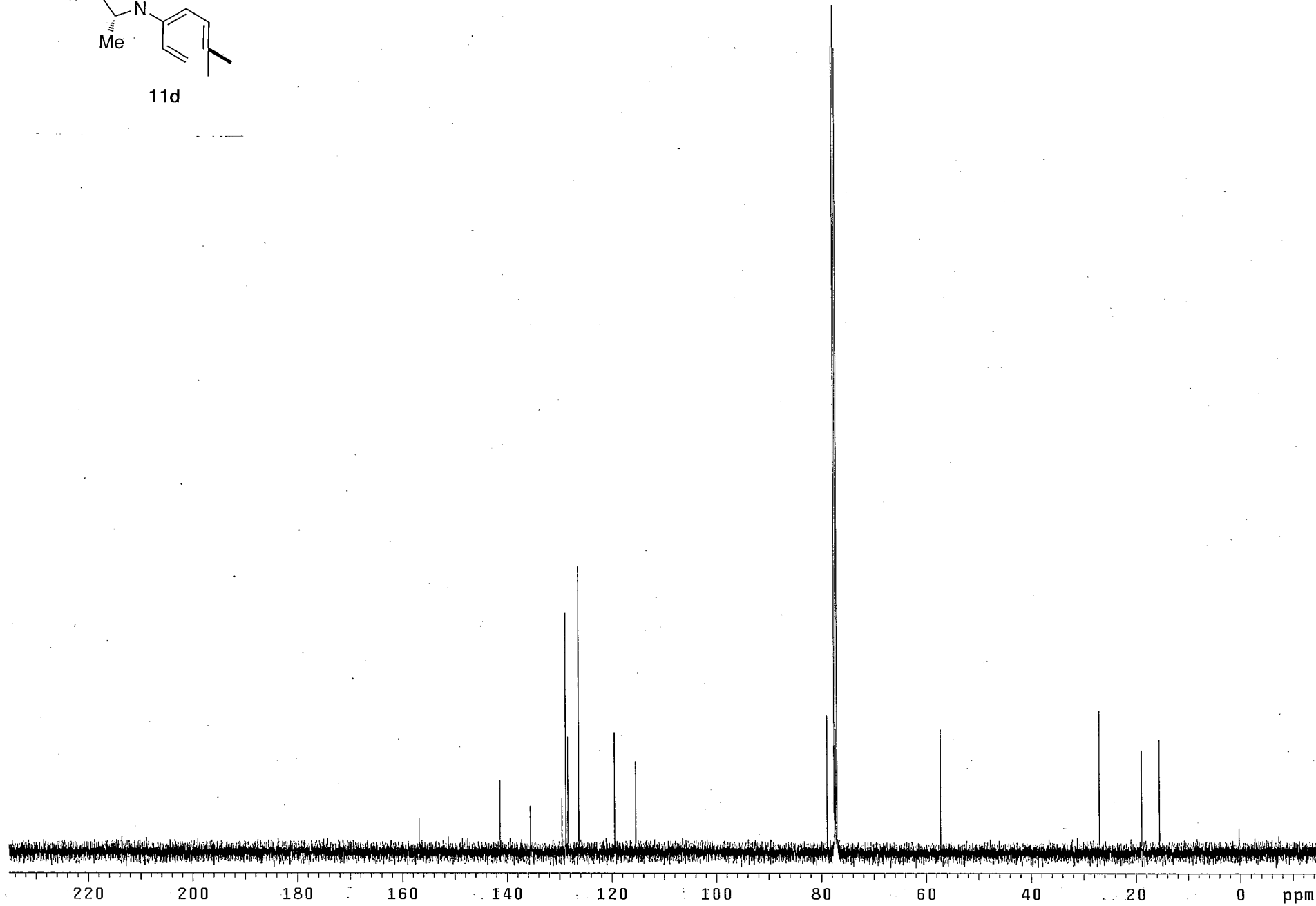


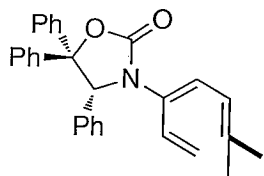
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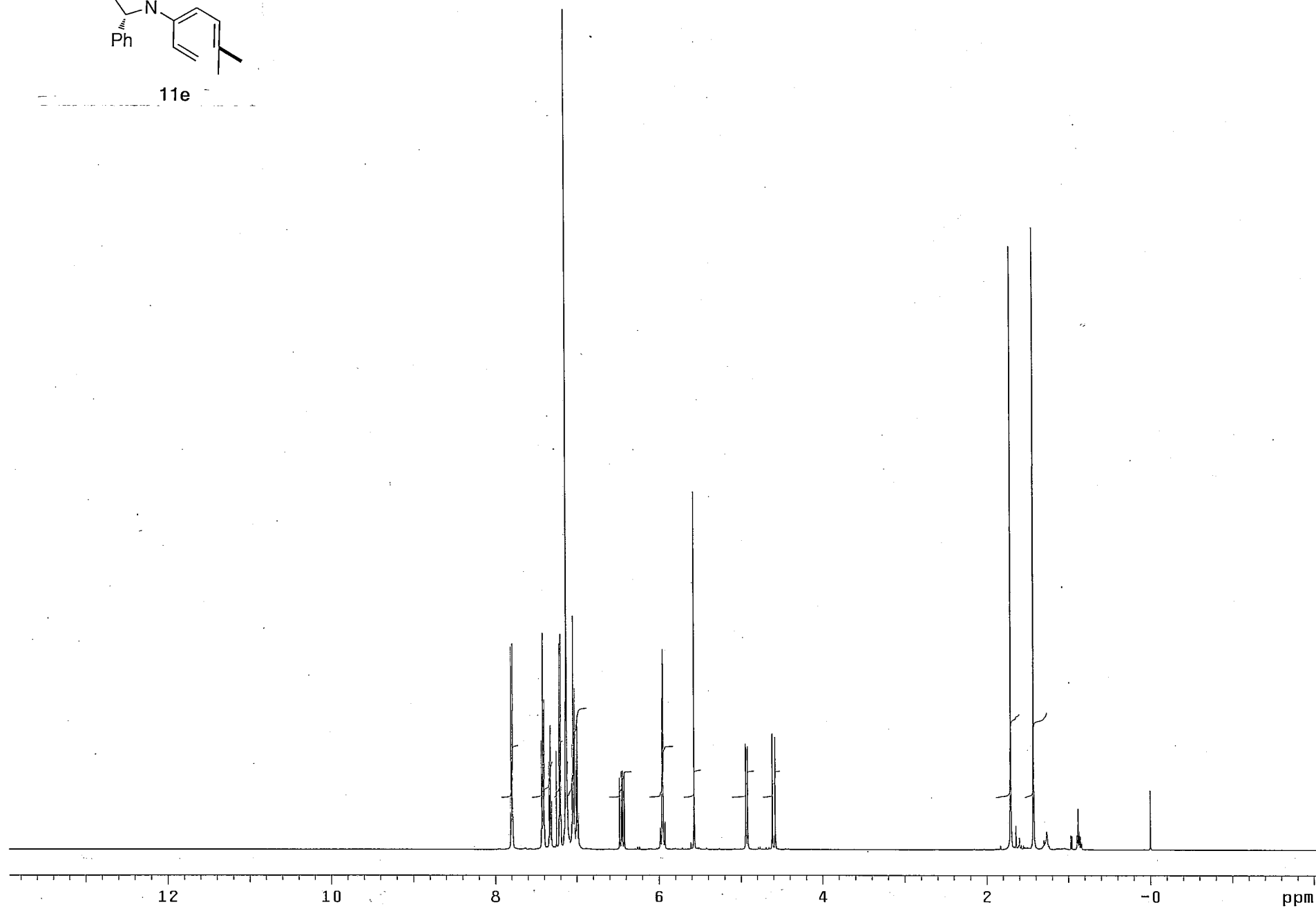


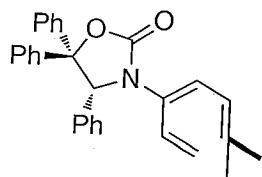
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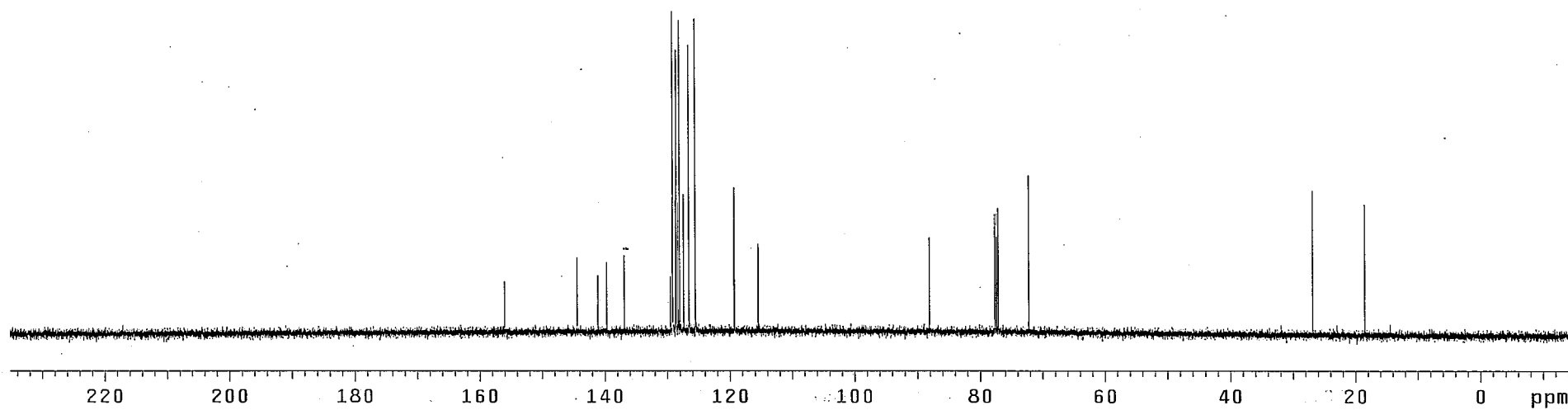


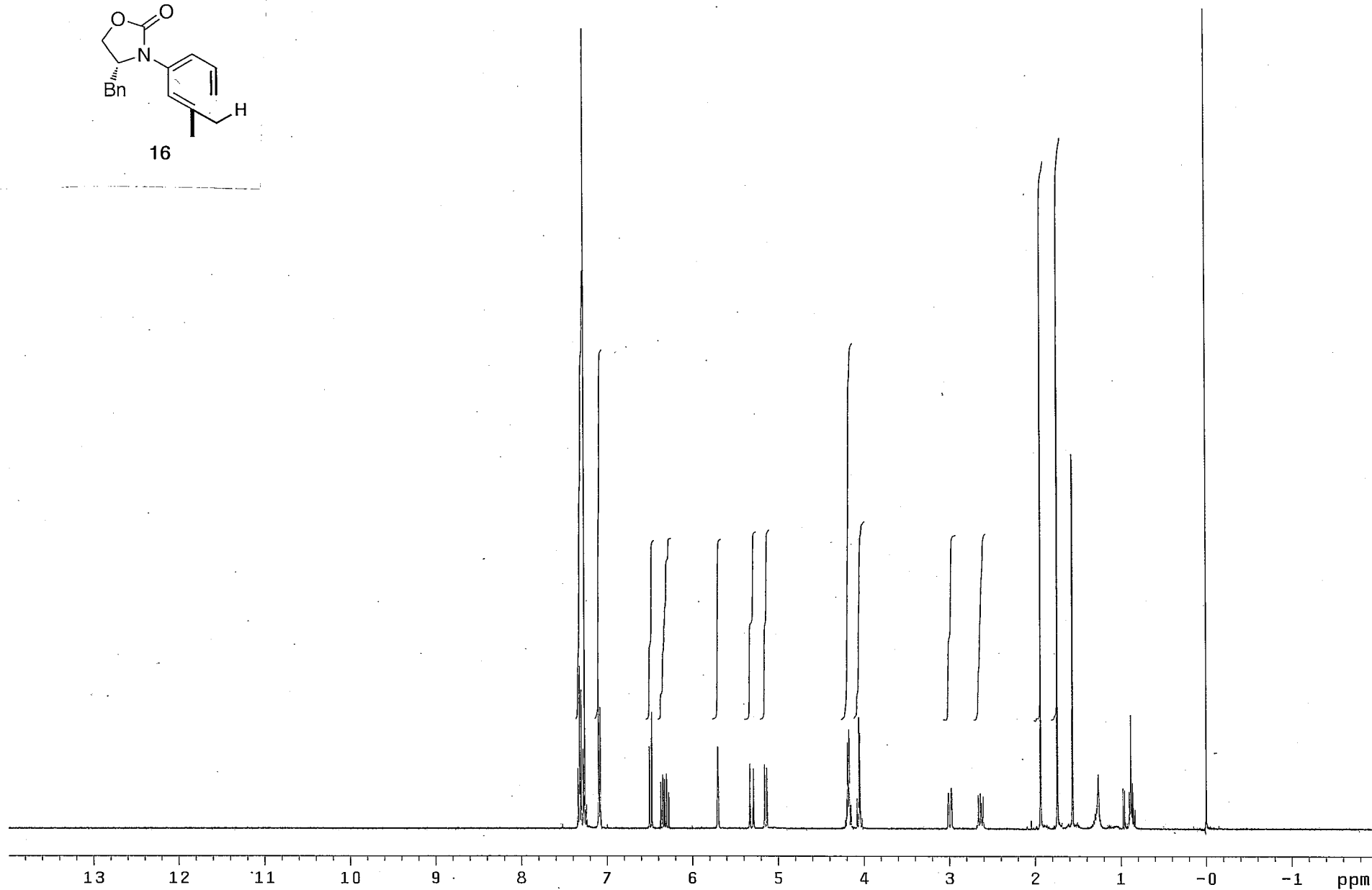
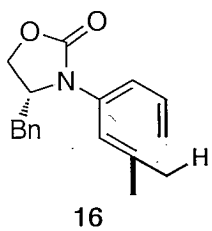
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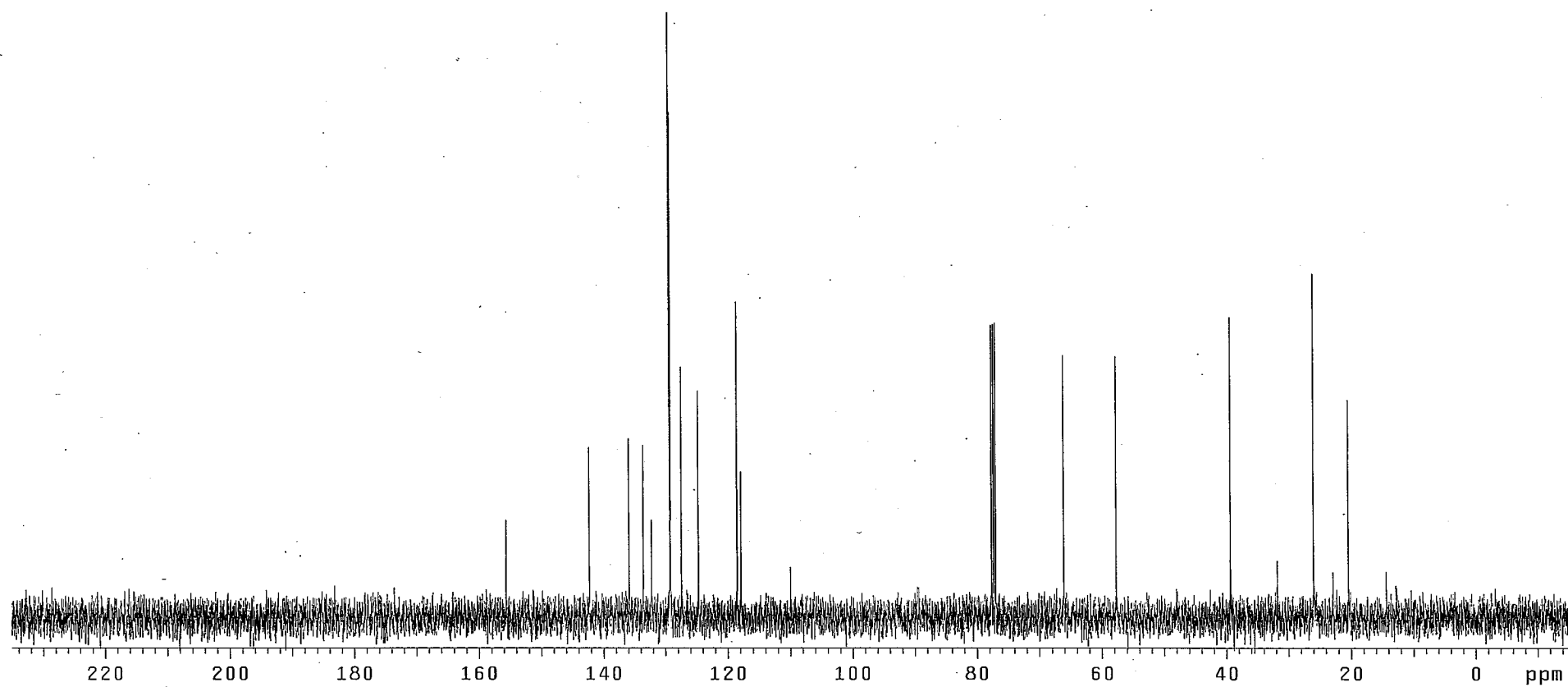
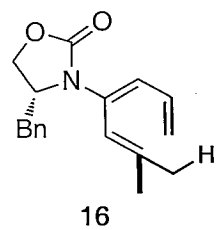


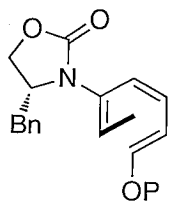


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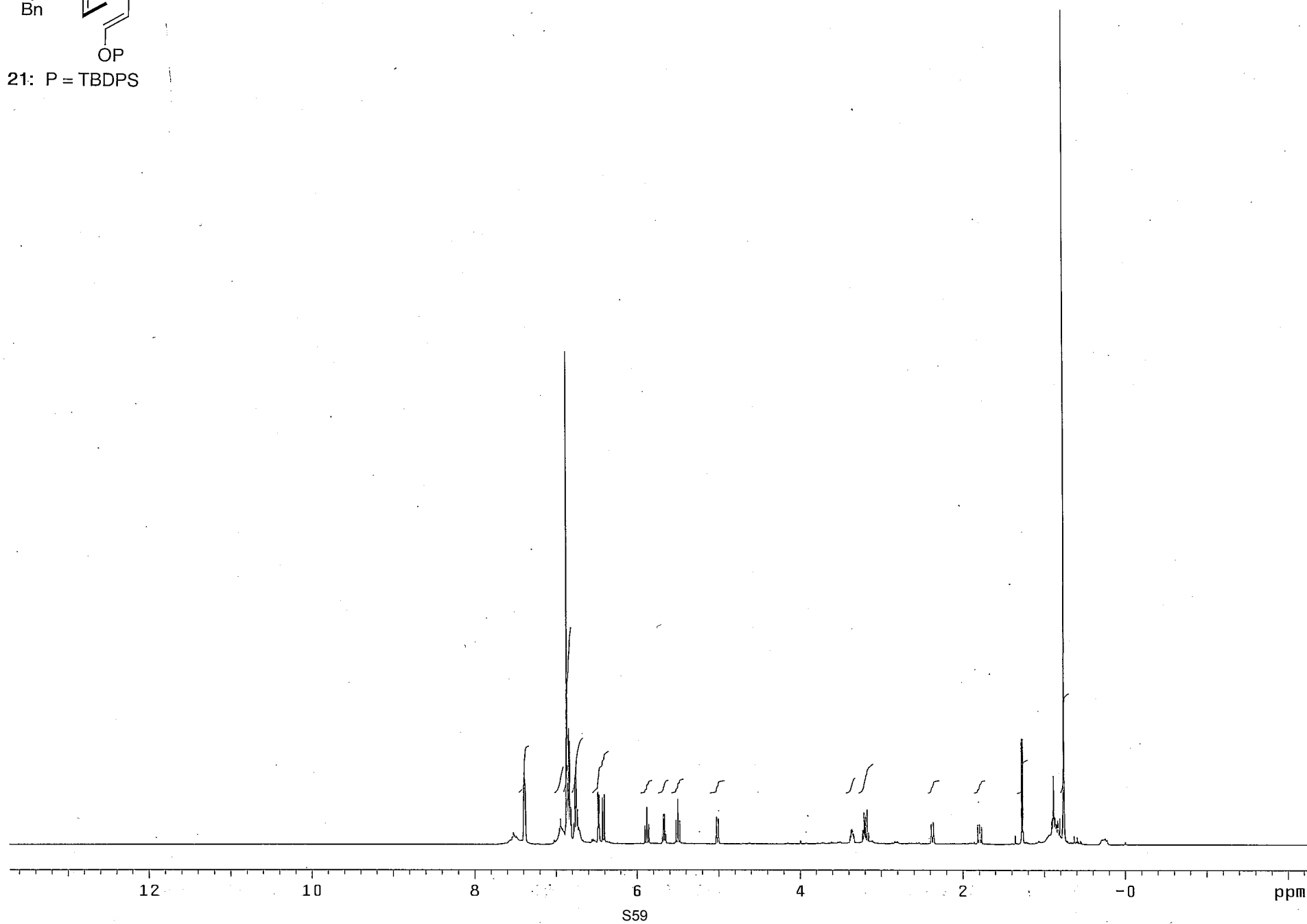


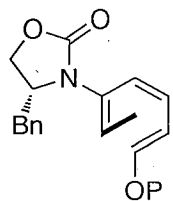




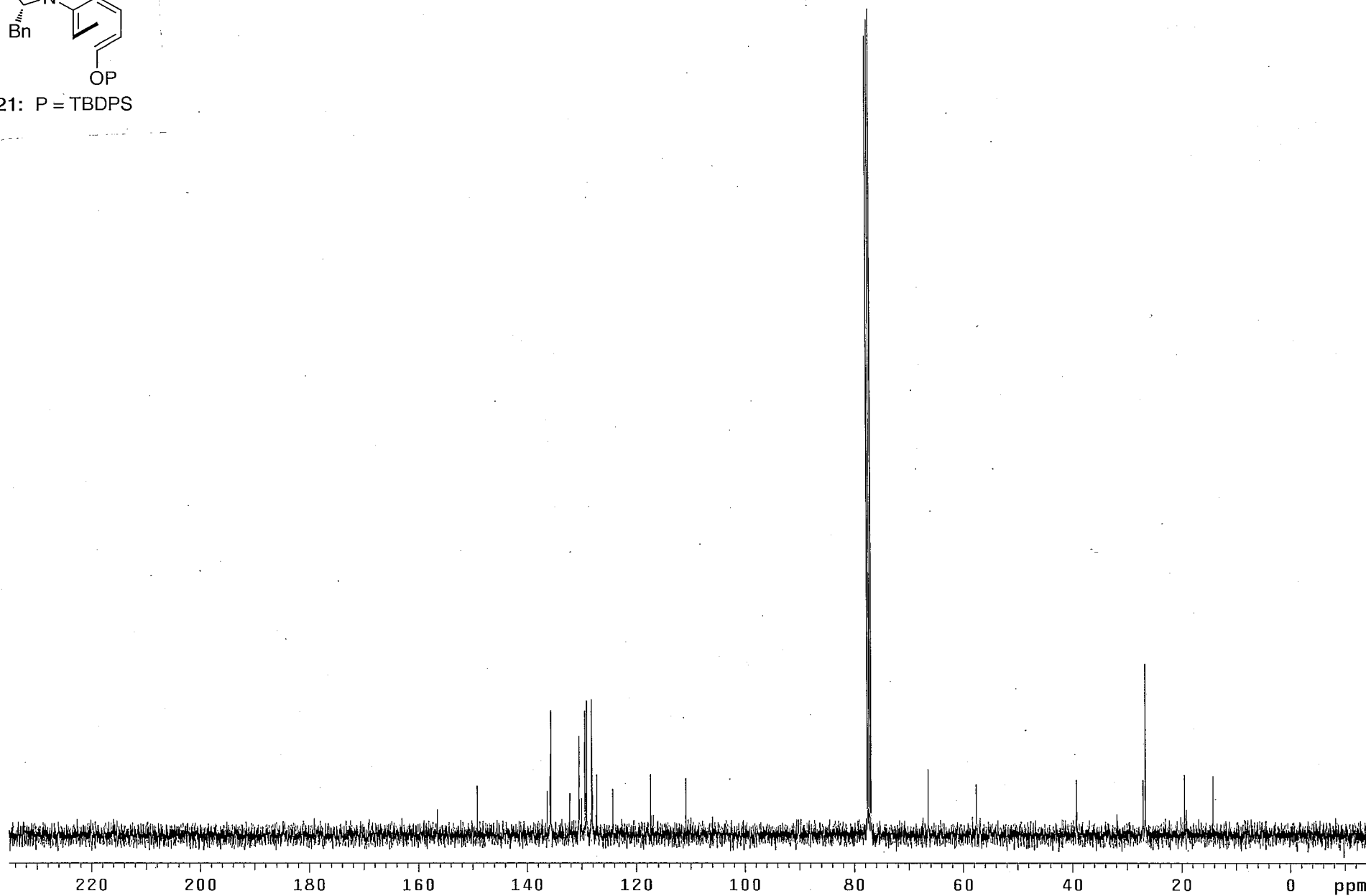


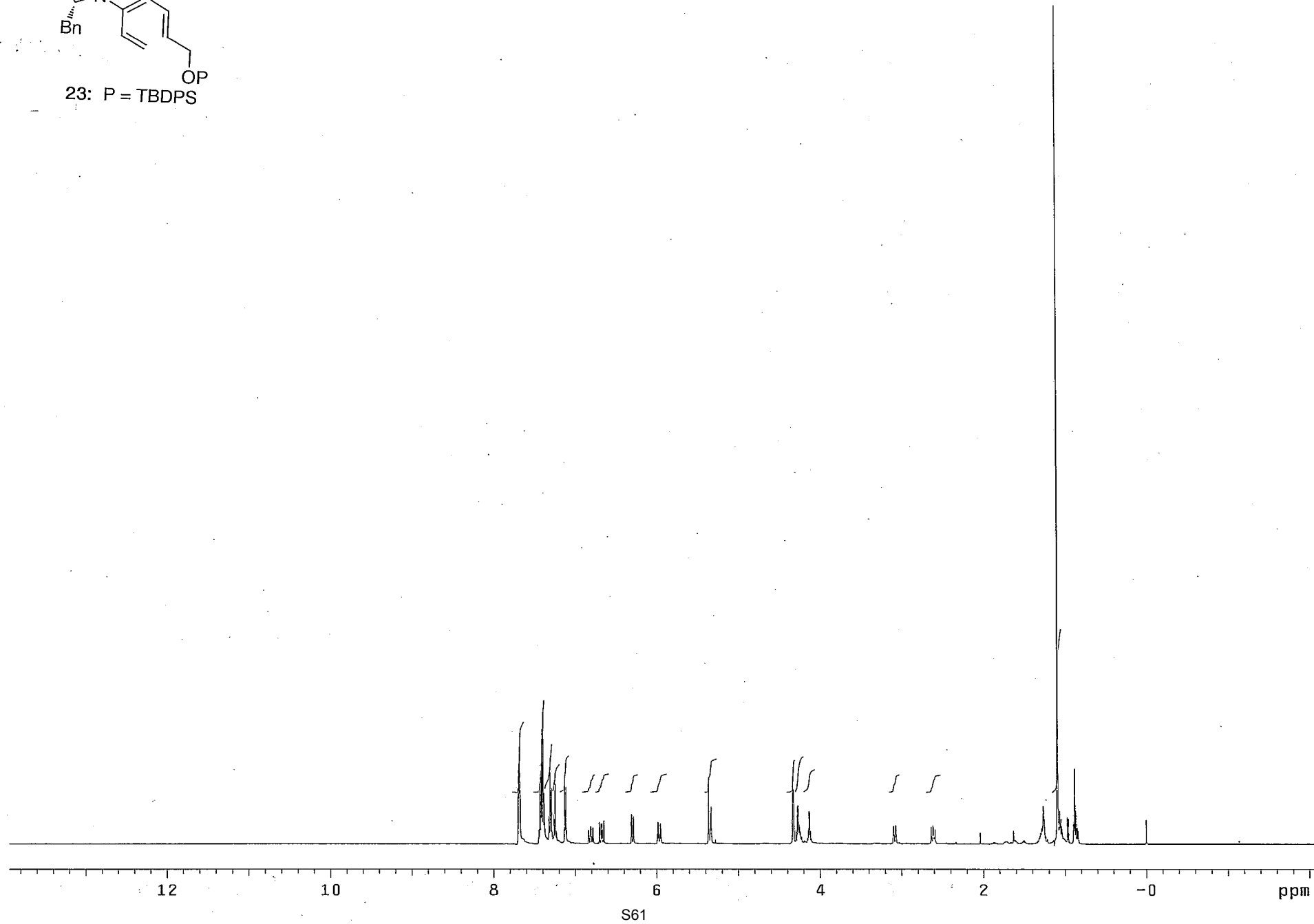
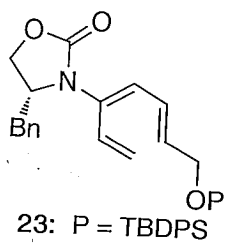
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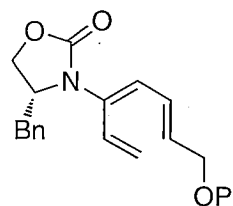




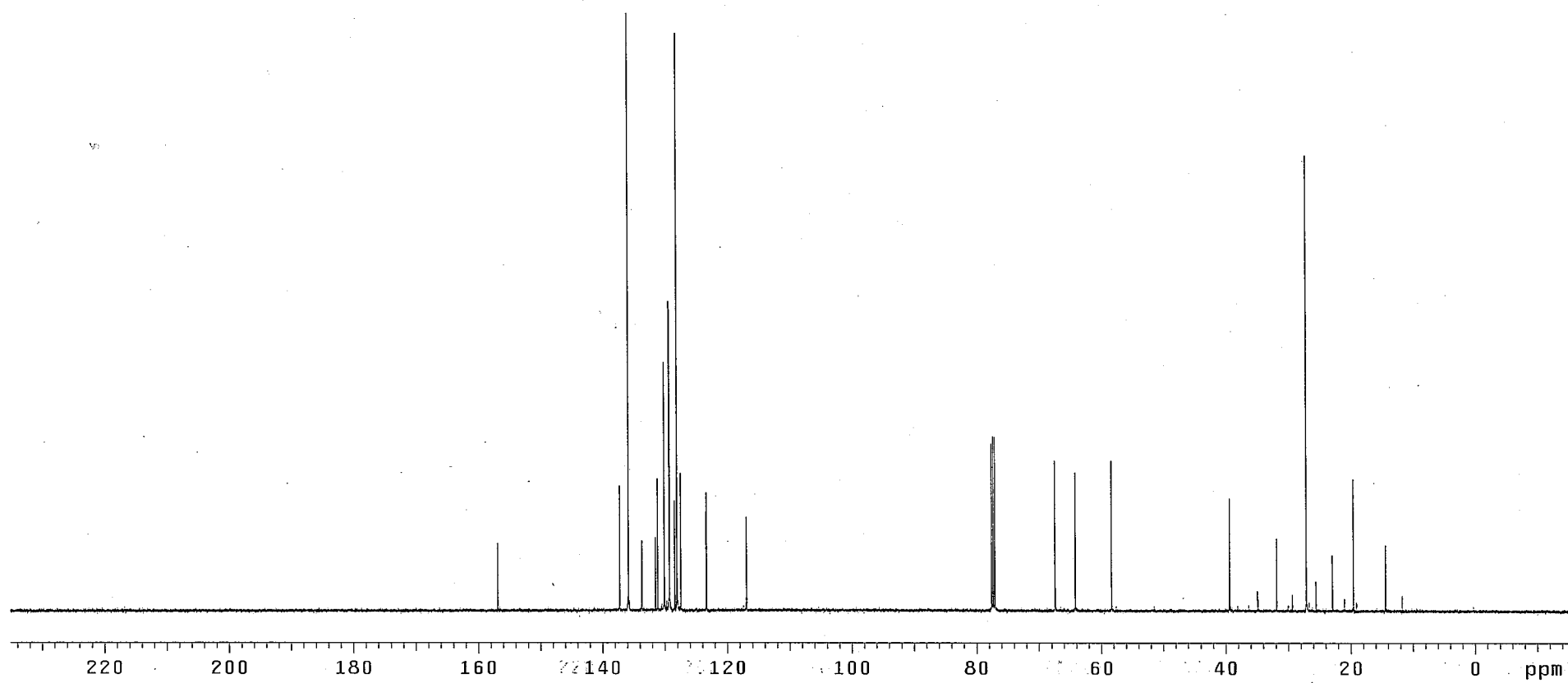
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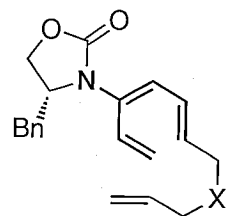




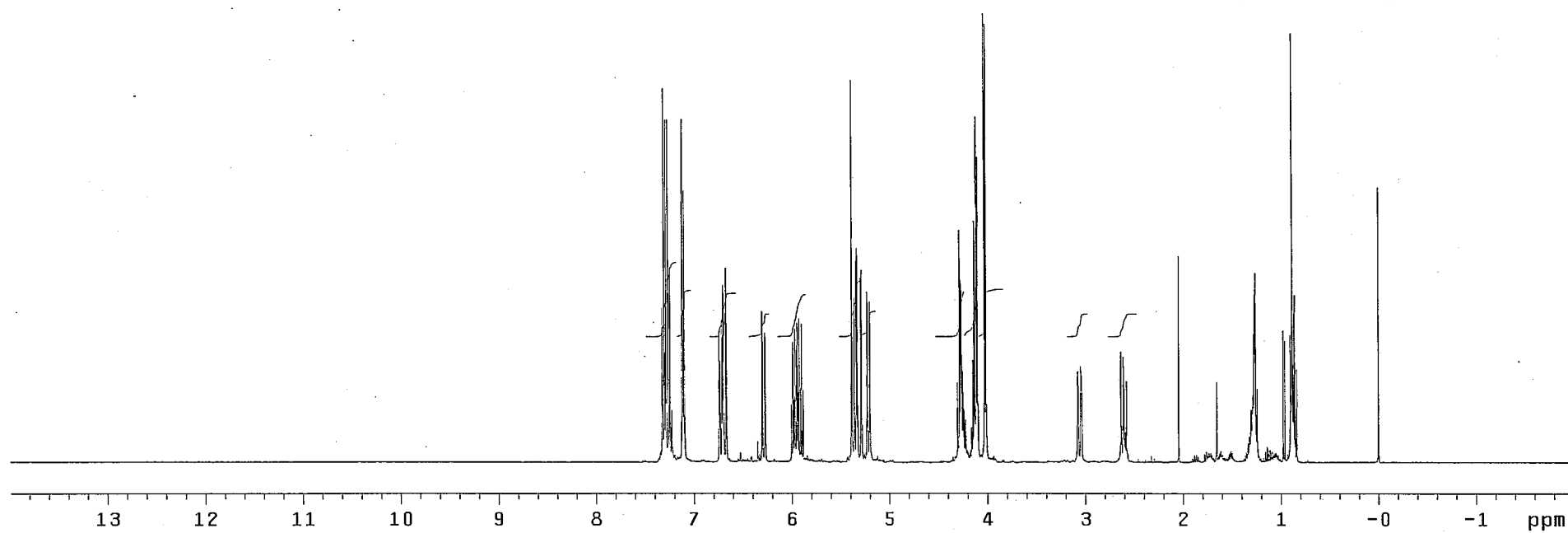


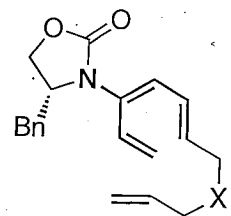
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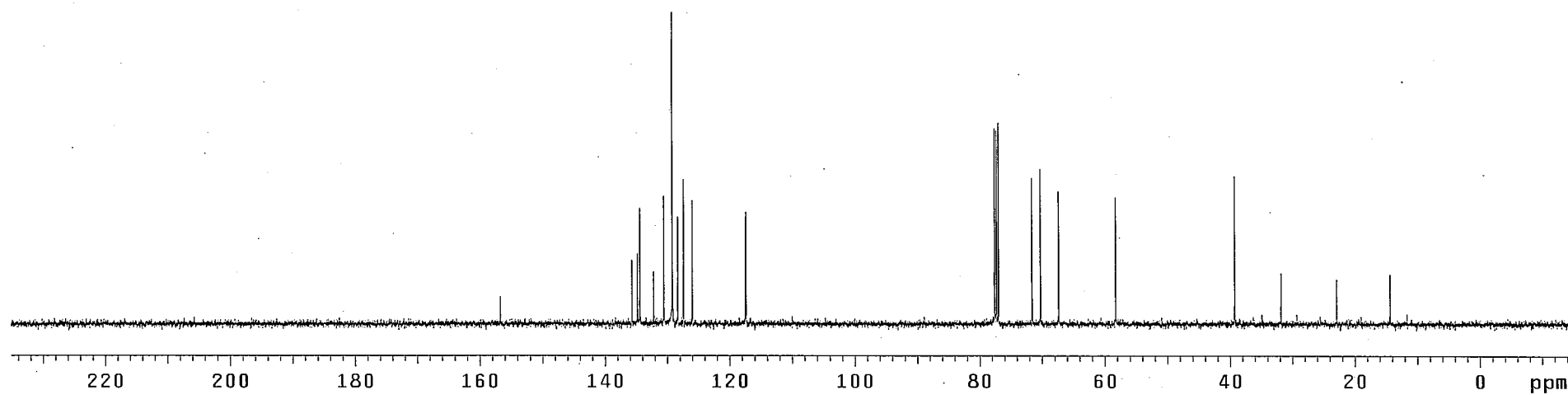


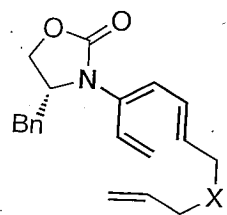
30a: X = O



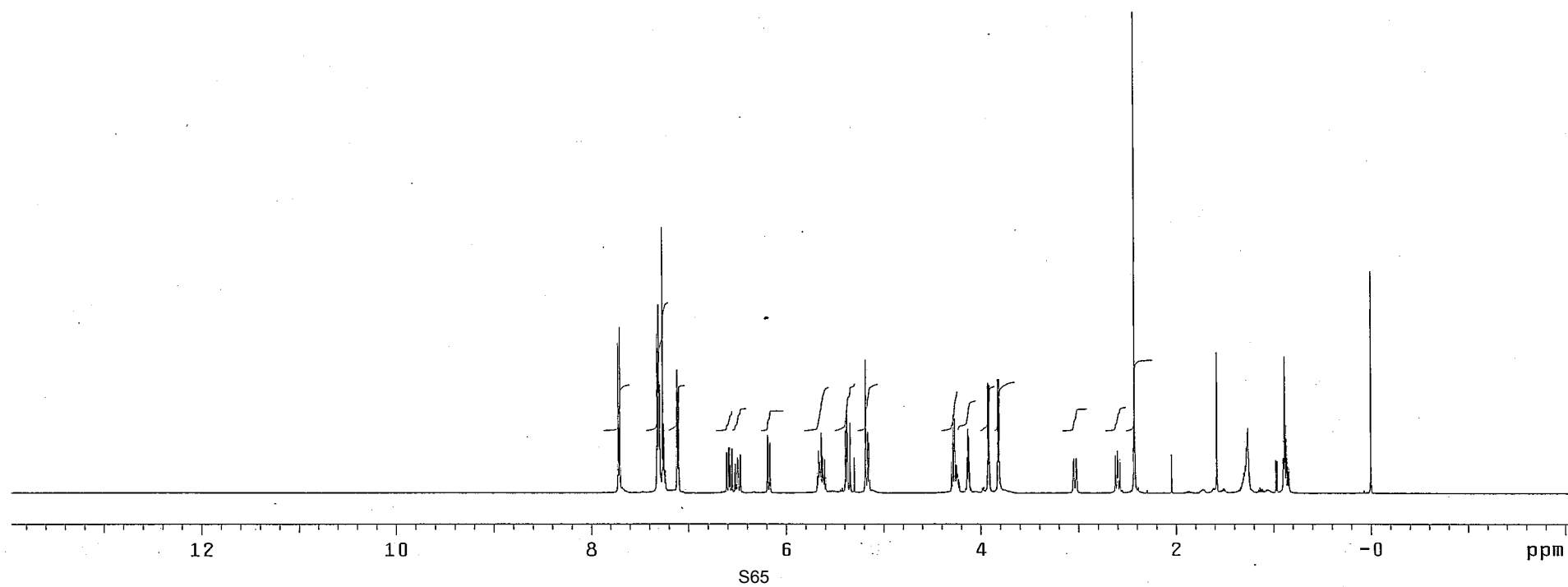


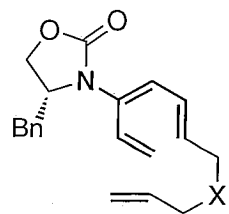
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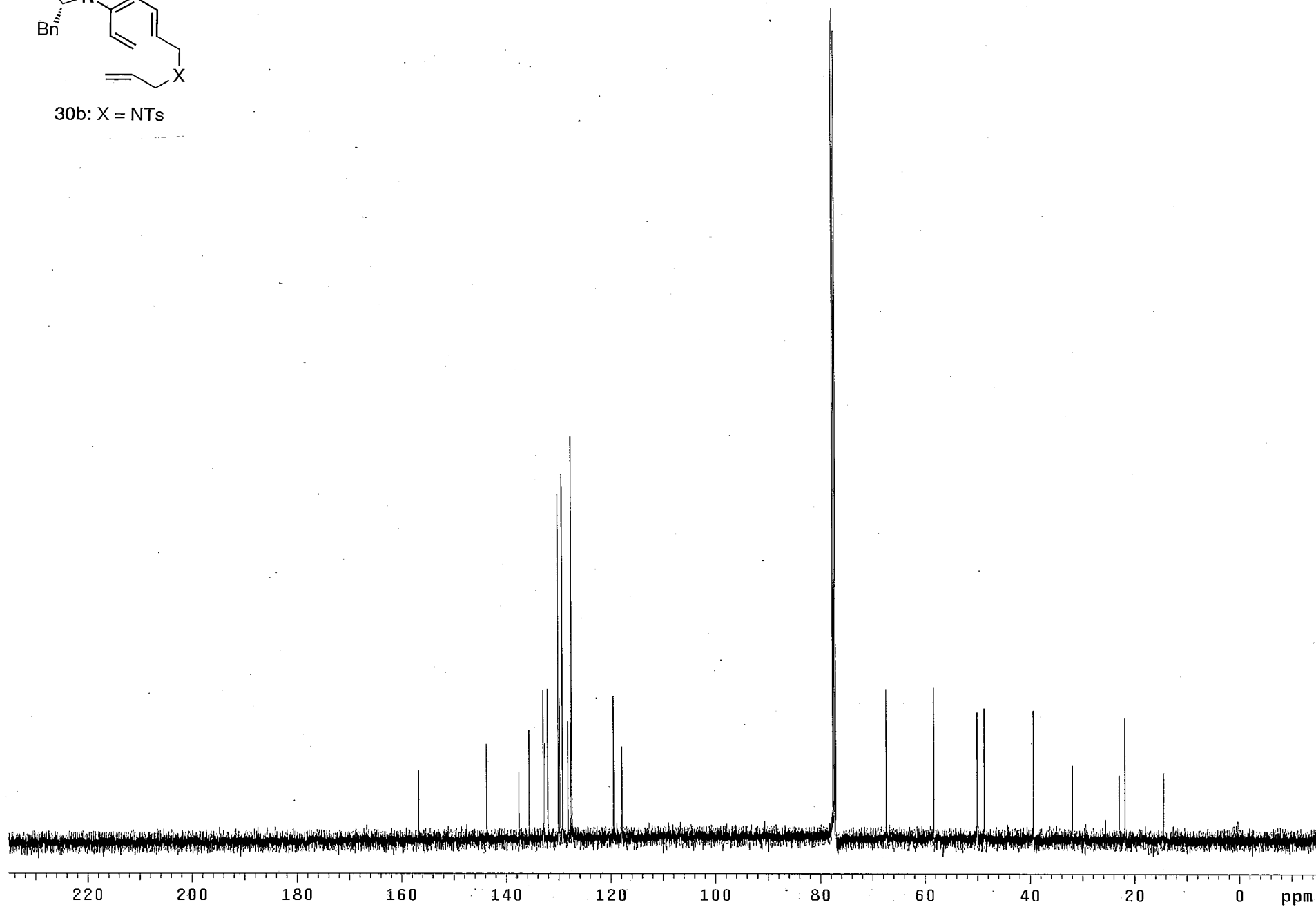


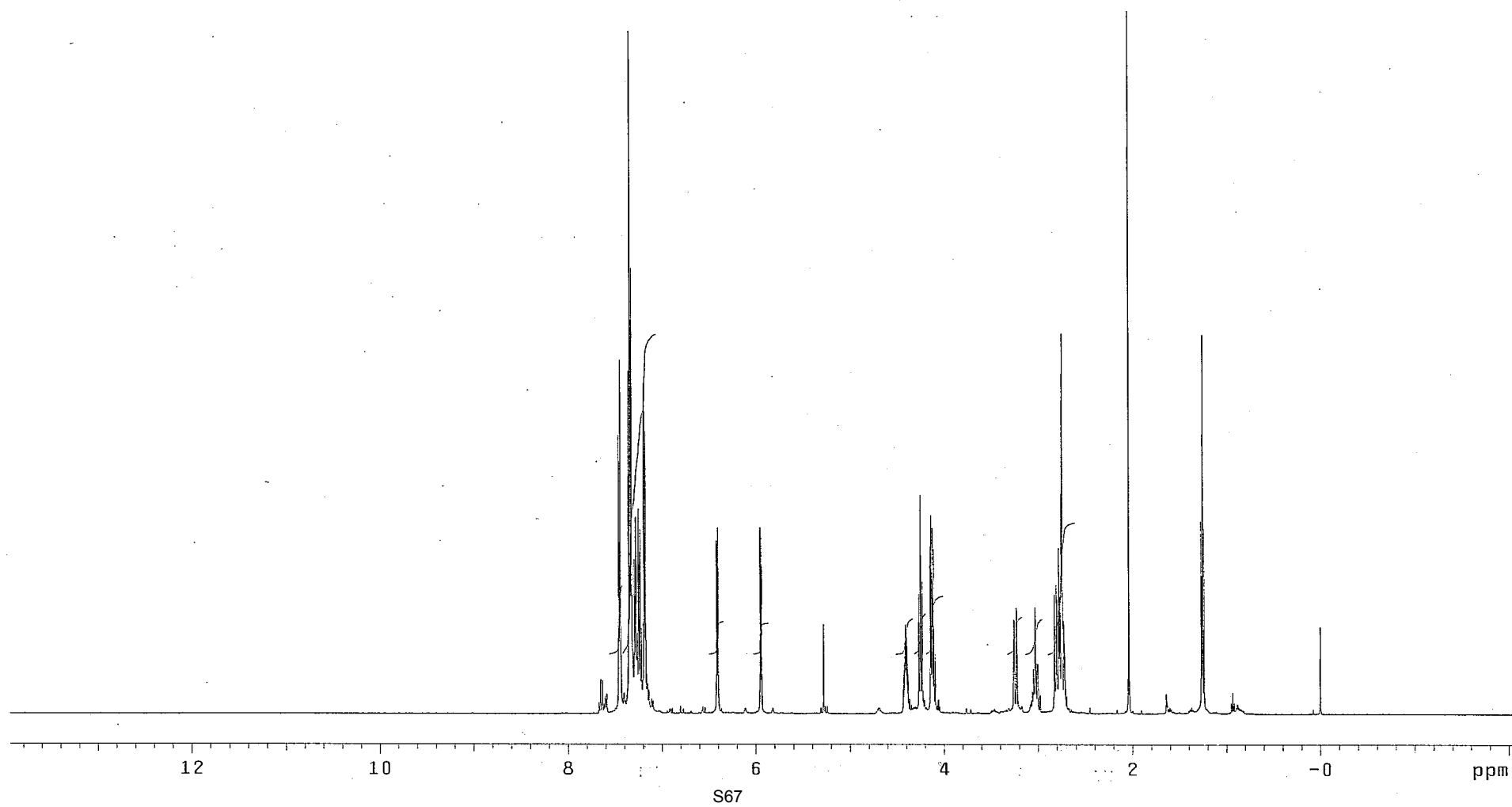
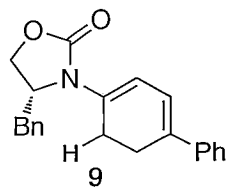
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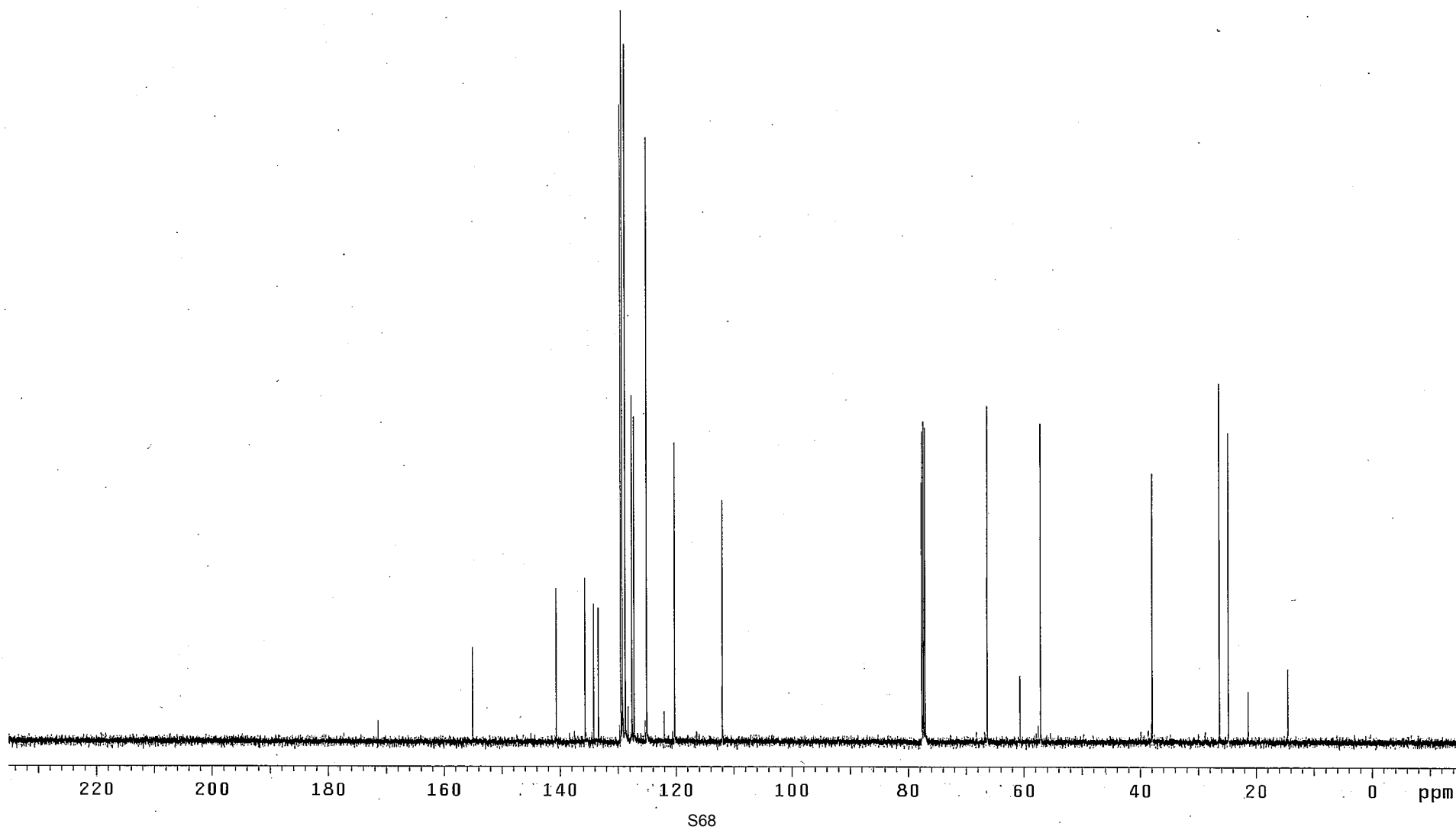
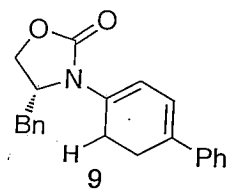


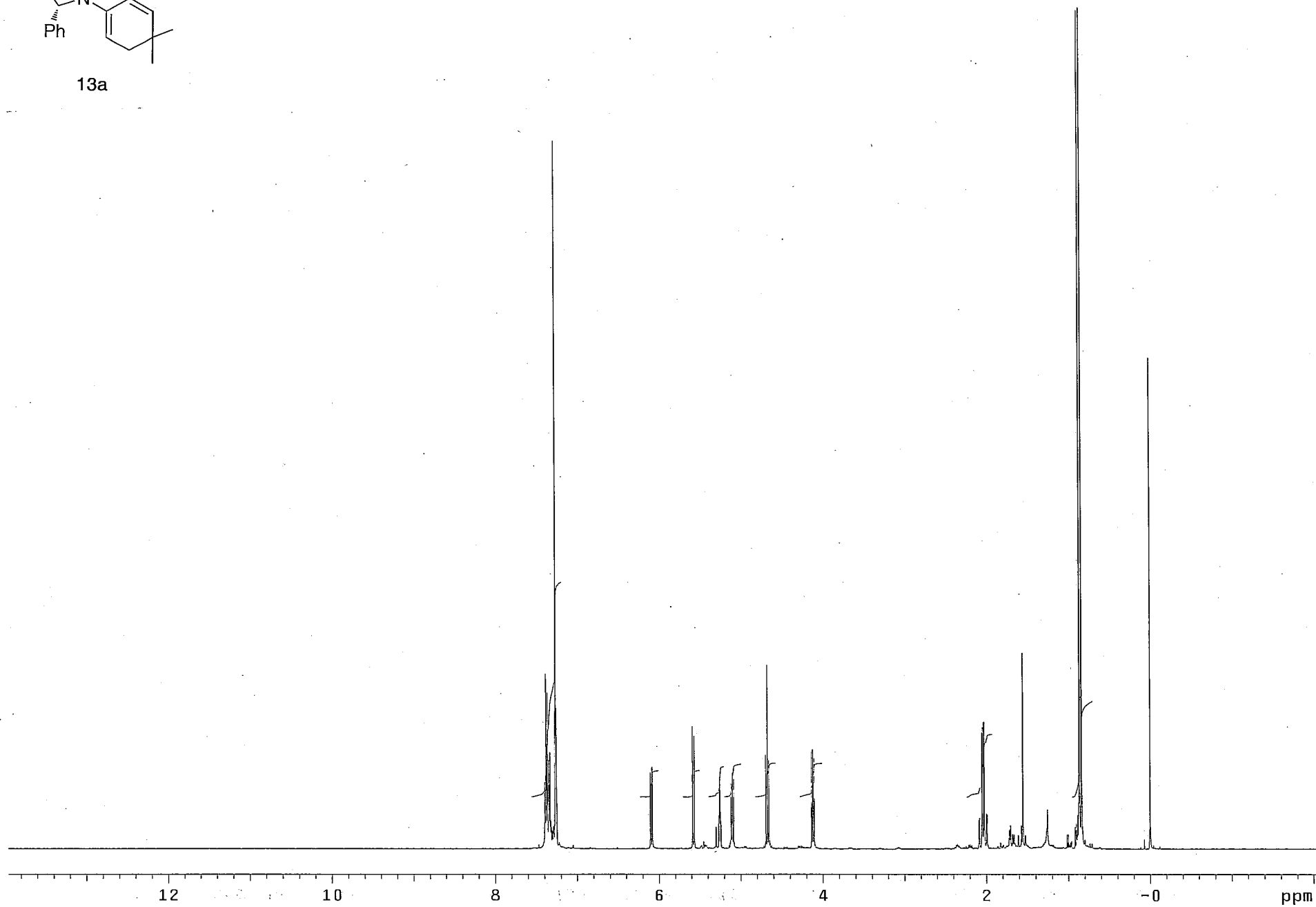
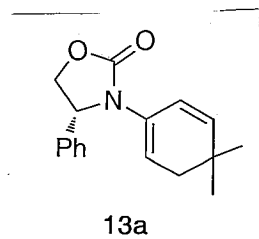


30b: X = NTs









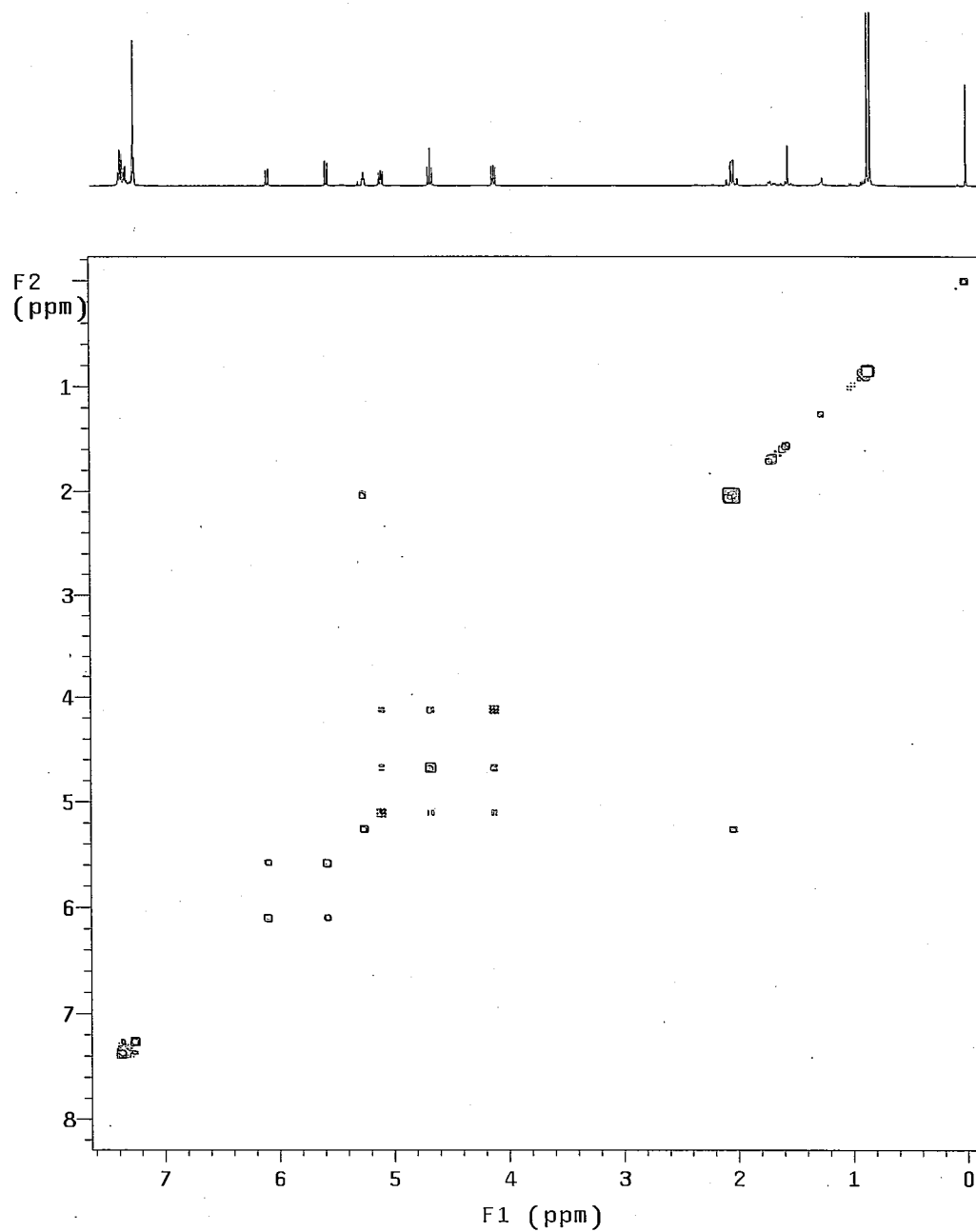
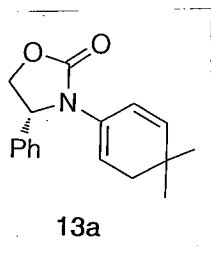
RH-2-185-1COSY_18Apr2009

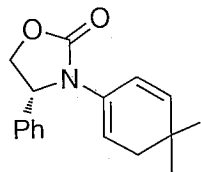
Archive directory: /export/home/ryuji/vnmrsys/data
Sample directory: RH-2-185-1COSY_18Apr2009

Pulse Sequence: gCOSY

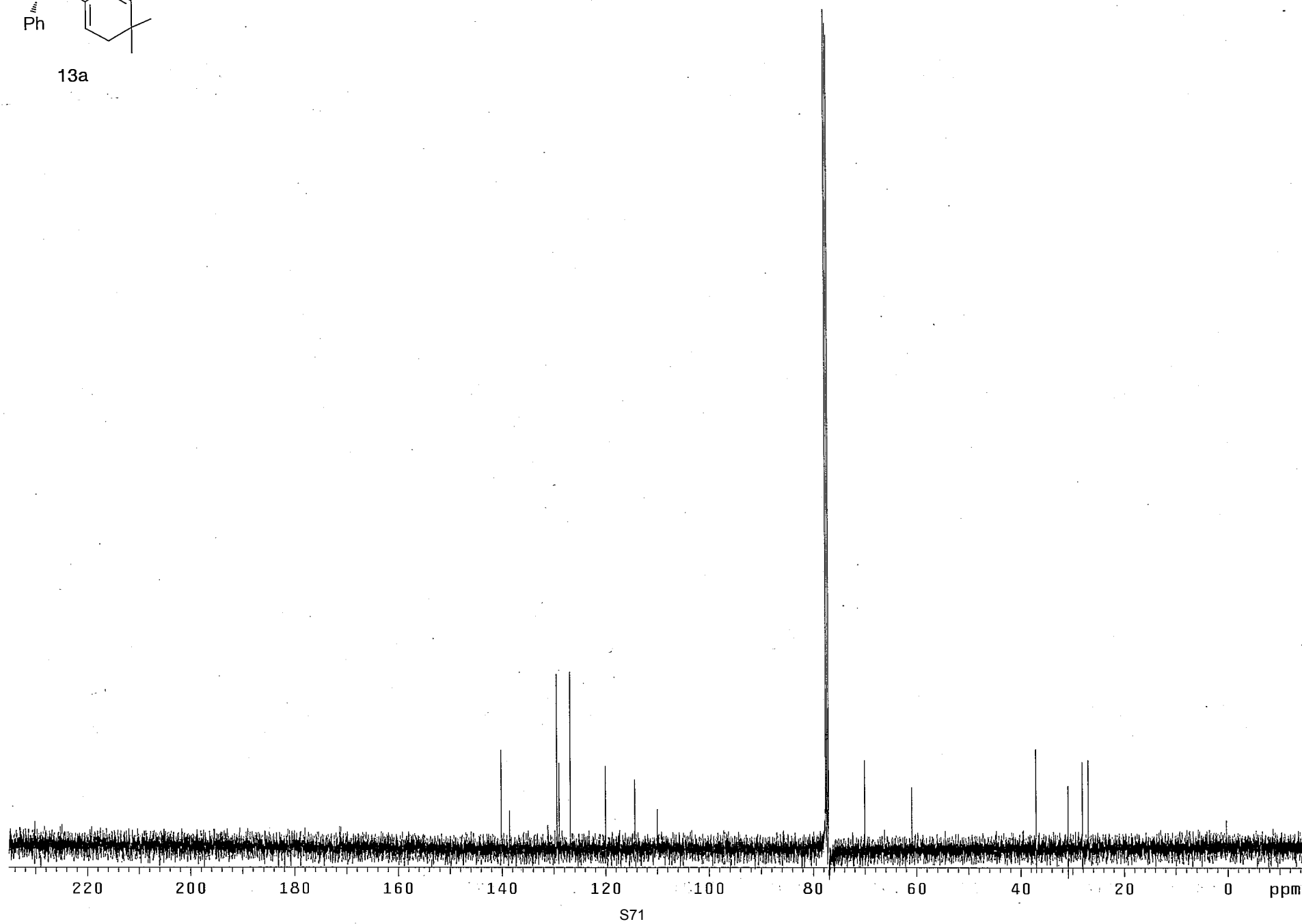
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

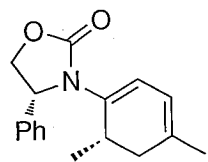
Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
Single scan
128 increments
OBSERVE H1, 499.7288168 MHz
DATA PROCESSING
Sq. sine bell 0.064 sec
F1 DATA PROCESSING
Sq. sine bell 0.016 sec
FT size 2048 x 2048
Total time 2 min, 45 sec



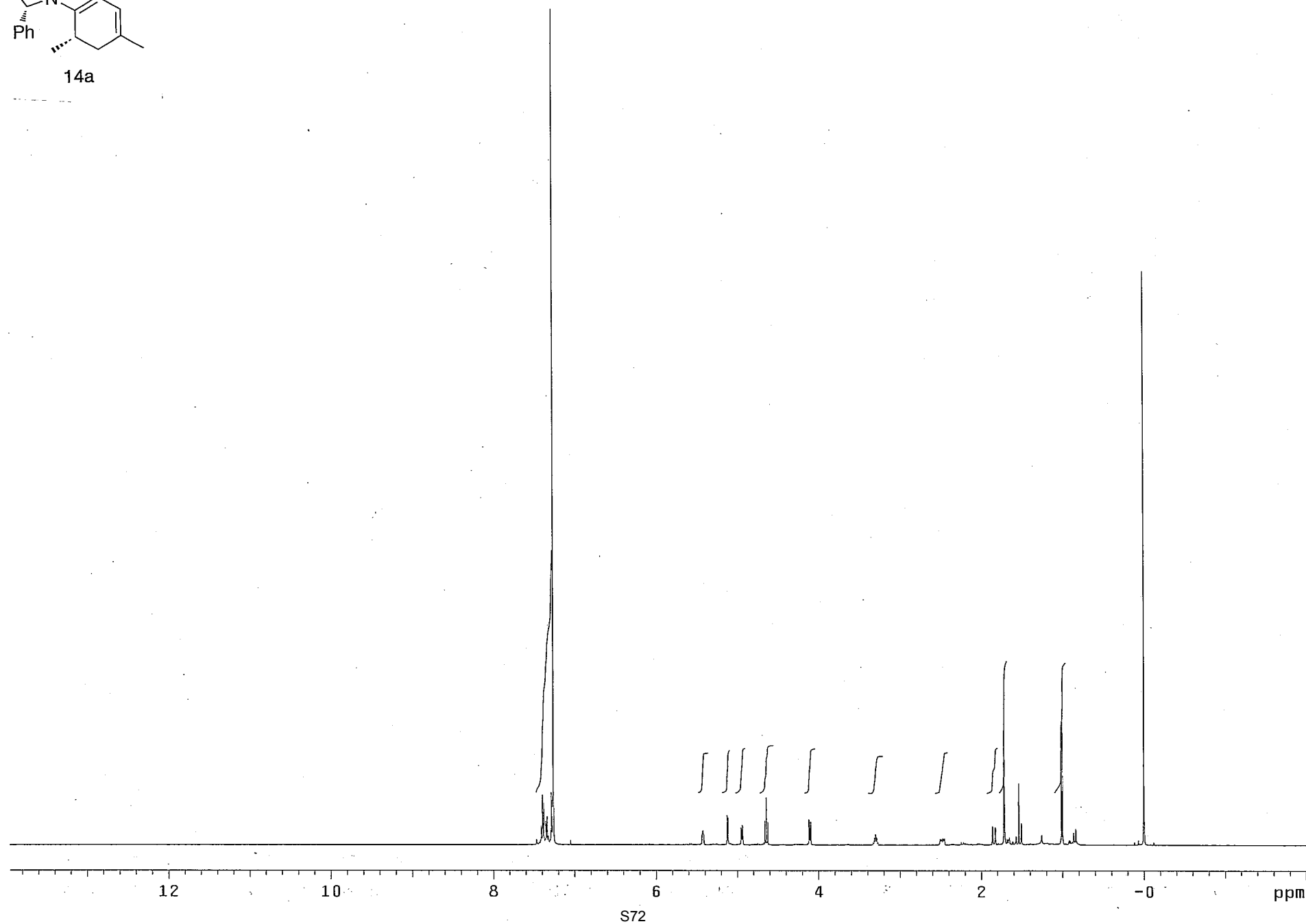


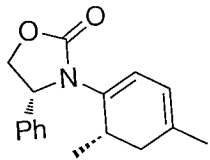
13a



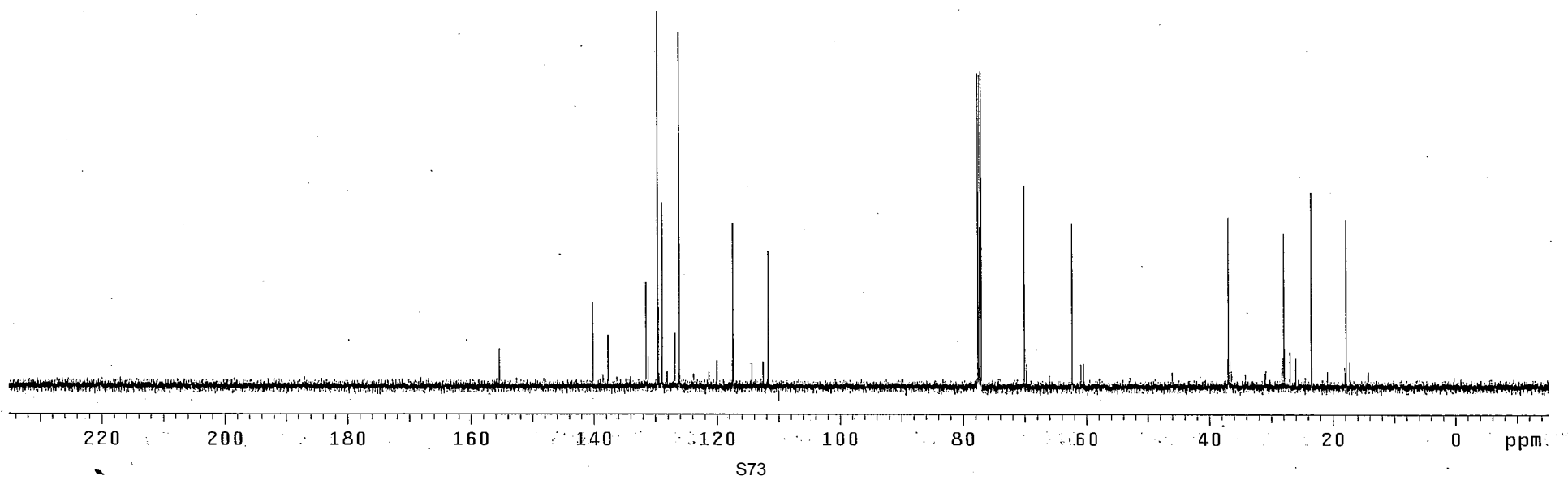


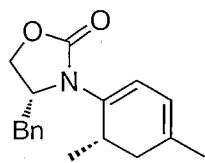
14a



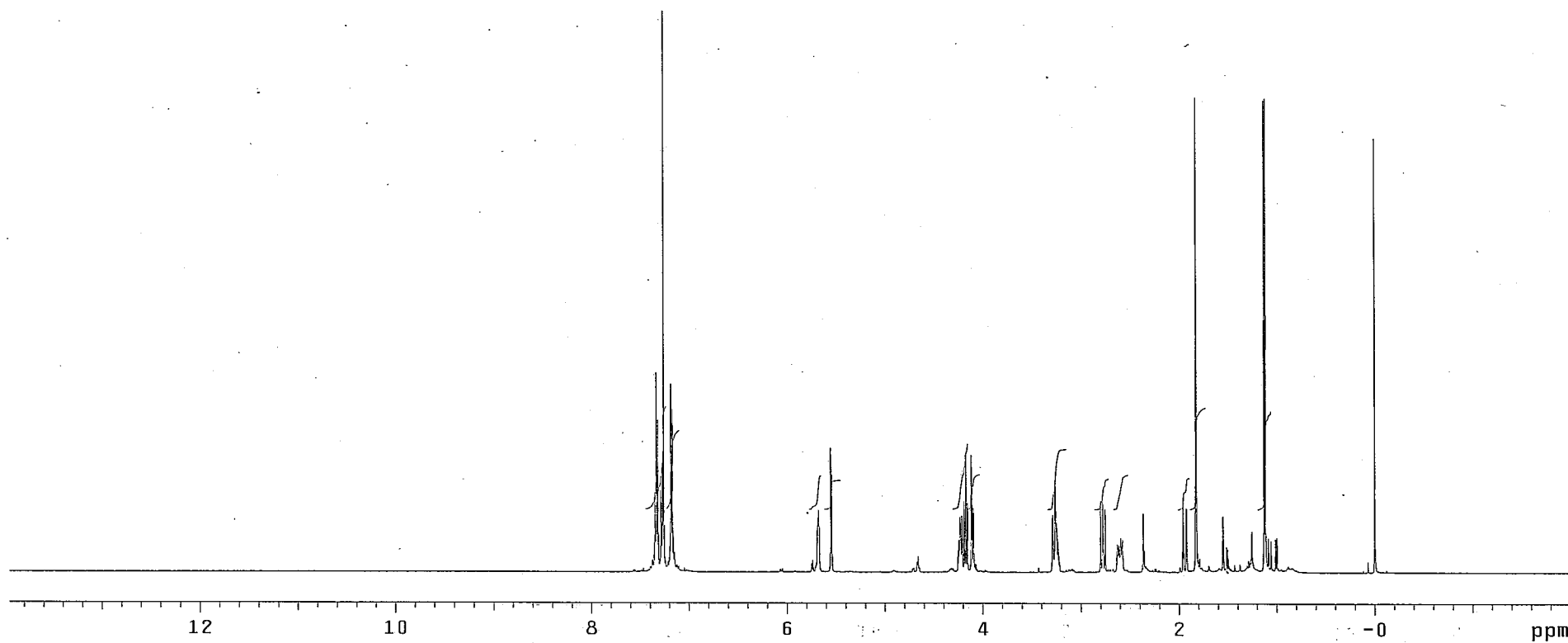


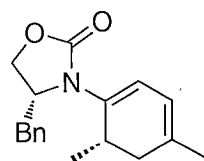
14a



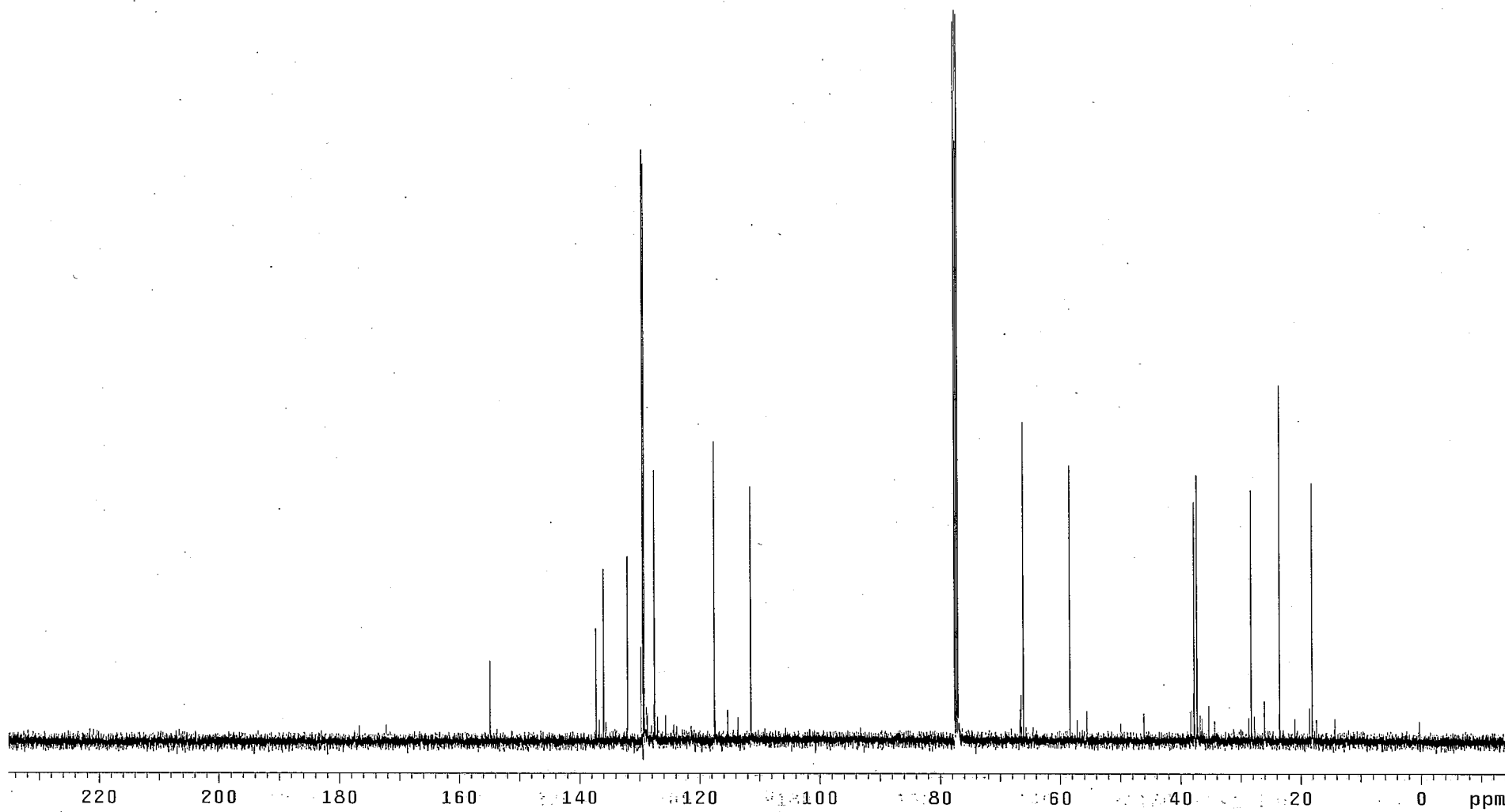


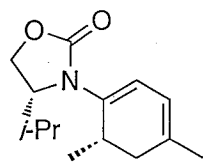
14b



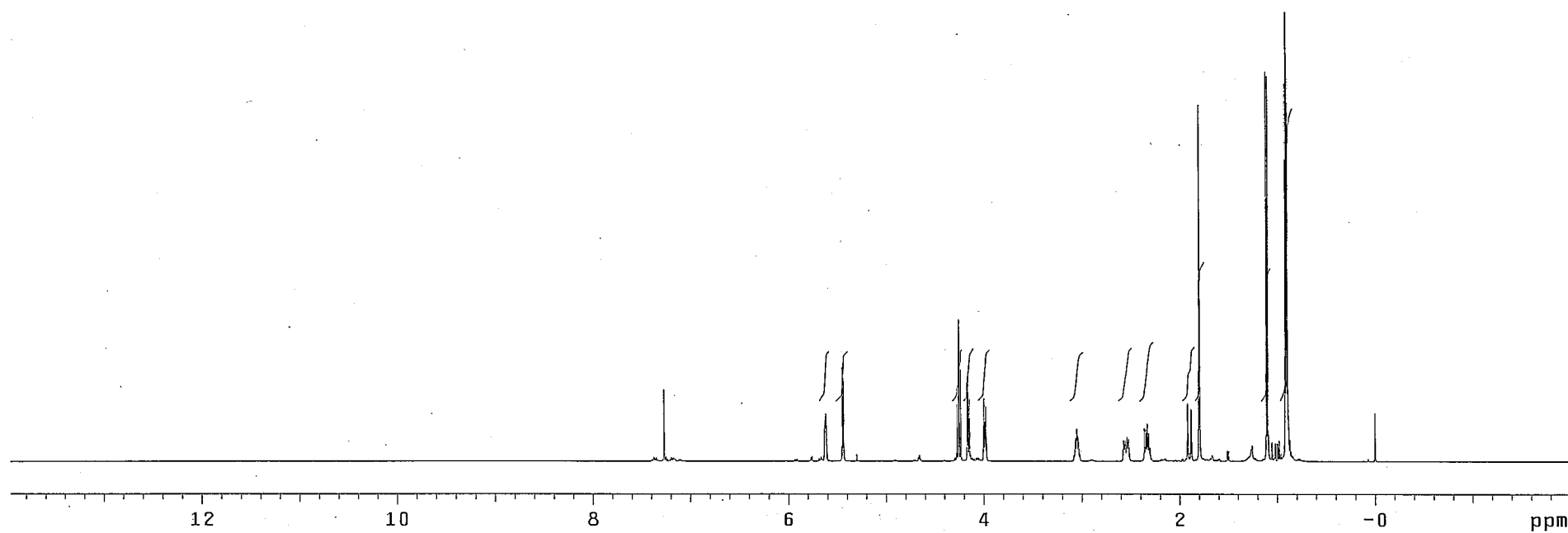


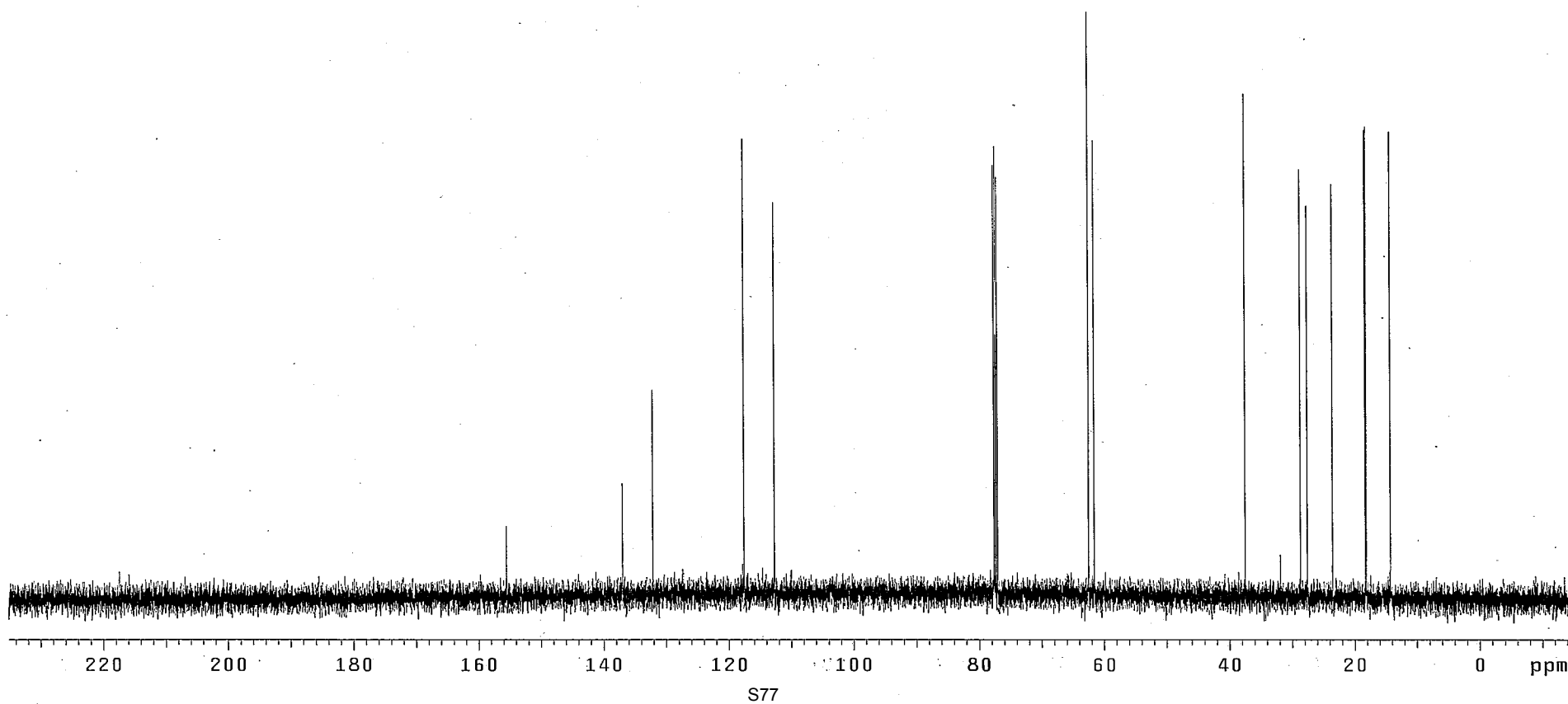
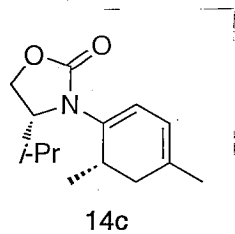
14b

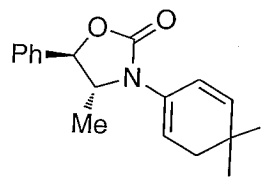




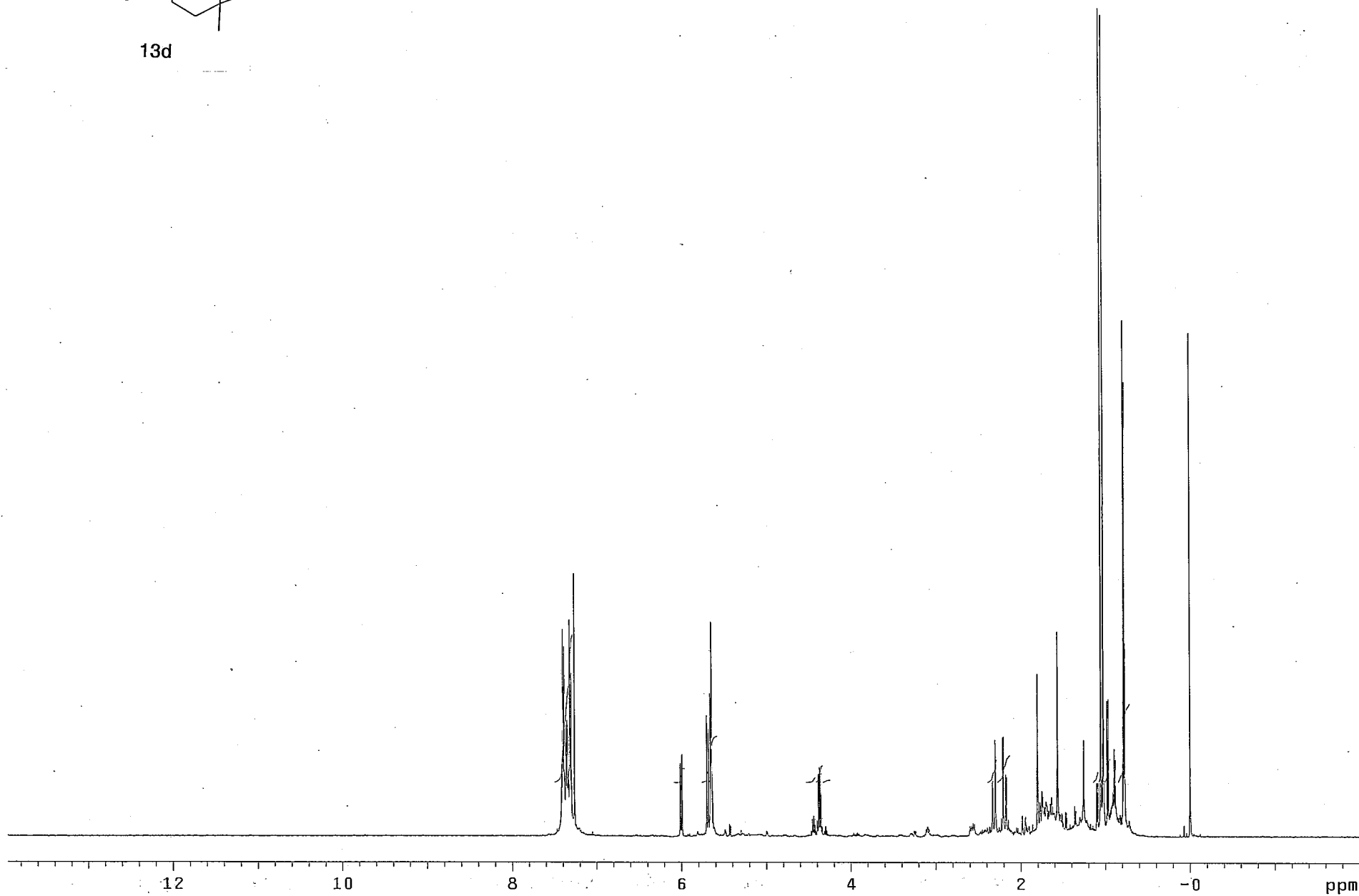
14c

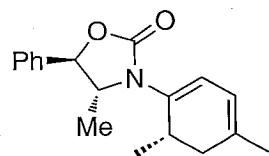




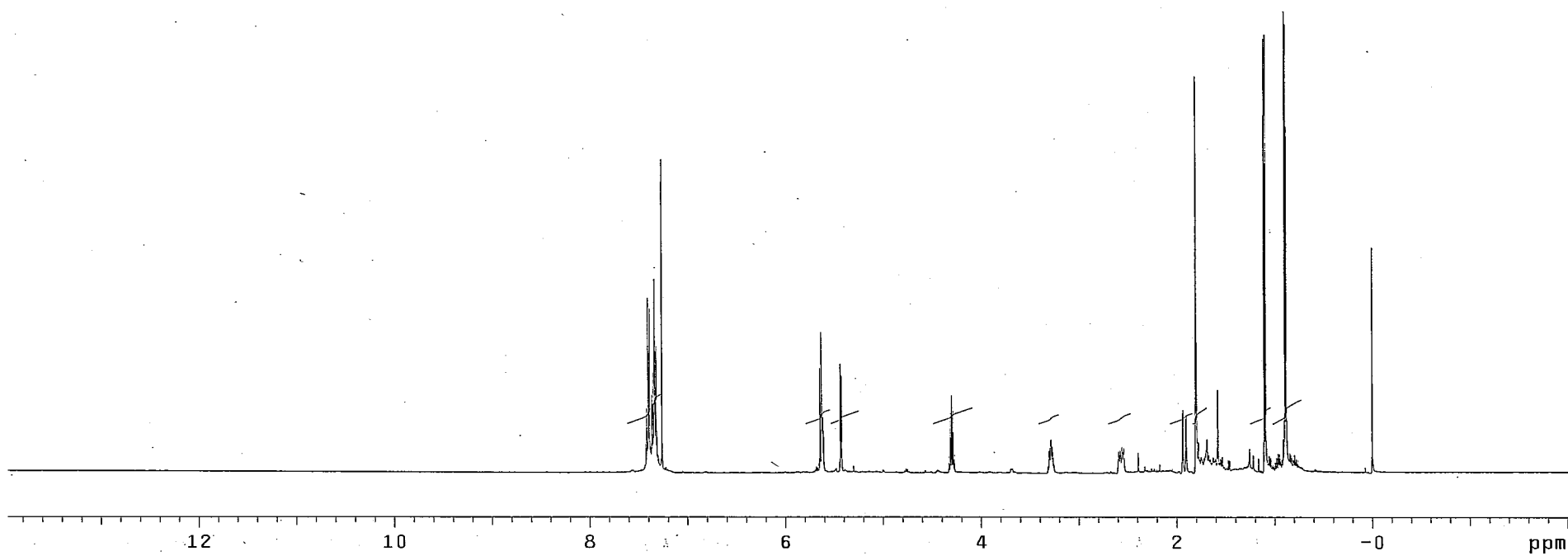


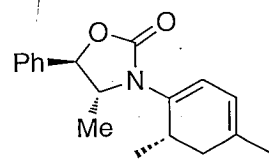
13d



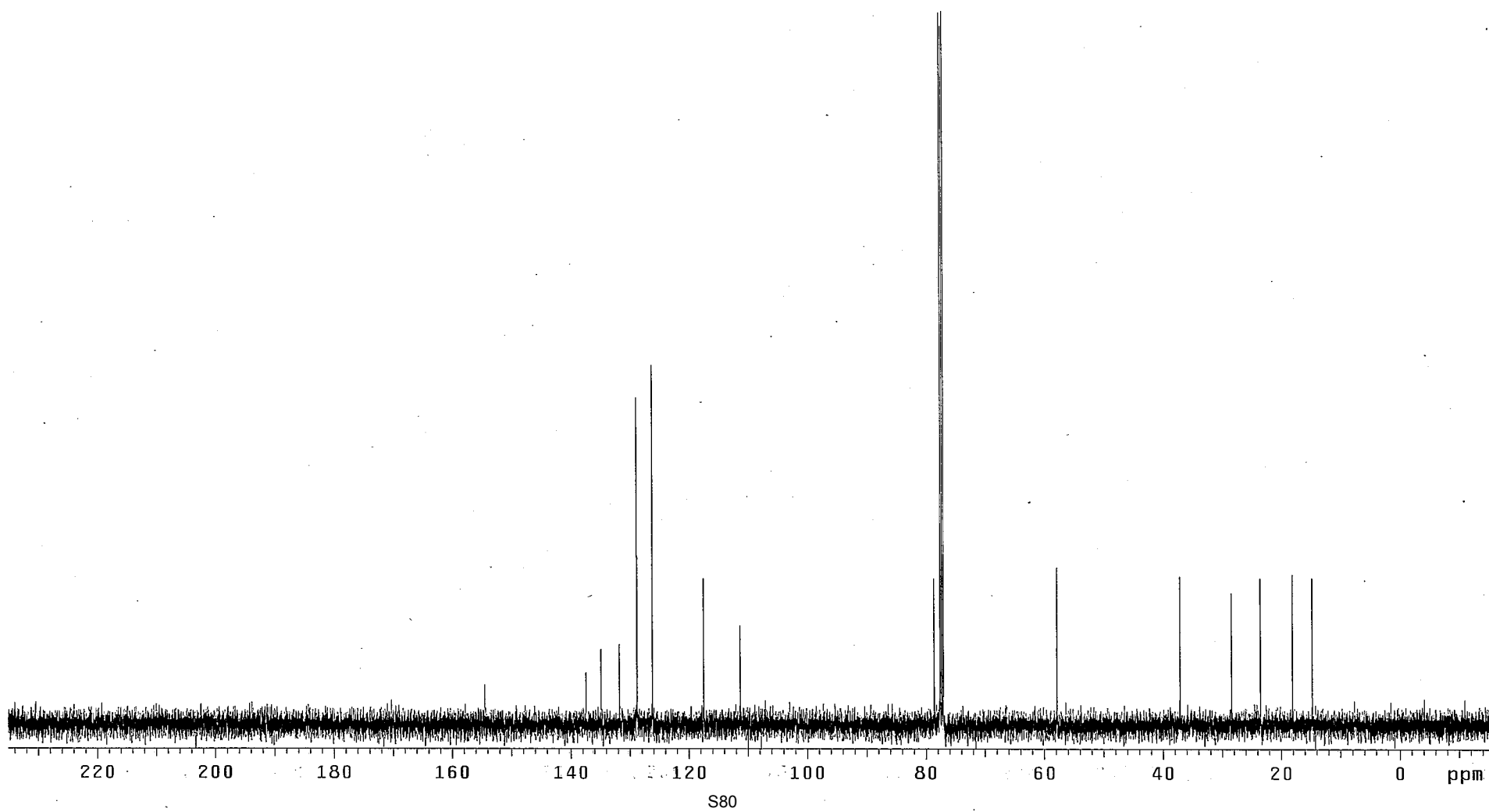


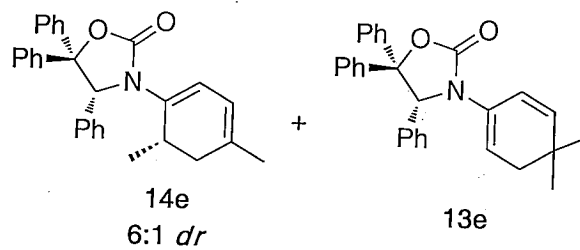
14d



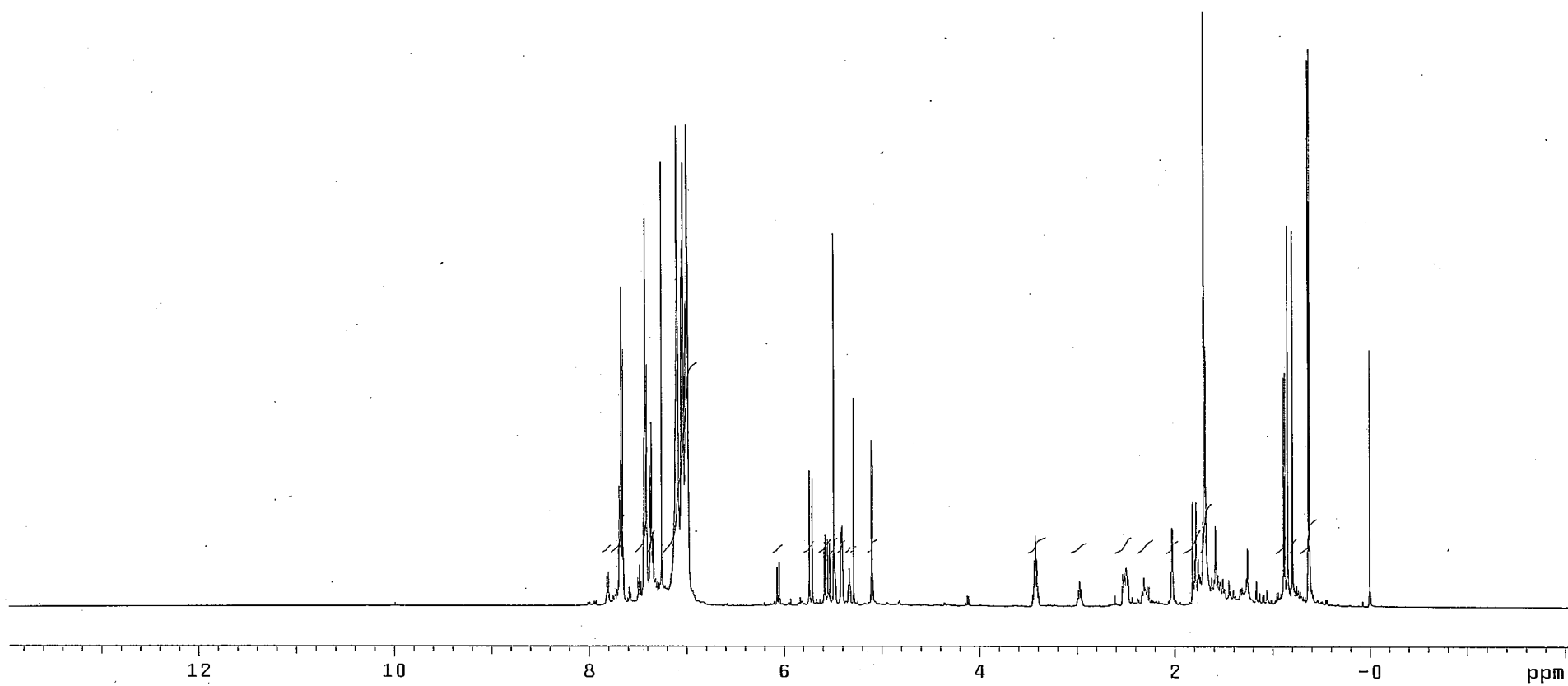


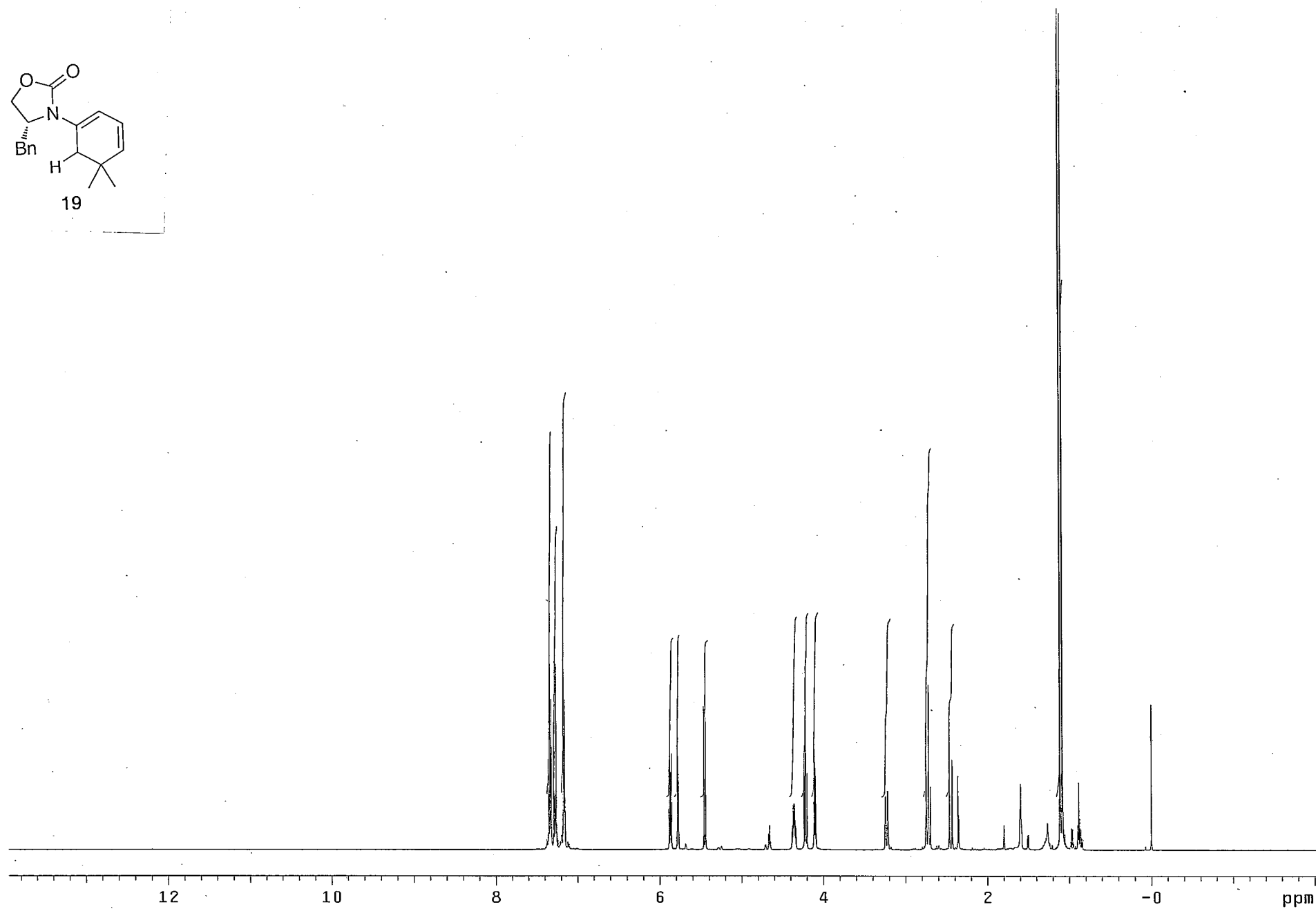
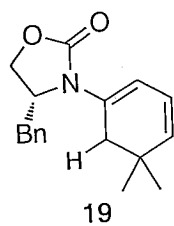
14d

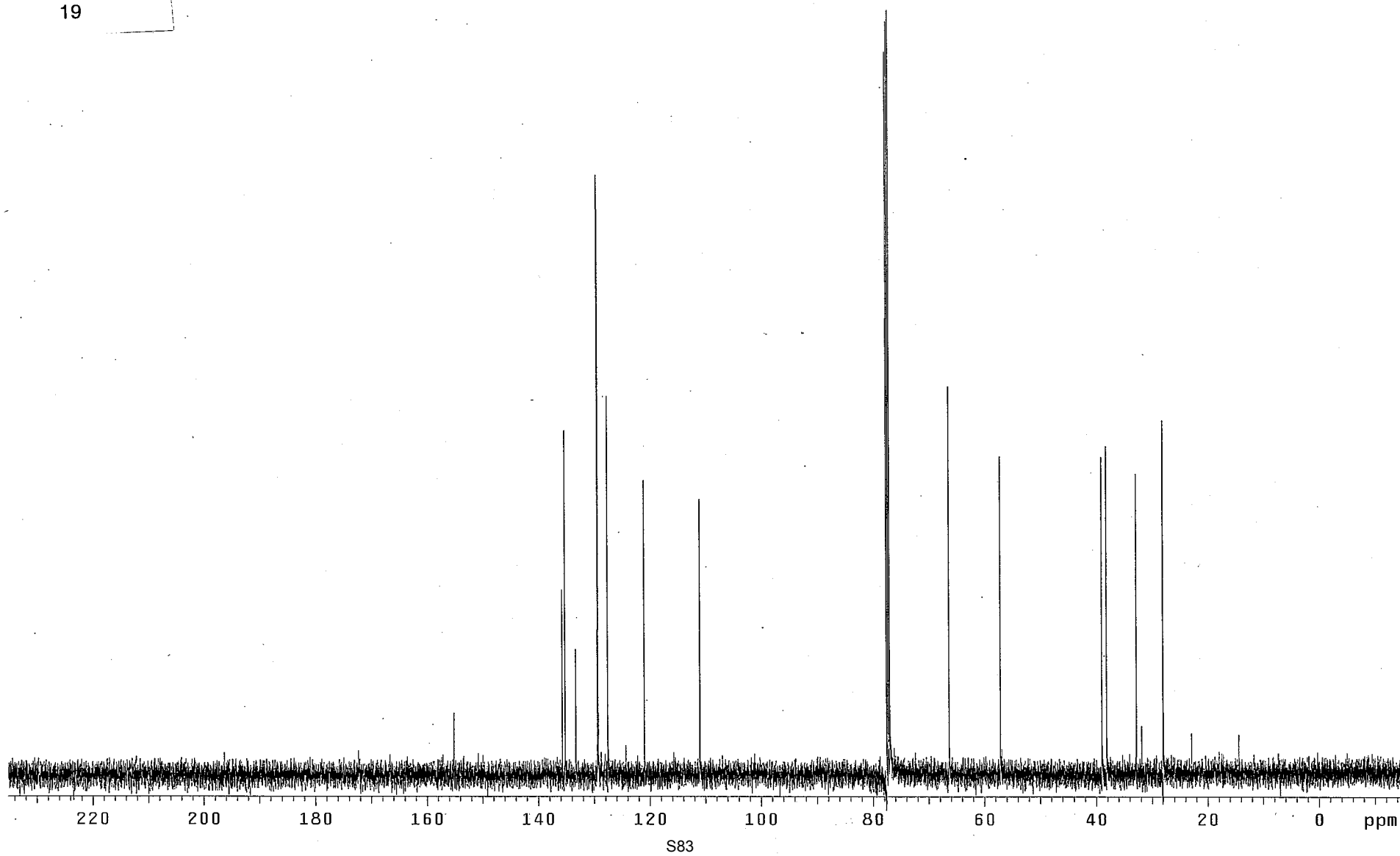
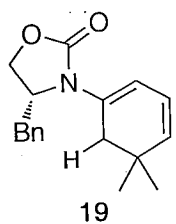


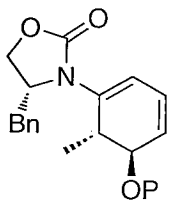


3 : 1
 14e : 13e

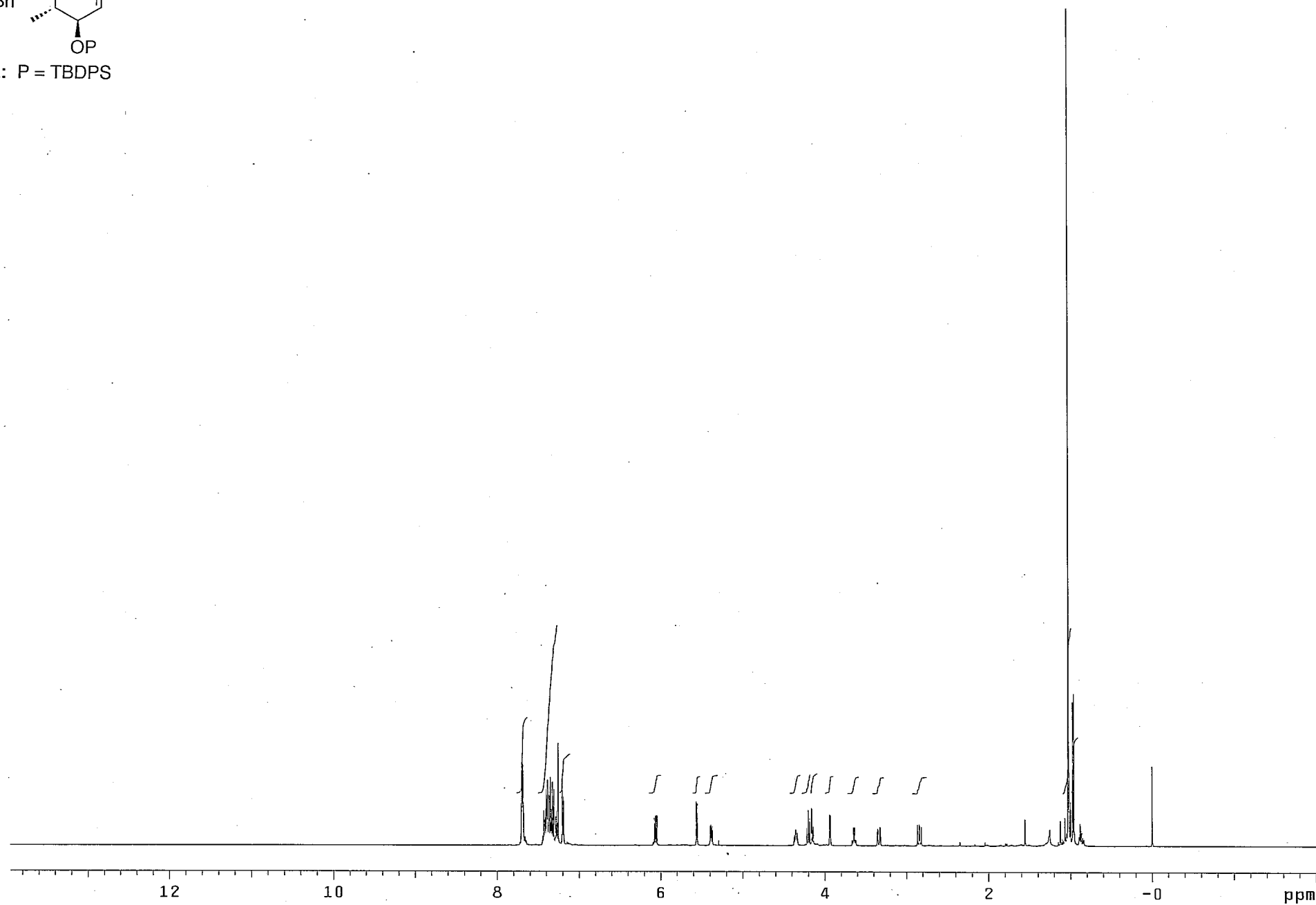








22: P = TBDPS



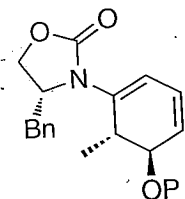
RH-2-148COSY_03Apr2009

Archive directory: /export/home/ryuji/vnmrsys/data
Sample directory: RH-2-148COSY_03Apr2009

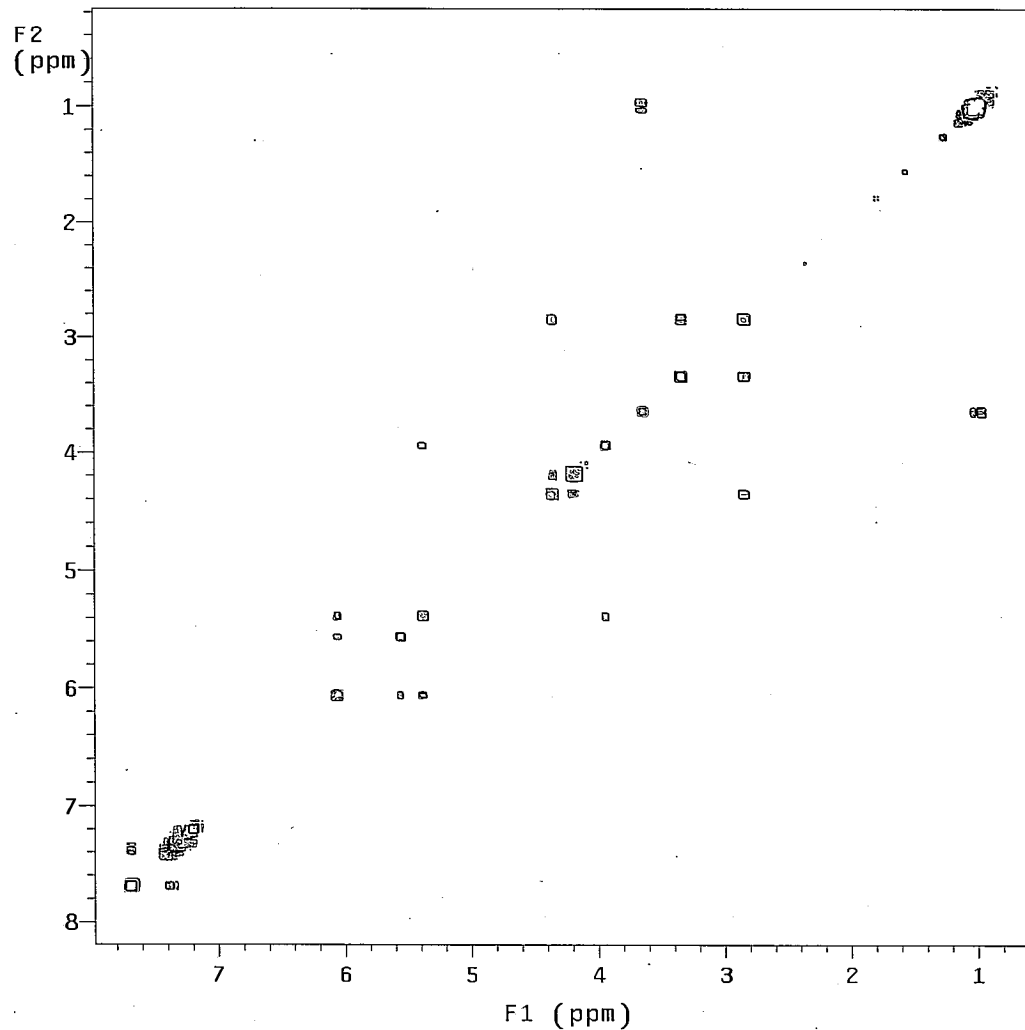
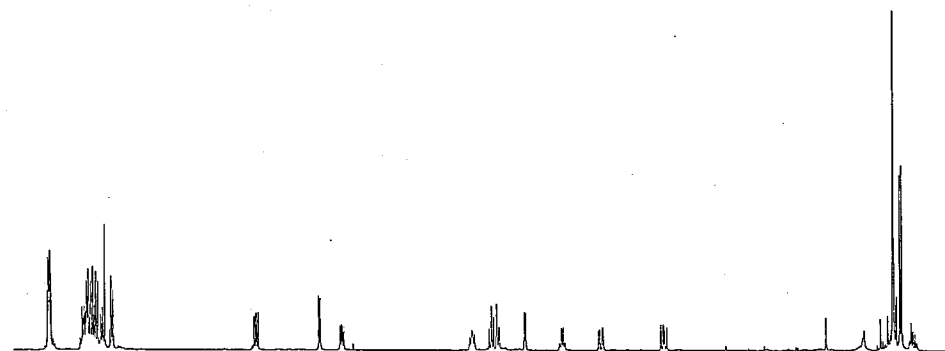
Pulse Sequence: gCOSY

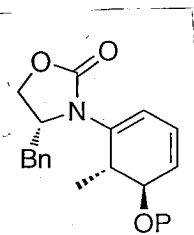
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

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, 499.7288200 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

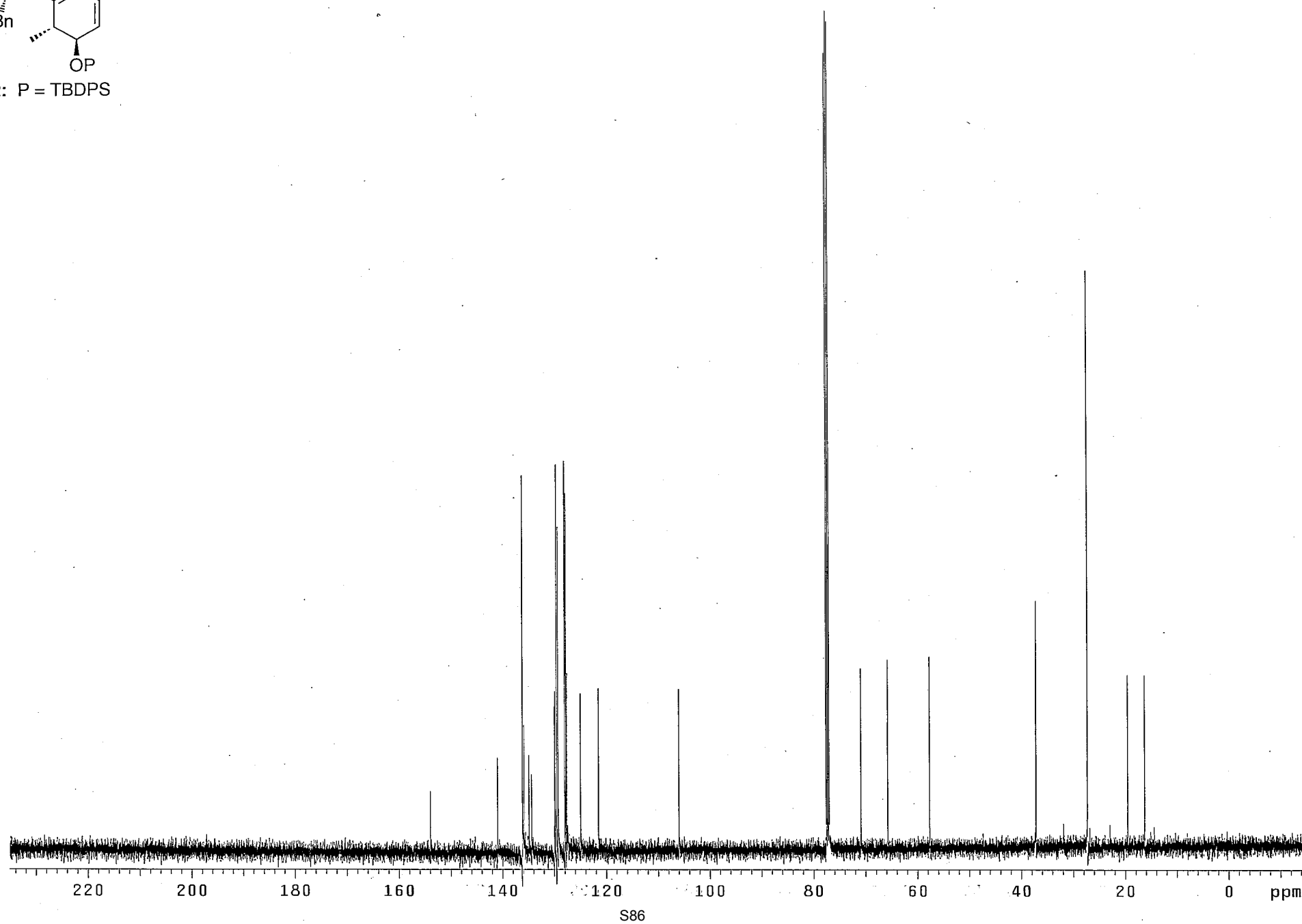


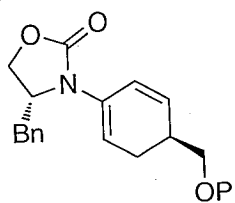
22: P = TBDPS



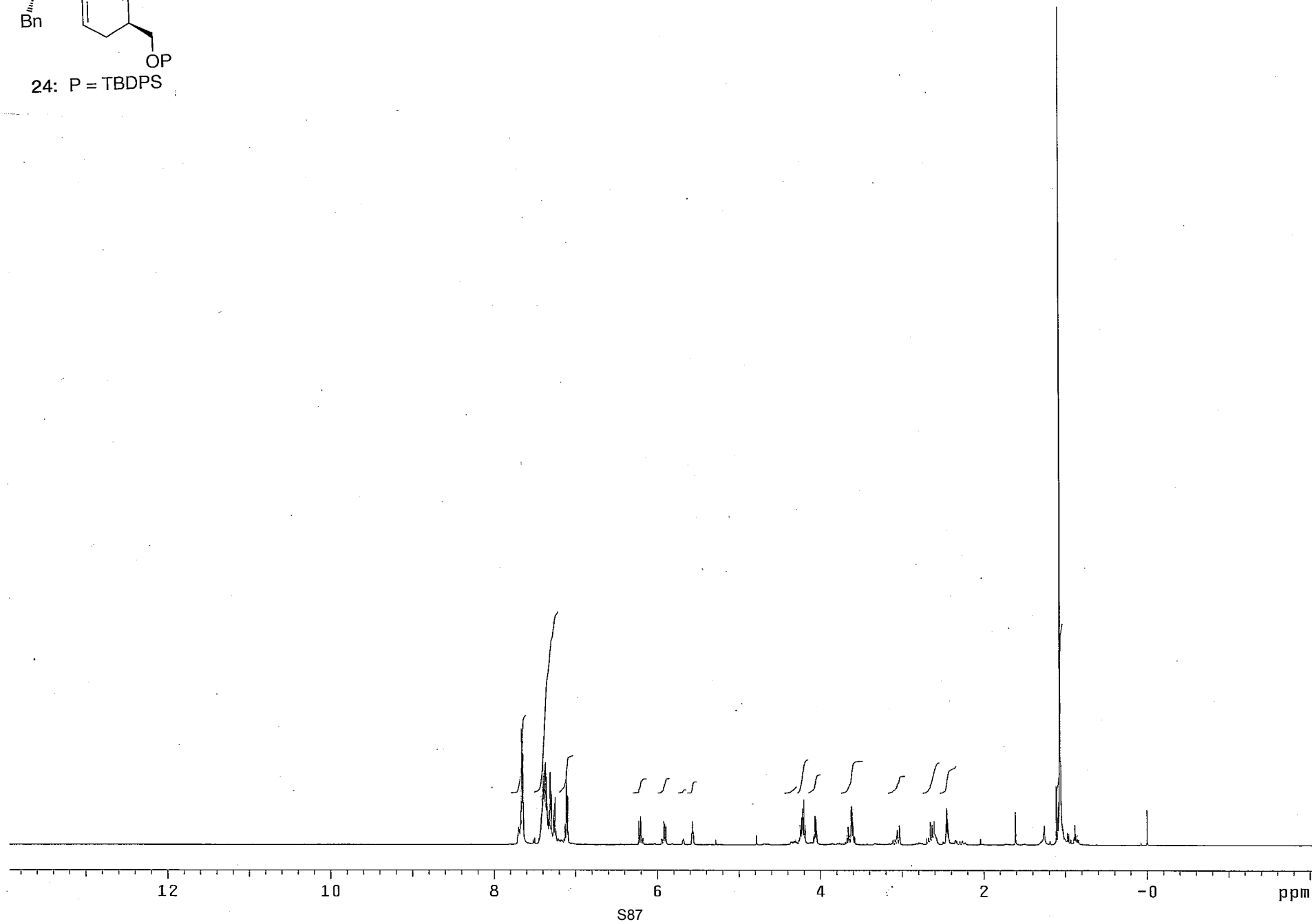


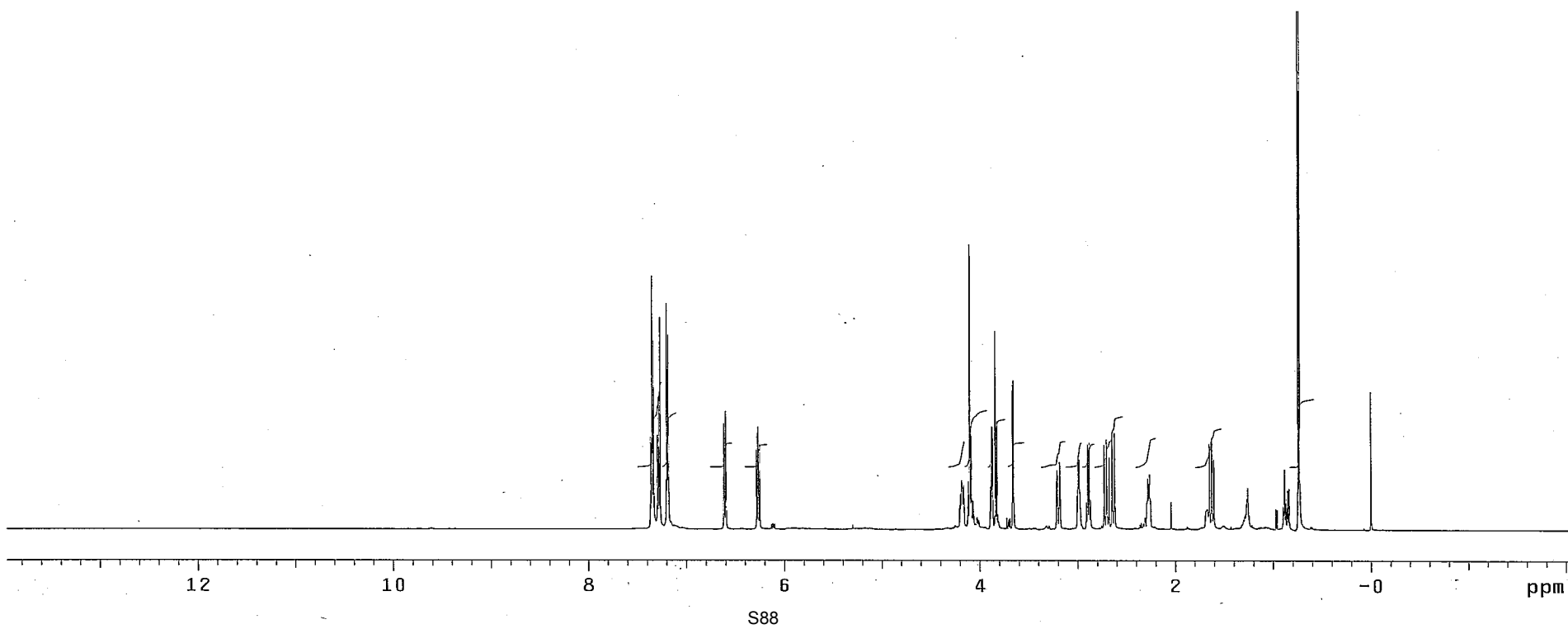
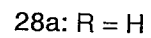
22: P = TBDPS





24: P = TBDPS





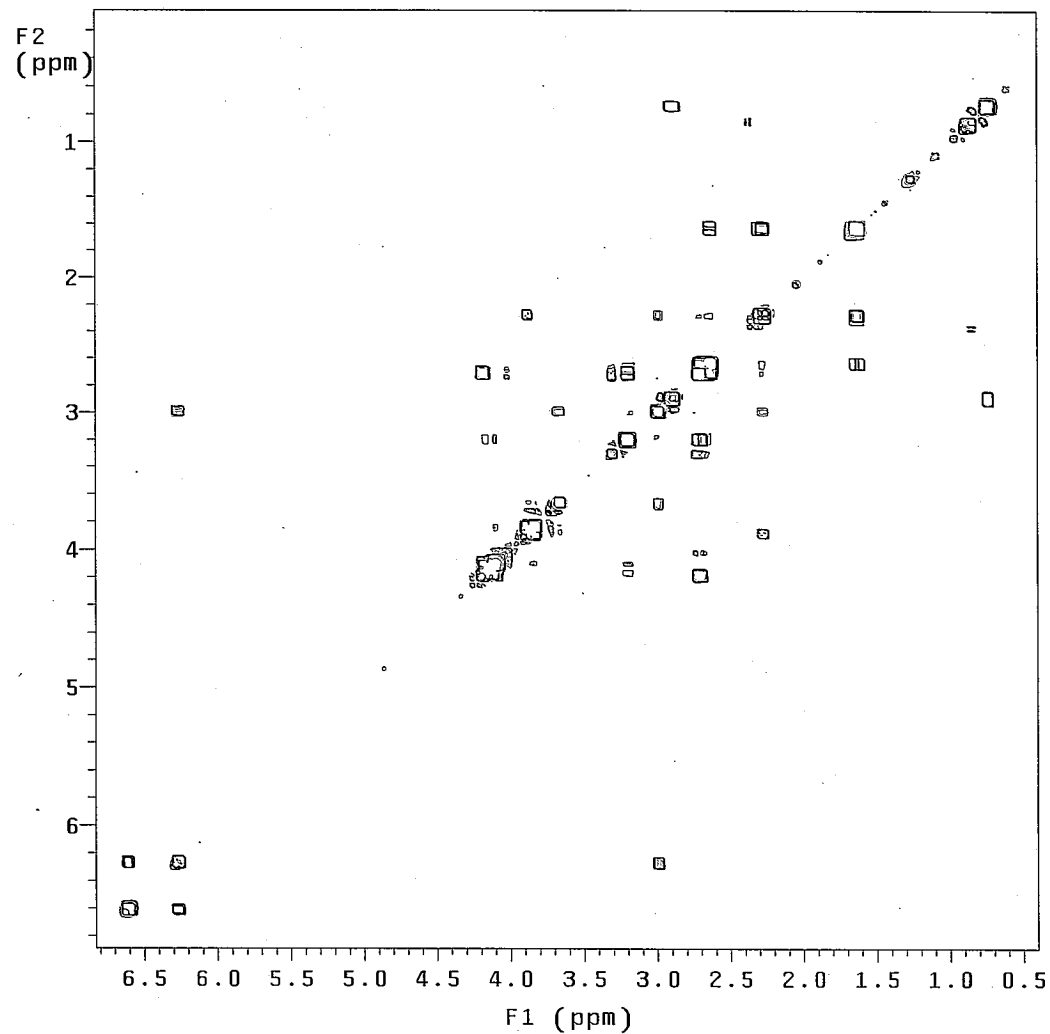
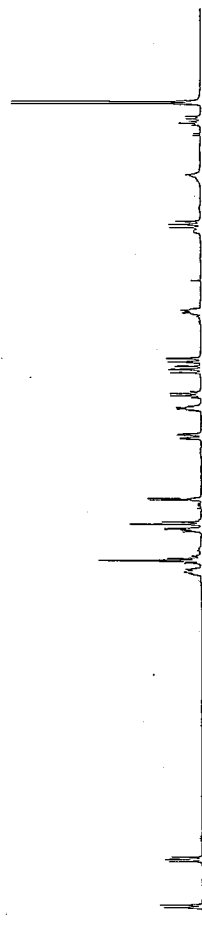
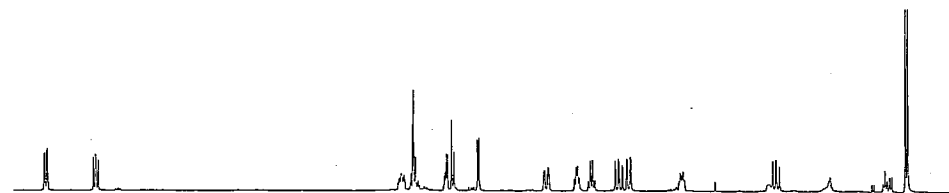
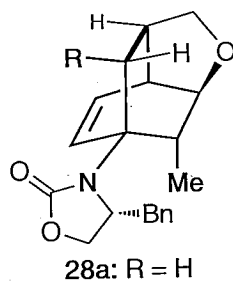
RH-2-228COSY_13May2009

Archive directory: /export/home/ryuji/vnmrsys/data
Sample directory: RH-2-228COSY_13May2009

Pulse Sequence: gCOSY

Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: gCOSY
INNOVA-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, 499.7288156 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



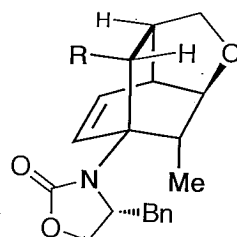
RH-2-228SINOESY-1_05Jun2009

Archive directory: /export/home/ryuji/vnmrsys/data
Sample directory: RH-2-228SINOESY-1_05Jun2009

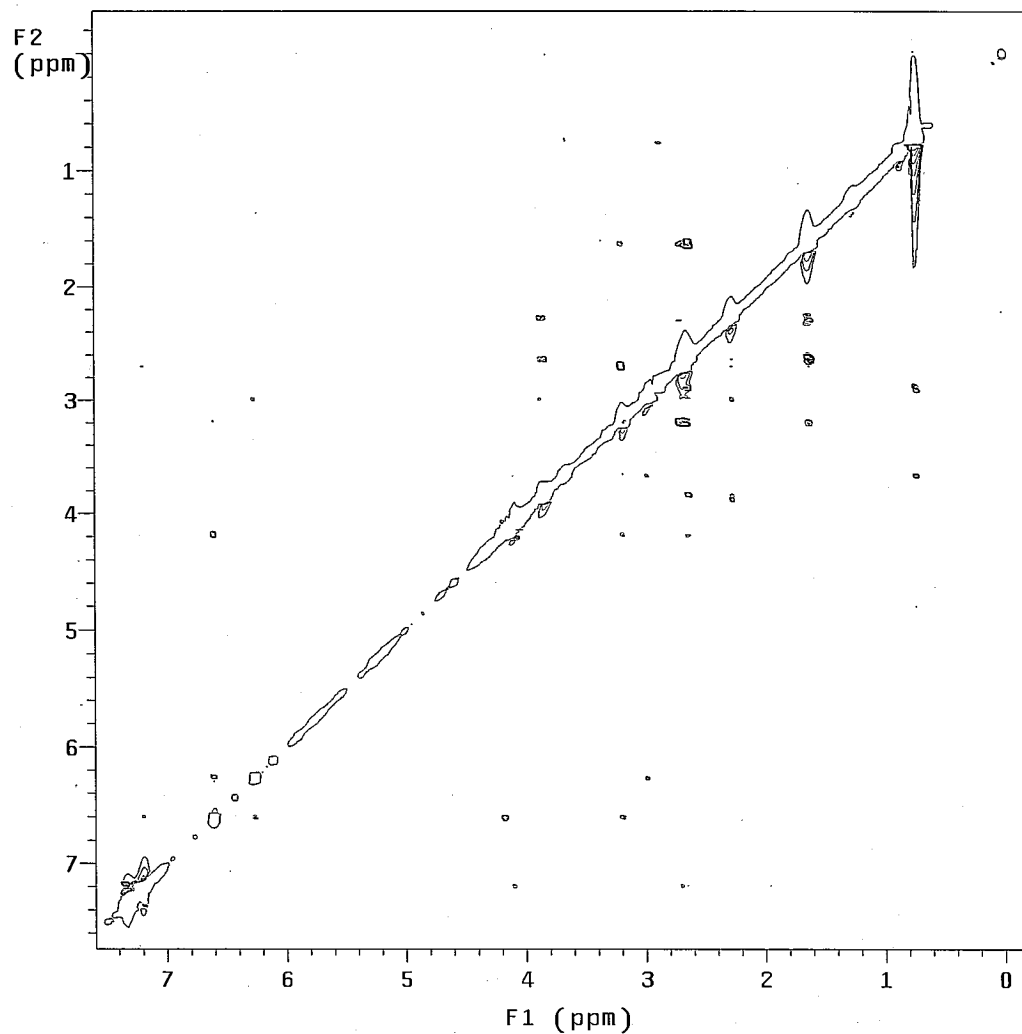
Pulse Sequence: NOESY

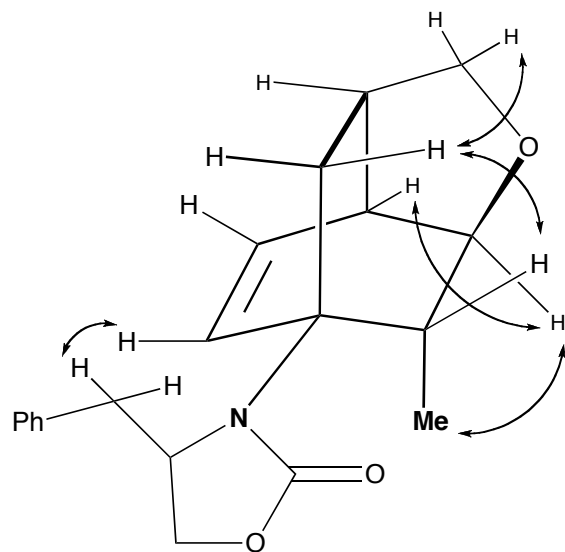
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
File: NOESY
INOVA-500 "nmr03"

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, 499.7288156 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, 32 min, 51 sec

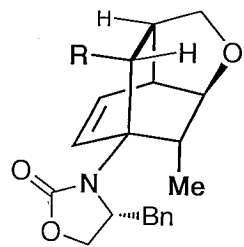


28a: R = H

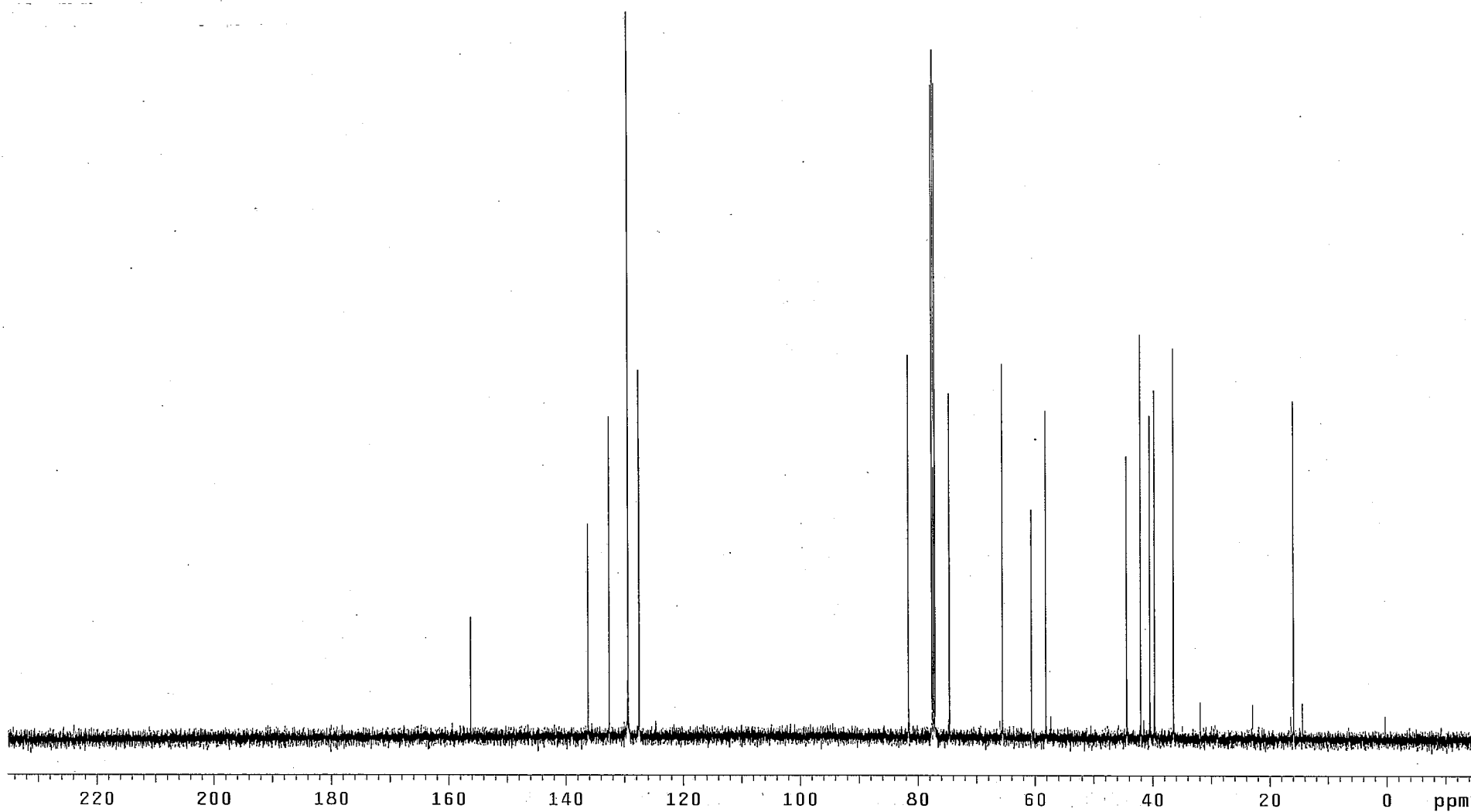


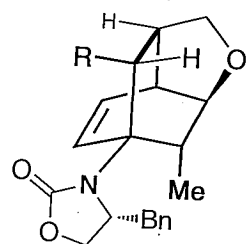


The key nOe

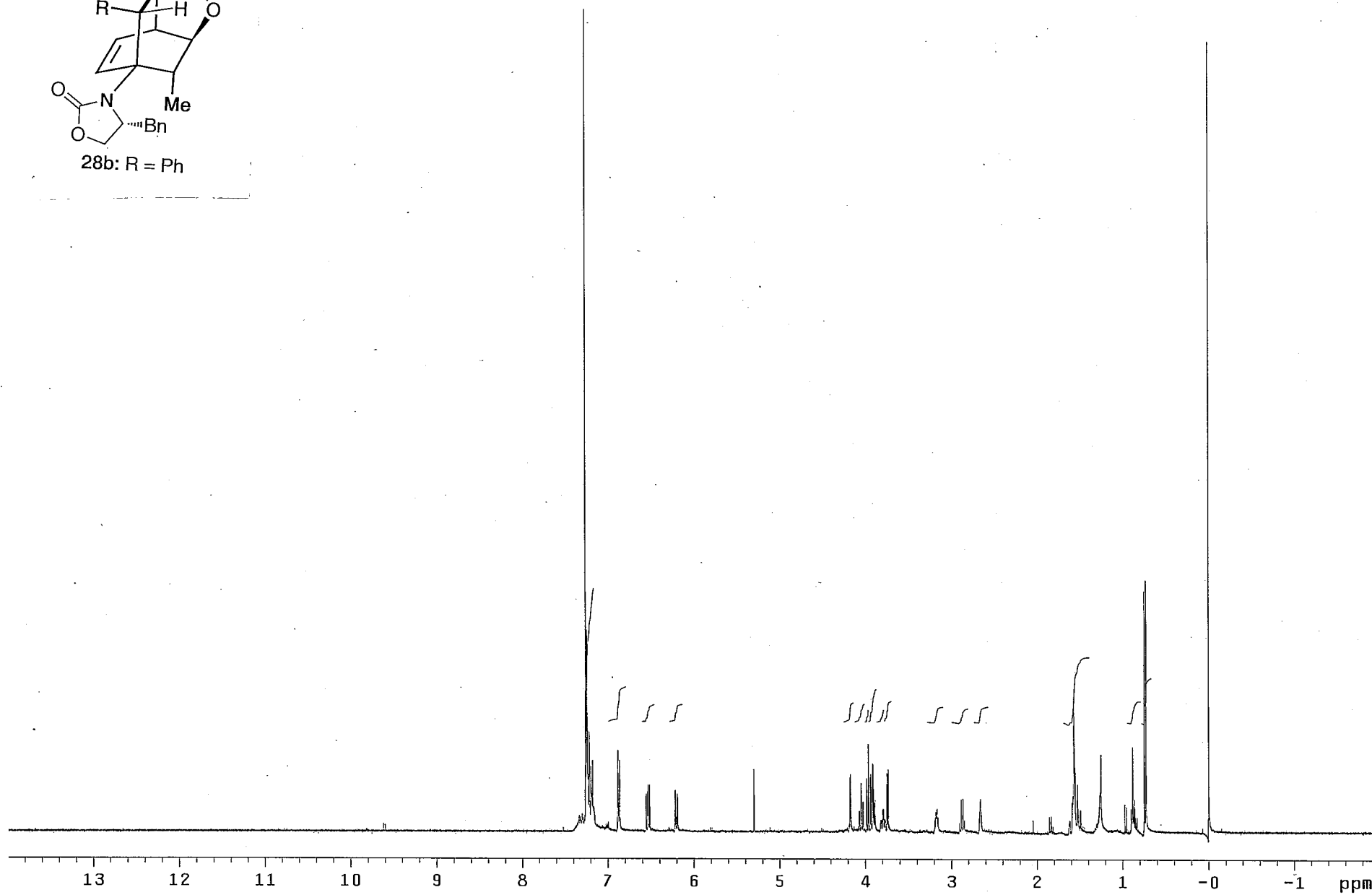


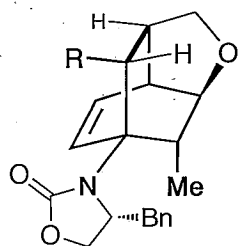
28a: R = H



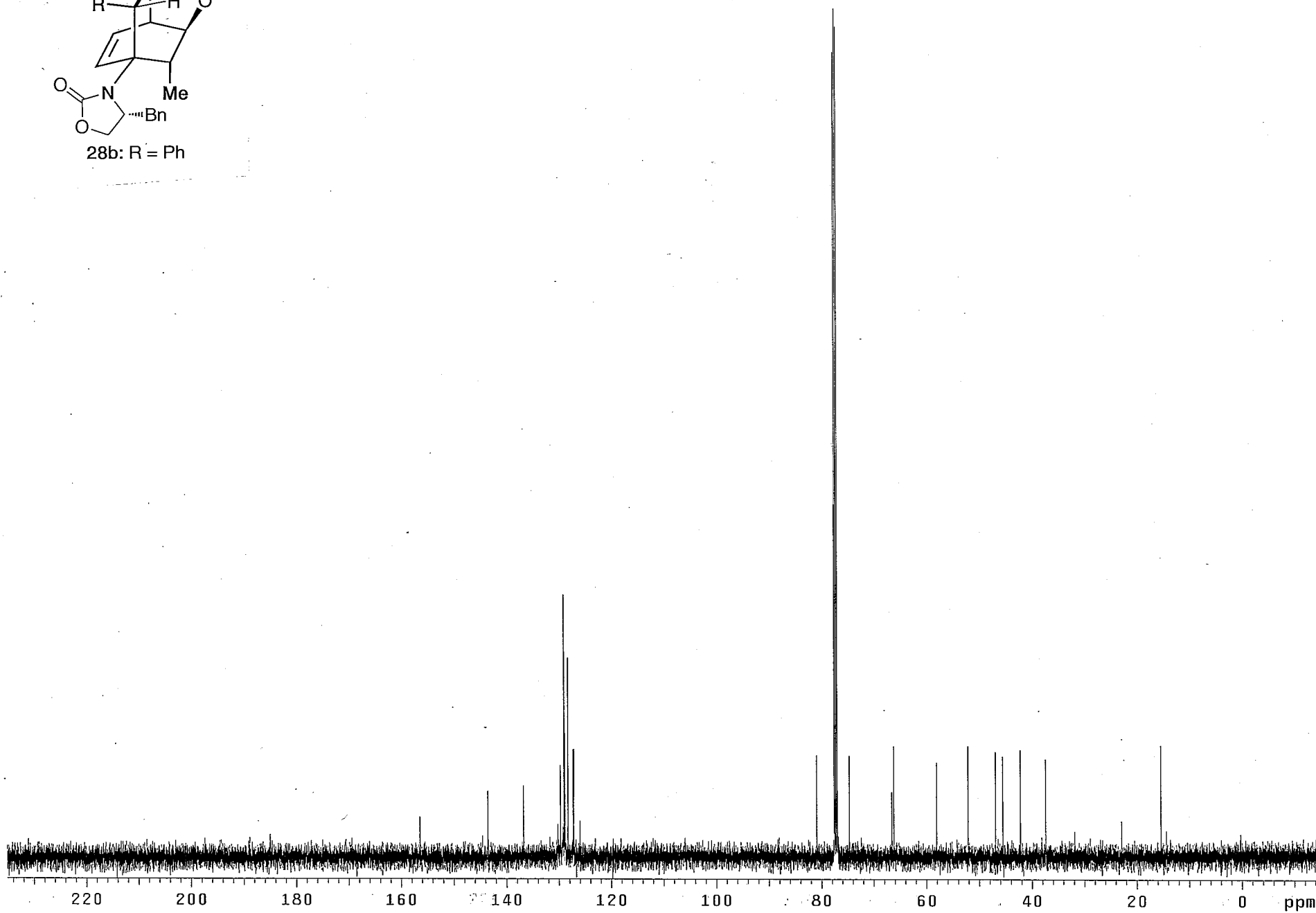


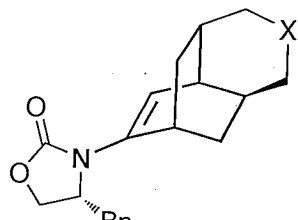
28b: R = Ph



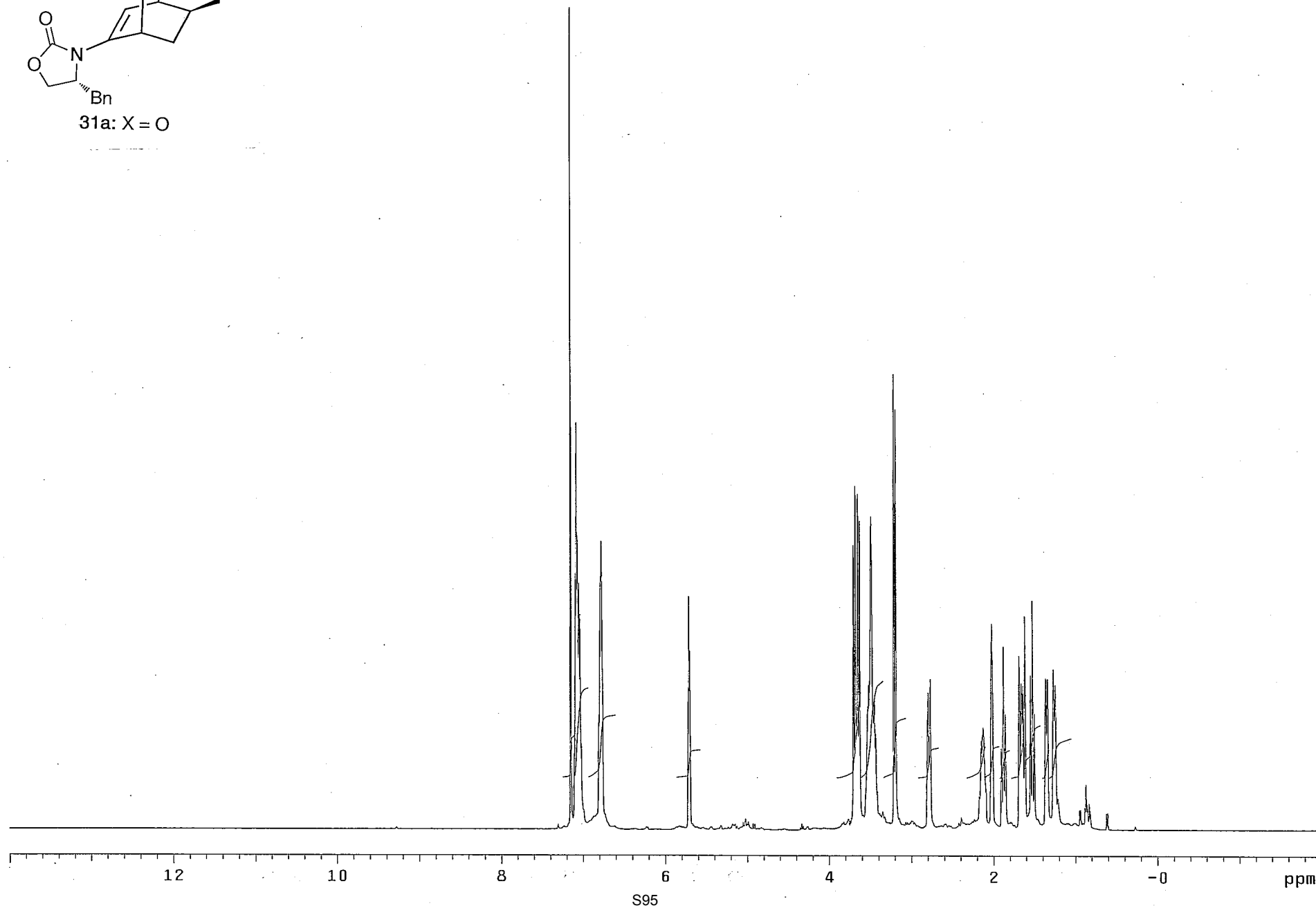


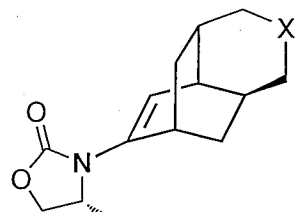
28b: R = Ph



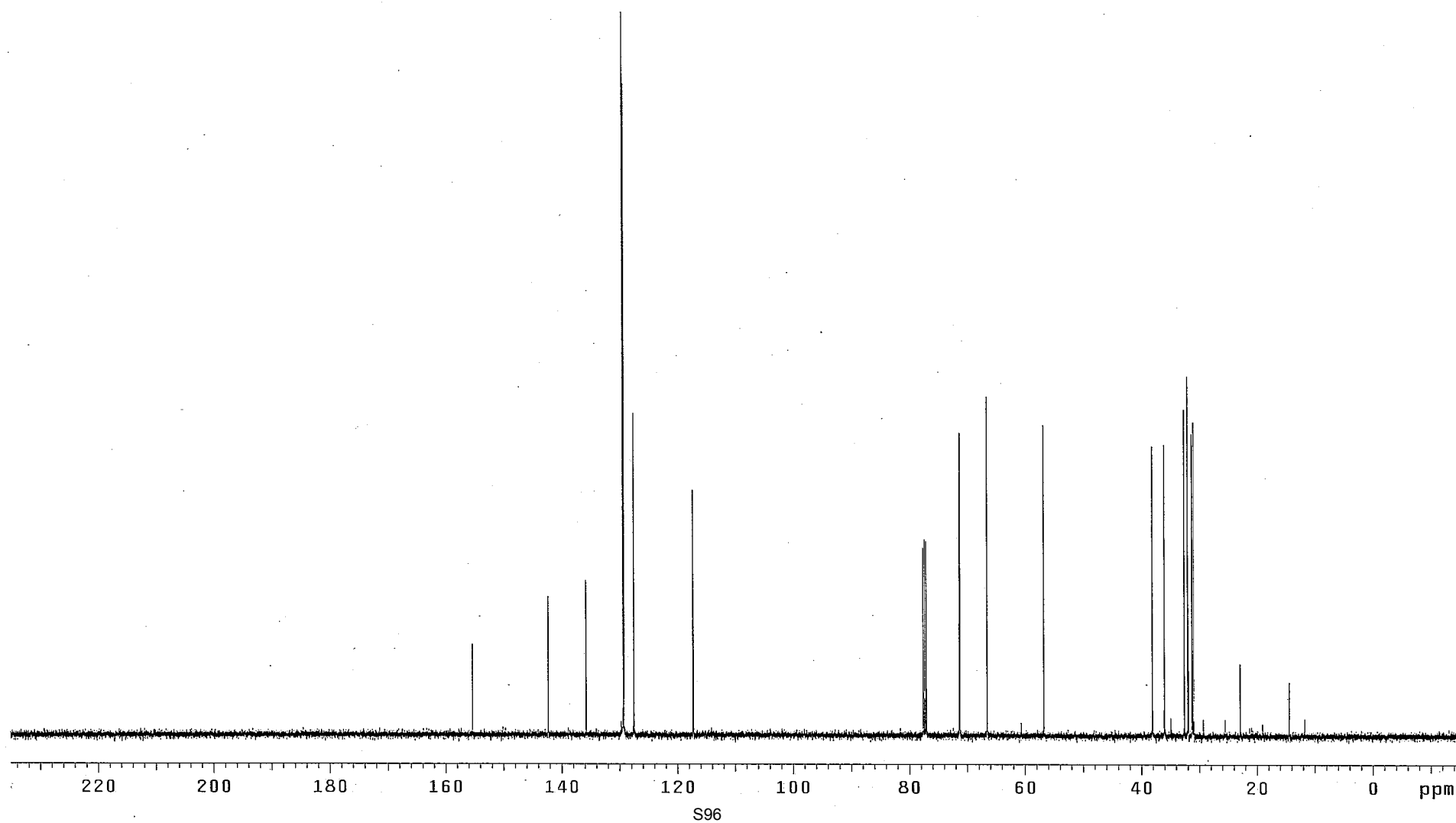


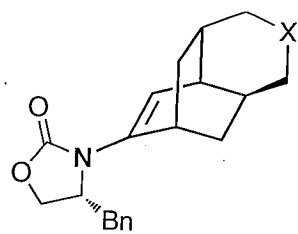
31a: X = O



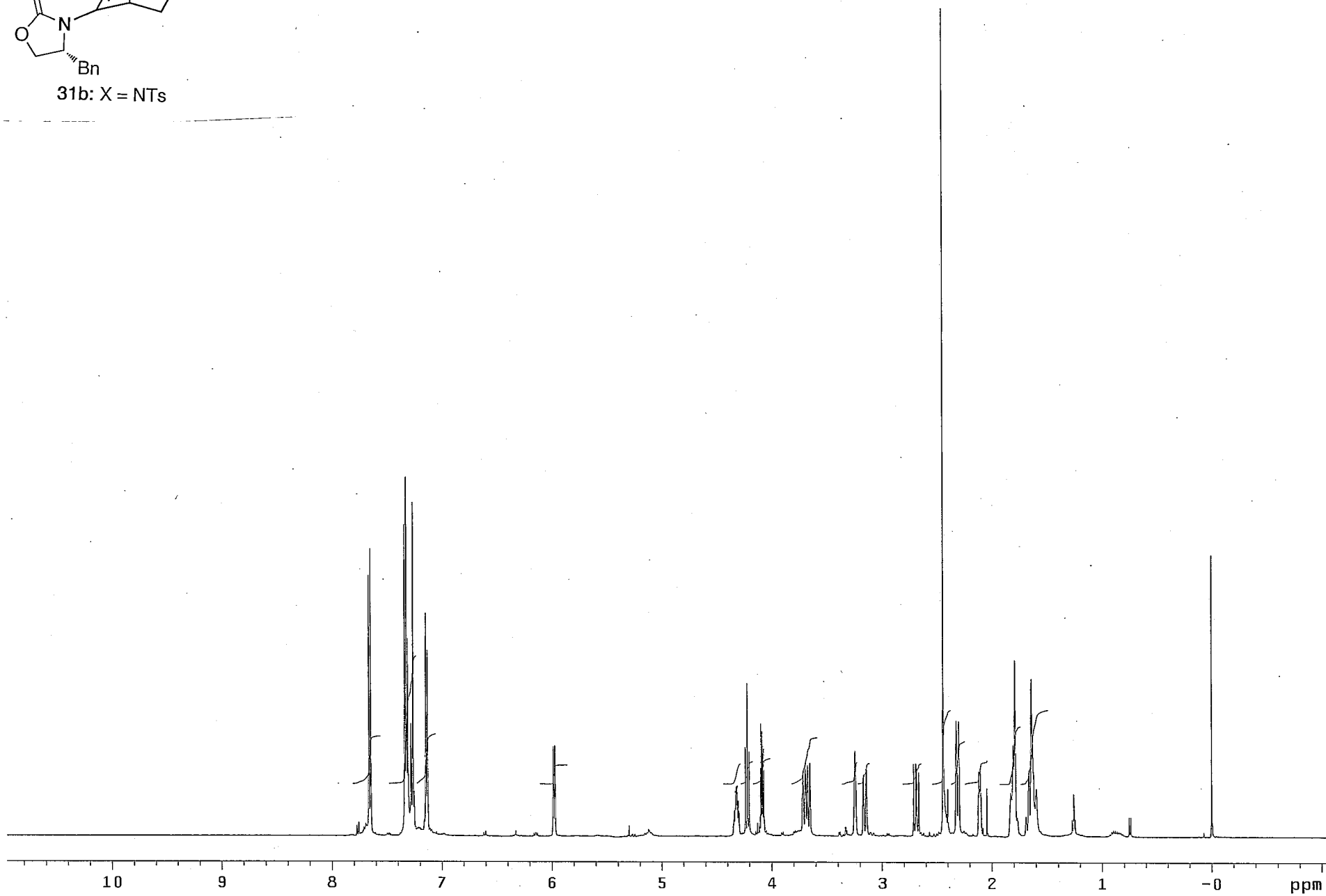


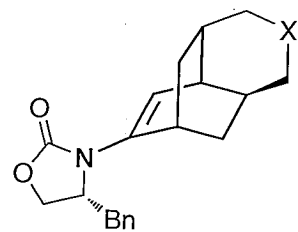
31a: X = O





31b: X = NTs





31b: X = NTs

