

SUPPORTING INFORMATION

PROTON NMR AND SELECTED CARBON NMR SPECTRA

for the
communication
entitled

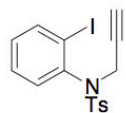
**An Approach to Cyclohepta[b]indoles Through
an Allenamide (4 + 3) Cycloaddition–Grignard Cyclization–Chugaev Elimination Sequence**

authored by

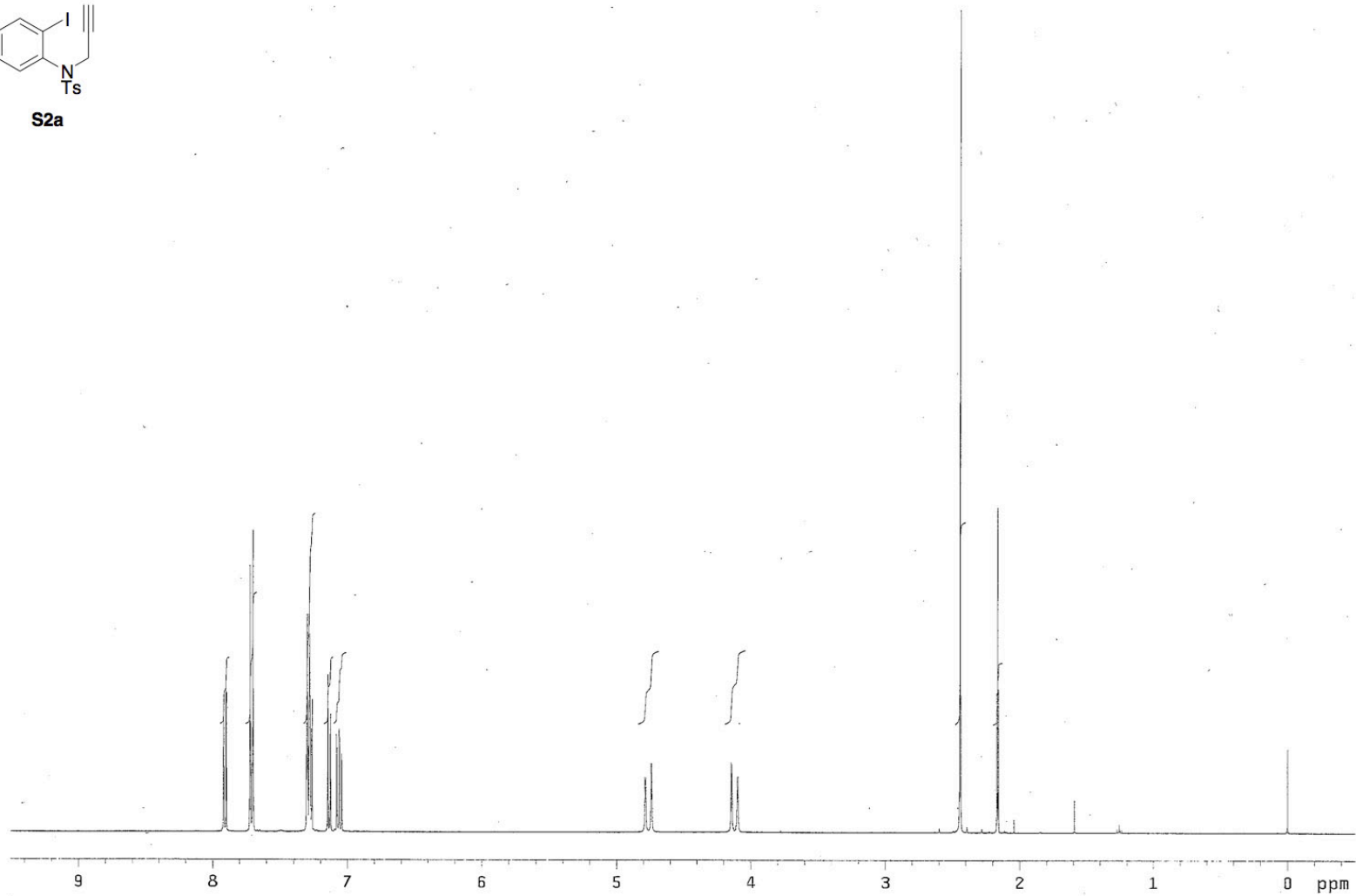
Shuzhong He, Richard P. Hsung,* William R. Presser, Zhi-Xiong Ma, and Bryan J. Haugen

*Division of Pharmaceutical Sciences, School of Pharmacy, and Department of Chemistry, University of Wisconsin,
Madison, WI 53705, United States*

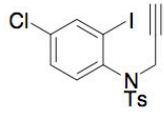
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Spectrometer: 399.79
Solvent: CDCl₃



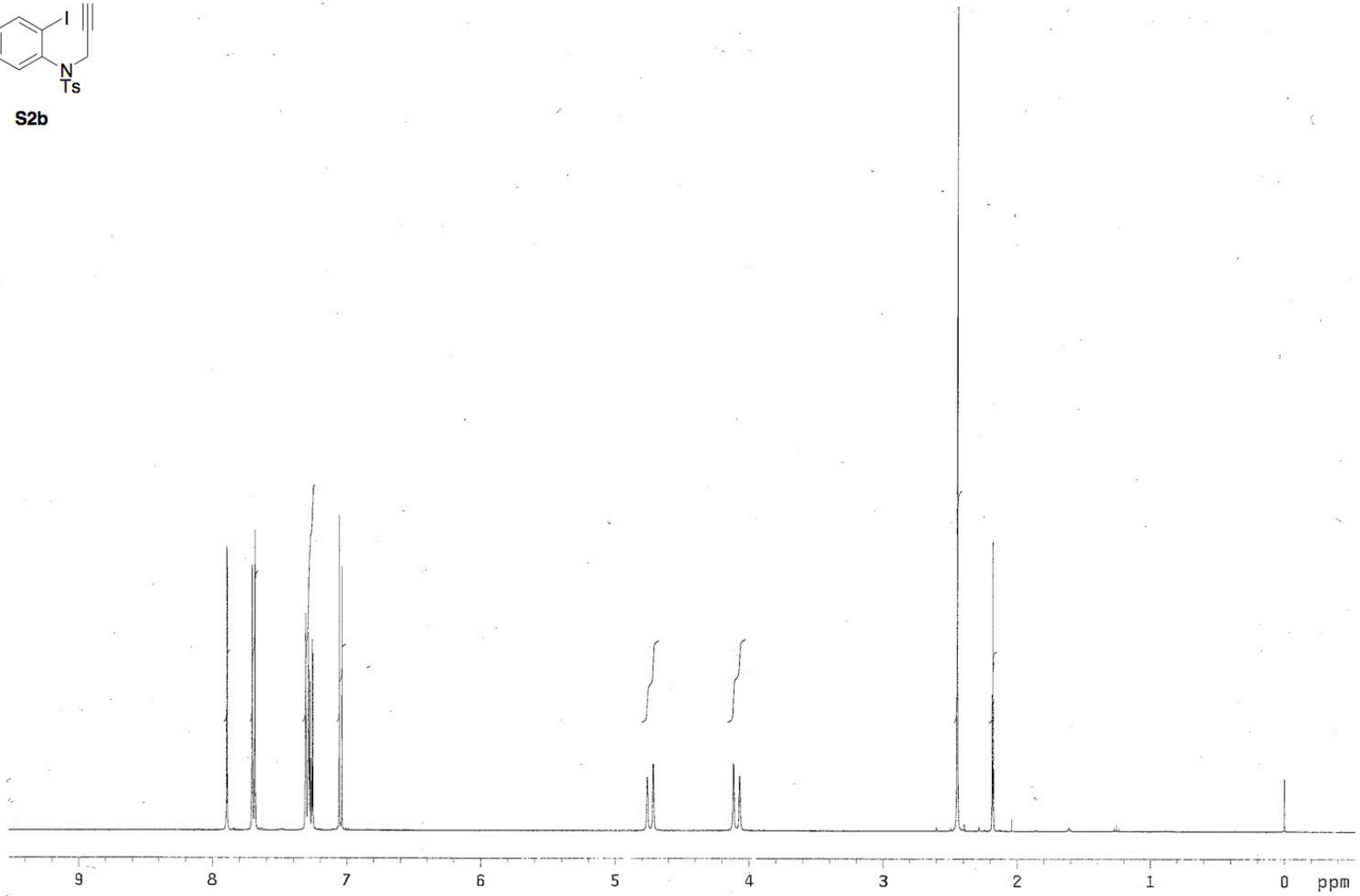
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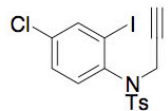
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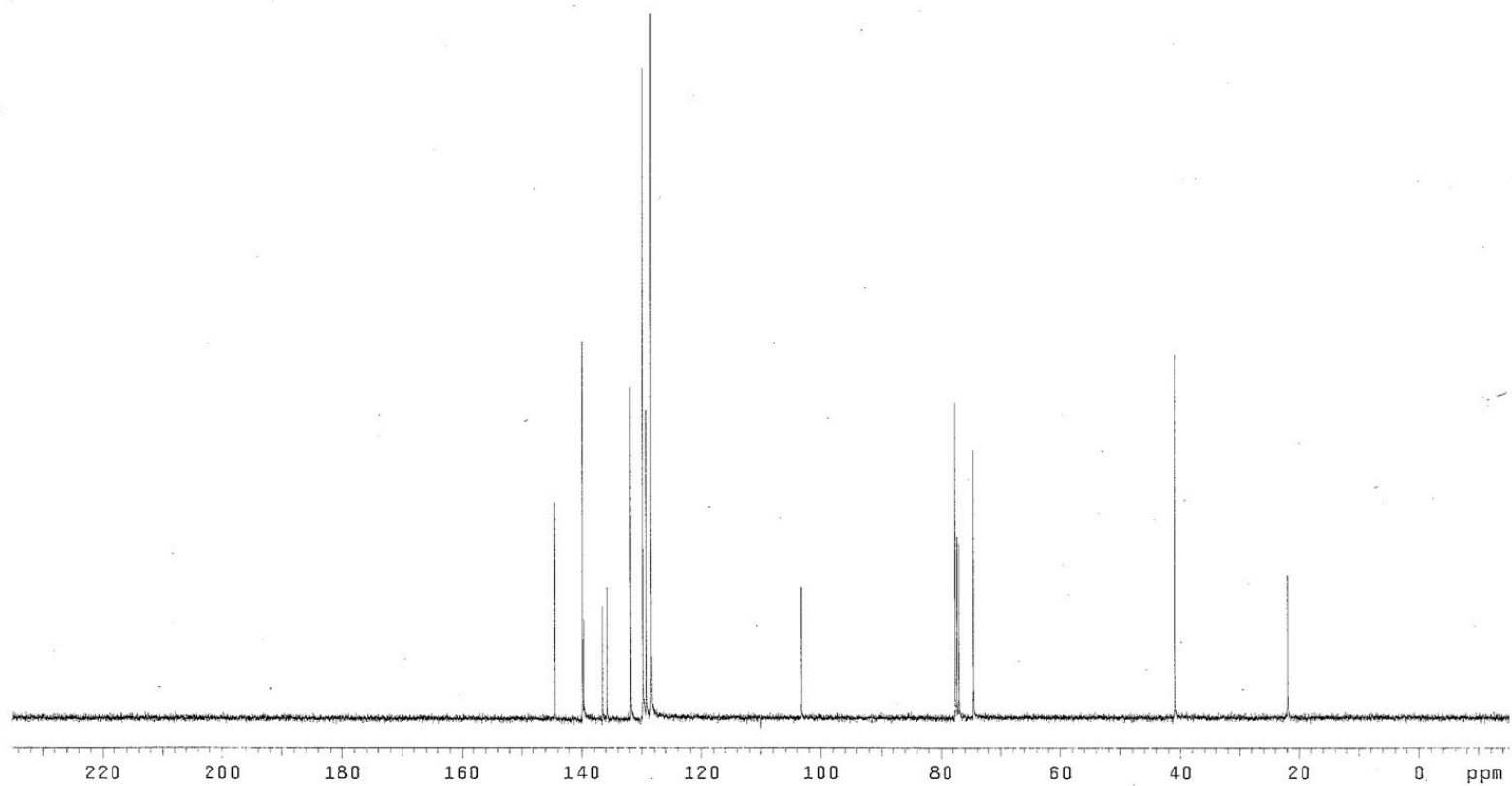
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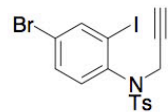
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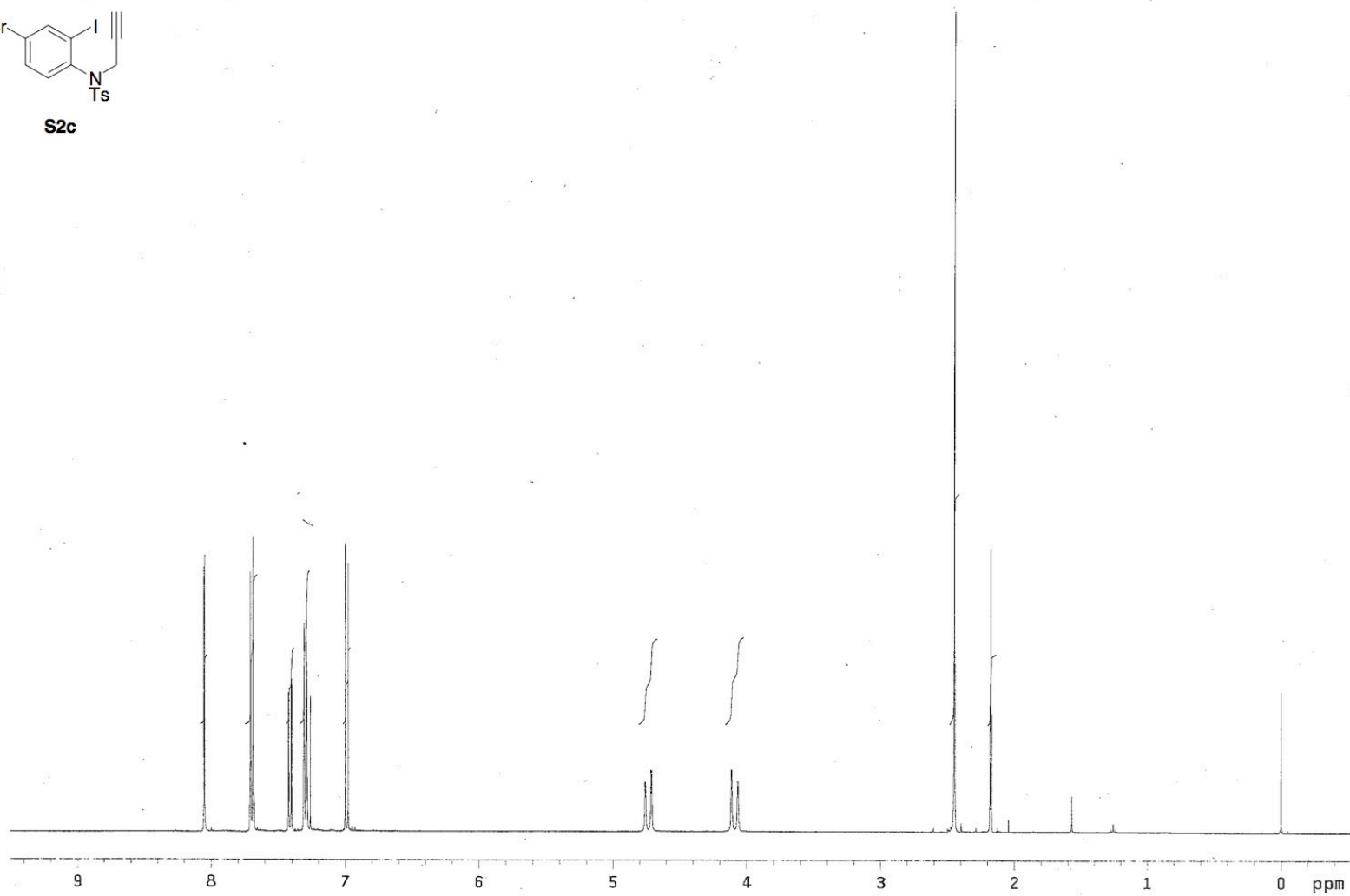
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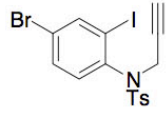
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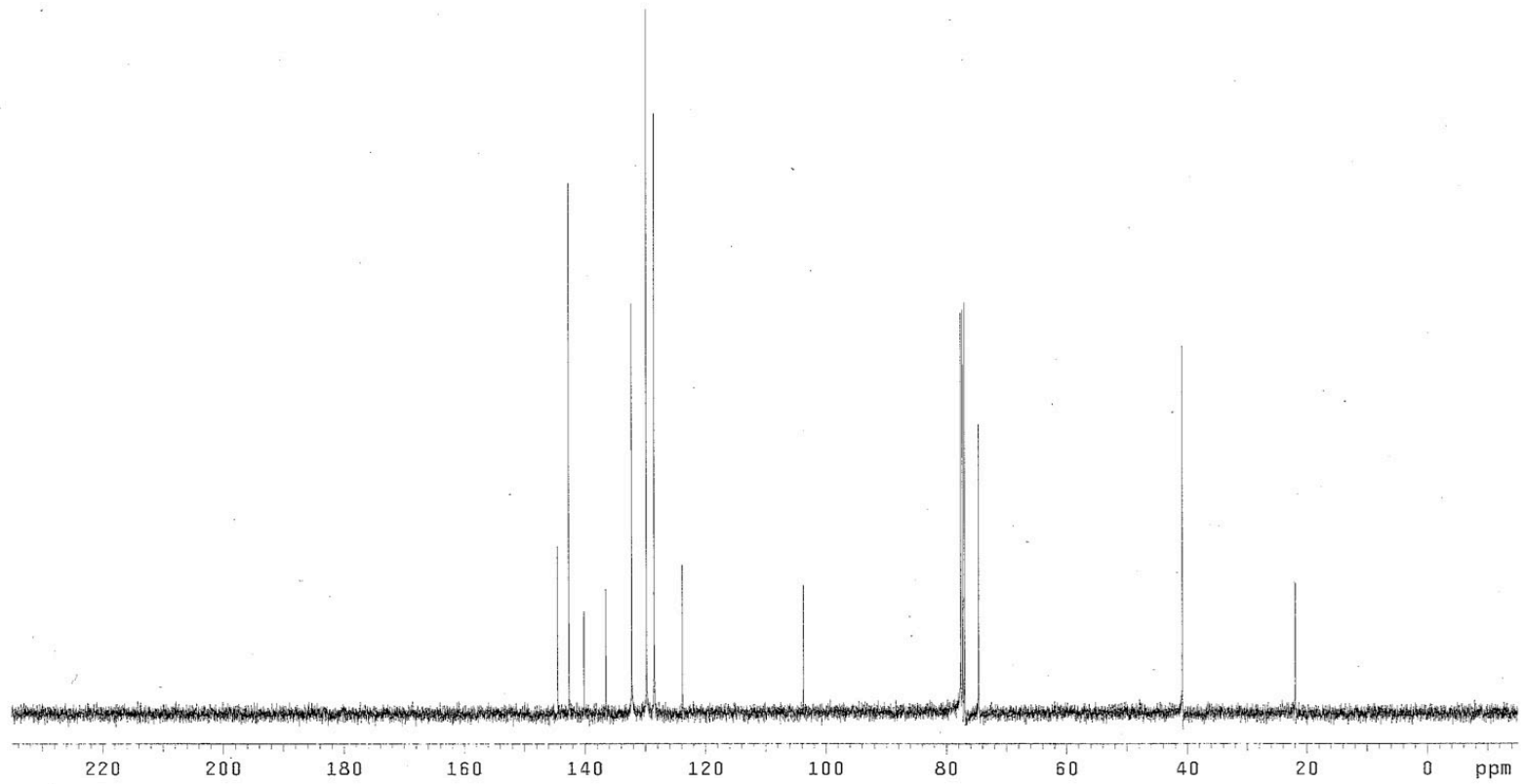
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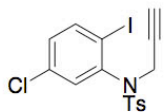
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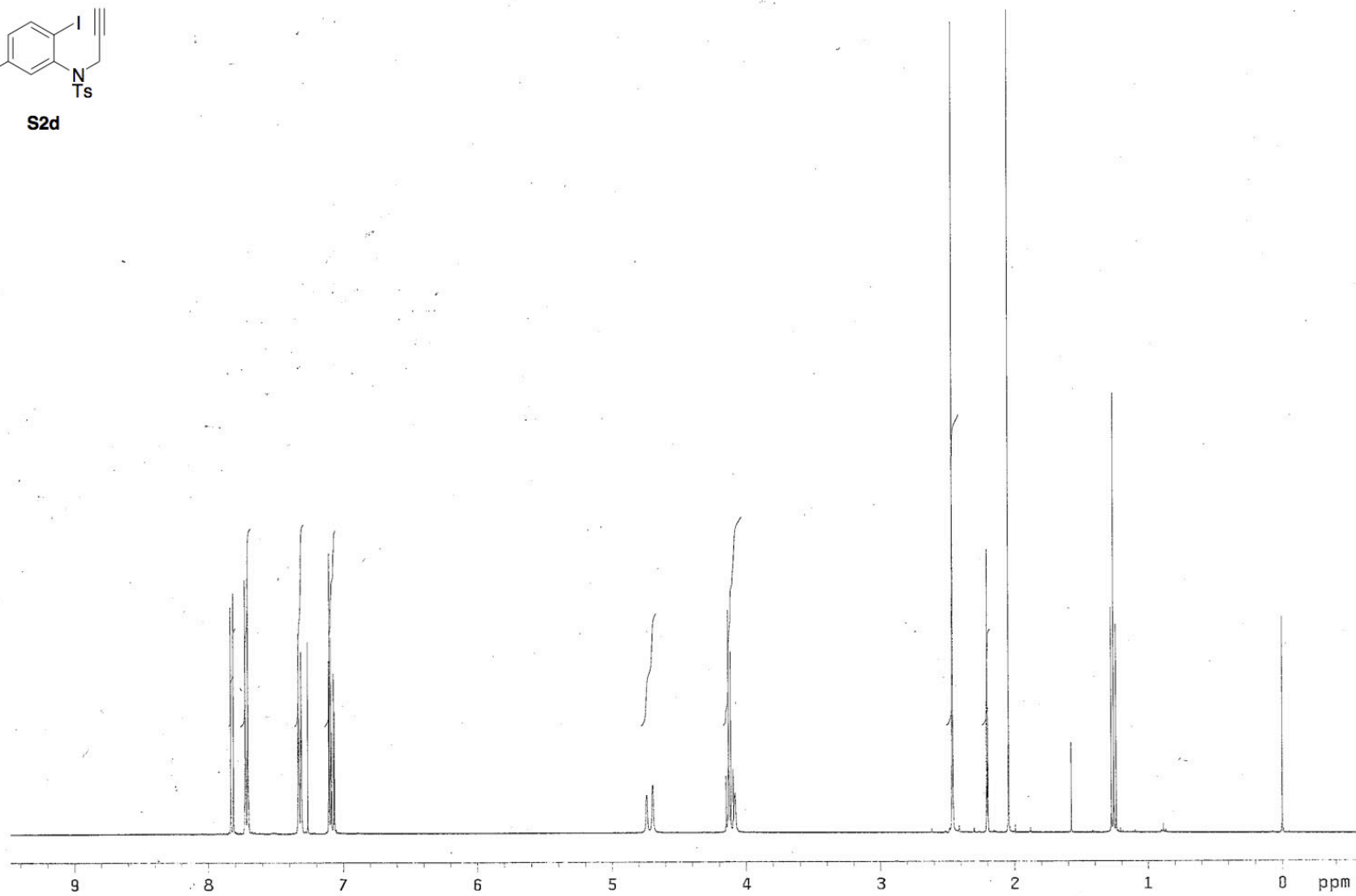
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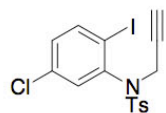
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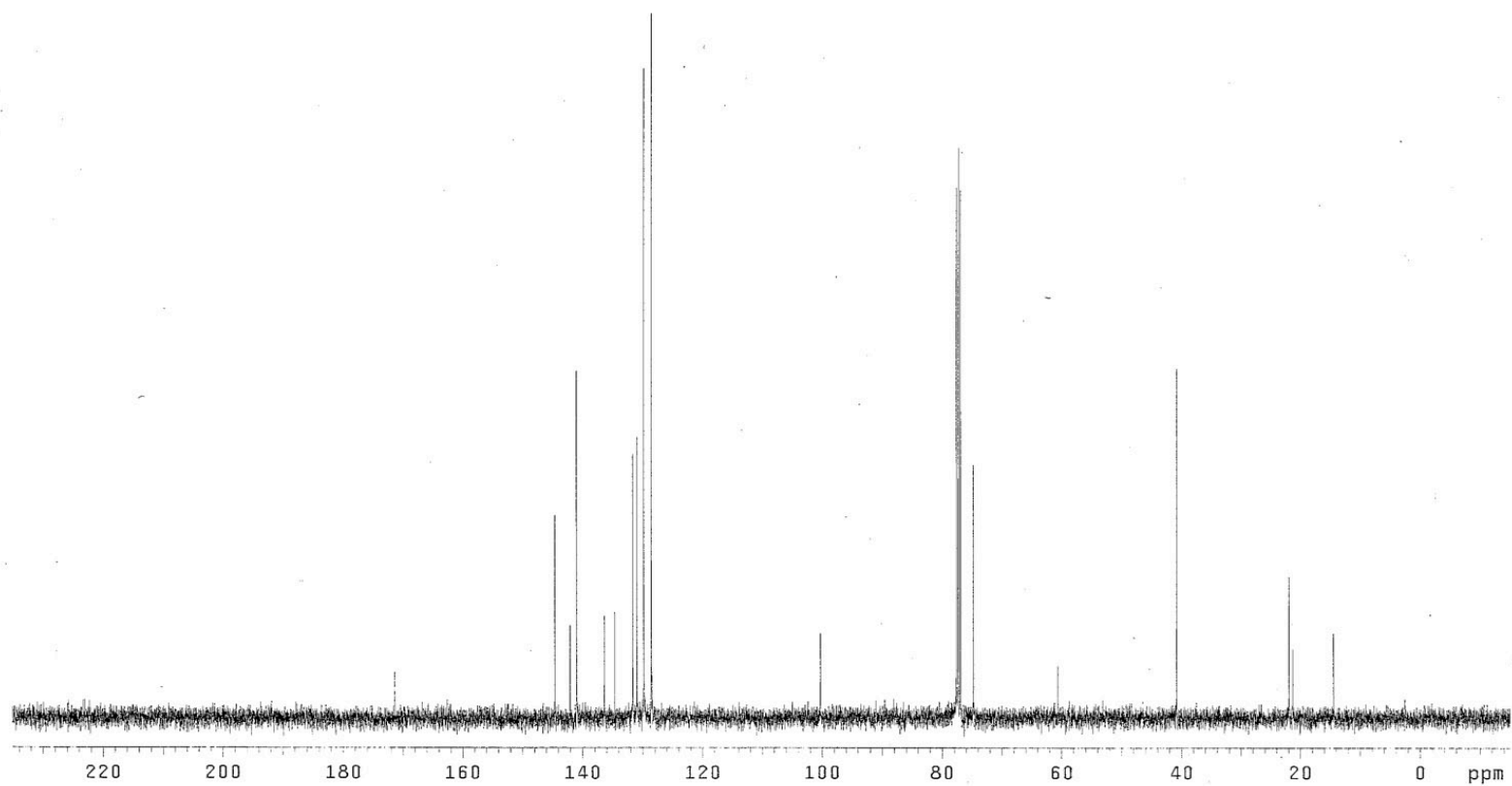
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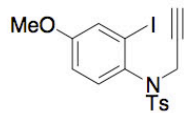
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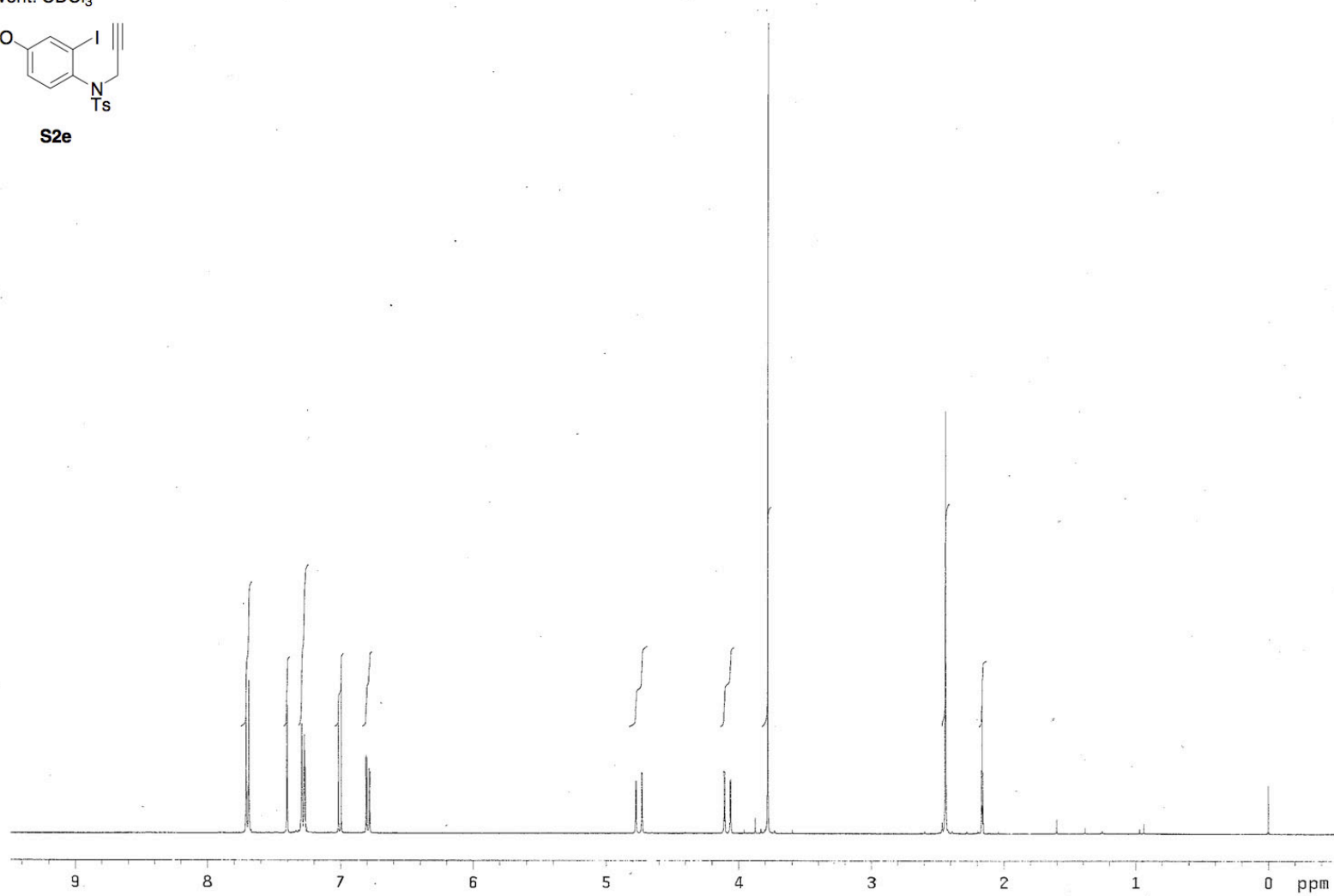
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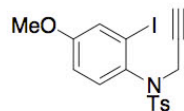
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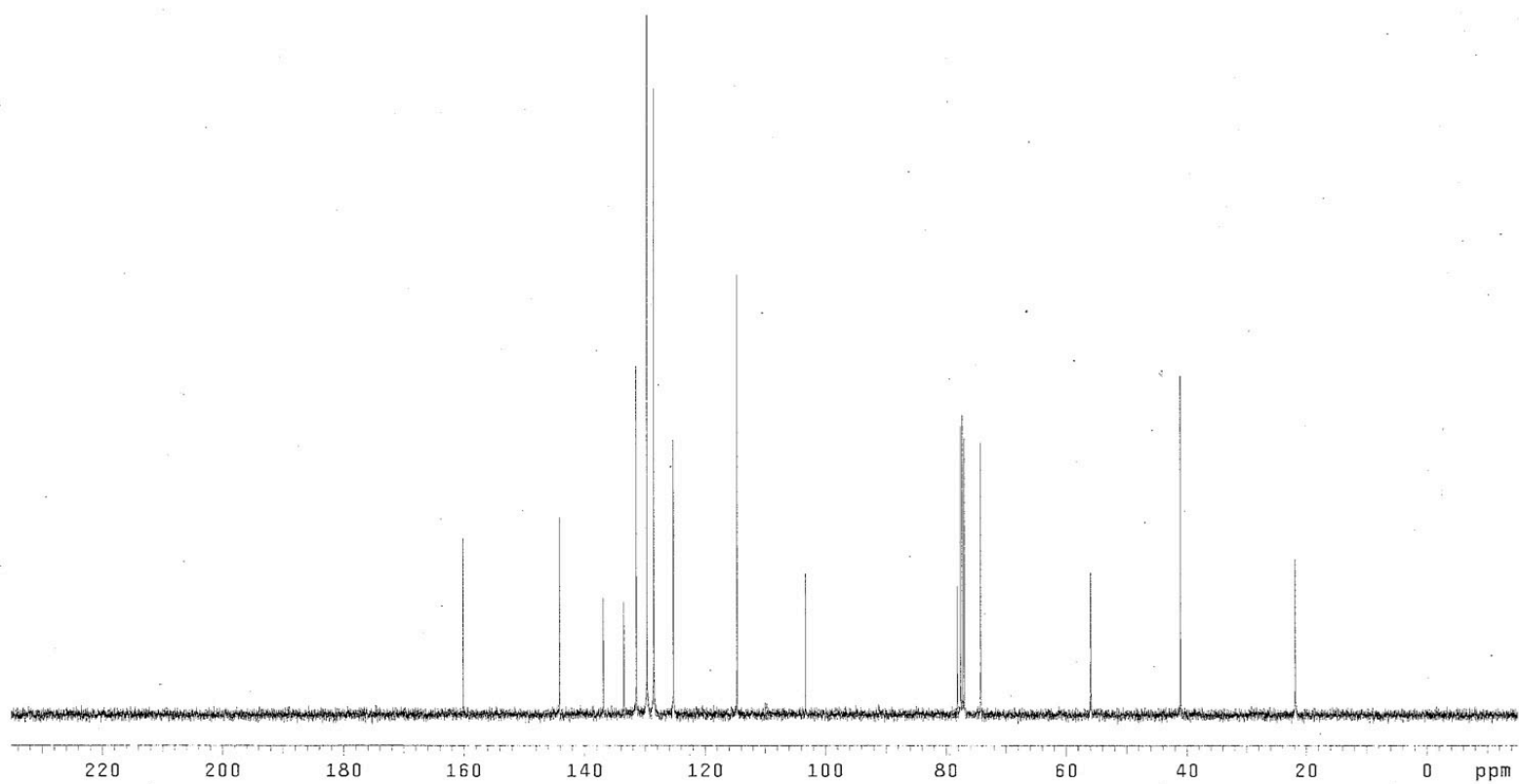
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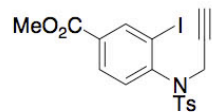
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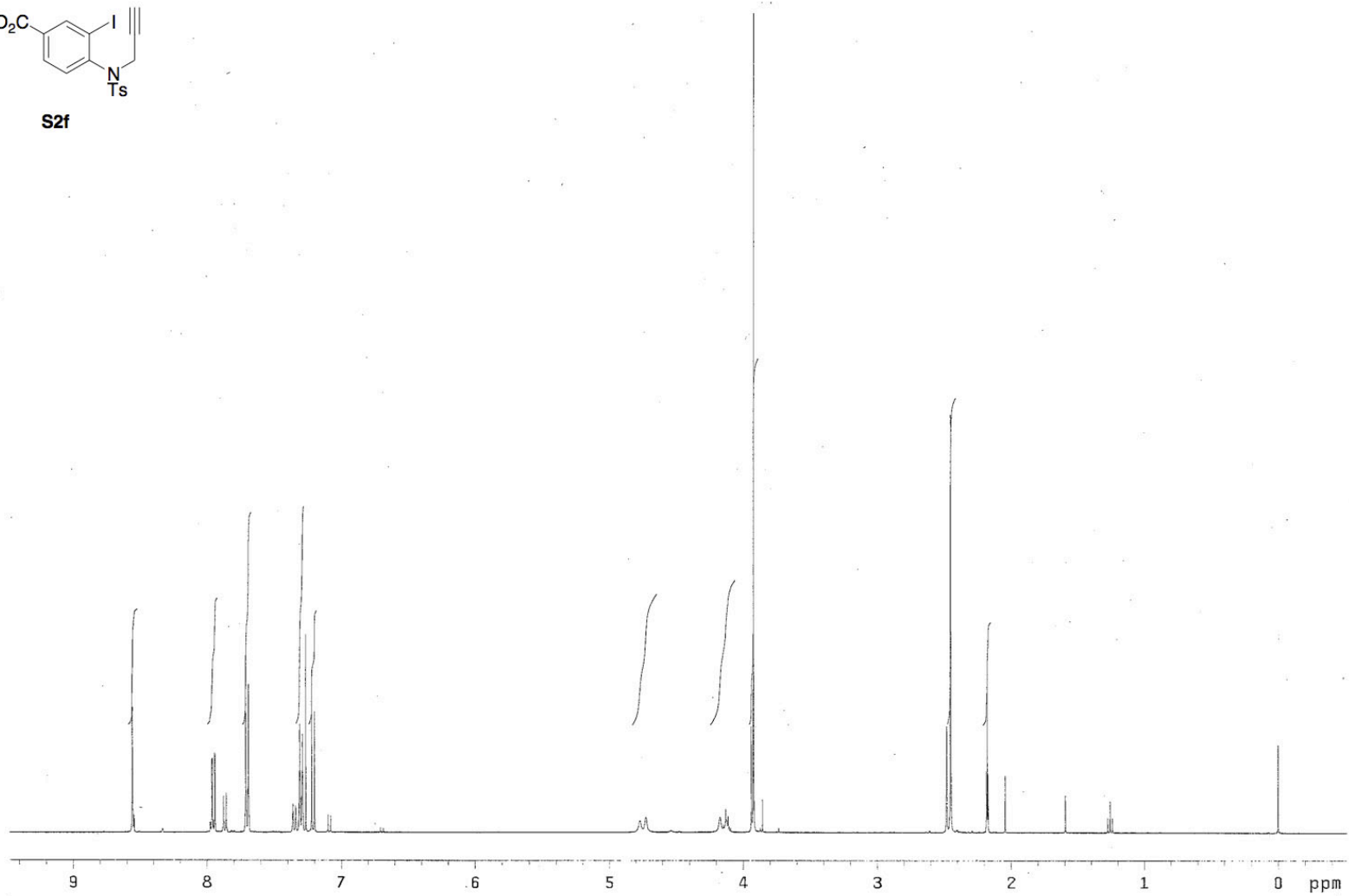
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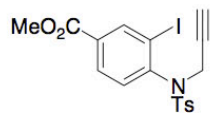
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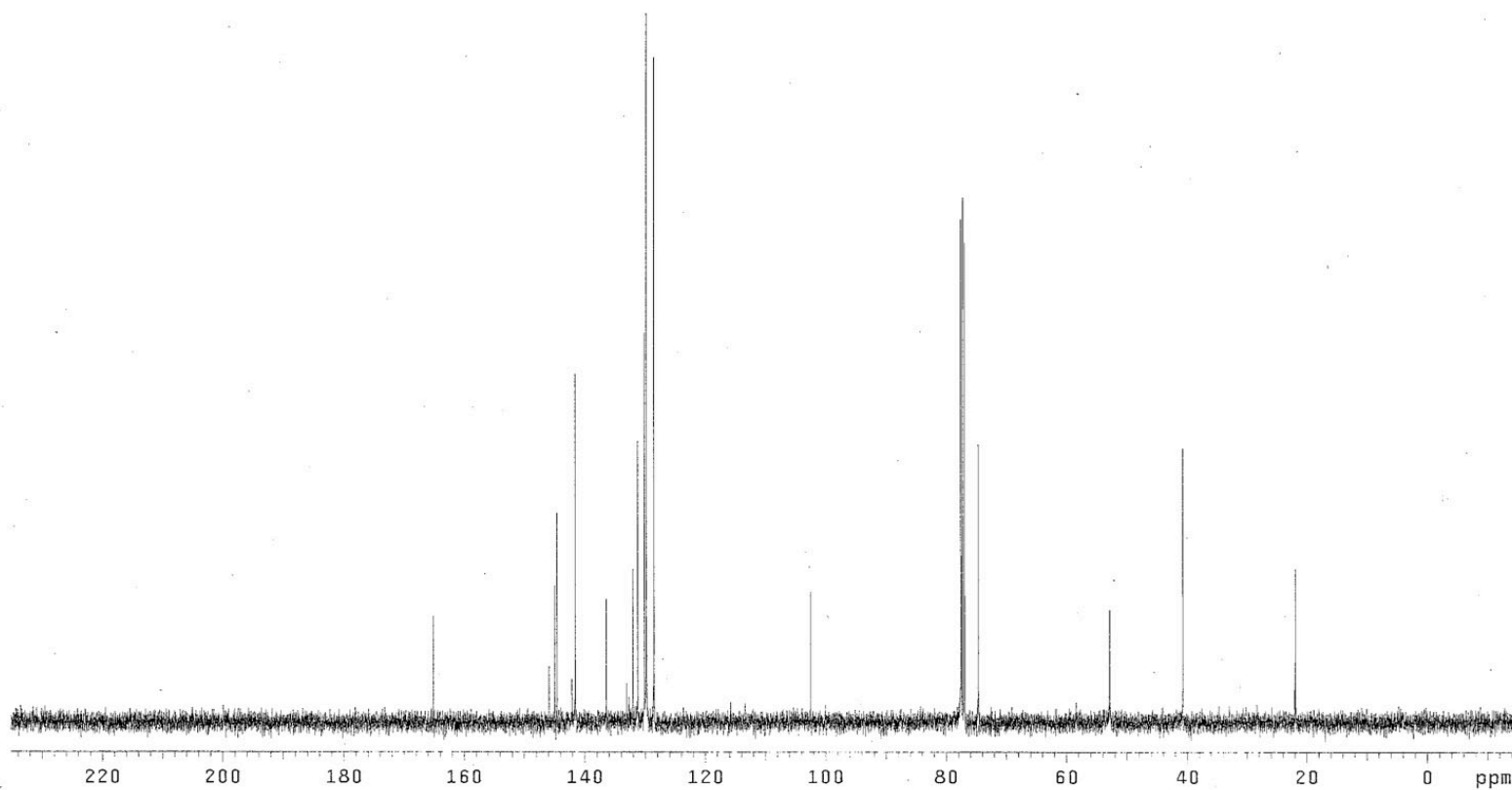
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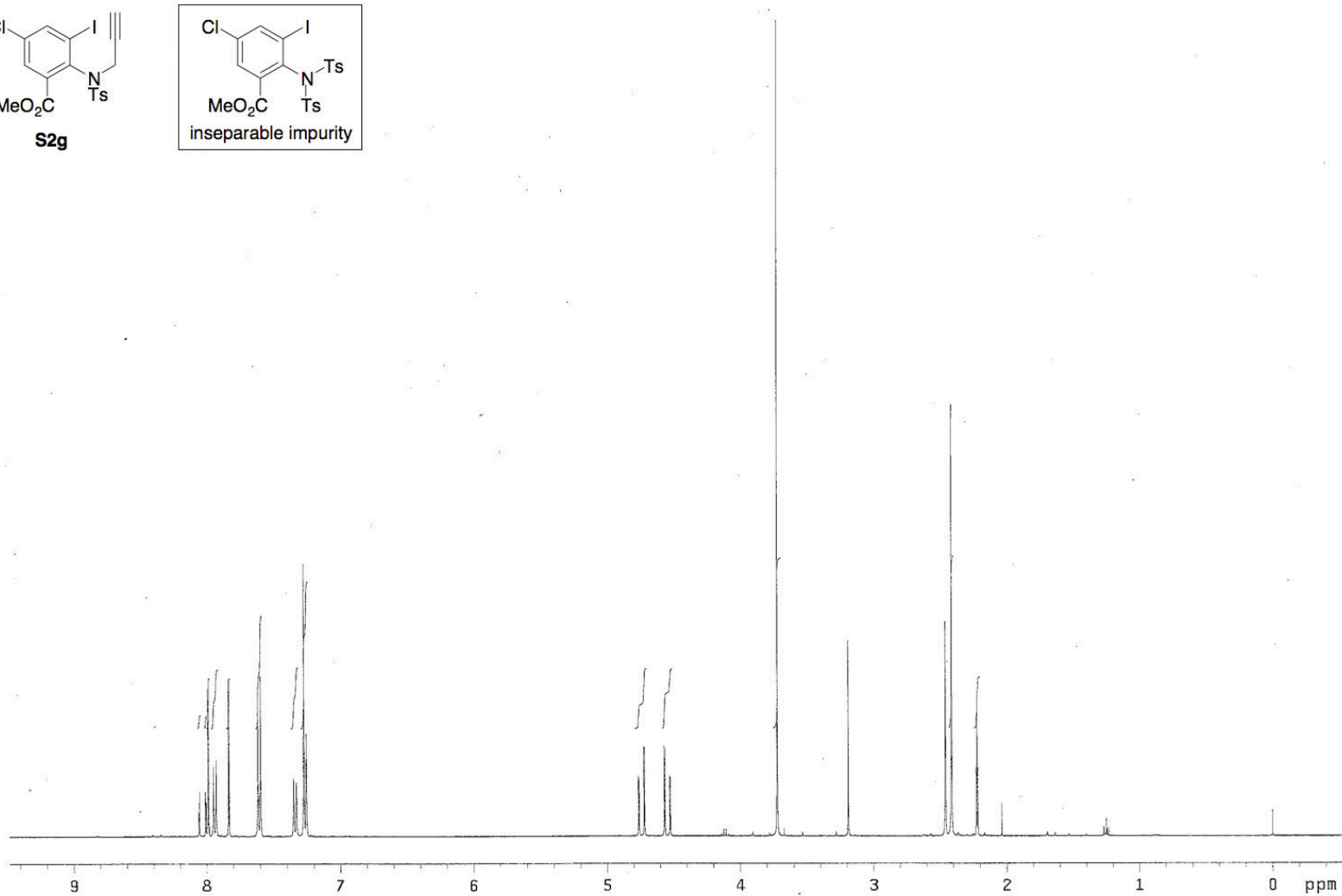
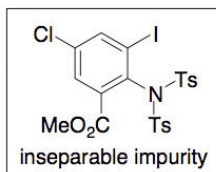
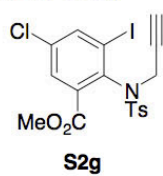
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Solvent: CDCl₃



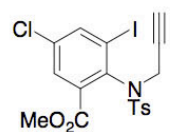
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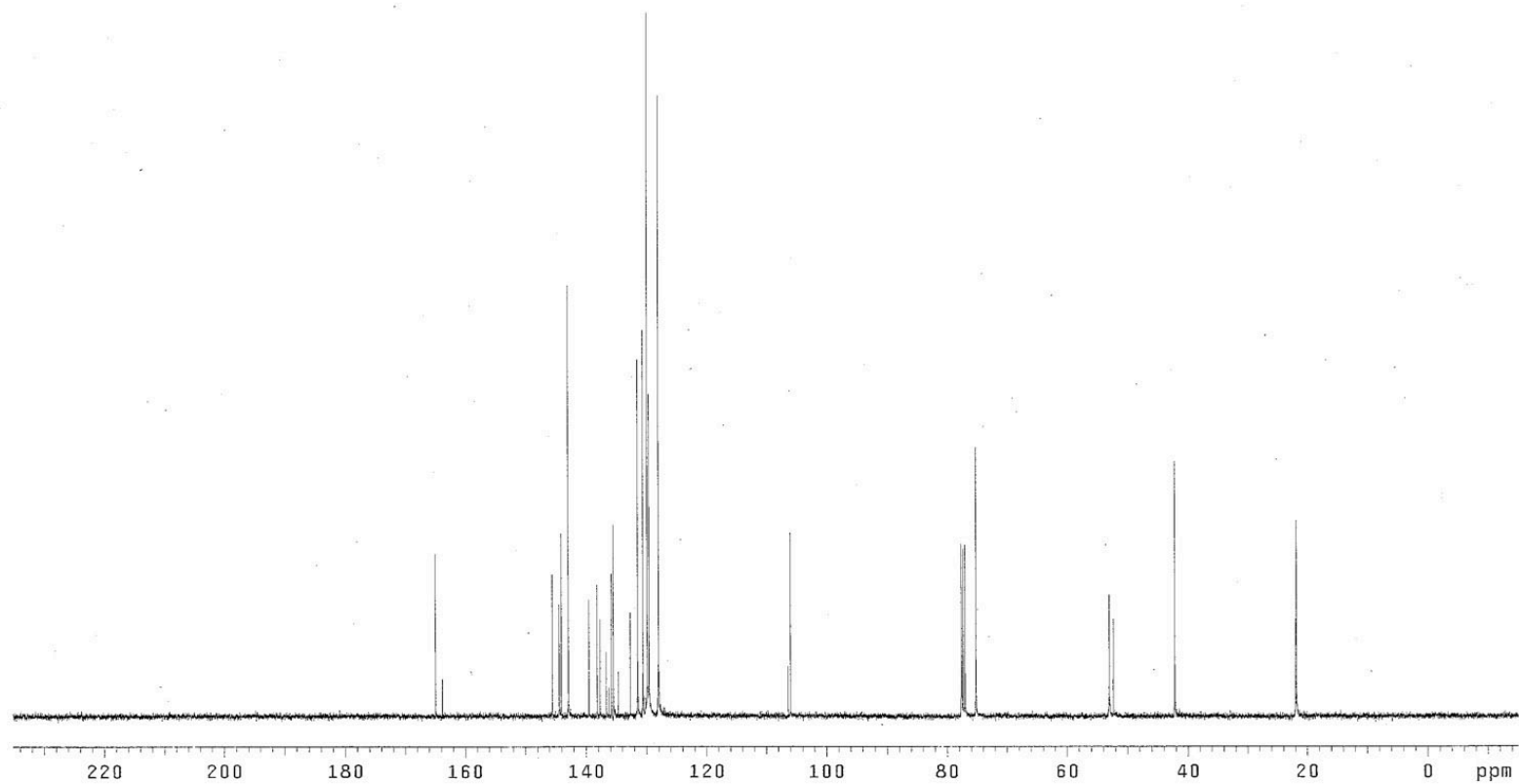
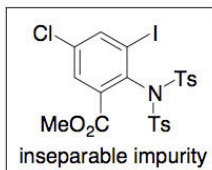
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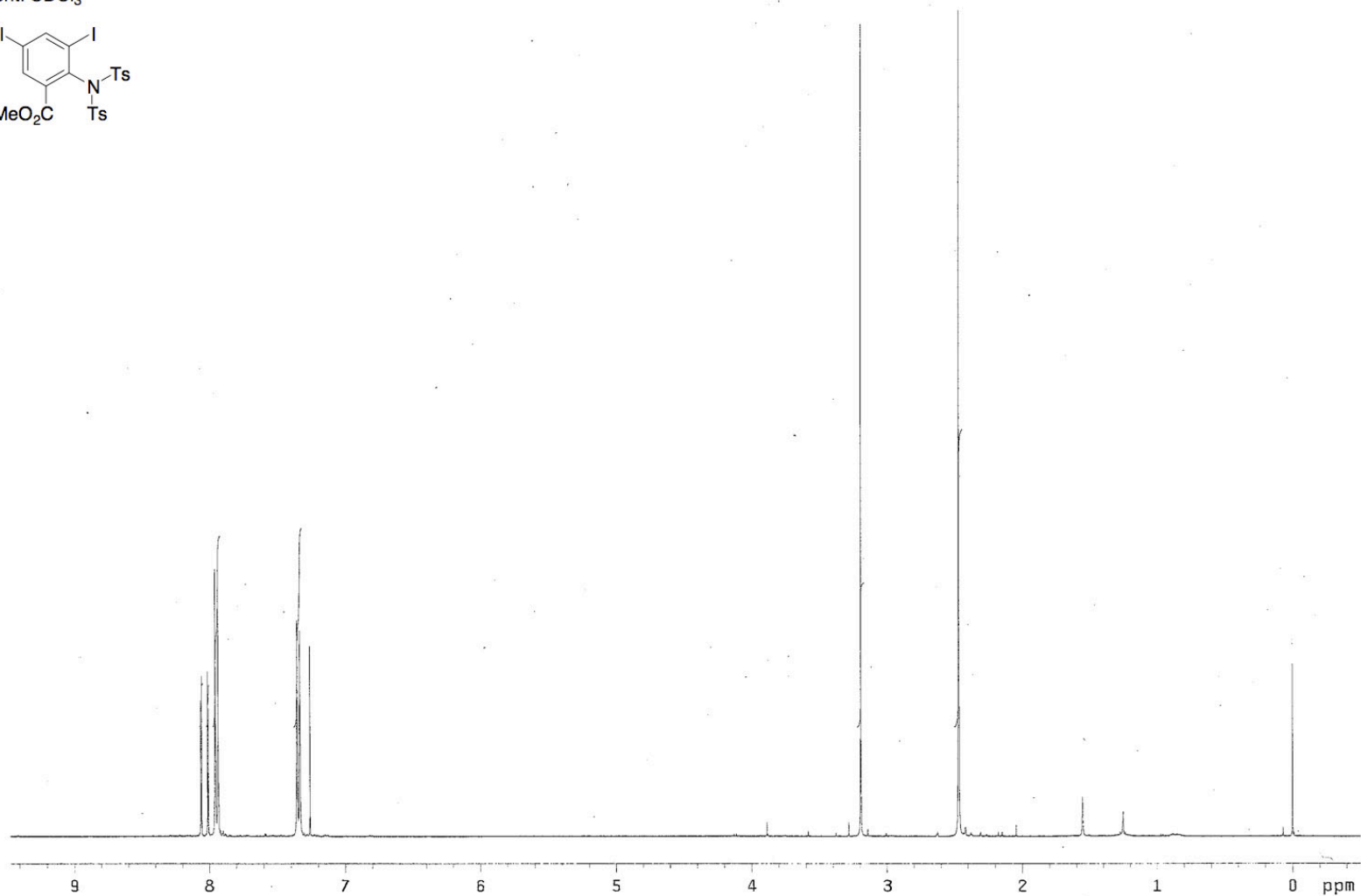
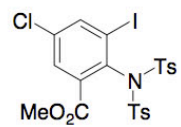
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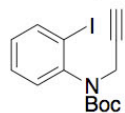
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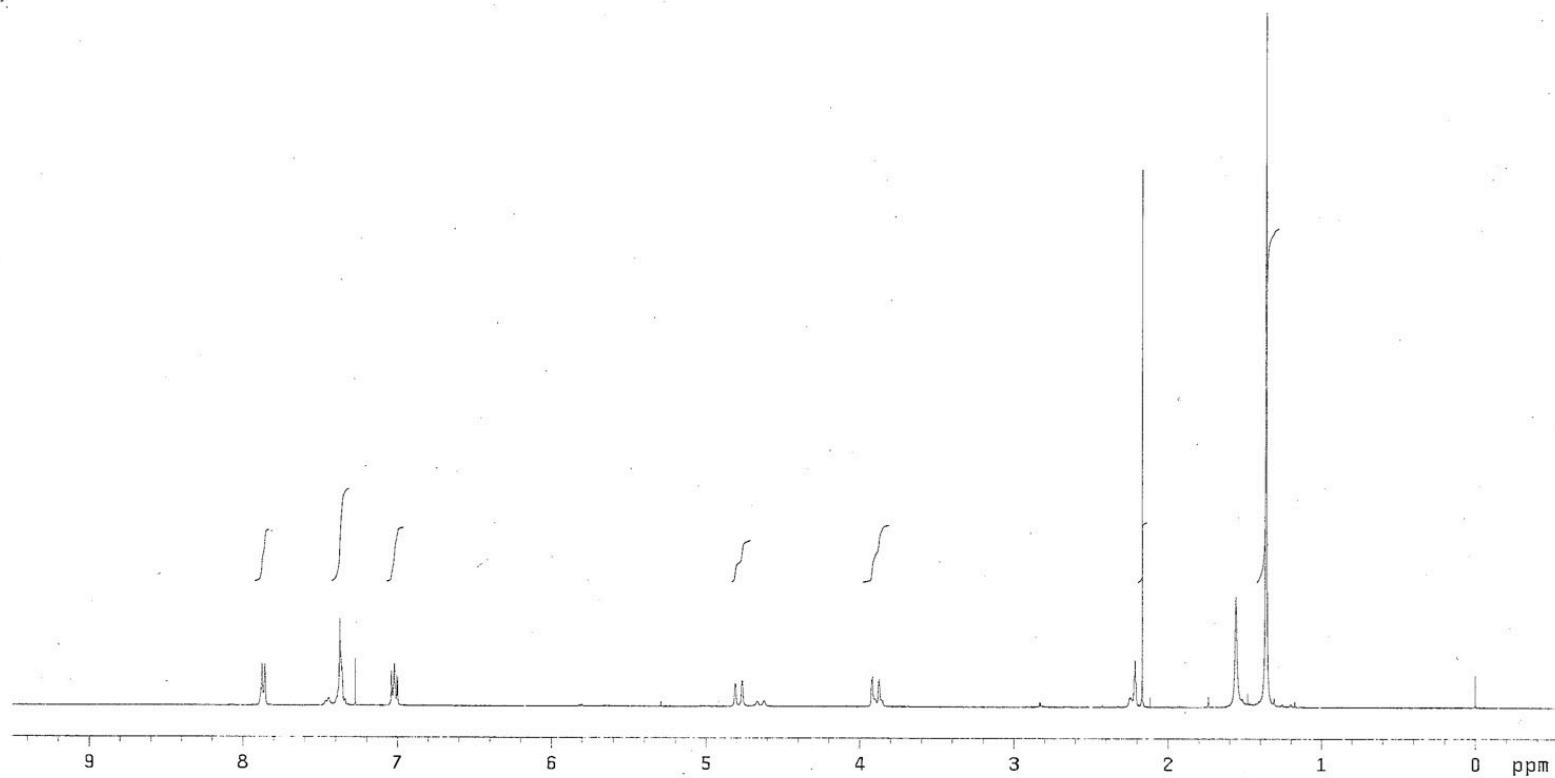
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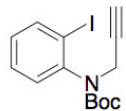
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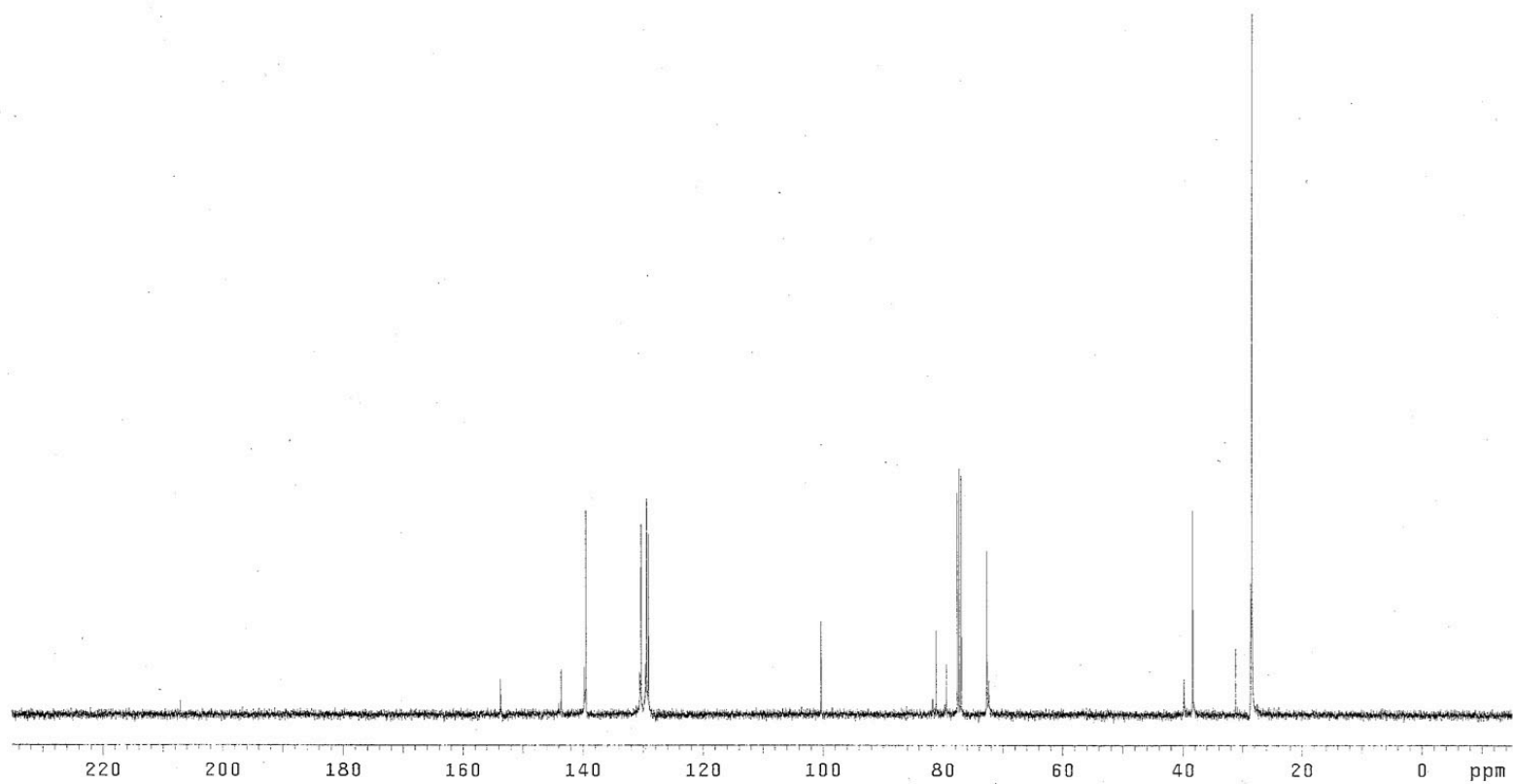
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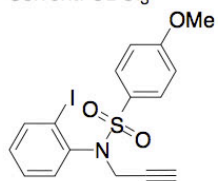
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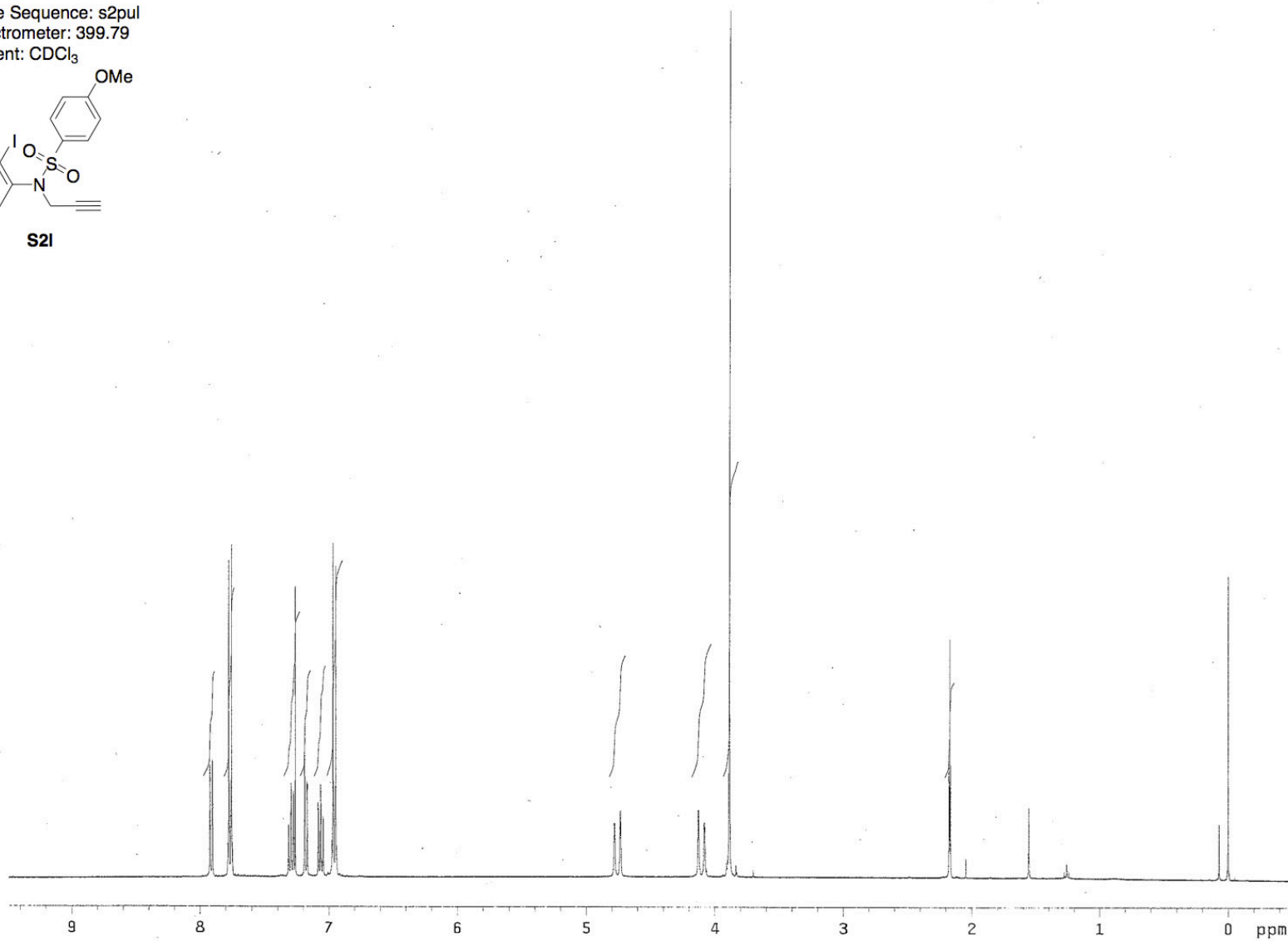
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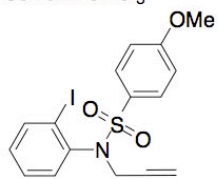
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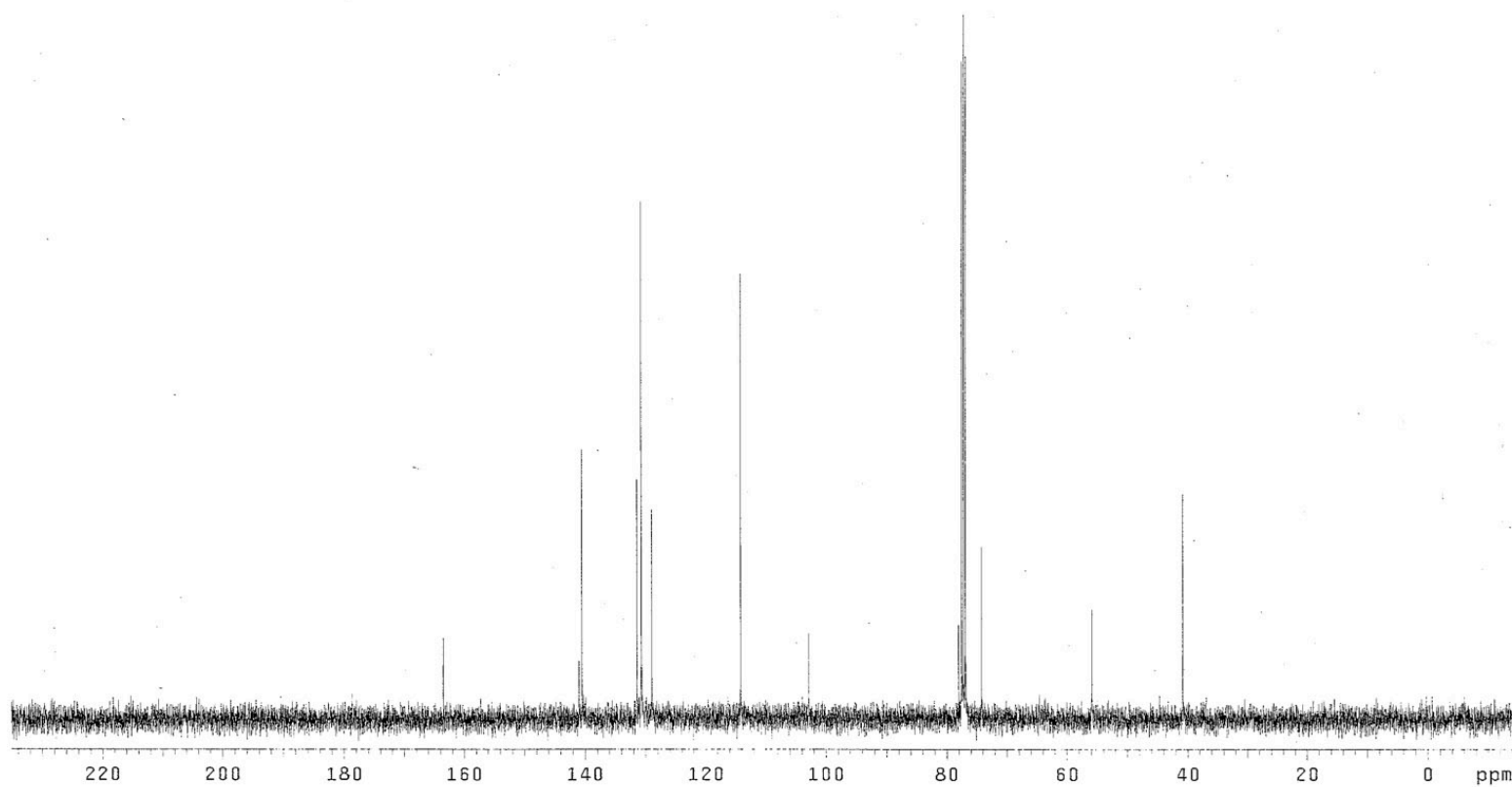
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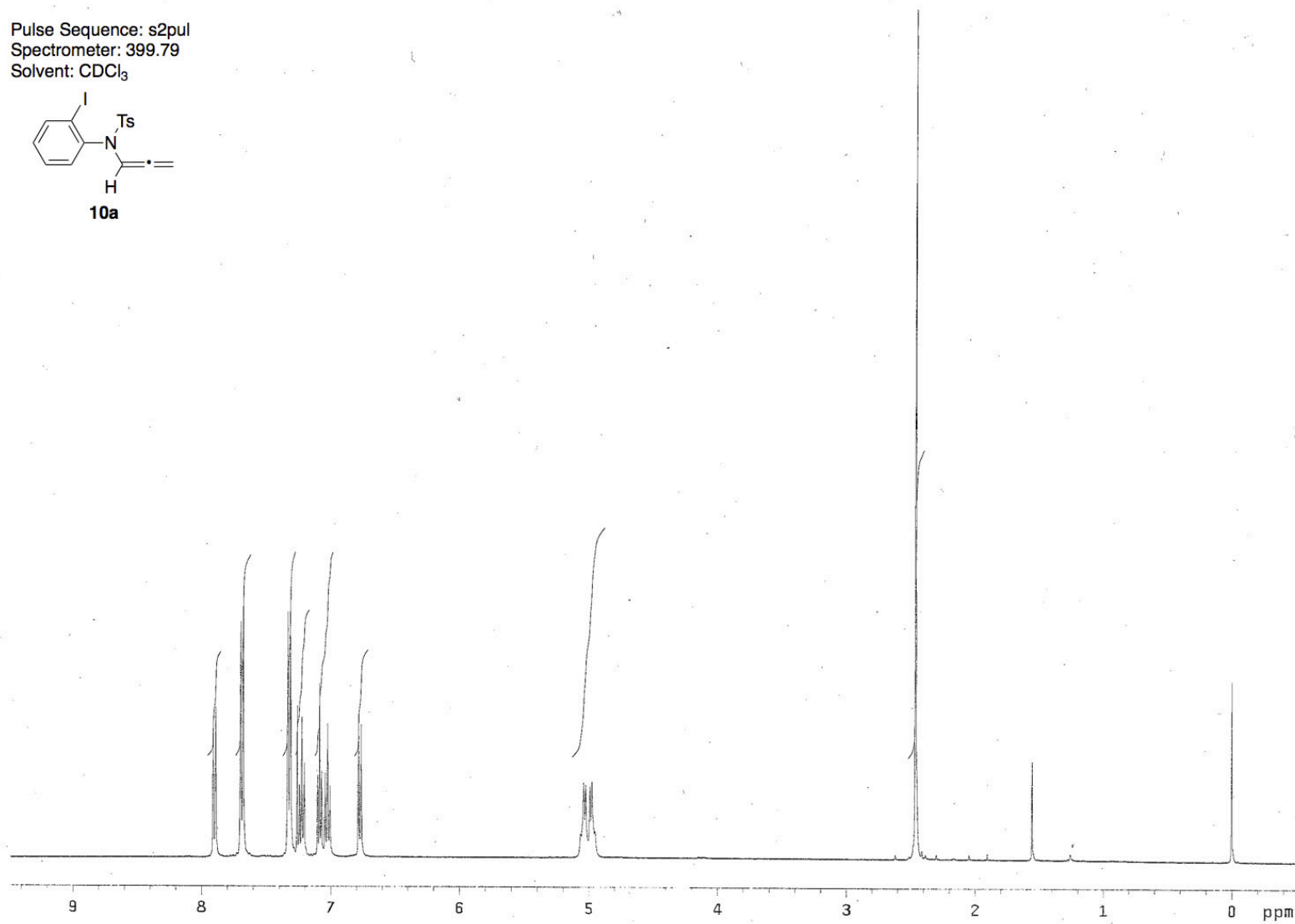
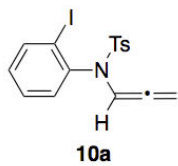
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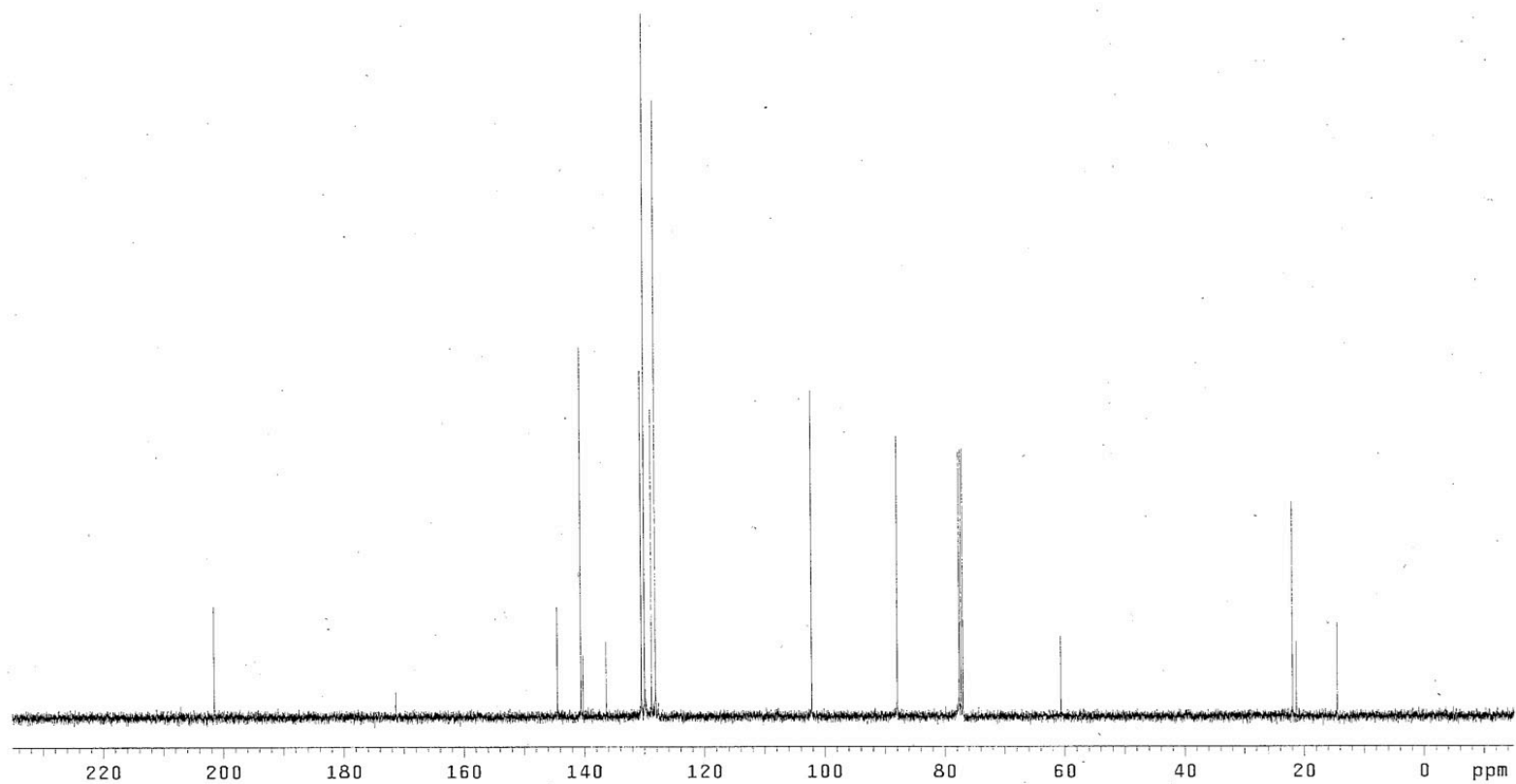
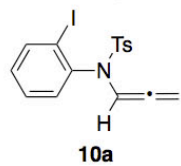
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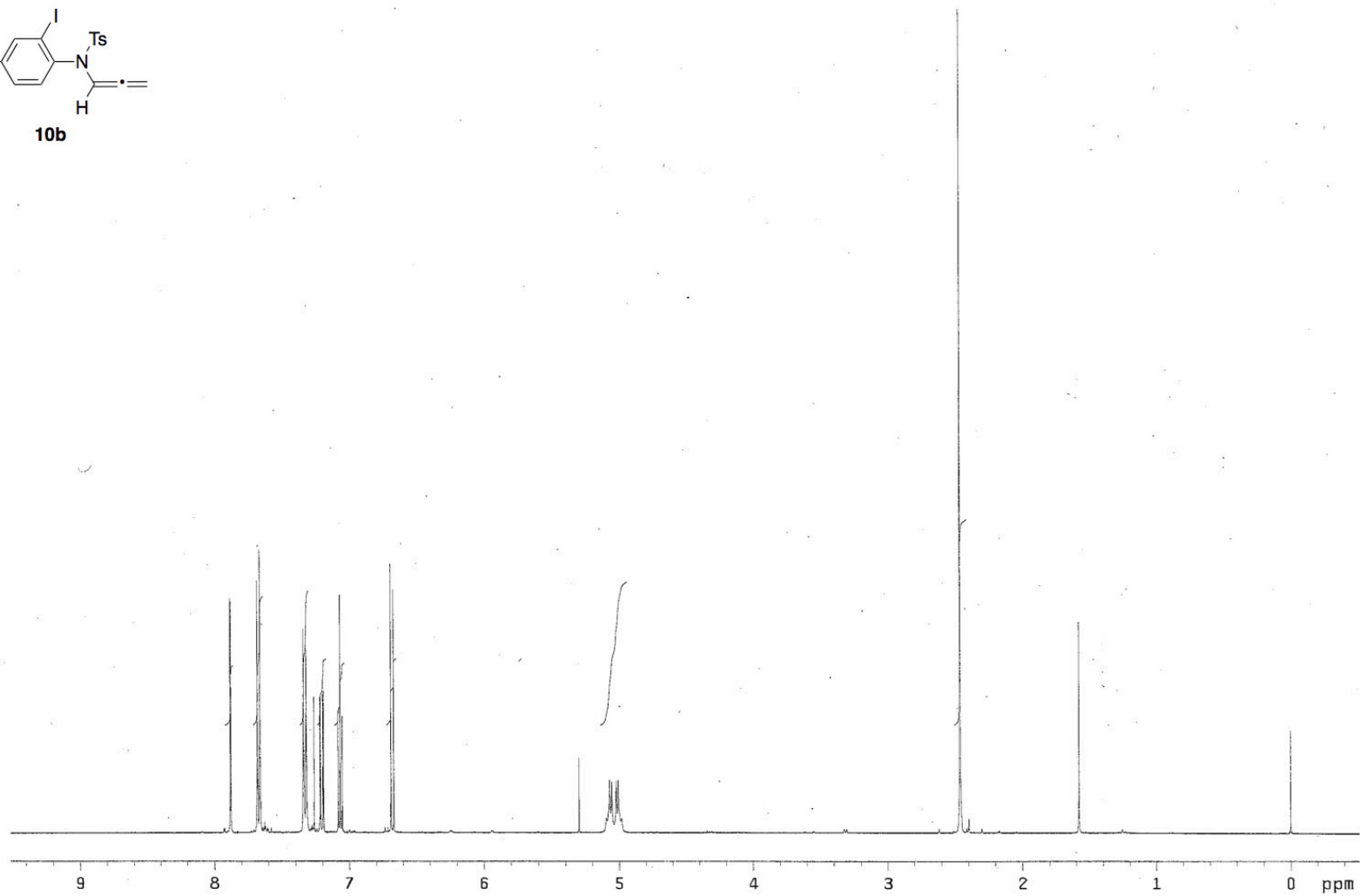
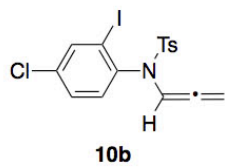
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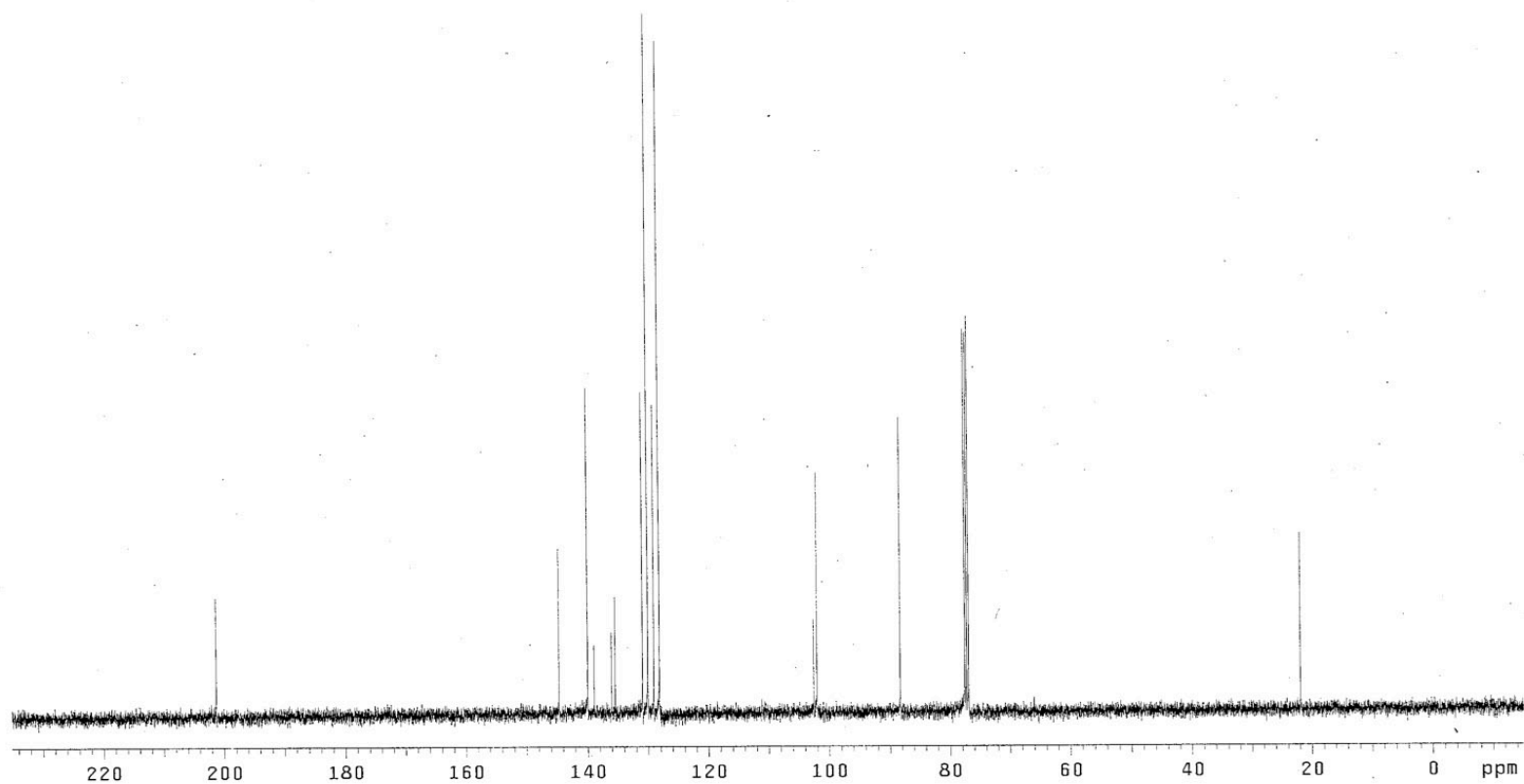
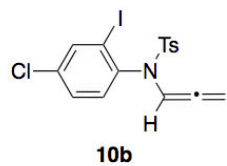
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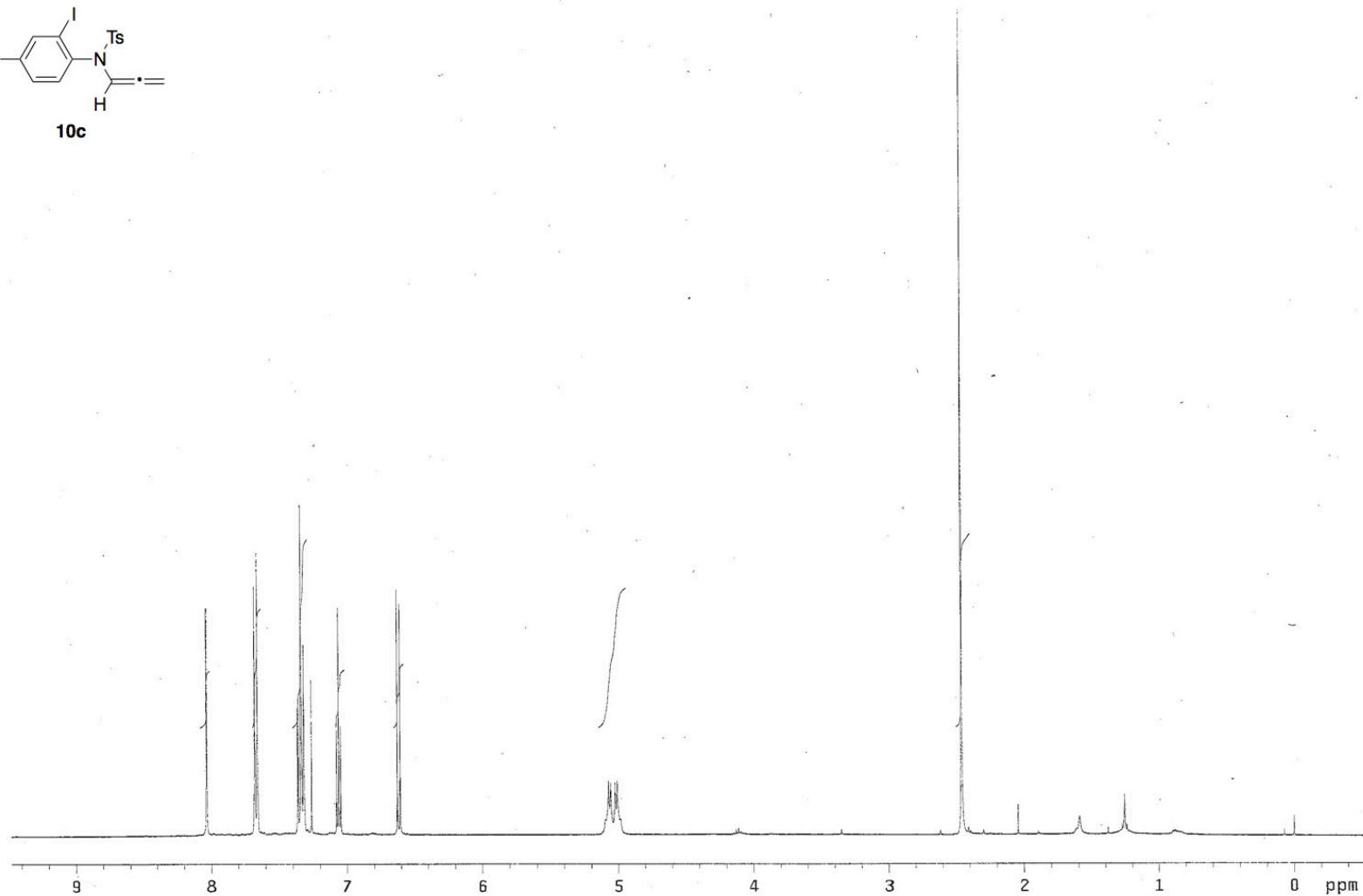
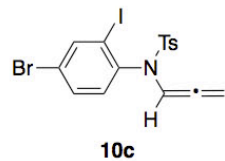
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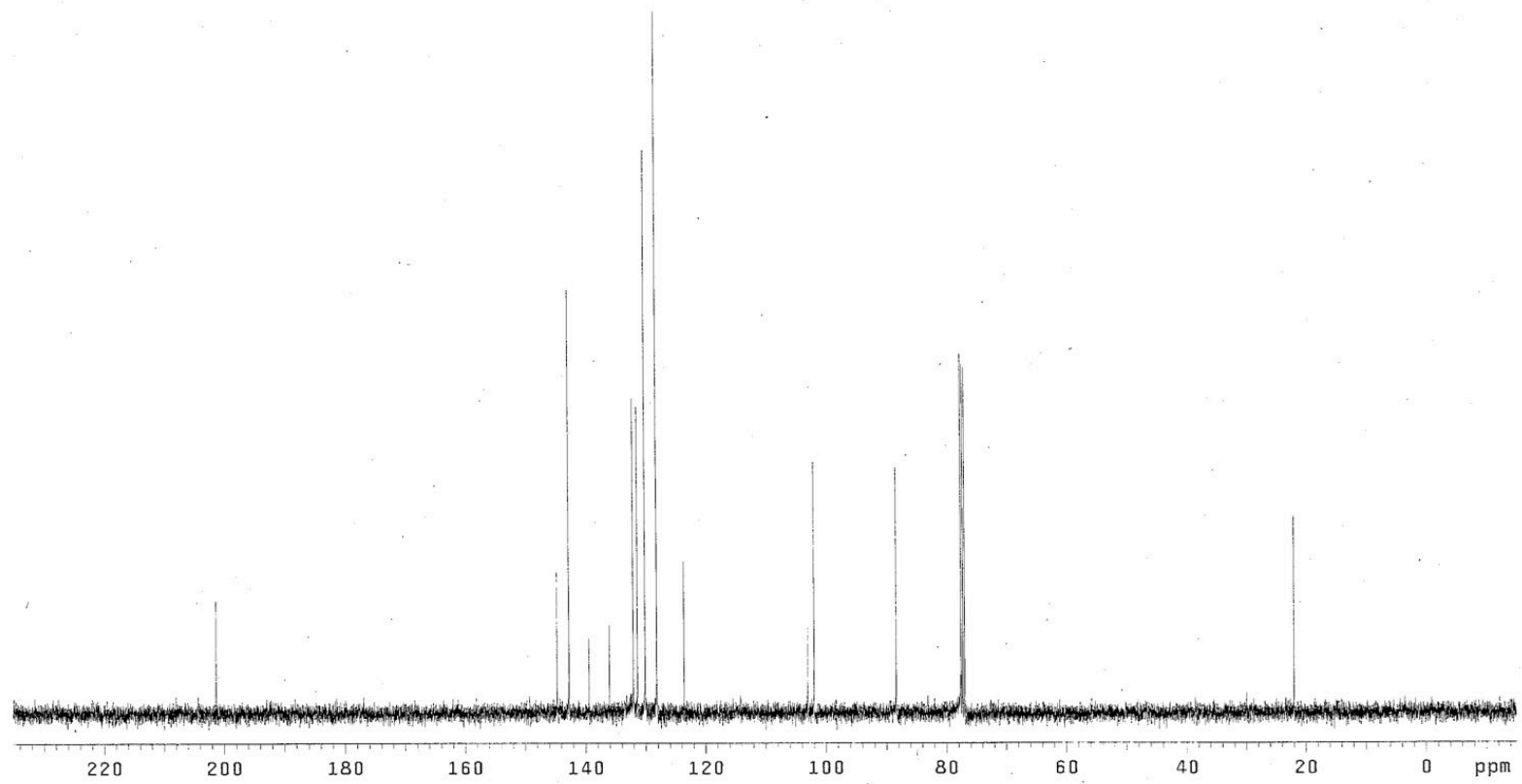
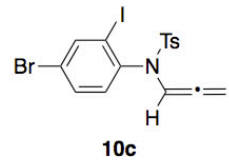
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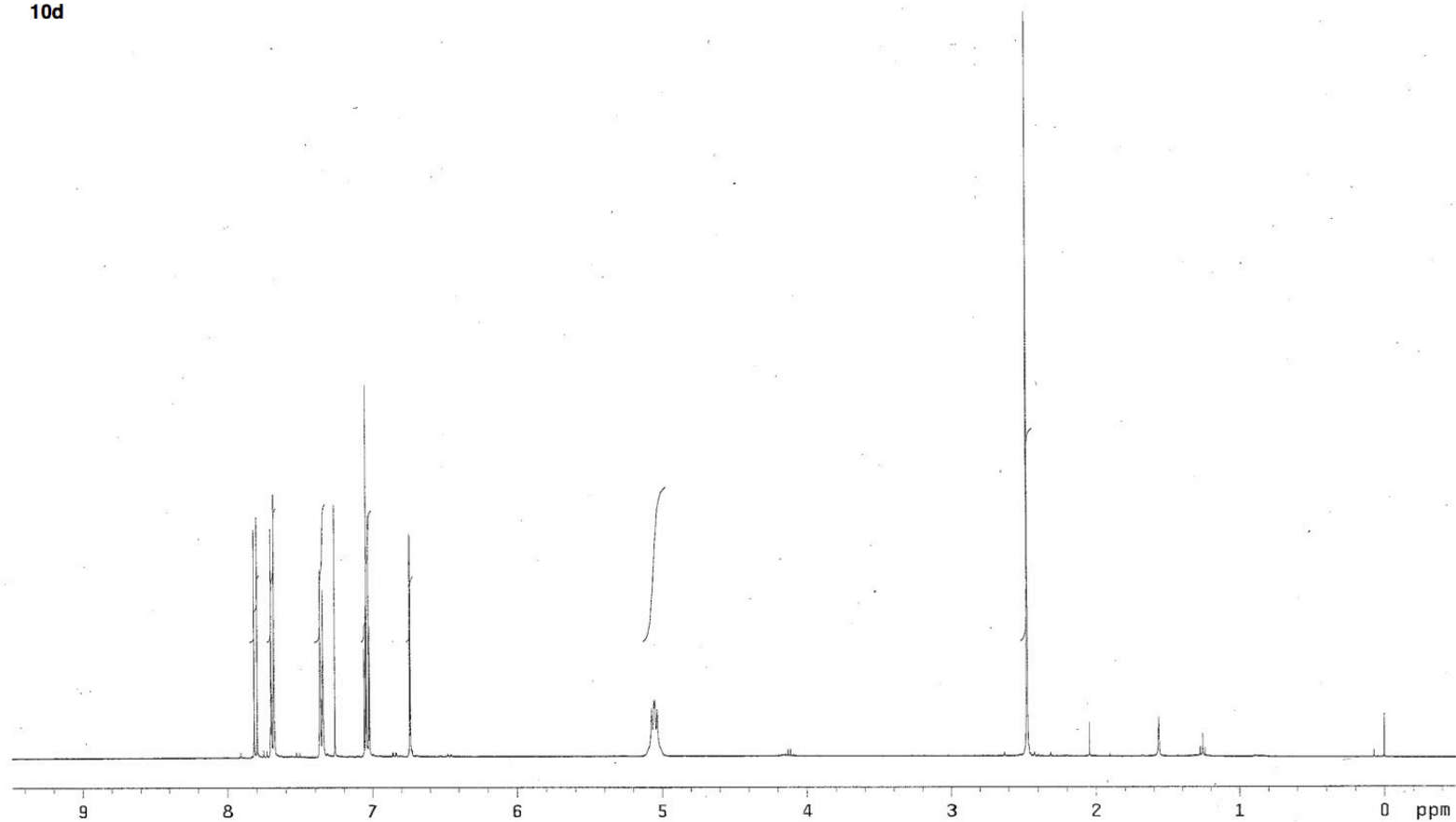
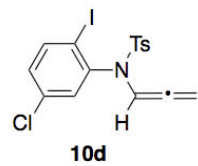
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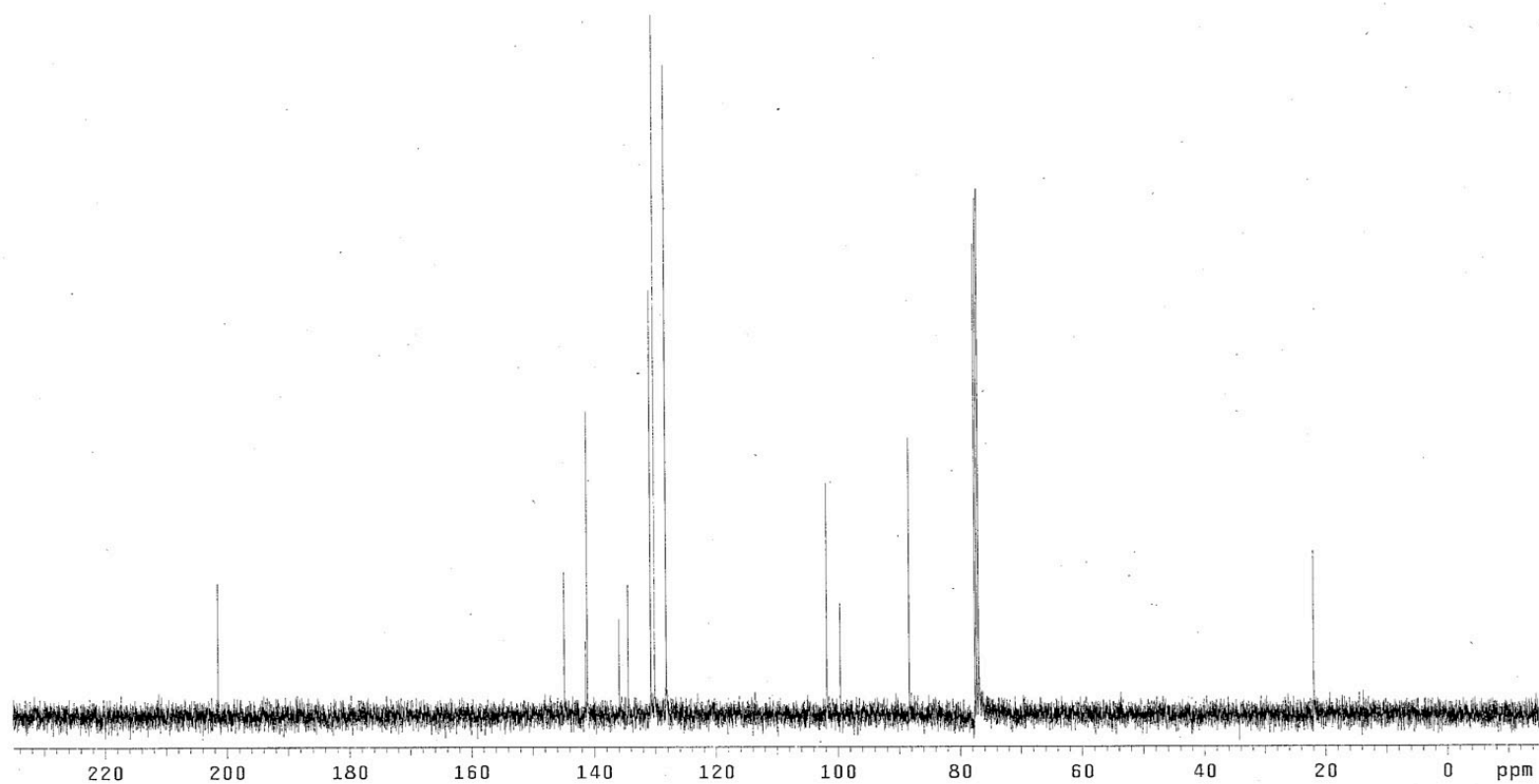
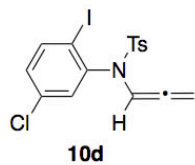
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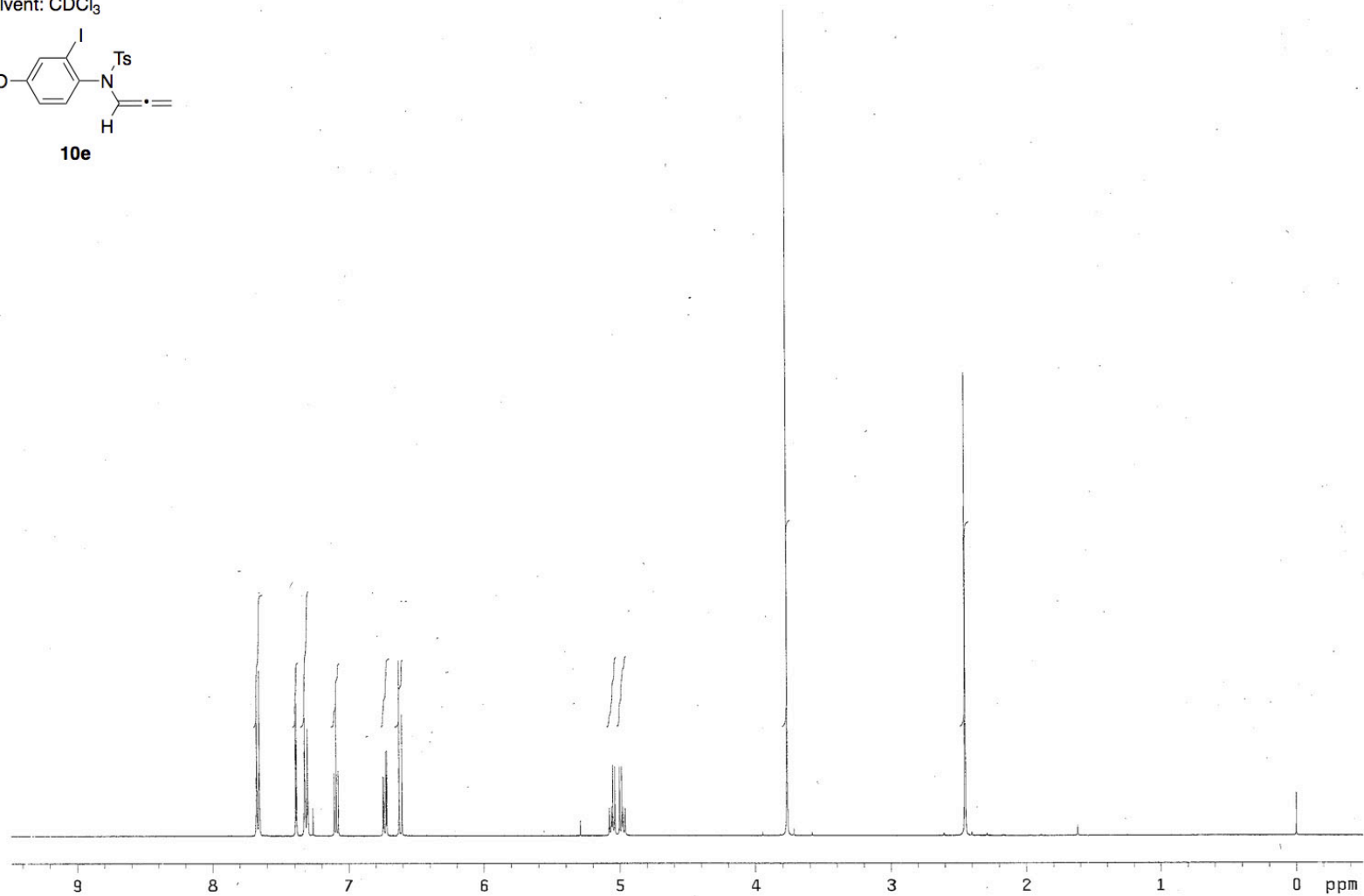
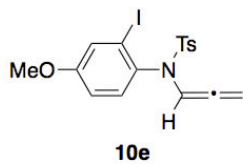
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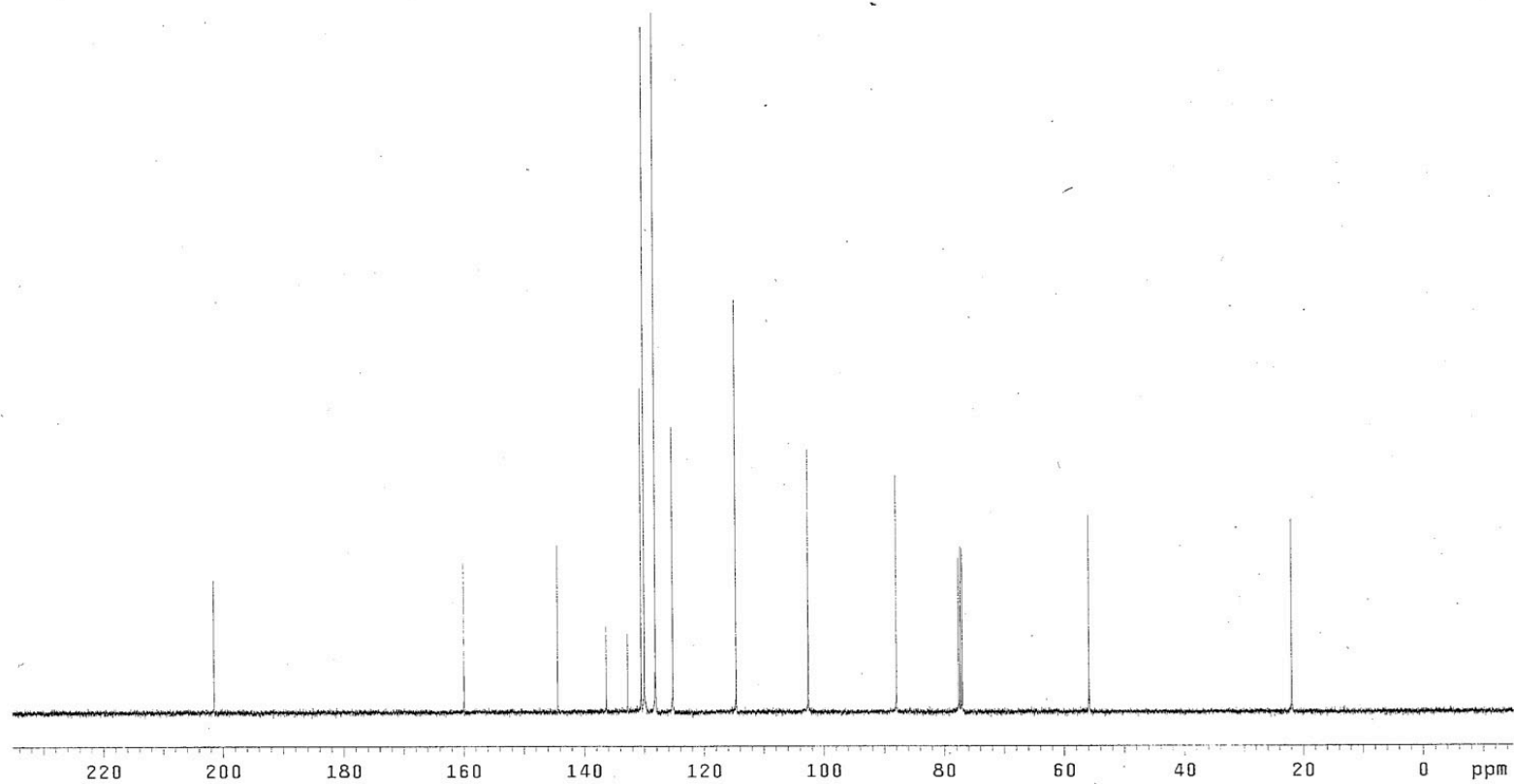
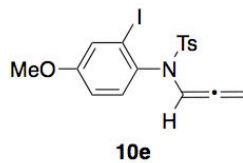
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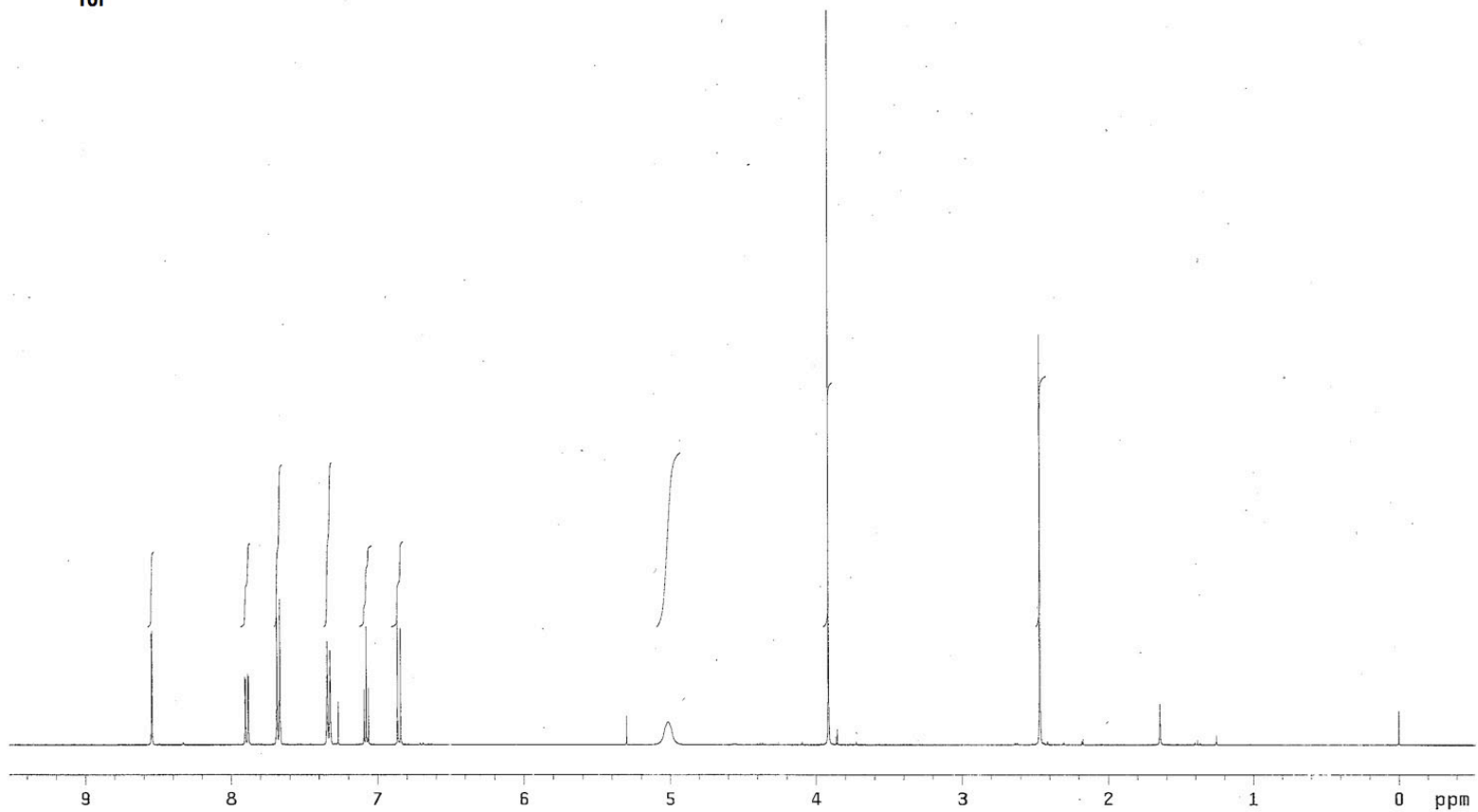
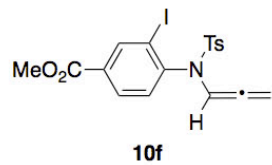
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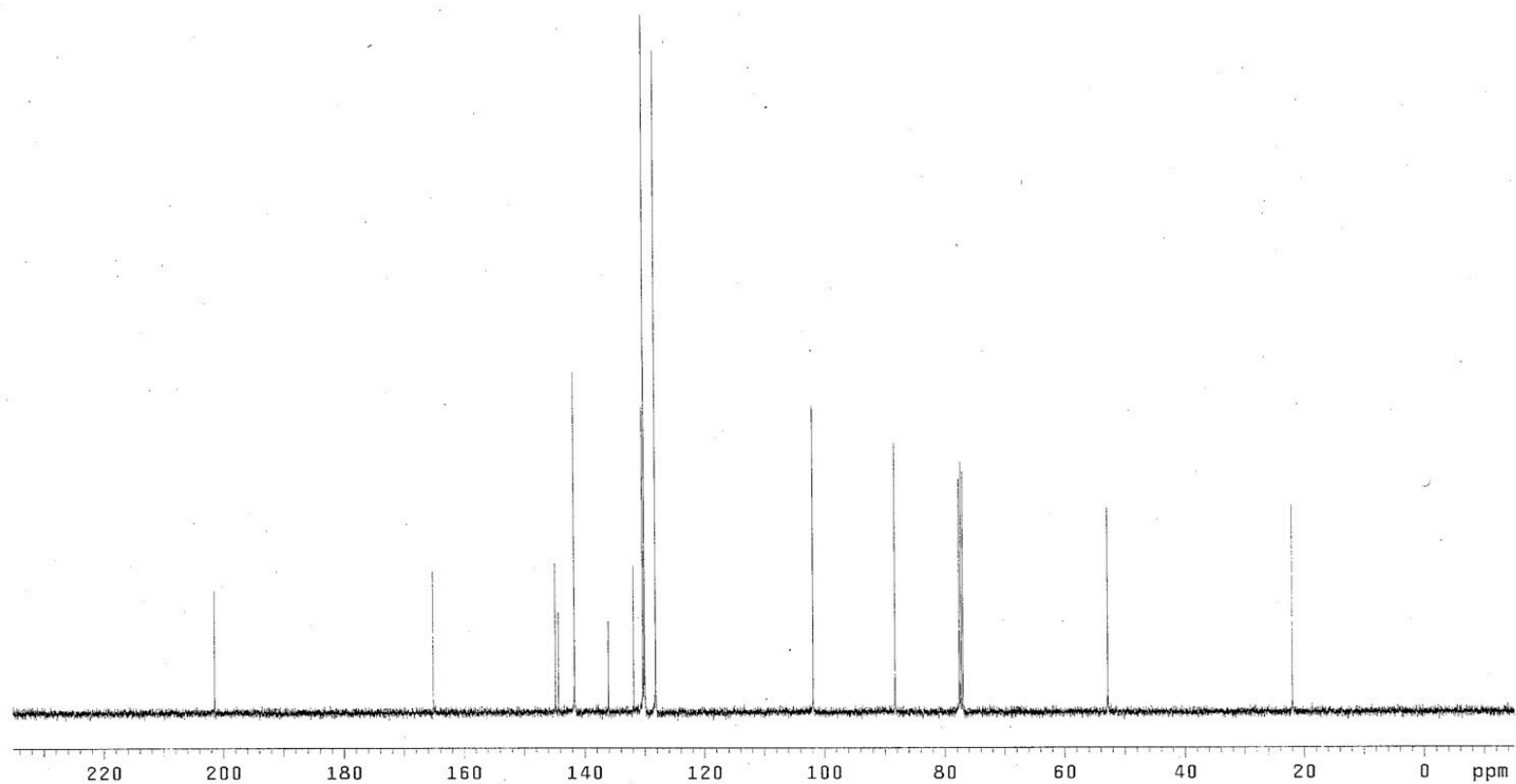
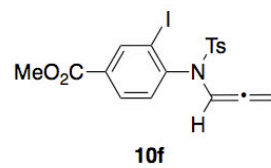
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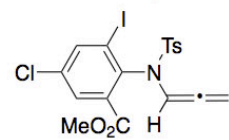
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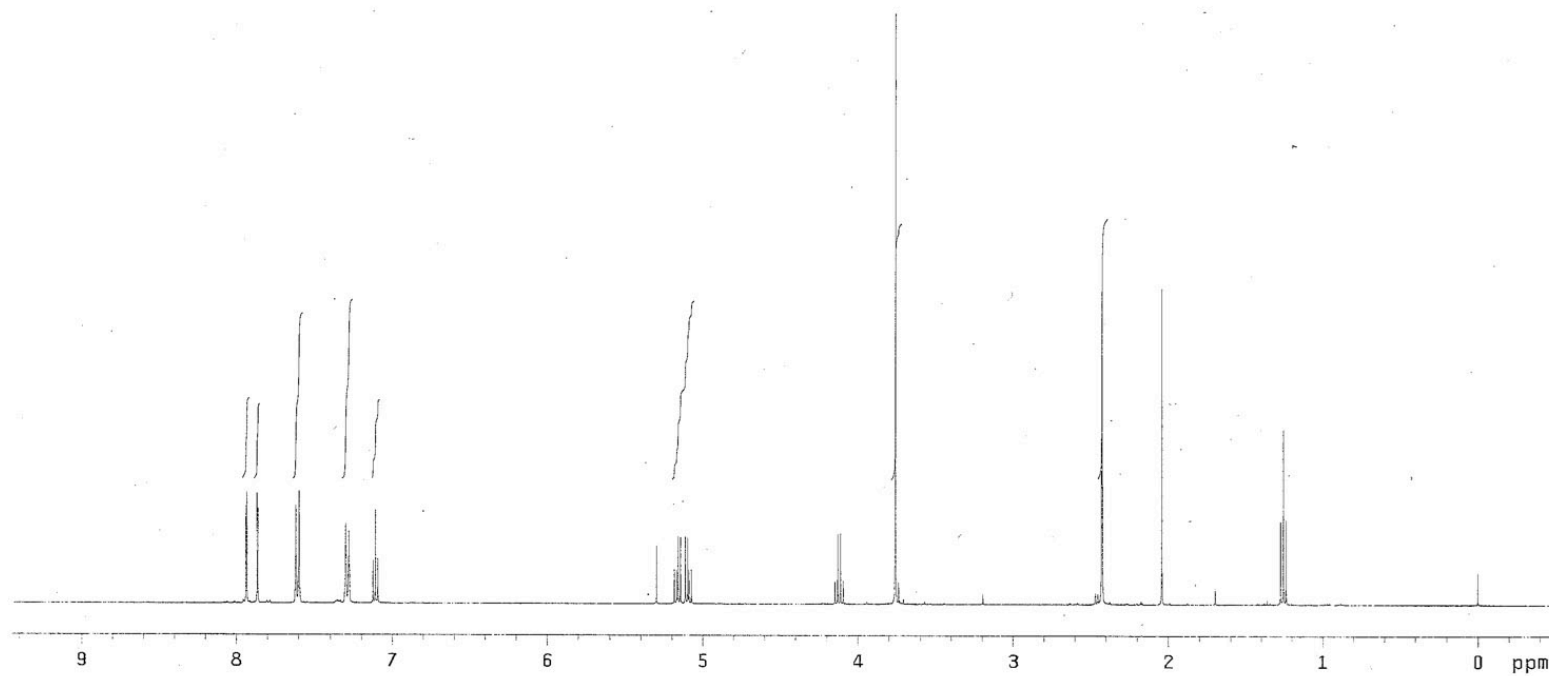
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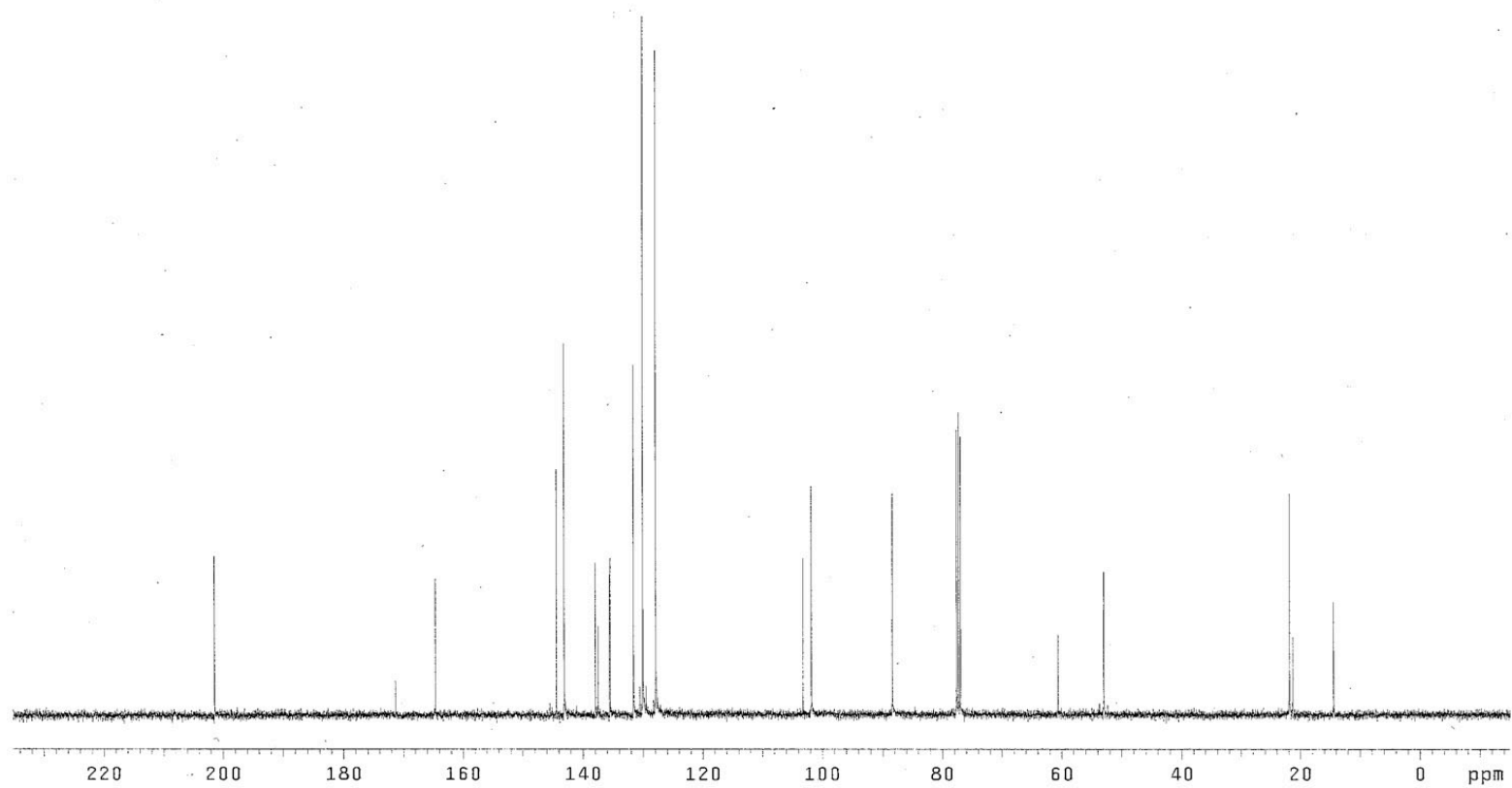
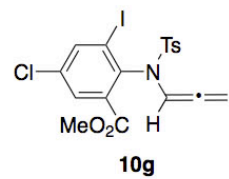
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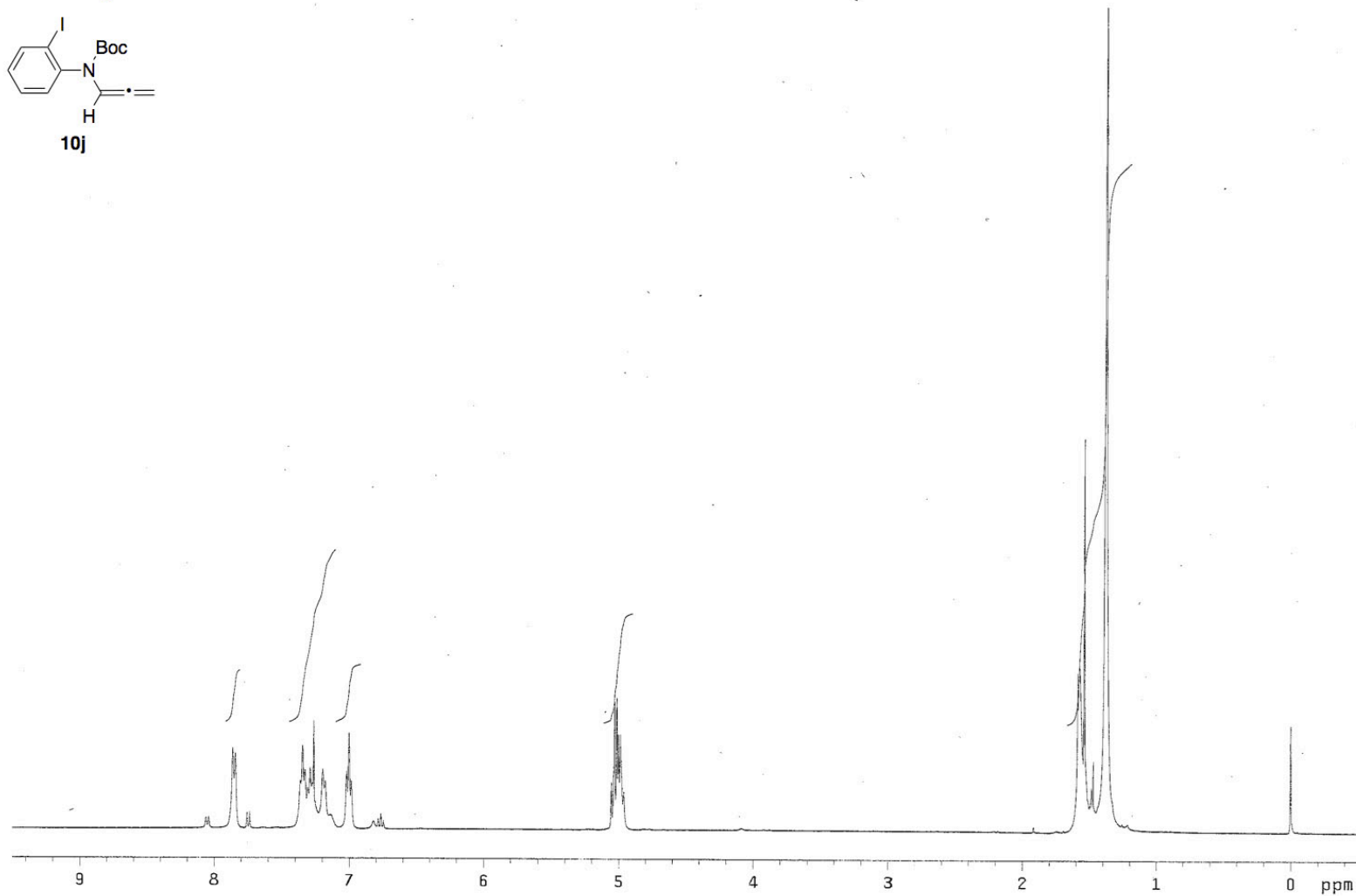
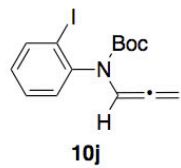
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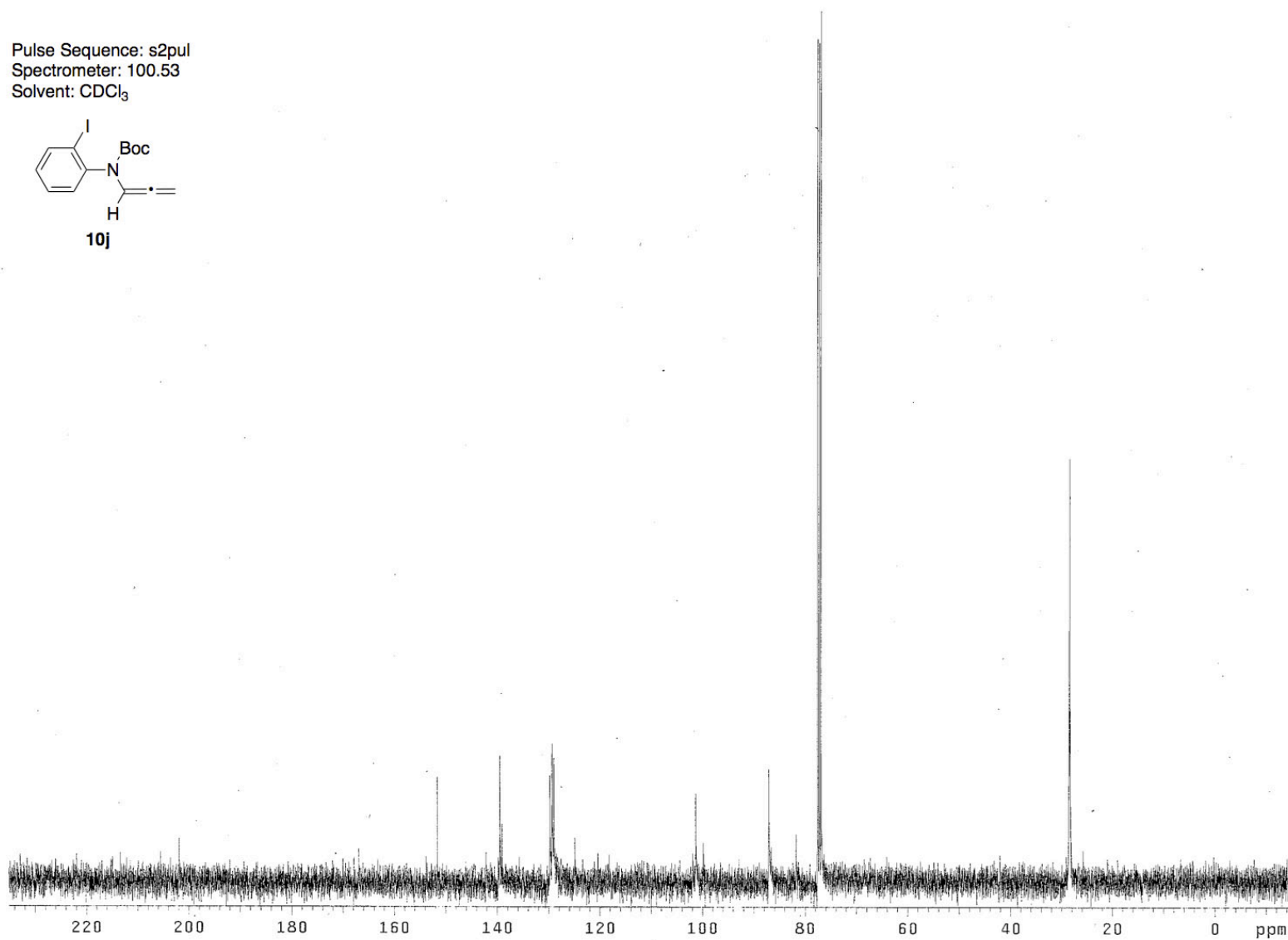
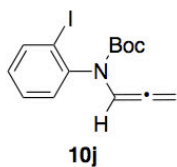
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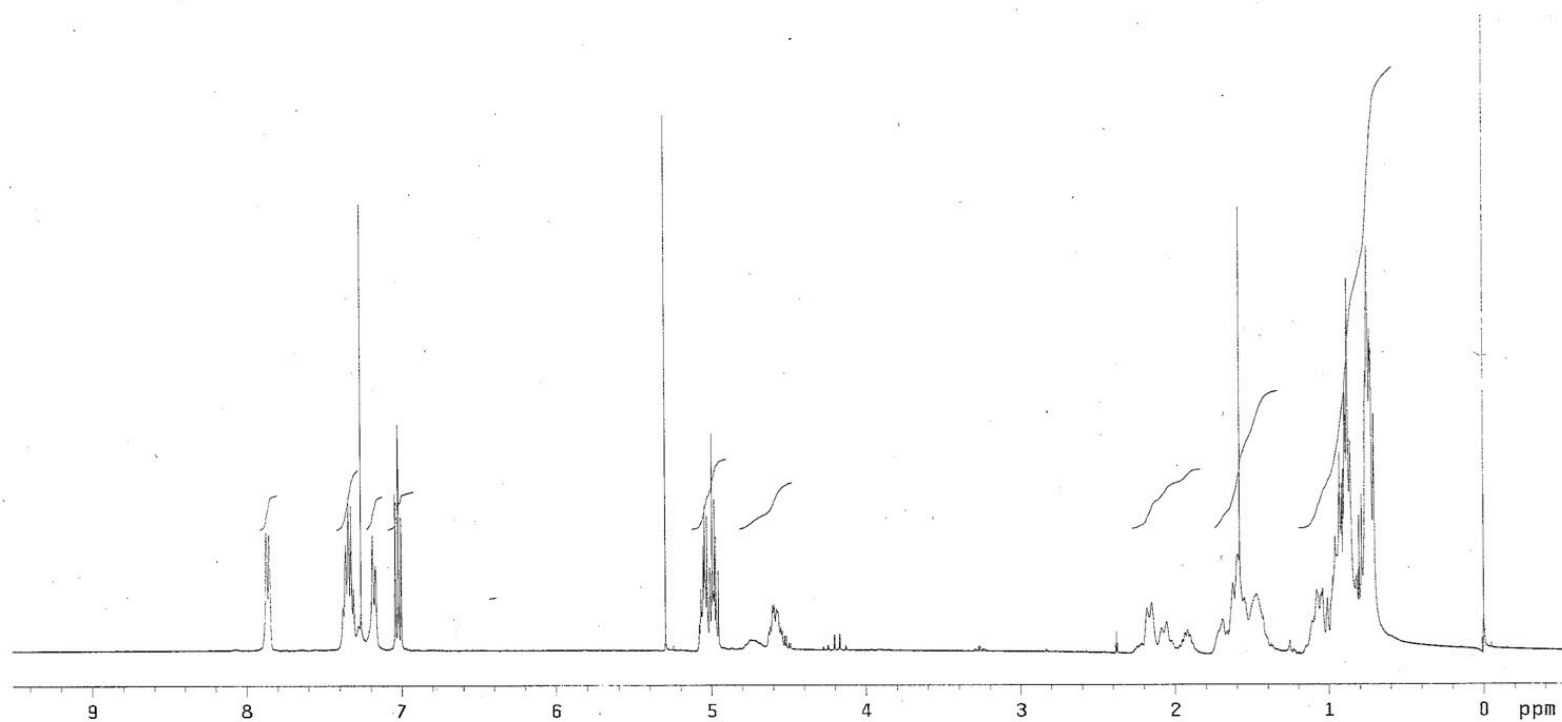
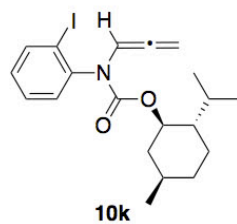
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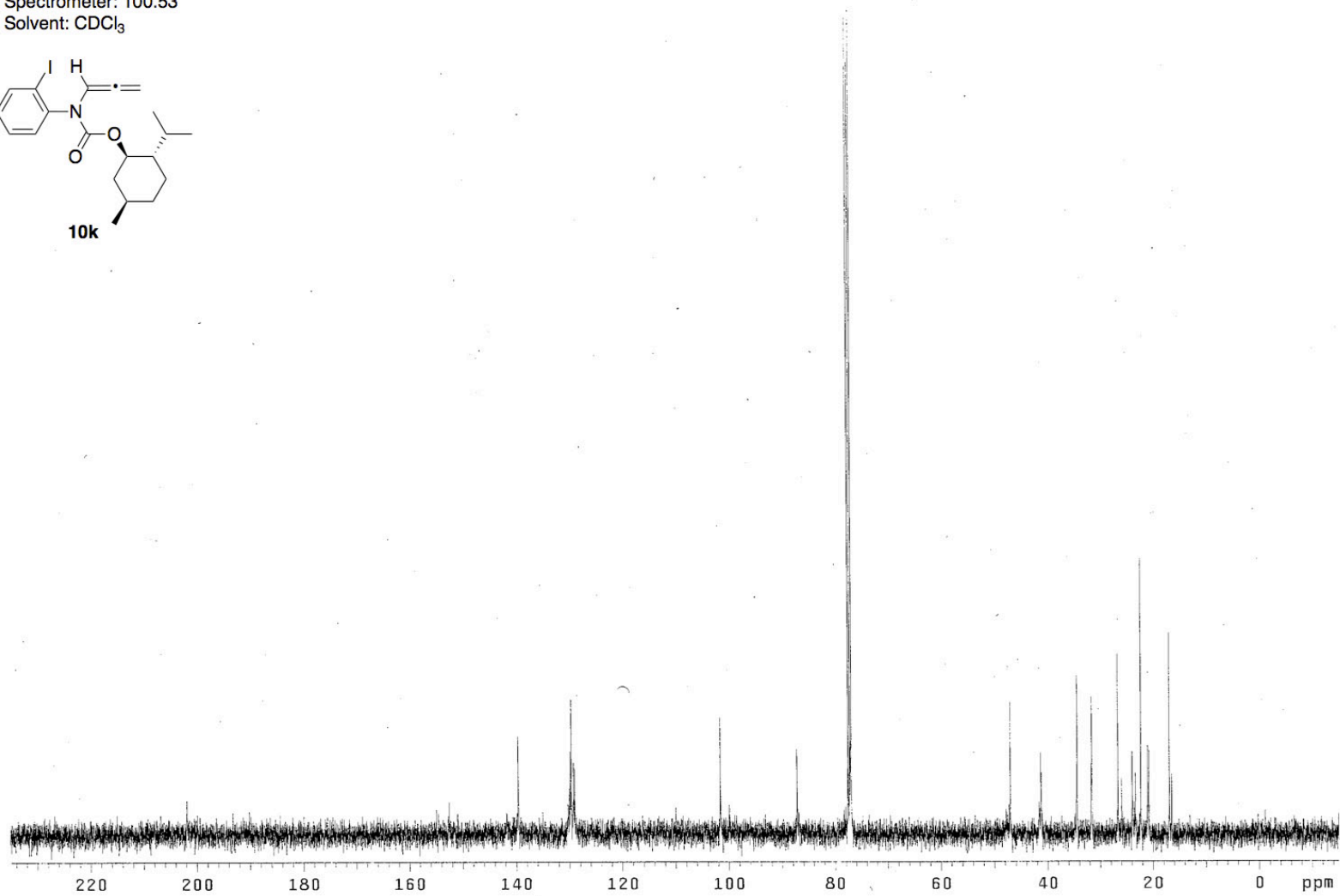
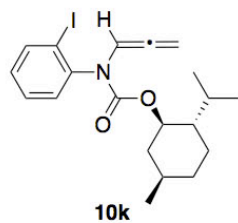
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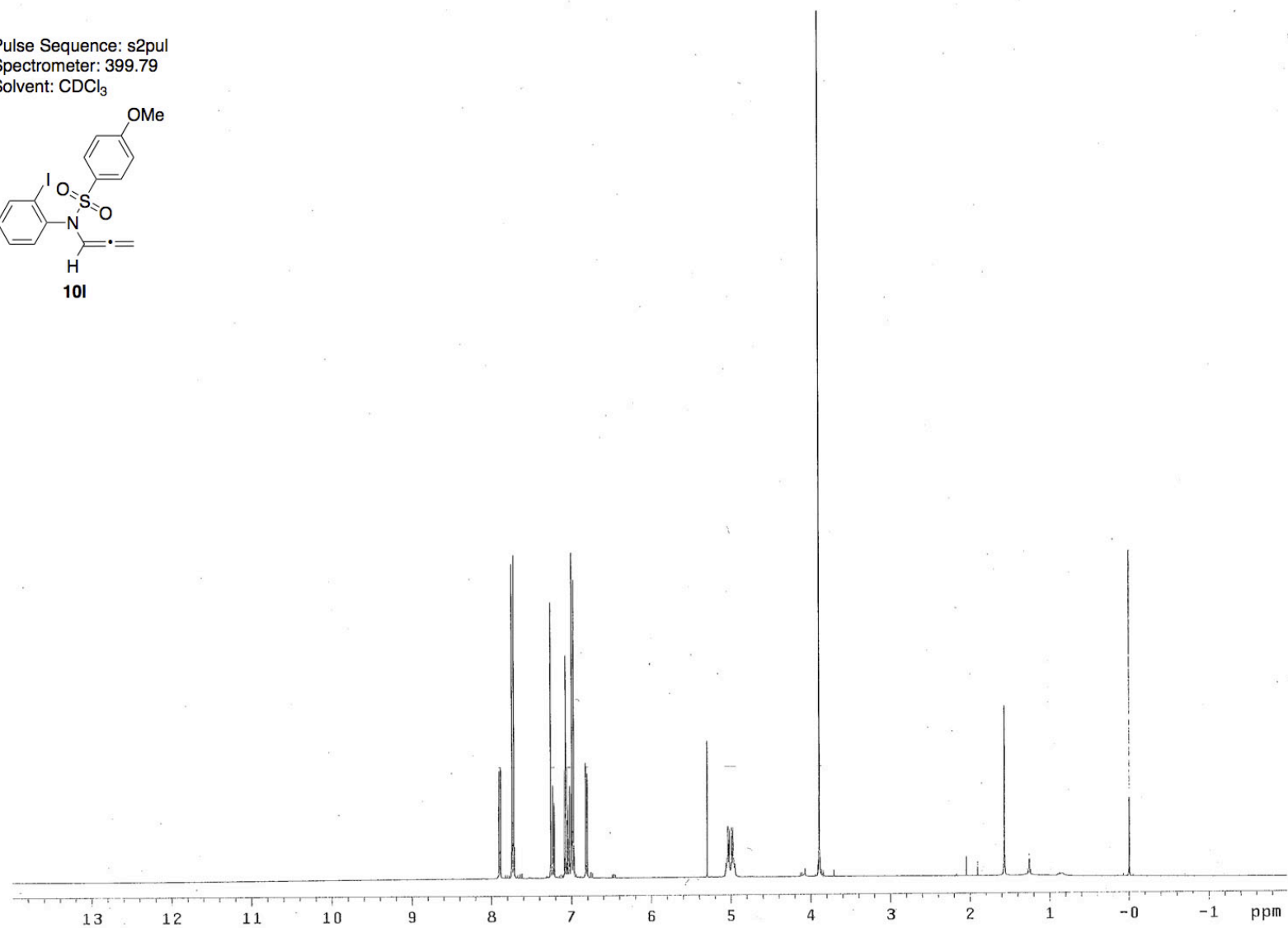
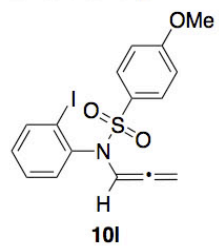
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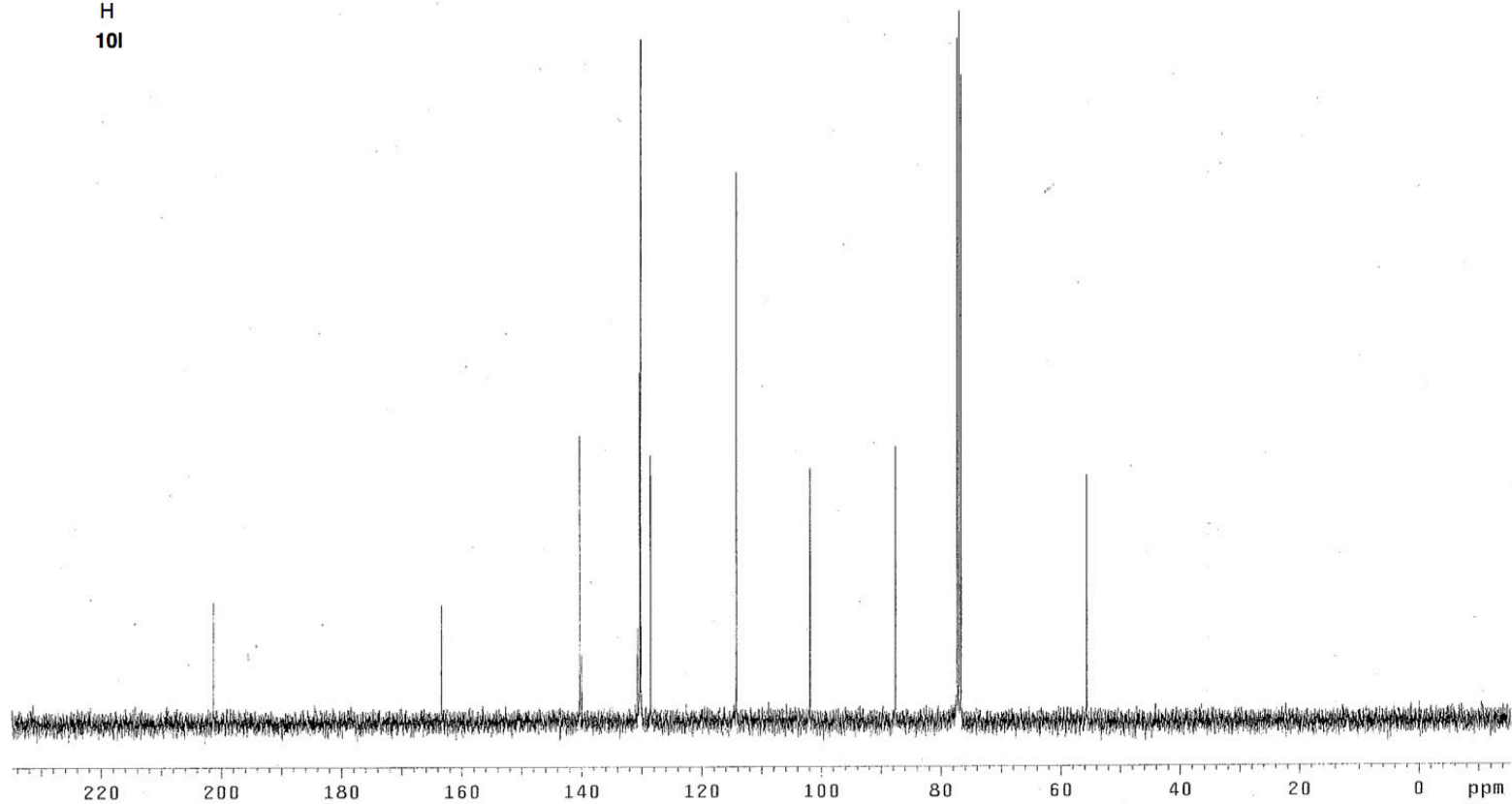
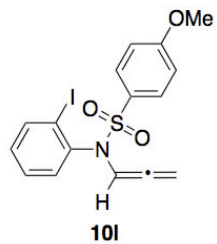
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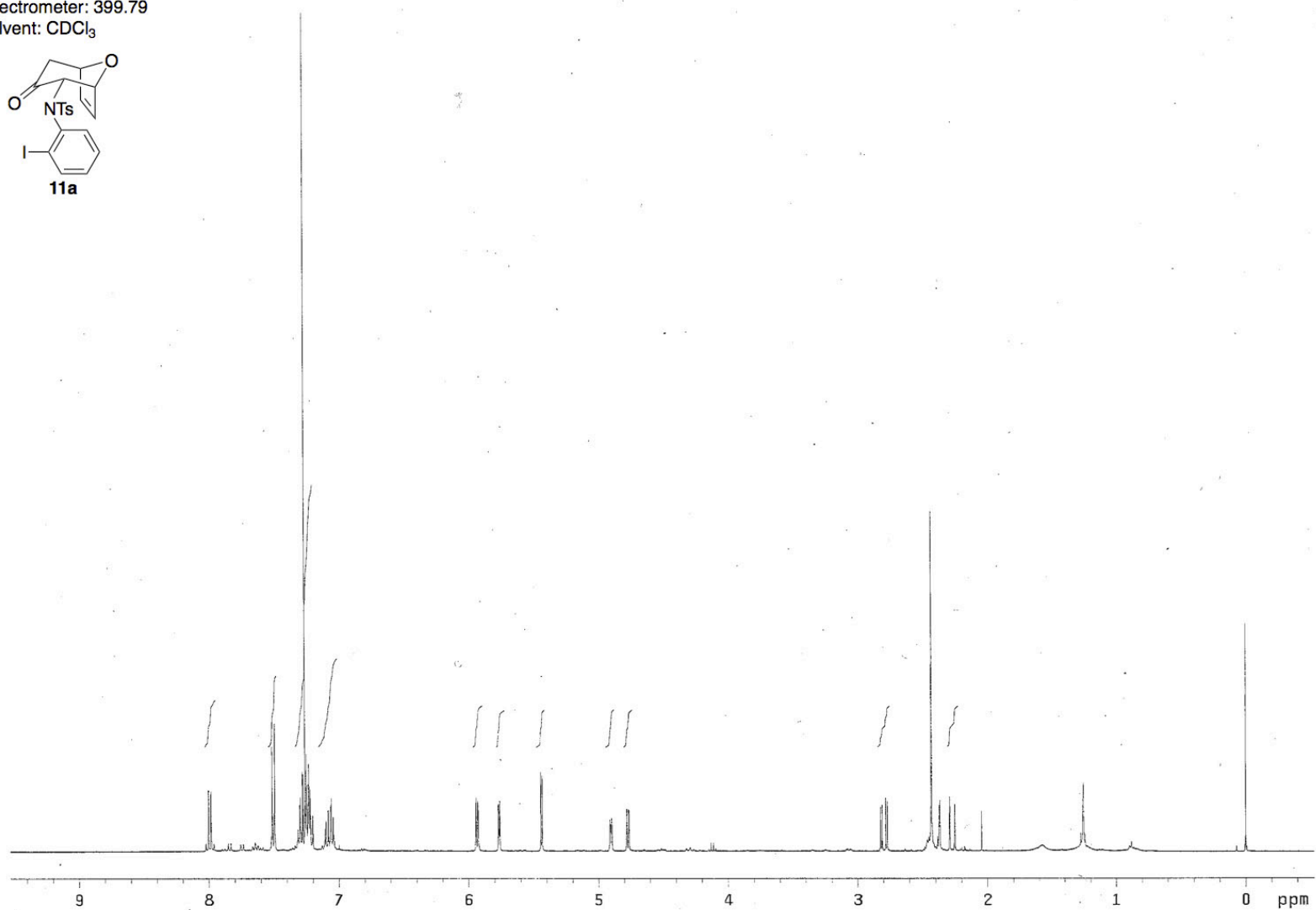
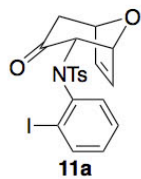
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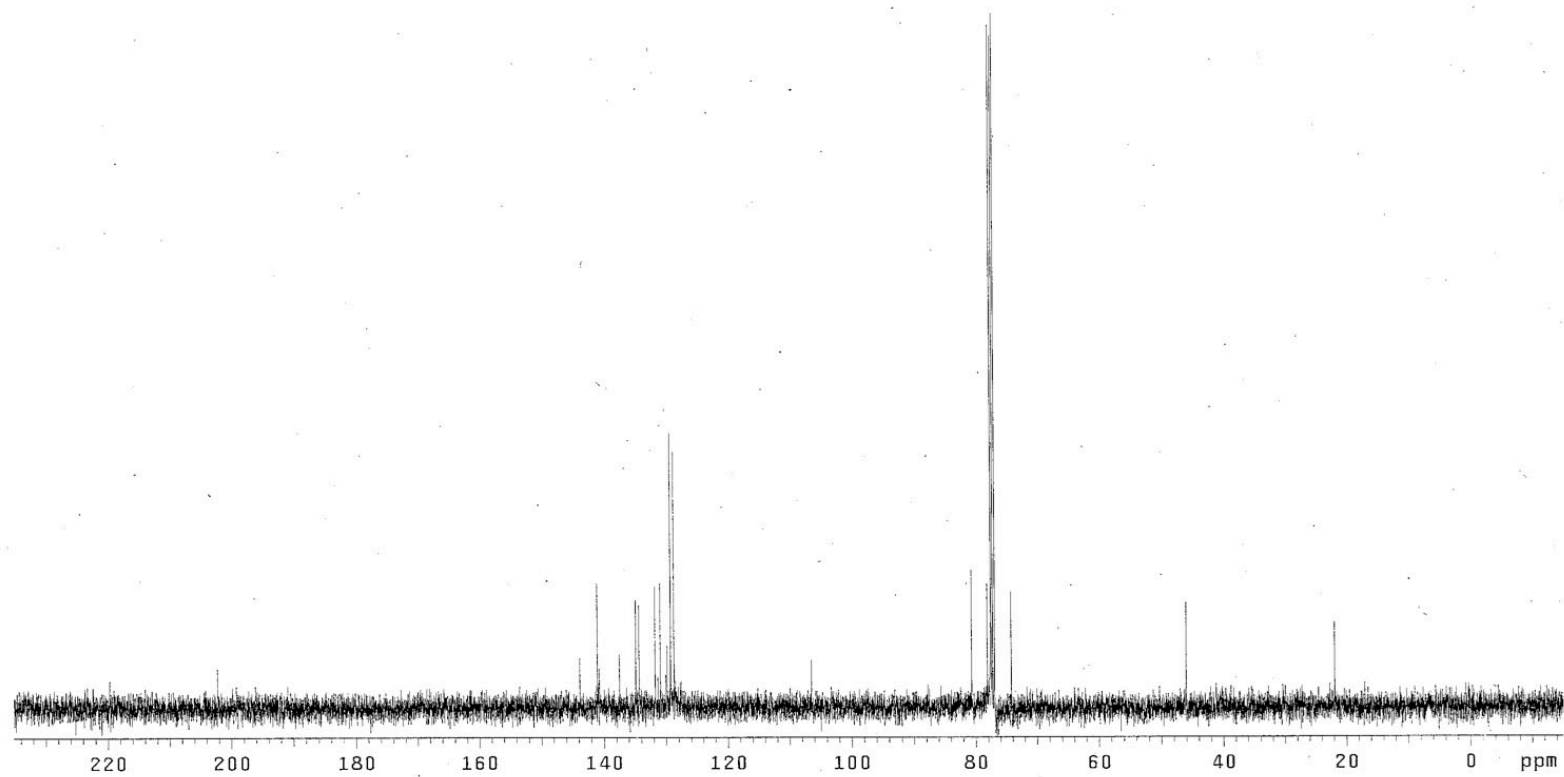
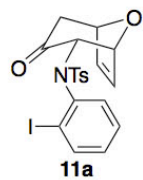
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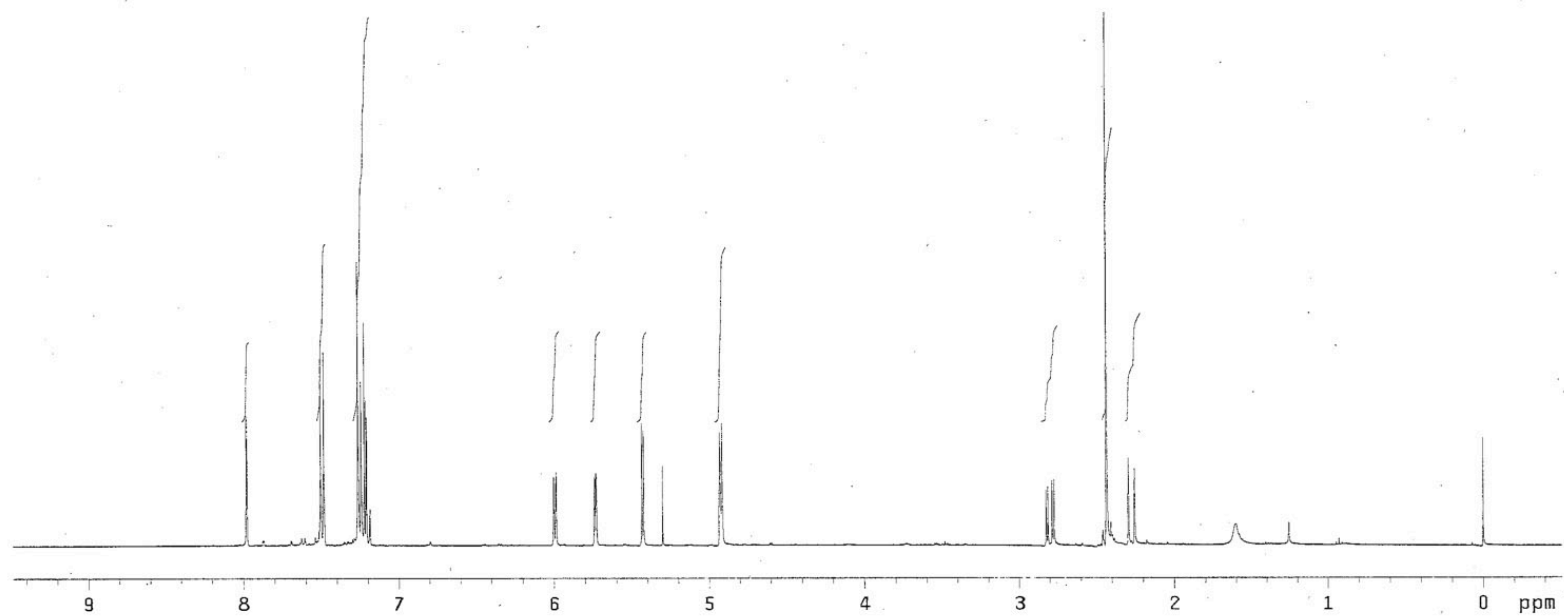
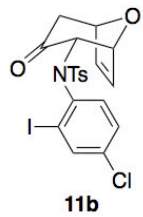
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



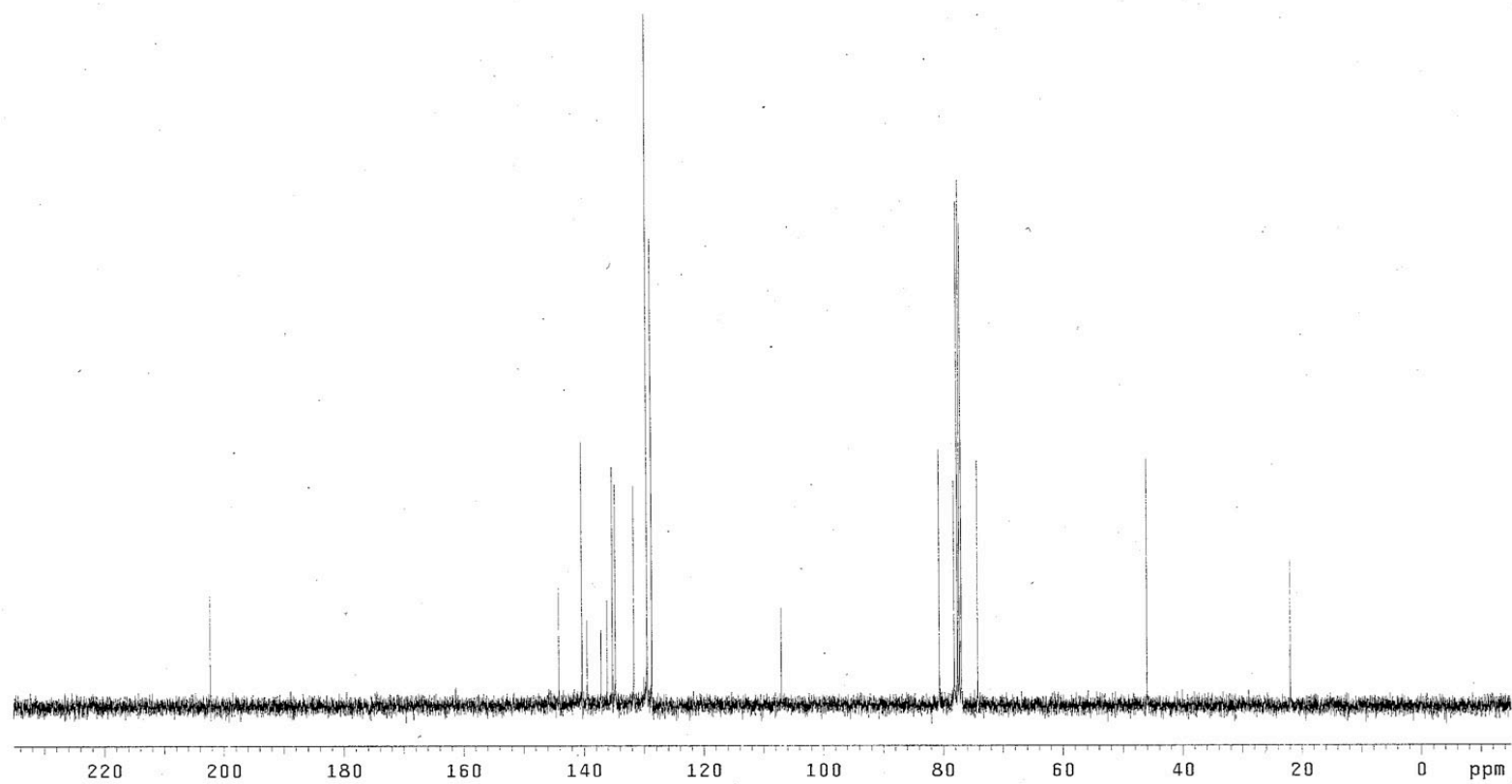
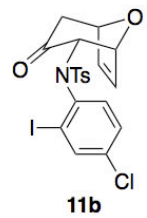
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



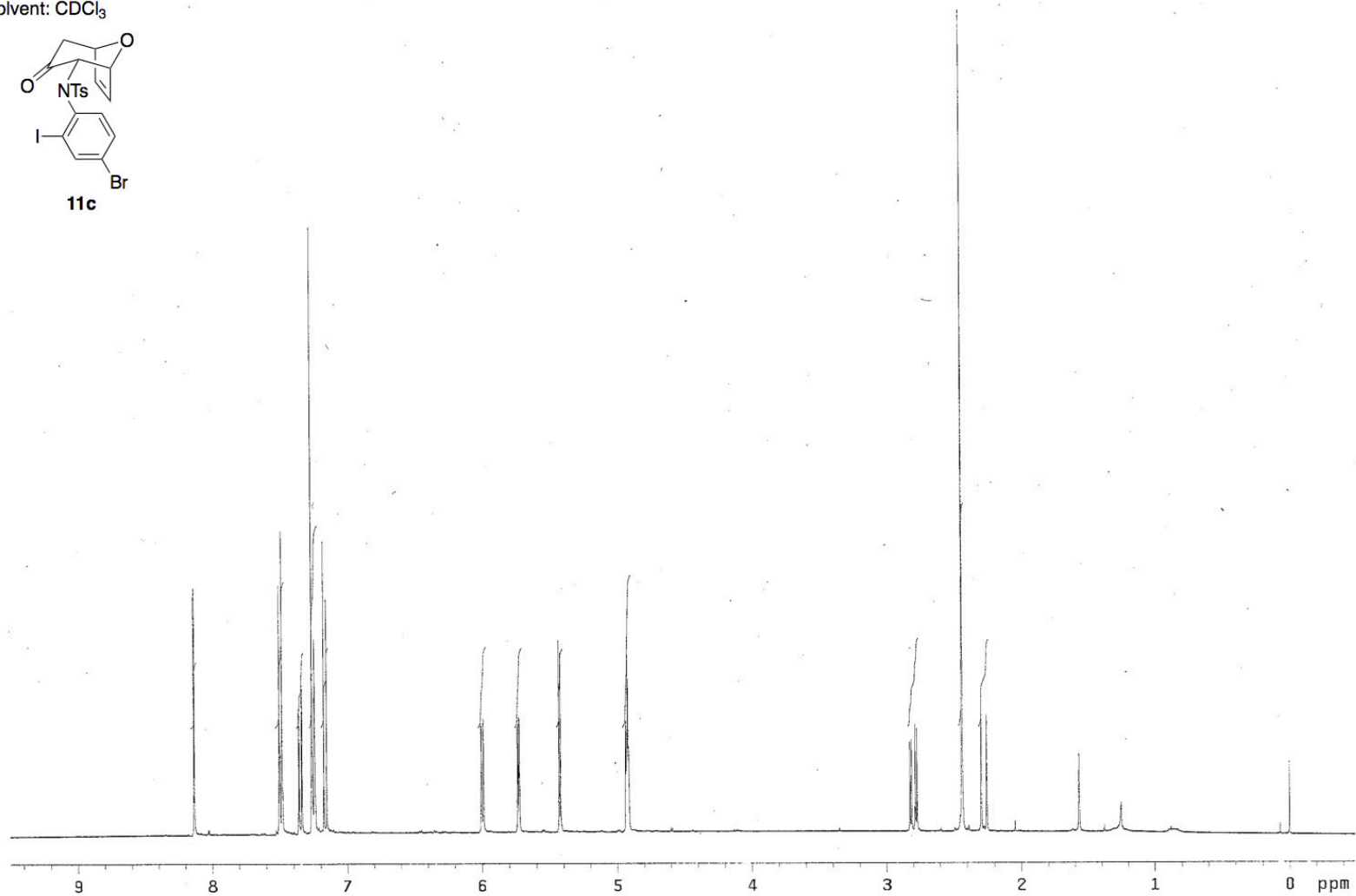
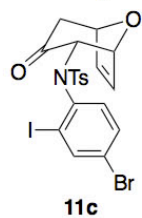
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



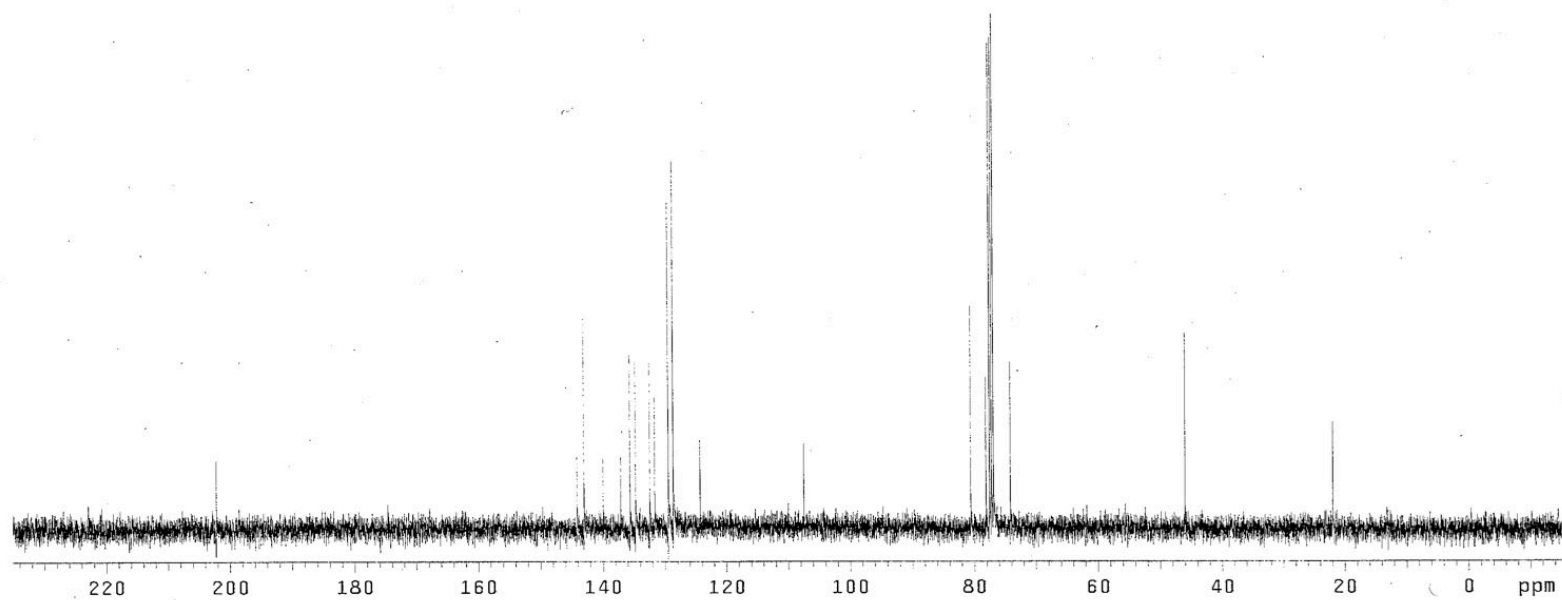
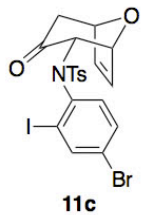
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



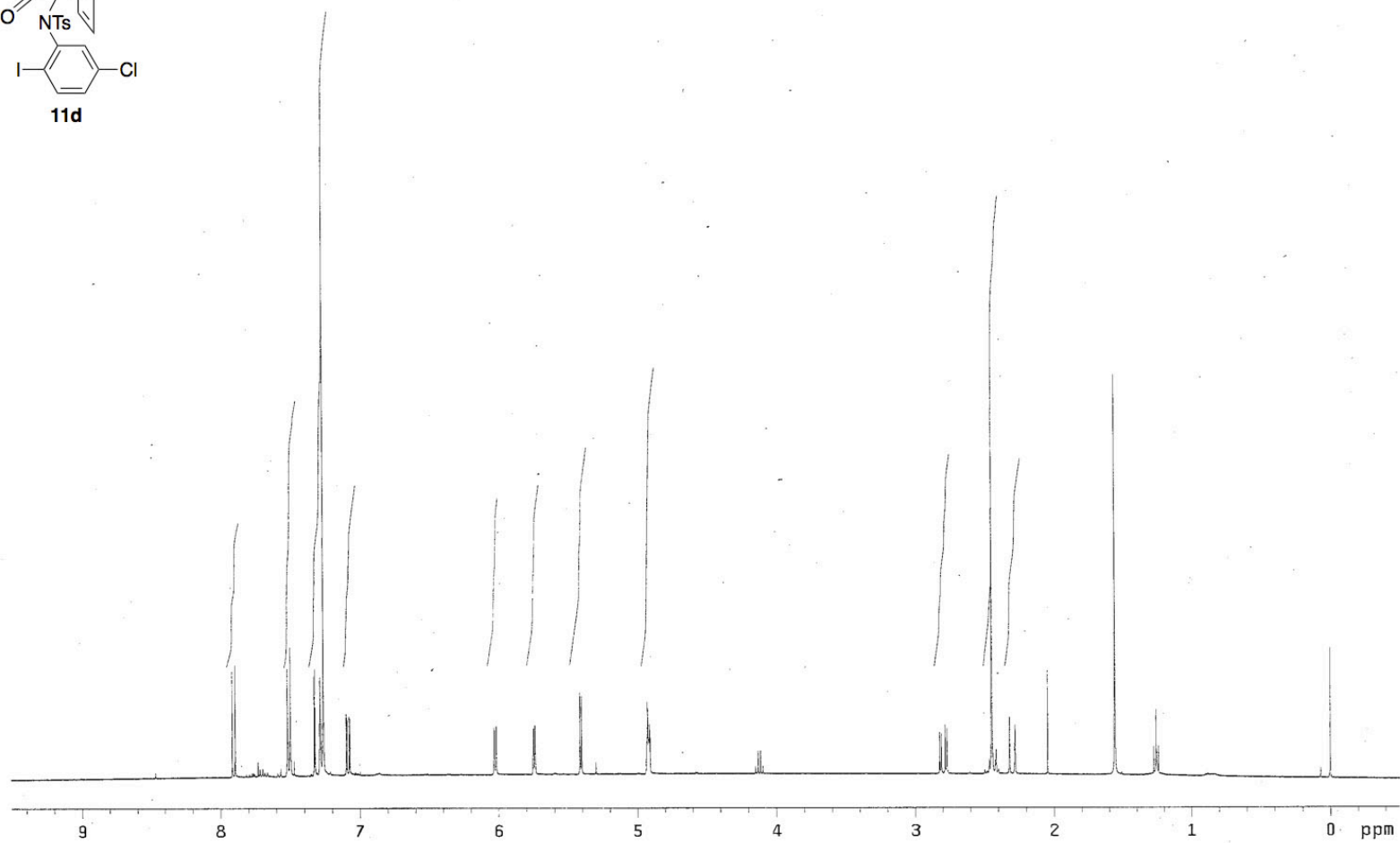
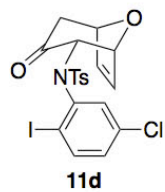
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



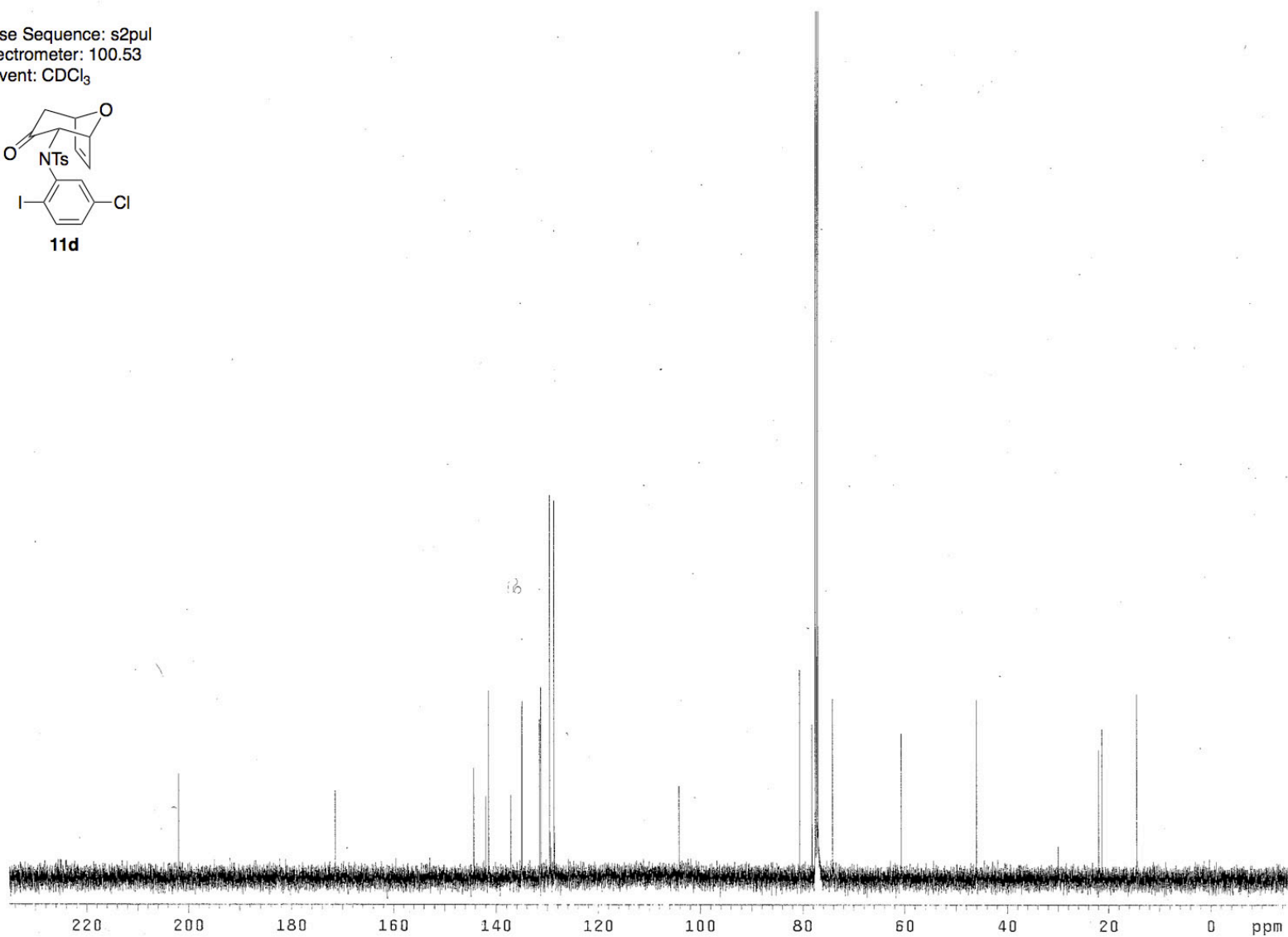
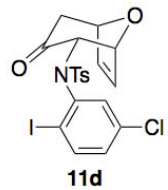
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



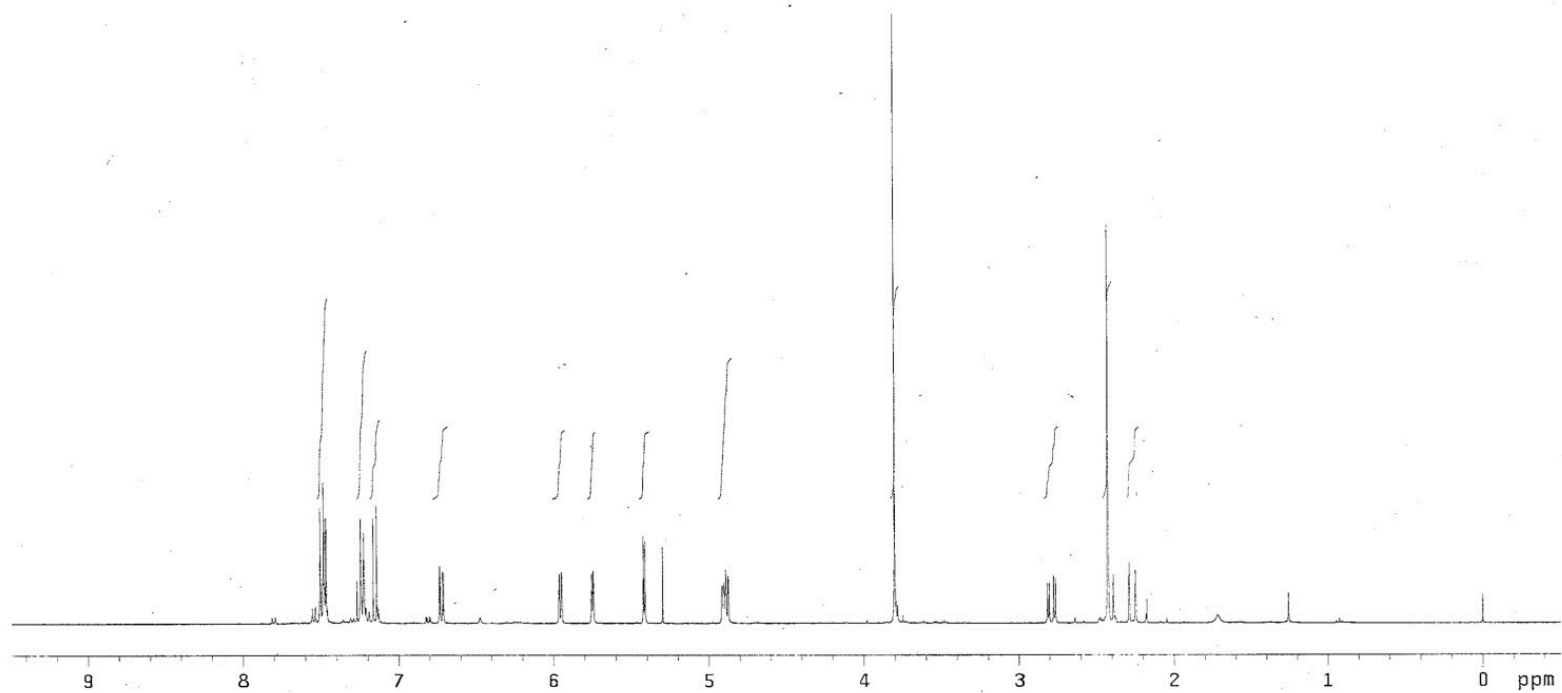
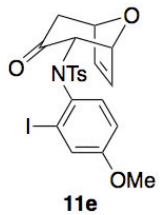
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



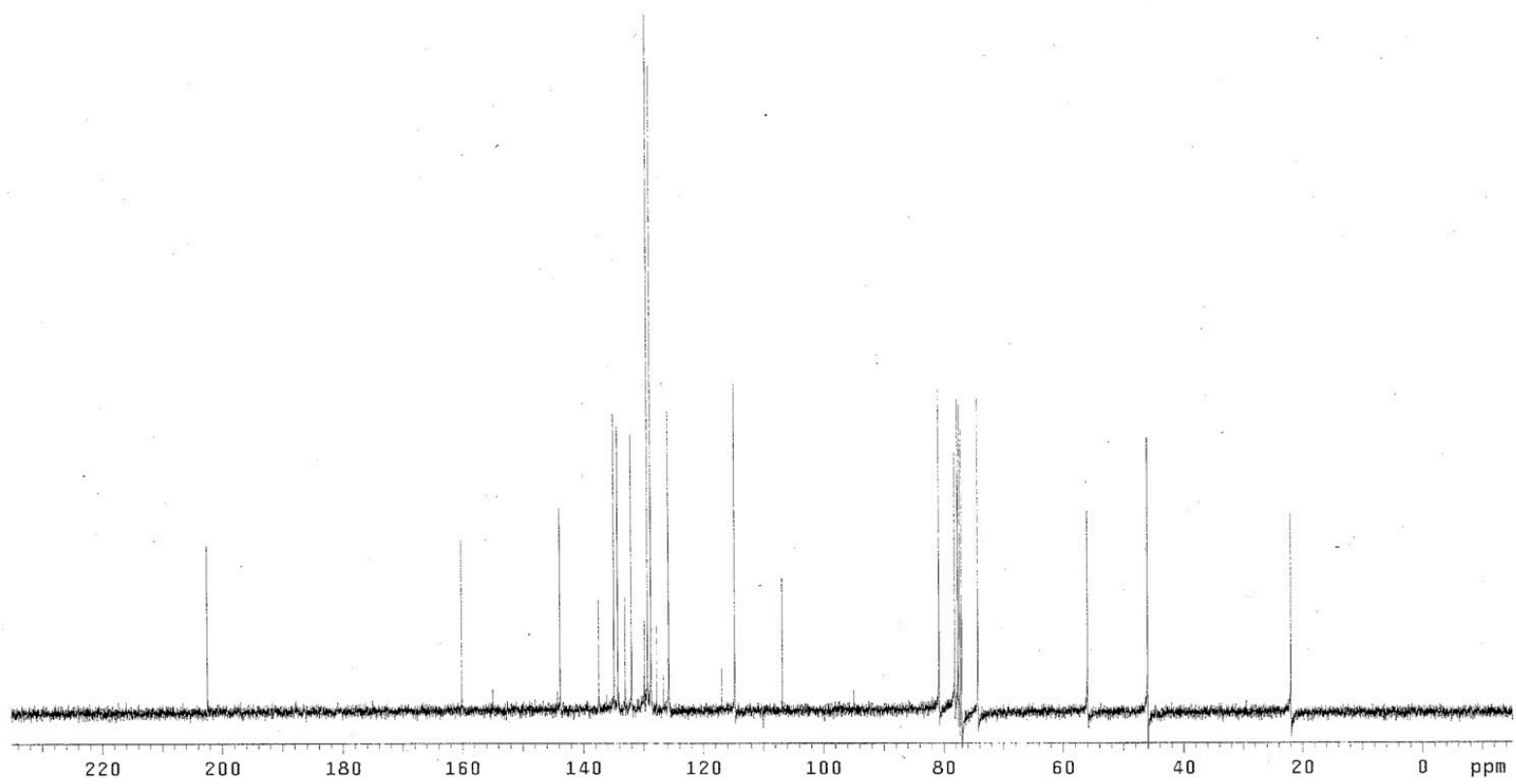
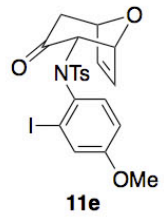
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



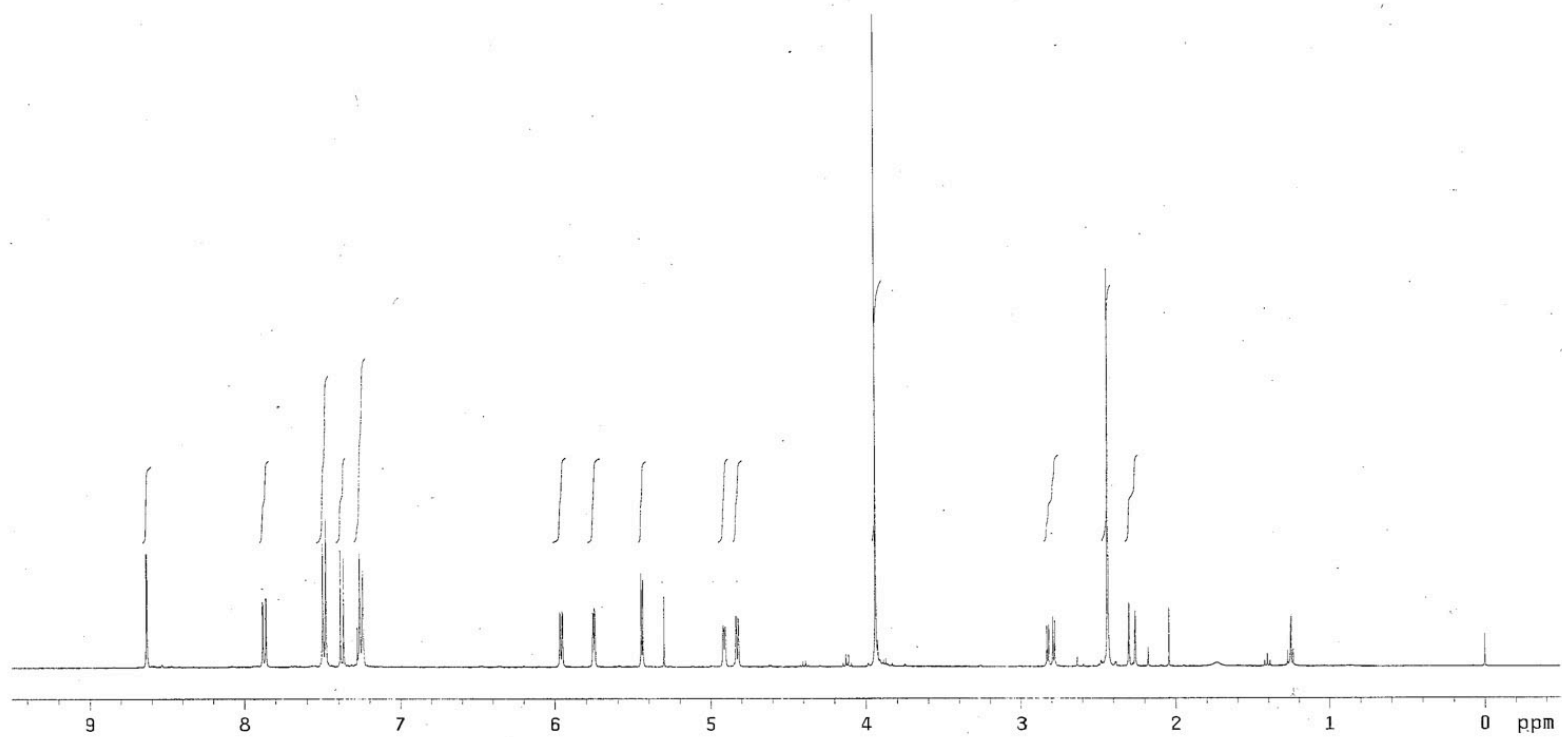
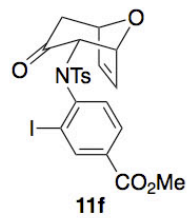
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



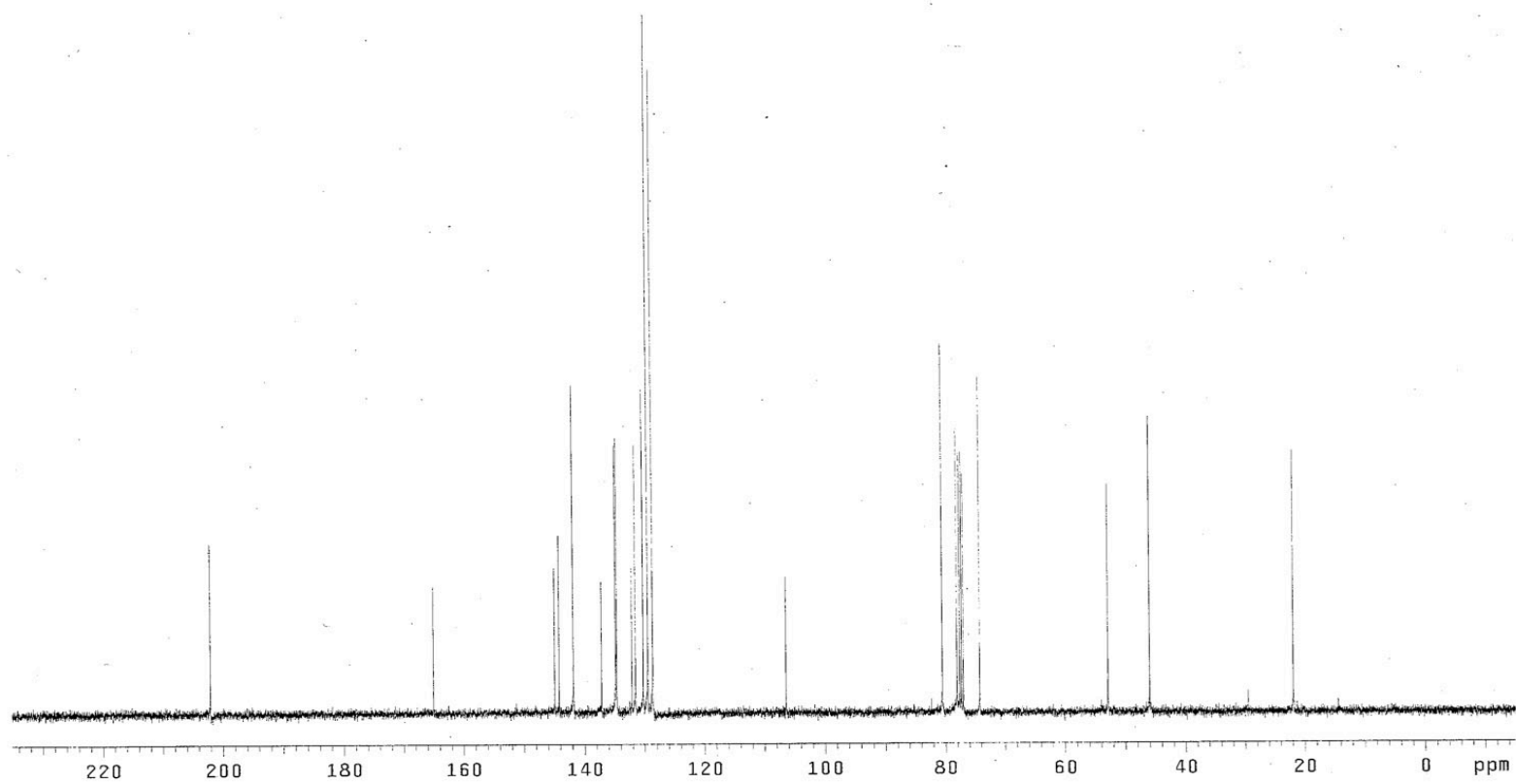
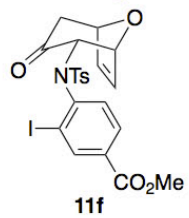
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



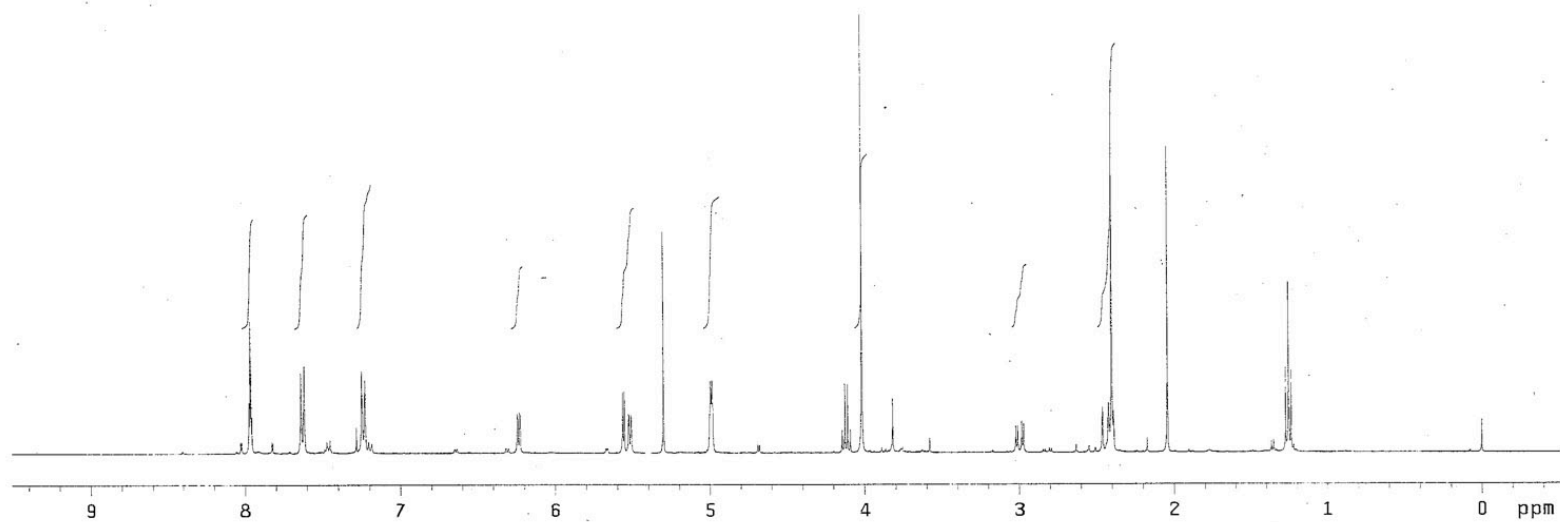
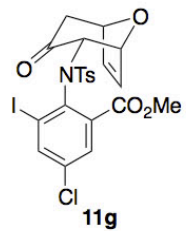
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



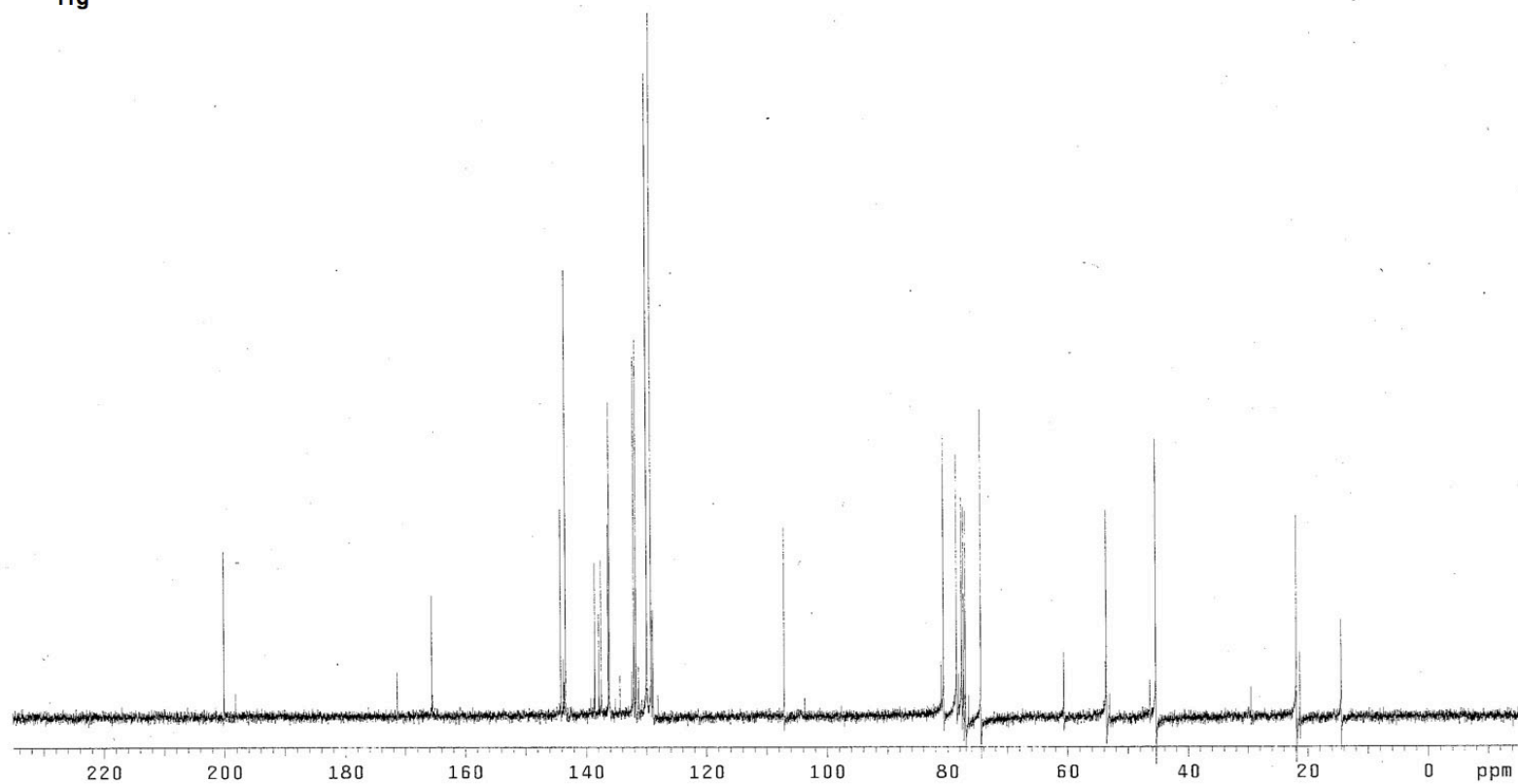
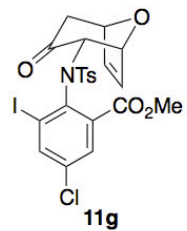
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



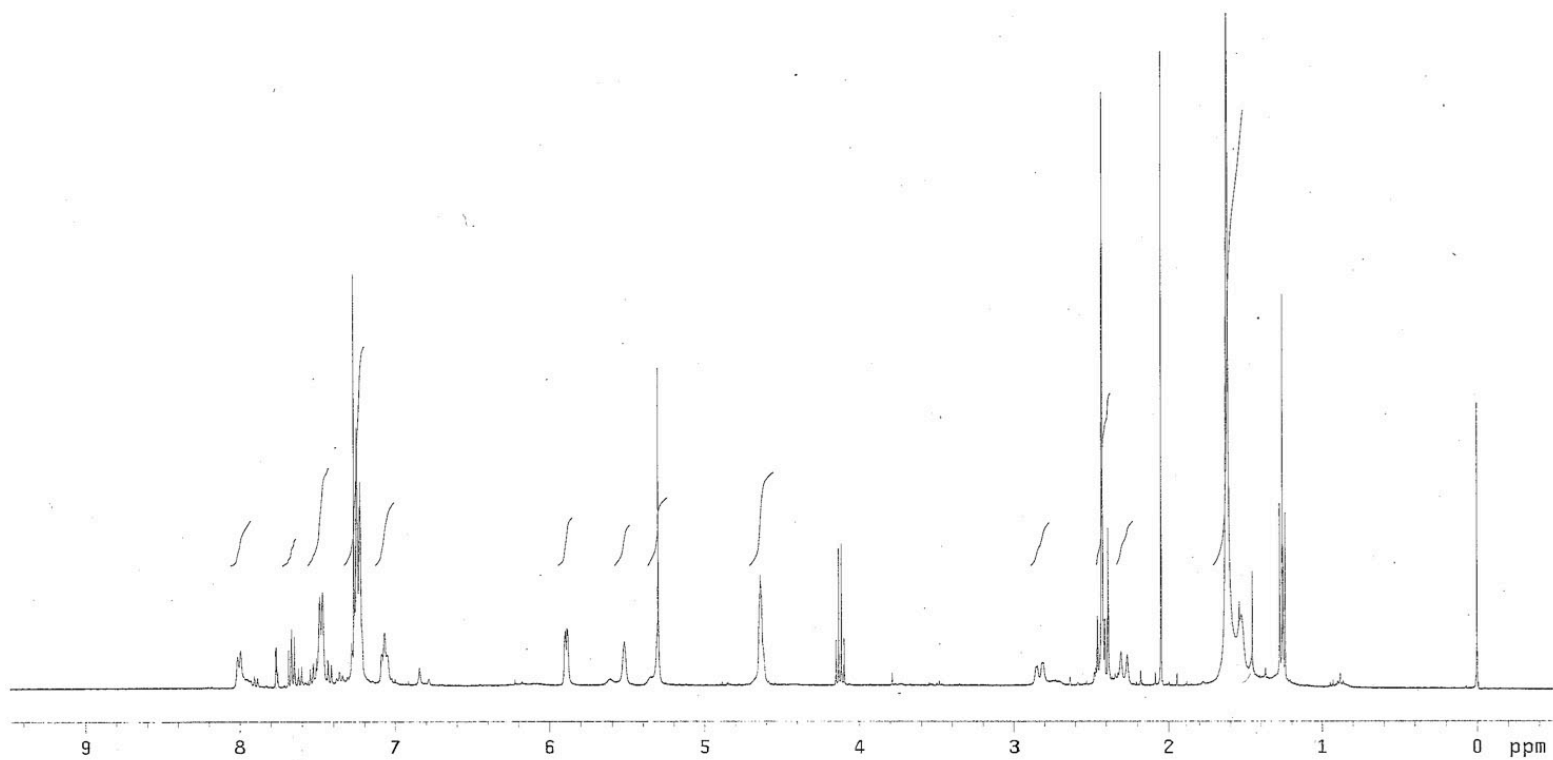
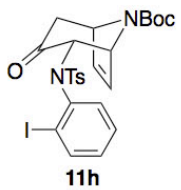
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



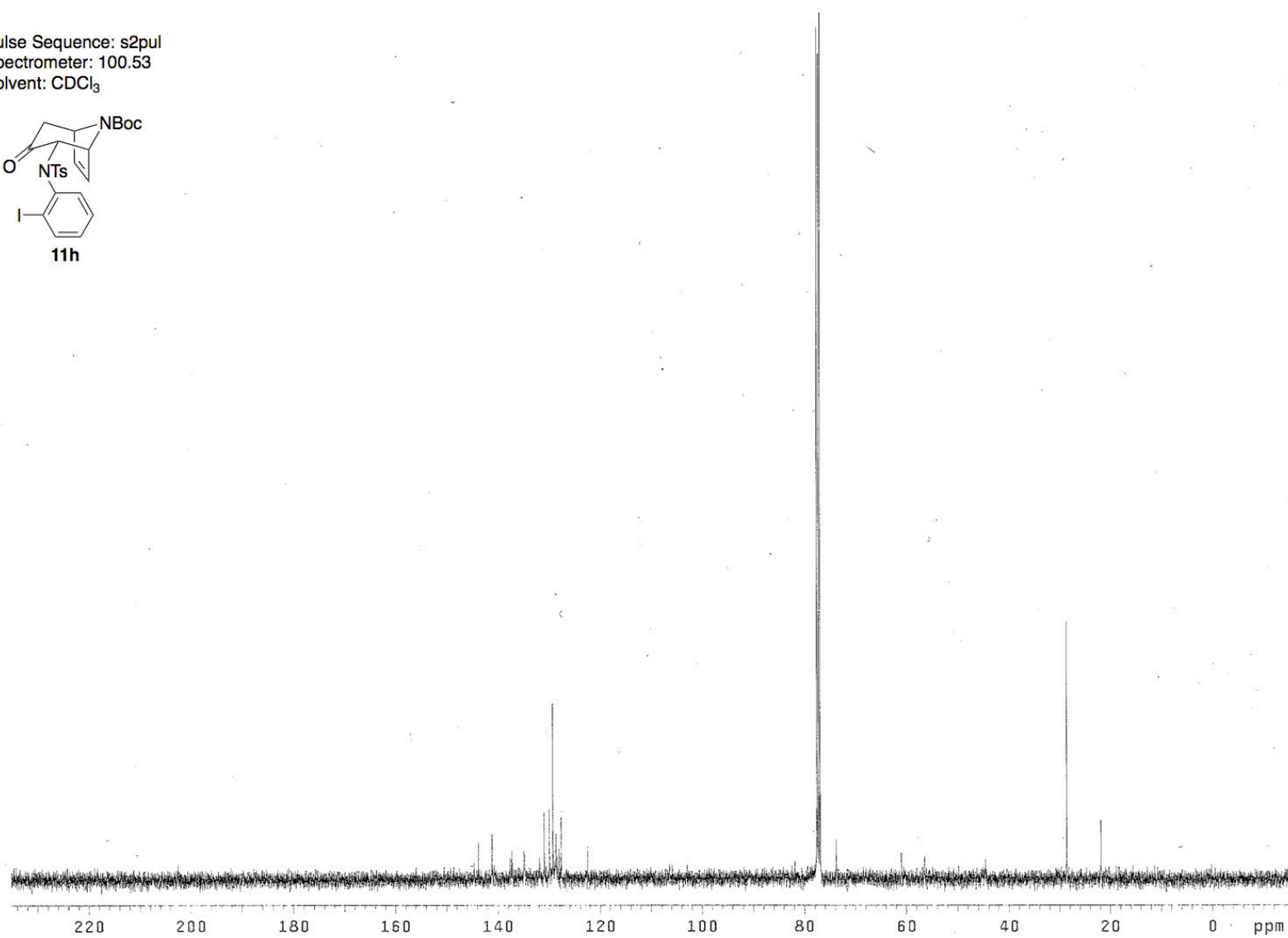
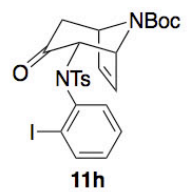
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



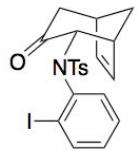
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



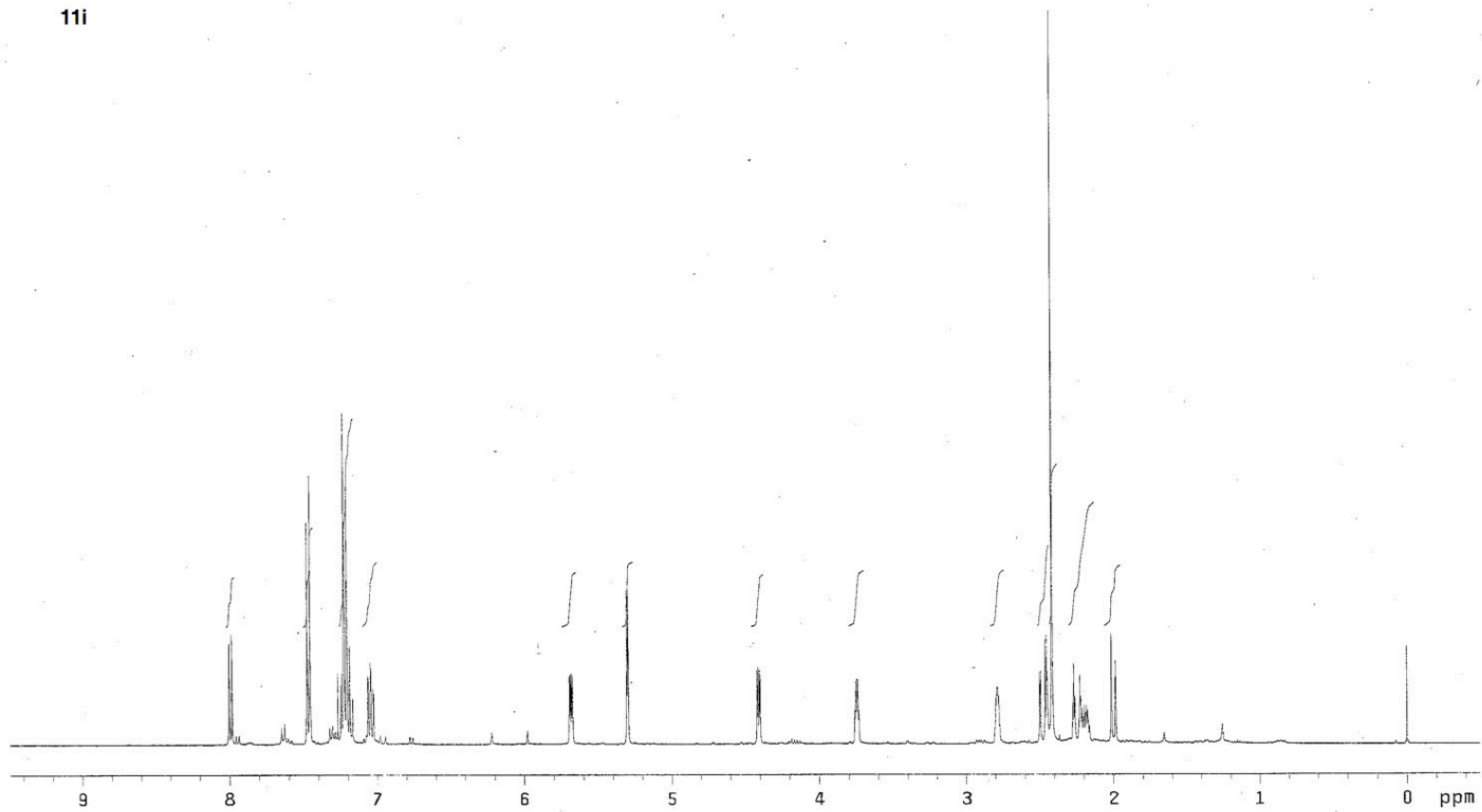
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



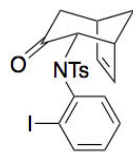
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



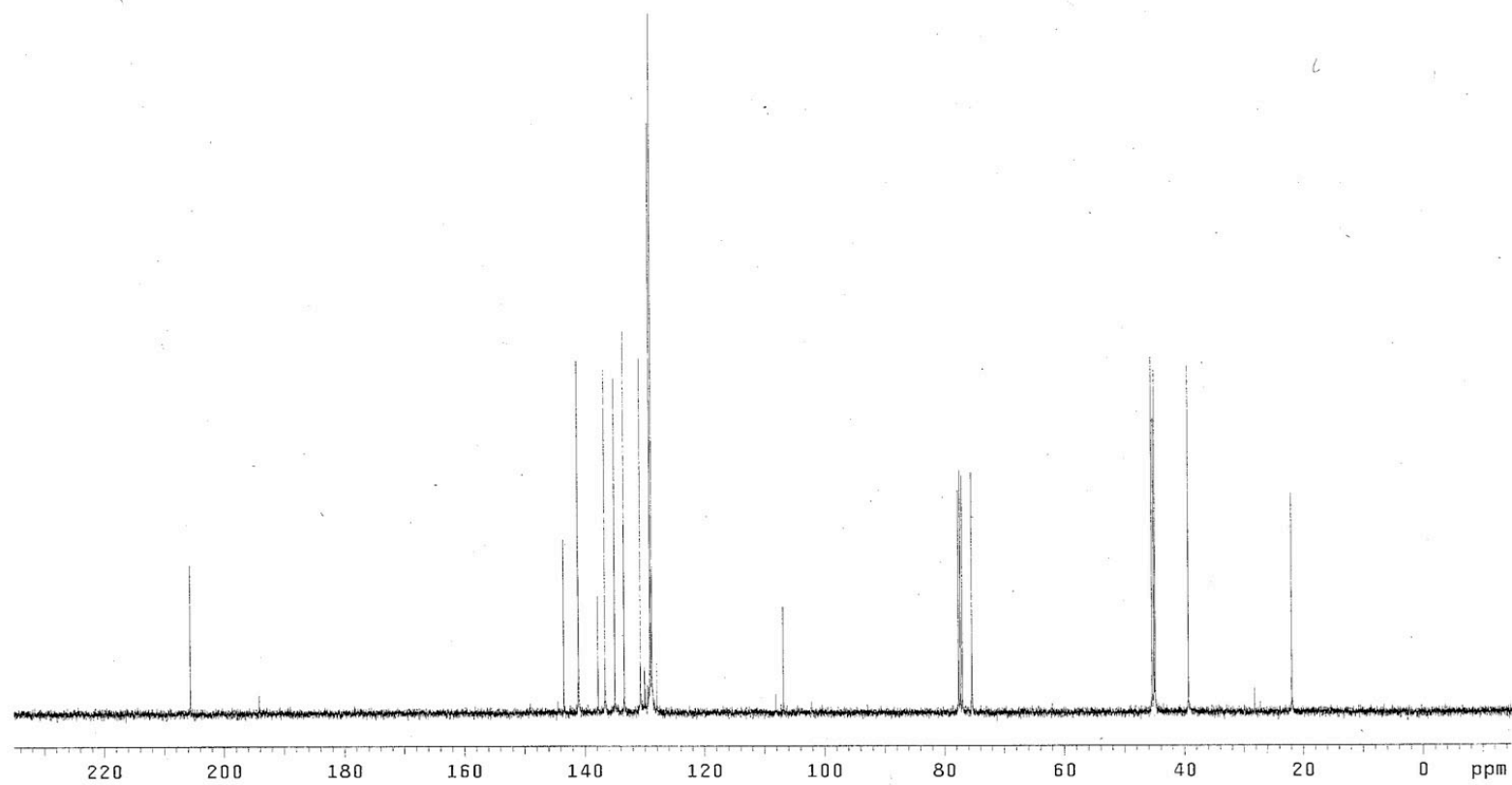
11i



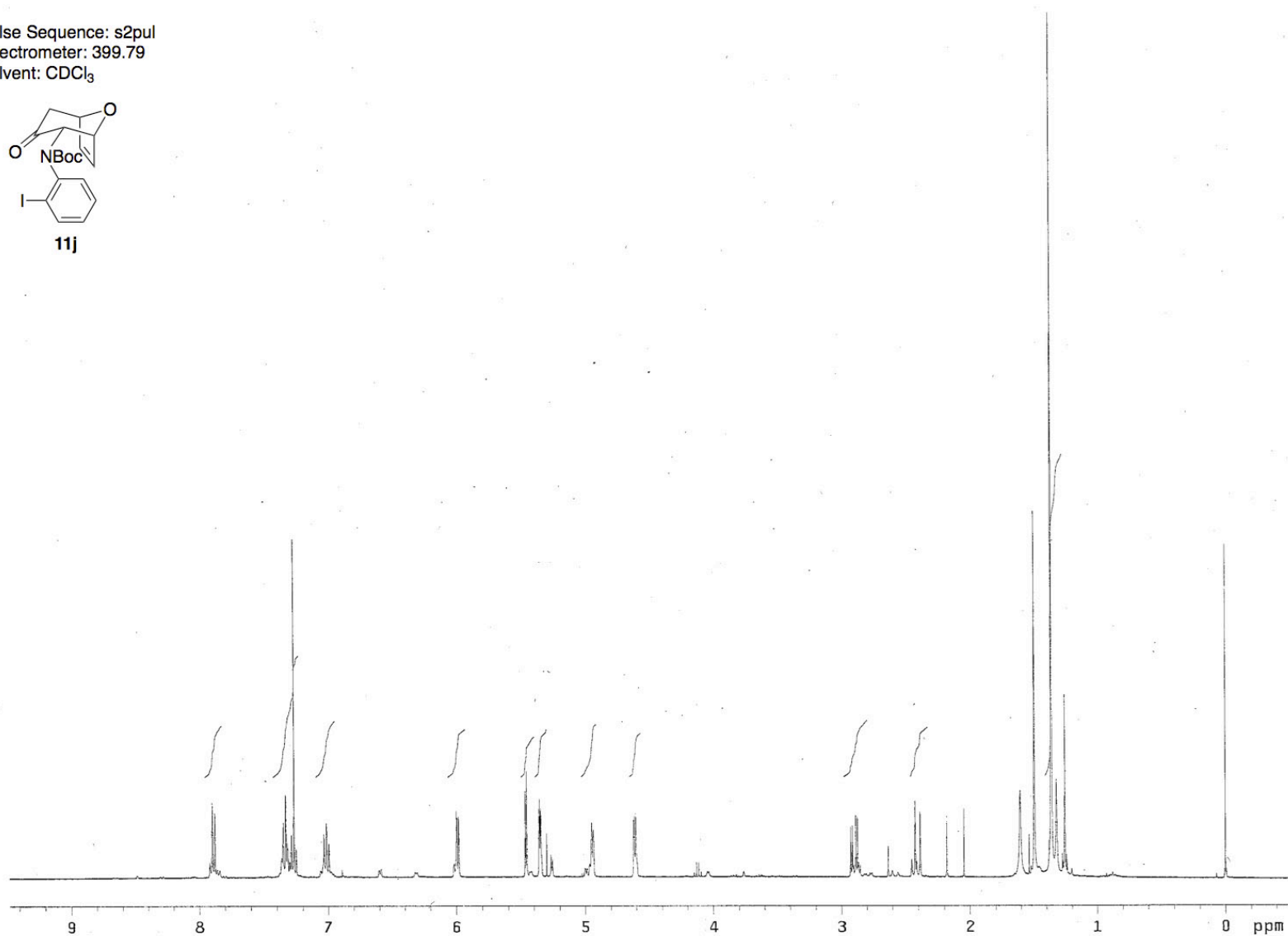
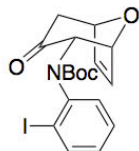
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



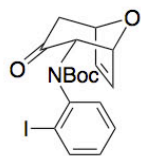
11i



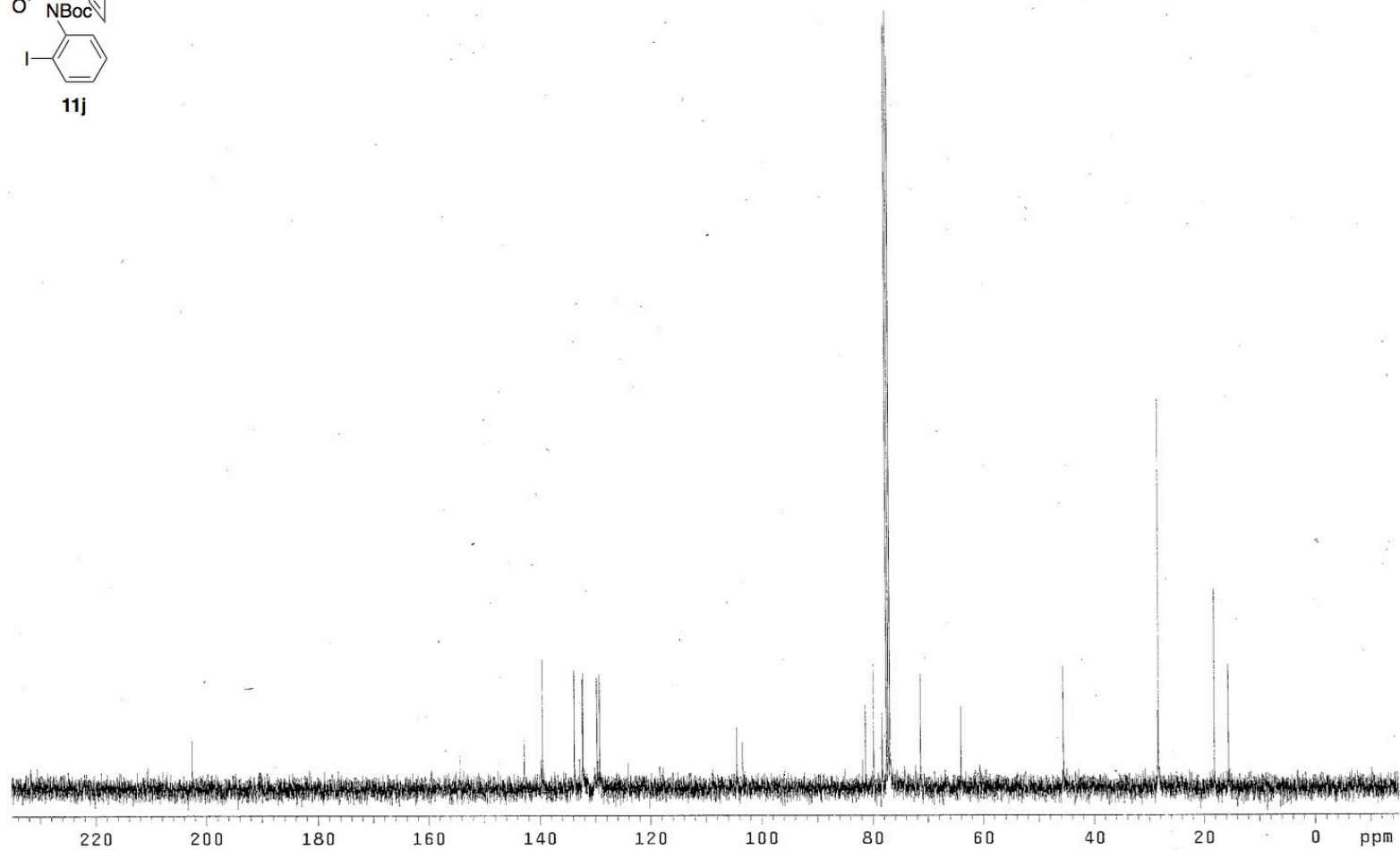
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



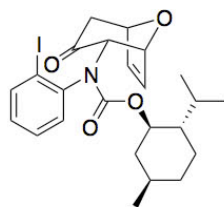
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



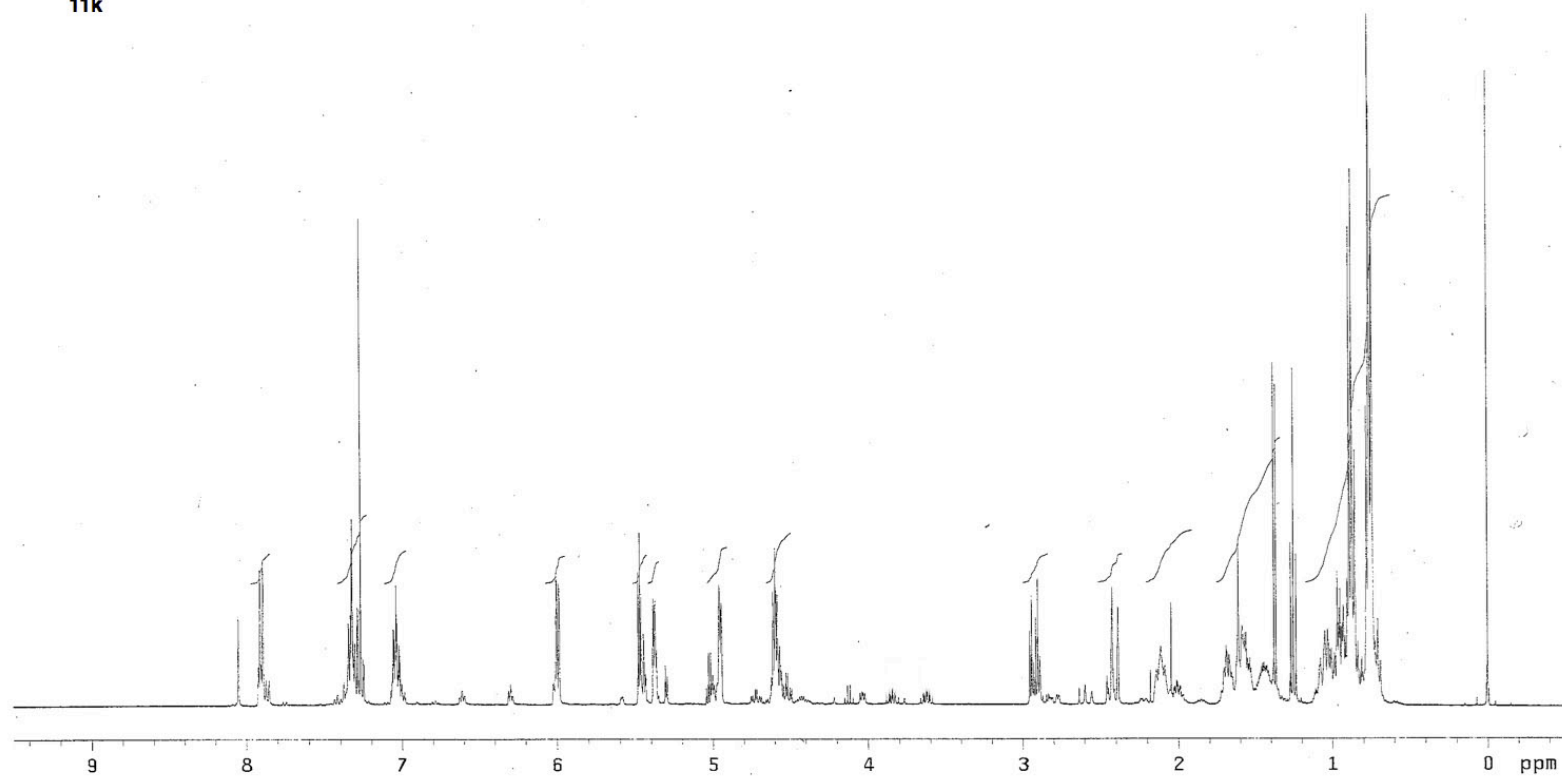
11j



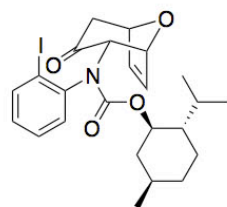
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



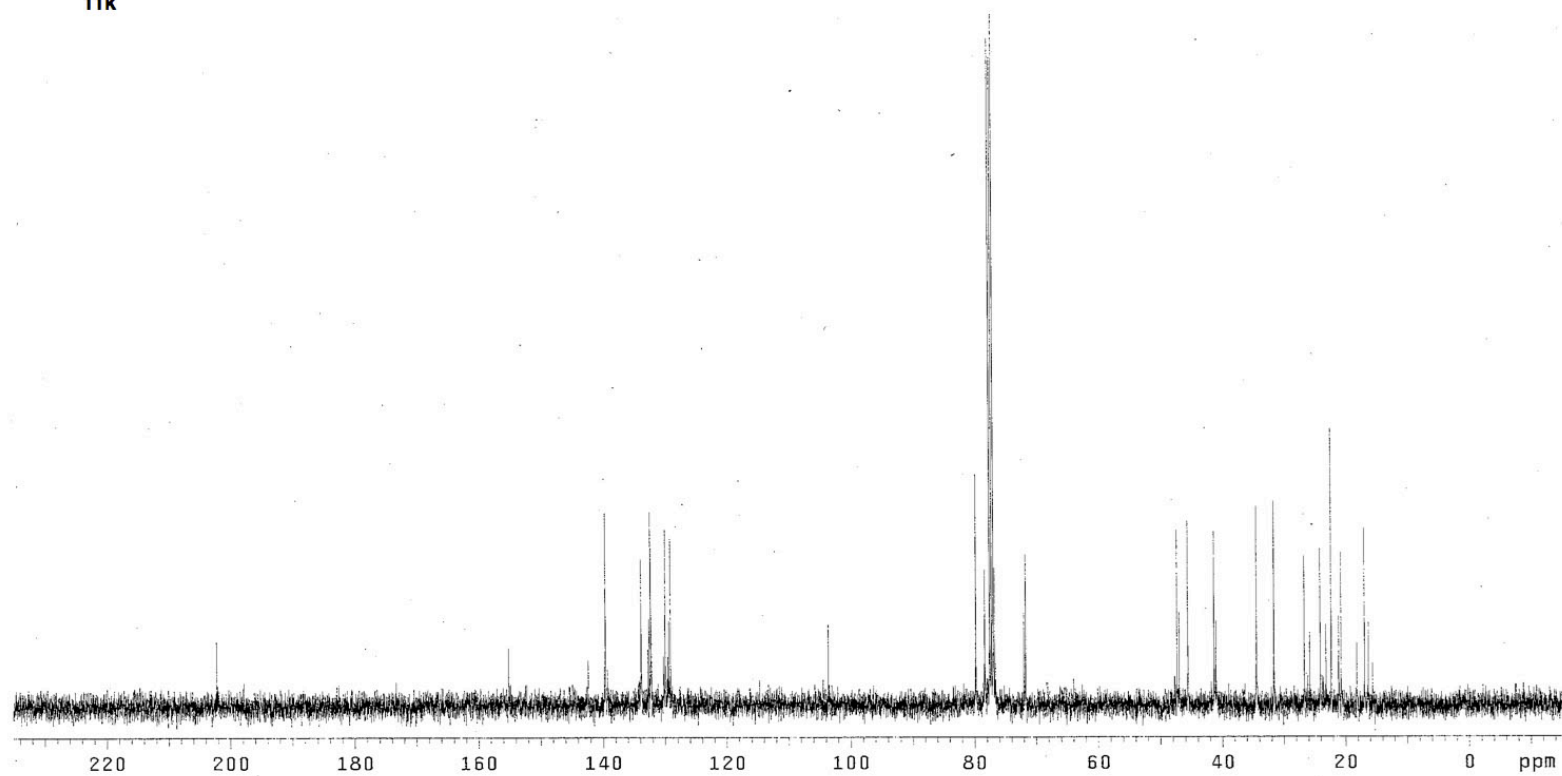
11k



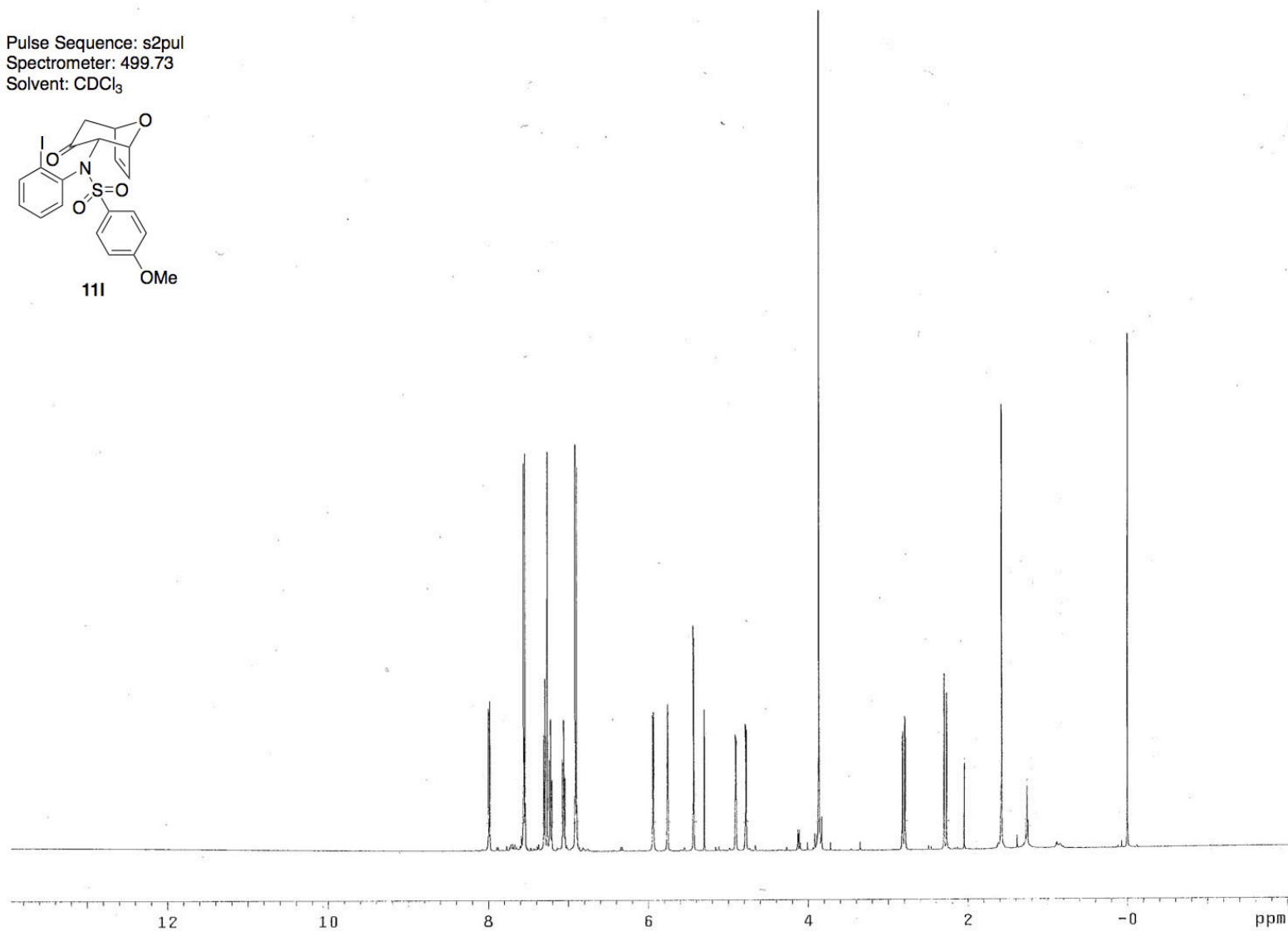
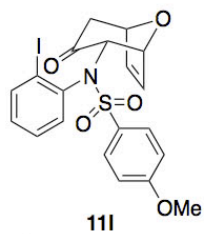
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



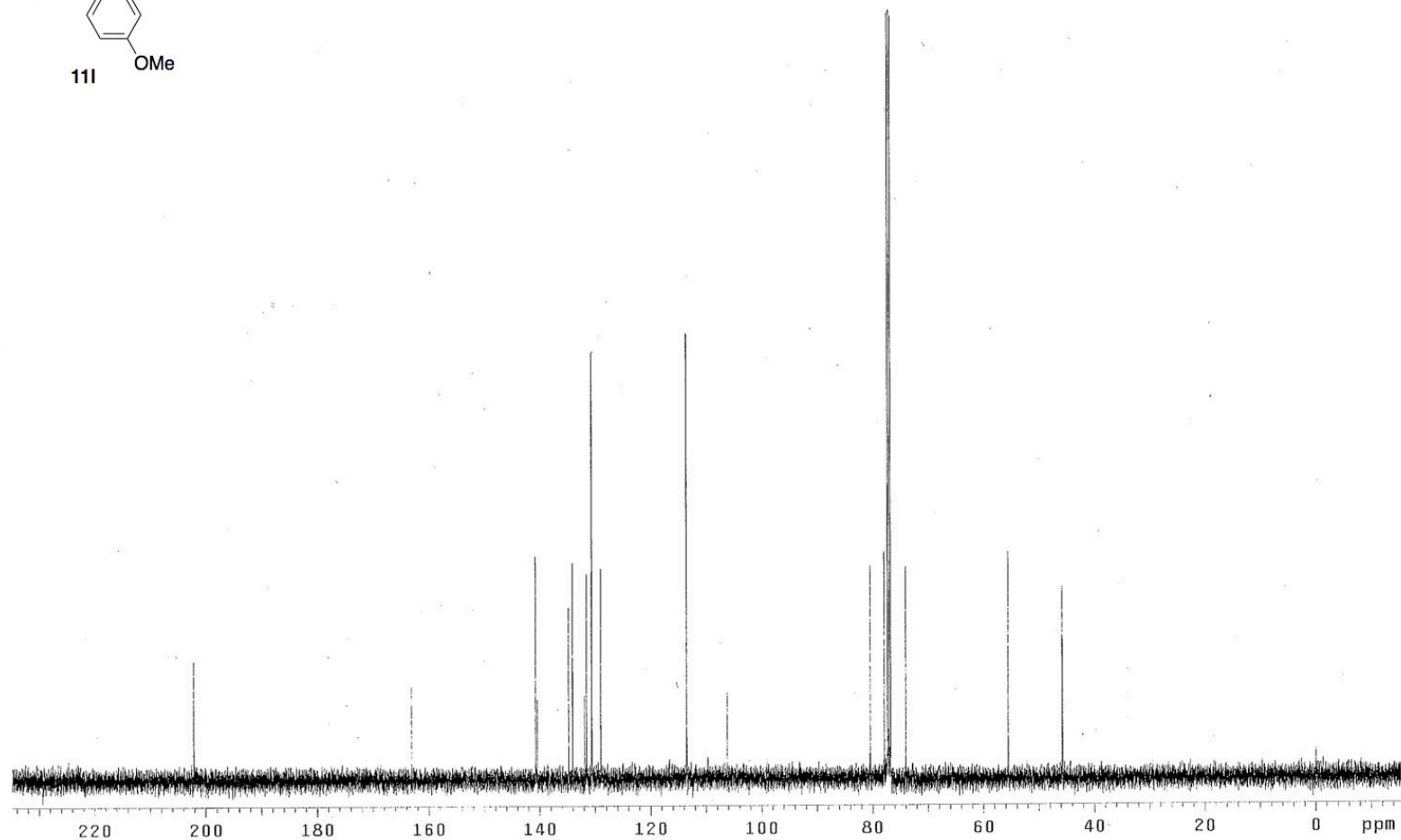
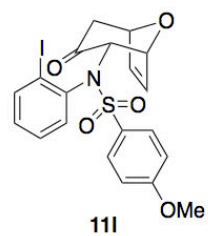
11k



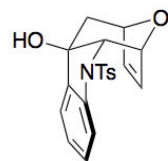
Pulse Sequence: s2pul
Spectrometer: 499.73
Solvent: CDCl₃



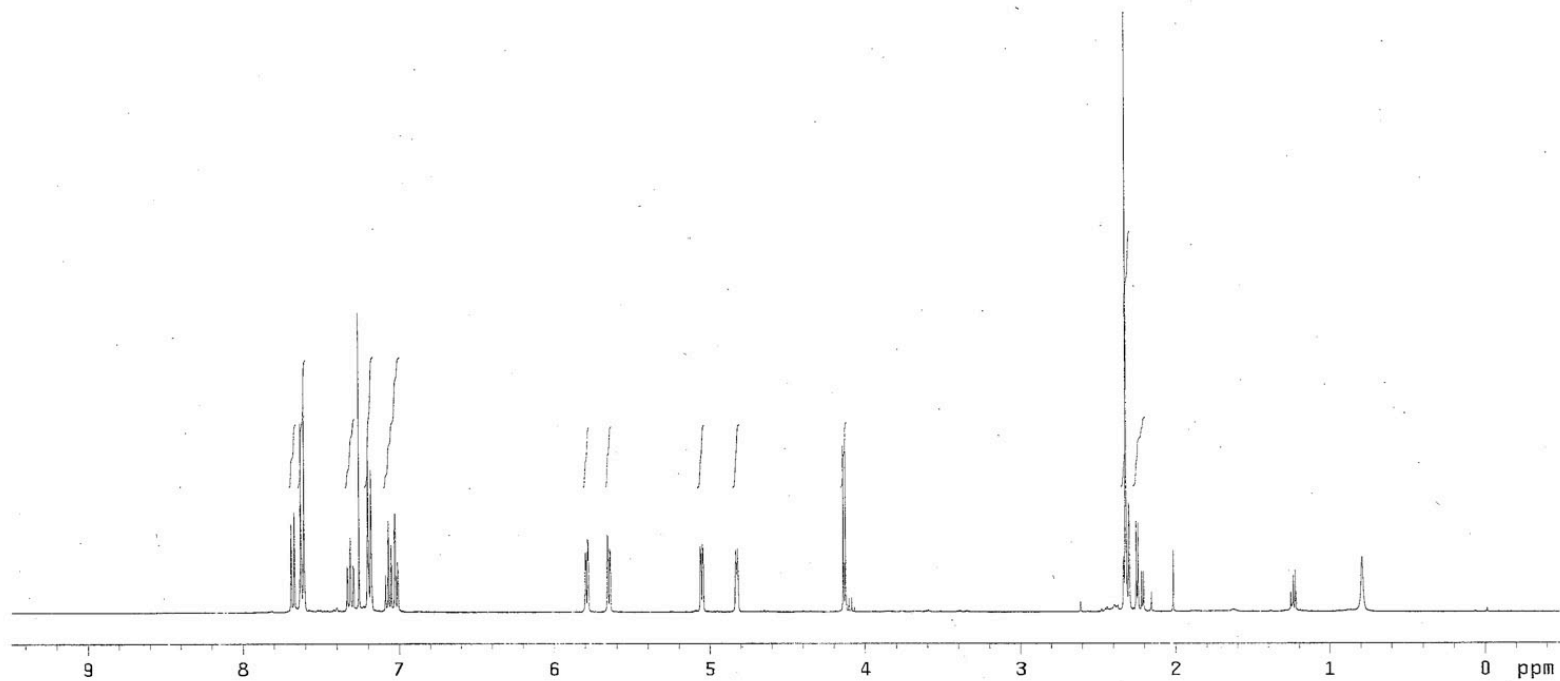
Pulse Sequence: s2pul
Spectrometer: 125.66
Solvent: CDCl₃



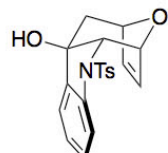
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



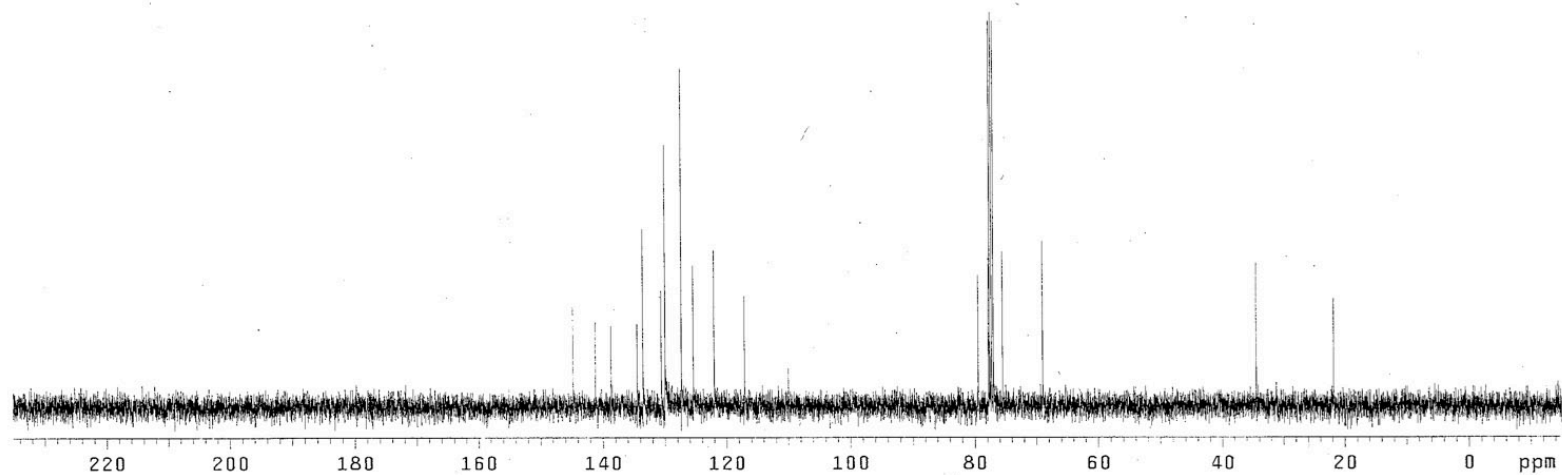
12a



Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃

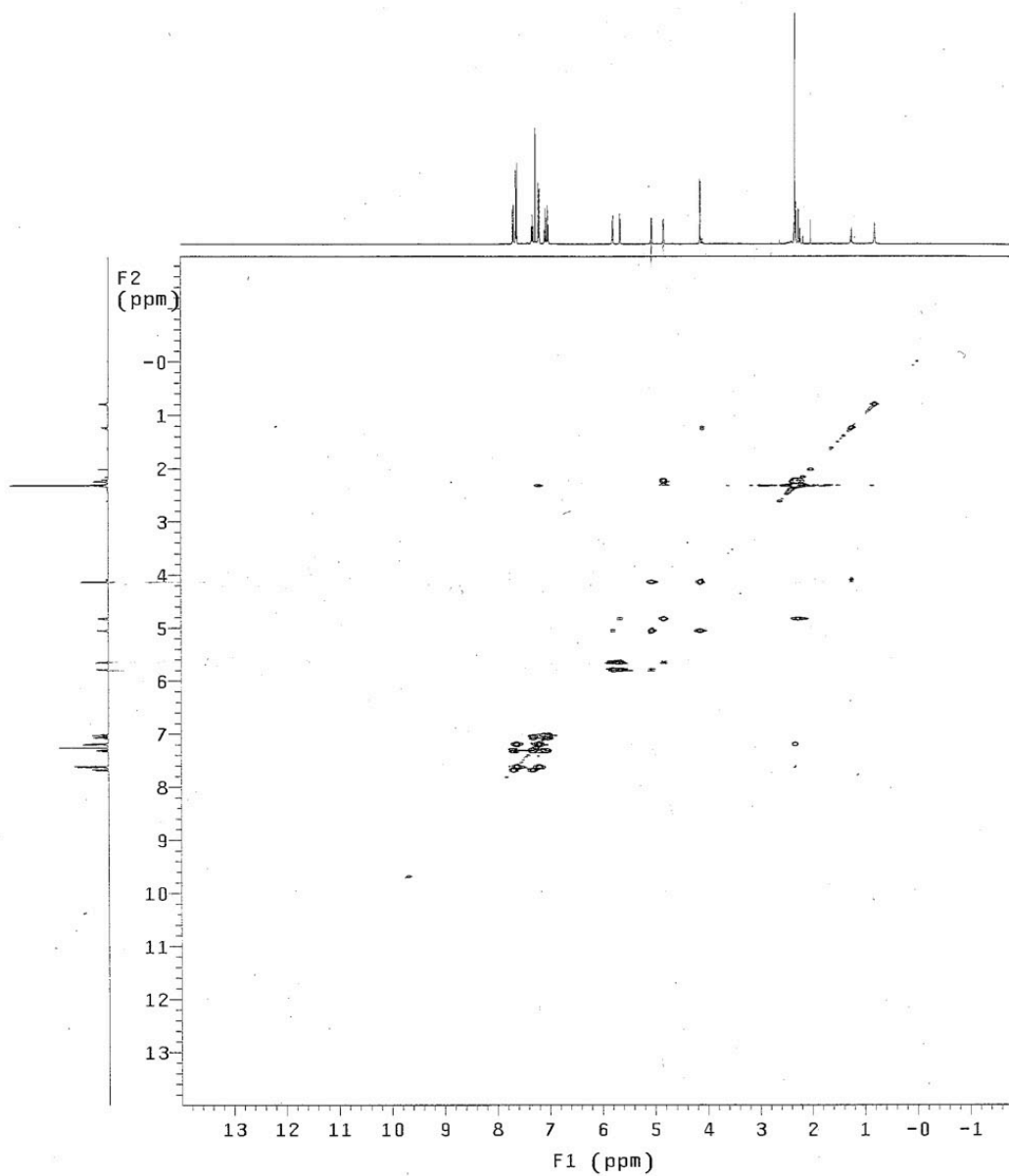
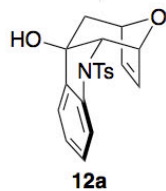


12a

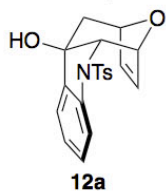


Pulse Sequence: gCOSY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

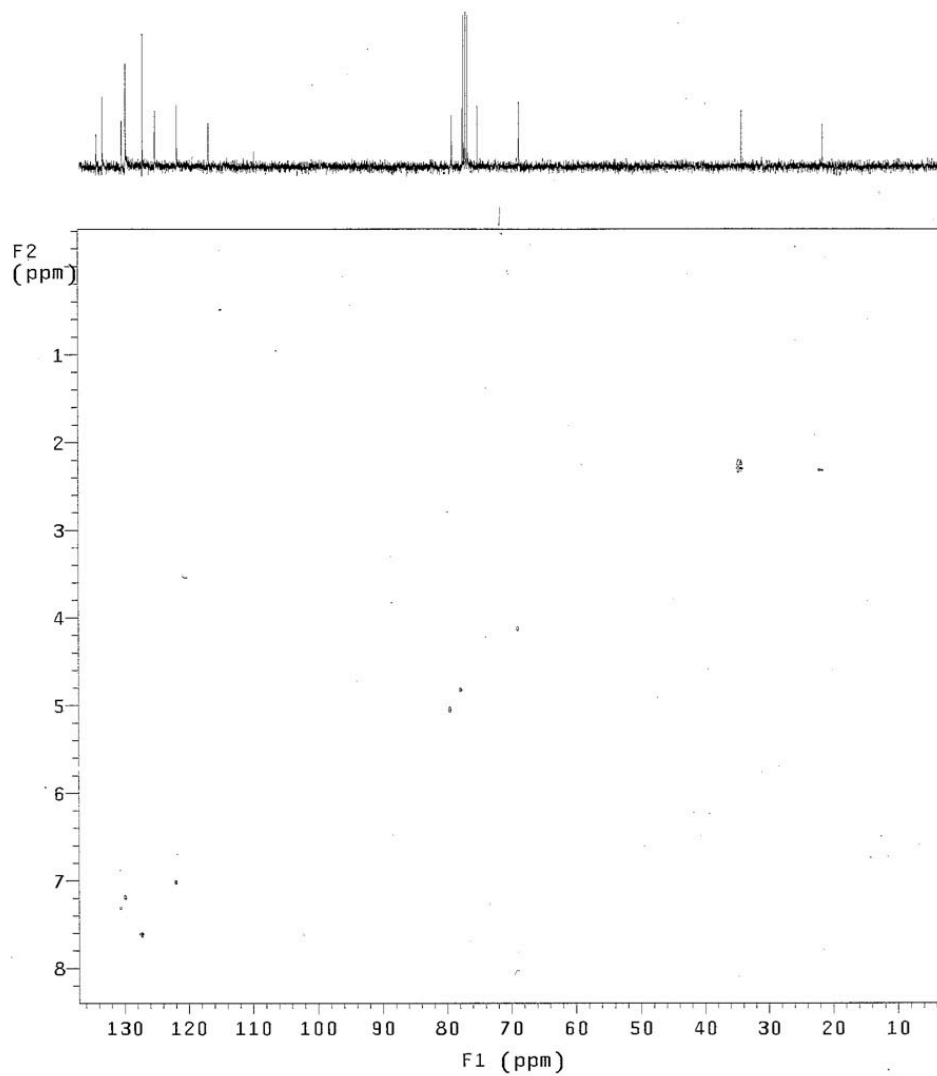
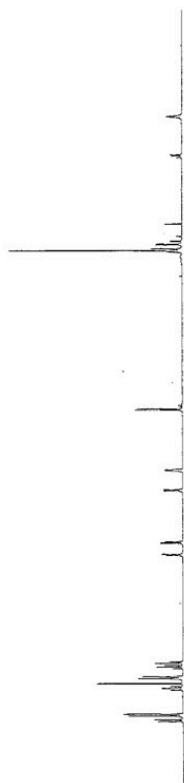
Relax. delay 1.000 sec
Acq. time 0.160 sec
Width 6387.7 Hz
2D Width 6387.7 Hz
2 repetitions
256 increments
OBSERVE H1, 399.7865251 MHz
DATA PROCESSING
Sq. sine bell 0.080 sec
F1 DATA PROCESSING
Sq. sine bell 0.040 sec
FT size 4096 x 4096
Total time 10 min, 29 sec



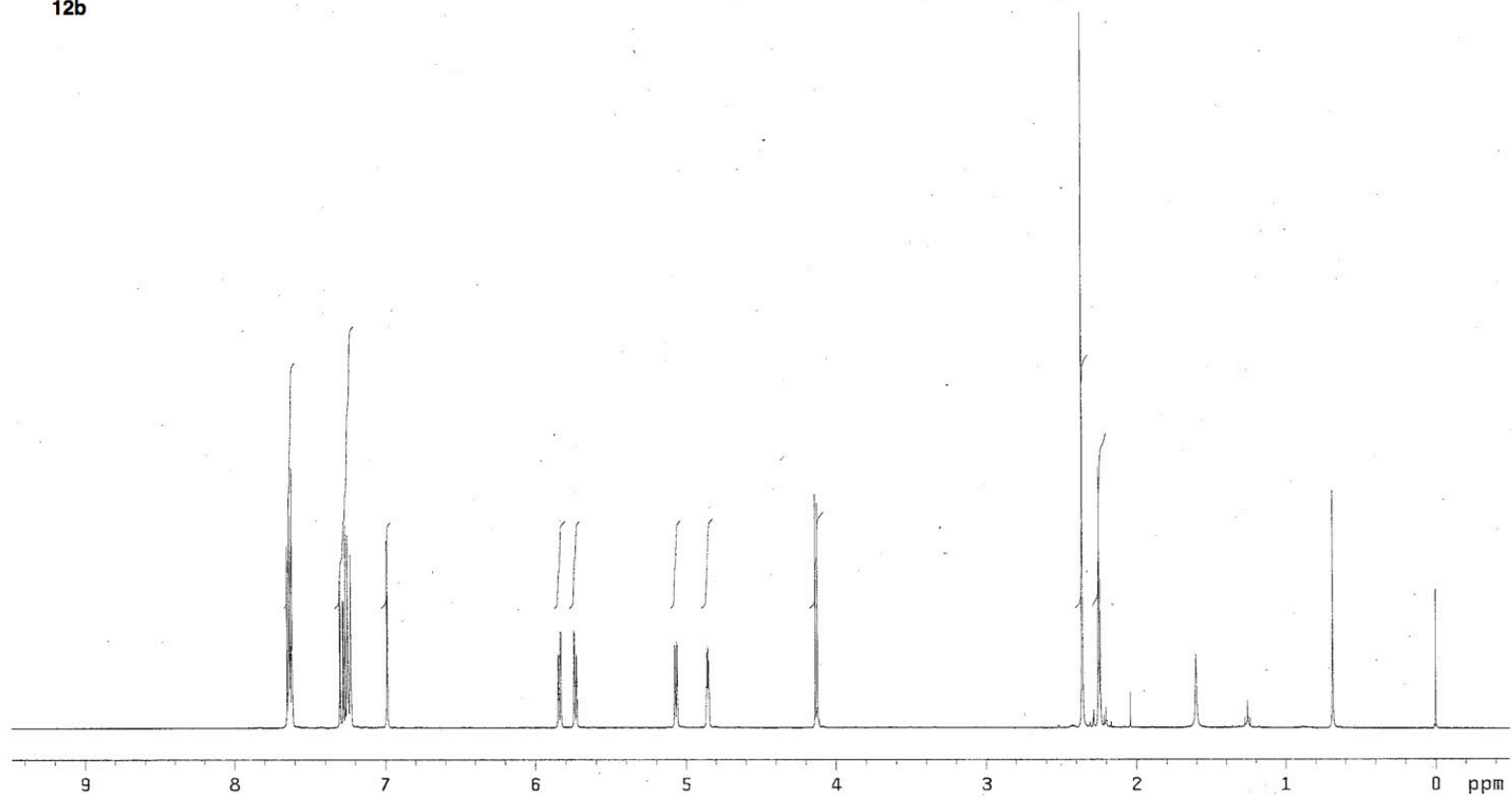
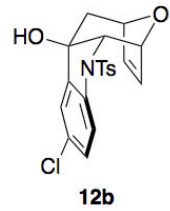
Pulse Sequence: gHSQC



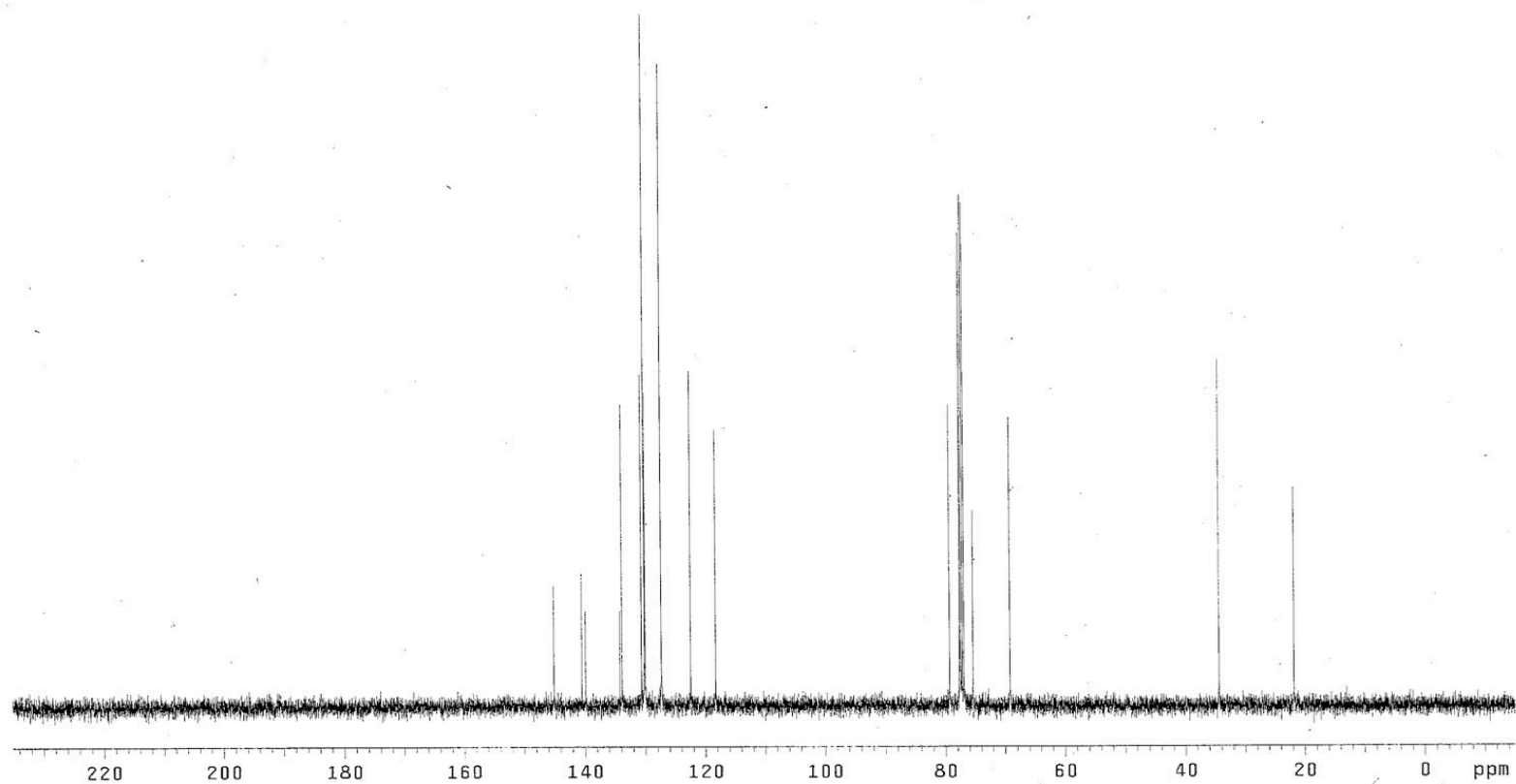
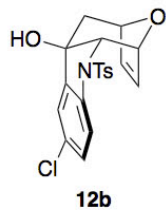
12a



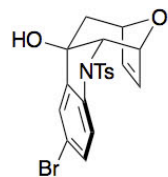
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



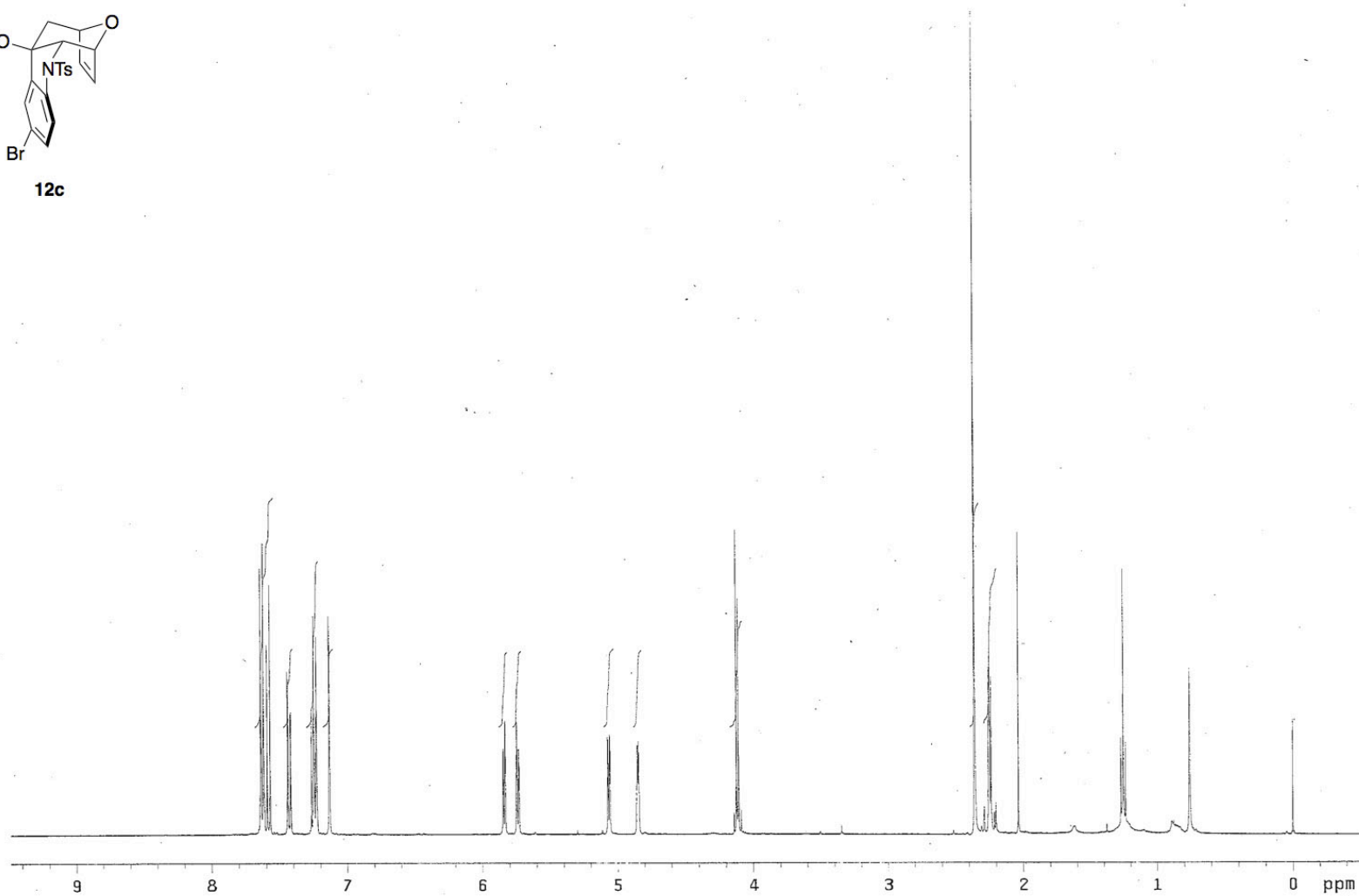
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



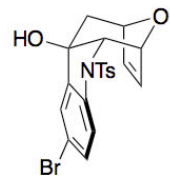
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



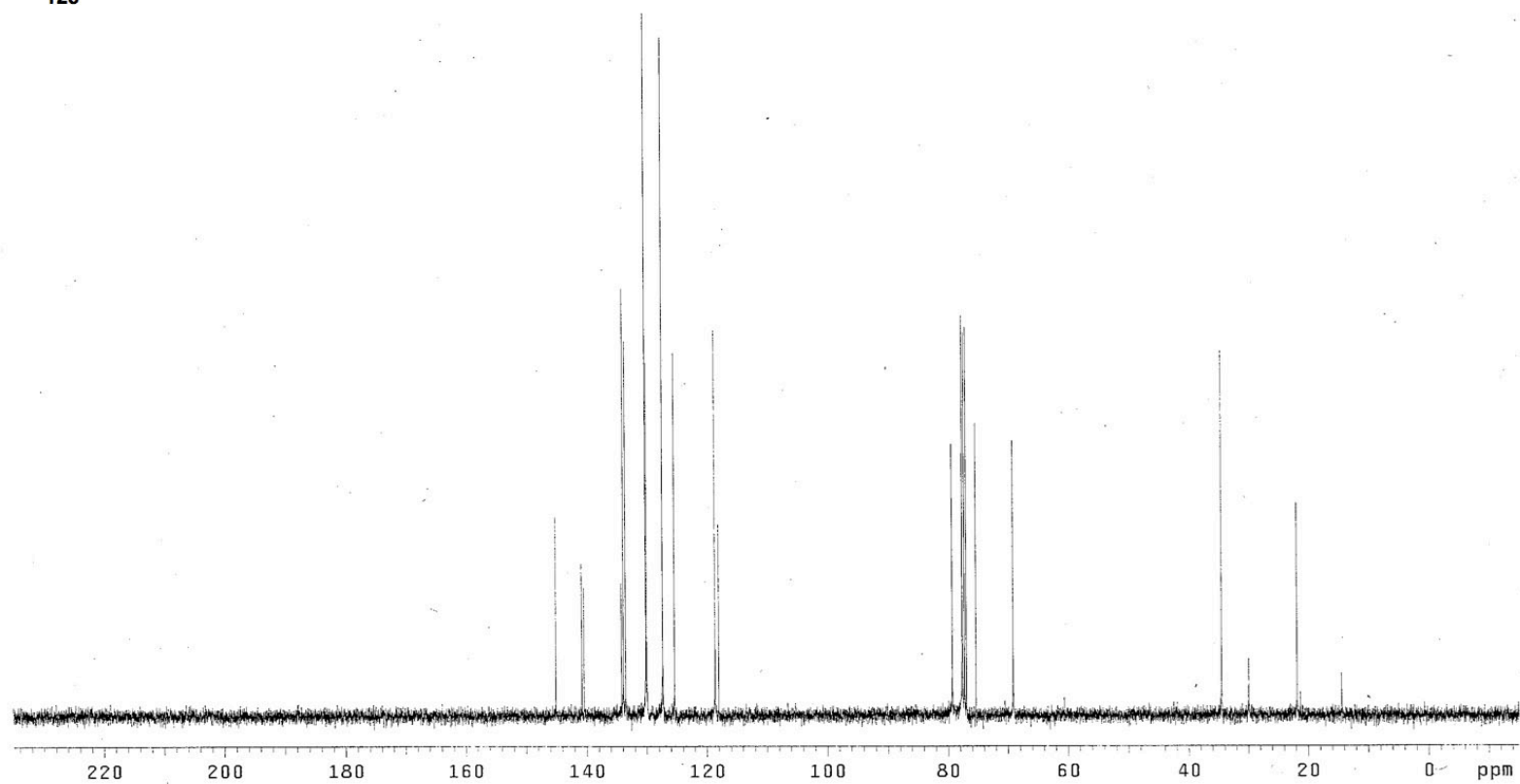
12c



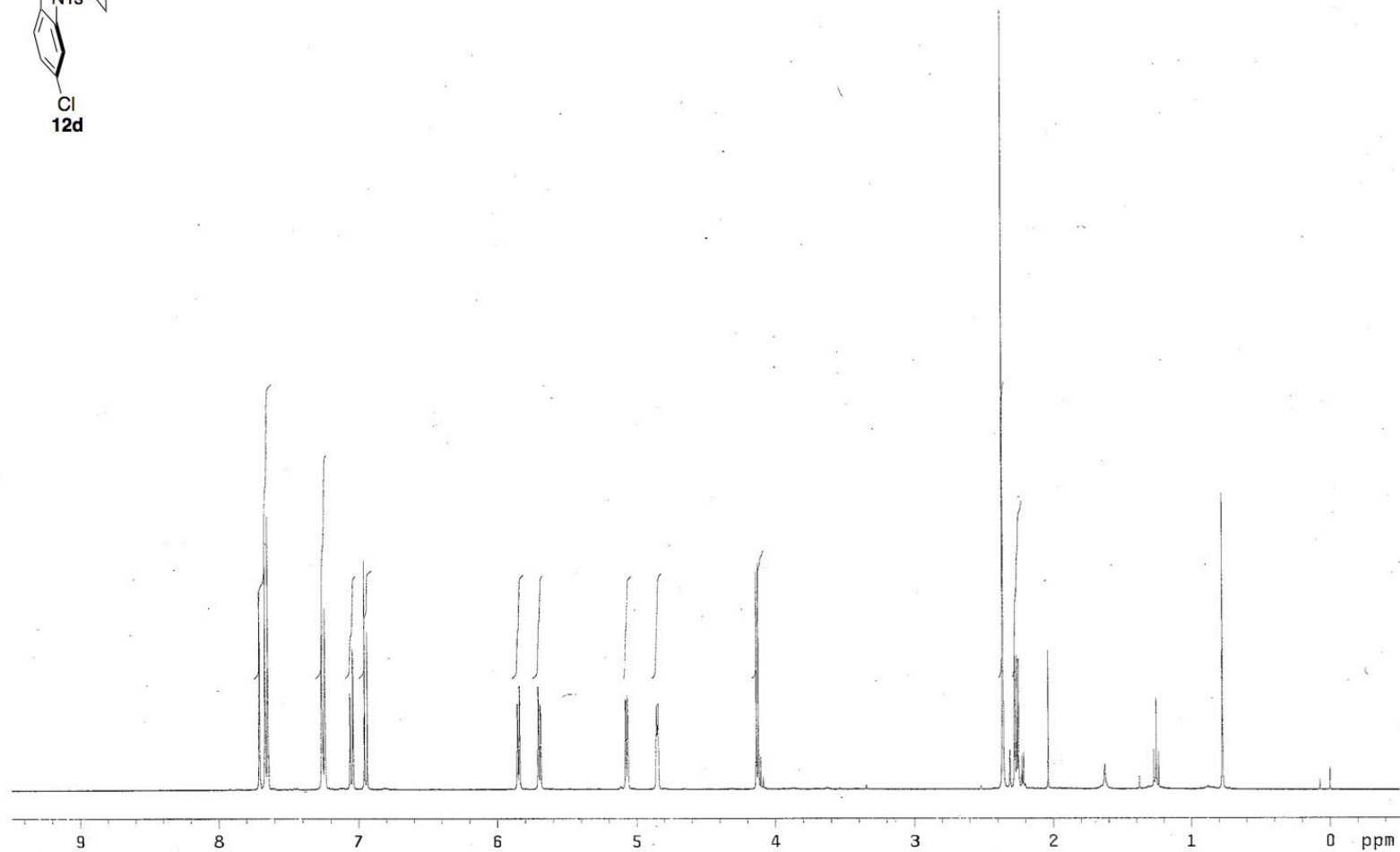
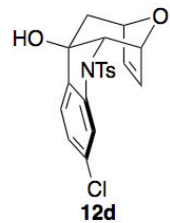
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



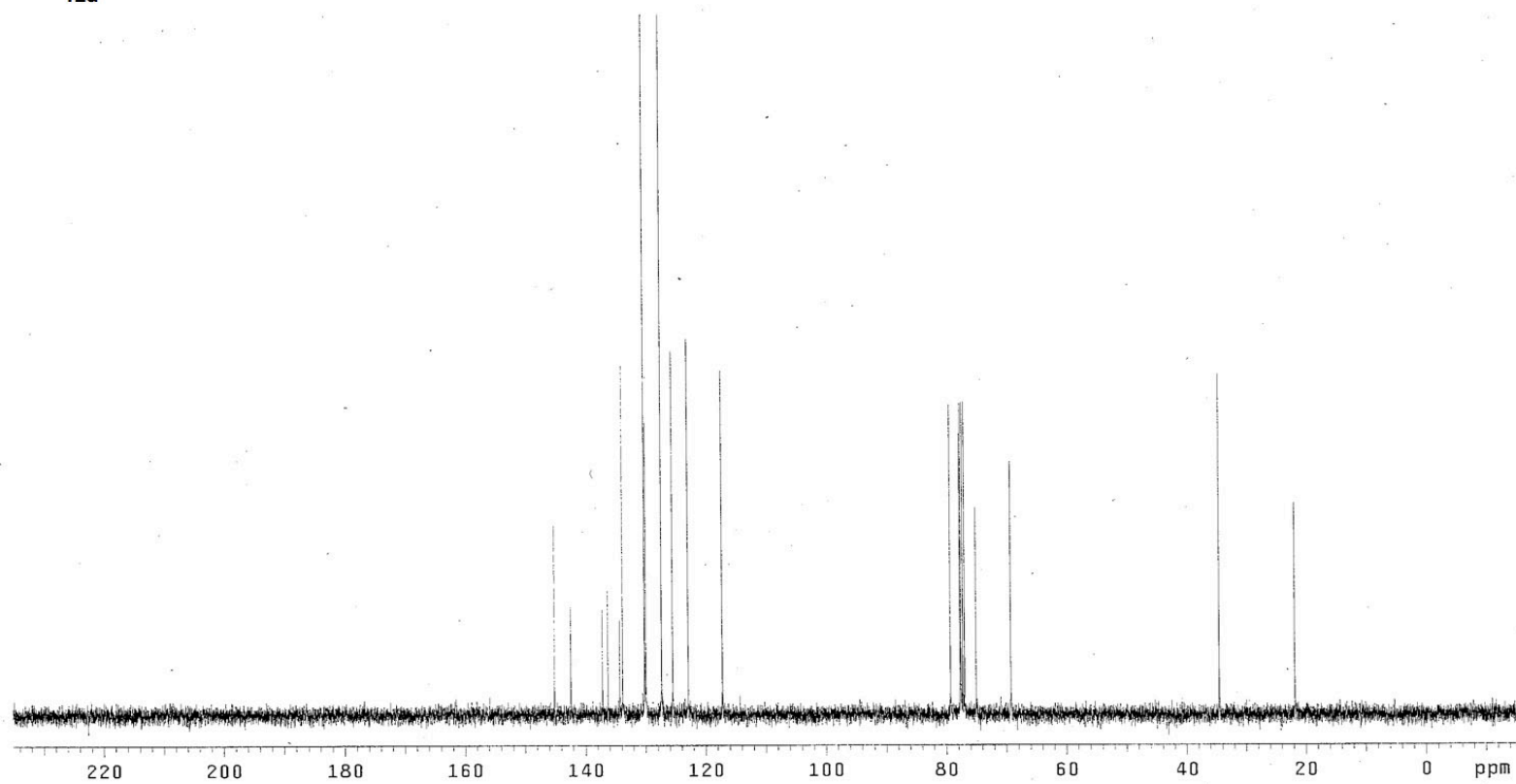
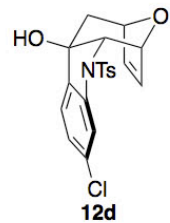
12c



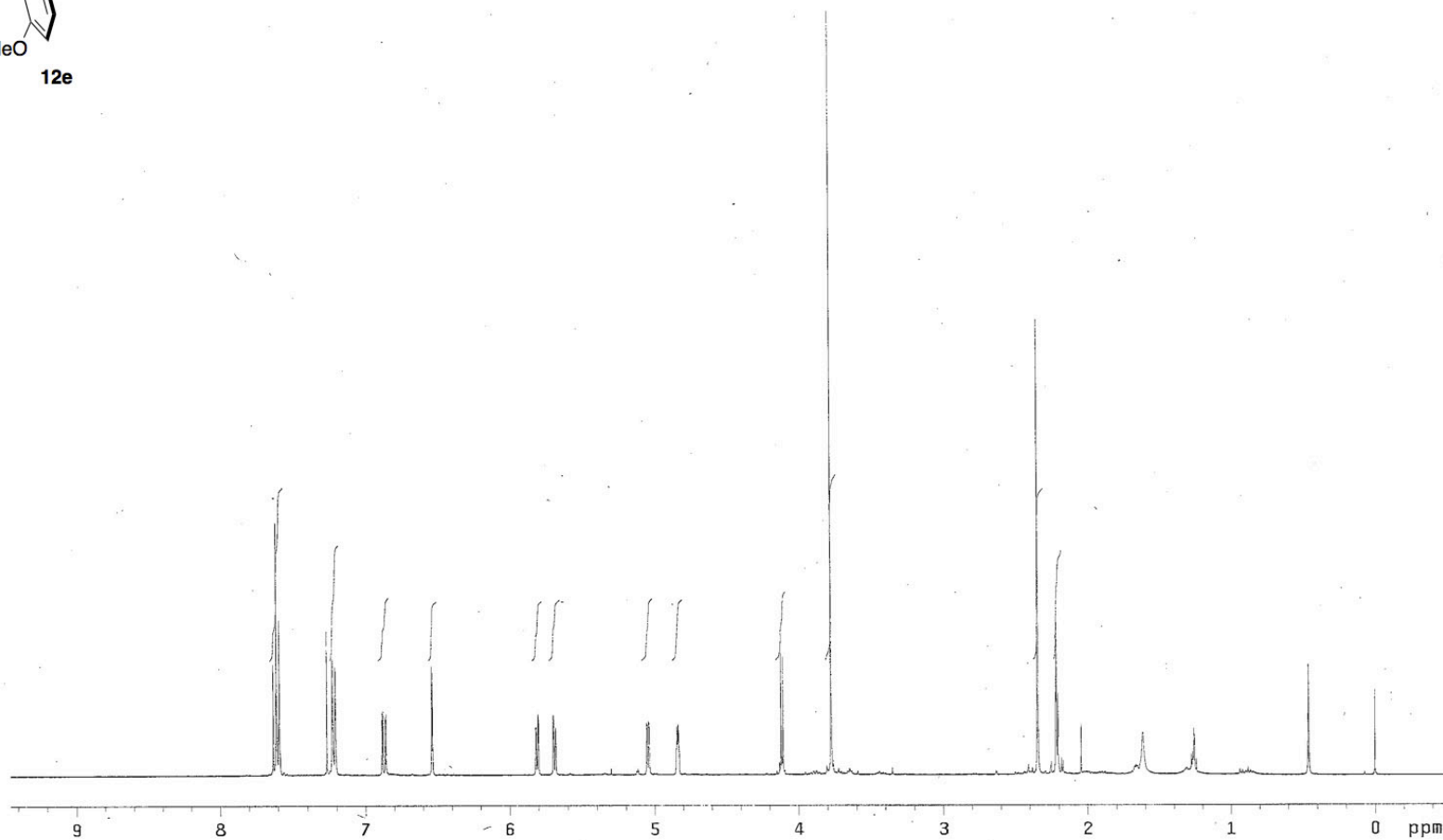
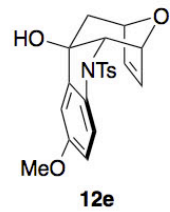
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



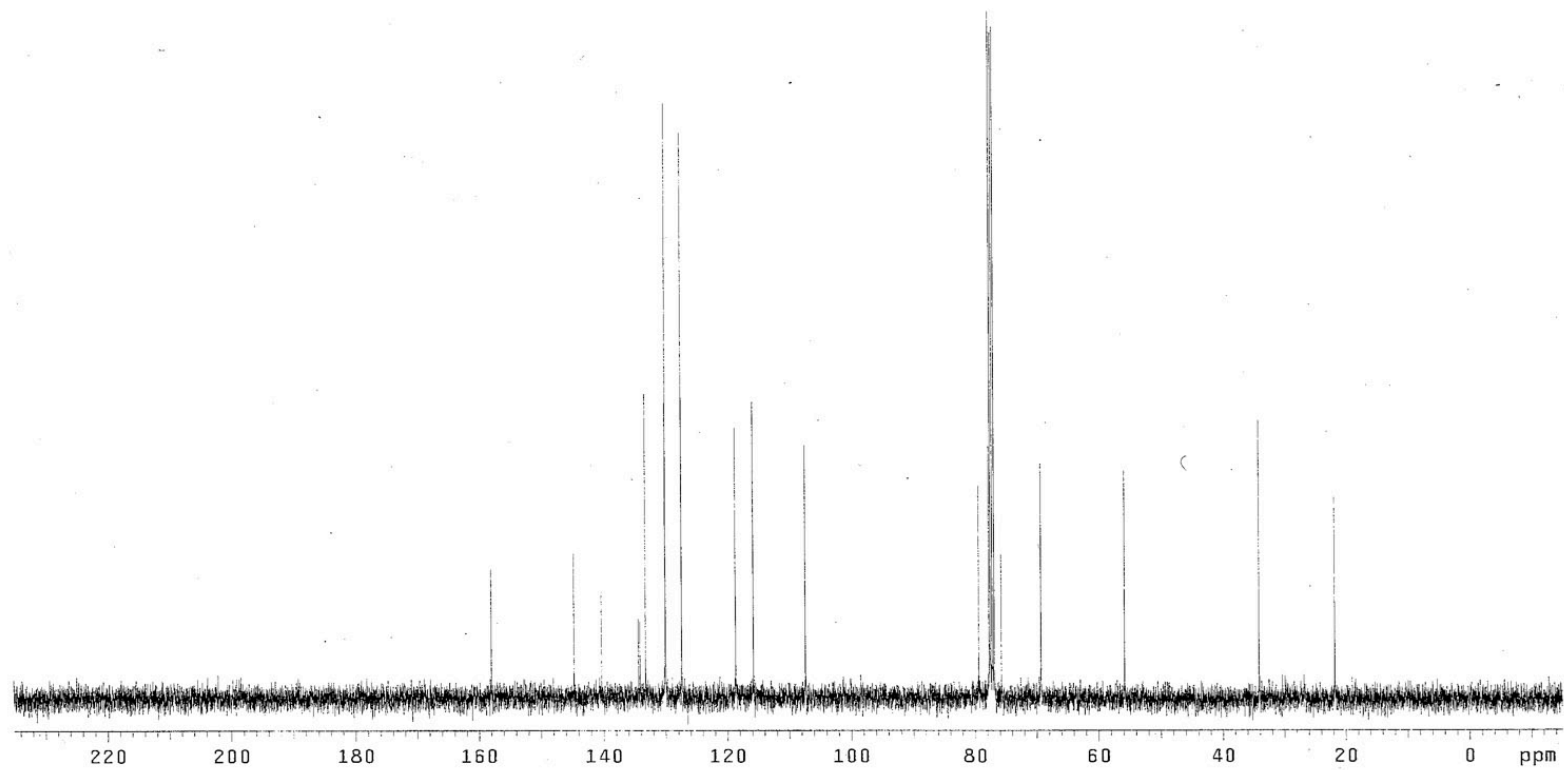
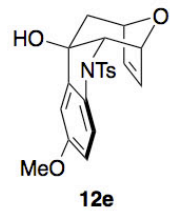
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



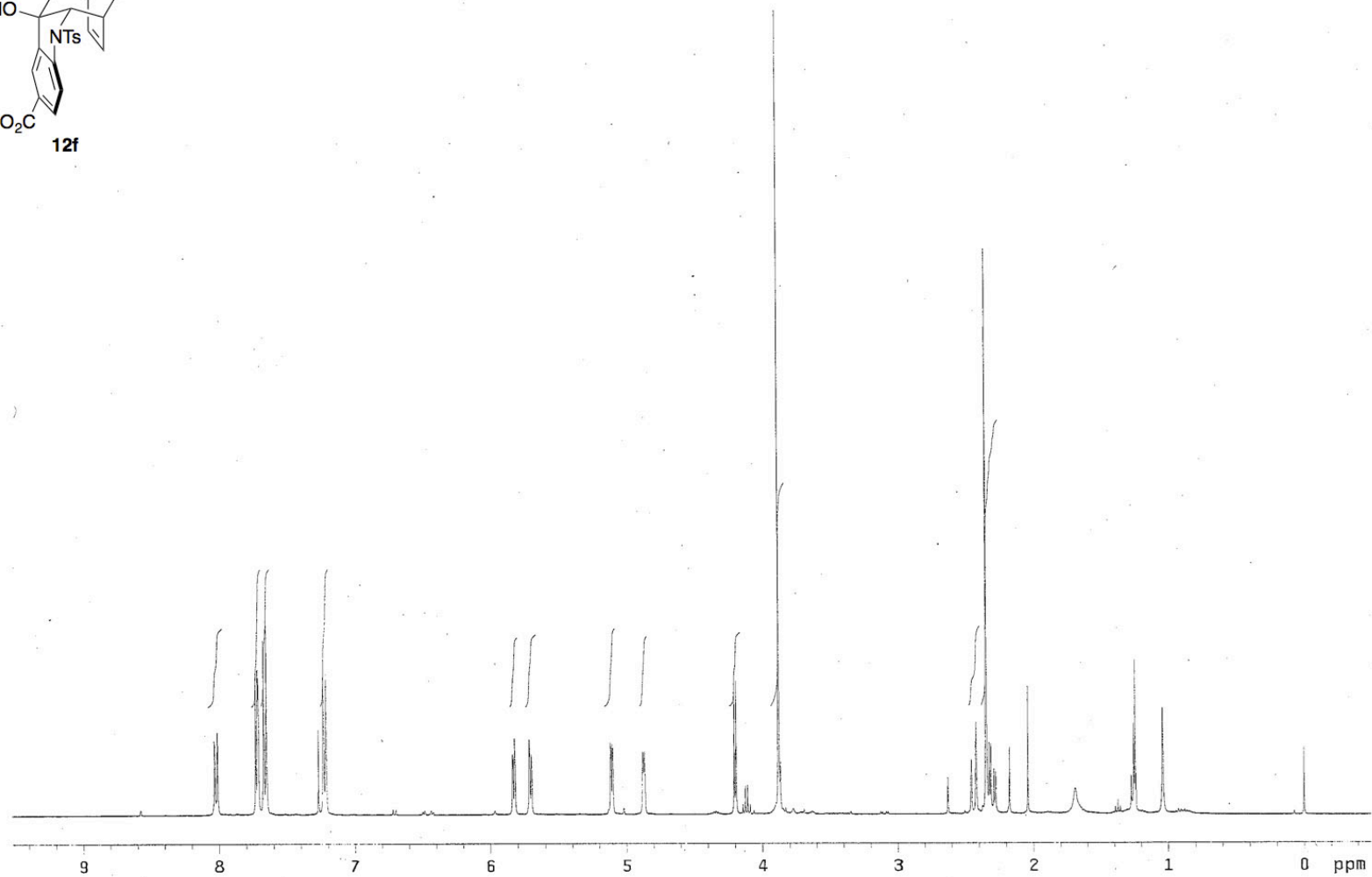
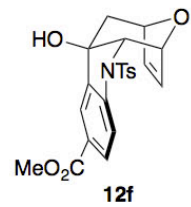
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



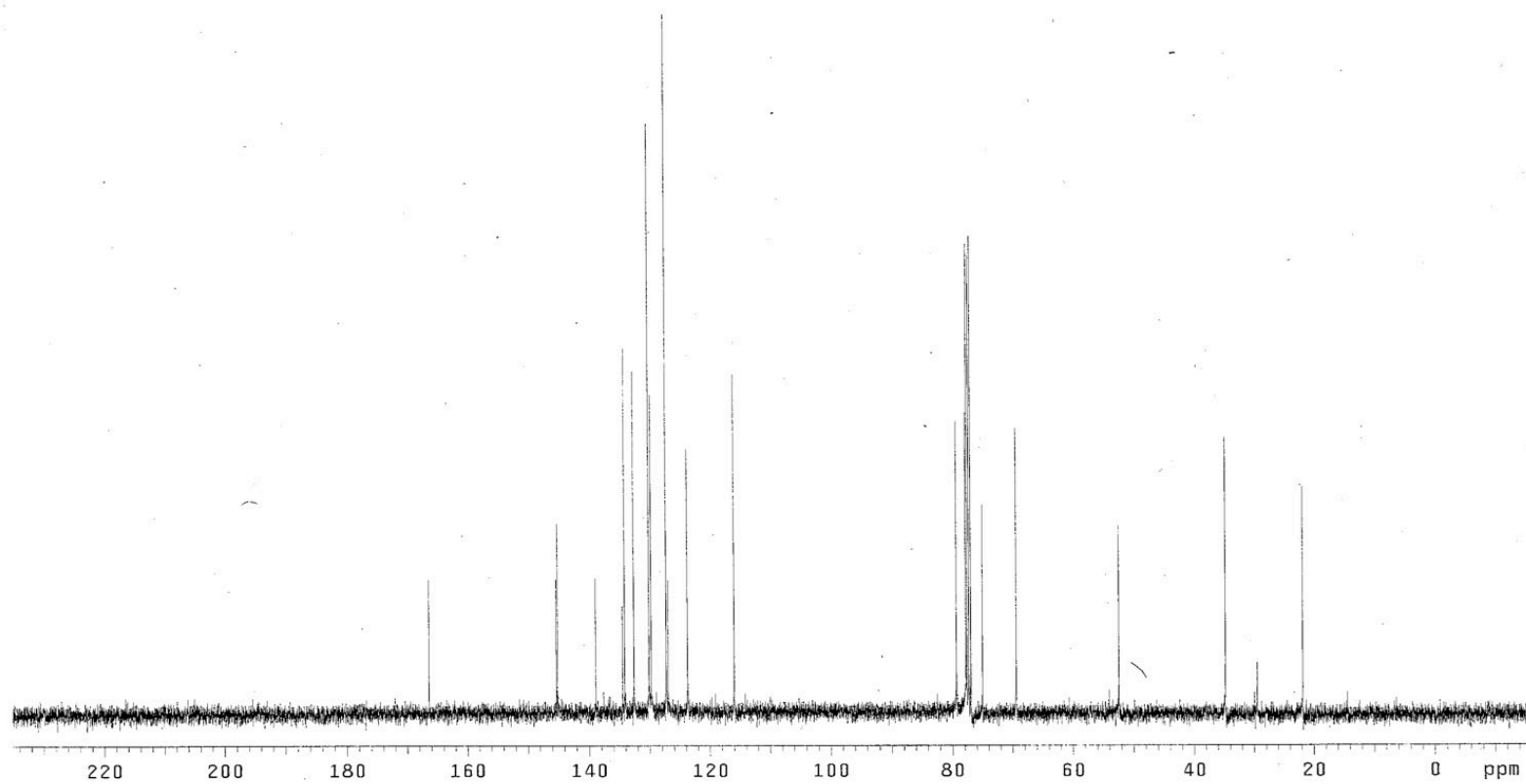
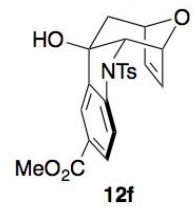
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



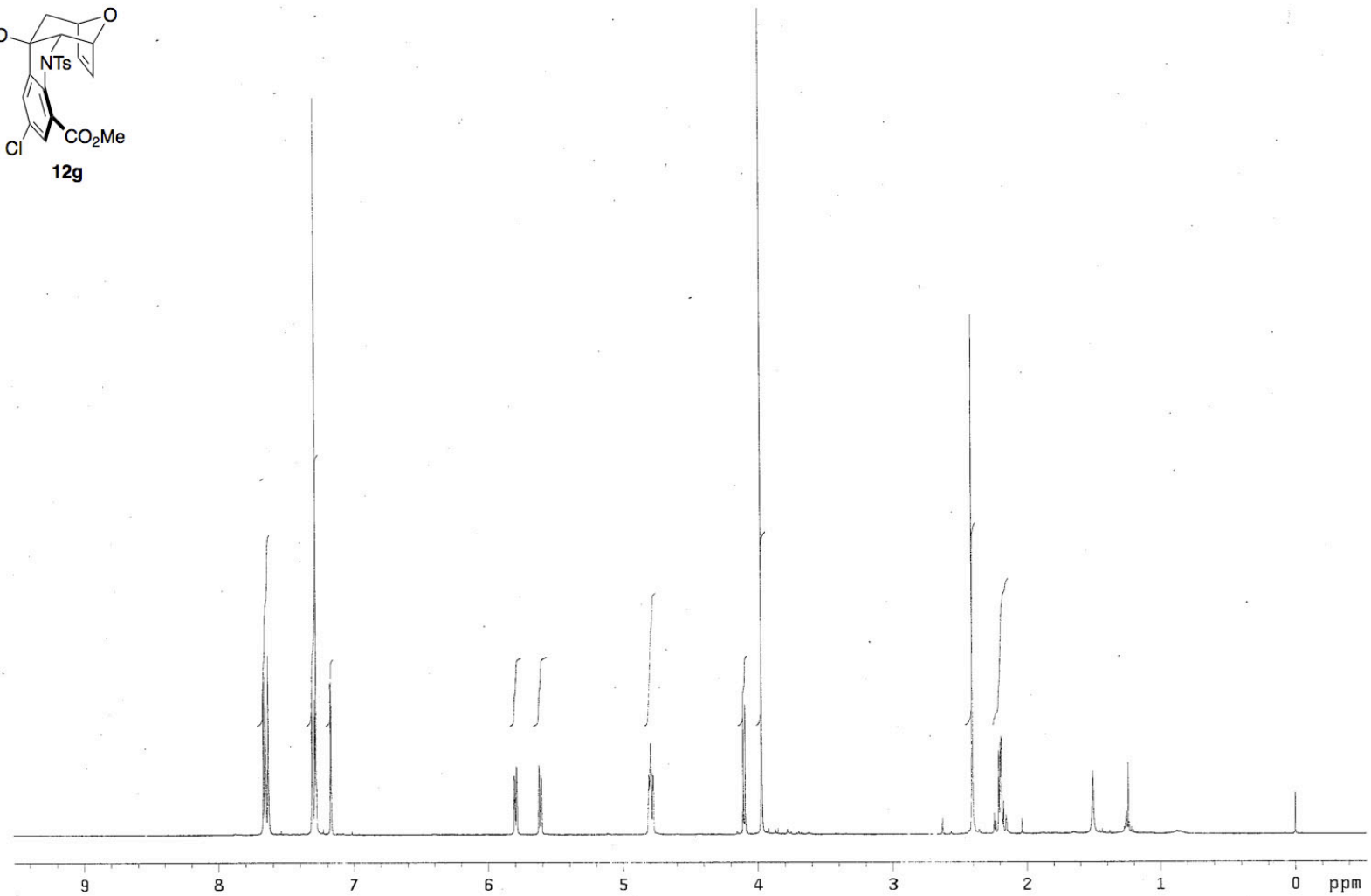
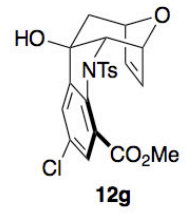
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



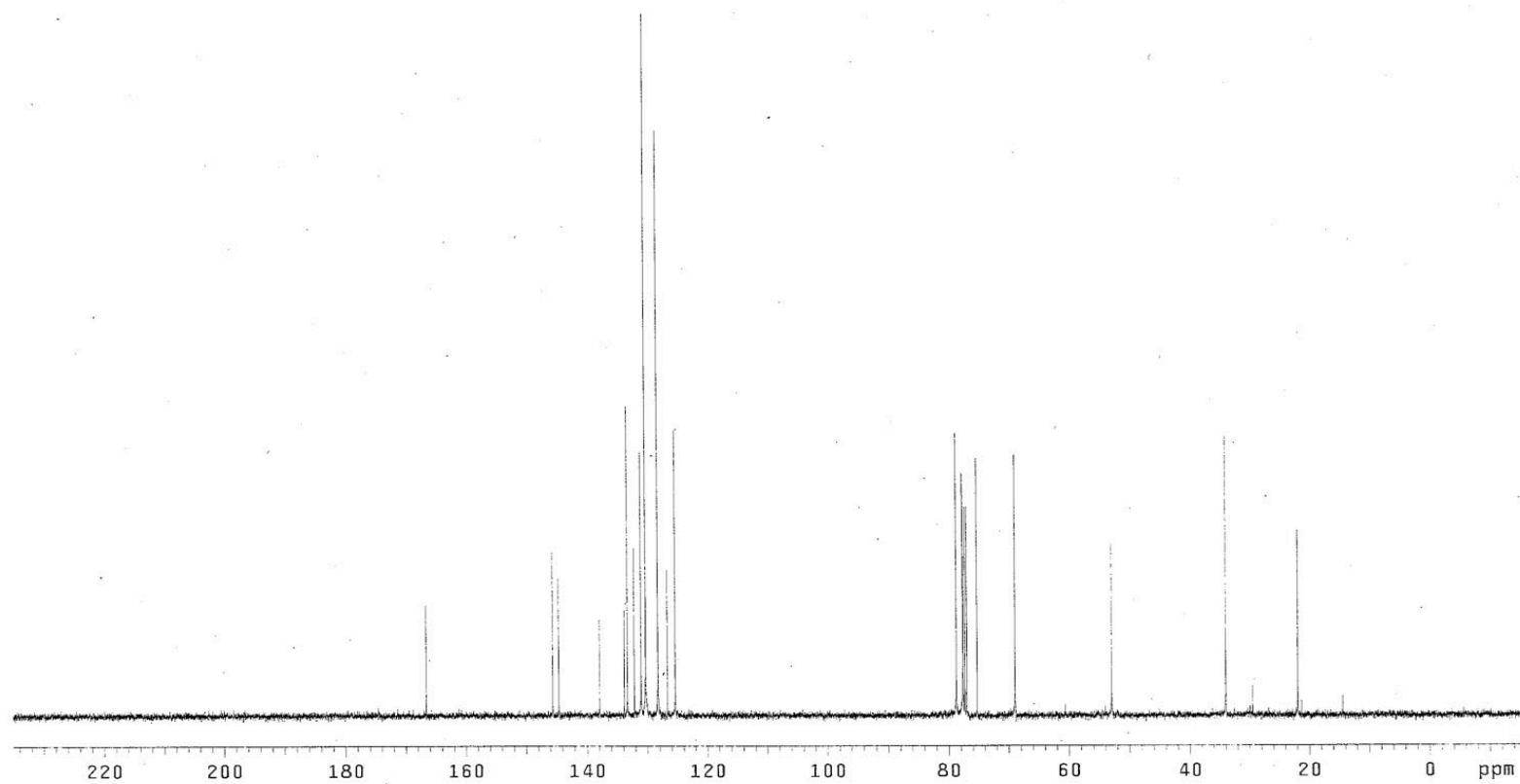
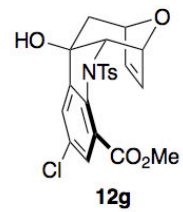
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



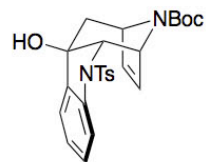
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



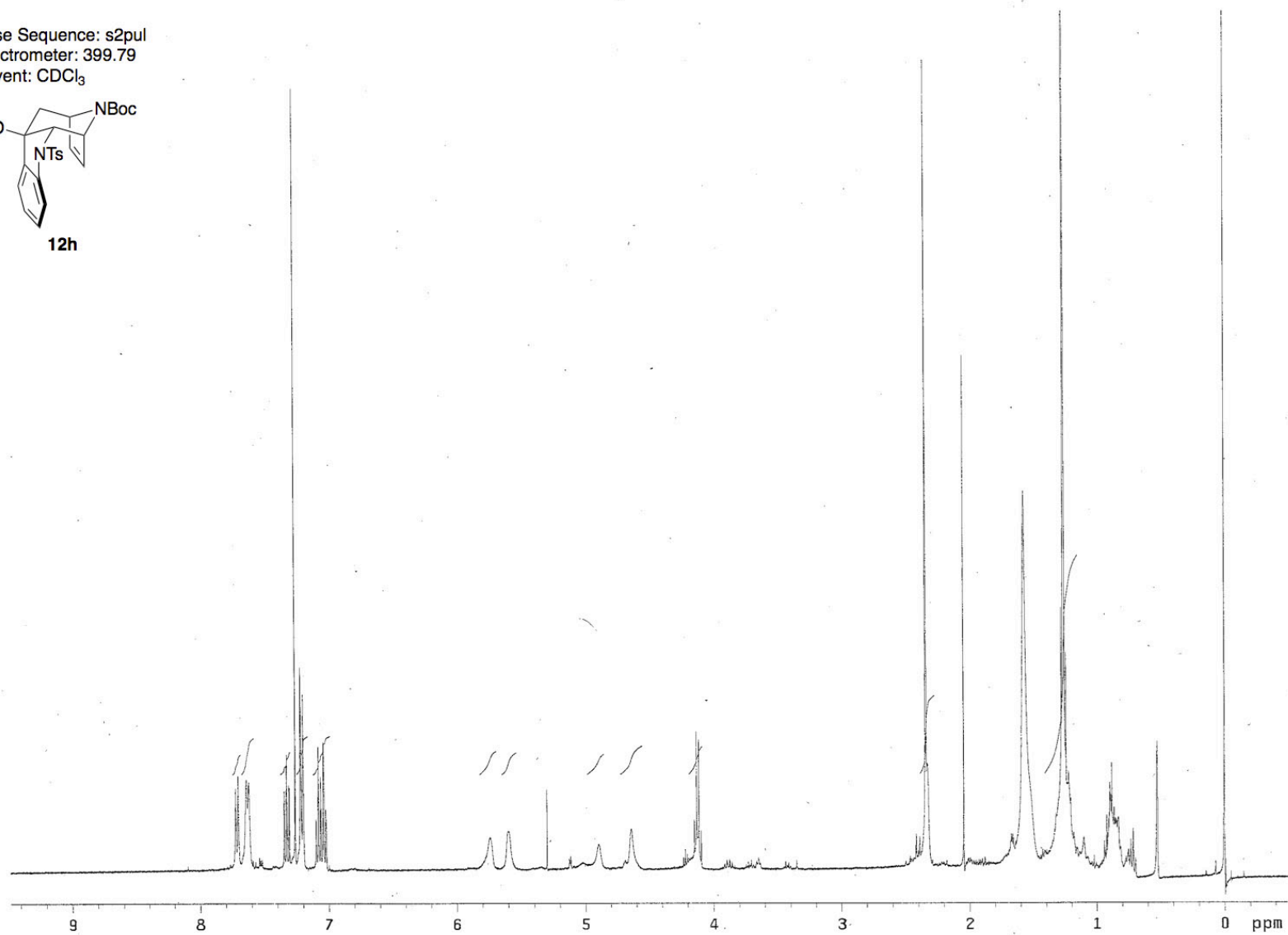
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



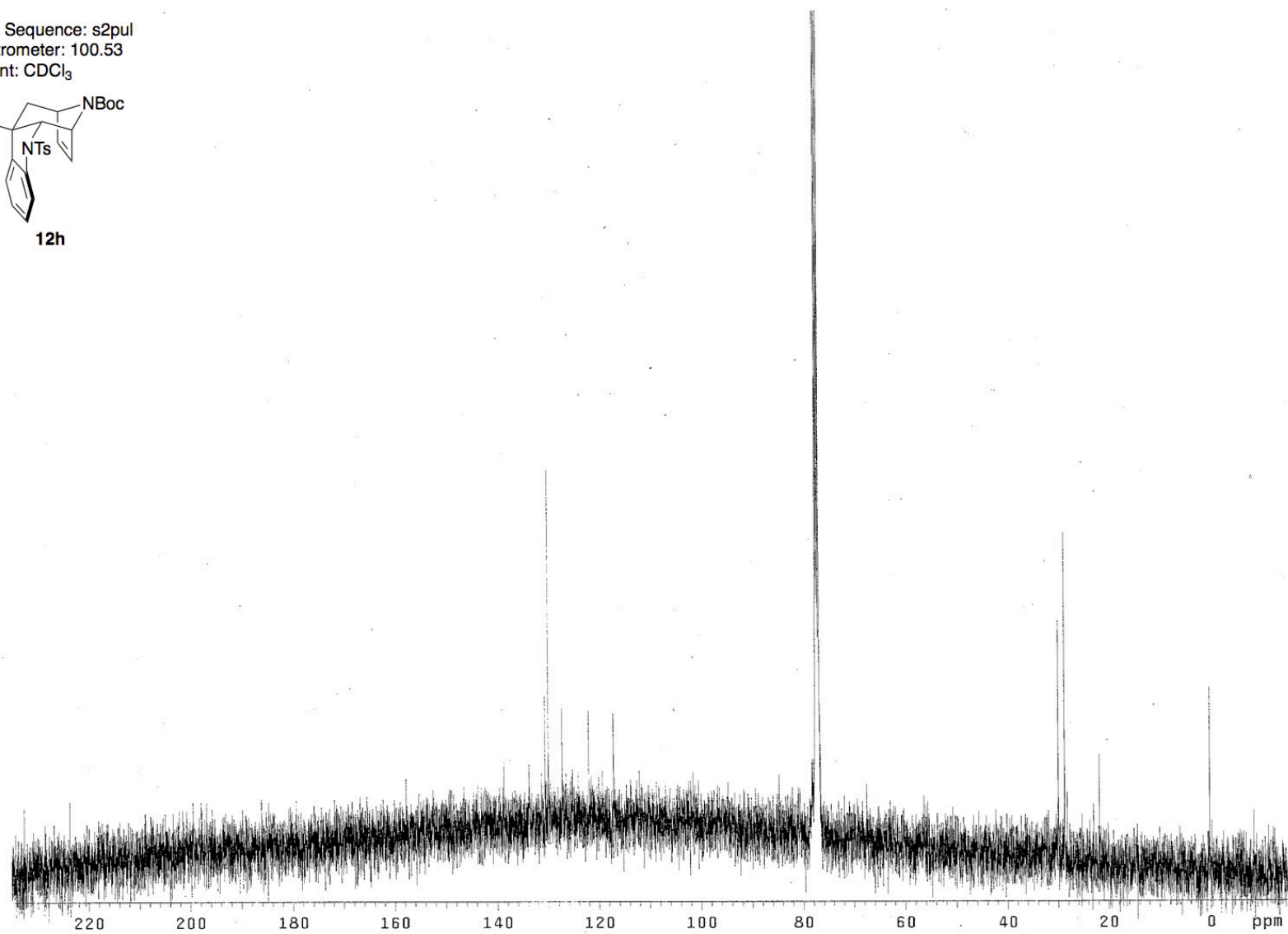
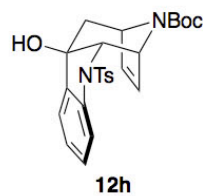
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



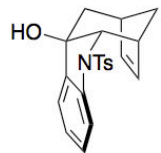
12h



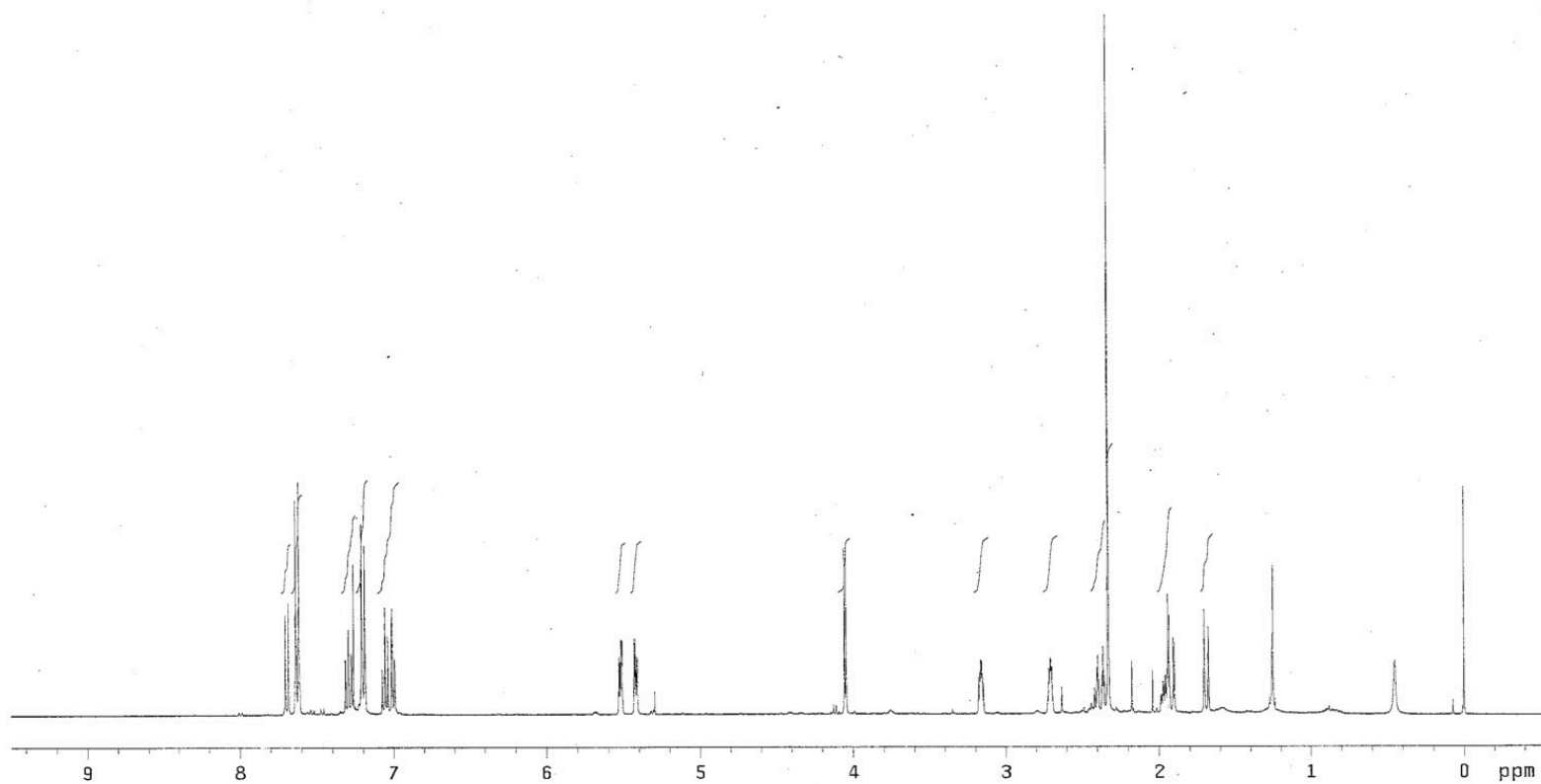
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



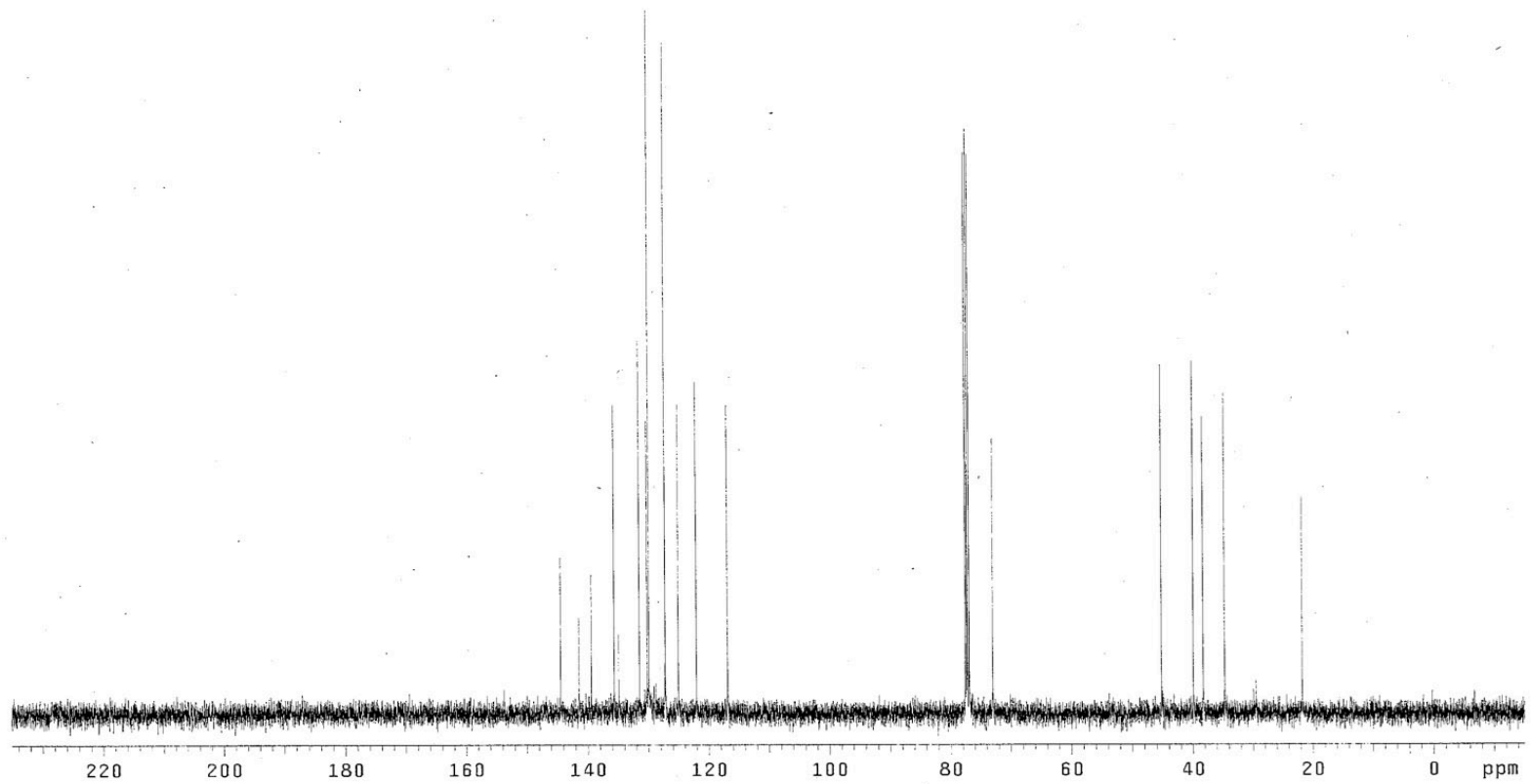
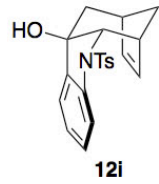
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



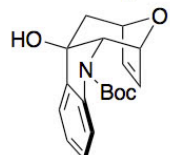
12i



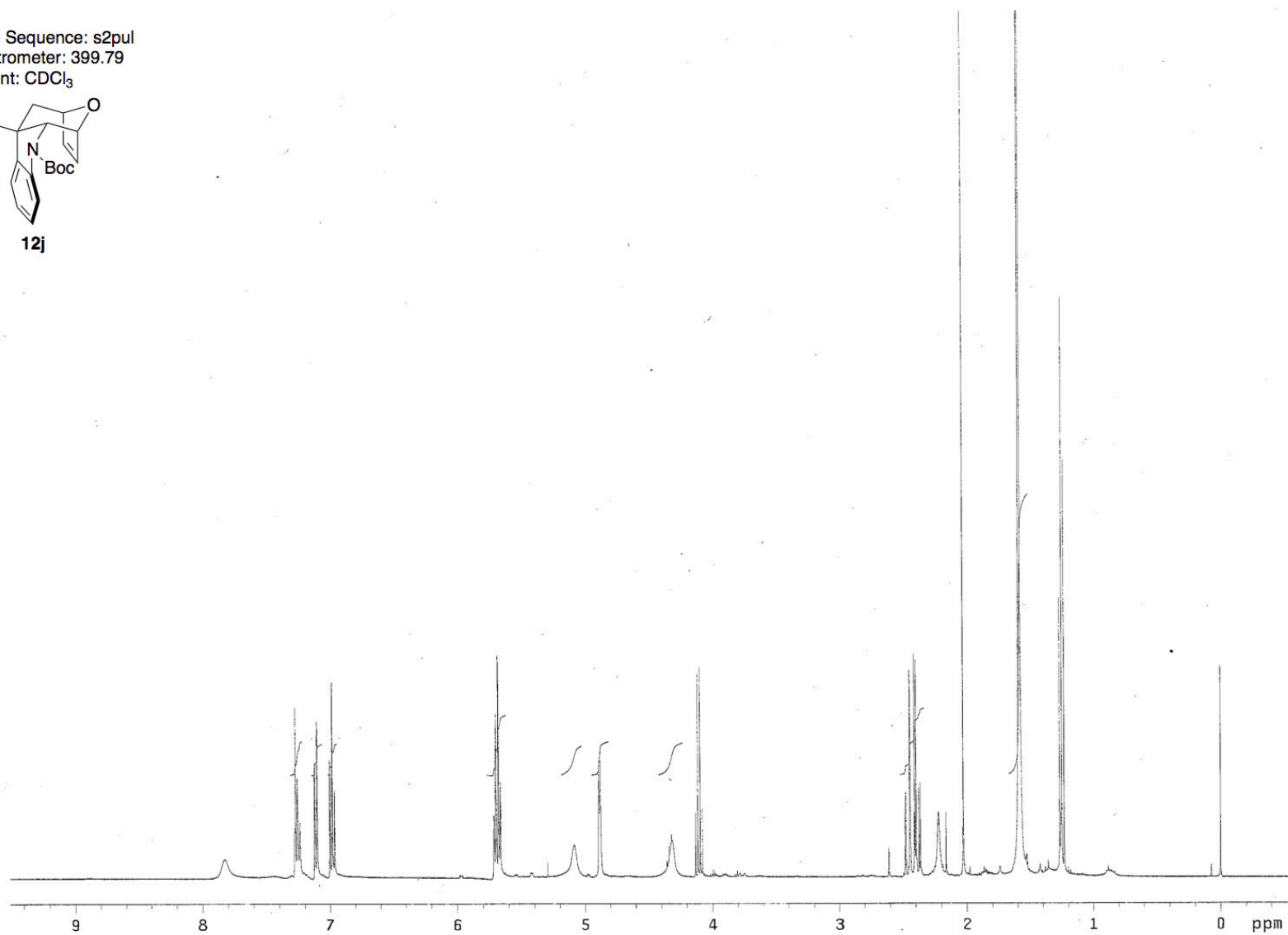
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



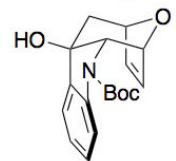
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



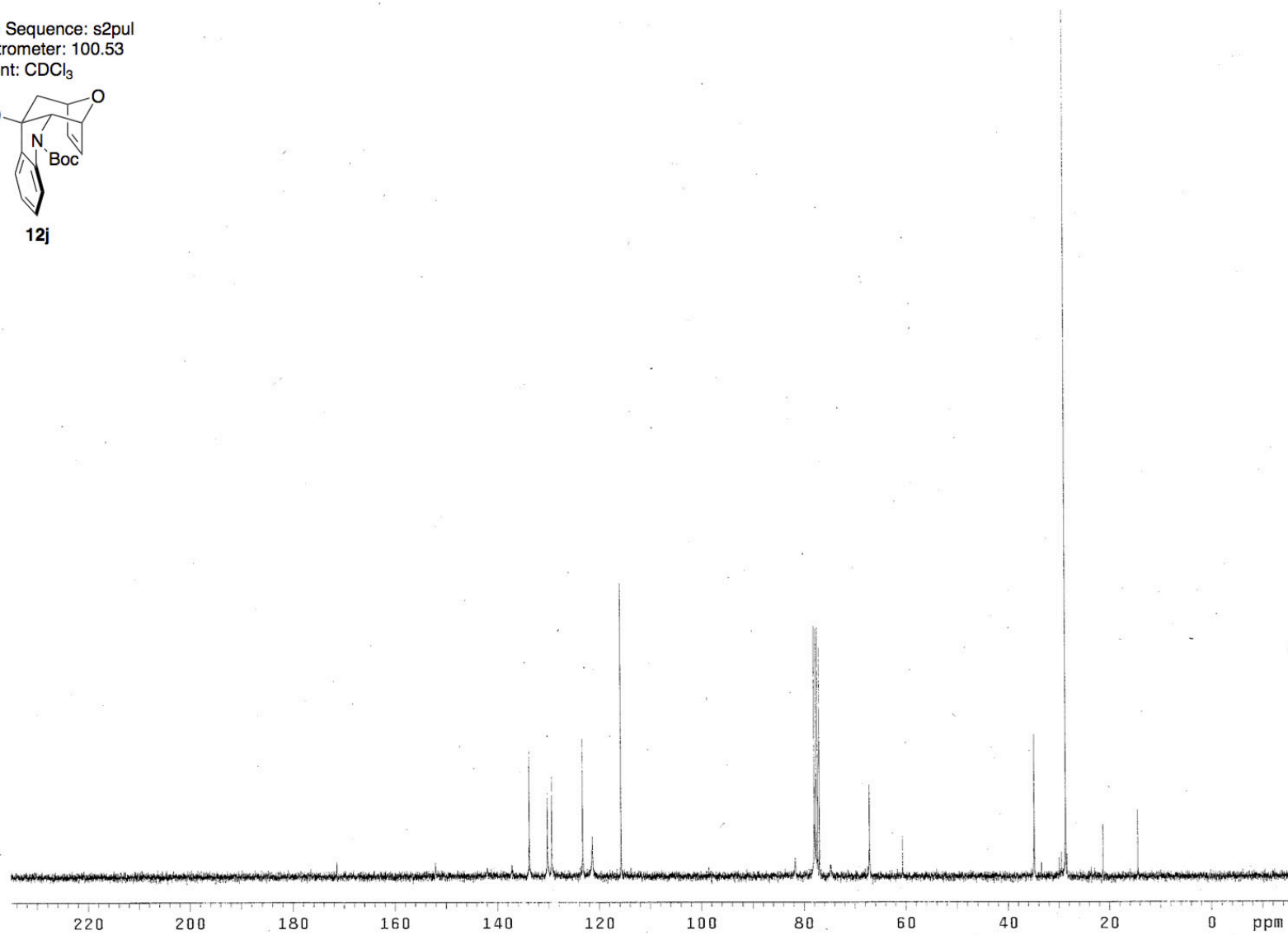
12j



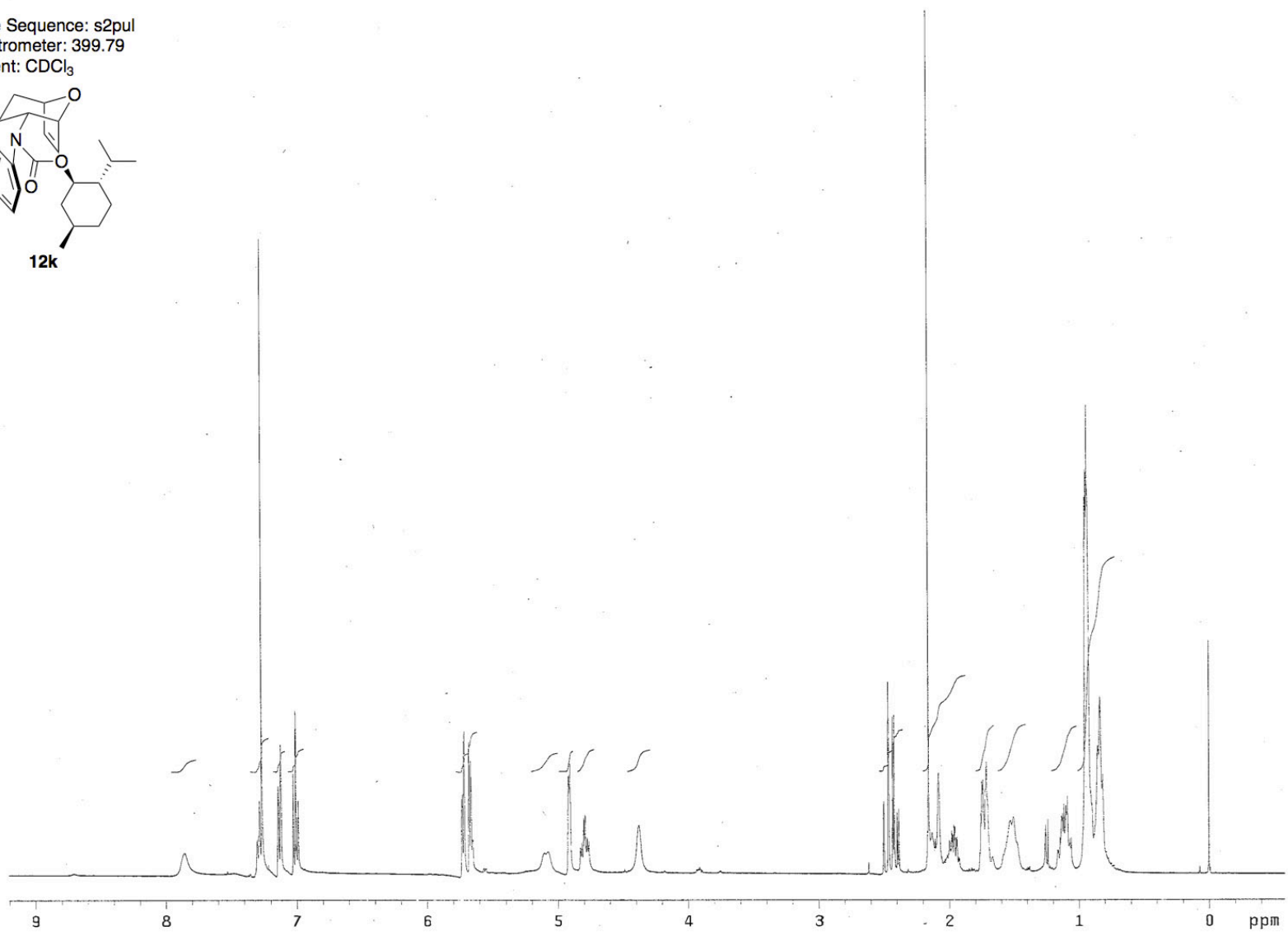
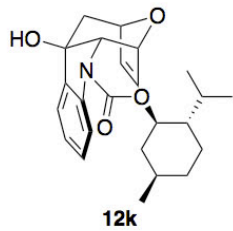
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



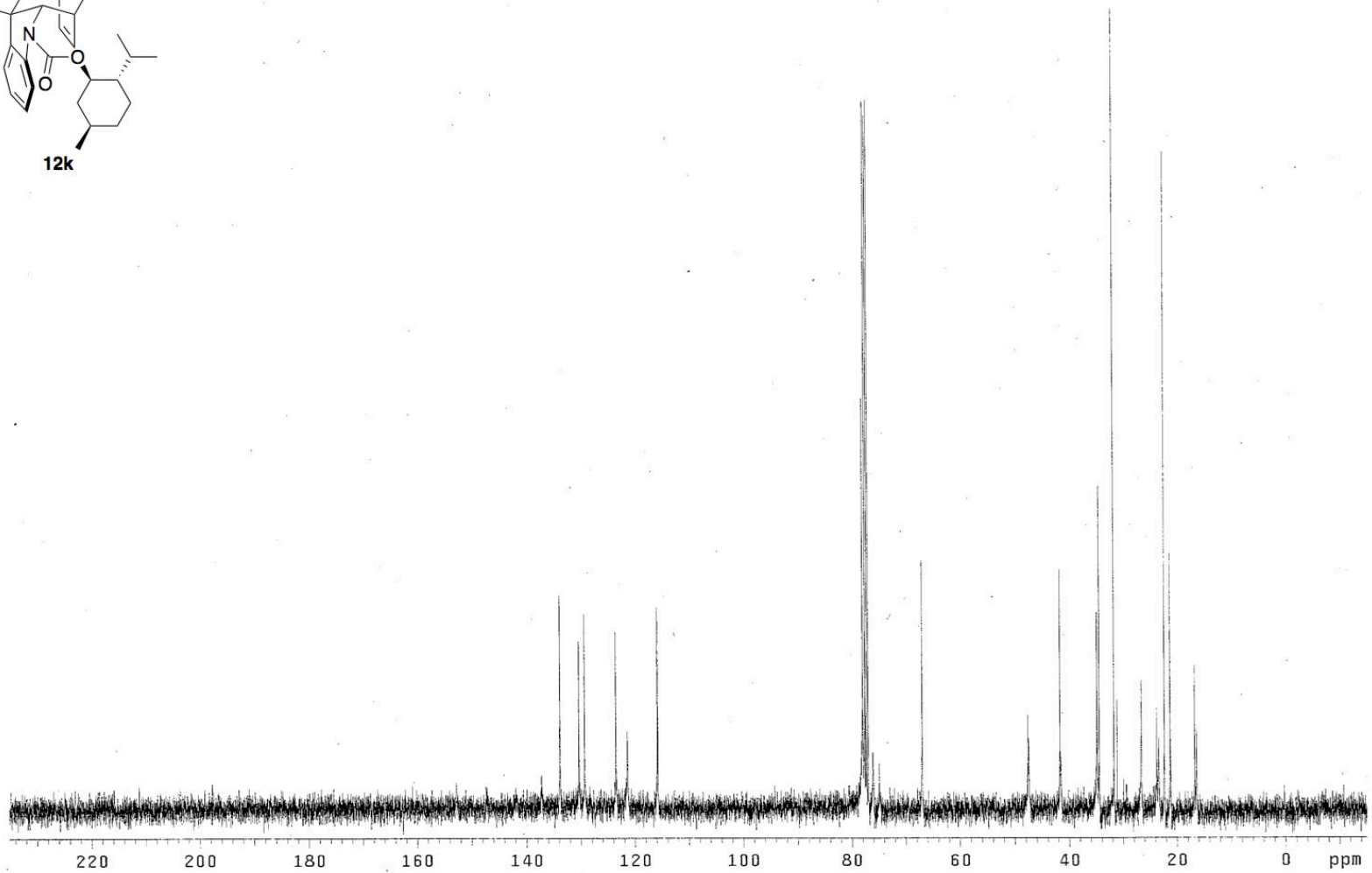
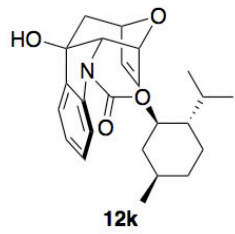
12j



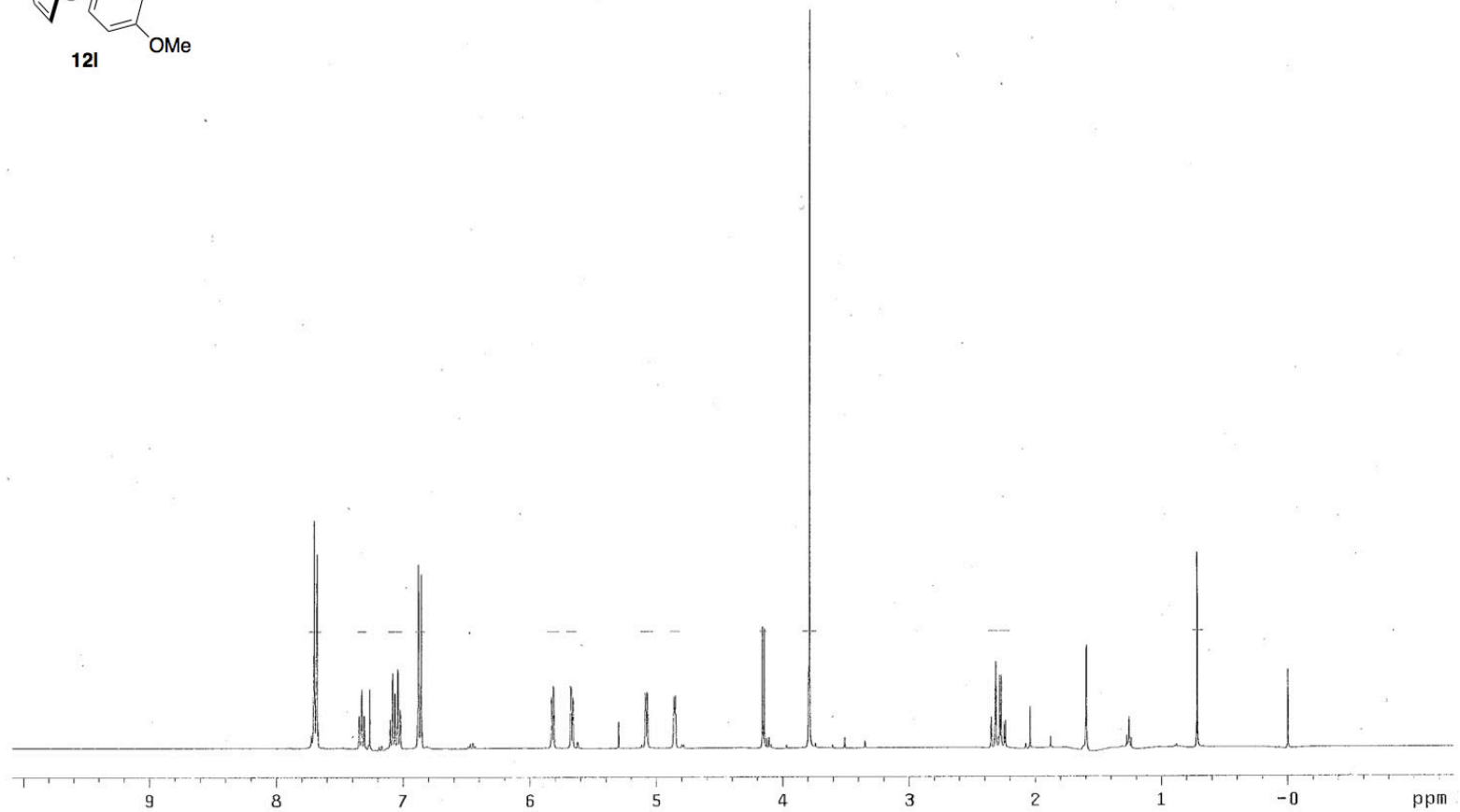
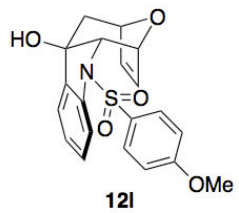
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



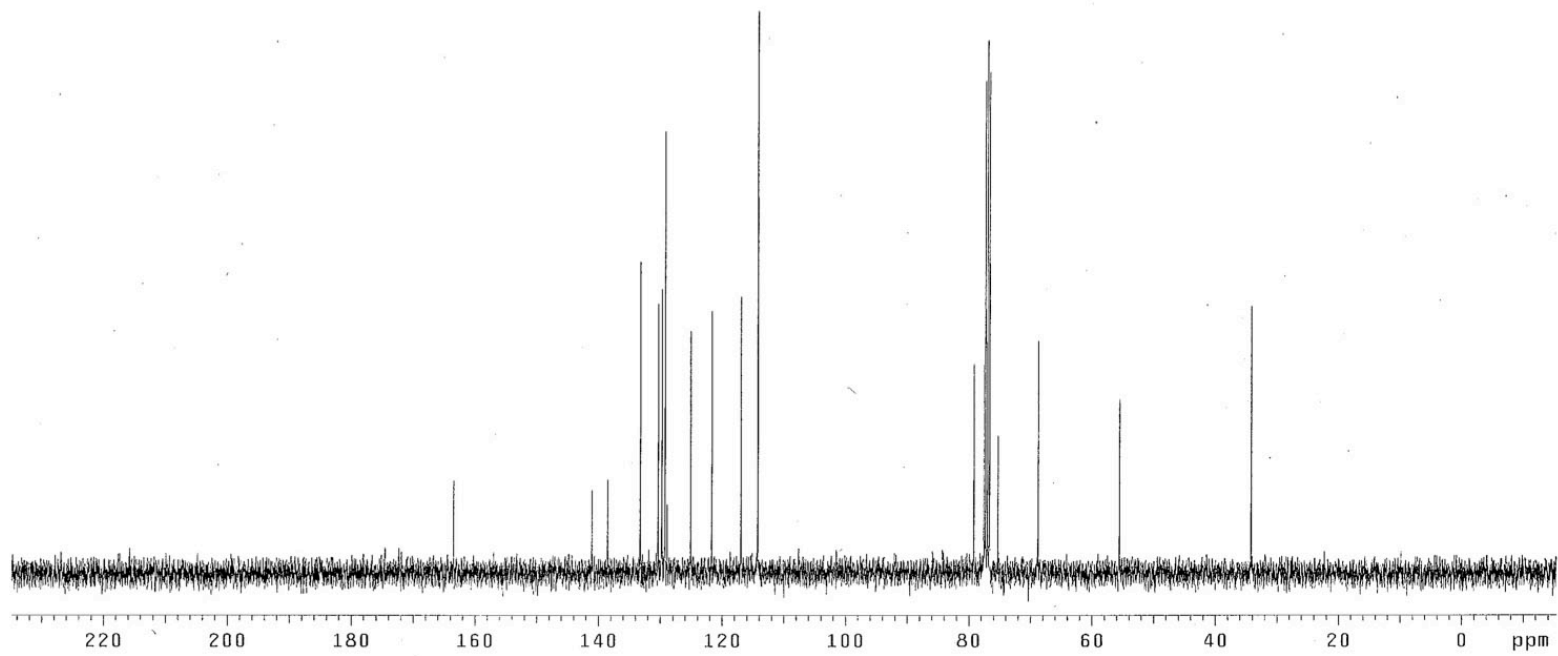
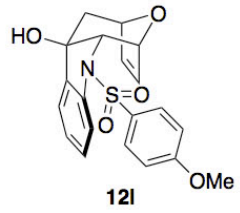
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



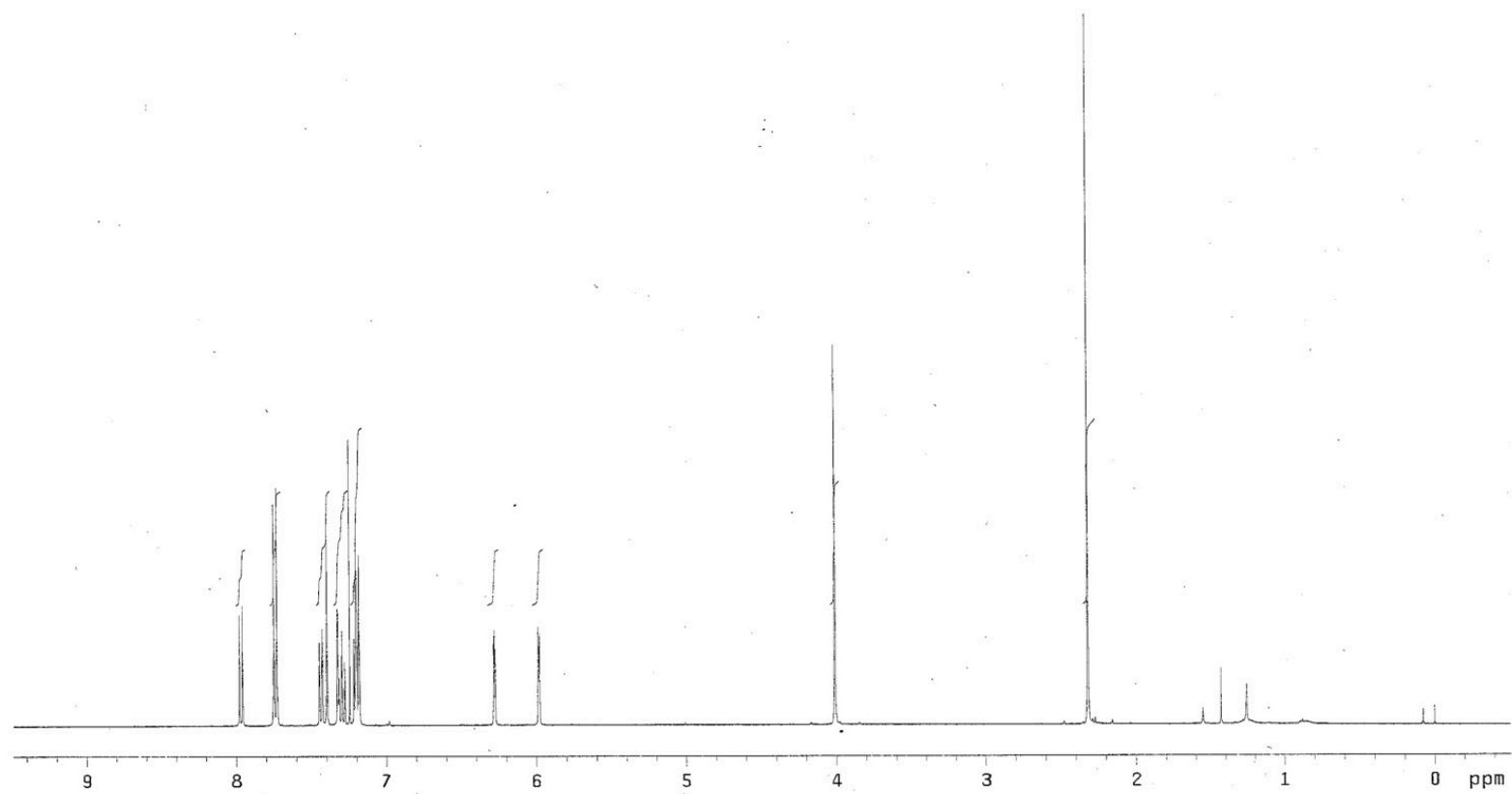
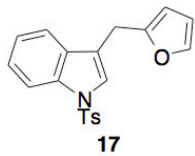
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



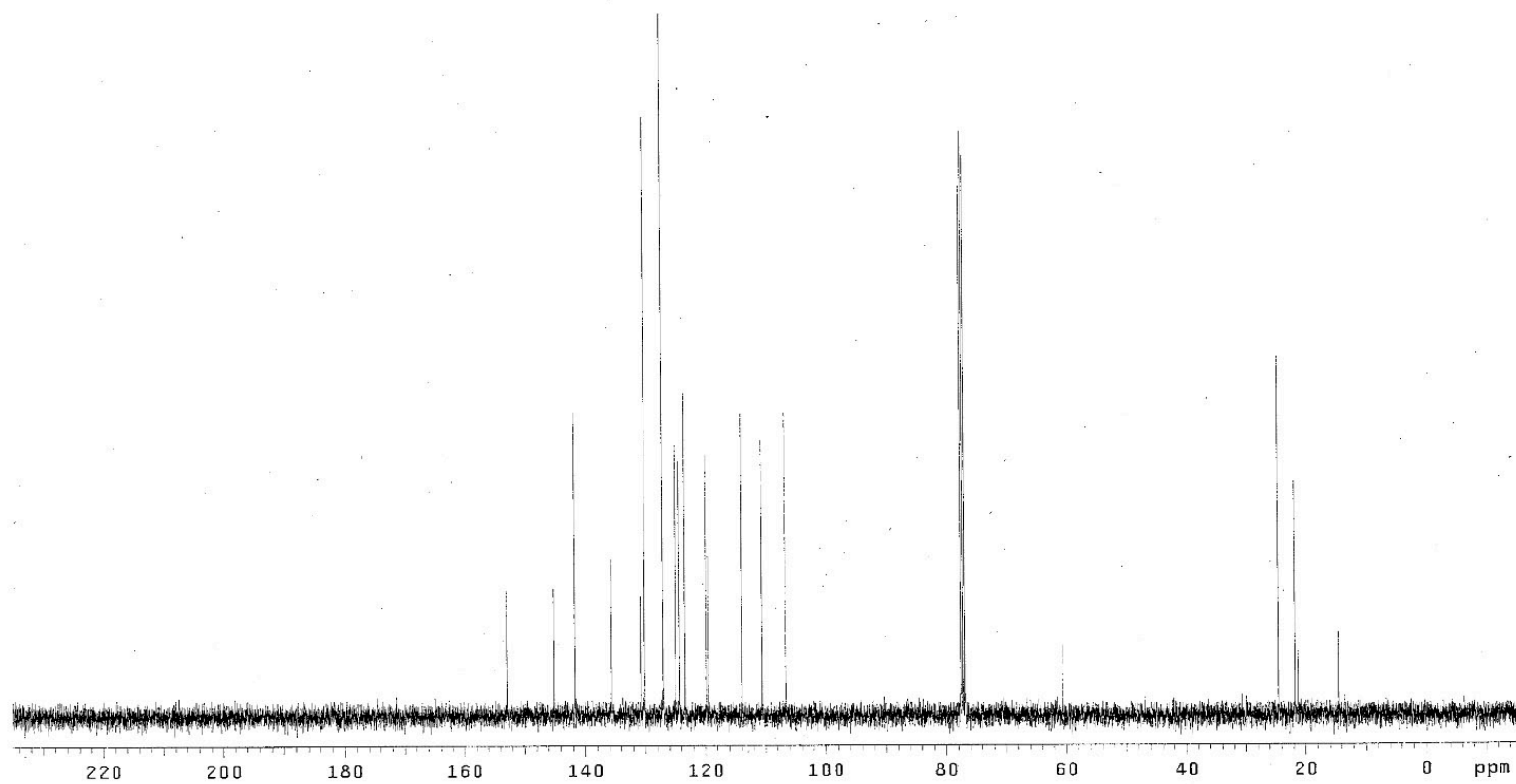
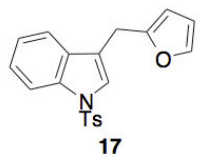
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃

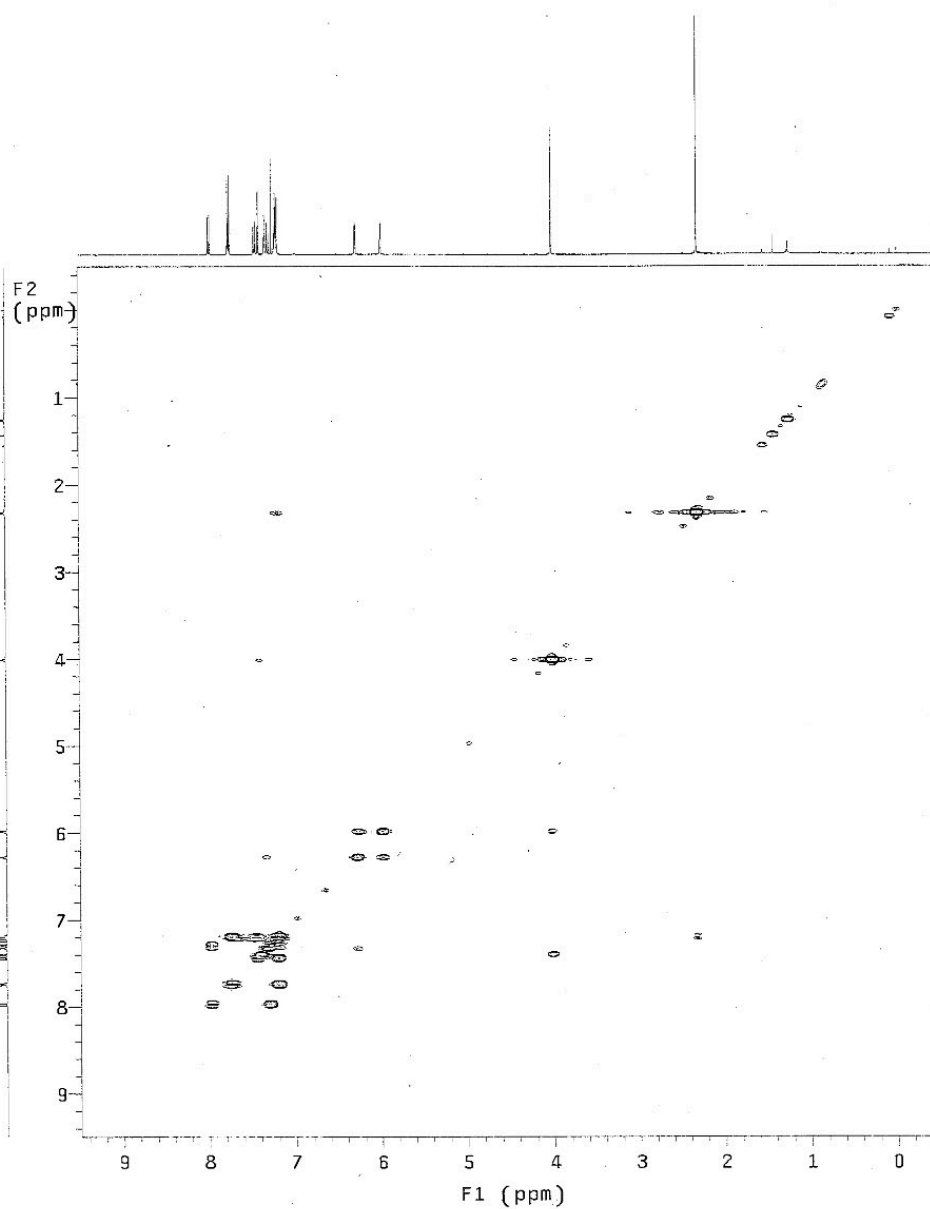
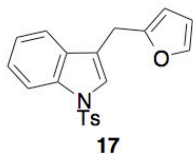


Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



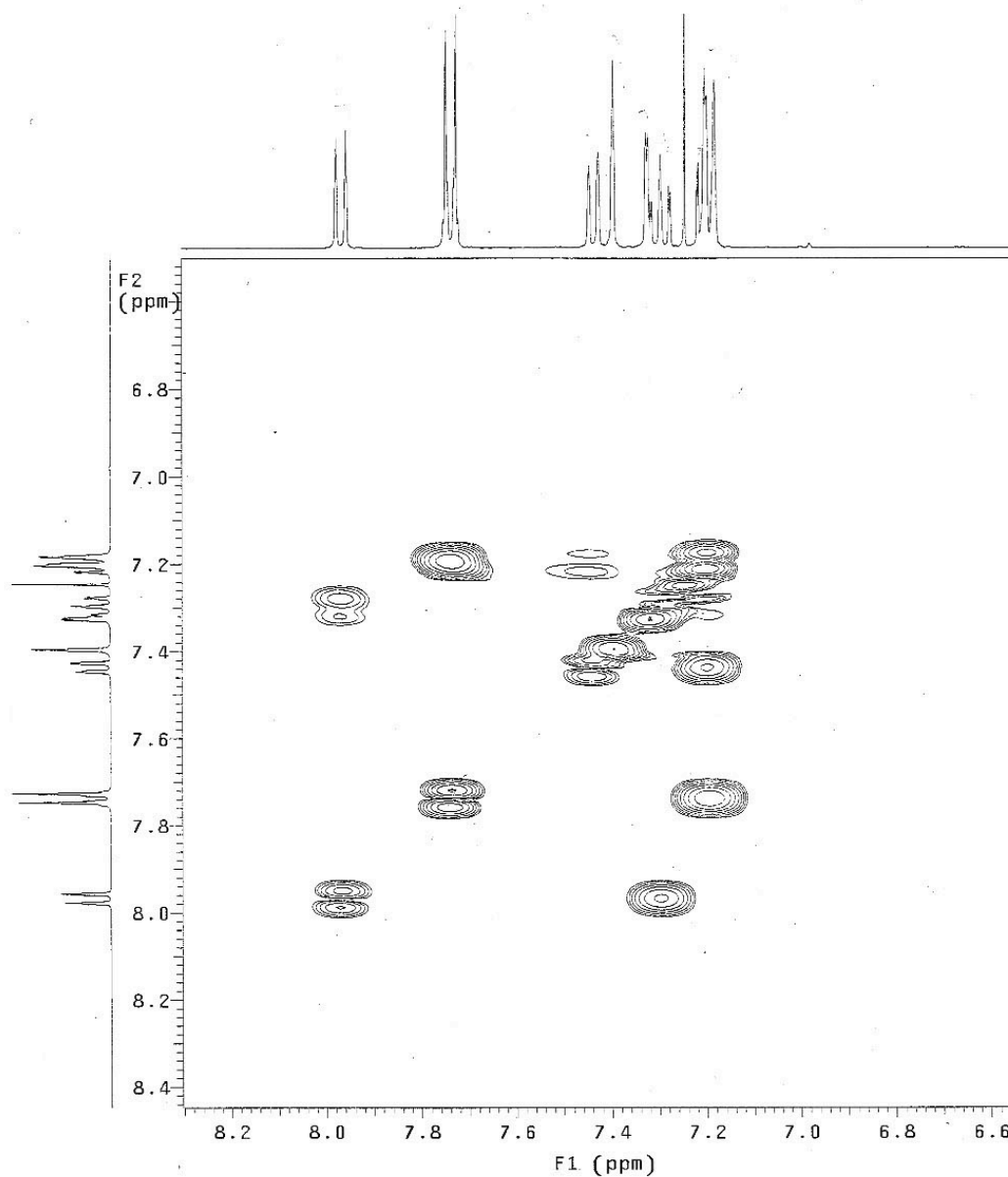
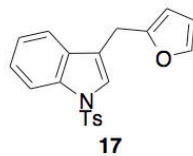
Pulse Sequence: gCOSY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: gCOSY
INOVA-500 "nmr03"

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 4000.4 Hz
2D Width 4001.6 Hz
2 repetitions
128 increments
OBSERVE H1, 399.7865296 MHz
DATA PROCESSING
Sq. sine bell 0.064 sec
F1 DATA PROCESSING
Sq. sine bell 0.032 sec
FT size 4096 x 2048
Total time 5 min, 14 sec

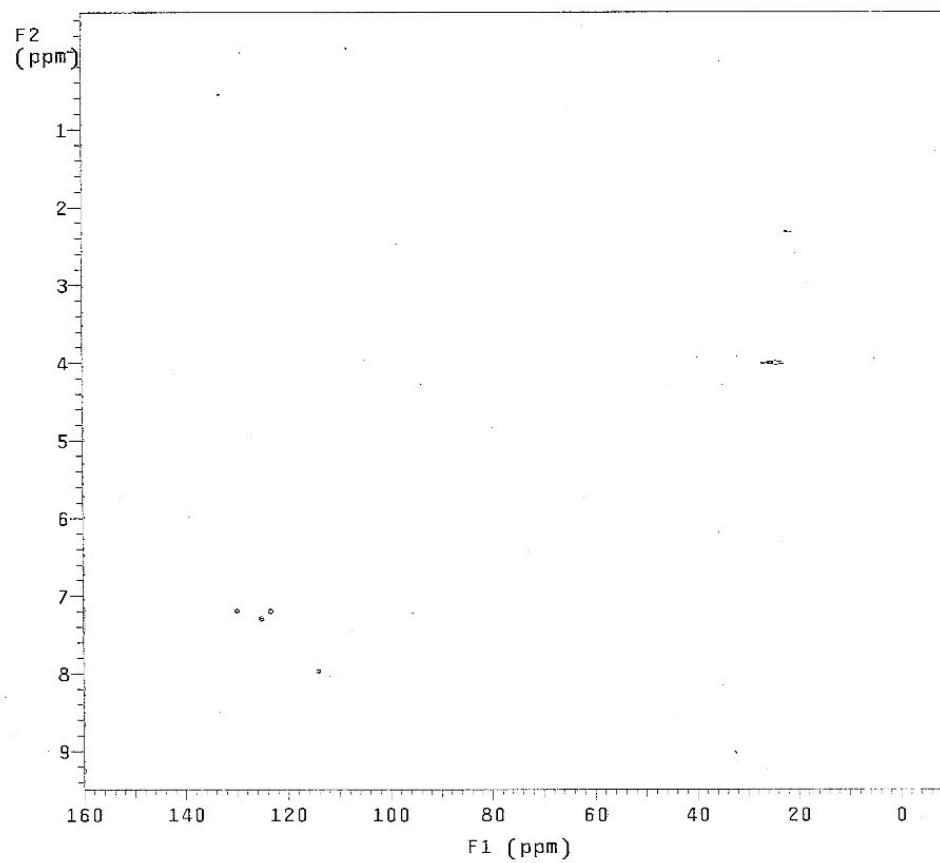
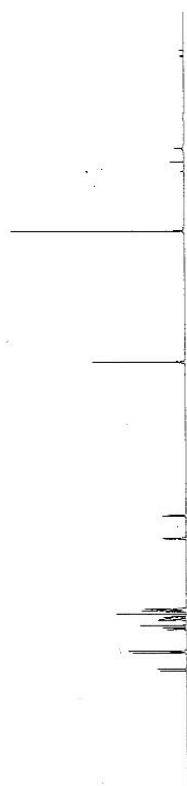
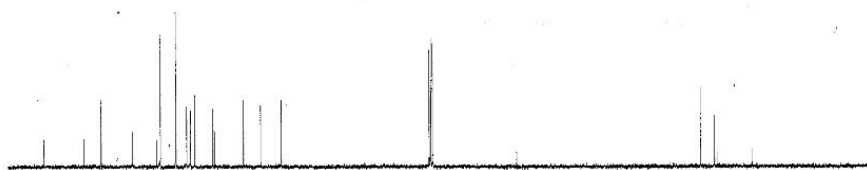
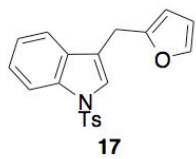


Pulse Sequence: gCOSY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: gCOSY
INNOVA-500 "nmr03"

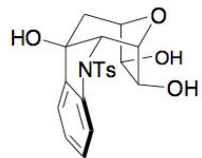
Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 4000.4 Hz
2D Width 4001.6 Hz
2 repetitions
128 increments
OBSERVE F1, 399.7865296 MHz
DATA PROCESSING
Sq. sine bell 0.064 sec
F1 DATA PROCESSING
Sq. sine bell 0.032 sec
FT size 4096 x 2048
Total time 5 min, 14 sec



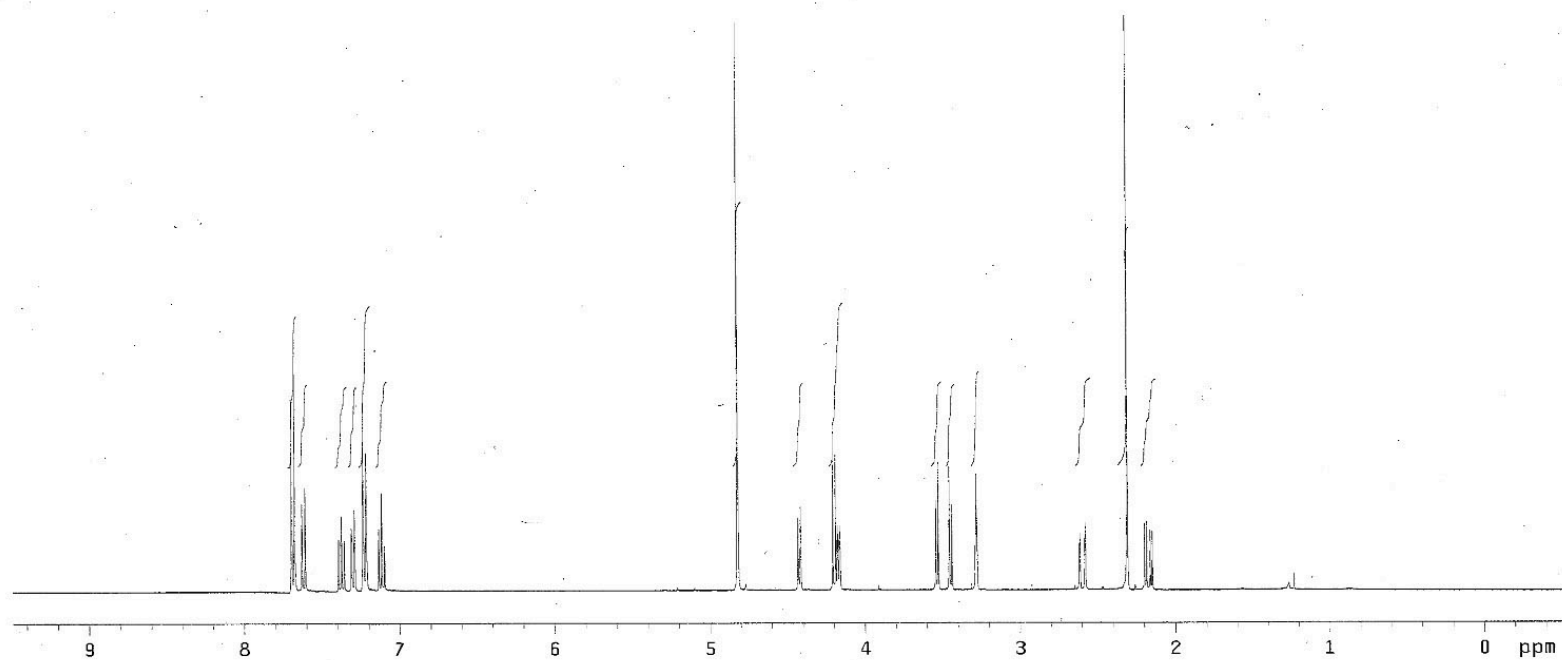
Pulse Sequence: gHSQC



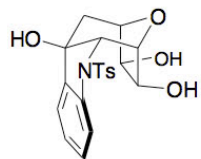
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CD₃OD



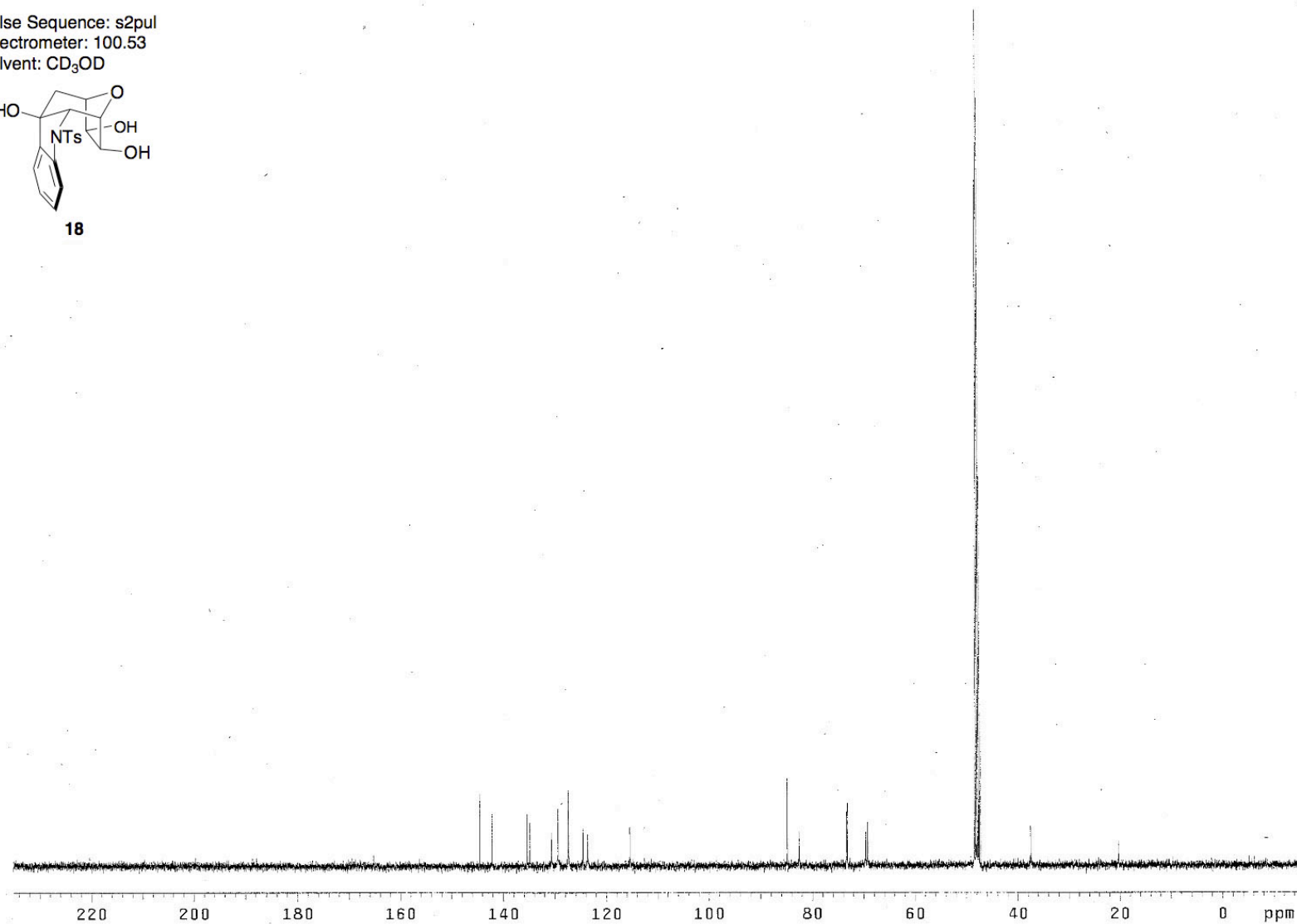
18



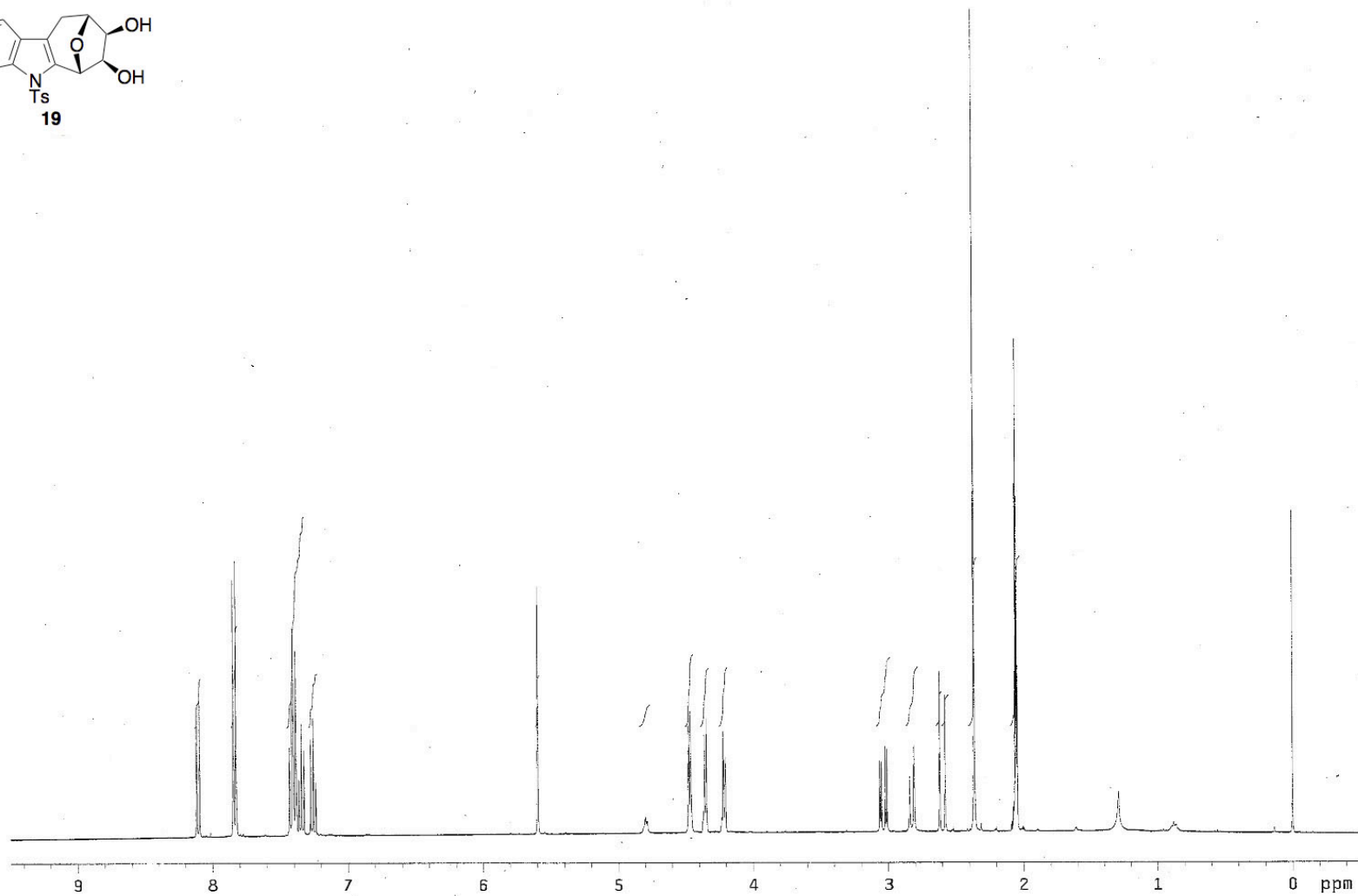
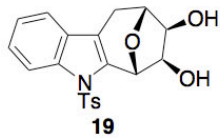
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CD₃OD



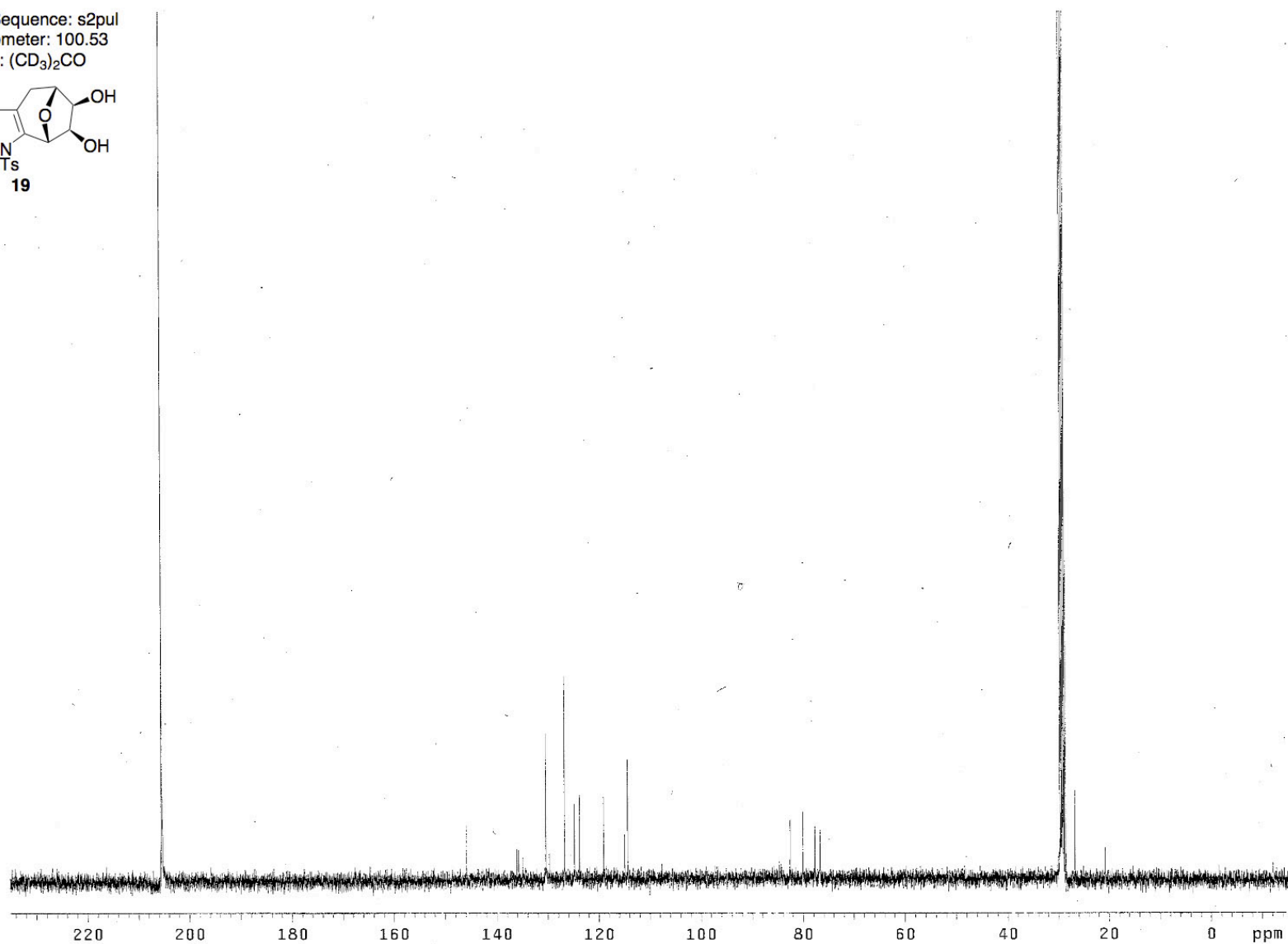
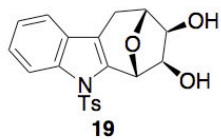
18



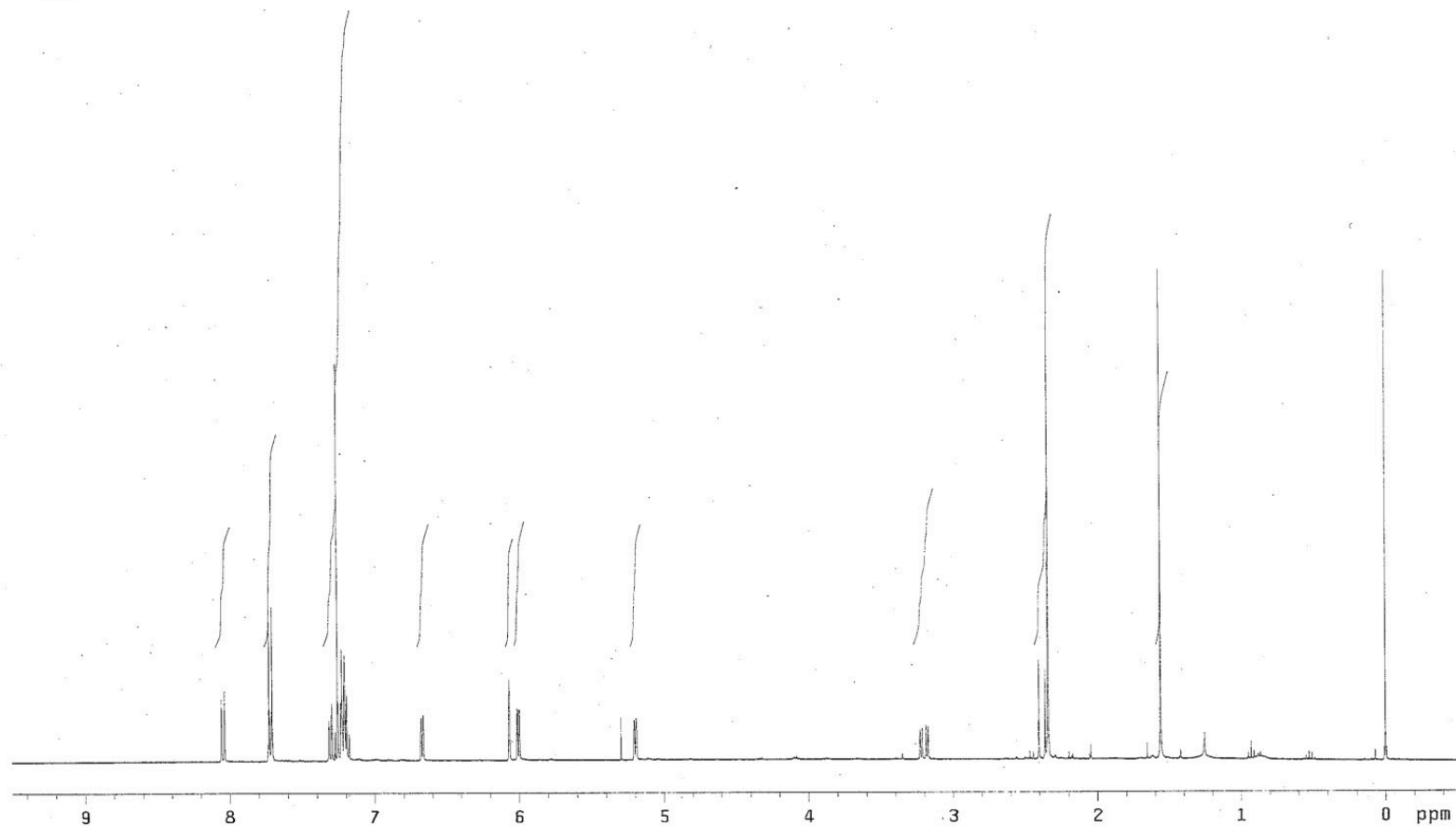
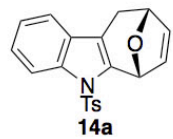
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: (CD₃)₂CO



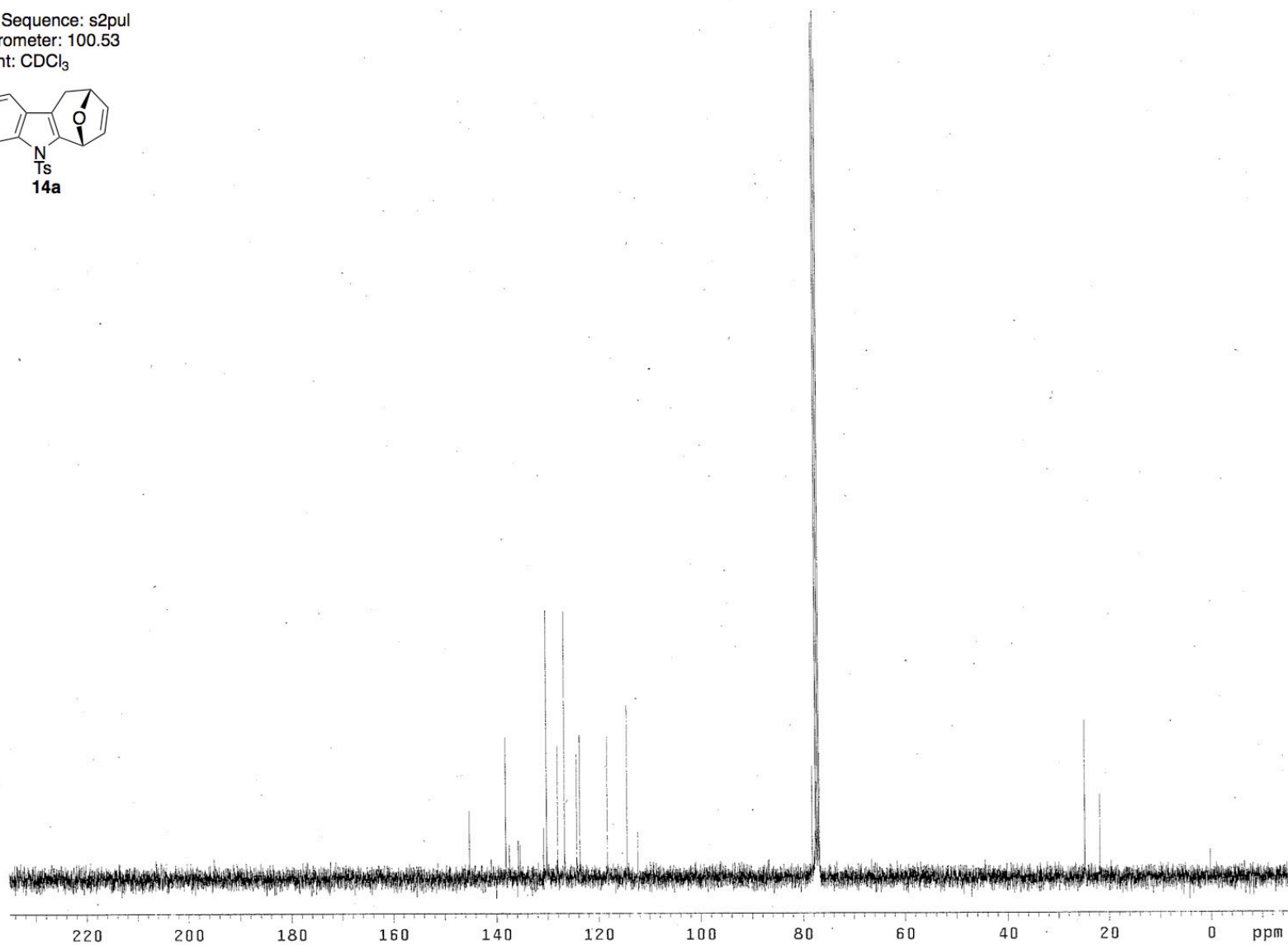
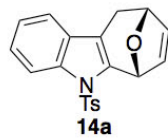
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: (CD₃)₂CO



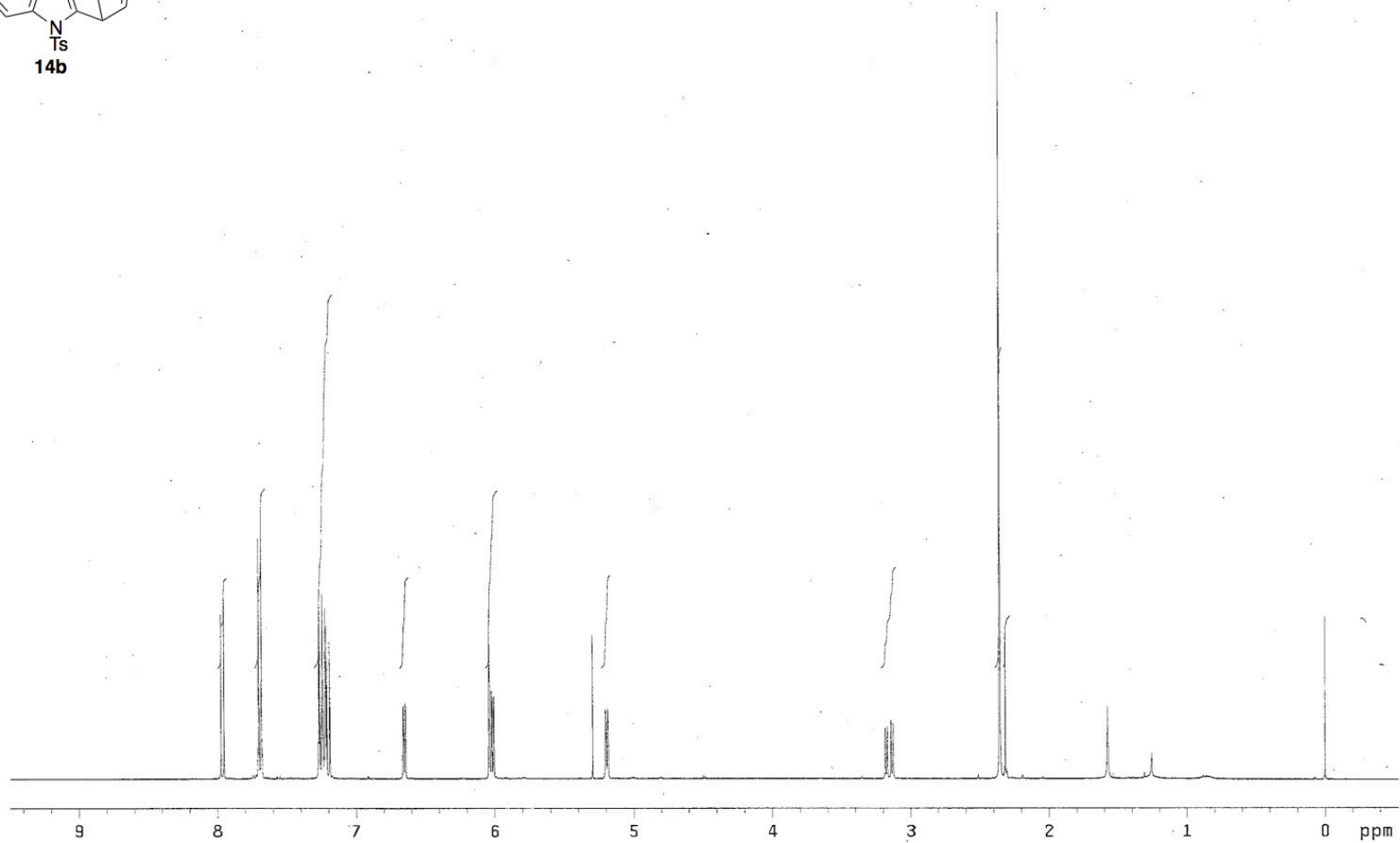
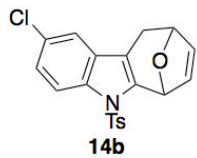
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



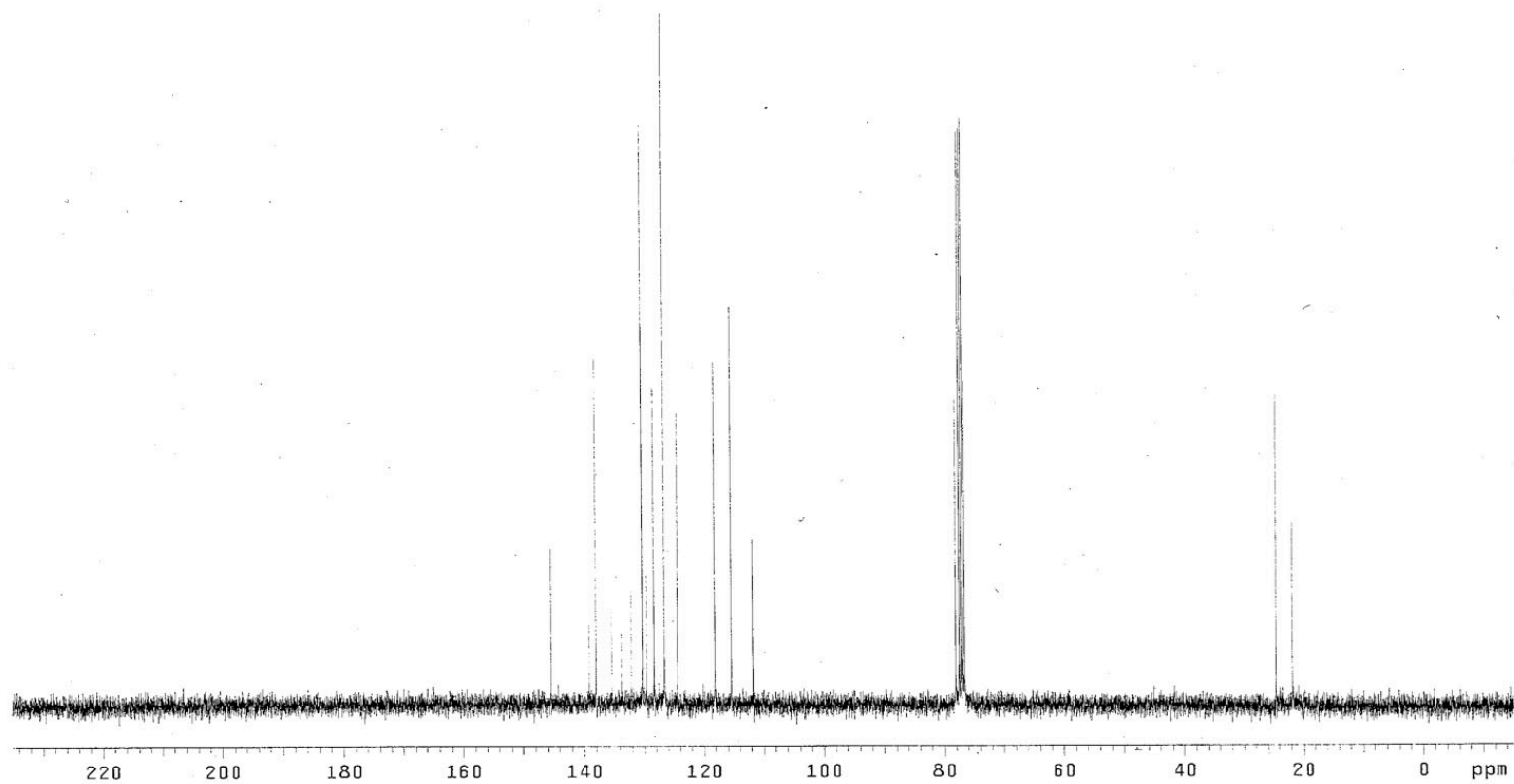
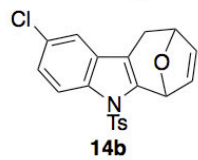
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



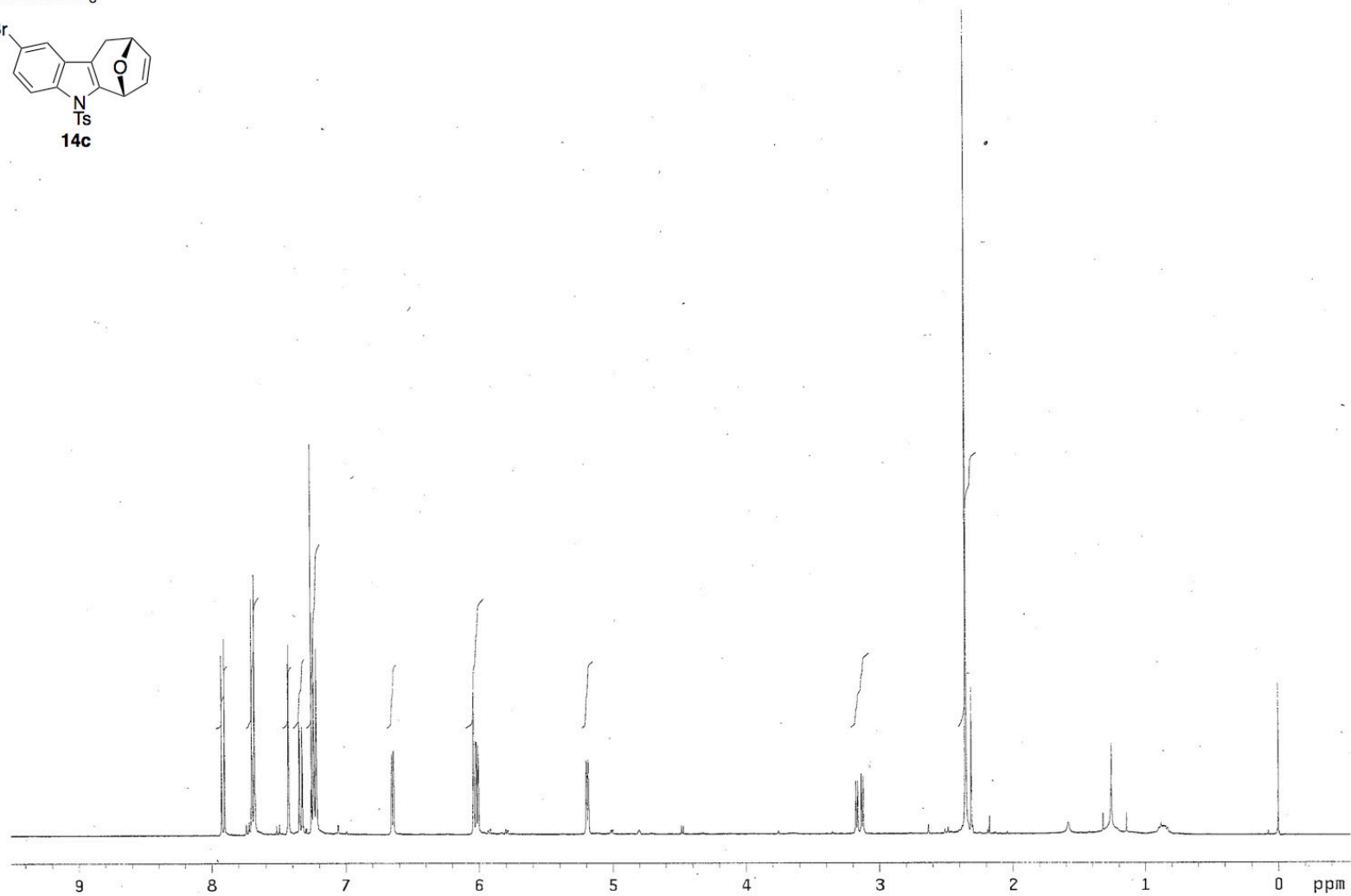
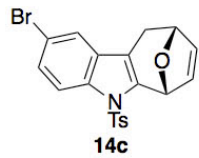
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



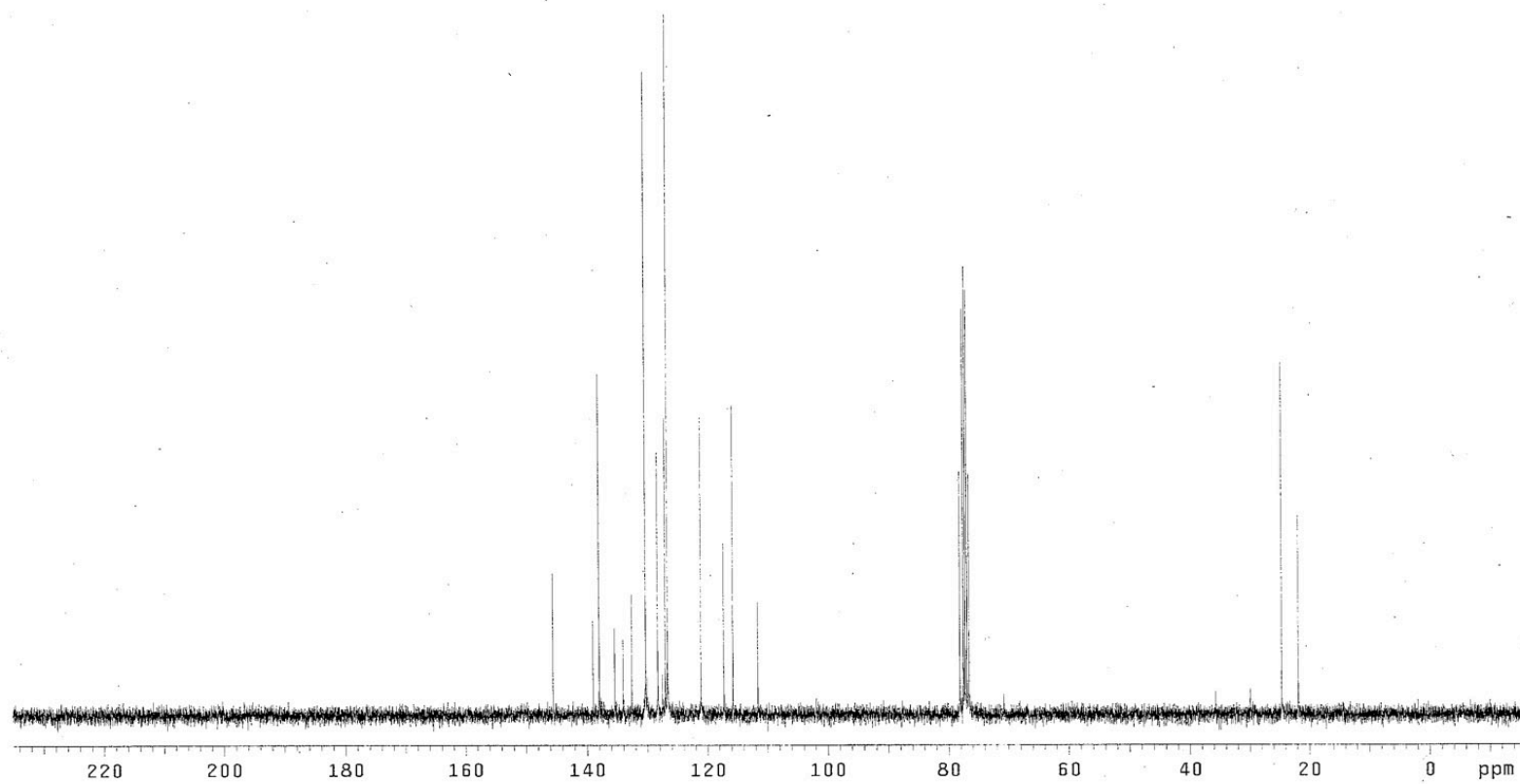
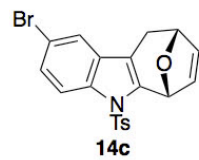
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



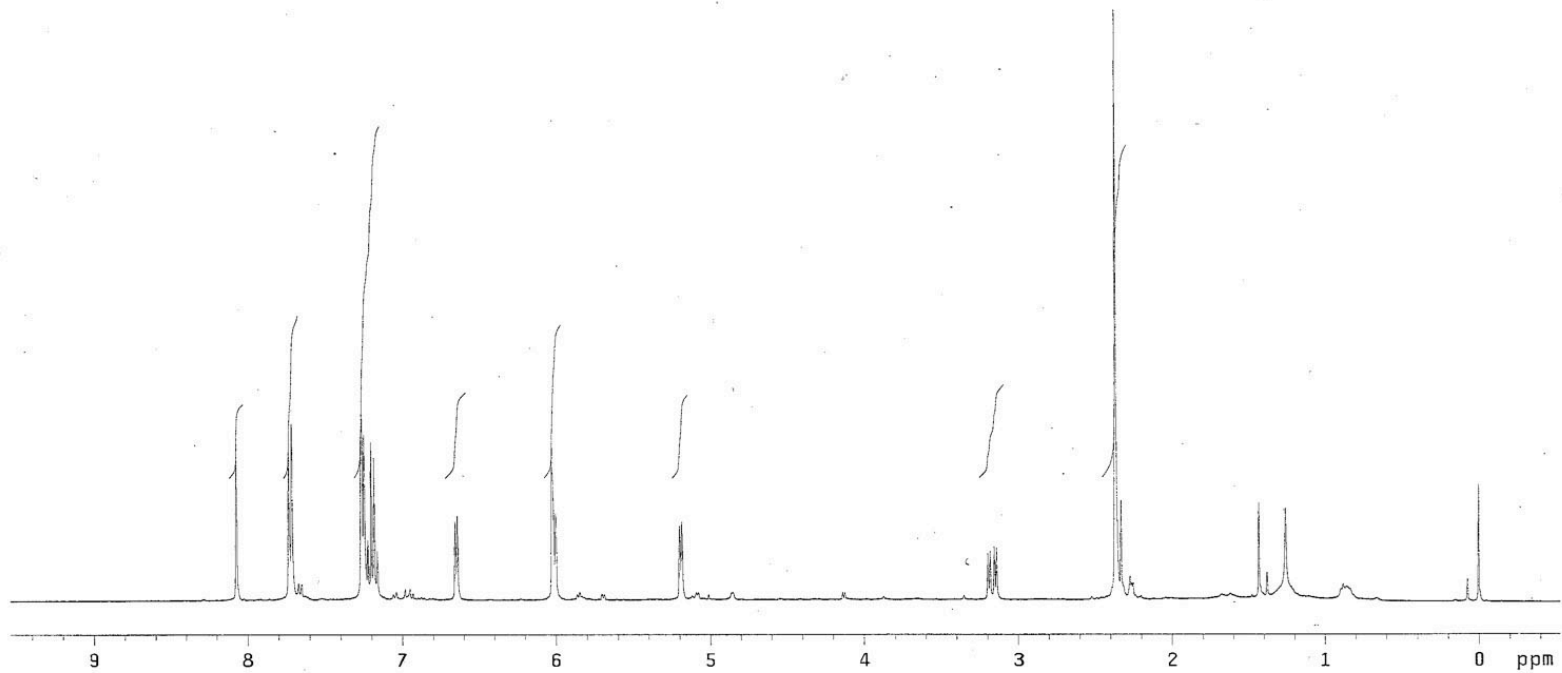
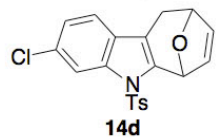
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



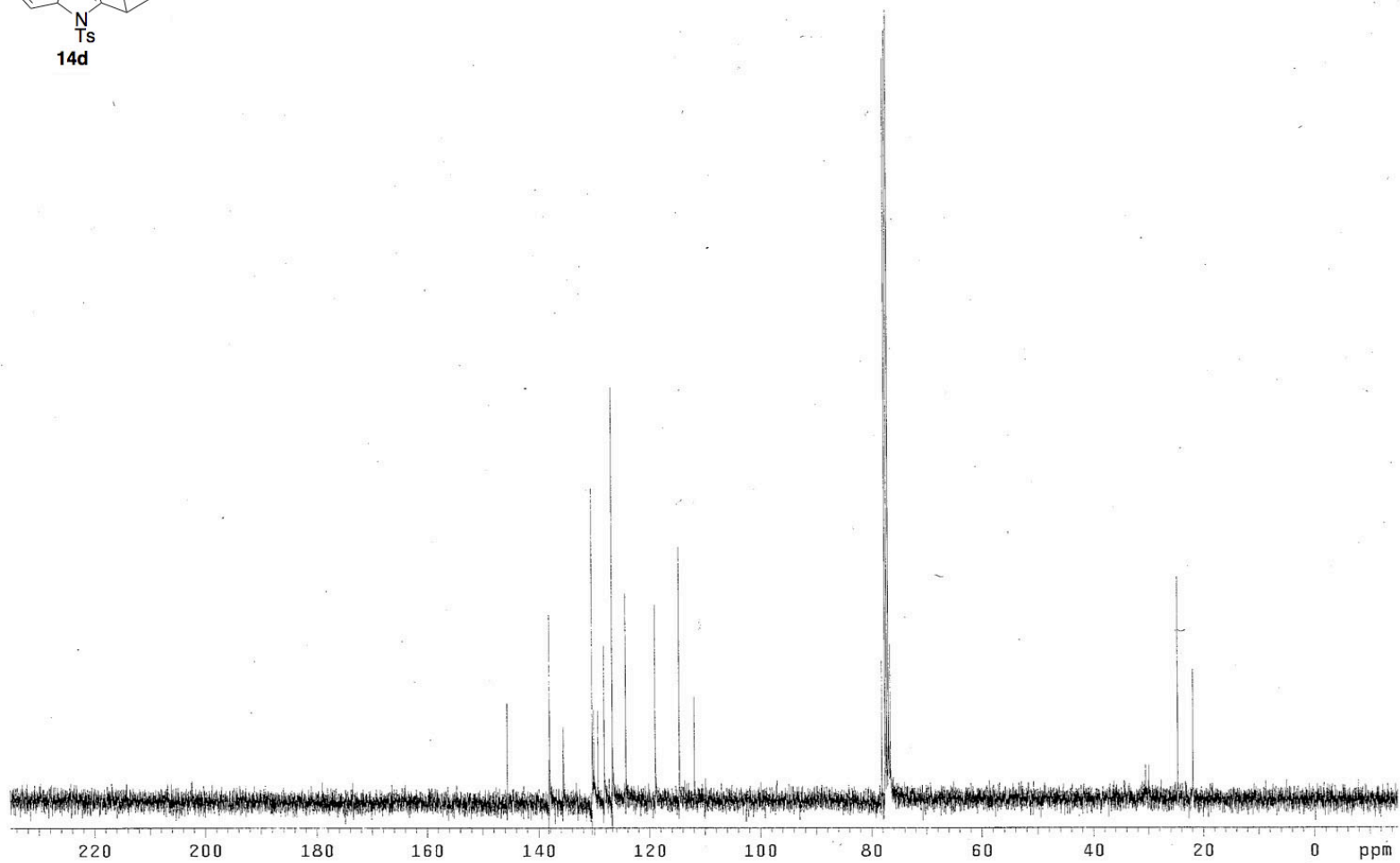
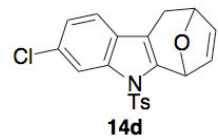
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



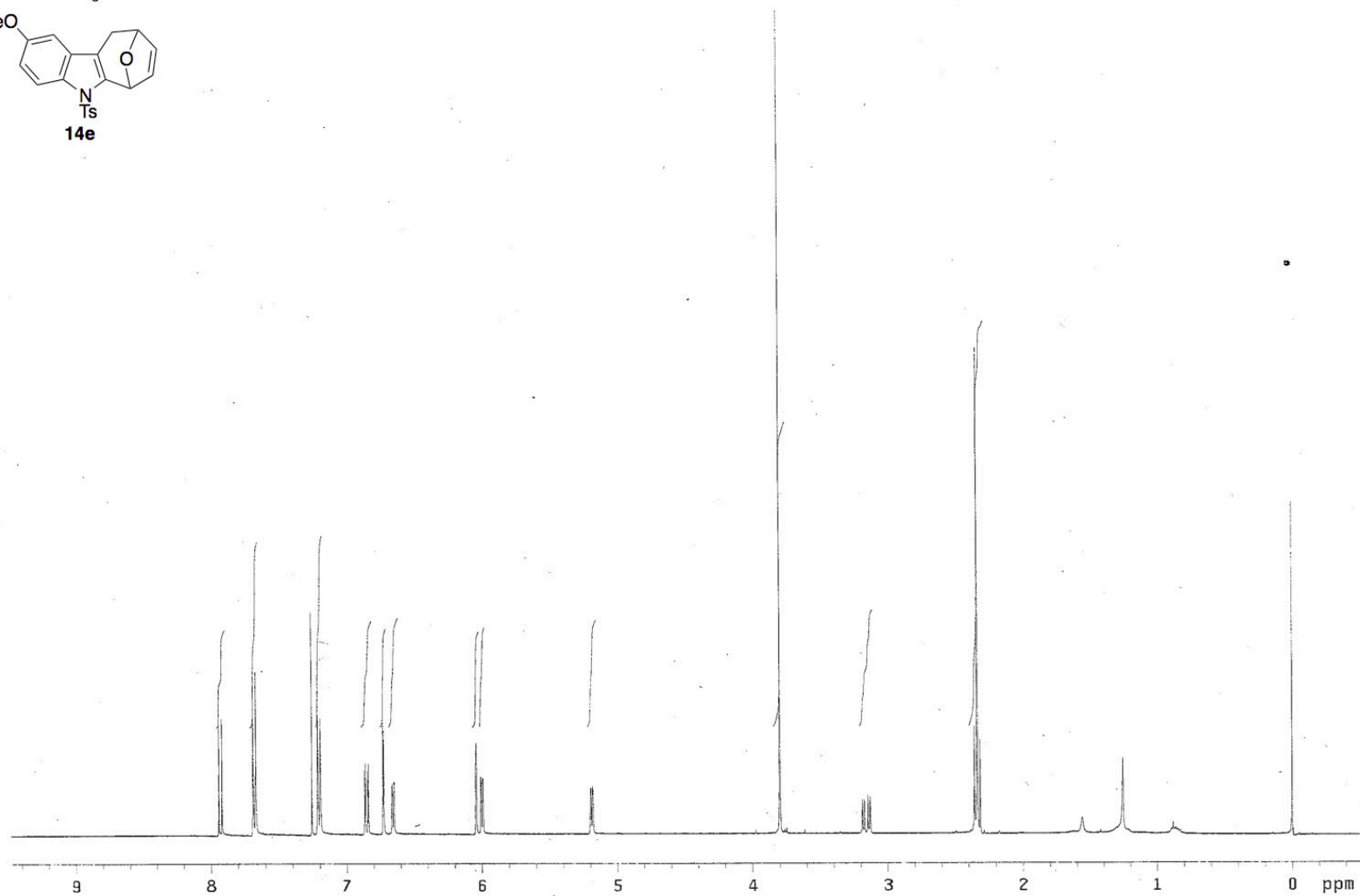
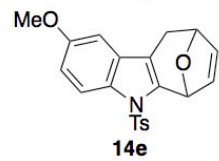
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



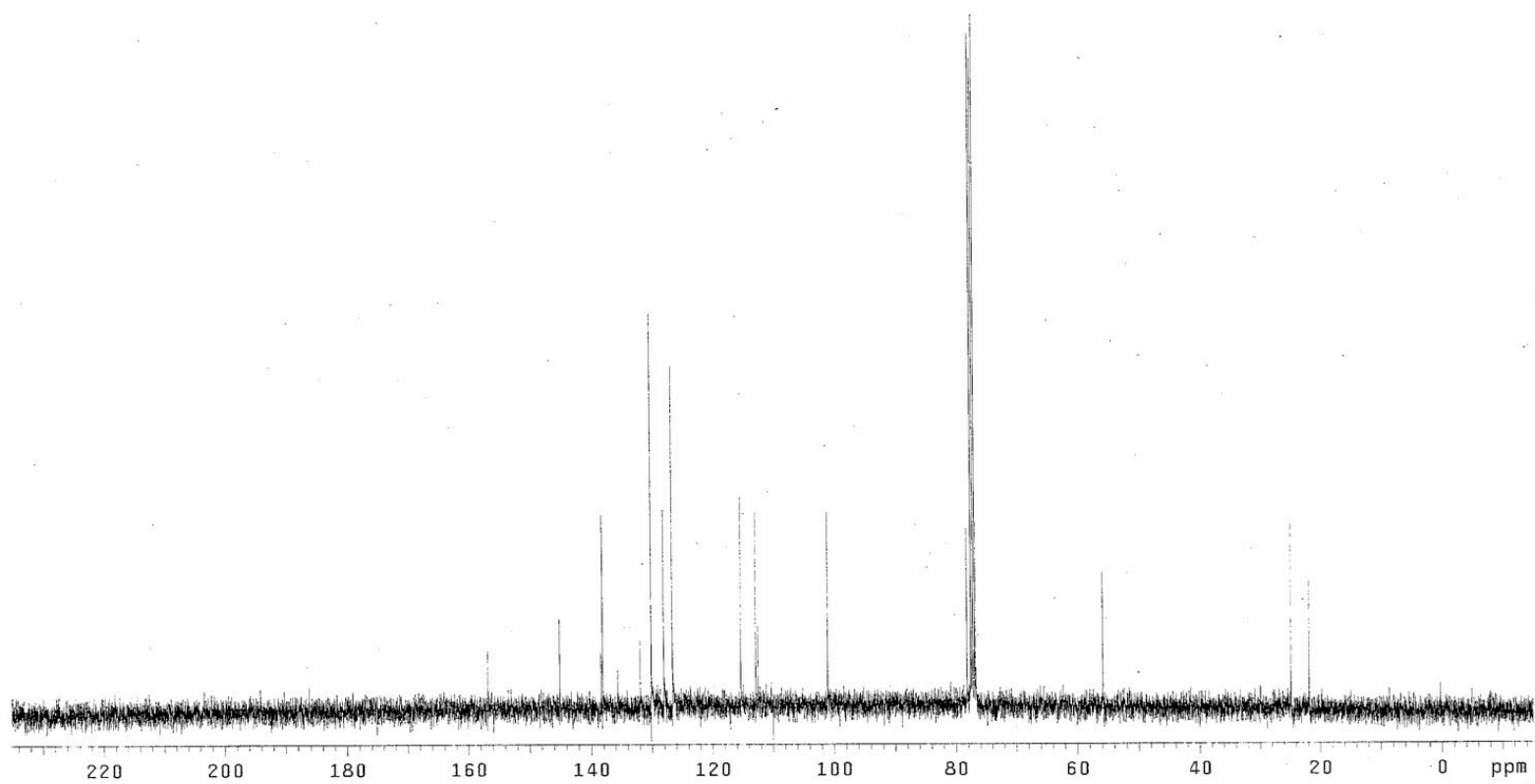
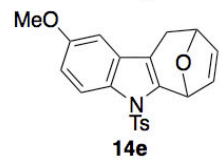
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



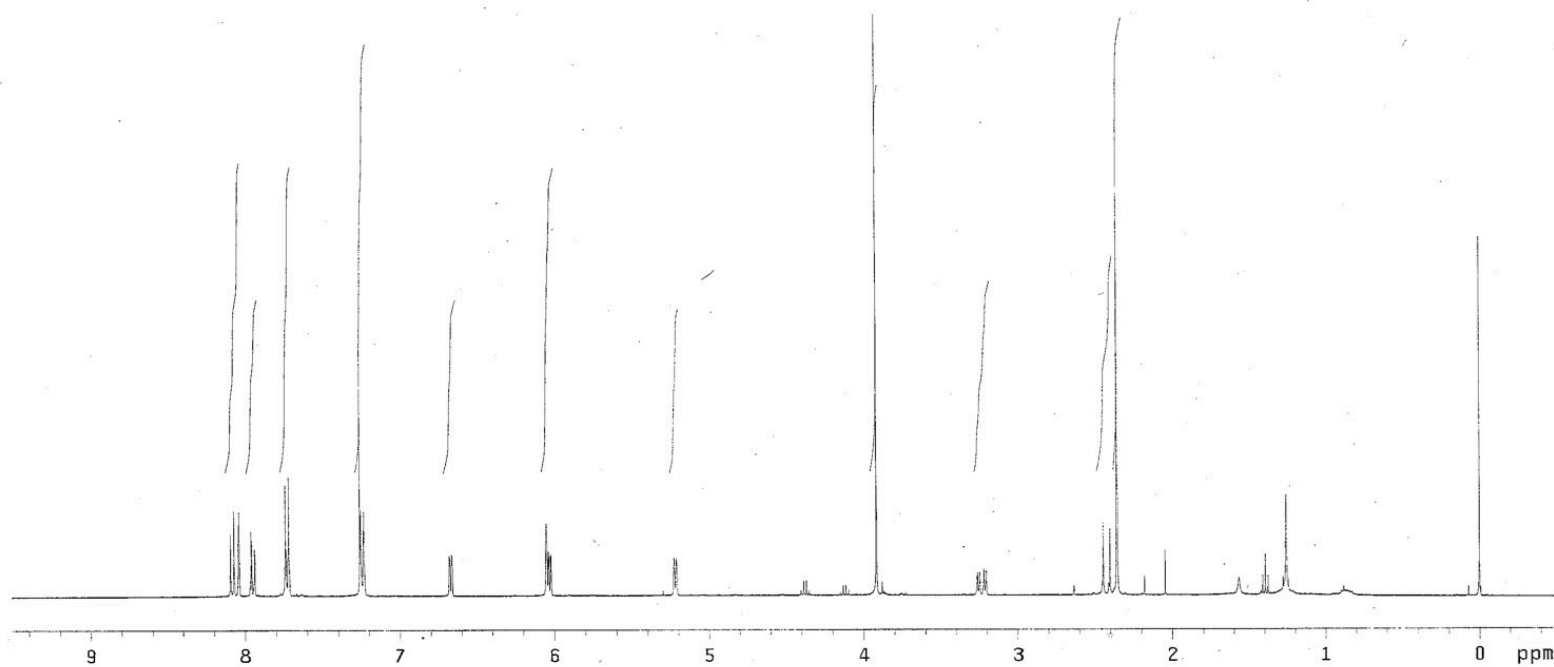
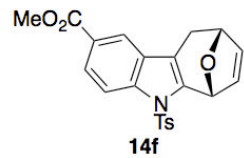
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



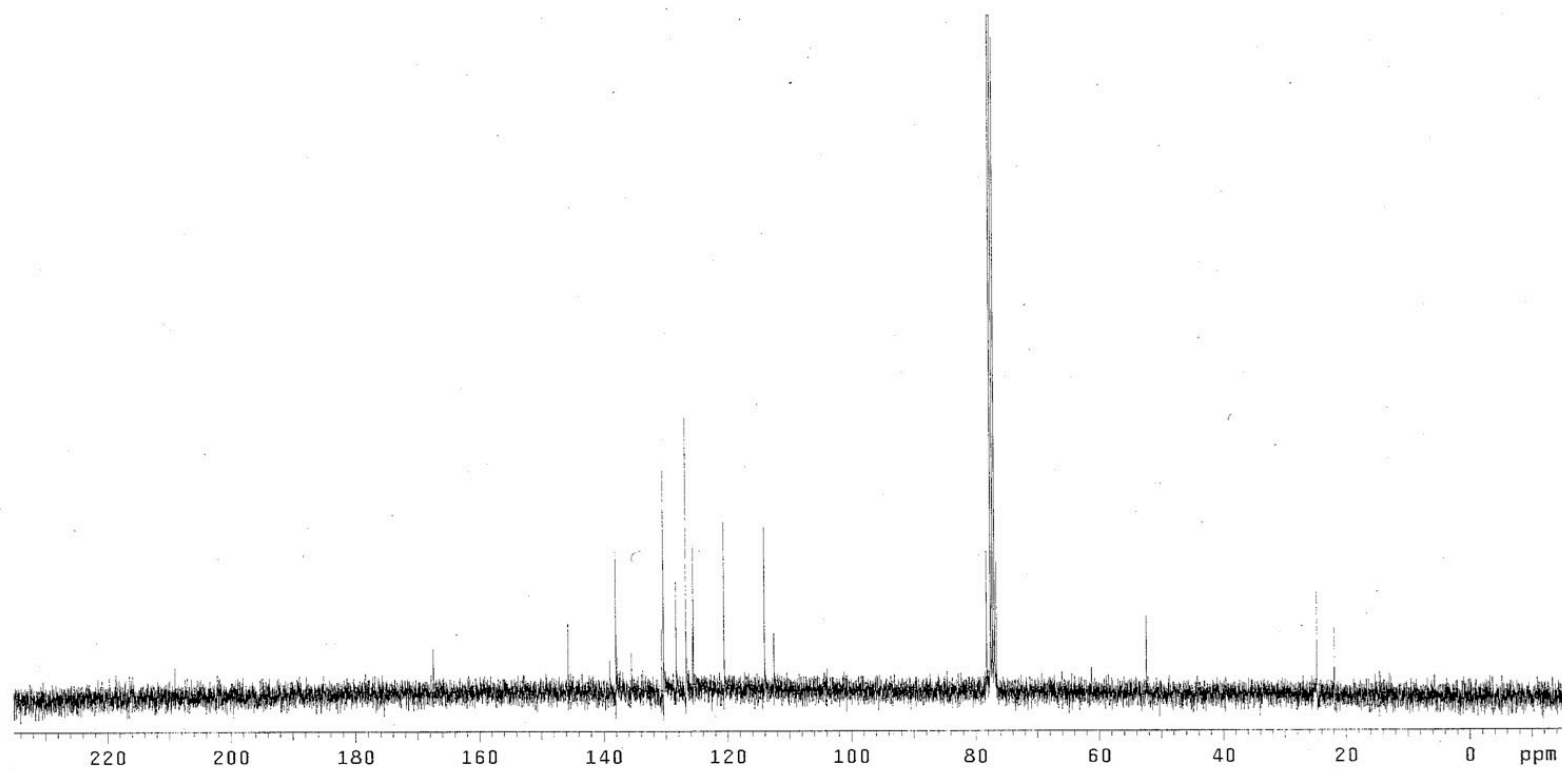
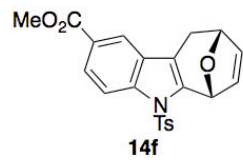
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



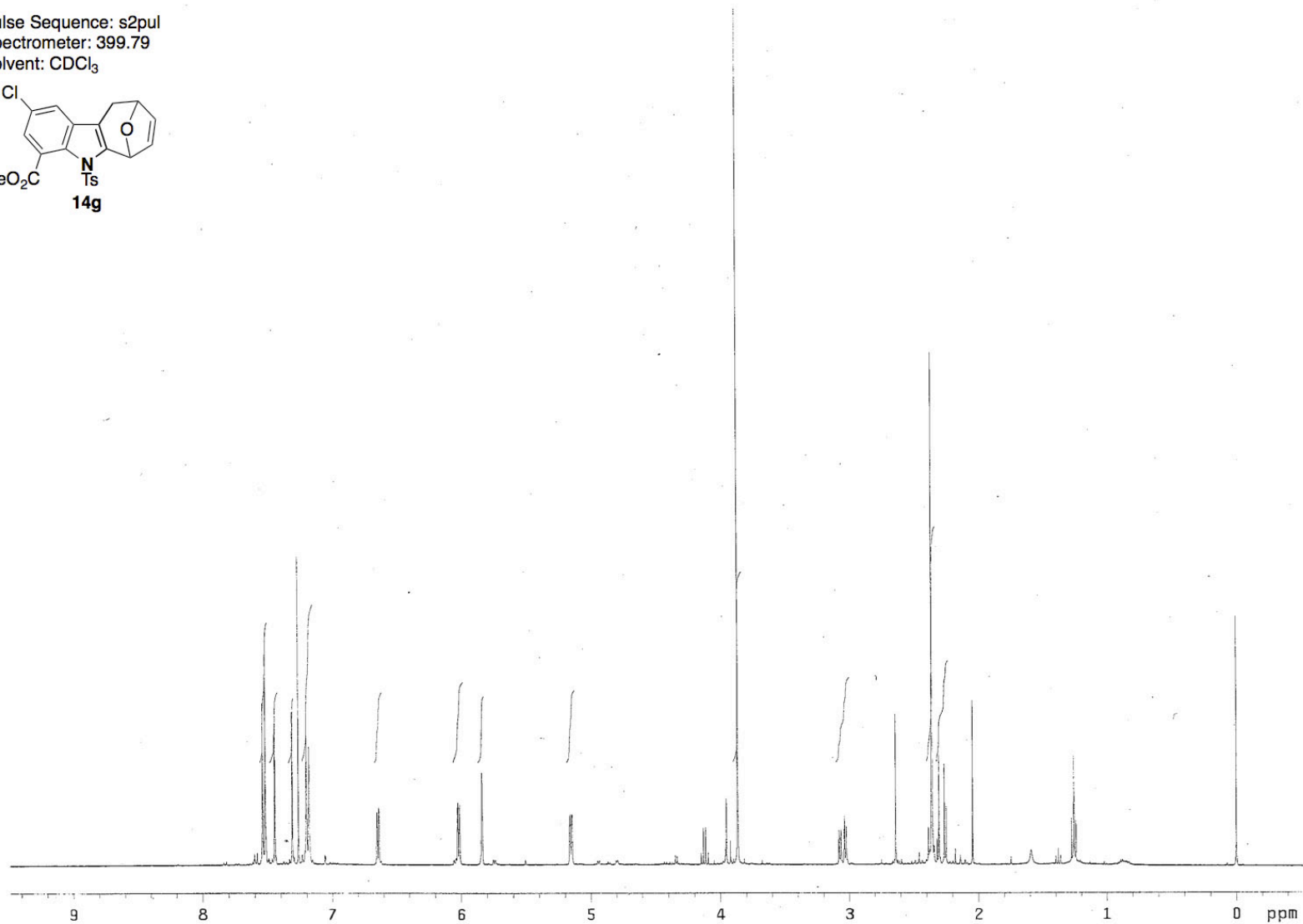
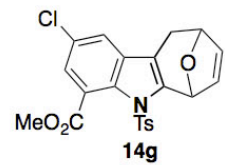
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



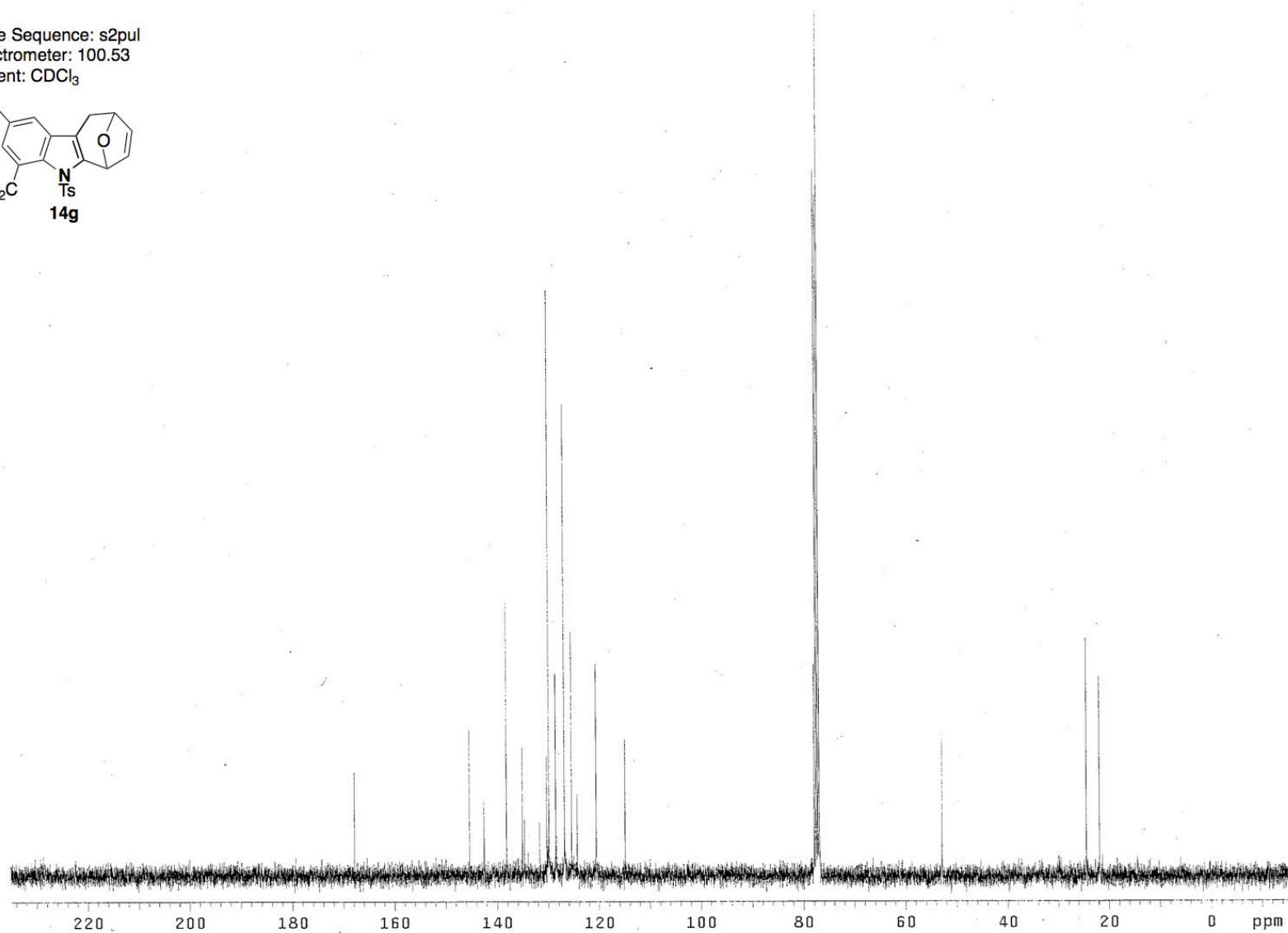
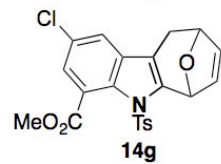
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



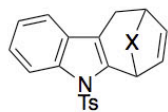
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



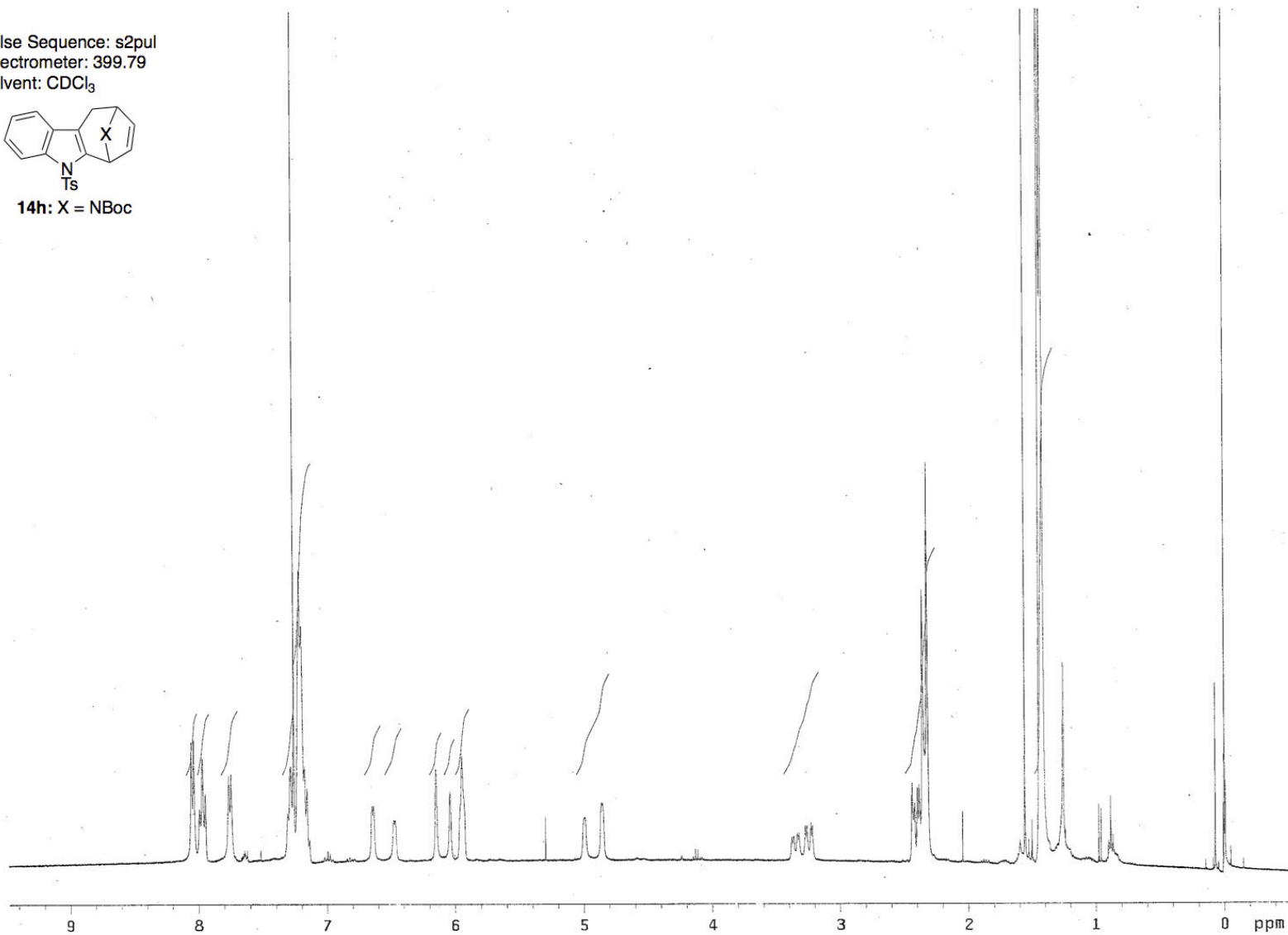
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



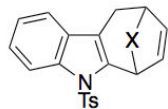
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



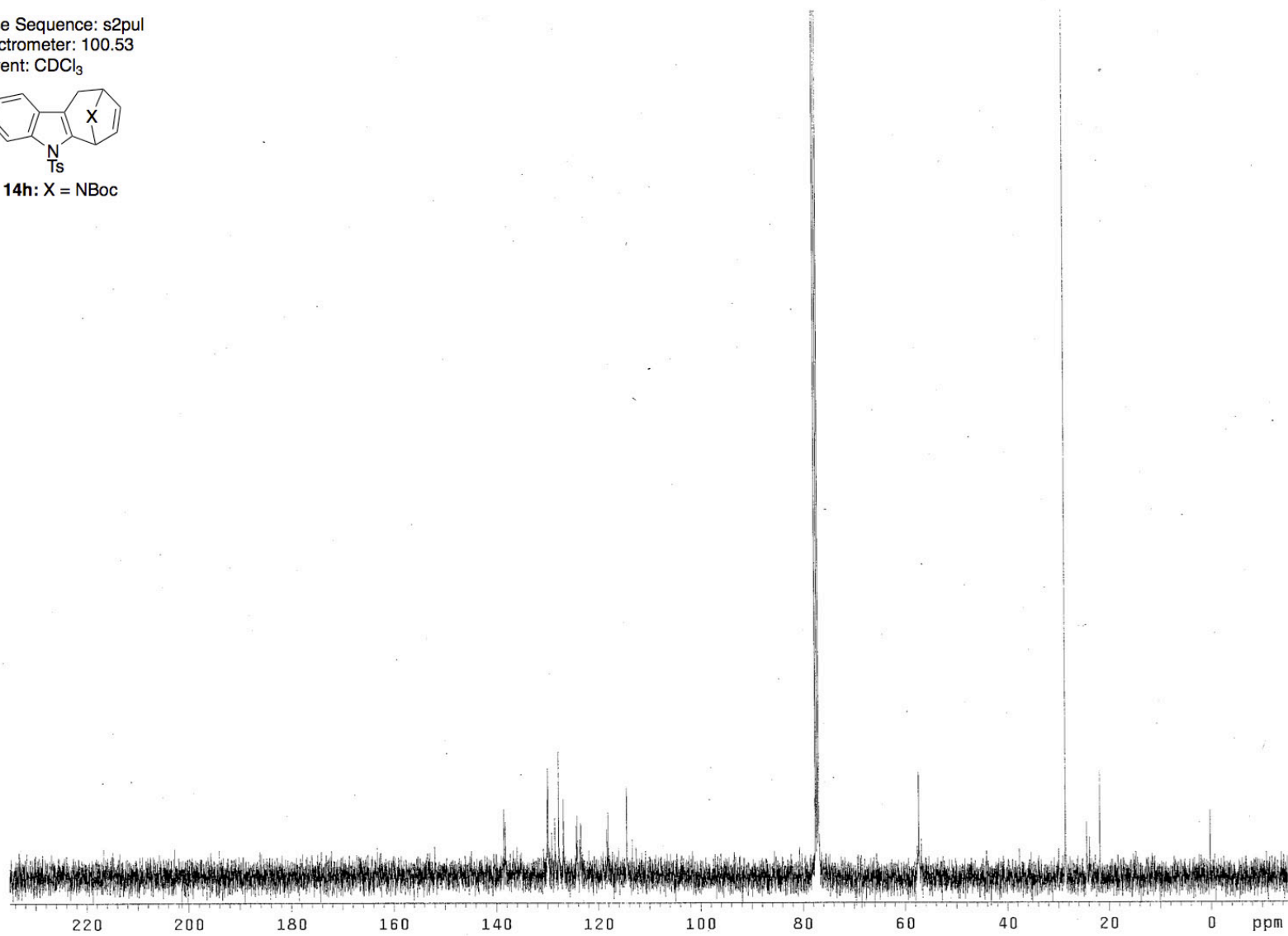
14h: X = NBoc



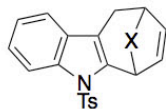
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



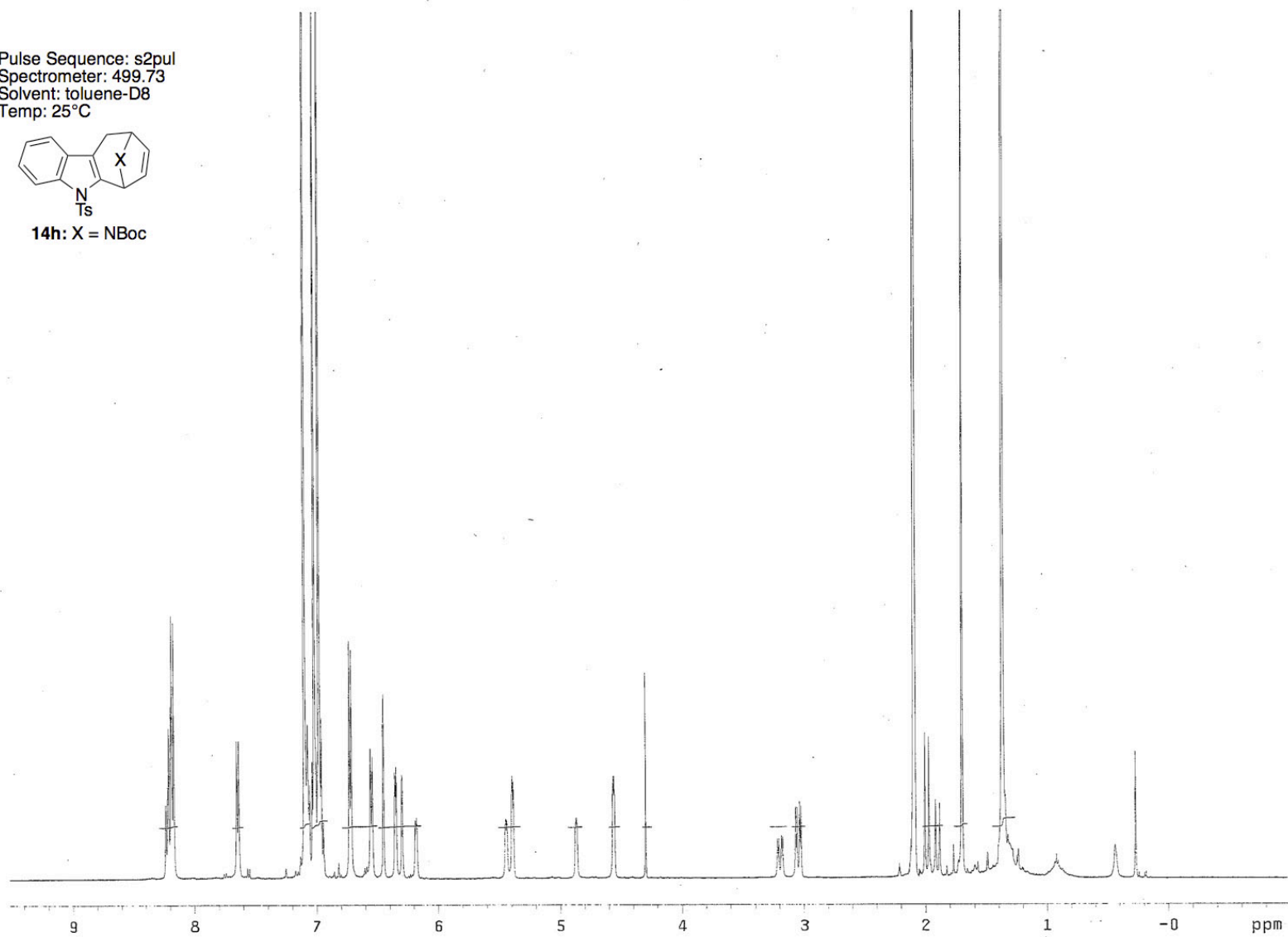
14h: X = NBoc



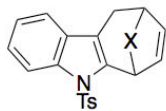
Pulse Sequence: s2pul
Spectrometer: 499.73
Solvent: toluene-D8
Temp: 25°C



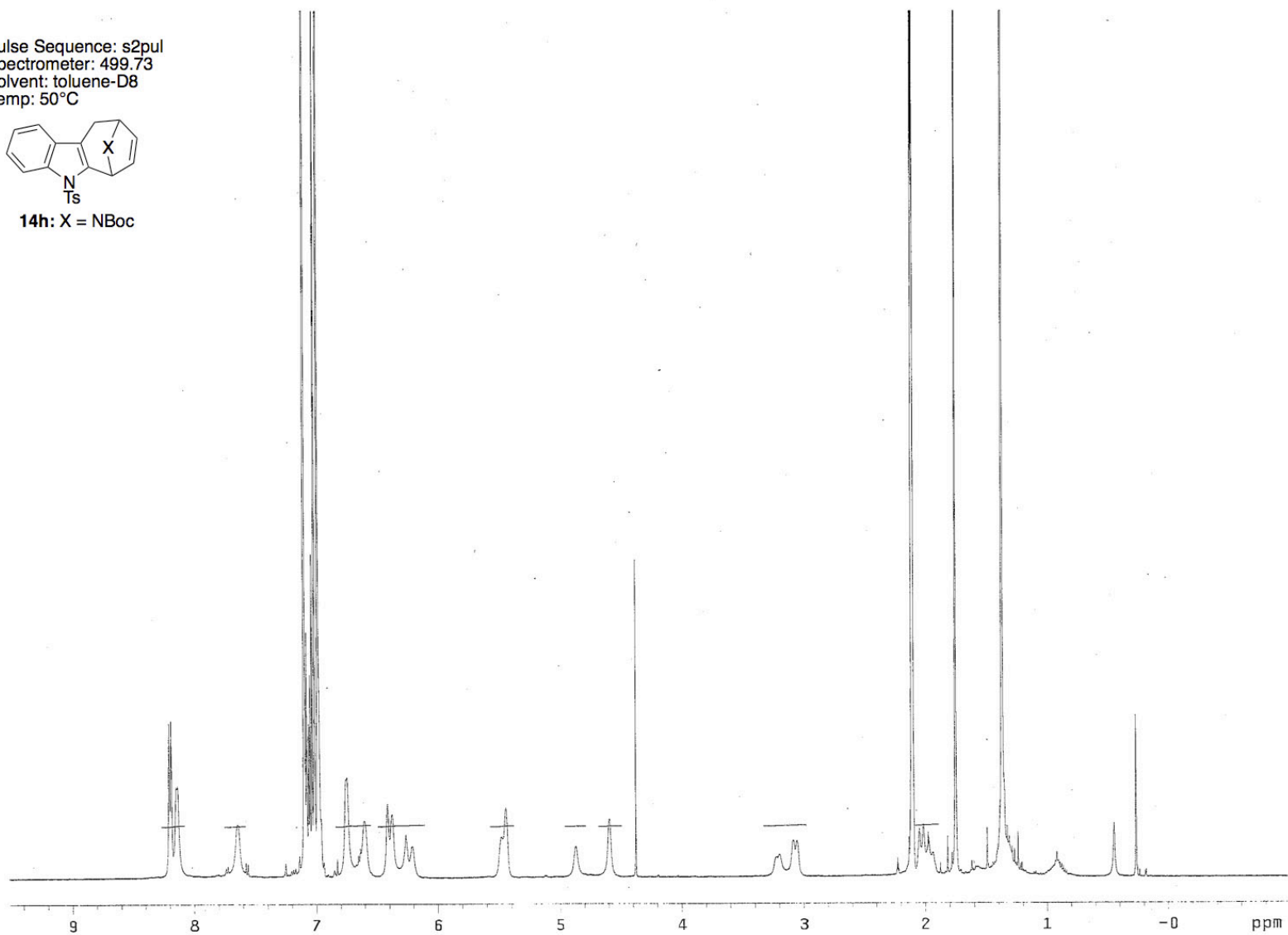
14h: X = NBoc



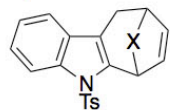
Pulse Sequence: s2pul
Spectrometer: 499.73
Solvent: toluene-D8
Temp: 50°C



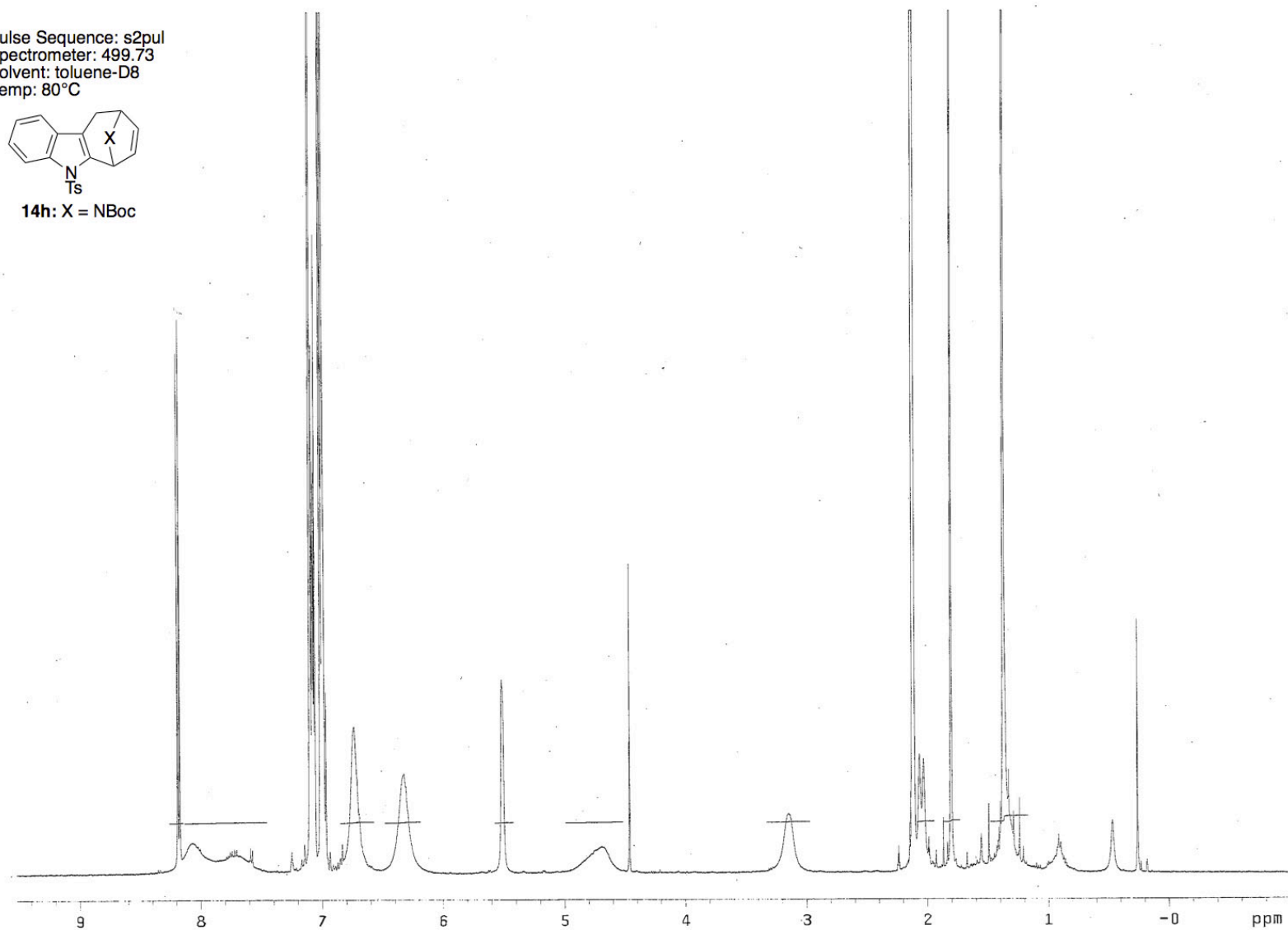
14h: X = NBoc



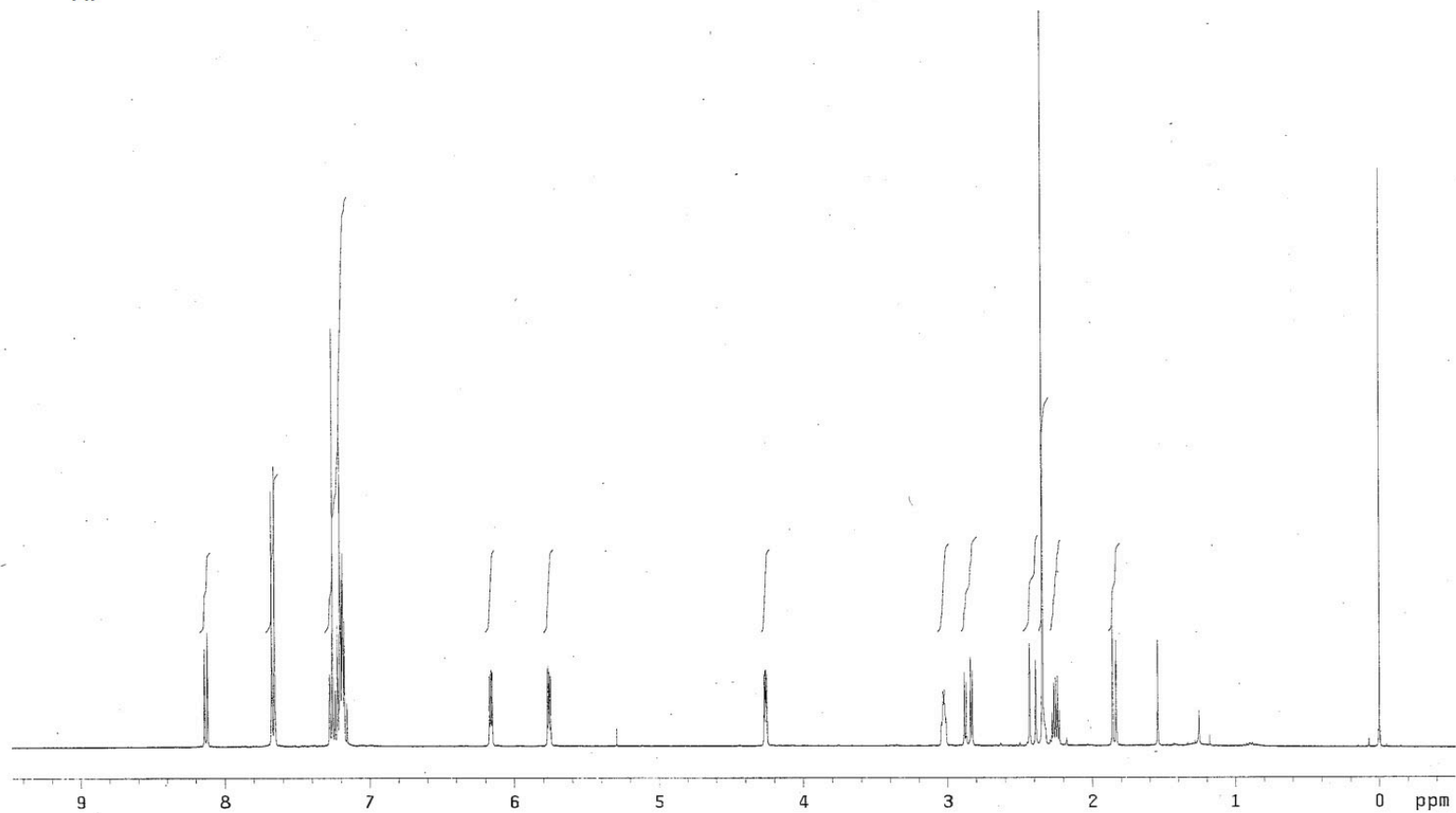
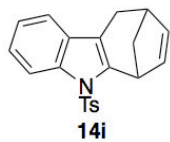
Pulse Sequence: s2pul
Spectrometer: 499.73
Solvent: toluene-D8
Temp: 80°C



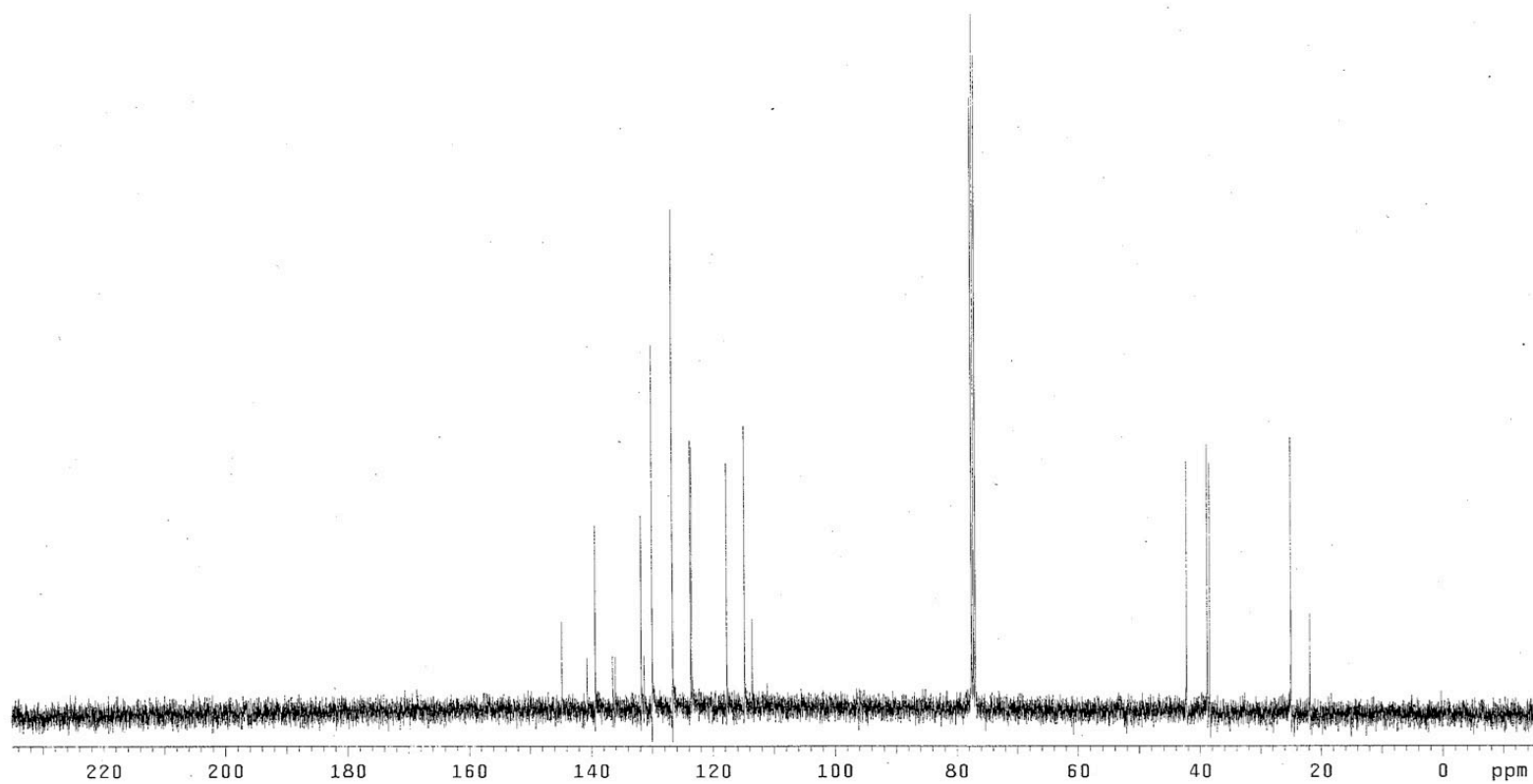
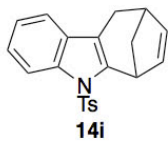
14h: X = NBoc



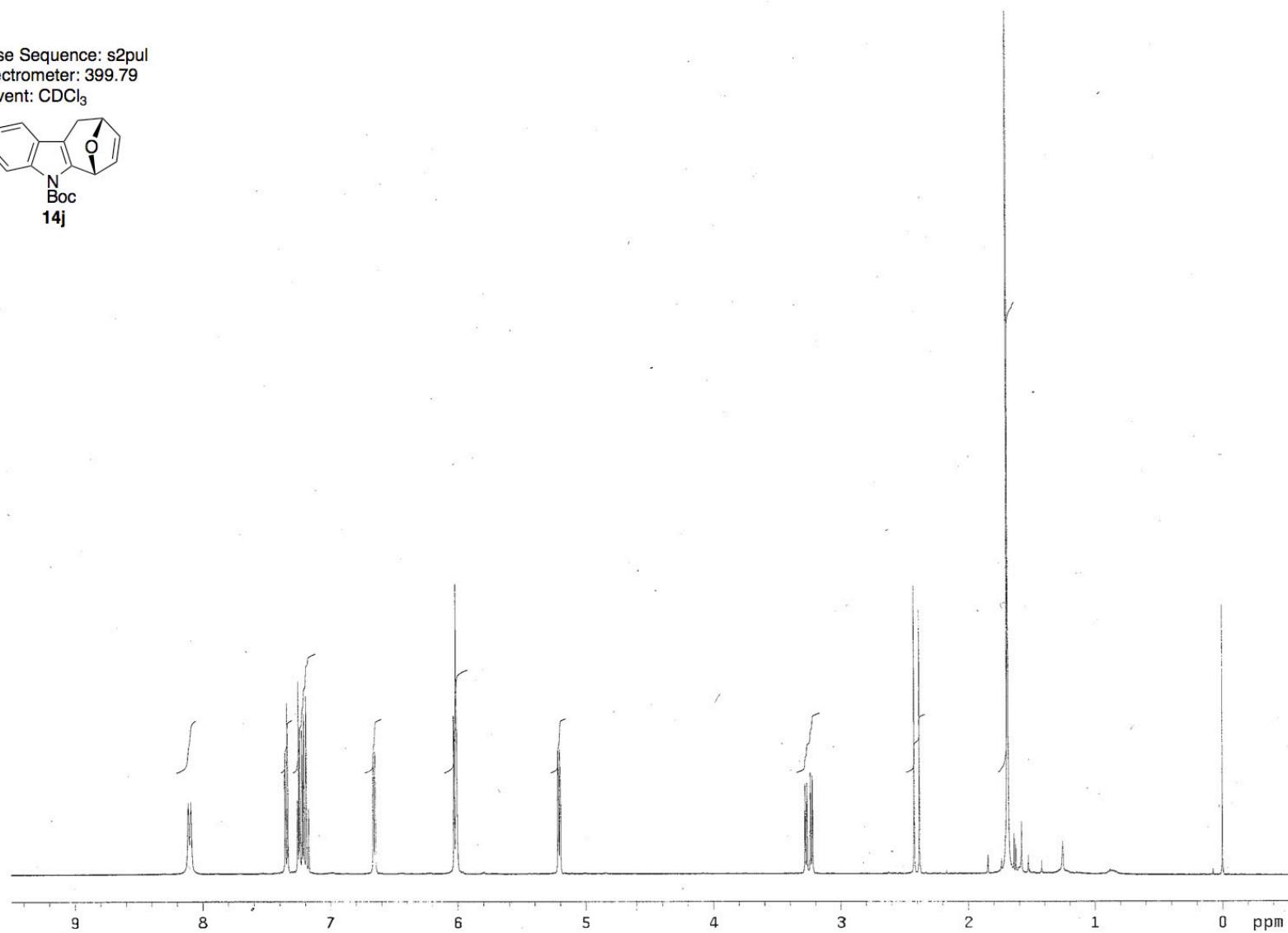
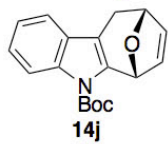
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



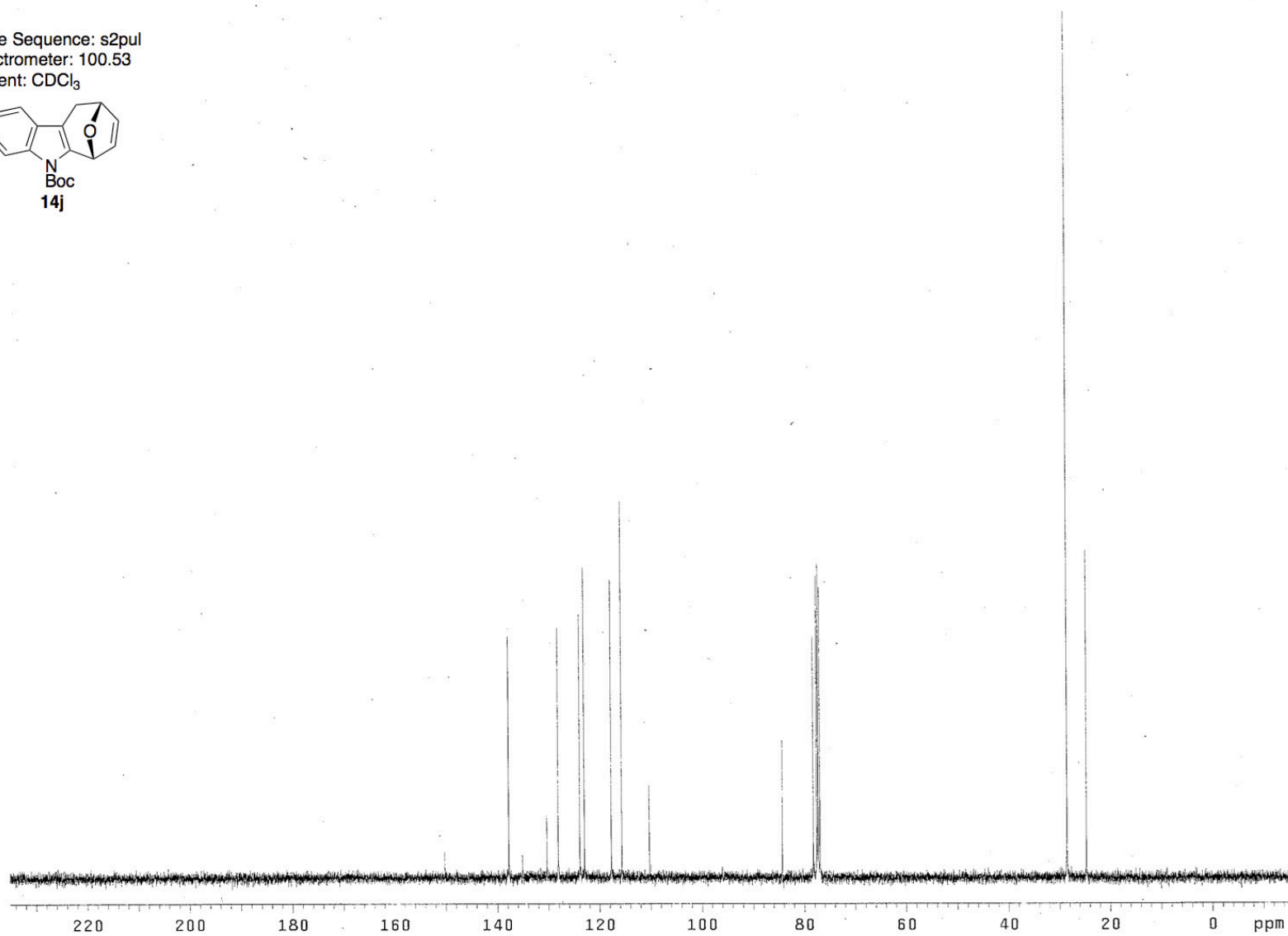
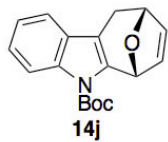
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



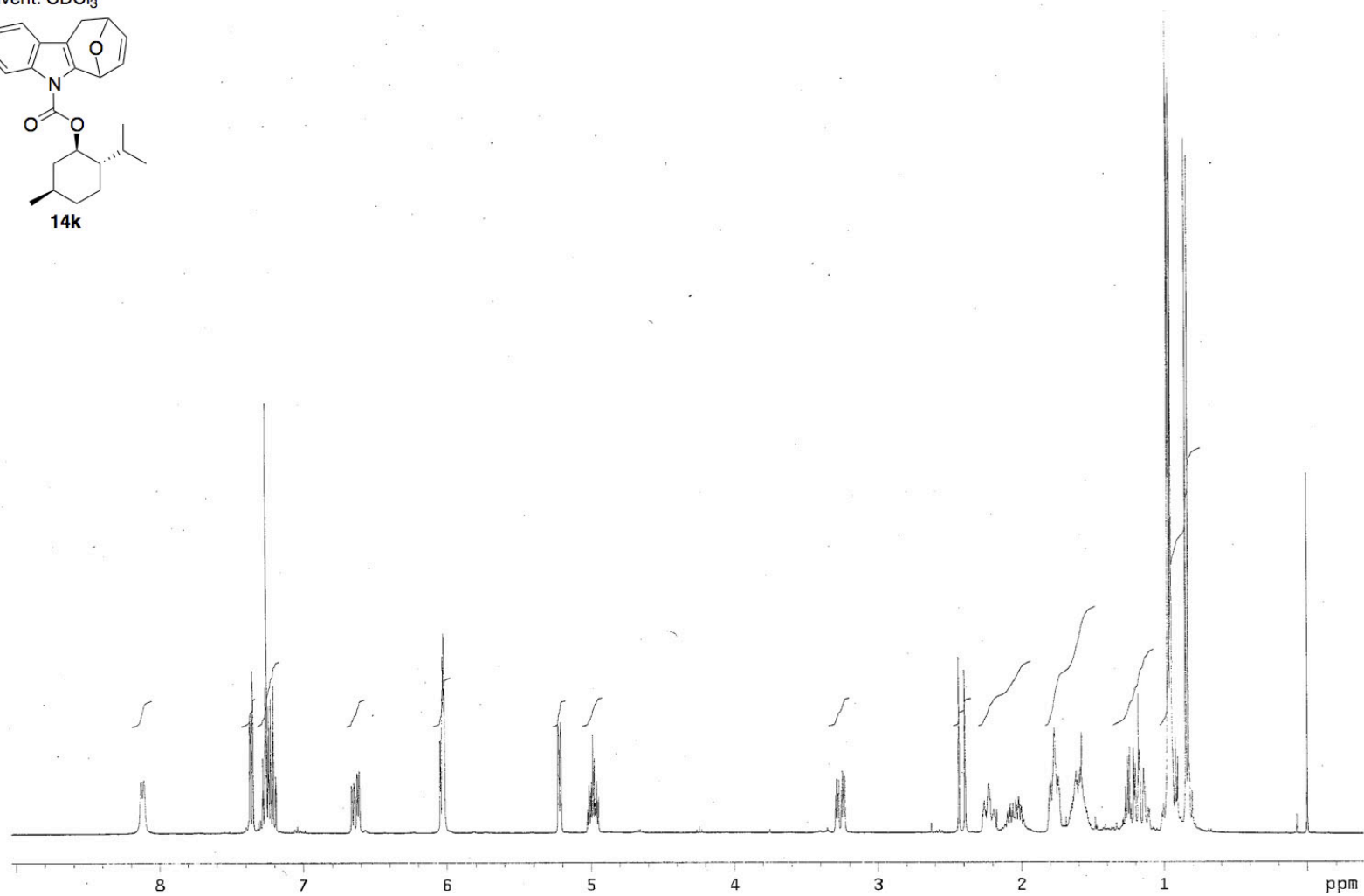
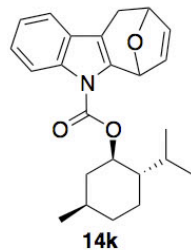
Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



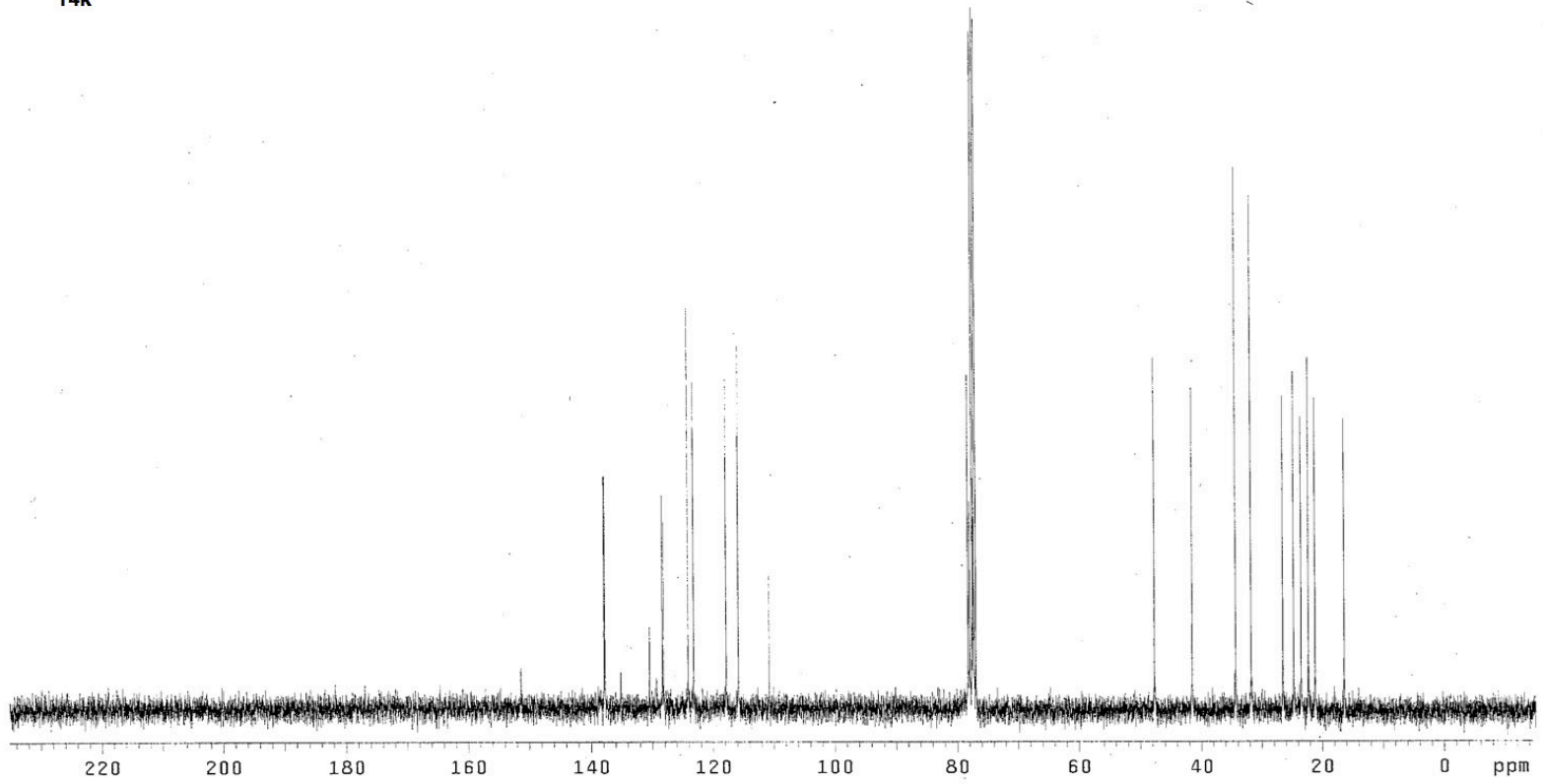
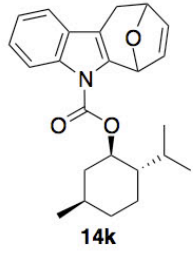
Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



Pulse Sequence: s2pul
Spectrometer: 399.79
Solvent: CDCl₃



Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃



Pulse Sequence: s2pul
Spectrometer: 100.53
Solvent: CDCl₃

