

Supporting Information

For

A New Approach for Fused Isoindolines via hexdehydro-Diels-Alder Reaction (HDDA) by Fe(0) Catalysis

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^aDepartment of Medicinal and Applied Chemistry

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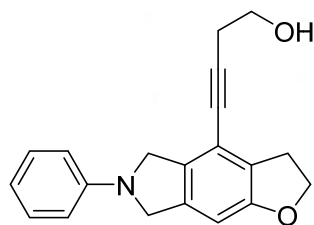
Kaohsiung Medical University, Kaohsiung, Taiwan.

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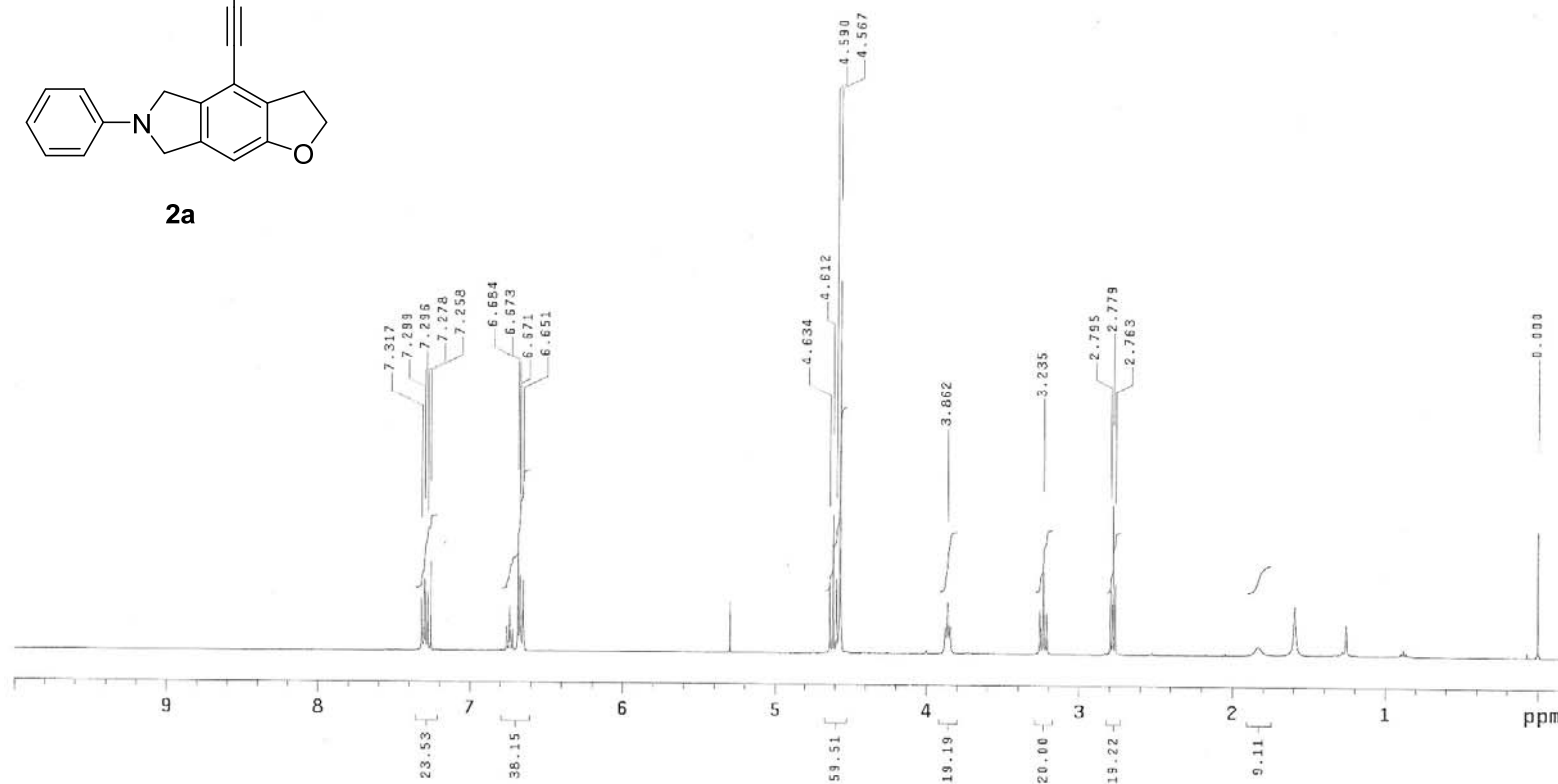
1. NMR Spectras.....	S1-S49
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Milu-ph-5-ring
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: M0335-1
Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees
Acq. time 4.002 sec
Width 5995.2 Hz
64 repetitions
OBSERVE H1, 400.3978971 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 7 sec



2a



Milu-ph-5-ring

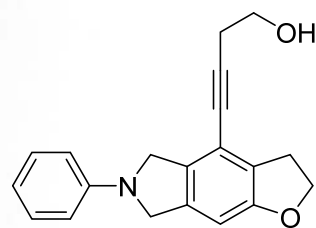
Pulse Sequence: s2pul

Solvent: CDCl₃

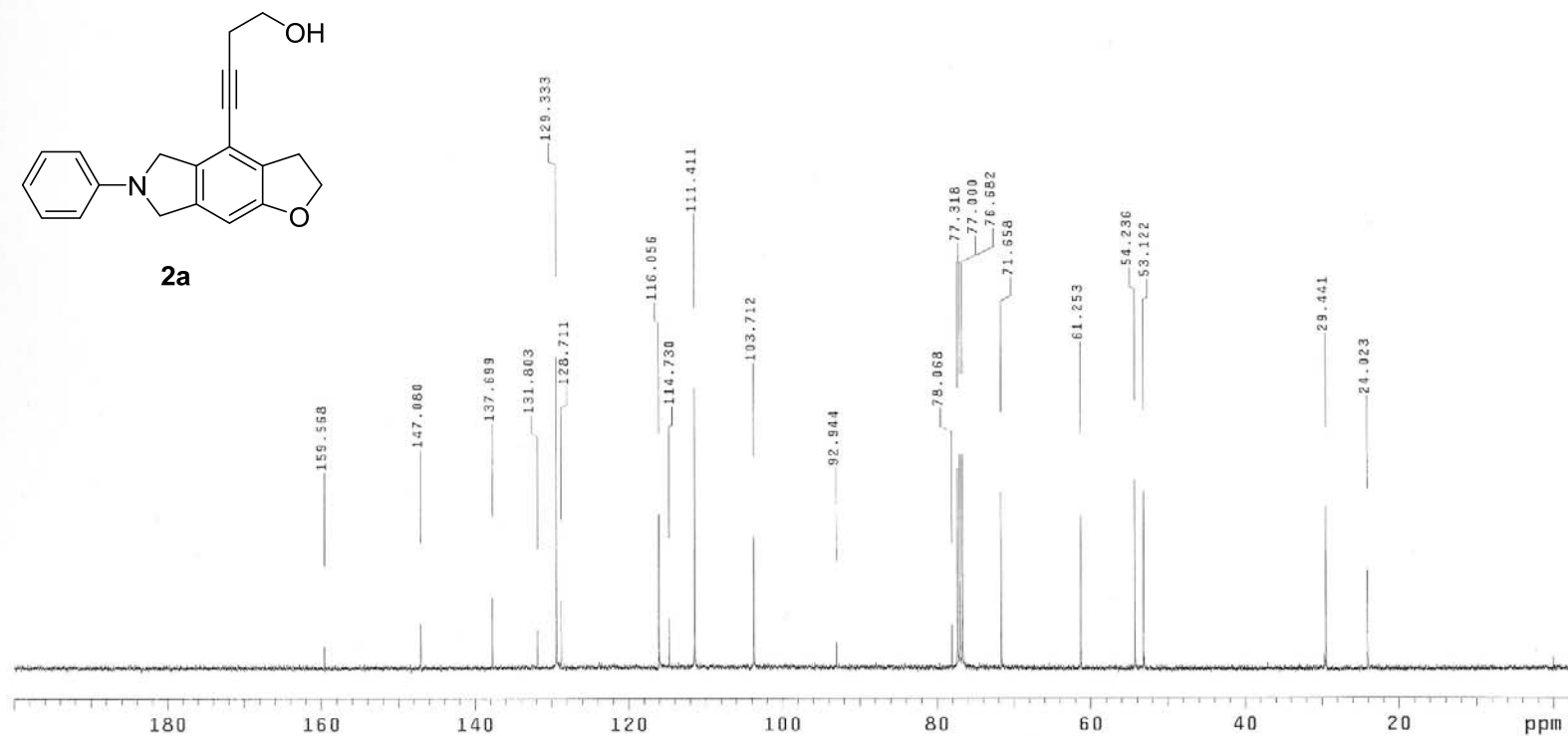
Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees
Acq. time 1.000 sec
Width 25000.0 Hz
64000 repetitions
OBSERVE C13, 100.6801330 MHz
DECOUPLE H1, 400.3999572 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 51 min, 34 sec

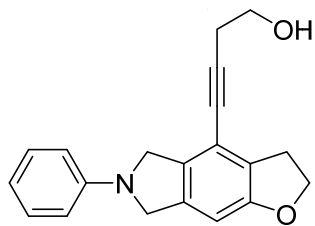


2a

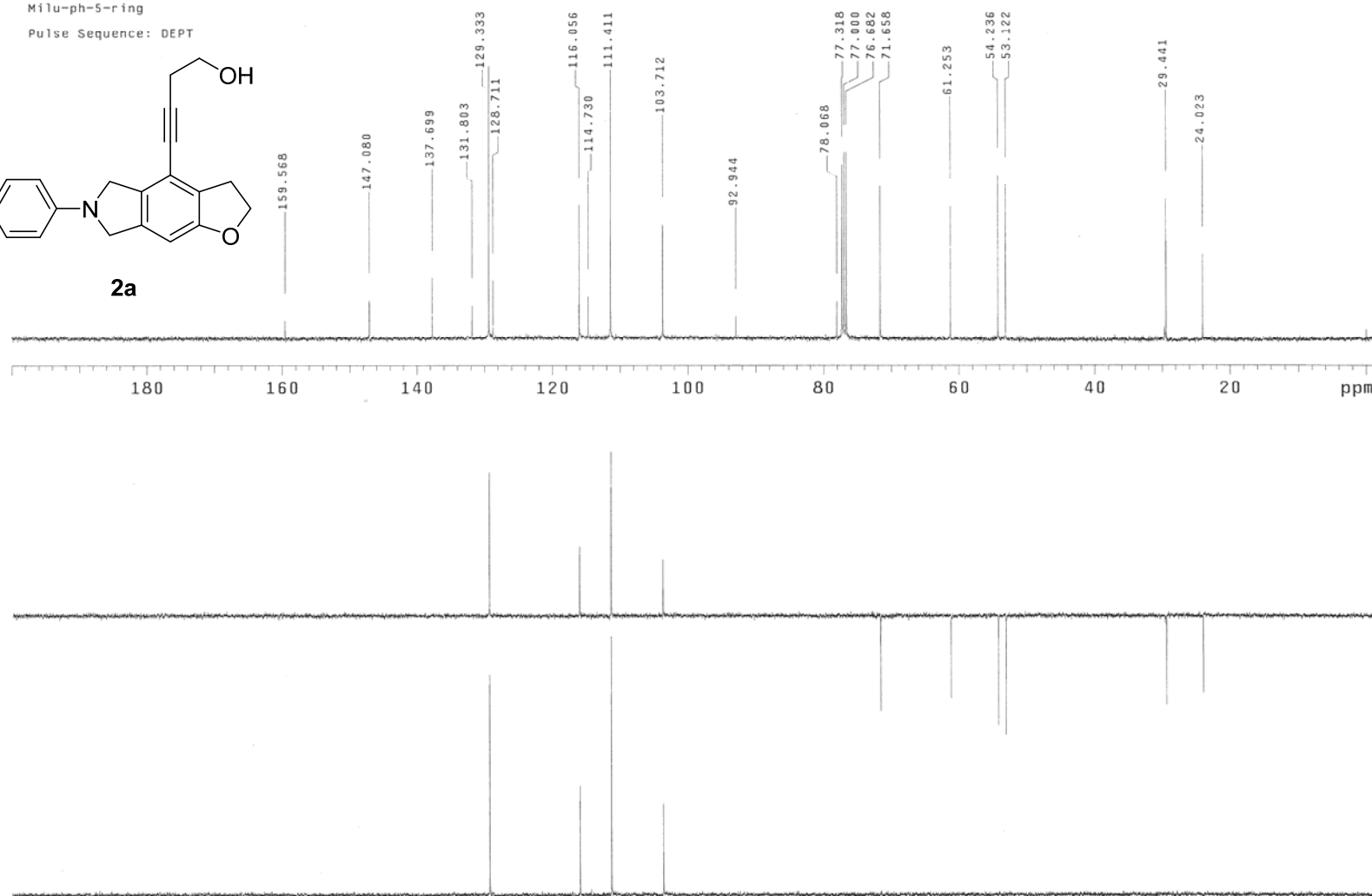


Milu-ph-5-ring

Pulse Sequence: DEPT



2a



102-1/90/90A

Pulse Sequence: s2pu1

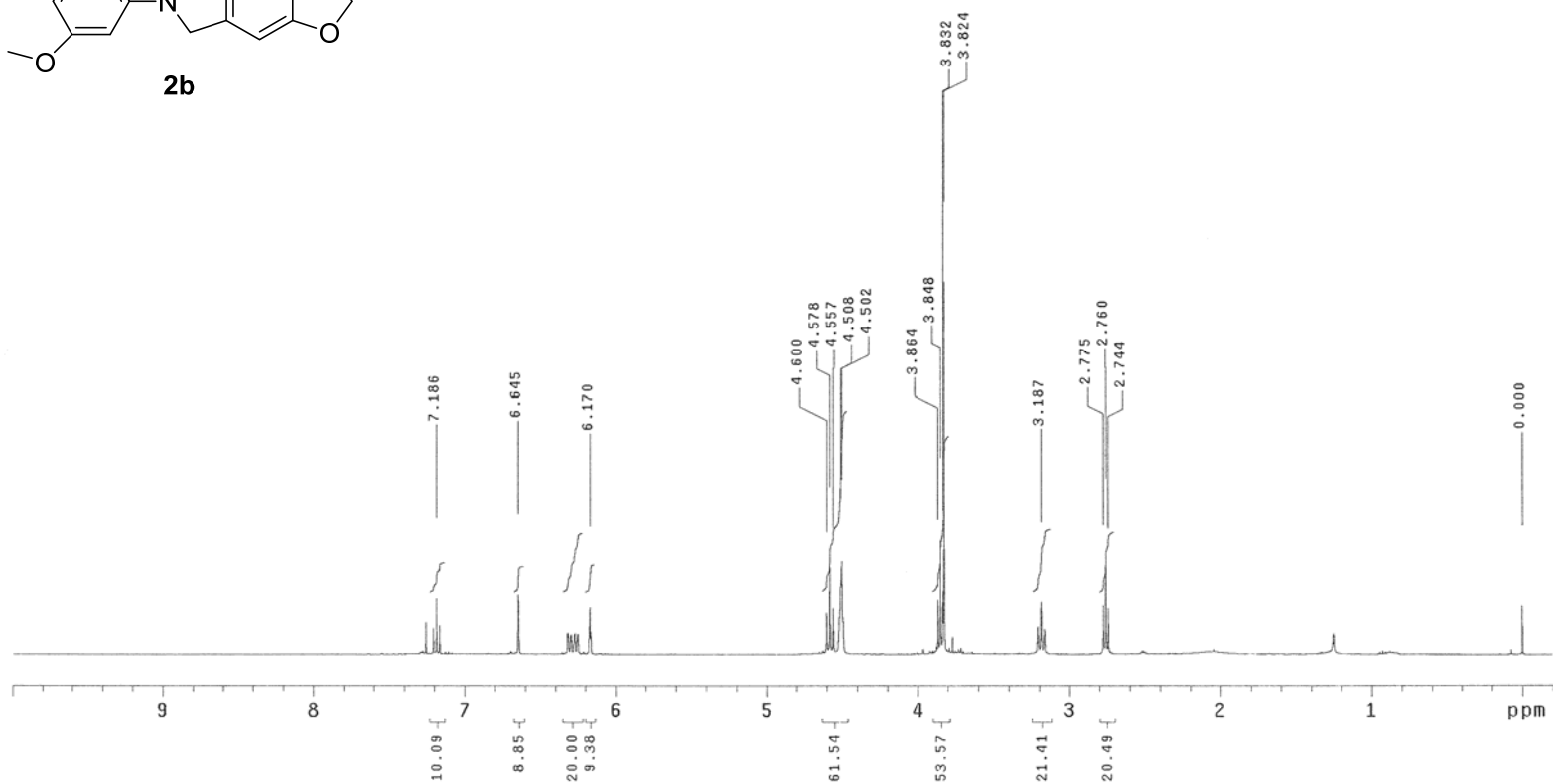
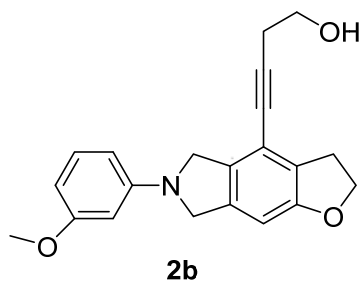
UNITYplus-400 "unity400"

Date: Oct 23 2013

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



102-1/90/90A

Pulse Sequence: s2pu1

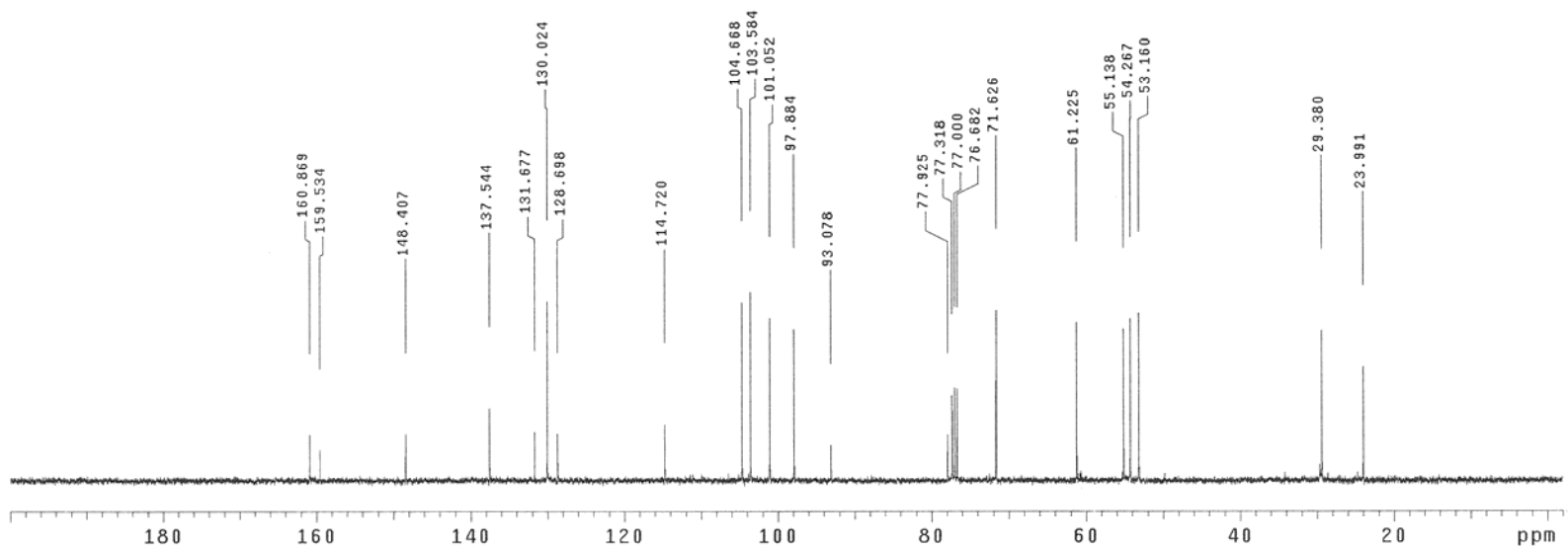
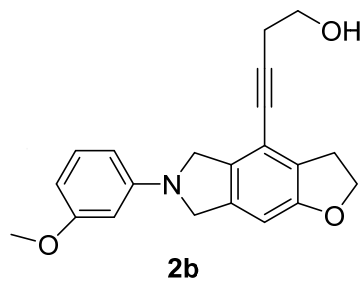
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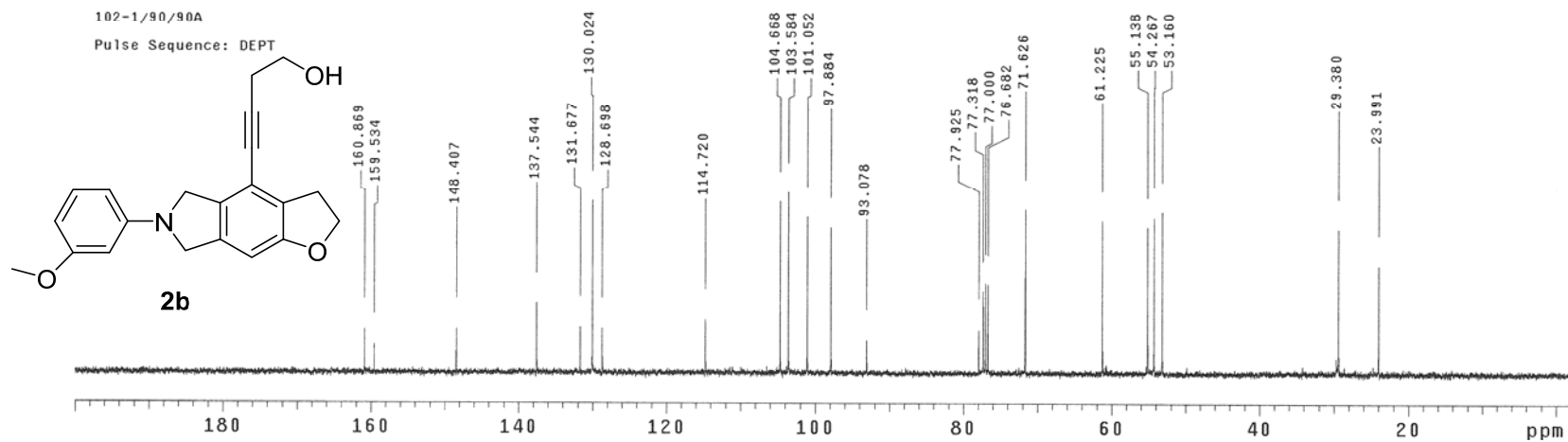
Date: Oct 23 2013

Solvent: CDCl₃

Ambient temperature

Total 2064 repetitions





Milu-4-Cl-5-ring

Pulse Sequence: s2pu1

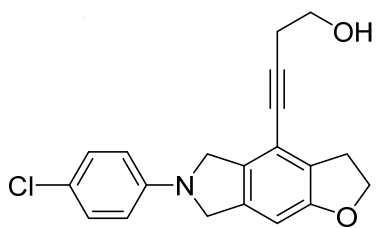
UNITYplus-400 "unity400"

Date: Jan 22 2014

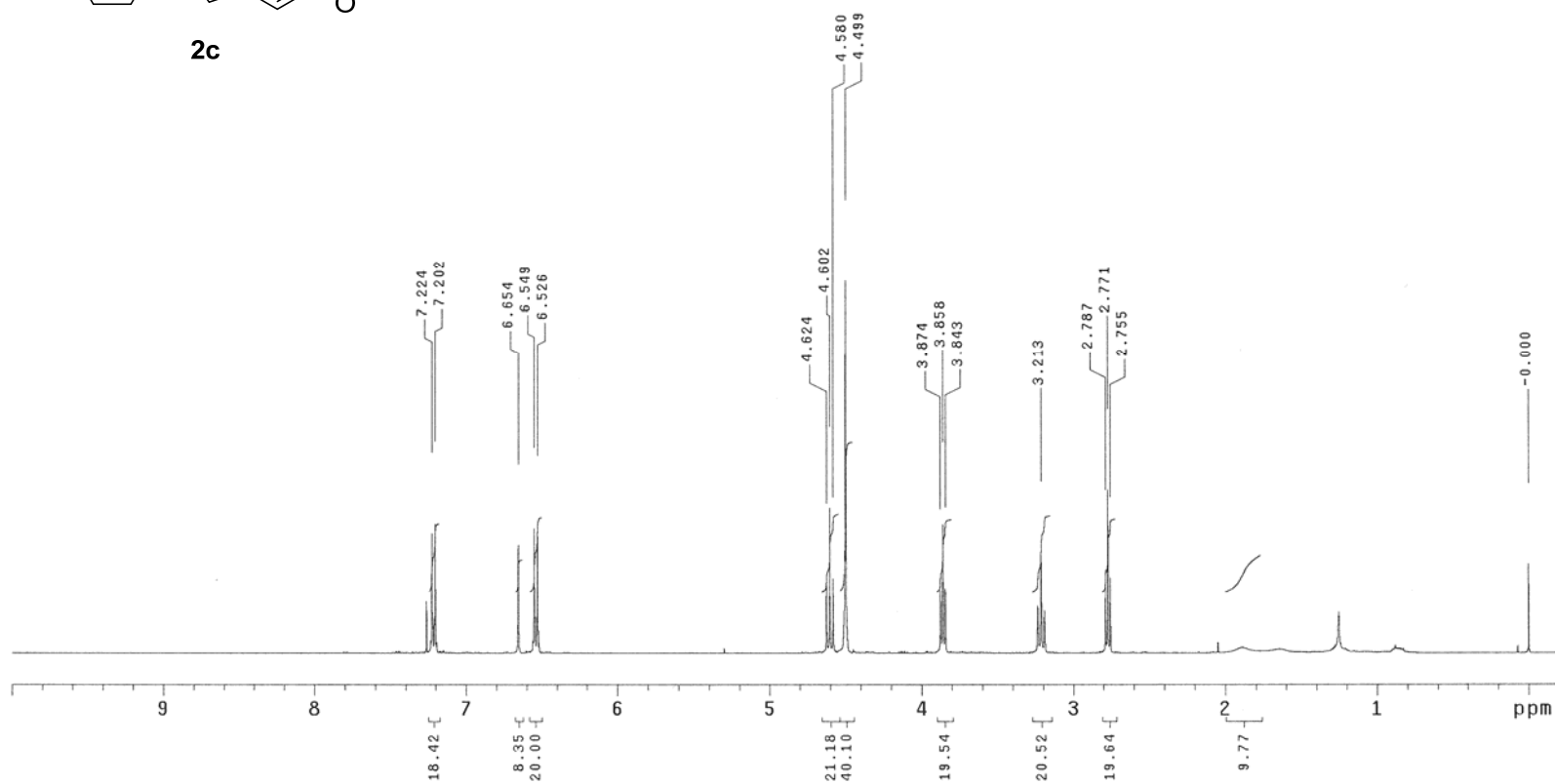
Solvent: CDC13

Ambient temperature

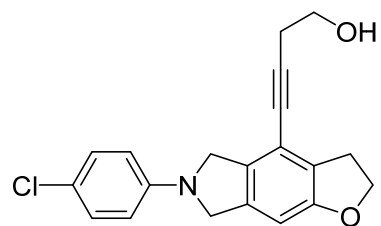
Total 64 repetitions



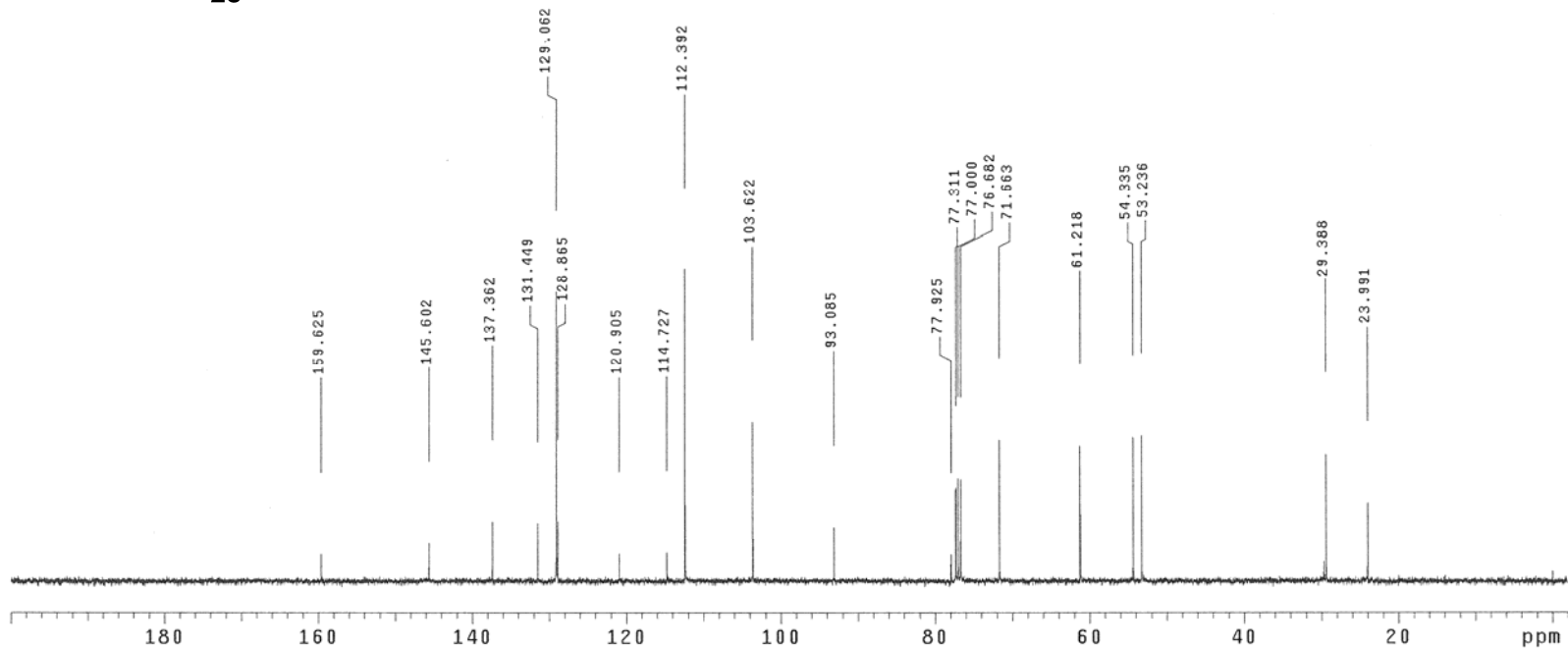
2c

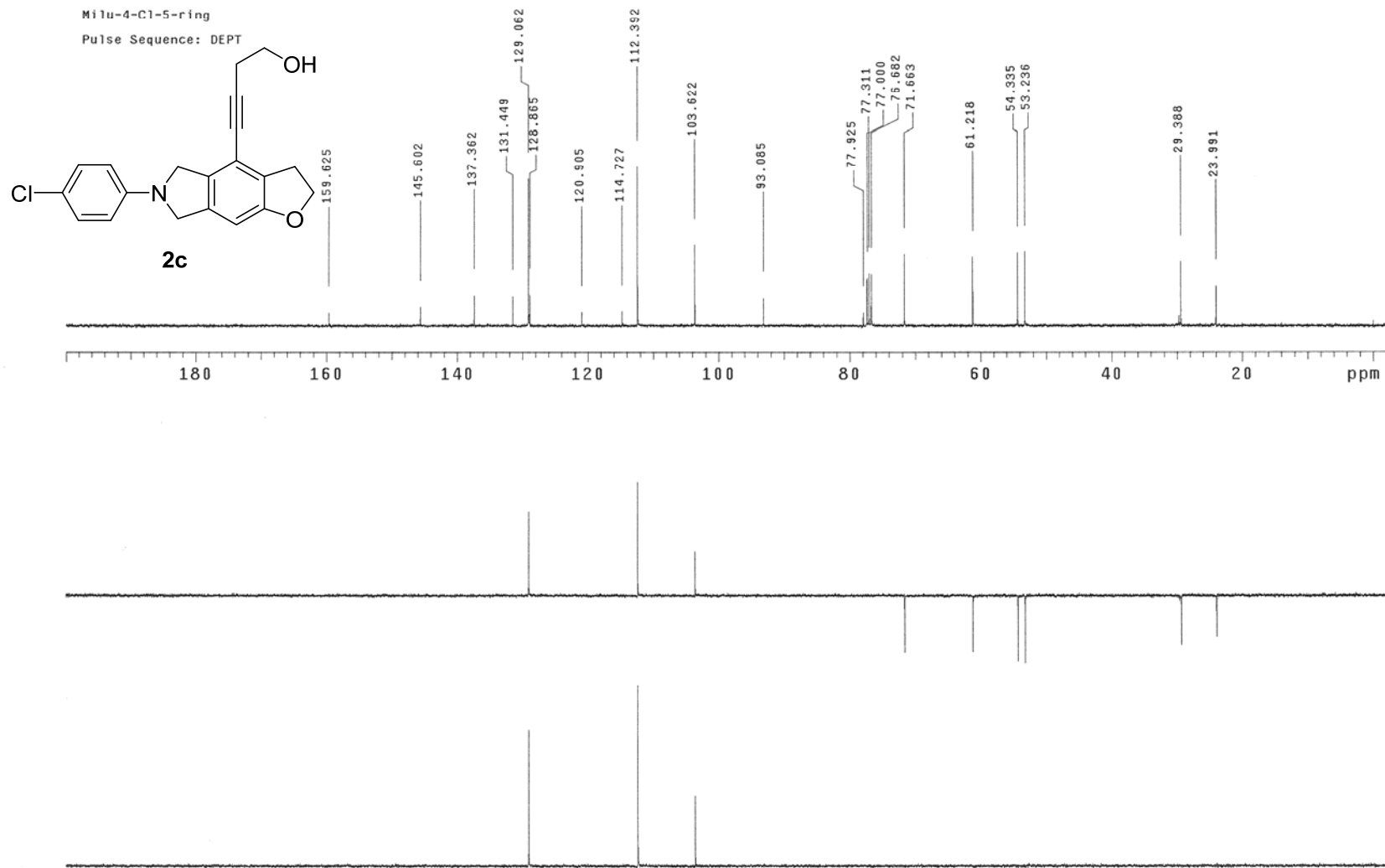


Milu-4-Cl-5-ring
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 22 2014
Solvent: CDCl₃
Ambient temperature
Total 2656 repetitions



2c





Milu-4-Br-Ph/5r

Pulse Sequence: s2pul

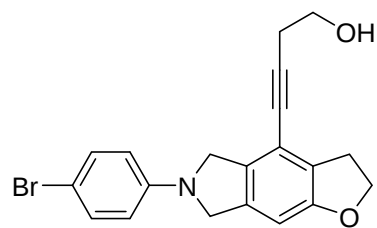
UNITYplus-400 "unity400"

Date: Feb 11 2014

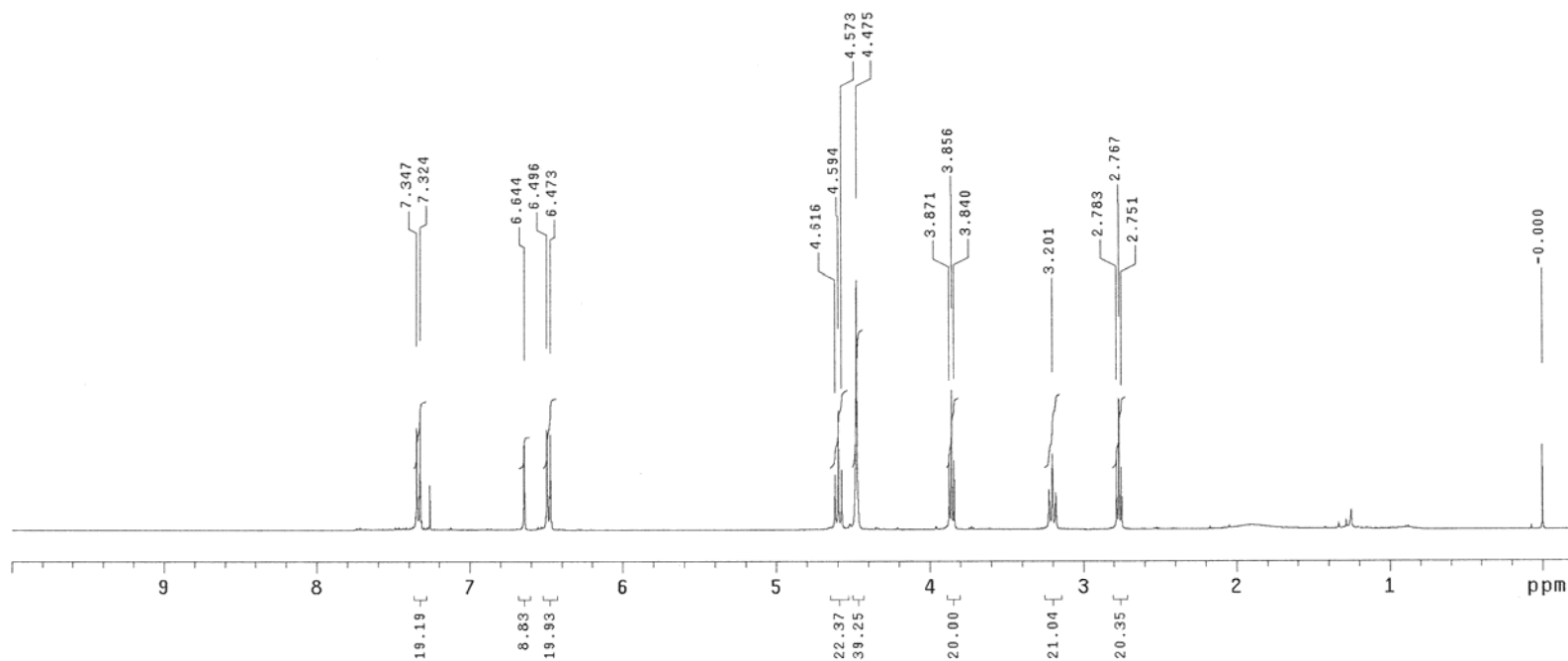
Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



2d



Milu-4-Br-Ph/5r

Pulse Sequence: s2pu1

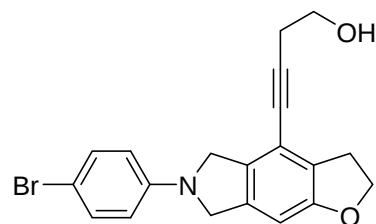
UNITYplus-400 "unity400"

Date: Feb 11 2014

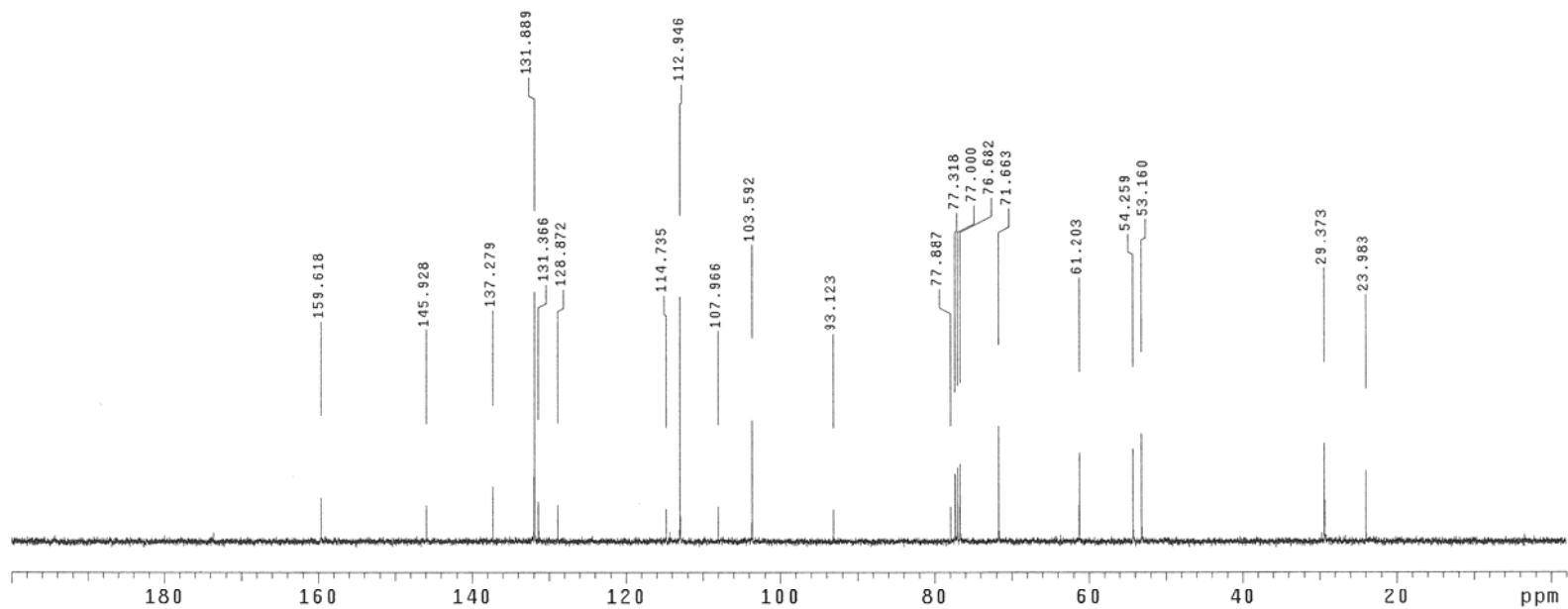
Solvent: CDCl₃

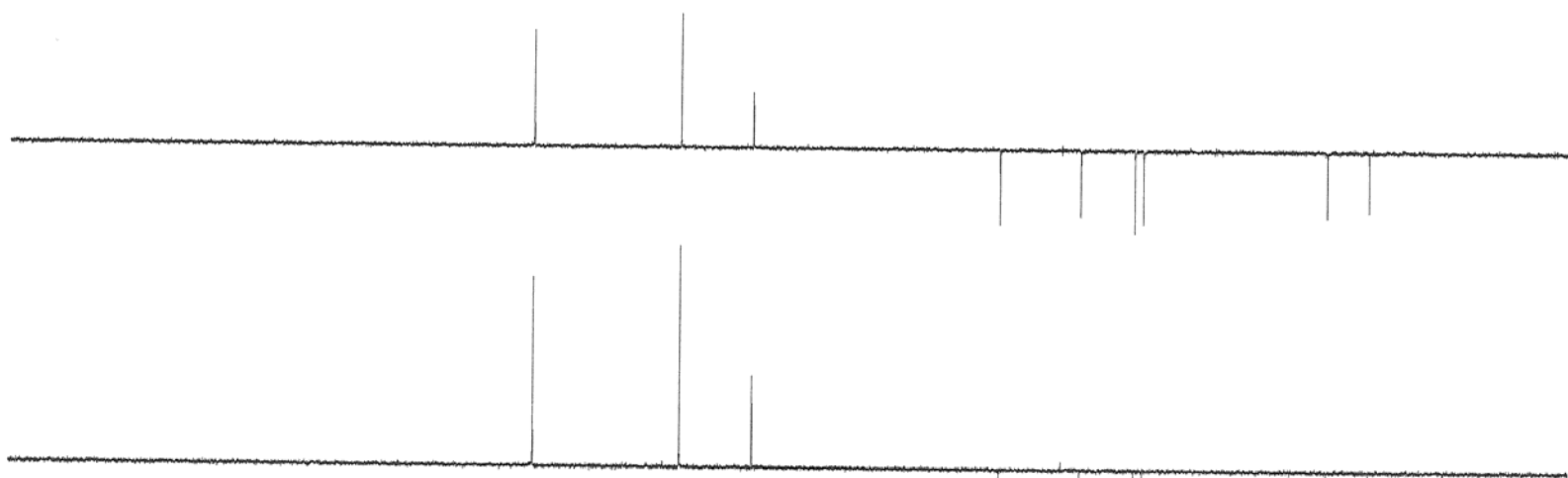
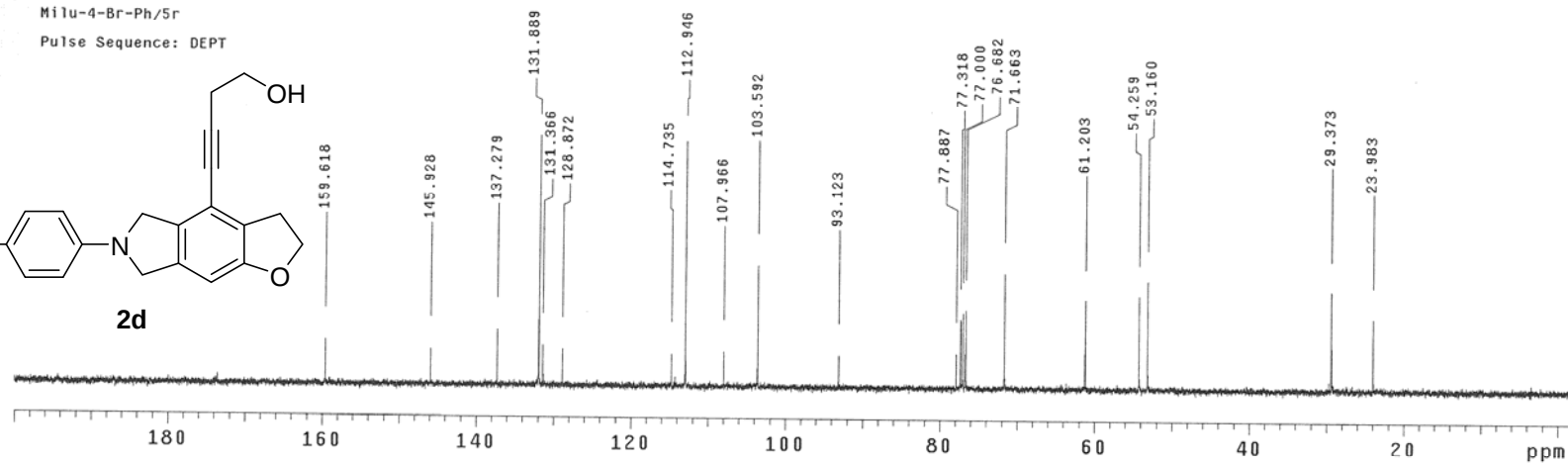
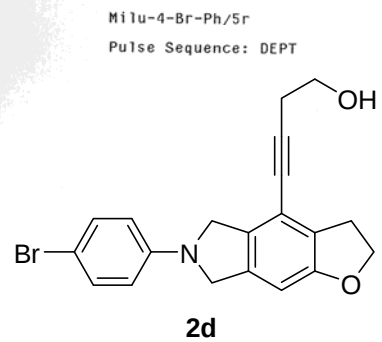
Ambient temperature

Total 1072 repetitions



2d





Milu-4-CH3-5-ring

Pulse Sequence: s2pu1

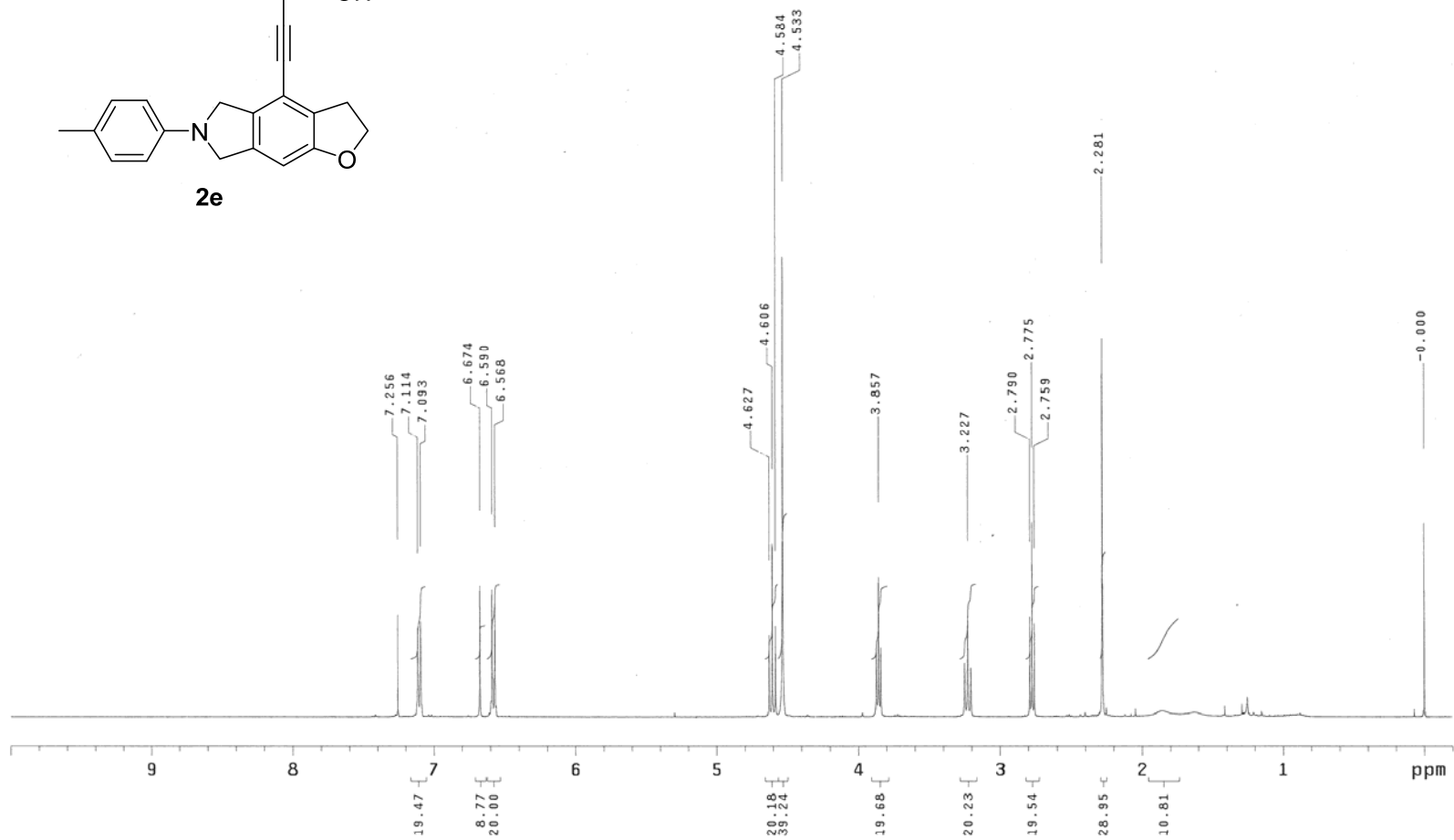
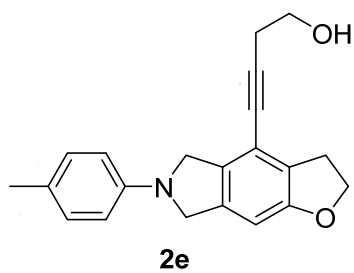
Mercury-400BB "MercuryPlus400"

Date: Jan 22 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Milu-4-CH3-5-ring

Pulse Sequence: s2pu1

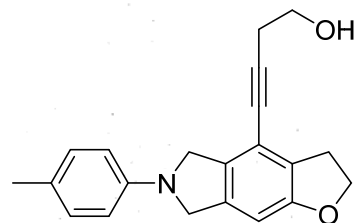
Mercury-400BB "MercuryPlus400"

Date: Jan 22 2014

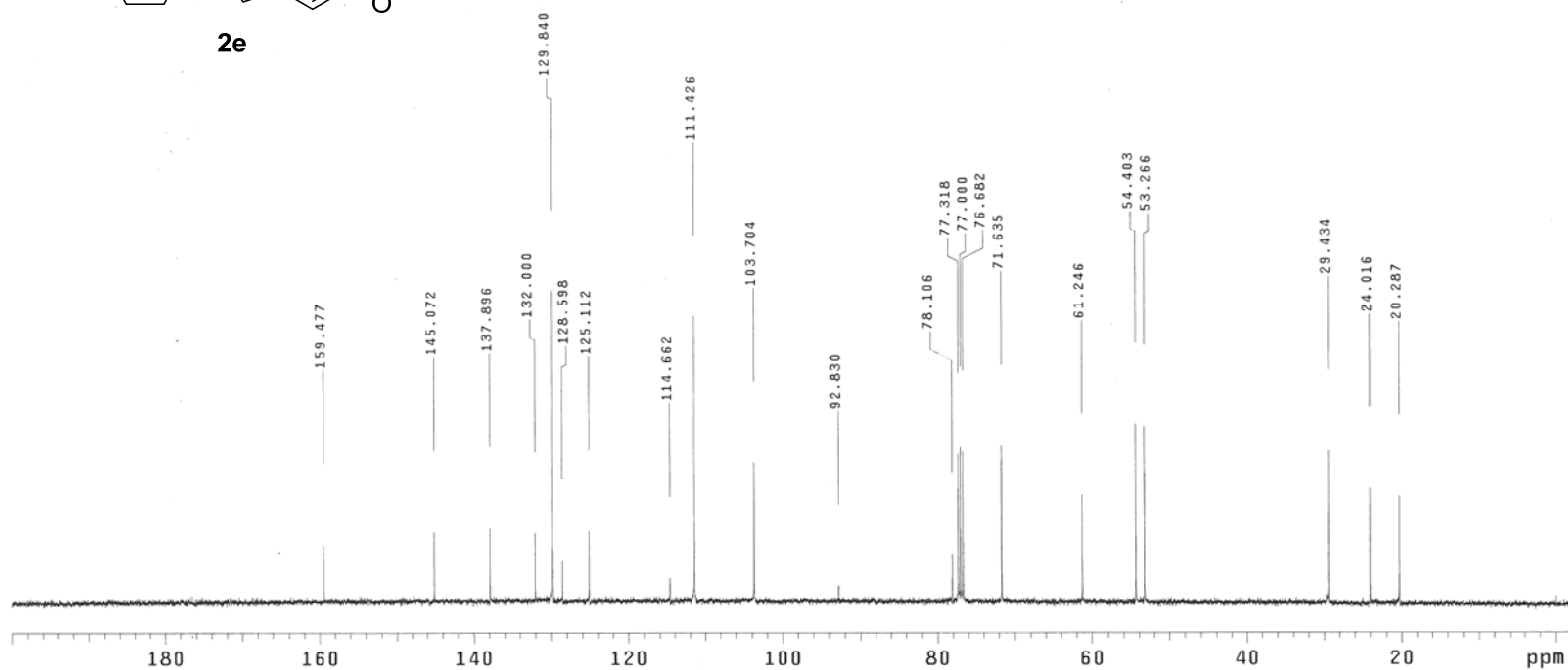
Solvent: CDCl₃

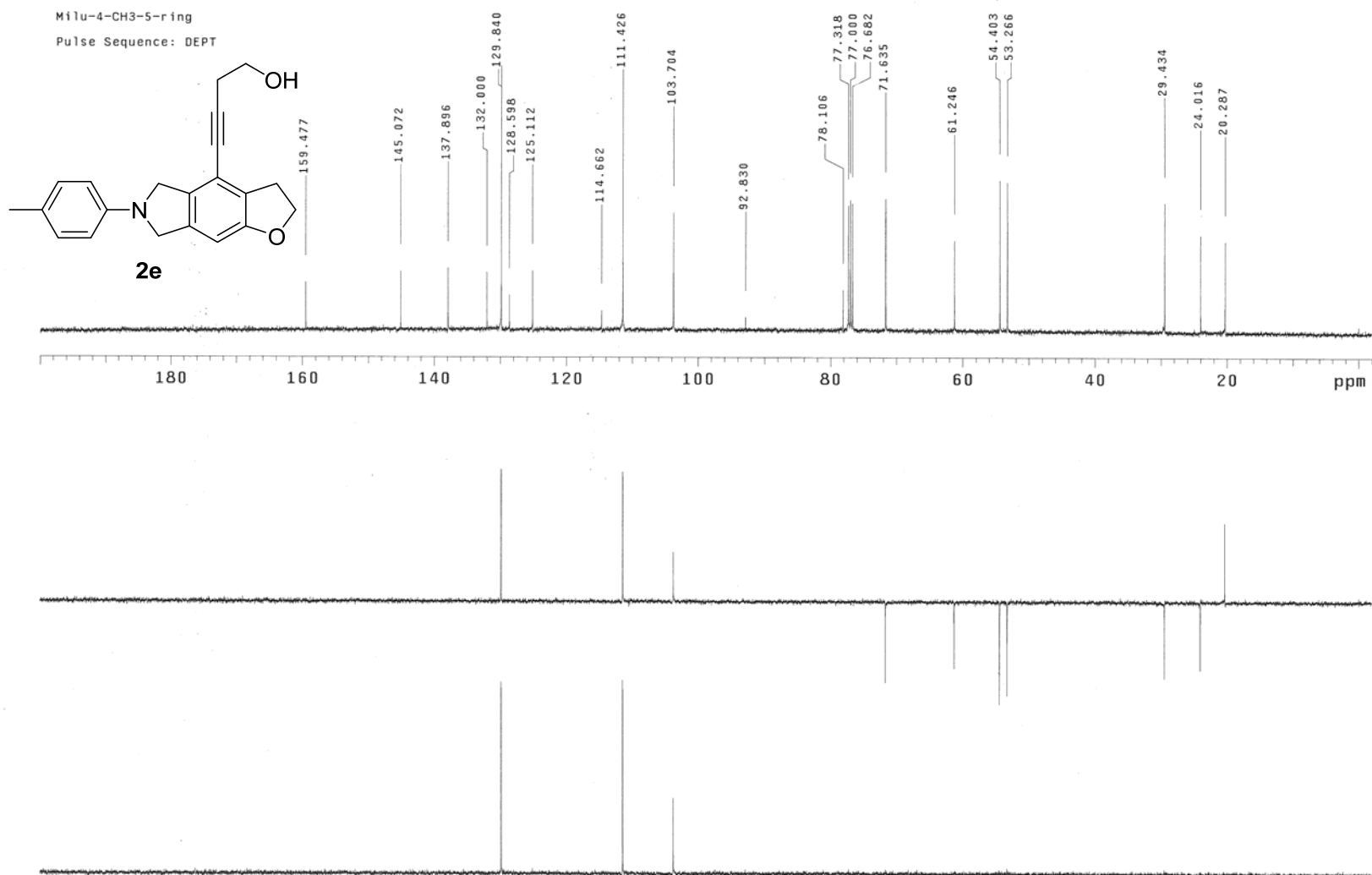
Ambient temperature

Total 432 repetitions



2e





102-1/32/32A

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees

Acq. time 4.002 sec

Width 5995.2 Hz

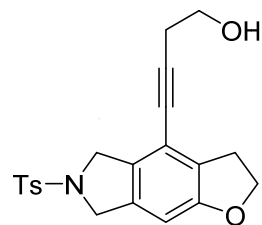
64 repetitions

OBSERVE H1, 400.3978947 MHz

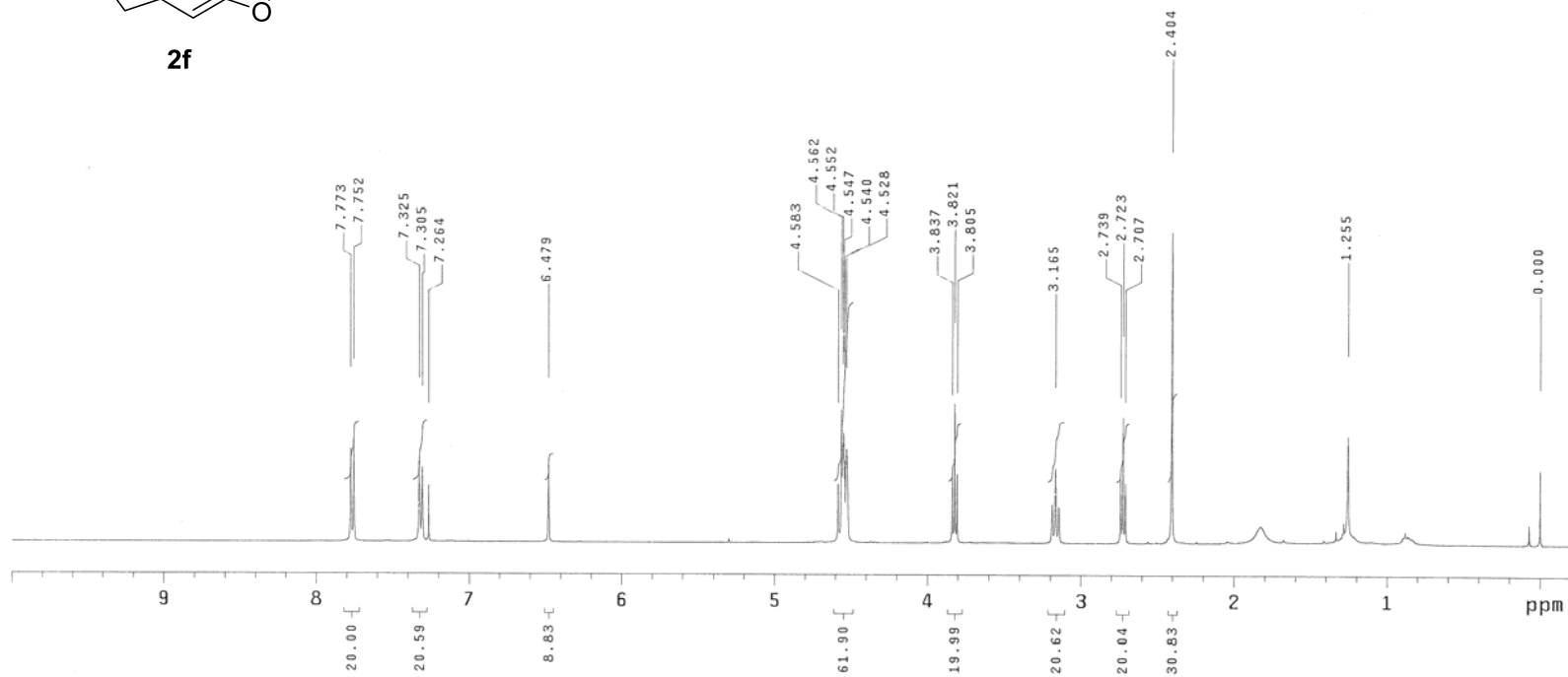
DATA PROCESSING

FT size 65536

Total time 5 min, 7 sec



2f



102-1/32/32A

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

3040 repetitions

OBSERVE C13, 100.6801323 MHz

DECOUPLE H1, 400.3999572 MHz

Power 38 dB

continuously on

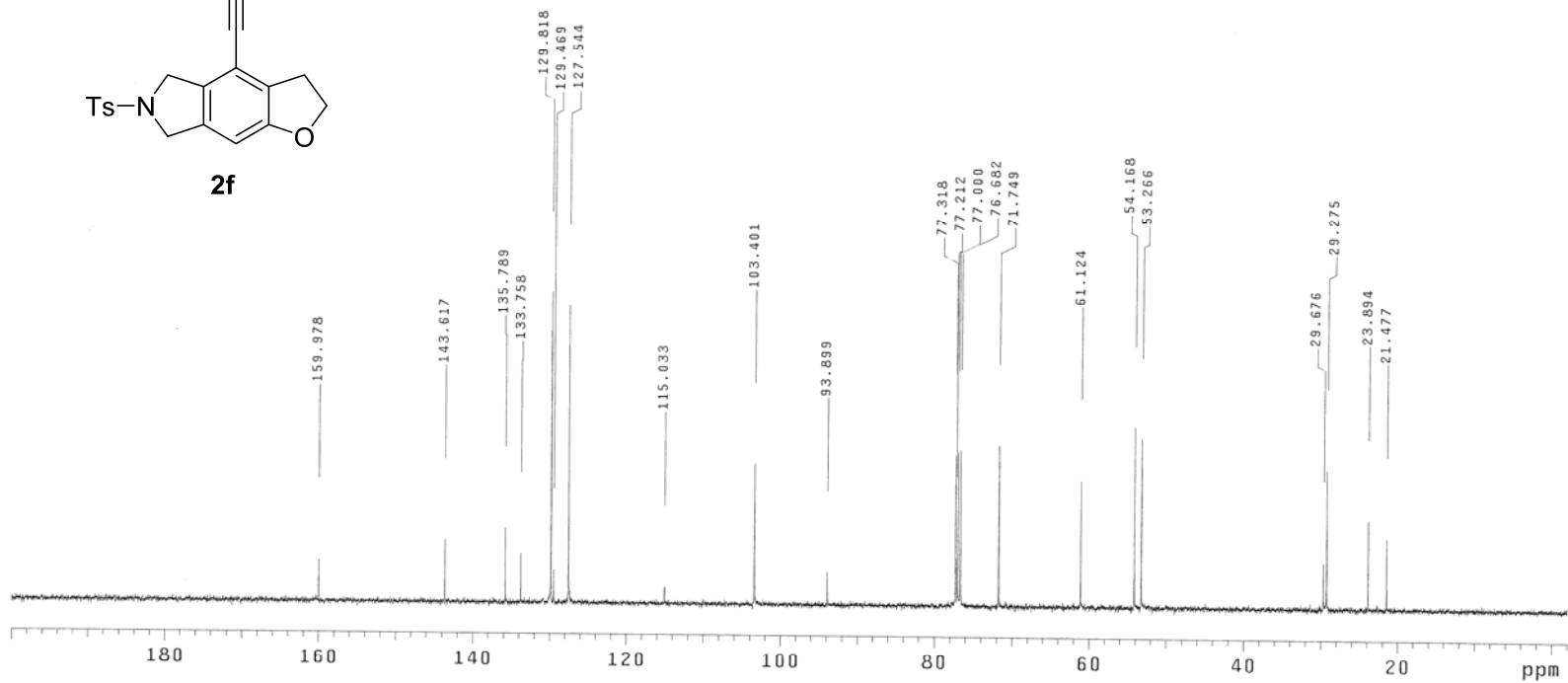
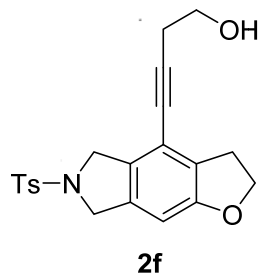
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

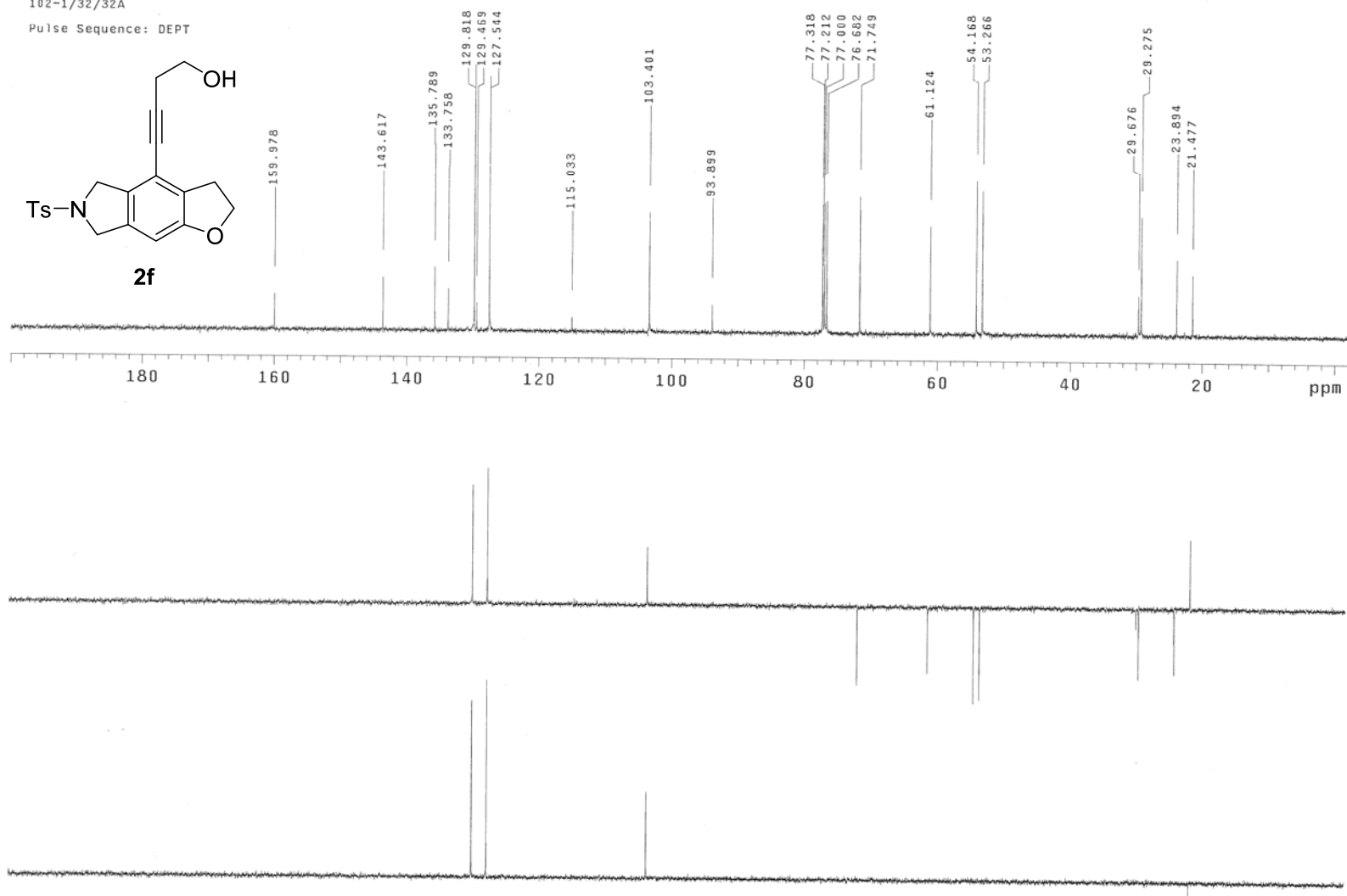
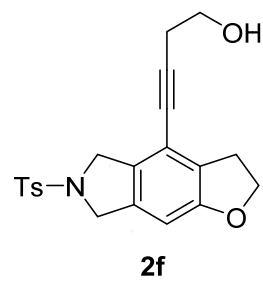
FT size 65536

Total time 21 hr, 51 min, 34 sec



102-1/32/32A

Pulse Sequence: DEPT



Milu-4-CF3-Ph/5r

Pulse Sequence: s2pu1

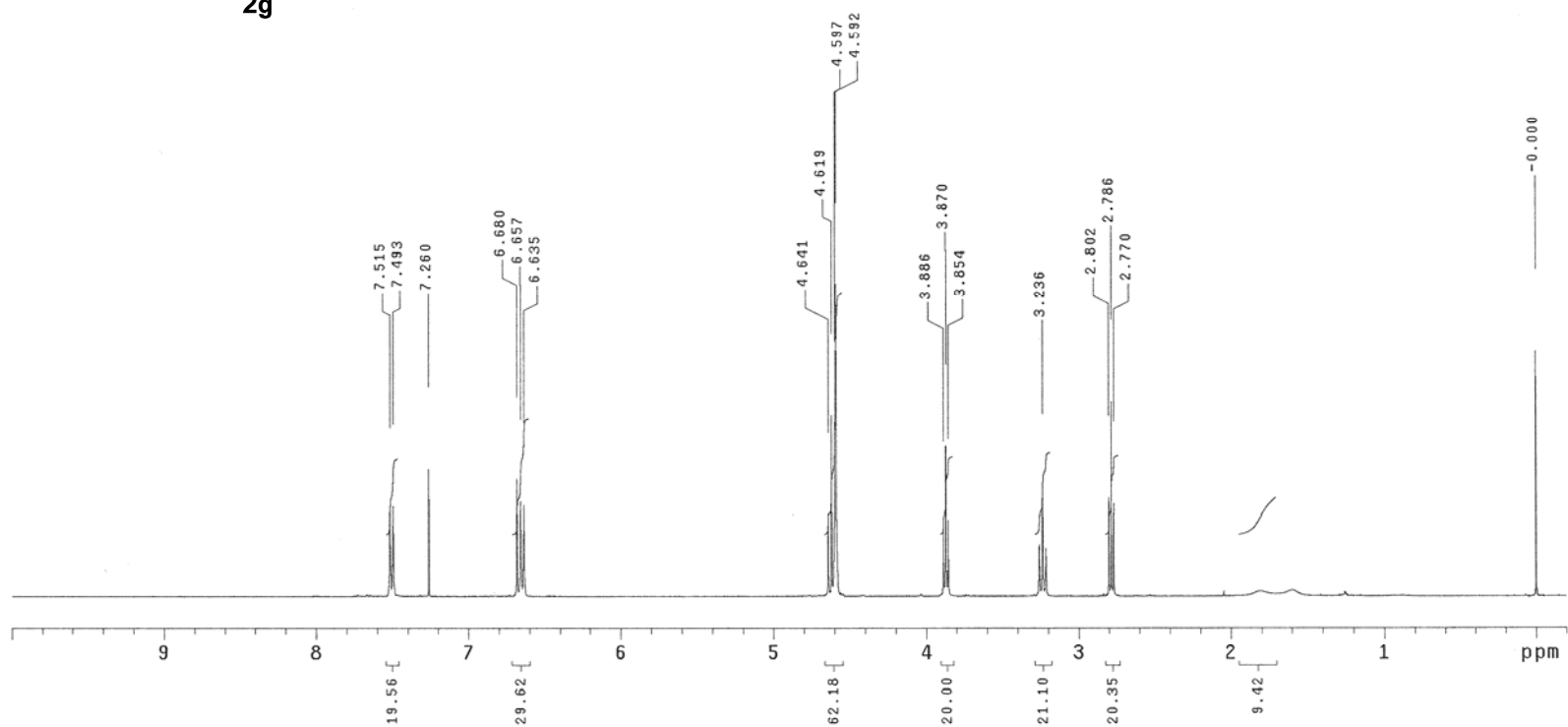
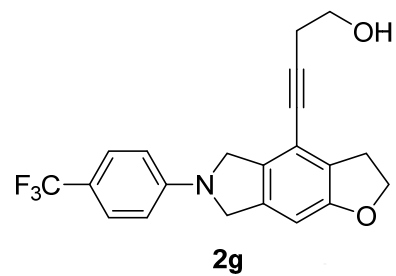
UNITYplus-400 "unity400"

Date: Mar 24 2014

Solvent: CDC13

Ambient temperature

Total 32 repetitions



Milu-4-CF₃-Ph/5r

Pulse Sequence: s2pu1

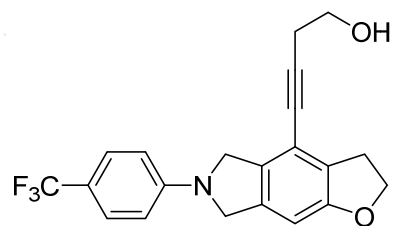
UNITYplus-400 "unity400"

Date: Mar 24 2014

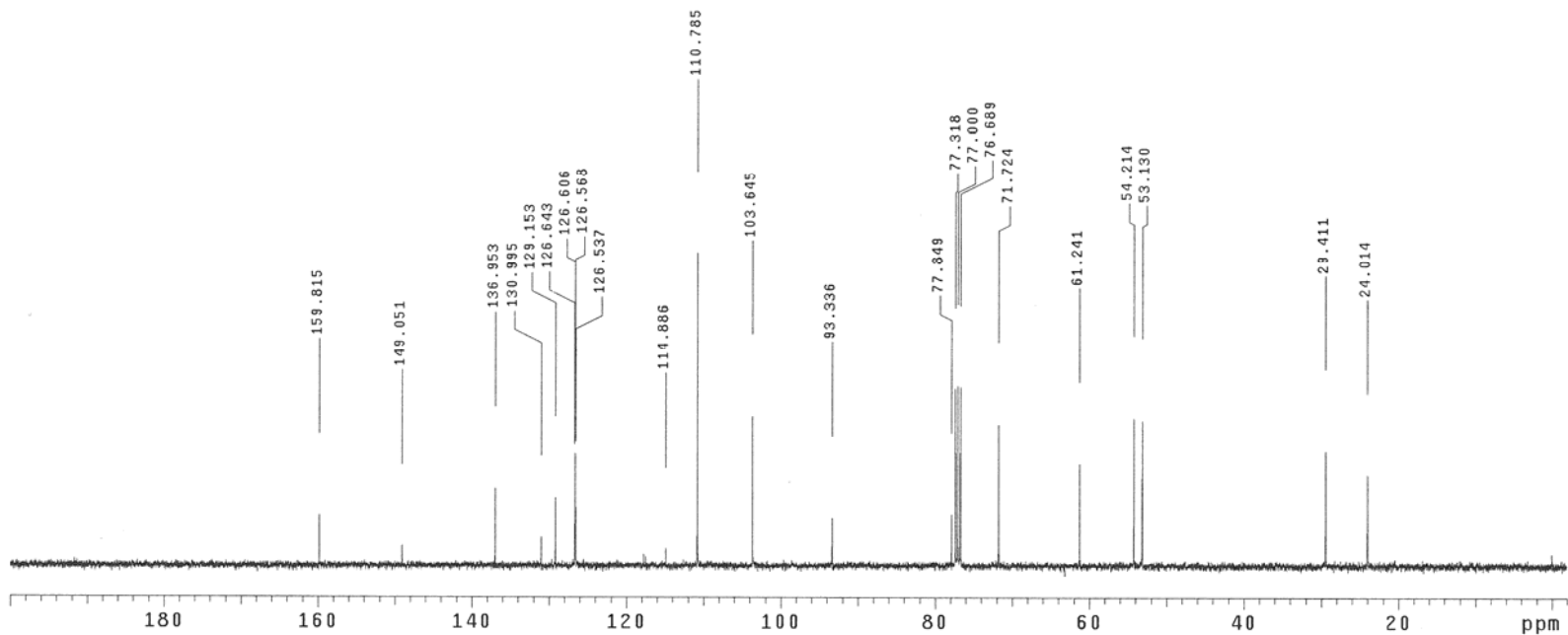
Solvent: CDCl₃

Ambient temperature

Total 6032 repetitions

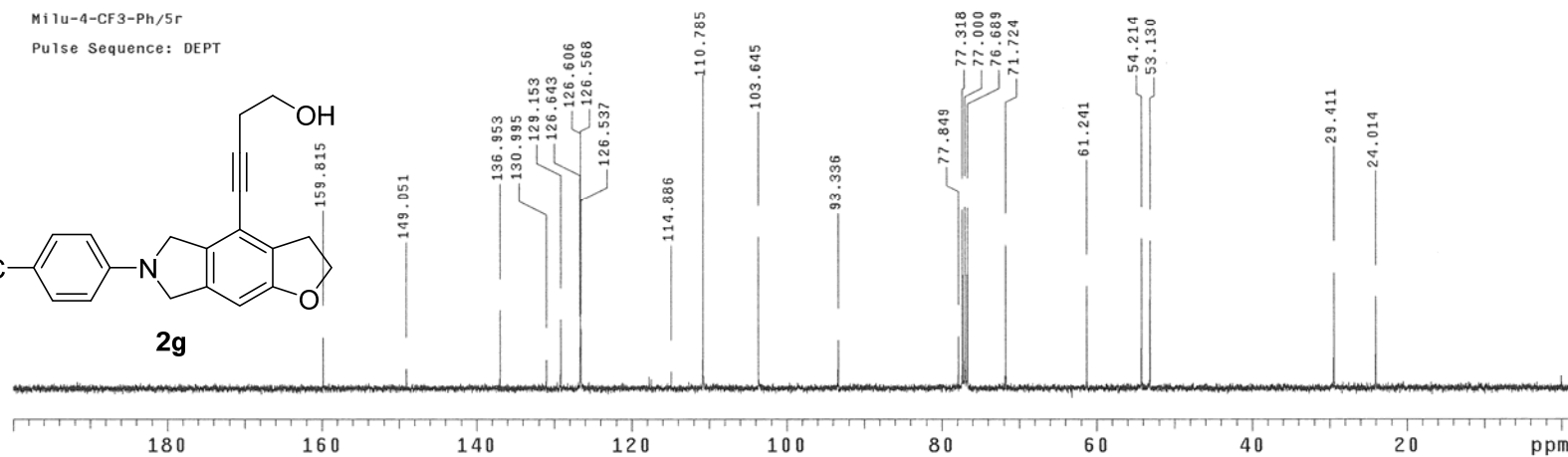
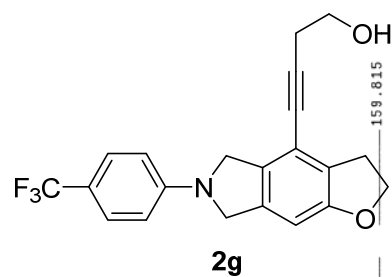


2g



Milu-4-CF₃-Ph/5r

Pulse Sequence: DEPT



Milu-Ph/6r

Pulse Sequence: s2pu1

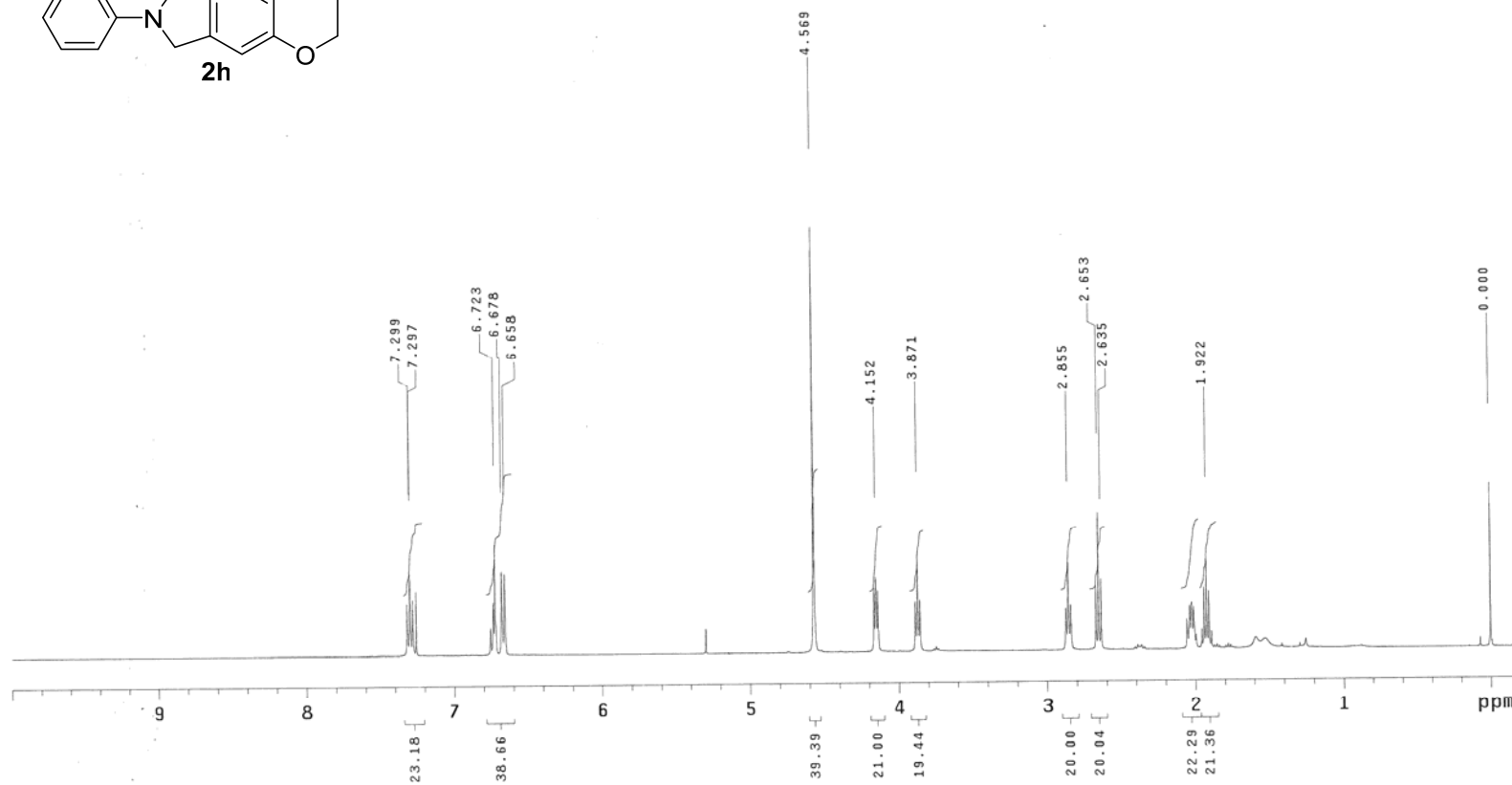
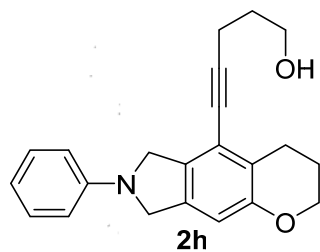
Mercury-400BB "MercuryPlus400"

Date: Mar 10 2014

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



Milu-Ph/6r

Pulse Sequence: s2pu1

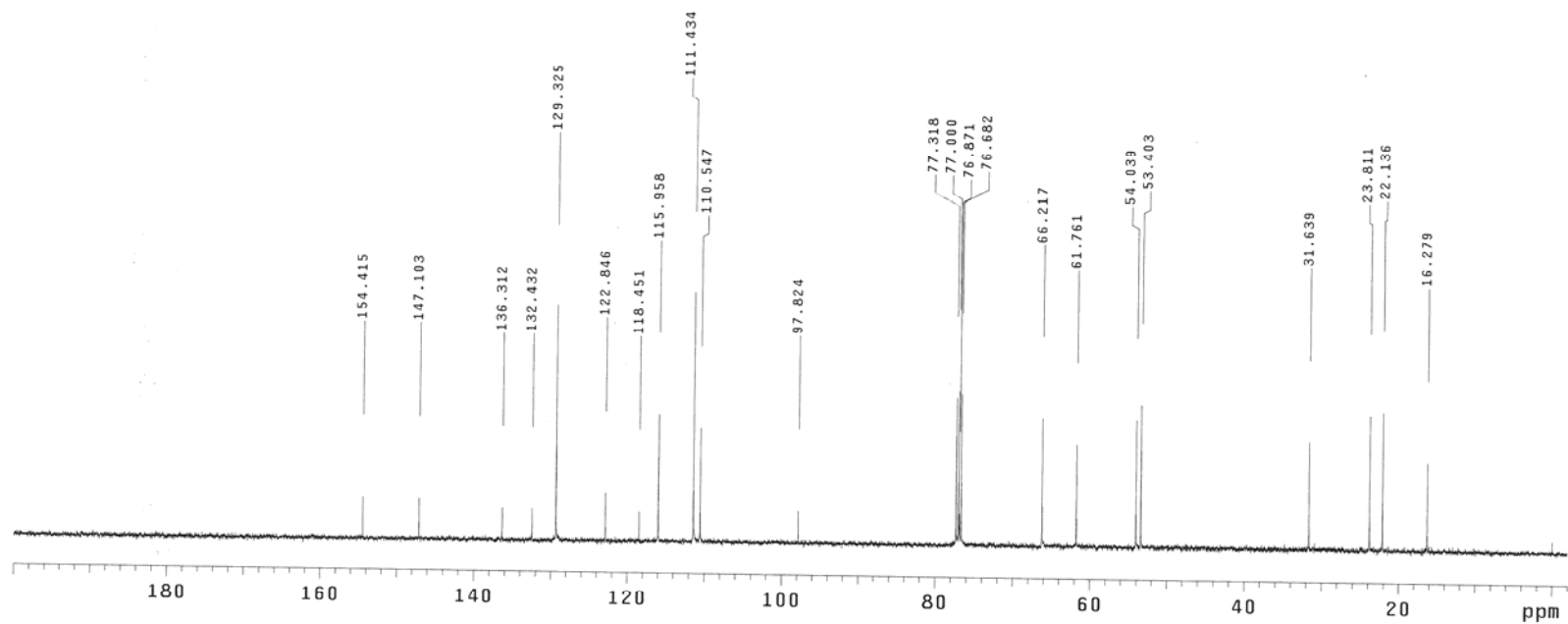
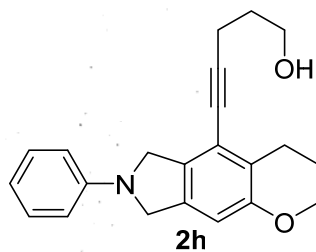
Mercury-400BB "MercuryPlus400"

Date: Mar 10 2014

Solvent: CDCl₃

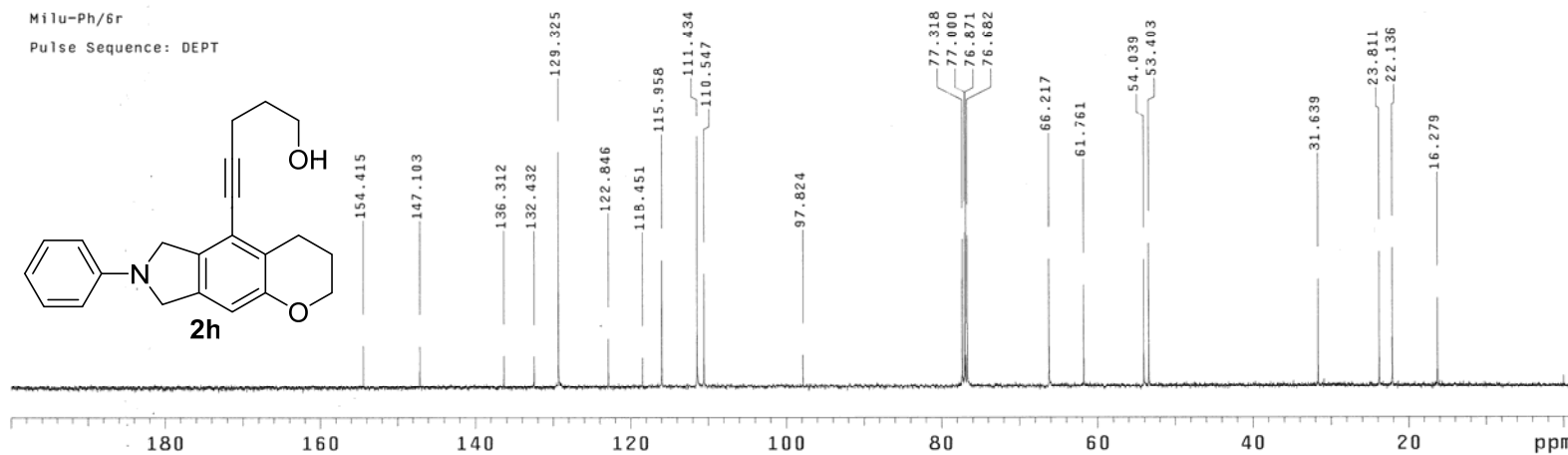
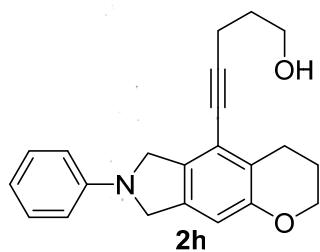
Ambient temperature

Total 2016 repetitions



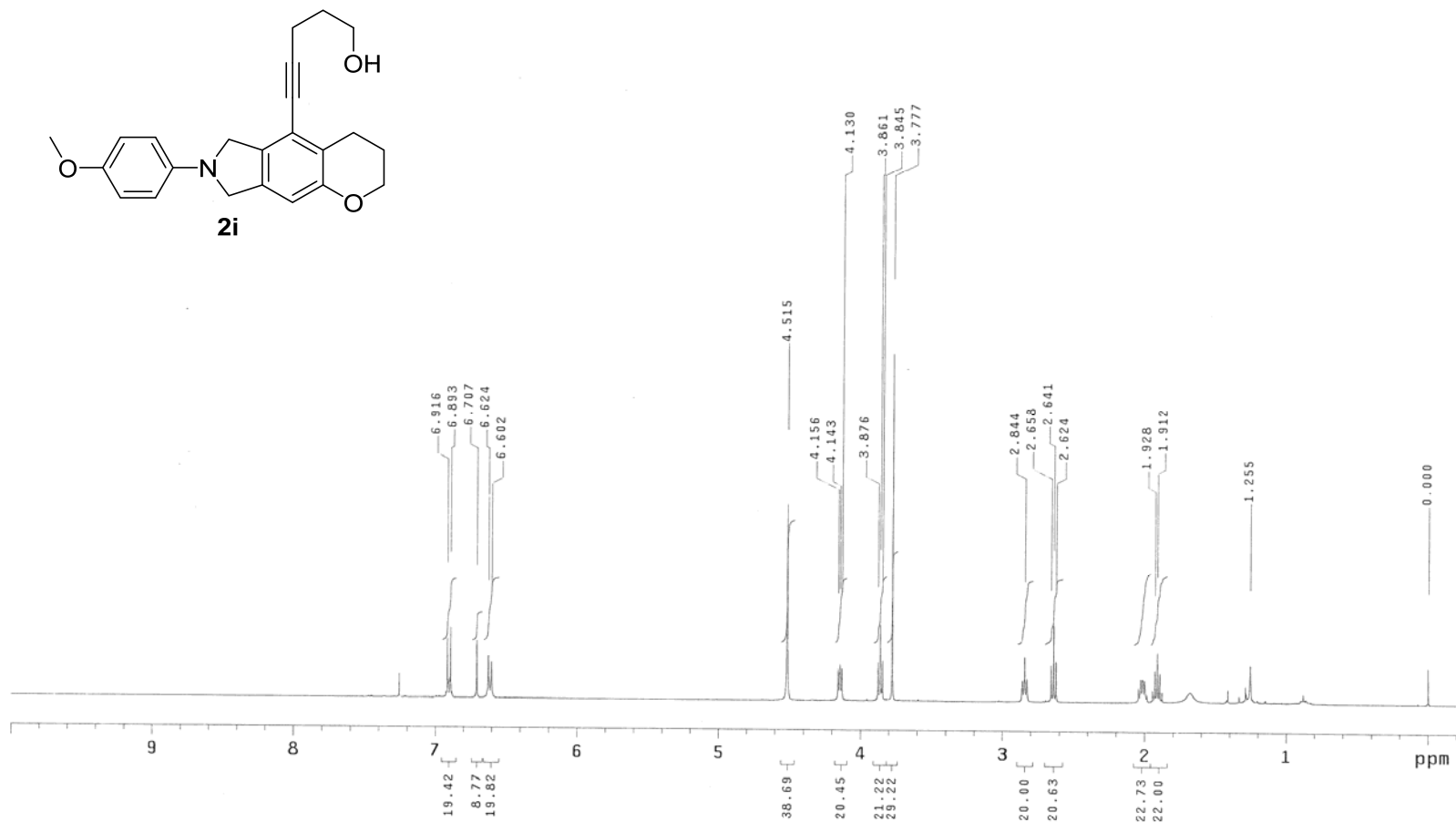
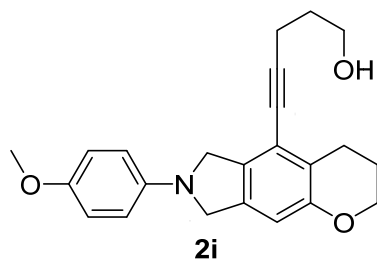
Milu-Ph/6r

Pulse Sequence: DEPT



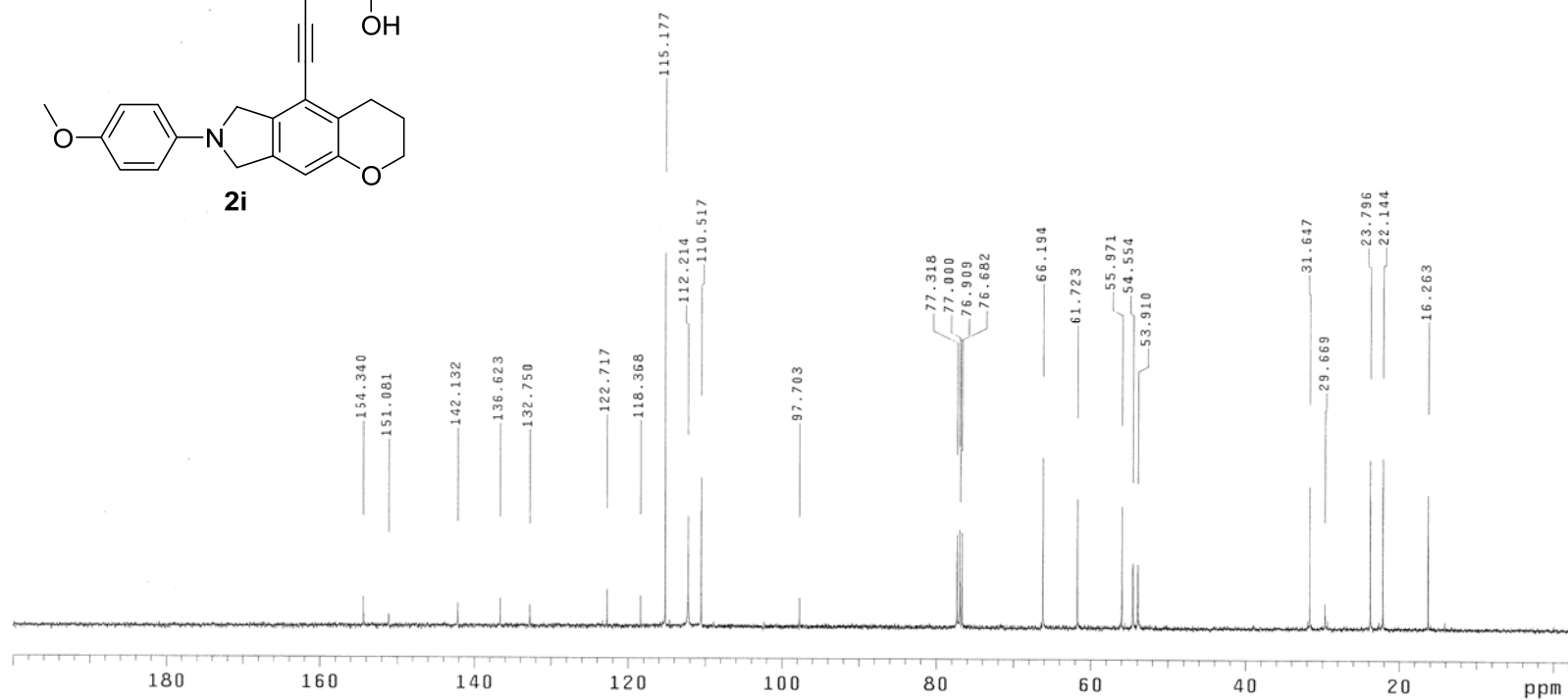
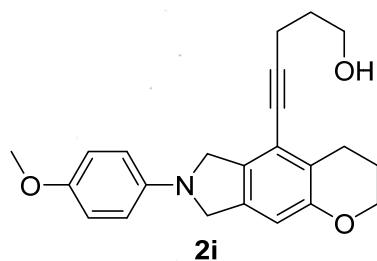
Milu-4-OMe-Ph/6-ring
Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees
Acq. time 4.002 sec
Width 5995.2 Hz
64 repetitions
OBSERVE H1, 400.3978976 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 7 sec



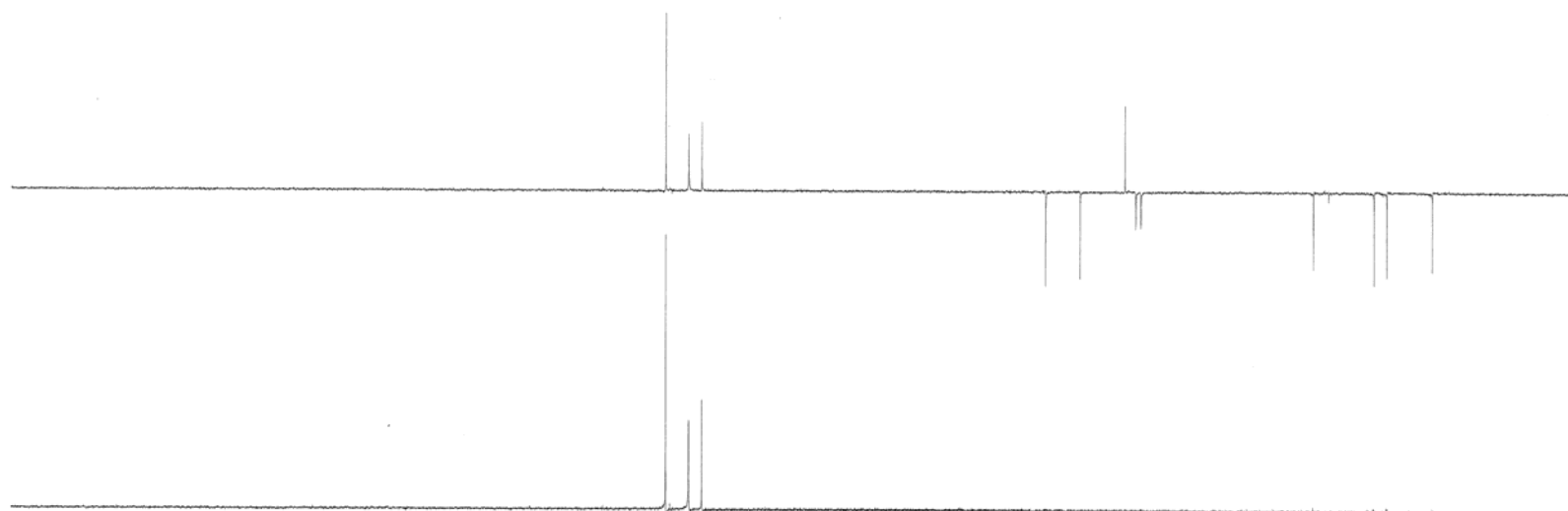
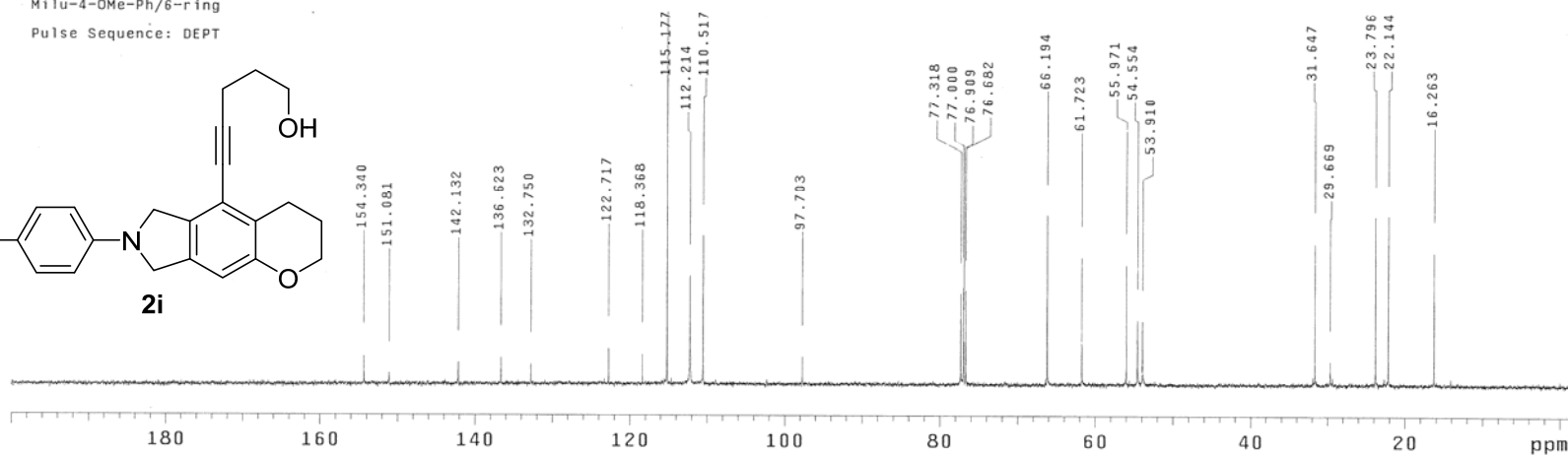
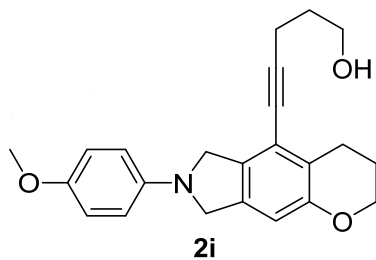
Milu-4-OMe-Ph/6-ring
Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
Mercury-400SB "MercuryPlus400"

Pulse 68.7 degrees
Acq. time 1.000 sec
Width 25000.0 Hz
4000 repetitions
OBSERVE C13, 100.6801338 MHz
DECOUPLE H1, 400.3999572 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 21 min, 58 sec



Milu-4-OMe-Ph/6-ring

Pulse Sequence: DEPT



Milu-3-OMe-Ph/6r

Pulse Sequence: s2pu1

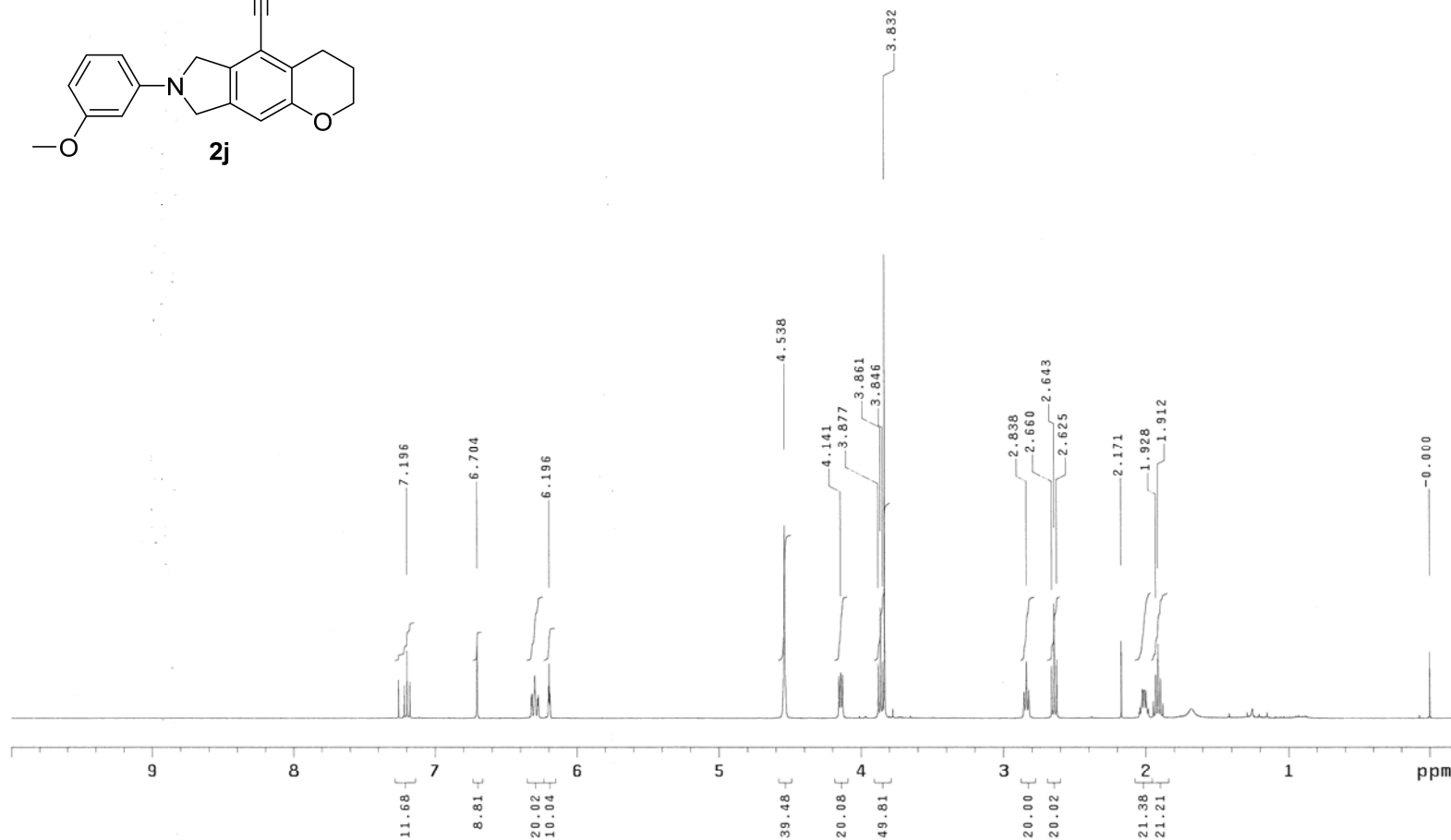
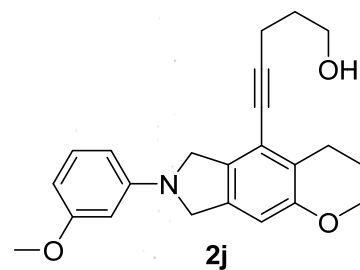
Mercury-400BB "MercuryPlus400"

Date: Mar 10 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Milu-3-OMe-Ph/6r

Pulse Sequence: s2pu1

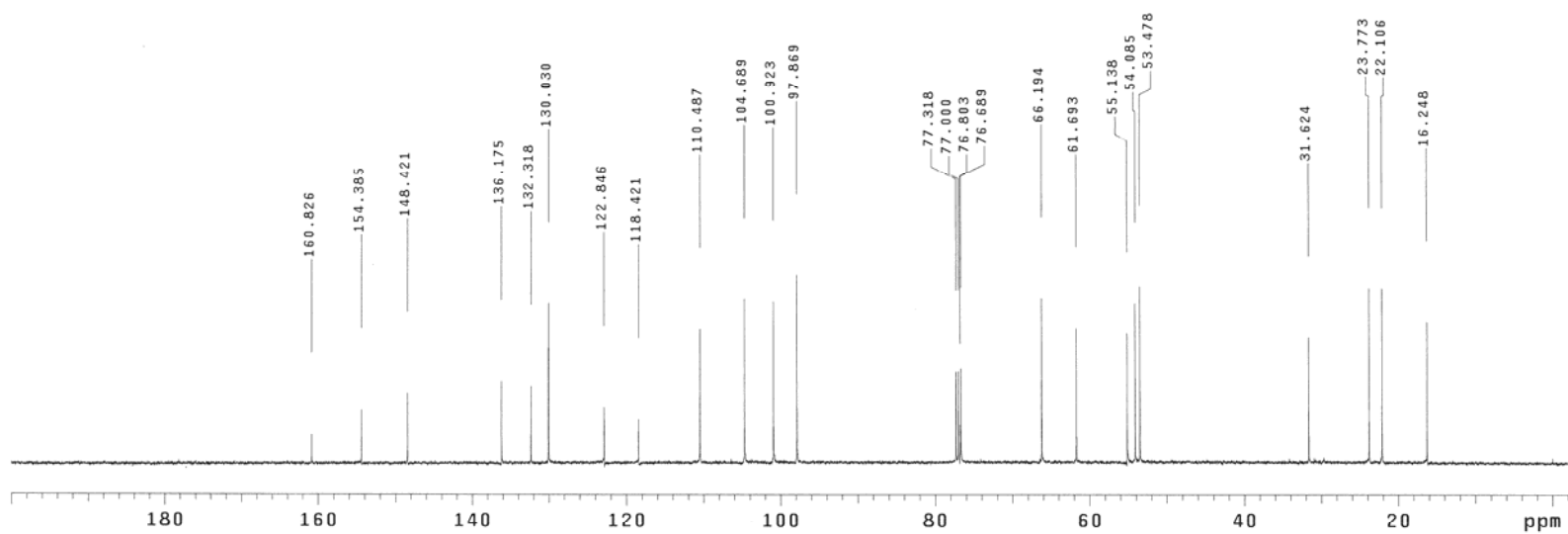
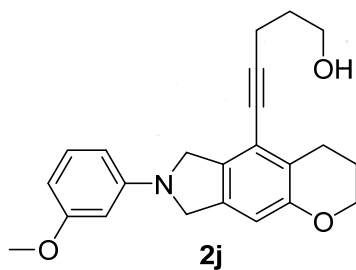
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Date: Mar 10 2014

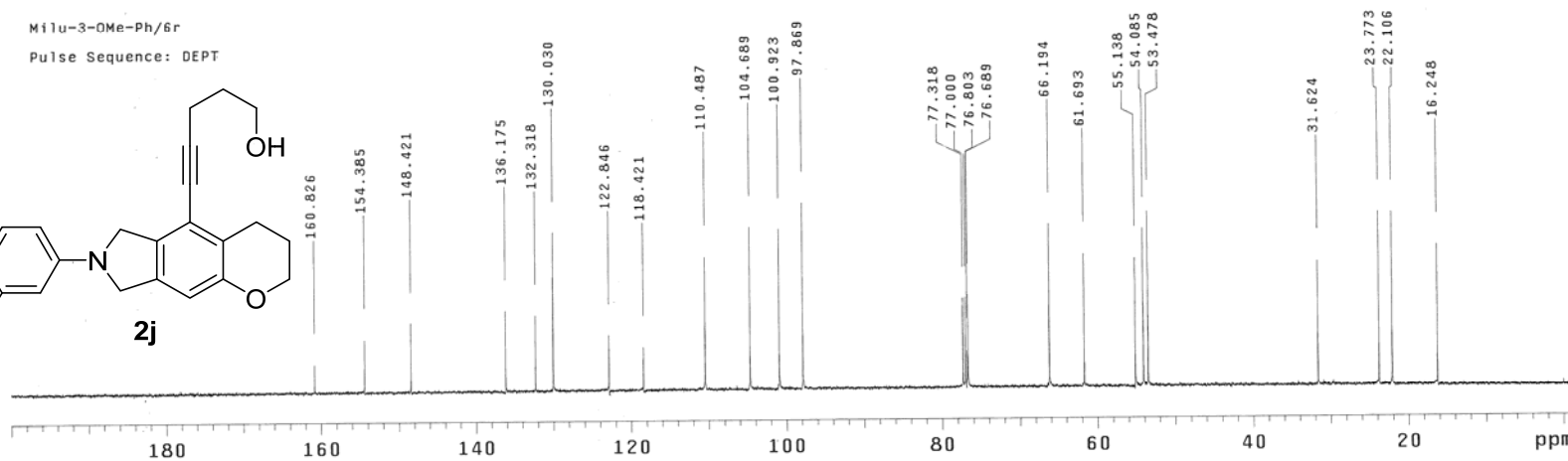
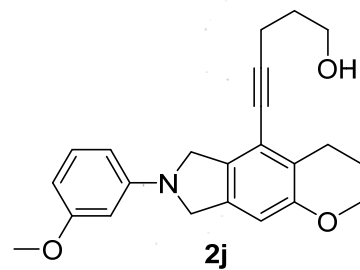
Solvent: CDCl₃

Ambient temperature

Total 64000 repetitions



Milu-3-OMe-Ph/6r
Pulse Sequence: DEPT



Milu-2-OMe-Ph/6r

Pulse Sequence: s2pu1

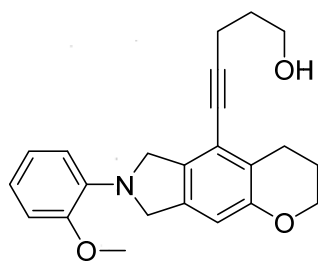
Mercury-400BB "MercuryPlus400"

Date: Mar 10 2014

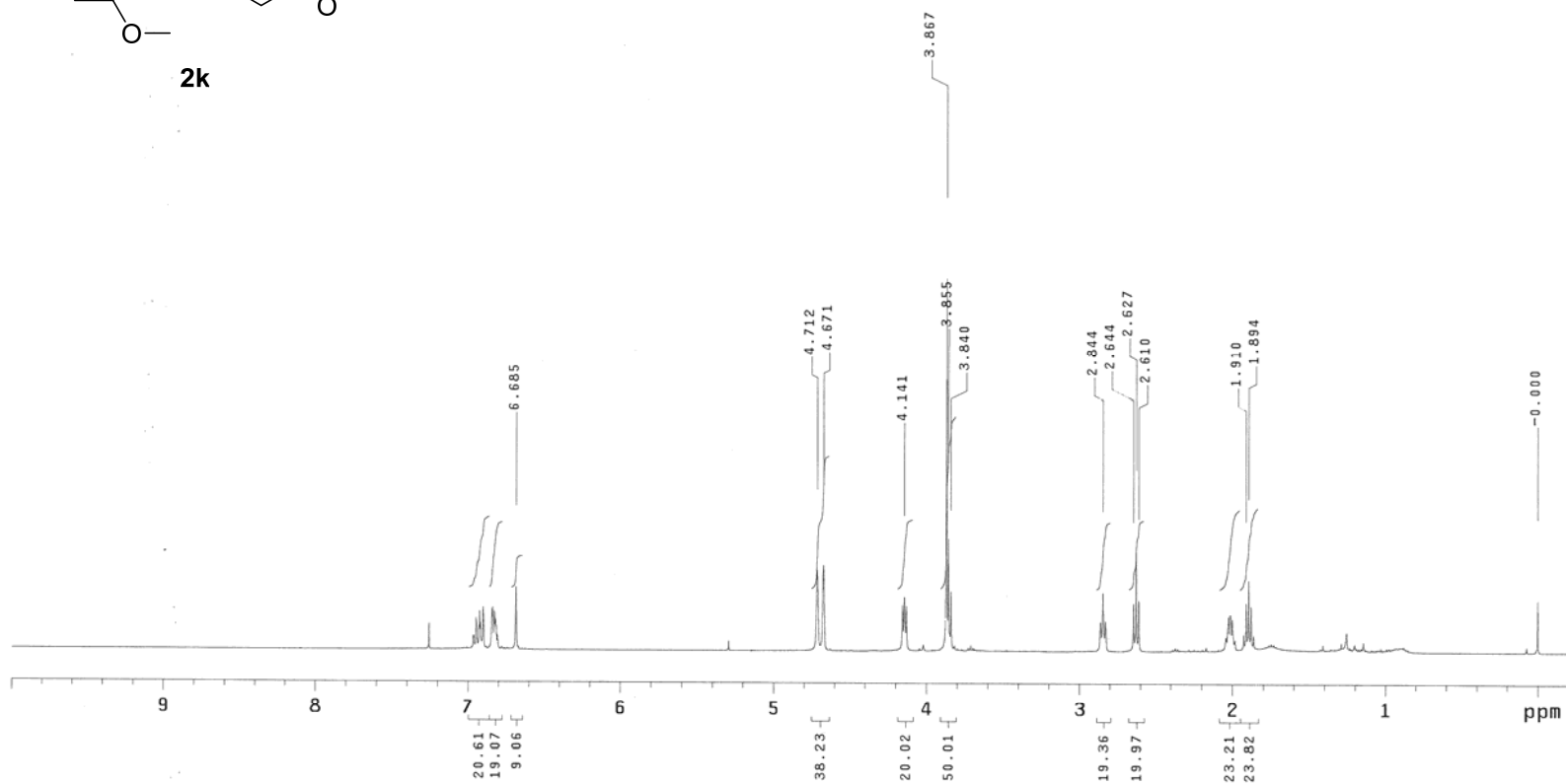
Solvent: CDCl₃

Ambient temperature

Total 40 repetitions



2k



Milu-2-OMe-Ph/6r

Pulse Sequence: s2pu1

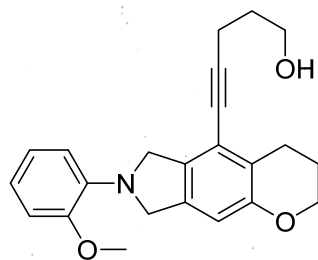
Mercury-400BB "MercuryPlus400"

Date: Mar 10 2014

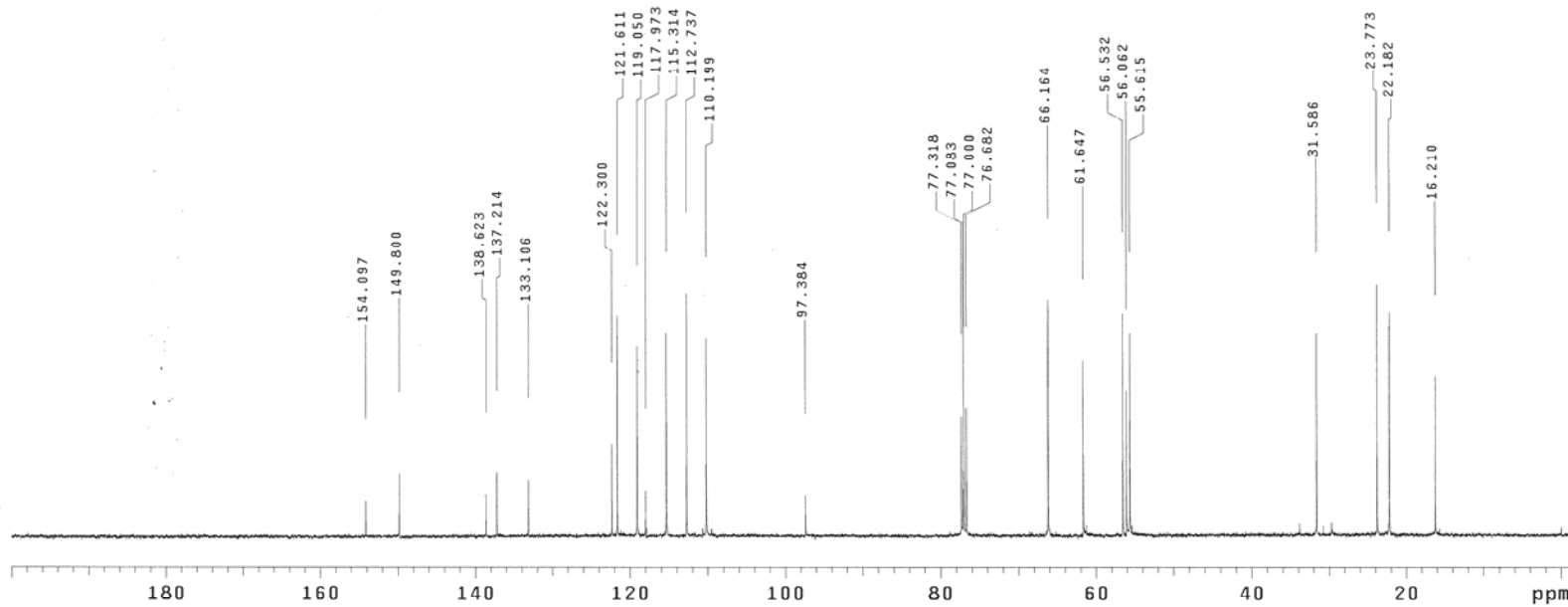
Solvent: CDCl₃

Ambient temperature

Total 3024 repetitions

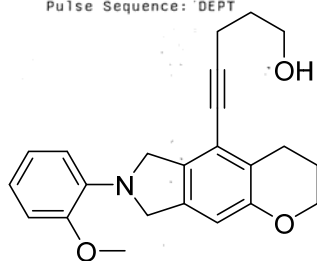


2k

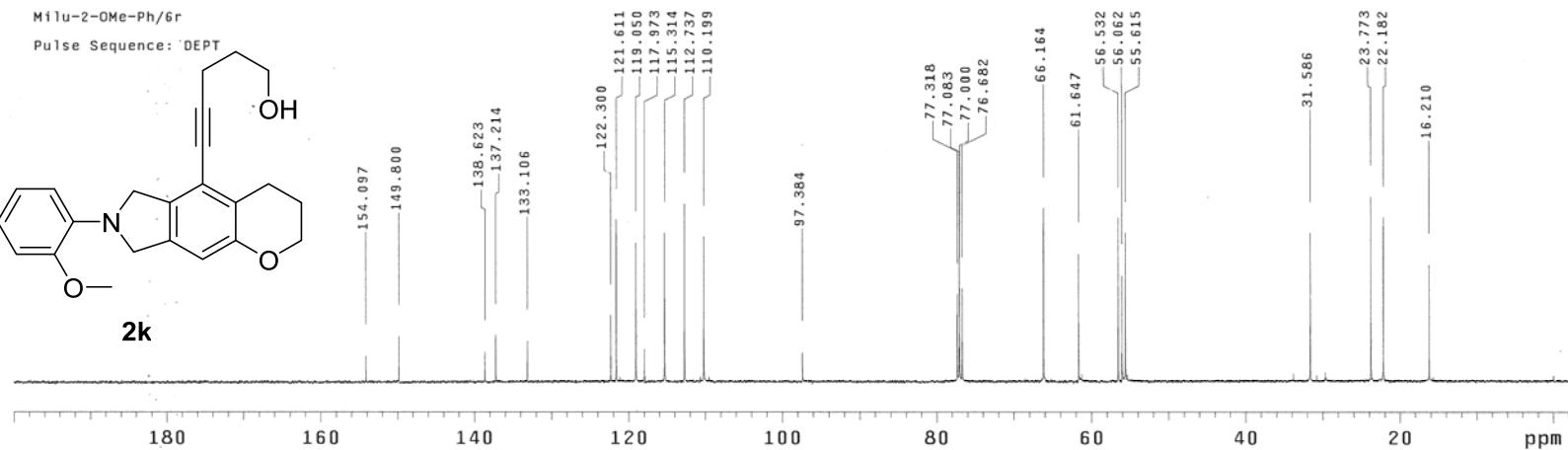


Milu-2-OMe-Ph/6r

Pulse Sequence: DEPT



2k



Milu-4-C1-6r

Pulse Sequence: s2pu1

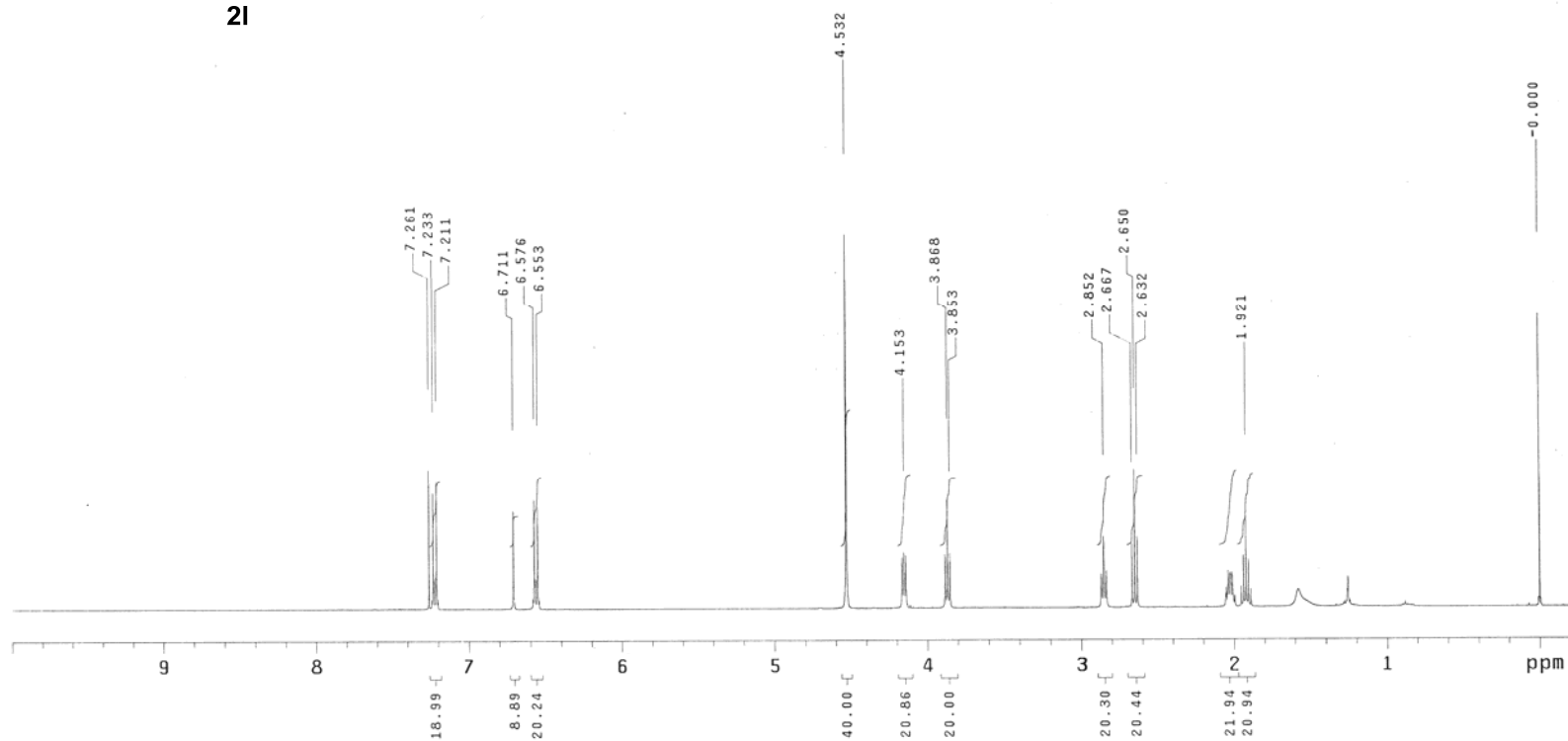
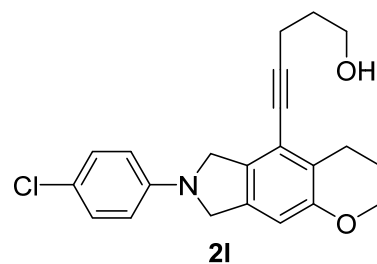
Mercury-400BB "MercuryPlus400"

Date: Dec 24 2013

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



Milu-4-Cl-6r

Pulse Sequence: s2pu1

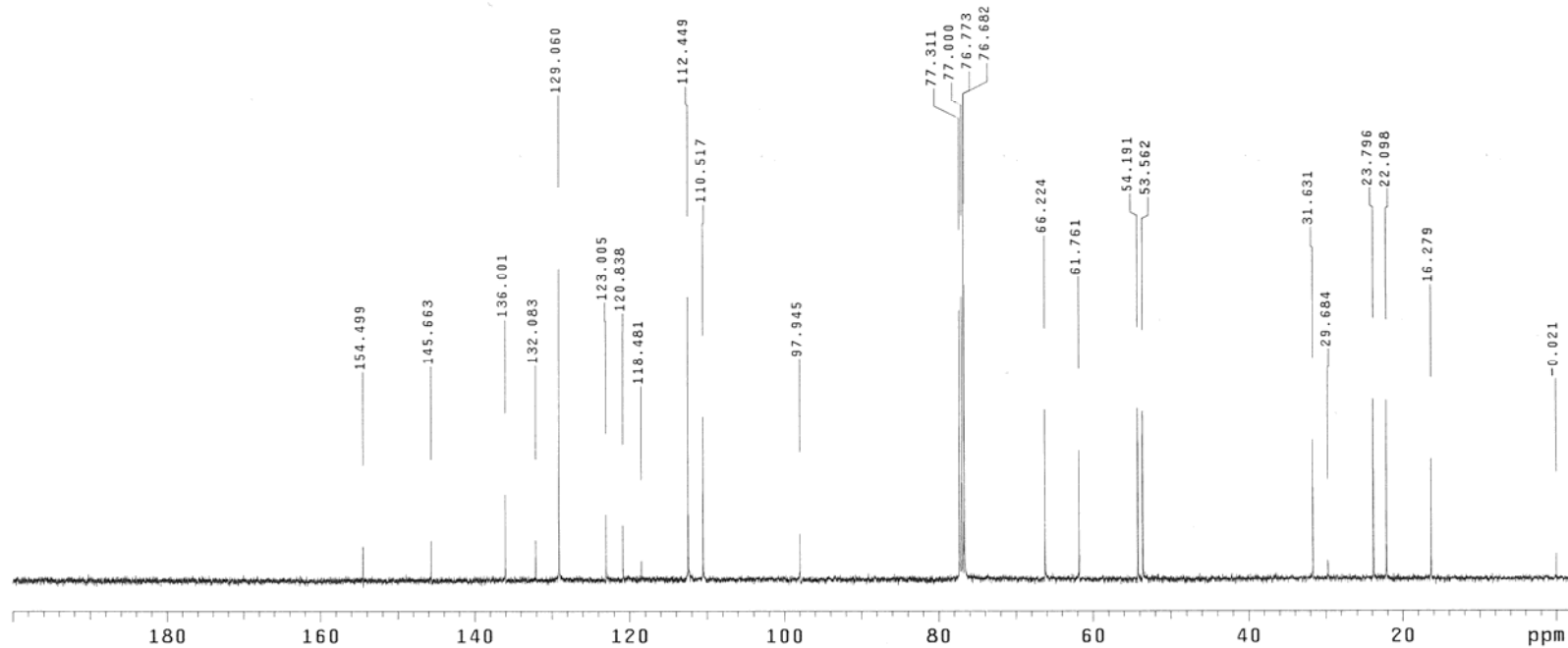
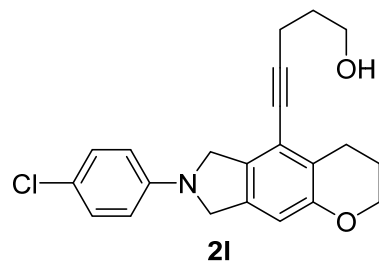
Mercury-400BB "MercuryPlus400"

Date: Dec 24 2013

Solvent: CDCl₃

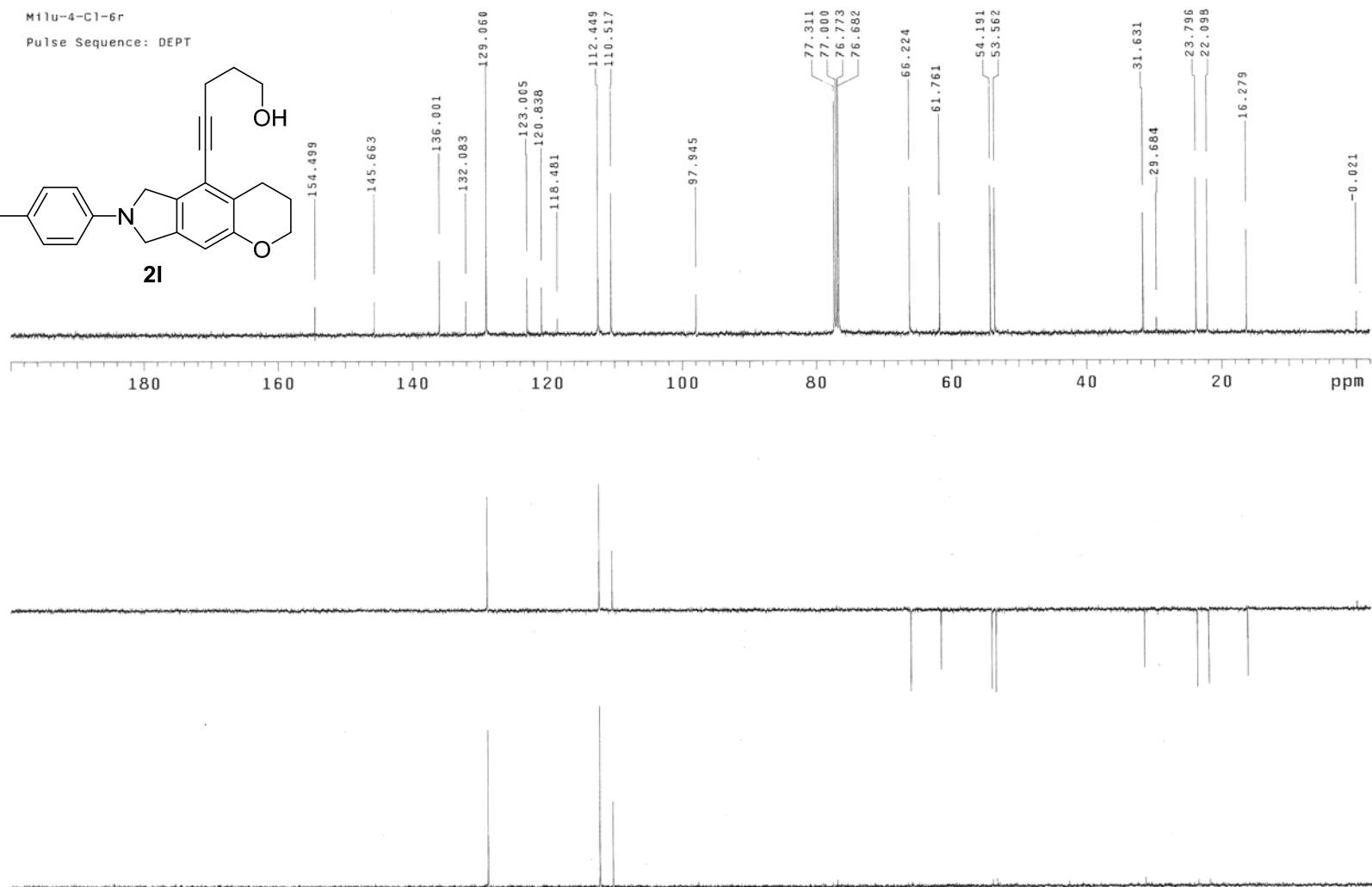
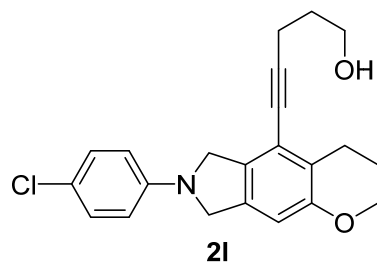
Ambient temperature

Total 4800 repetitions



M11u-4-Cl-6r

Pulse Sequence: DEPT



Milu-Br-Ph/6r

Pulse Sequence: s2pu1

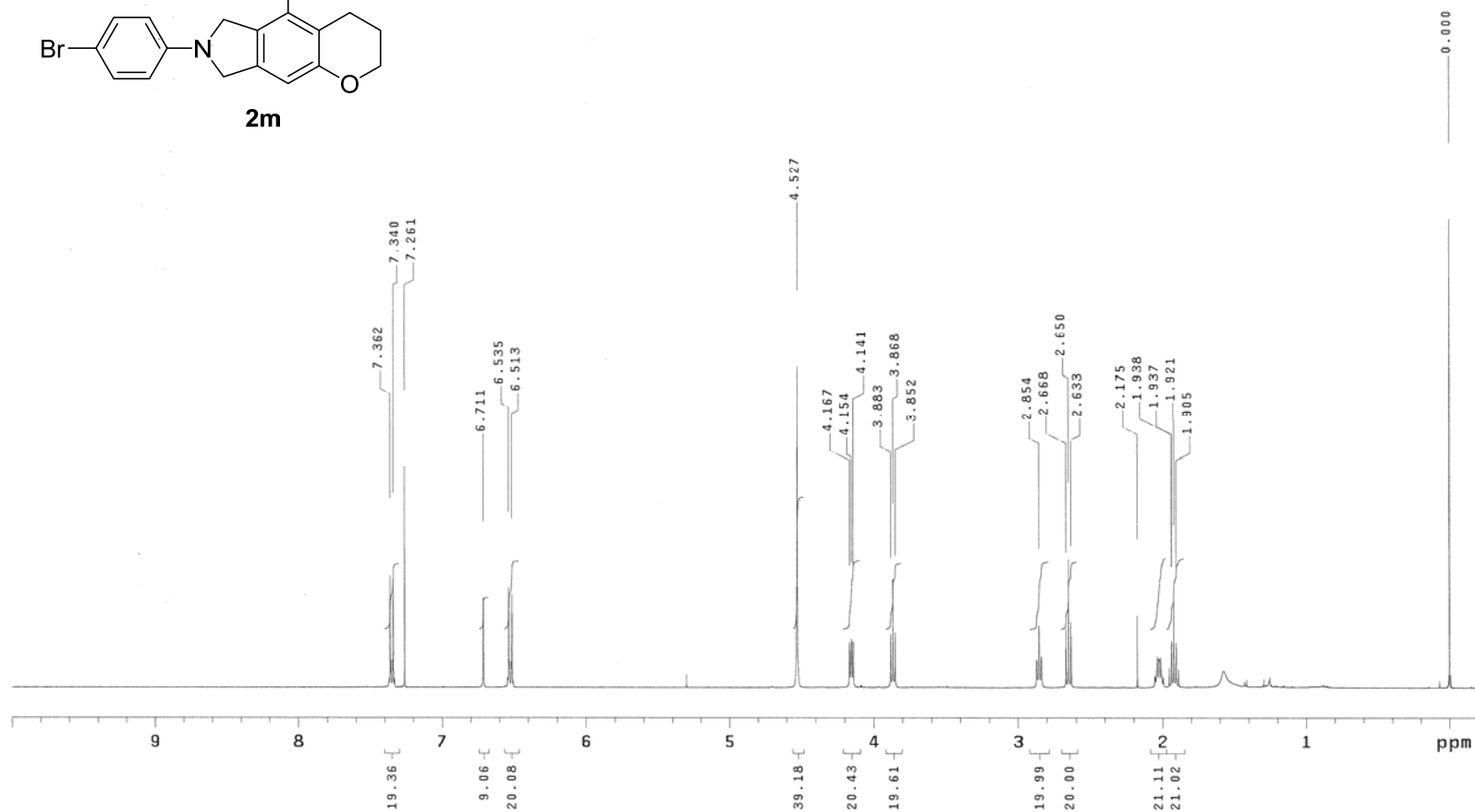
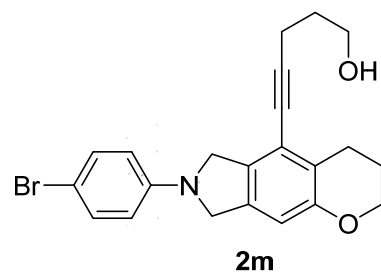
Mercury-400BB "MercuryPlus400"

Date: Mar 10 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Milu-Br-Ph/6r

Pulse Sequence: s2pu1

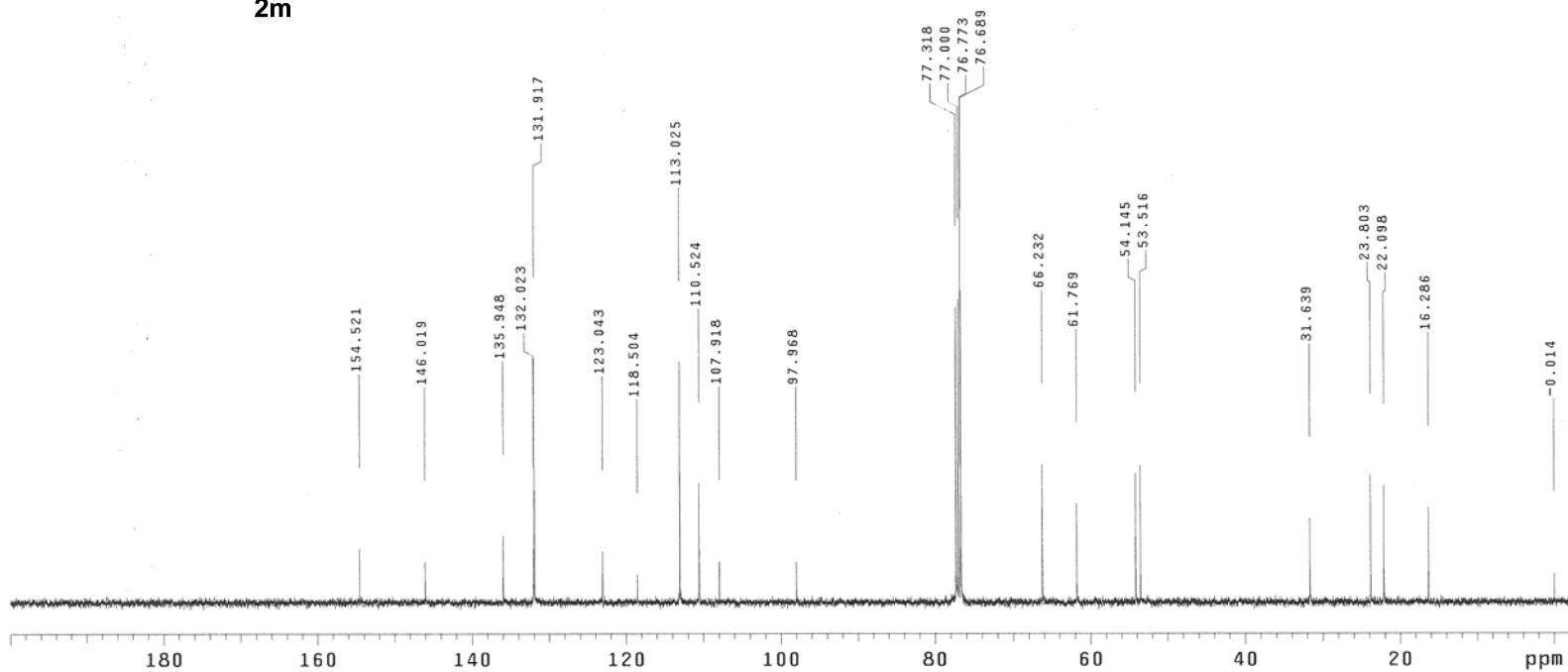
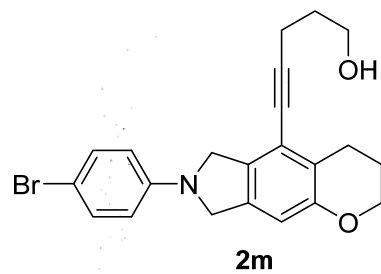
Mercury-400BB "MercuryPlus400"

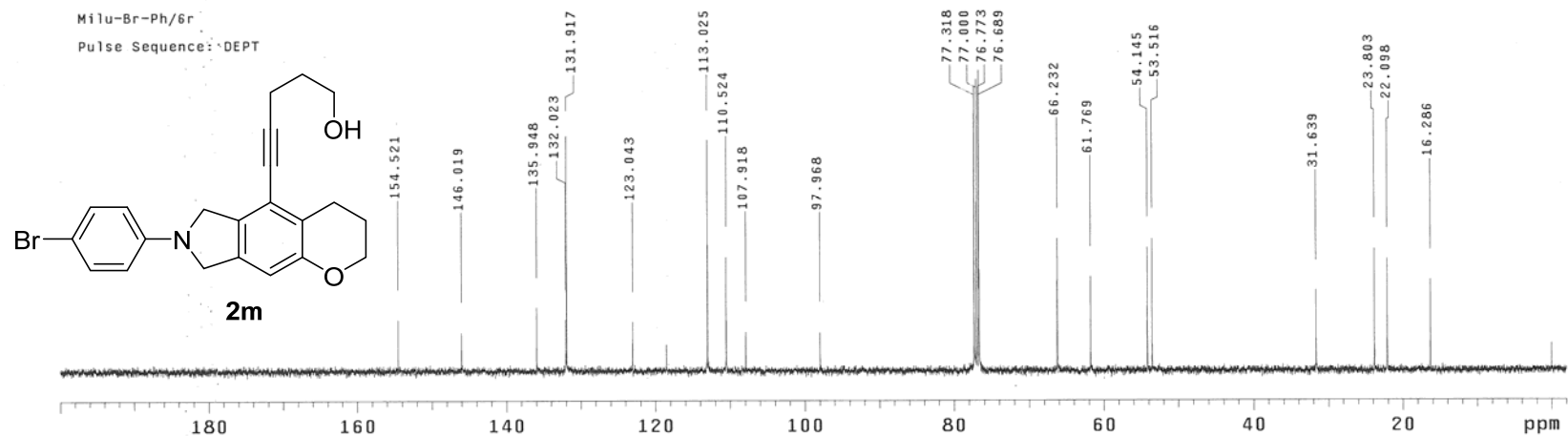
Date: Mar 10 2014

Solvent: CDCl₃

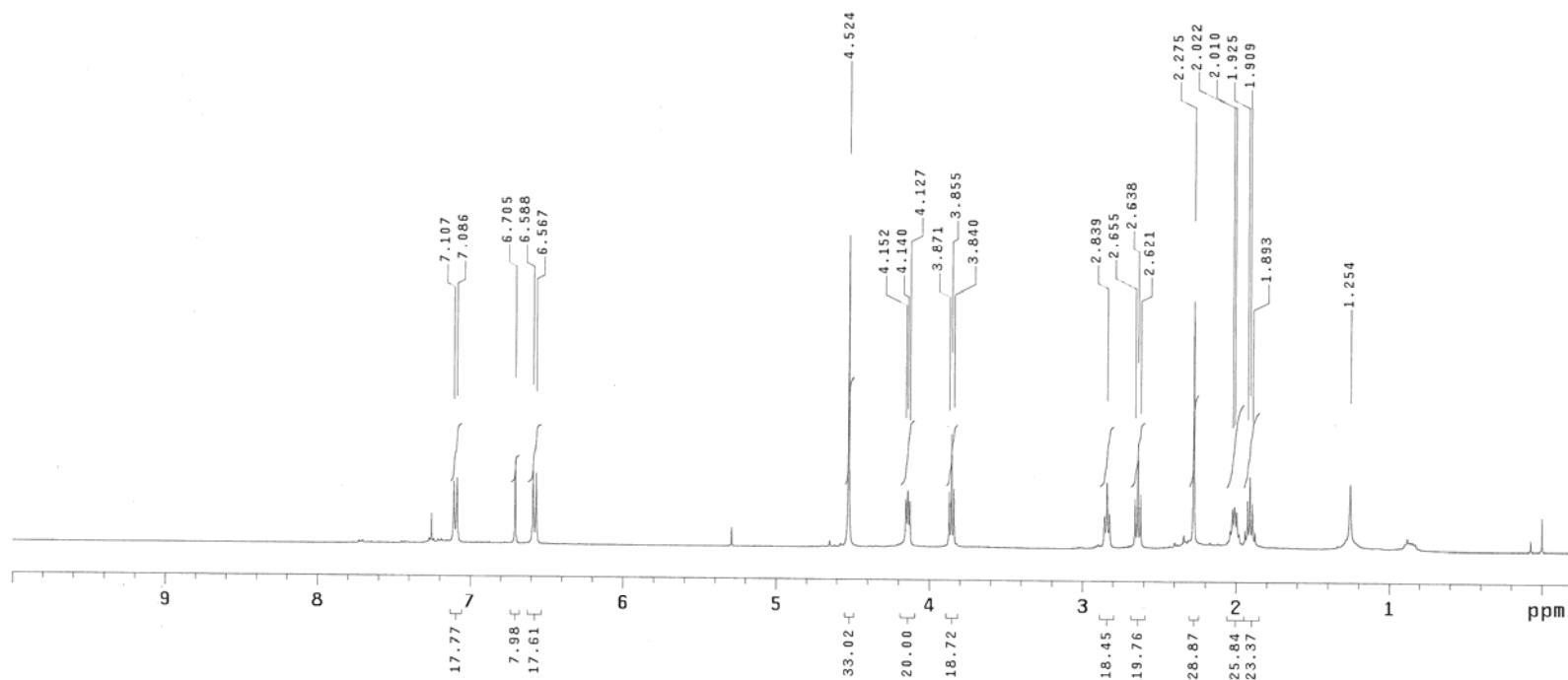
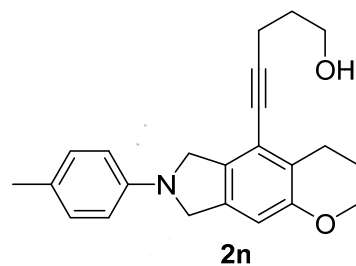
Ambient temperature

Total 3056 repetitions

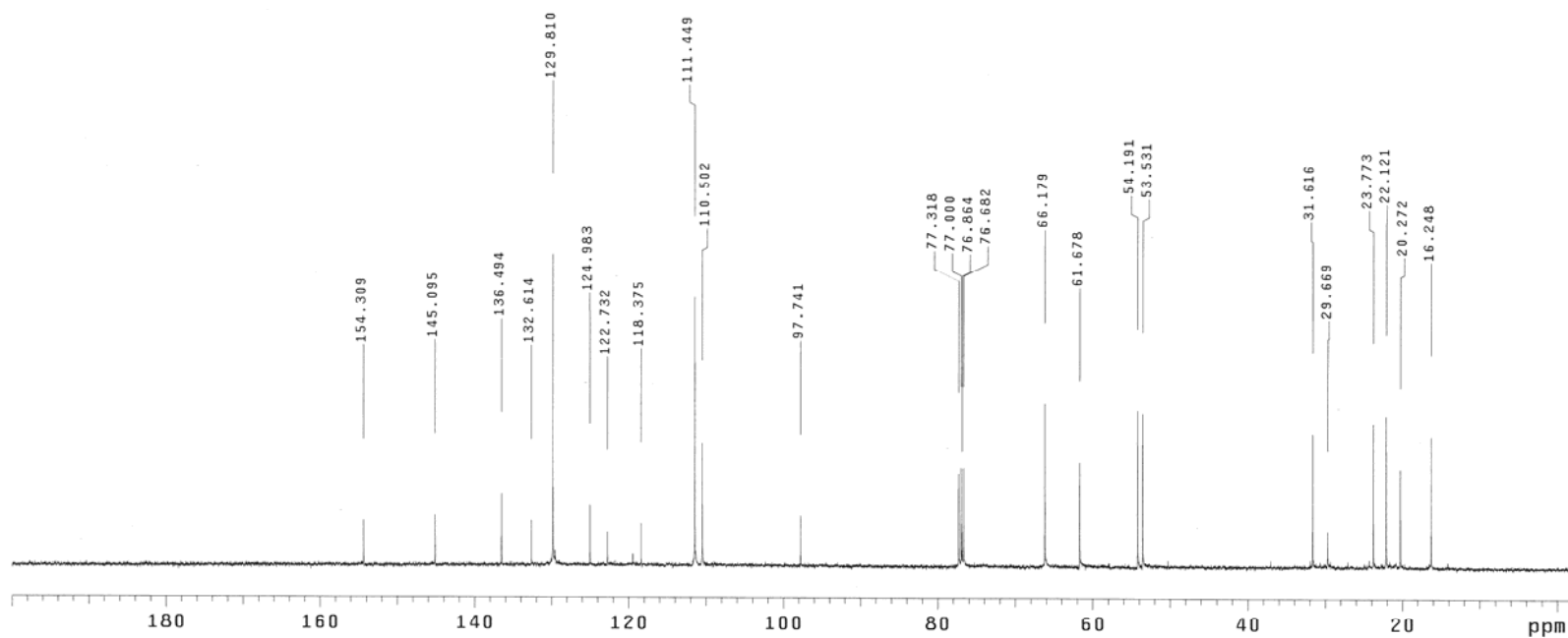
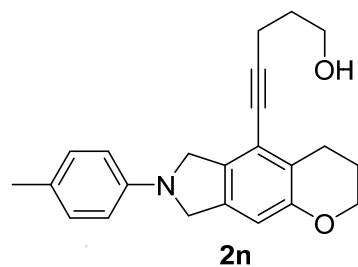




Milu-4-CH3-Ph/6r
Pulse Sequence: s2pu1
Mercury-400BB "MercuryPlus400"
Date: Feb 11 2014
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

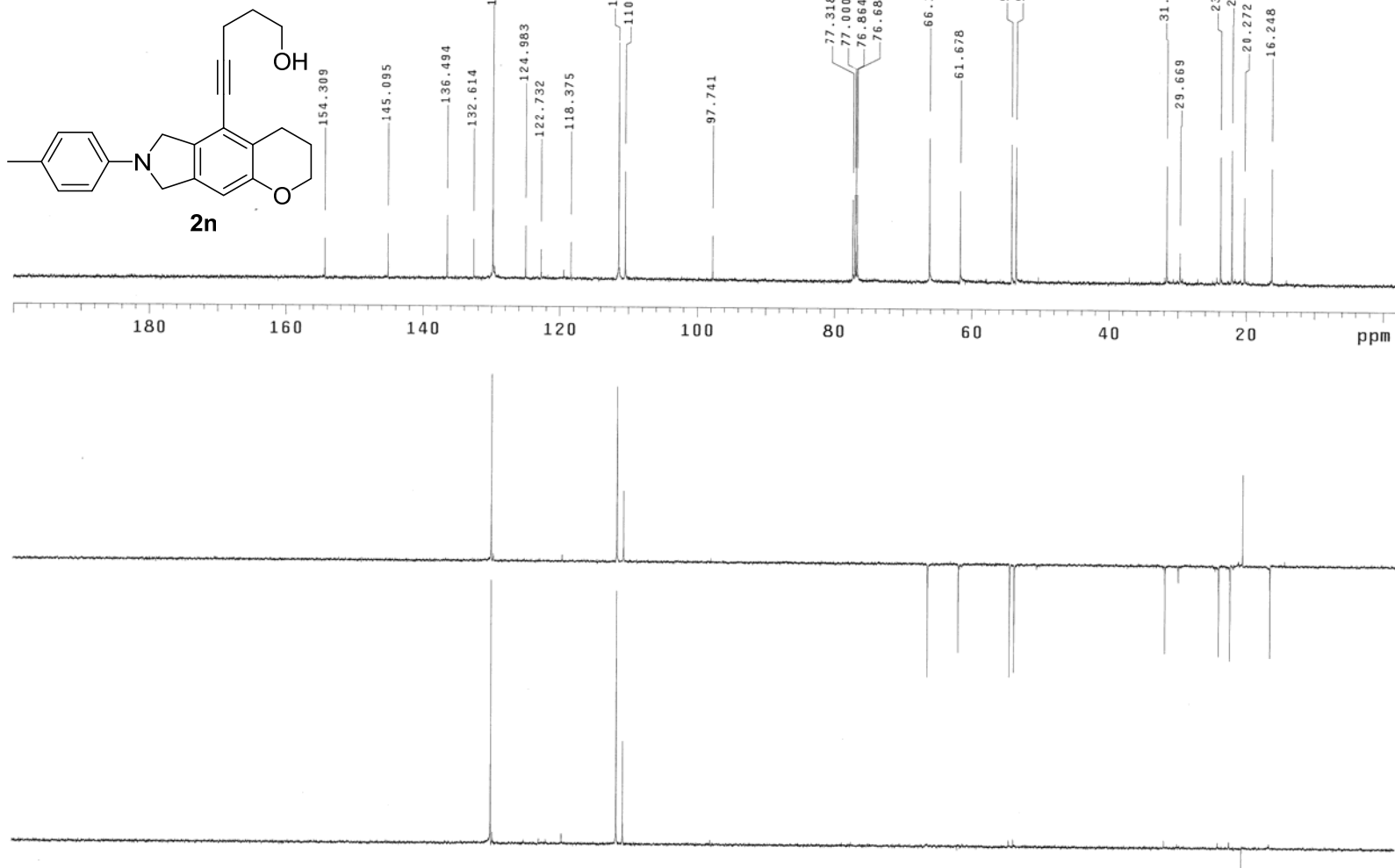


Milu-4-CH3-Ph/6r
Pulse Sequence: s2pu1
Mercury-400BB "MercuryPlus400"
Date: Feb 11 2014
Solvent: CDCl3
Ambient temperature
Total 784 repetitions



Milu-4-CH3-Ph/6r

Pulse Sequence: DEPT



102-1/47/47A

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees

Acq. time 4.002 sec

Width 5995.2 Hz

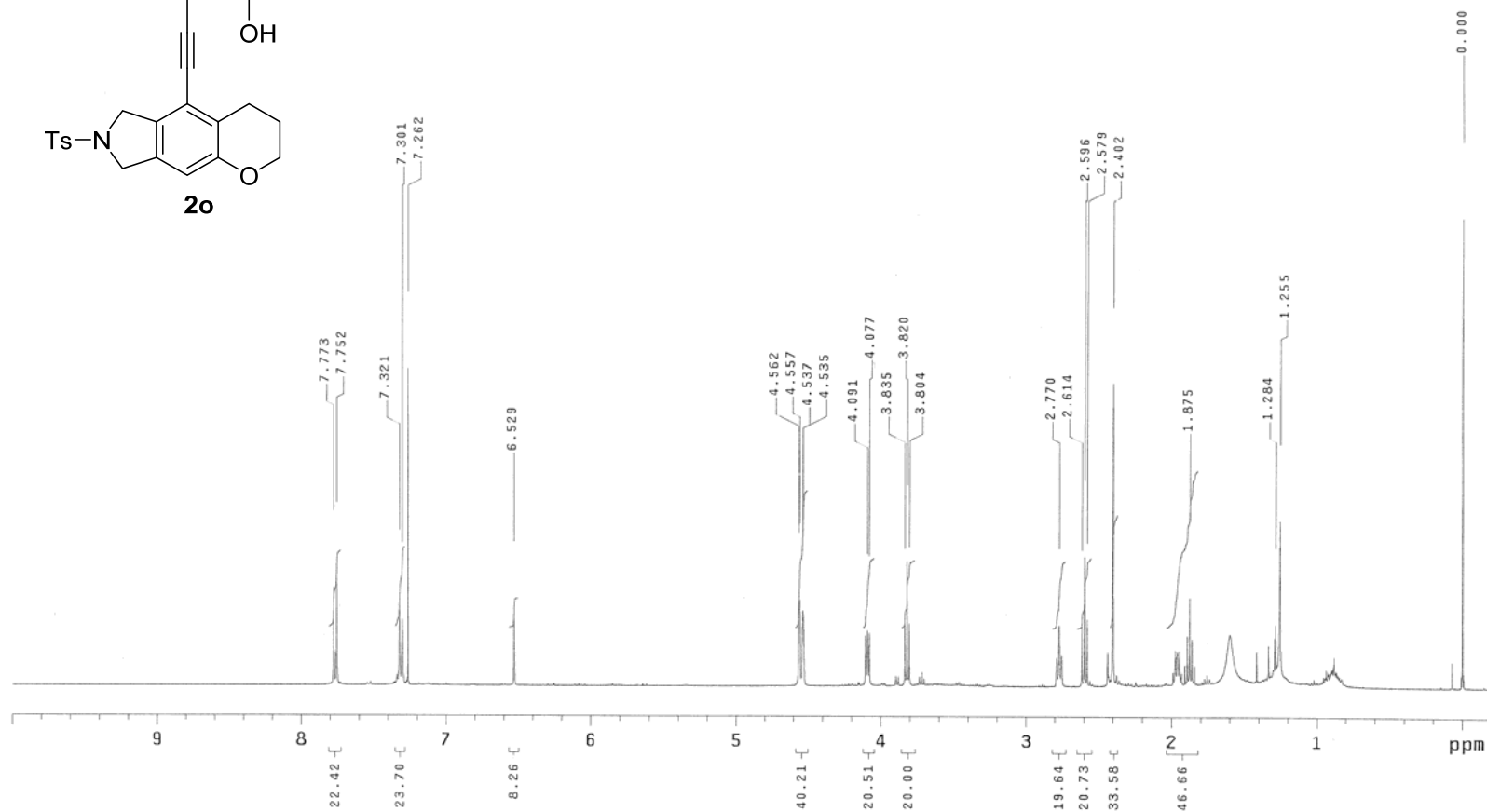
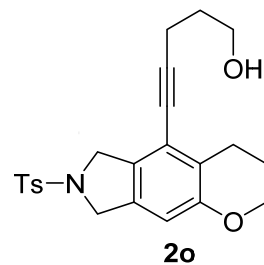
80 repetitions

OBSERVE H1, 400.3978954 MHz

DATA PROCESSING

FT size 65536

Total time 6 min, 23 sec



102-1/47/47A

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

Mercury-400BB "MercuryPlus400"

Relax. delay 0.500 sec

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

16000 repetitions

OBSERVE C13, 100.6801315 MHz

DECOUPLE H1, 400.3999572 MHz

Power 38 dB

continuously on

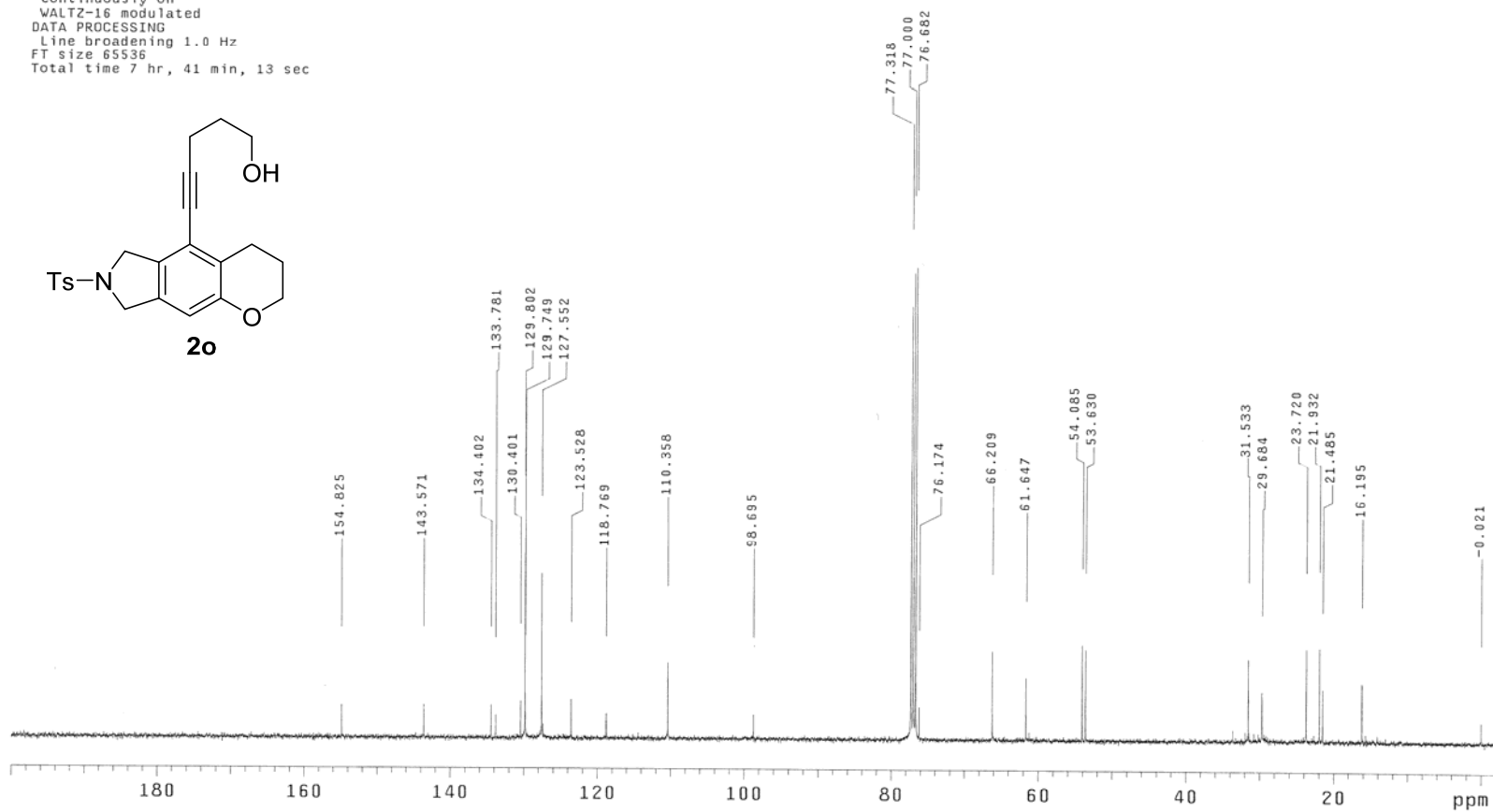
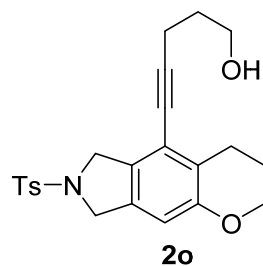
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

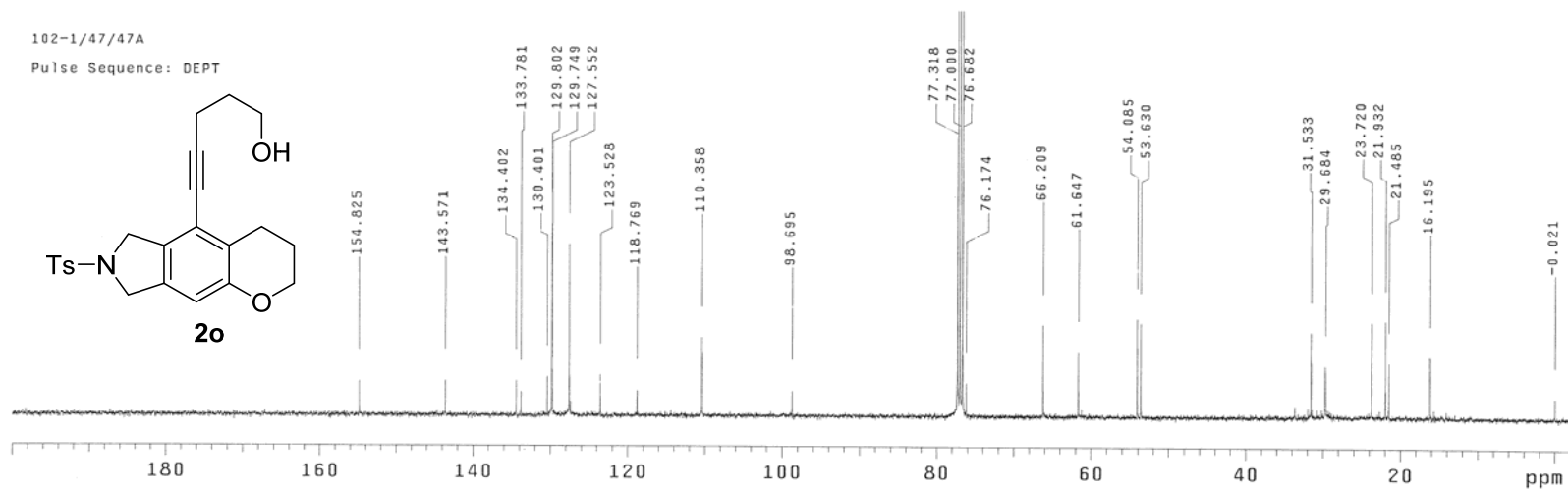
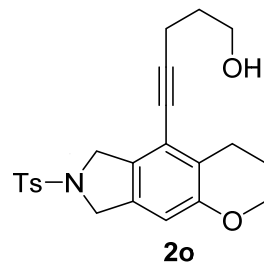
FT size 65536

Total time 7 hr, 41 min, 13 sec



102-1/47/47A

Pulse Sequence: DEPT



Milu-CF3-Ph/6r

Pulse Sequence: s2pu1

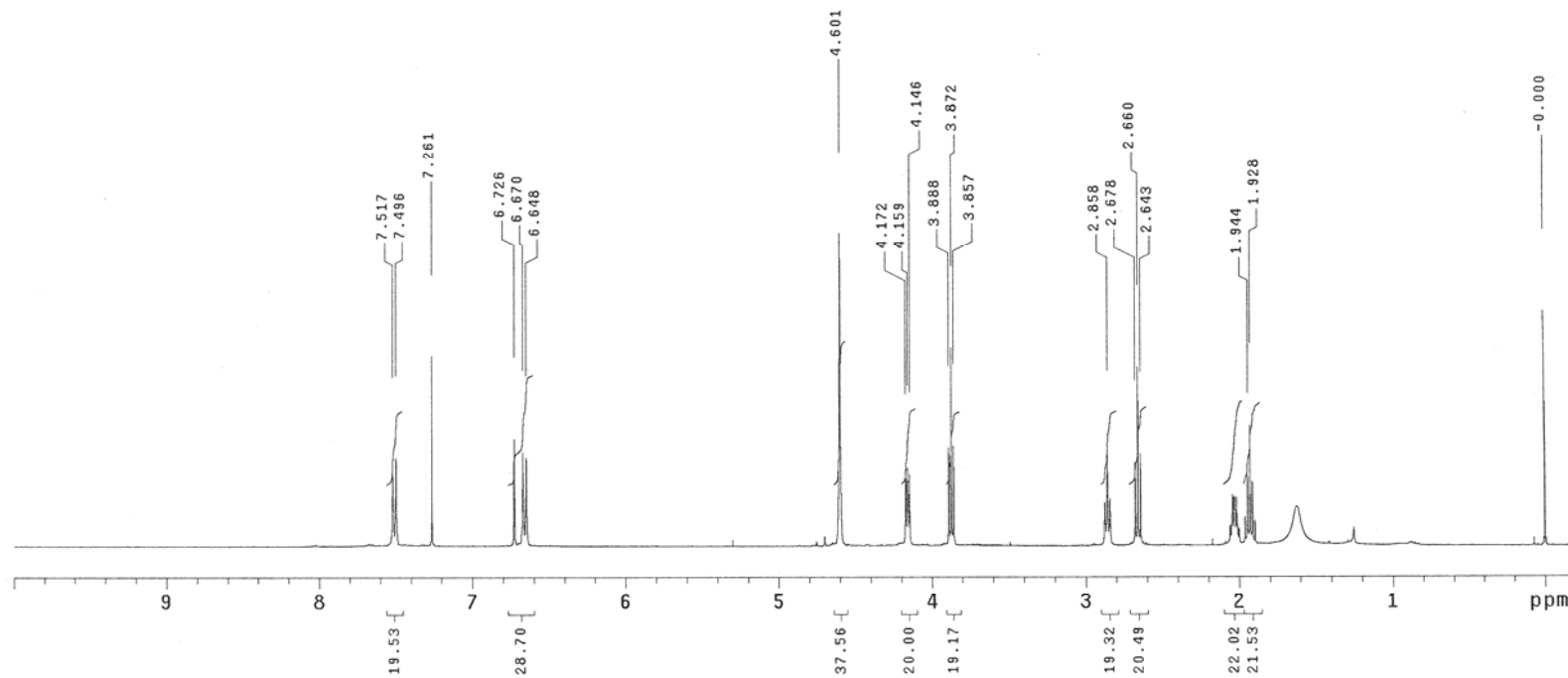
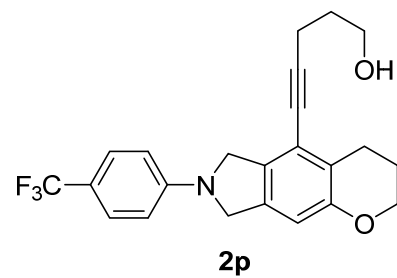
UNITYplus-400 "unity400"

Date: Mar 26 2014

Solvent: CDCl3

Ambient temperature

Total 80 repetitions



Milu-CF3-Ph/6r

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: Mar 26 2014

Solvent: CDC13

Ambient temperature

Total 8048 repetitions

