

# **Aza-Wittig Rearrangements of *N*-Benzyl and *N*-Allyl Glycine Methyl Esters. Discovery of a Surprising Cascade Aza-Wittig Rearrangement/Hydroboration Reaction.**

**Renata K. Everett and John P. Wolfe\***

*Department of Chemistry, University of Michigan, 930 N. University Avenue, Ann Arbor, Michigan 48109-1055*

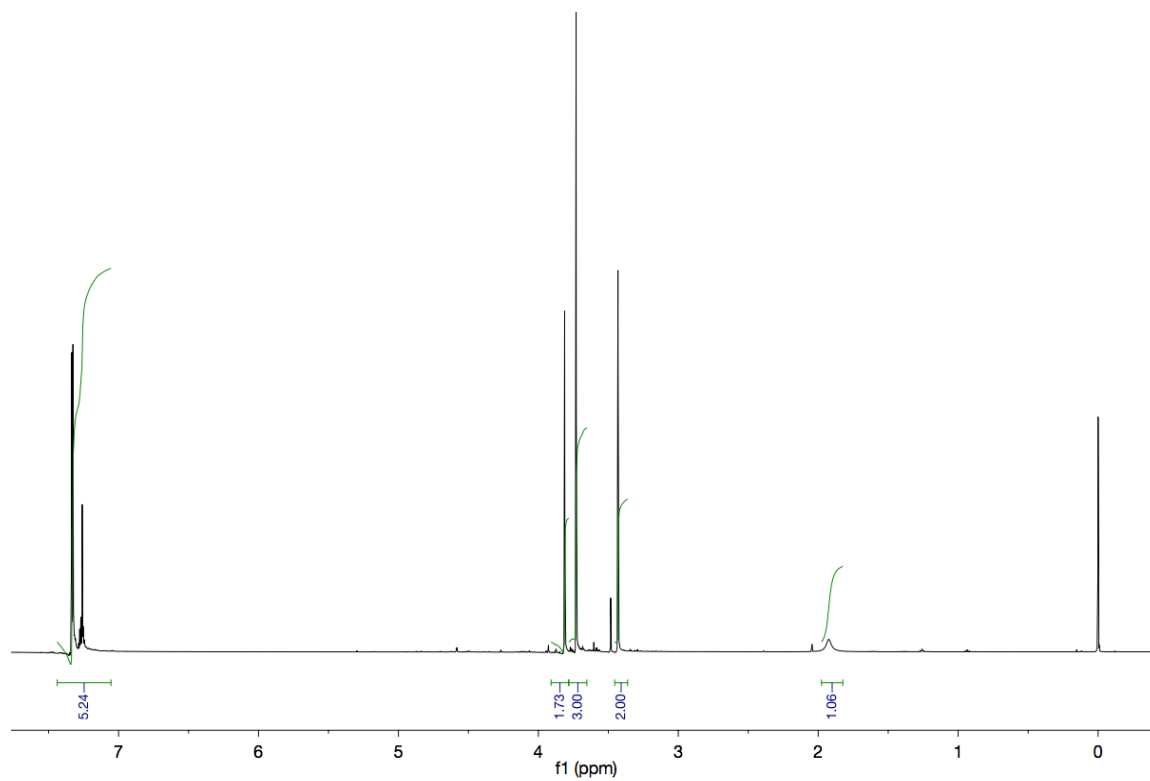
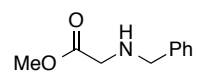
## **Supporting Information**

### **Table of Contents**

**Copies of  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra**

**S2**

RE-2-145  
STANDARD Deuterium PARAMETERS  
Using lock coil



STANDARD Deuterium PARAMETERS  
Using lock coil

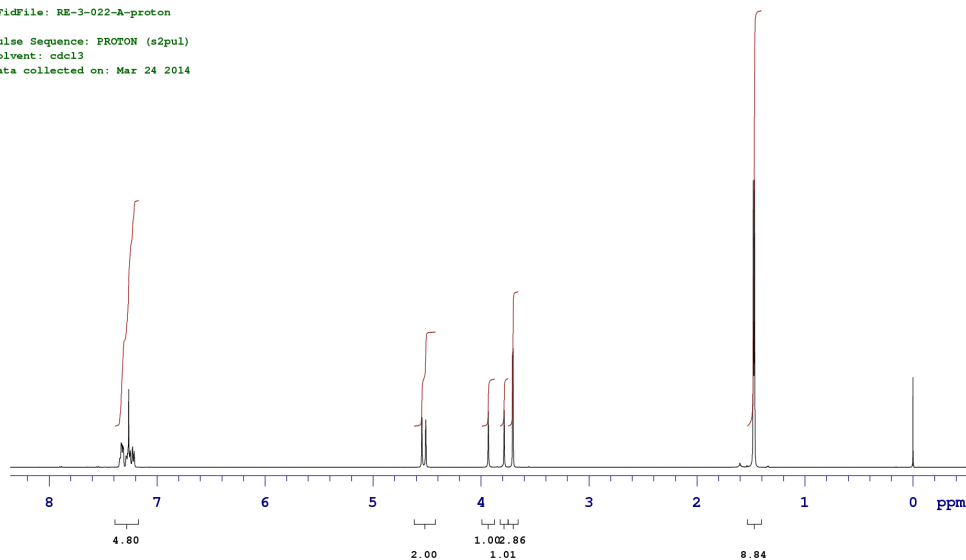
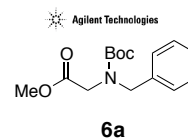
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Sample directory:

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Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 24 2014



STANDARD PROTON PARAMETERS  
Atropine

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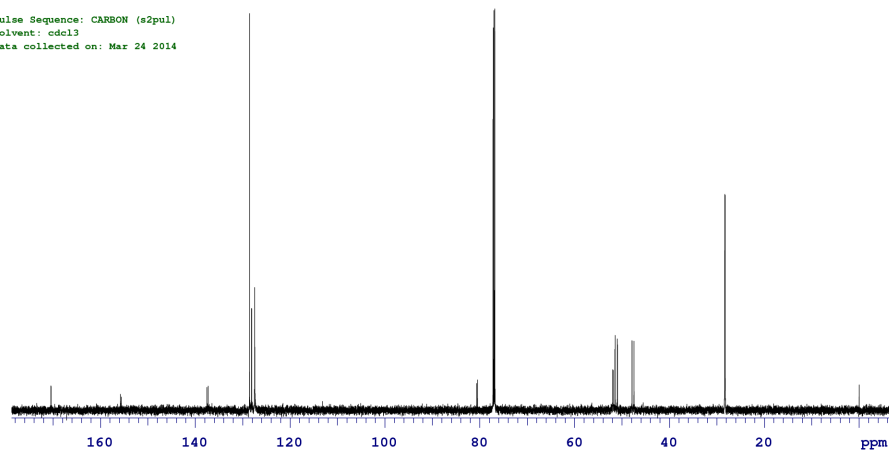
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Solvent: cdcl3  
Data collected on: Mar 24 2014

Agilent Technologies



Gradient Shimming

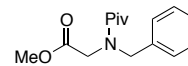
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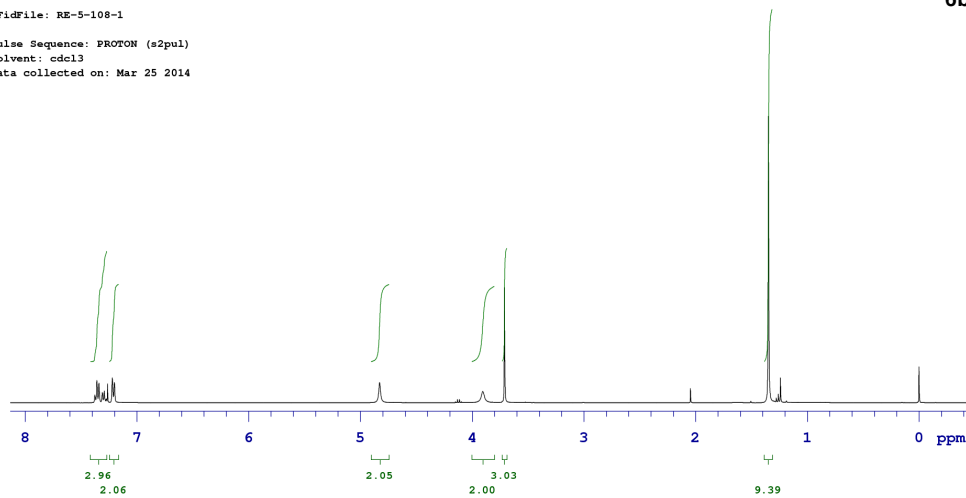
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Data collected on: Mar 25 2014

Agilent Technologies



**6b**



STANDARD 1H OBSERVE - profile

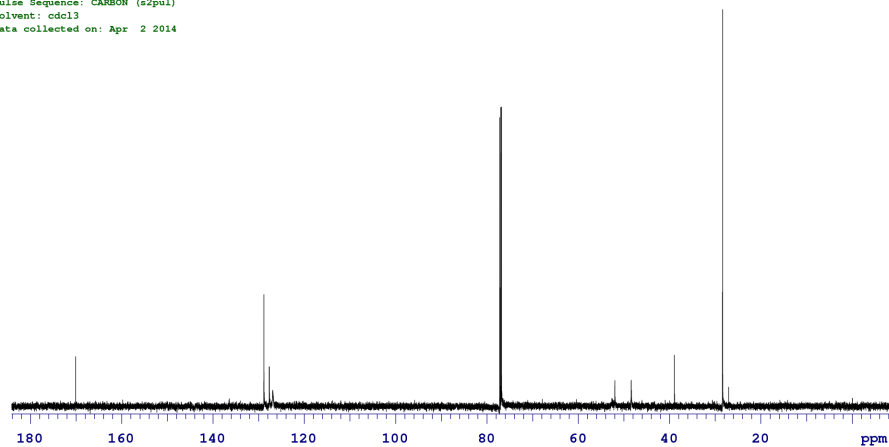
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Solvent: cdcl3  
Data collected on: Apr 2 2014

Agilent Technologies





Proton Spectrum

Sample Name:

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Archive directory:

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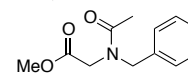
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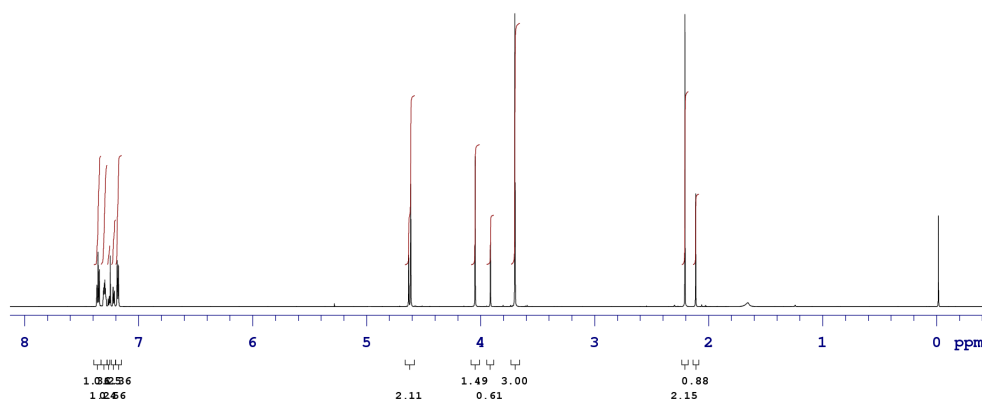
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Data collected on: Jul 1 2014

Agilent Technologies



6c



Carbon-13

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Archive directory:

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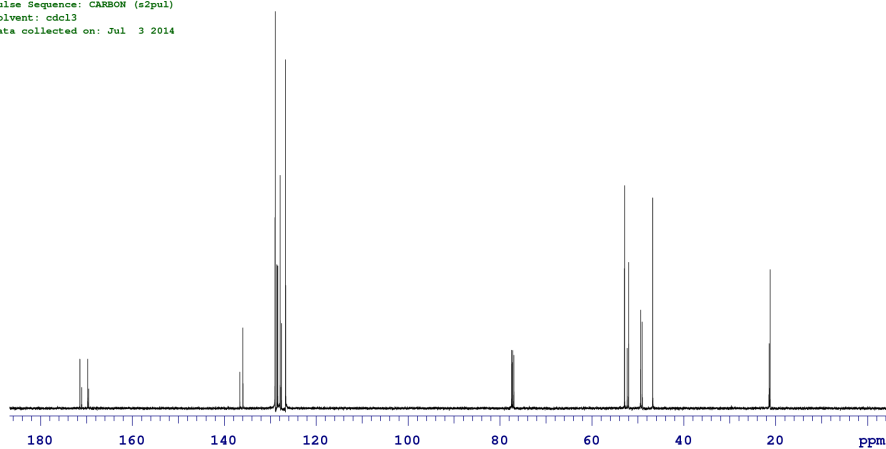
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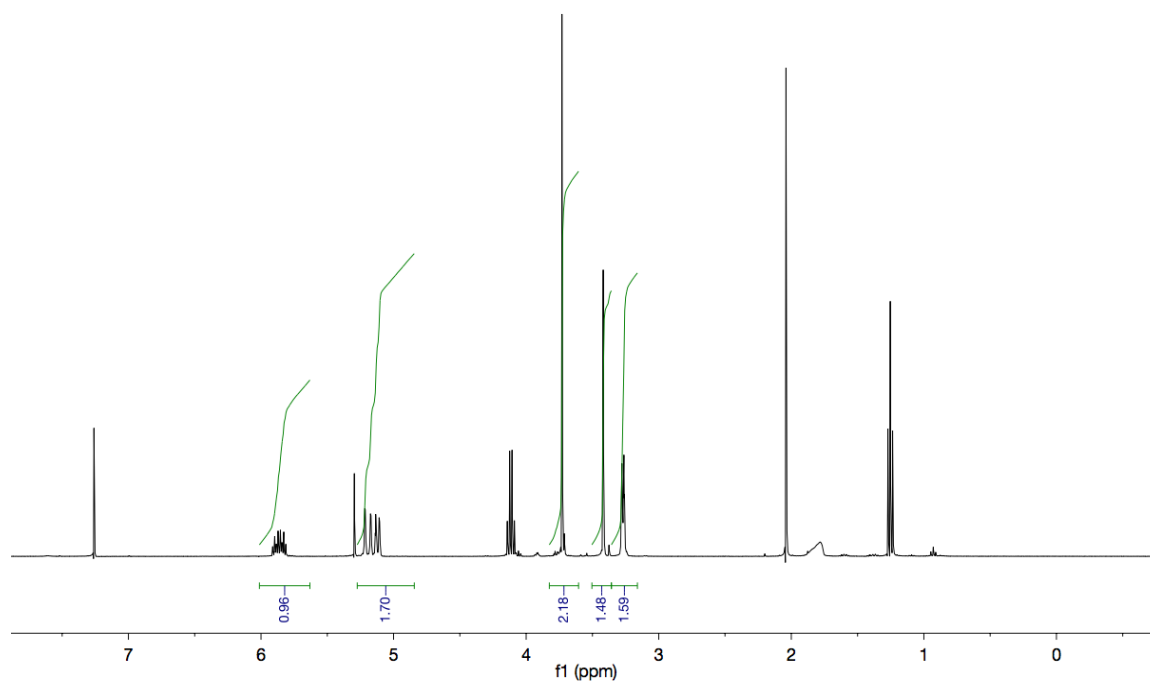
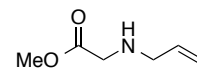
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Data collected on: Jul 3 2014

Agilent Technologies



RE-2-169  
STANDARD 1H OBSERVE - profile



Gradient Shimming

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Archive directory:

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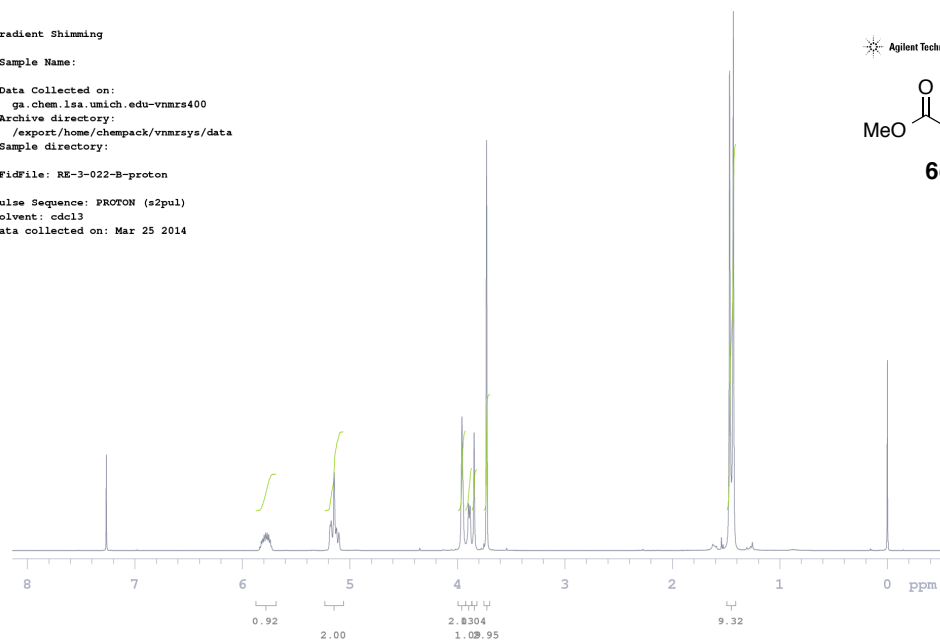
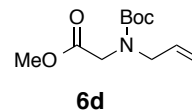
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Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 25 2014

Agilent Technologies



STANDARD 1H OBSERVE - profile

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Archive directory:

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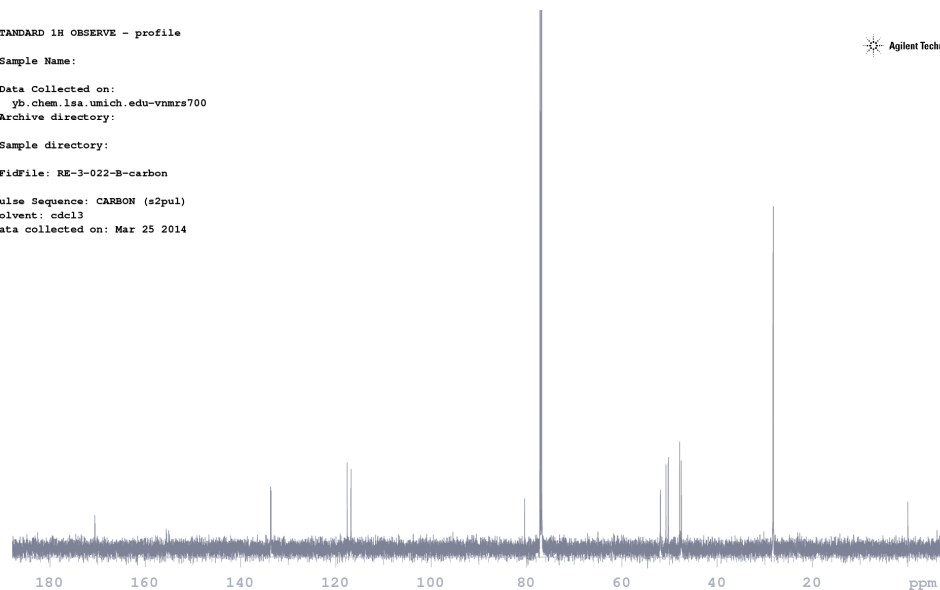
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Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 25 2014

Agilent Technologies



Proton Spectrum

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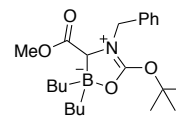
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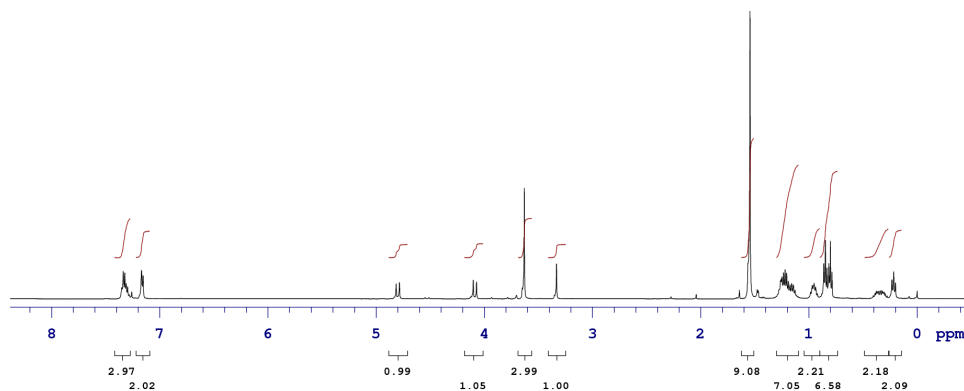
Solvent: cdcl3

Data collected on: Aug 1 2014

Agilent Technologies



7a



Carbon-13

Sample Name:

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Archive directory:

Sample directory:

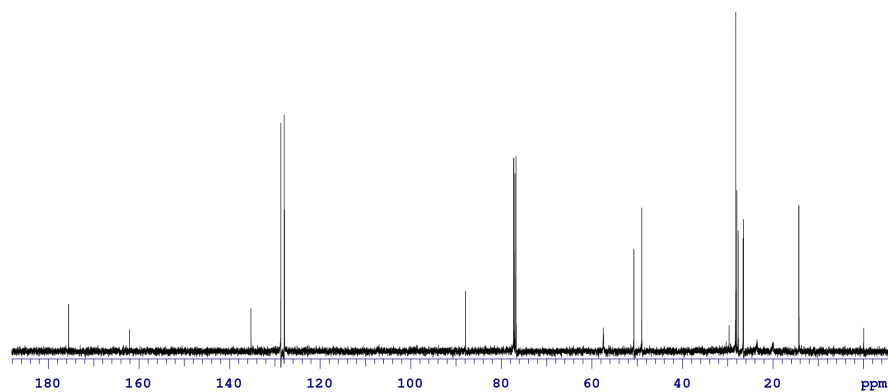
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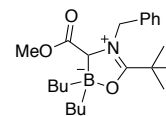
Agilent Technologies



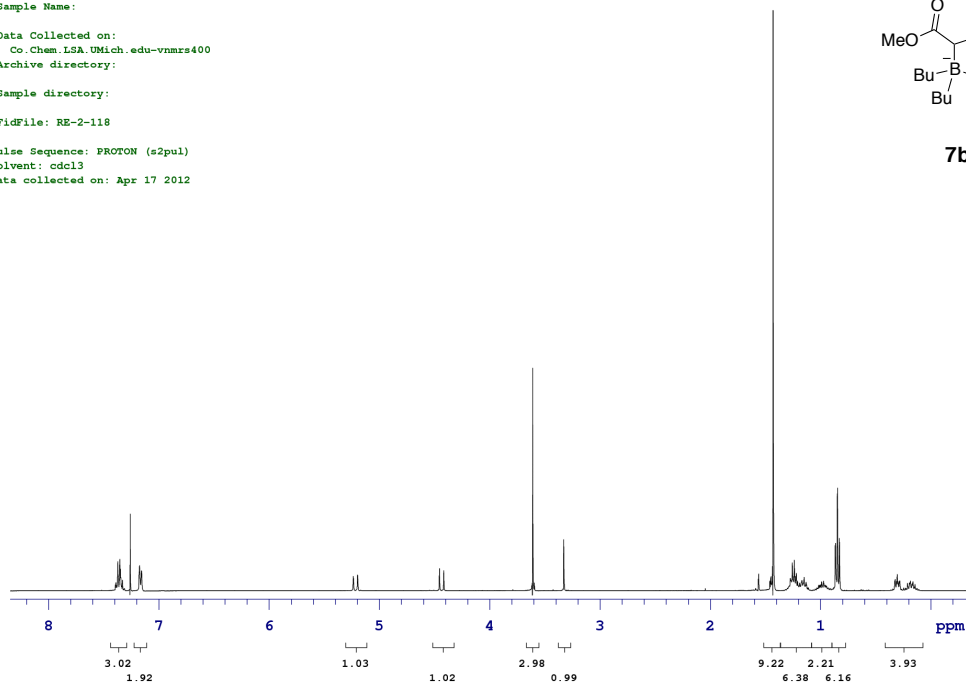
STANDARD 1H OBSERVE - profile

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 Data collected on: Apr 17 2012

Agilent Technologies



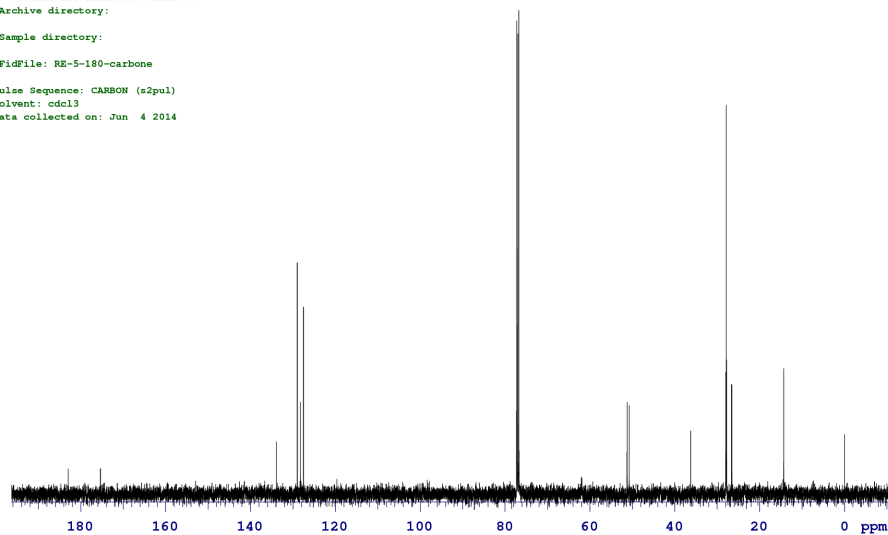
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Carbon-13

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 Solvent: cdcl3  
 Data collected on: Jun 4 2014

Agilent Technologies



Proton Spectrum

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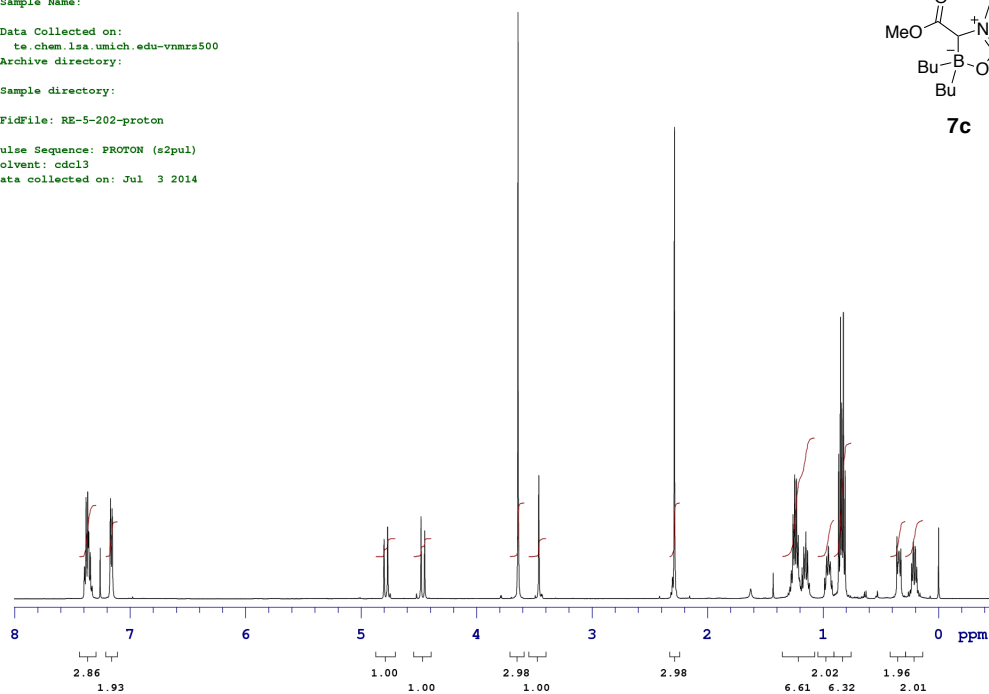
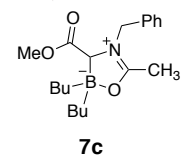
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Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 3 2014

Agilent Technologies



Carbon-13

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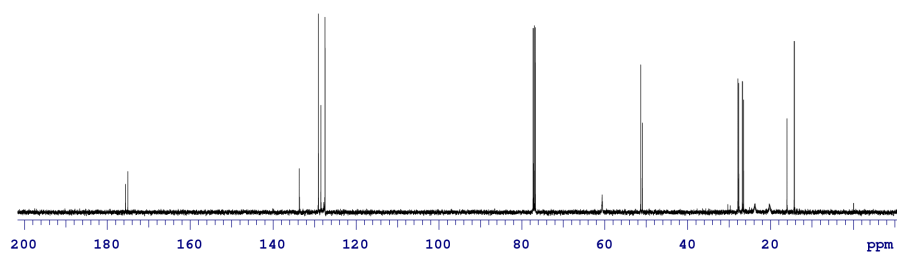
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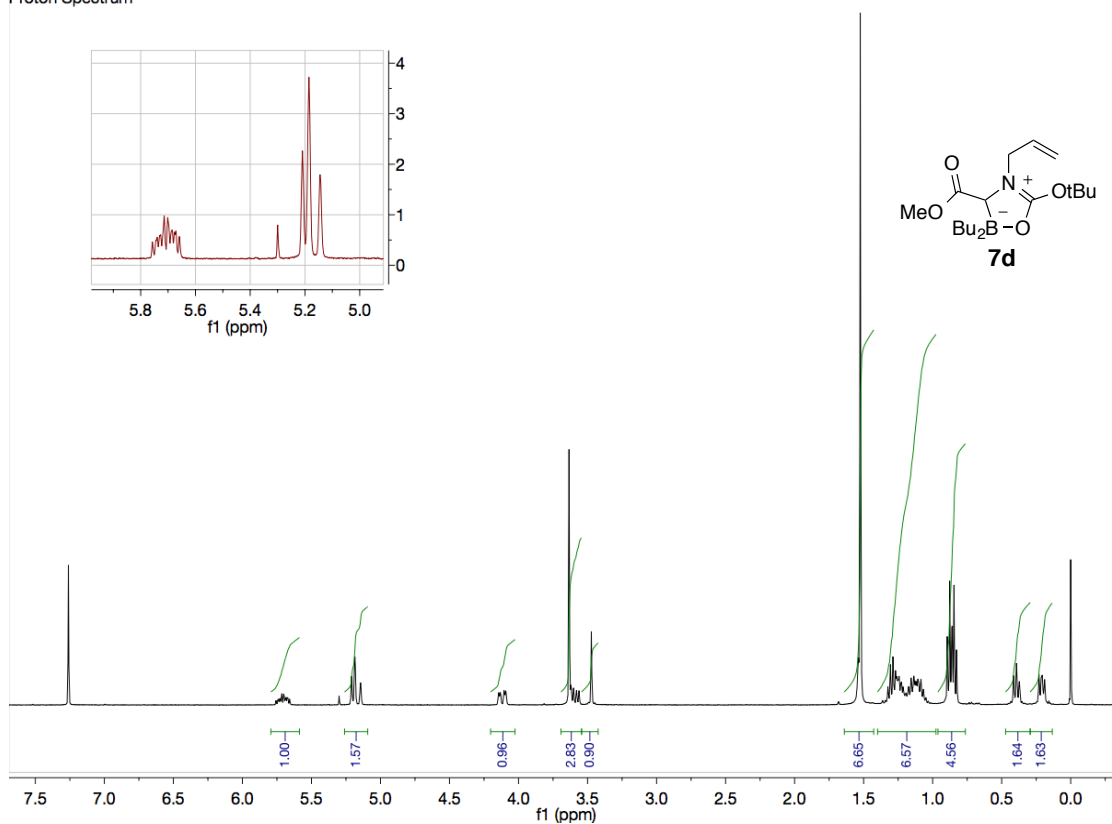
Solvent: cdcl3

Data collected on: Jul 3 2014

Agilent Technologies



RE-2-207B  
Proton Spectrum



Carbon-13

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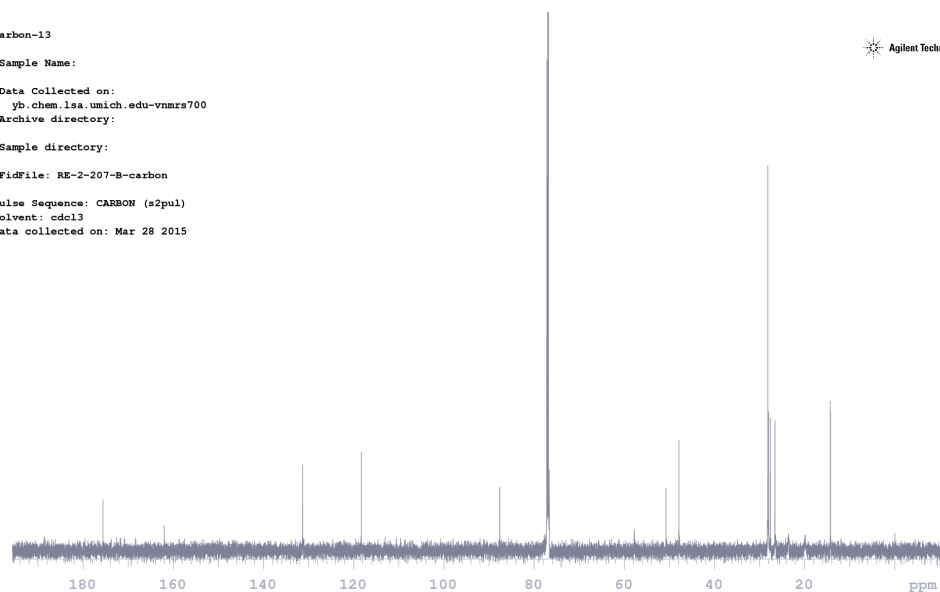
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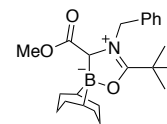
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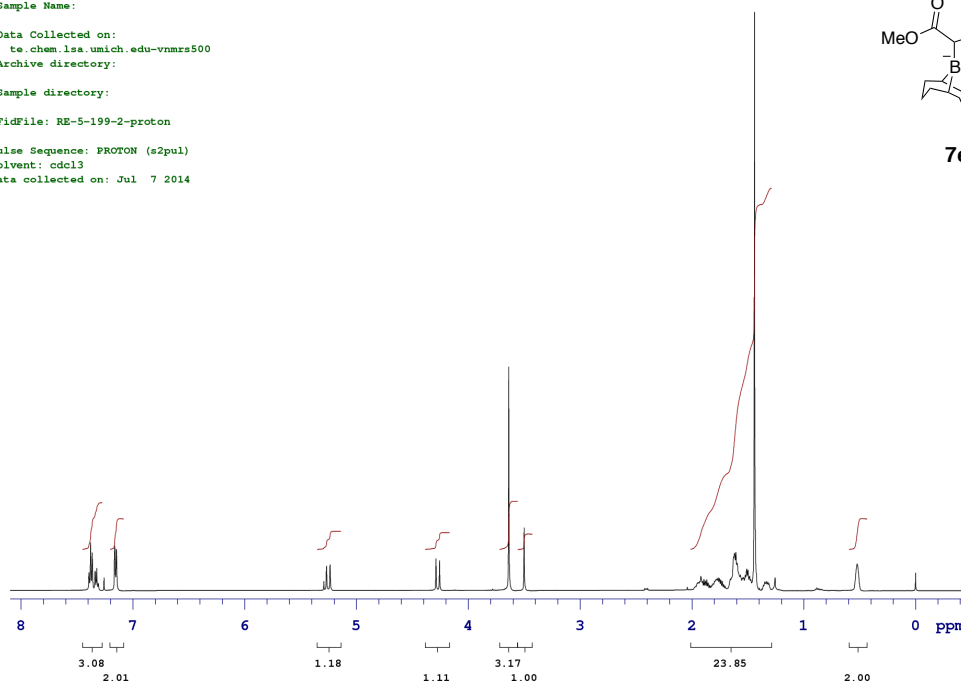
Proton Spectrum

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 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Jul 7 2014

Agilent Technologies



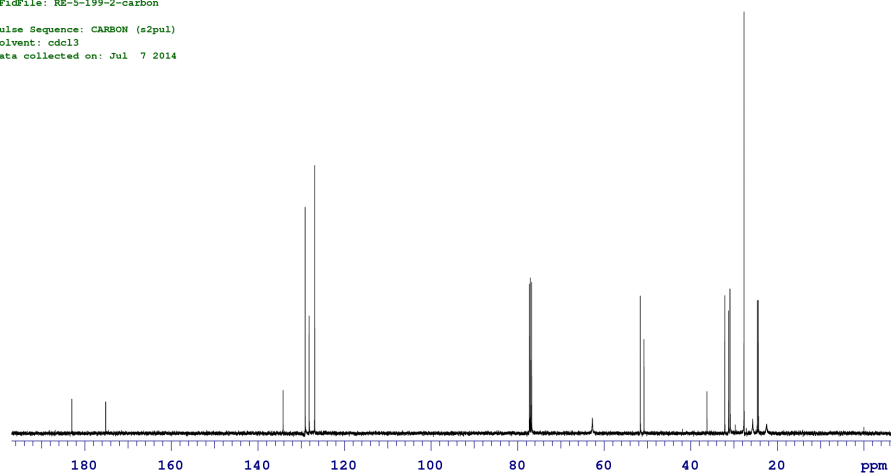
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Carbon-13

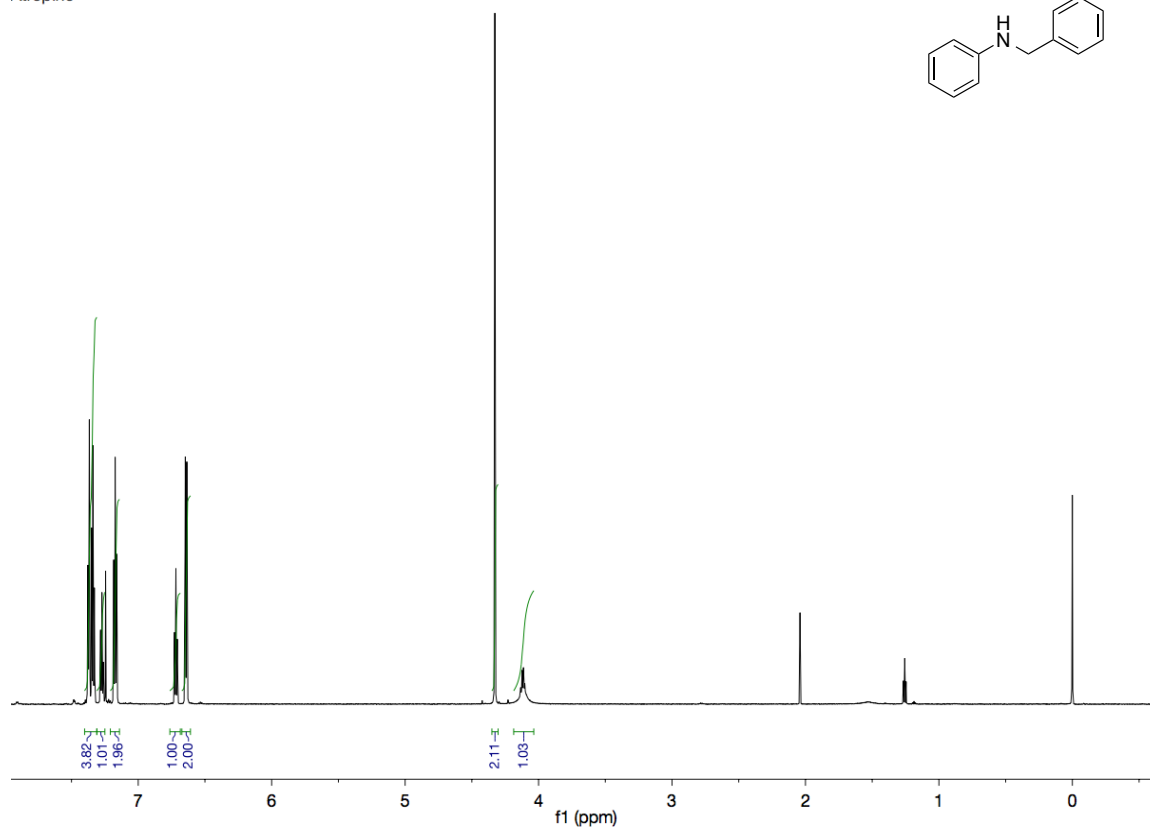
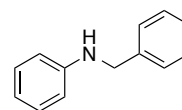
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 Data collected on: Jul 7 2014

Agilent Technologies

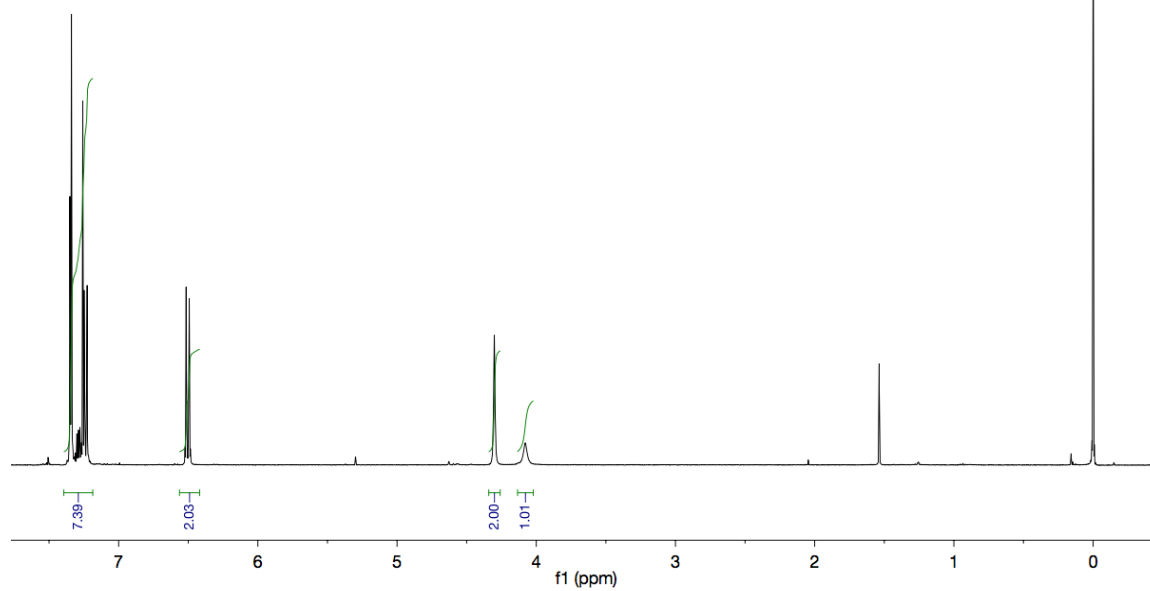
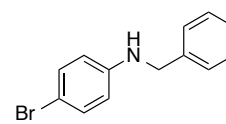




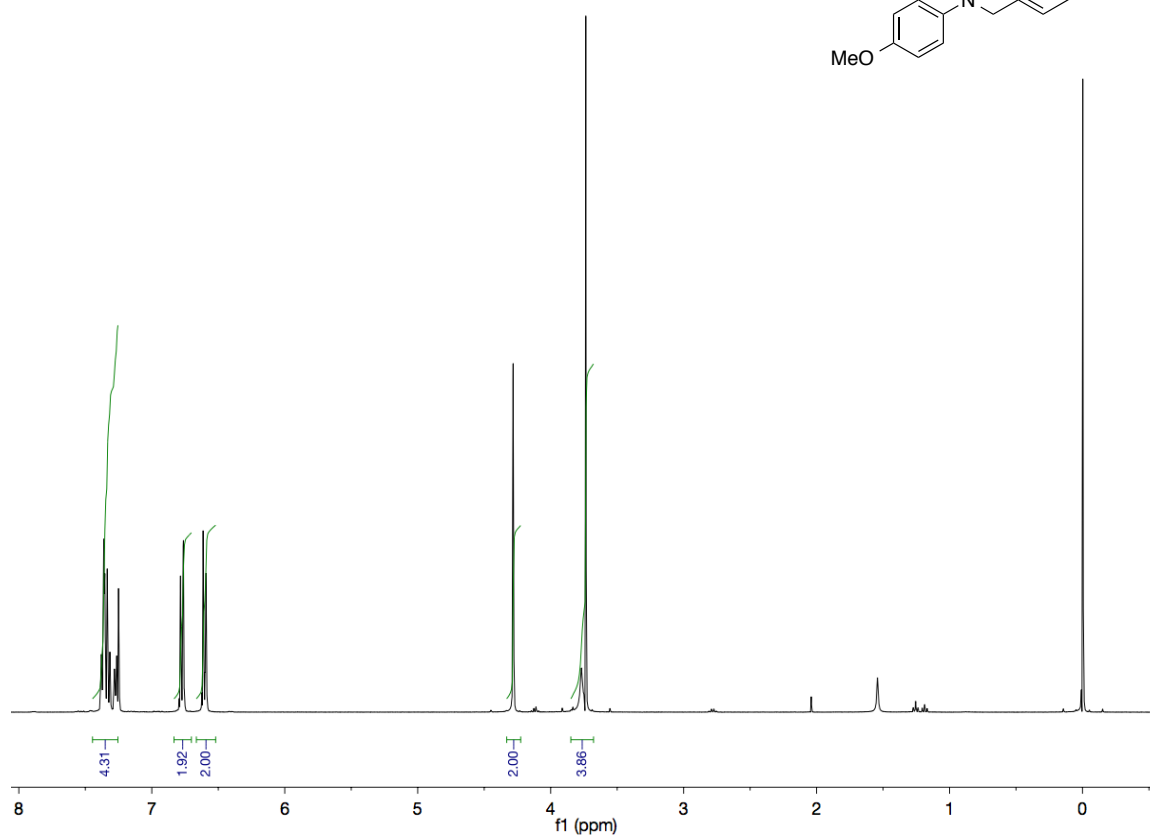
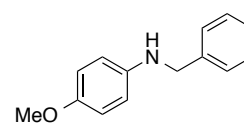
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STANDARD PROTON PARAMETERS  
Atropine



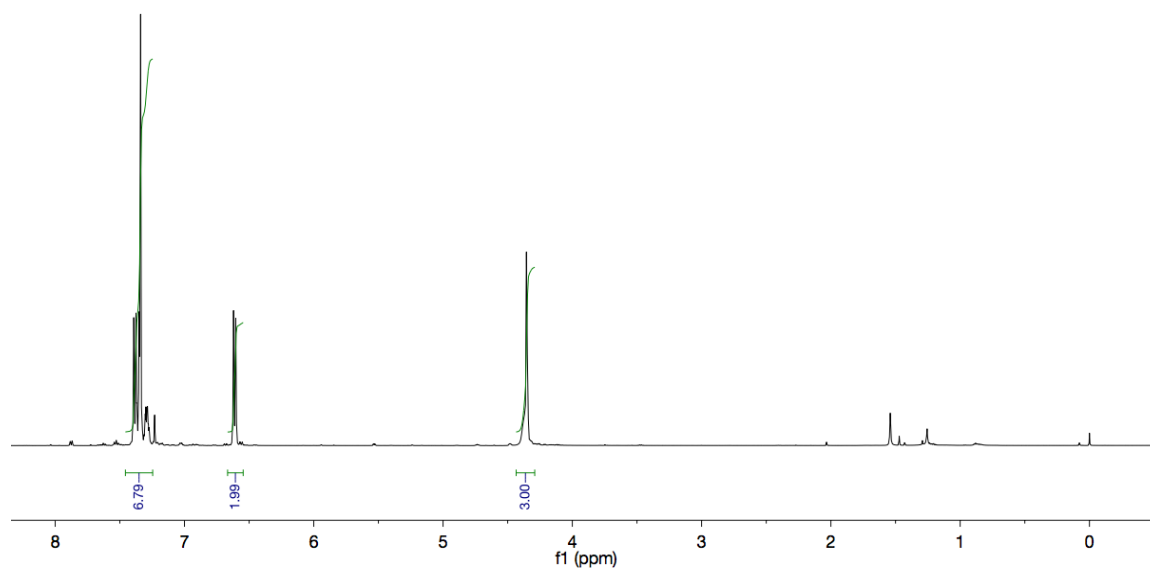
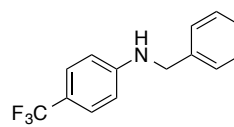
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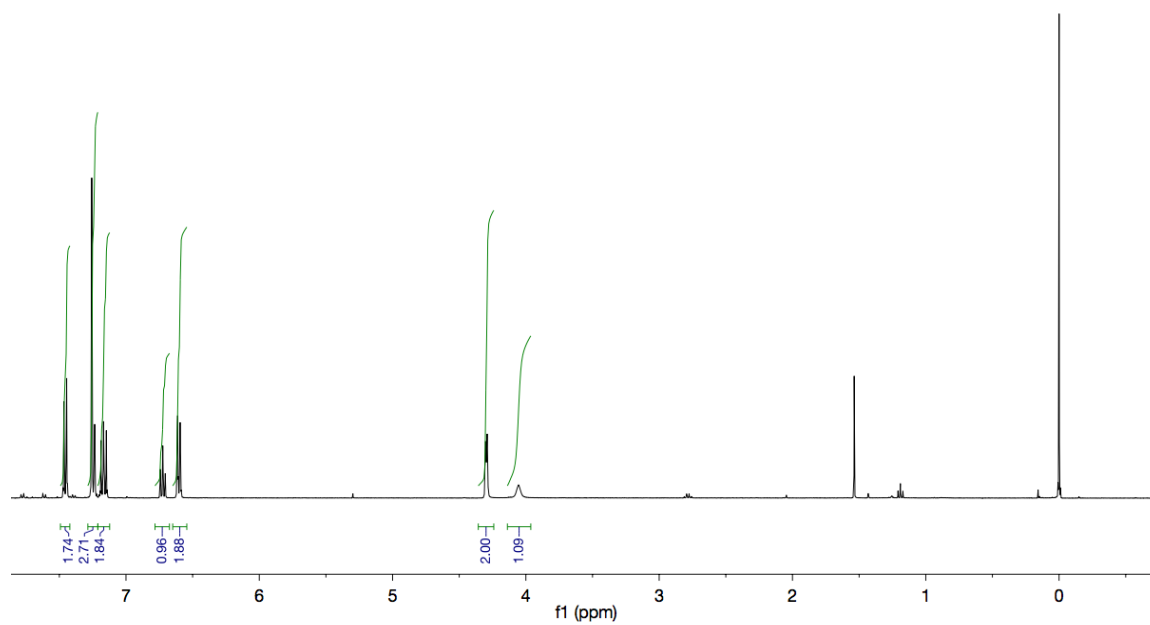
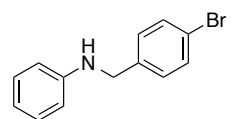
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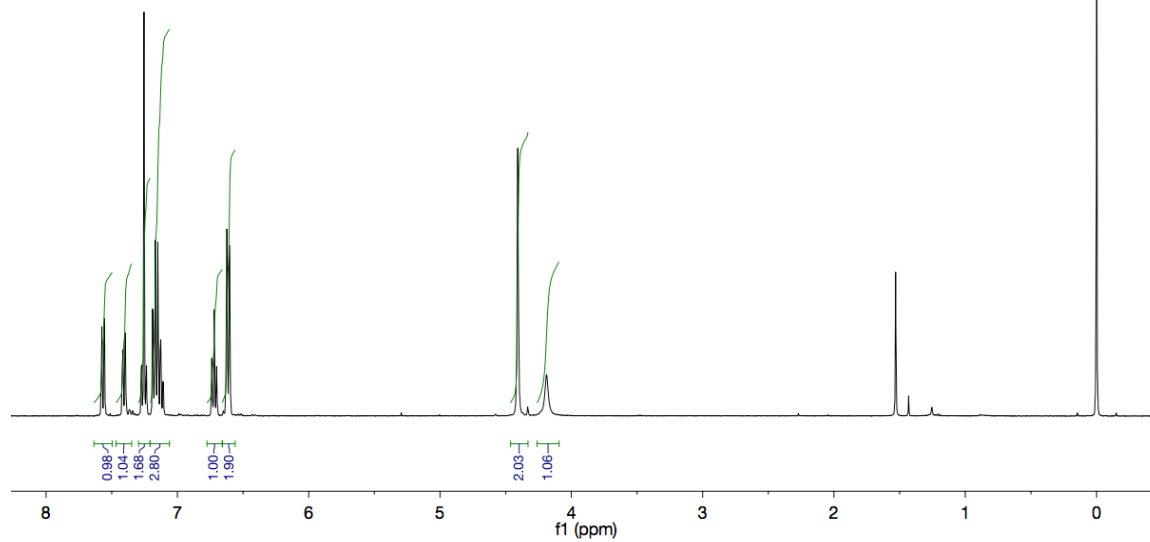
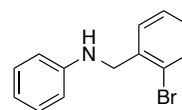
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Proton Spectrum



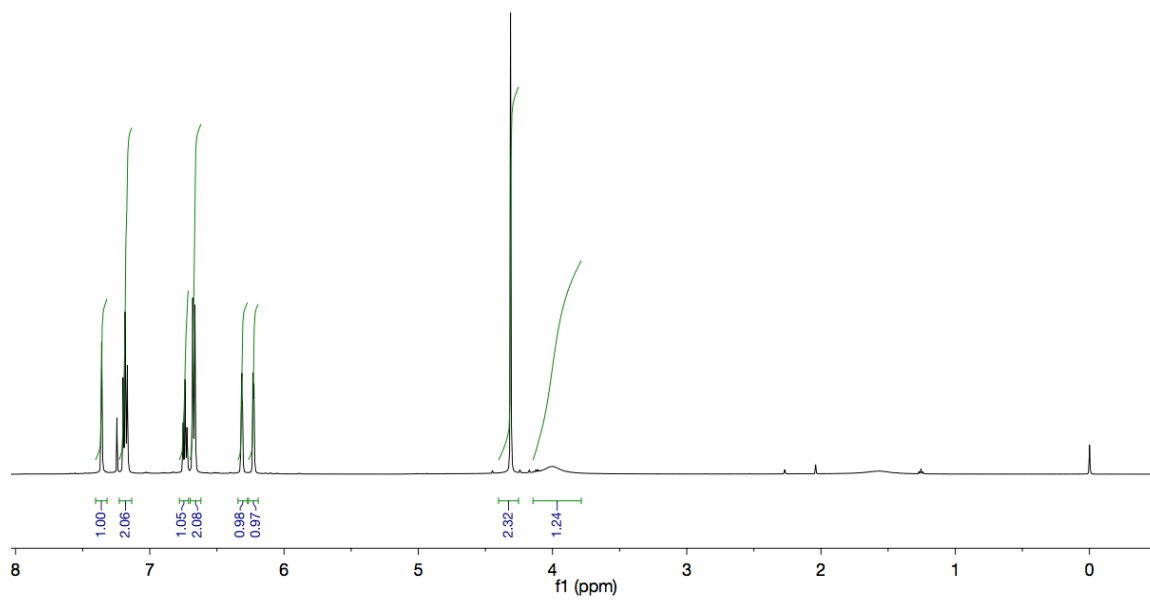
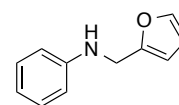
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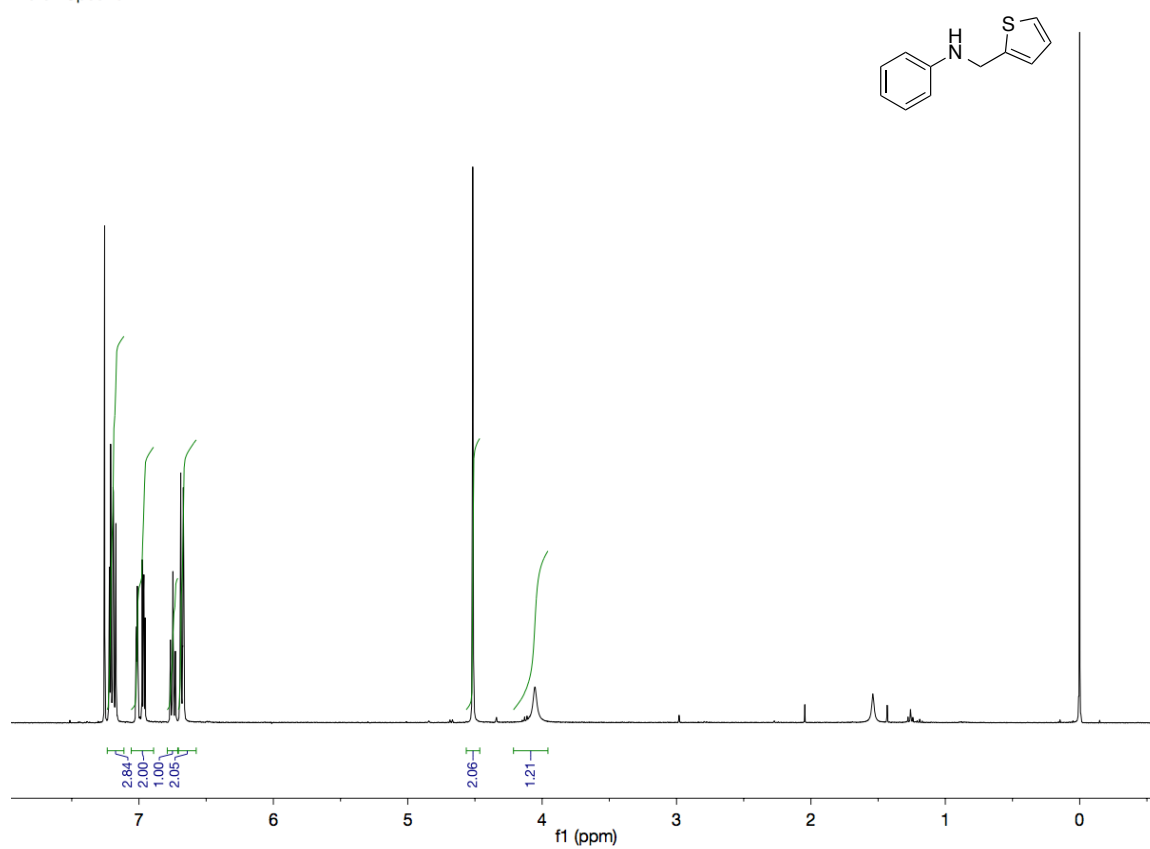
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Proton Spectrum



RE-5-114-1-1H-JRB-1  
Proton Spectrum

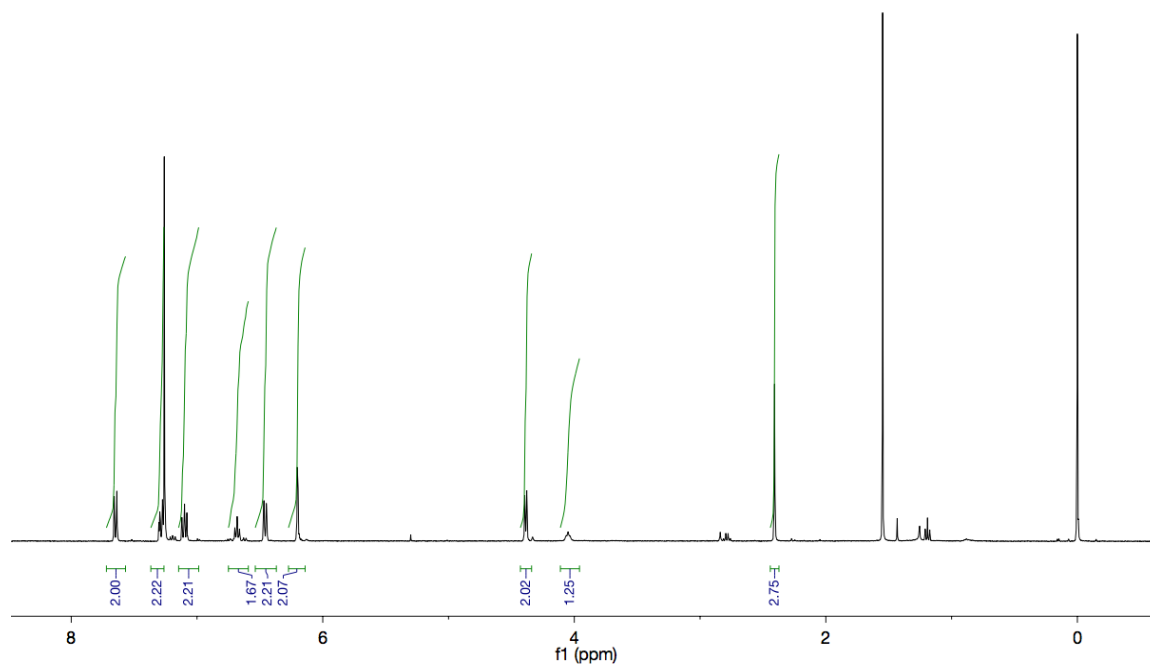
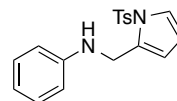


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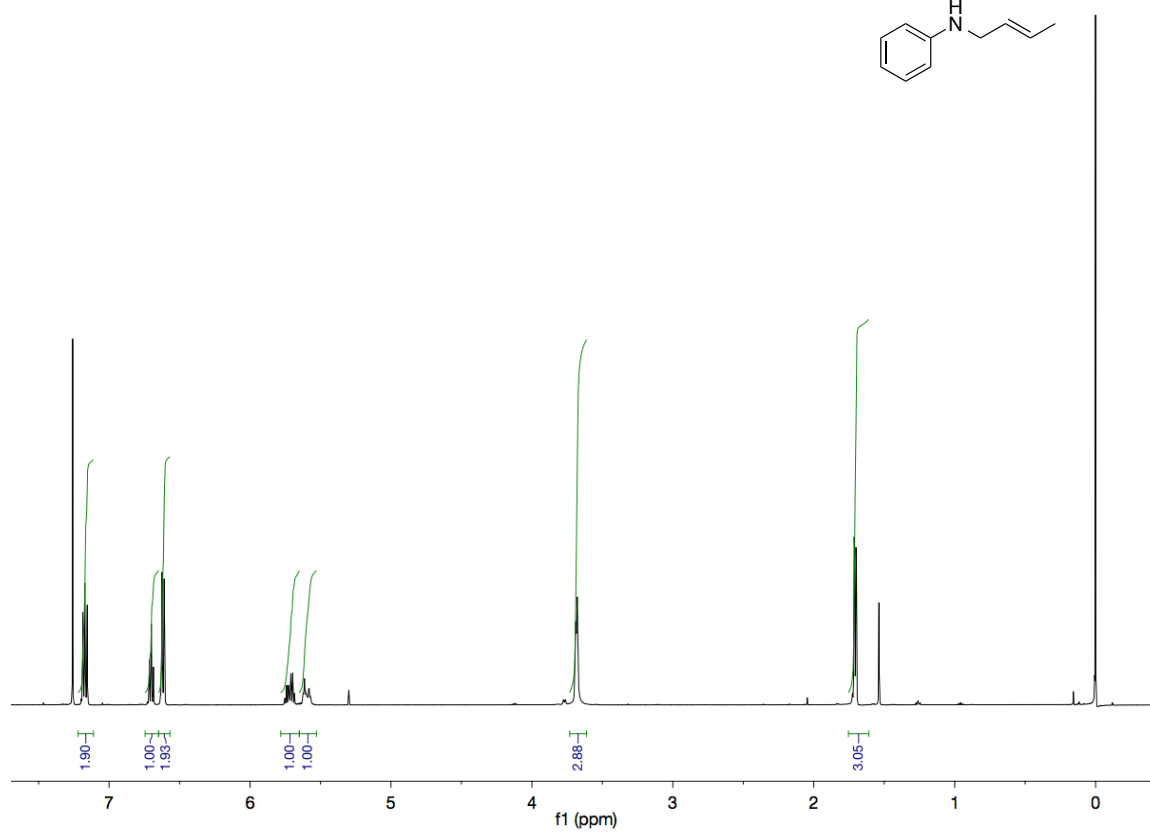
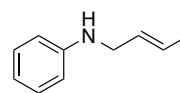




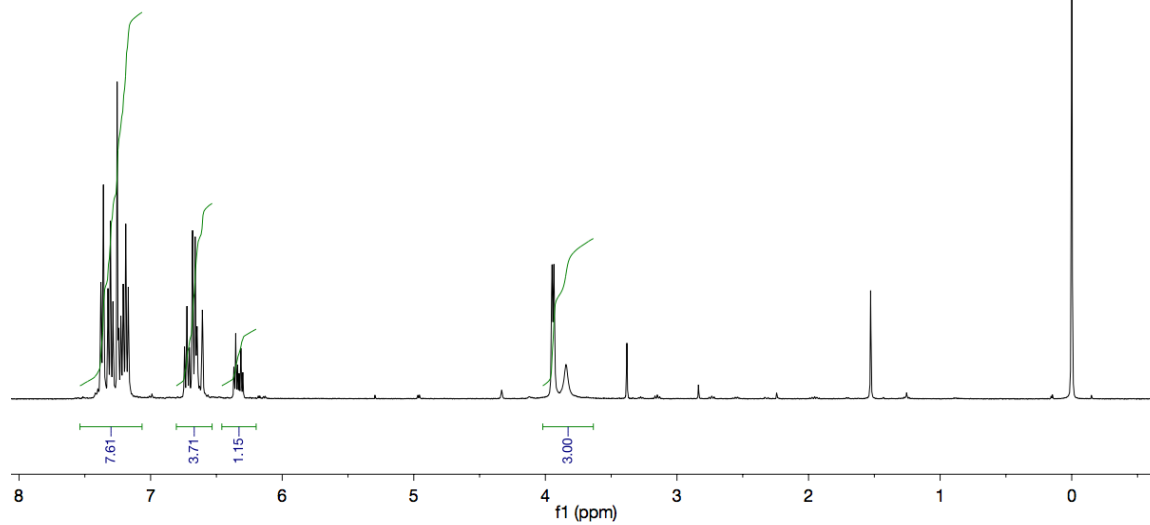
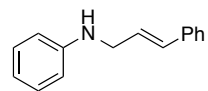
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Proton Spectrum



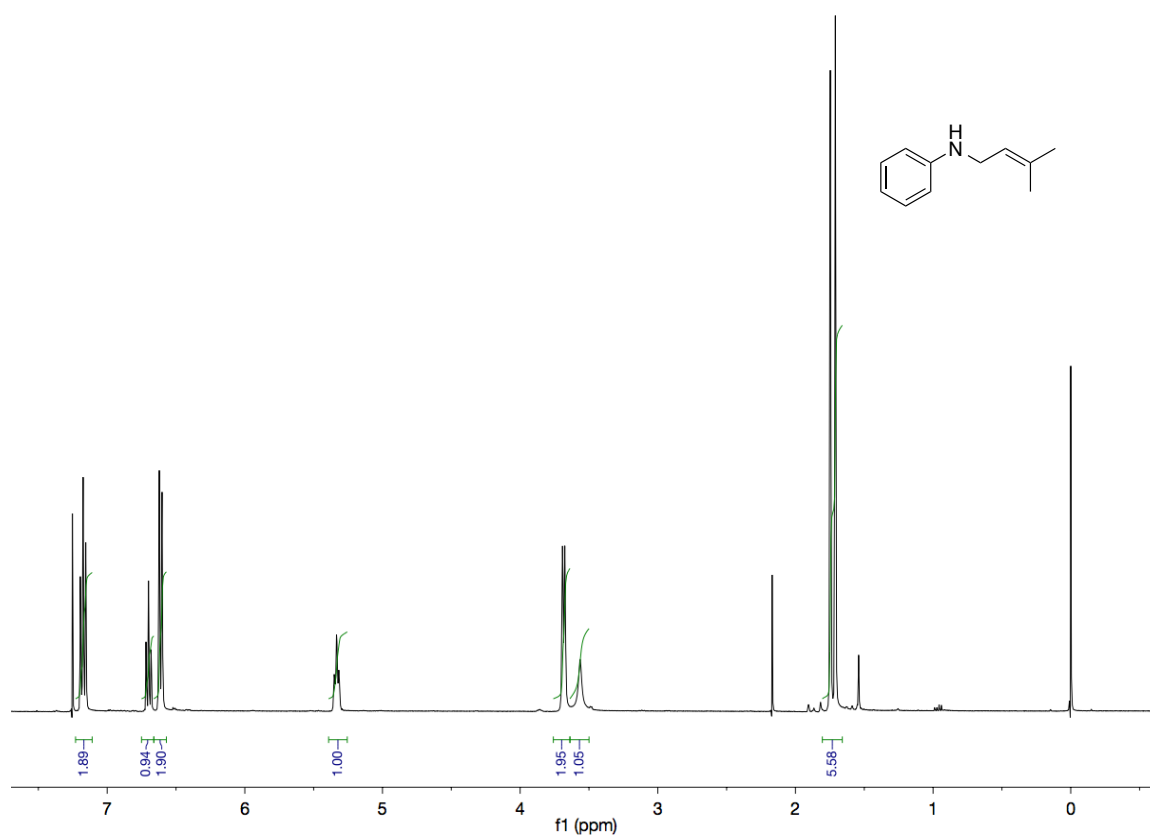
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Automated Probe tuning parameter



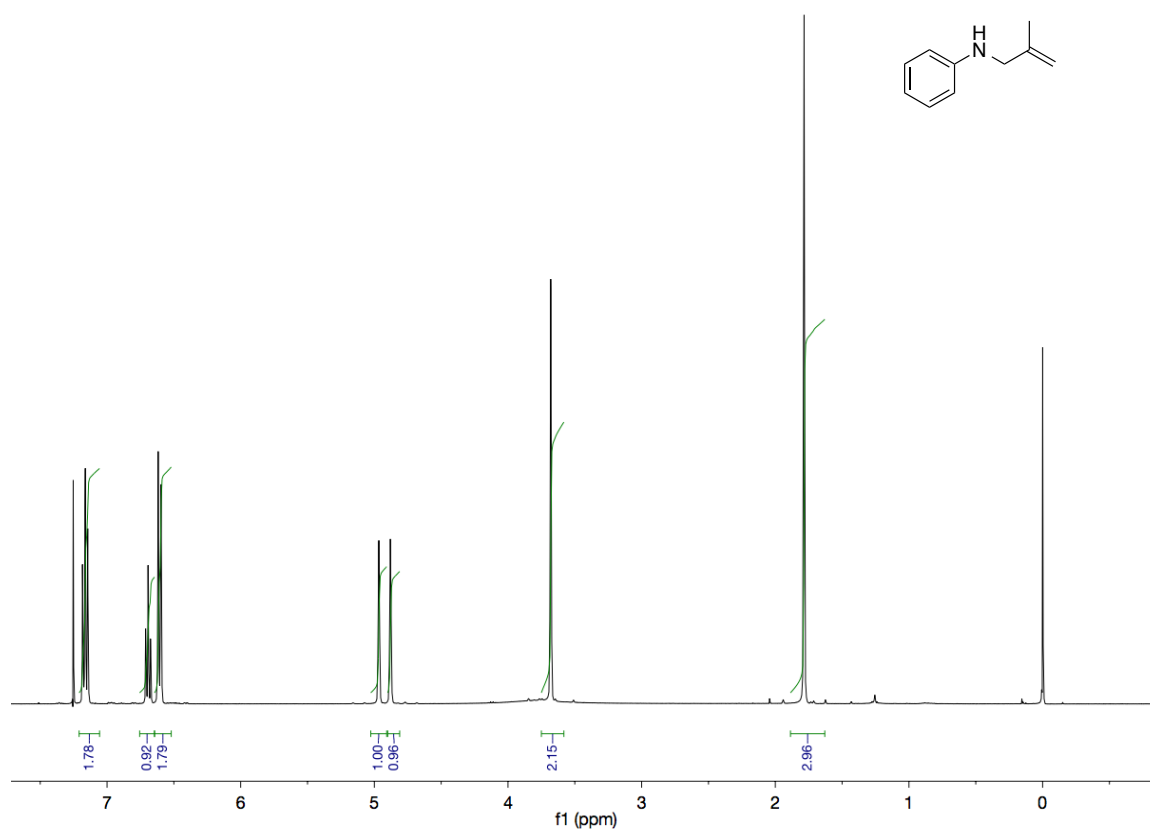
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Proton Spectrum



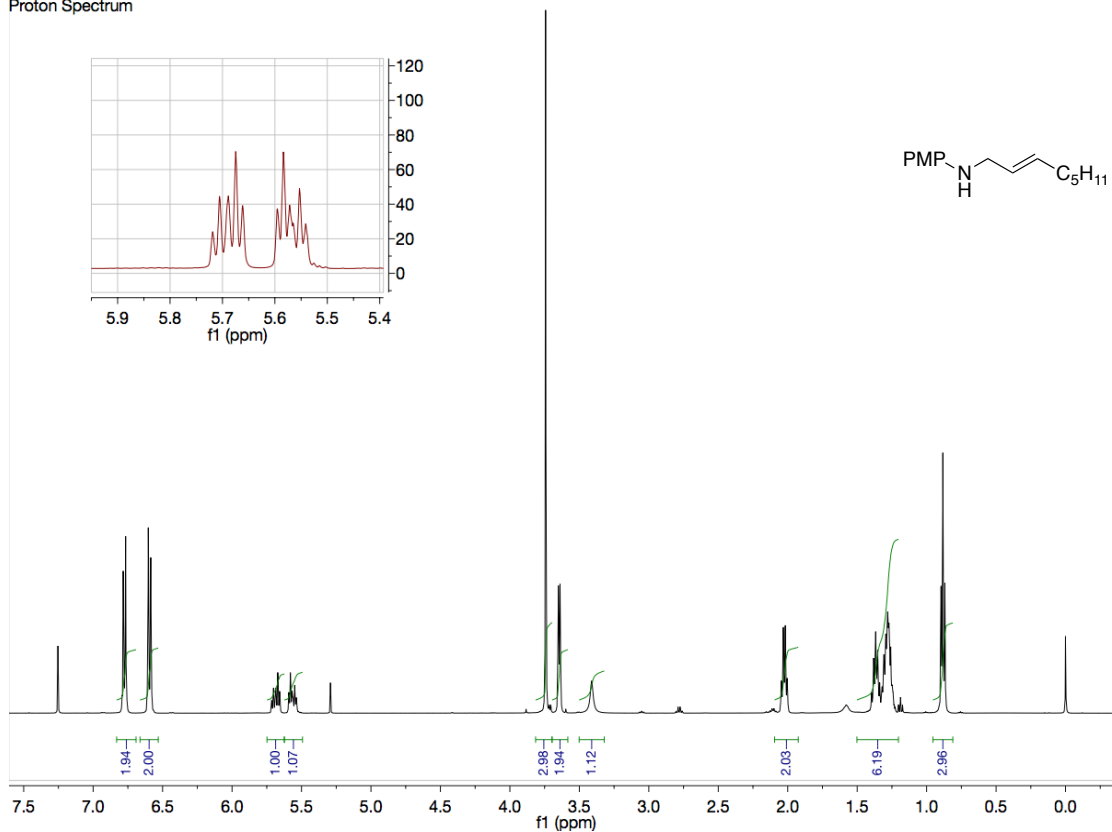
RE-6-053-proton  
Proton Spectrum



RE-5-113-1  
Gradient Shimming



RE-6-012-proton  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

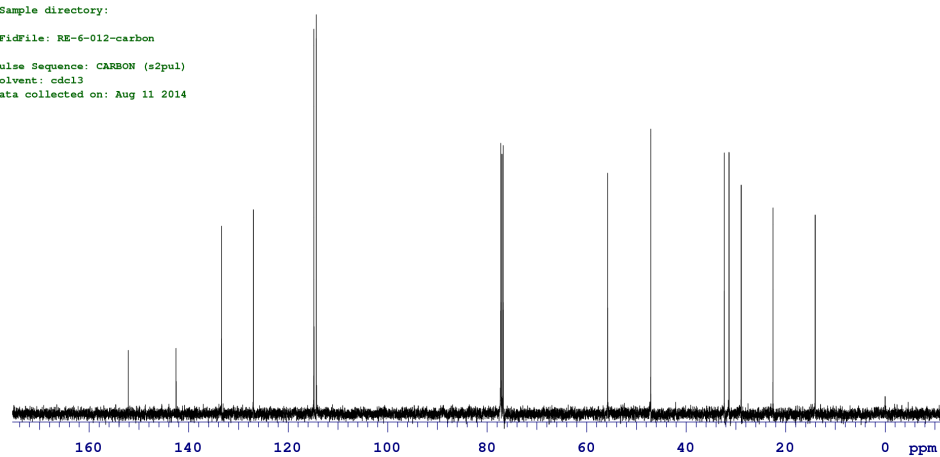
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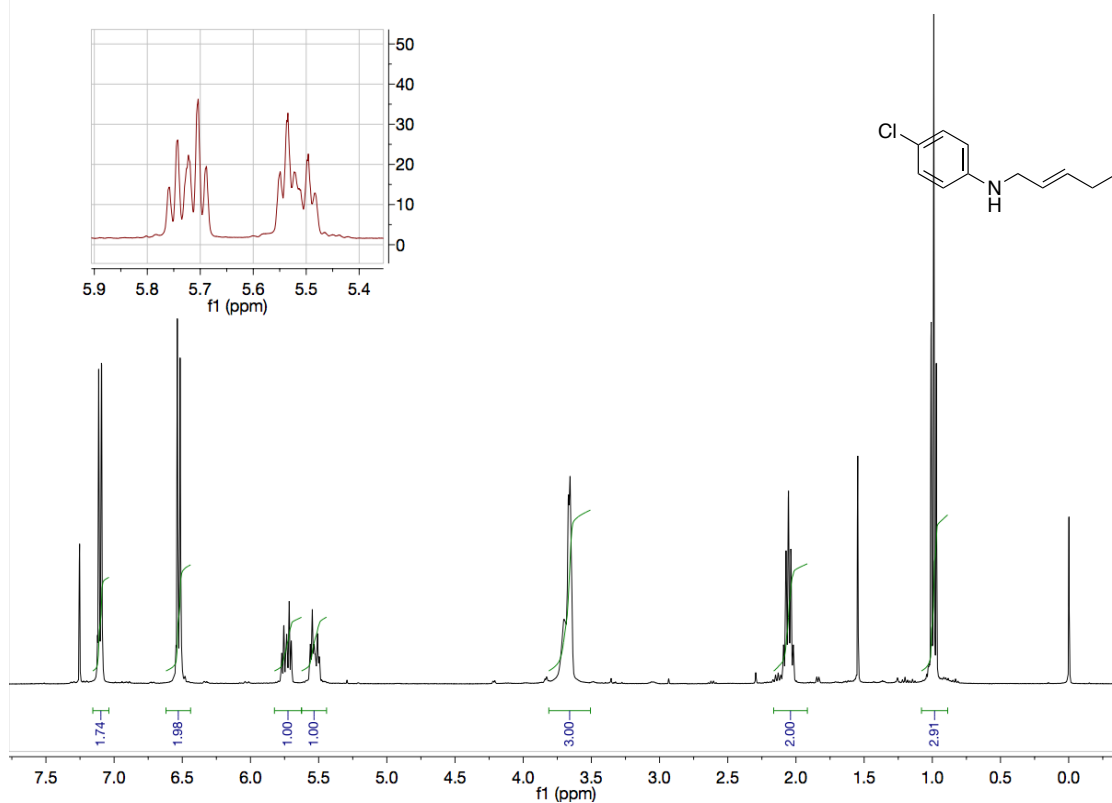
Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 11 2014



RE-6-016  
Proton Spectrum



Carbon-13

Sample Name:

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te.chem.lsa.umich.edu-vnmrs500

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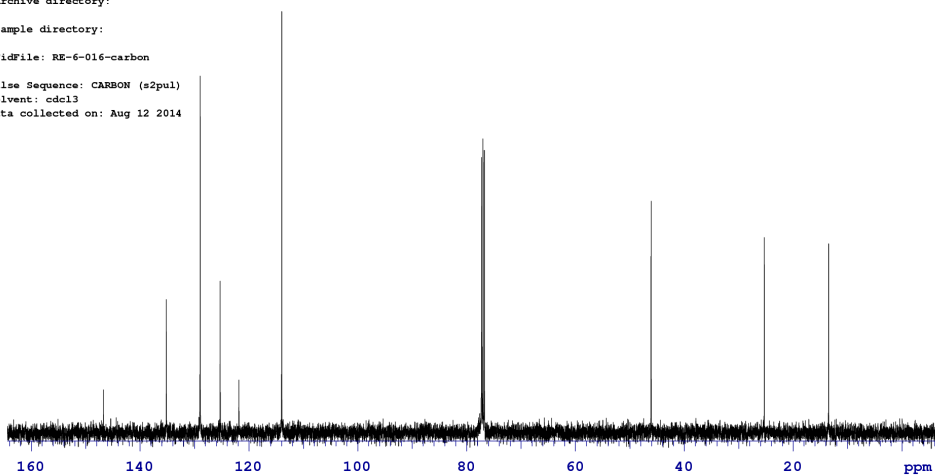
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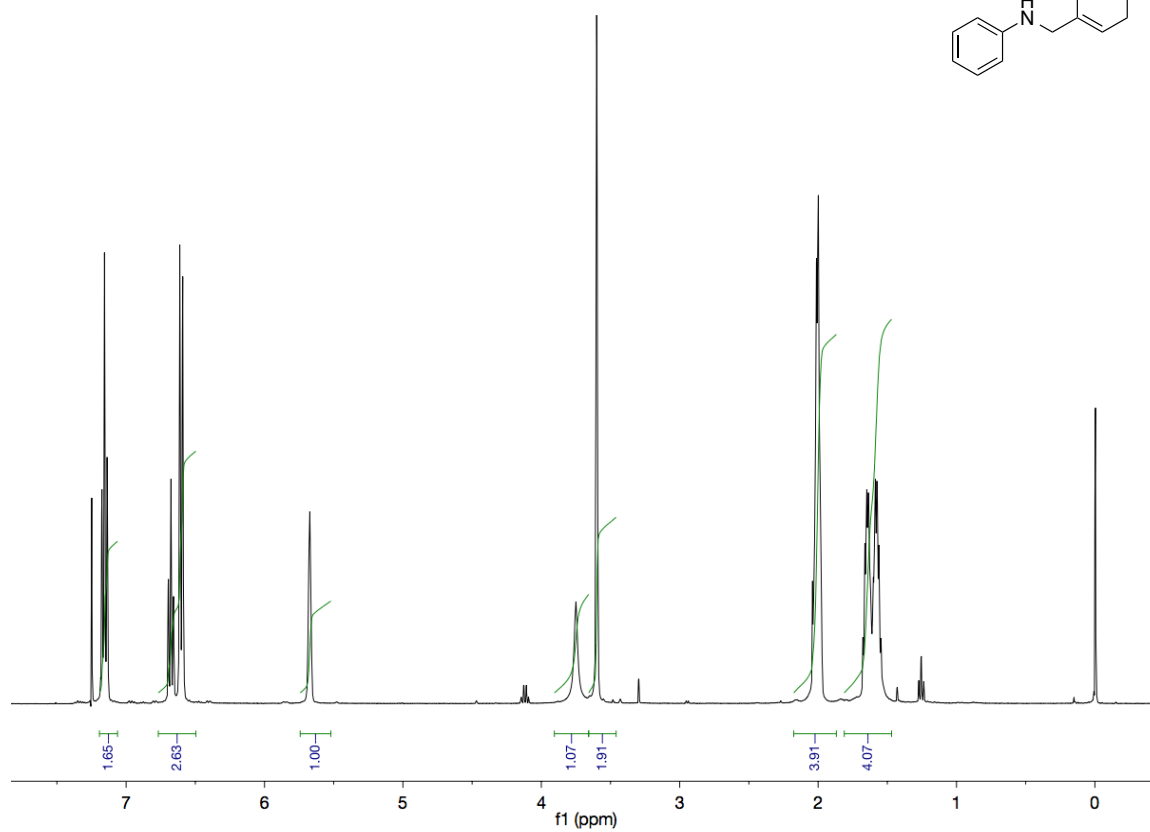
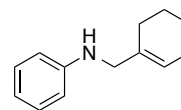
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Solvent: cdcl3

Data collected on: Aug 12 2014



RE-5-118  
Gradient Shimming

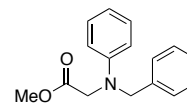




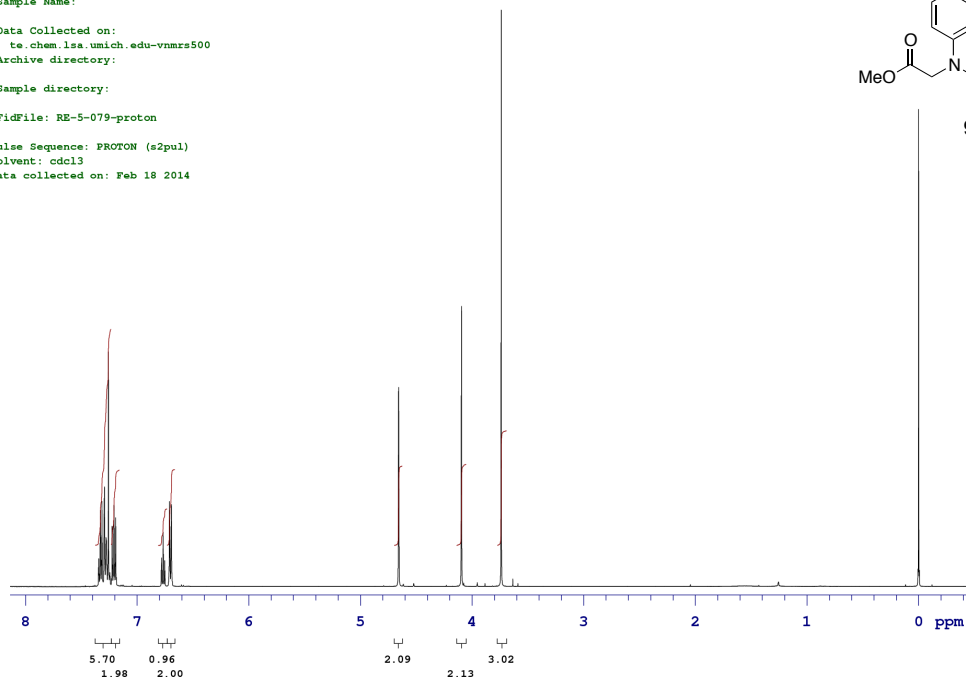
Automated Probe tuning parameter

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Archive directory:  
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Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

Agilent Technologies



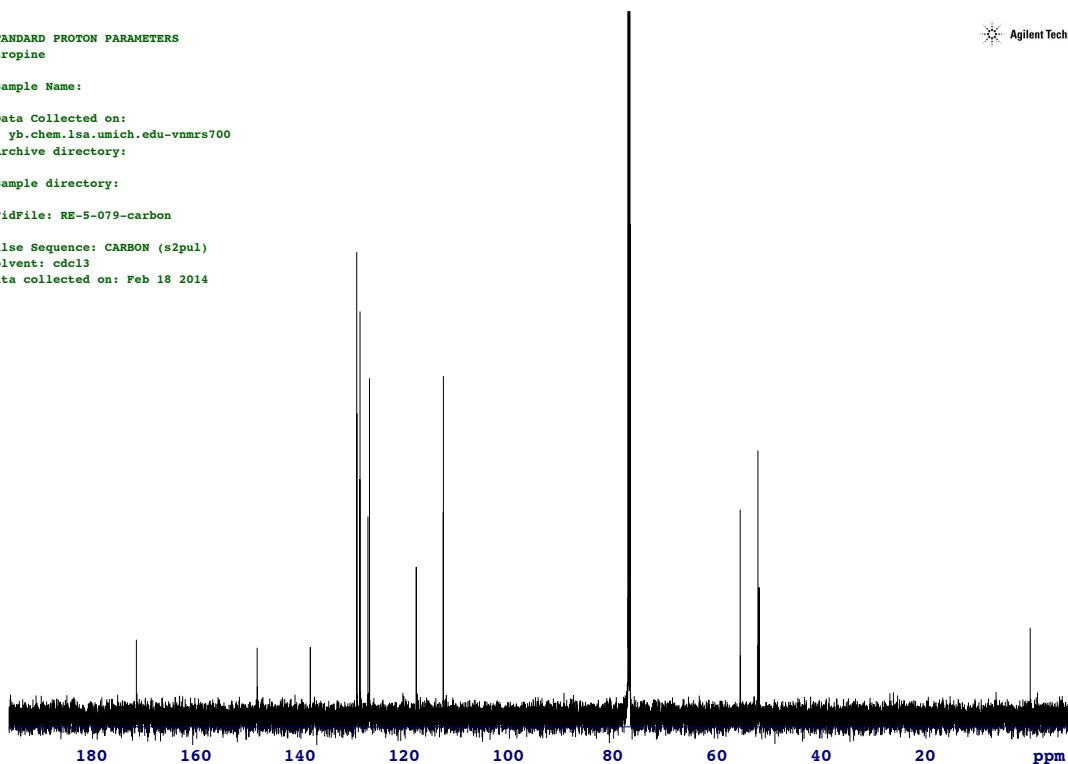
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STANDARD PROTON PARAMETERS  
Atropine

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Archive directory:  
Sample directory:  
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Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

Agilent Technologies



Automated Probe tuning parameter

Sample Name:

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Archive directory:

Sample directory:

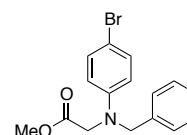
FidFile: RE-5-045-2-proton

Pulse Sequence: PROTON (s2pul)

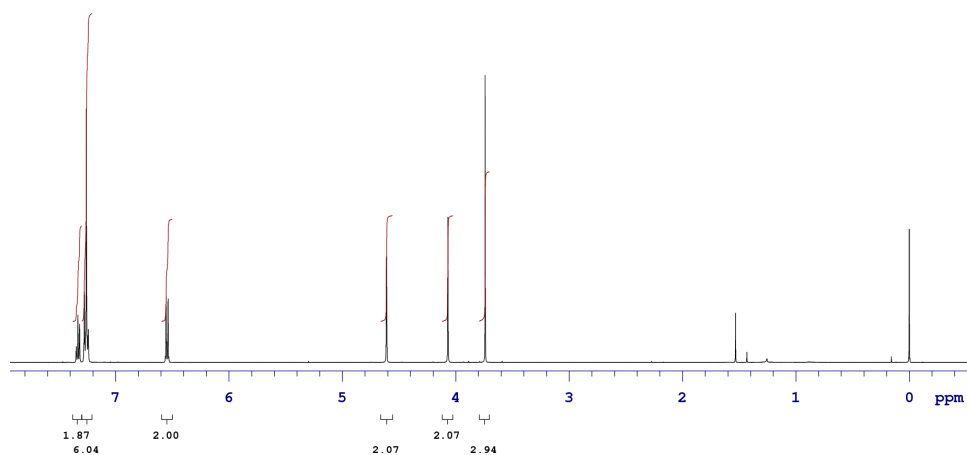
Solvent: cdcl3

Data collected on: Feb 13 2014

Agilent Technologies



9b



STANDARD PROTON PARAMETERS

Atropine

Sample Name:

Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

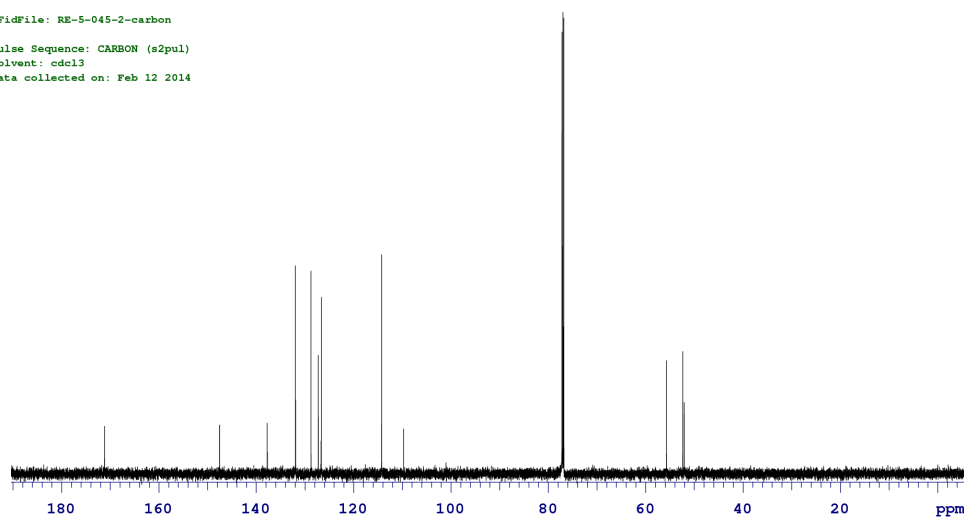
FidFile: RE-5-045-2-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 12 2014

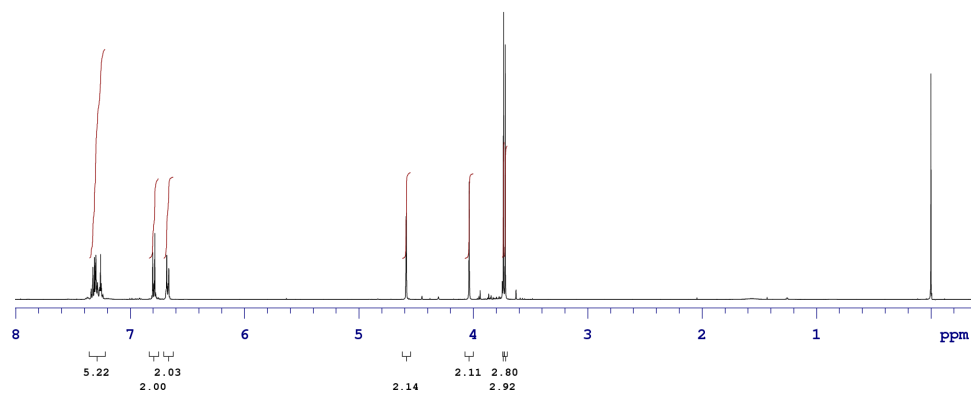
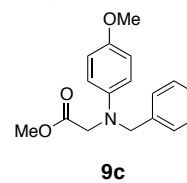
Agilent Technologies



Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-045-1-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

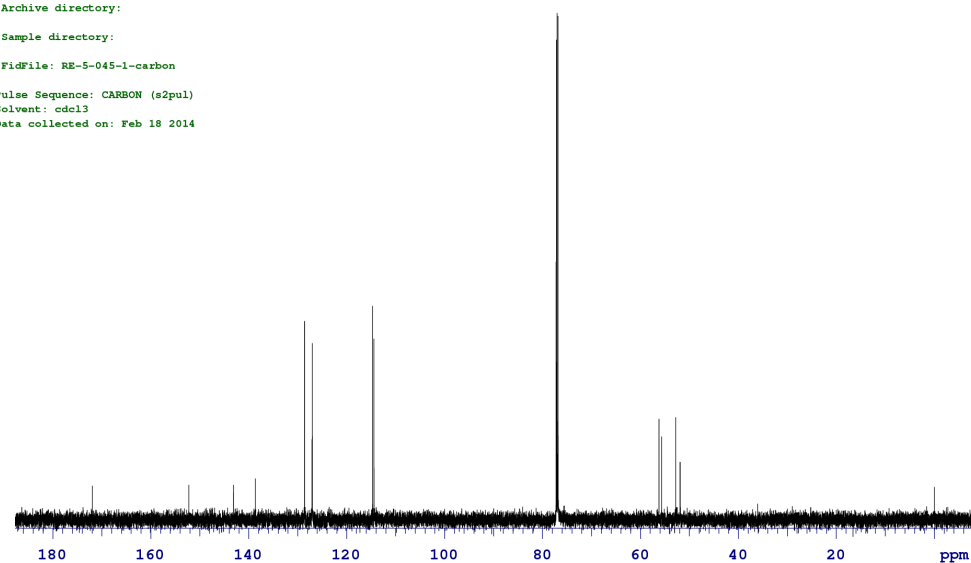
Agilent Technologies



STANDARD PROTON PARAMETERS  
Atropine

Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-045-1-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

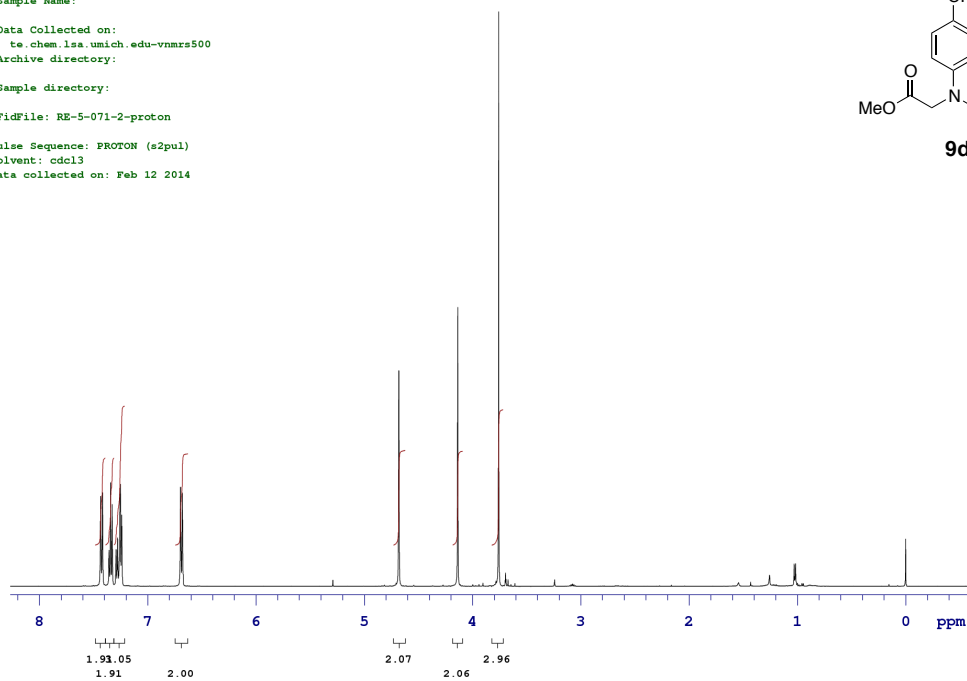
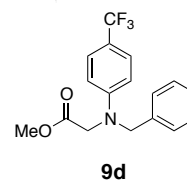
Agilent Technologies



Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-071-2-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 12 2014

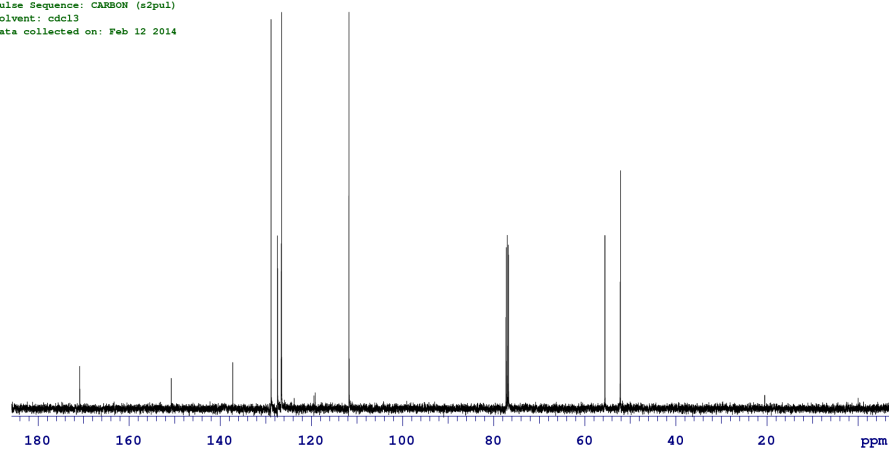
Agilent Technologies



Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-071-2-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 12 2014

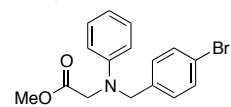
Agilent Technologies



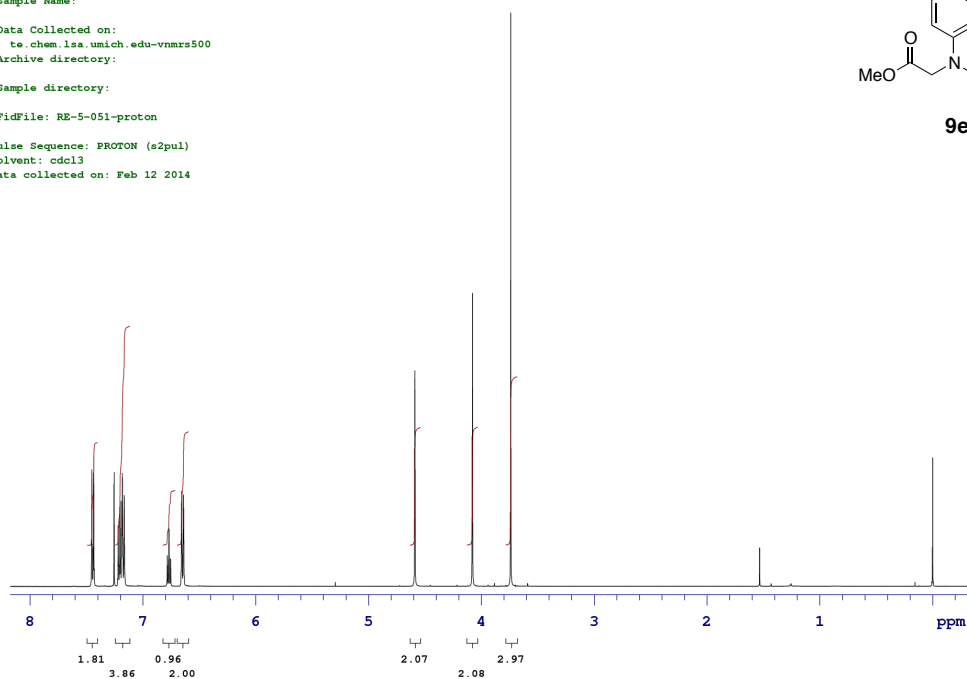
Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-051-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 12 2014

Agilent Technologies



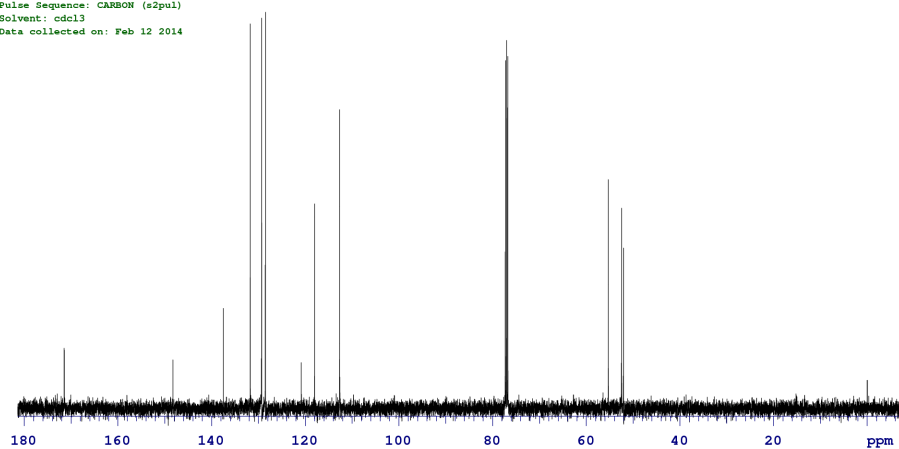
9e



Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-051-carbone  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 12 2014

Agilent Technologies



Automated Probe tuning parameter

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

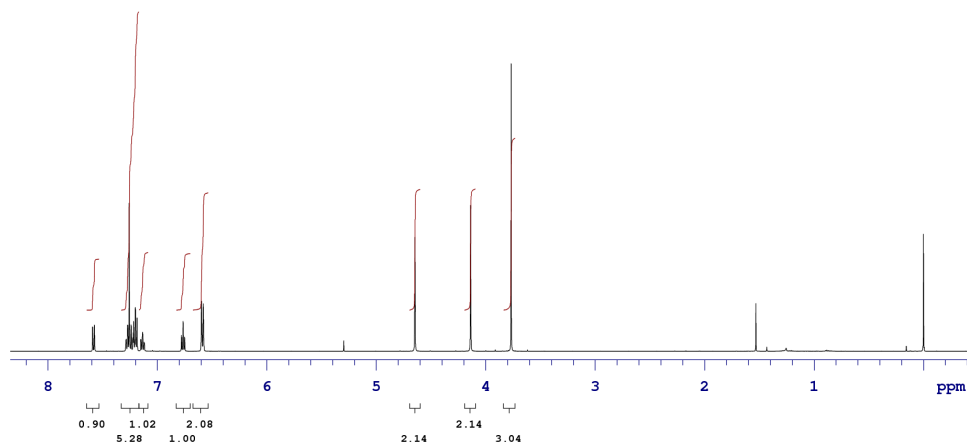
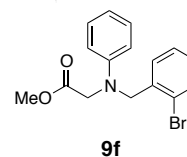
FidFile: RE-5-058-proton

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 13 2014

Agilent Technologies



Automated Probe tuning parameter

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

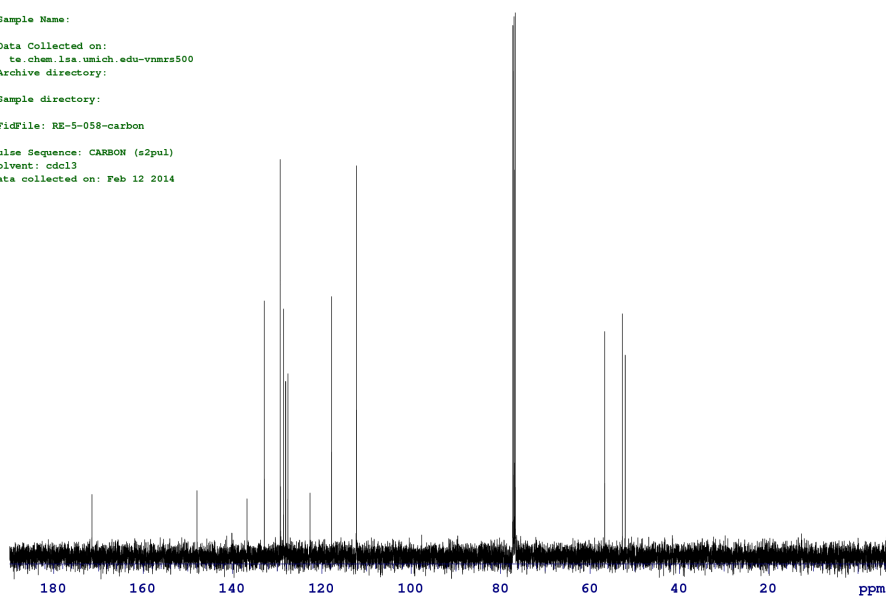
FidFile: RE-5-058-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 12 2014

Agilent Technologies



STANDARD 1H OBSERVE - profile

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

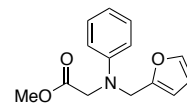
FidFile: RE-5-114-2-proton

Pulse Sequence: PROTON (s2pul)

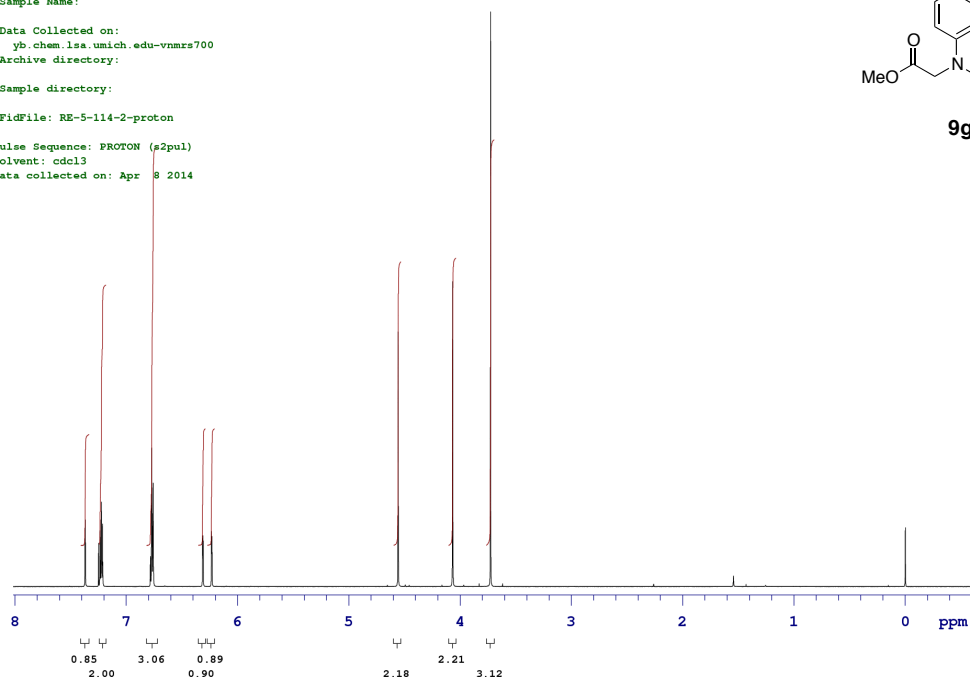
Solvent: cdcl3

Data collected on: Apr 8 2014

Agilent Technologies



9g



STANDARD 1H OBSERVE - profile

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

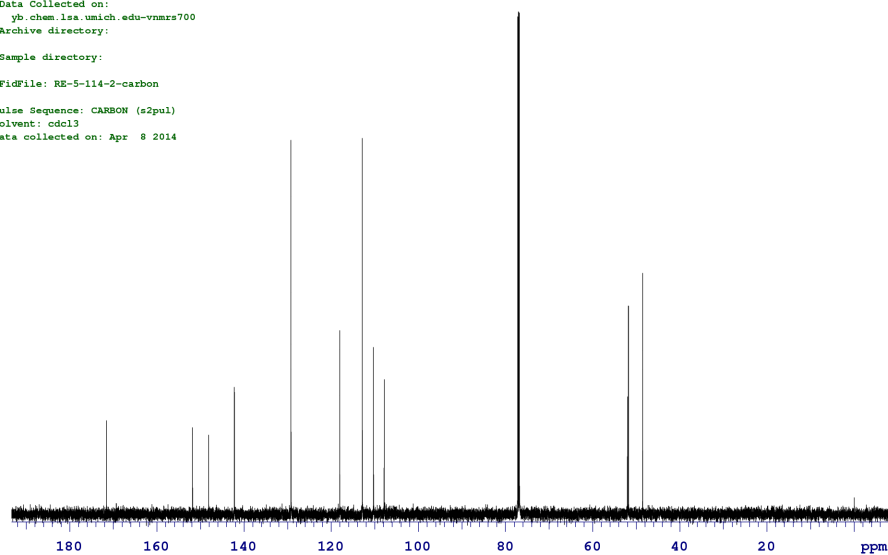
FidFile: RE-5-114-2-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Apr 8 2014

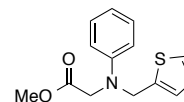
Agilent Technologies



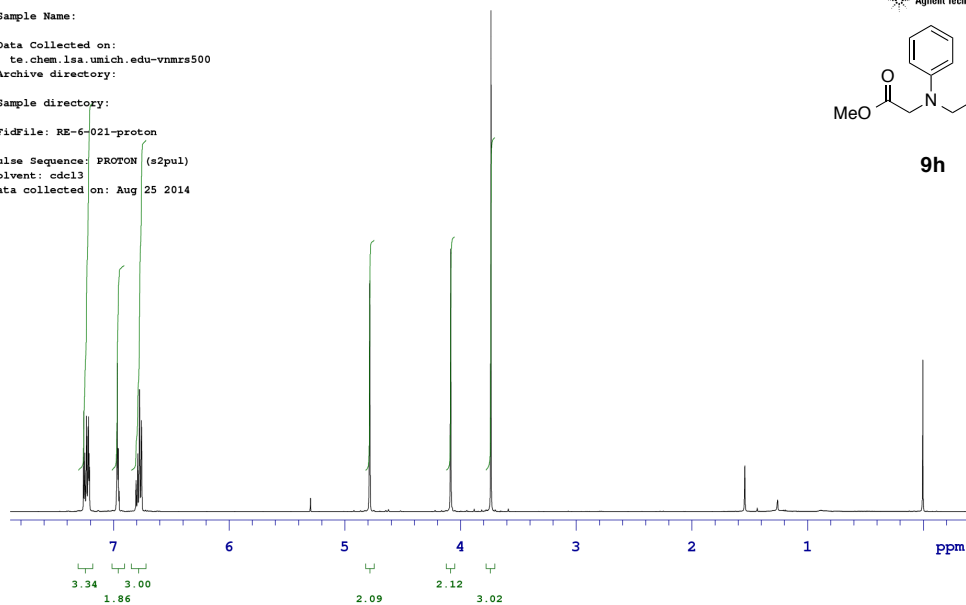
Proton Spectrum

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-6-021-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Aug 25 2014

Agilent Technologies



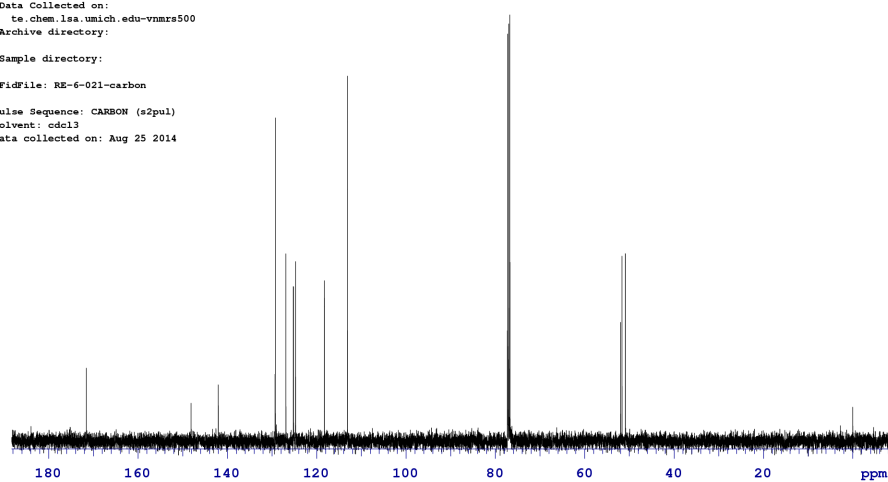
9h



Carbon-13

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-6-021-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Aug 25 2014

Agilent Technologies





Proton Spectrum

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

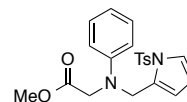
FidFile: RE-6-045-proton

Pulse Sequence: PROTON (s2pul)

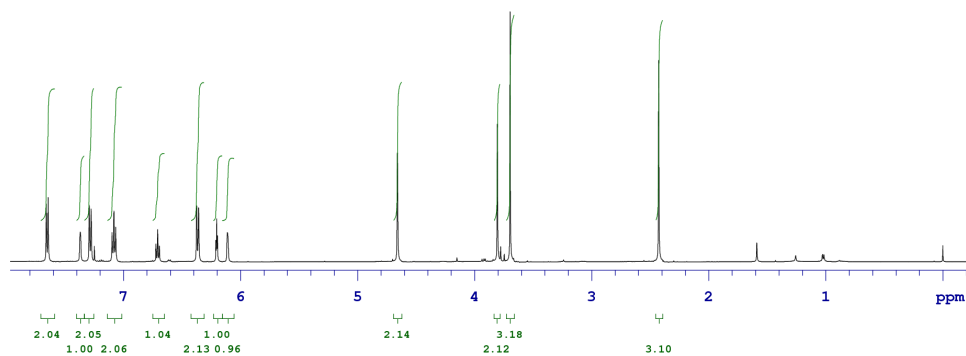
Solvent: cdcl3

Data collected on: Sep 9 2014

Agilent Technologies



9i



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

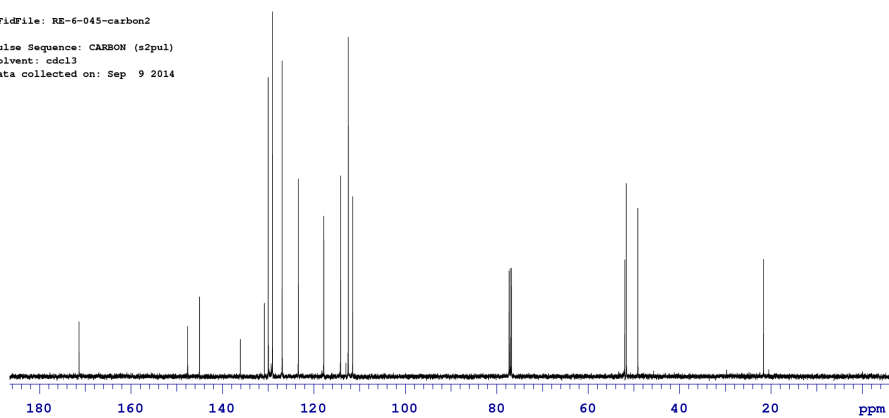
FidFile: RE-6-045-carbon2

Pulse Sequence: CARBON (s2pul)

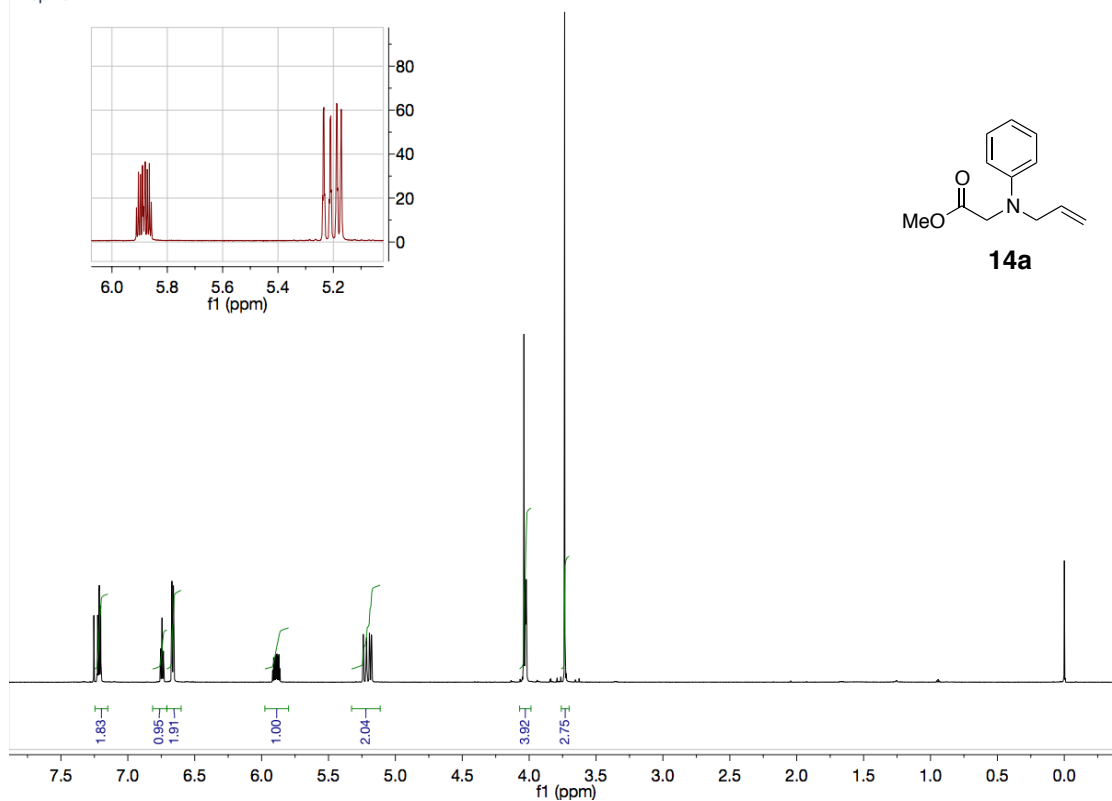
Solvent: cdcl3

Data collected on: Sep 9 2014

Agilent Technologies



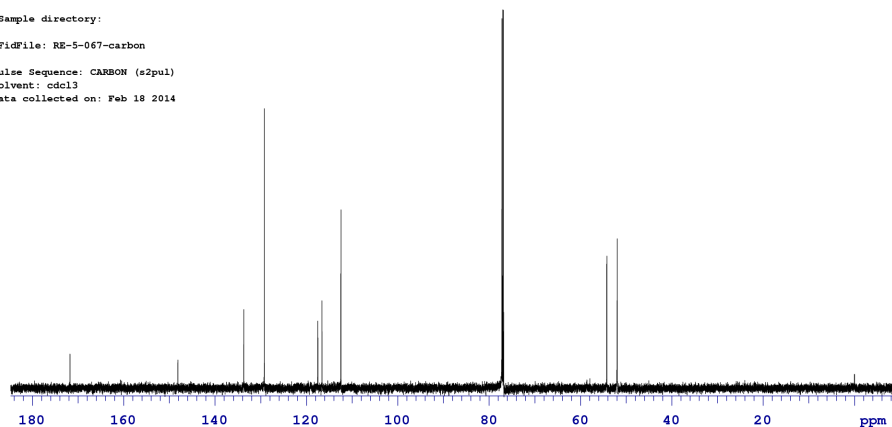
RE-5-067-proton  
STANDARD PROTON PARAMETERS  
Atropine



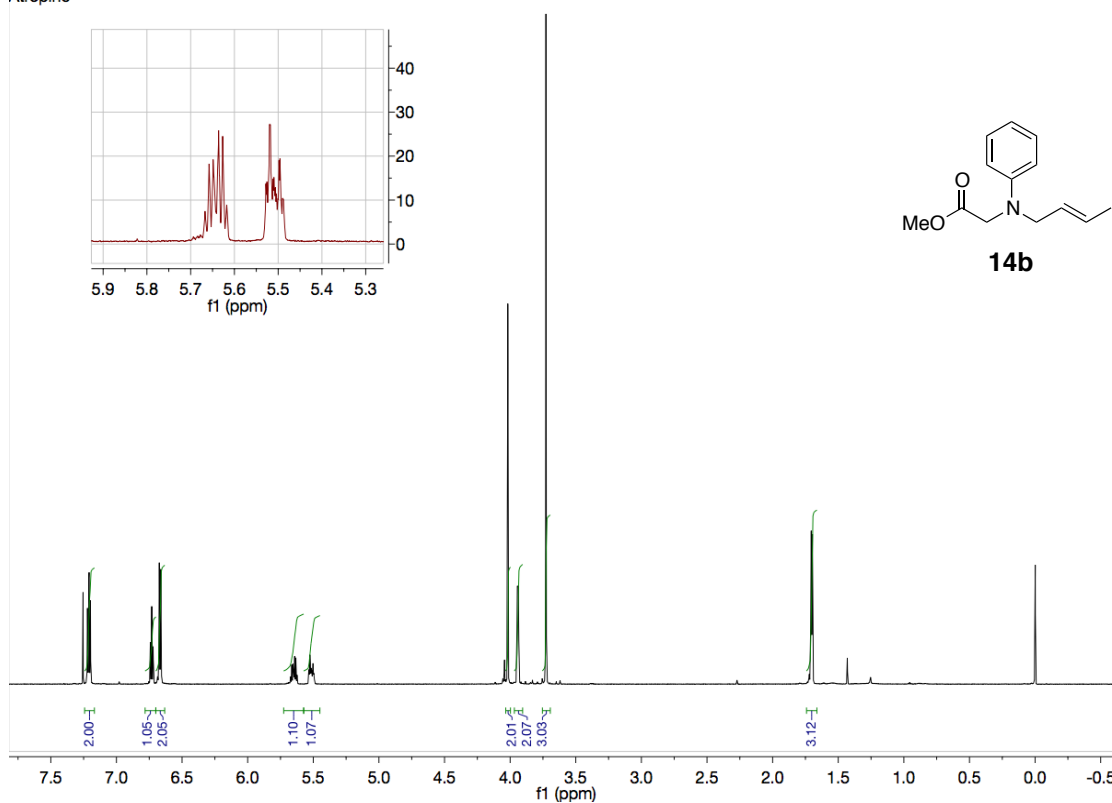
STANDARD PROTON PARAMETERS  
Atropine

Agilent Technologies

Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-067-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014



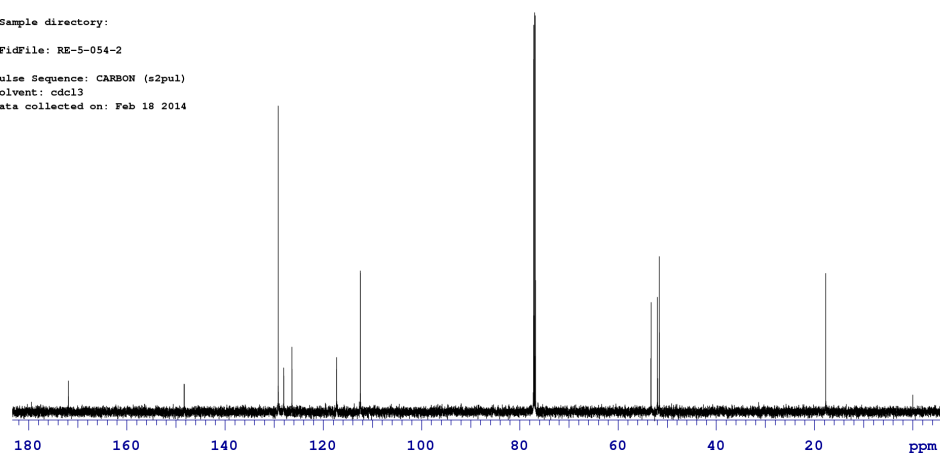
RE-5-054-2-proton  
STANDARD PROTON PARAMETERS  
Atropine



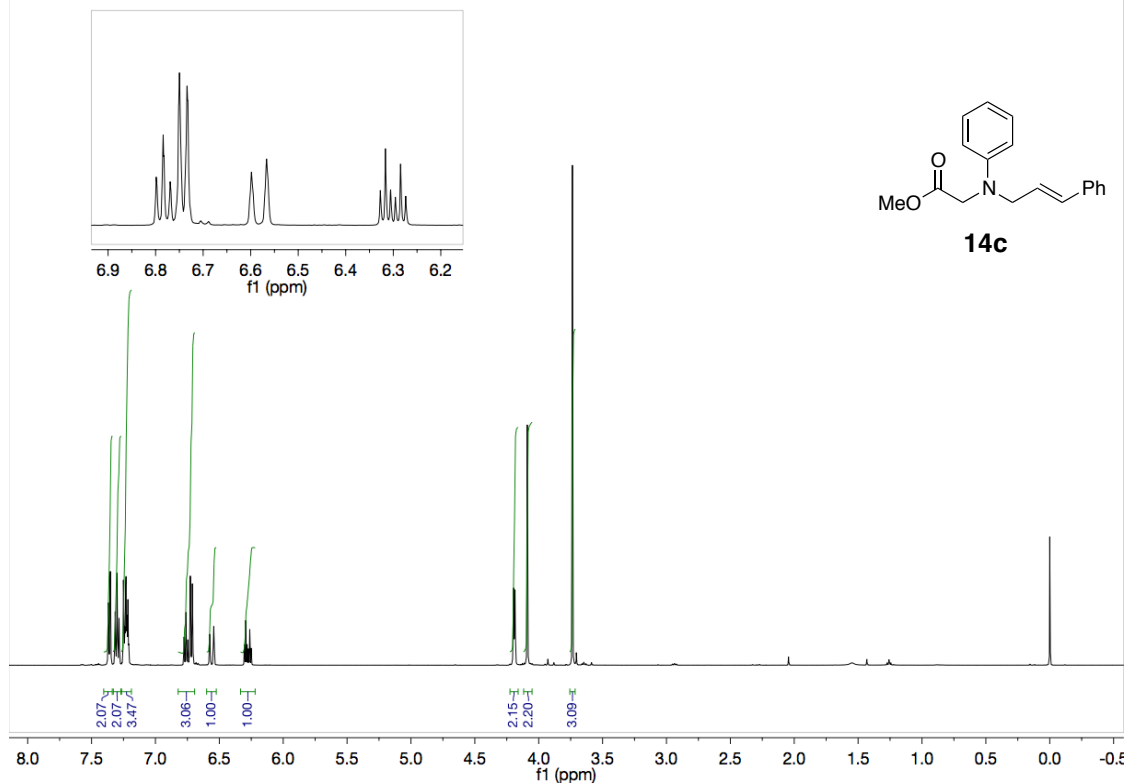
STANDARD PROTON PARAMETERS  
Atropine



Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-054-2  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014



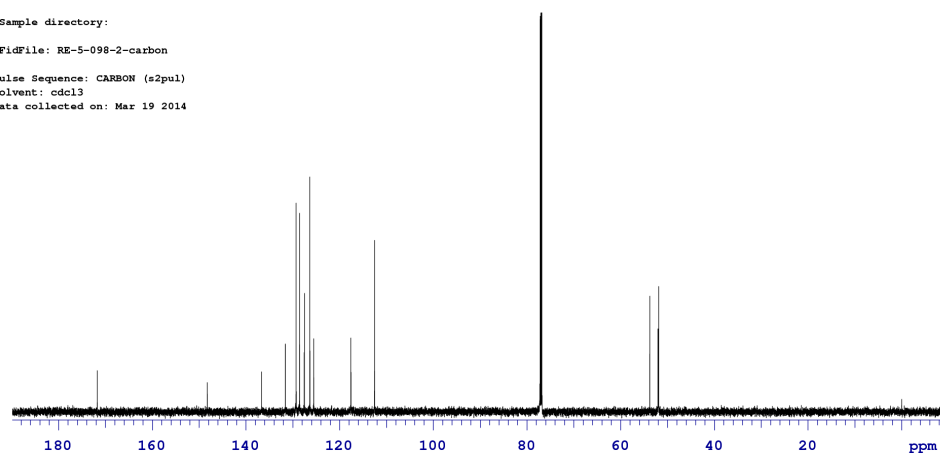
RE-5-098-2-proton  
STANDARD Deuterium PARAMETERS  
Using lock coil



STANDARD PROTON PARAMETERS  
Atropine



Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-098-2-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 19 2014



Proton Spectrum

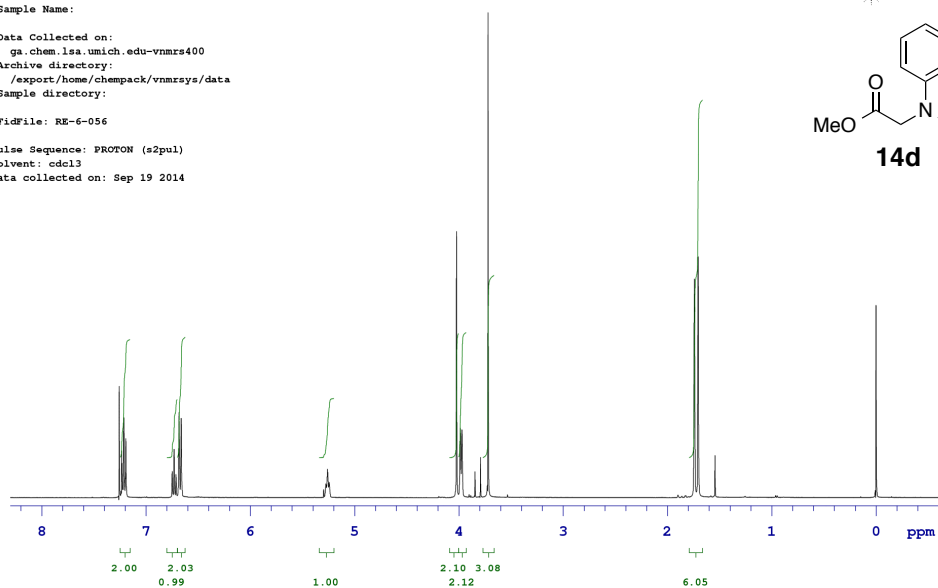
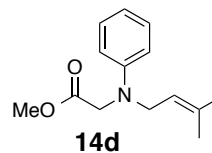
Sample Name:

Data Collected on:  
ga.chem.lsa.umich.edu-vnmrs400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: RK-6-056

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 19 2014

Agilent Technologies



Carbon-13

Sample Name:

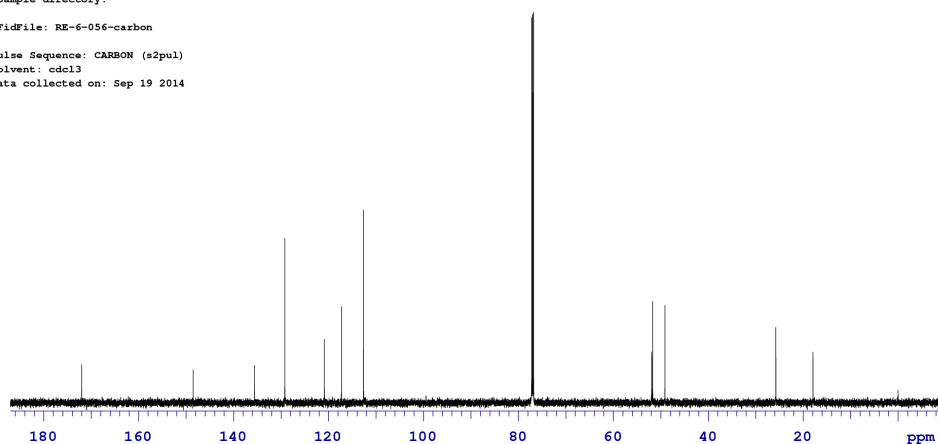
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

FidFile: RK-6-056-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 19 2014

Agilent Technologies



Gradient Shimming

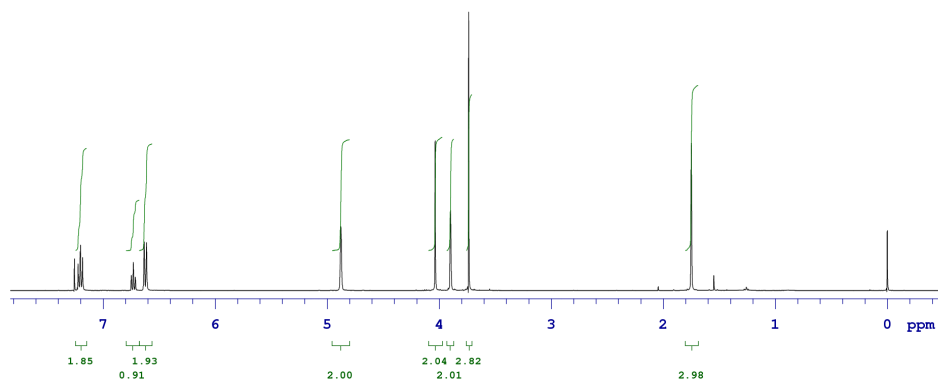
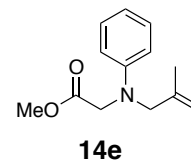
Sample Name:

Data Collected on:  
ga.chem.lsa.umich.edu-vnmrs400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: RK-5-113-2

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 2 2014

Agilent Technologies



Automated Probe tuning parameter

Sample Name:

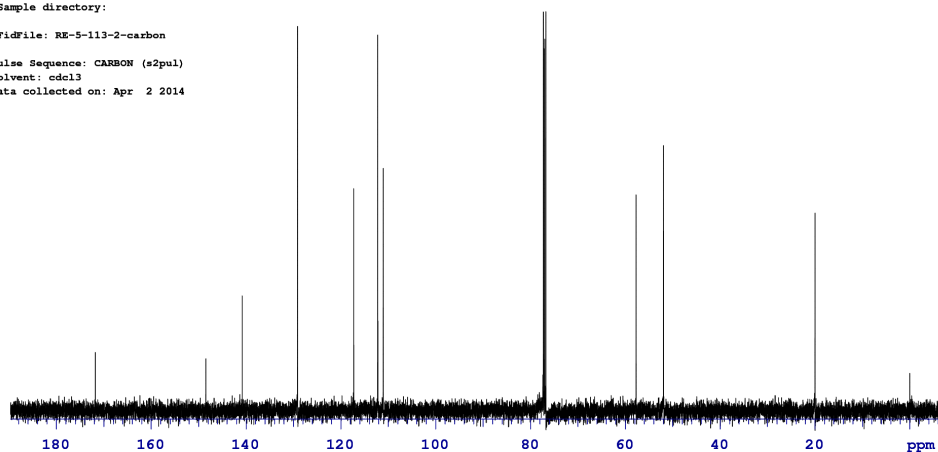
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

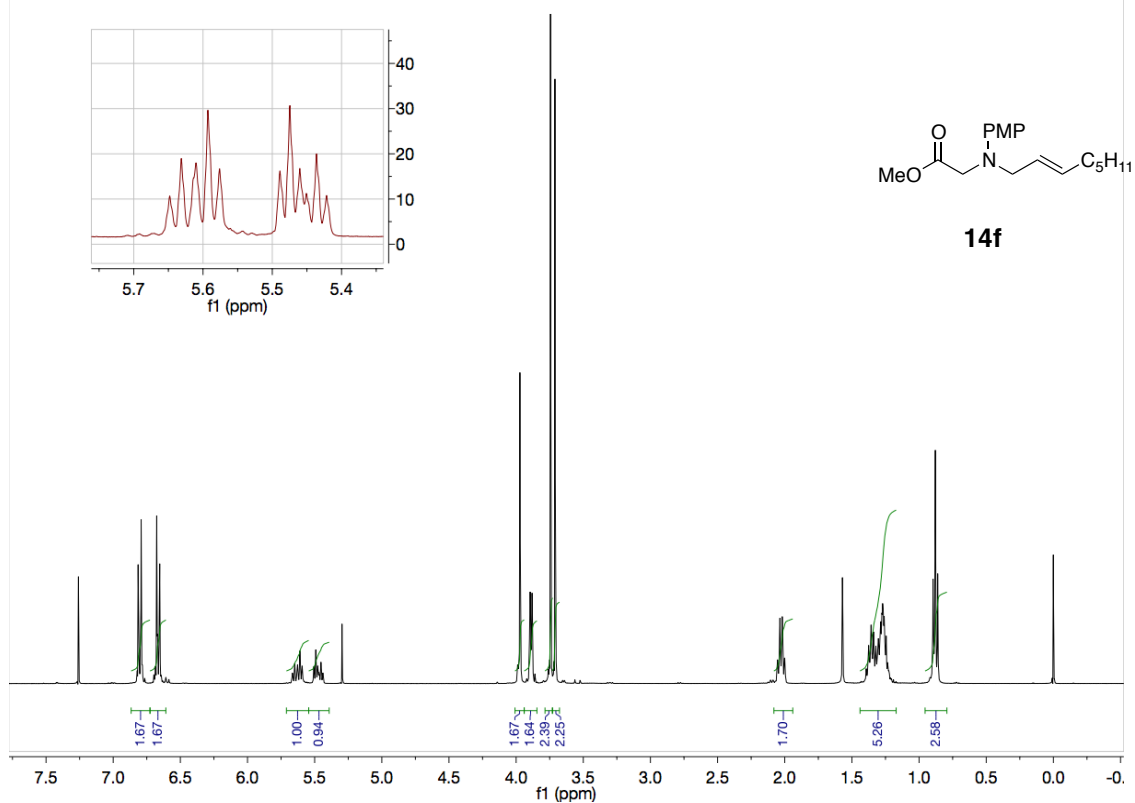
FidFile: RK-5-113-2-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 2 2014

Agilent Technologies



RE-6-013  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

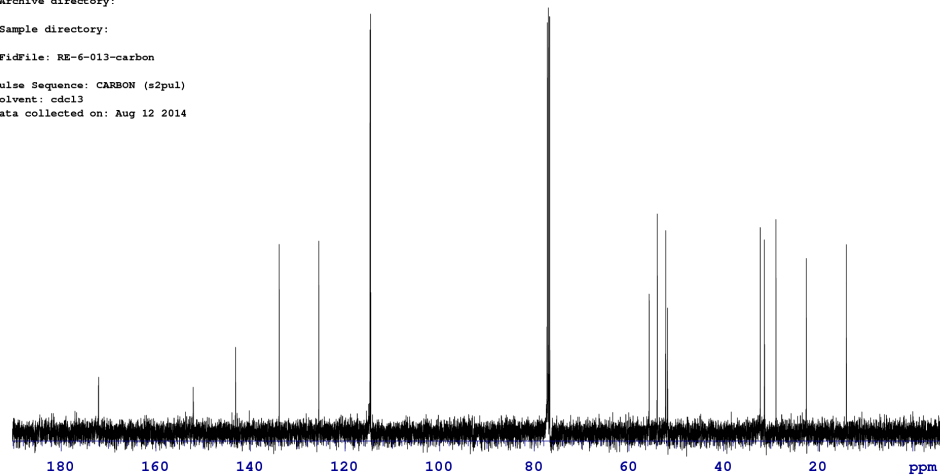
Sample directory:

FidFile: RE-6-013-carbon

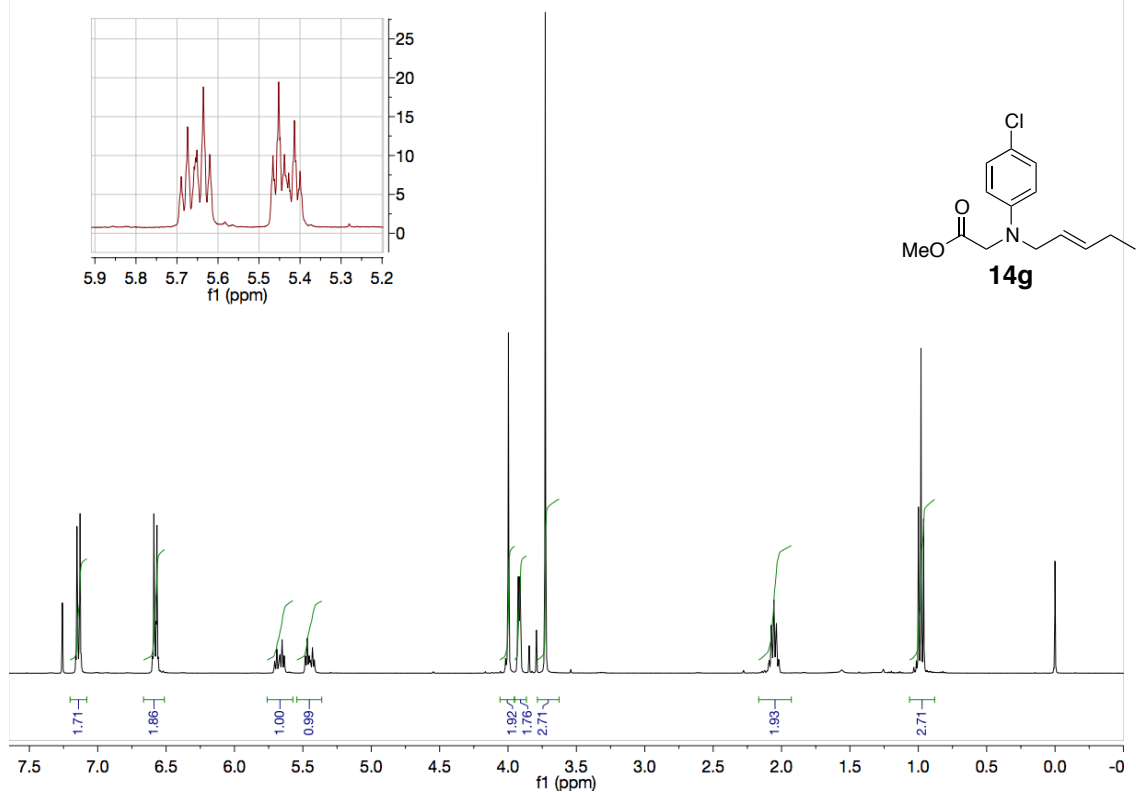
Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 12 2014



RE-6-019  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vmrs700

Archive directory:

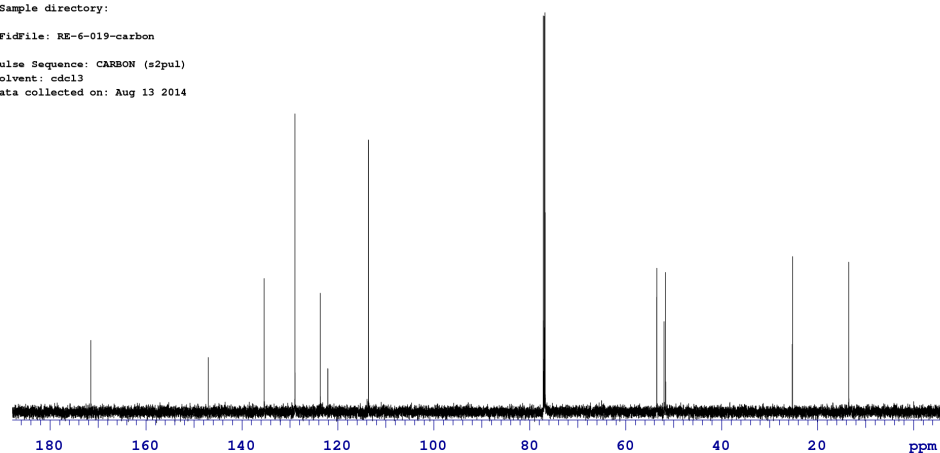
Sample directory:

FidFile: RE-6-019-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 13 2014





STANDARD 1H OBSERVE - profile

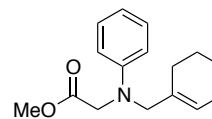
Sample Name:

Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

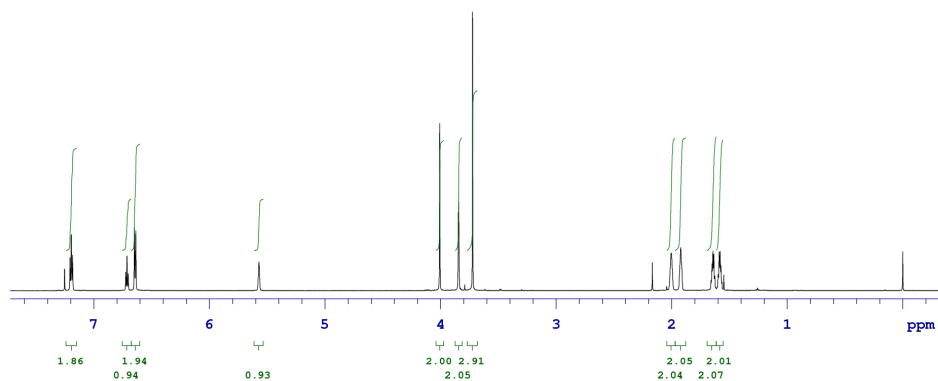
Sample directory:

FidFile: RK-5-118-2-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 9 2014



14h



STANDARD 1H OBSERVE - profile

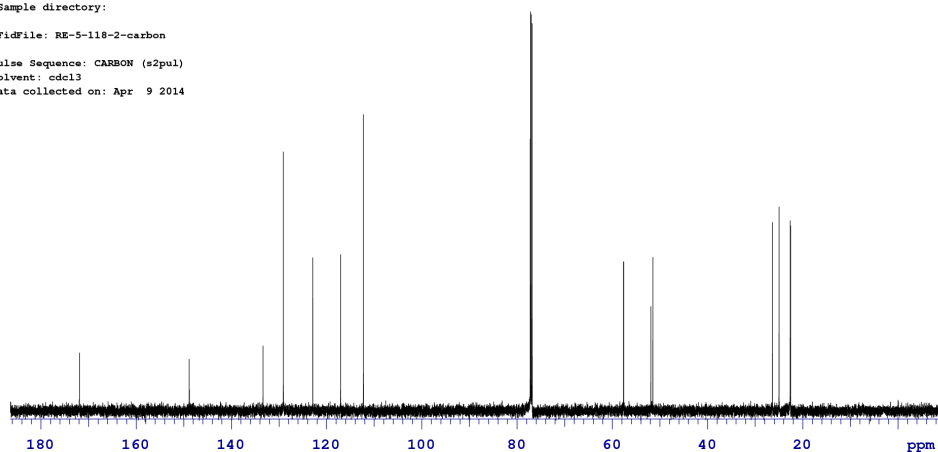
Sample Name:

Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

FidFile: RK-5-118-2-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 9 2014



Proton Spectrum

Sample Name:

Data Collected on:

co.chem.lsa.umich.edu-vnmrs400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

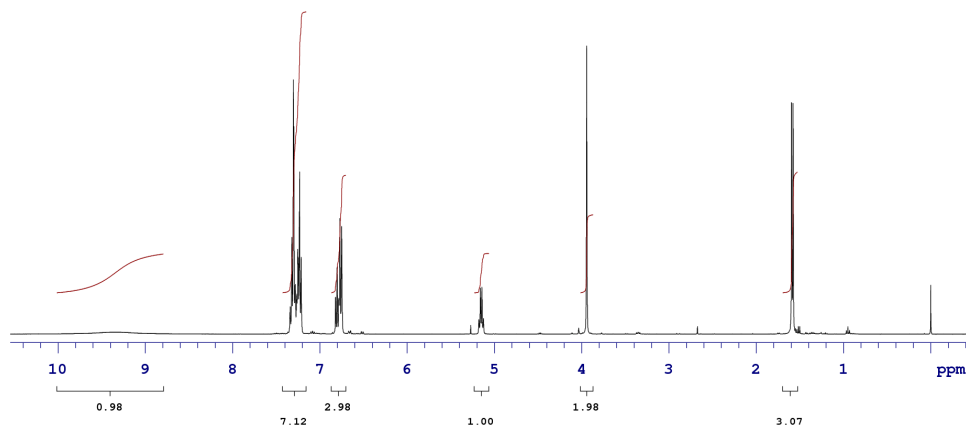
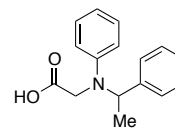
FidFile: RE-5-161-2-proton

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 3 2014

Agilent Technologies



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

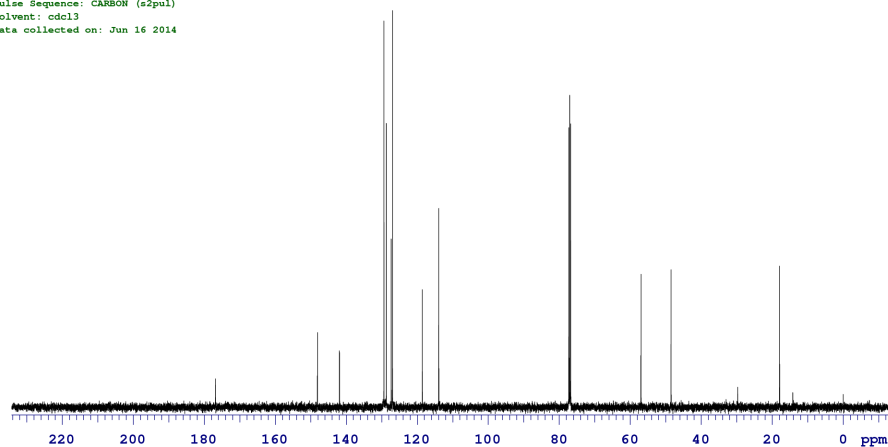
FidFile: RE-5-169-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 16 2014

Agilent Technologies



STANDARD Deuterium PARAMETERS  
Using lock coil

Sample Name:

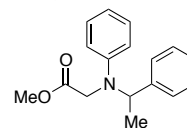
Data Collected on:  
sn.chem.lsa.umich.edu-inova500  
Archive directory:

Sample directory:

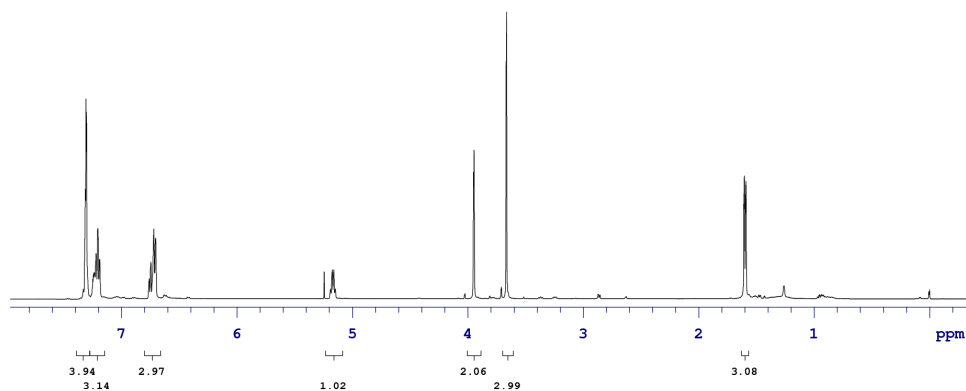
FidFile: RE-5-207

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 9 2014

Agilent Technologies



11



Carbon-13

Agilent Technologies

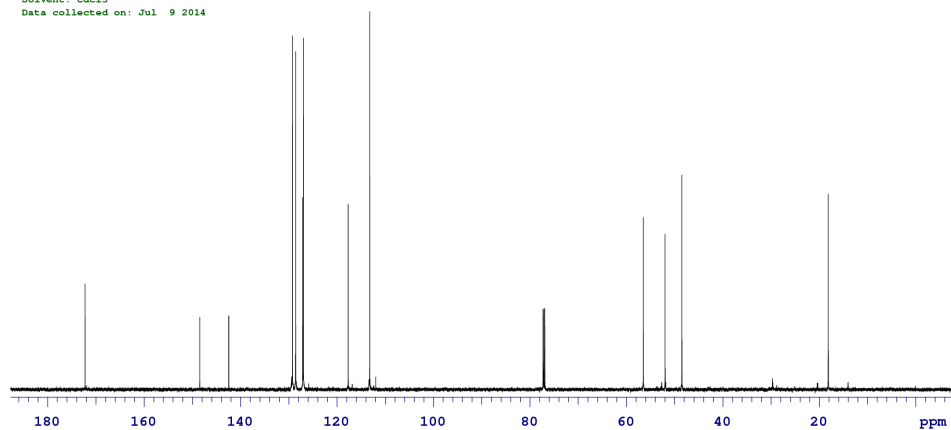
Sample Name:

Data Collected on:  
yb.chem.lsa.umich.edu-vmrs700  
Archive directory:

Sample directory:

FidFile: RE-5-207-carbon

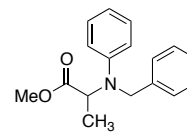
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 9 2014



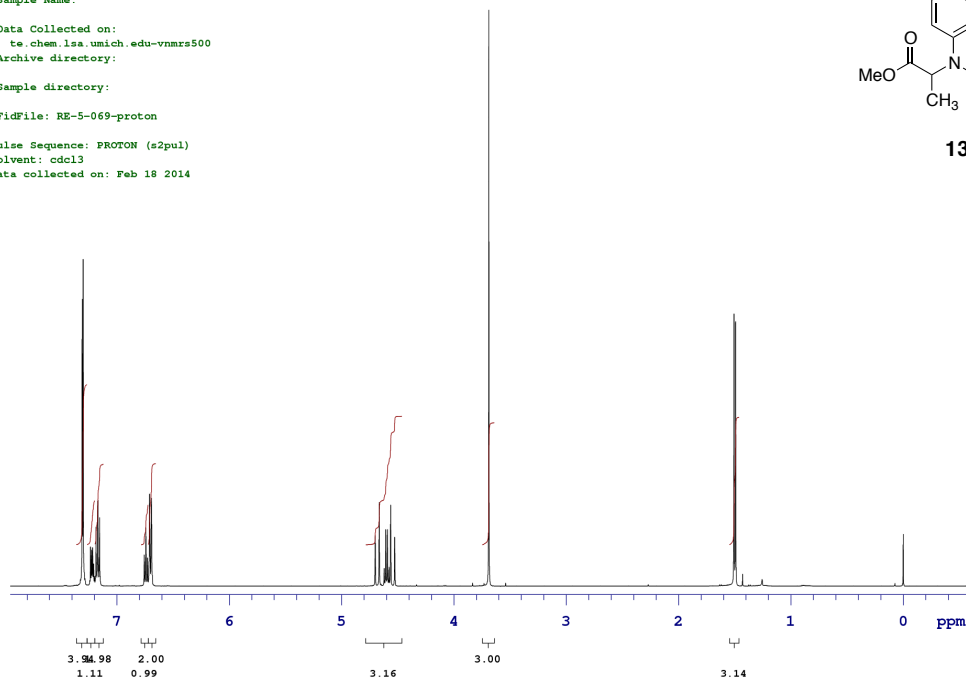
Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-069-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

Agilent Technologies



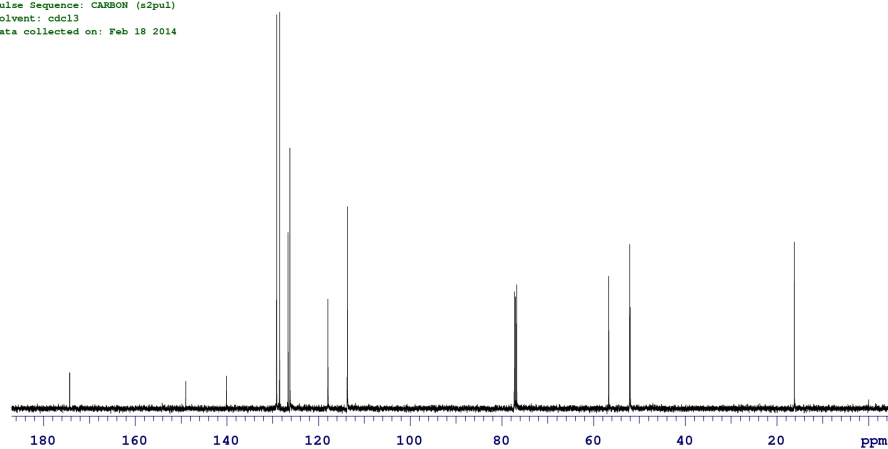
13



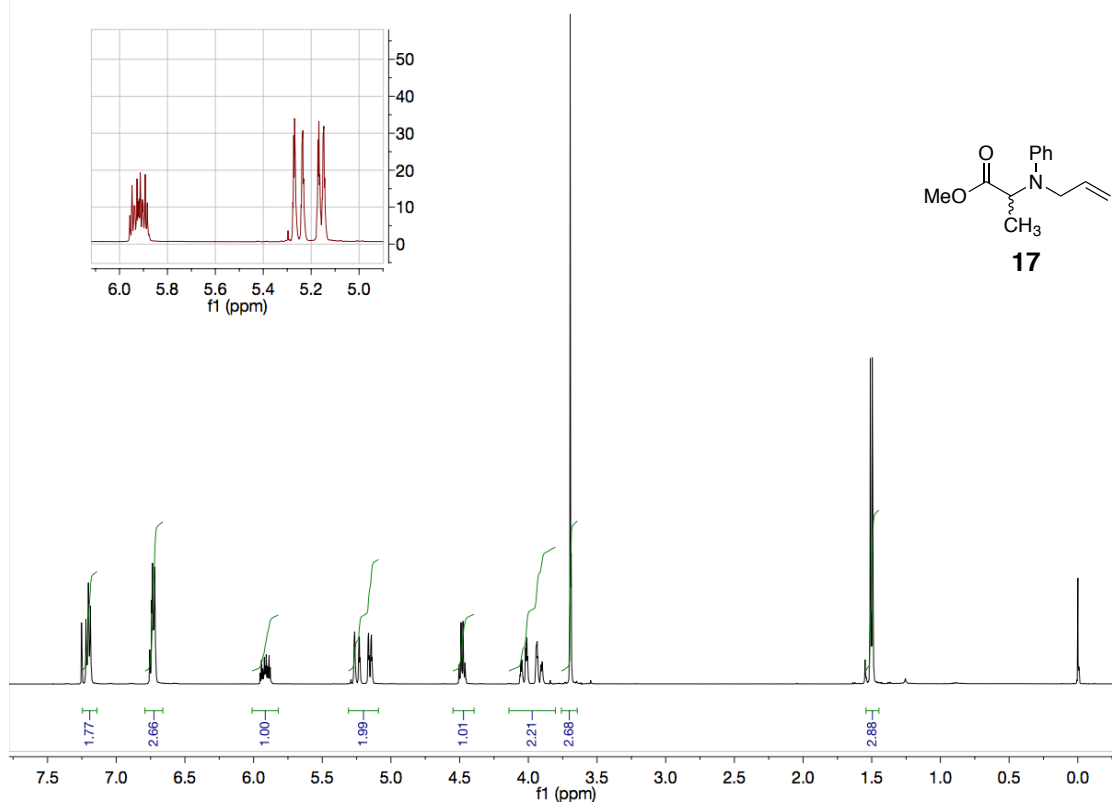
Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-069-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

Agilent Technologies



RE-6-027-proton  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vmrs500

Archive directory:

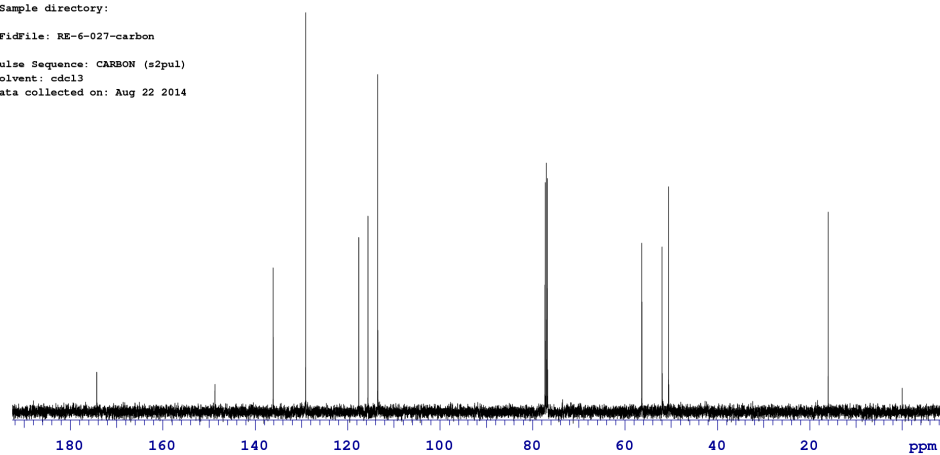
Sample directory:

FidFile: RE-6-027-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 22 2014





Proton Spectrum

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

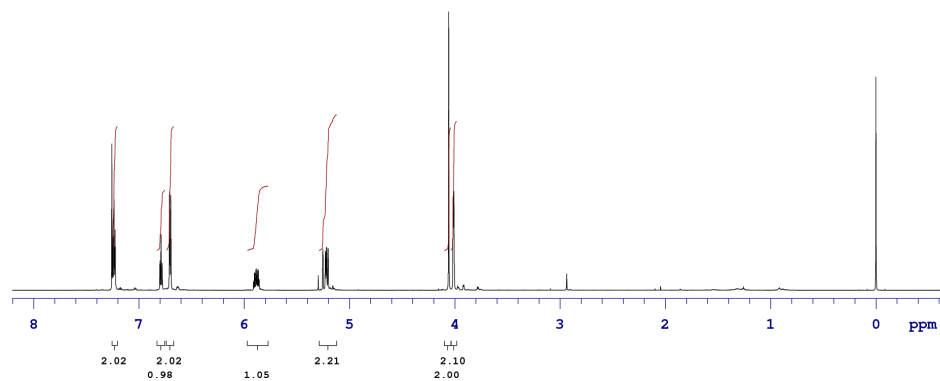
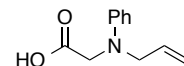
FidFile: RE-6-007-proton2

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 7 2014

Agilent Technologies



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

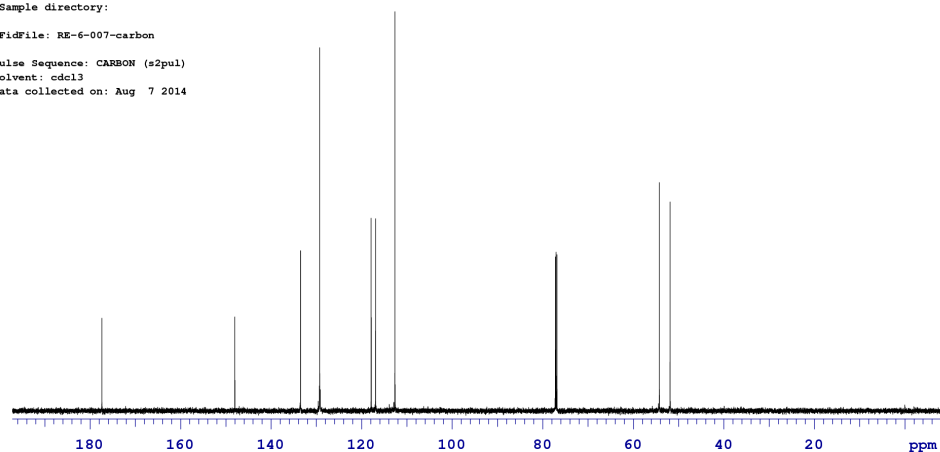
FidFile: RE-6-007-carbon

Pulse Sequence: CARBON (s2pul)

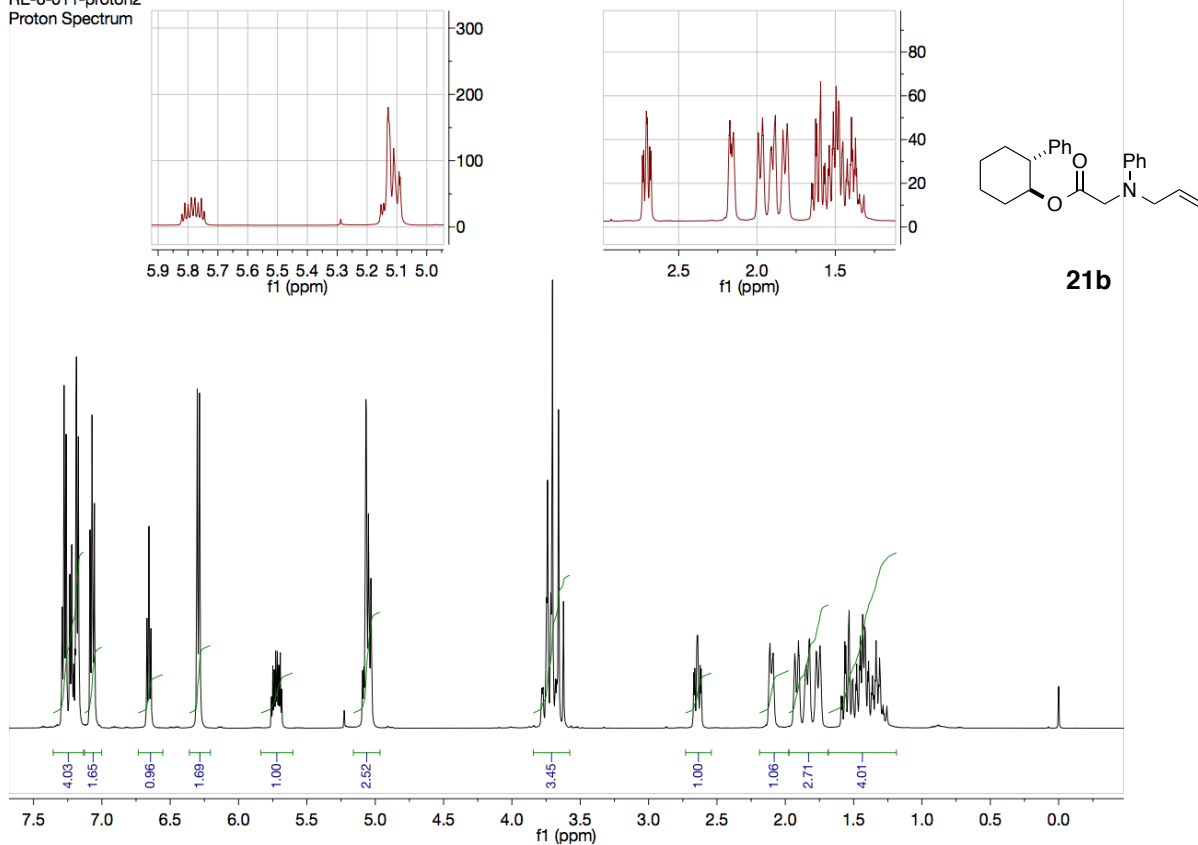
Solvent: cdcl3

Data collected on: Aug 7 2014

Agilent Technologies



RE-6-011-proton2  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vmrs500

Archive directory:

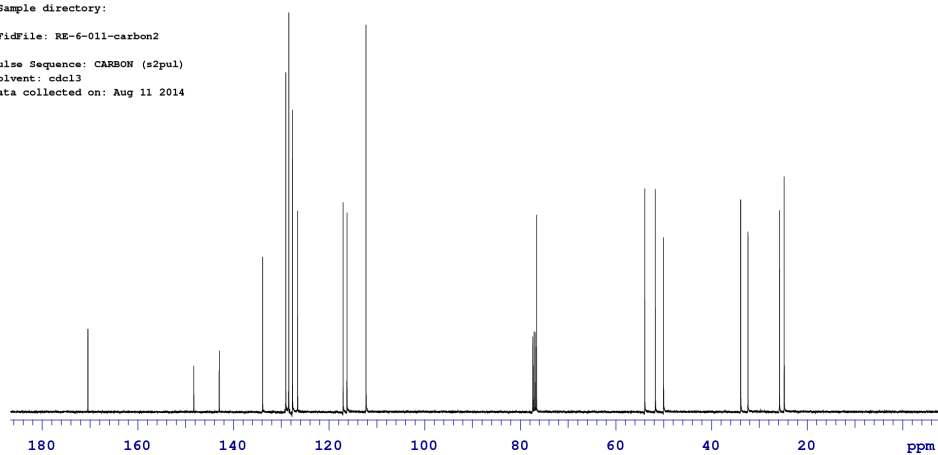
Sample directory:

FidFile: RE-6-011-carbon2

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 11 2014





STANDARD PROTON PARAMETERS  
 Atropine

Sample Name:

Data Collected on:  
 yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

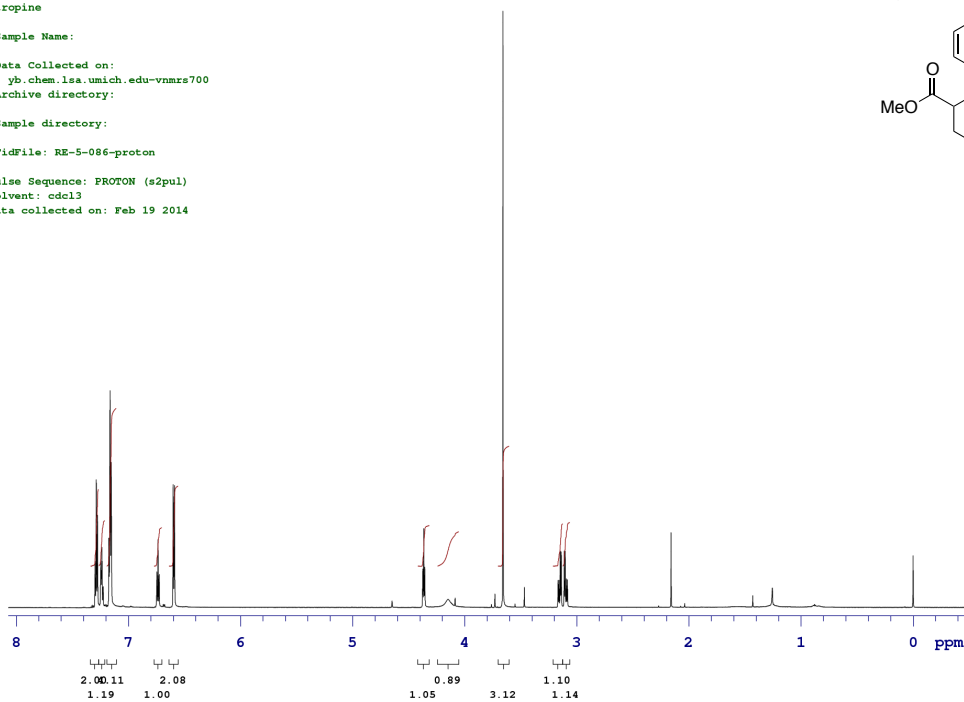
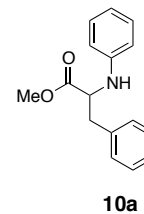
FidFile: RE-5-086-proton

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 19 2014

Agilent Technologies



STANDARD PROTON PARAMETERS  
 Atropine

Sample Name:

Data Collected on:  
 yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

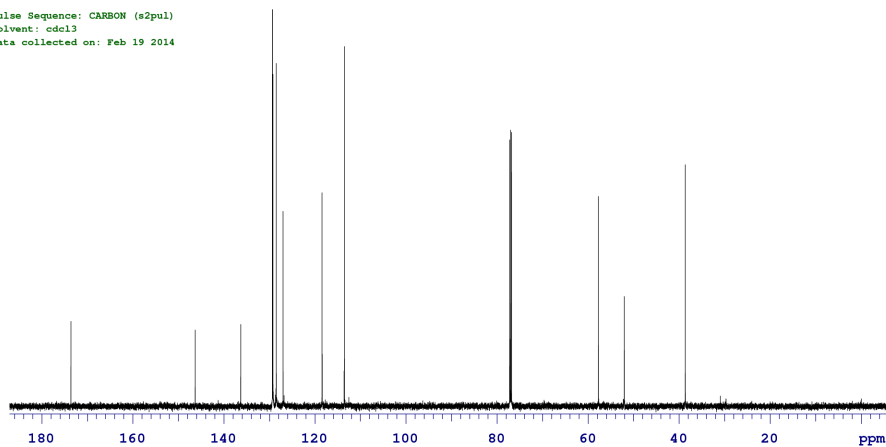
FidFile: RE-5-086-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 19 2014

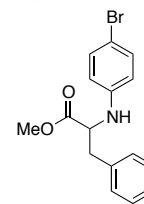
Agilent Technologies



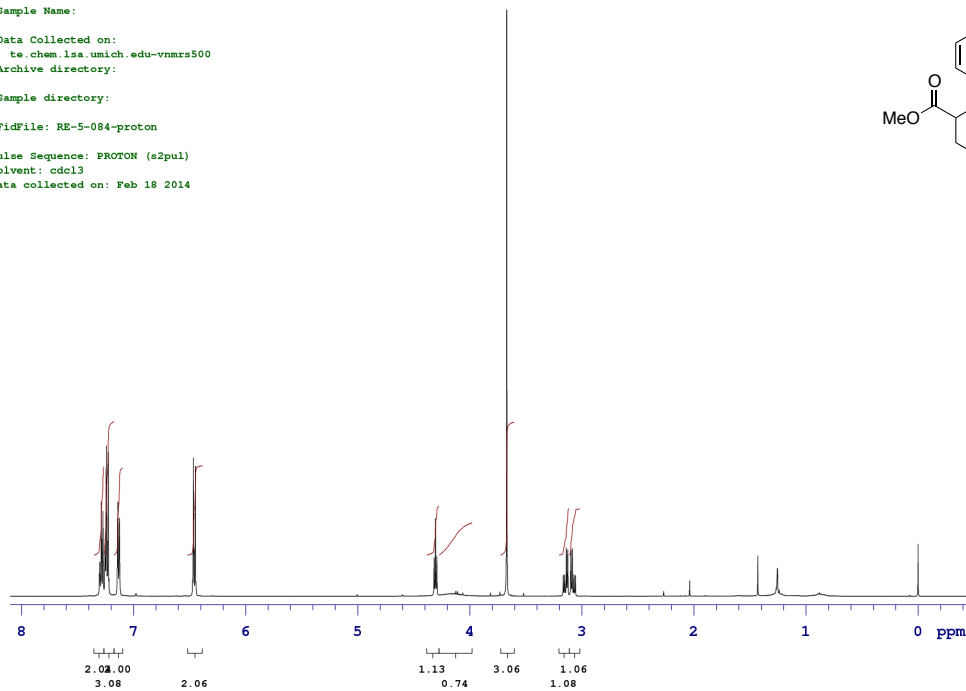
Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-084-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

Agilent Technologies



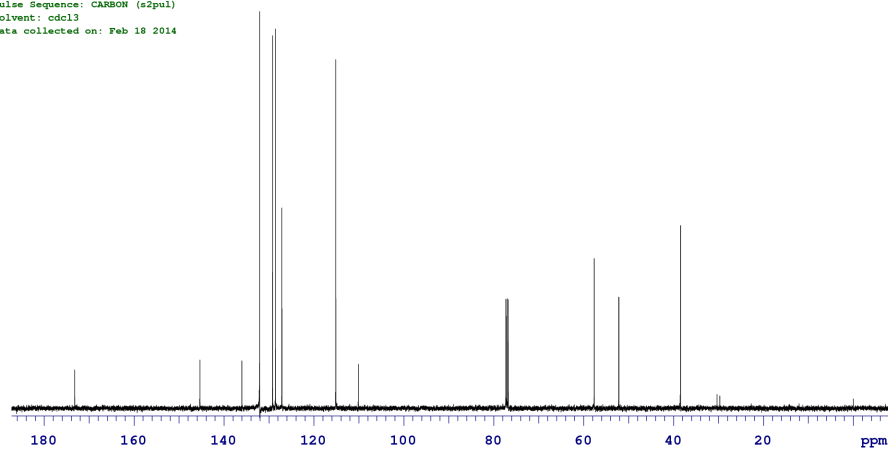
10b



Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-084-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

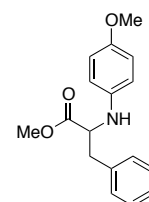
Agilent Technologies



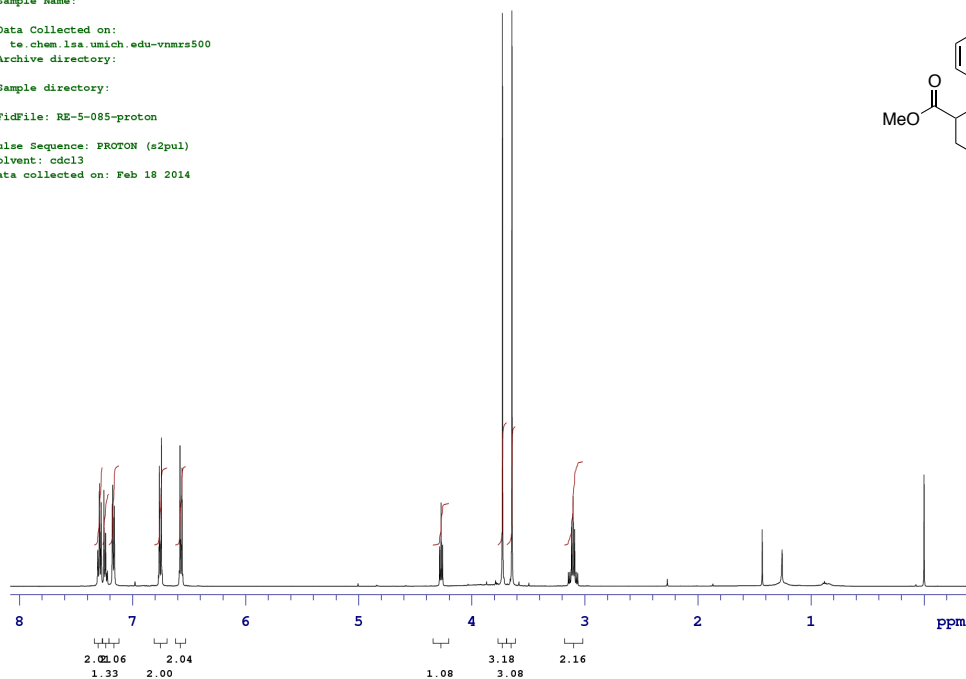
Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-085-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

Agilent Technologies



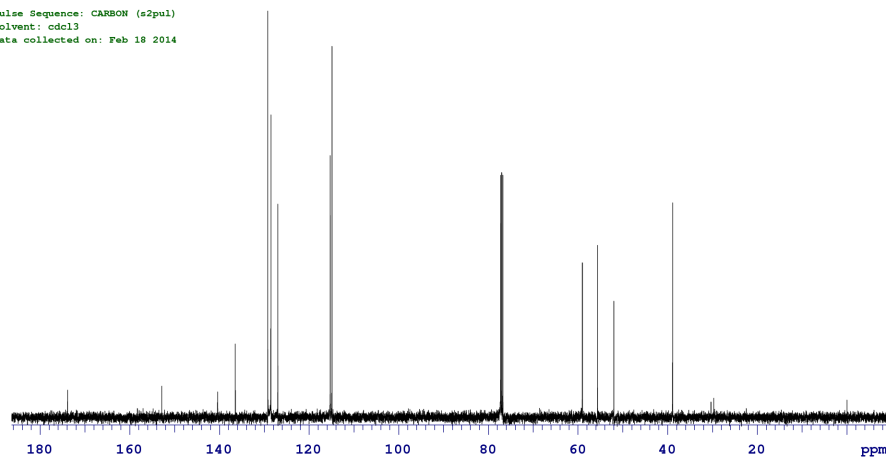
10c



Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-085-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 18 2014

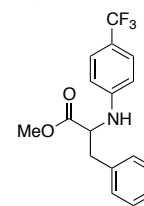
Agilent Technologies



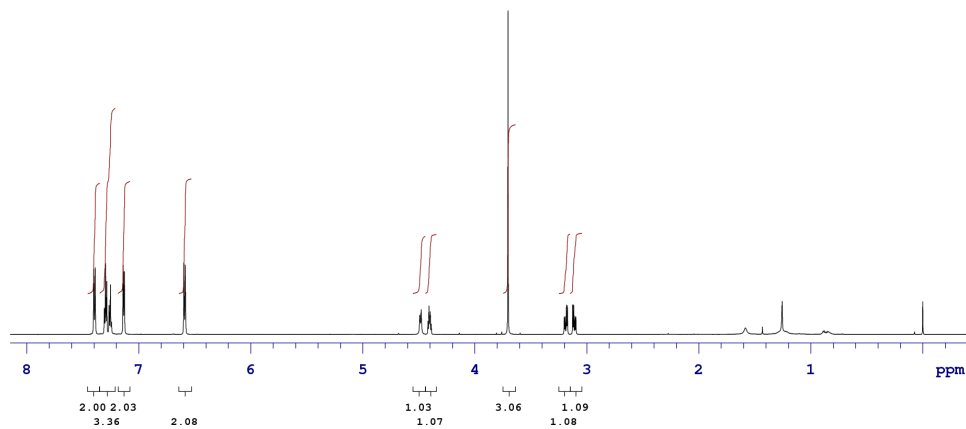
Proton Spectrum

Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-209  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 23 2014

Agilent Technologies



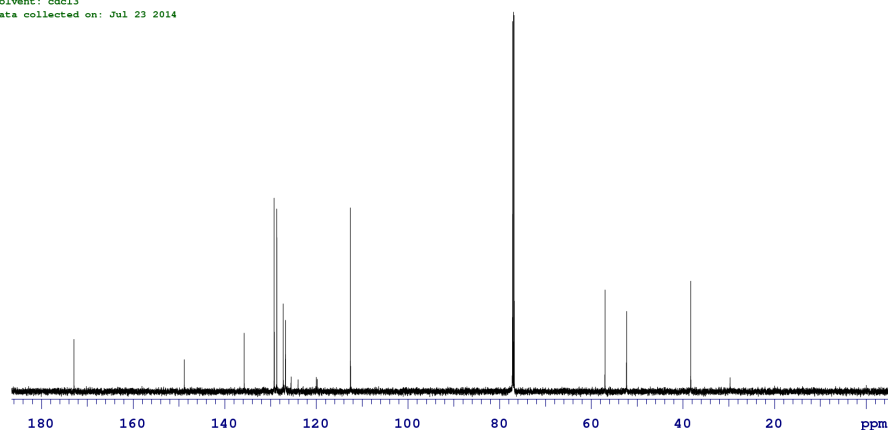
10d



Carbon-13

Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-209-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 23 2014

Agilent Technologies



STANDARD PROTON PARAMETERS  
Atropine

Sample Name:

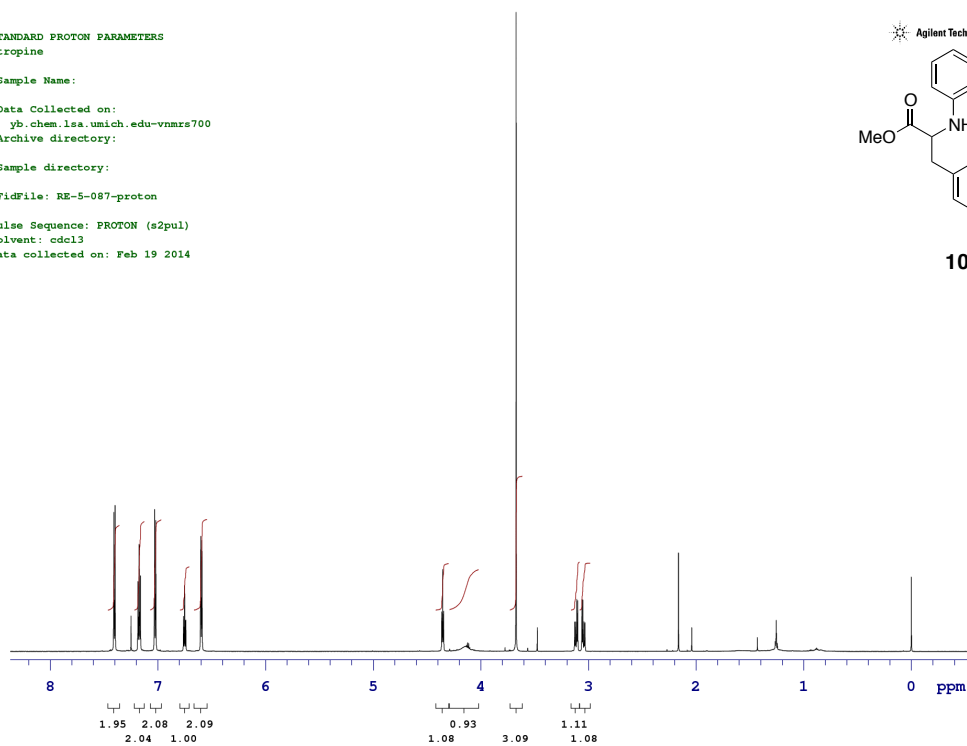
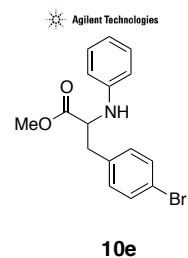
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

FidFile: RE-5-087-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 19 2014



STANDARD PROTON PARAMETERS  
Atropine

Sample Name:

Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700

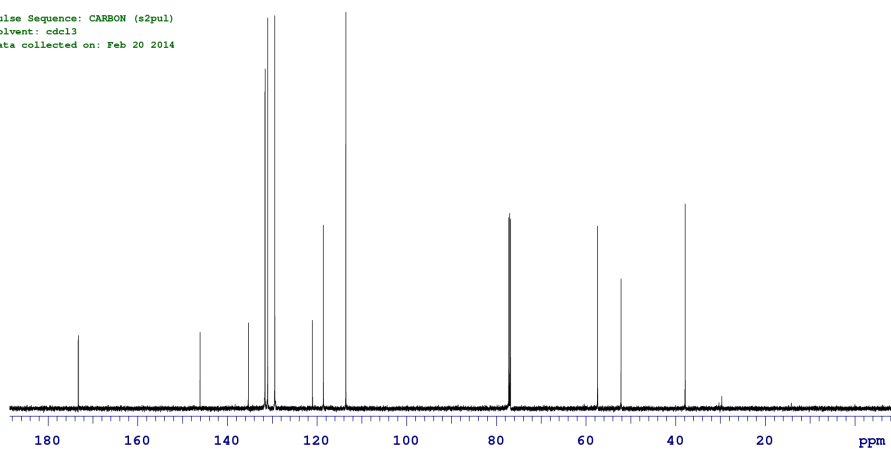
Archive directory:

Sample directory:

FidFile: RE-5-087-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 20 2014

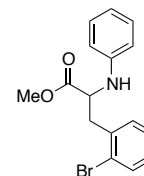
Agilent Technologies



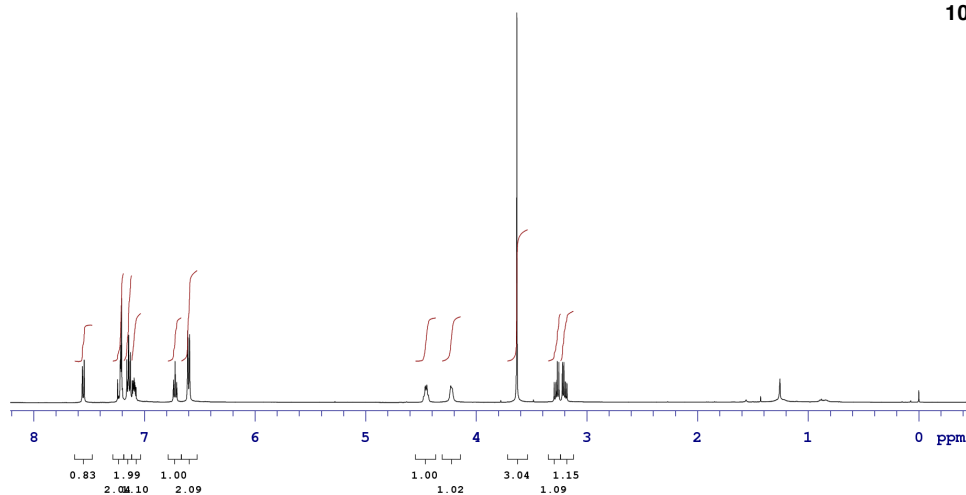
Automated Probe tuning parameter

Sample Name:  
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:  
Sample directory:  
FidFile: RE-5-082-proton  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 13 2014

Agilent Technologies



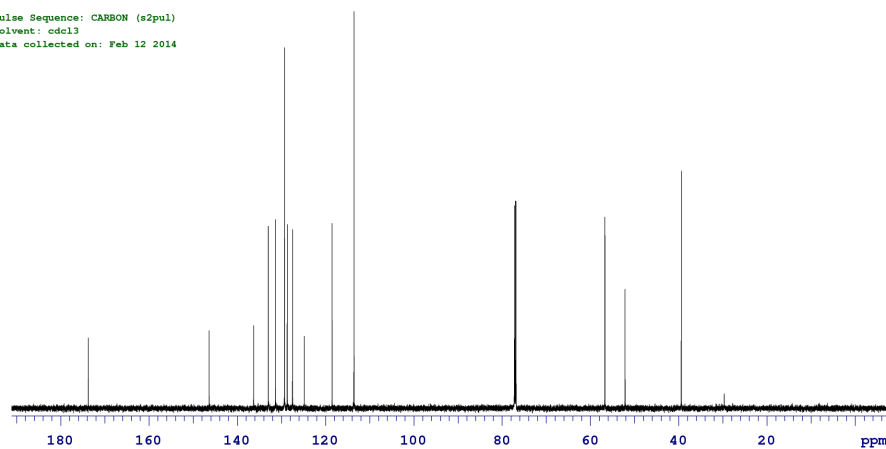
10f



STANDARD PROTON PARAMETERS  
Atropine

Sample Name:  
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:  
Sample directory:  
FidFile: RE-5-082-carbon  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 12 2014

Agilent Technologies



Gradient Shimming

Sample Name:

Data Collected on:

ga.chem.lsa.umich.edu-vnmrs400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

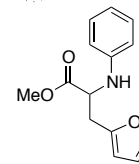
FidFile: RE-5-138-2

Pulse Sequence: PROTON (s2pul)

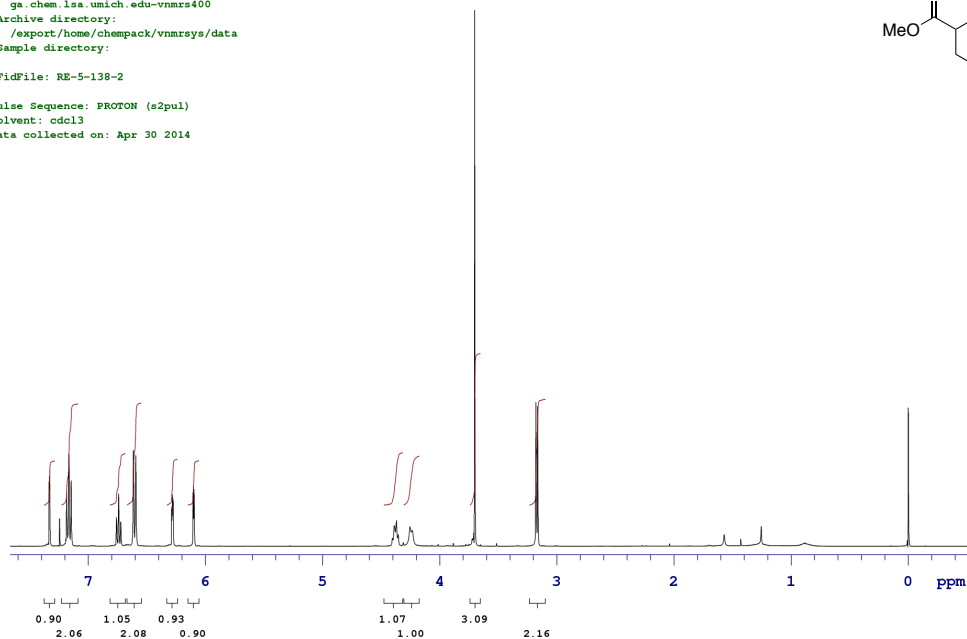
Solvent: cdcl3

Data collected on: Apr 30 2014

Agilent Technologies



10g



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

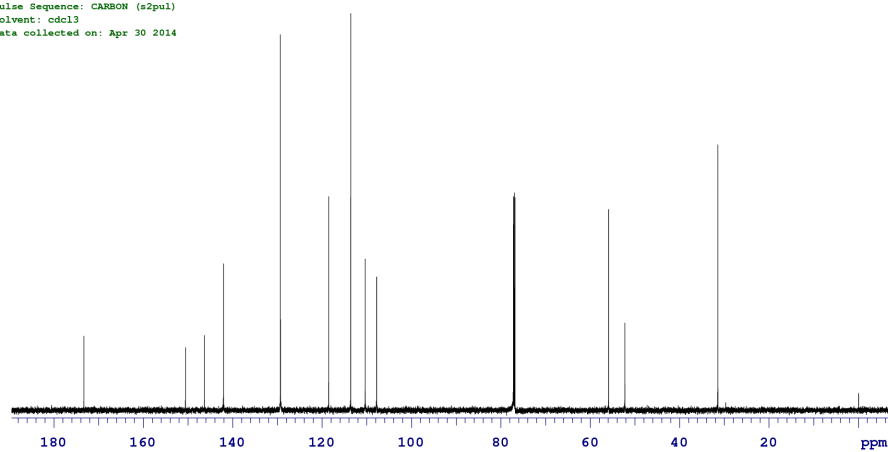
FidFile: RE-5-138-2-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Apr 30 2014

Agilent Technologies



Proton Spectrum

Sample Name:

Data Collected on:

ga.chem.lsa.umich.edu-vnmrs400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

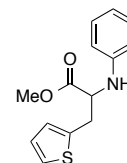
FidFile: RE-6-040-clean

Pulse Sequence: PROTON (s2pul)

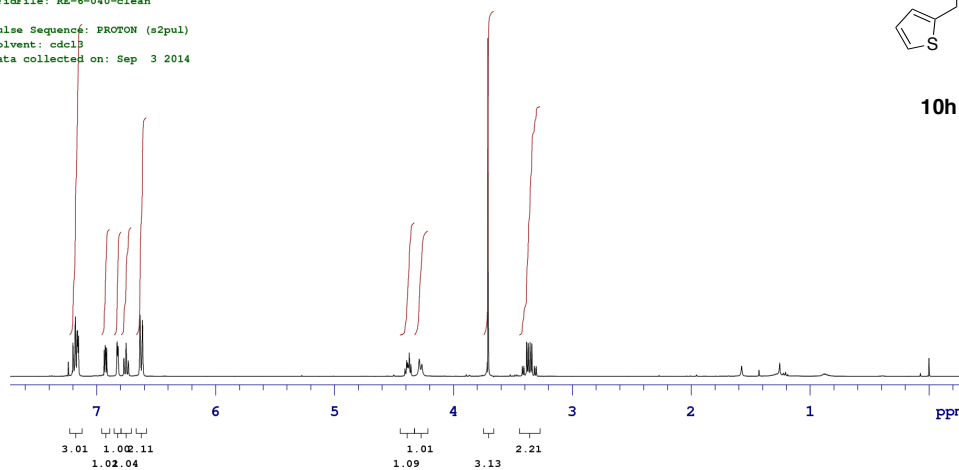
Solvent: cdcl3

Data collected on: Sep 3 2014

Agilent Technologies



10h



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

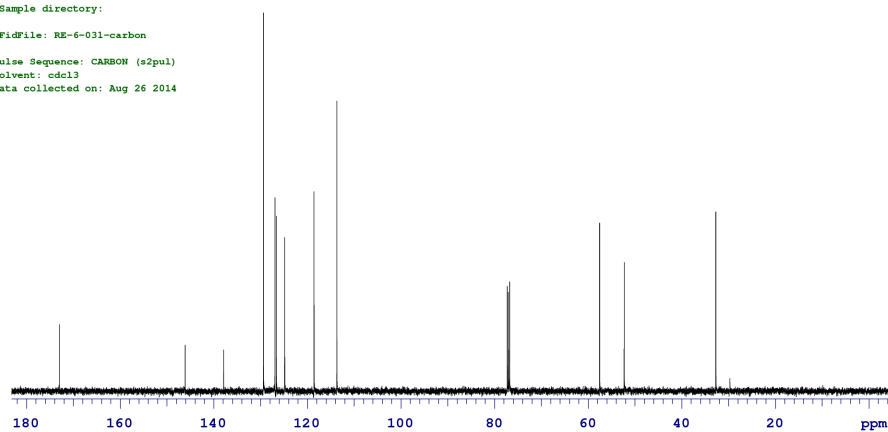
FidFile: RE-6-031-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 26 2014

Agilent Technologies

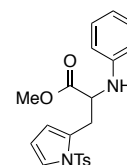




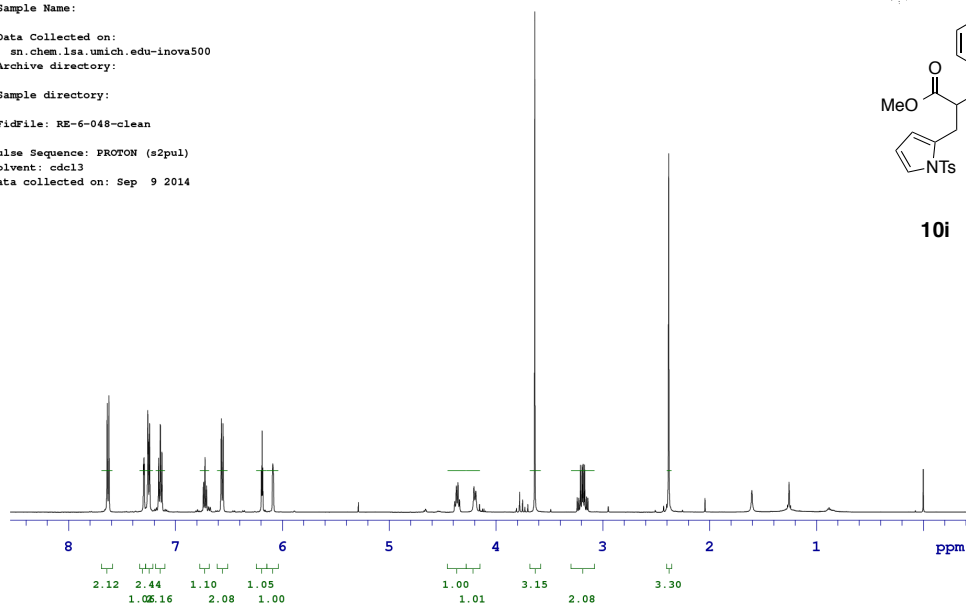
Proton Spectrum

Sample Name:  
 Data Collected on:  
 sn.chem.lsa.umich.edu-inova500  
 Archive directory:  
 Sample directory:  
 FidFile: RE-6-048-clean  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Sep 9 2014

Agilent Technologies



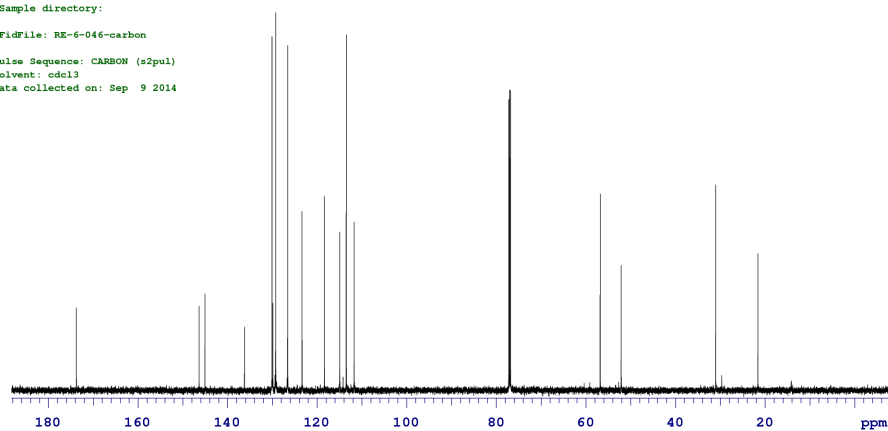
10i



Carbon-13

Sample Name:  
 Data Collected on:  
 yb.chem.lsa.umich.edu-vnmr700  
 Archive directory:  
 Sample directory:  
 FidFile: RE-6-046-carbon  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Sep 9 2014

Agilent Technologies



STANDARD Deuterium PARAMETERS  
Using lock coil

Sample Name:

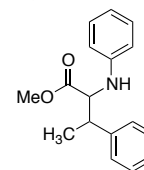
Data Collected on:  
sn.chem.lsa.umich.edu-inova500  
Archive directory:

Sample directory:

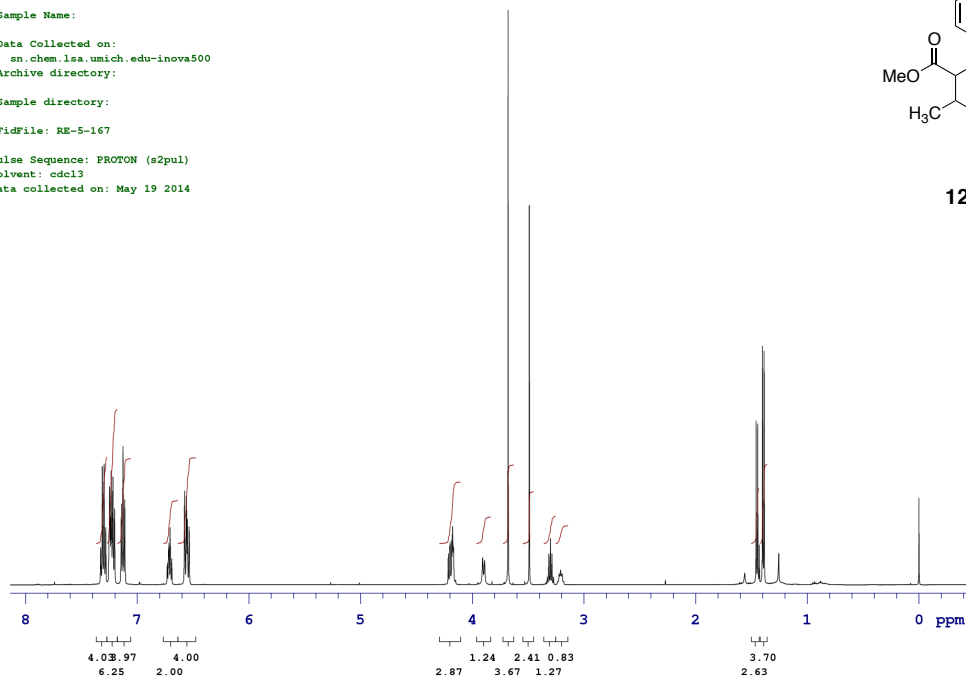
FidFile: RE-5-167

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: May 19 2014

Agilent Technologies



12



Carbon-13

Sample Name:

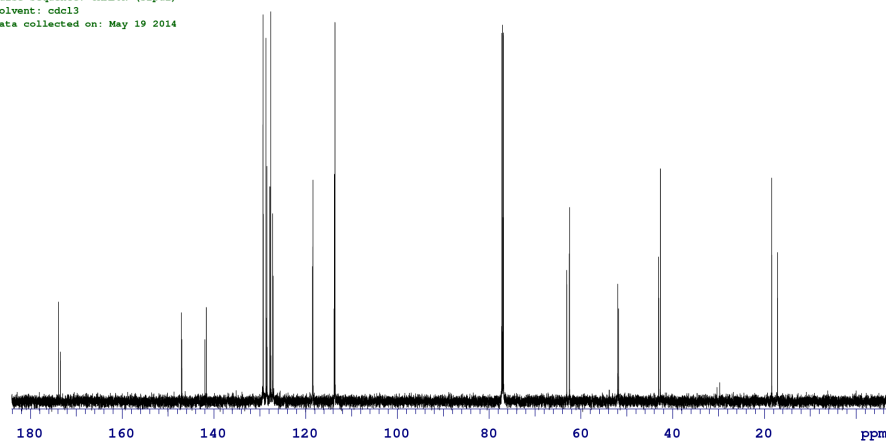
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

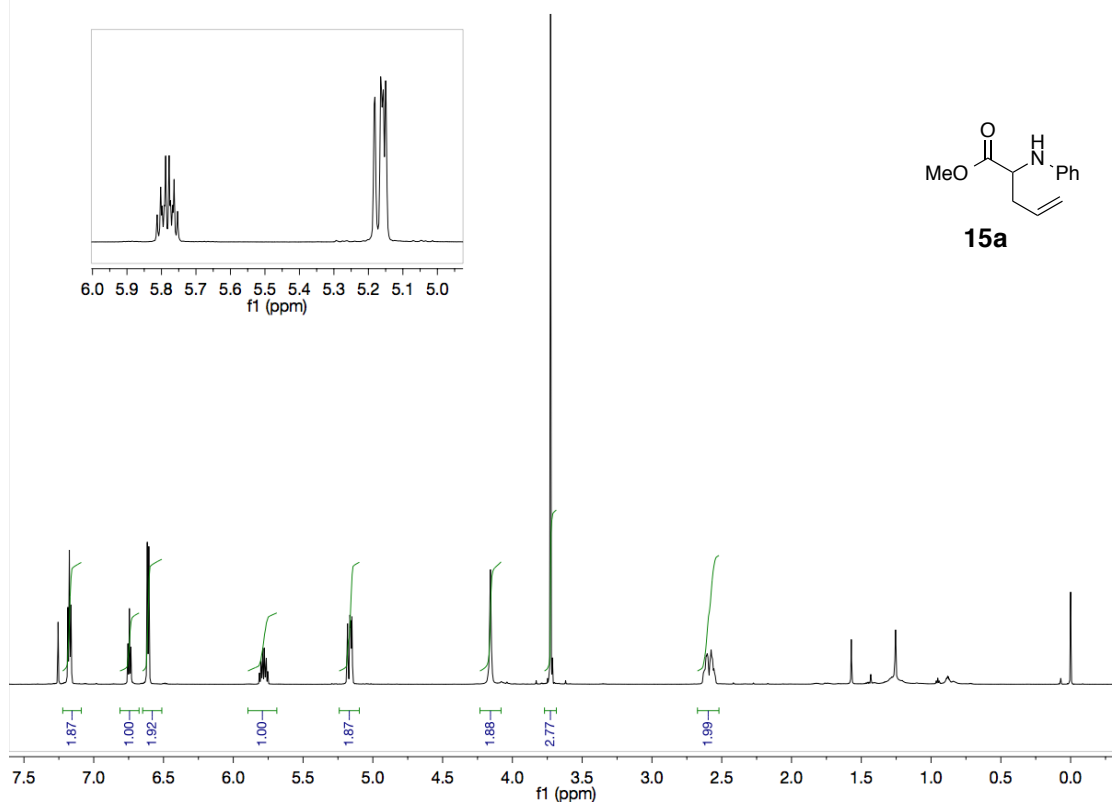
FidFile: RE-5-167-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: May 19 2014

Agilent Technologies



RE-6-050-1-A-proton  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vmrs700

Archive directory:

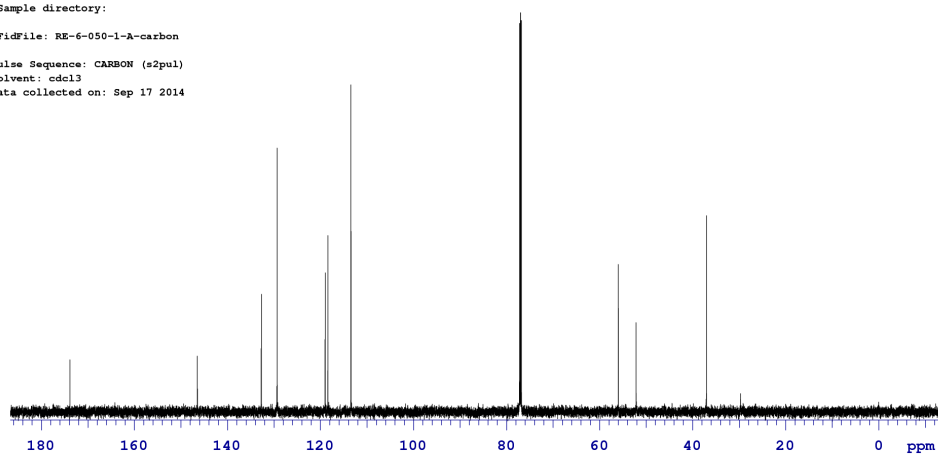
Sample directory:

FidFile: RE-6-050-1-A-carbon

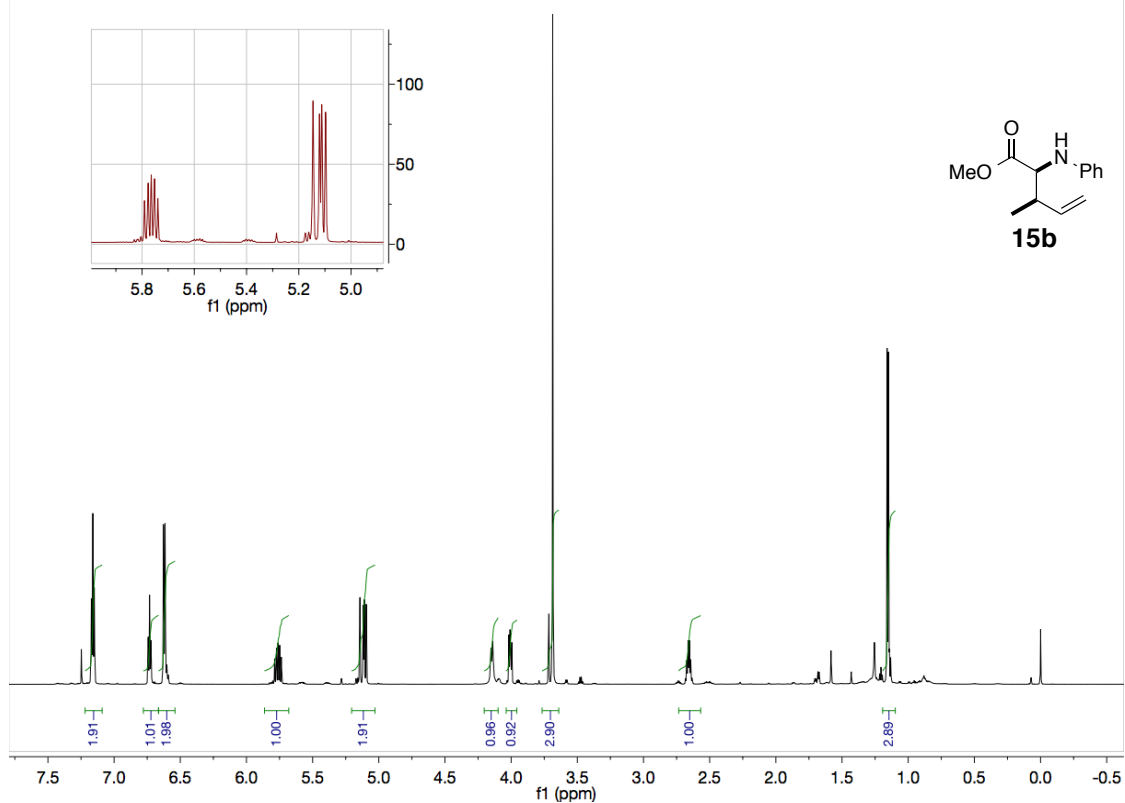
Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 17 2014



RE-6-062-proton  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vmrs700

Archive directory:

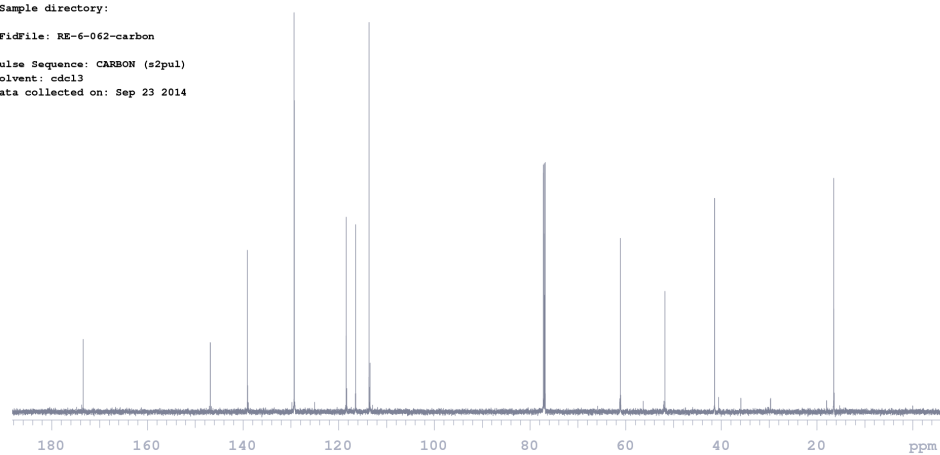
Sample directory:

FidFile: RE-6-062-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 23 2014



Proton Spectrum

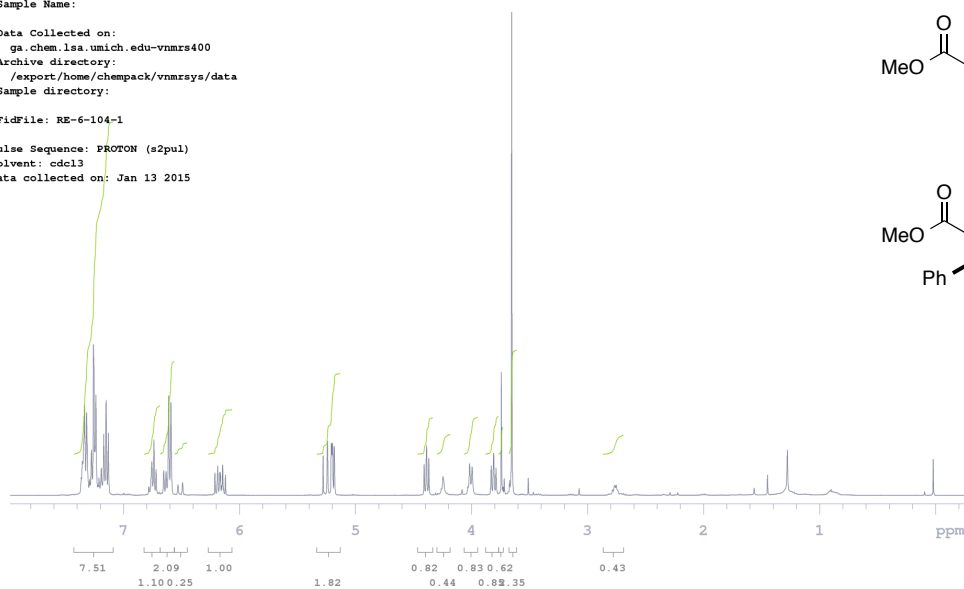
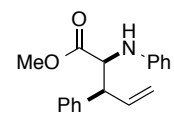
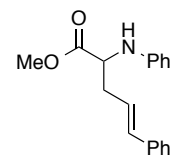
Sample Name:

Data Collected on:  
ga.chem.lsa.umich.edu-vnmrs400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

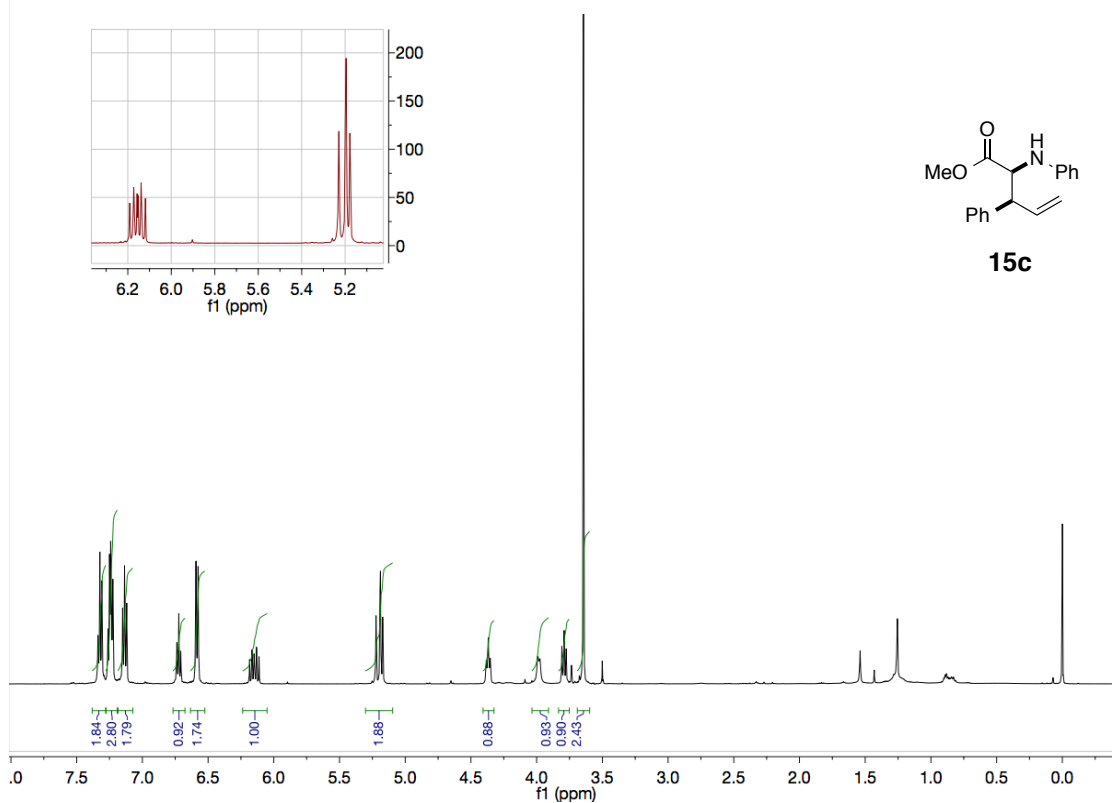
FidFile: RE-6-104-1

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 13 2015

Agilent Technologies



RE-6-083-A-proton  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

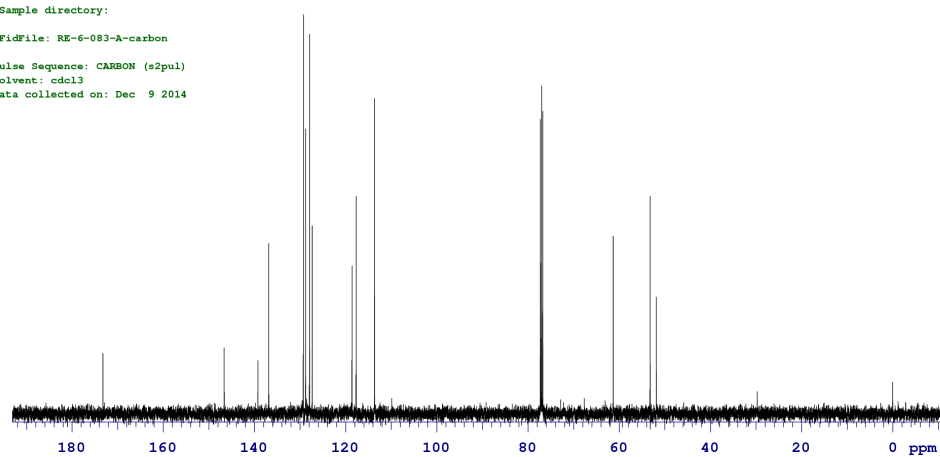
Sample directory:

FidFile: RE-6-083-A-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Dec 9 2014



Proton Spectrum

Sample Name:

Data Collected on:

ga.chem.lsa.umich.edu-vnmrs400

Archive directory:

/export/home/chempack/vnmrsvs/data

Sample directory:

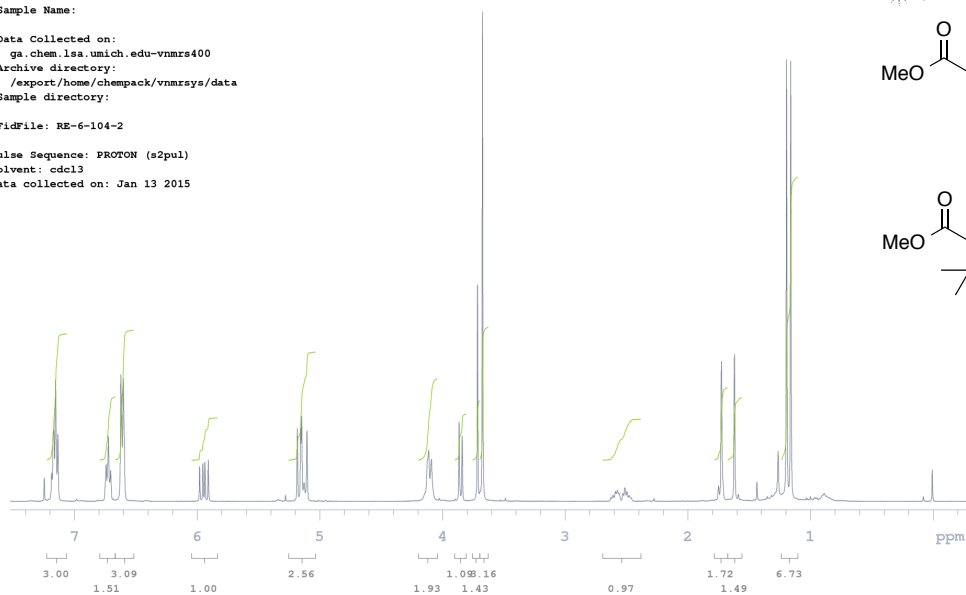
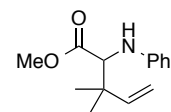
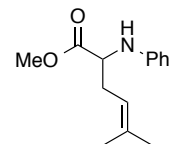
FidFile: RE-6-104-2

Pulse Sequence: PROTON (s2pul)

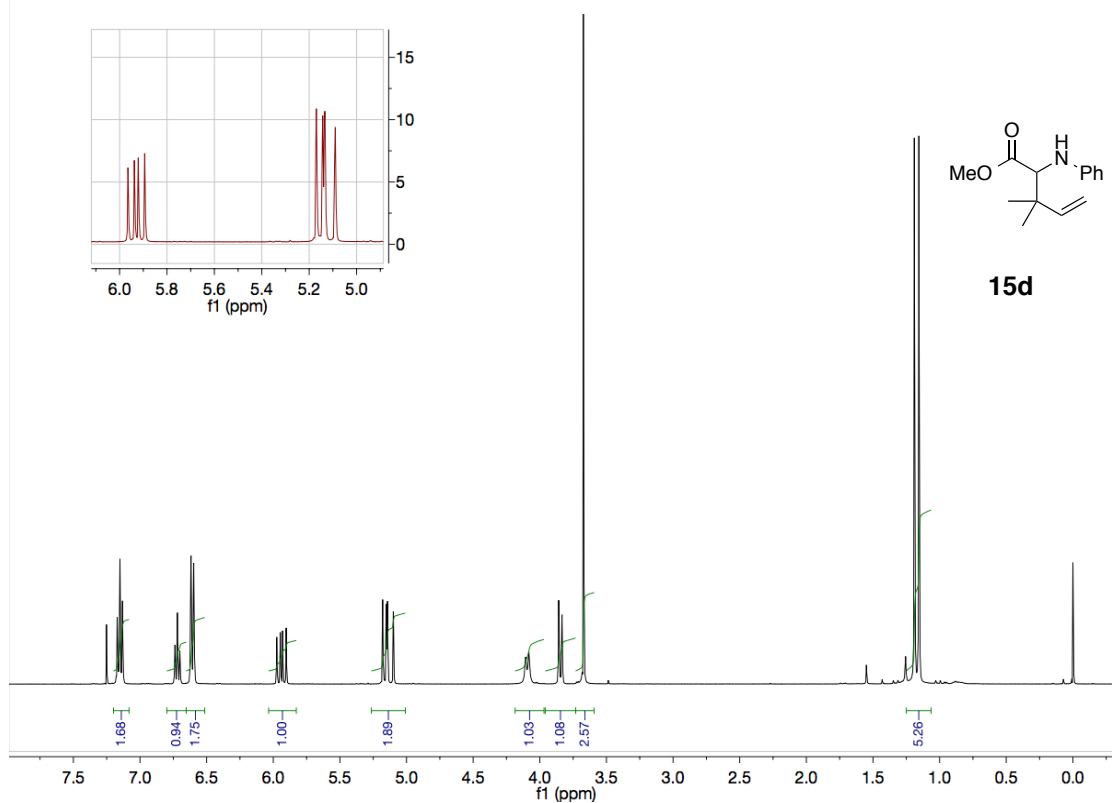
Solvent: cdcl3

Data collected on: Jan 13 2015

Agilent Technologies



RE-6-090-1  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

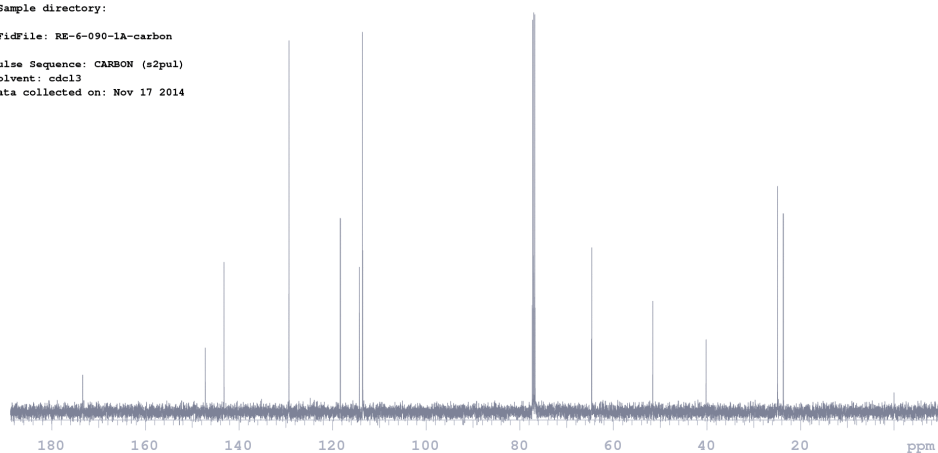
FidFile: RE-6-090-1A-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Nov 17 2014

Agilent Technologies





Proton Spectrum

Sample Name:

Data Collected on:

ga.chem.lsa.umich.edu-vnmrs400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

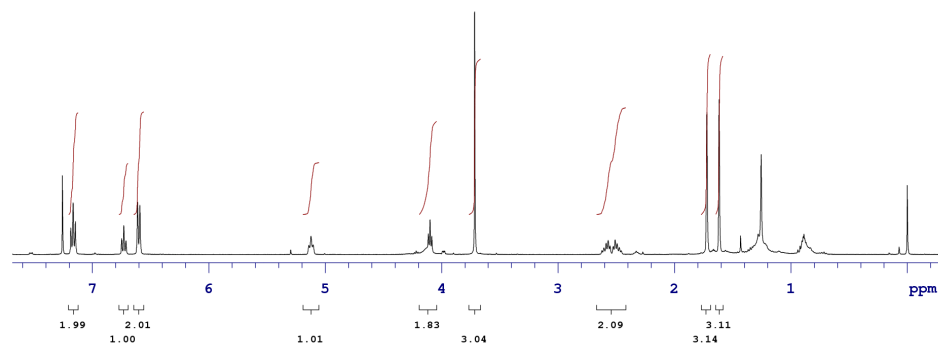
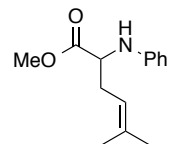
FidFile: RK-6-104-2B

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 28 2015

Agilent Technologies



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

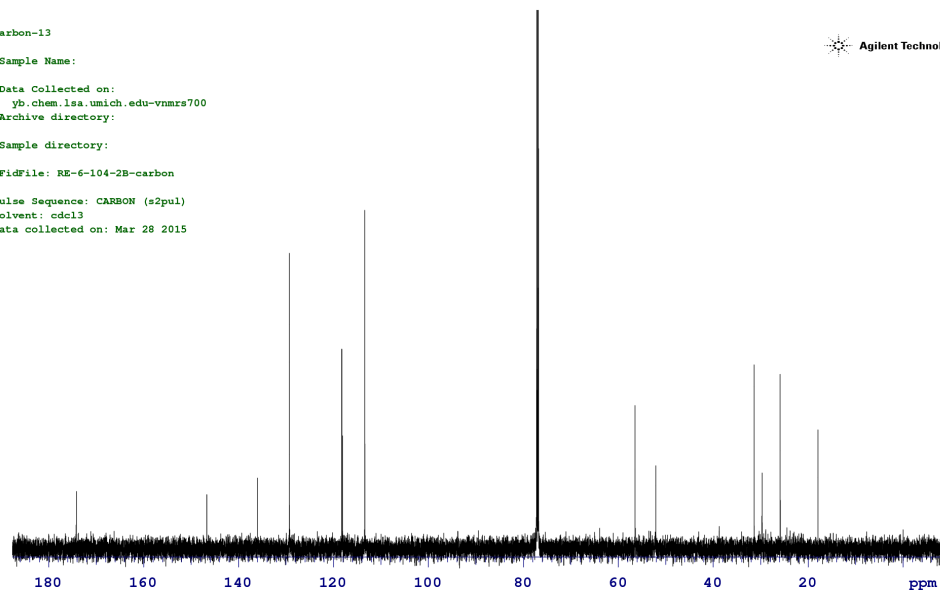
FidFile: RK-6-104-2B-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 28 2015

Agilent Technologies



Proton Spectrum

Sample Name:

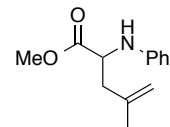
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

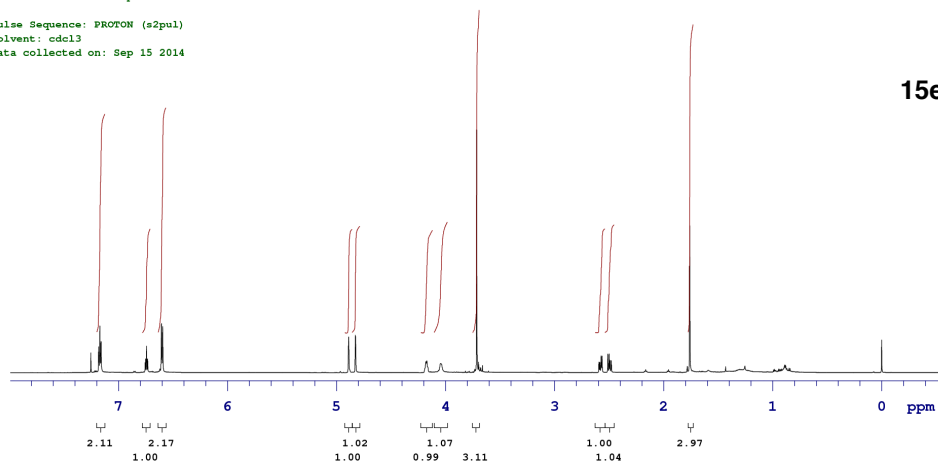
FidFile: RK-6-014-A-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 15 2014

Agilent Technologies



15e



Carbon-13

Sample Name:

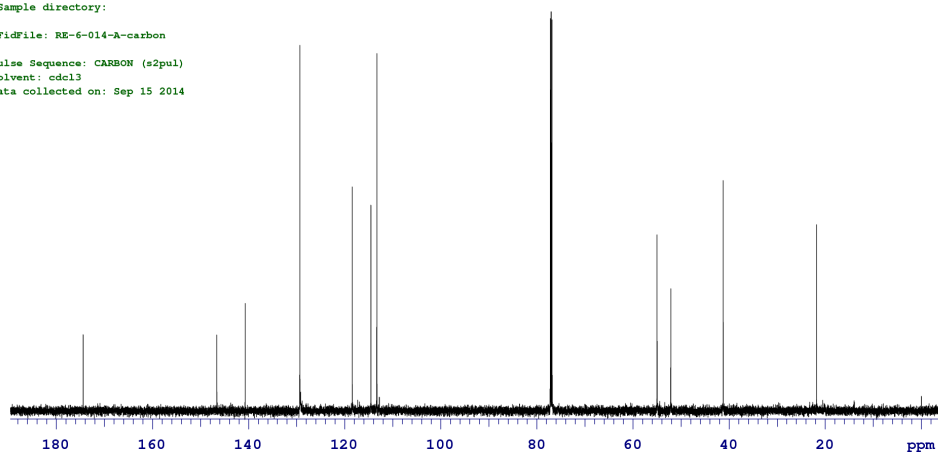
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

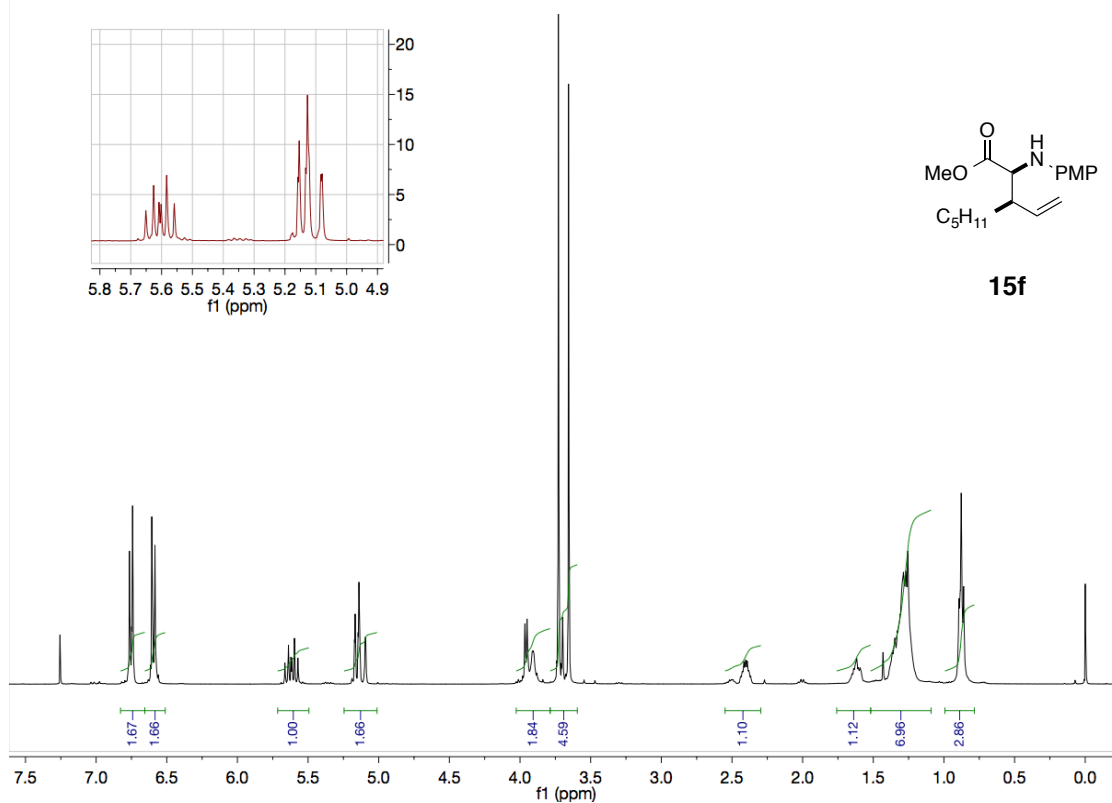
FidFile: RK-6-014-A-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 15 2014

Agilent Technologies



RE-6-090-2  
Proton Spectrum



Carbon-13

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vmrs500

Archive directory:

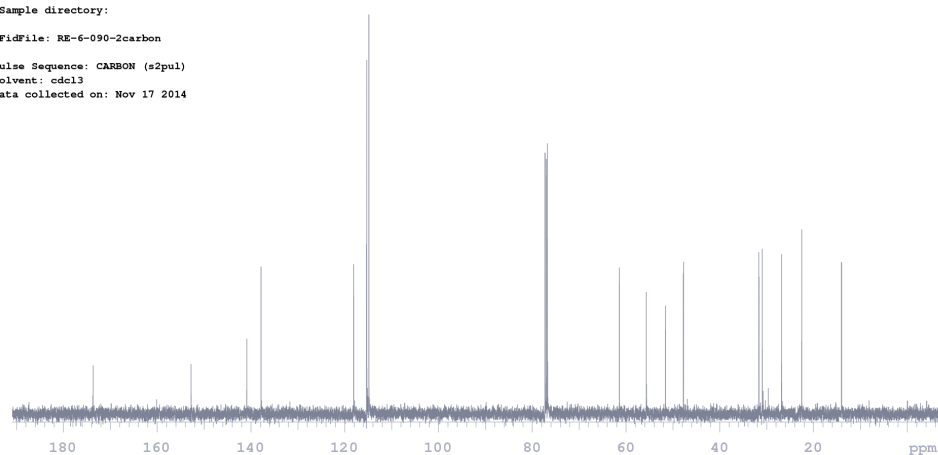
Sample directory:

FidFile: RE-6-090-2carbon

Pulse Sequence: CARBON (s2pul)

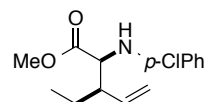
Solvent: cdcl3

Data collected on: Nov 17 2014

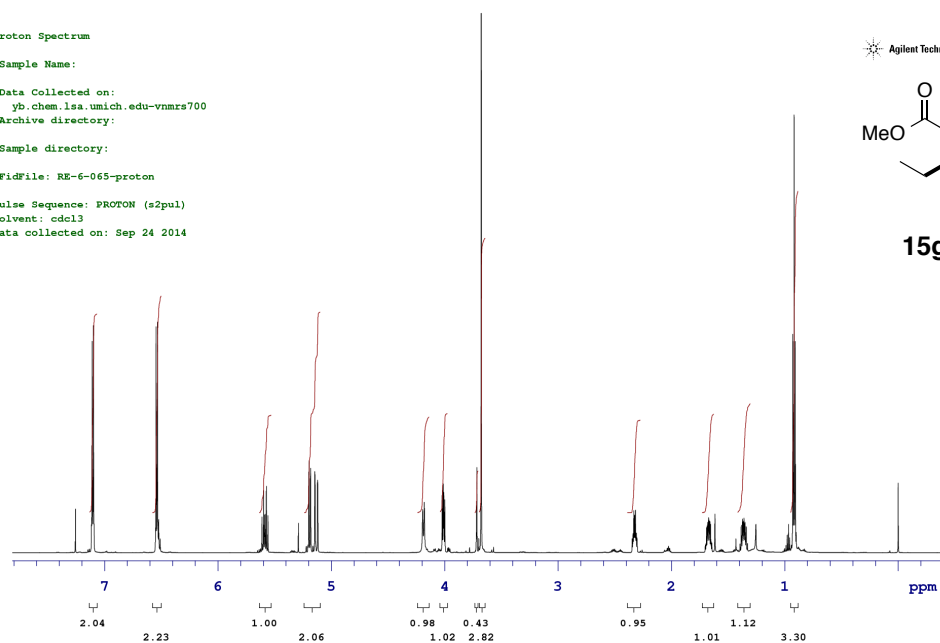


Proton Spectrum  
 Sample Name:  
 Data Collected on:  
 yb.chem.lsa.umich.edu-vnmrs700  
 Archive directory:  
 Sample directory:  
 FidFile: RK-6-065-proton  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Sep 24 2014

Agilent Technologies

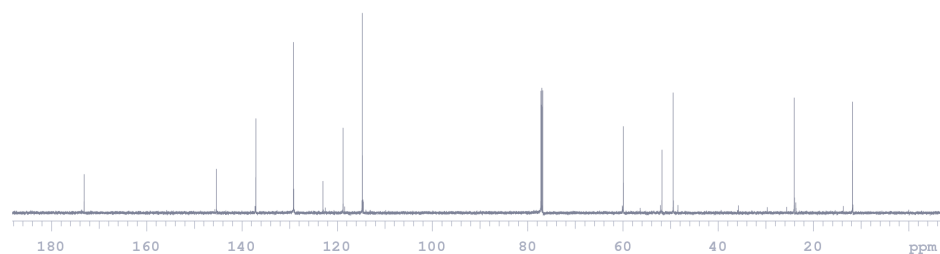


15g



Carbon-13  
 Sample Name:  
 Data Collected on:  
 yb.chem.lsa.umich.edu-vnmrs700  
 Archive directory:  
 Sample directory:  
 FidFile: RK-6-065-carbon  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Sep 24 2014

Agilent Technologies



Proton Spectrum

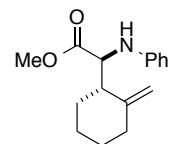
Sample Name:

Data Collected on:  
ga.chem.lsa.umich.edu-vnmrs400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

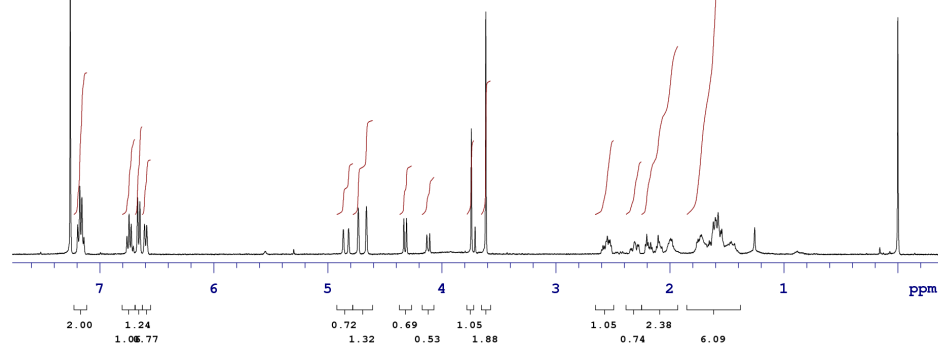
FidFile: RK-6-109-fr20

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 28 2015

Agilent Technologies



15h



Carbon-13

Sample Name:

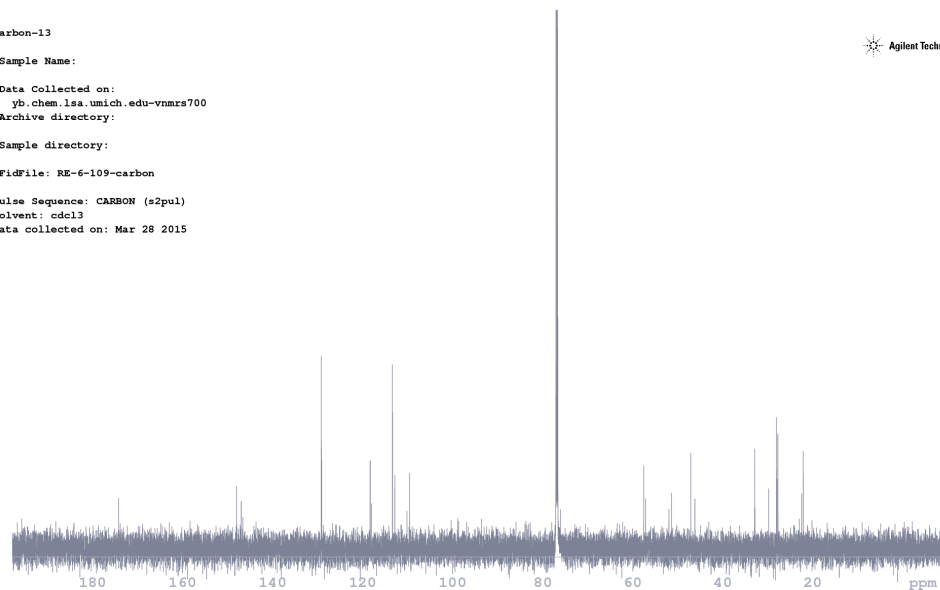
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

FidFile: RK-6-109-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 28 2015

Agilent Technologies



Proton Spectrum

Sample Name:

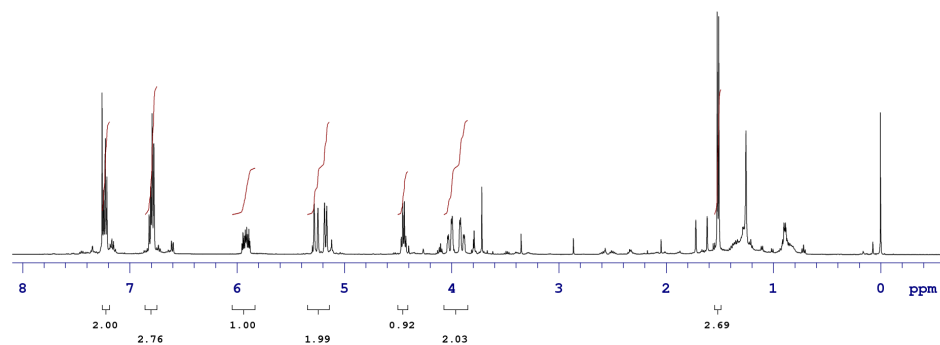
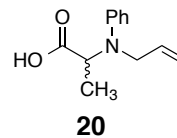
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: Re-6-120-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 20 2015

Agilent Technologies



Carbon-13

Sample Name:

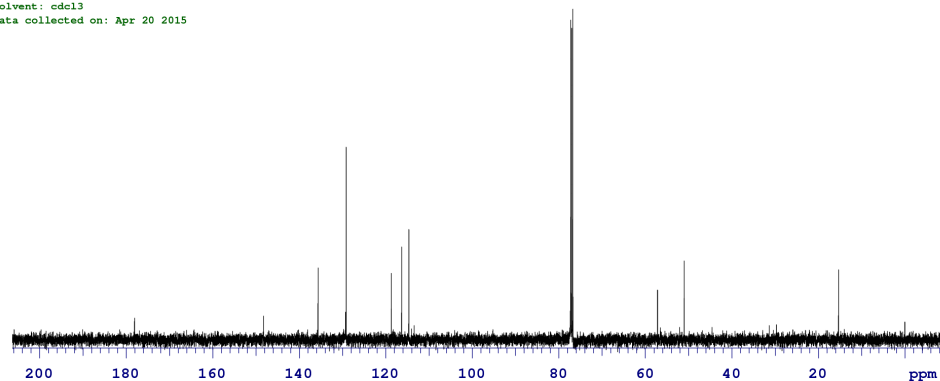
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: RE-6-120-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 20 2015

Agilent Technologies



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

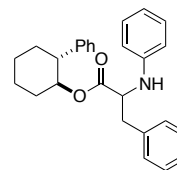
FidFile: RE-5-163-proton2

Pulse Sequence: PROTON (s2pul)

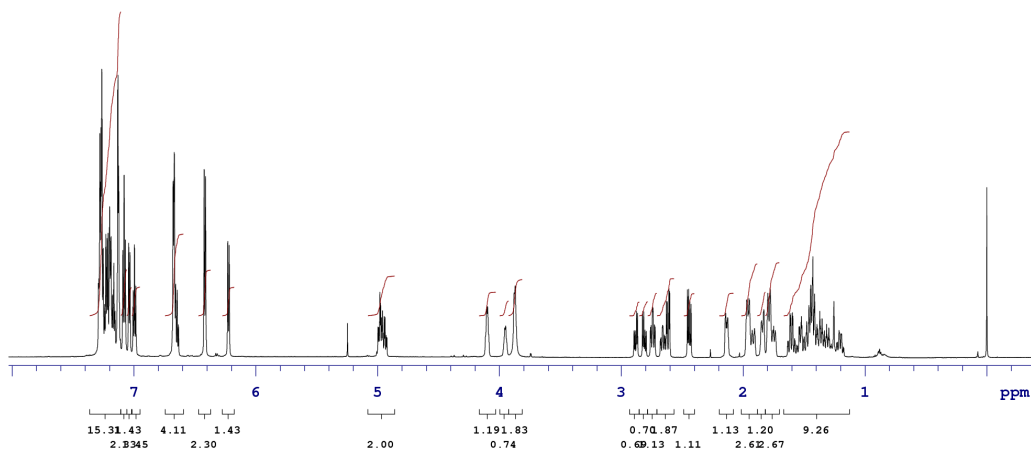
Solvent: cdcl3

Data collected on: May 16 2014

Agilent Technologies



22a



Carbon-13

Sample Name:

Data Collected on:

yb.chem.lsa.umich.edu-vnmrs700

Archive directory:

Sample directory:

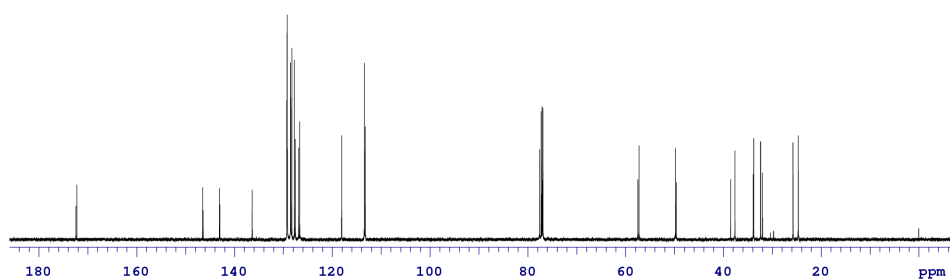
FidFile: RE-5-163-carbon2

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 16 2014

Agilent Technologies



Proton Spectrum

Sample Name:

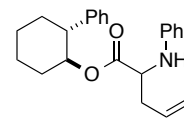
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

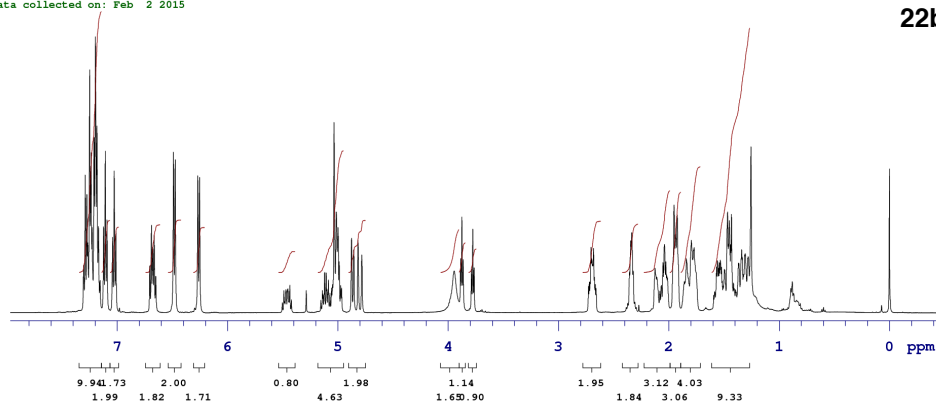
FidFile: RK-6-107-2-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 2 2015

Agilent Technologies



22b



Carbon-13

Sample Name:

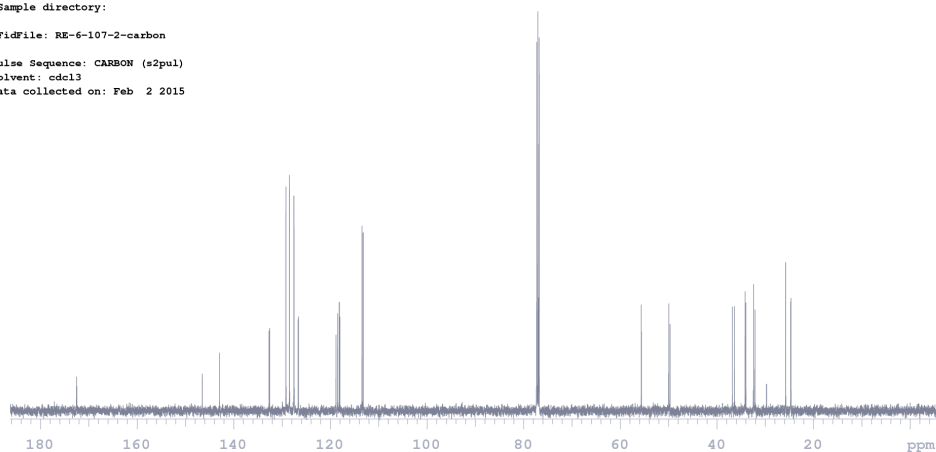
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: RK-6-107-2-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 2 2015

Agilent Technologies





Proton Spectrum

Sample Name:

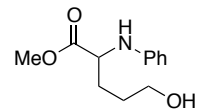
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

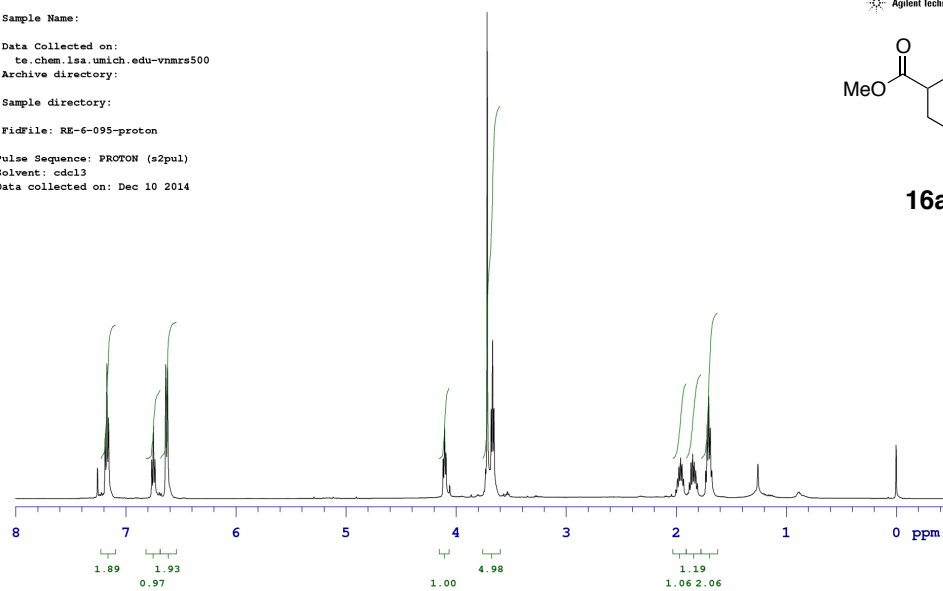
FidFile: RK-6-095-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 10 2014

Agilent Technologies



16a



Carbon-13

Sample Name:

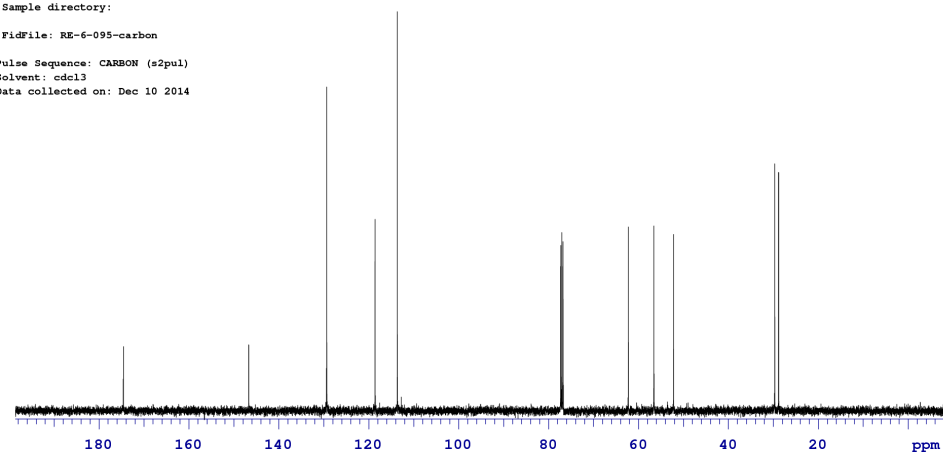
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: RK-6-095-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 10 2014

Agilent Technologies



Proton Spectrum

Sample Name:

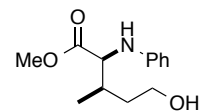
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

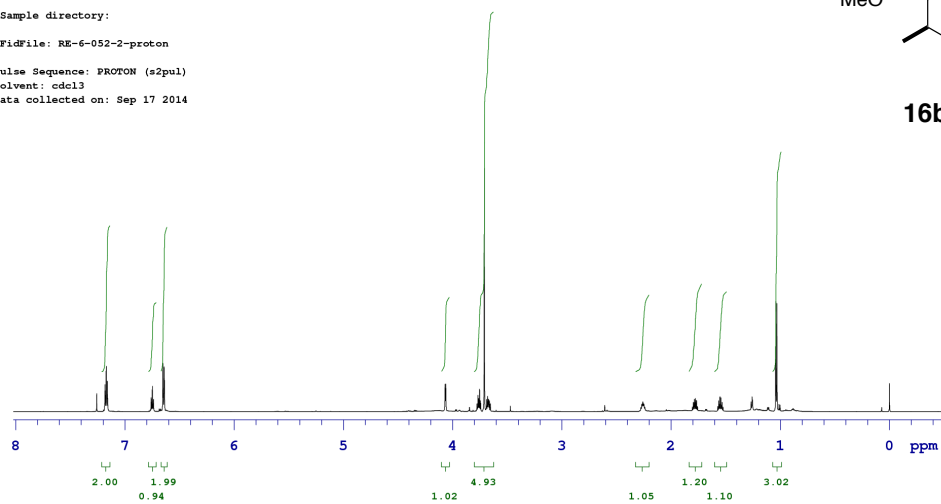
FidFile: RK-6-052-2-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 17 2014

Agilent Technologies



16b



Carbon-13

Sample Name:

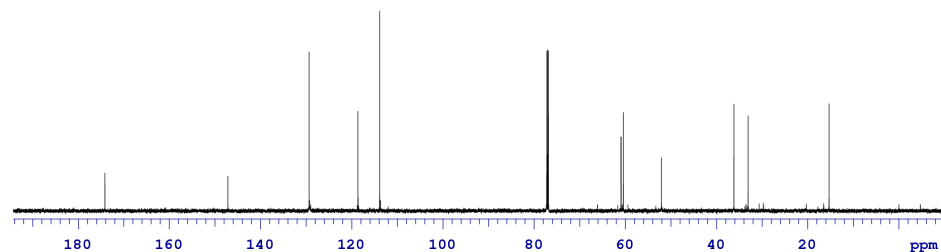
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

FidFile: RK-6-052-2-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 17 2014

Agilent Technologies



Proton Spectrum

Sample Name:

Data Collected on:

ga.chem.lsa.umich.edu-vnmrs400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

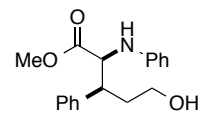
FidFile: RK-6-102-2-proton

Pulse Sequence: PROTON (s2pul)

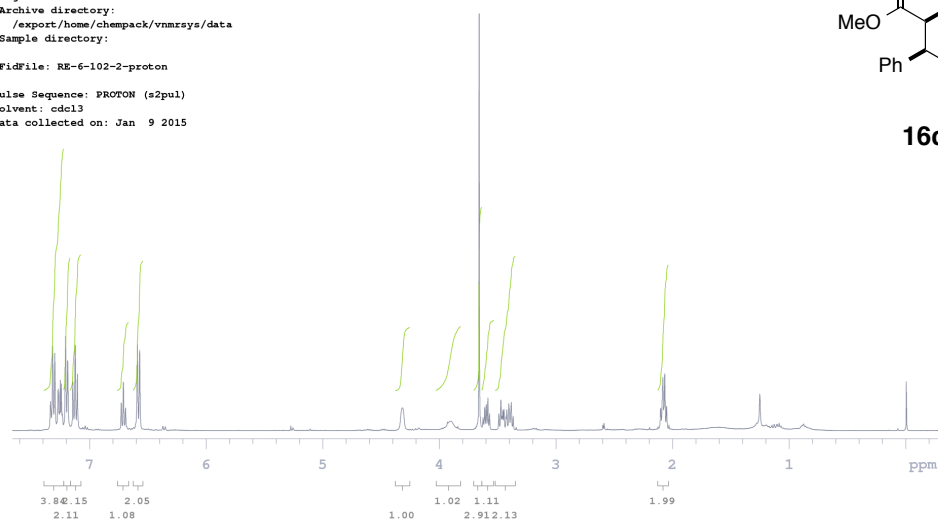
Solvent: cdcl3

Data collected on: Jan 9 2015

Agilent Technologies



**16c**



Automated Probe tuning parameter

Sample Name:

Data Collected on:

te.chem.lsa.umich.edu-vnmrs500

Archive directory:

Sample directory:

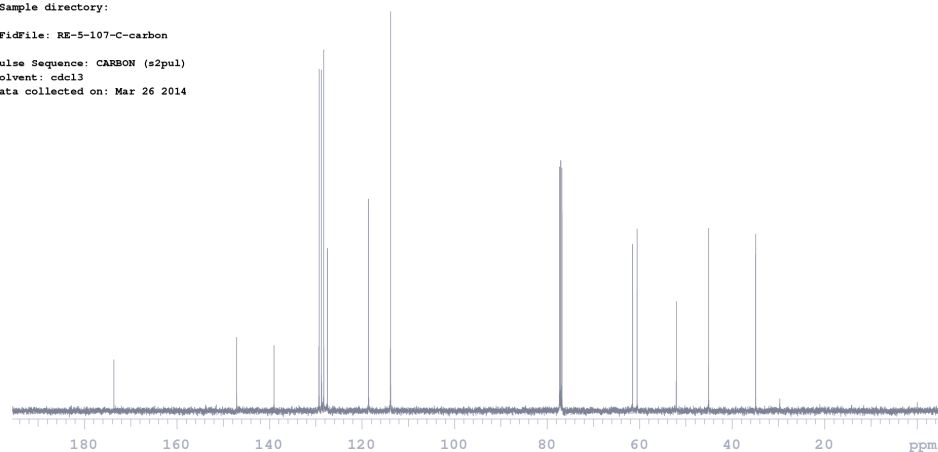
FidFile: RK-5-107-C-carbon

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 26 2014

Agilent Technologies



Proton Spectrum

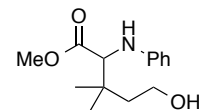
Sample Name:

Data Collected on:  
ga.chem.lsa.umich.edu-vnmrs400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: RK-6-059

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 23 2014

Agilent Technologies



16d

Carbon-13

Sample Name:

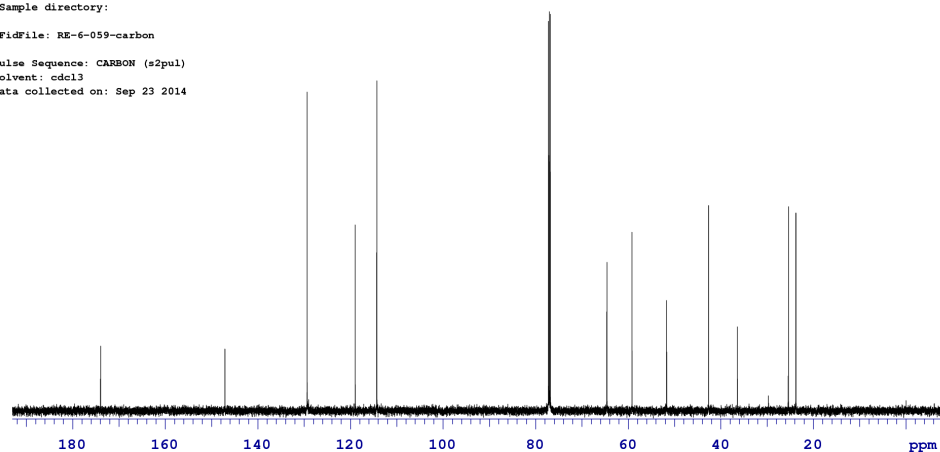
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

FidFile: RK-6-059-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 23 2014

Agilent Technologies



Proton Spectrum

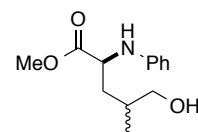
Sample Name:

Data Collected on:  
ga.chem.lsa.umich.edu-vnmrs400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

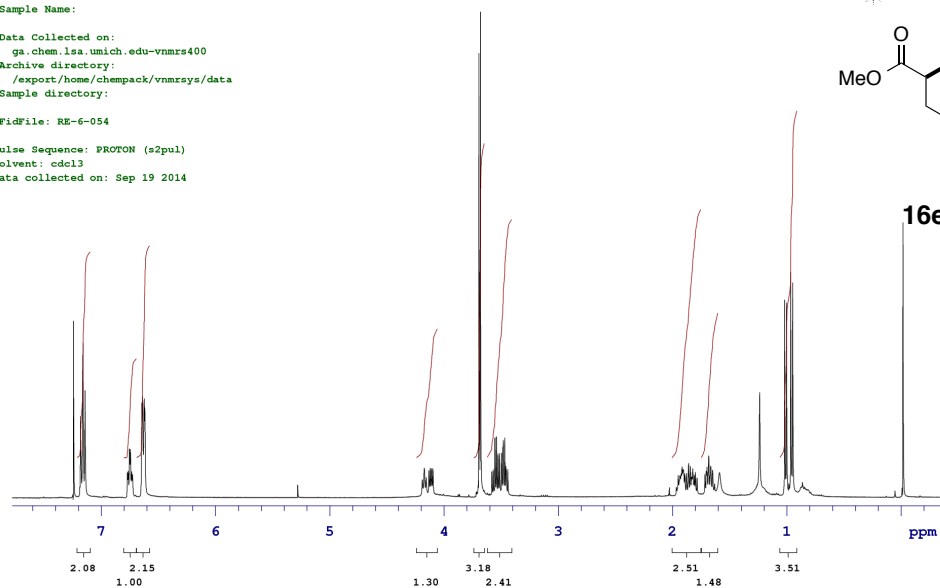
FidFile: RK-6-054

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 19 2014

Agilent Technologies



16e



Carbon-13

Sample Name:

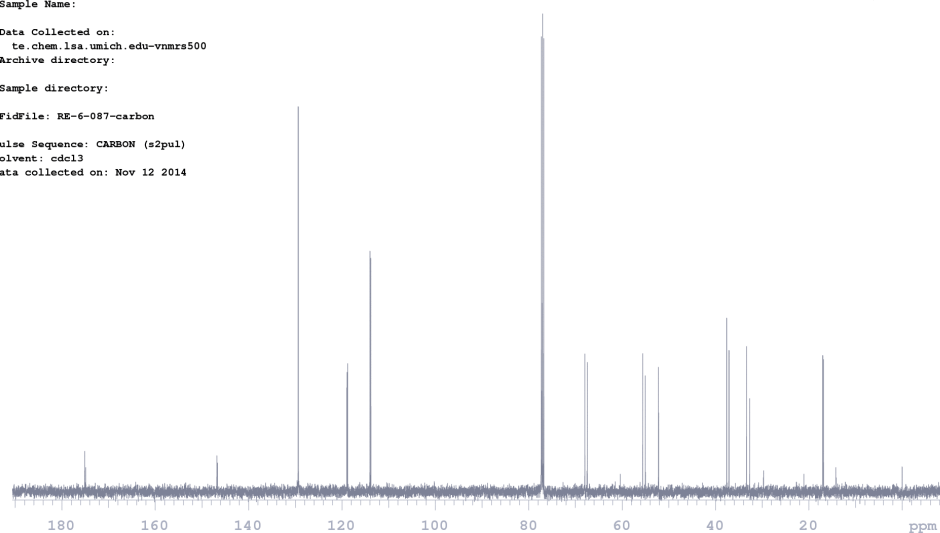
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: RK-6-087-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 12 2014

Agilent Technologies



Proton Spectrum

Sample Name:

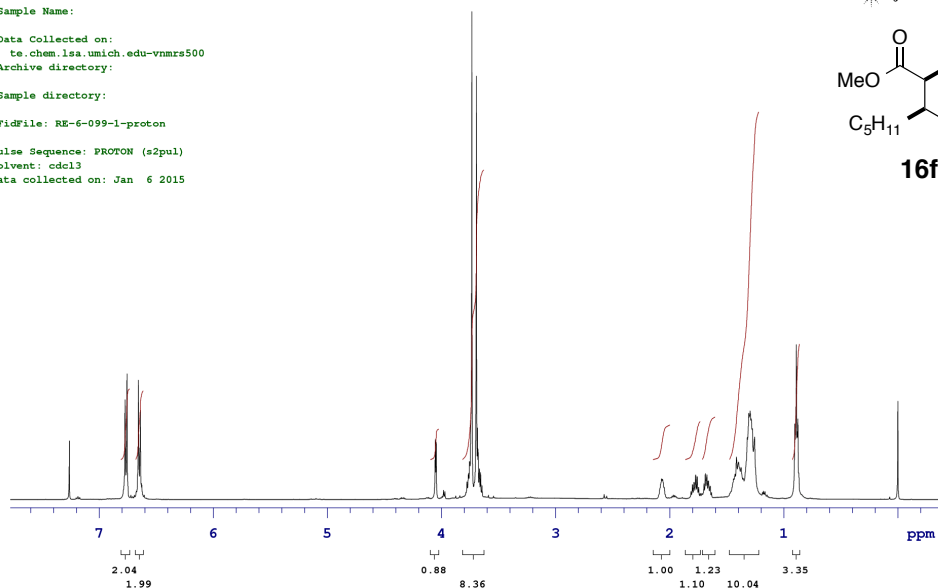
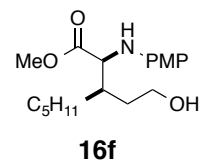
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: RK-6-099-1-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 6 2015

Agilent Technologies



Carbon-13

Sample Name:

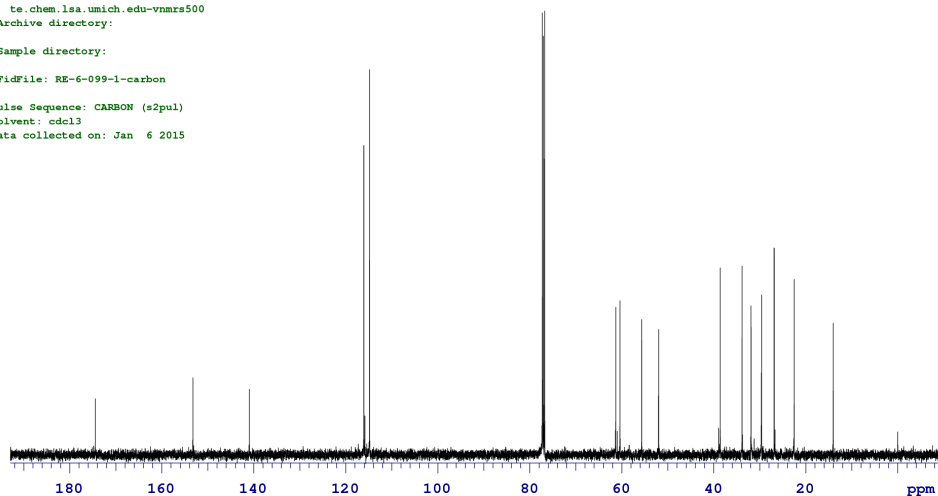
Data Collected on:  
te.chem.lsa.umich.edu-vnmrs500  
Archive directory:

Sample directory:

FidFile: RK-6-099-1-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 6 2015

Agilent Technologies



Proton Spectrum

Sample Name:

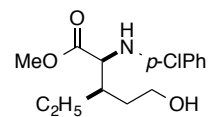
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

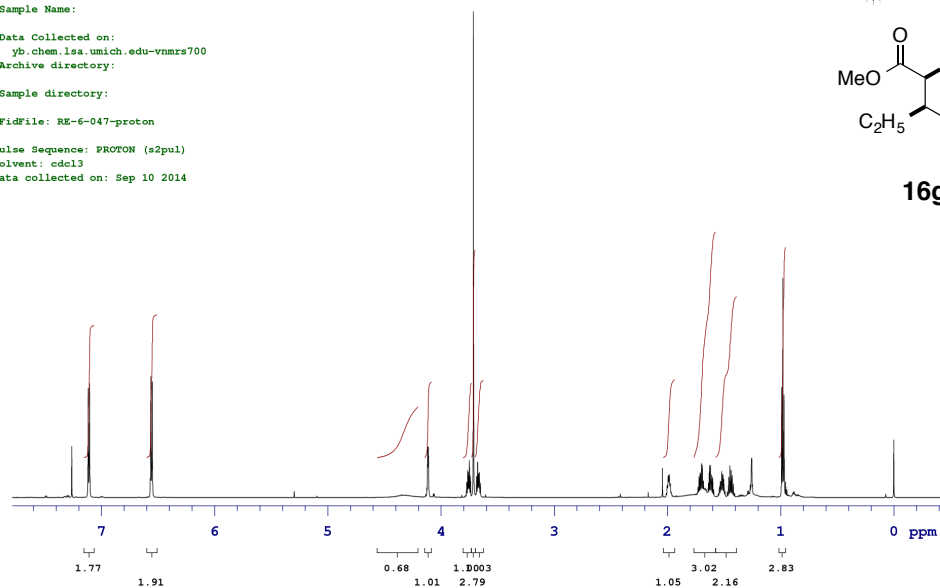
FidFile: RK-6-047-proton

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 10 2014

Agilent Technologies



16g



Carbon-13

Sample Name:

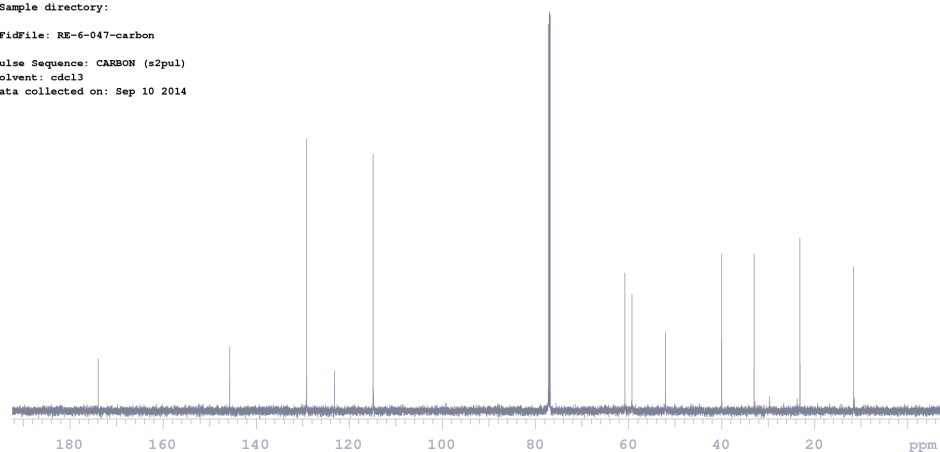
Data Collected on:  
yb.chem.lsa.umich.edu-vnmrs700  
Archive directory:

Sample directory:

FidFile: RK-6-047-carbon

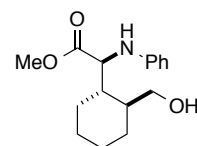
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 10 2014

Agilent Technologies

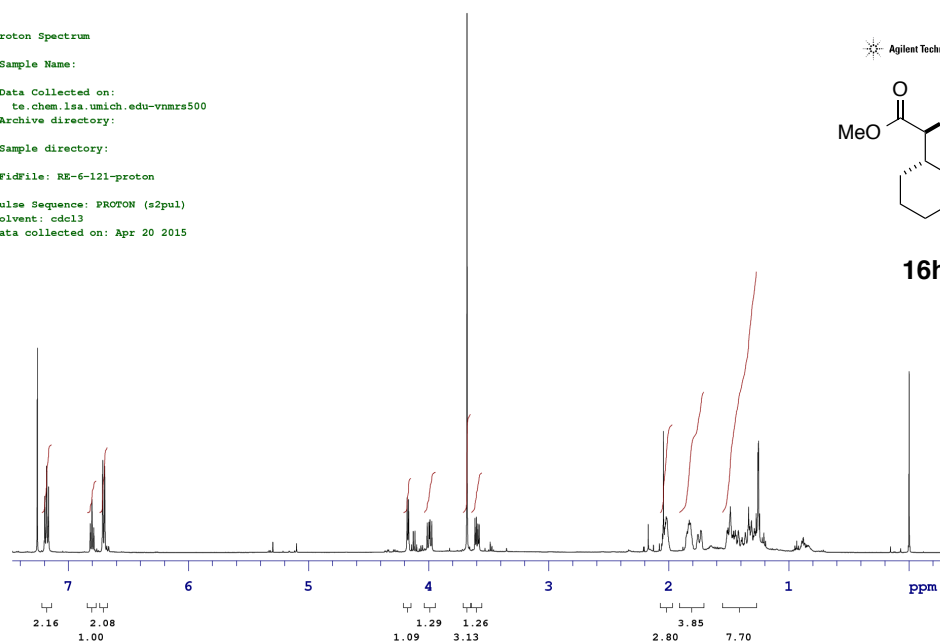


Proton Spectrum  
 Sample Name:  
 Data Collected on:  
 te.chem.lsa.umich.edu-vnmrs500  
 Archive directory:  
 Sample directory:  
 FidFile: RK-6-121-proton  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Apr 20 2015

Agilent Technologies



**16h**



Carbon-13  
 Sample Name:  
 Data Collected on:  
 te.chem.lsa.umich.edu-vnmrs500  
 Archive directory:  
 Sample directory:  
 FidFile: RK-6-121-carbon  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Apr 20 2015

Agilent Technologies

