

Three-Step Synthesis of 2,5,7-Trisubstituted Indoles from *N*-Acetyl-2,4,6-trichloroaniline Using Pd-Catalyzed Site-Selective Cross-Couplings

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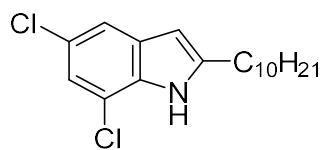
Email: manabe@u-shizuoka-ken.ac.jp

Supporting Information

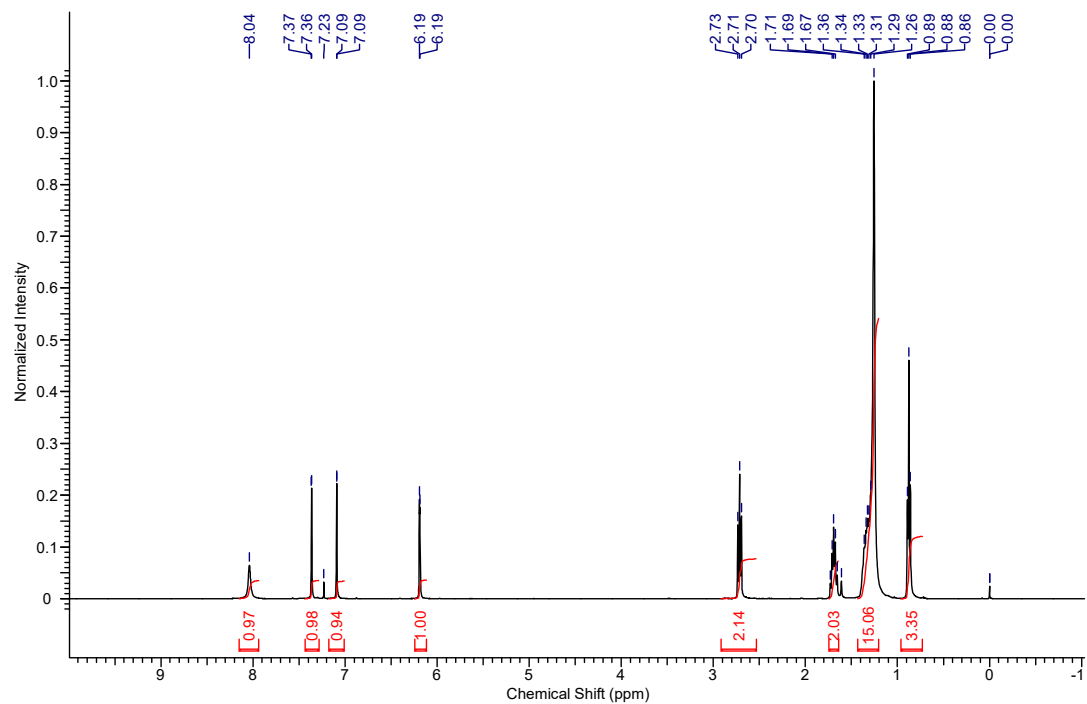
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1. NMR spectra of the products

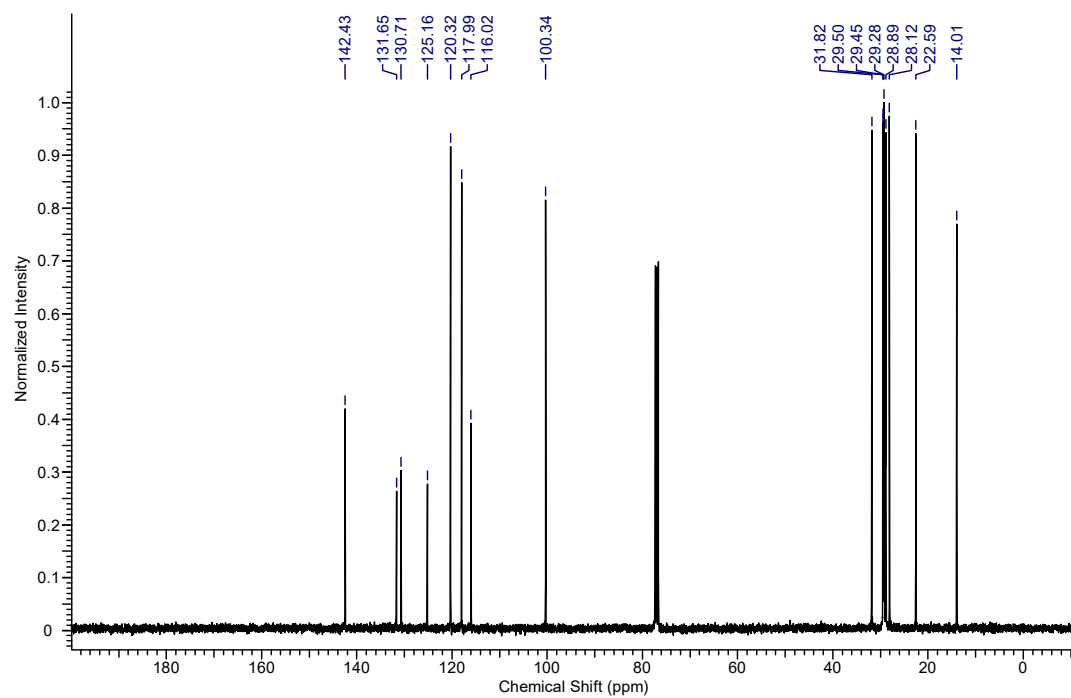


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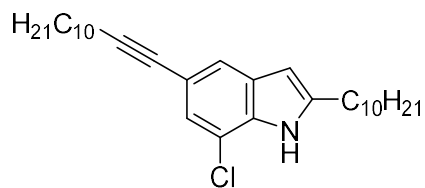
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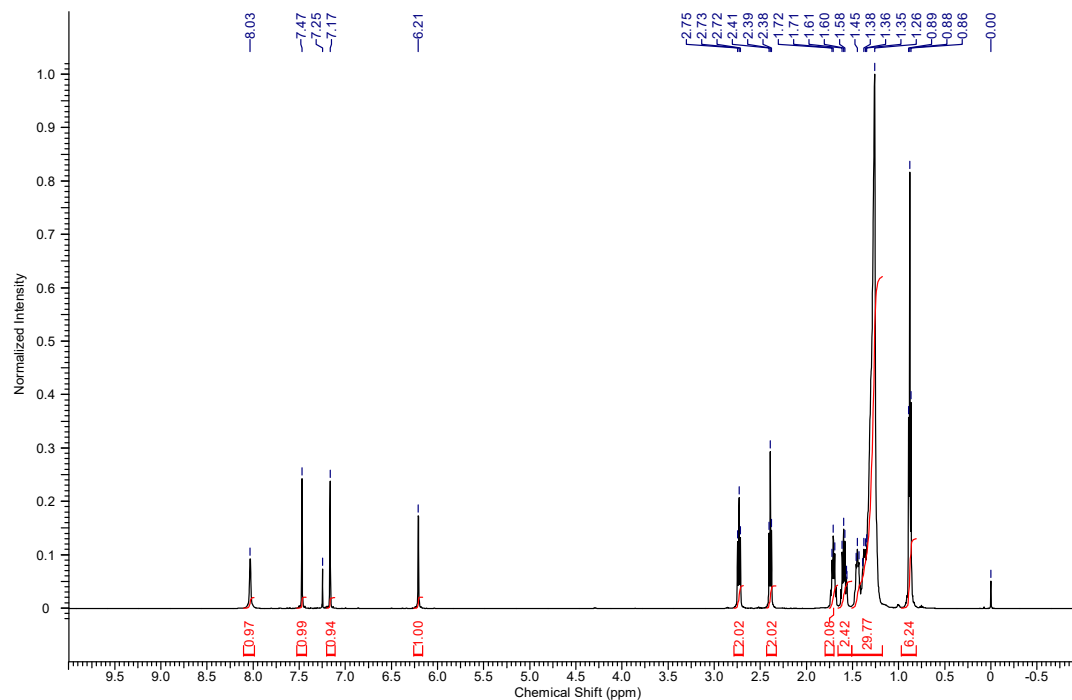


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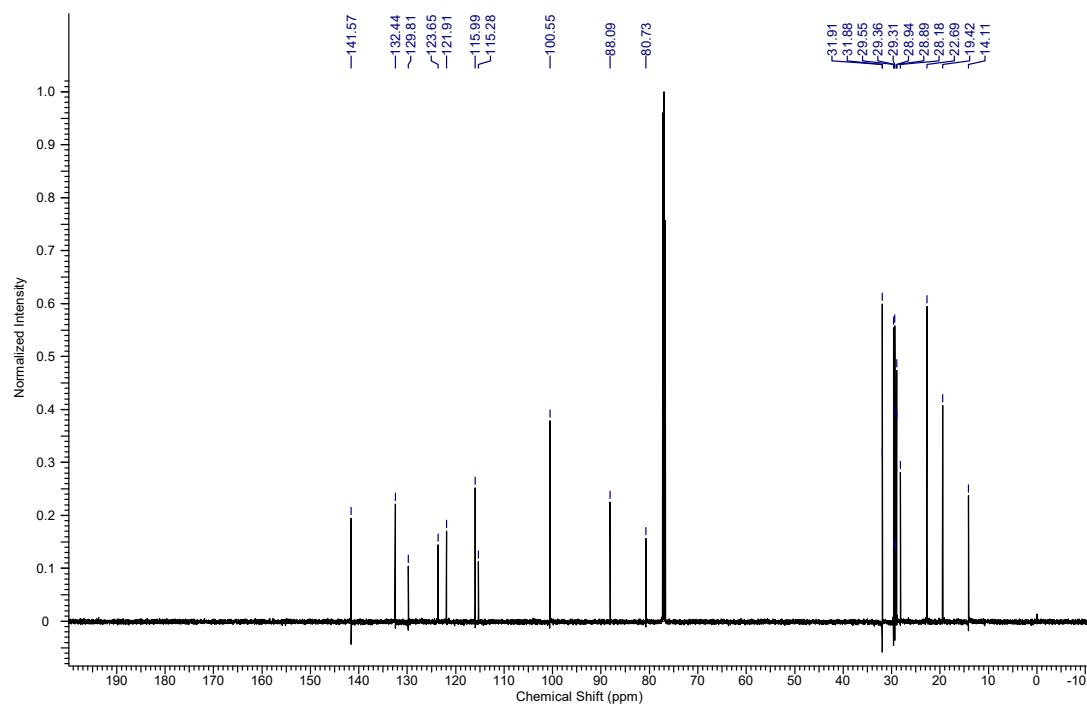


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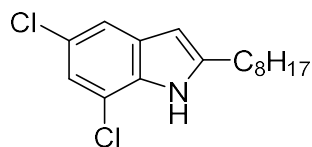
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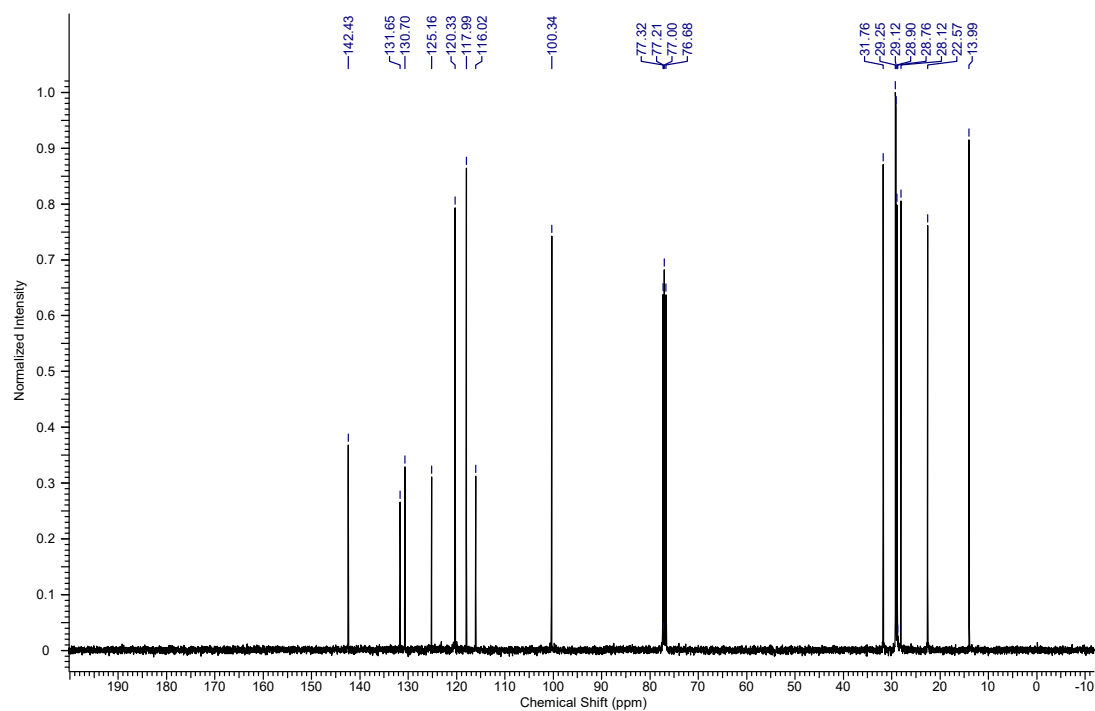
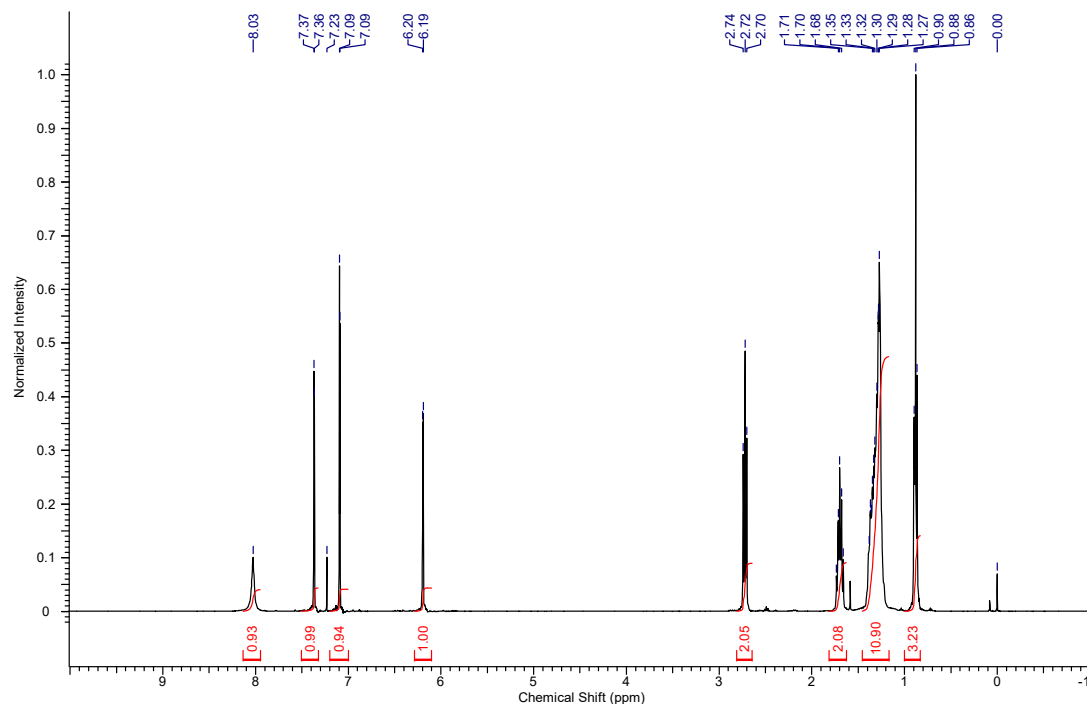


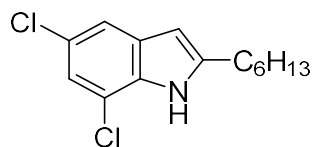
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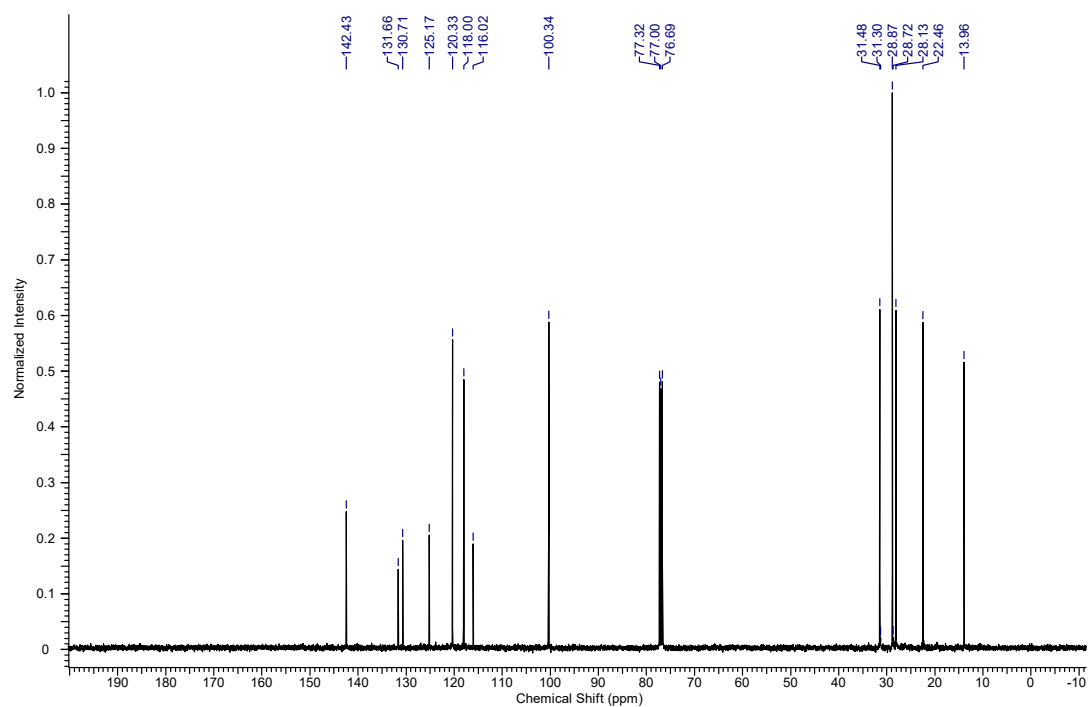
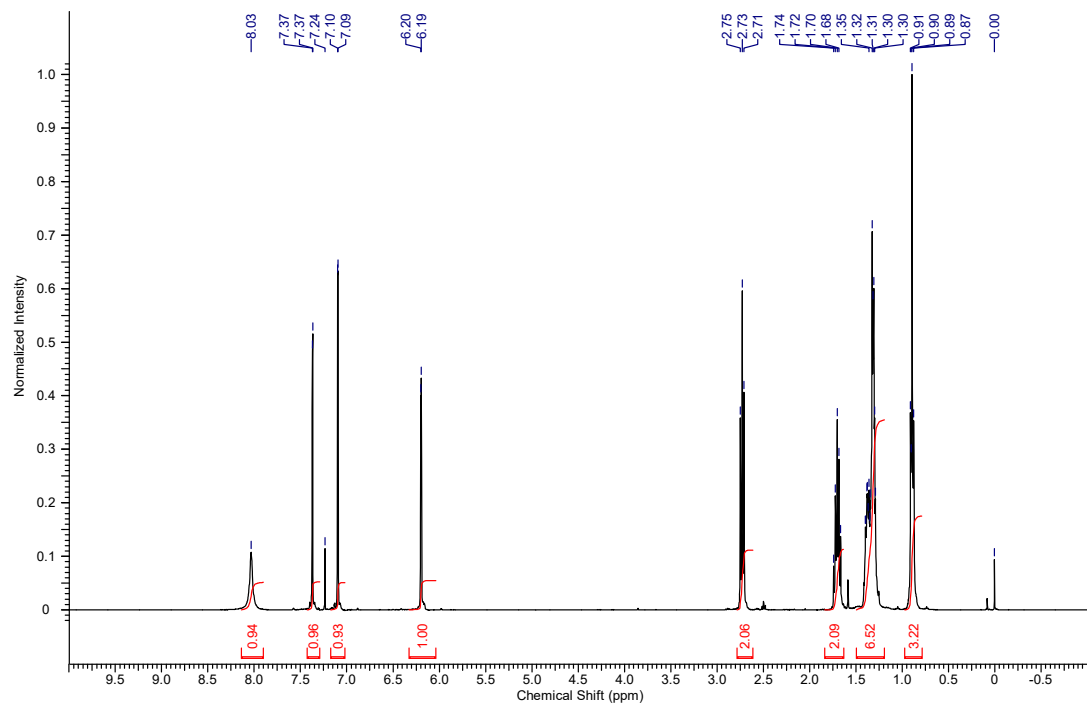


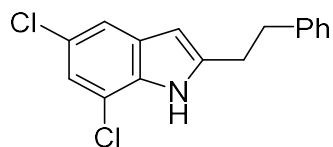
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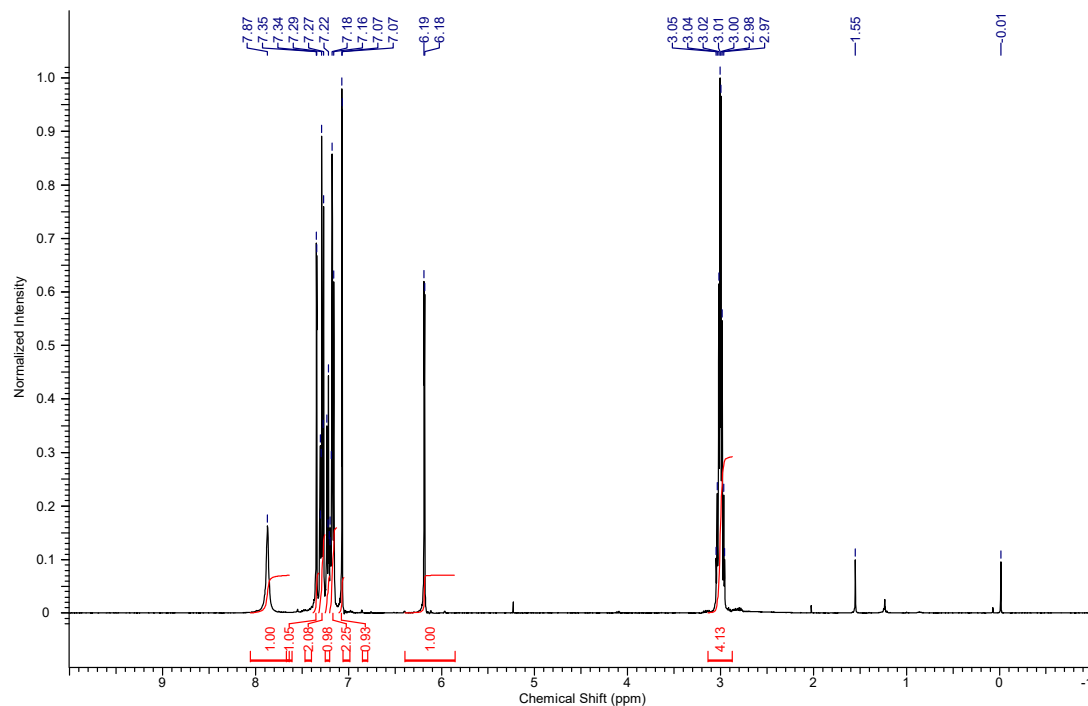


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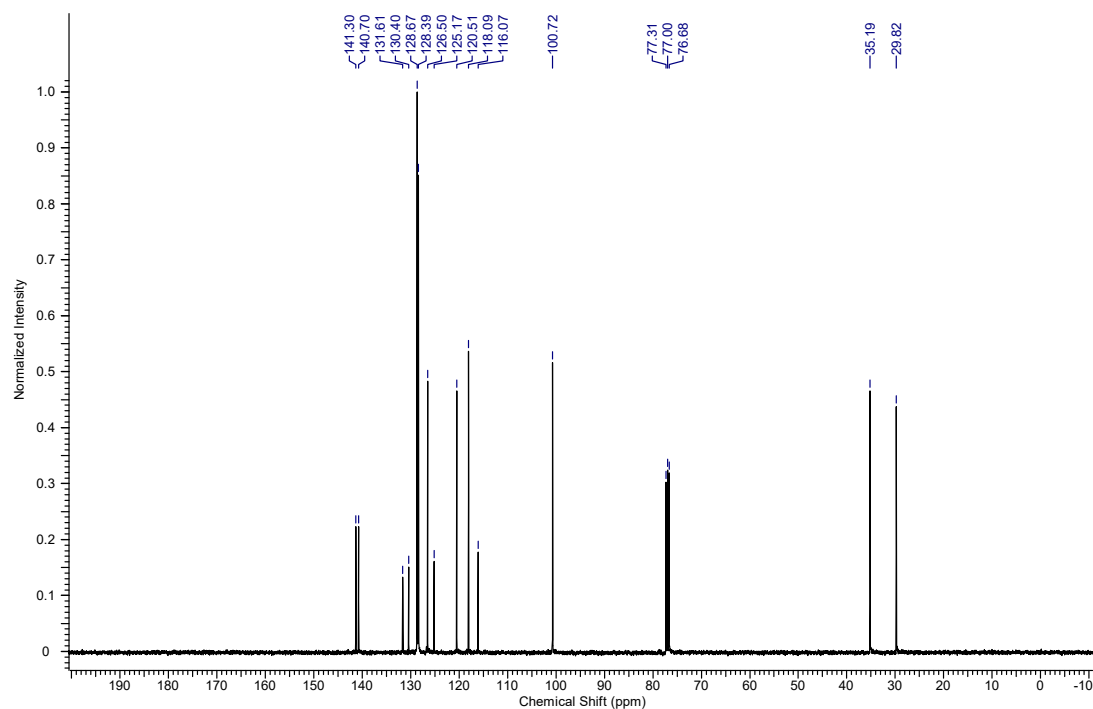


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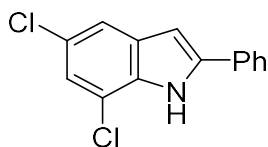
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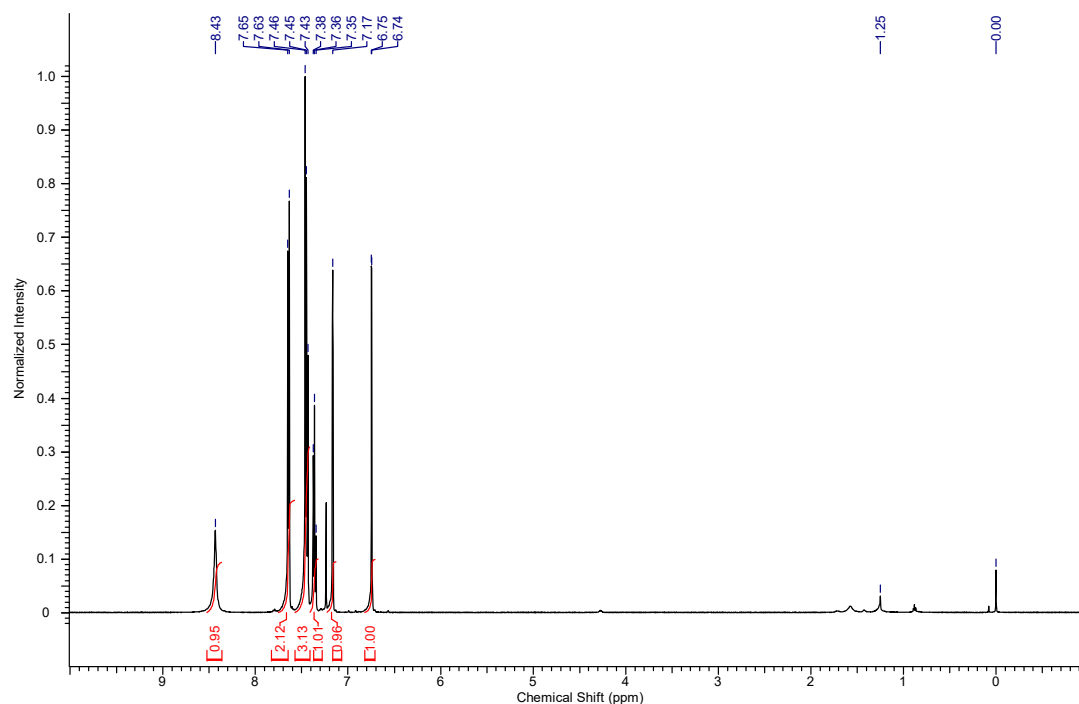


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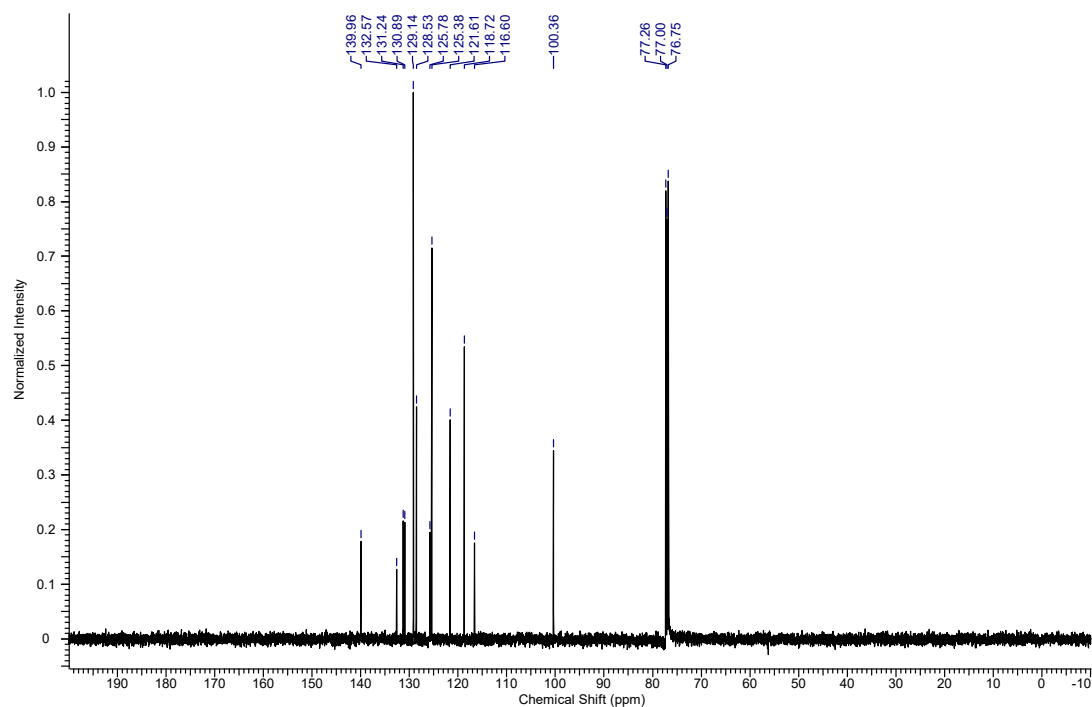
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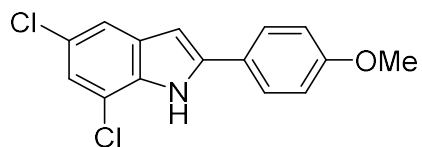
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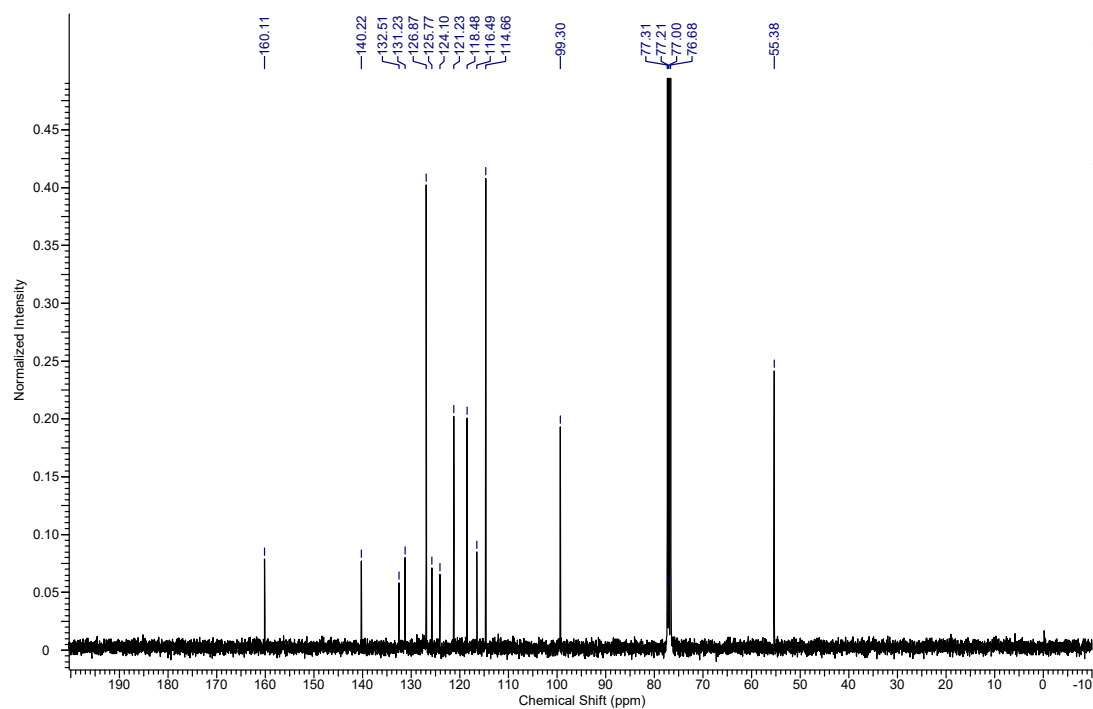
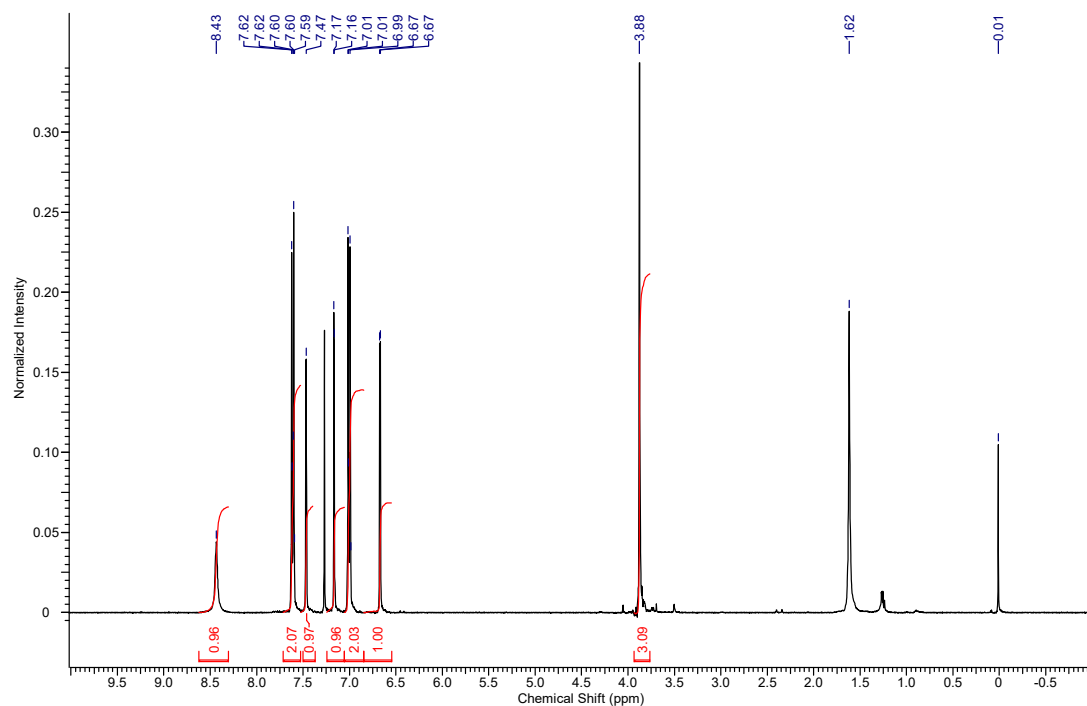
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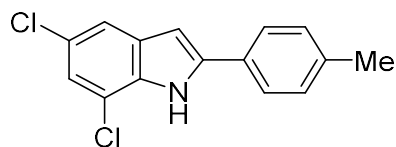


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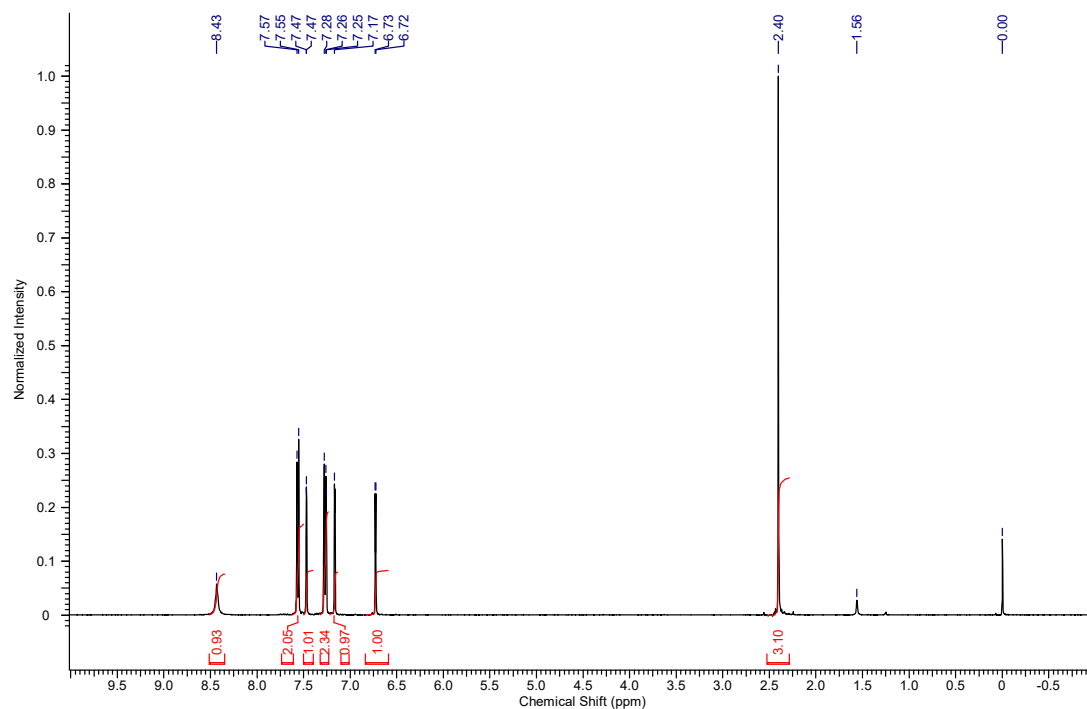


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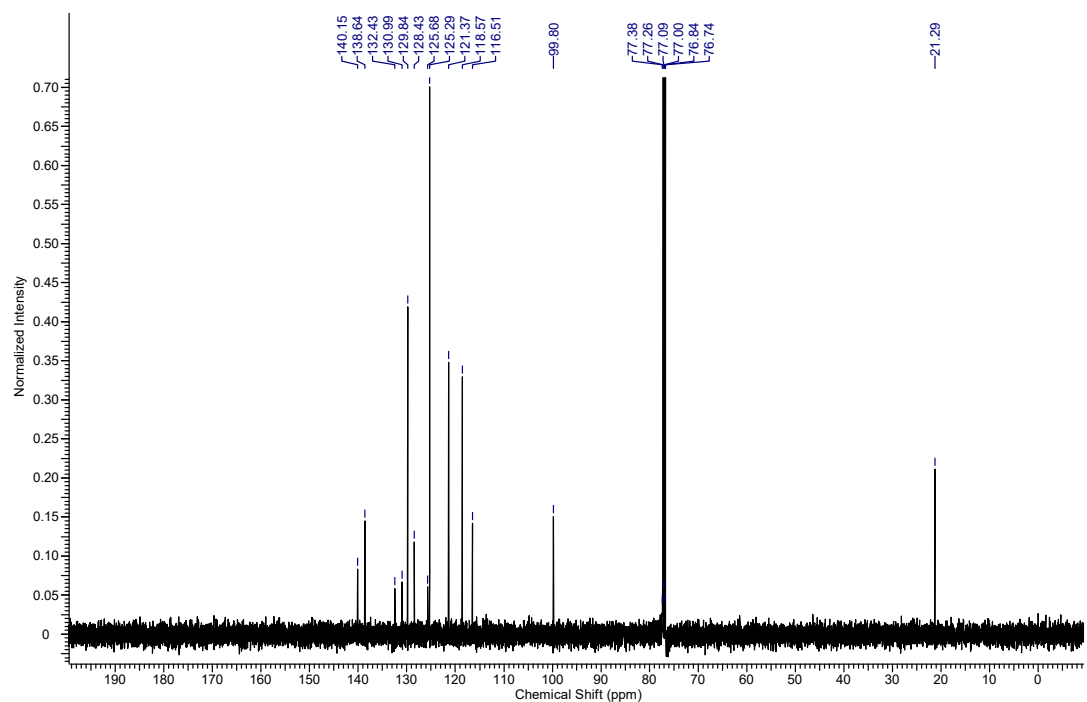




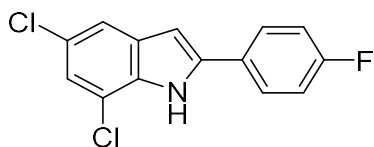
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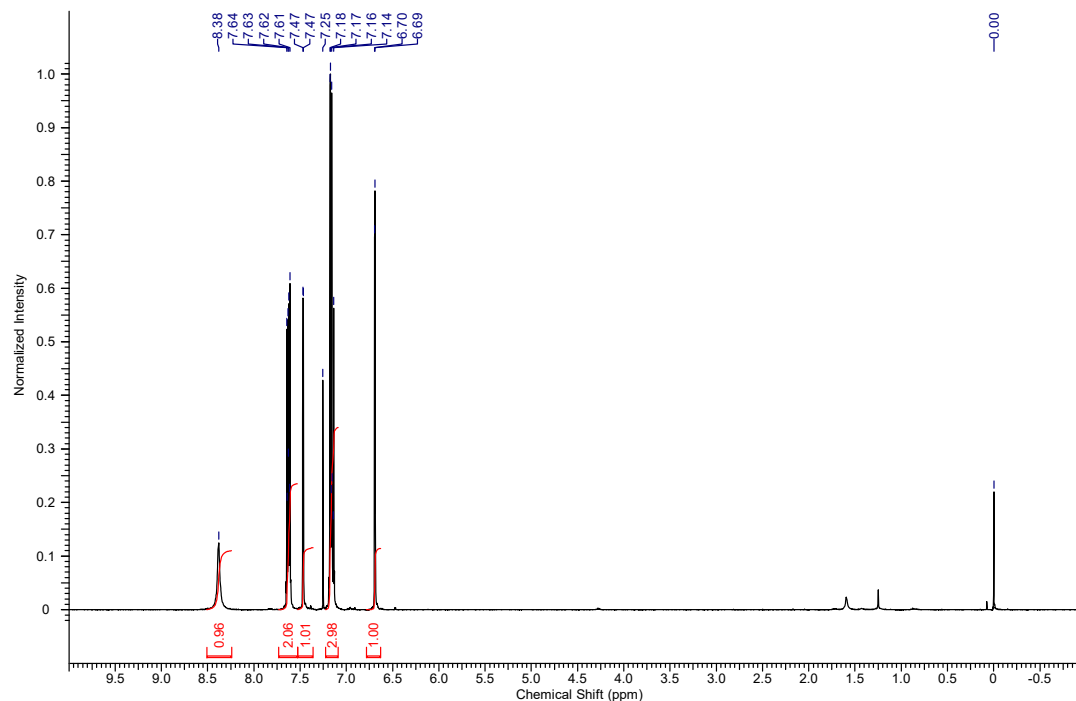
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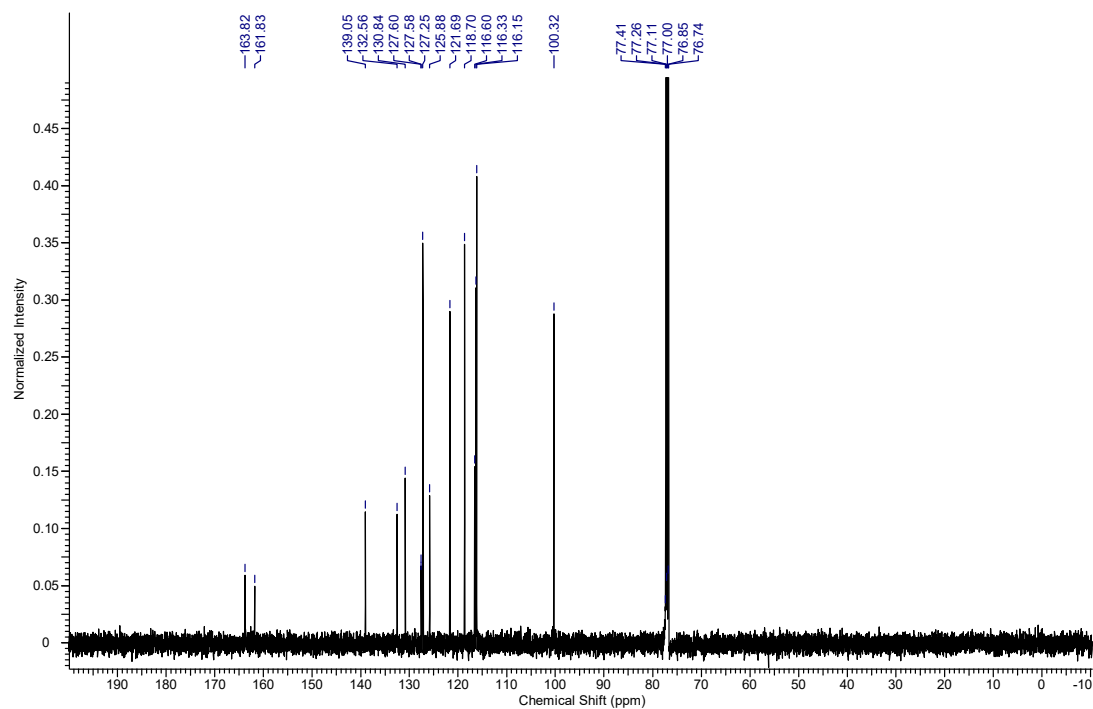
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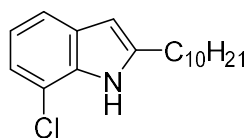
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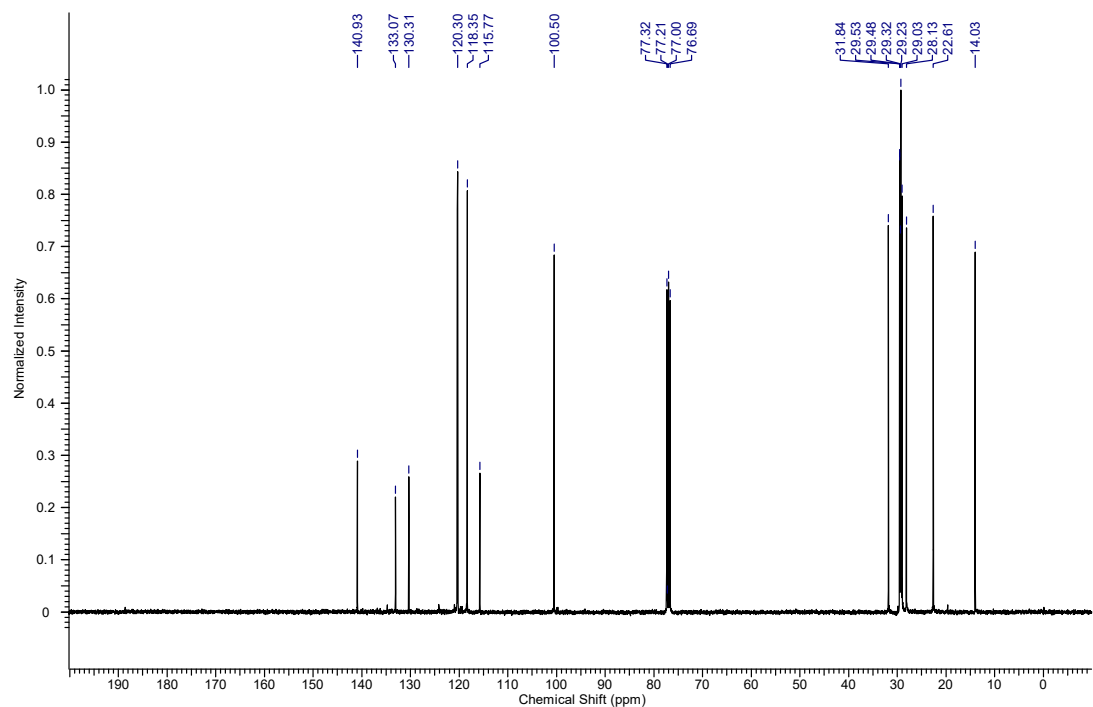
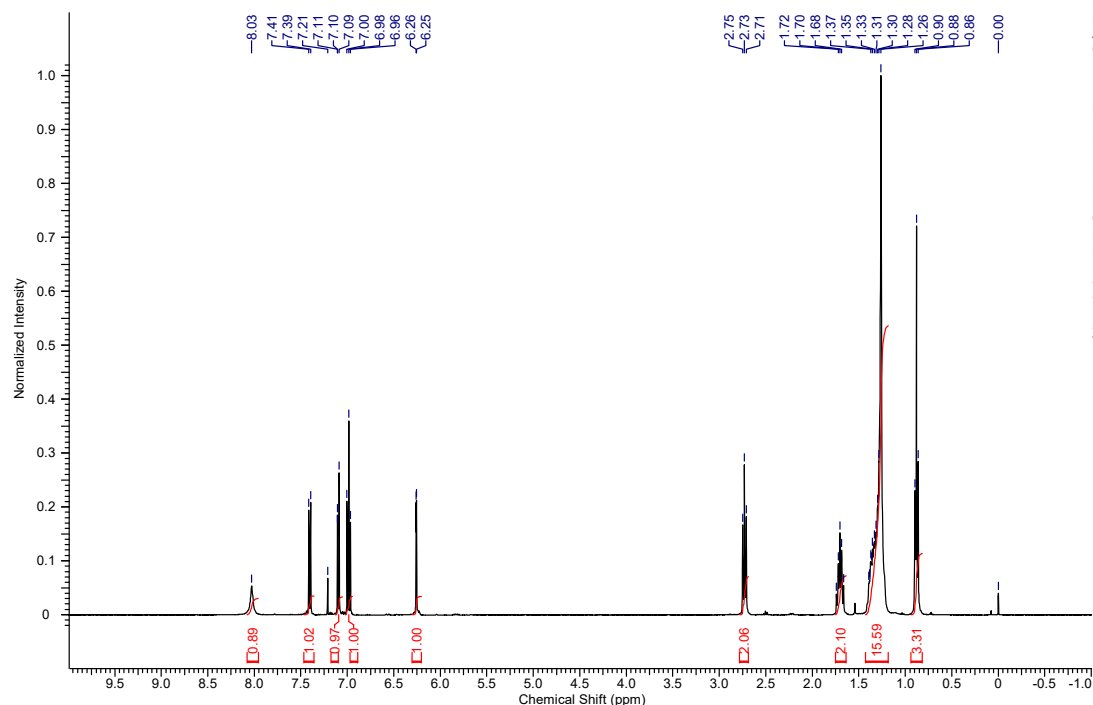
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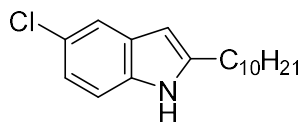


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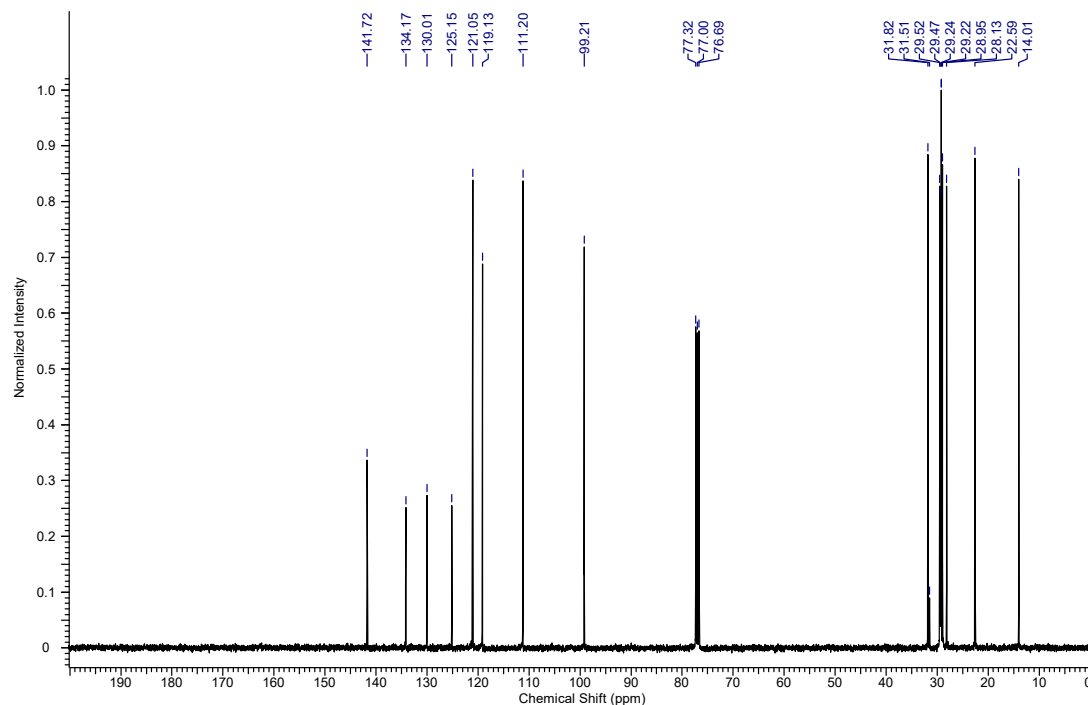
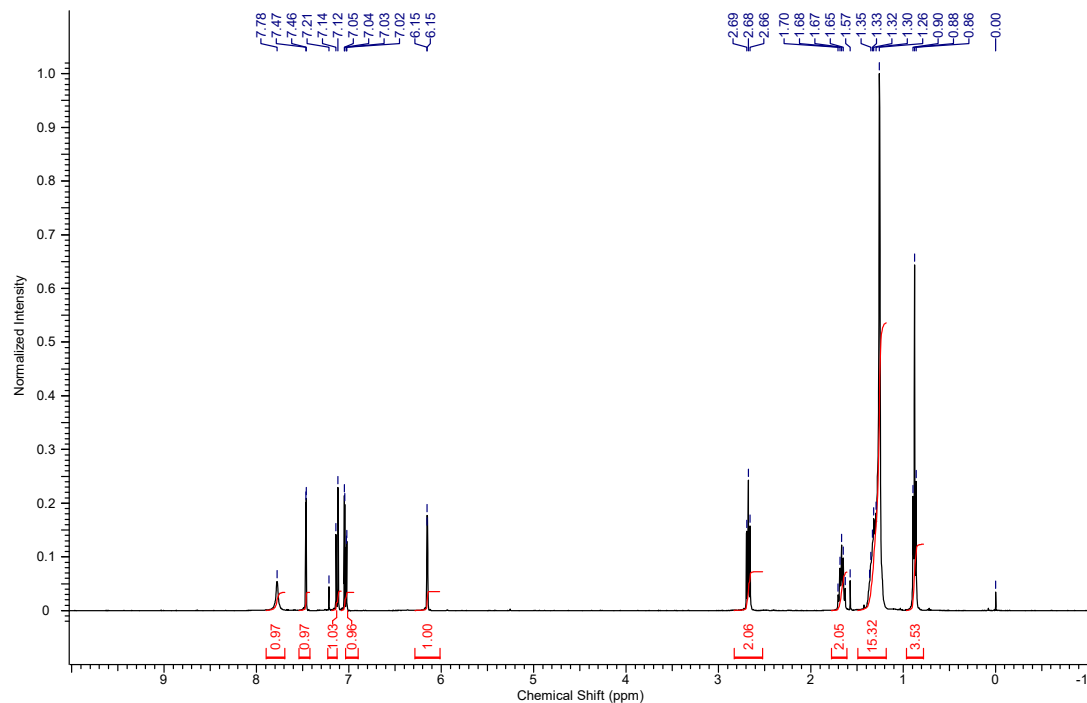


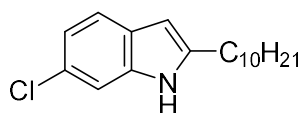
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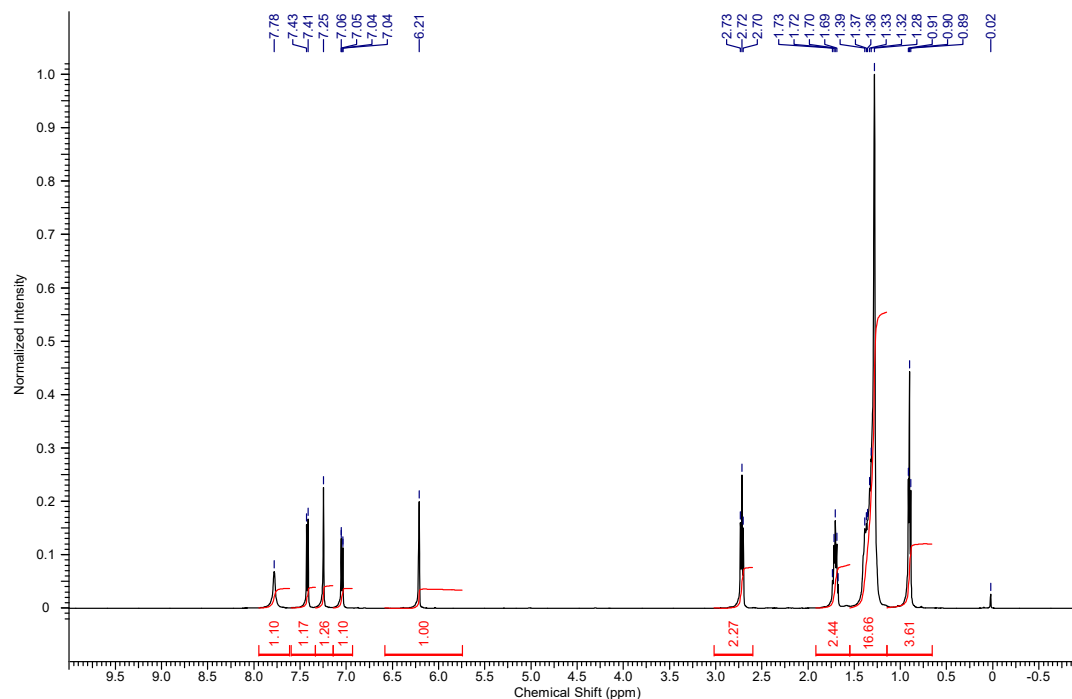


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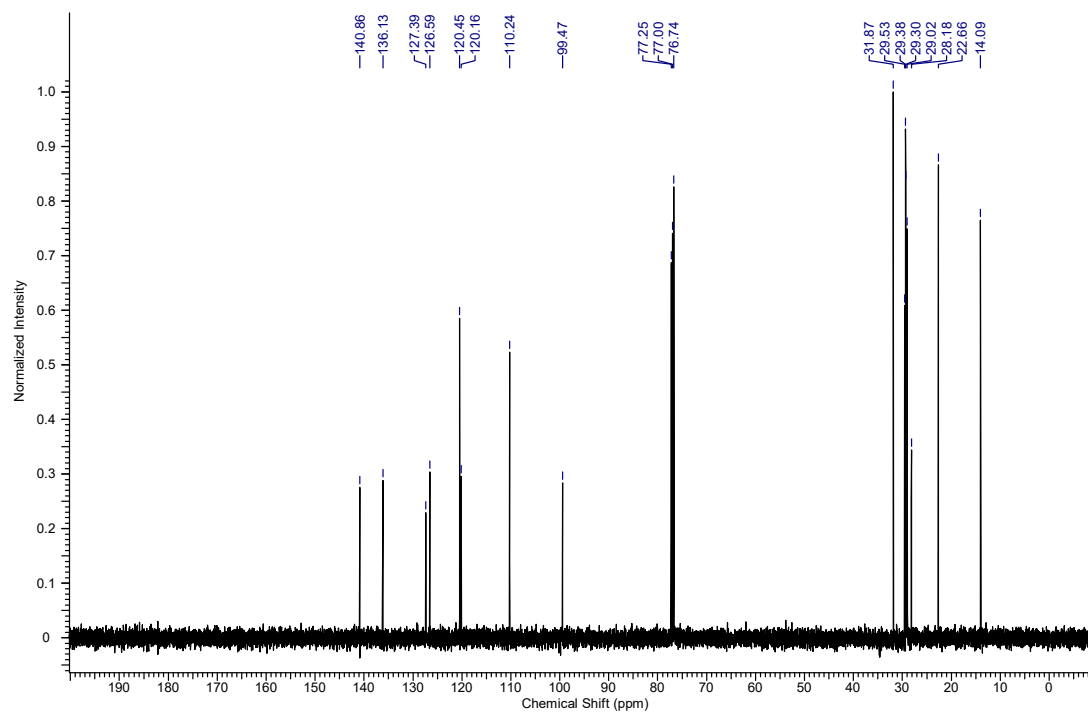


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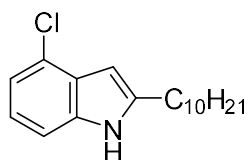
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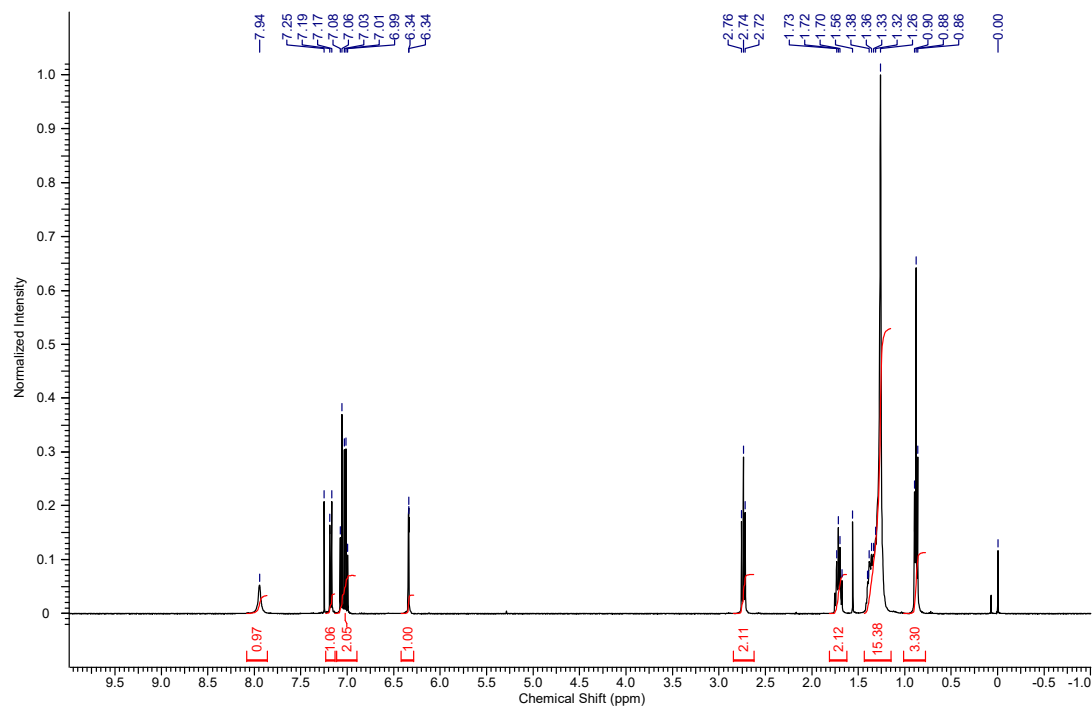


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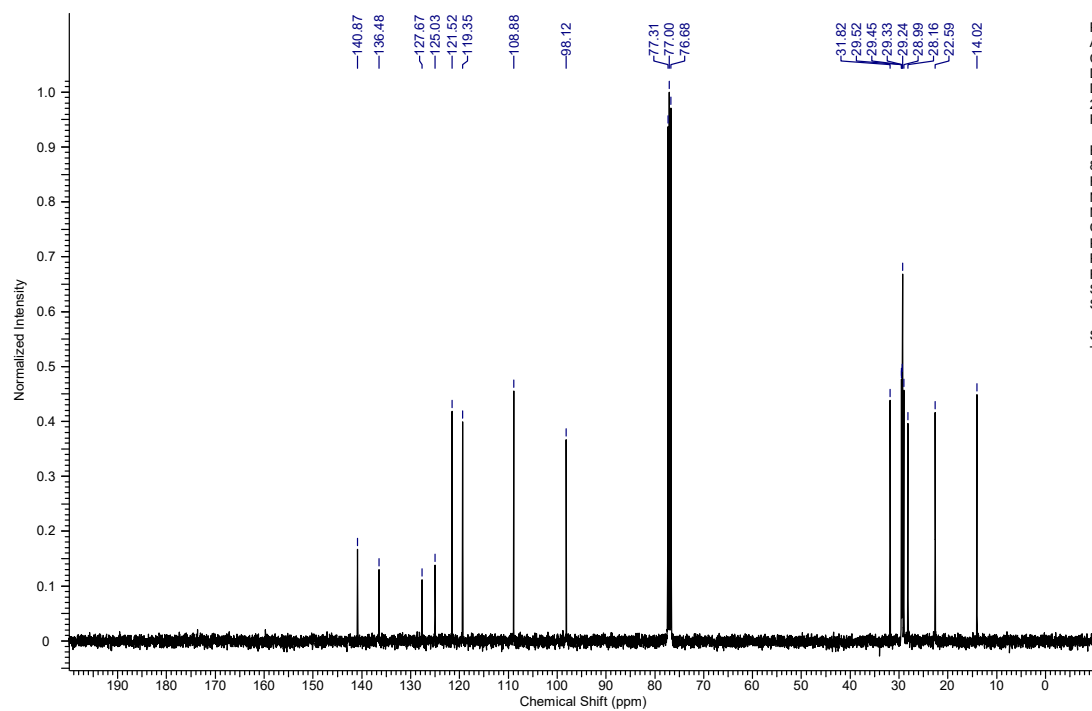
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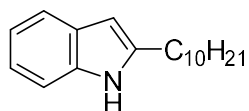
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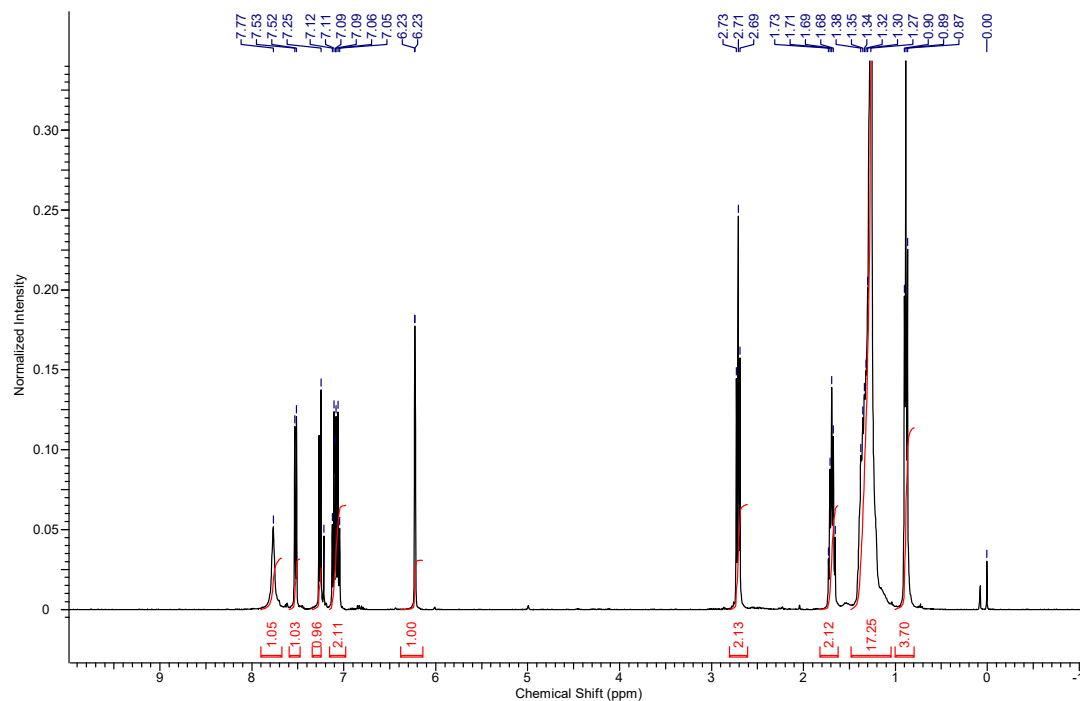
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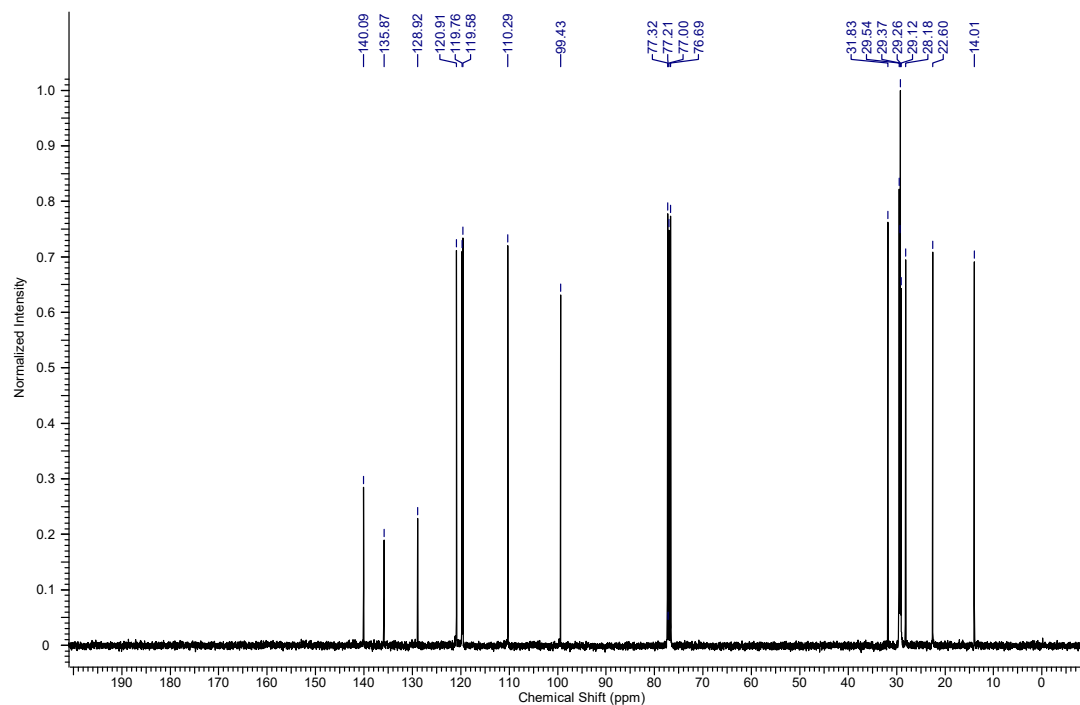


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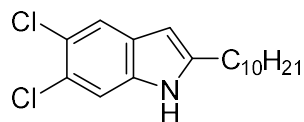
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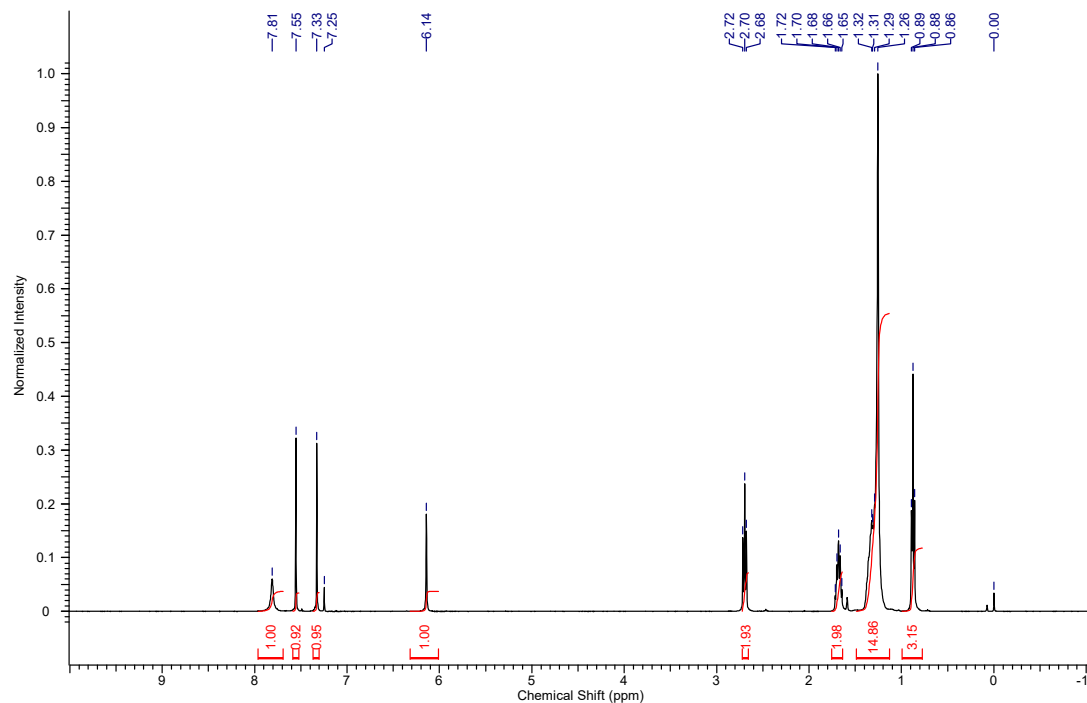


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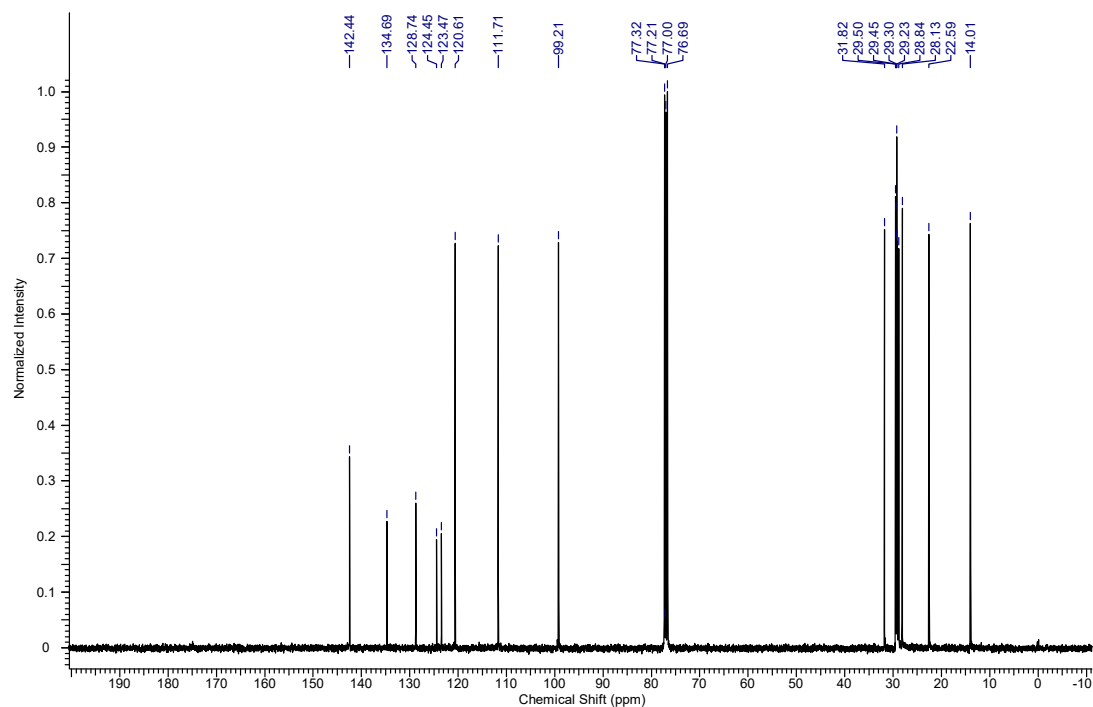
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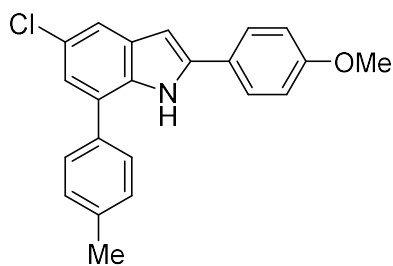
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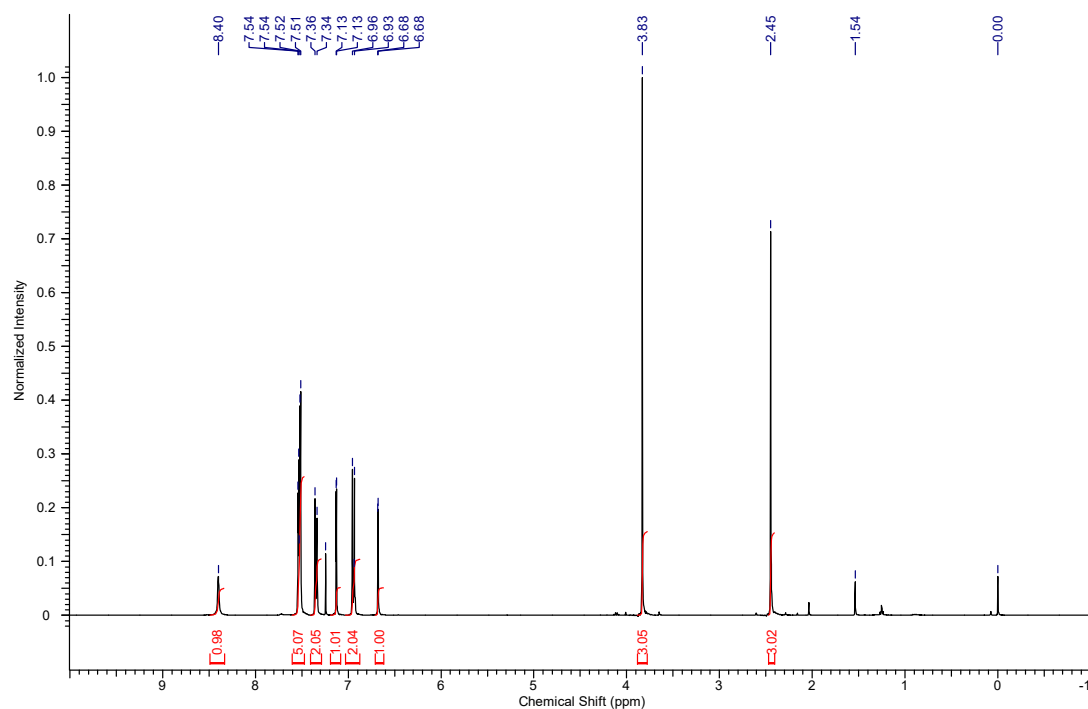
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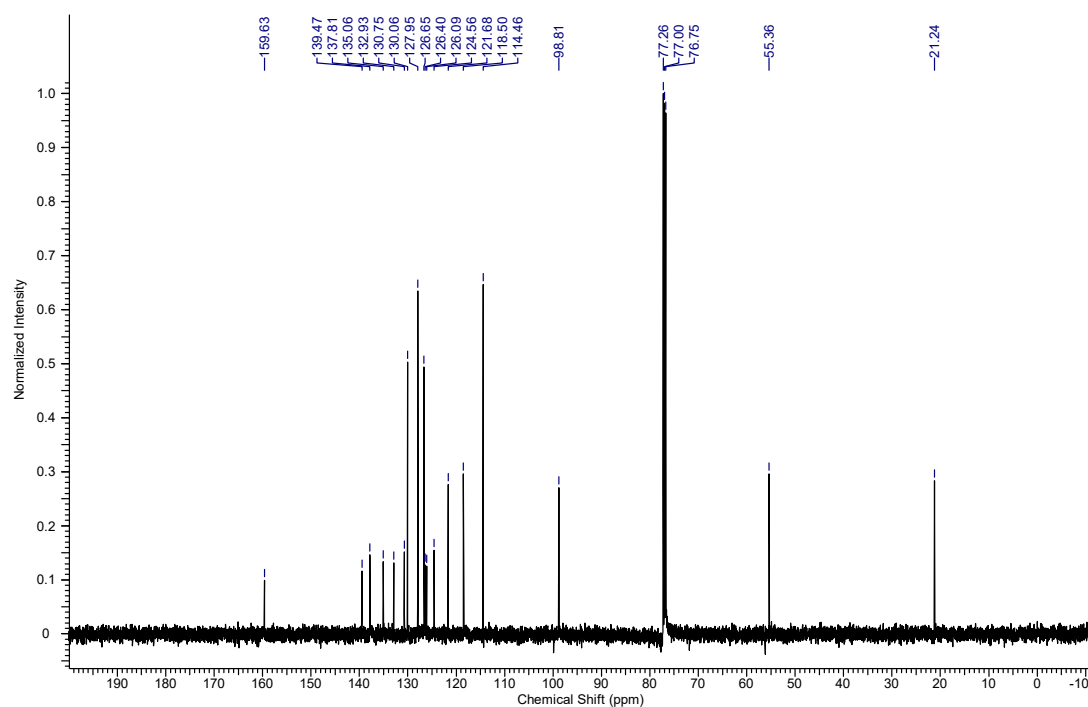
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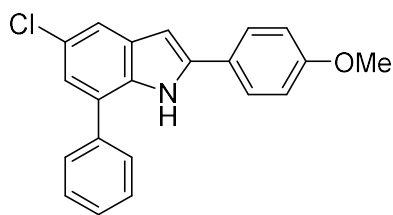
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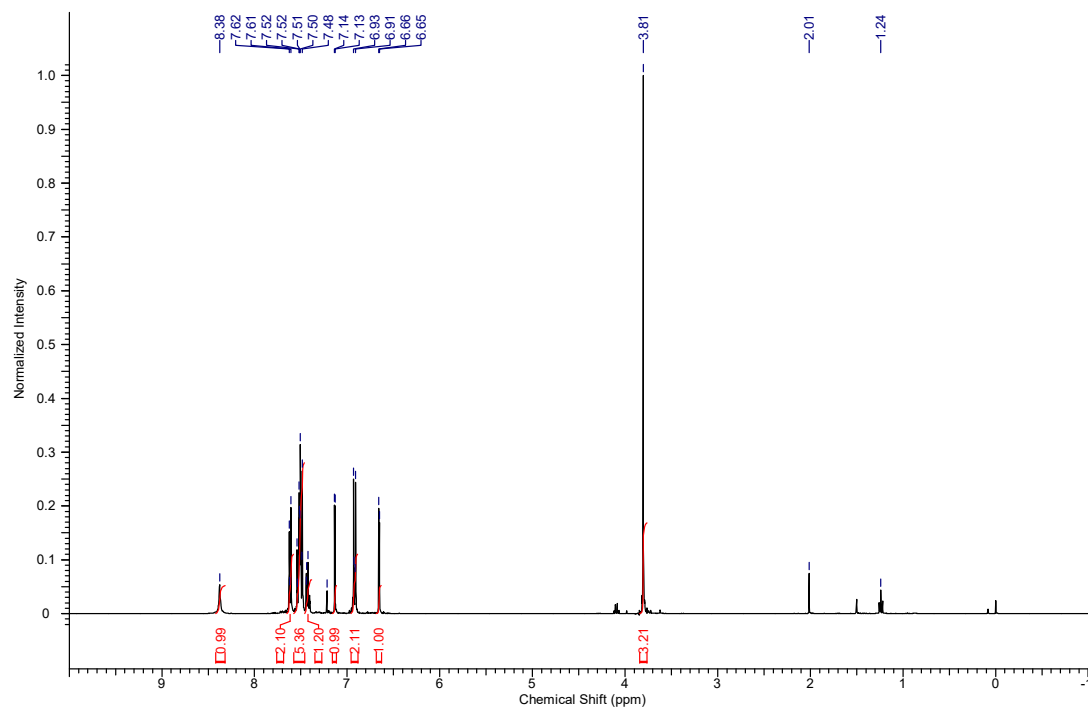
Parameter Value
 Acquisition Time (sec) 2.0500
 Comment MY964PTLC1-1
 Date 21 Jan 2017 19:41:58
 Date Stamp Sat Jan 21 19:41:55 2017
 File Name
 E:\NMRdata\yamaguchi\2017\MY964-2-11\NON_E3_FT.als
 Frequency (MHz) 399.65
 Nucleus ¹H
 Number of Transients 8
 Original Points Count 16384
 Points Count 16384
 Pulse Sequence NON
 Receiver Gain 14.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz) 1985.3193
 Sweep Width (Hz) 7992.01
 Temperature (degree C) 16.400



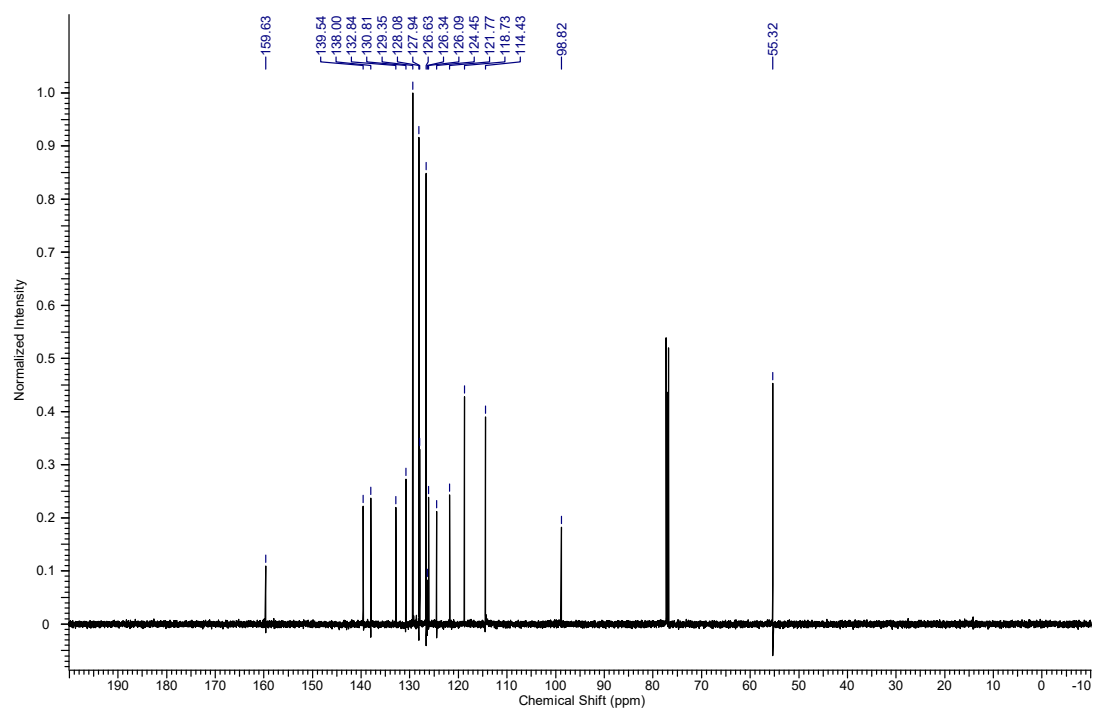
Parameter Value
 Acquisition Time (sec) 0.8389
 Comment single pulse decoupled gated NOE
 Date 21 Jan 2017 16:17:26
 Date Stamp 21 Jan 2017 15:52:12
 File Name
 E:\NMRdata\yamaguchi\2017\MY964-2-1-13C-1.jdf
 Frequency (MHz) 124.50
 Nucleus ¹³C
 Number of Transients 500
 Origin ECA 500
 Original Points Count 32768
 Owner delta
 Points Count 32768
 Pulse Sequence single_pulse_dec
 Receiver Gain 56.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz) 12433.9775
 Spectrum Type STANDARD
 Sweep Width (Hz) 39062.50
 Temperature (degree C) 21.800



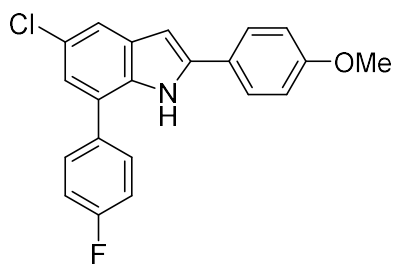
23



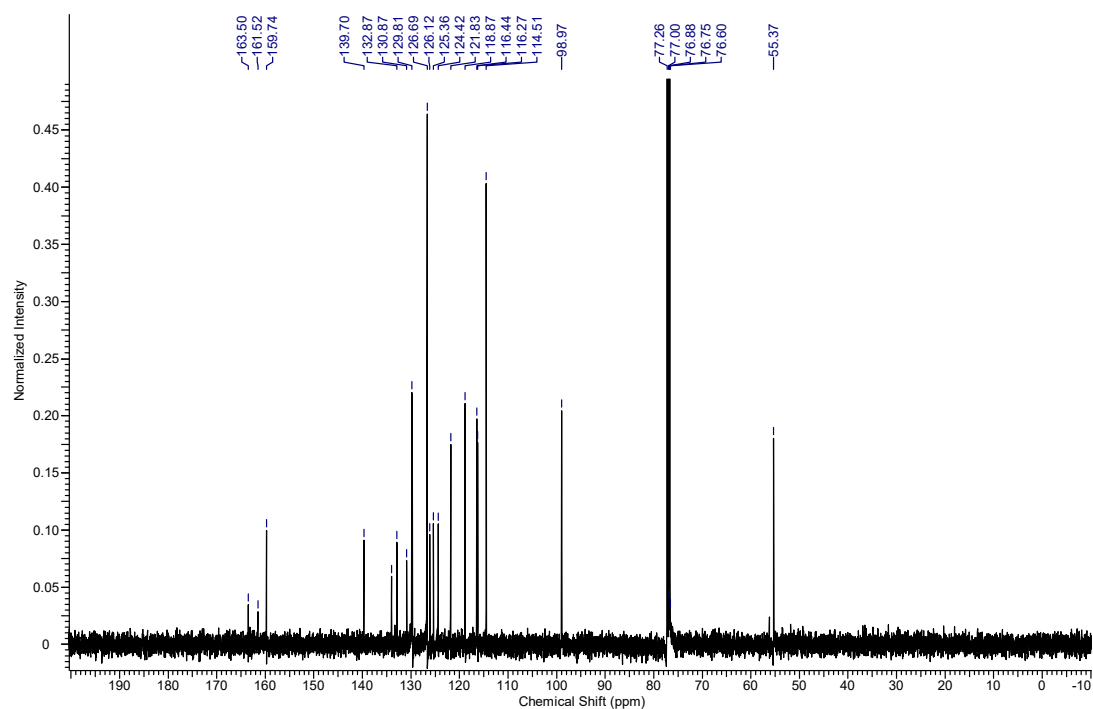
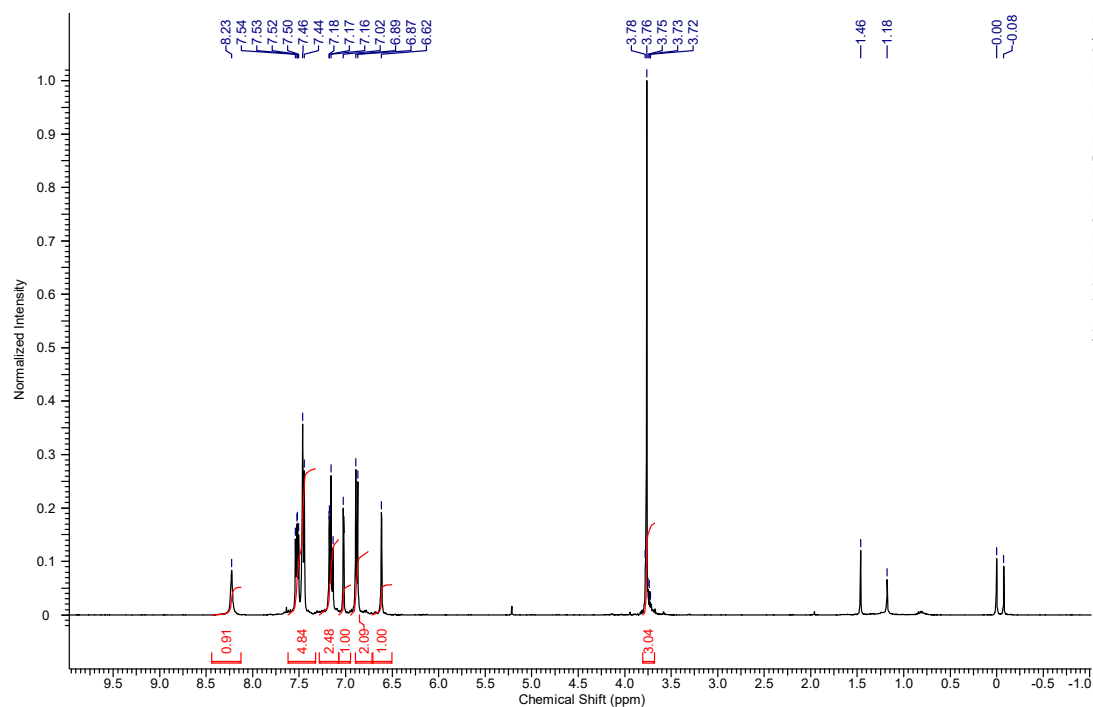
Parameter Value
 Acquisition Time (sec) 2.0500
 Comment MY977PTLC1-1
 Date 03 Feb 2017 09:31:14
 Date Stamp Fri Feb 03
 09:31:11 2017
 File Name
 E:\NMRdata\yamaguchi\2017\MY9
 77-2-11NON_E2_FT.als
 Frequency (MHz) 399.65
 Nucleus 1H
 Number of Transients 8
 Original Points Count 16384
 Points Count 16384
 Pulse Sequence NON
 Receiver Gain 11.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz)
 1976.0513
 Sweep Width (Hz) 7992.01
 Temperature (degree C) 20.800

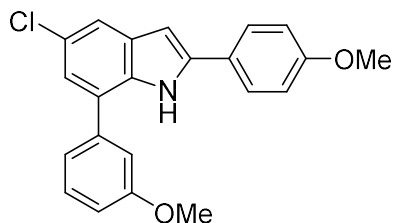


Parameter Value
 Acquisition Time (sec) 0.8336
 Comment single pulse decoupled
 gated NOE
 Date 03 Feb 2017 08:04:13
 Date Stamp 03 Feb 2017
 07:57:39
 File Name
 E:\NMRdata\yamaguchi\2017\MY9
 77-2-1-13C.1
 Frequency (MHz) 125.77
 Nucleus 13C
 Number of Transients 500
 Origin ECA500
 Owner delta
 Points Count 32768
 Pulse Sequence
 single_pulse_dec
 Receiver Gain 60.00
 Solvent CHLOROFORM-D
 Spectrum Offset (Hz)
 12555.2344
 Spectrum Type STANDARD
 Sweep Width (Hz) 39308.18
 Temperature (degree C) 21.700

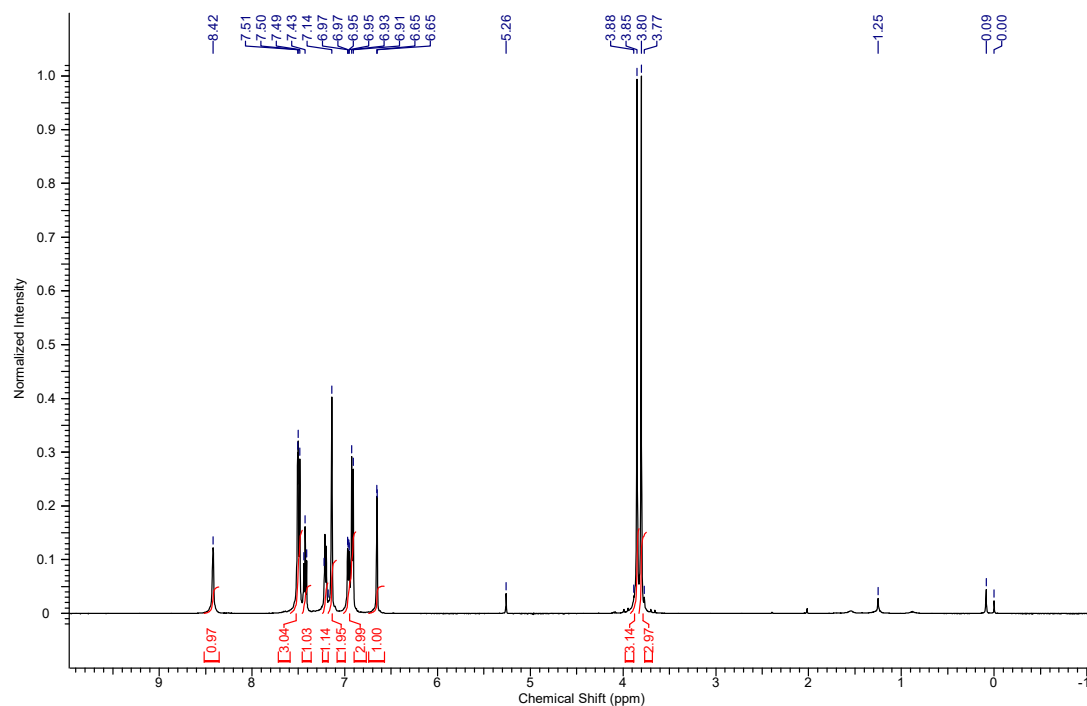


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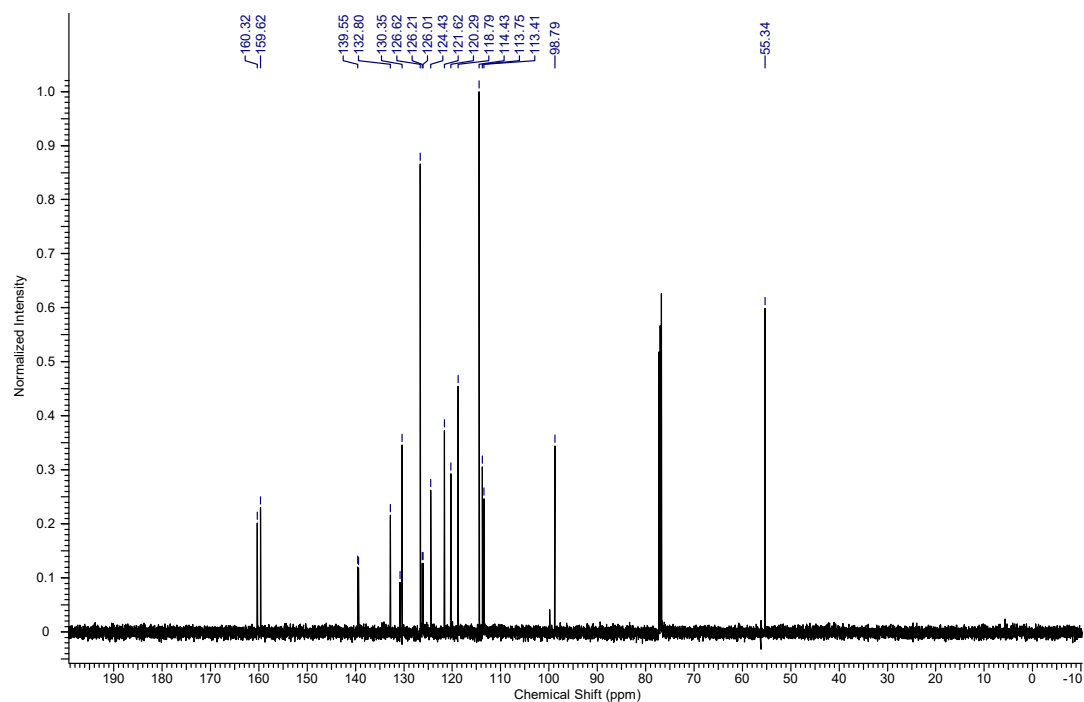


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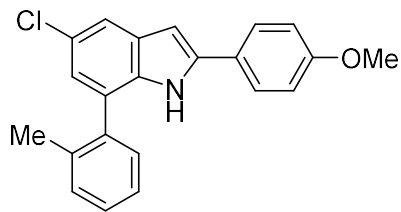
Parameter Value
Acquisition Time (sec) 1.7642
Comment single_pulse
Date 03 Mar 2017 16:51:02
Date Stamp 03 Mar 2017 16:23:36
File Name

E:\NMRdata\yamaguchi\2017\MY1006-2-1-1.jdf
Frequency (MHz) 495.13
Nucleus ¹H
Number of Transients 8
Original Points Count 16384
Owner delta
Points Count 16384
Pulse Sequence single_pulse.ex2
Receiver Gain 30.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz) 2459.8645
Spectrum Type STANDARD
Sweep Width (Hz) 9286.78
Temperature (degree C) 21.300

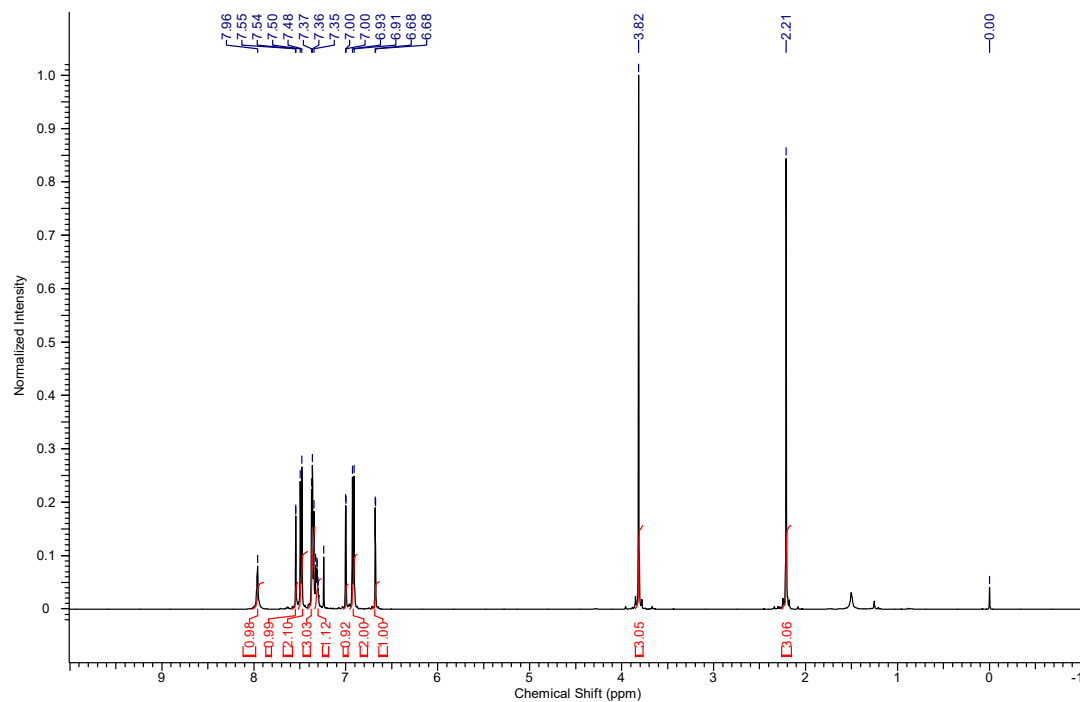


Parameter Value
Acquisition Time (sec) 0.8389
Comment single pulse decoupled gated NOE
Date 03 Mar 2017 17:12:55
Date Stamp 03 Mar 2017 16:45:29
File Name

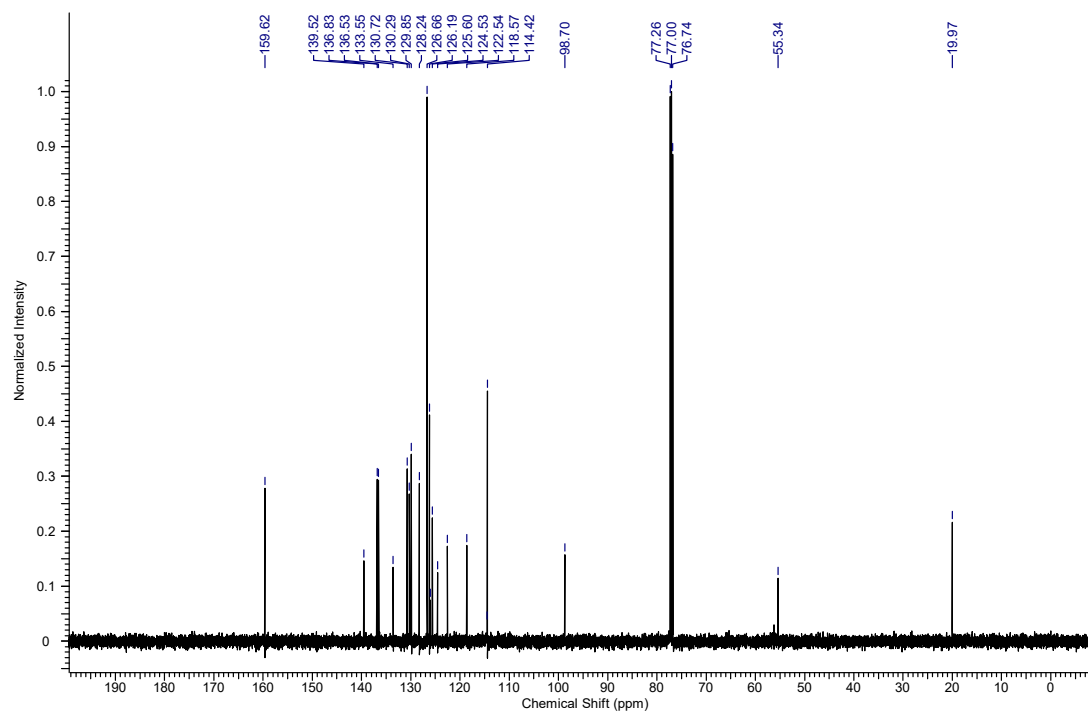
E:\NMRdata\yamaguchi\2017\MY1006-2-1-13C-1.jdf
Frequency (MHz) 124.50
Nucleus ¹³C
Number of Transients 500
Original Points Count 32768
Owner delta
Points Count 32768
Pulse Sequence single_pulse_dec
Receiver Gain 50.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz) 12428.0186
Spectrum Type STANDARD
Sweep Width (Hz) 39062.50
Temperature (degree C) 21.800



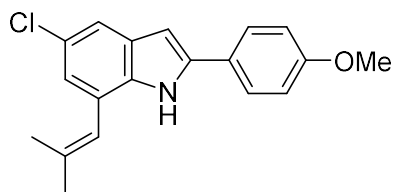
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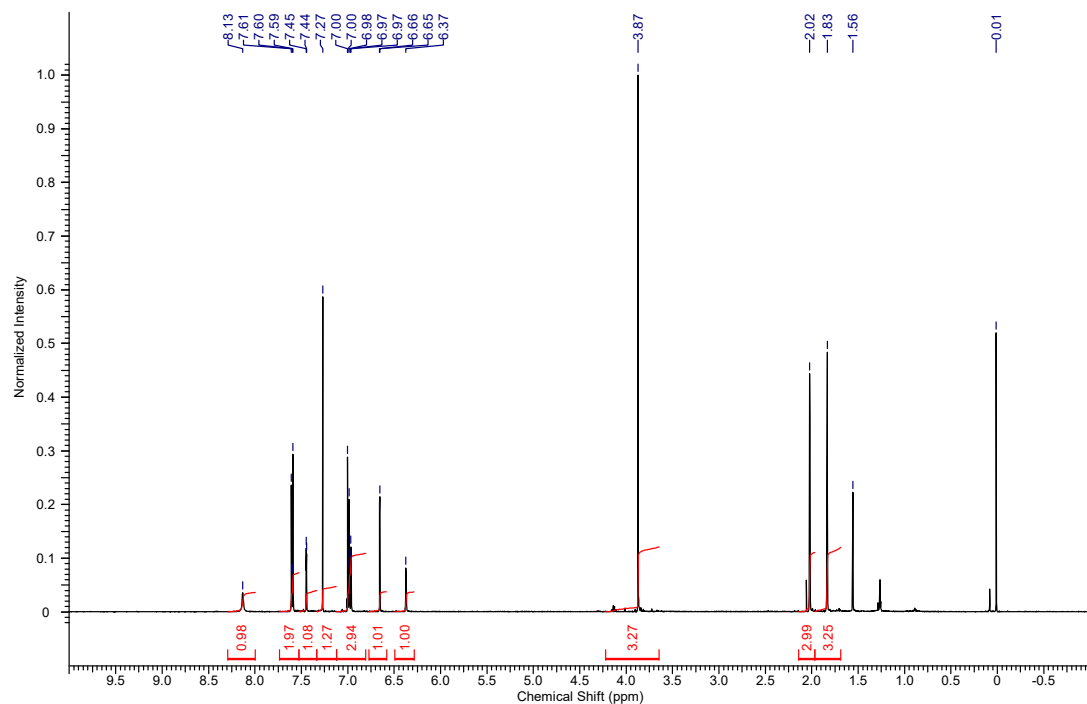
Parameter Value
 Acquisition Time (sec) 1.7642
 Comment single_pulse
 Date 21 Apr 2017 17:08:58
 Date Stamp 21 Apr 2017 16:42:23
 File Name F:\MY1028-3-1-2nd-1.jdf
 Frequency (MHz) 495.13
 Nucleus ¹H
 Number of Transients 8
 Origin ECA 500
 Original Points Count 16384
 Owner delta
 Points Count 16384
 Pulse Sequence single_pulse.ex2
 Receiver Gain 34.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz) 2497.8438
 Spectrum Type STANDARD
 Sweep Width (Hz) 9286.78
 Temperature (degree C) 21.900



Parameter Value
 Acquisition Time (sec) 0.8389
 Comment single pulse decoupled gated NOE
 Date 21 Apr 2017 17:45:03
 Date Stamp 21 Apr 2017 17:18:29
 File Name F:\MY1028-3-1-13C-1.jdf
 Frequency (MHz) 124.50
 Nucleus ¹³C
 Number of Transients 1000
 Origin ECA 500
 Original Points Count 32768
 Owner delta
 Points Count 32768
 Pulse Sequence single_pulse_dec
 Receiver Gain 50.00
 Solvent CHLOROFORM-D
 Spectrum Offset (Hz) 12439.9385
 Spectrum Type STANDARD
 Sweep Width (Hz) 39062.50
 Temperature (degree C) 22.100

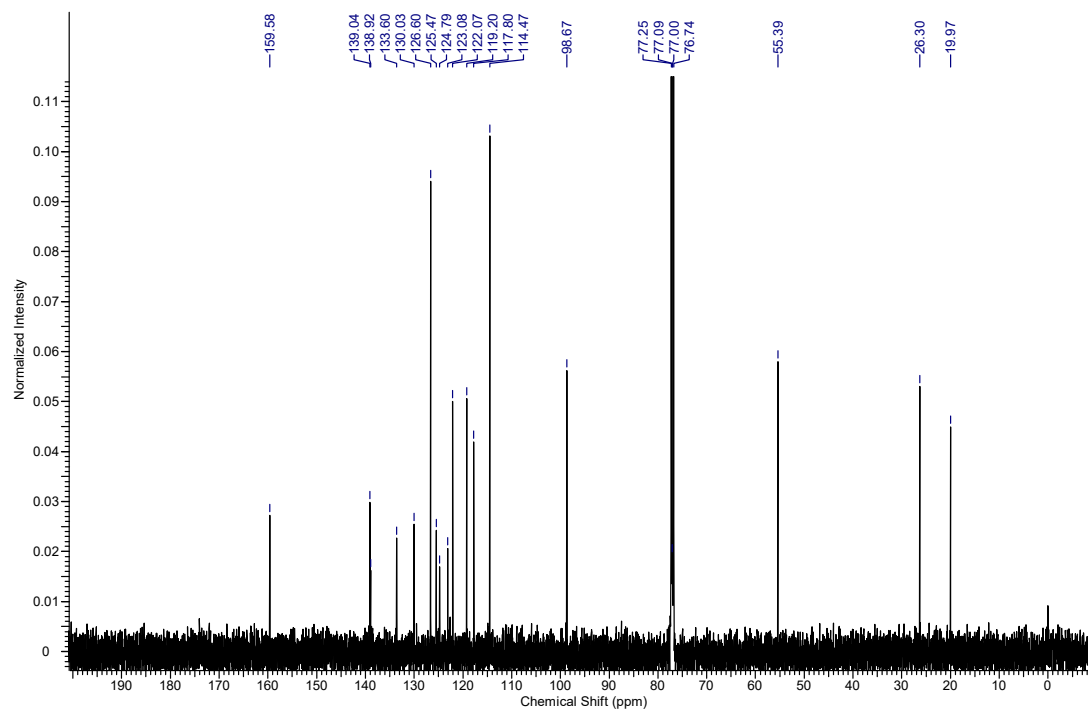


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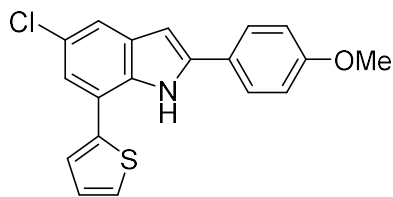
Parameter Value
Acquisition Time (sec) 1.7459
Comment single_pulse
Date 03 Feb 2017 08:12:42
Date Stamp 03 Feb 2017
08:06:08
File Name

E:\NMRdata\yamaguchi\2017\MY9
78-2-1.1
Frequency (MHz) 500.16
Nucleus ¹H
Number of Transients 8
Origin ECA500
Original Points Count 16384
Owner delta
Points Count 16384
Pulse Sequence
single_pulse.ex2
Receiver Gain 48.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
2508.5813
Spectrum Type STANDARD
Sweep Width (Hz) 9384.38
Temperature (degree C) 21.200

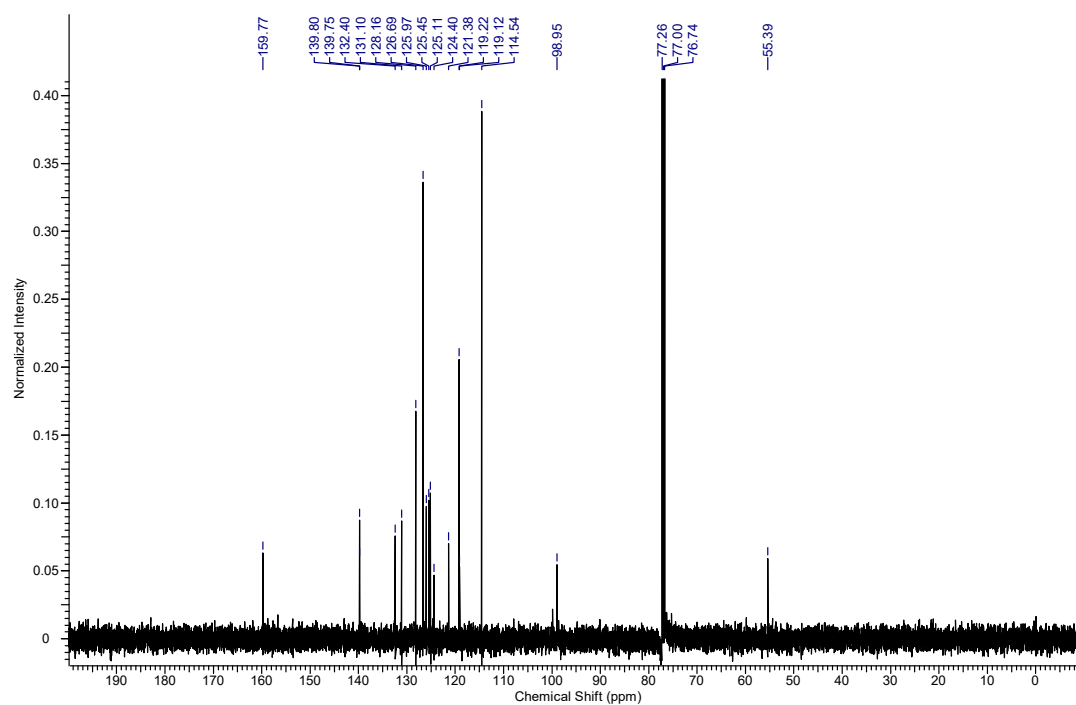
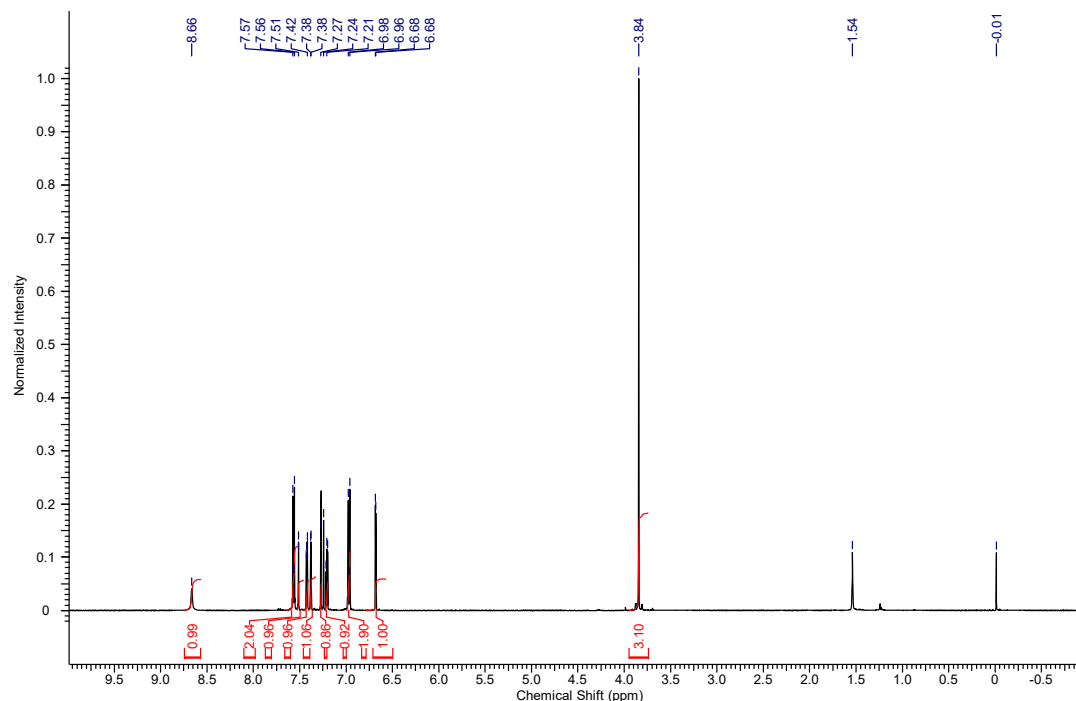


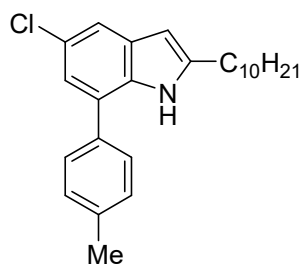
Parameter Value
Acquisition Time (sec) 0.8336
Comment single pulse decoupled
gated NOE
Date 03 Feb 2017 08:49:17
Date Stamp 03 Feb 2017
08:42:42
File Name

E:\NMRdata\yamaguchi\2017\MY9
78-2-1-13C.1
Frequency (MHz) 125.77
Nucleus ¹³C
Number of Transients 1000
Origin ECA500
Original Points Count 32768
Owner delta
Points Count 32768
Pulse Sequence
single_pulse_dec
Receiver Gain 60.00
Solvent CHLOROFORM-d
Spectrum Offset (Hz)
12562.4326
Spectrum Type STANDARD
Sweep Width (Hz) 39308.18
Temperature (degree C) 21.900

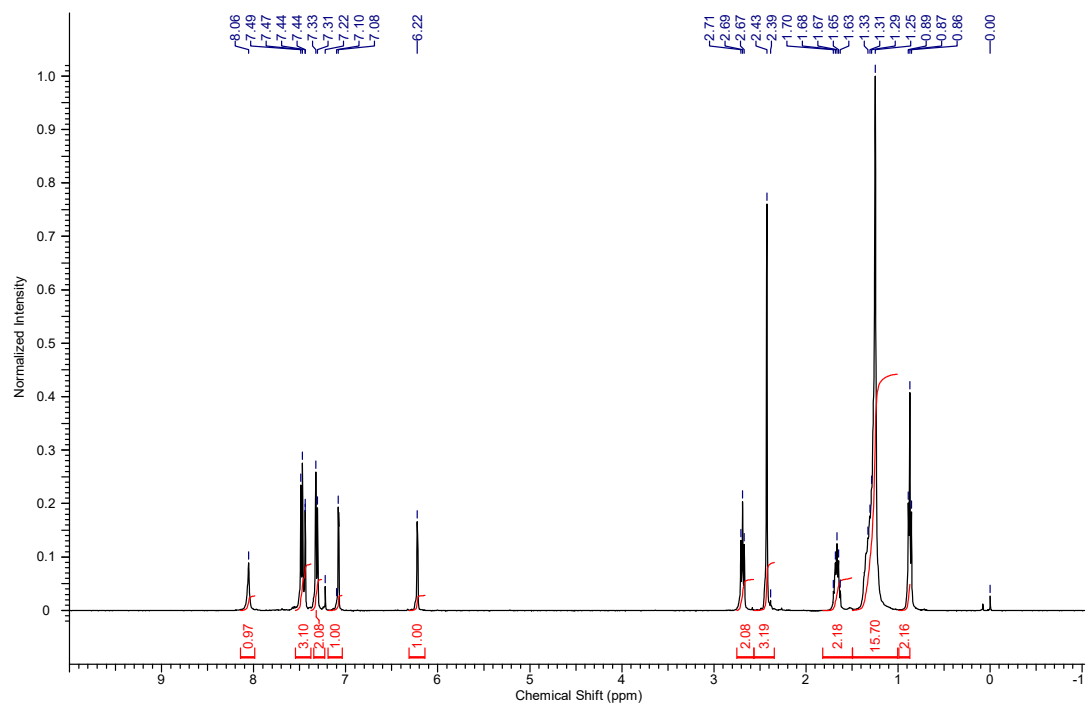


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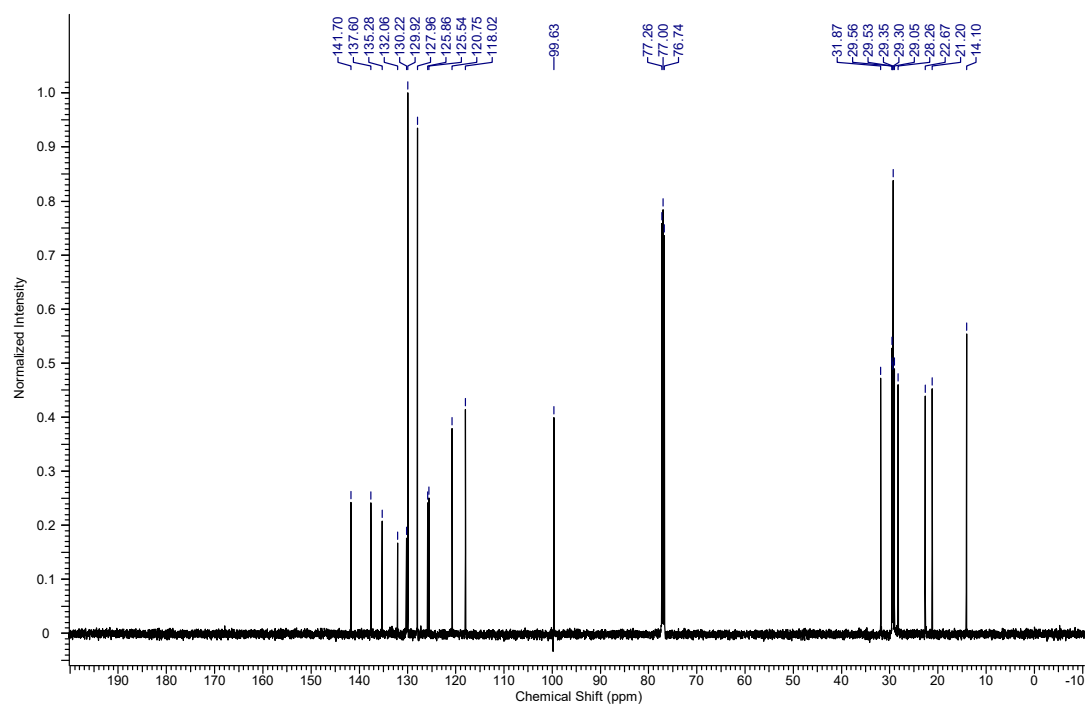




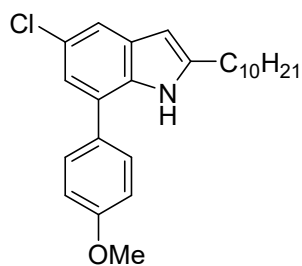
29



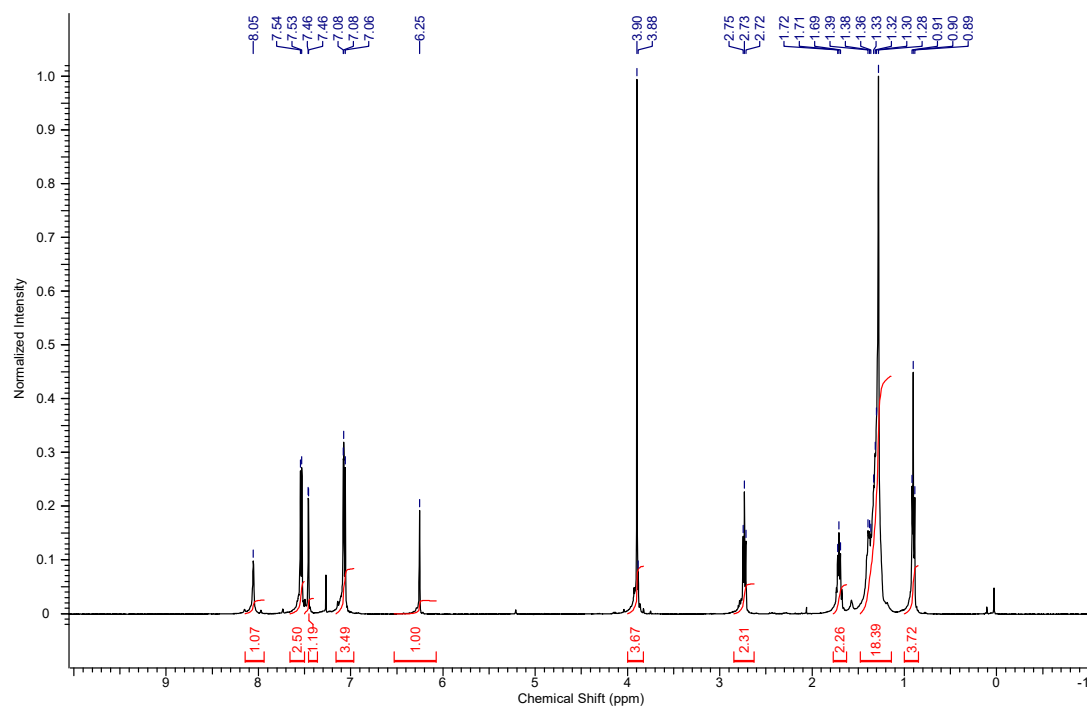
Parameter Value
 Acquisition Time (sec) 2.0500
 Comment MY988PTLC1-1
 Date 13 Feb 2017 09:44:12
 Date Stamp Mon Feb 13
 09:44:11 2017
 File Name
 E:\NMRdata\yamaguchi\2017\MY9
 88-2-11NON_E7_FT.als
 Frequency (MHz) 399.65
 Nucleus ¹H
 Number of Transients 8
 Original Points Count 16384
 Points Count 16384
 Pulse Sequence NON
 Receiver Gain 9.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz)
 1977.0269
 Sweep Width (Hz) 7992.01
 Temperature (degree C) 14.400



Parameter Value
 Acquisition Time (sec) 0.8389
 Comment single pulse decoupled
 gated NOE
 Date 13 Feb 2017 15:16:59
 Date Stamp 13 Feb 2017
 14:50:36
 File Name
 E:\NMRdata\yamaguchi\2017\MY98
 8-2-1-13C-1.jdf
 Frequency (MHz) 124.50
 Nucleus ¹³C
 Number of Transients 1000
 Origin ECA 500
 Original Points Count 32768
 Owner delta
 Points Count 32768
 Pulse Sequence
 single_pulse_dec
 Receiver Gain 50.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz)
 12431.5947
 Spectrum Type STANDARD
 Sweep Width (Hz) 39062.50
 Temperature (degree C) 22.800

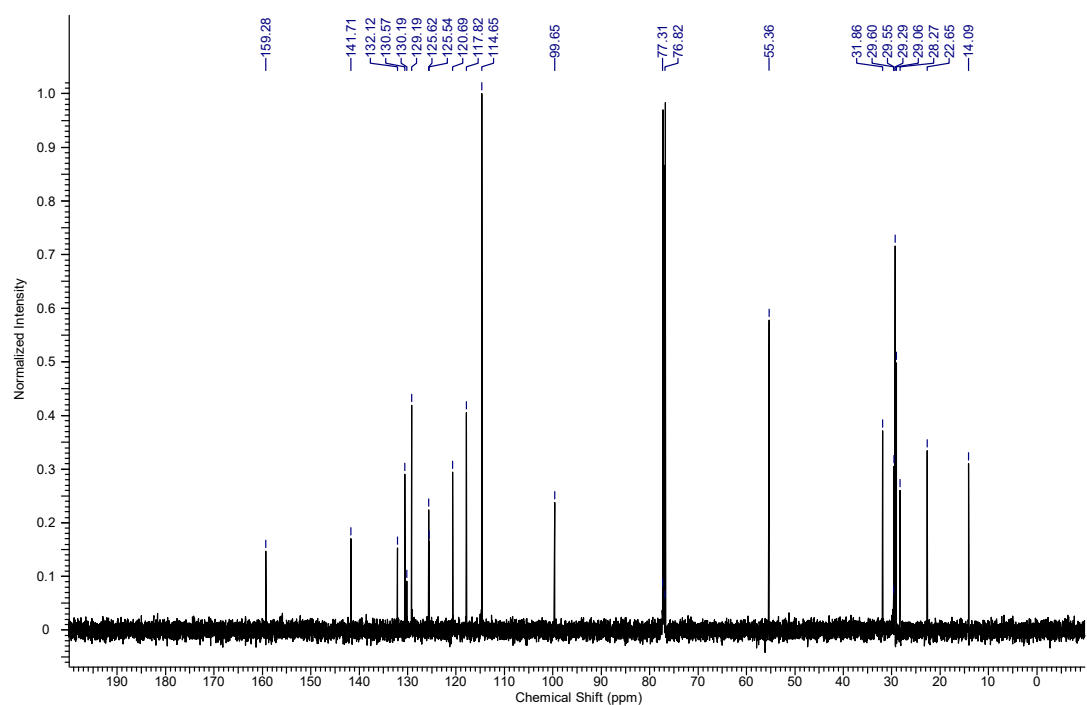


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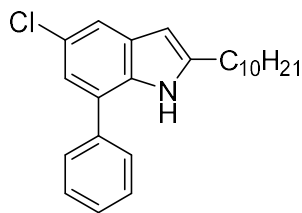
Parameter Value
Acquisition Time (sec) 1.7642
Comment single_pulse
Date 17 Feb 2017 16:29:46
Date Stamp 17 Feb 2017
16:02:28
File Name

E:\NMRdata\yamaguchi\2017\MY9
93-2-2-2nd-1.jdf
Frequency (MHz) 495.13
Nucleus ¹H
Number of Transients 8
Origin ECA 500
Original Points Count 16384
Owner delta
Points Count 16384
Pulse Sequence
single_pulse.ex2
Receiver Gain 30.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
2483.1895
Spectrum Type STANDARD
Sweep Width (Hz) 9286.78
Temperature (degree C) 23.700

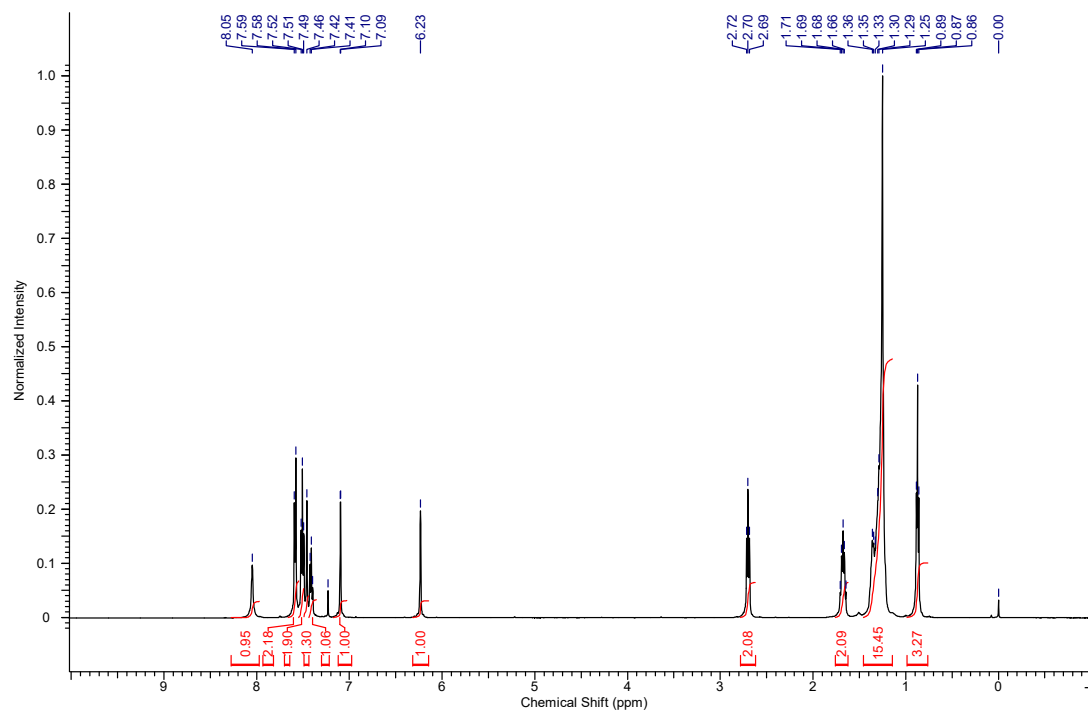


Parameter Value
Acquisition Time (sec) 0.8389
Comment single_pulse decoupled
gated NOE
Date 17 Feb 2017 17:11:02
Date Stamp 17 Feb 2017
16:43:44
File Name

E:\NMRdata\yamaguchi\2017\MY9
93-2-2-13C-1.jdf
Frequency (MHz) 124.50
Nucleus ¹³C
Number of Transients 1000
Origin ECA 500
Original Points Count 32768
Owner delta
Points Count 32768
Pulse Sequence
single_pulse_dec
Receiver Gain 50.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
12433.9775
Spectrum Type STANDARD
Sweep Width (Hz) 39062.50
Temperature (degree C) 23.900

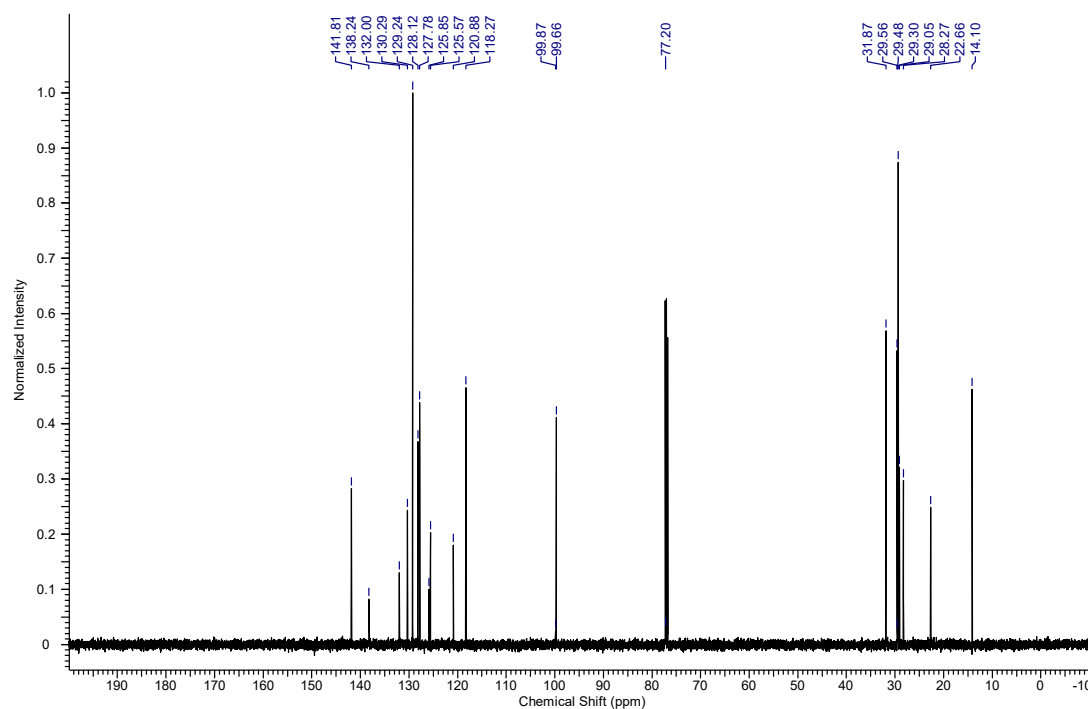


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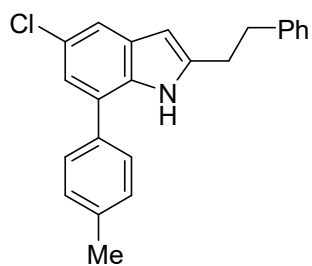
Parameter Value
Acquisition Time (sec) 1.7642
Comment single_pulse
Date 08 Mar 2017 13:25:13
Date Stamp 08 Mar 2017
12:57:52
File Name

E:\NMRdata\yamaguchi\2017\IMY1
004-4-1-1.jdf
Frequency (MHz) 495.13
Nucleus 1H
Number of Transients 8
Origin ECA 500
Original Points Count 16384
Owner delta
Points Count 16384
Pulse Sequence
single_pulse.ex2
Receiver Gain 30.00
Solvent CHLOROFORM-d
Spectrum Offset (Hz)
2463.8325
Spectrum Type STANDARD
Sweep Width (Hz) 9286.78
Temperature (degree C) 21.800

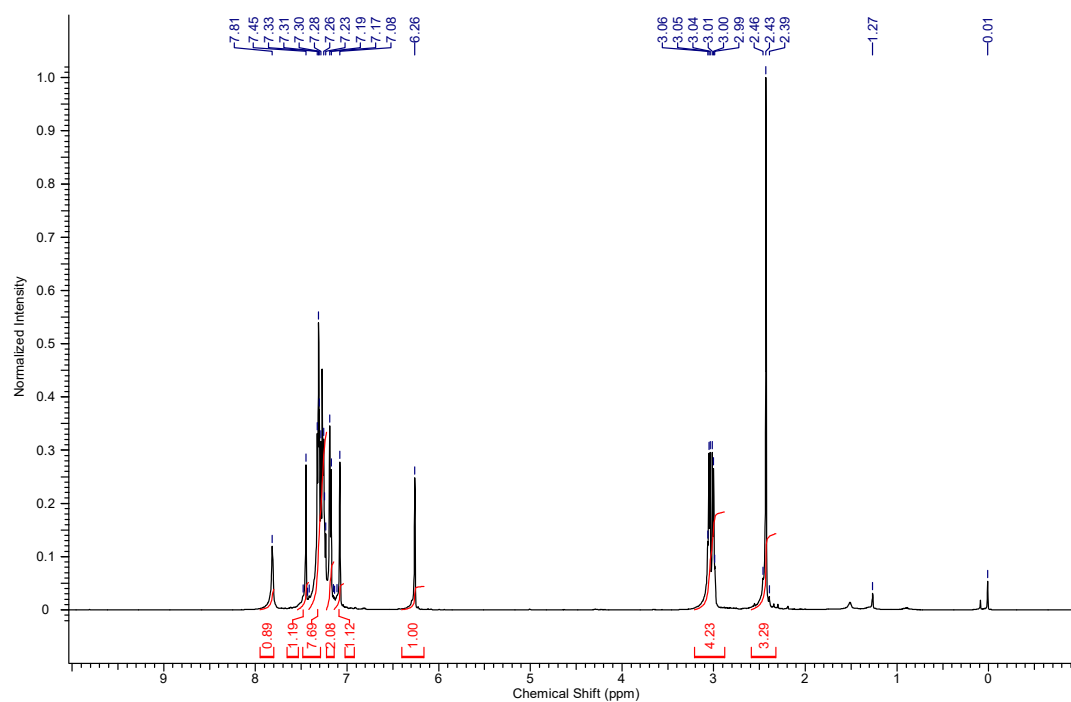


Parameter Value
Acquisition Time (sec) 0.8389
Comment single pulse decoupled
gated NOE
Date 08 Mar 2017 14:06:21
Date Stamp 08 Mar 2017
13:39:00
File Name

E:\NMRdata\yamaguchi\2017\IMY1
1004-4-1-13C-1.jdf
Frequency (MHz) 124.50
Nucleus 13C
Number of Transients 1000
Origin ECA 500
Original Points Count 32768
Owner delta
Points Count 32768
Pulse Sequence
single_pulse_dec
Receiver Gain 52.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
12432.7861
Spectrum Type STANDARD
Sweep Width (Hz) 39062.50
Temperature (degree C) 22.000

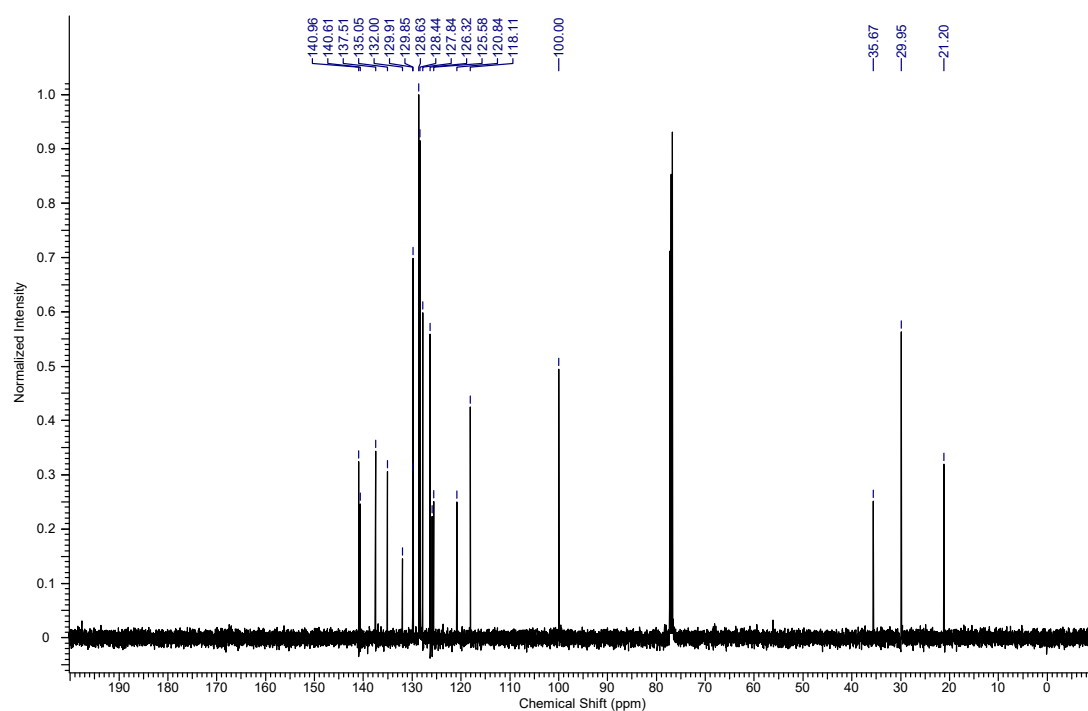


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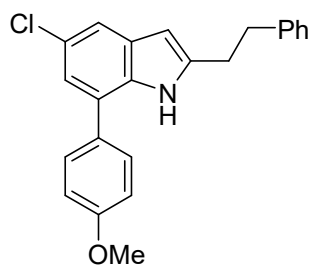
Parameter Value
Acquisition Time (sec) 1.7642
Comment single_pulse
Date 17 Feb 2017 12:38:28
Date Stamp 17 Feb 2017
12:11:09
File Name

E:\NMRdata\yamaguchi\2017\MY99
1-2-1-3rd-1.jdf
Frequency (MHz) 495.13
Nucleus 1H
Number of Transients 8
Origin ECA 500
Original Points Count 16384
Owner delta
Points Count 16384
Pulse Sequence
single_pulse.ex2
Receiver Gain 34.00
Solvent CHLOROFORM-d
Spectrum Offset (Hz)
2466.1838
Spectrum Type STANDARD
Sweep Width (Hz) 9286.78
Temperature (degree C) 23.700

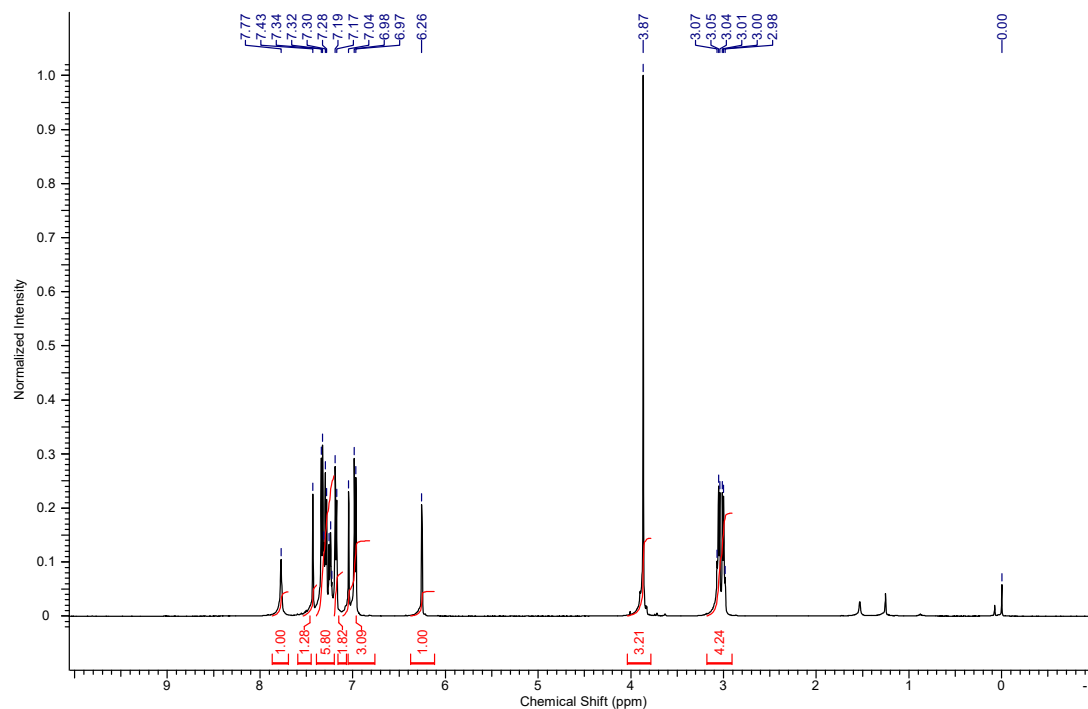


Parameter Value
Acquisition Time (sec) 0.8389
Comment single pulse decoupled
gated NOE
Date 17 Feb 2017 13:19:18
Date Stamp 17 Feb 2017
12:51:59
File Name

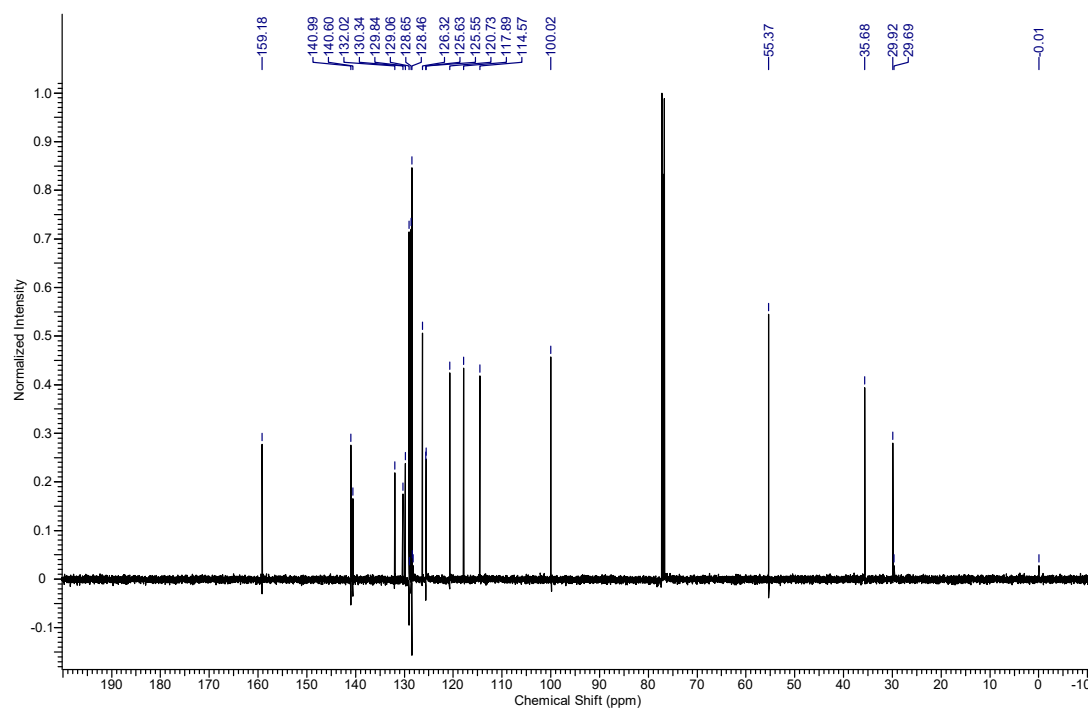
E:\NMRdata\yamaguchi\2017\MY9
91-2-1-13C-1.jdf
Frequency (MHz) 124.50
Nucleus 13C
Number of Transients 1000
Origin ECA 500
Original Points Count 32768
Owner delta
Points Count 32768
Pulse Sequence
single_pulse_dec
Receiver Gain 50.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
12431.5947
Spectrum Type STANDARD
Sweep Width (Hz) 39062.50
Temperature (degree C) 24.100



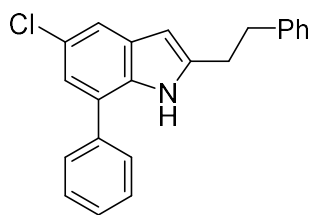
33



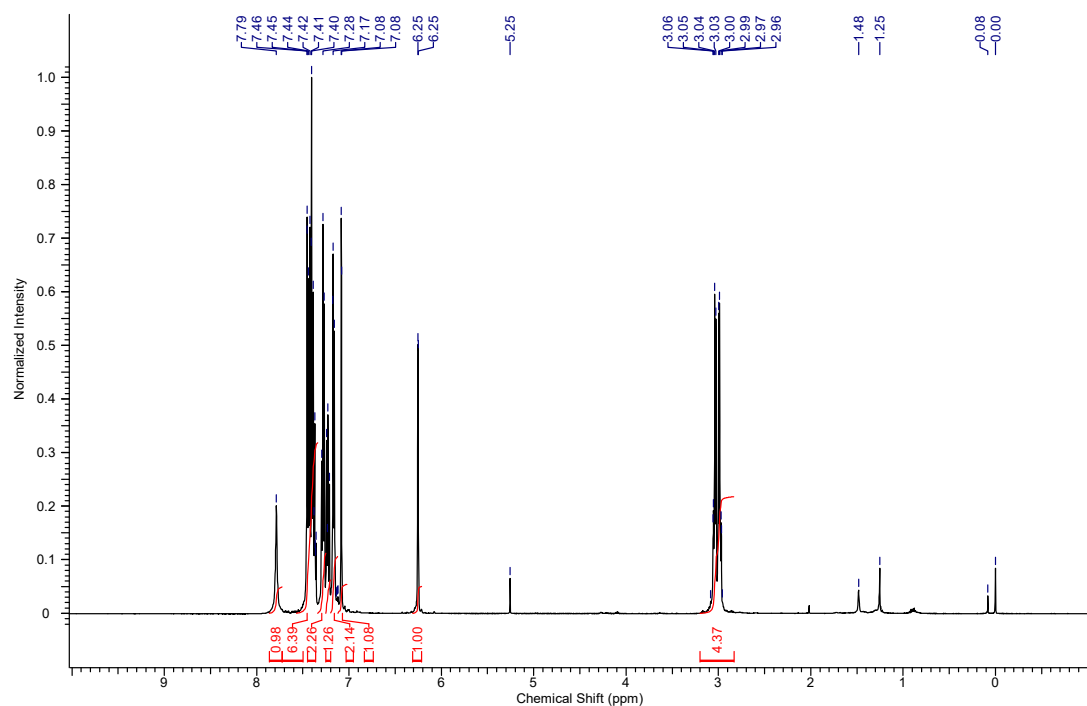
Parameter Value
 Acquisition Time (sec) 1.7642
 Comment single_pulse
 Date 21 Feb 2017 07:35:24
 Date Stamp 21 Feb 2017
 07:07:58
 File Name
 E:\NMRdata\yamaguchi\2017\MY9
 94-2-1-2nd-1.jdf
 Frequency (MHz) 495.13
 Nucleus 1H
 Number of Transients 8
 Origin ECA 500
 Original Points Count 16384
 Owner delta
 Points Count 16384
 Pulse Sequence
 single_pulse.ex2
 Receiver Gain 40.00
 Solvent CHLOROFORM-d
 Spectrum Offset (Hz)
 2467.2336
 Spectrum Type STANDARD
 Sweep Width (Hz) 9286.78
 Temperature (degree C) 20.900



Parameter Value
 Acquisition Time (sec) 0.8336
 Comment single pulse decoupled
 gated NOE
 Date 21 Feb 2017 08:30:01
 Date Stamp 21 Feb 2017
 08:23:49
 File Name
 E:\NMRdata\yamaguchi\2017\MY9
 94-2-1-13C-1
 Frequency (MHz) 125.77
 Nucleus 13C
 Number of Transients 1000
 Origin ECA500
 Original Points Count 32768
 Owner delta
 Points Count 32768
 Pulse Sequence
 single_pulse_dec
 Receiver Gain 60.00
 Solvent CHLOROFORM-D
 Spectrum Offset (Hz)
 12558.8340
 Spectrum Type STANDARD
 Sweep Width (Hz) 39308.18
 Temperature (degree C) 20.600

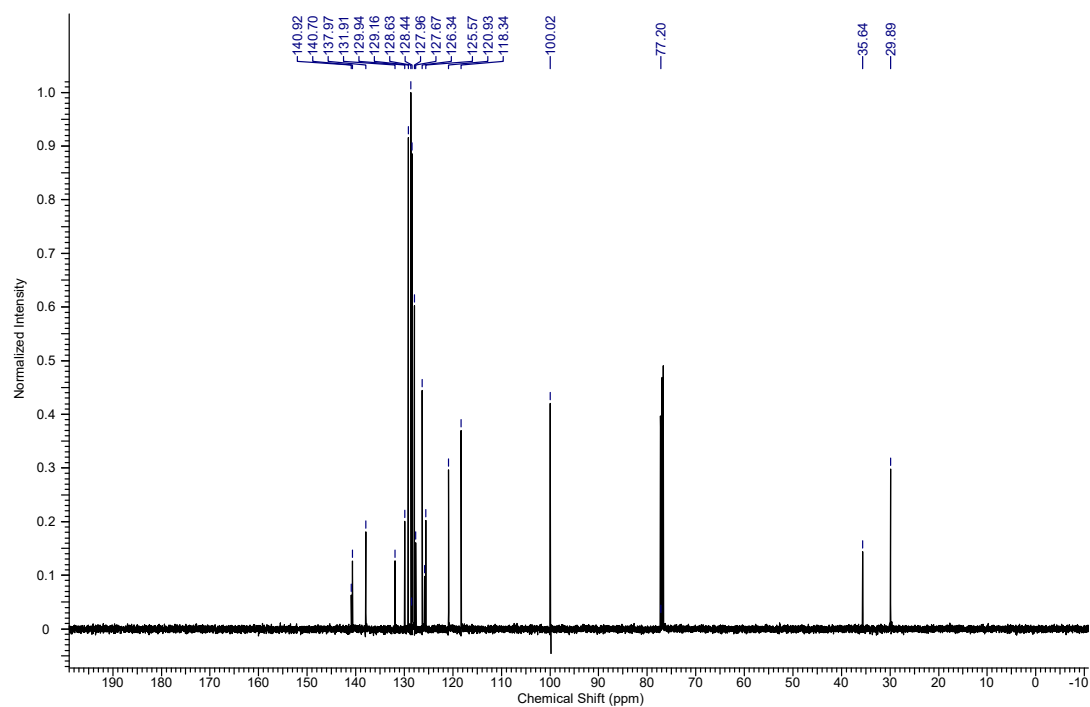


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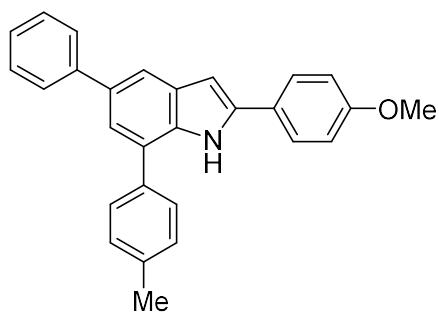
Parameter Value
Acquisition Time (sec) 1.7642
Comment single_pulse
Date 28 Feb 2017 16:34:33
Date Stamp 28 Feb 2017
16:07:03
File Name

E:\NMRdata\yamaguchi\2017\MY10
02-2-1-3rd-1.jdf
Frequency (MHz) 495.13
Nucleus ¹H
Number of Transients 8
Origin ECA 500
Original Points Count 16384
Owner delta
Points Count 16384
Pulse Sequence
single_pulse.ex2
Receiver Gain 34.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
2454.1960
Spectrum Type STANDARD
Sweep Width (Hz) 9286.78
Temperature (degree C) 21.000

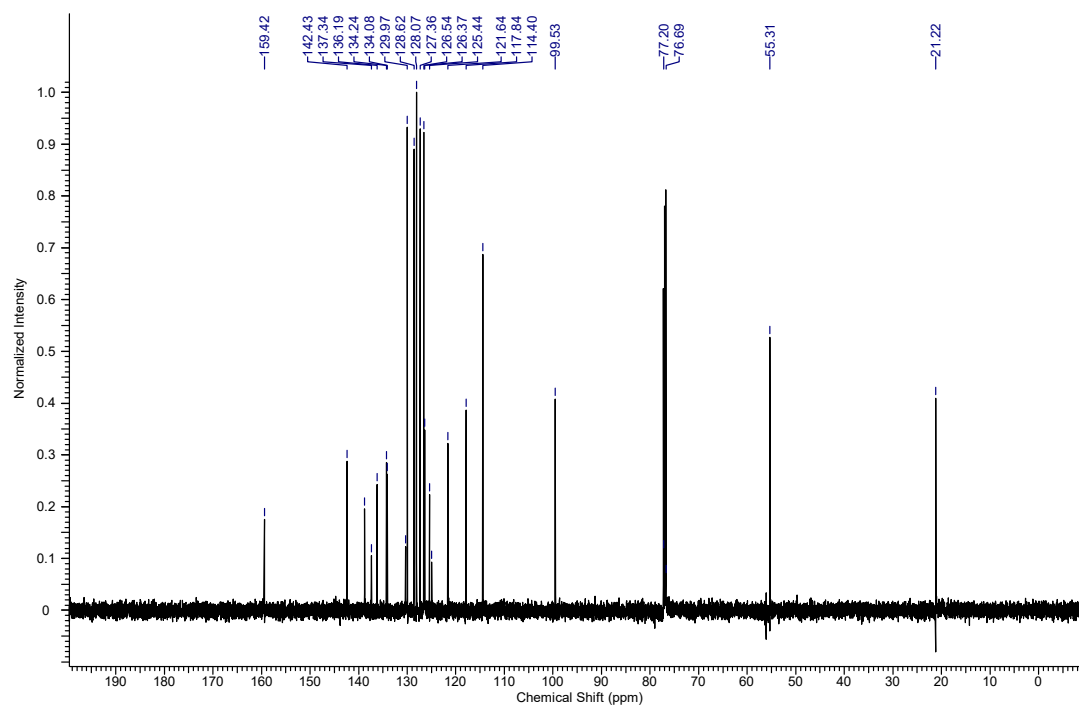
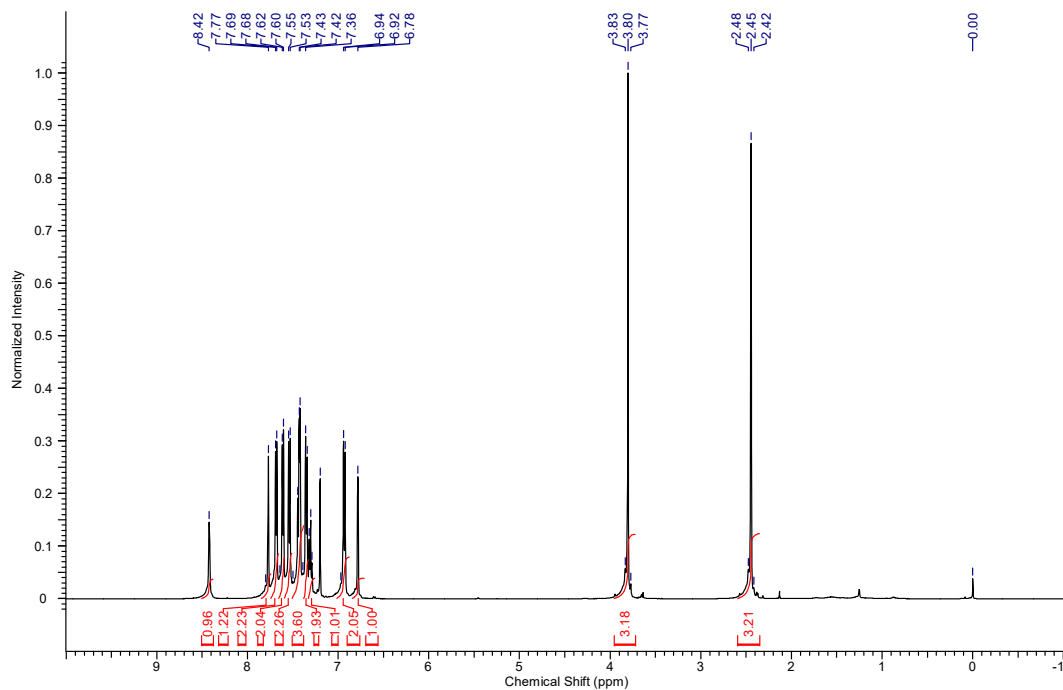


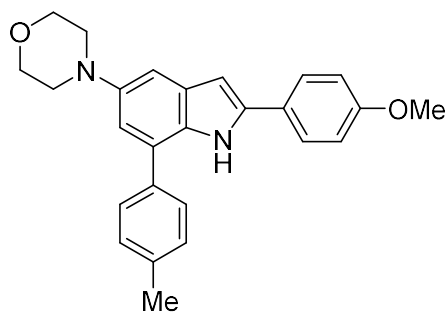
Parameter Value
Acquisition Time (sec) 0.8389
Comment single pulse decoupled
gated NOE
Date 28 Feb 2017 17:15:17
Date Stamp 28 Feb 2017
16:47:48
File Name

E:\NMRdata\yamaguchi\2017\MY10
02-2-1-13C-1.jdf
Frequency (MHz) 124.50
Nucleus ¹³C
Number of Transients 1000
Origin ECA 500
Original Points Count 32768
Owner delta
Points Count 32768
Pulse Sequence
single_pulse_dec
Receiver Gain 50.00
Solvent CHLOROFORM-D
Spectrum Offset (Hz)
12428.0186
Spectrum Type STANDARD
Sweep Width (Hz) 39062.50
Temperature (degree C) 21.200



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