

Short Paper

DESIGN, SYNTHESIS, PHYSICAL PROPERTIES AND INDOLEAMINE 2, 3-DIOXYGENASE 1 INHIBITORY ACTIVITY OF SUBSTITUED INDOLE DERIVATIVES WITH *N*-H, *N*-METOHY METHYL, OR *N*-MEHYLTHIOMETHYL GROUPS TOWARD FRAGMENT-BASED DRUG DISCOVERY¹

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¹ This paper is dedicated to Dr. Yasuyuki Kita on the occasion of his 77th birthday.

1. Docking model of compound **1af**

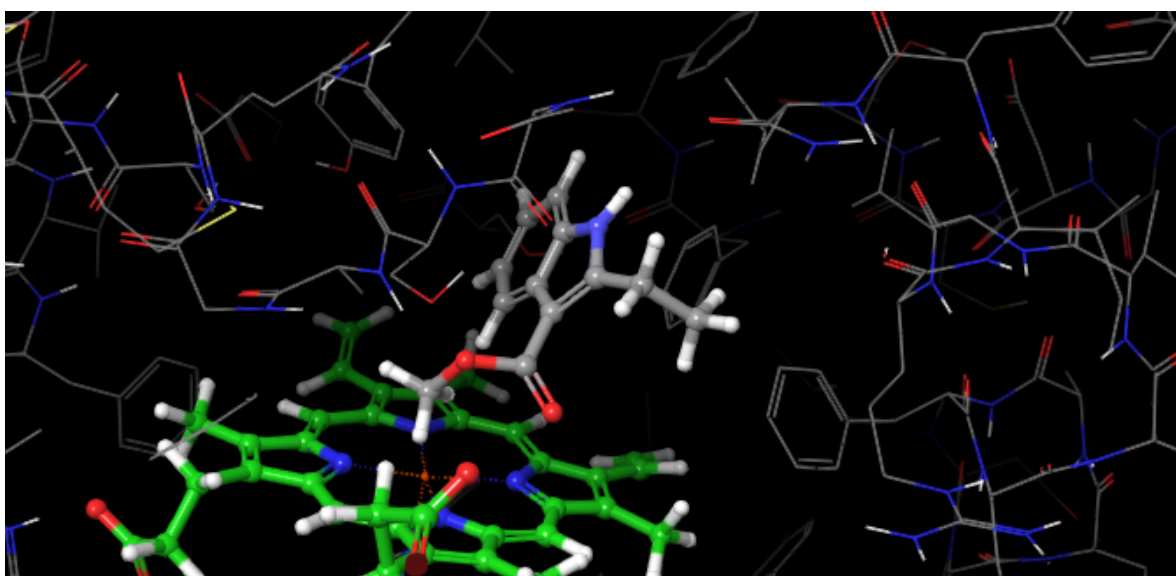
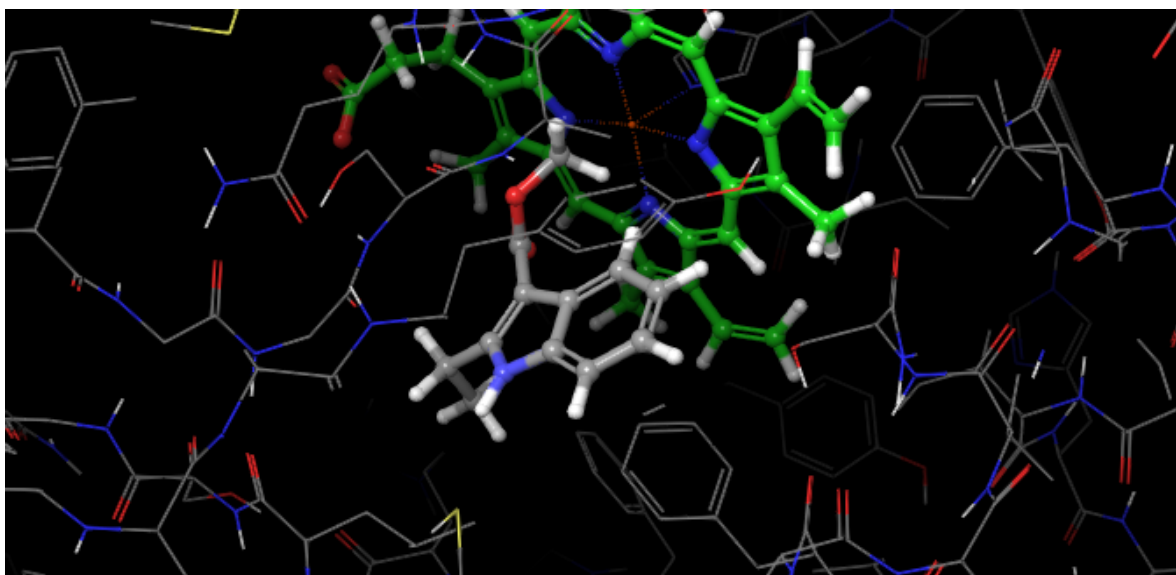
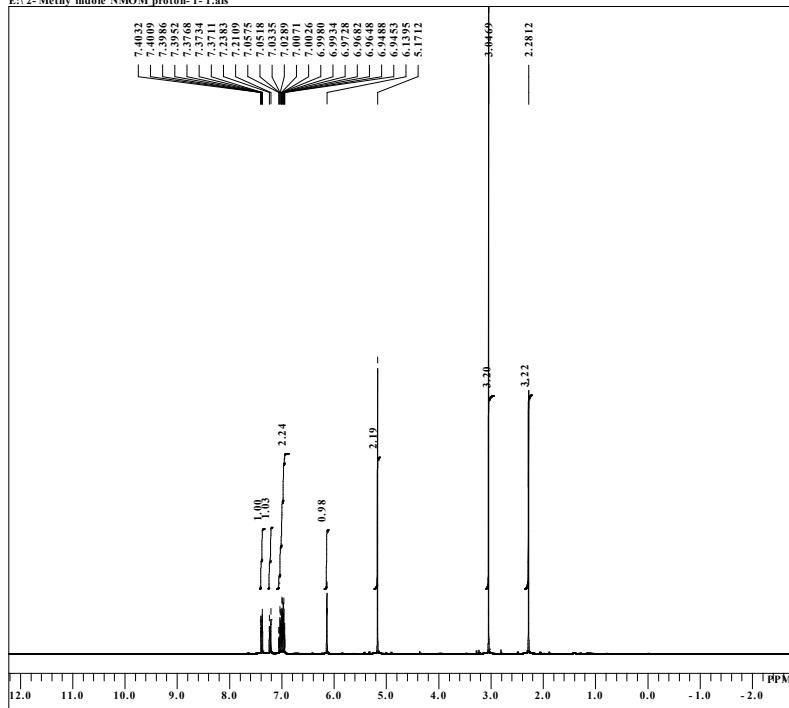


Figure S1. Docking model of compound **1af**.

2. ¹H, ¹³C, ¹⁹F NMR Spectra

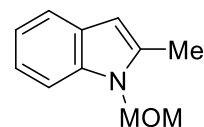
single pulse

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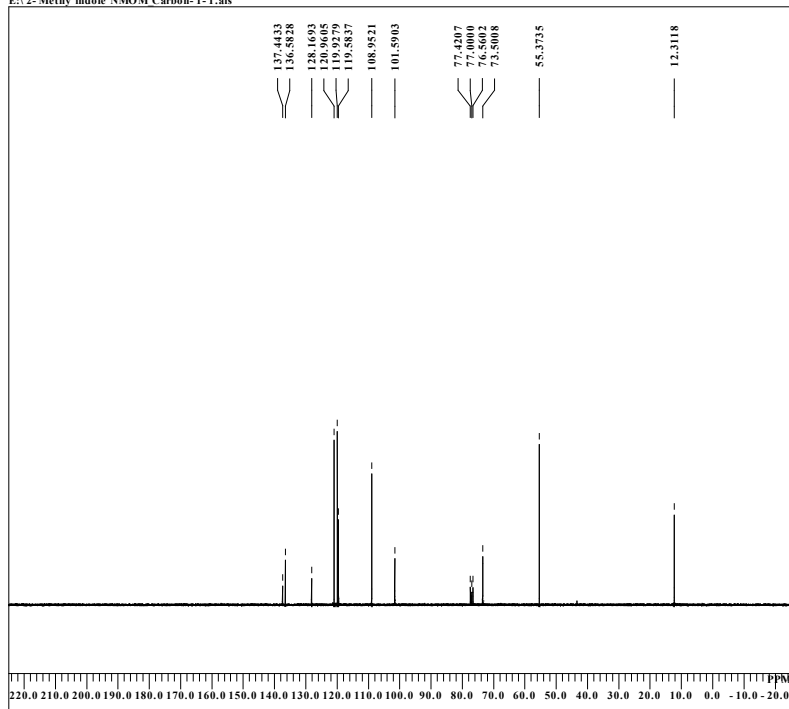
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OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
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PD 2.0000 sec
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CTEMP 18.6 c
SLVNT CDCL3
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BF 0.12 Hz
RGAIN 22
    
```



1b

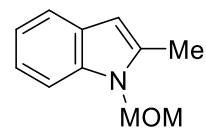
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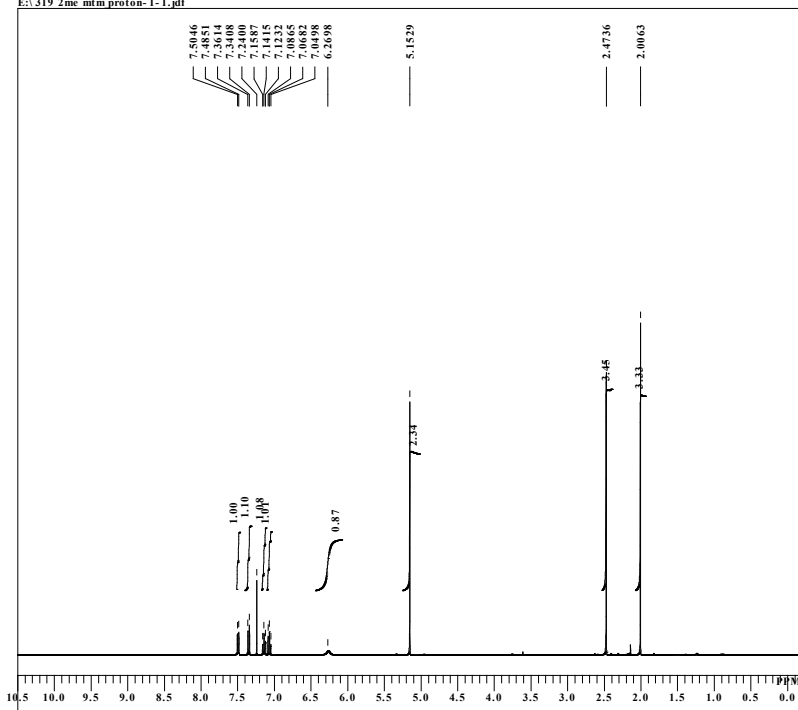
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OBSET 5.79 kHz
OBFIN 1.08 Hz
POINT 13107
FREQU 18939.39 Hz
SCANS 133
ACQTM 0.6921 sec
PD 1.0000 sec
PWI 3.73 usec
IRNUC 1H
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SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60
    
```



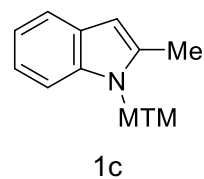
1b

single_pulse

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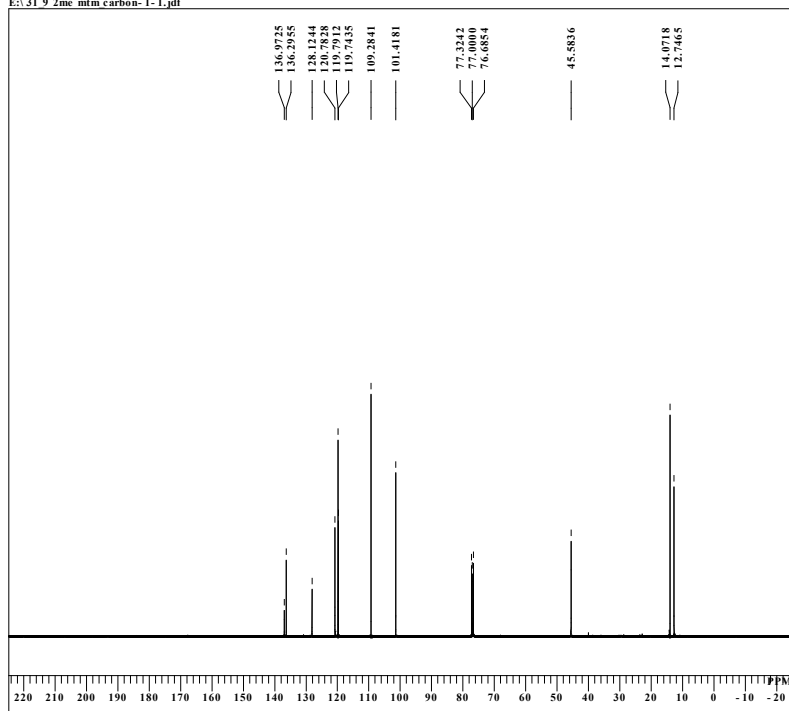


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 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 16384
 FREQU 7503.00 Hz
 SCANS 16
 ACQTM 2.1837 sec
 PD 2.0000 sec
 PWI 6.40 usec
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 CTEMP 20.3 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 46

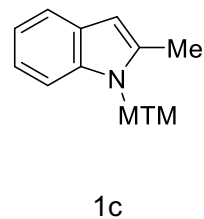


single pulse decoupled gated NOE

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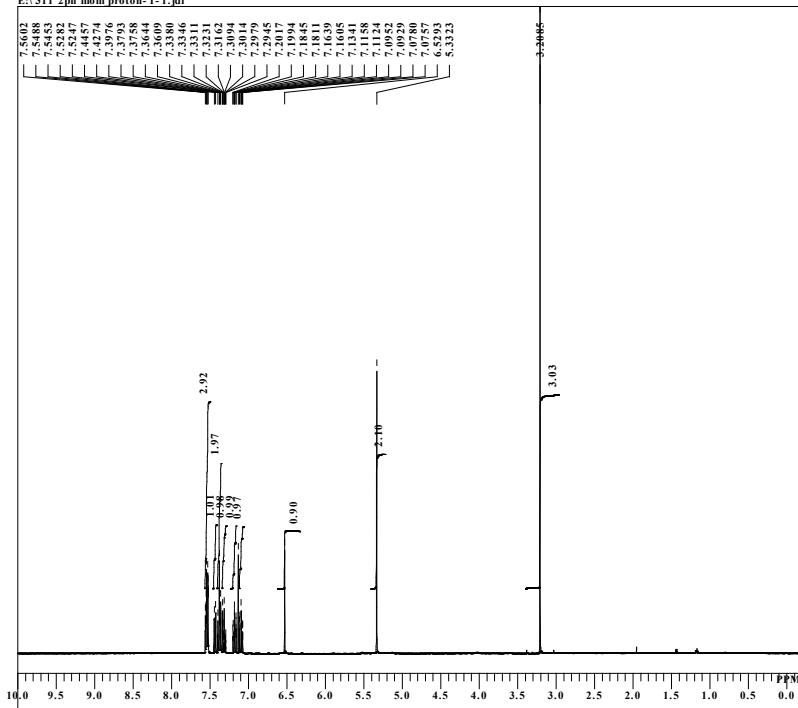


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 RGAIN 60

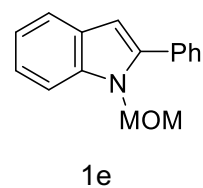


single pulse

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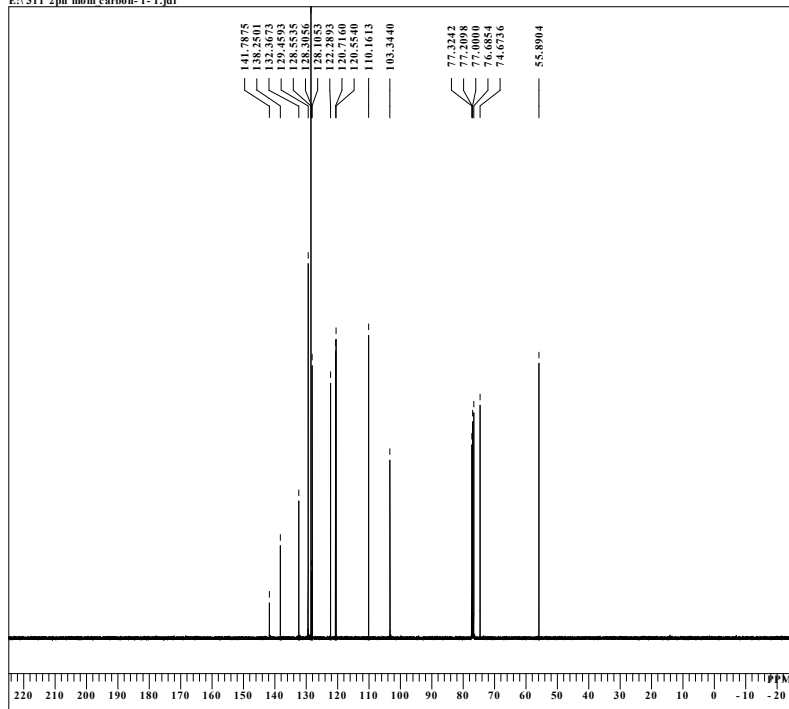


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POINT 16384
FREQU 7503.00 Hz
SCANS 16
ACQTM 2.1837 sec
PD 2.0000 sec
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SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 32

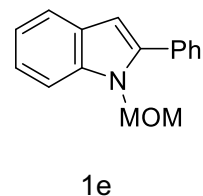


single pulse decoupled gated NOE

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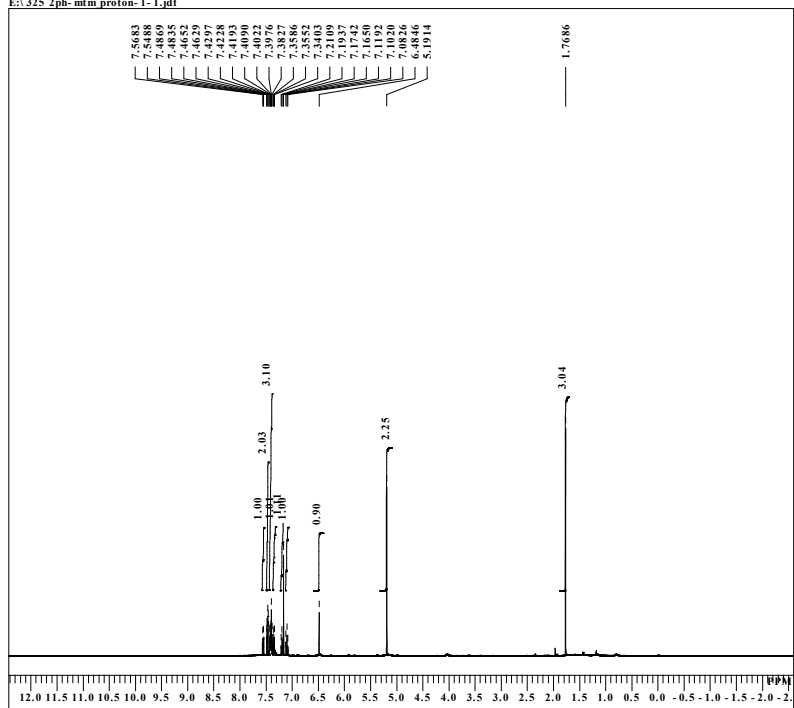


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OBFIN 5.86 Hz
POINT 32767
FREQU 31407.04 Hz
SCANS 1024
ACQTM 1.0433 sec
PD 2.0000 sec
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SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60

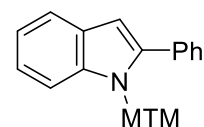


single_pulse

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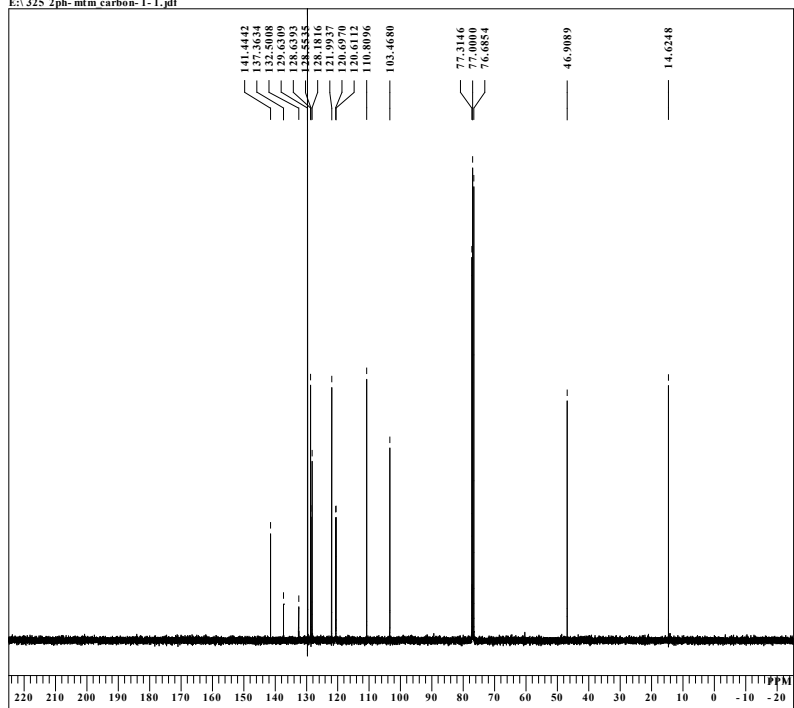
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 OBFIN 7.29 Hz
 POINT 16384
 FREQU 7503.00 Hz
 SCANS 16
 ACQTM 2.1837 sec
 PD 1.0000 sec
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 CTEMP 20.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 38



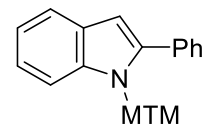
1f

single_pulse decoupled gated NOE

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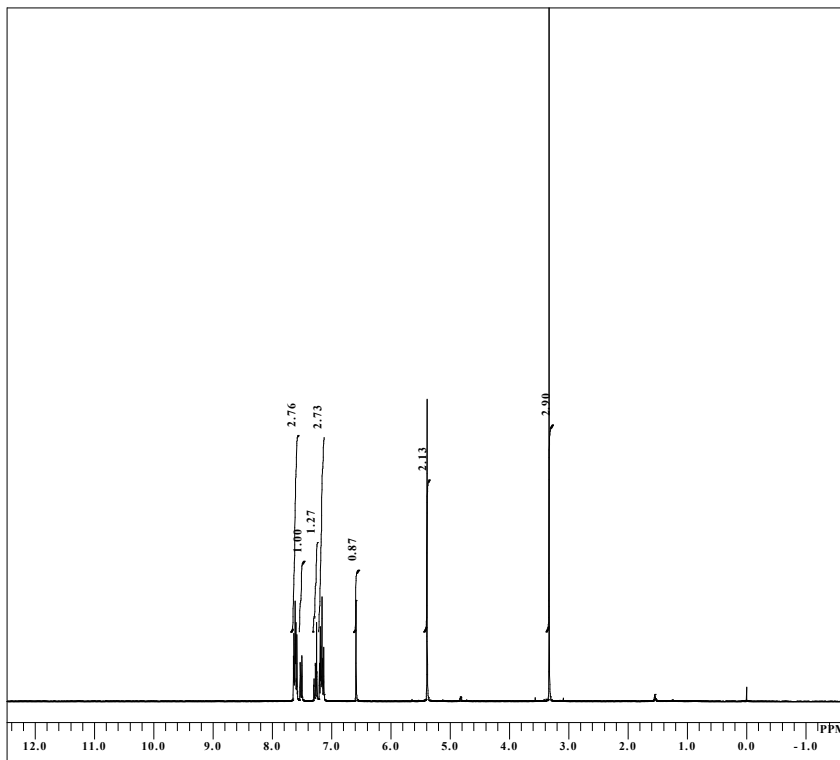


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 OBSET 5.35 kHz
 OBFIN 5.86 Hz
 POINT 32767
 FREQU 31407.04 Hz
 SCANS 601
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PWI 2.87 usec
 IRNUC 1H
 CTEMP 20.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60

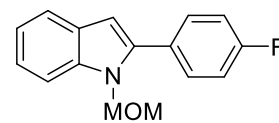


1f

single_pulse

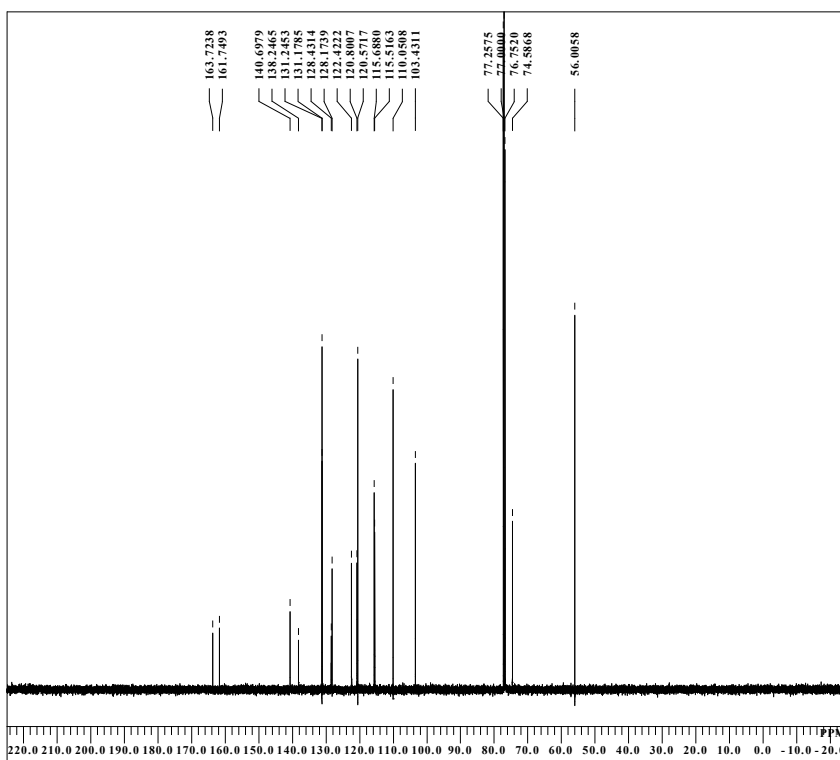


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 FREQU 9025.27 Hz
 SCANS 32
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 BF 0.12 Hz
 RGAIN 36

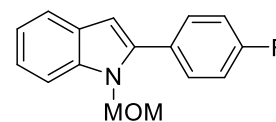


1h

single_pulse decoupled gated NOE



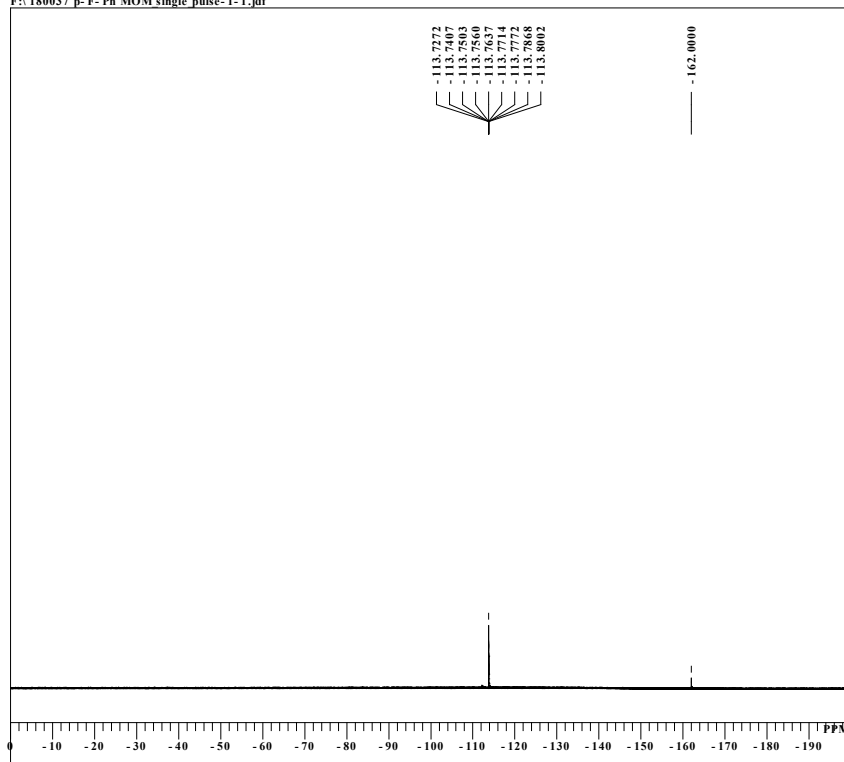
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 POINT 26214
 FREQU 31446.54 Hz
 SCANS 1000
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 CTEMP 19.0 c
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 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



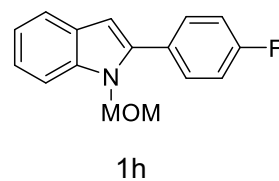
1h

single_pulse

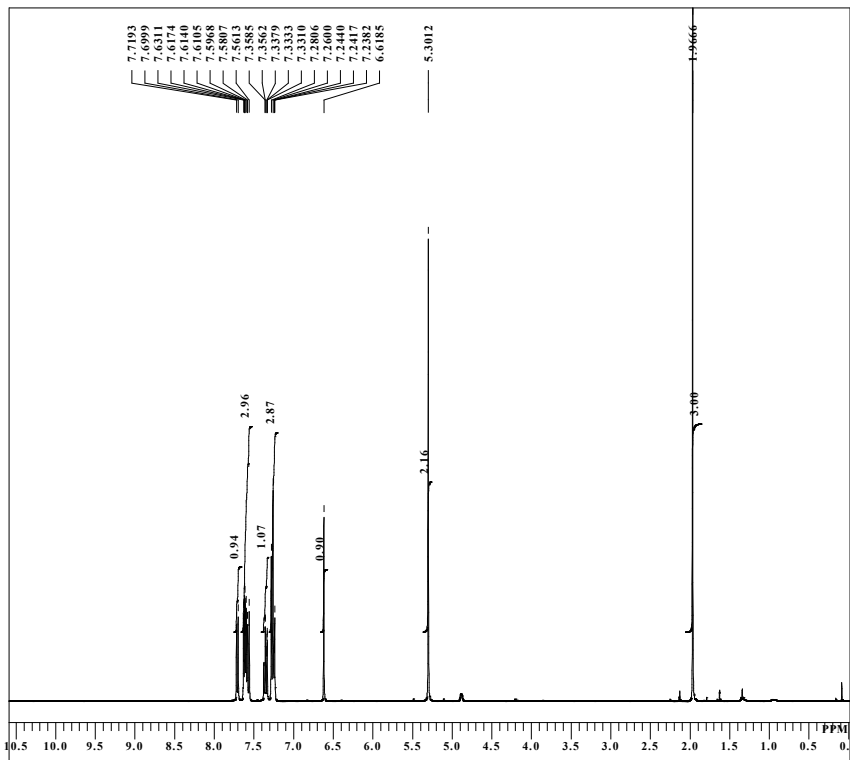
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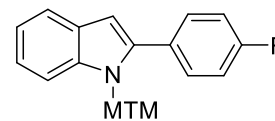
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OBFREQ 376.13 MHz
OBSETE 3.43 kHz
OBFEN 6.82 Hz
POINT 131071
FREQU 94696.97 Hz
SCANS 16
ACQTM 1.3841 sec
PD 2.0000 sec
PWI 7.80 usec
IRNUC 19F
CTEMP 20.6 c
SLVNT CDCL3
XREF -162.00 ppm
BF 0.12 Hz
RGAIN 46



single_pulse

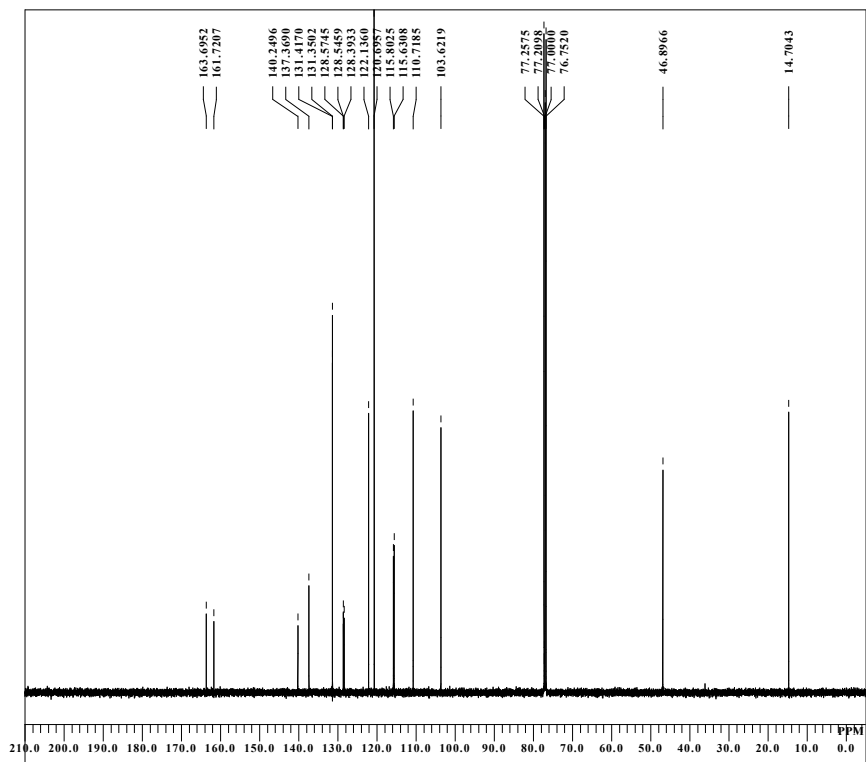


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EXMOD proton.jsp
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OBSET 4.19 kHz
OBFEN 7.29 Hz
POINT 13107
FREQU 6002.40 Hz
SCANS 8
ACQTM 2.1837 sec
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IRNUC 1H
CTEMP 20.6 c
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XREF 7.26 ppm
BF 0.12 Hz
RGAIN 40

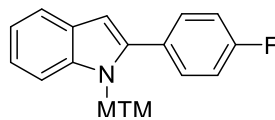


1i

single_pulse decoupled gated NOE



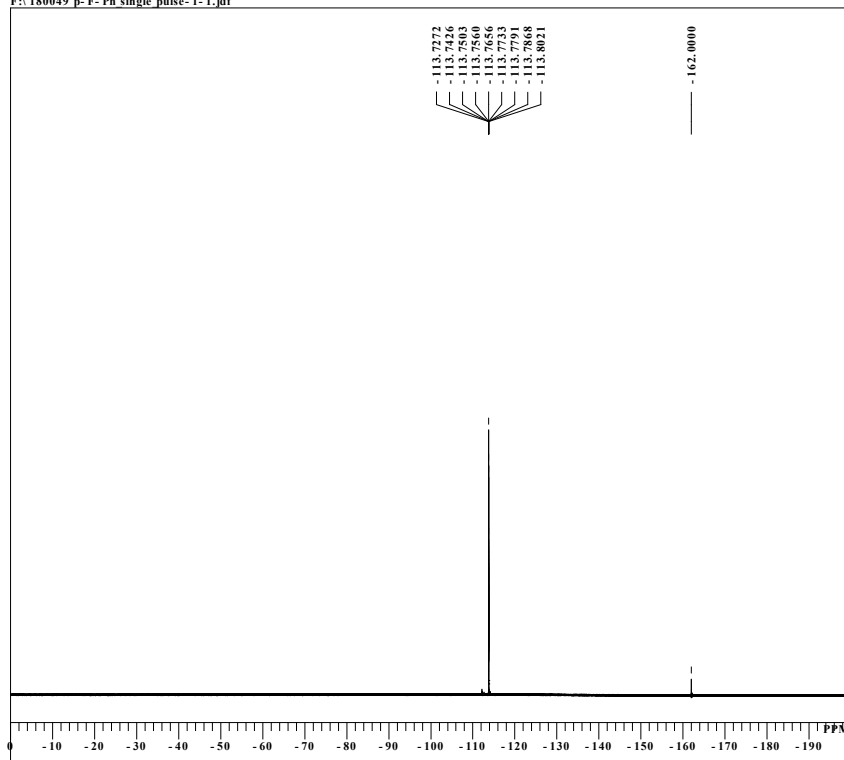
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OBSET 7.87 kHz
OBFEN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 1053
ACQTM 0.8336 sec
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XREF 77.00 ppm
BF 0.12 Hz
RGAIN 60



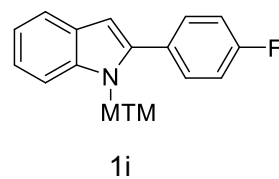
1i

single_pulse

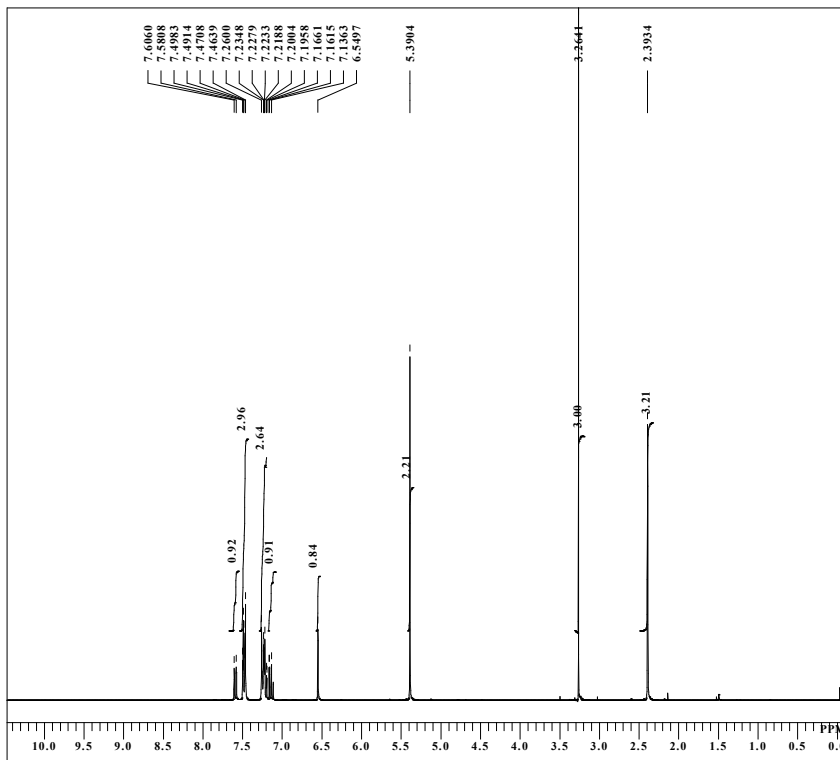
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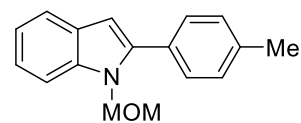
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OBSET 3.43 kHz
OBFEN 6.82 Hz
POINT 131071
FREQU 94696.97 Hz
SCANS 16
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 7.80 usec
IRNUC 19F
CTEMP 20.3 c
SLVNT CDCL3
XREF -162.00 ppm
BF 0.12 Hz
RGAIN 46



single_pulse

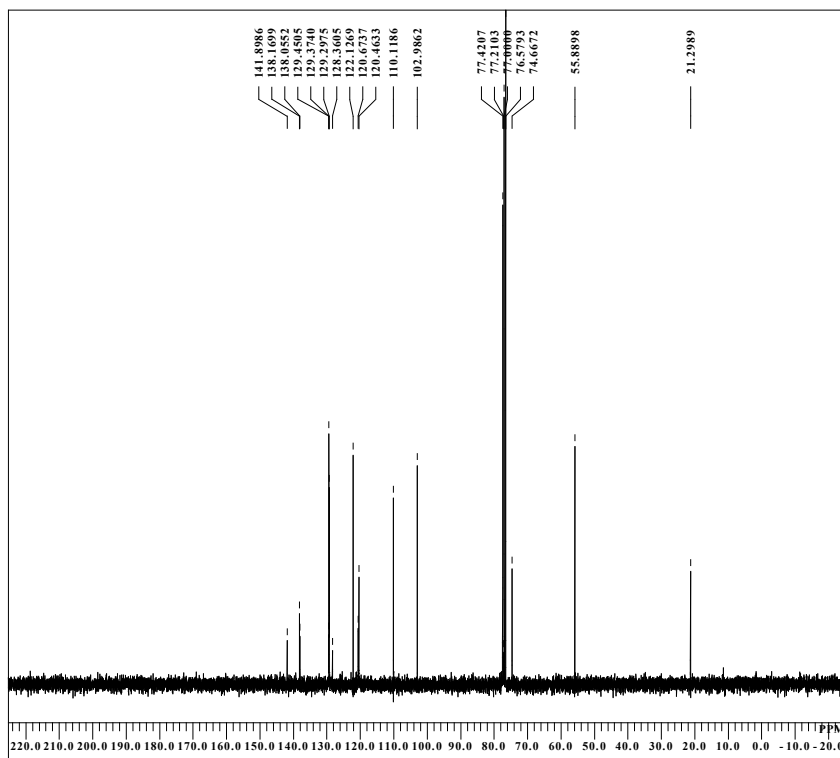


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OBFIN 8.57 Hz
POINT 13107
FREQU 9025.27 Hz
SCANS 16
ACQTM 1.4523 sec
PD 1.0000 sec
PWI 5.50 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
XREF 7.26 ppm
BF 0.12 Hz
RGAIN 36

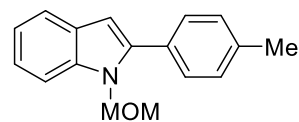


1k

single_pulse decoupled gated NOE

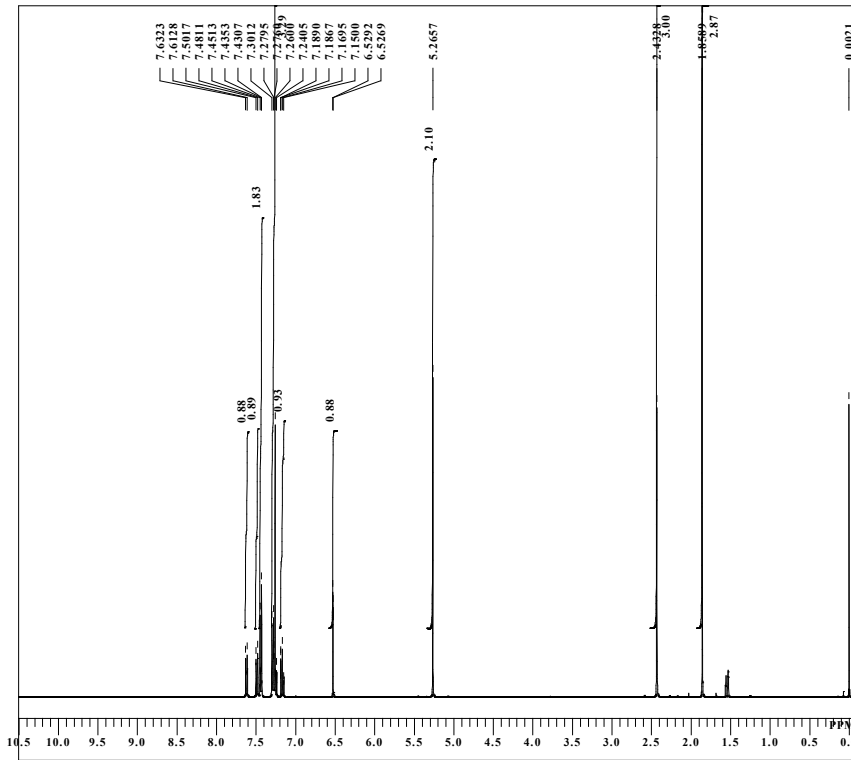


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OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 13107
FREQU 18939.39 Hz
SCANS 1024
ACQTM 0.6921 sec
PD 2.0000 sec
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CTEMP 19.4 c
SLVNT CDCL3
XREF 77.00 ppm
BF 0.12 Hz
RGAIN 60

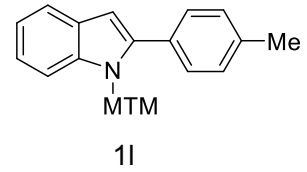


1k

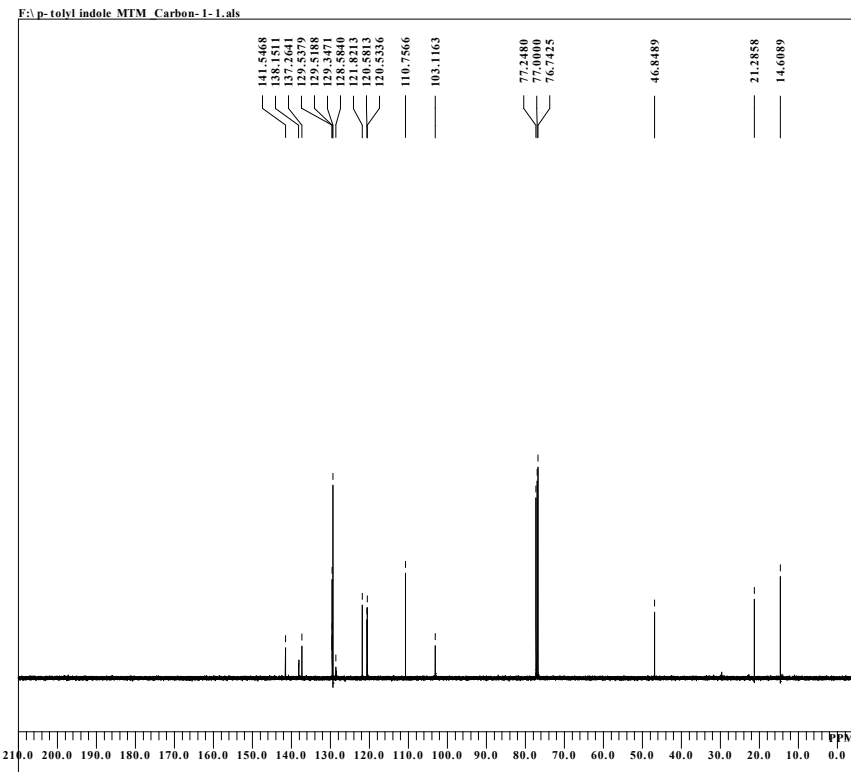
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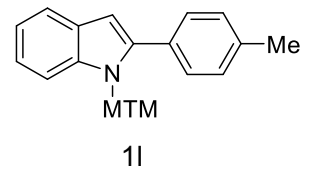
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 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 16
 ACQTM 2.1837 sec
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 CTEMP 21.3 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 50



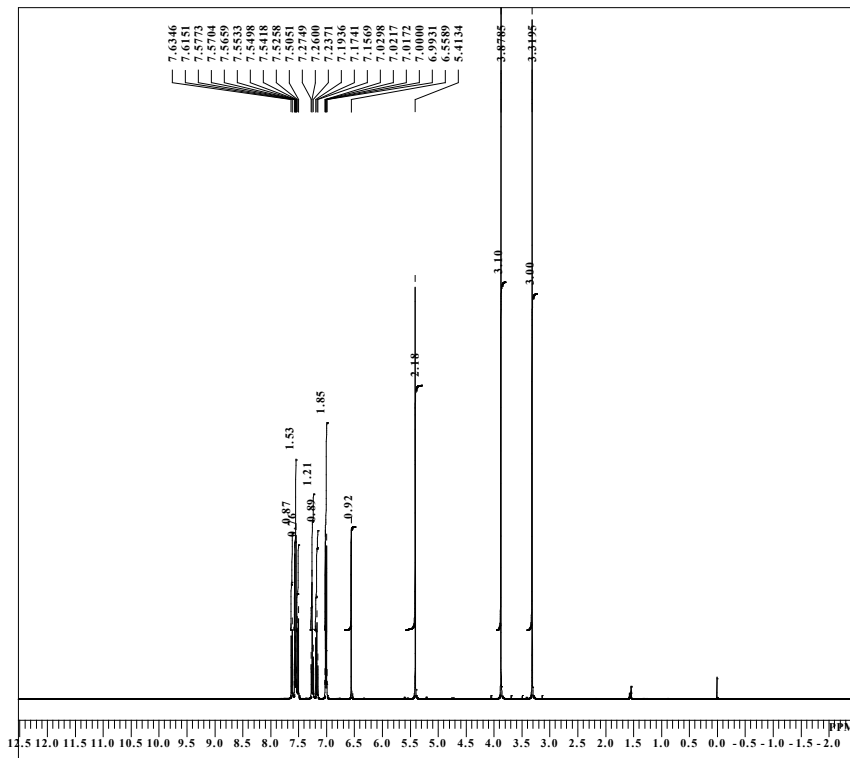
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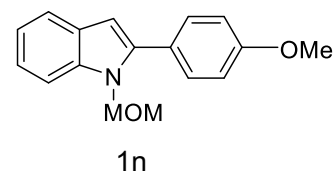
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 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 281
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PWI 3.27 usec
 IRNUC 1H
 CTEMP 19.6 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50



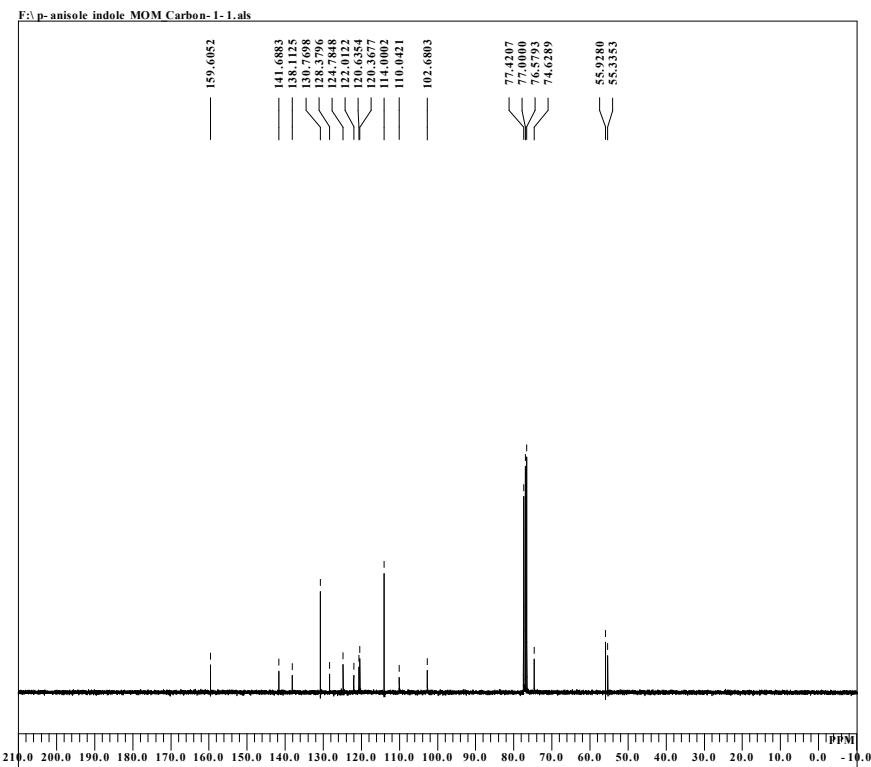
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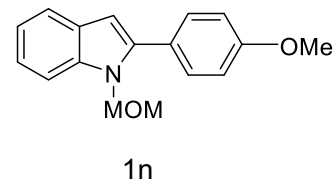
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 EXMOD proton.jsp
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 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 16
 ACQTM 2.1837 sec
 PD 1.0000 sec
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 IRNUC 1H
 CTEMP 21.3 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 44



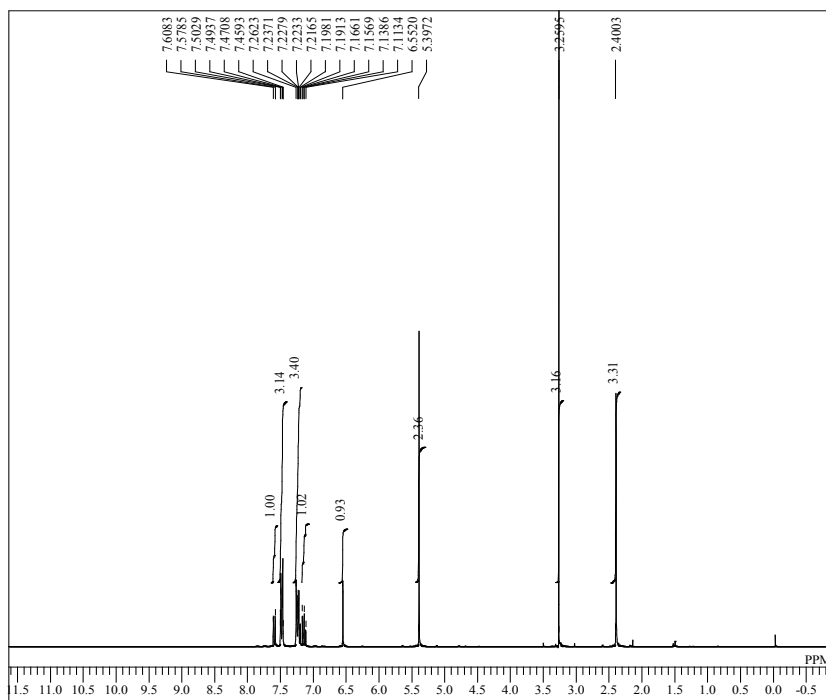
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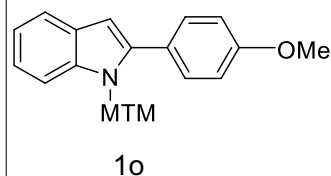
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 OBSET 5.79 KHz
 OBFIN 1.08 Hz
 POINT 13107
 FREQU 18939.39 Hz
 SCANS 1130
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 PD 2.5000 sec
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 IRNUC 1H
 CTEMP 20.5 c
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 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



single_pulse

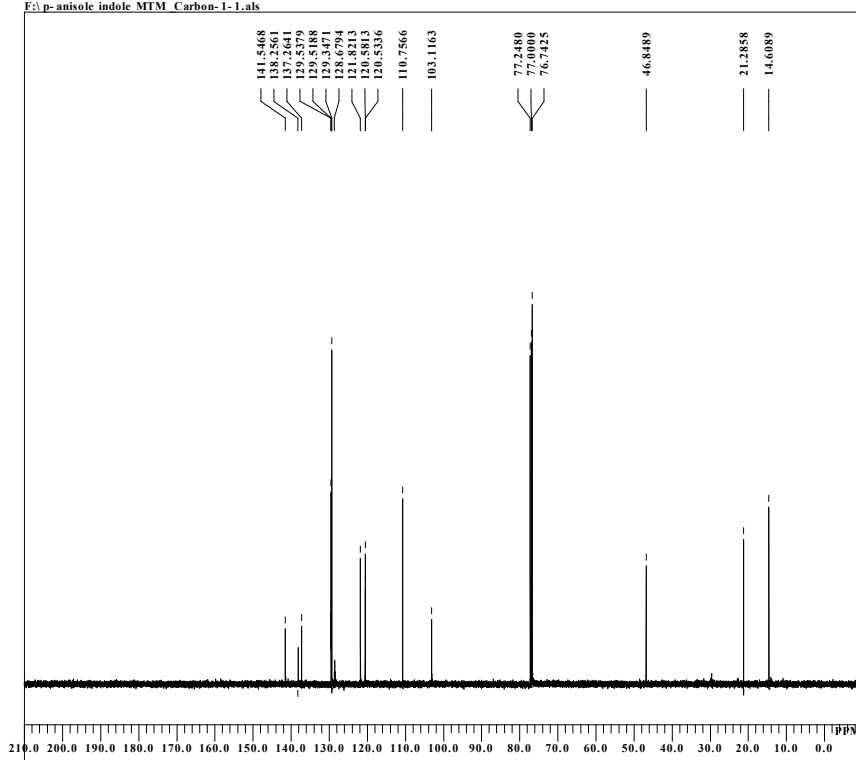


DFILE 180048 p-anisole indole mtm_proton-1-1.a
COMNT single_pulse
DATIM 2019-03-28 16:55:49
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 9025.27 Hz
SCANS 16
ACQTM 1.4523 sec
PD 1.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 36

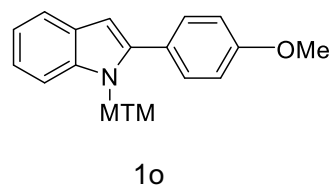


single pulse decoupled gated NOE

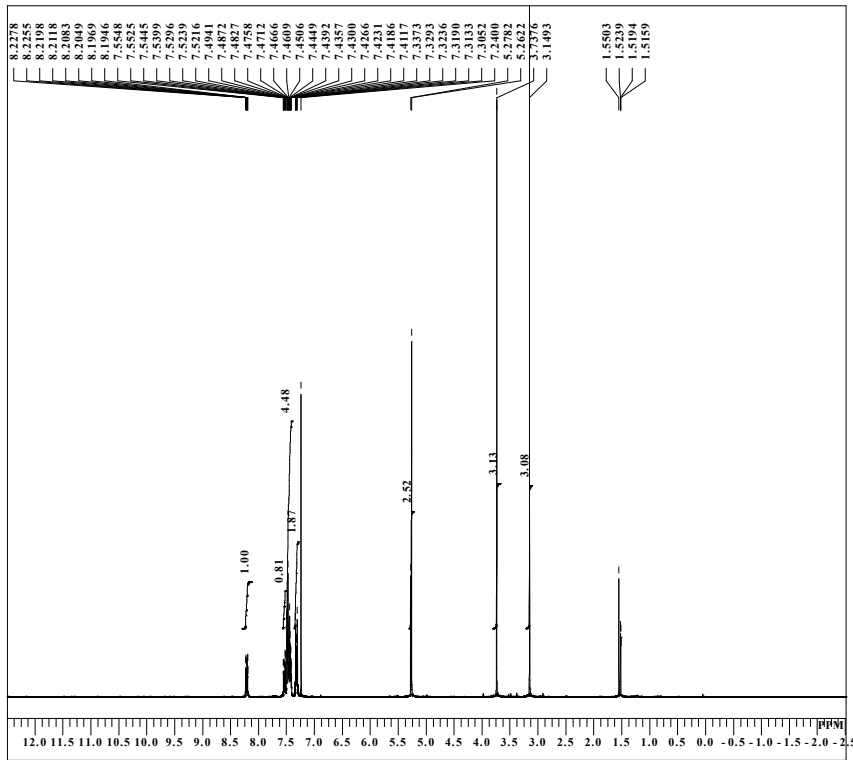
F2: p-anisole indole MTM Carbon-1-1.als



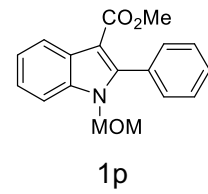
DFILE p-anisole indole MTM Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2019-04-19 12:24:19
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 281
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 19.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



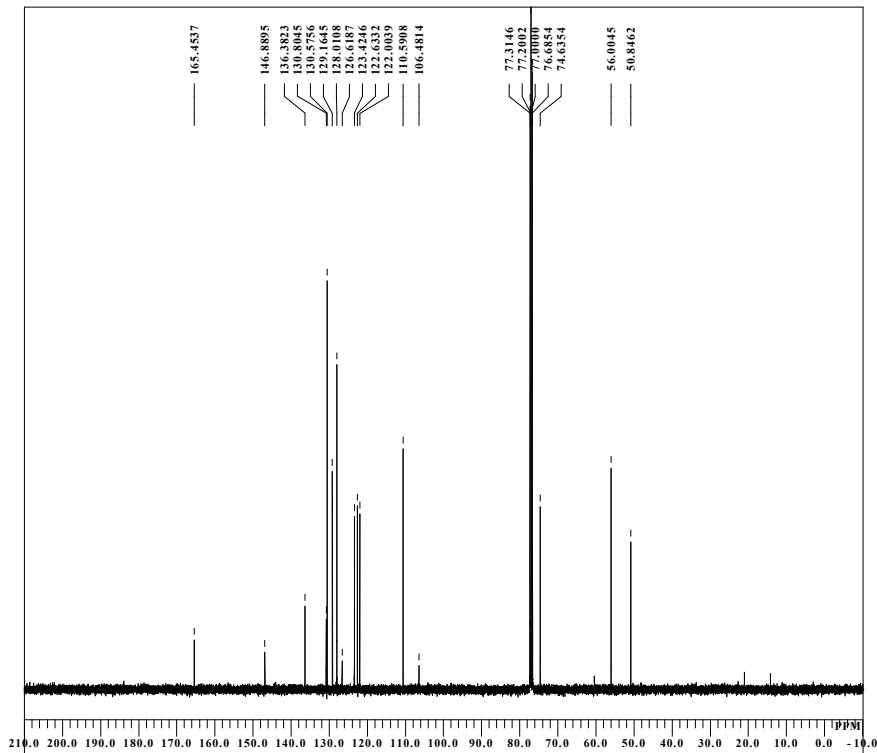
single_pulse



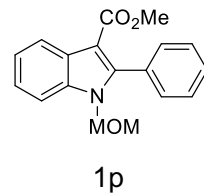
DFILE 59 2- Ph 3-COOme MOM proton-1-1.
 COMNT single_pulse
 DATIM 2019-07-03 16:59:26
 ORNUC 1H
 EXMOD proton.jsp
 OBFREQ 300.53 MHz
 OBSET 1.15 KHz
 OBFIN 8.57 Hz
 POINT 13107
 FREQU 4508.57 Hz
 SCANS 16
 ACQTM 2.9072 sec
 PD 2.0000 sec
 PWI 5.50 usec
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 42



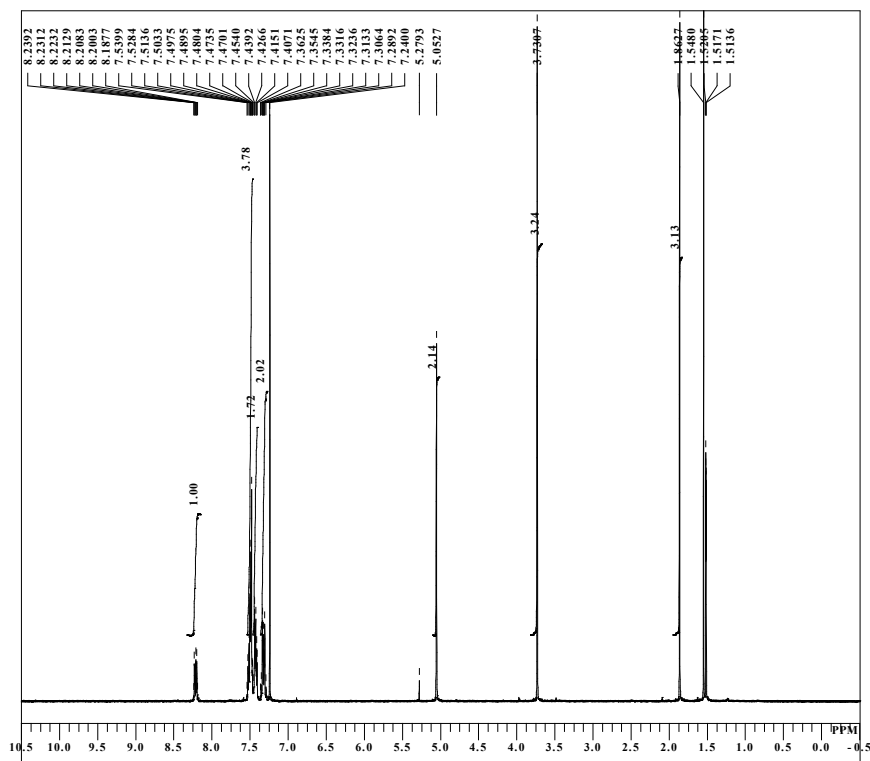
single_pulse decoupled gated NOE



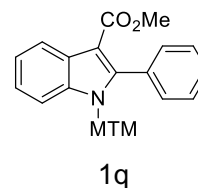
DFILE 59 2- Ph 3-COOme MOM carbon-1-1.
 COMNT single_pulse decoupled gated NOE
 DATIM 2019-06-26 17:49:35
 ORNUC 13C
 EXMOD carbon.jsp
 OBFREQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PWI 3.17 usec
 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



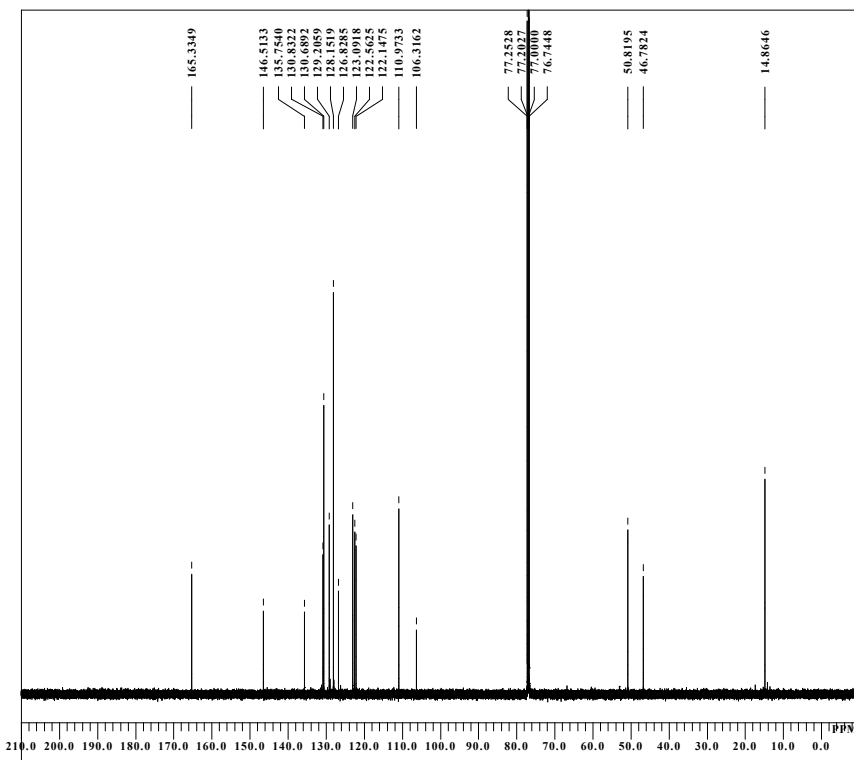
single_pulse



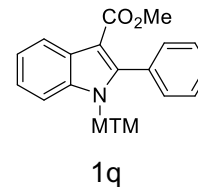
DFILE 60 2- Ph 3-COOMe MTM proton-1-1.
 COMNT single_pulse
 DATIM 2019-07-03 17:06:20
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 300.53 MHz
 OBSET 1.15 KHz
 OBFIN 8.57 Hz
 POINT 13107
 FREQU 4508.57 Hz
 SCANS 16
 ACQTM 2.9072 sec
 PD 2.0000 sec
 PWI 5.50 usec
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 44



single_pulse decoupled gated NOE

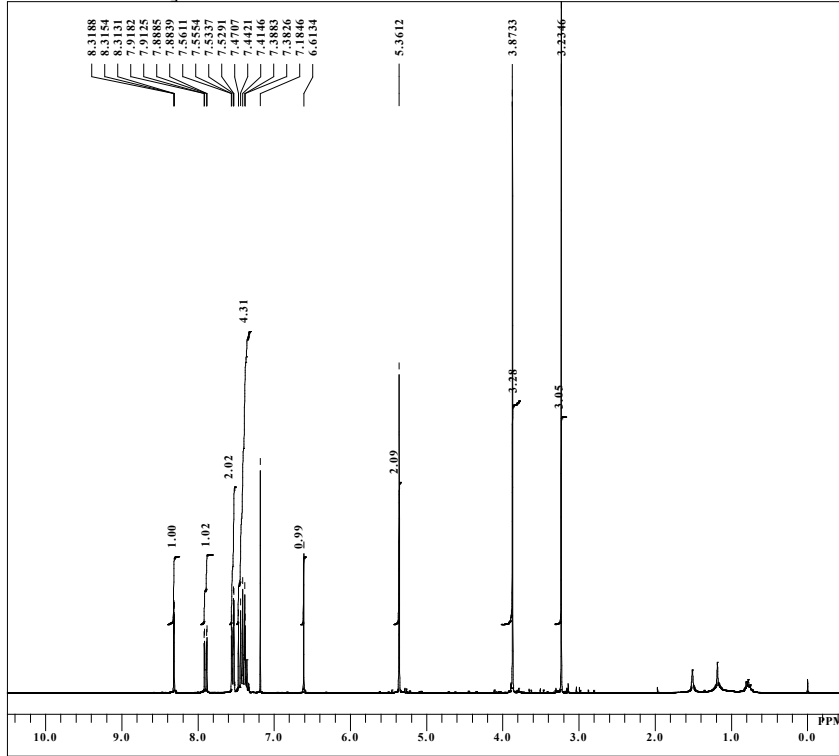


DFILE 60 2- Ph 3-COOMe MTM Carbon-1-1.
 COMNT single_pulse decoupled gated NOE
 DATIM 2019-06-27 10:39:47
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 104857
 FREQU 31446.54 Hz
 SCANS 601
 ACQTM 3.3345 sec
 PD 2.0000 sec
 PWI 3.27 usec
 IRNUC 1H
 CTEMP 23.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 54

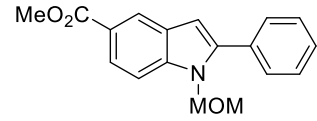


single_pulse

E:\63 2-Ph 5-COOMe MOM proton-1-1.als



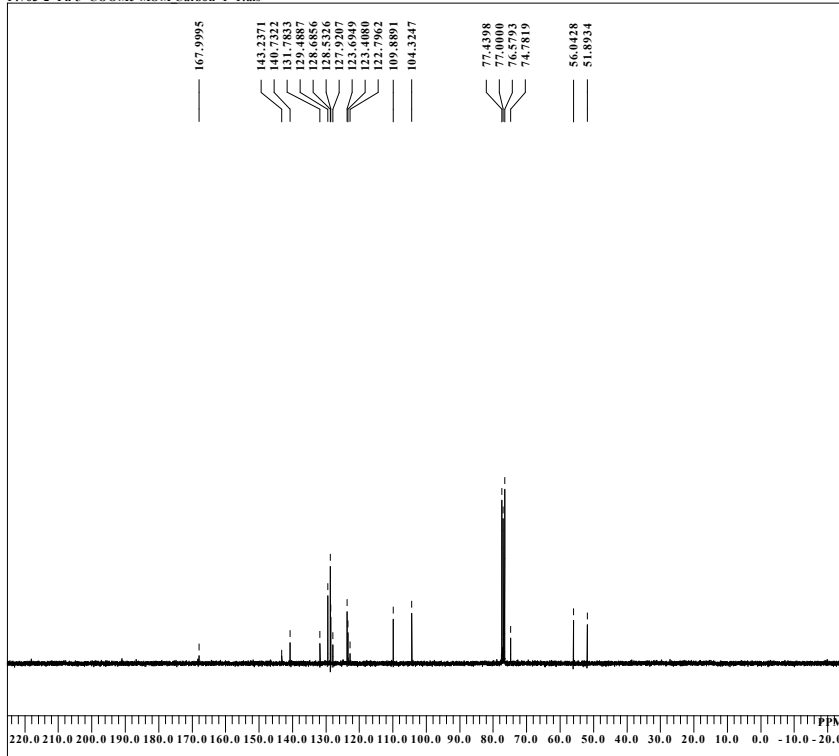
DFILE 63 2-Ph 5-COOMe MOM proton-1-1.
 COMNT single_pulse
 DATIM 2019-06-28 15:28:45
 ORNUC 1H
 EXMOD proton.jsp
 OBFREQ 300.53 MHz
 OBSET 1.15 KHz
 OBFIN 8.57 Hz
 POINT 13107
 FREQU 4508.57 Hz
 SCANS 16
 ACQTM 2.9072 sec
 PD 2.0000 sec
 PWI 5.50 usec
 IRNUC 1H
 CTEMP 23.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 40



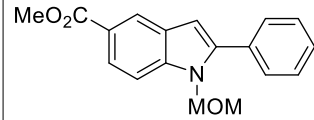
1r

single_pulse decoupled gated NOE

E:\63 2-Ph 5-COOMe MOM Carbon-1-1.als



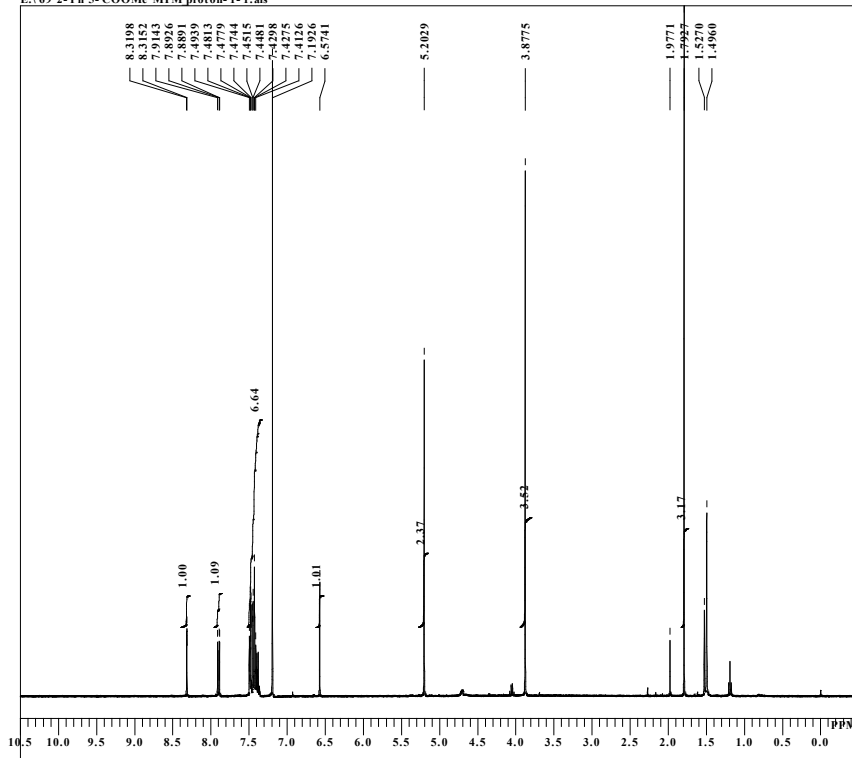
DFILE 63 2-Ph 5-COOMe MOM Carbon-1-1
 COMNT single_pulse decoupled gated NOE
 DATIM 2019-06-28 15:32:18
 ORNUC 13C
 EXMOD carbon.jsp
 OBFREQ 75.57 MHz
 OBSET 5.79 KHz
 OBFIN 1.08 Hz
 POINT 13107
 FREQU 18939.39 Hz
 SCANS 1024
 ACQTM 0.6921 sec
 PD 2.5000 sec
 PWI 3.73 usec
 IRNUC 1H
 CTEMP 23.8 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60



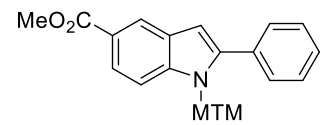
1r

single_pulse

E:\69 2-Ph 5-COOMe MTM proton-1-1.als



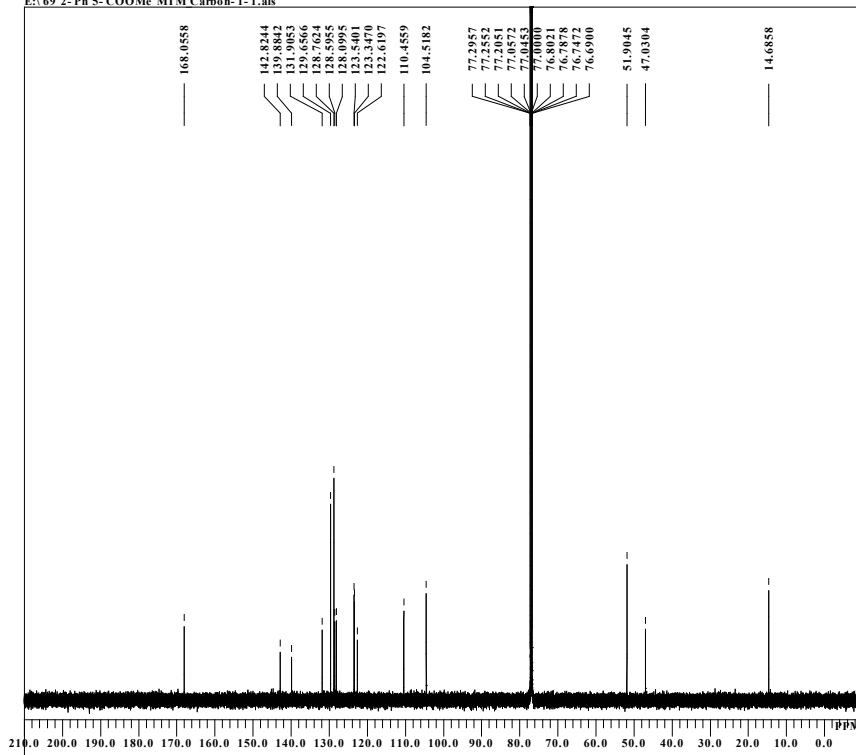
DFILE 69 2-Ph 5-COOMe MTM proton-1-1.
 COMNT single_pulse
 DATIM 2019-06-28 19:01:26
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 1.0000 sec
 PWI 7.25 usec
 IRNUC 1H
 CTEMP 22.6 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 56



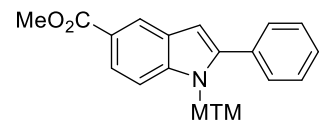
1s

single pulse decoupled gated NOE

E:\69 2-Ph 5-COOMe MTM Carbon-1-1.als

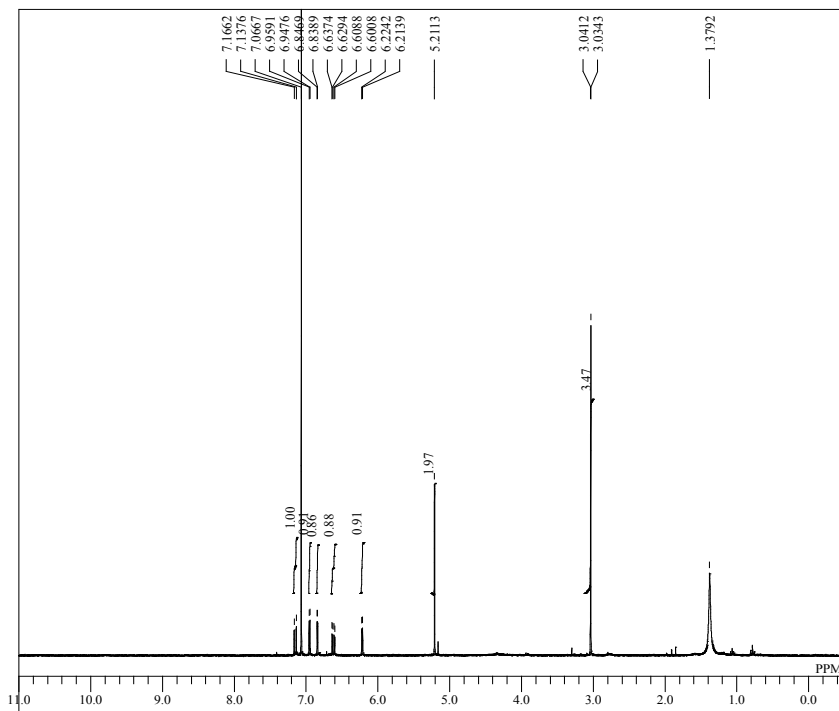


DFILE 69 2-Ph 5-COOMe MTM Carbon-1-1.
 COMNT single pulse decoupled gated NOE
 DATIM 2019-06-29 10:20:42
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 104857
 FREQU 31446.54 Hz
 SCANS 1717
 ACQTM 3.3345 sec
 PD 1.0000 sec
 PWI 3.27 usec
 IRNUC 1H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 56

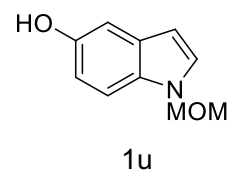


1s

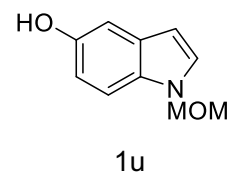
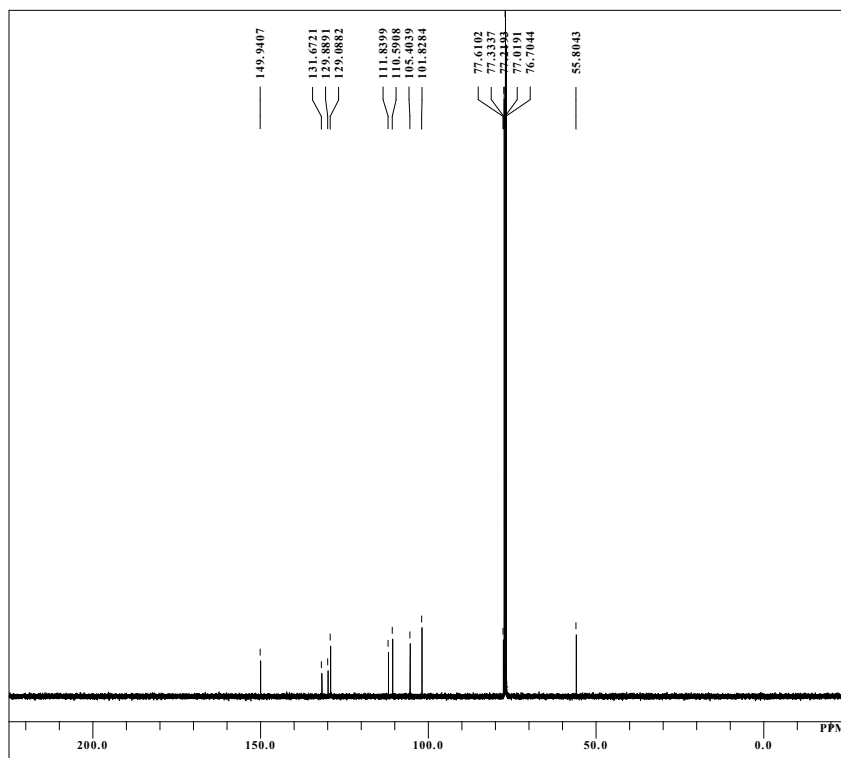
single_pulse



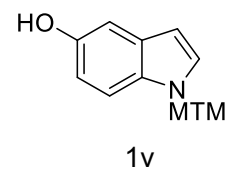
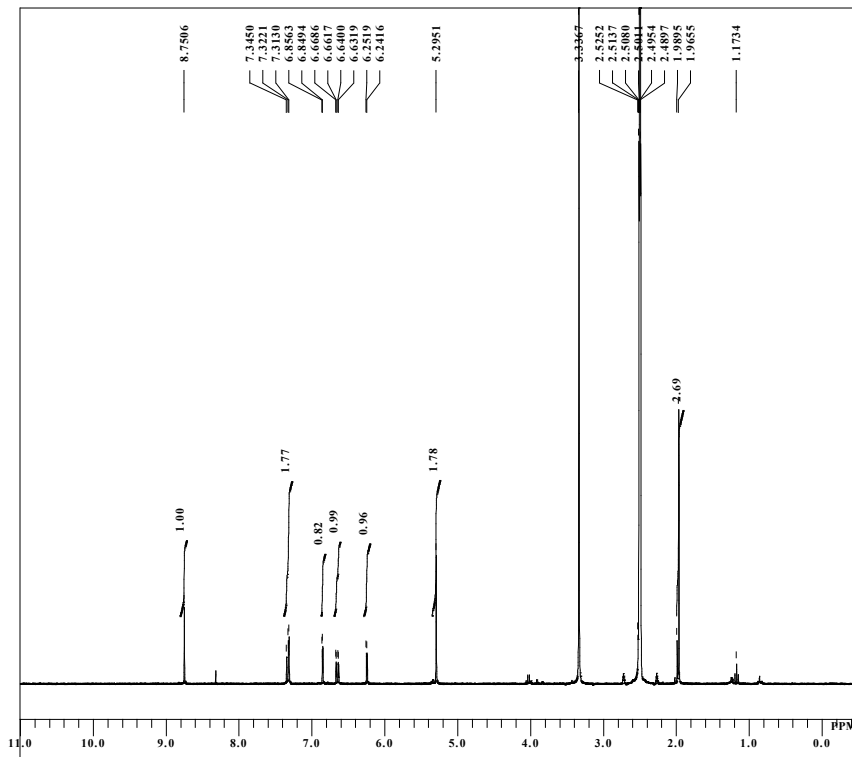
DFILE 109 OH MOM_proton-1-1.als
COMNT single_pulse
DATIM 2019-11-05 19:02:01
OBNUC 1H
EXMOD proton.jpg
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 16
ACQTM 2.9072 sec
PD 2.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 44



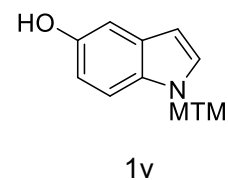
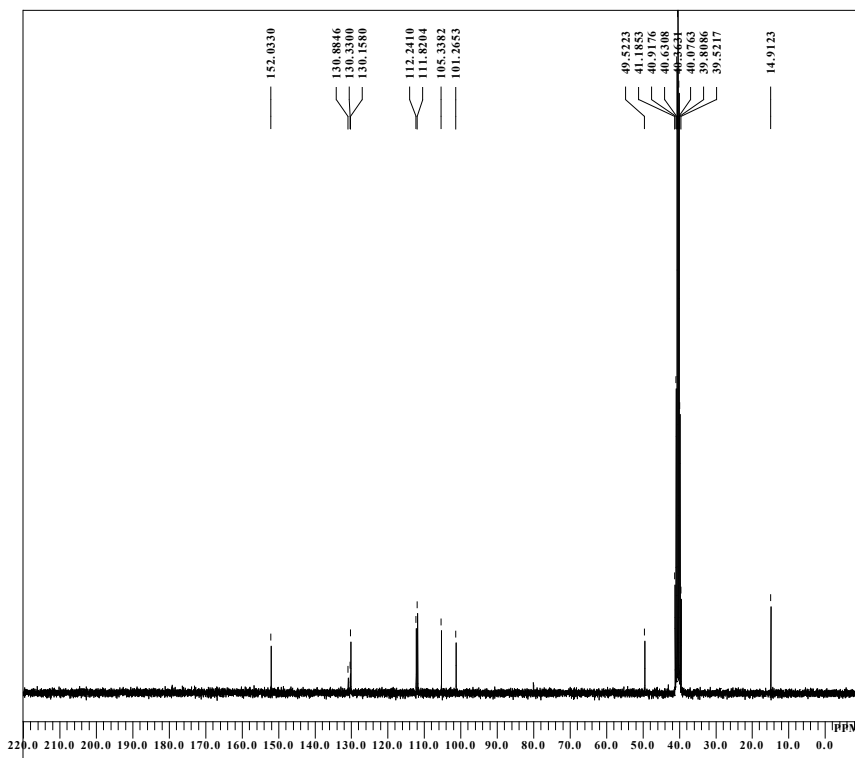
single_pulse decoupled gated NOE



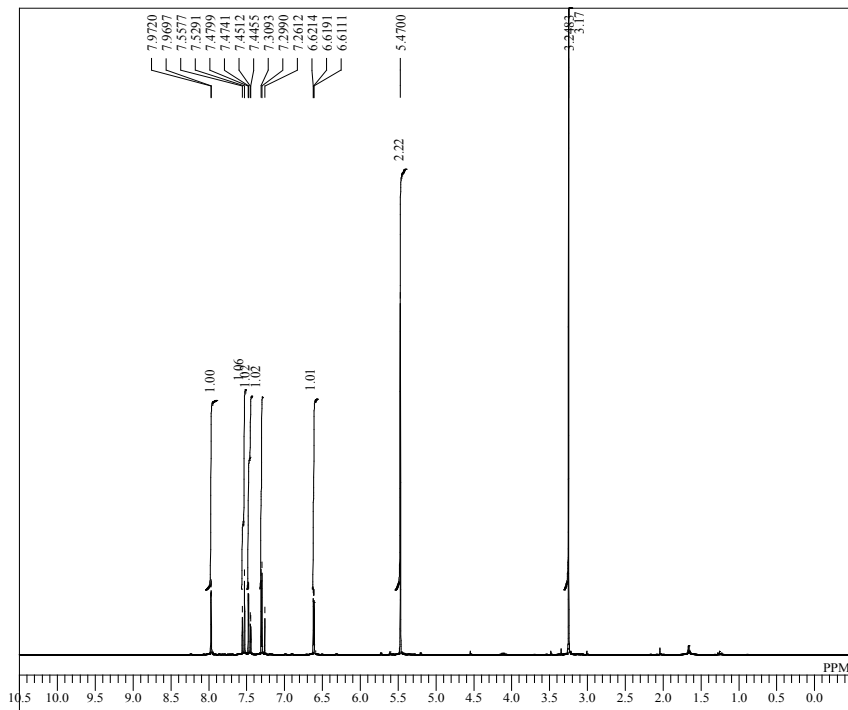
single pulse



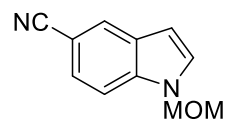
single pulse decoupled gated NOE



single_pulse

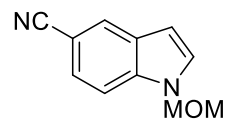
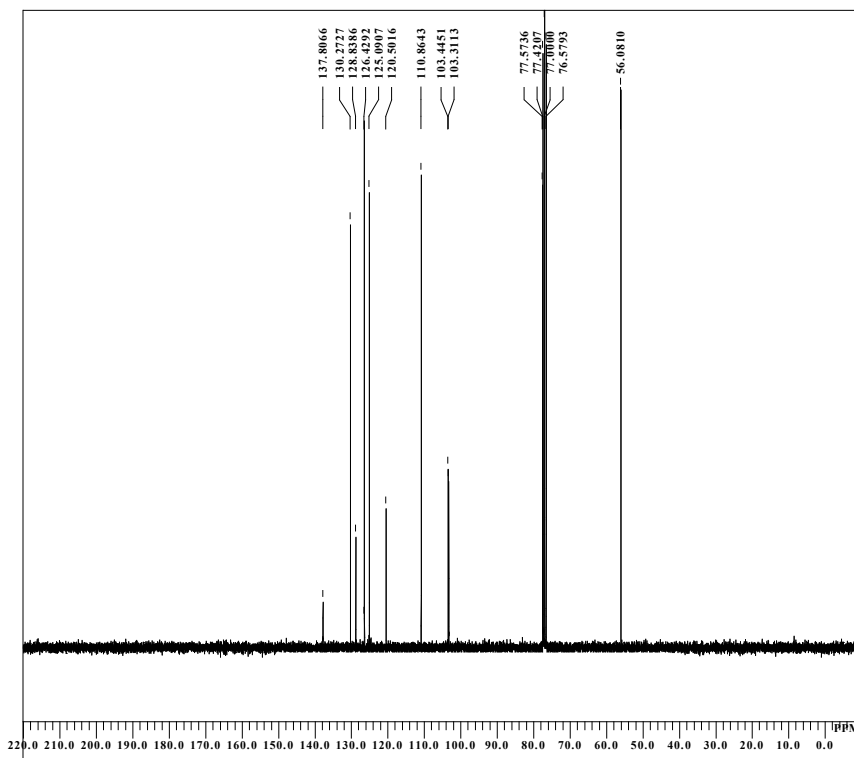


DFILE 104 CN MOM_proton-1-1.als
COMNT single_pulse
DATIM 2019-10-29 18:22:55
OBNUC 1H
EXMOD proton.jpg
OBFRQ 300.53 MHz
OBSEI 1.15 kHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 8
ACQTM 2.9072 sec
PD 2.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 36



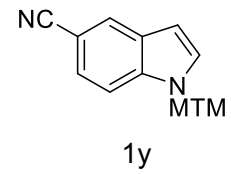
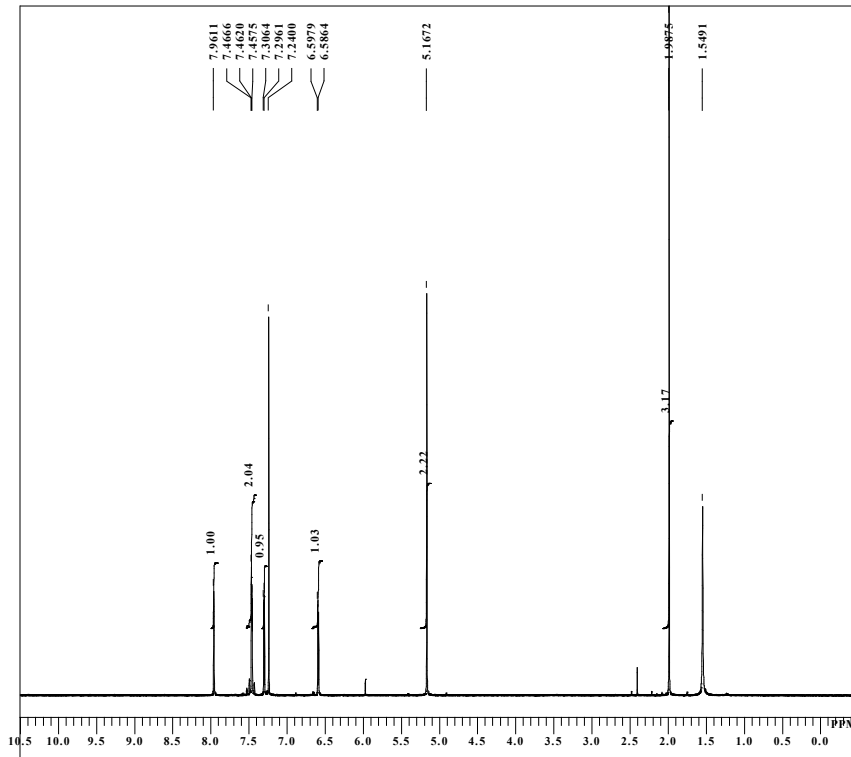
1x

single_pulse decoupled gated NOE



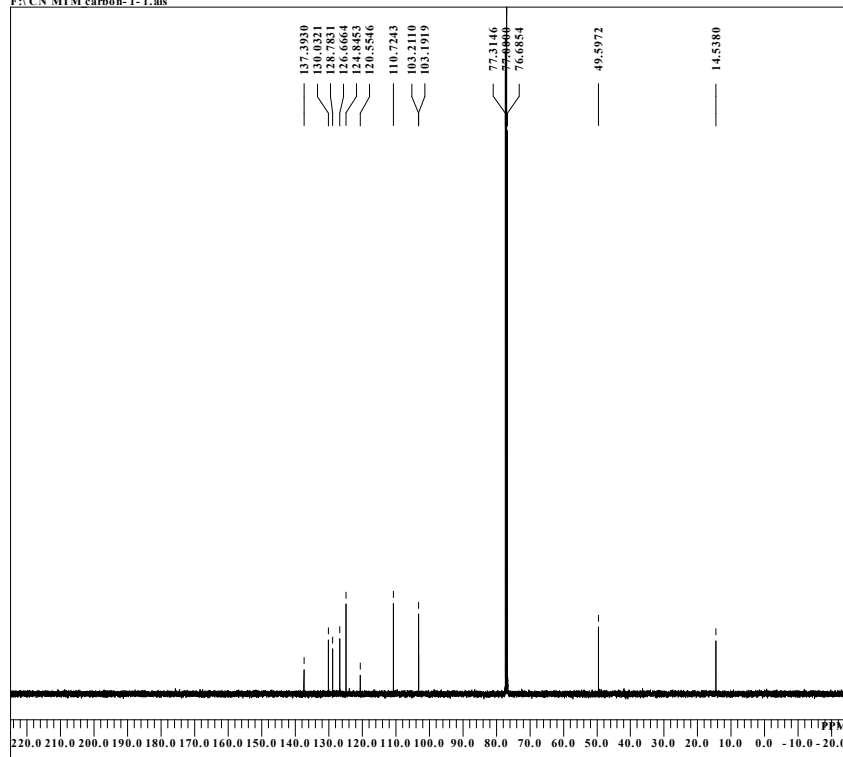
1x

single_pulse

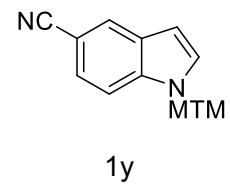


single pulse decoupled gated NOE

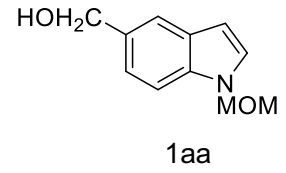
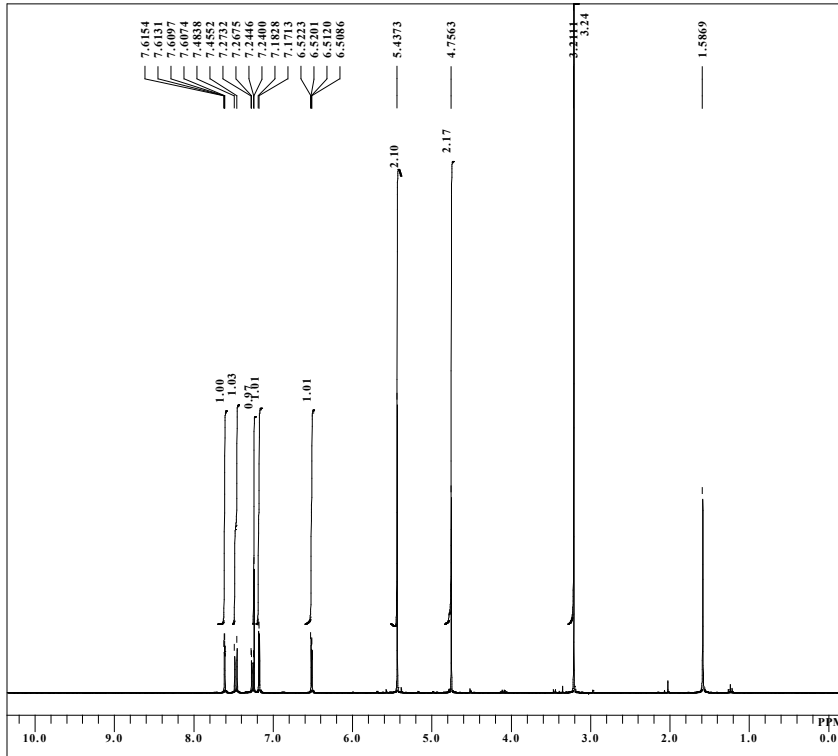
F:\CN MTM carbon-1-1.als



DFILE CN MTM carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2019-11-08 17:57:00
OBNUC 13C
EXMOD carbon_jpp
OBFRO 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 2496
ACQTM 1.0433 sec
PD 1.0000 sec
PWI 3.17 usec
IRNUC 1H
CTEMP 19.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60

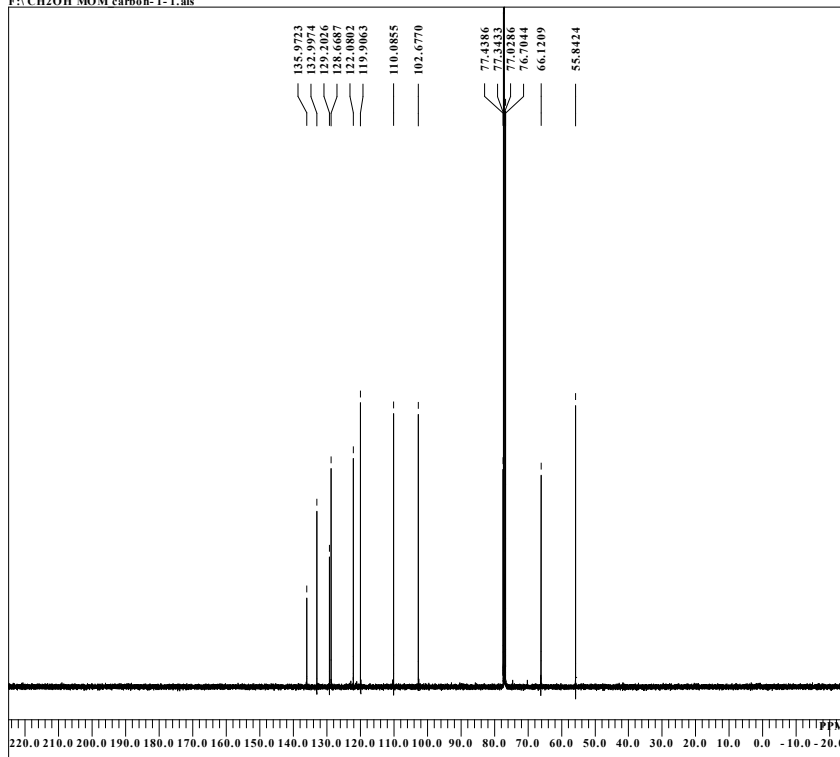


single pulse

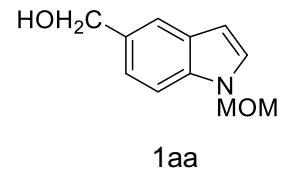


single pulse decoupled gated NOE

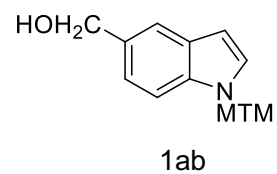
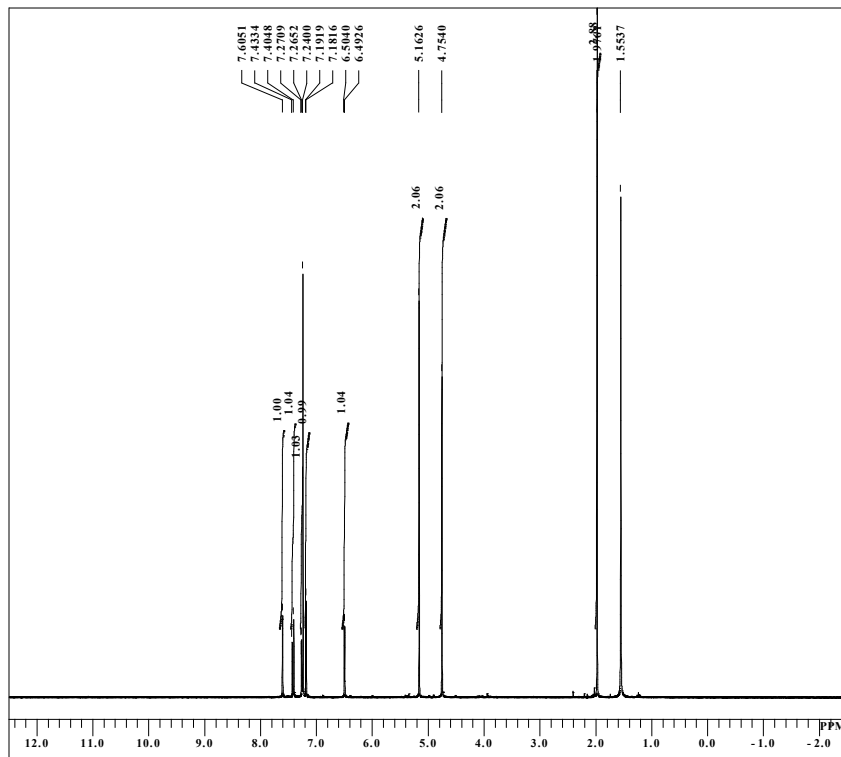
F:\CH2OH MOM carbon-1-1.als



DFILE CH2OH MOM carbon-1-1.als
 COMNT single pulse decoupled gated NOE
 DATIM 2019-10-31 15:52:58
 13C
 EXMOD carbon_jsp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFEN 5.86 Hz
 POINT 26214
 FREOU 25125.63 Hz
 SCANS 3500
 ACQTM 1.0433 sec
 PD 1.0000 sec
 PWI 3.17 usec
 1H
 IRNUC
 CTEMP 19.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60

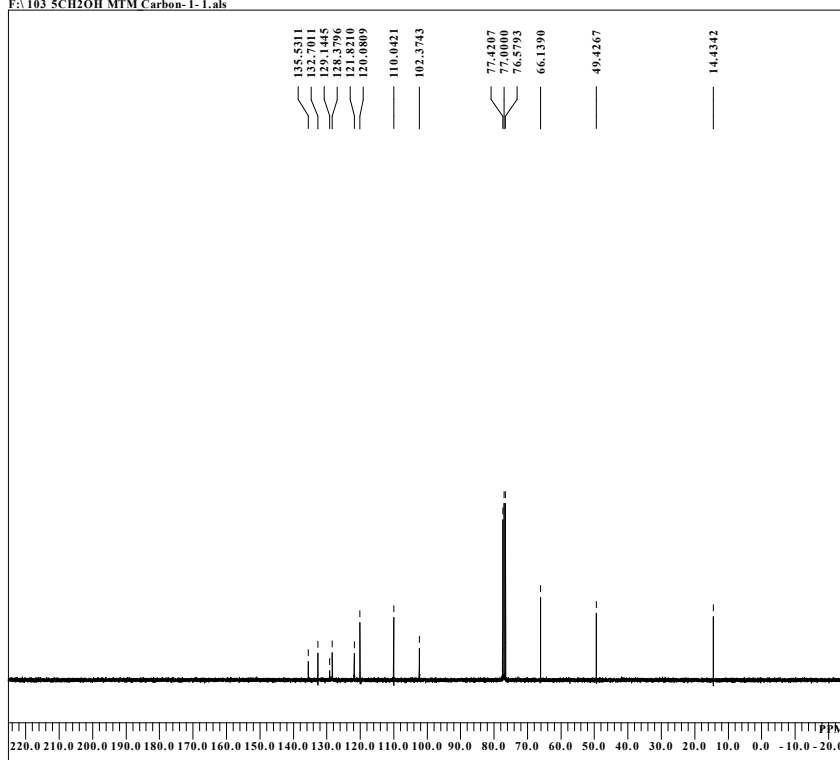


single_pulse

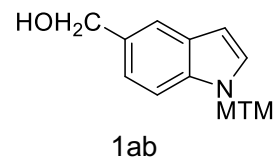


single pulse decoupled gated NOE

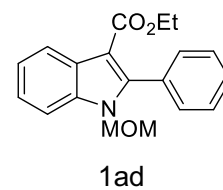
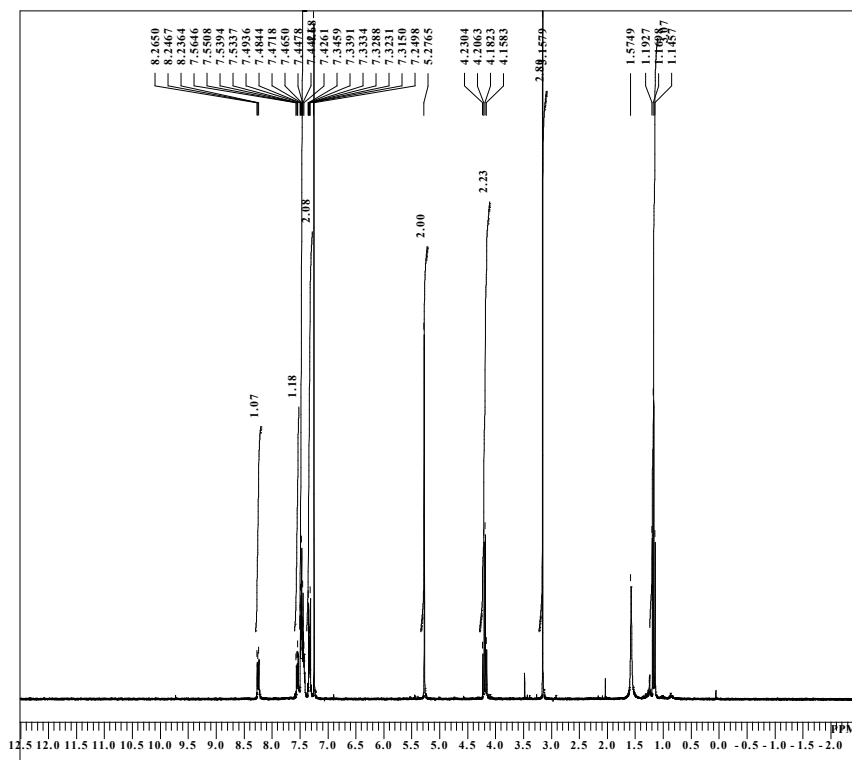
F:\103_5CH2OH_MTM_Carbon-1-1.als



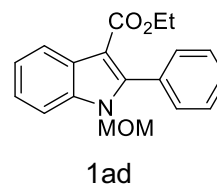
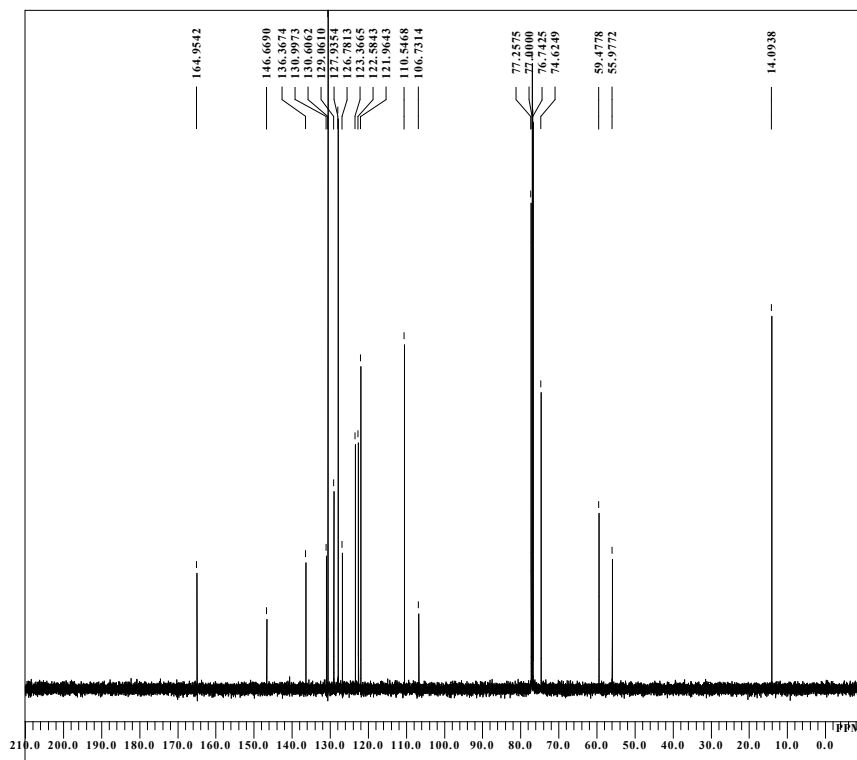
DFILE 103_5CH2OH_MTM_Carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2019-10-28 18:23:07
13C
EXMOD carbon.jsp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 13107
FREOU 18939.39 Hz
SCANS 960
ACQTM 0.6921 sec
PD 2.0000 sec
PWI 3.73 usec
1H
IRNUC
CTEMP 20.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60



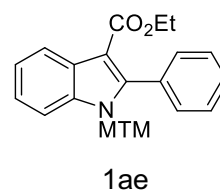
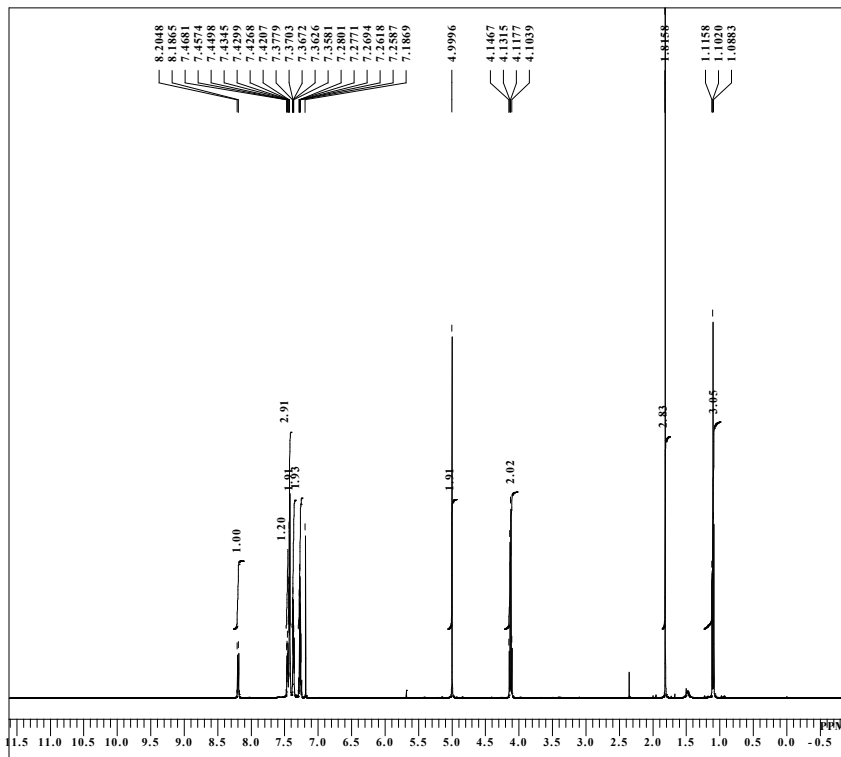
single pulse



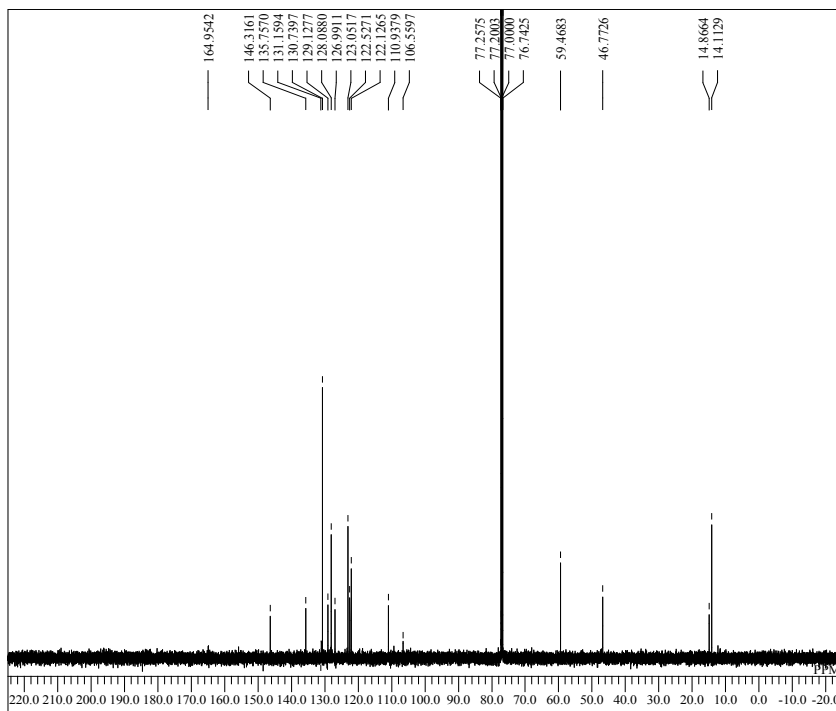
single pulse decoupled gated NOE



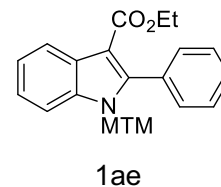
single pulse



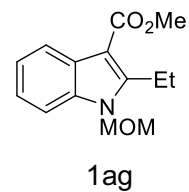
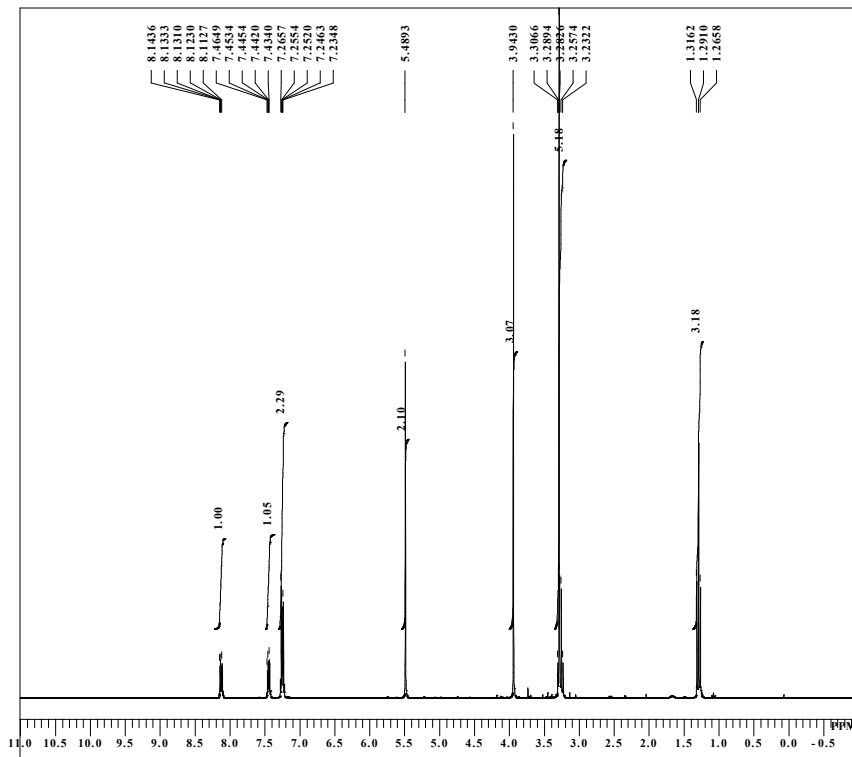
single pulse decoupled gated NOE



DFILE 121 Ph COOEt MTM_Carbon-1-L.als
 COMNT single pulse decoupled gated NOE
 DATIM 2019-12-12 16:25:36
 OBNUC 13C
 EXMOD carbon_jxp
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 336
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.27 usec
 IRNUC 1H
 CTEMP 21.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 60

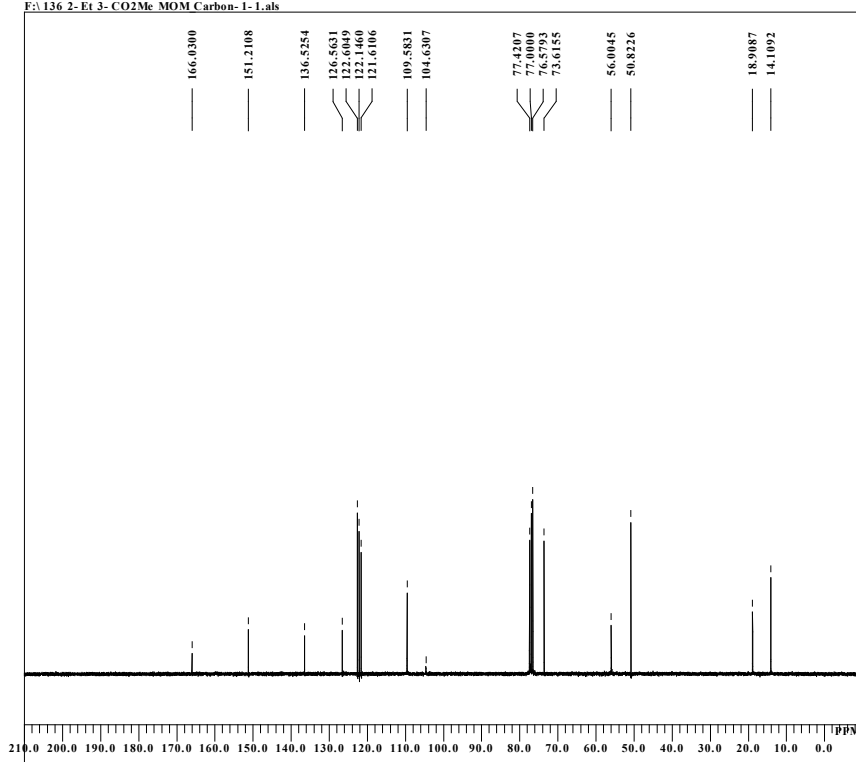


single pulse

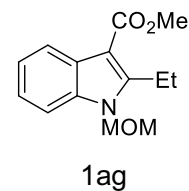


single pulse decoupled gated NOE

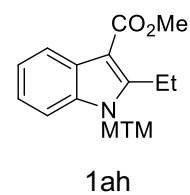
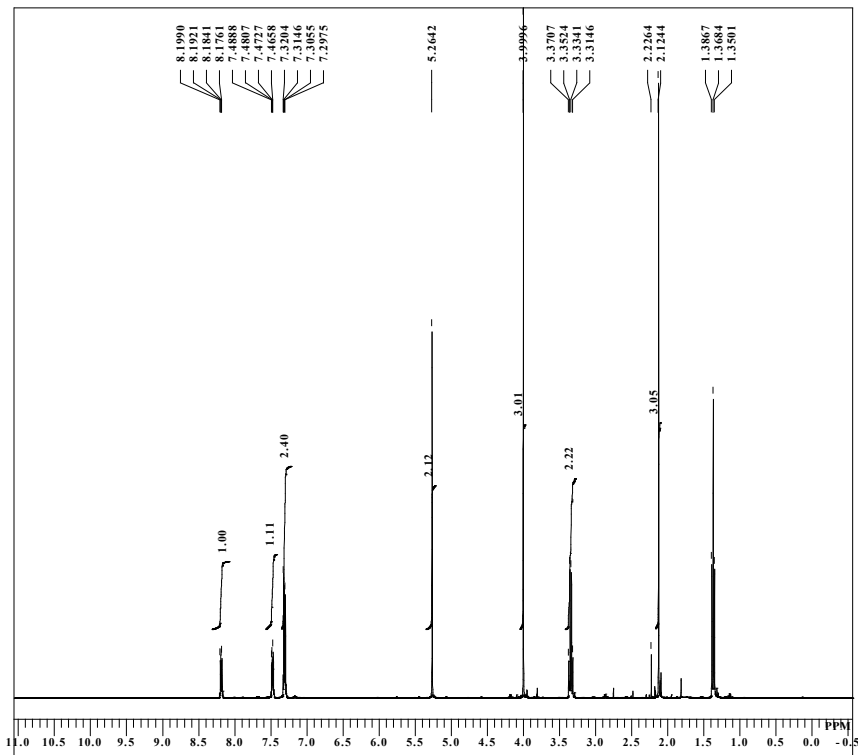
F:\136 2-Et 3-CO2Me MOM Carbon-1-1.als



DFILE 136 2-Et 3-CO2Me MOM Carbon-1-1
 COMNT single pulse decoupled gated NOE
 DATIM 2019-12-21 09:49:03
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 75.57 MHz
 OBSET 5.79 KHz
 OBFIN 1.08 Hz
 POINT 13107
 FREQU 18939.39 Hz
 SCANS 2867
 ACQTM 0.6921 sec
 PD 1.0000 sec
 PWI 3.73 usec
 IH 1H
 IRNUC 19.1 c
 CTEMP CDCL3
 SLVNT 77.00 ppm
 EXREF 0.12 Hz
 BF 60
 RGAIN



single_pulse



single_pulse decoupled gated NOE

