

Supplementary Information

Total Synthesis of (–)-Kainic Acid and (+)-*allo*-Kainic Acid through SmI₂-Mediated Intramolecular Coupling between Allyl Chloride and an α,β -Unsaturated Ester

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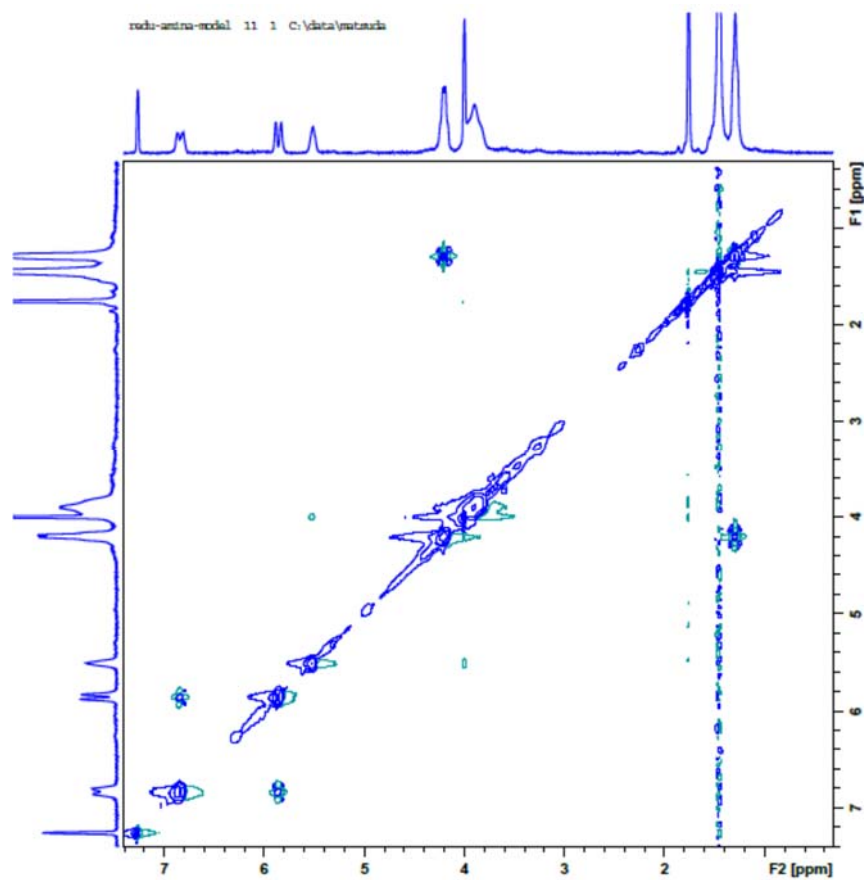
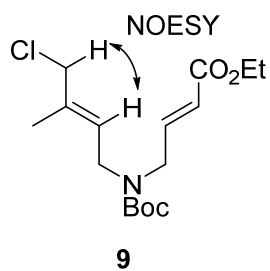
N10W5 Sapporo 060-0810, Japan

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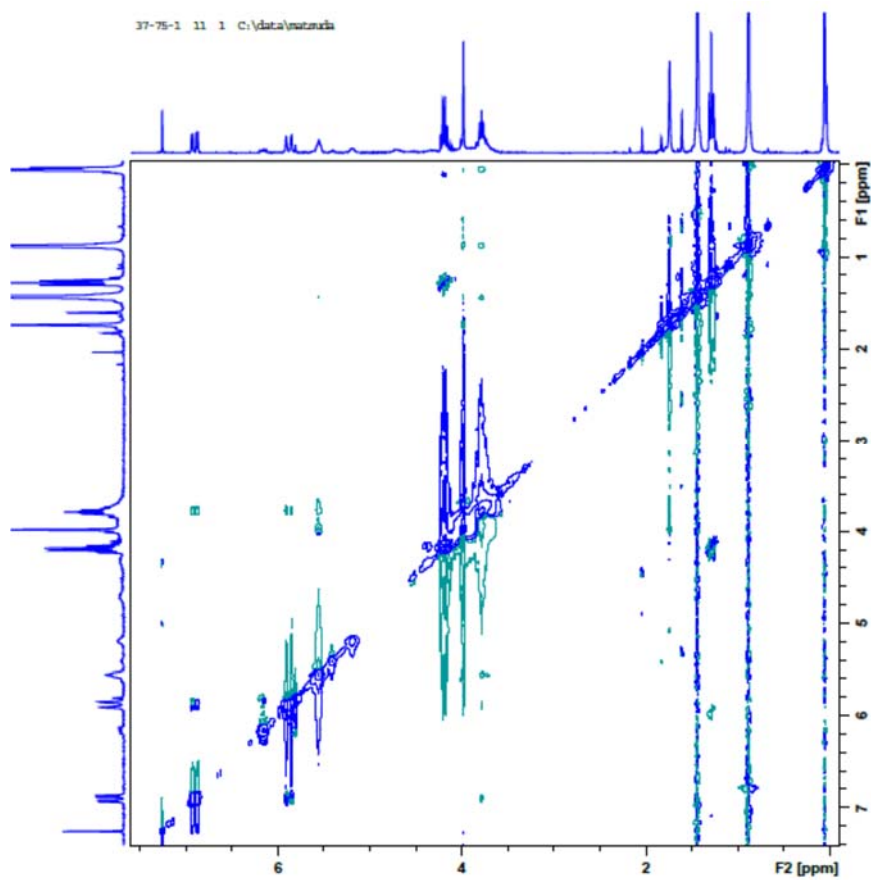
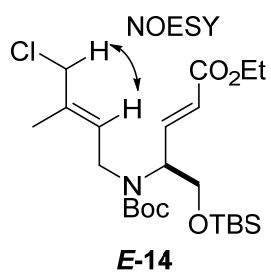
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Determination of geometry of allyl chloride

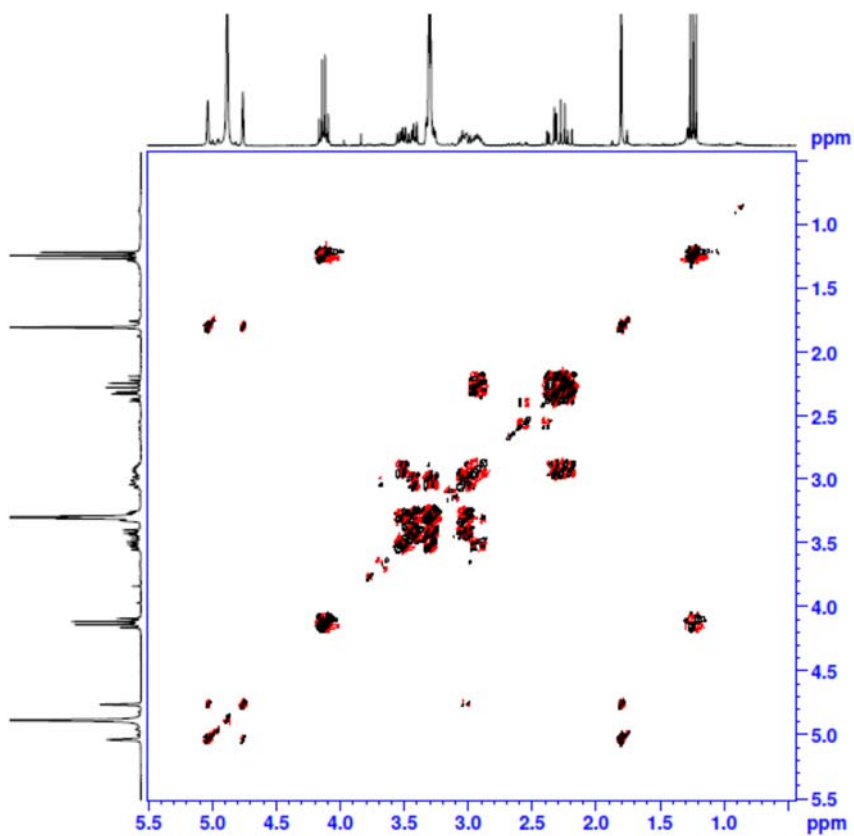
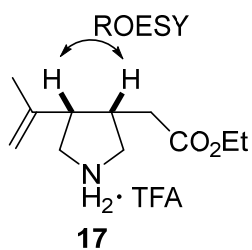
NOESY Spectrum of **9**



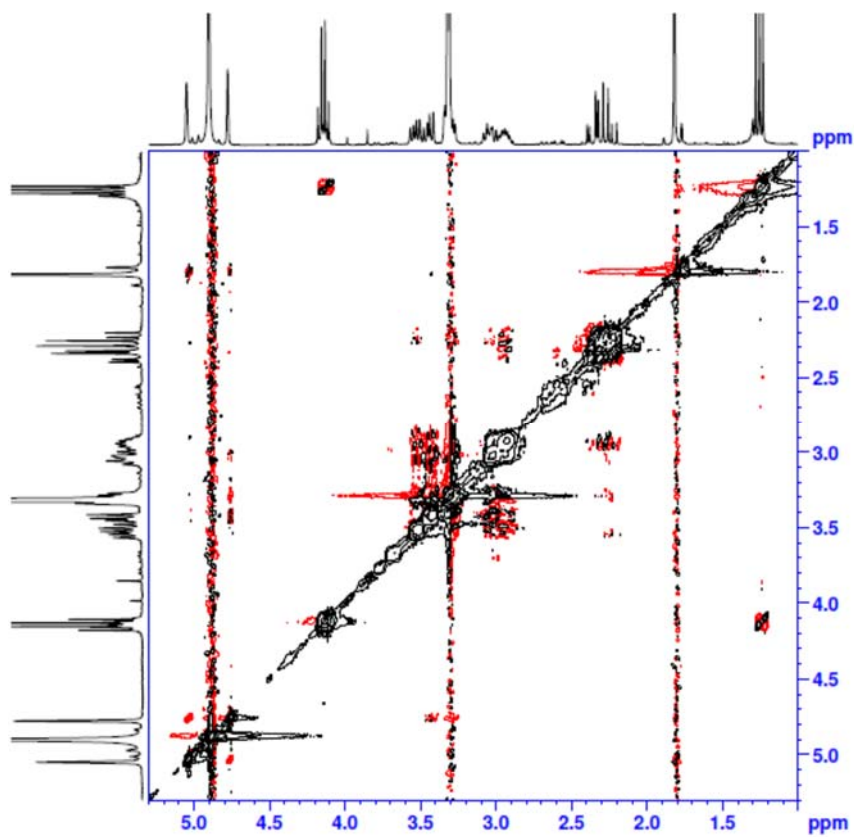
NOESY Spectrum of *E-14*



Determination of relative configuration of 17

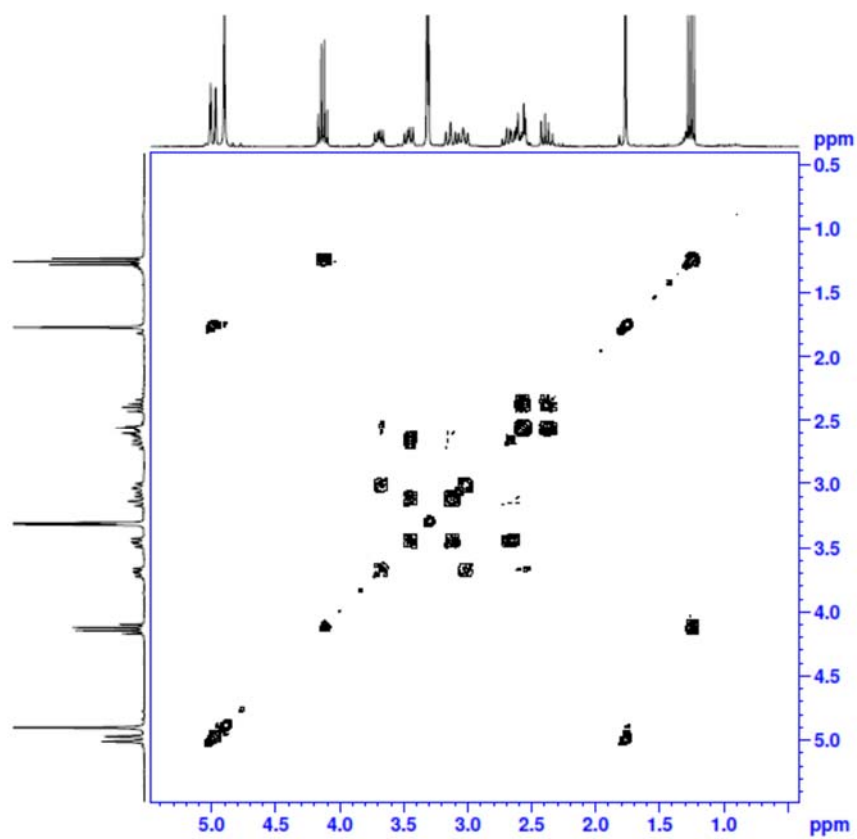
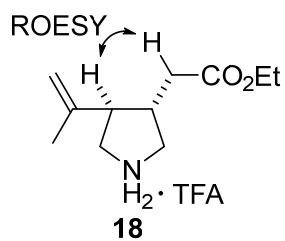


COSY Spectrum

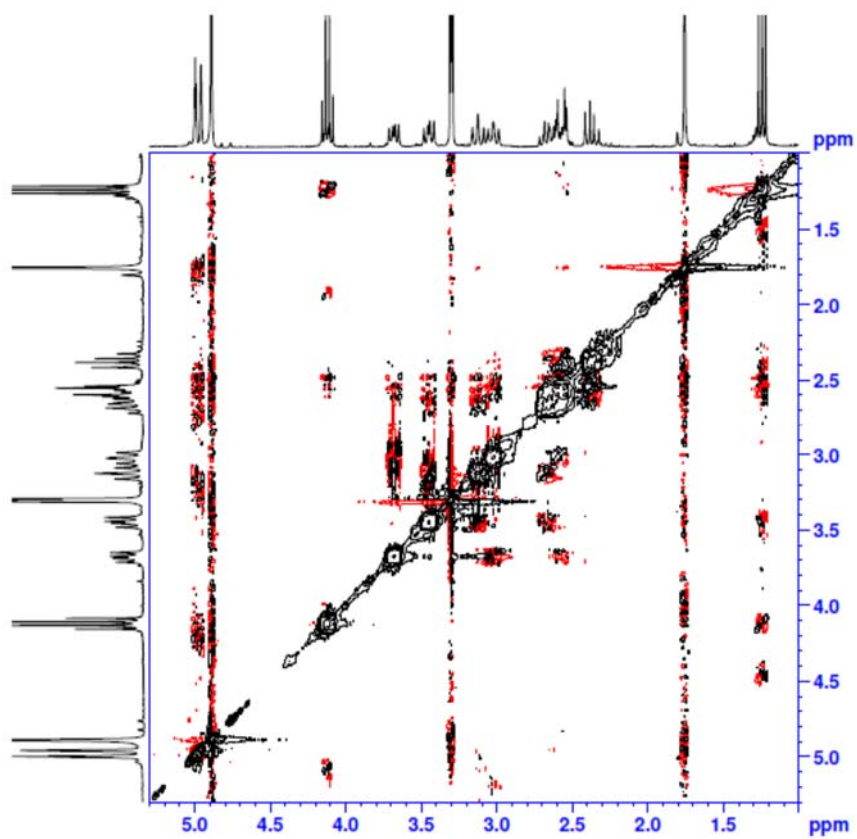


ROESY Spectrum

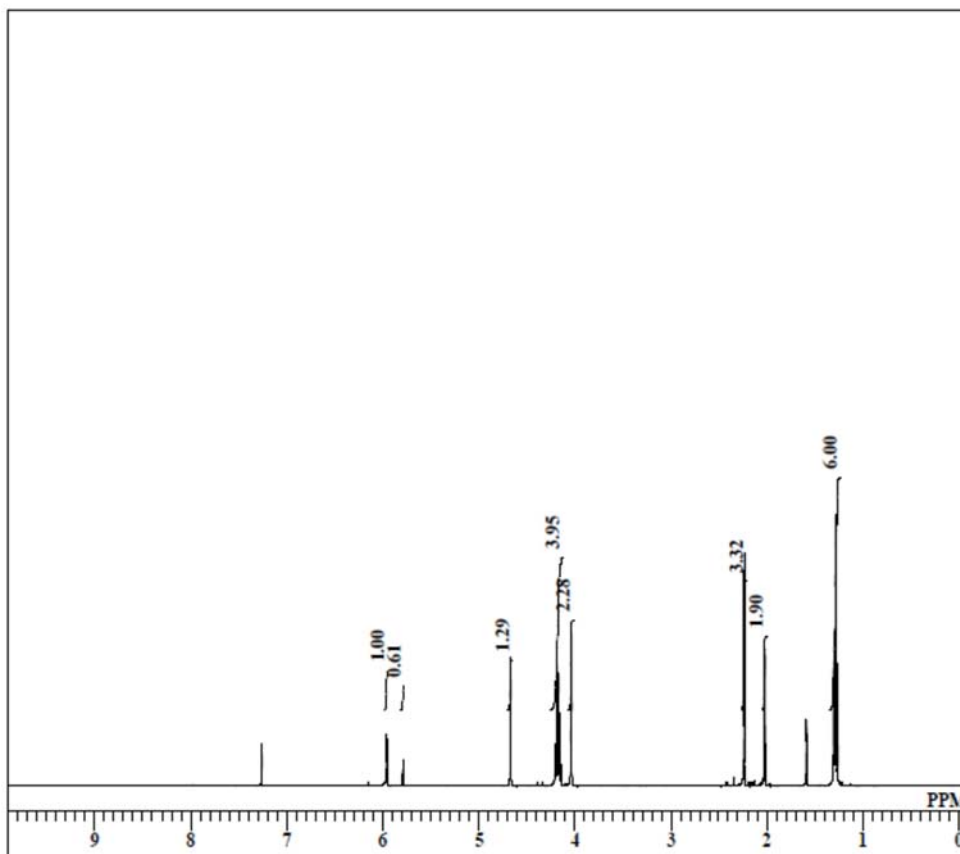
Determination of relative configuration of **18**



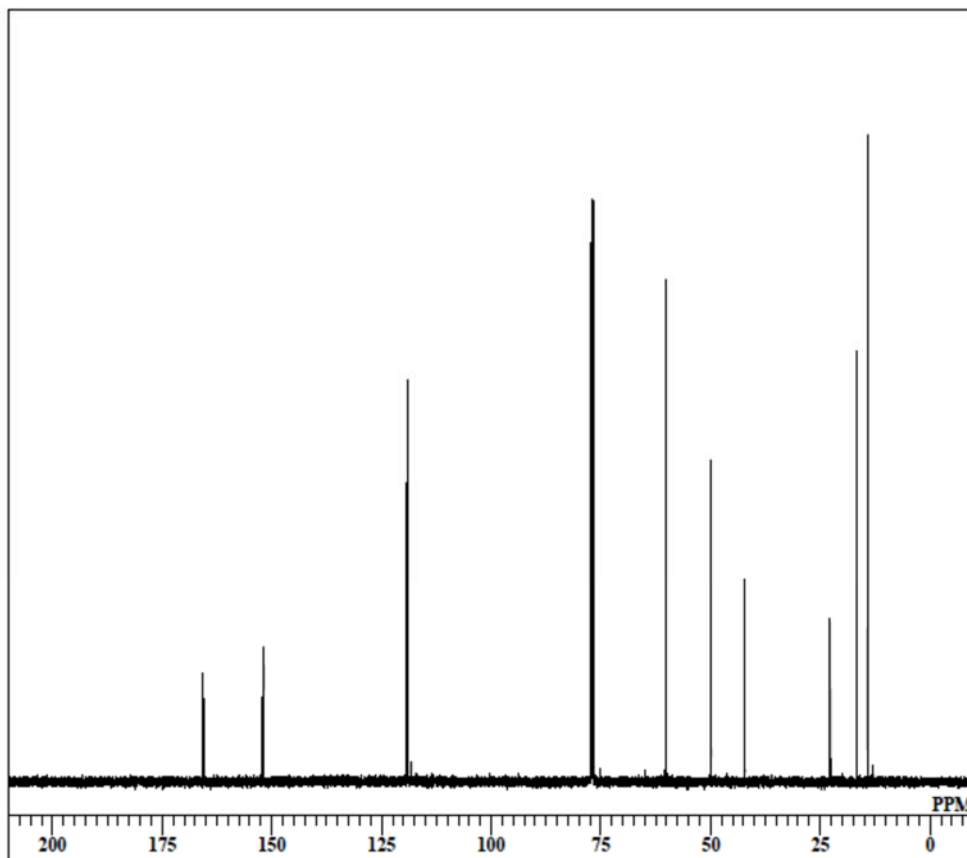
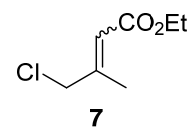
COSY Spectrum



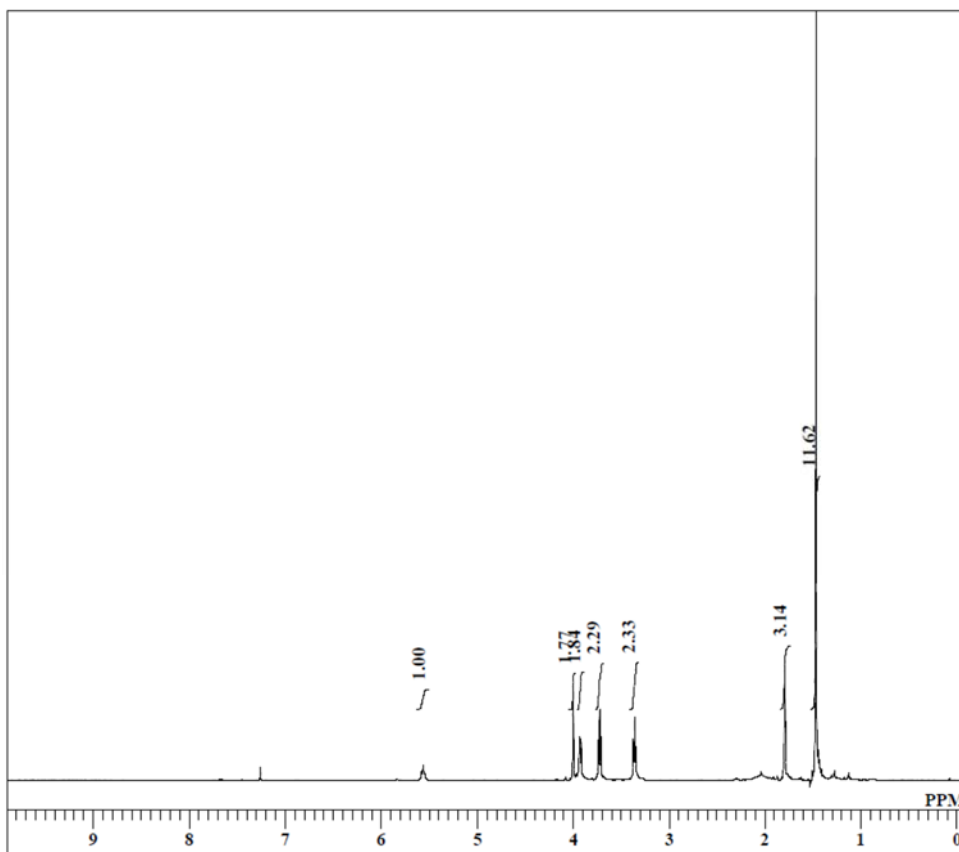
ROESY Spectrum



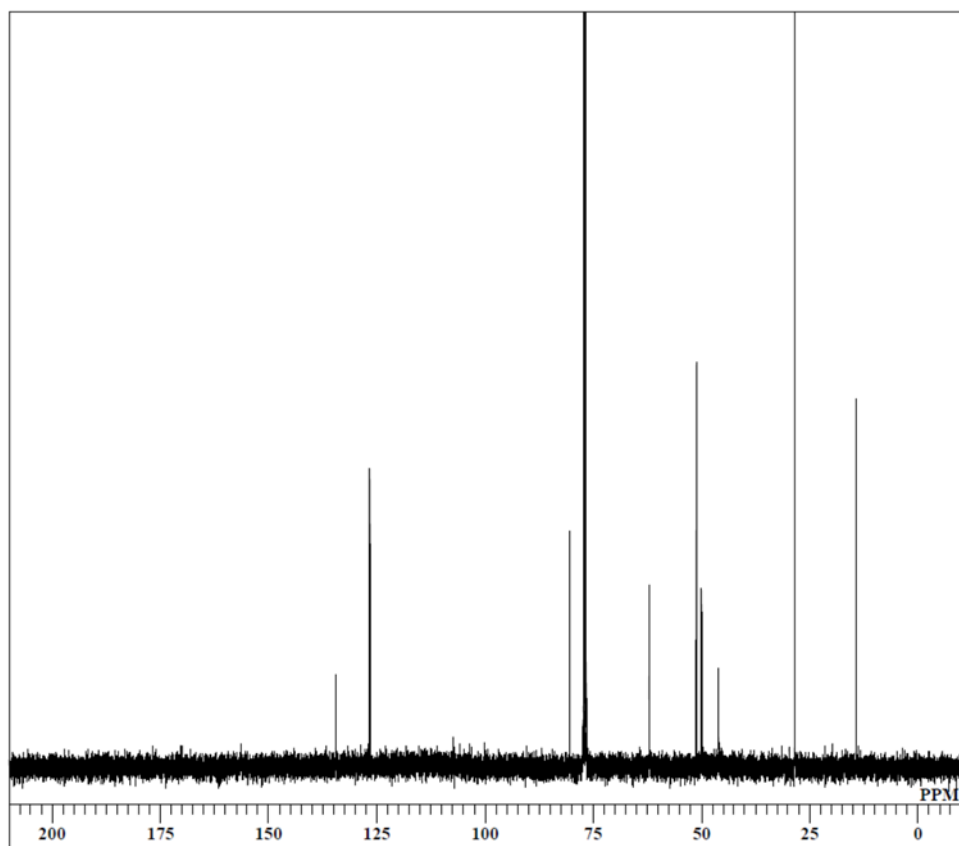
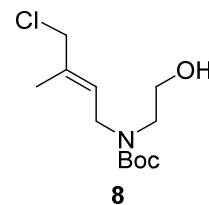
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 SCANS 8
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PWI 6.10 usec
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 19



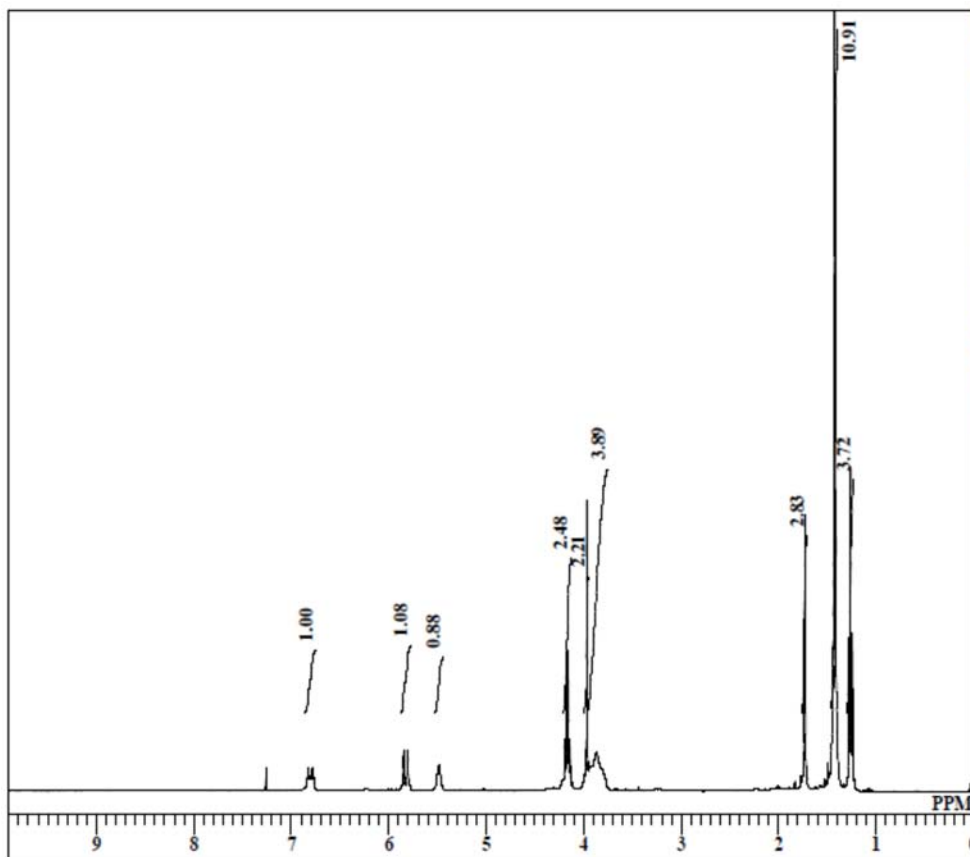
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 FREQU 27118.64 Hz
 SCANS 1711
 ACQTM 1.2083 sec
 PD 1.7920 sec
 PWI 4.40 usec
 IRNUC 1H
 CTEMP 22.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



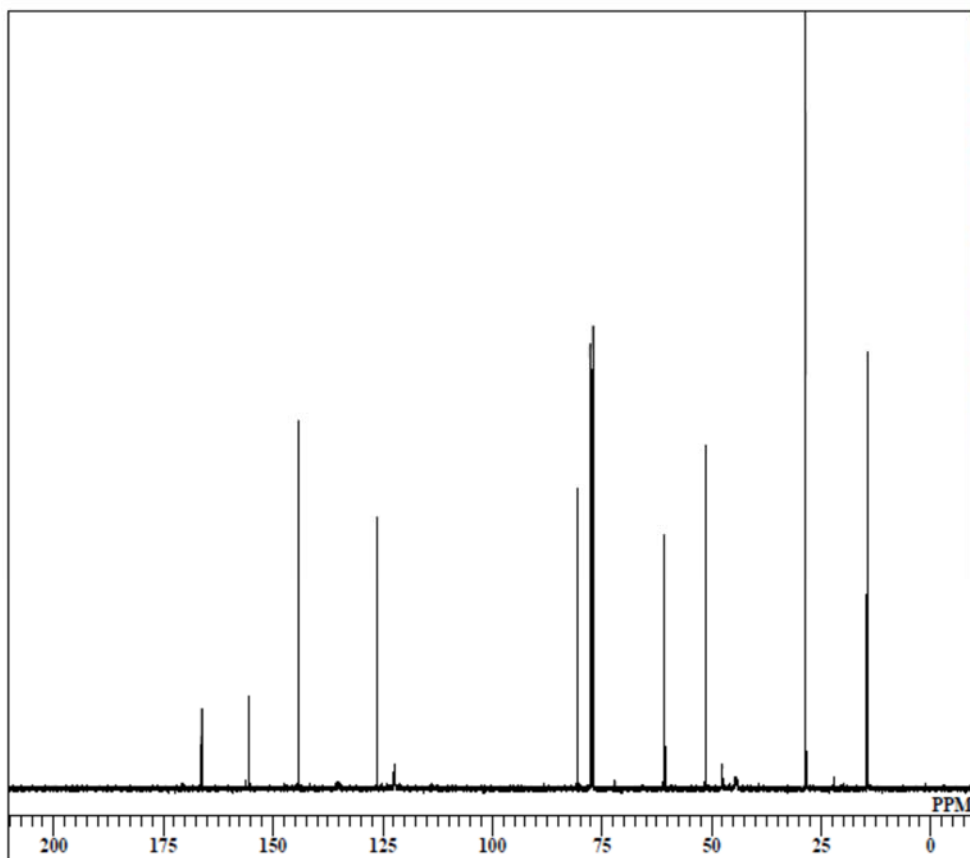
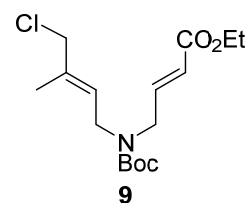
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 FREQU 7992.01 Hz
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 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 12.10 usec
 IRNUC 1H
 CTEMP 69.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 14



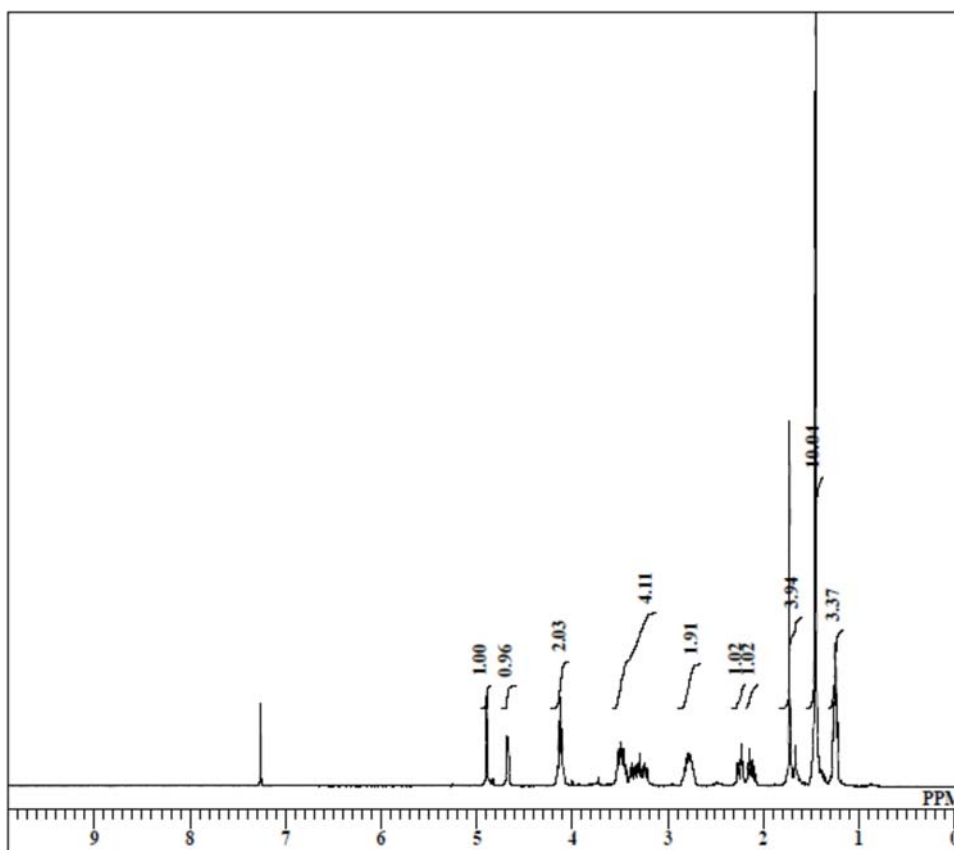
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 POINT 32768
 FREQU 27118.64 Hz
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 ACQTM 1.2083 sec
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 PW1 4.40 usec
 IRNUC 1H
 CTEMP 69.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 31



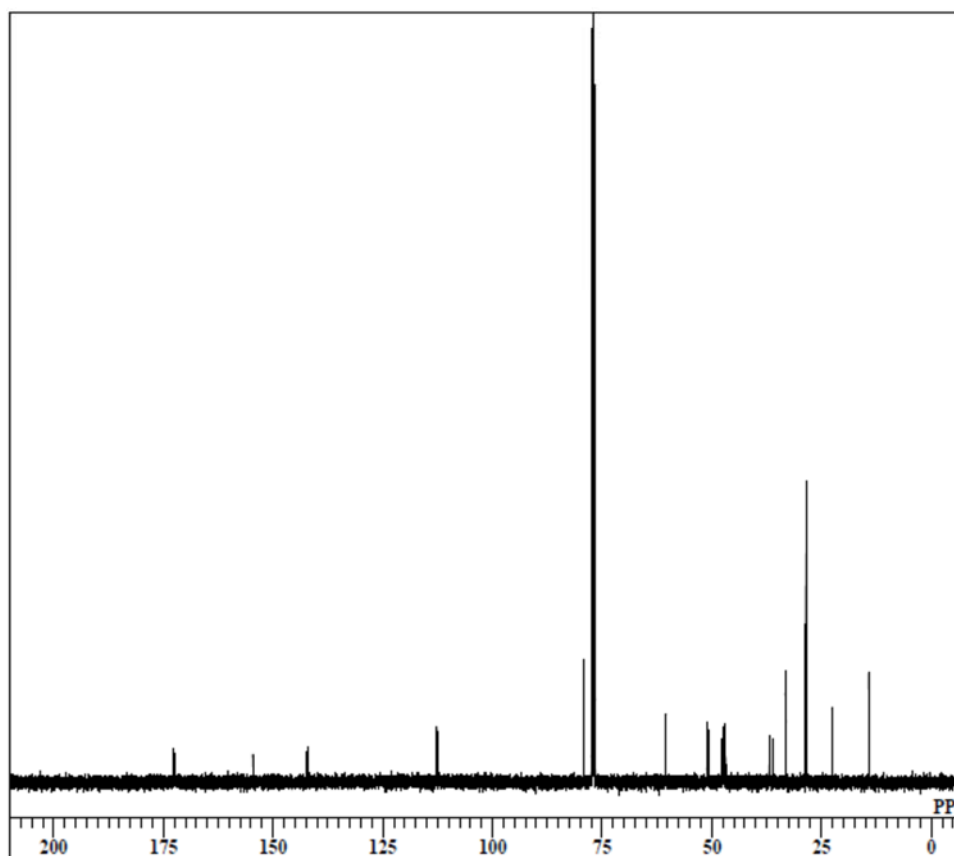
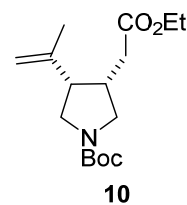
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 FREQU 7992.01 Hz
 SCANS 8
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 12.10 usec
 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 11



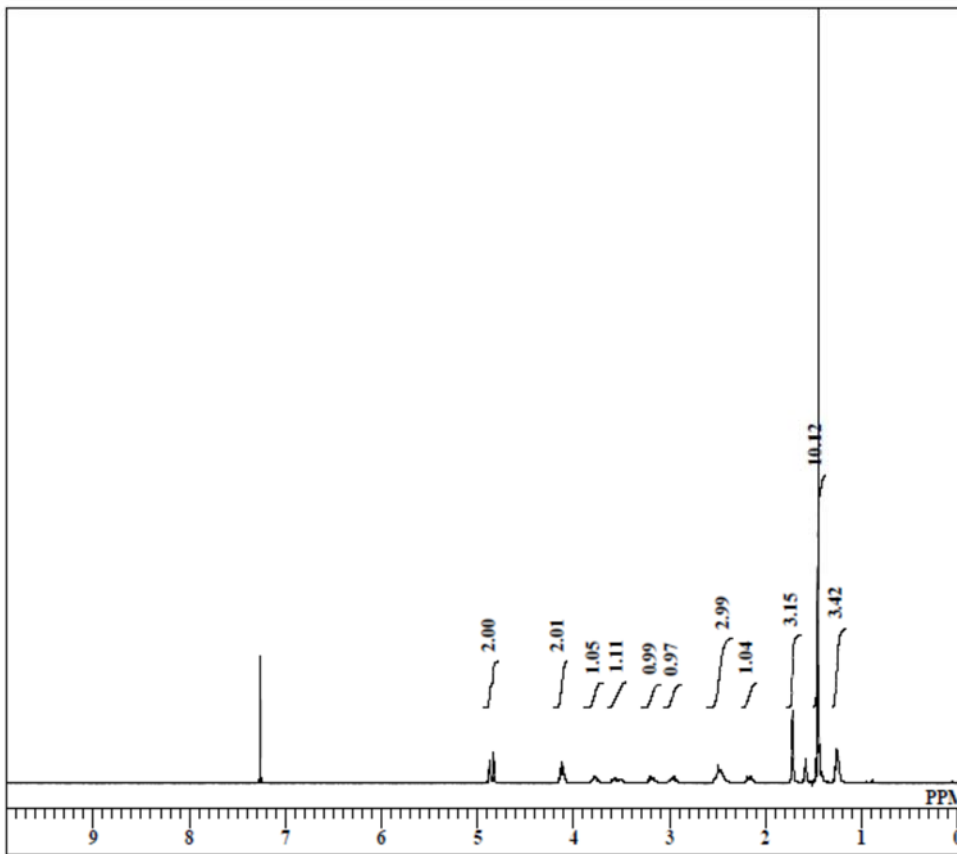
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 POINT 32768
 FREQU 27118.64 Hz
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 ACQTM 1.2083 sec
 PD 1.7920 sec
 PW1 4.40 usec
 IRNUC 1H
 CTEMP 22.6 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



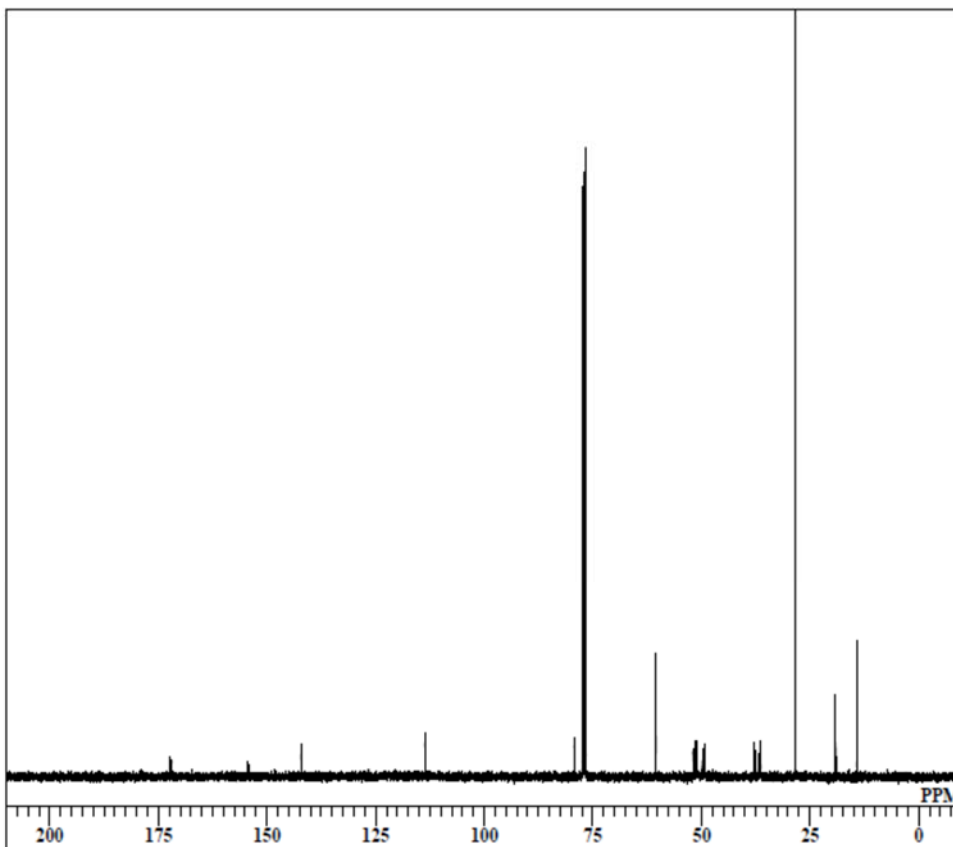
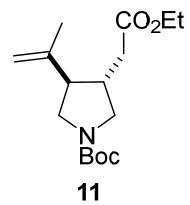
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 ACQTM 2.0500 sec
 PD 4.9500 sec
 PWI 12.10 usec
 IRNUC 1H
 CTEMP 22.9 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 15



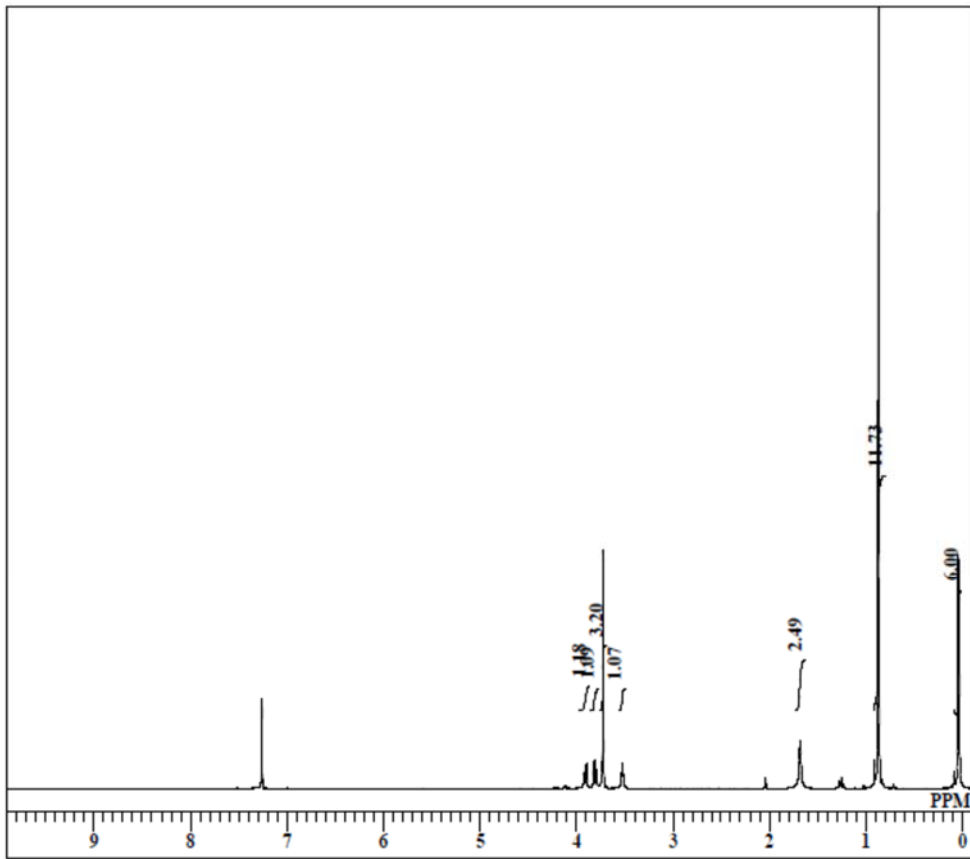
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 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 2221
 ACQTM 1.2083 sec
 PD 1.7920 sec
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 CTEMP 23.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



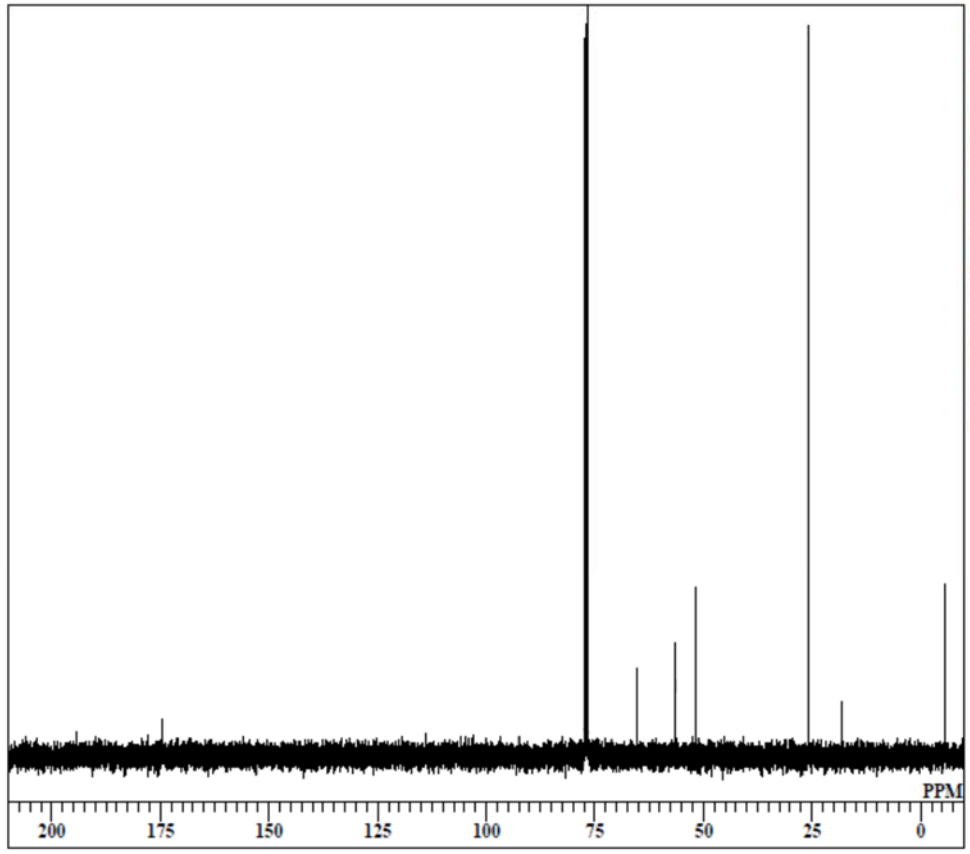
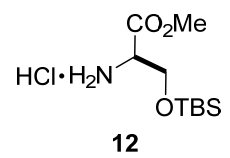
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 POINT 16384
 FREQU 7992.01 Hz
 SCANS 4
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PWI 12.10 usec
 IRNUC 1H
 CTEMP 22.8 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 20



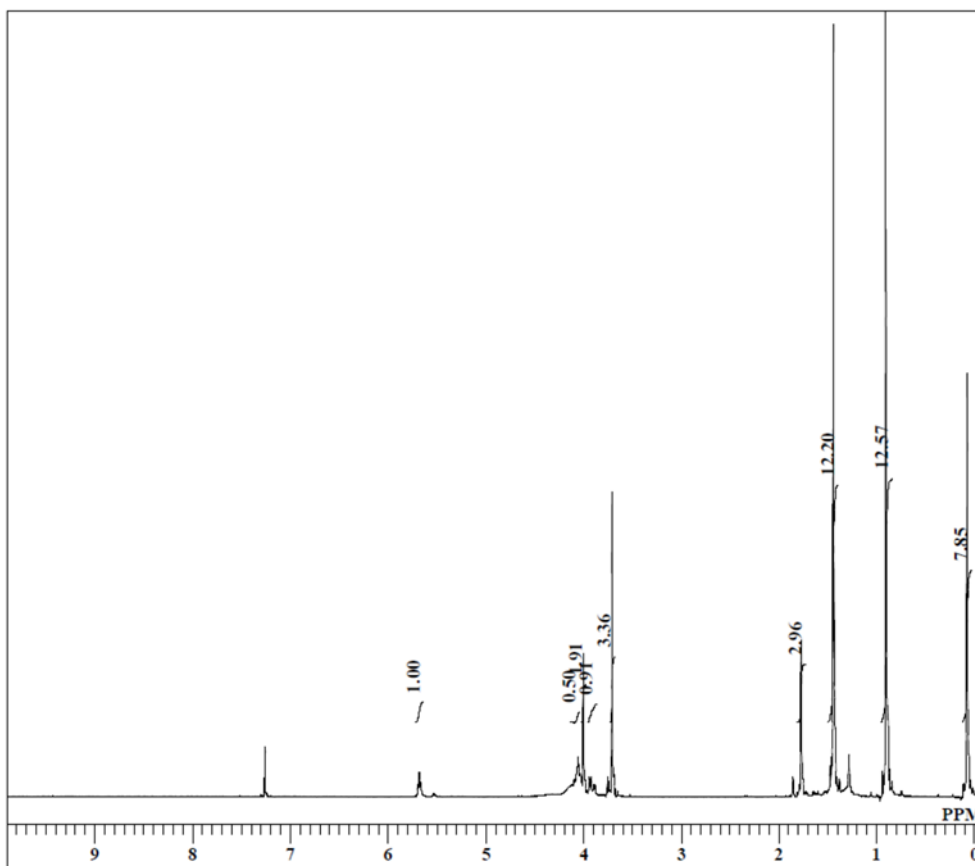
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 POINT 32768
 FREQU 27118.64 Hz
 SCANS 2270
 ACQTM 1.2083 sec
 PD 1.7920 sec
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 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



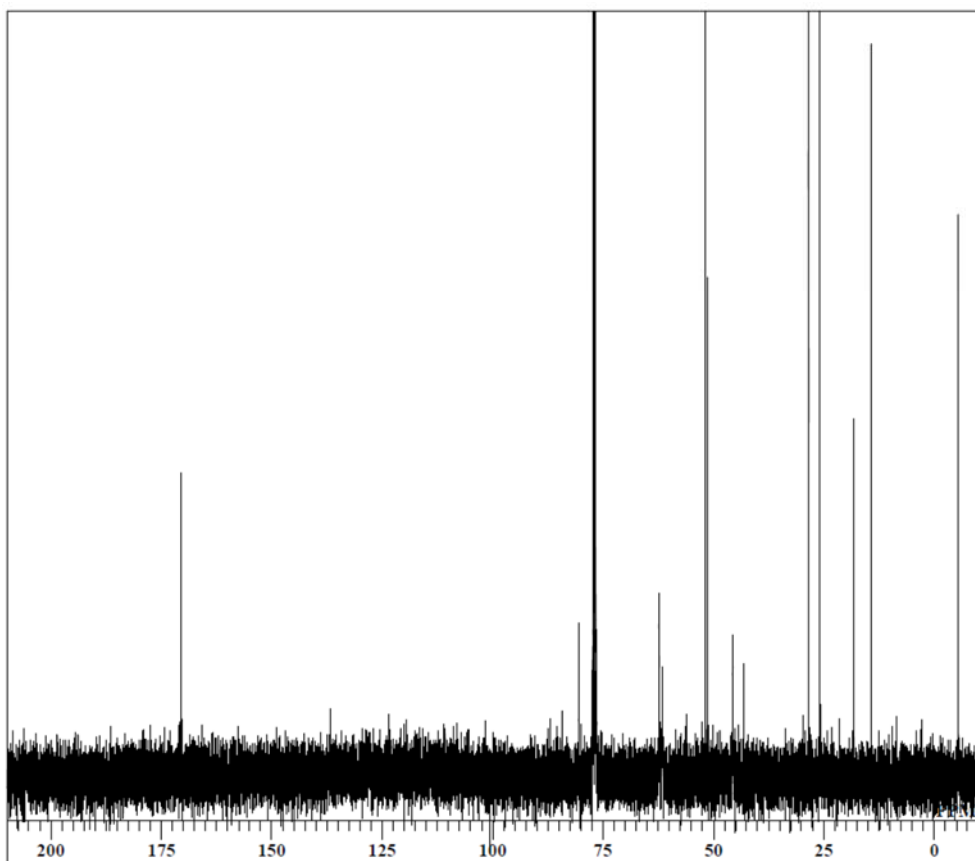
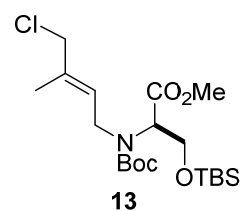
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 EXMOD NON
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 OBFIN 64.90 Hz
 POINT 16384
 FREQU 7992.01 Hz
 SCANS 8
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PWI 12.10 usec
 IRNUC 1H
 CTEMP 22.4 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 18



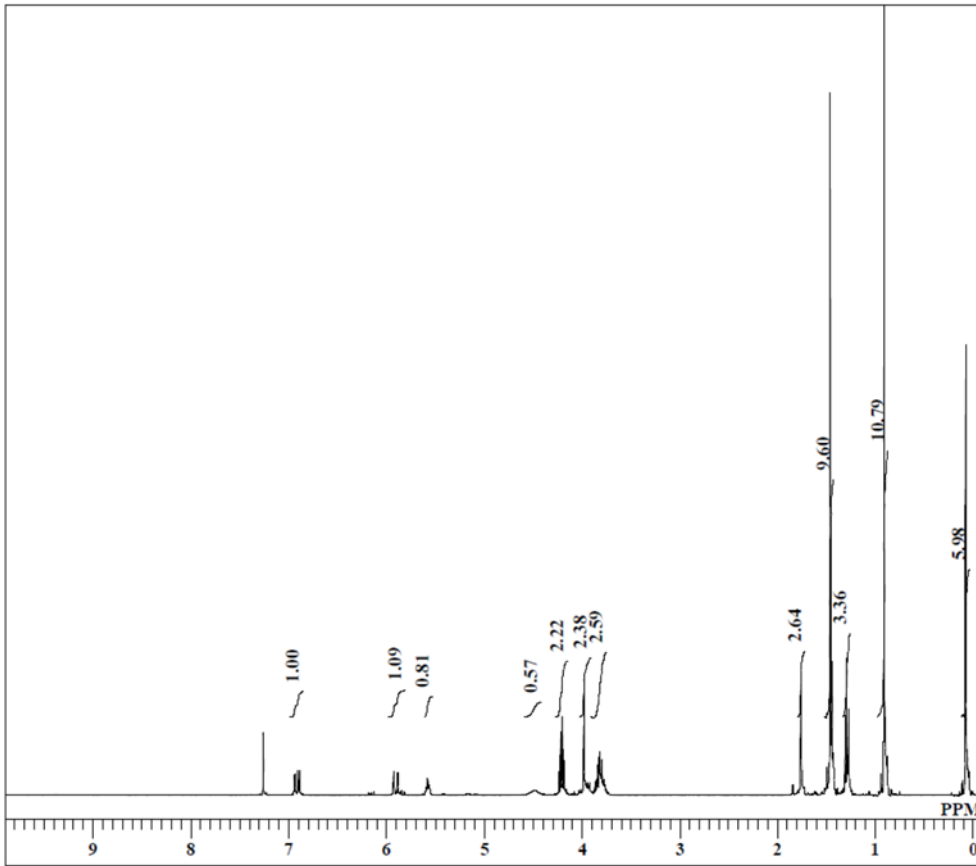
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 EXMOD BCM
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 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 360
 ACQTM 1.2083 sec
 PD 1.7920 sec
 PWI 4.40 usec
 IRNUC 1H
 CTEMP 23.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



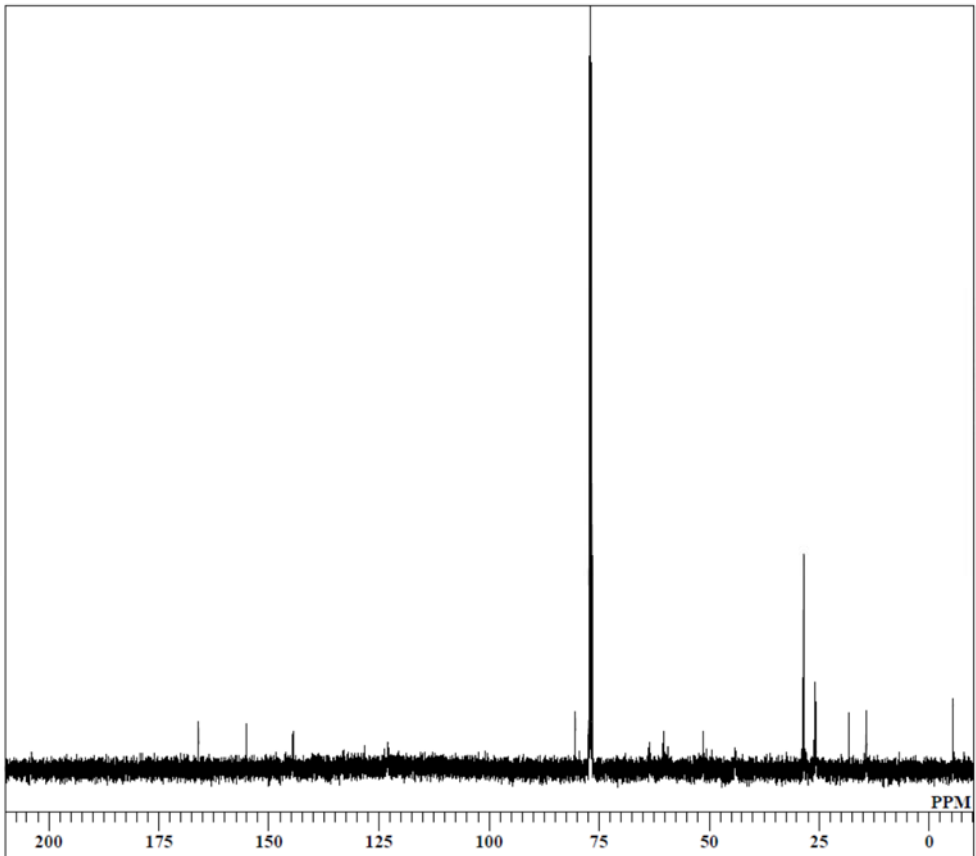
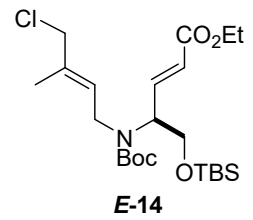
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 OBFIN 10500.00 Hz
 POINT 16384
 FREQU 7992.01 Hz
 SCANS 4
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 6.60 usec
 IRNUC 1H
 CTEMP 69.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 18



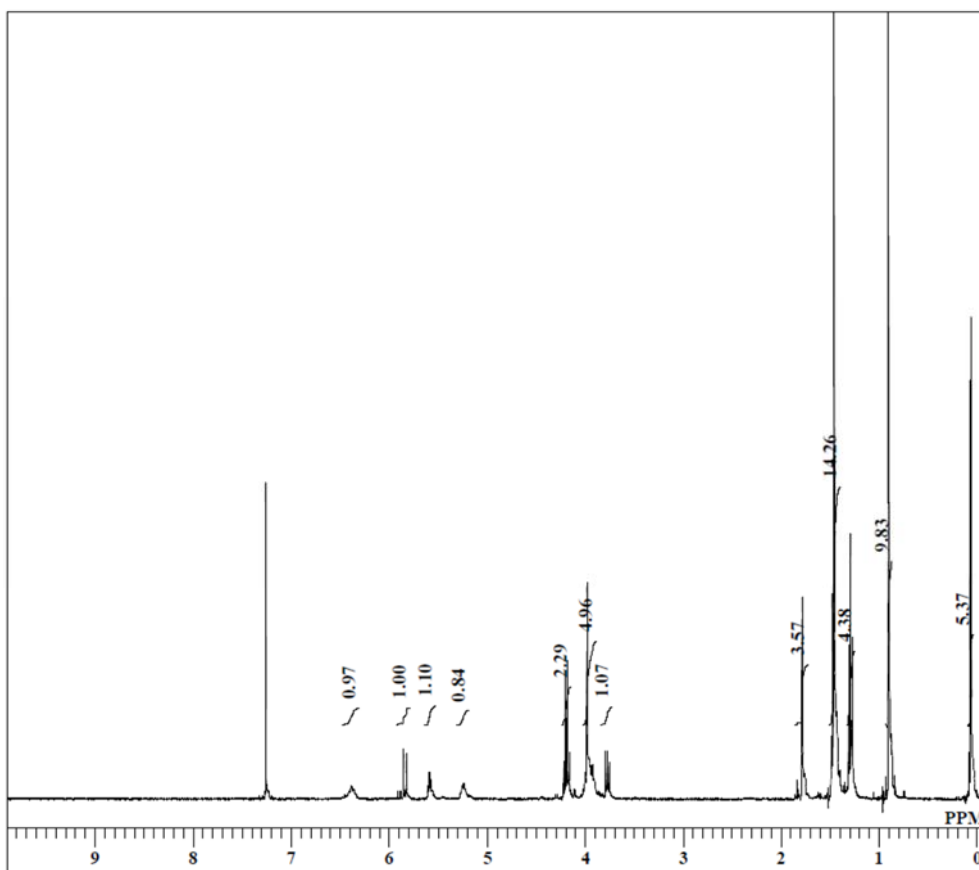
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 POINT 32768
 FREQU 27118.64 Hz
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 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 31



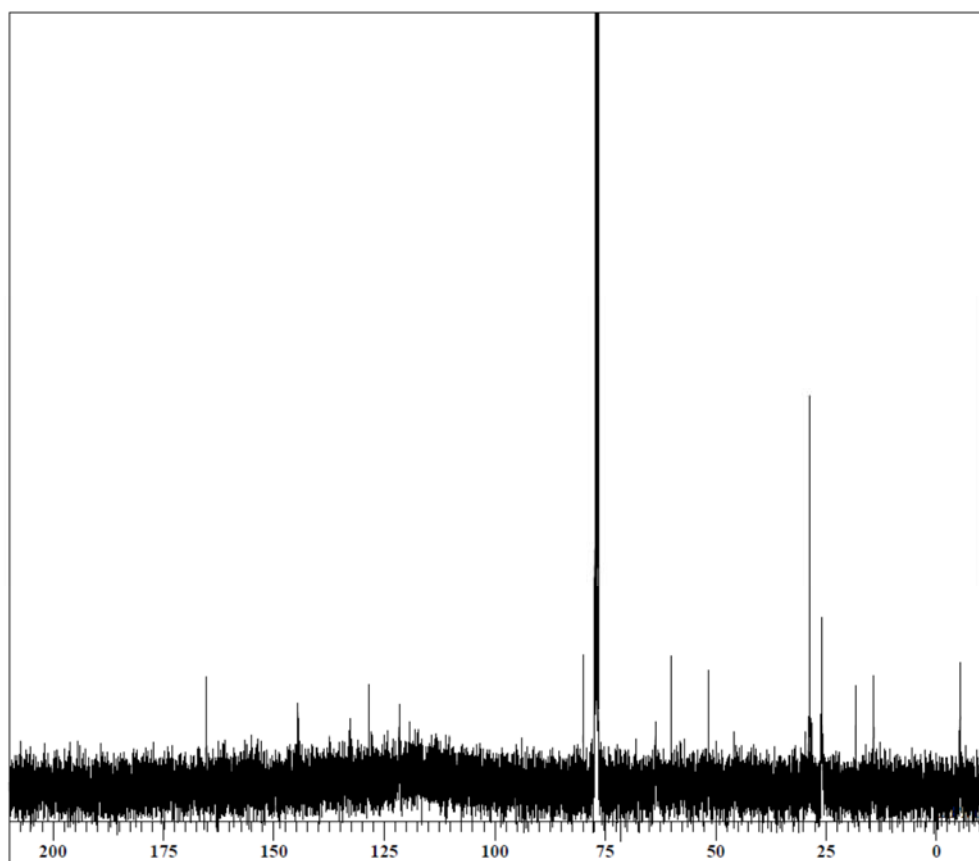
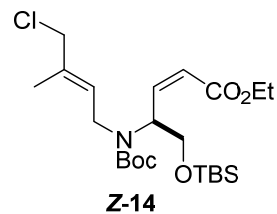
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 OBFIN 10500.00 Hz
 POINT 16384
 FREQU 7992.01 Hz
 SCANS 4
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 6.60 usec
 IRNUC 1H
 CTEMP 69.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 18



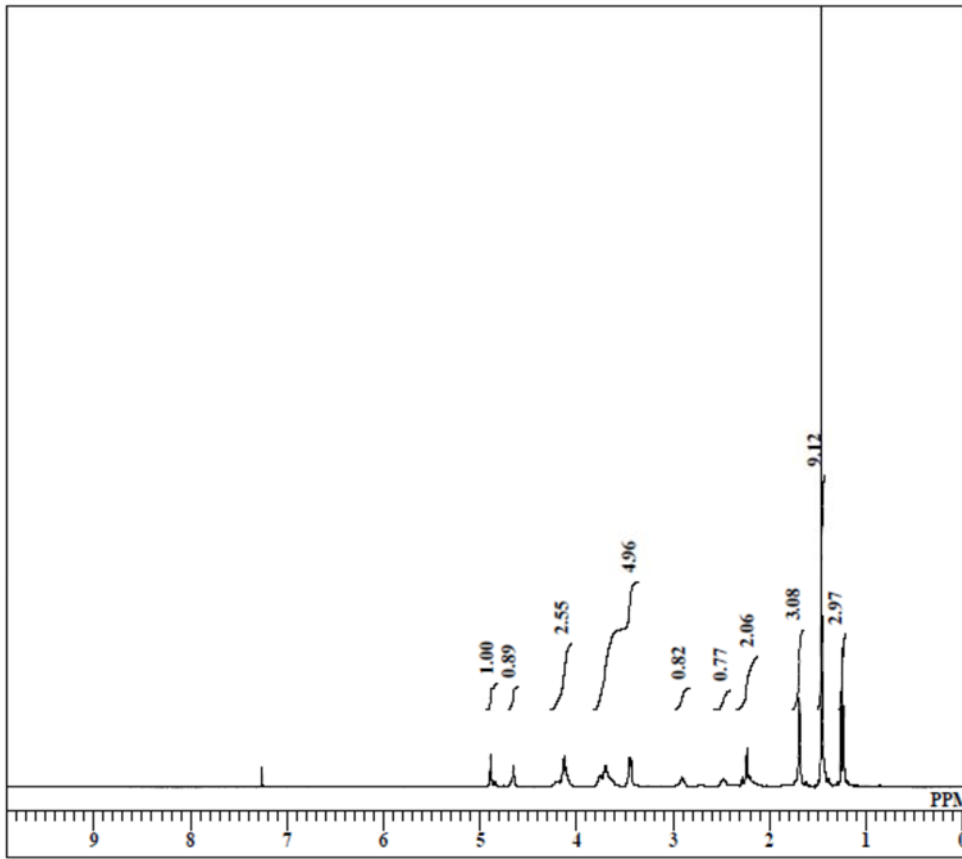
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 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 4844
 ACQTM 1.2083 sec
 PD 1.7920 sec
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 CTEMP 69.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



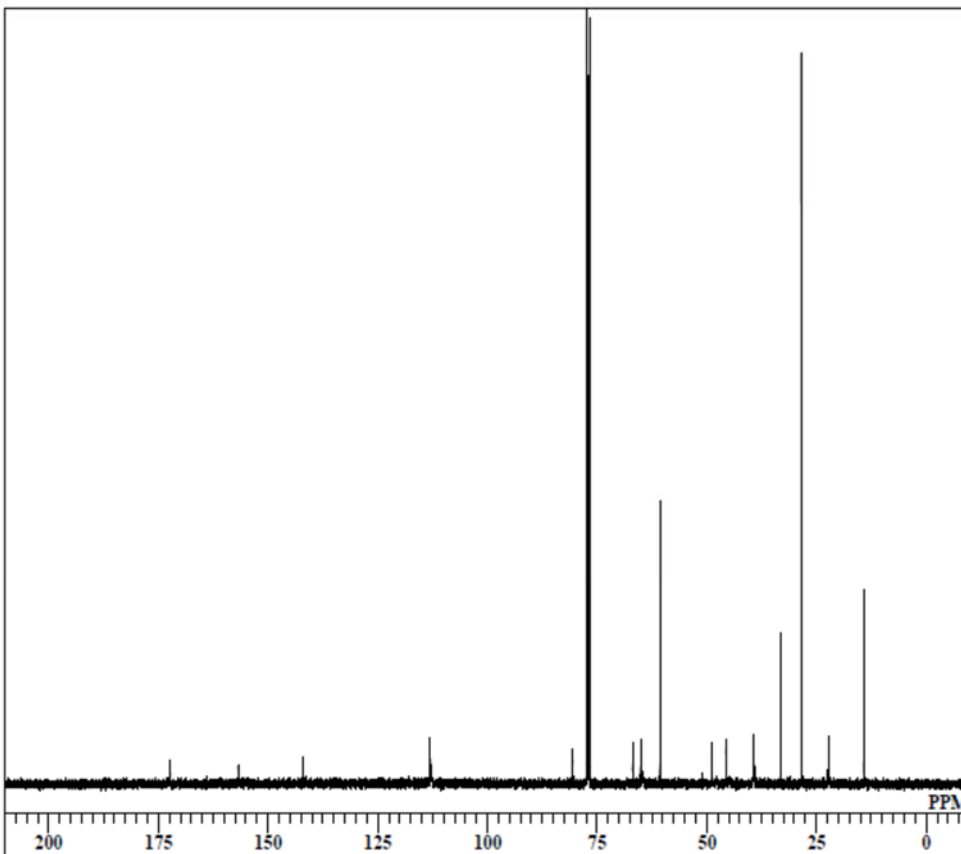
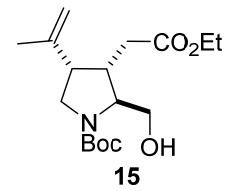
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 ACQTM 2.0500 sec
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 SLVNT CDCL3
 EXREF 7.26 ppm
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 RGAIN 21



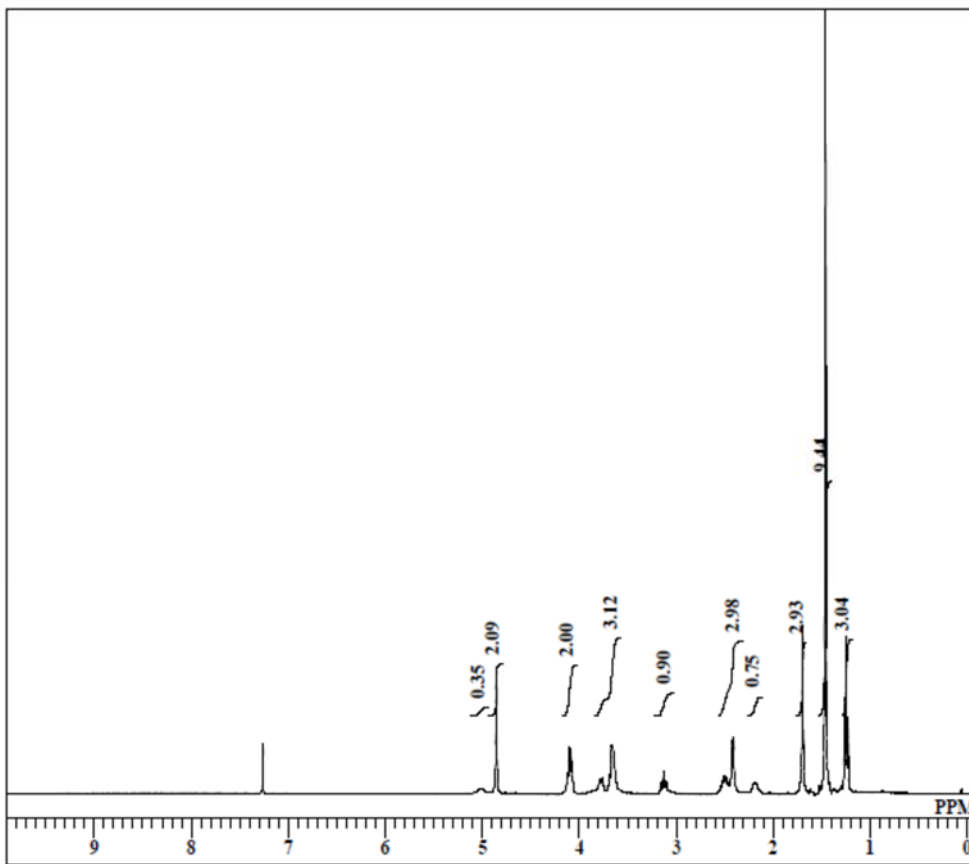
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 EXMOD BCM
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 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 14196
 ACQTM 1.2083 sec
 PD 1.7920 sec
 PW1 4.40 usec
 IRNUC 1H
 CTEMP 69.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



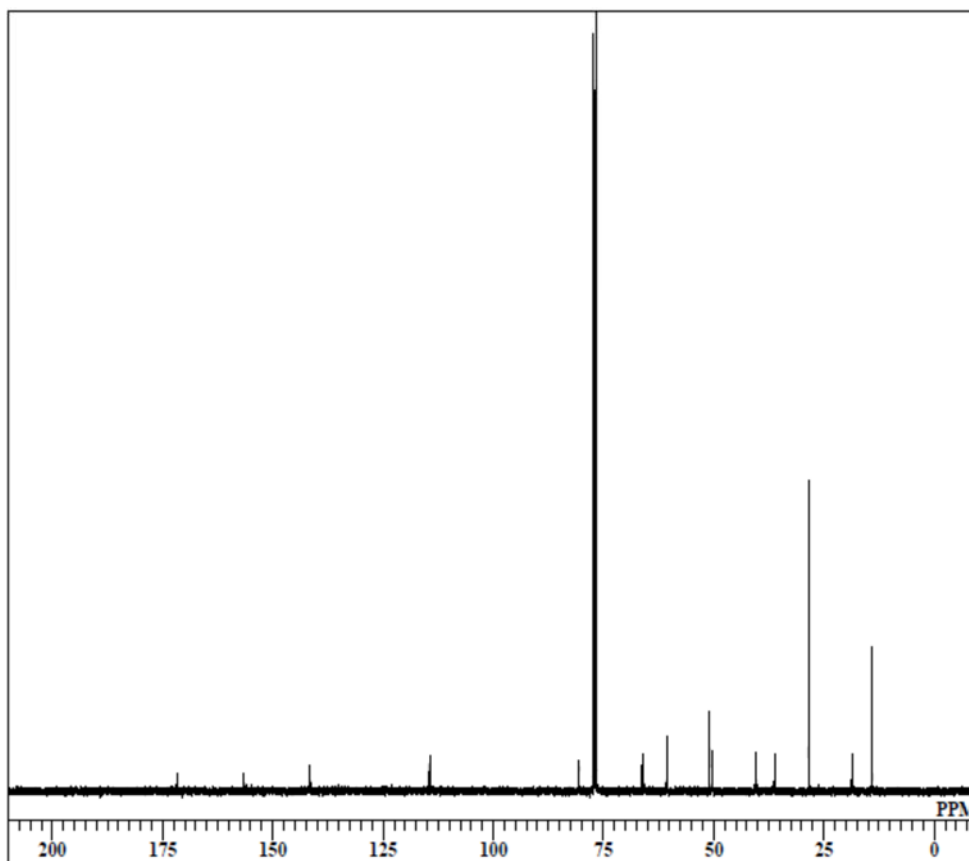
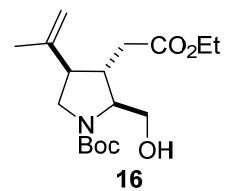
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 POINT 16384
 FREQU 7992.01 Hz
 SCANS 8
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PWI 12.10 usec
 IRNUC 1H
 CTEMP 23.3 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 14



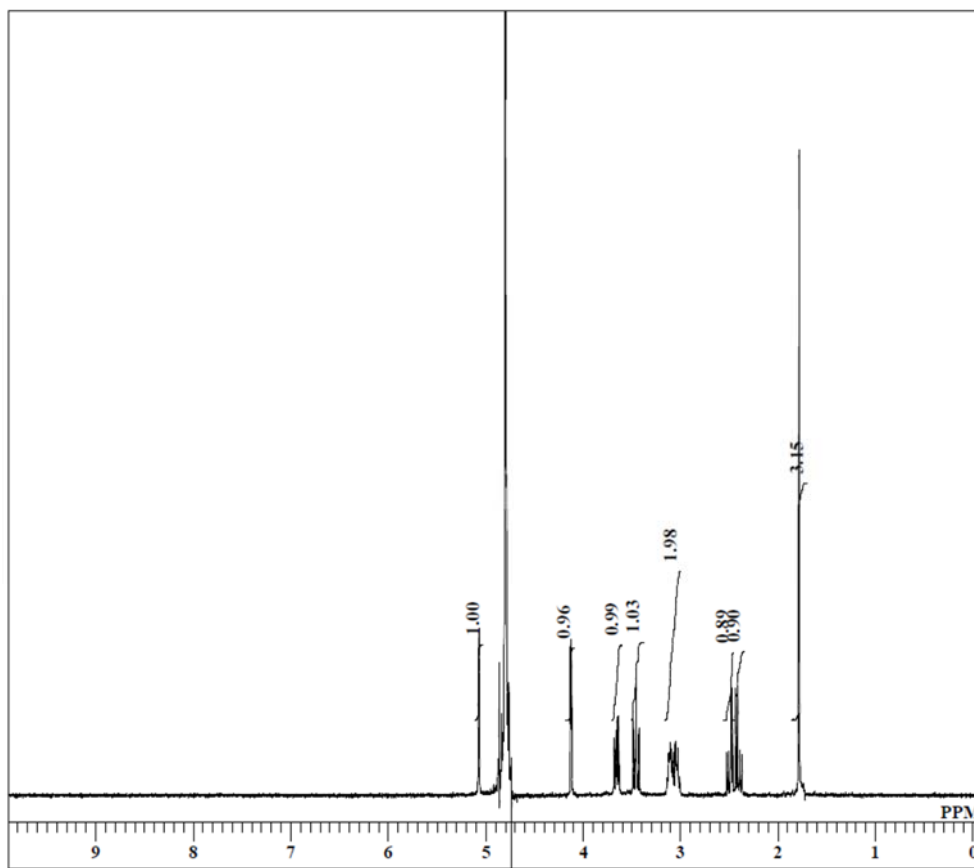
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 POINT 32768
 FREQU 27118.64 Hz
 SCANS 3000
 ACQTM 1.2083 sec
 PD 1.7920 sec
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 IRNUC 1H
 CTEMP 22.9 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 31



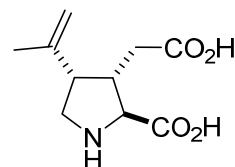
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 FREQU 7992.01 Hz
 SCANS 4
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 12.10 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 16



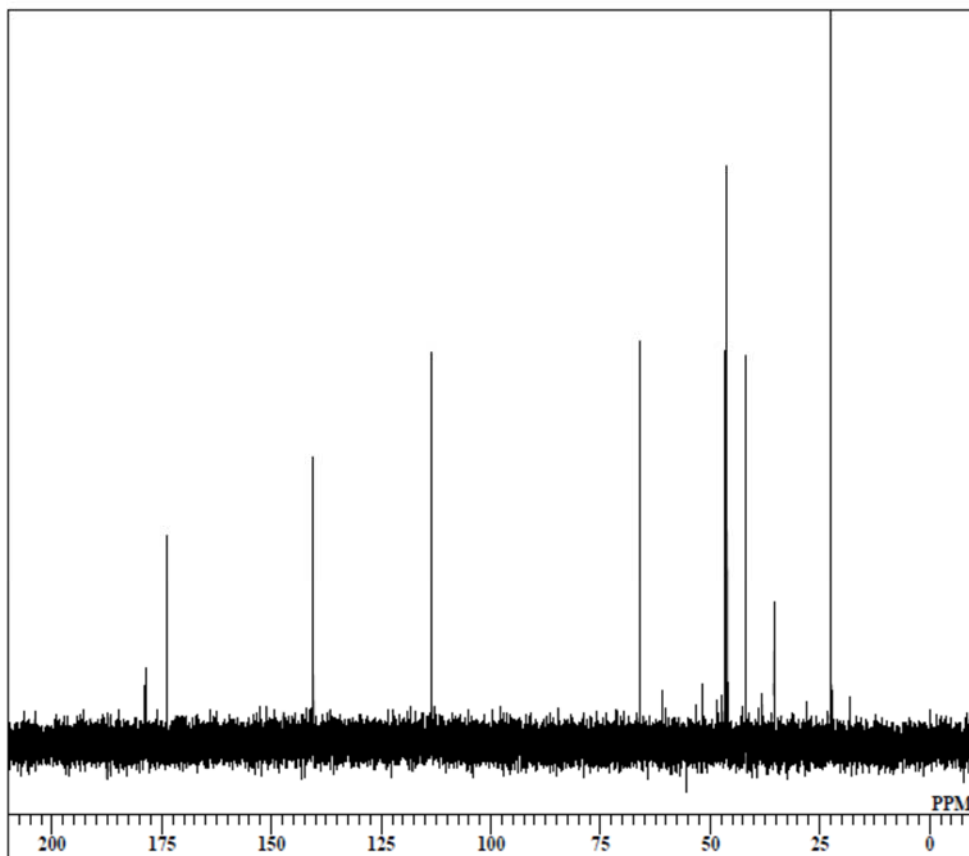
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 CTEMP 18.7 c
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 RGAIN 31



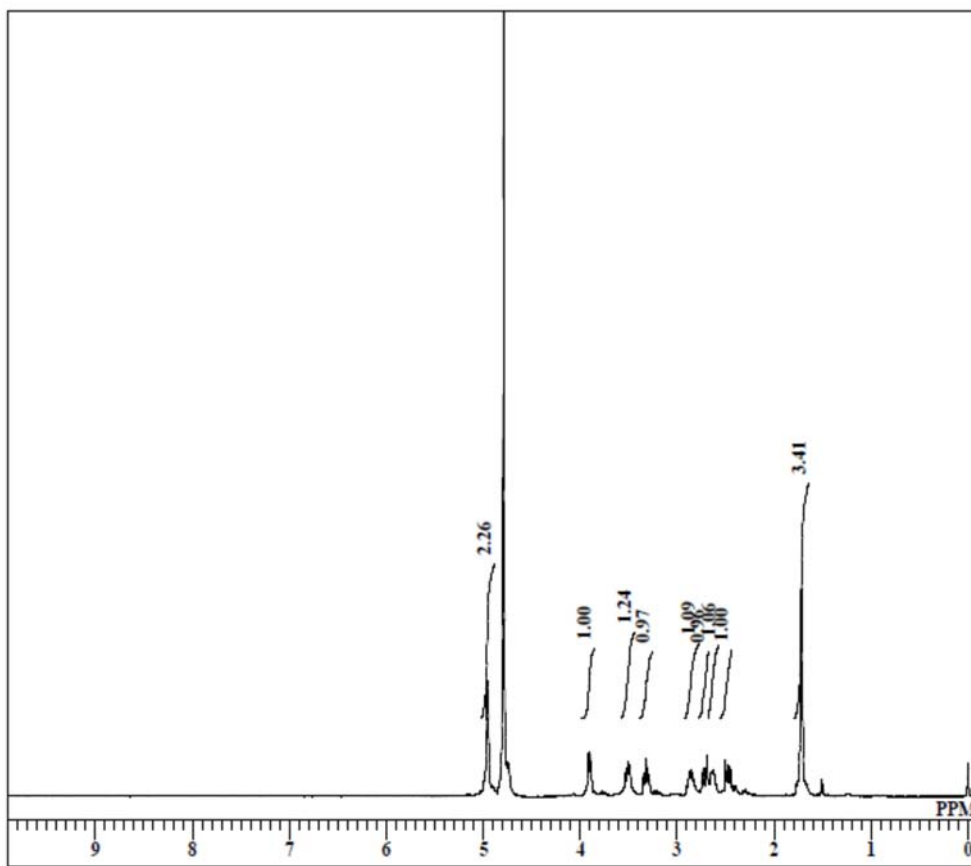
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 EXMOD NON
 OBFRQ 399.65 MHz
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 POINT 16384
 FREQU 7992.01 Hz
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 PW1 6.60 usec
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT D2O
 EXREF 4.80 ppm
 BF 0.10 Hz
 RGAIN 23



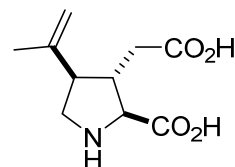
1



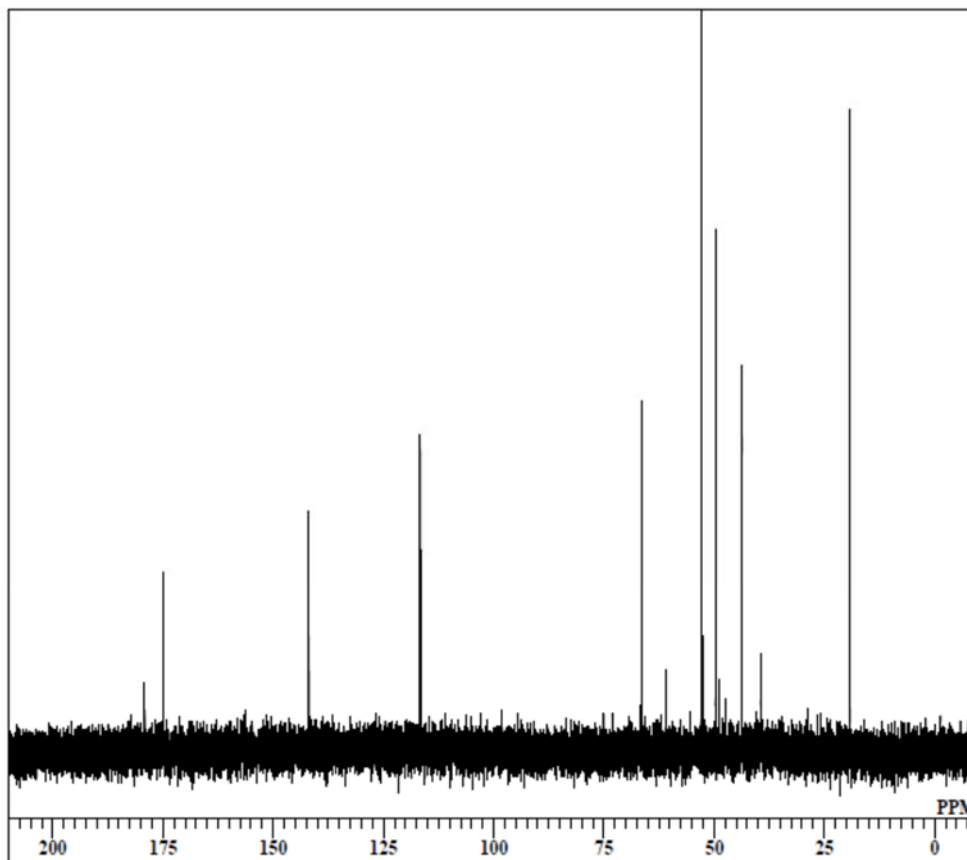
DFILE 39-21-4-C.als
 COMNT 39-21-4-C
 DATIM Sun Oct 09 10:05:07 2016
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 2919
 ACQTM 1.2083 sec
 PD 1.7920 sec
 PW1 4.40 usec
 IRNUC 1H
 CTEMP 22.0 c
 SLVNT D2O
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 31



DFILE 39-19-4.als
 COMNT 39-19-3
 DATIM Thu Oct 06 18:27:02 2016
 OBNUC 1H
 EXMOD NON
 OBFREQ 399.65 MHz
 OBSET 134.40 KHz
 OBFIN 64.90 Hz
 POINT 16384
 FREQU 7992.01 Hz
 SCANS 8
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 12.10 usec
 IRNUC 1H
 CTEMP 22.2 c
 SLVNT D2O
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 18



2



DFILE 39-19-4-C.als
 COMNT 39-19-4-C
 DATIM Sat Oct 08 09:14:38 2016
 OBNUC 13C
 EXMOD BCM
 OBFREQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 2868
 ACQTM 1.2083 sec
 PD 1.7920 sec
 PW1 4.40 usec
 IRNUC 1H
 CTEMP 22.3 c
 SLVNT D2O
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 31

