

Total Synthesis of Fargesine Using a Platinum-Catalyzed Intramolecular Friedel-Crafts-Type C–H Coupling–Allylic Amination Cascade

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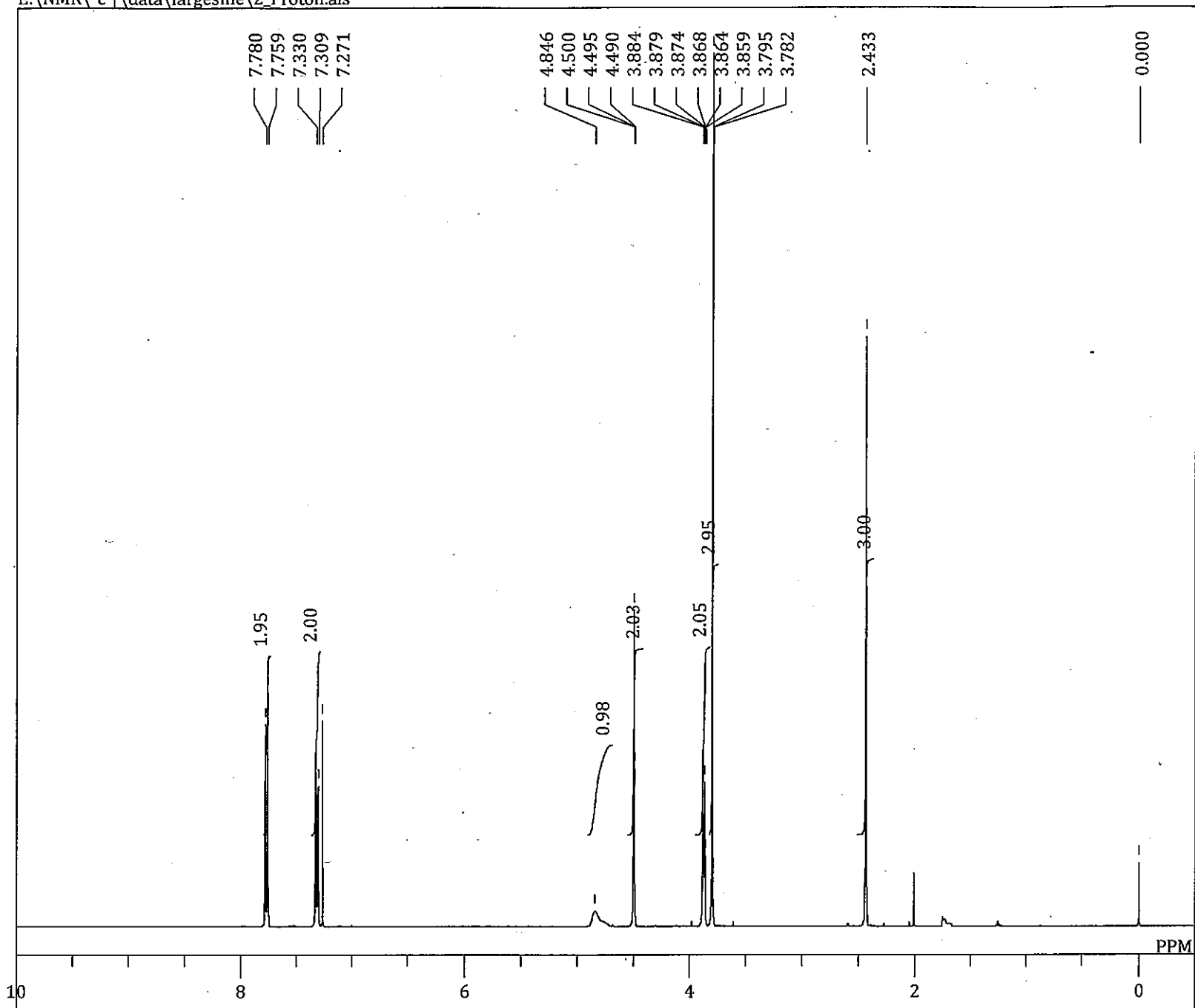
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Supporting Information

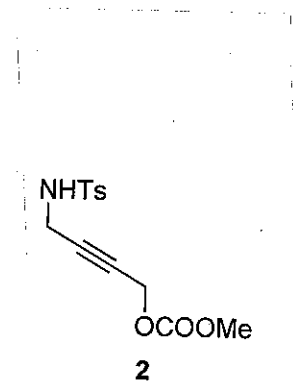
- 1. ¹H and ¹³C NMR Charts of Synthetic Intermediates and Fargesine (S-2–S-21)**

Compound 2

E:\NMR\c+\data\argesine\2_Proton.als



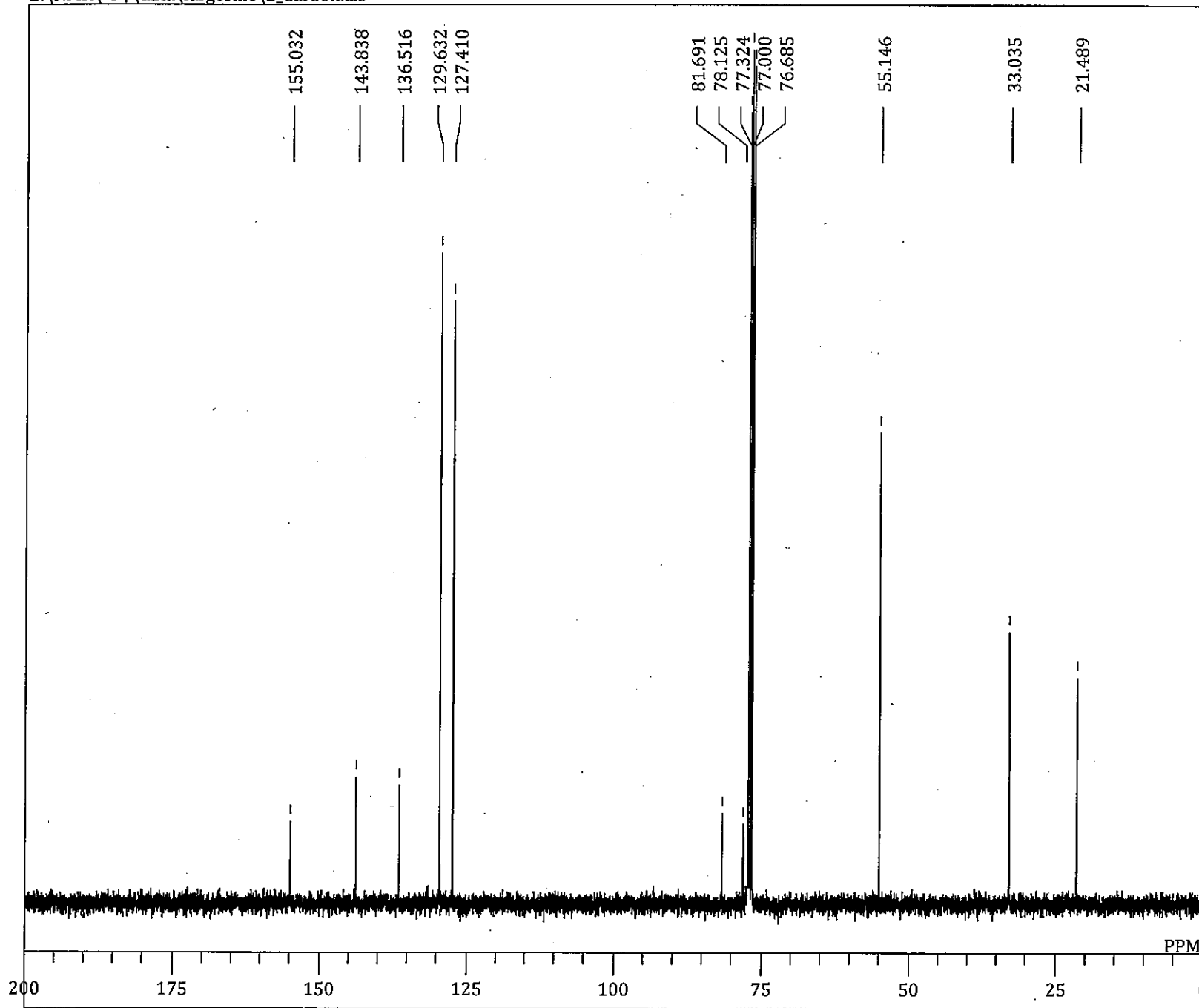
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 OBNUC 1H
 EXMOD proton.jpg
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 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.01 usec
 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 38



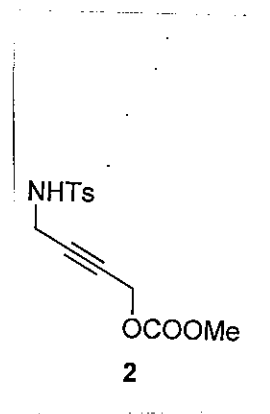
S 2

Compound 2

E:\NMR\c+\data\fargesine\2_Carbon.als



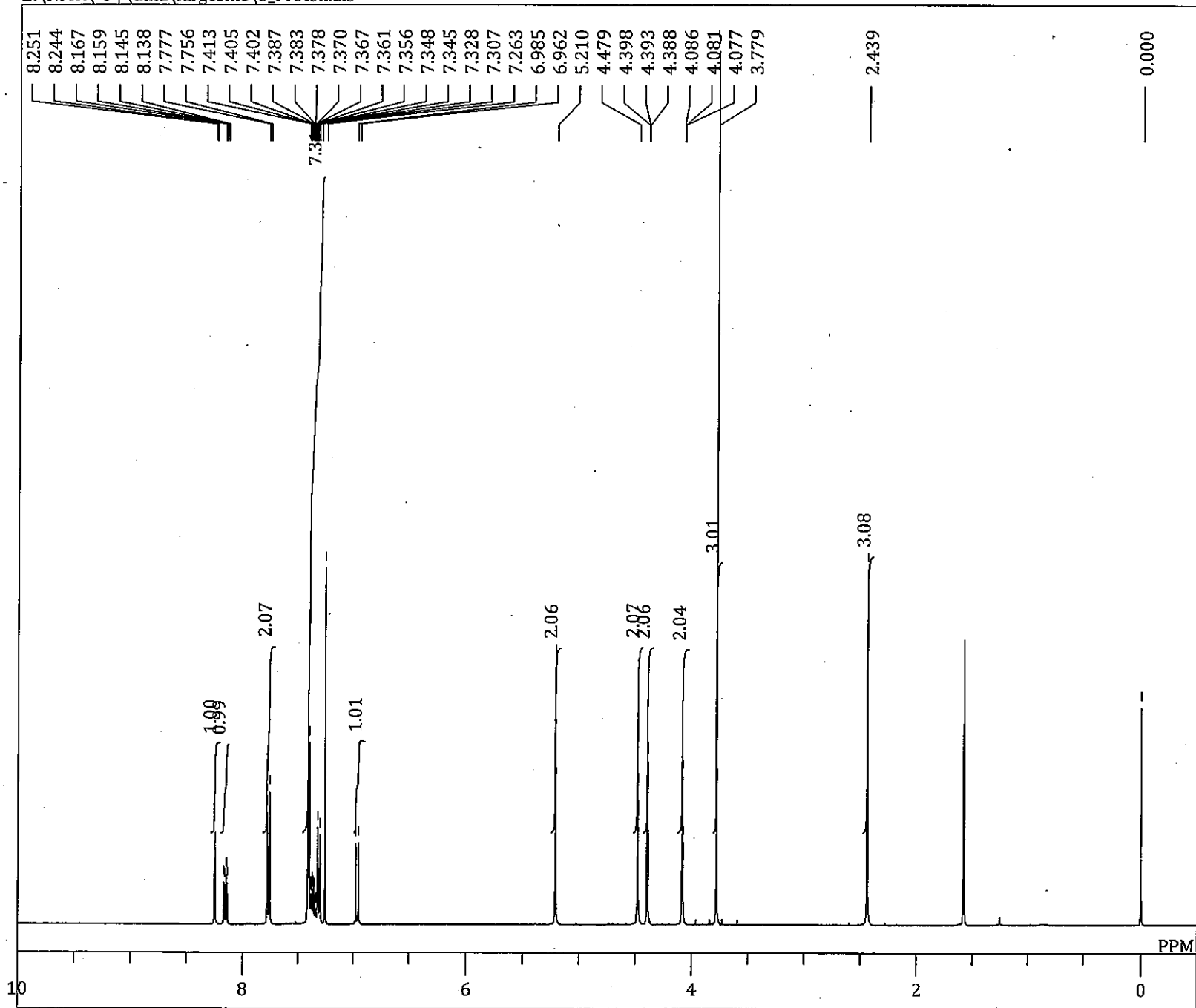
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EXMOD carbon.jsp
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OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 129
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 2.77 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 50



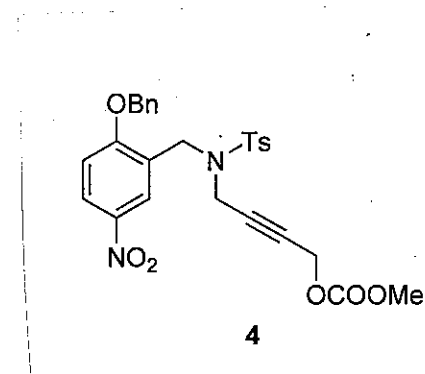
S 3

Compound 4

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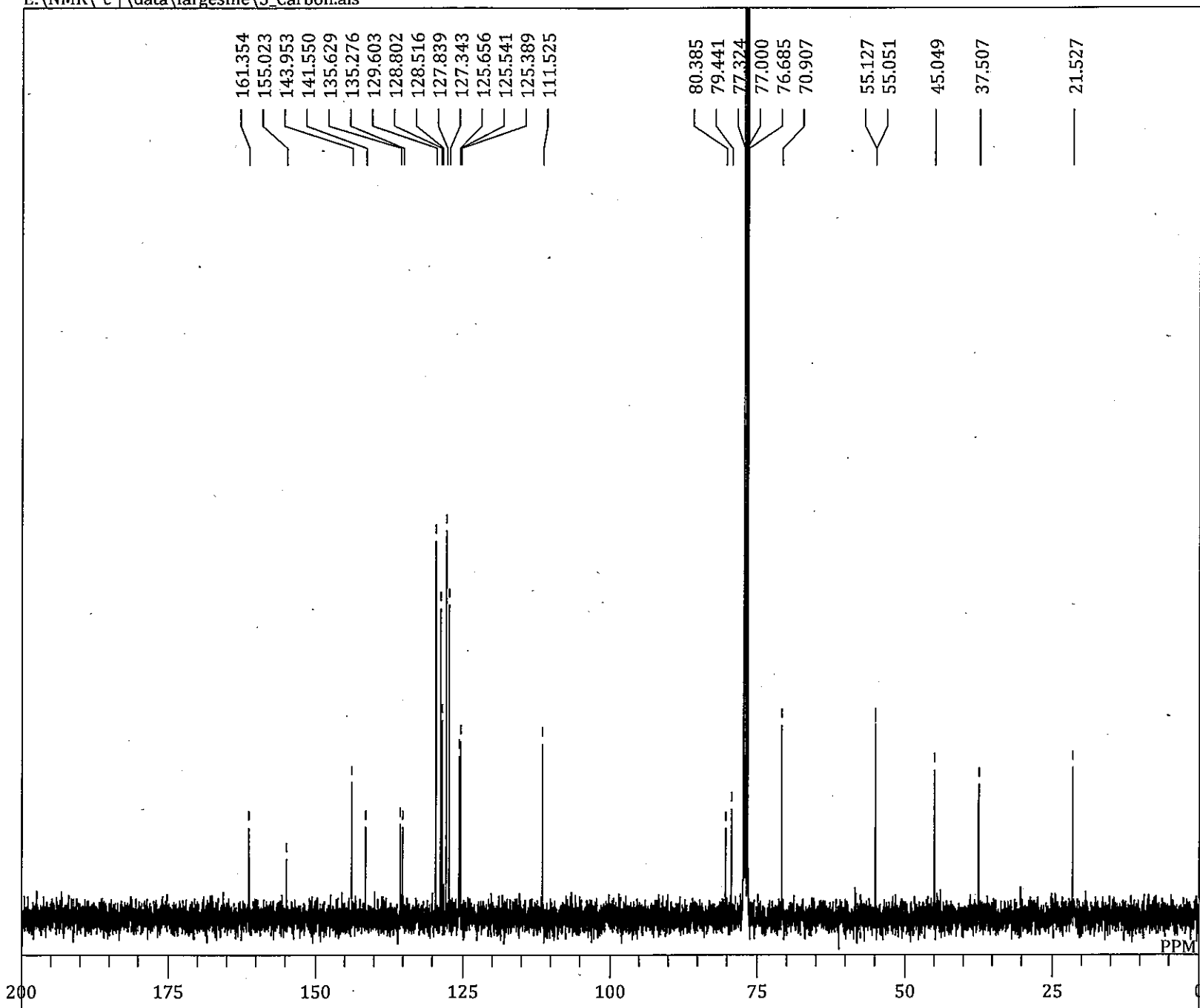


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 OBNUC 1H
 EXMOD proton.jpg
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 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.01 usec
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 46

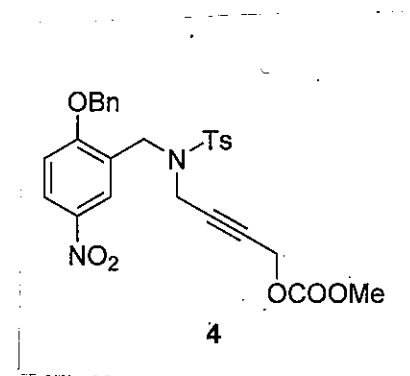


Compound 4

E:\NMR\c+\data\fargesine\3_Carbon.als

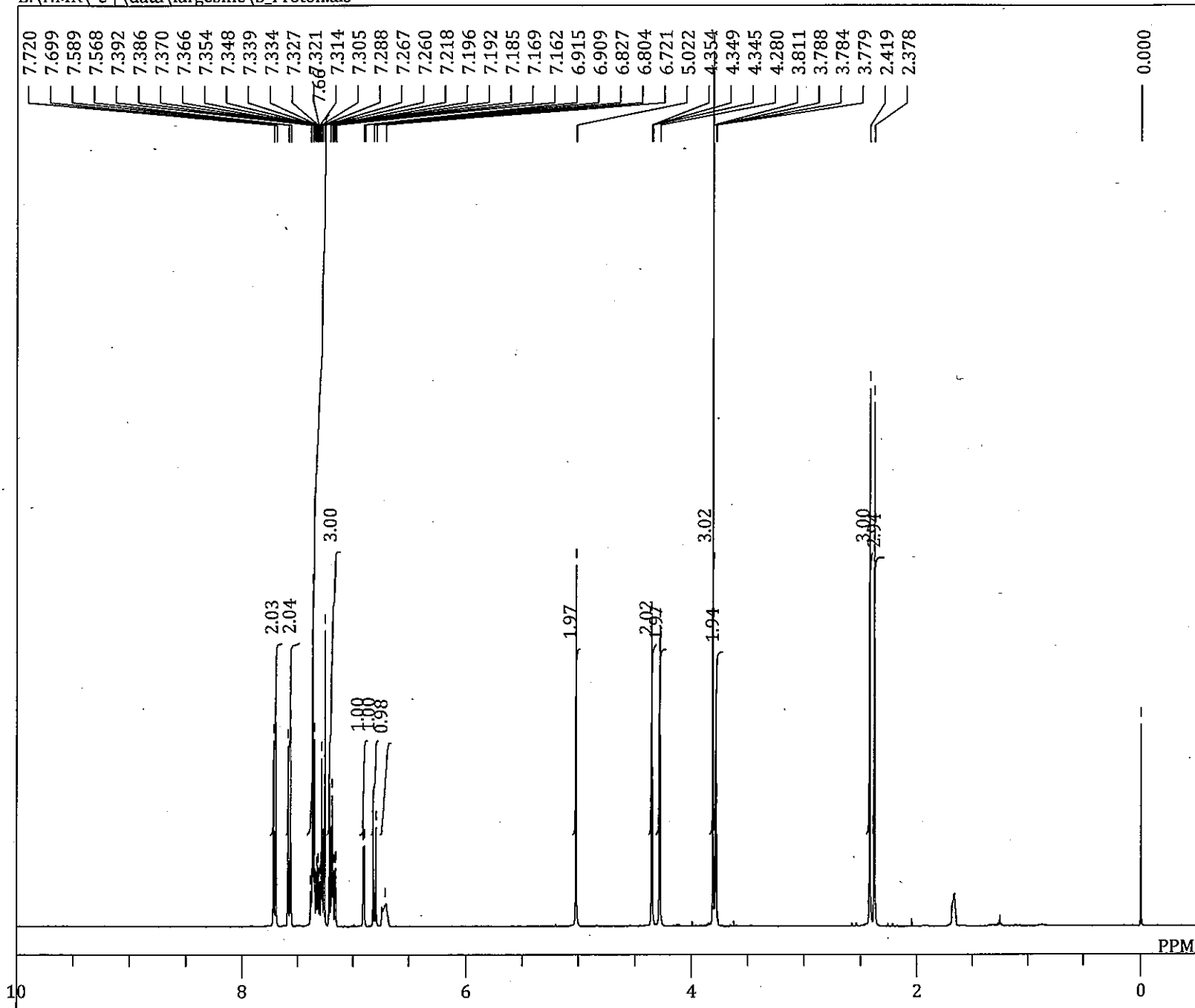


DFILE 3_Carbon.als
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 OBNUC 13C
 EXMOD carbon.jxp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 512
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.77 usec
 IRNUC 1H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 50

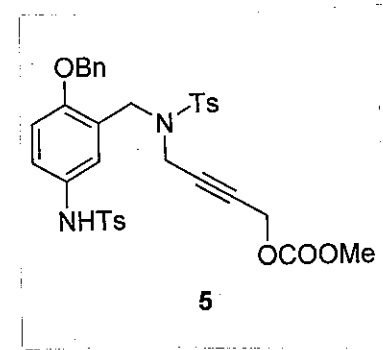


Compound 5

E:\NMR\c+\data\fargesine\5_Proton.als

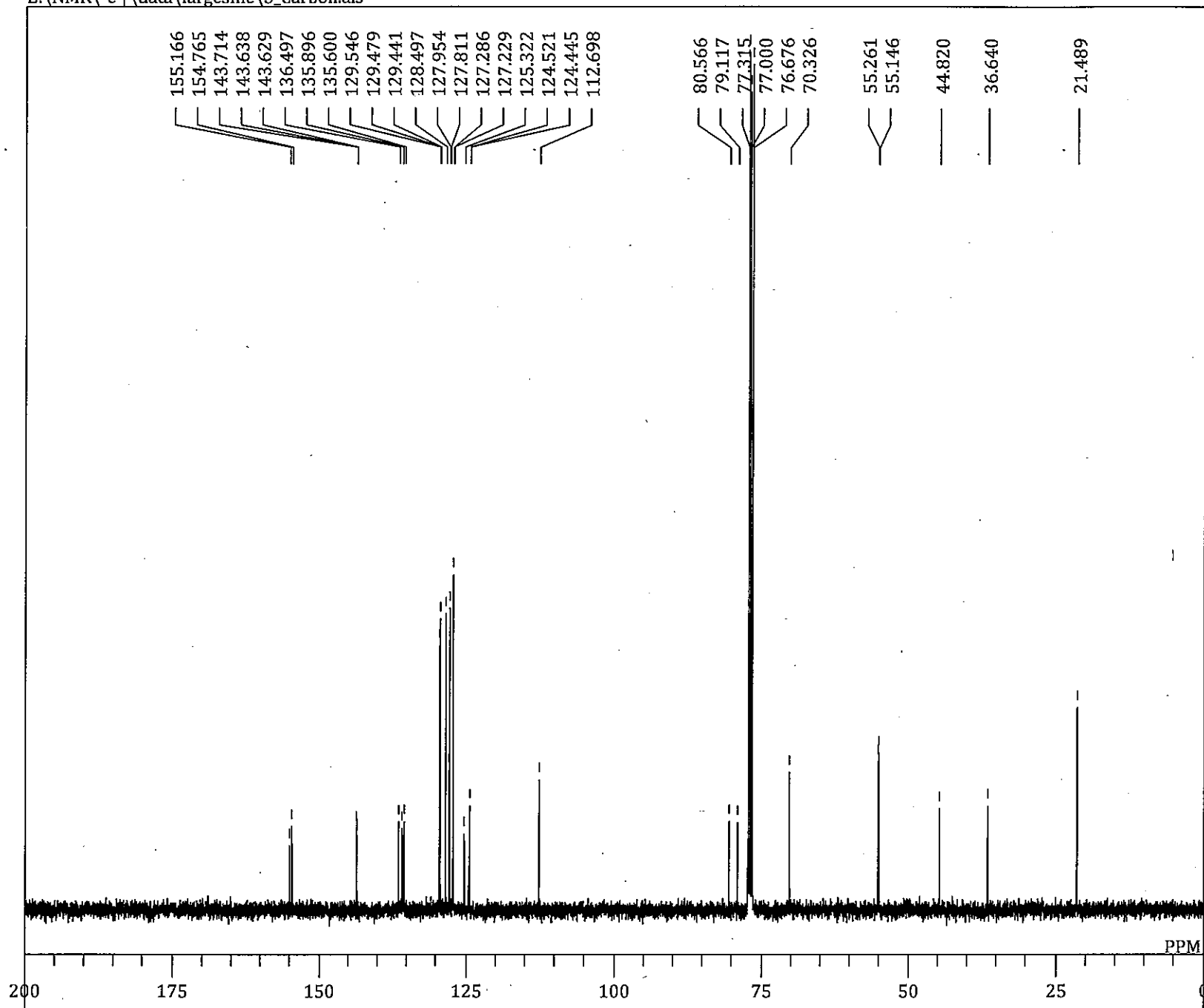


DFILE 5_Proton.als
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 DATIM 2015-07-28 11:05:09
 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.01 usec
 IRNUC 1H
 CTEMP 23.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 38

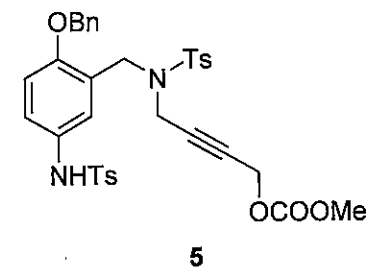


Compound 5

E:\NMR\c+\data\fargesine\5_Carbon.als

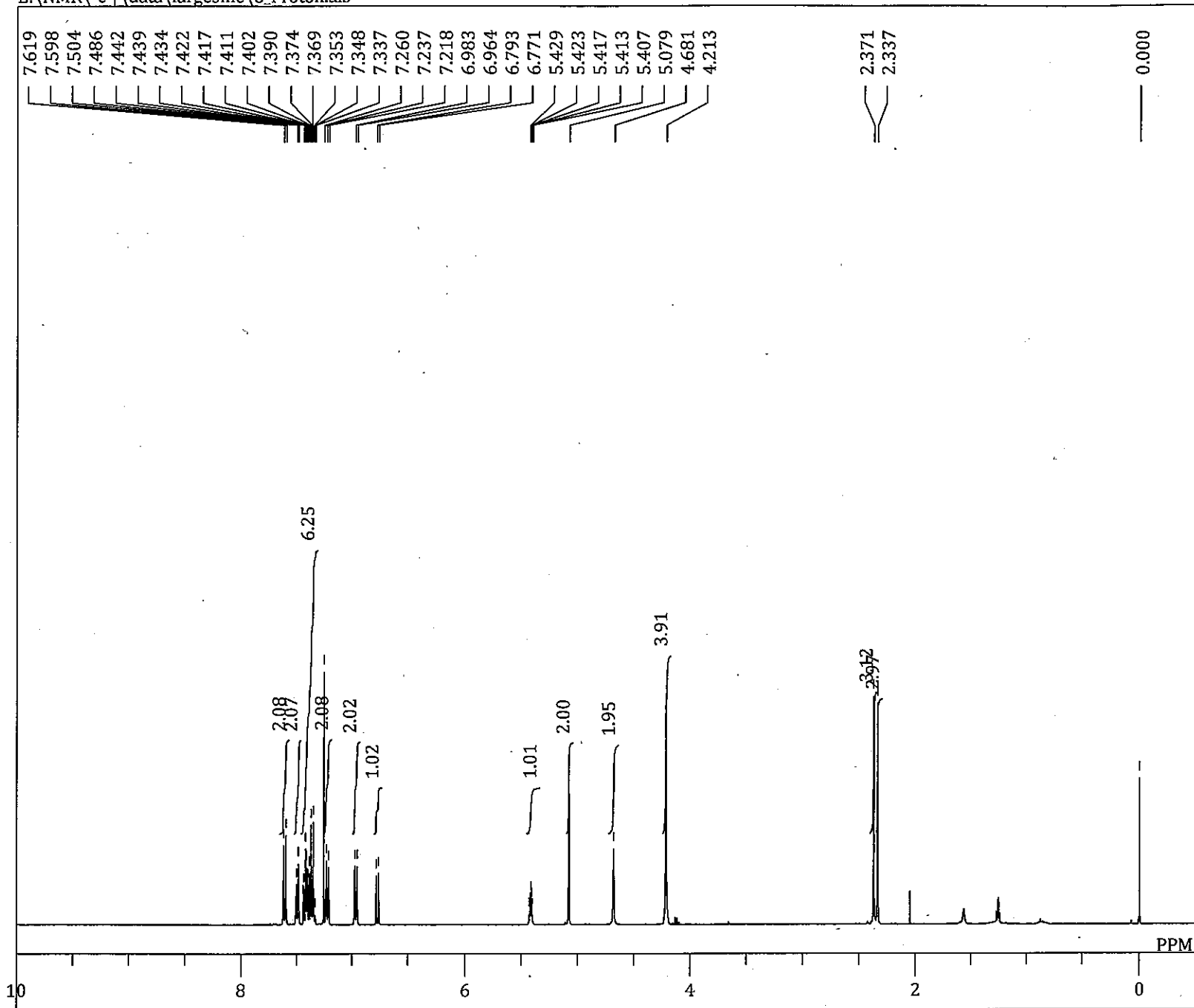


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 OBNUC 13C
 EXMOD carbon.jxp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 227
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.77 usec
 IRNUC 1H
 CTEMP 23.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 50

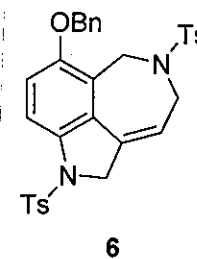


Compound 6

E:\NMR\c+\data\fargesine\6_Proton.als



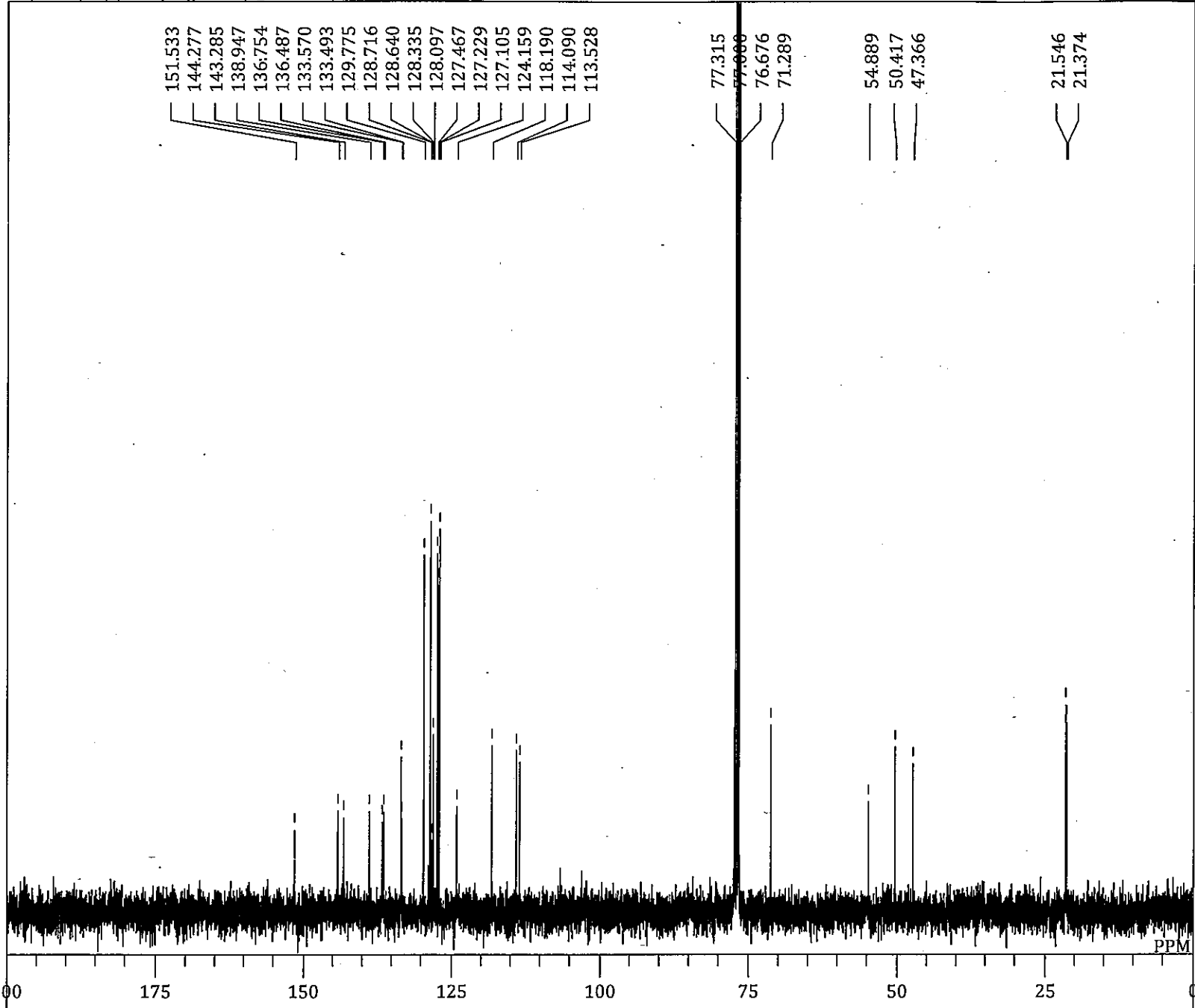
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 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.01 usec
 IRNUC 1H
 CTEMP 22.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 44



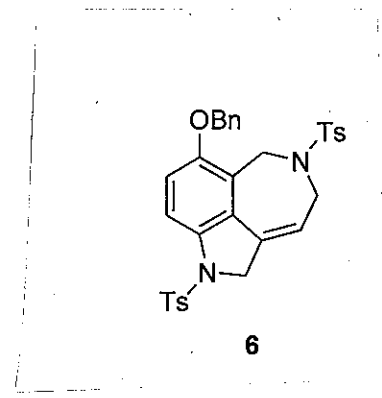
S 8

Compound 6

E:\NMR\c+\data\fargesine\6_Carbon.als



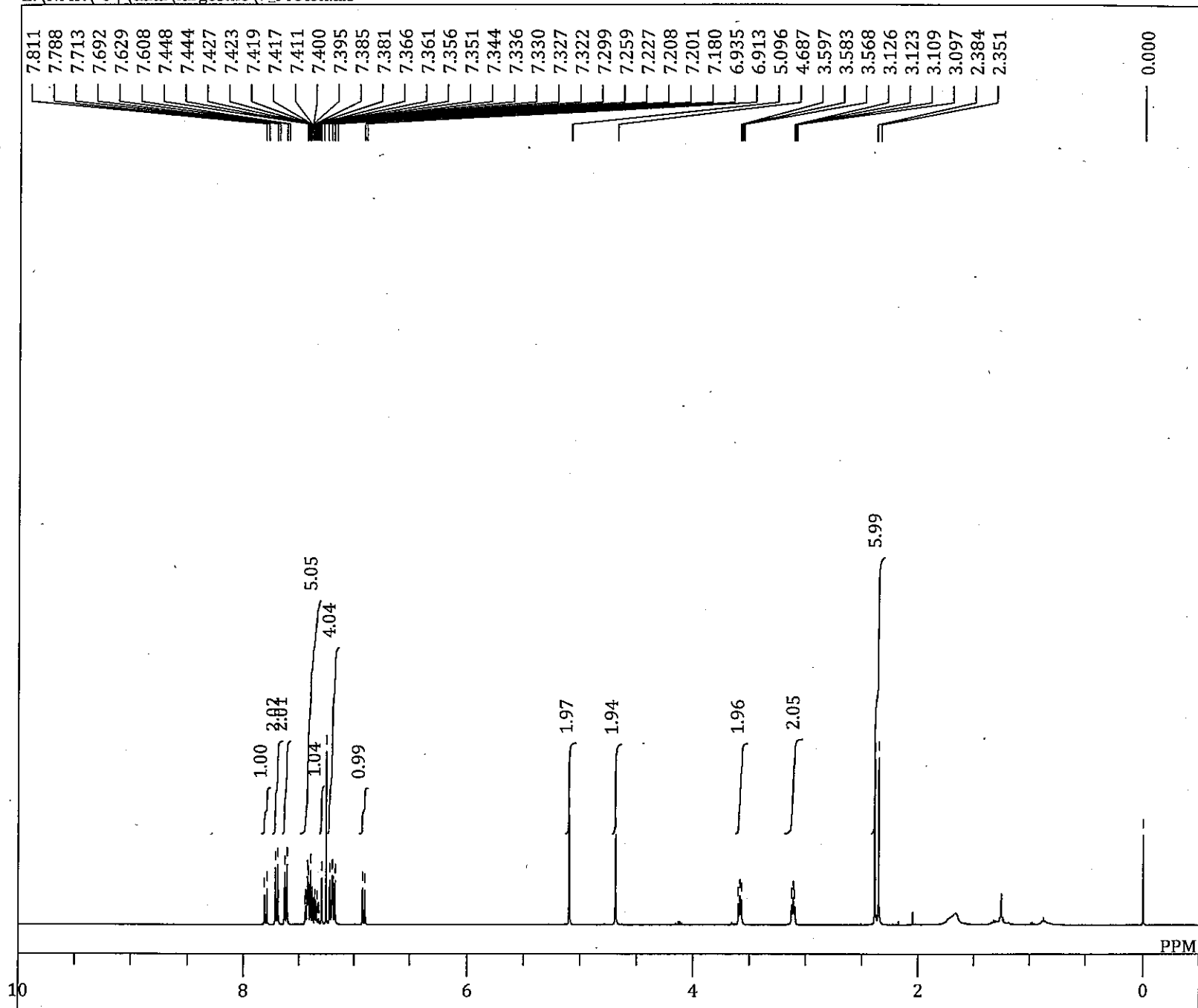
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 OBNUC 13C
 EXMOD carbon.jxp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 256
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.77 usec
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 50



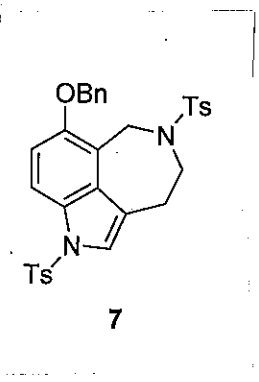
S 9

Compound 7

E:\NMR\c+\data\fargesine\7_Proton.als

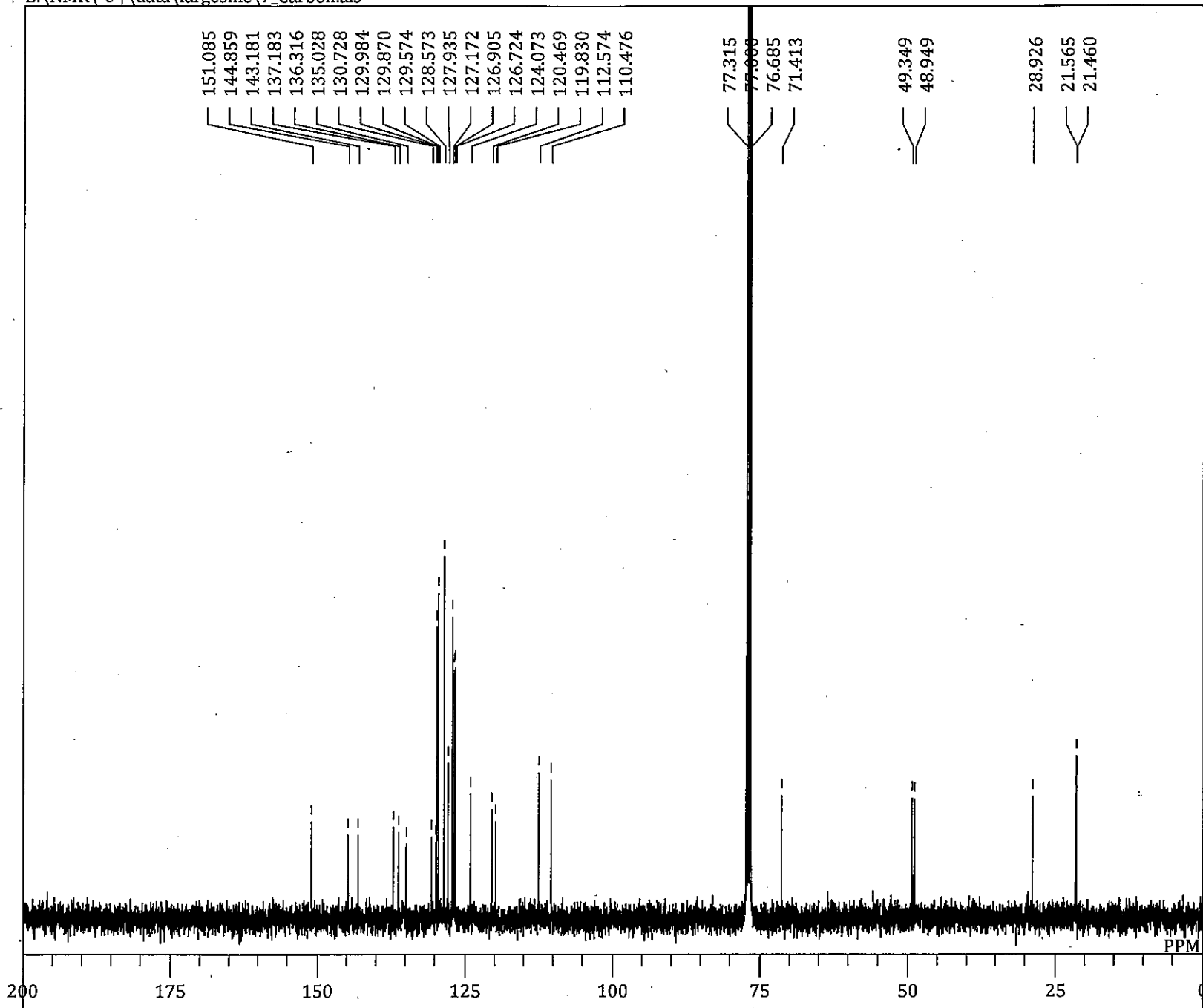


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 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.01 usec
 IRNUC 1H
 CTEMP 23.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 46

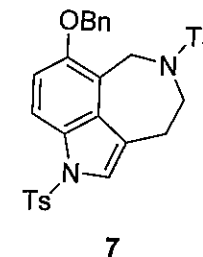


Compound 7

E:\NMR\c+\data\fargesine\7_Carbon.als



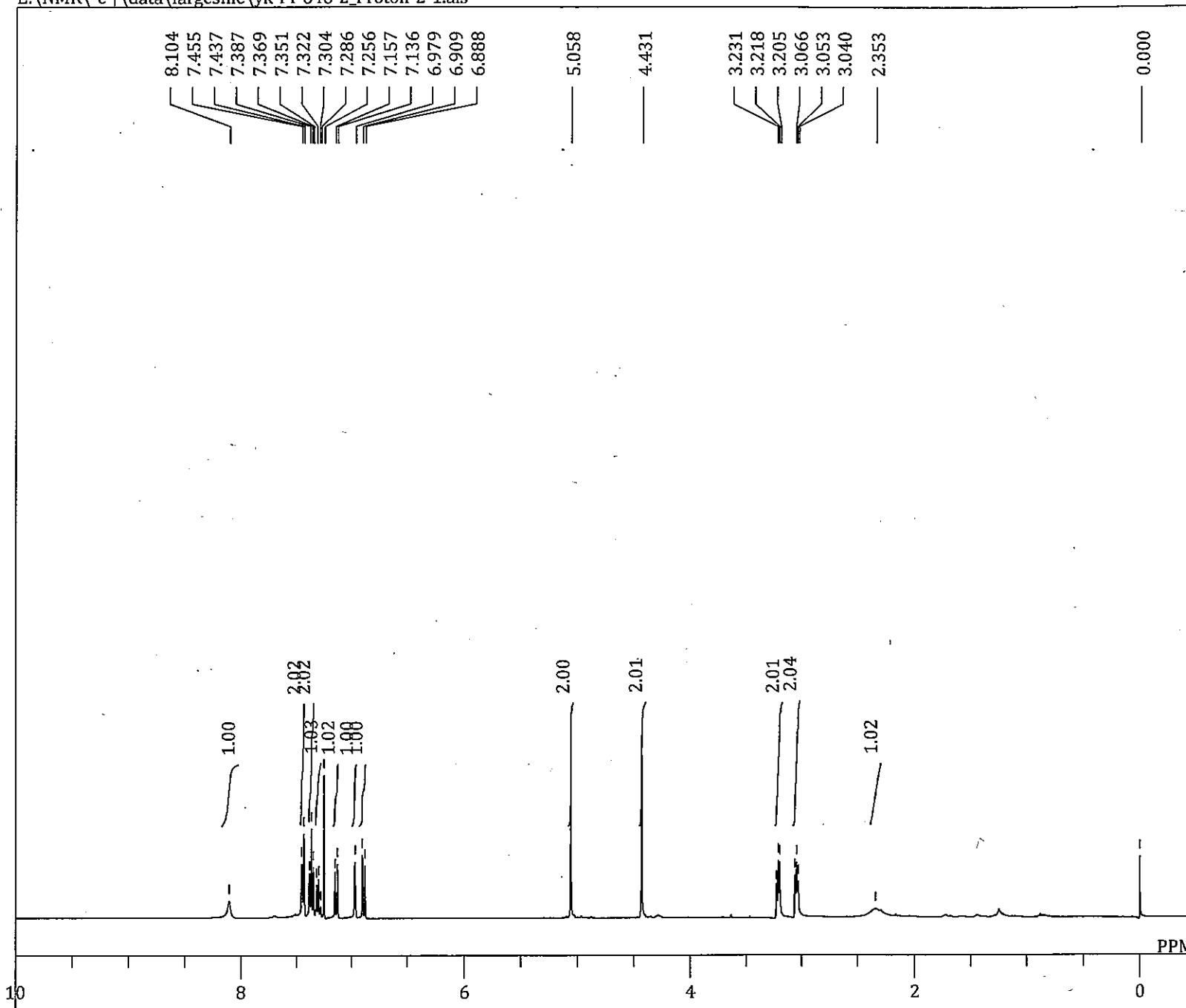
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 EXMOD carbon.jxp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 624
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.77 usec
 IRNUC 1H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 50



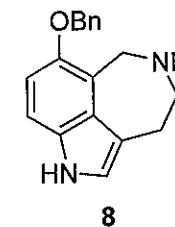
S 11

Compound 8

E:\NMR\c+\data\fargesine\yk-YT-646-2_Proton-2-1.als

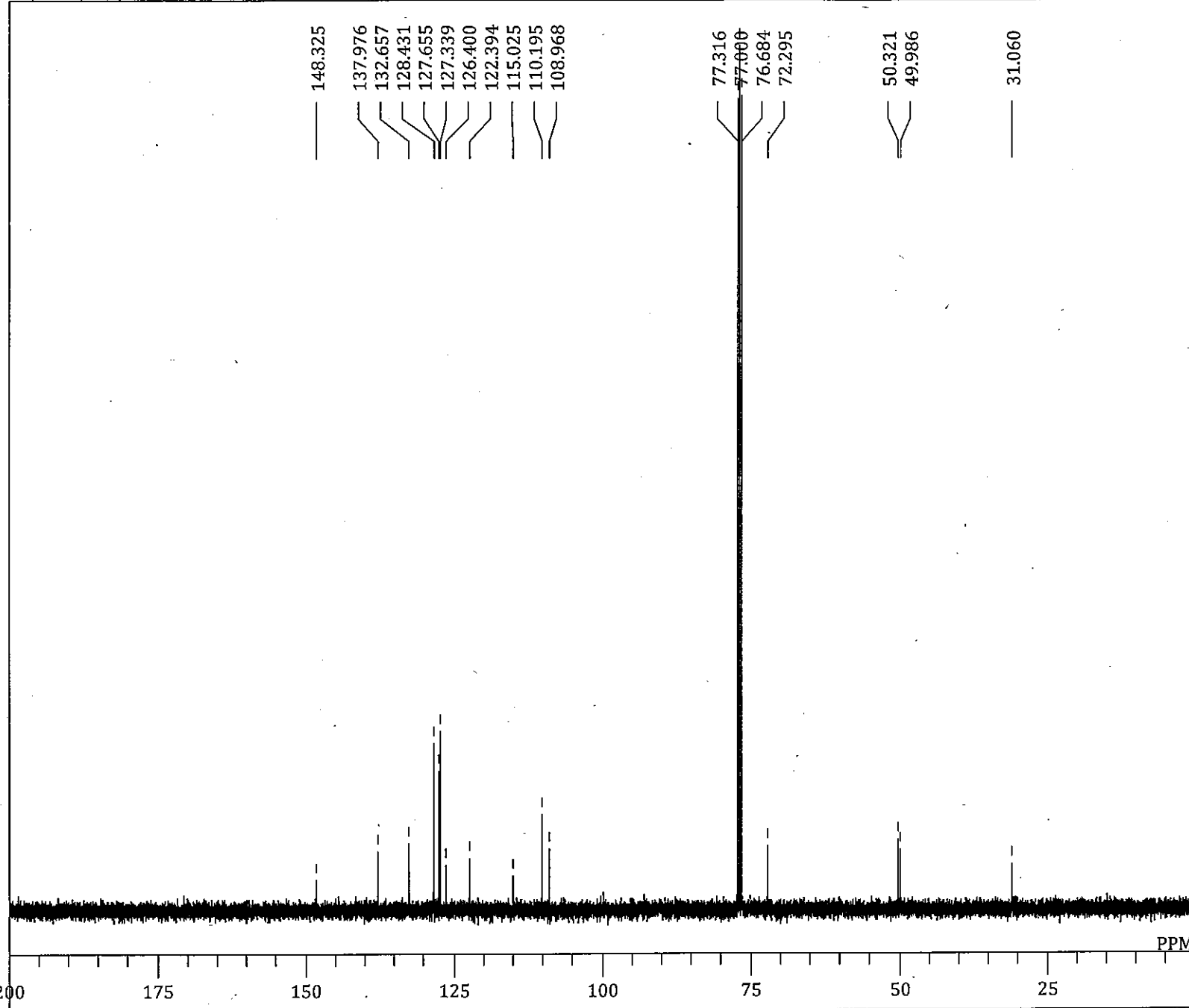


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 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 5995.20 Hz
 SCANS 8
 ACQTM 2.1863 sec
 PD 5.0000 sec
 PW1 2.72 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 56

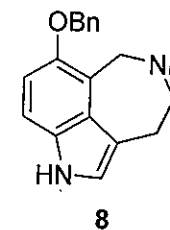


Compound 8

E:\NMR\c+f\data\fargesine\yk-yt-646-2_Carbon-1-1.als

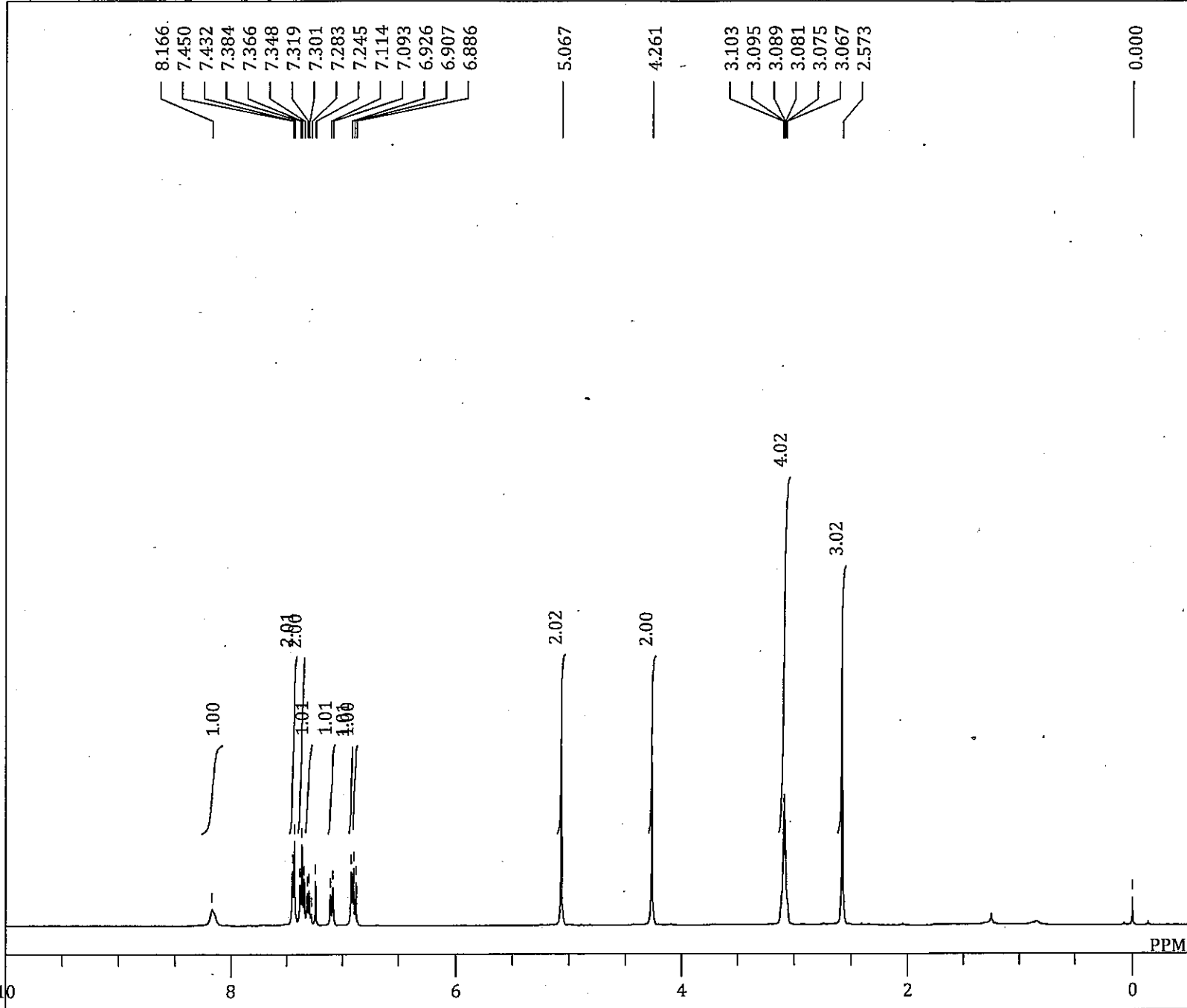


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 COMNT Compound 8
 DATIM 2016-02-18 15:15:57
 OBNUC 13C
 EXMOD carbon.jxp
 OBFREQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25252.53 Hz
 SCANS 526
 ACQTM 1.0381 sec
 PD 2.0000 sec
 PW1 3.52 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50

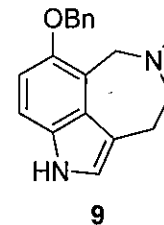


Compound 9

E:\NMR\c+\data\fargesine\yk-yt-644-2_Proton-1-1.als

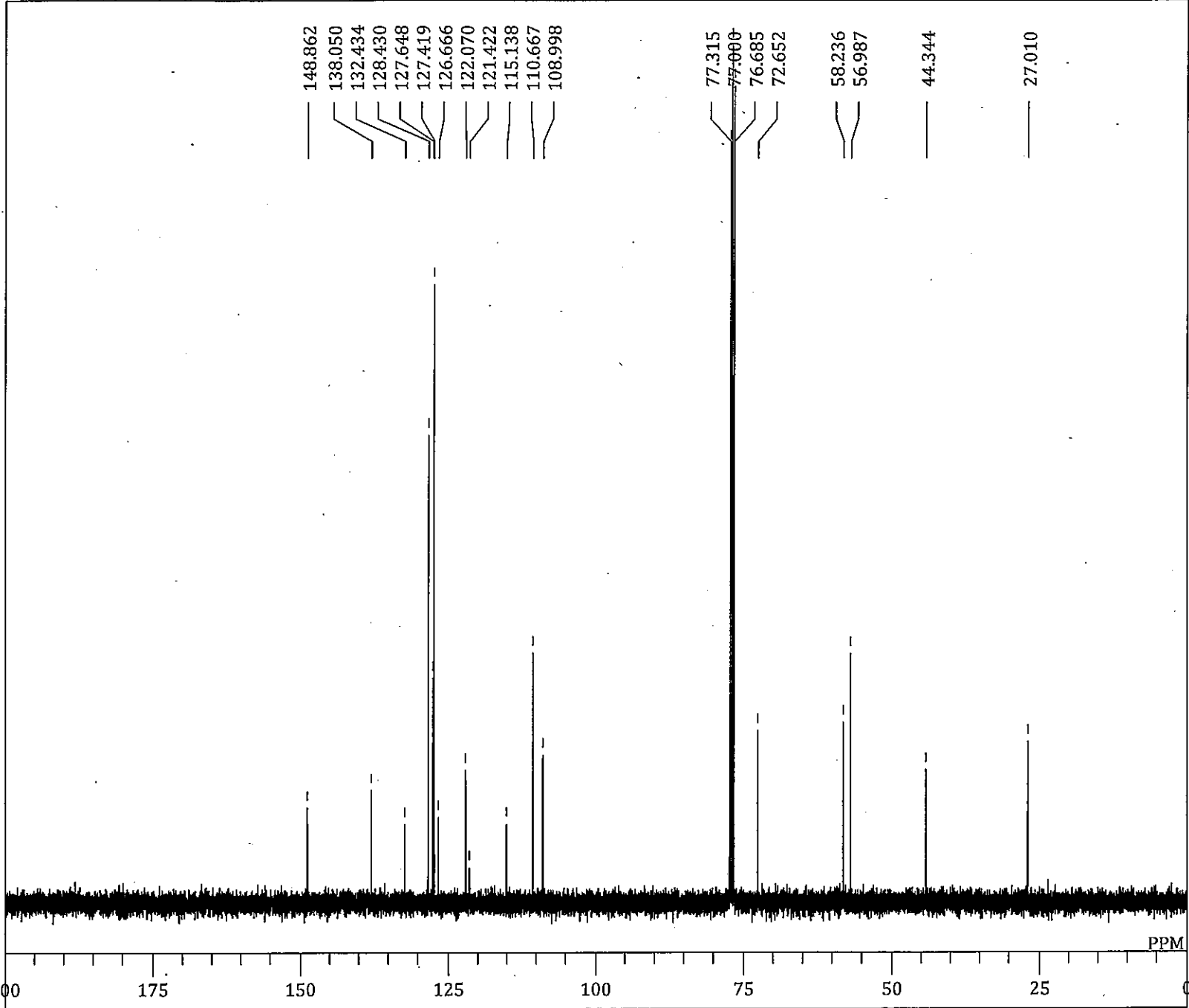


DFILE yk-yt-644-2_Proton-1-1.als
 COMNT Compound 9
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 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.01 usec
 IRNUC 1H
 CTEMP 23.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 38

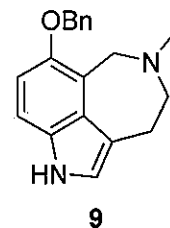


Compound 9

E:\NMR\c+\data\fargesine\yk-yt-644-2_Carbon-1-1.jdf



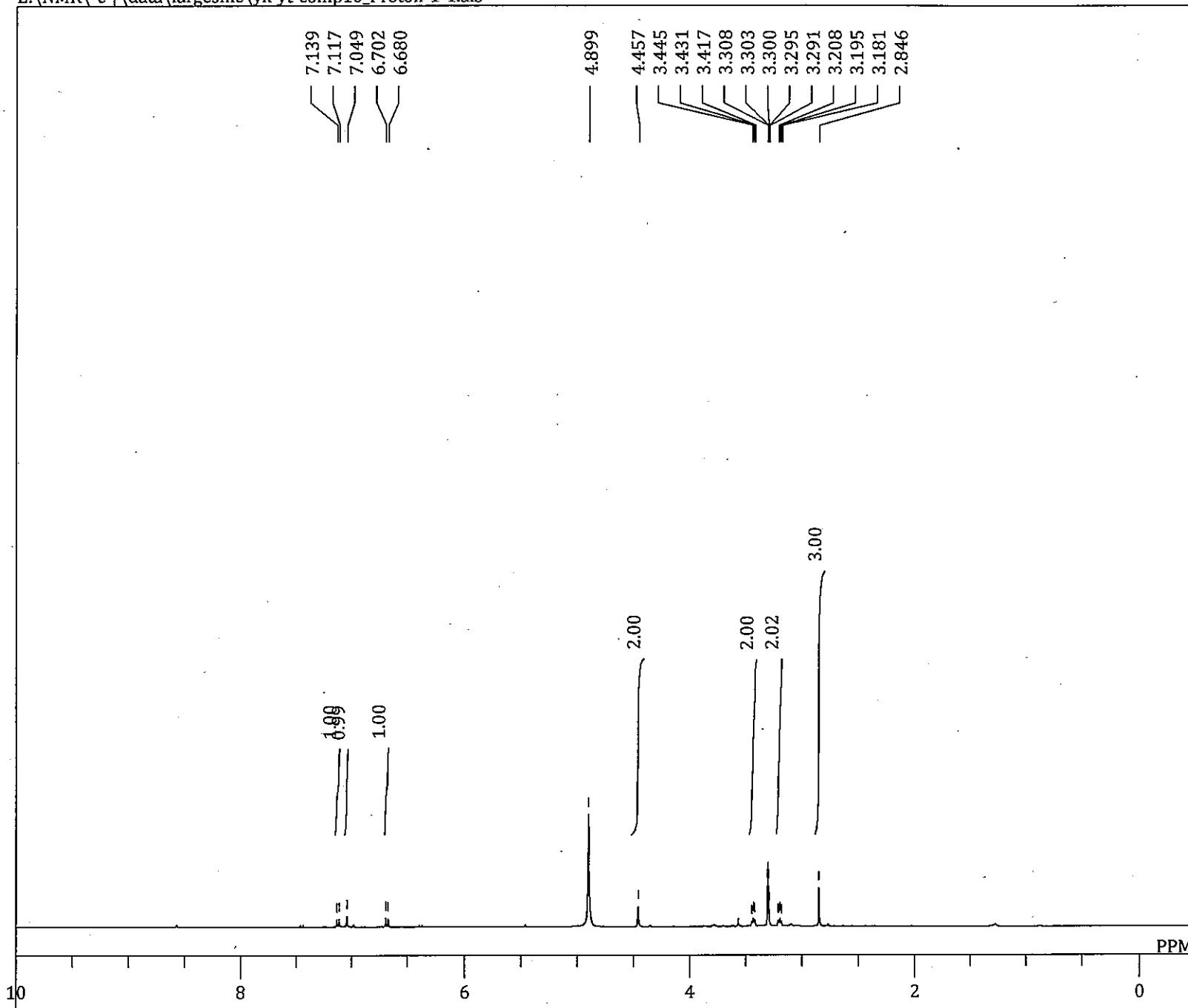
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 EXMOD carbon.jxp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32767
 FREQU 31407.04 Hz
 SCANS 257
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.77 usec
 IRNUC 1H
 CTEMP 23.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50



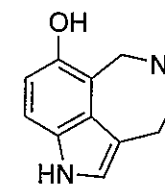
S 15

Compound 10

E:\NMR\c+\data\fargesine\yk-yt-comp10_Proton-1-1.als



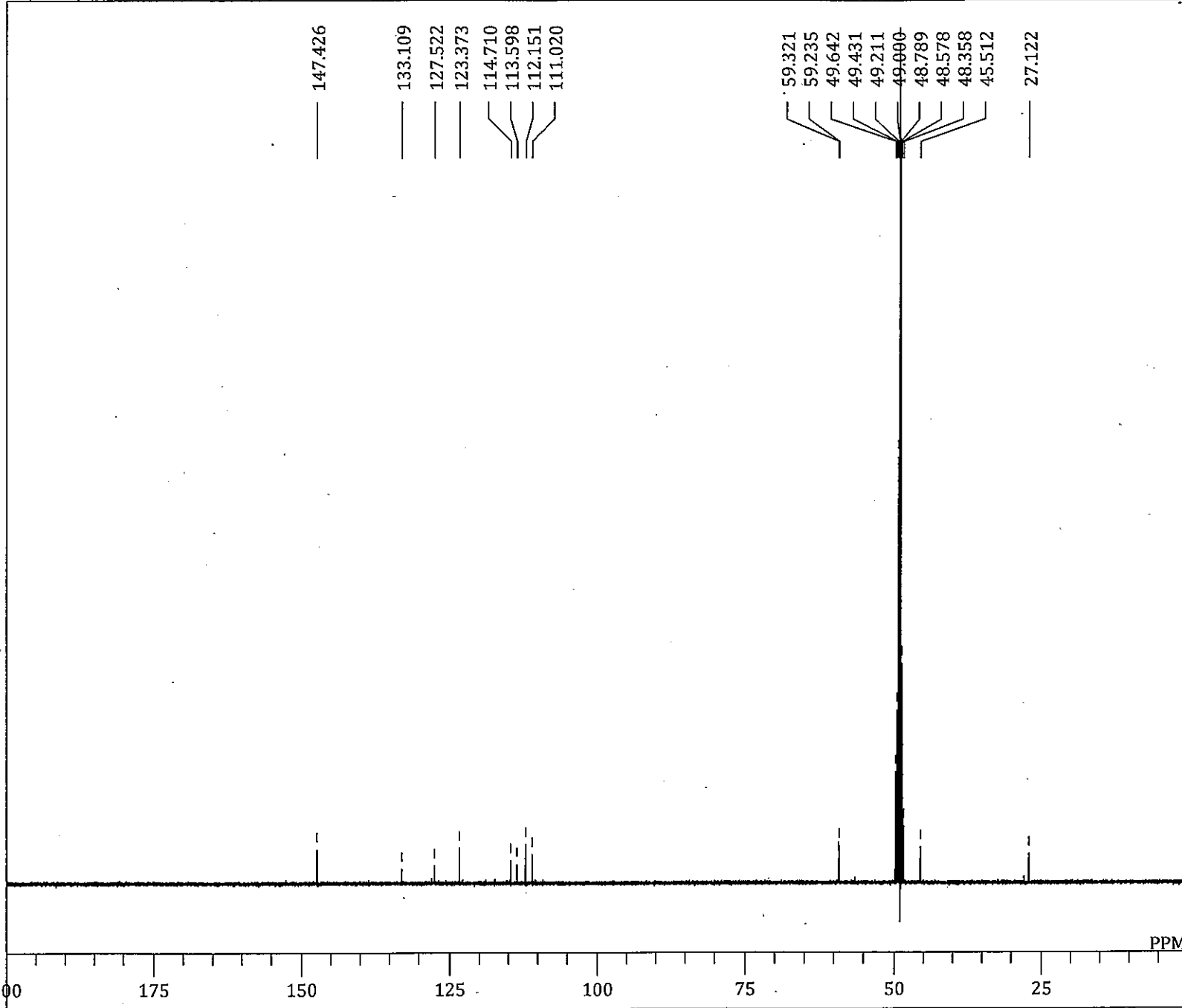
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 EXMOD proton.jxp
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 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.00 usec
 IRNUC 1H
 CTEMP 19.7 c
 SLVNT CD3OD
 EXREF 3.30 ppm
 BF 0.12 Hz
 RGAIN 44



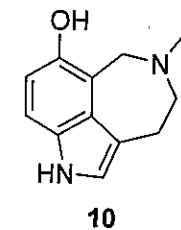
10

Compound 10

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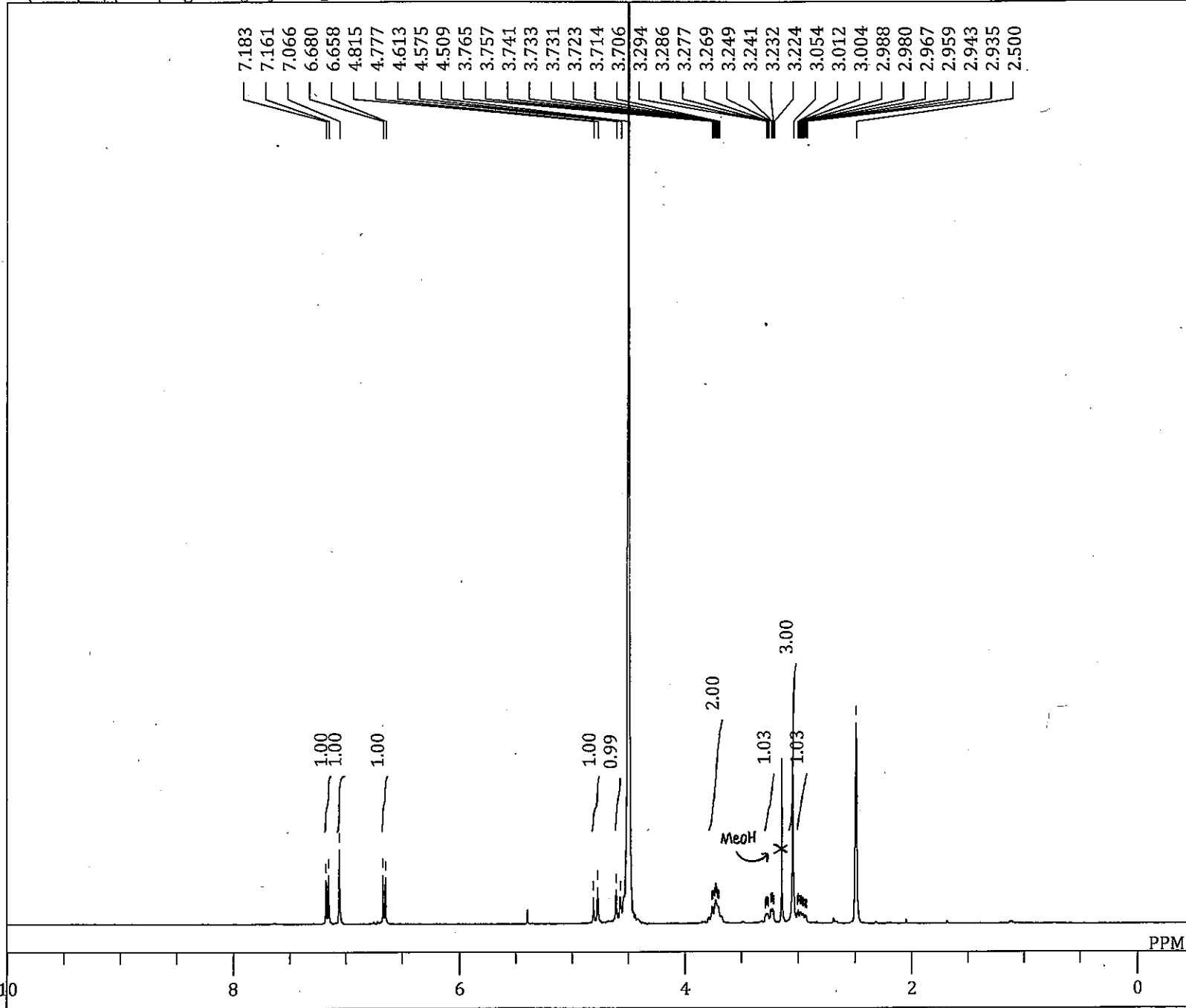


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OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 1024
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 19.0 c
SLVNT CD3OD
EXREF 49.00 ppm
BF 0.12 Hz
RGAIN 50

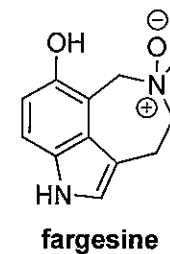


fargesine

E:\NMR\c+f\data\fargesine\yk-yt-721_Proton-1-1.als



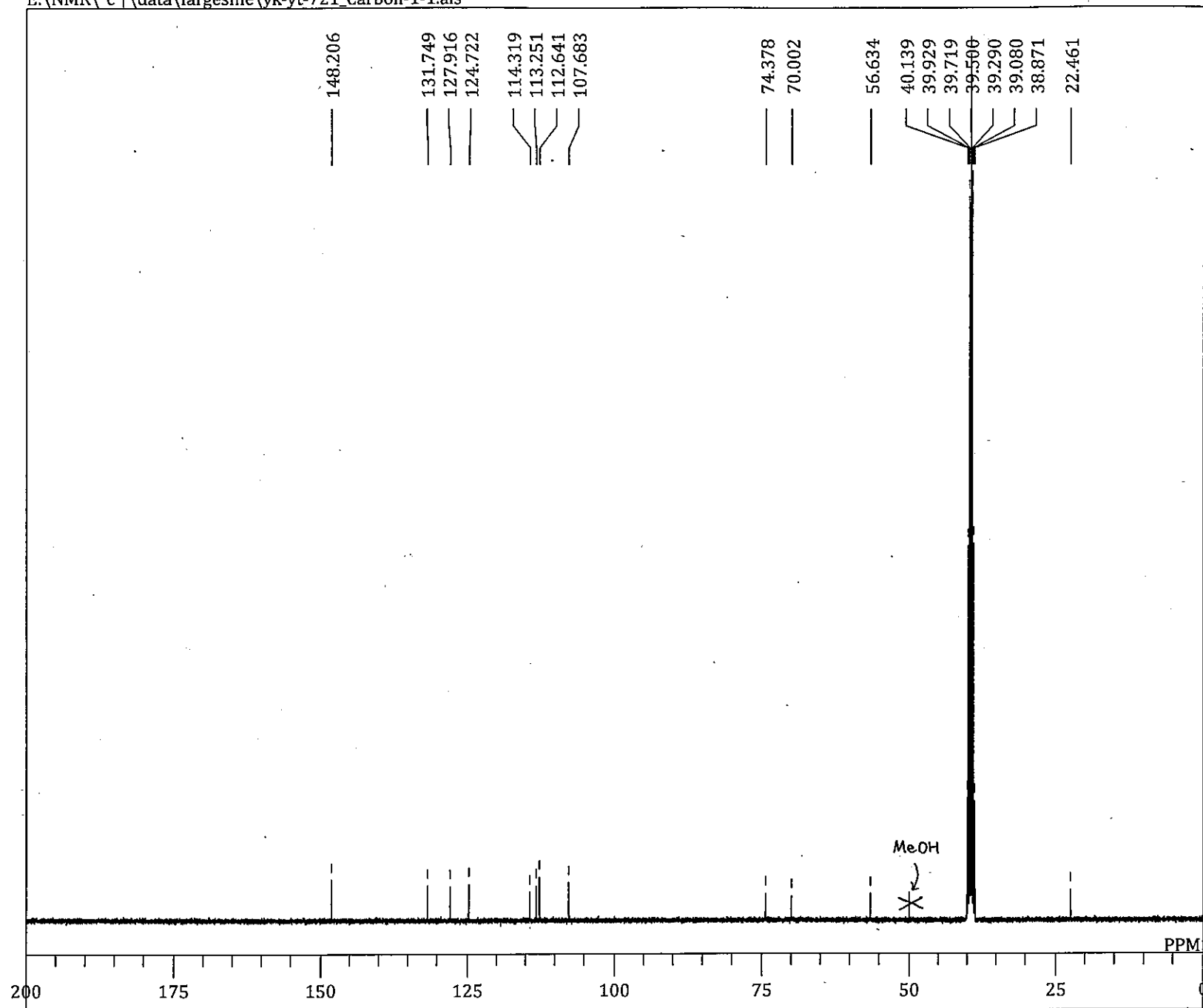
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 EXMOD proton.jxp
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 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.00 usec
 IRNUC 1H
 CTEMP 19.5 c
 SLVNT DMSO
 EXREF 2.50 ppm
 BF 0.12 Hz
 RGAIN 40



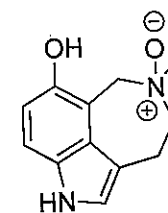
in DMSO-d₆ - D₂O

fargesine

E:\NMR\c+\data\fargesine\yk-yt-721_Carbon-1-1.als



DFILE yk-yt-721_Carbon-1-1.als
 COMNT fargesine
 DATIM 2016-06-16 23:10:40
 OBNUC 13C
 EXMOD carbon.jxp
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 8192
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.87 usec
 IRNUC 1H
 CTEMP 19.8 c
 SLVNT DMSO
 EXREF 39.50 ppm
 BF 0.12 Hz
 RGAIN 50

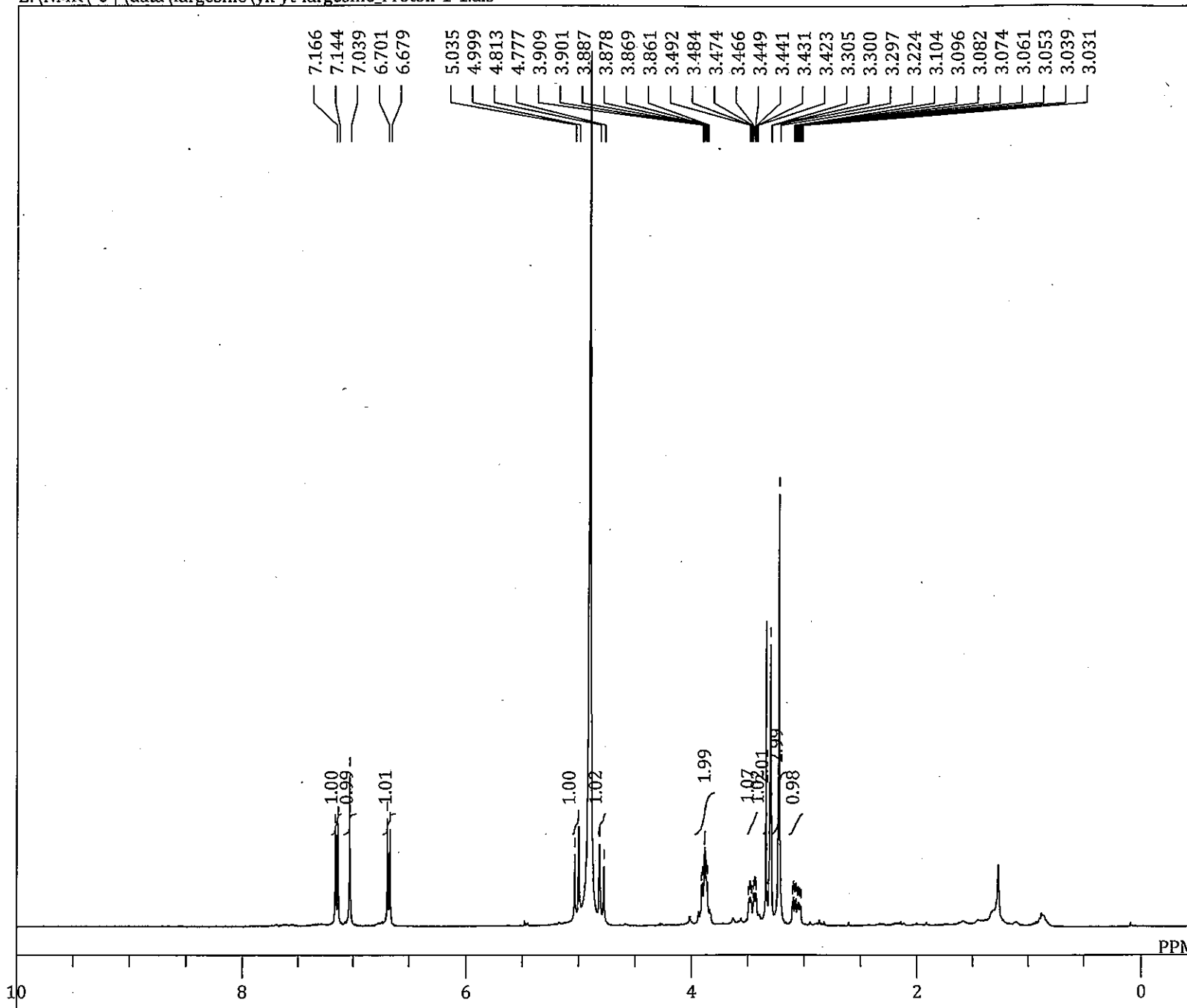


fargesine

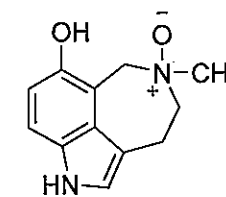
in DMSO-d₆ - D₂O

fargesine

E:\NMR\c+\data\fargesine\yk-yt-fargesine_Proton-1-1.als



DFILE yk-yt-fargesine_Proton-1-1.als
 COMNT fargesine
 DATIM 2016-05-31 17:22:49
 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PW1 5.00 usec
 IRNUC 1H
 CTEMP 20.1 c
 SLVNT CD3OD
 EXREF 3.30 ppm
 BF 0.12 Hz
 RGAIN 40

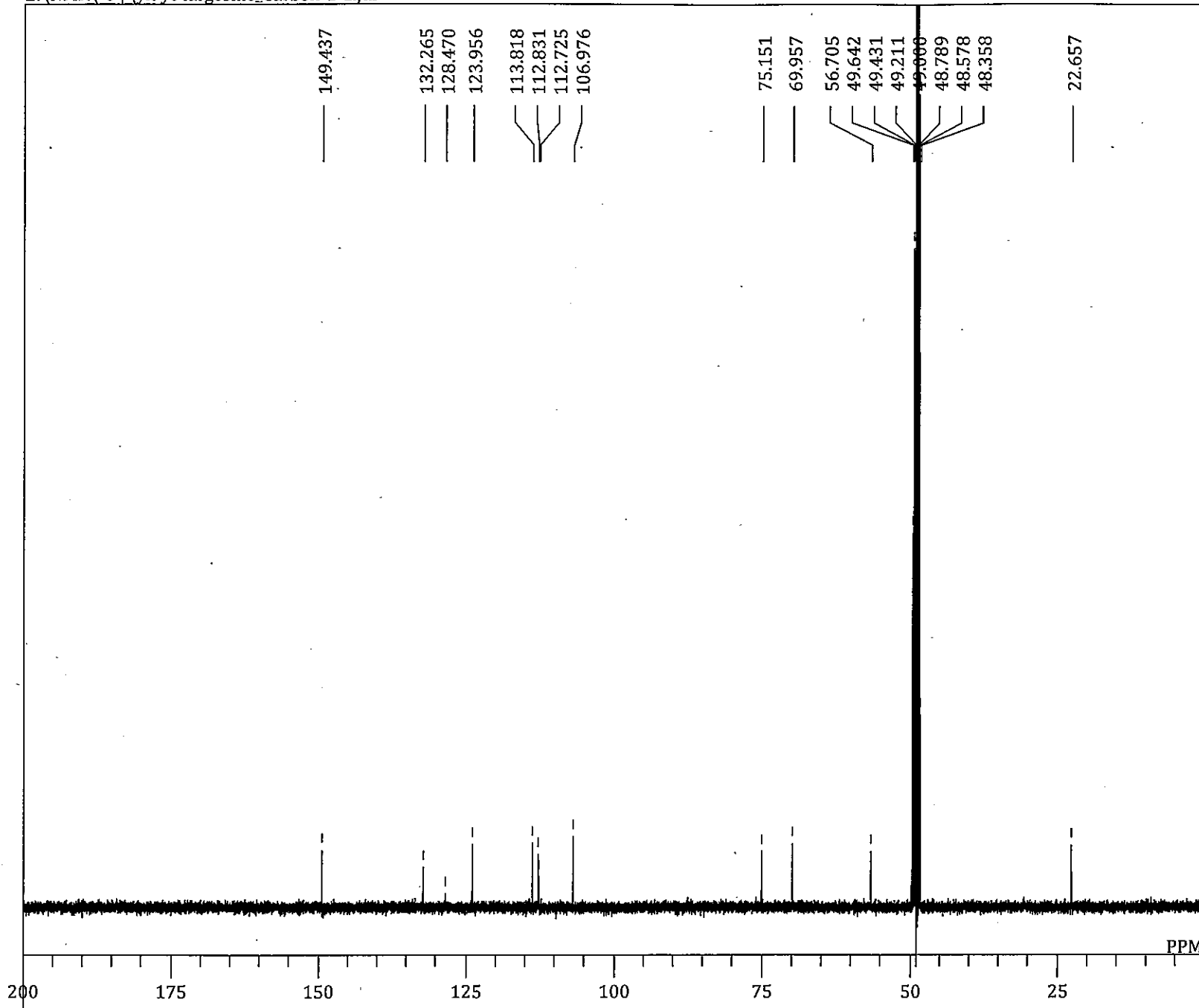


fargesine

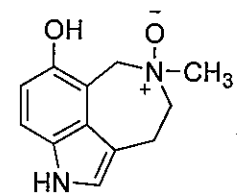
in CD₃OD

fargesine

E:\NMR\c+\yk-yt-fargesine_Carbon-1-1.jdf



DFILE yk-yt-fargesine_Carbon-1-1.jdf
COMNT fargesine
DATIM 2016-05-31 18:12:28
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 890
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CD3OD
EXREF 49.00 ppm
BF 0.12 Hz
RGAIN 50



fargesine

in CD₃OD

S 21