

Electronic Supplementary Information

Synthesis of [^{18}F]pitavastatin using a Suzuki Reaction and its application in positron emission tomography imaging

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f) Sugiyama Laboratory, RIKEN Innovation Center, RIKEN Research Cluster for Innovation, RIKEN, 1-7-22 Suehiro-cho, Tsurumi-ku, Yokohama, Kanagawa, 230-0045, Japan

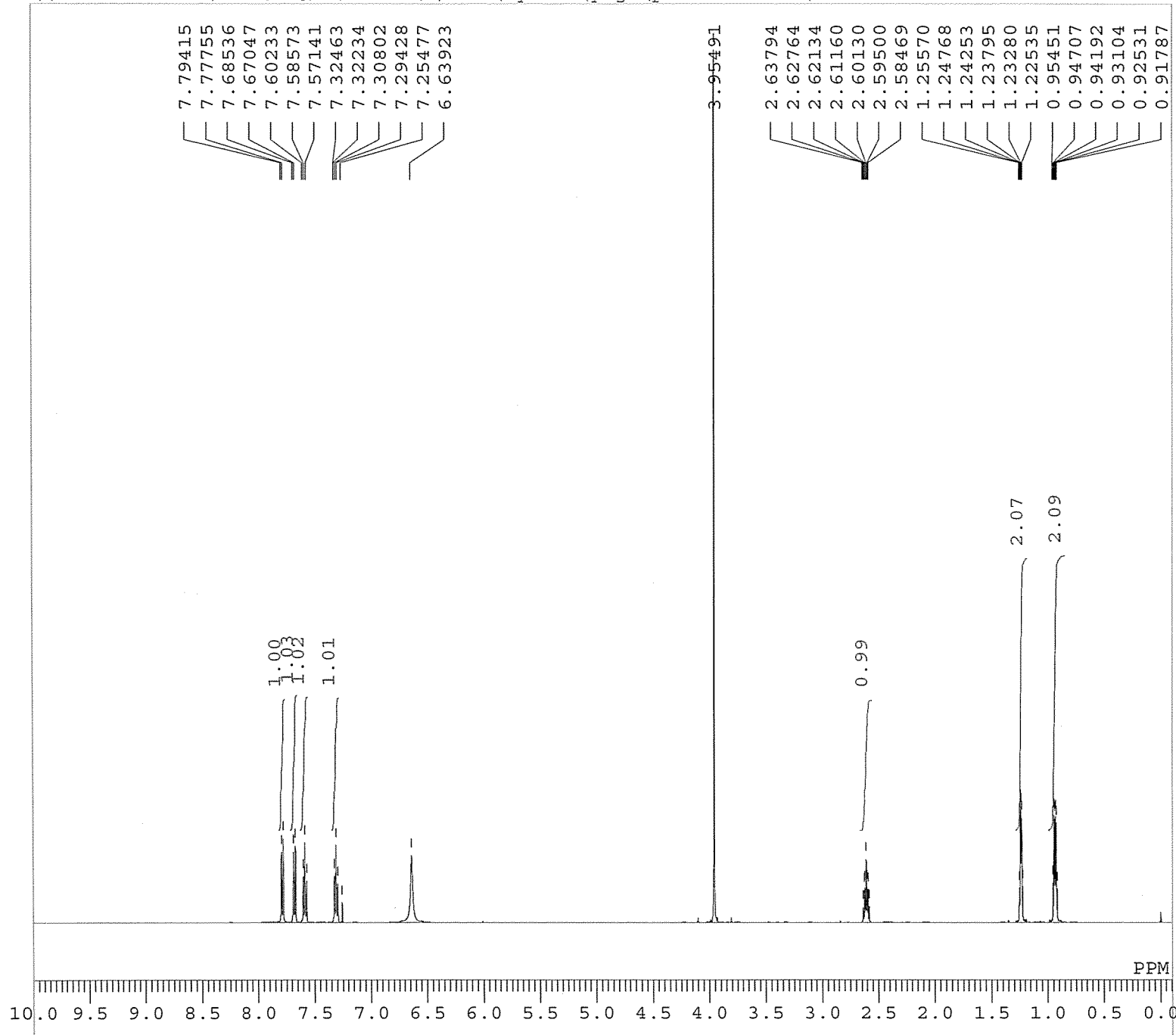
Content

1. ^1H , and ^{13}C NMR spectra

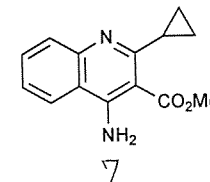
S2

Compound 7

\\10.242.96.55\< 冪-Lff[] [f^ (nmr400) \data\byotai\yagi\pitavastatin\Pitavastatin-NH2-CO2Me-1.als

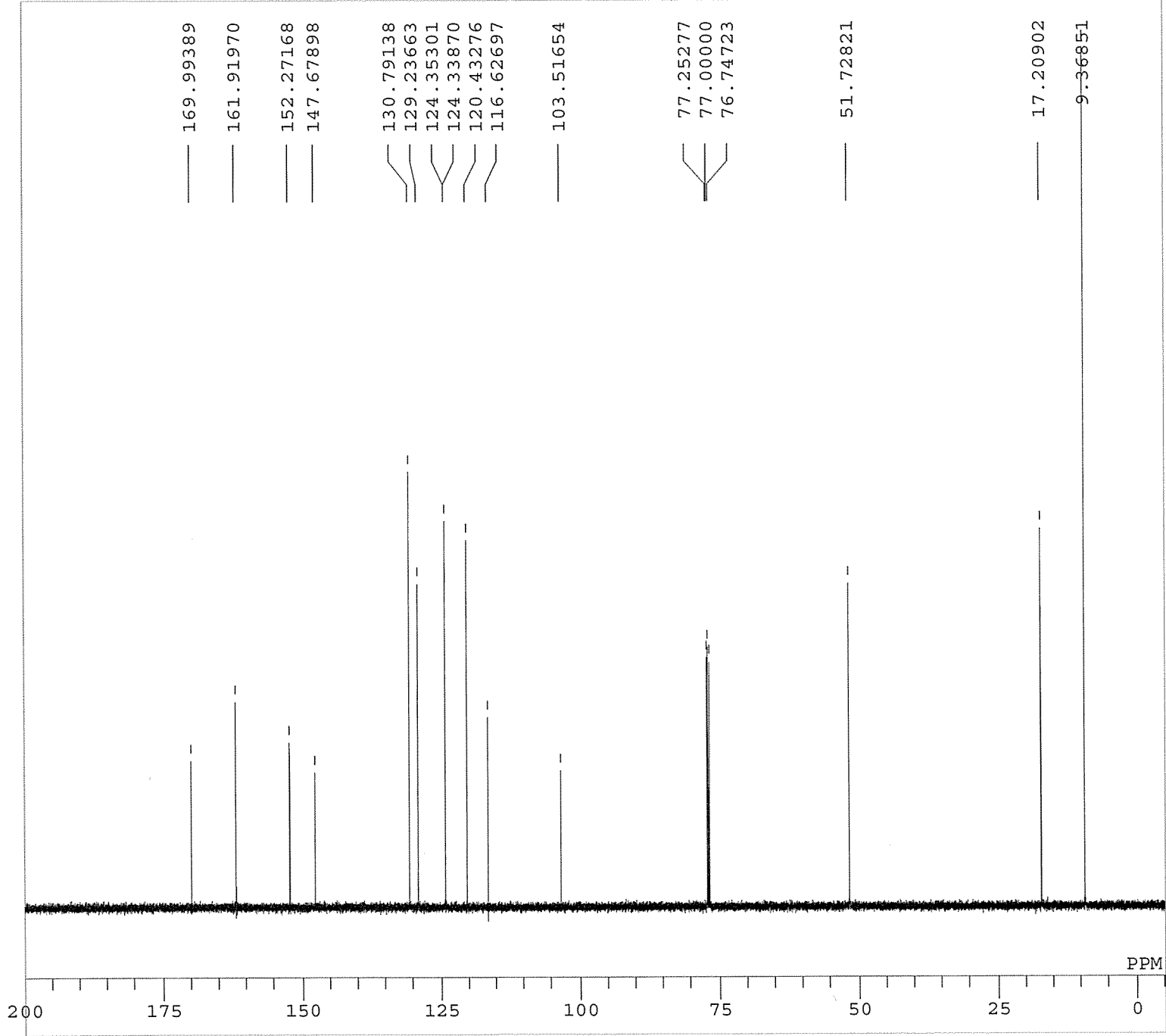


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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 402.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 34

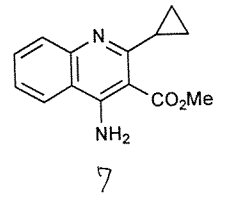


Compound 7

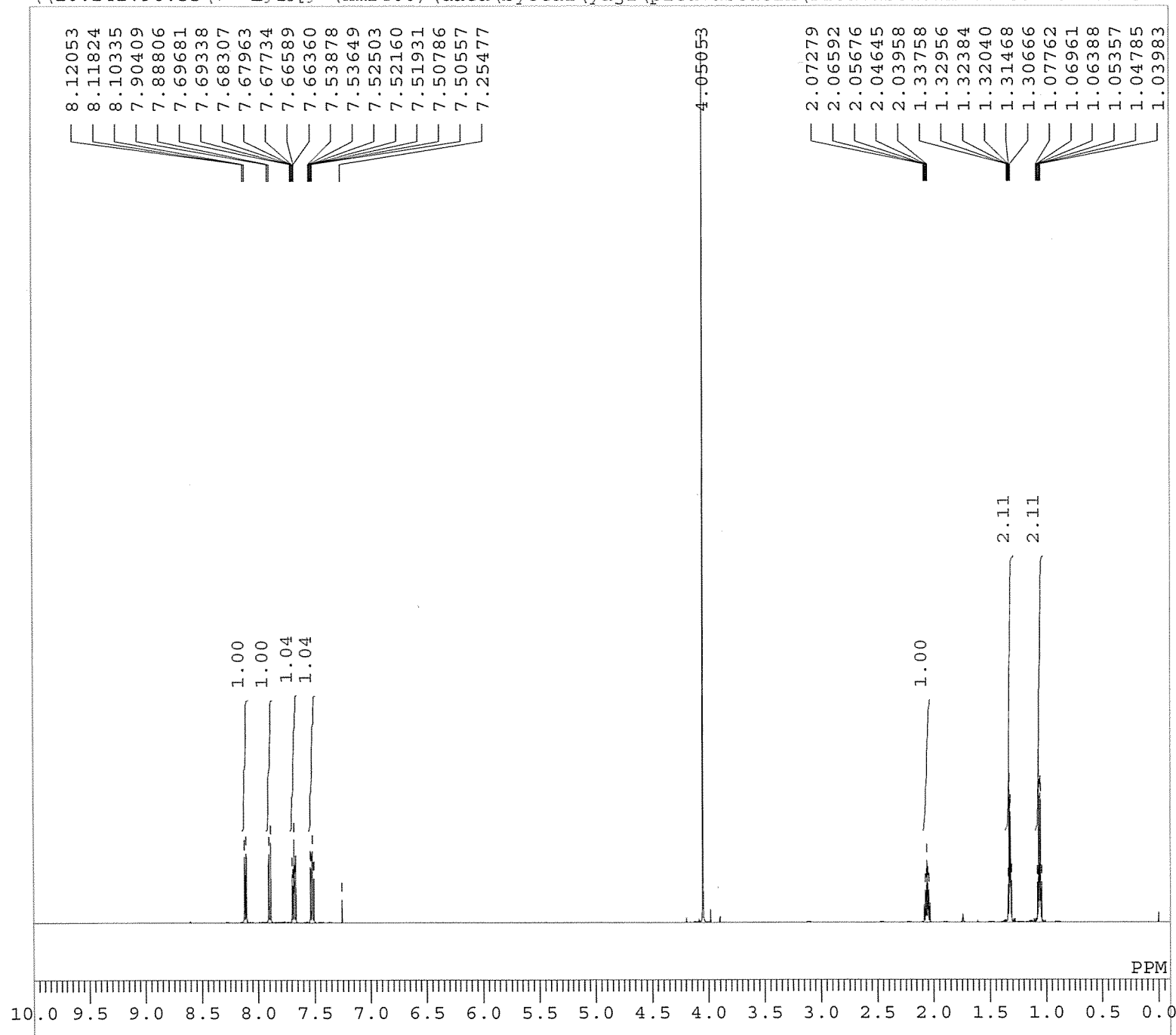
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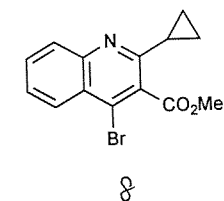
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OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 52428
FREQU 31446.06 Hz
SCANS 153
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.73 usec
IRNUC 1H
CTEMP 402.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 54



\\10.242.96.55\<µ-Lff[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-Br-CO2Me-2.als

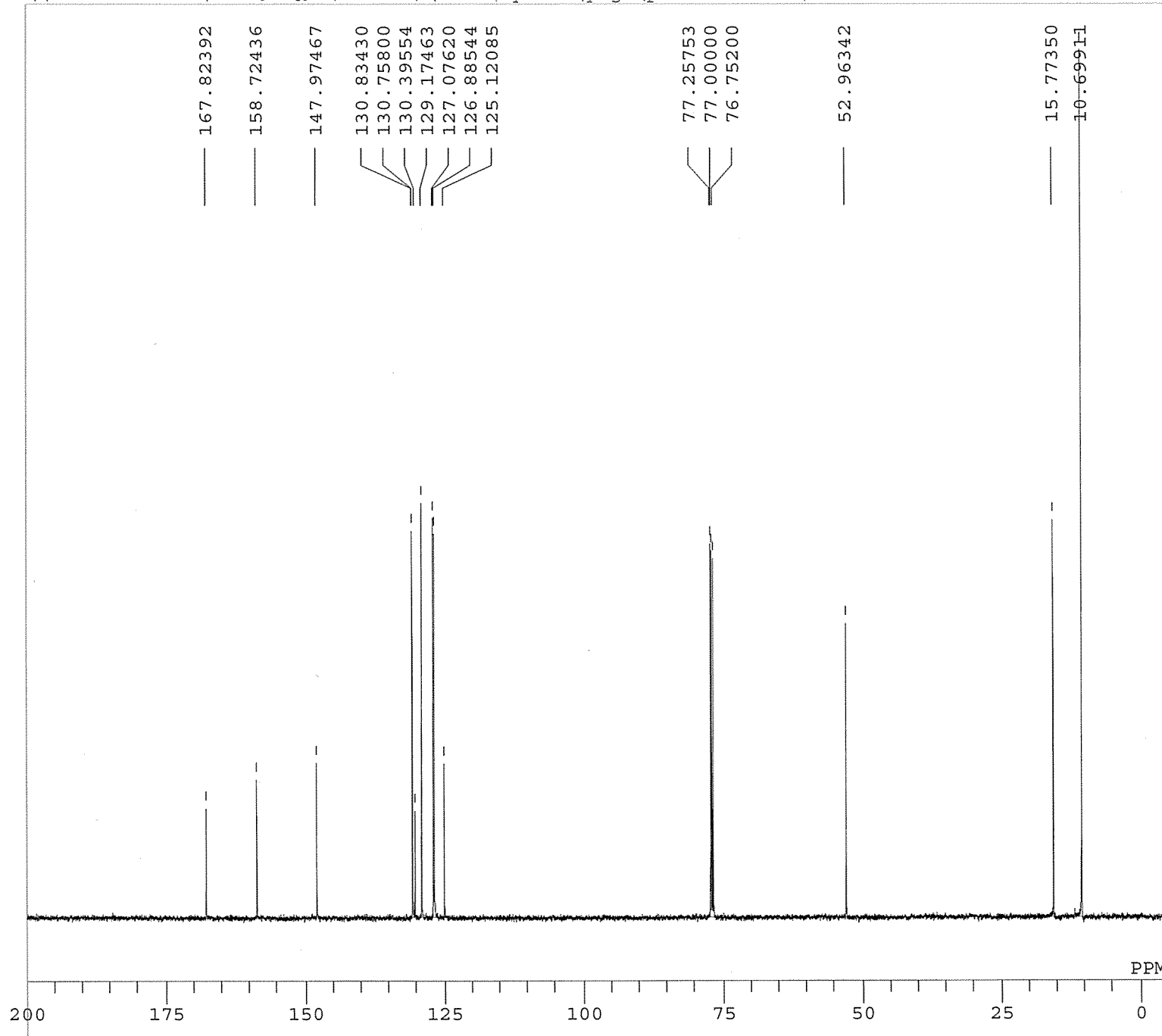


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 EXMOD single_pulse.ex2
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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 16
 ACQTM 1.7459 sec
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 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 34

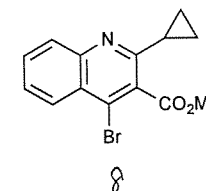


Compound 8

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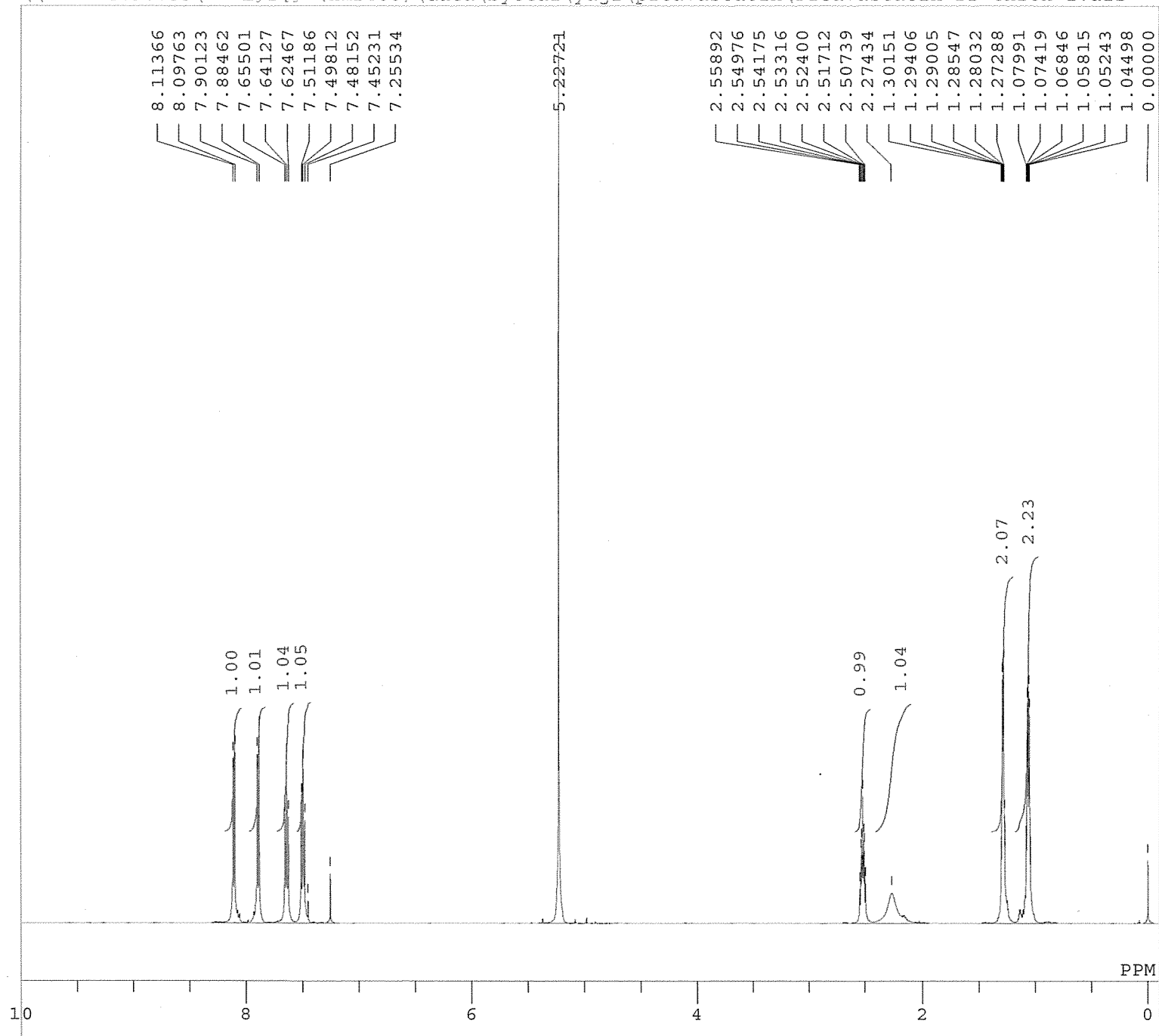


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 POINT 32768
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 BF 0.12 Hz
 RGAIN 54

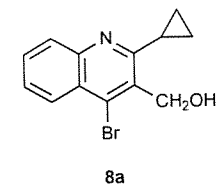


Compound 8a

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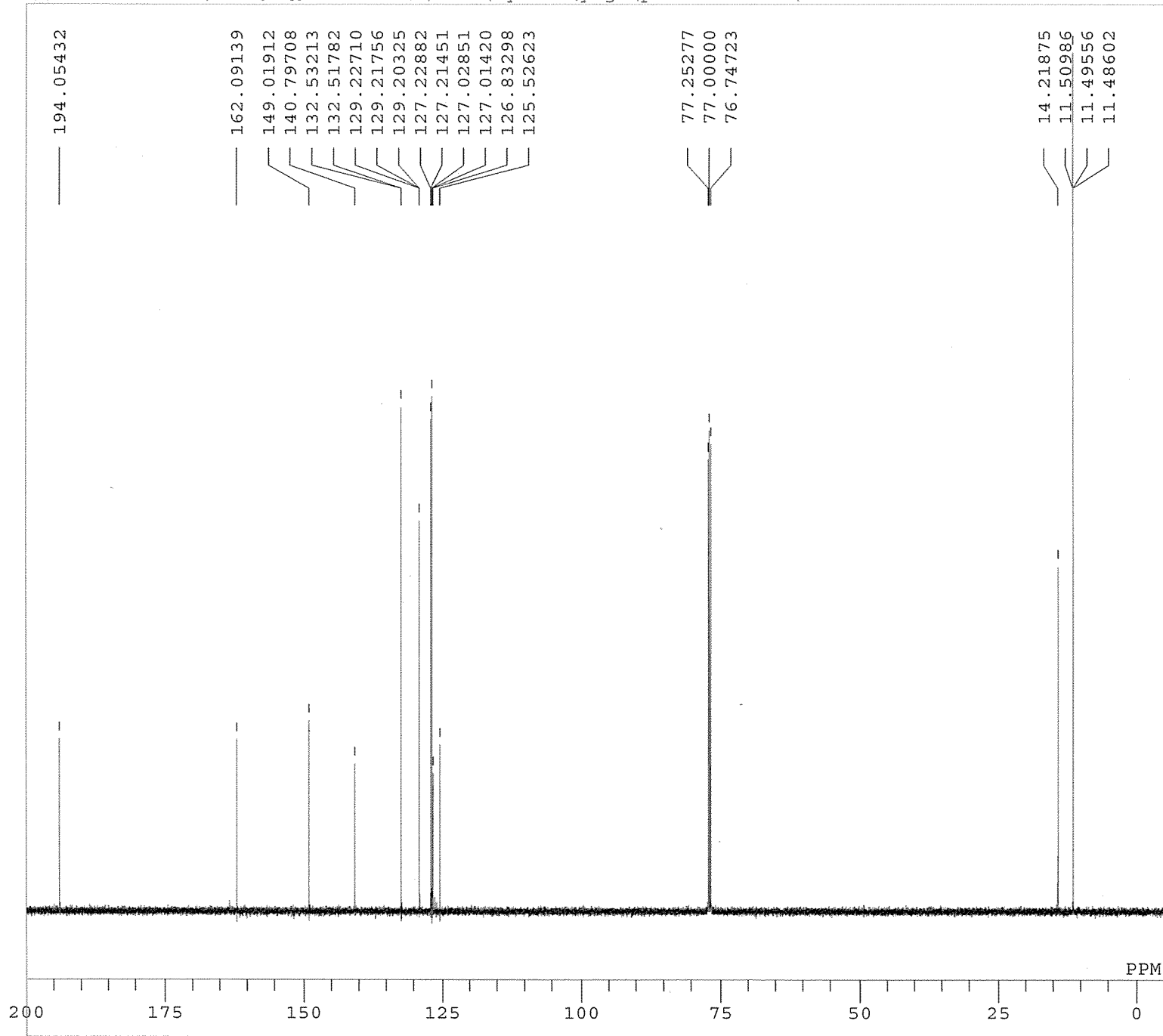


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 OBSET 2.41 KHz
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 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.82 usec
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 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 40

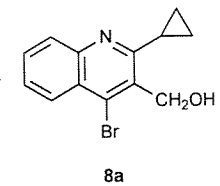


Compound 8a

\\10.242.96.55\< 卣-Lff[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-Br-CHO-C13-1.als

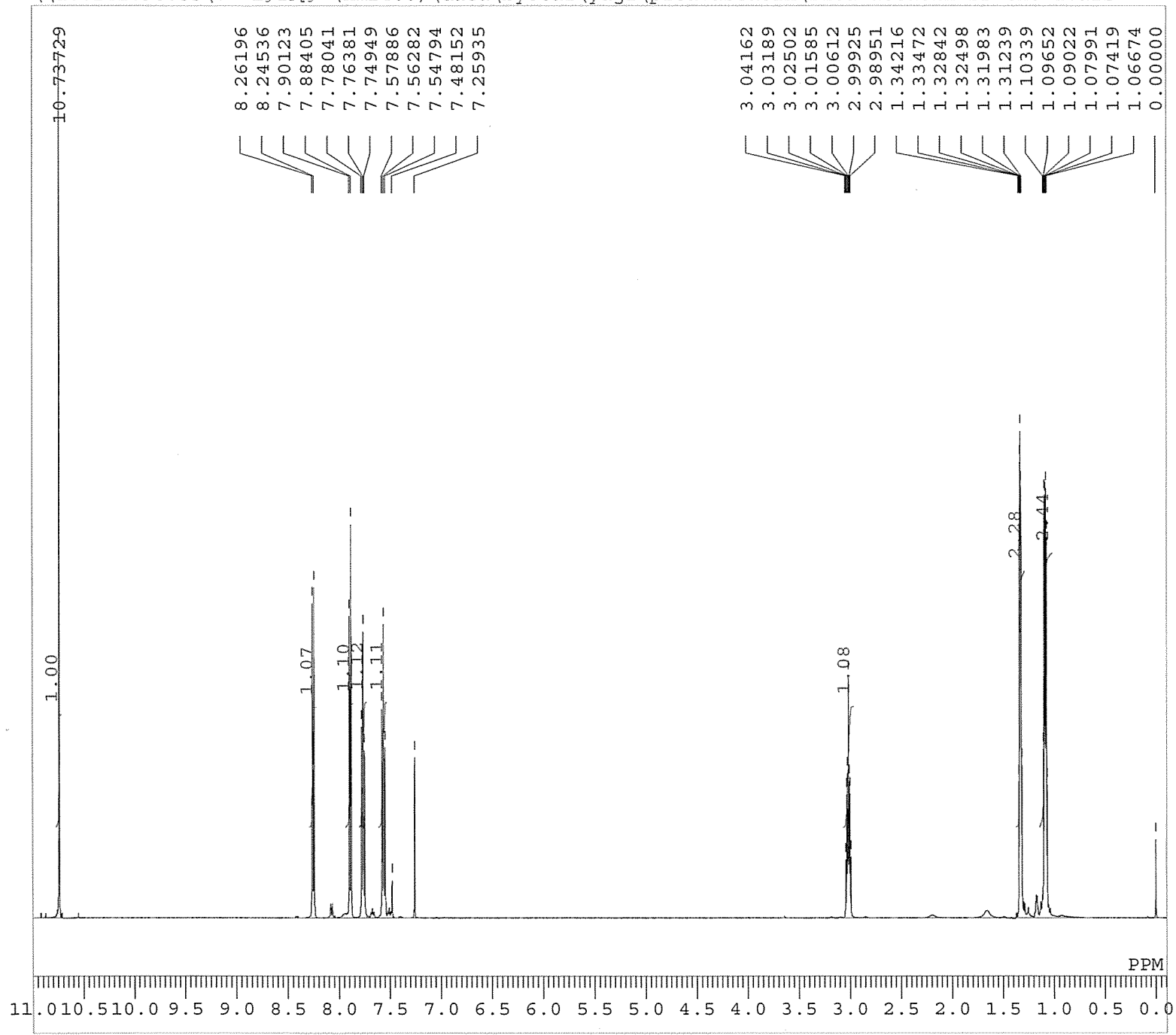


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EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 52428
FREQU 31446.06 Hz
SCANS 640
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.73 usec
IRNUC 1H
CTEMP 25.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 54

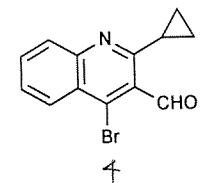


Compound 4

\\10.242.96.55\< 卐-Lffll[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-Br-CHO-1.als

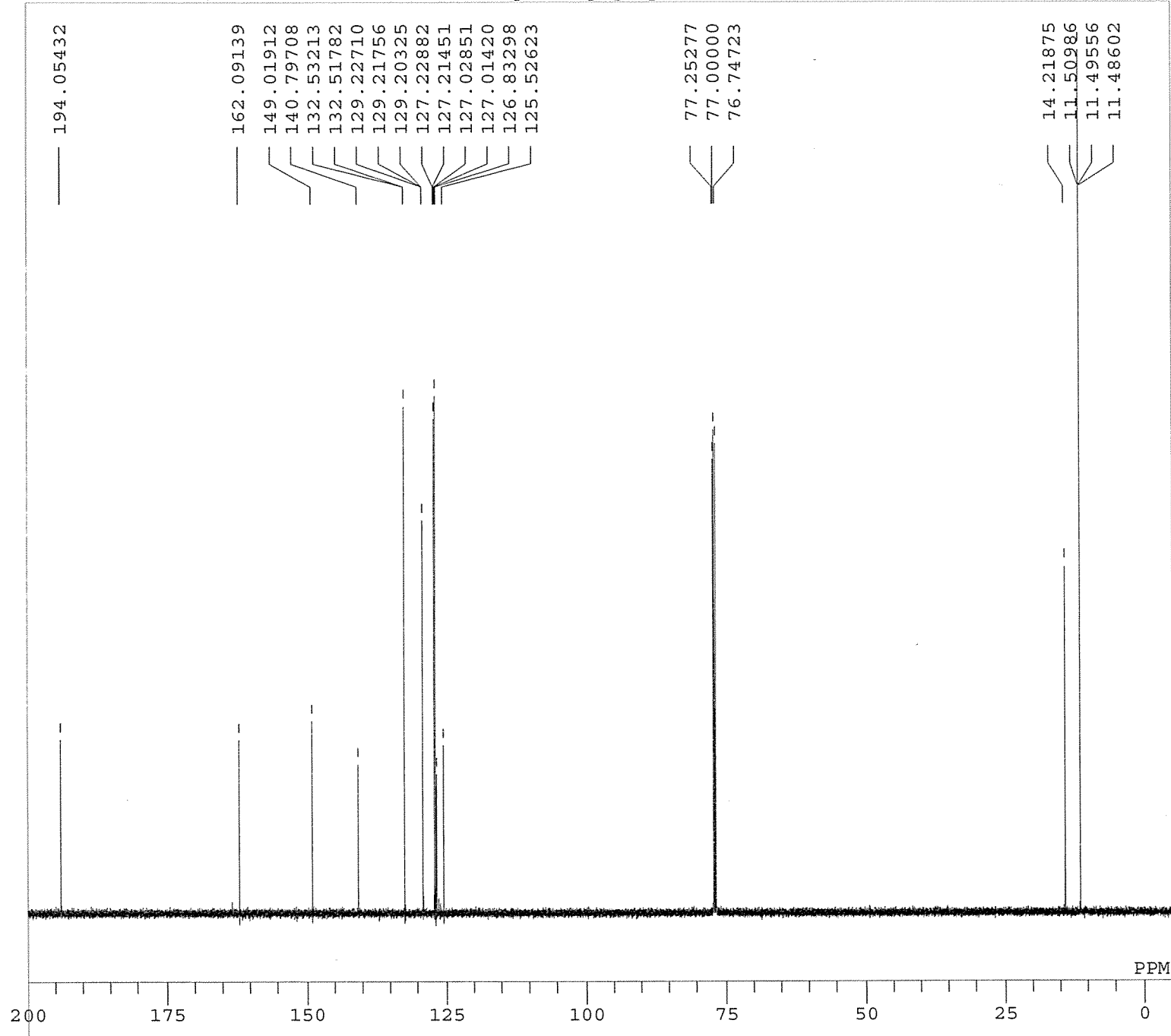


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 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 25.6 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 40

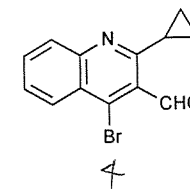


Compound 4

\\10.242.96.55\< n-Lffl[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-Br-CHO-C13-1.als

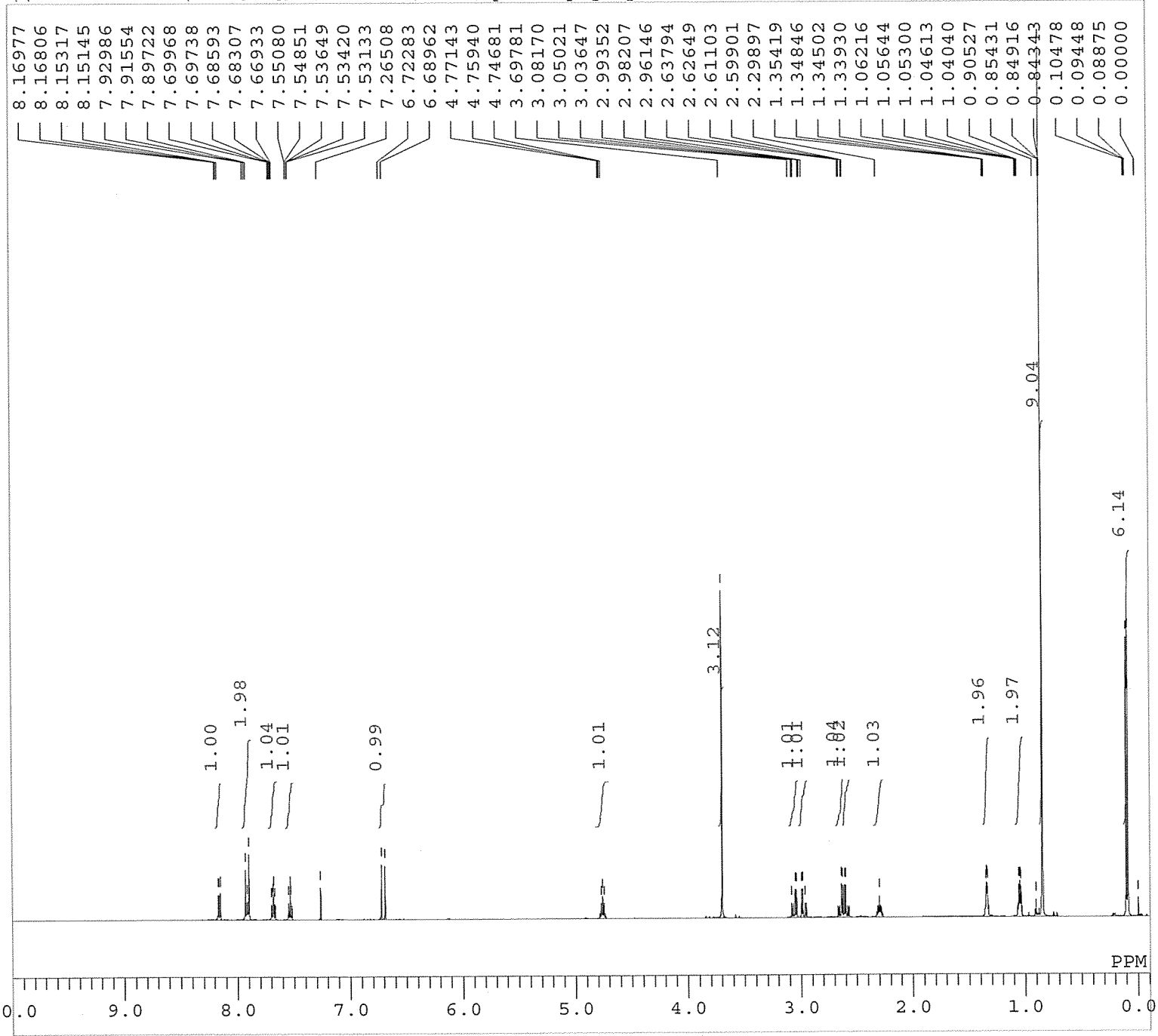


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 OBNUC 13C
 EXMOD single_pulse_dec
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 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 52428
 FREQU 31446.06 Hz
 SCANS 640
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.73 usec
 IRNUC 1H
 CTEMP 25.8 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 54

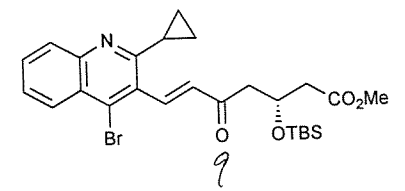


Compound 9

\\10.242.96.55\<µ-Lffl[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-C=O-OTBS-1.als

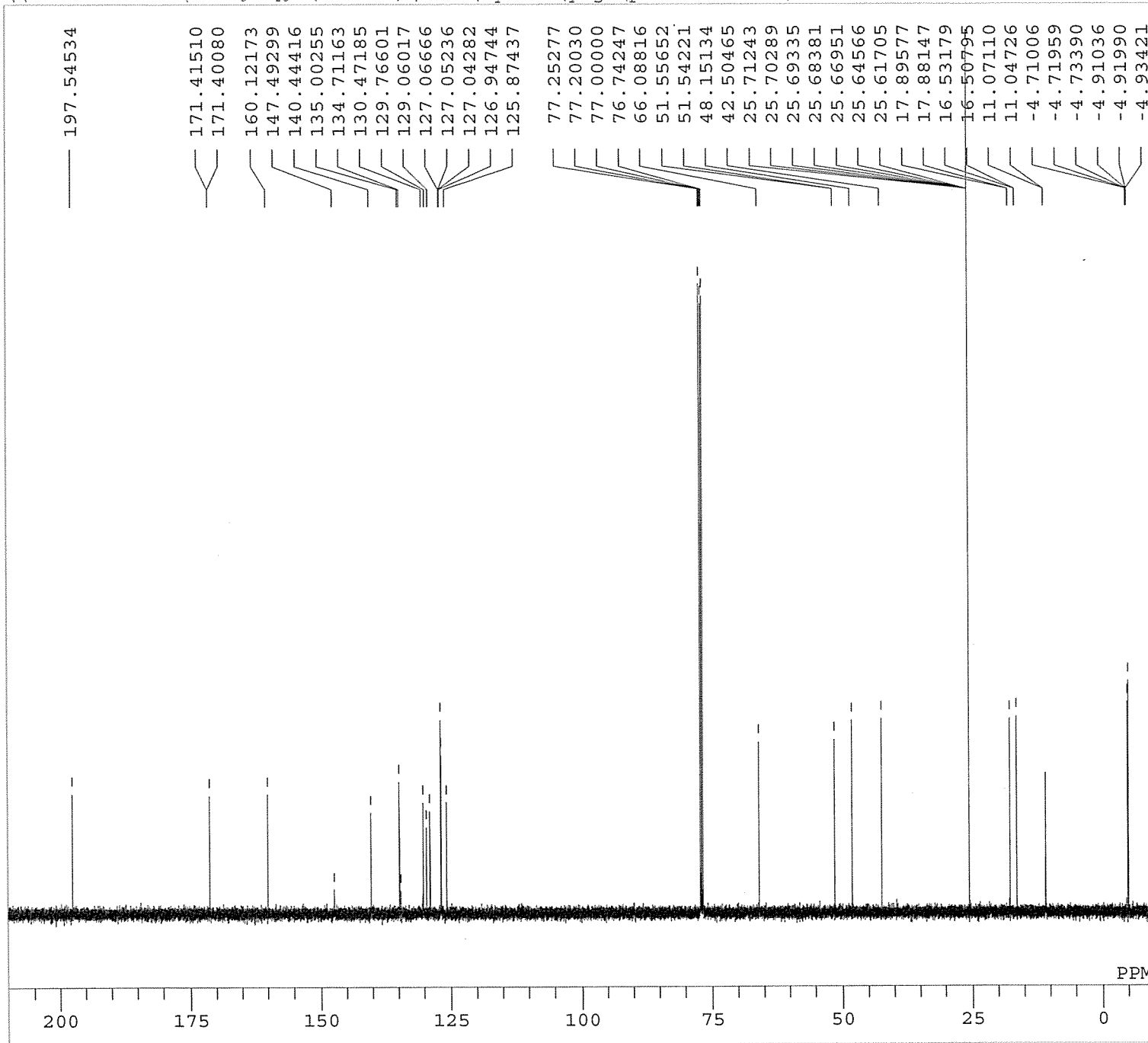


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 EXMOD single_pulse.ex2
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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 25.0 c
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 BF 0.12 Hz
 RGAIN 36

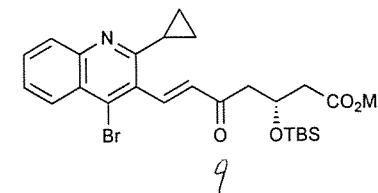


Compound 9

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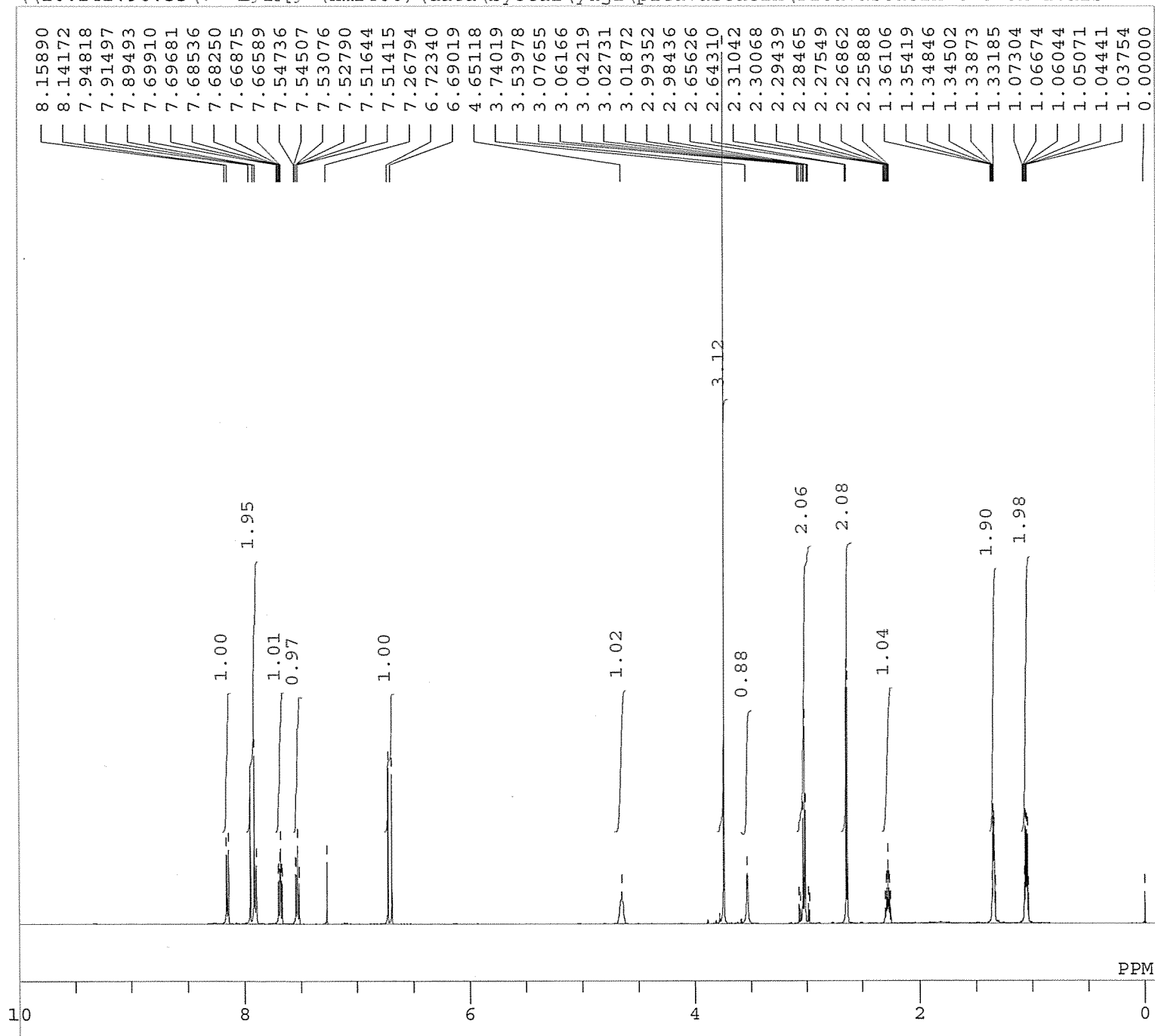


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 EXMOD single_pulse_dec
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 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 52428
 FREQU 31446.06 Hz
 SCANS 261
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.73 usec
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 BF 0.12 Hz
 RGAIN 54

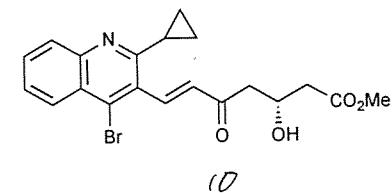


Compound 10

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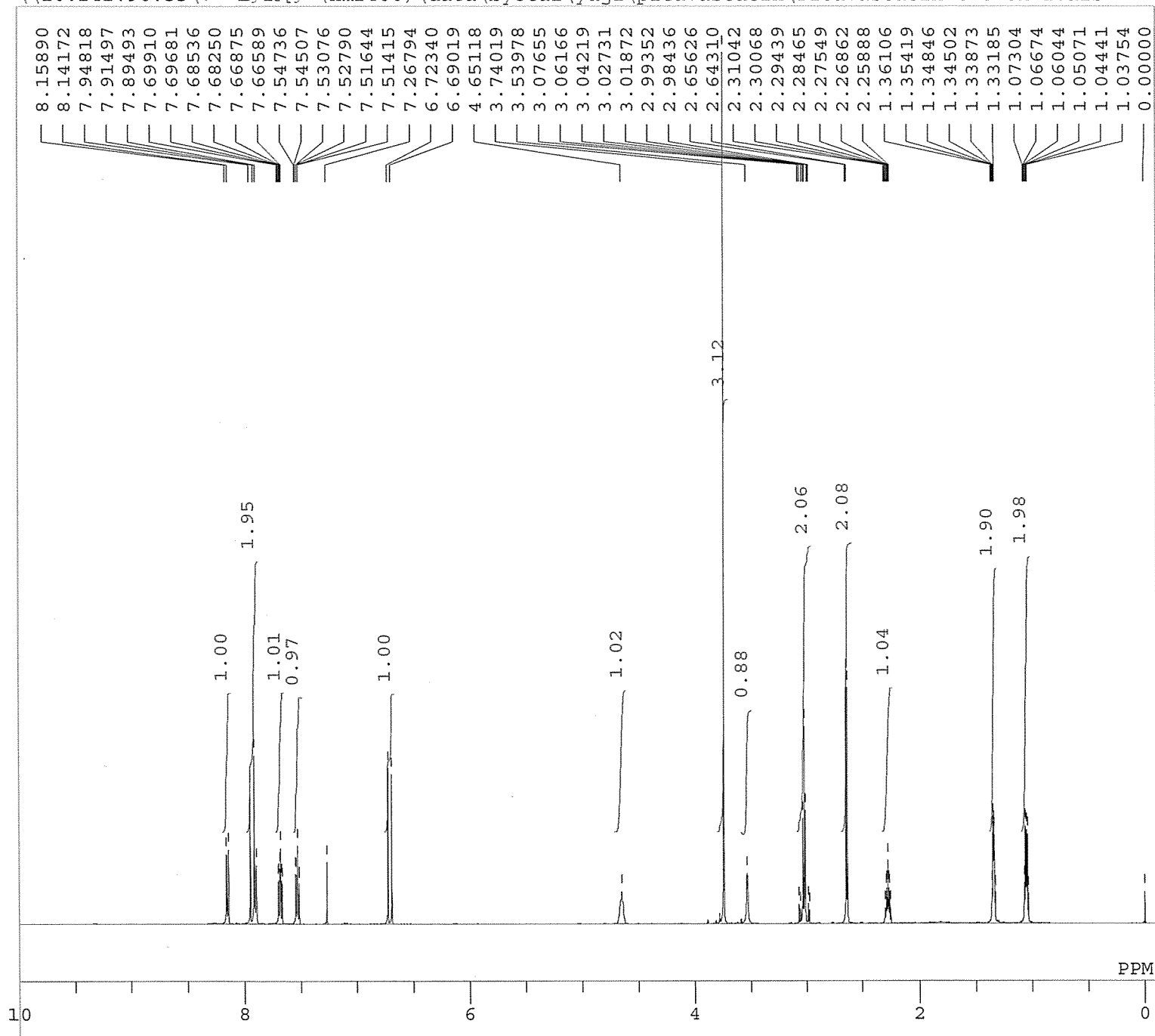


DFILE Pitavastatin-C=O-OH-1.als
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 EXMOD single_pulse.ex2
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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 24.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 40

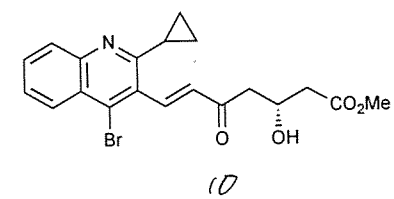


Compound 10

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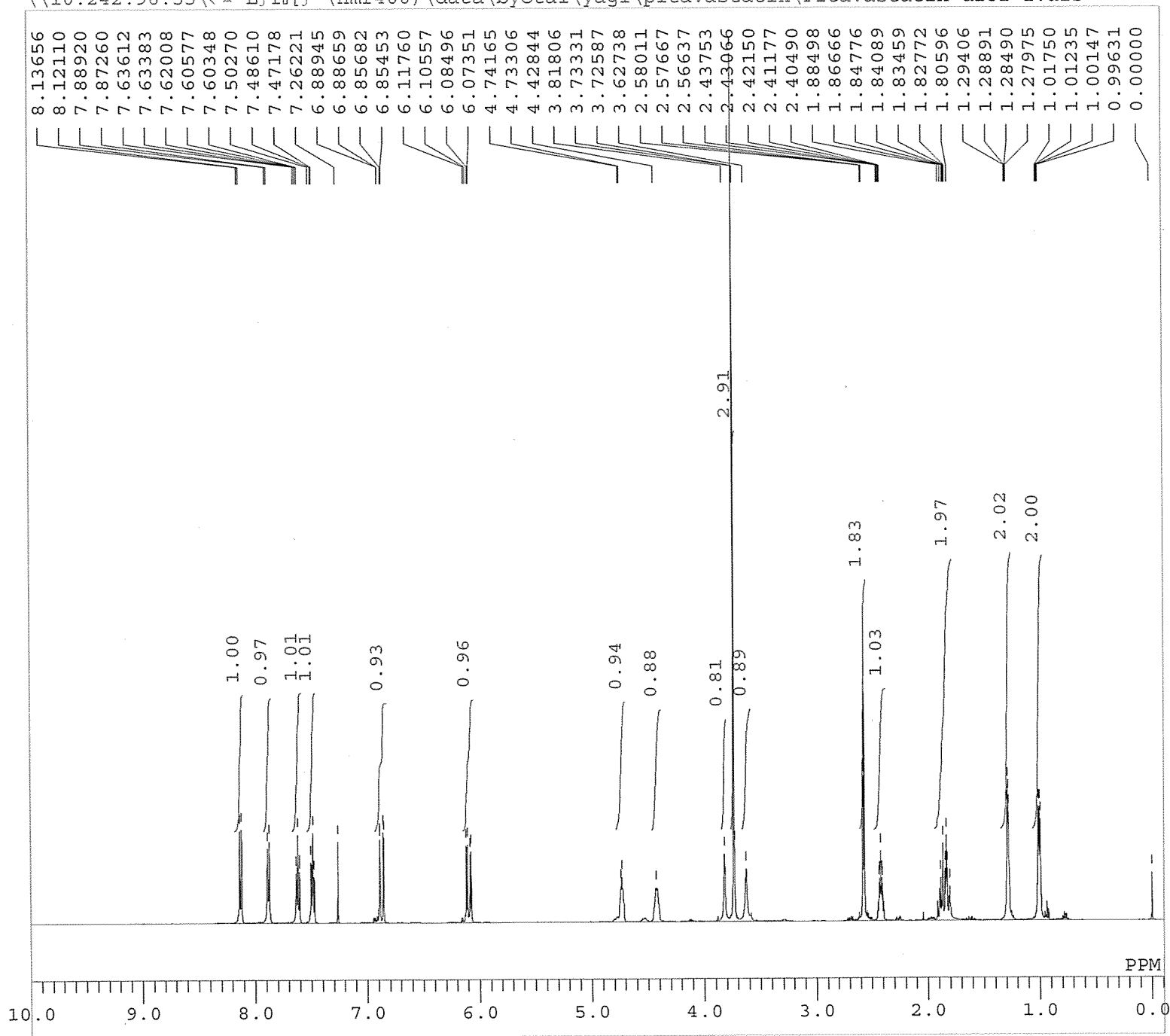


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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 24.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 40



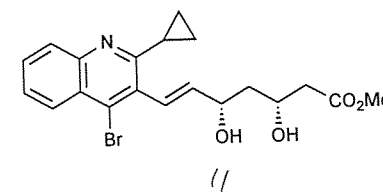
Compound 11

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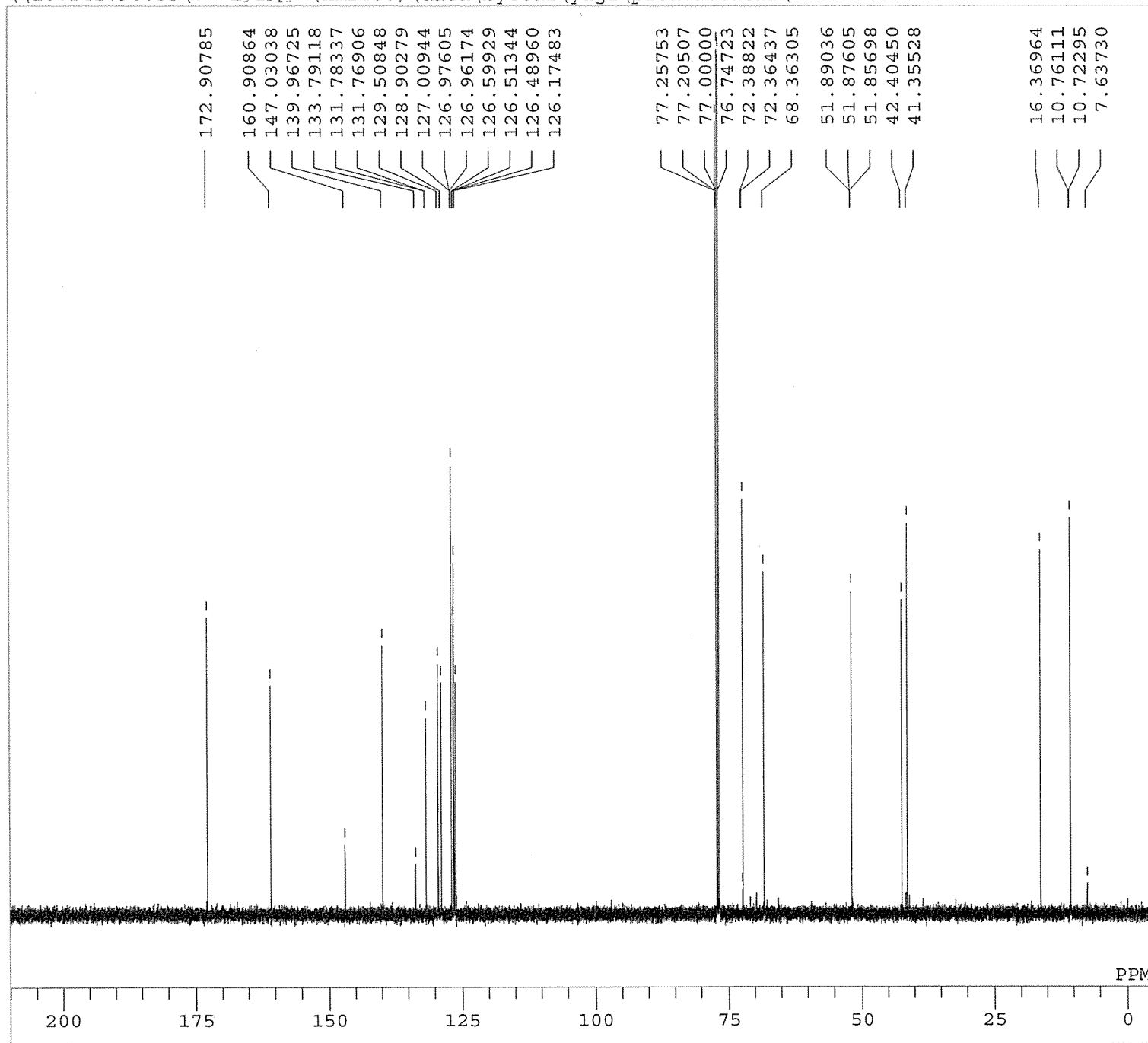
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.39 Hz
SCANS 16
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 6.50 usec
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CTEMP 25.4 c
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BF 0.12 Hz
RGAIN 38
    
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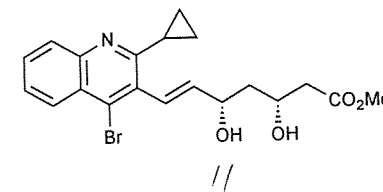


Compound 11

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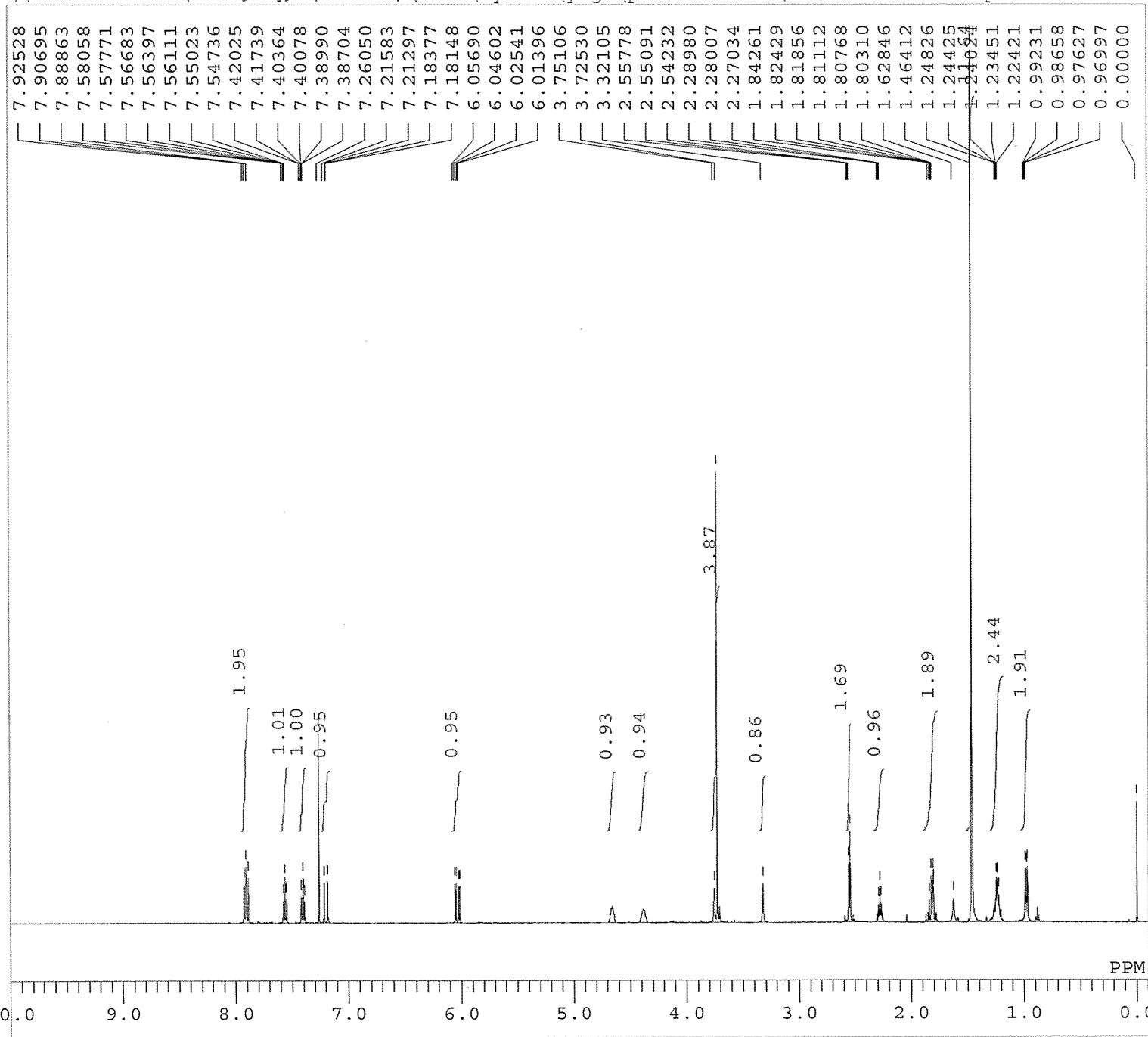


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 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 52428
 FREQU 31446.06 Hz
 SCANS 602
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.73 usec
 IRNUC 1H
 CTEMP 25.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 54

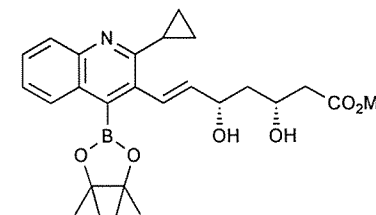


Compound 2

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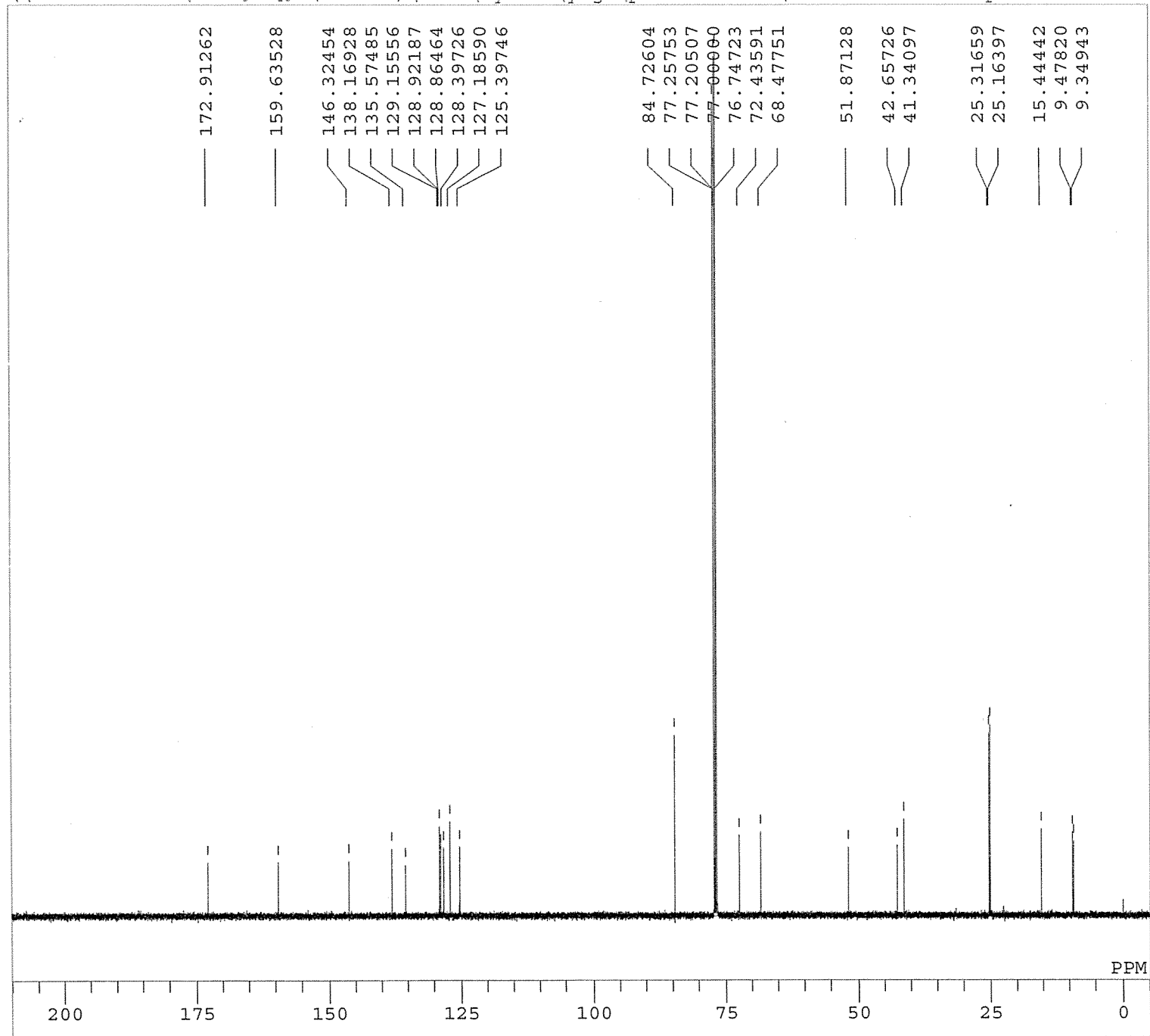


DFILE Pitavastatin-Comp24-1.als
 COMNT single_pulse
 DATIM 2013-04-23 14:13:44
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 401.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 44

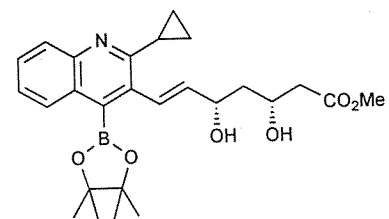


Compound 2

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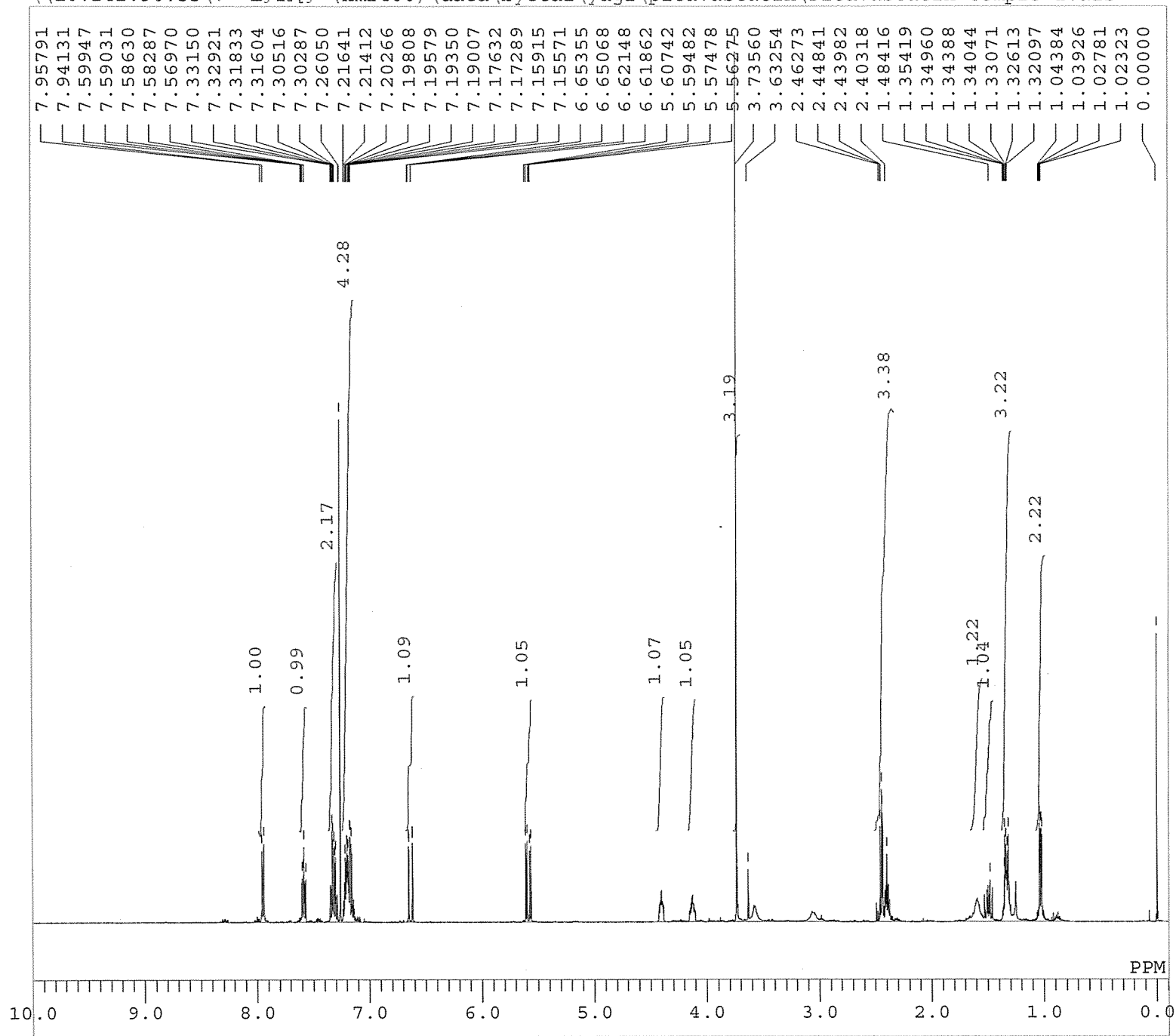


DFILE Pitavastatin-Comp24-C13-1
 COMNT single pulse decoupled ga
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 EXMOD single_pulse_dec
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 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 52428
 FREQU 31446.06 Hz
 SCANS 2853
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.73 usec
 IRNUC 1H
 CTEMP 402.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 54

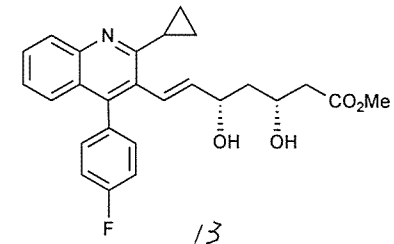


2

\\10.242.96.55\<µ-Lffl[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-Comp25-1.als

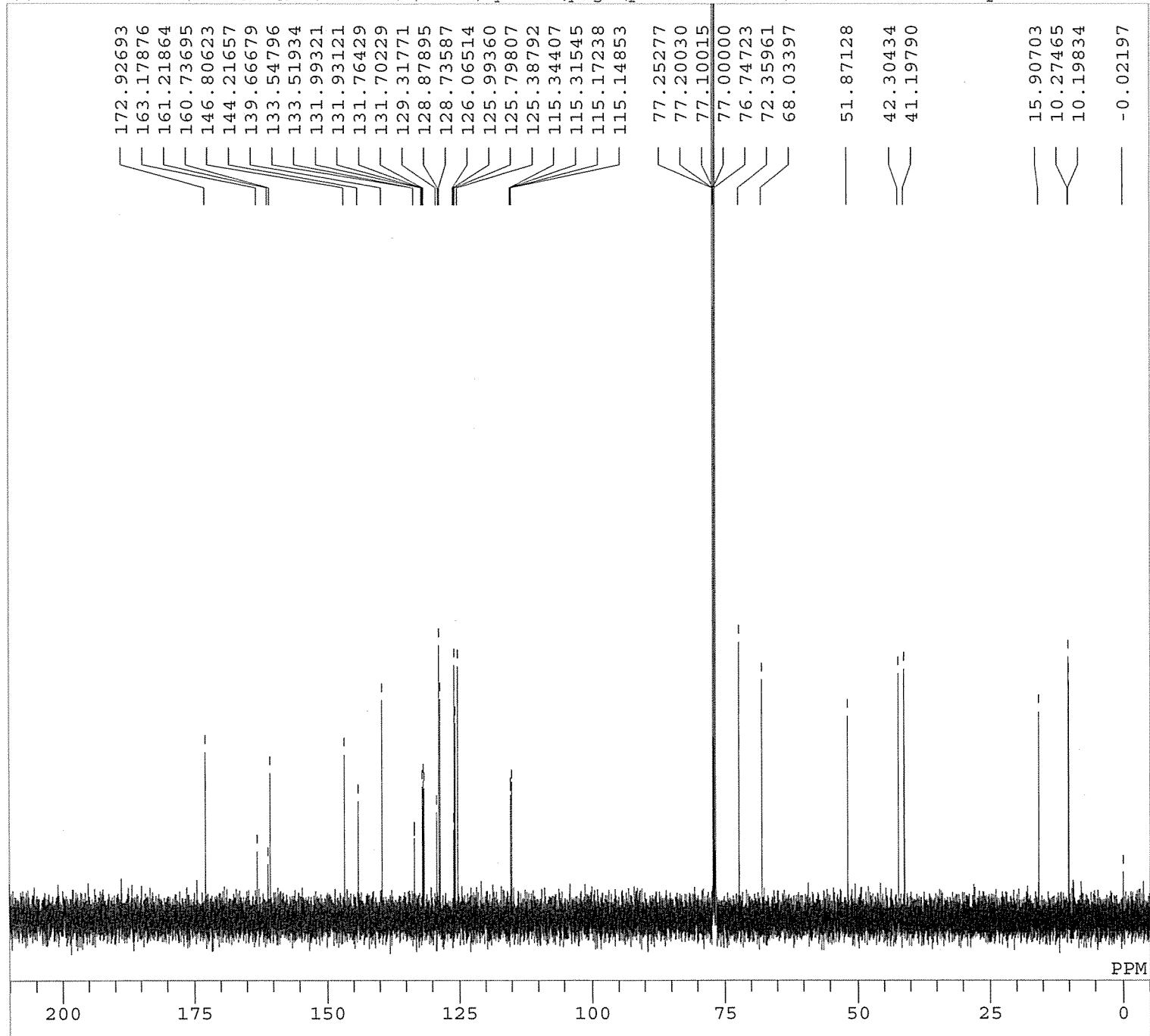


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 DATIM 2013-04-05 21:45:12
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 25.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 48

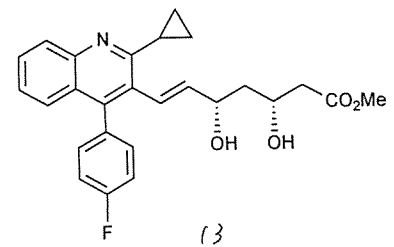


Compound 13

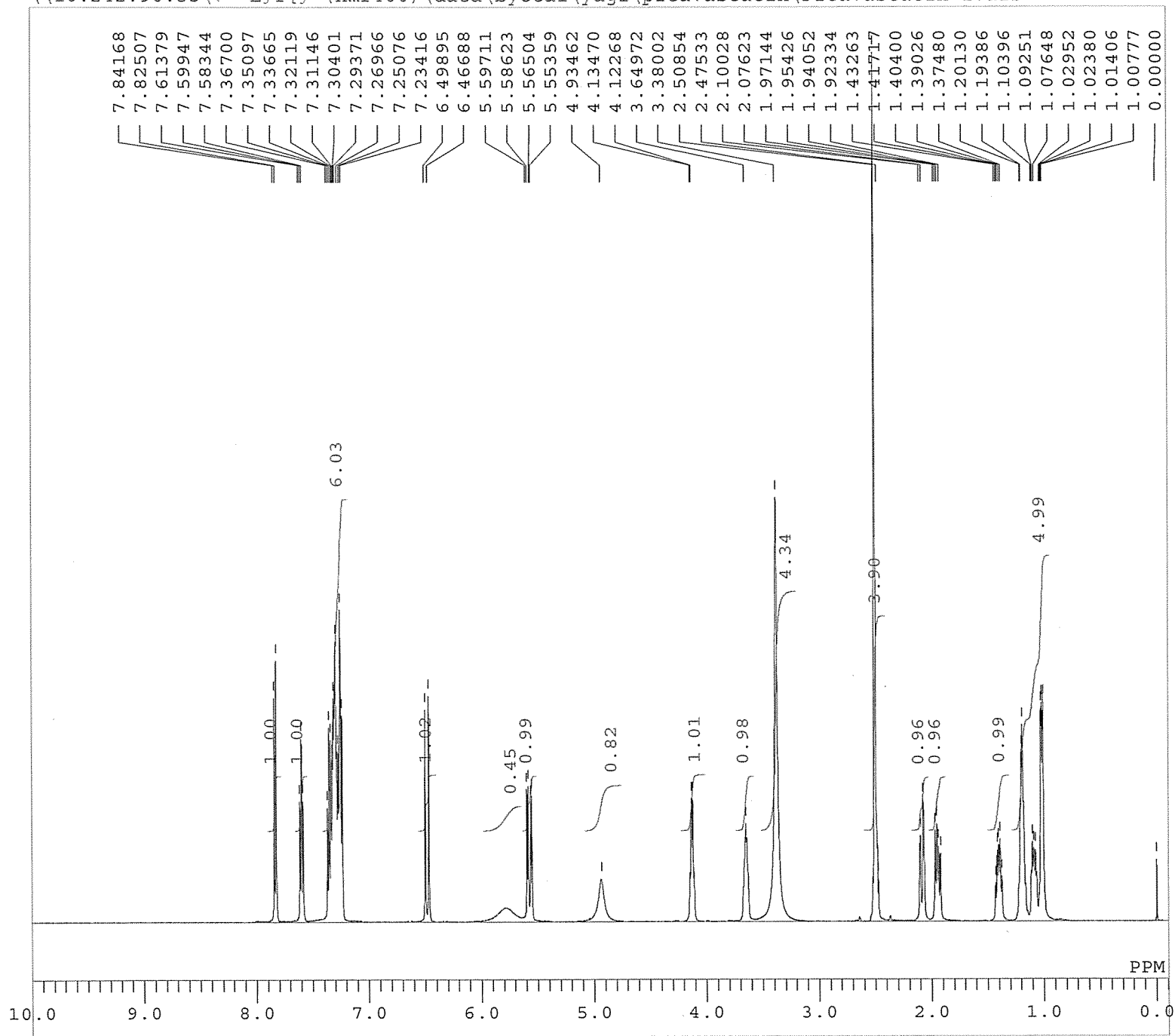
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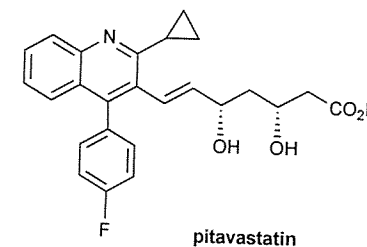
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 DATIM 2013-04-05 22:34:02
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 52428
 FREQU 31446.06 Hz
 SCANS 1000
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.73 usec
 IRNUC 1H
 CTEMP 25.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 56



\\10.242.96.55\< 日-Lff[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-1.als

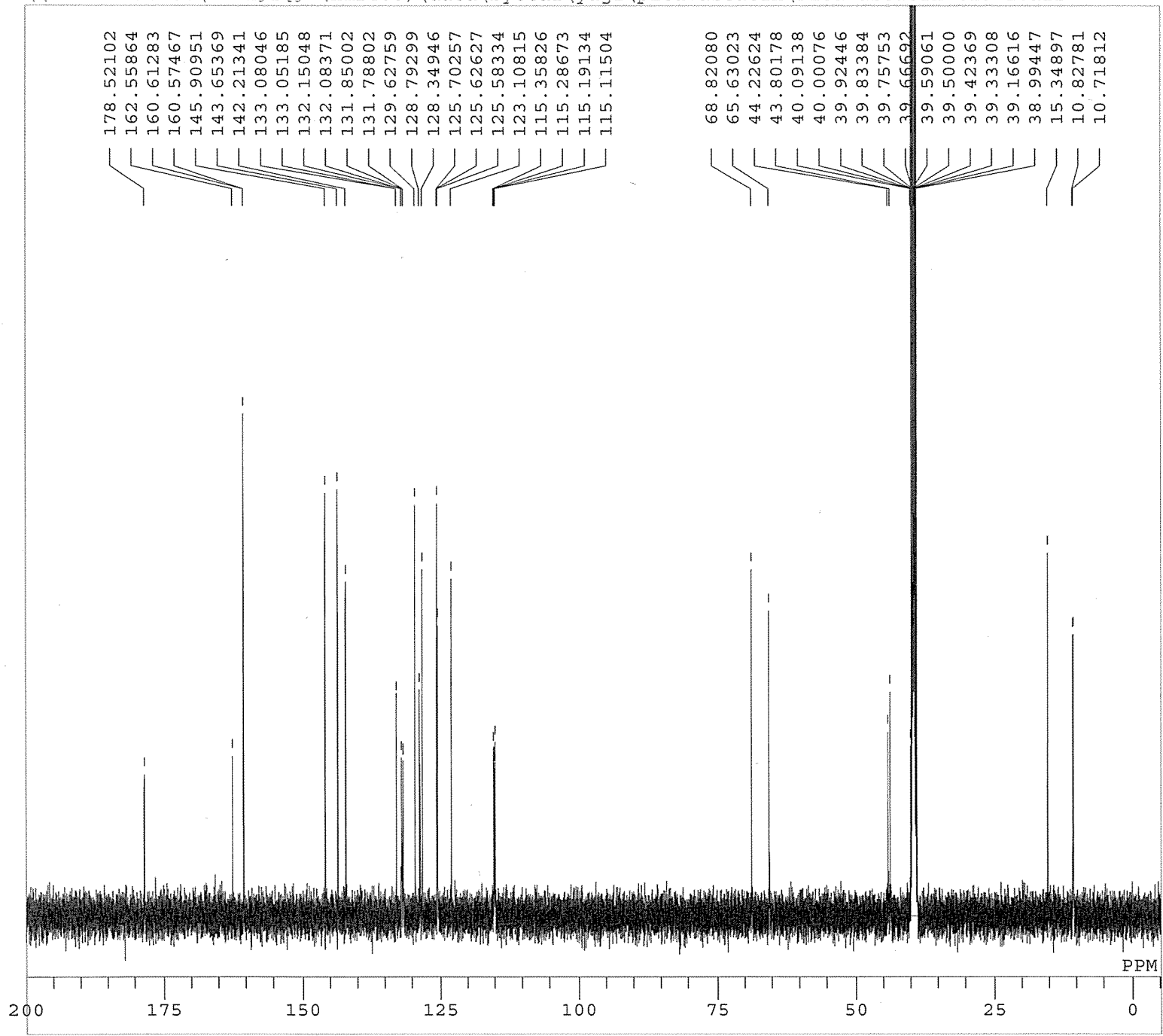


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 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.39 Hz
 SCANS 16
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 20.6 c
 SLVNT DMSO
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 40



pitavastatin

\\10.242.96.55\< ¼-Lff[f^(nmr400)\data\byotai\yagi\pitavastatin\Pitavastatin-C13-1.als



DFILE Pitavastatin-C13-1.als
 COMNT single pulse decoupled ga
 DATIM 2014-03-04 18:39:39
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 52428
 FREQU 31446.06 Hz
 SCANS 1819
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.73 usec
 IRNUC 1H
 CTEMP 21.0 c
 SLVNT DMSO
 EXREF 39.50 ppm
 BF 0.12 Hz
 RGAIN 54

