

Supporting Information

Part 2

Mo-Au Combo Catalysis for Rapid 1,3-Rearrangement of Propargyl Alcohols into α,β -Unsaturated Carbonyl Compounds

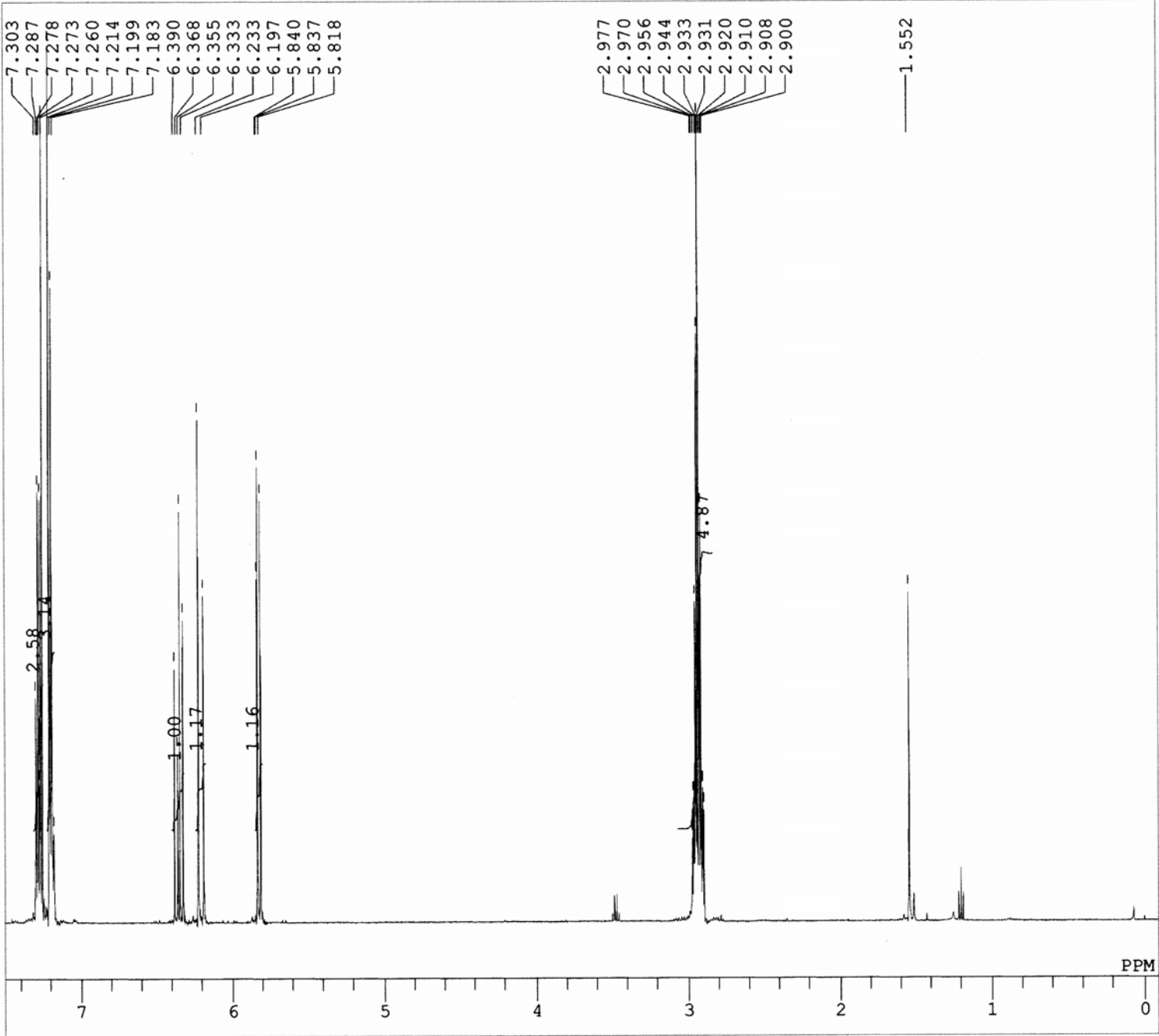
Masahiro Egi, Yoshiko Yamaguchi, Noboru Fujiwara, Shuji Akai*

School of Pharmaceutical Sciences, University of Shizuoka, 52-1, Yada, Suruga-ku, Shizuoka,
Shizuoka 422-8526, Japan

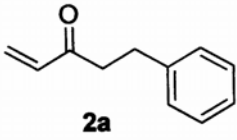
Contents

^1H and ^{13}C NMR chart for α,β -unsaturated carbonyl compounds 2a–s	S2–S47
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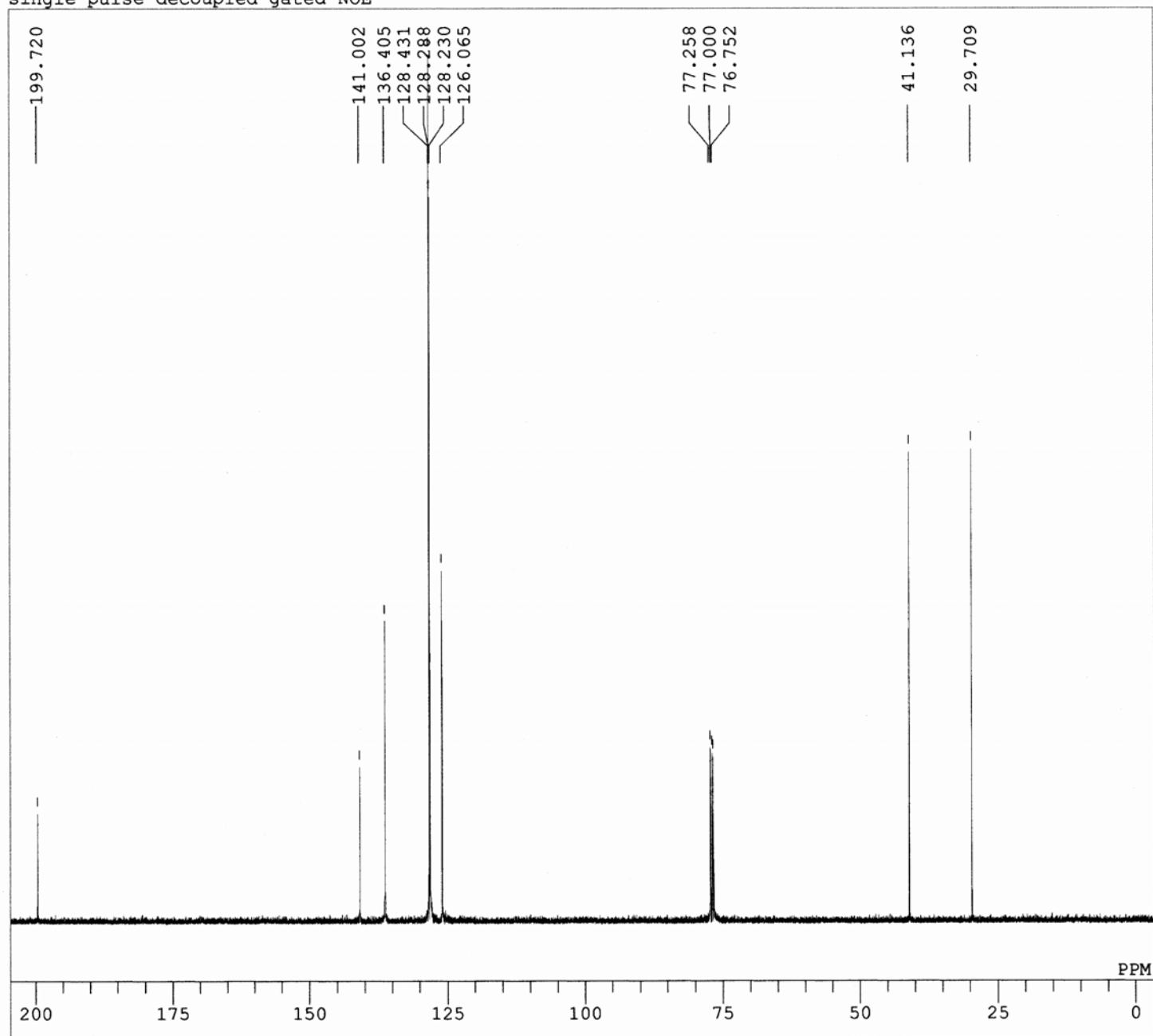
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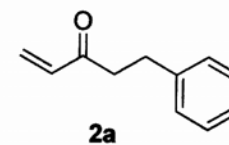
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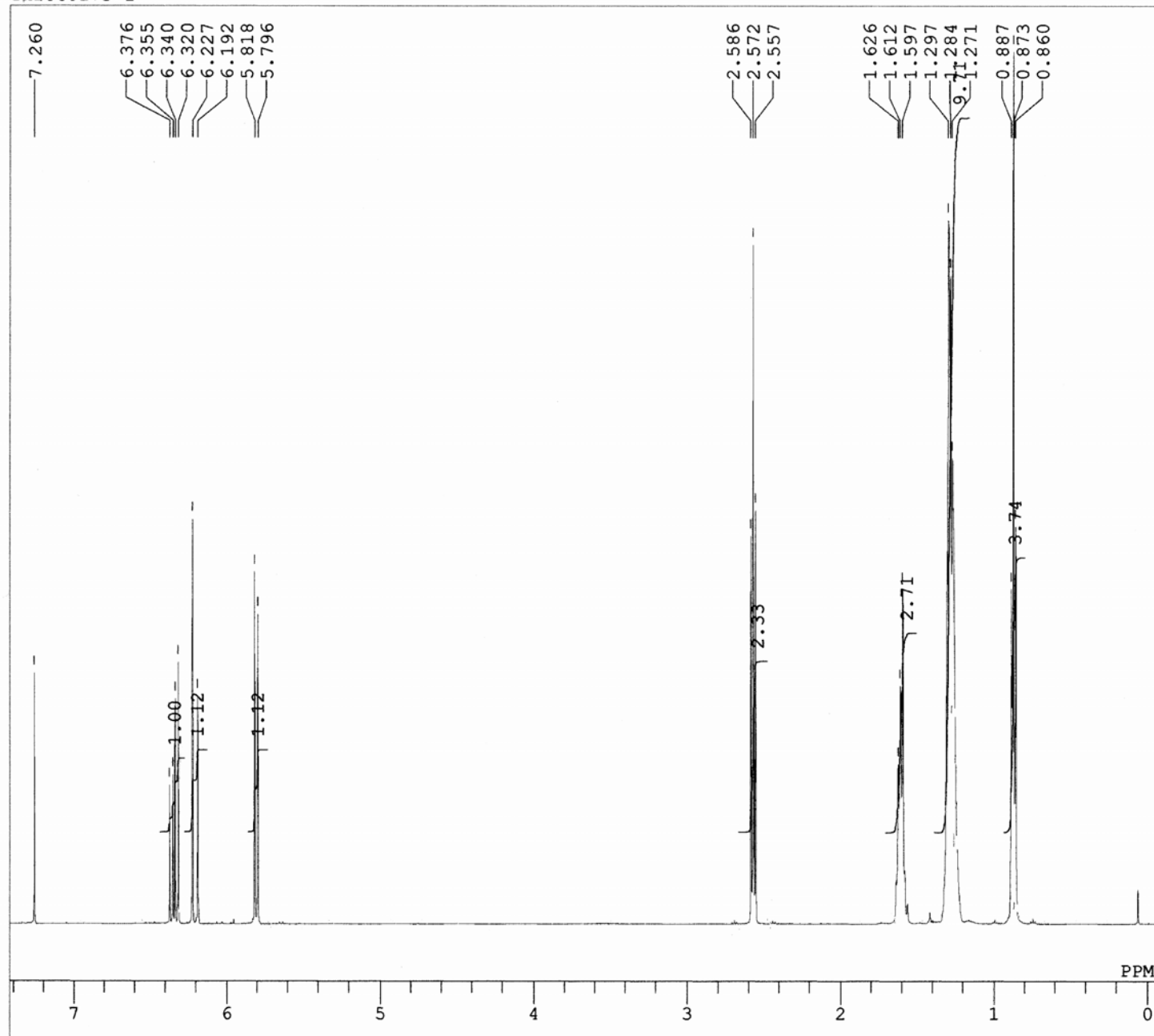
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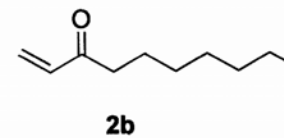
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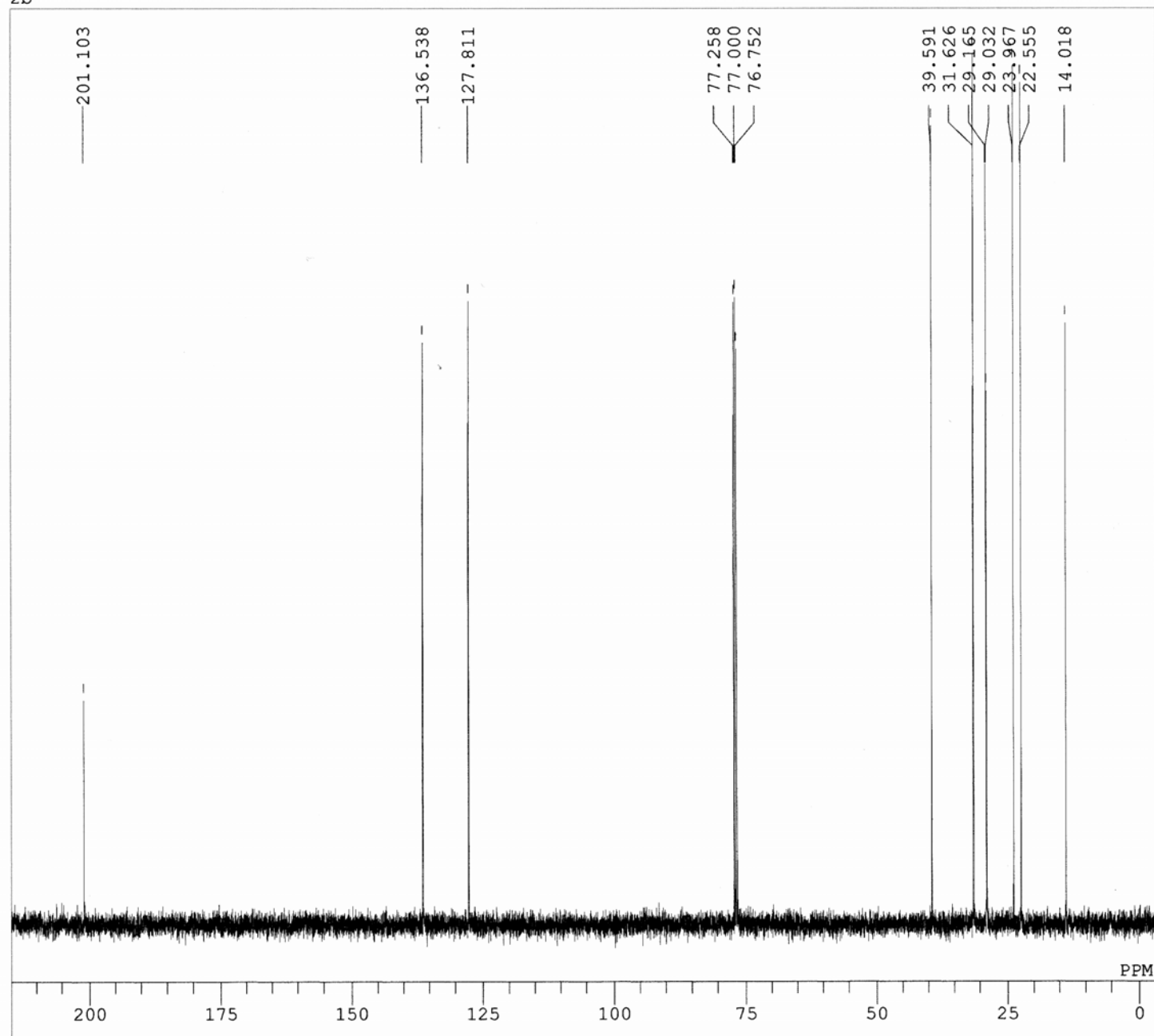
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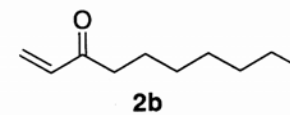
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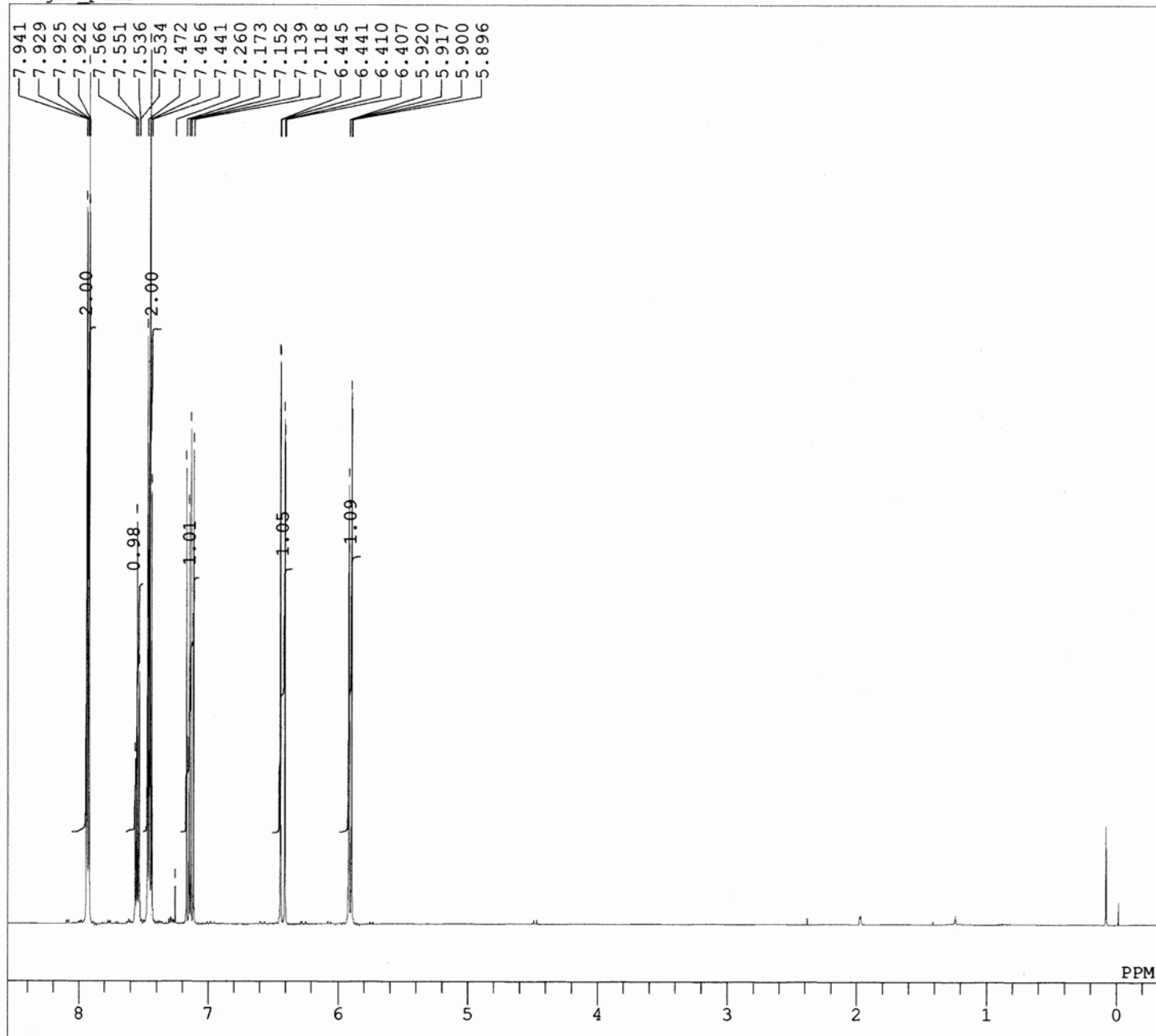
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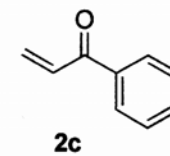
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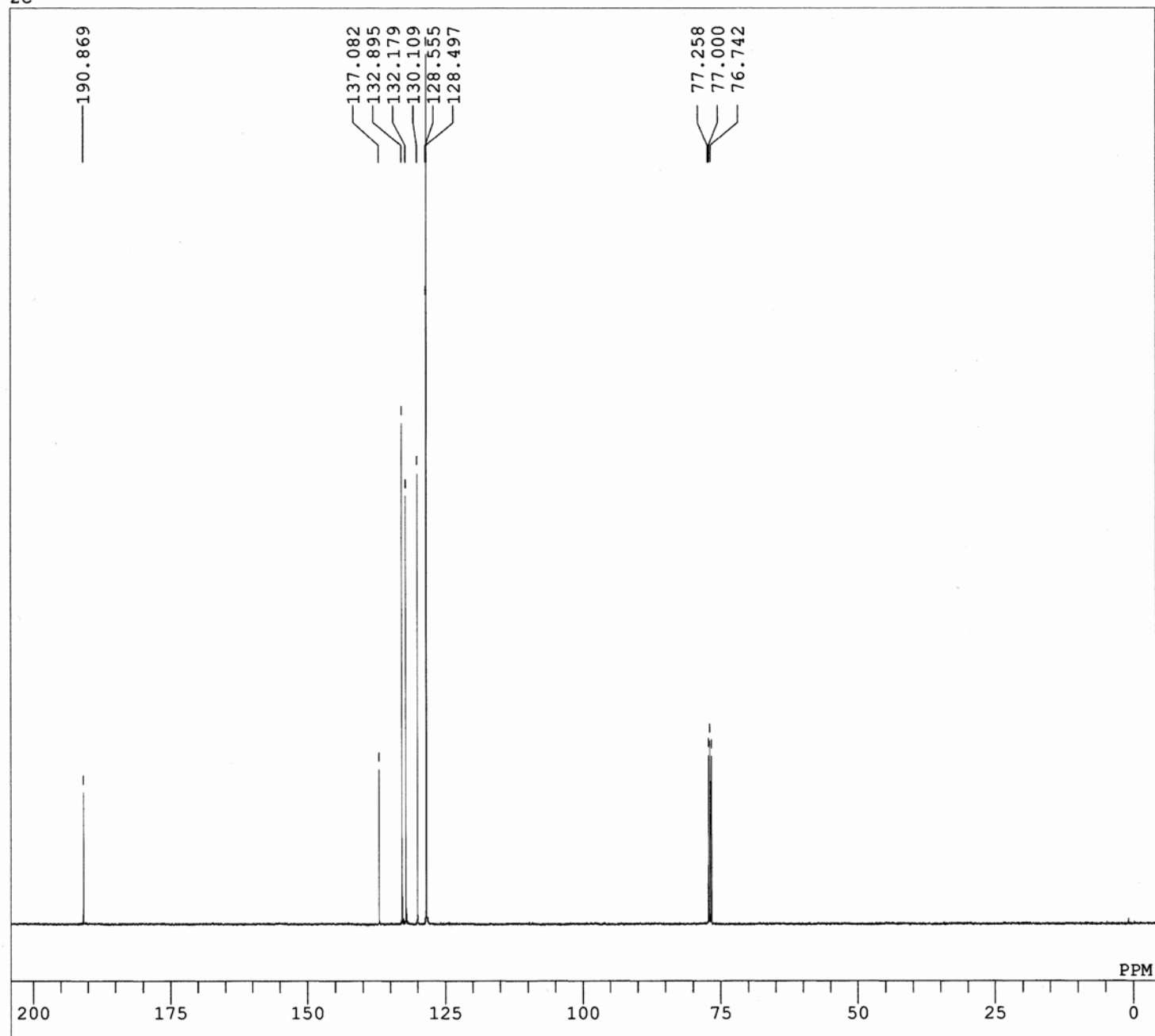
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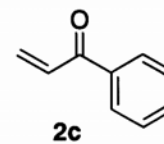
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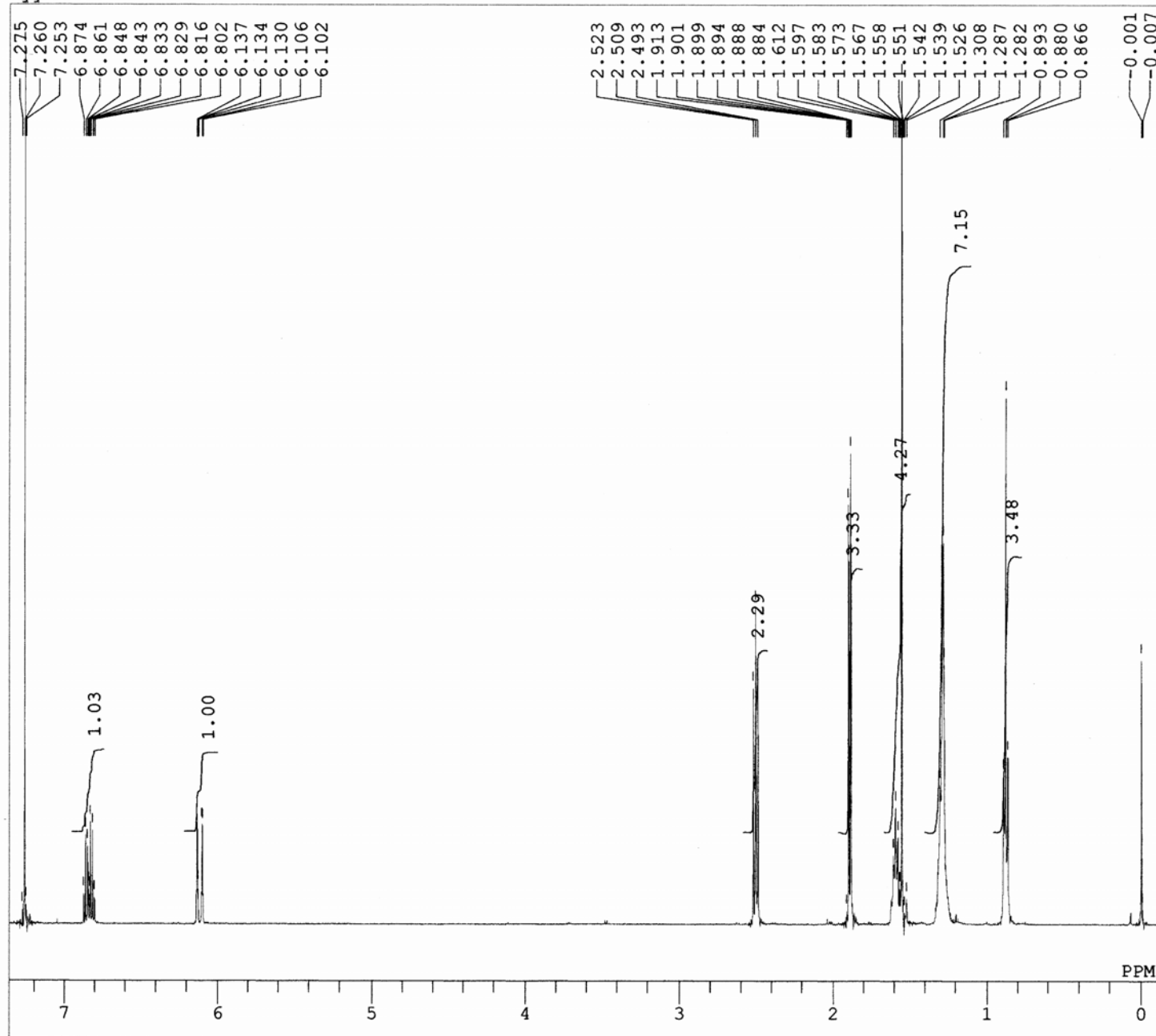


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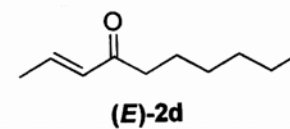


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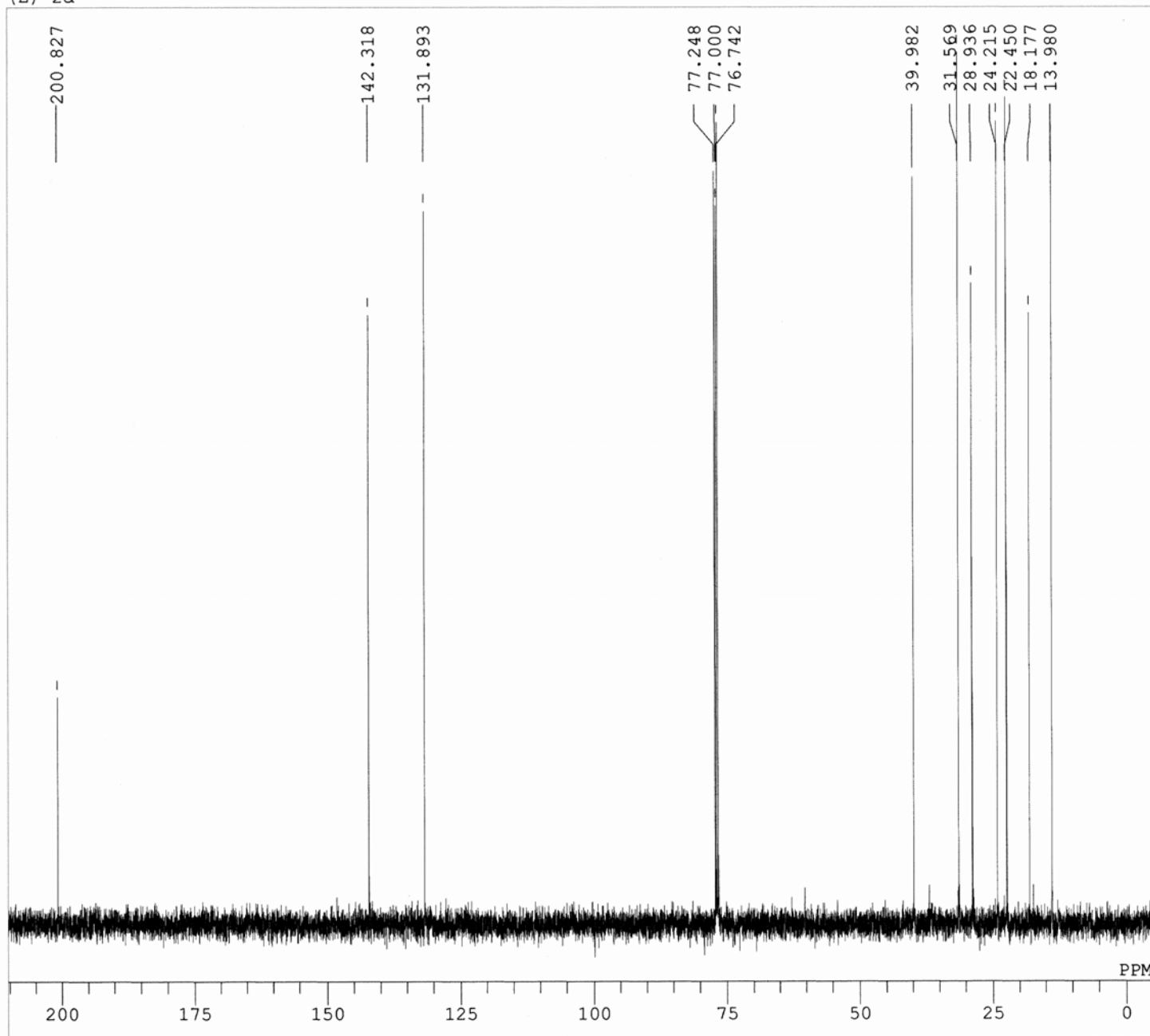




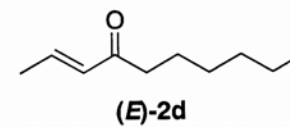
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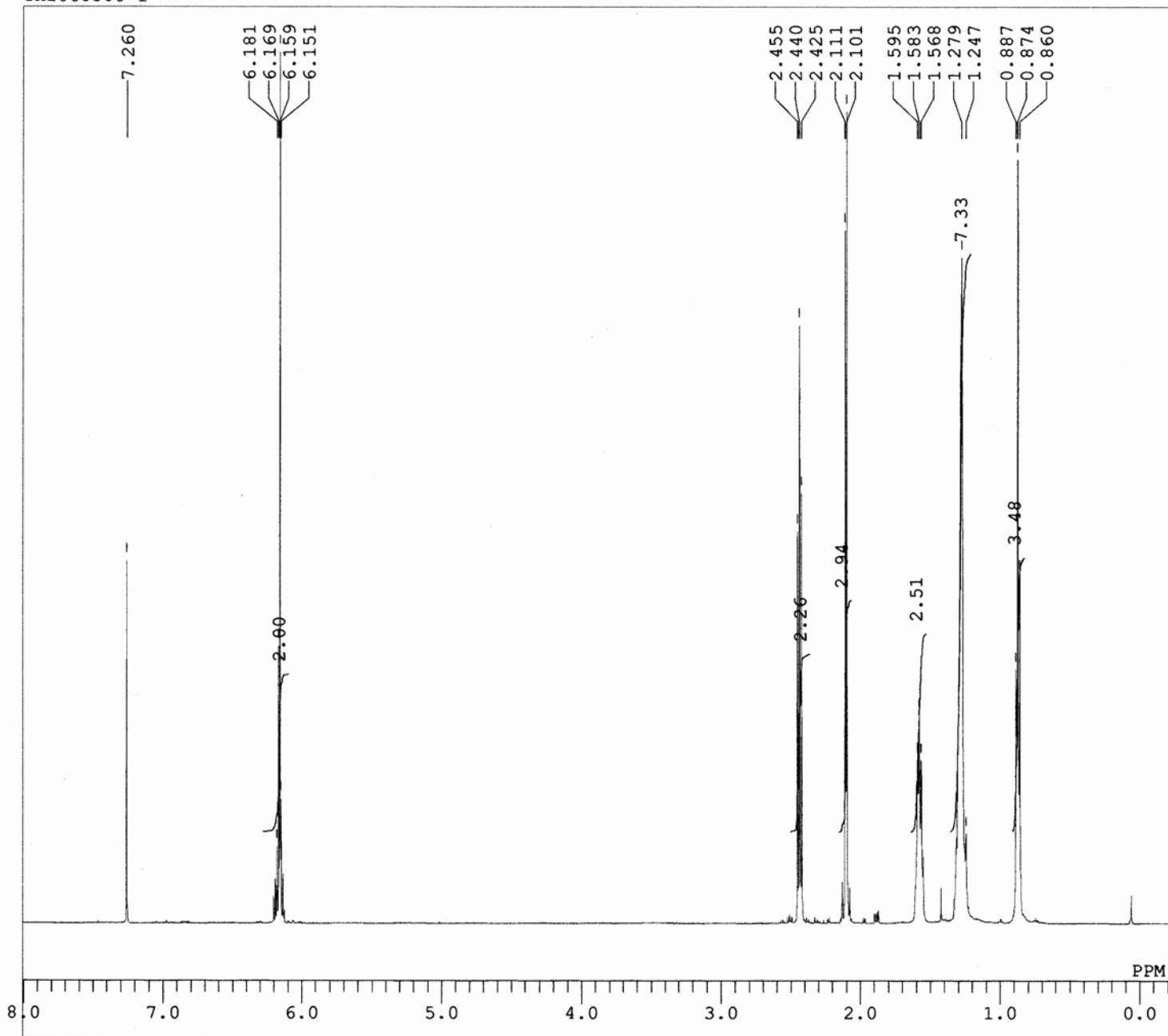
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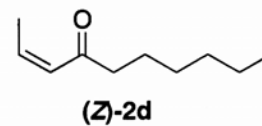
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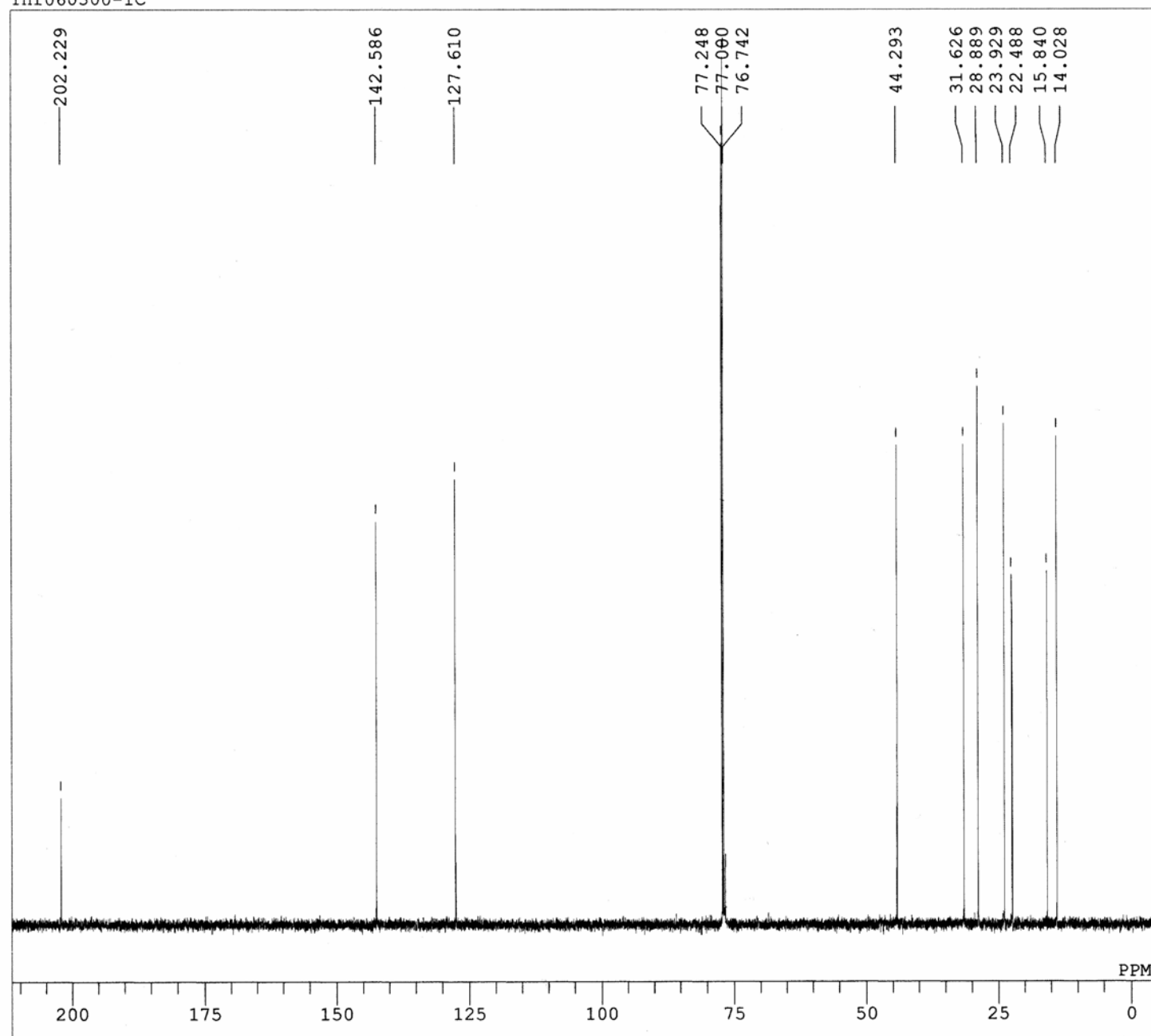
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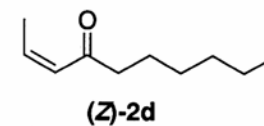
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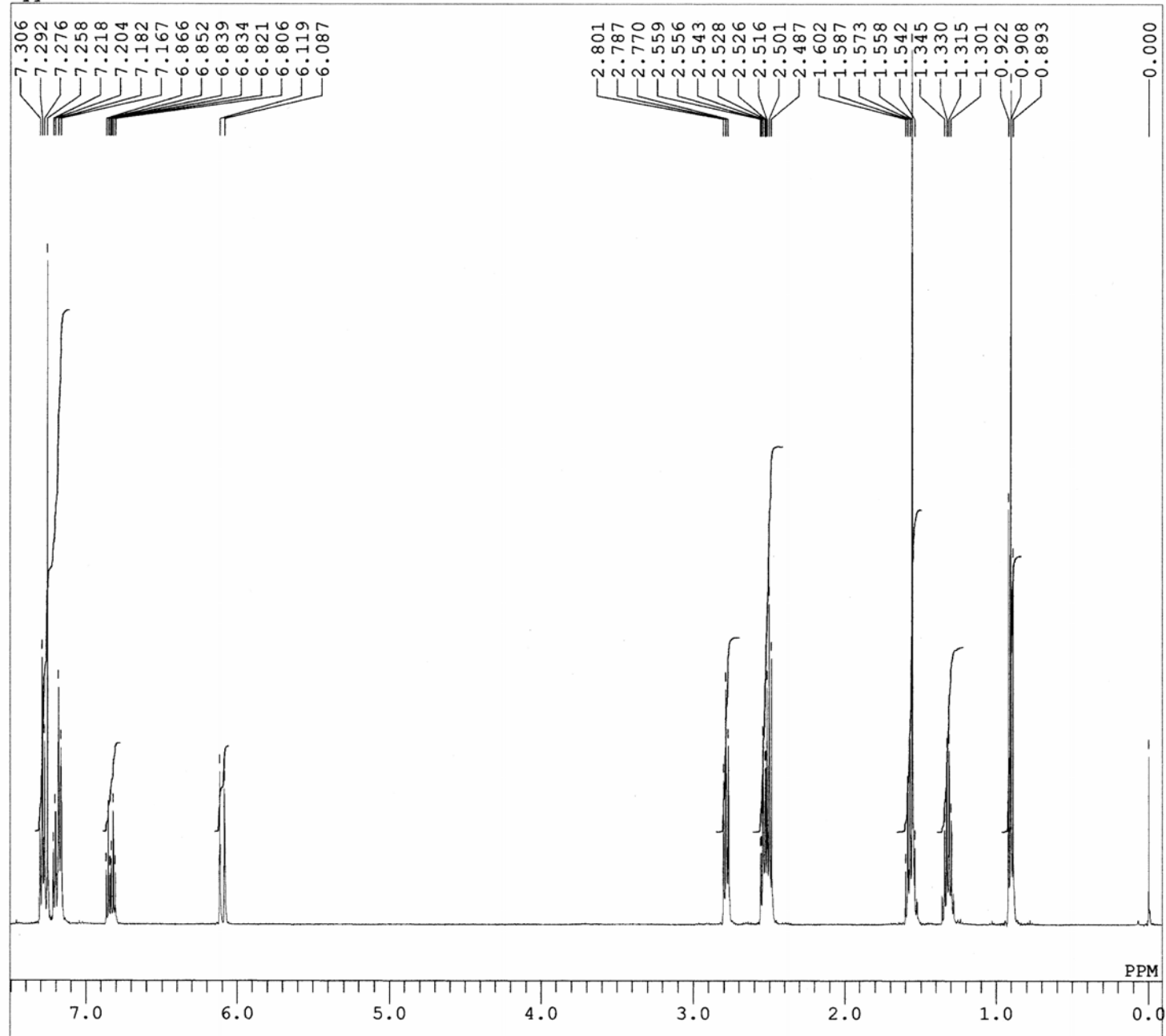
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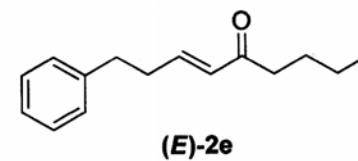
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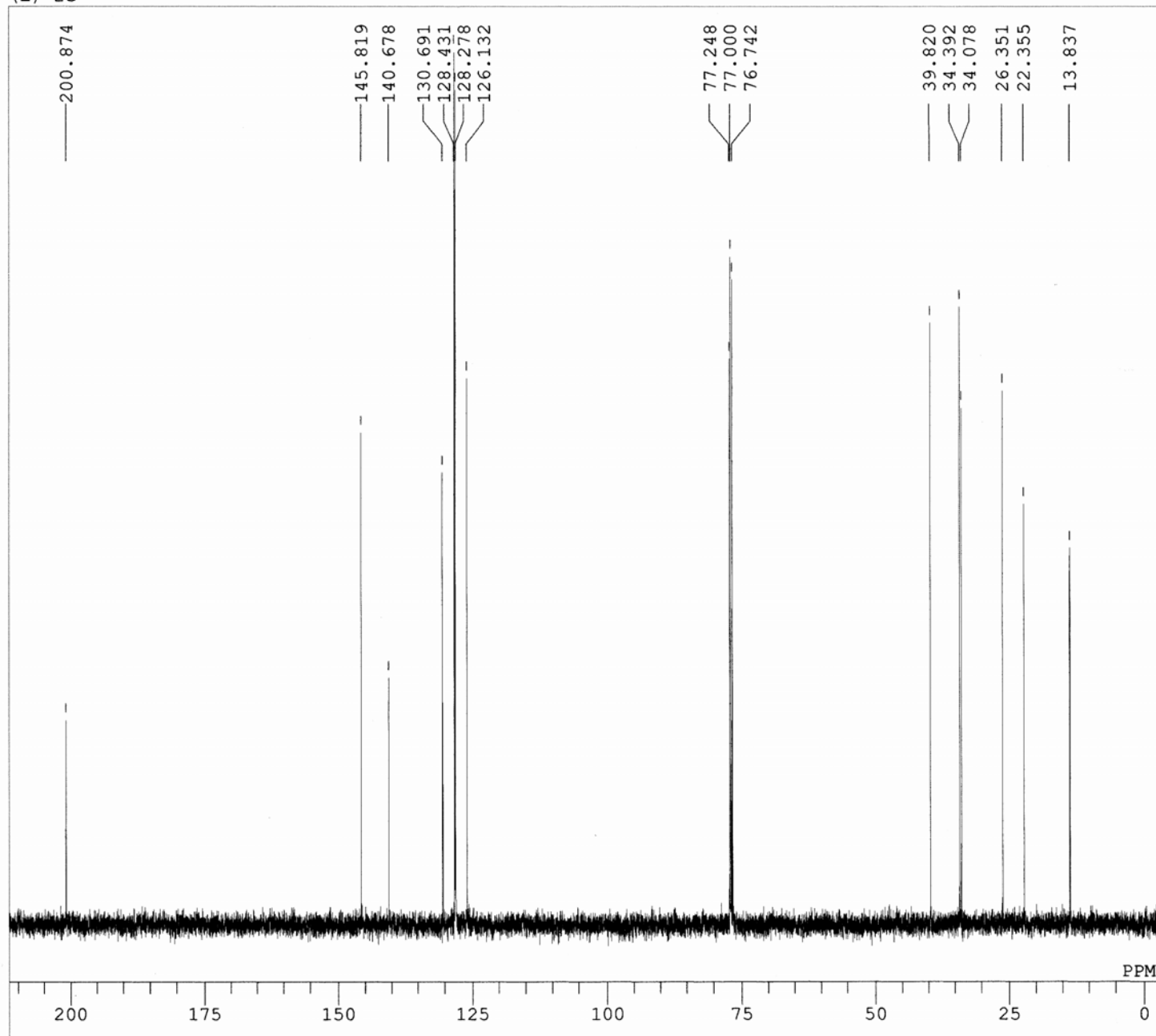
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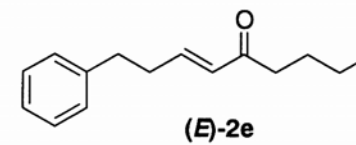
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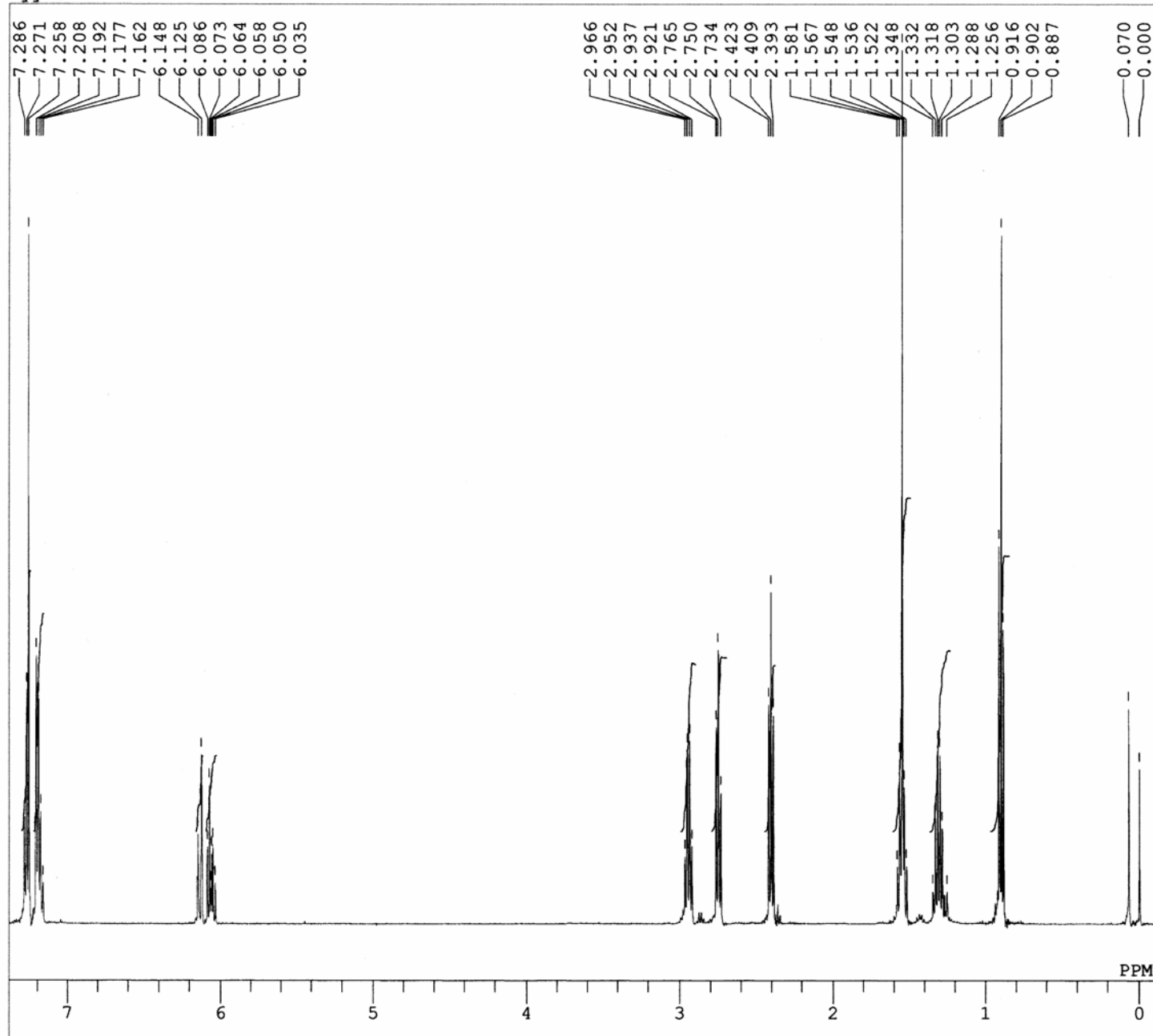
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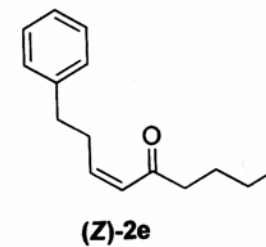
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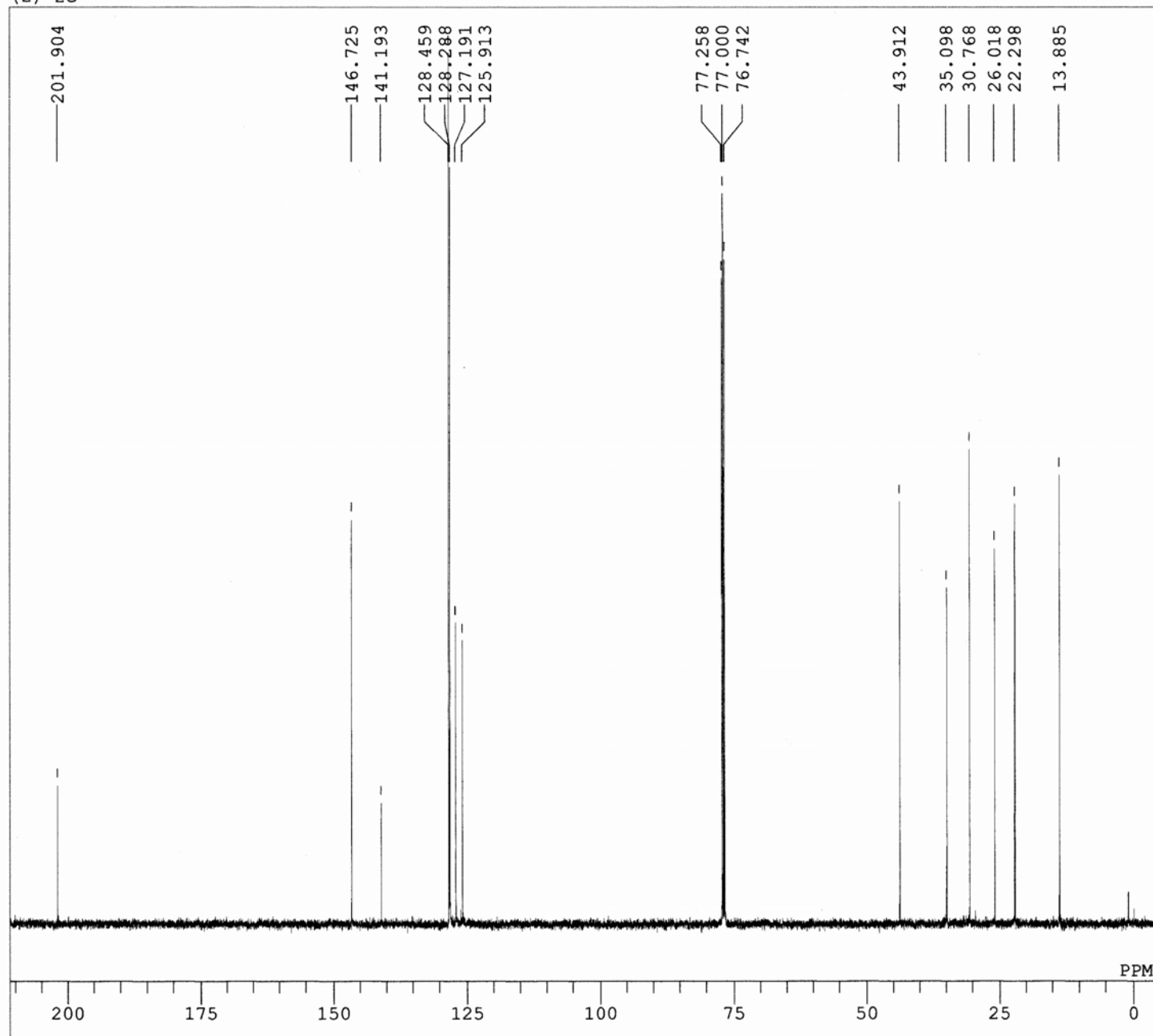
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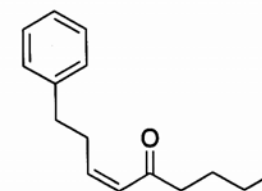
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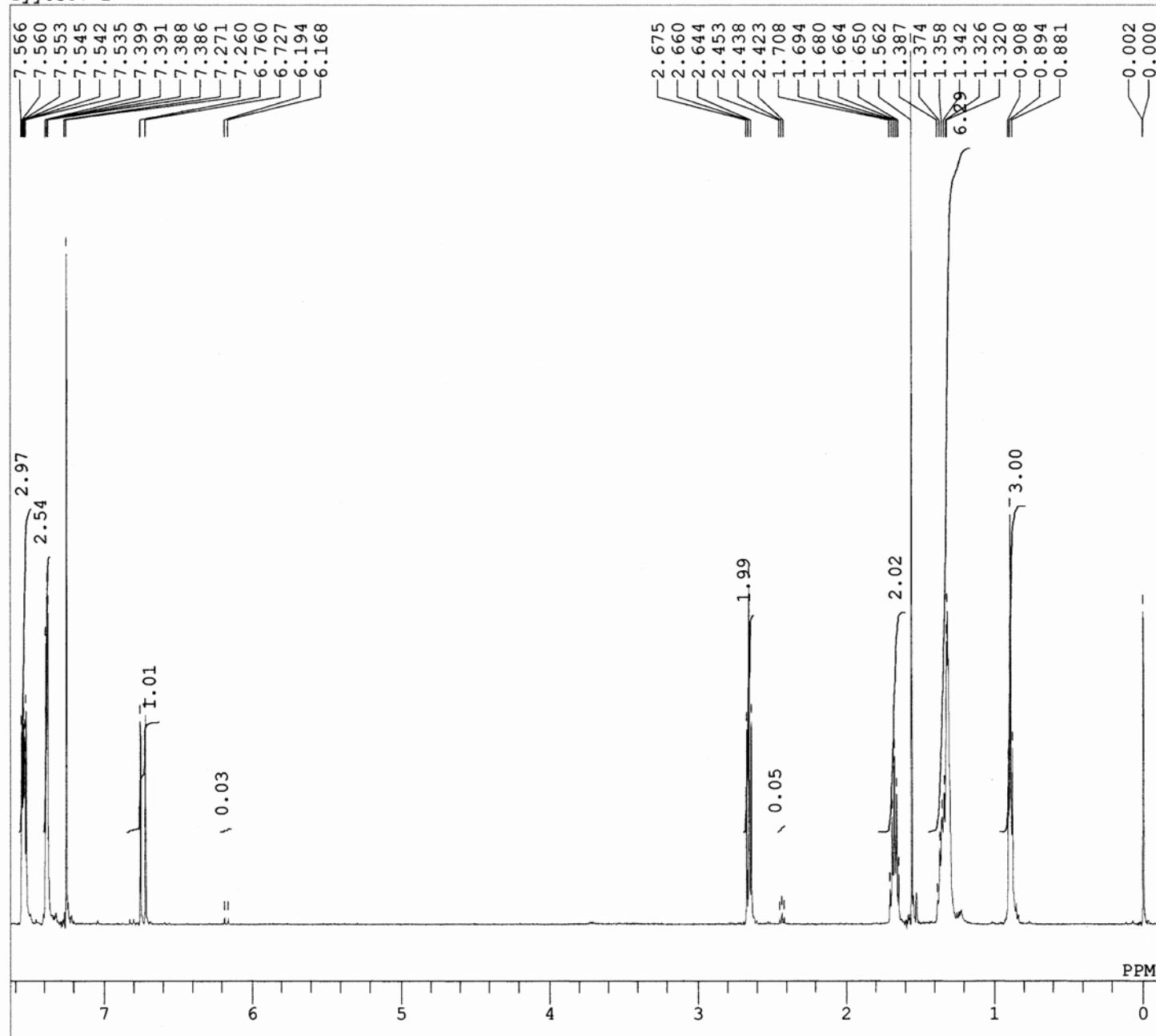


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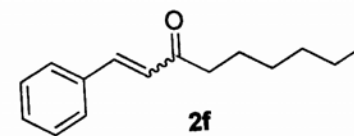


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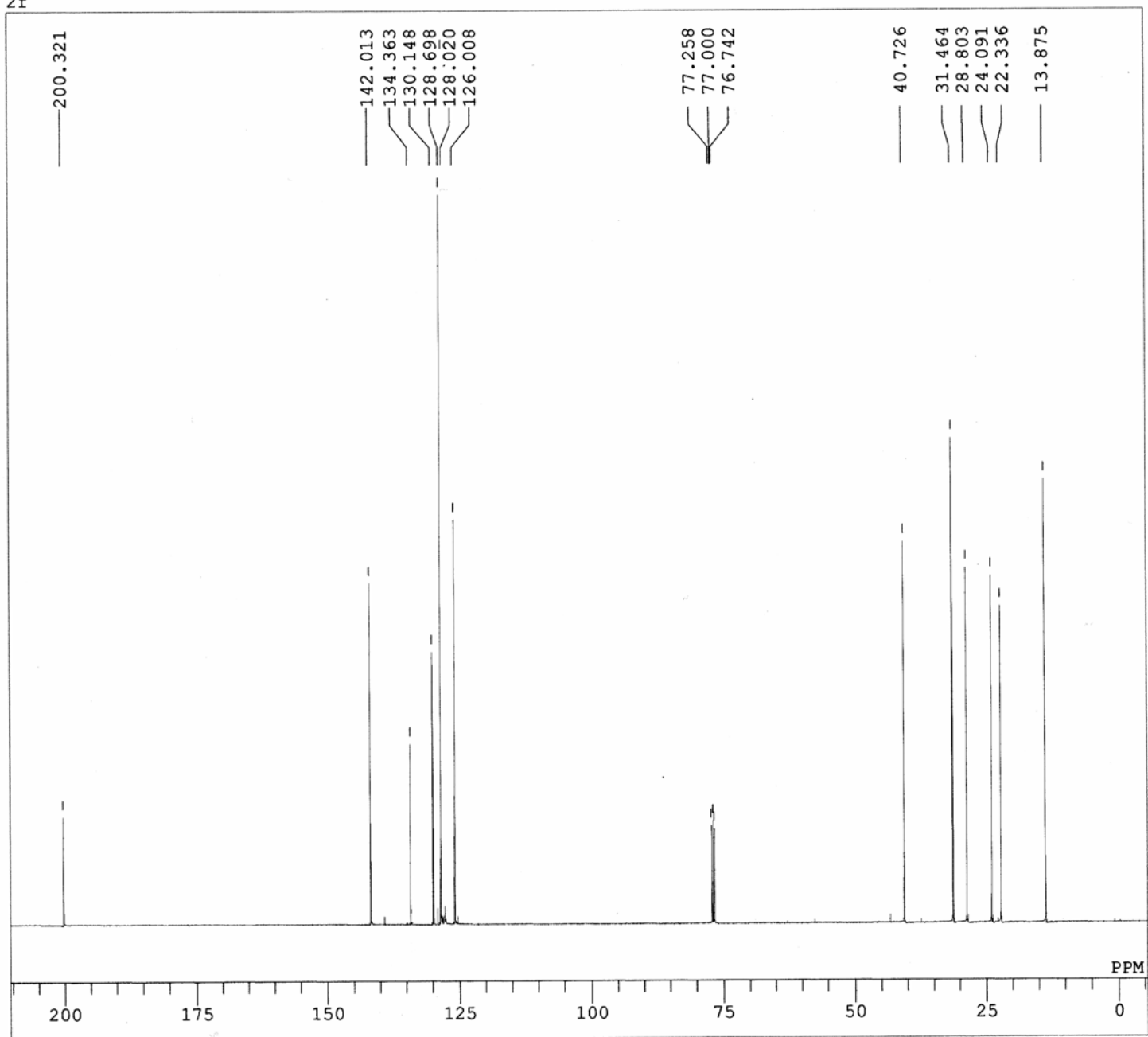
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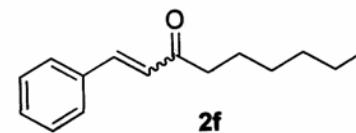
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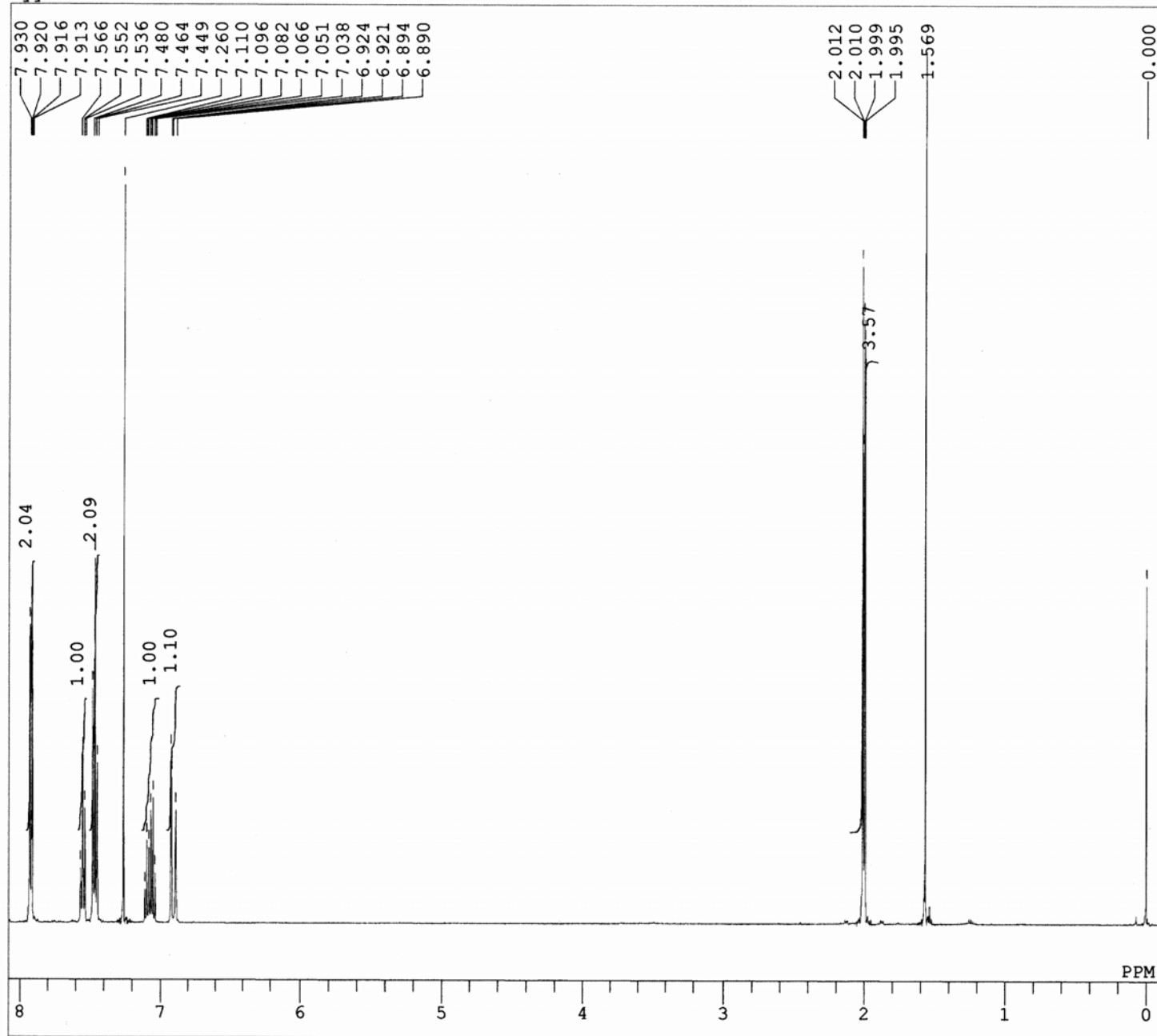
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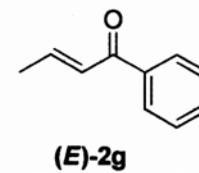
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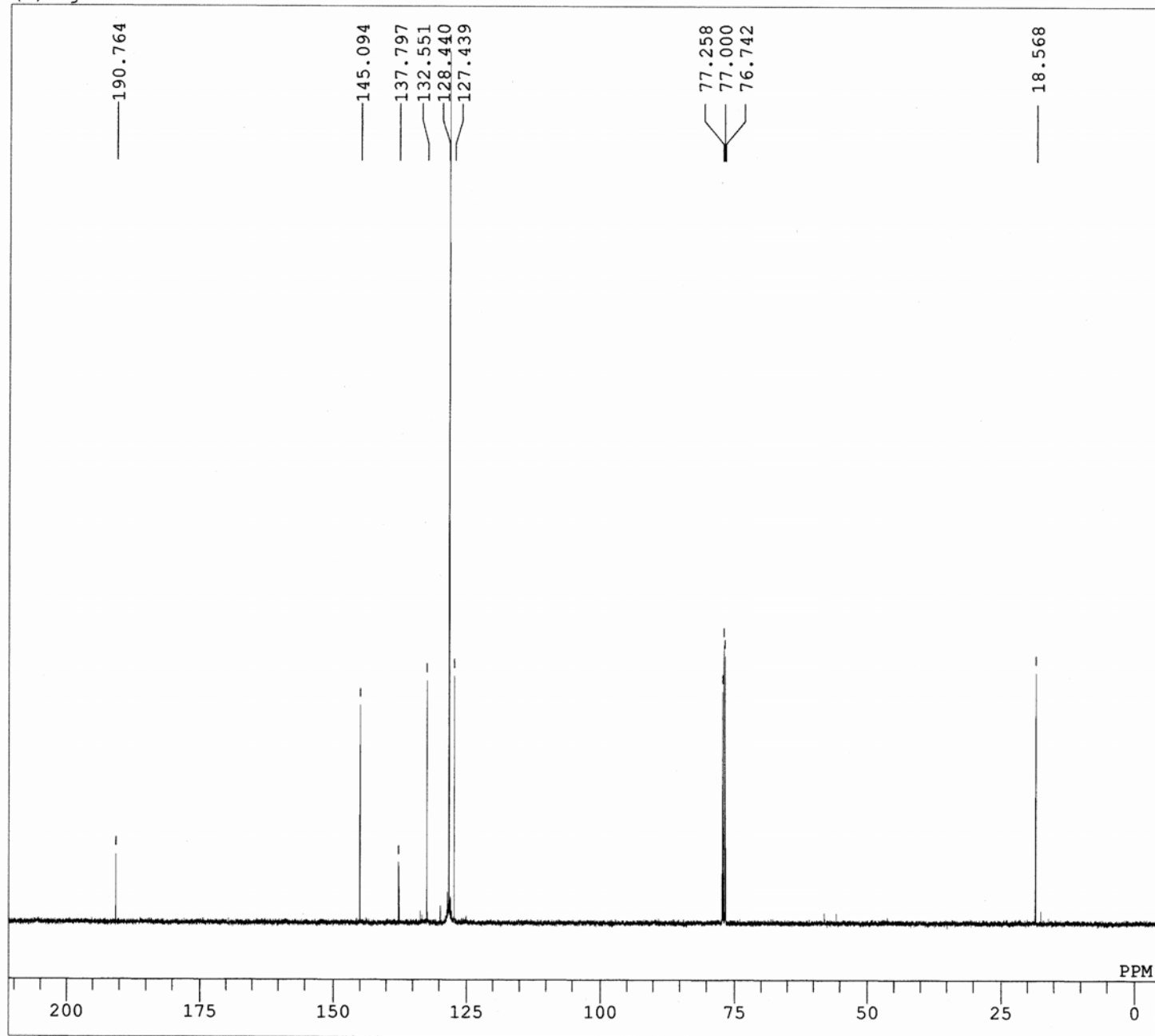
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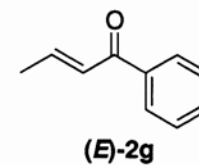
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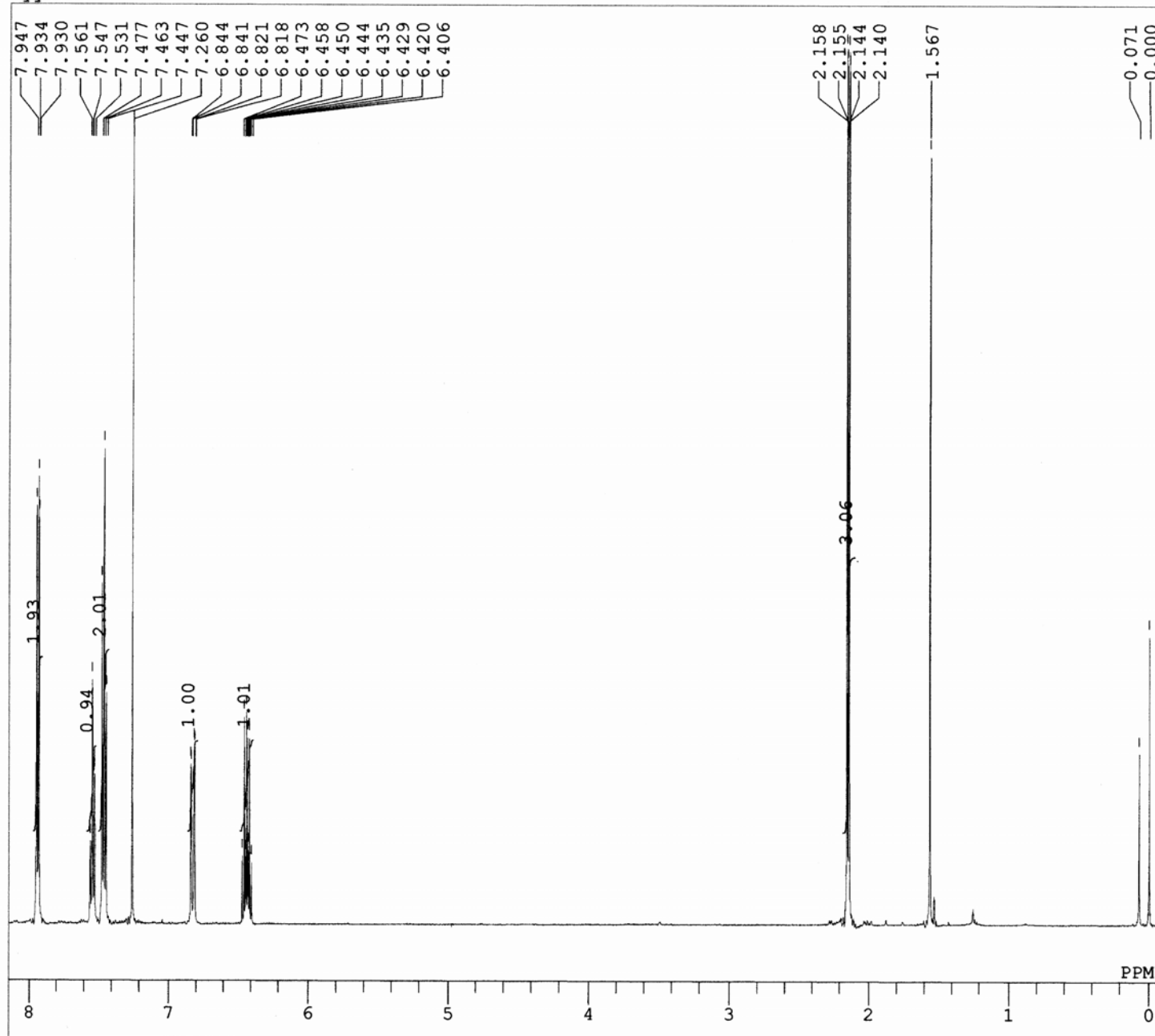
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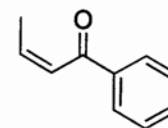
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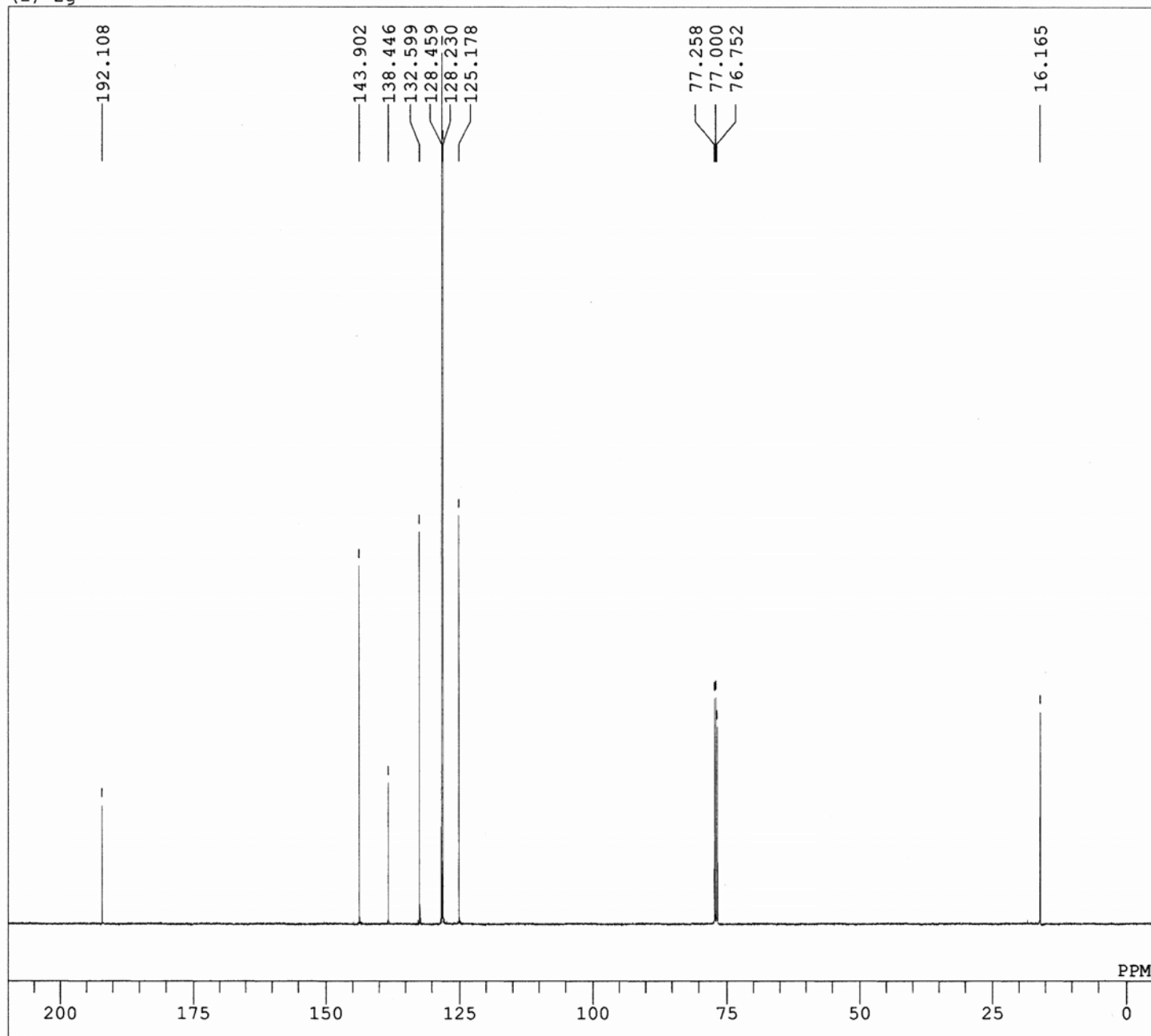


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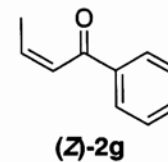


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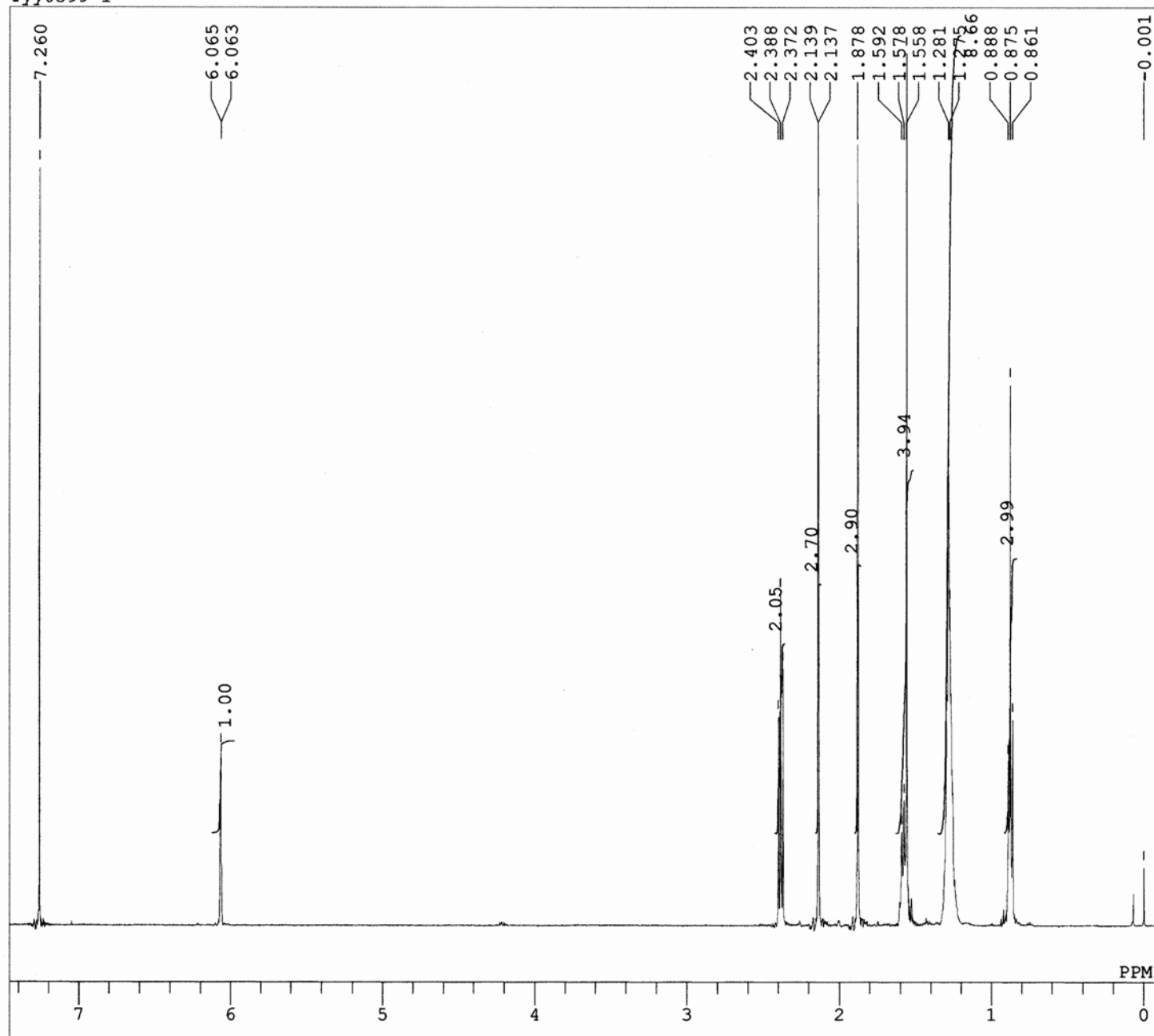
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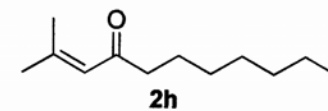
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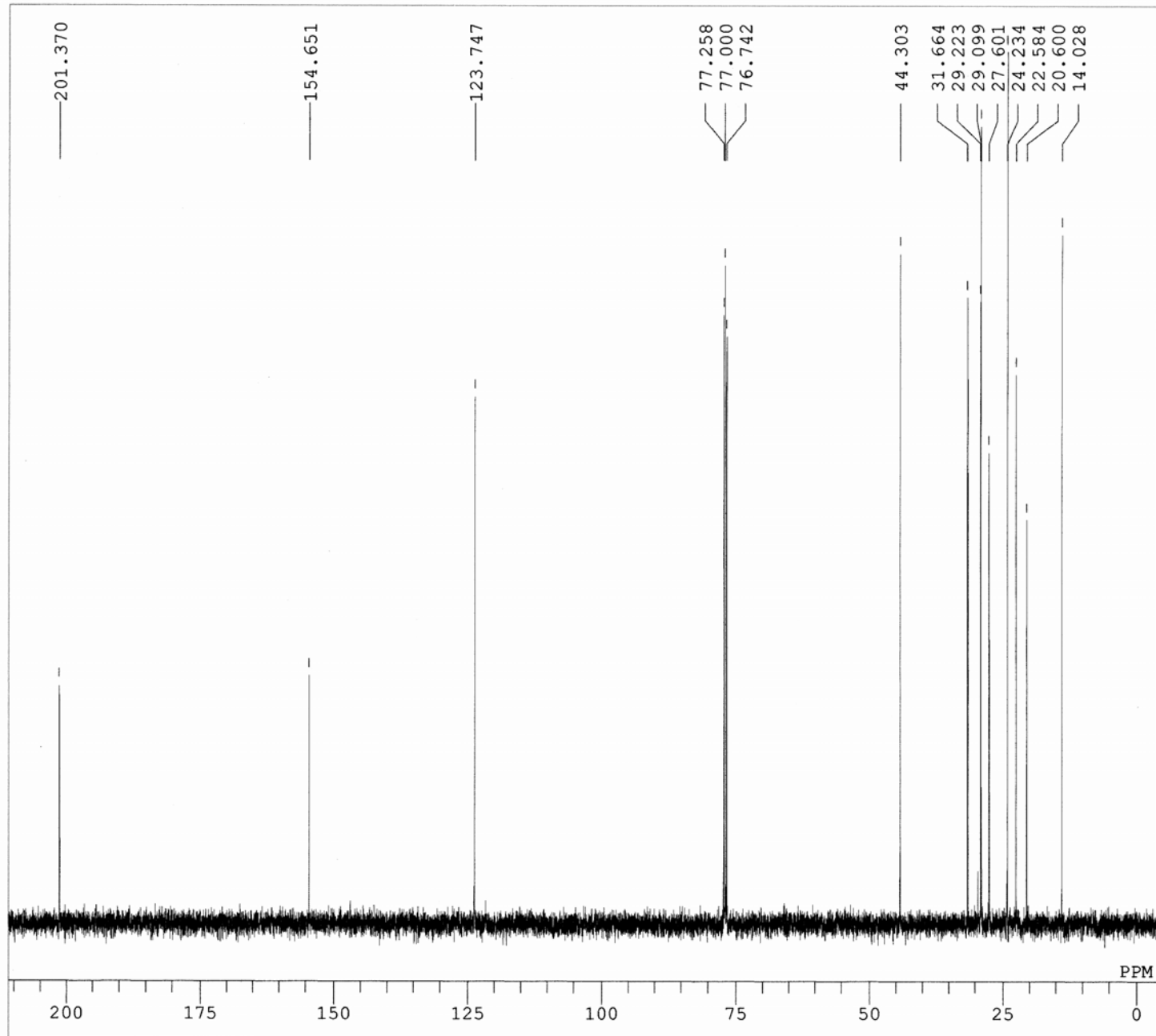
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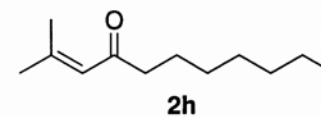
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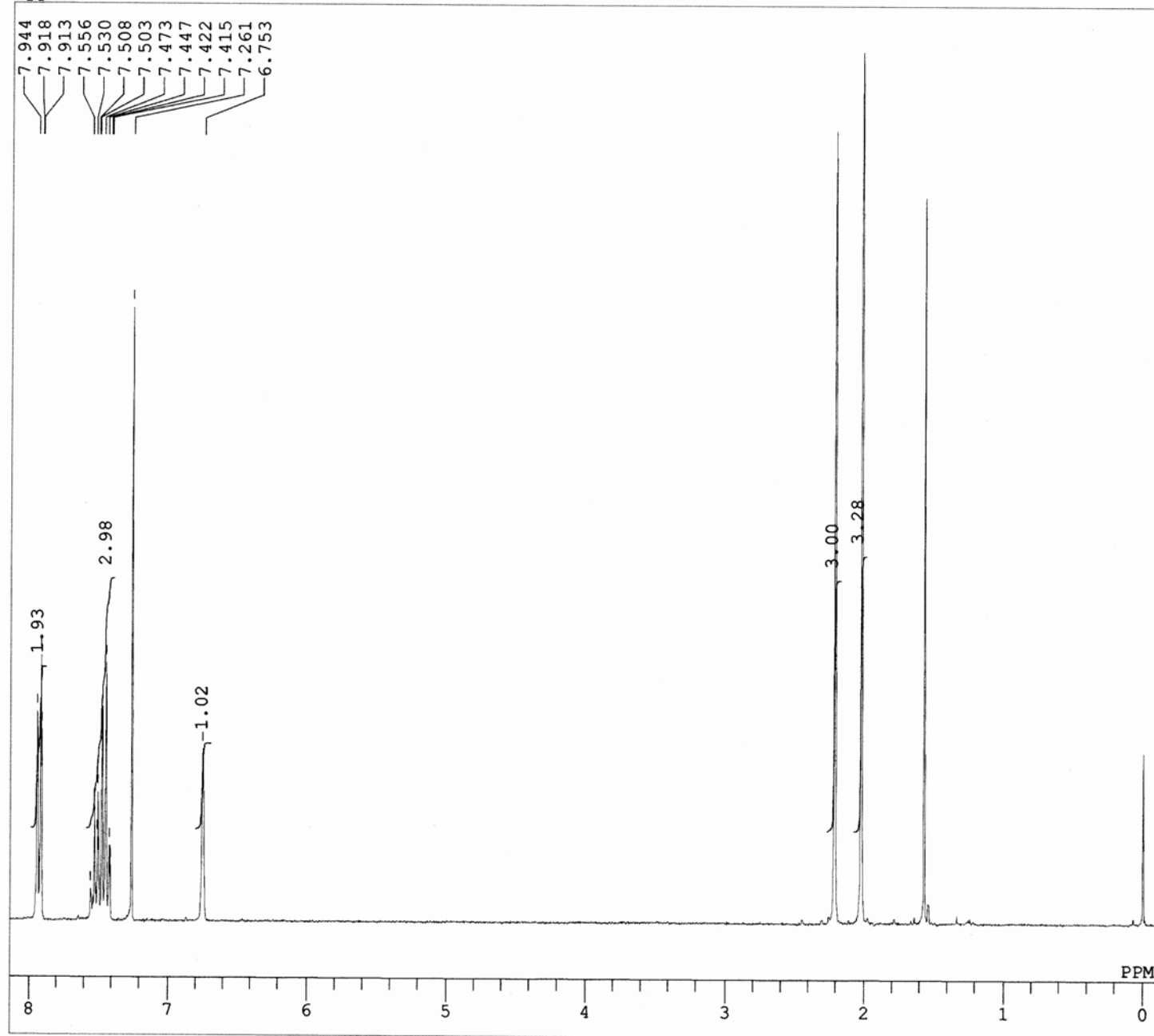
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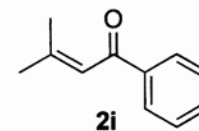
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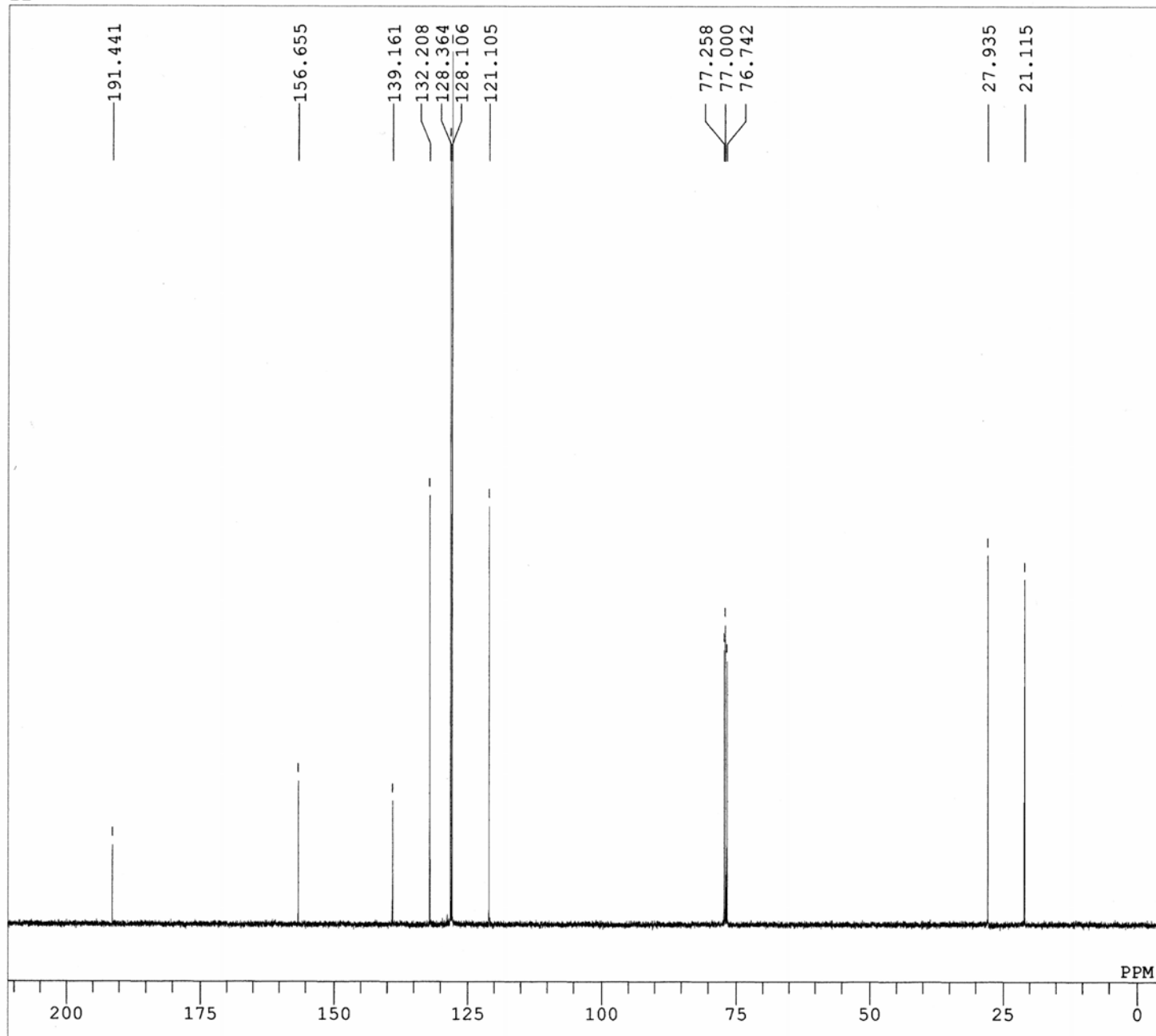
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Yyy0394-1



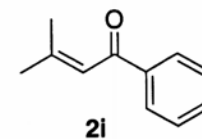
DFILE E:\30H\
COMNT Yyy0394-1
DATIM Tue Jul 10 21:07:44 2007
OBNUC 1H
EXMOD NON
OBFRQ 270.05 MHz
OBSET 112.00 KHz
OBFIN 5800.00 Hz
POINT 8192
FREQU 5401.76 Hz
SCANS 8
ACQTM 1.5165 sec
PD 1.0000 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 23.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22



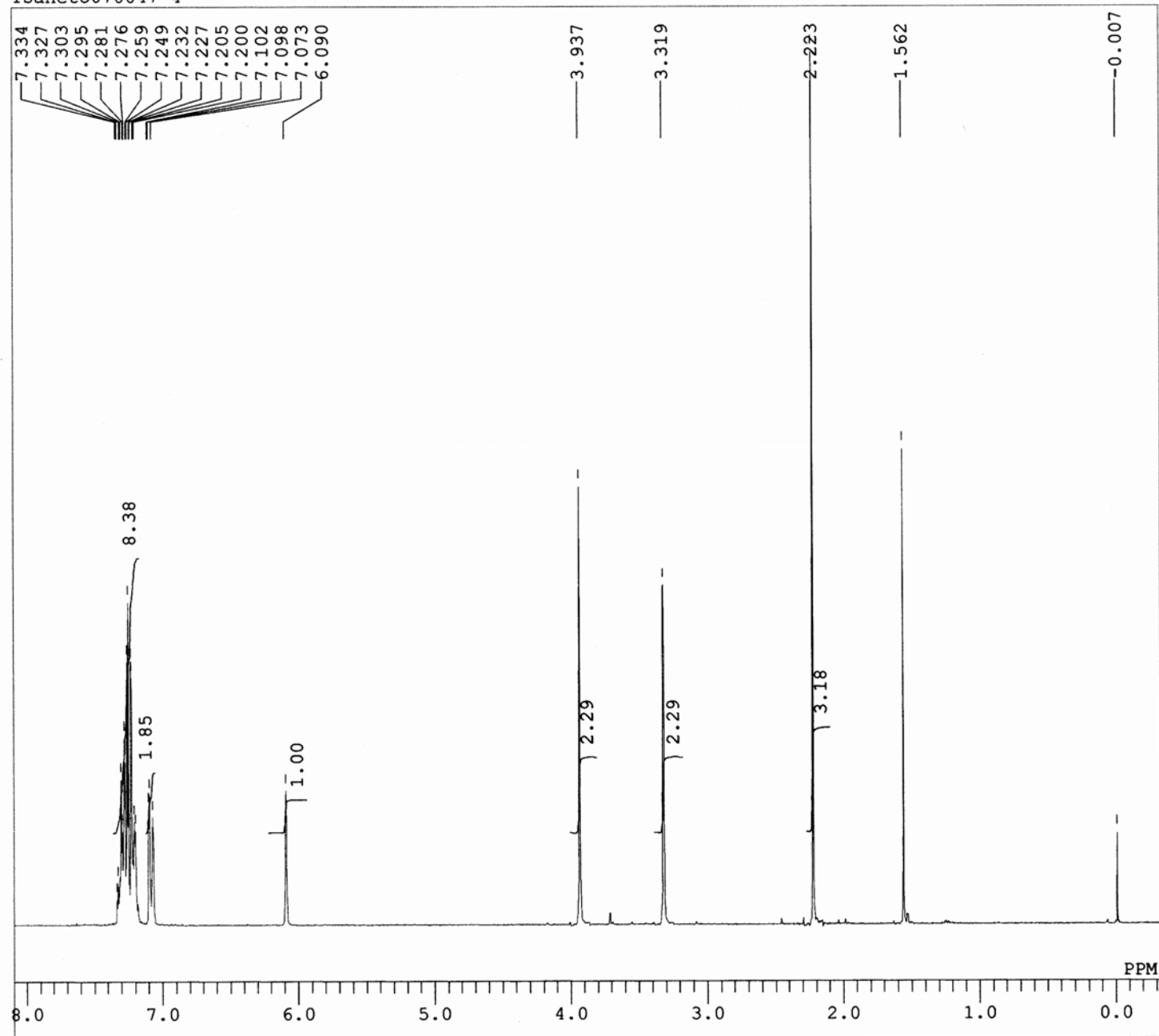
2i



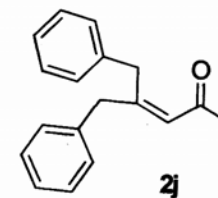
DFILE E:\2i.1
COMNT 2i
DATIM 13-11-2007 14:29:55
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 200
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 19.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



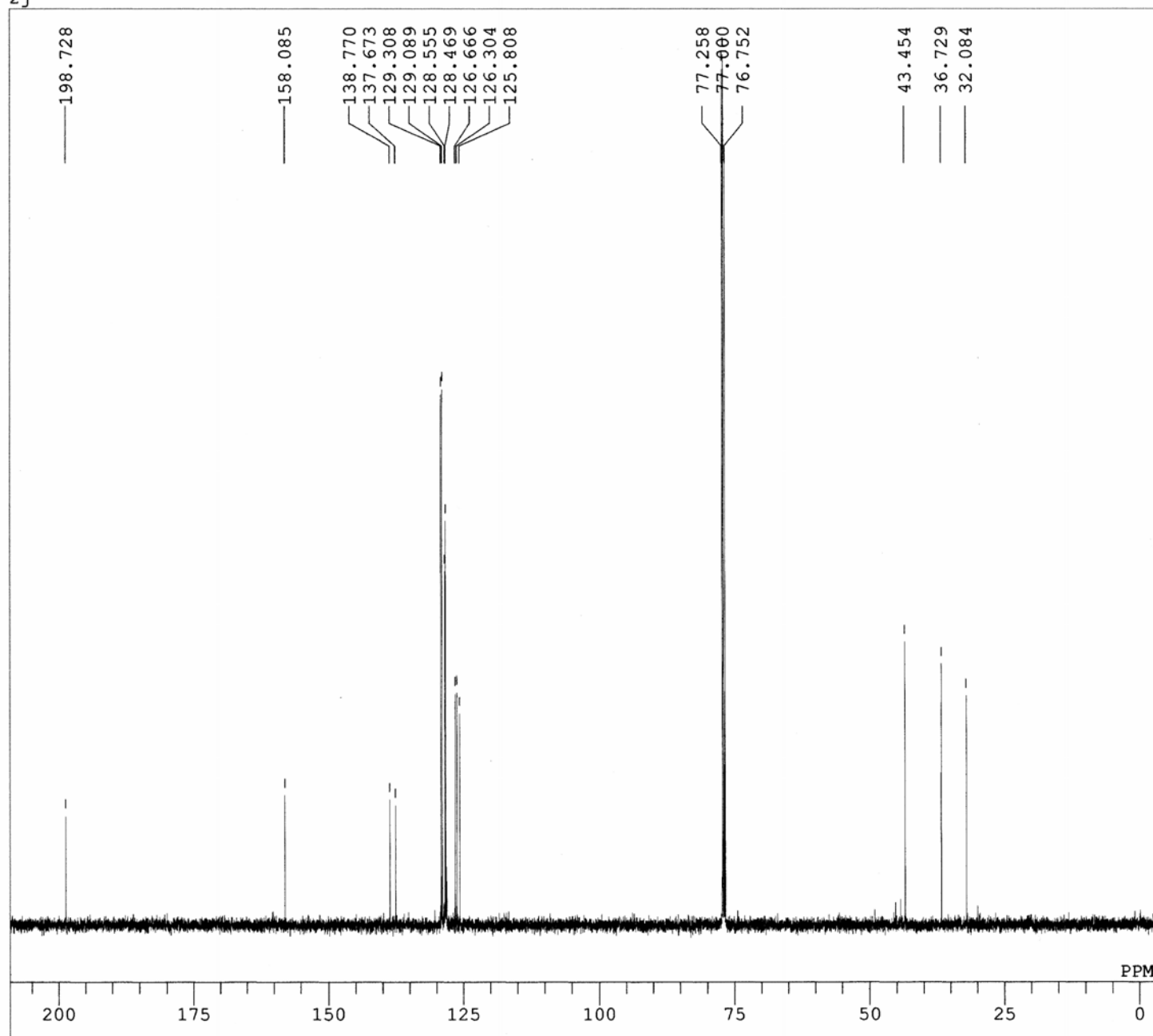
E:\0300-\Yyy0393-2.als
Ysaneto070047-4



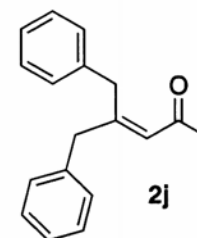
DFILE E:\0300-\Yyy0393-2.als
 COMNT Ysaneto070047-4
 DATIM Tue Jul 10 21:03:27 2007
 OBNUC 1H
 EXMOD NON
 OBFRQ 270.05 MHz
 OBSET 112.00 KHz
 OBFIN 5800.00 Hz
 POINT 8192
 FREQU 5401.76 Hz
 SCANS 8
 ACQTM 1.5165 sec
 PD 1.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 23.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 21



2j

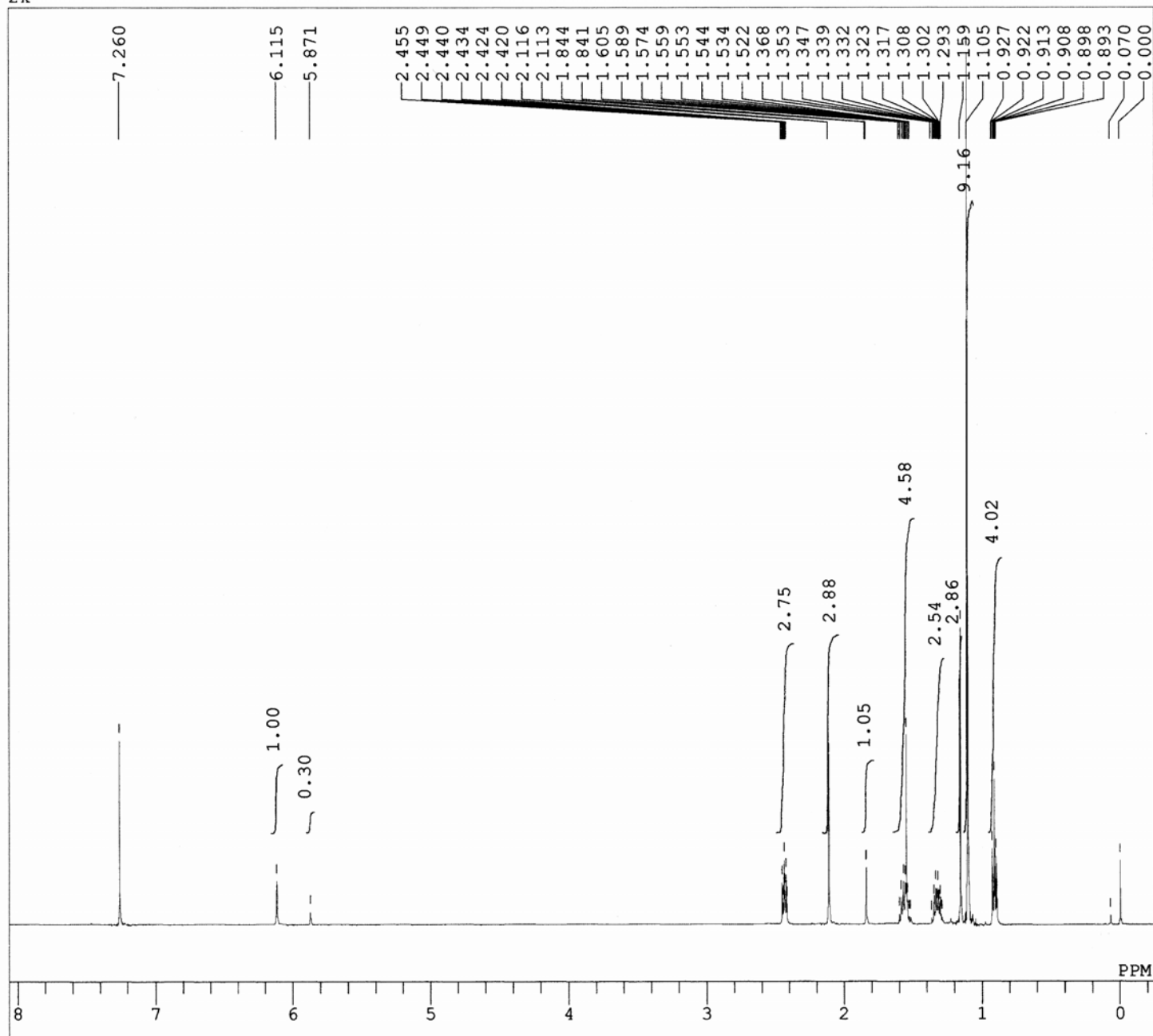


DFILE E:\M.Egi\2j.1
COMNT 2j
DATIM 24-11-2007 15:28:51
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 304
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 18.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60

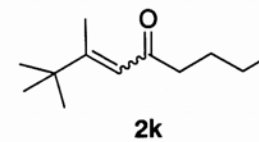


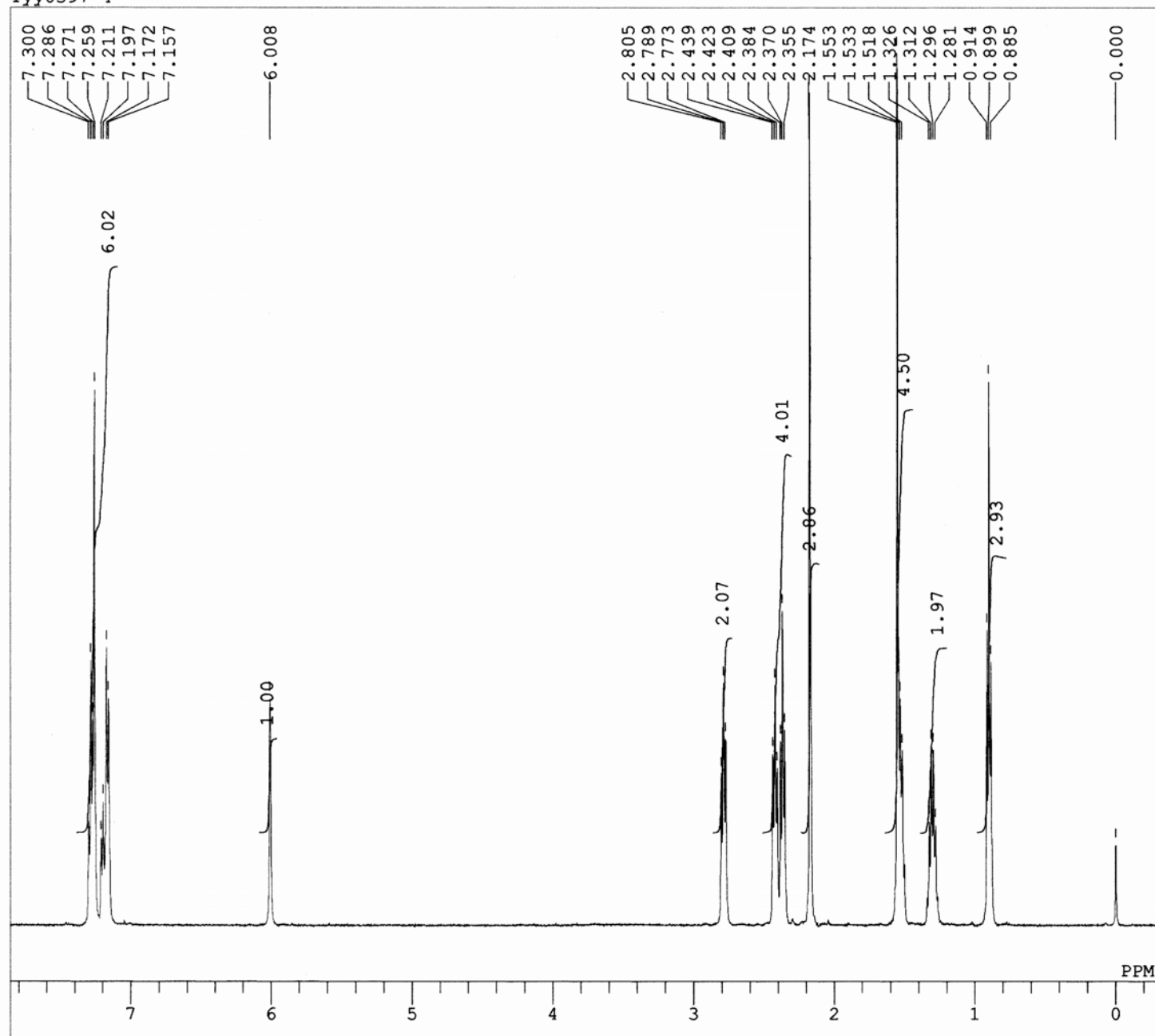
2j

2k

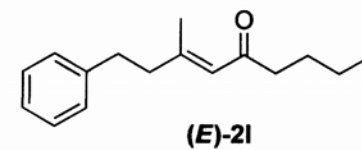


DFILE C:\Documents and Settings\Studer
 COMNT 2k
 DATIM Mon Jul 09 21:43:53 2007
 OBNUC 1H
 EXMOD SINGL
 OBFRQ 499.10 MHz
 OBSET 0.00 KHz
 OBFIN 125250.00 Hz
 POINT 16384
 FREQU 9980.04 Hz
 SCANS 8
 ACQTM 1.6417 sec
 PD 2.0000 sec
 PW1 5.50 usec
 IRNUC 1H
 CTEMP -204.8 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 23

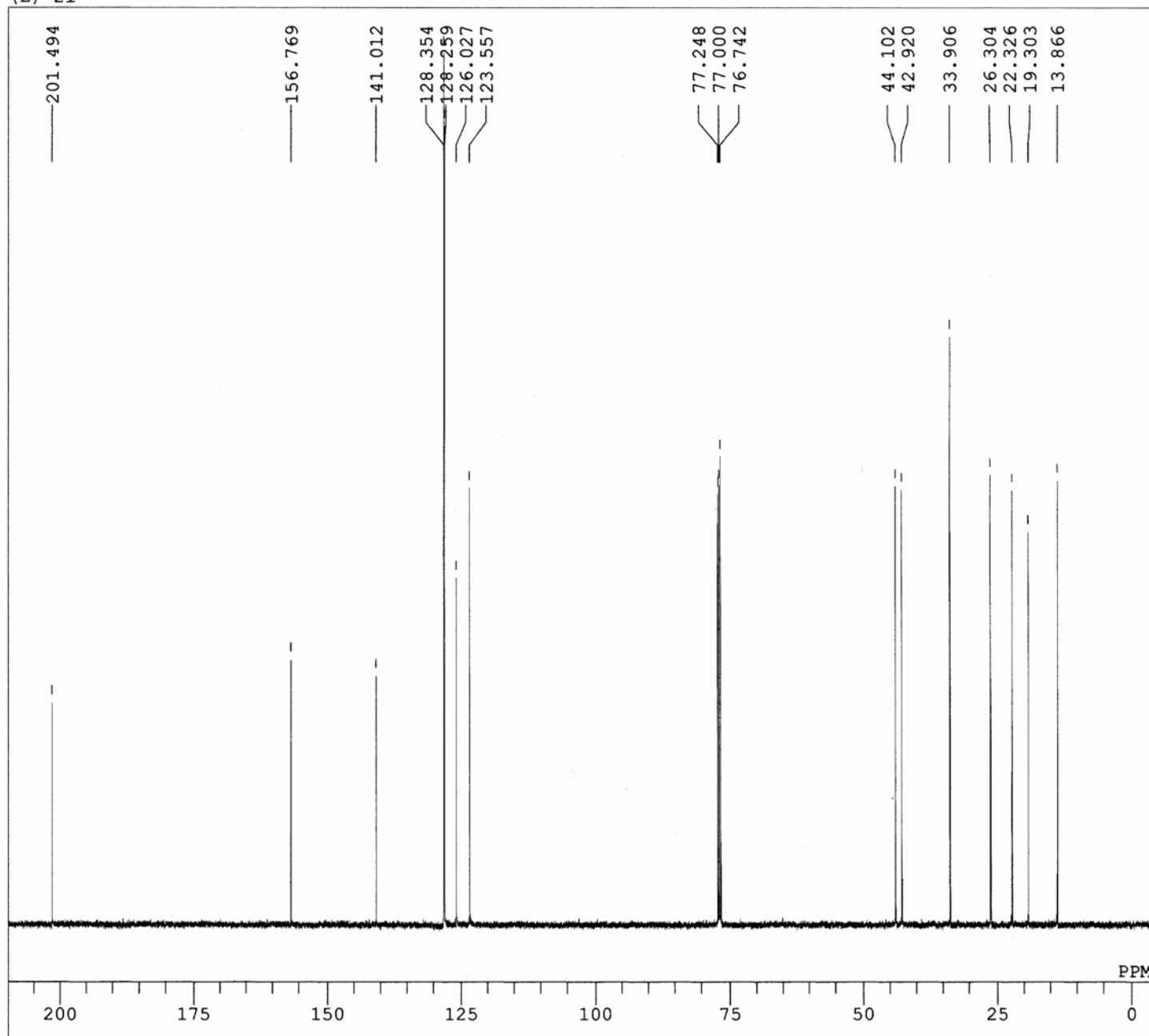




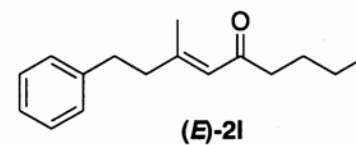
DFILE E:\0300-\Yyy0397-41NON_E9.als
COMNT Yyy0397-4
DATIM Thu Jul 12 21:26:14 2007
OBNUC 1H
EXMOD SINGL
OBFRQ 499.10 MHz
OBSET 0.00 KHz
OBFIN 125250.00 Hz
POINT 16384
FREQU 9980.04 Hz
SCANS 8
ACQTM 1.6417 sec
PD 2.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP -204.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 24



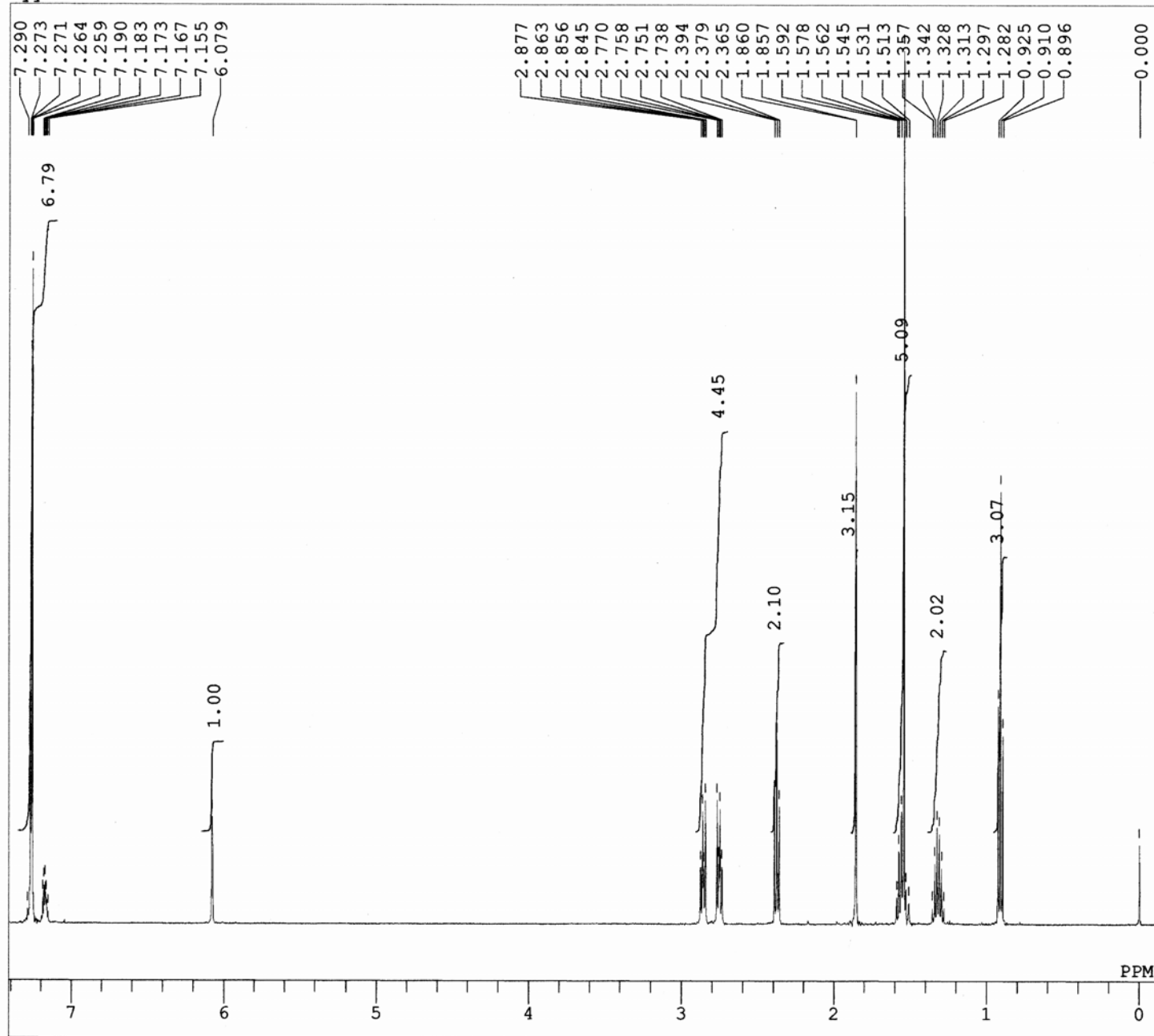
(E)-21



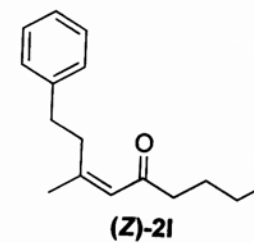
DFILE E:\M.Egi\21 (E).1
COMNT (E)-21
DATIM 15-11-2007 16:11:49
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 391
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



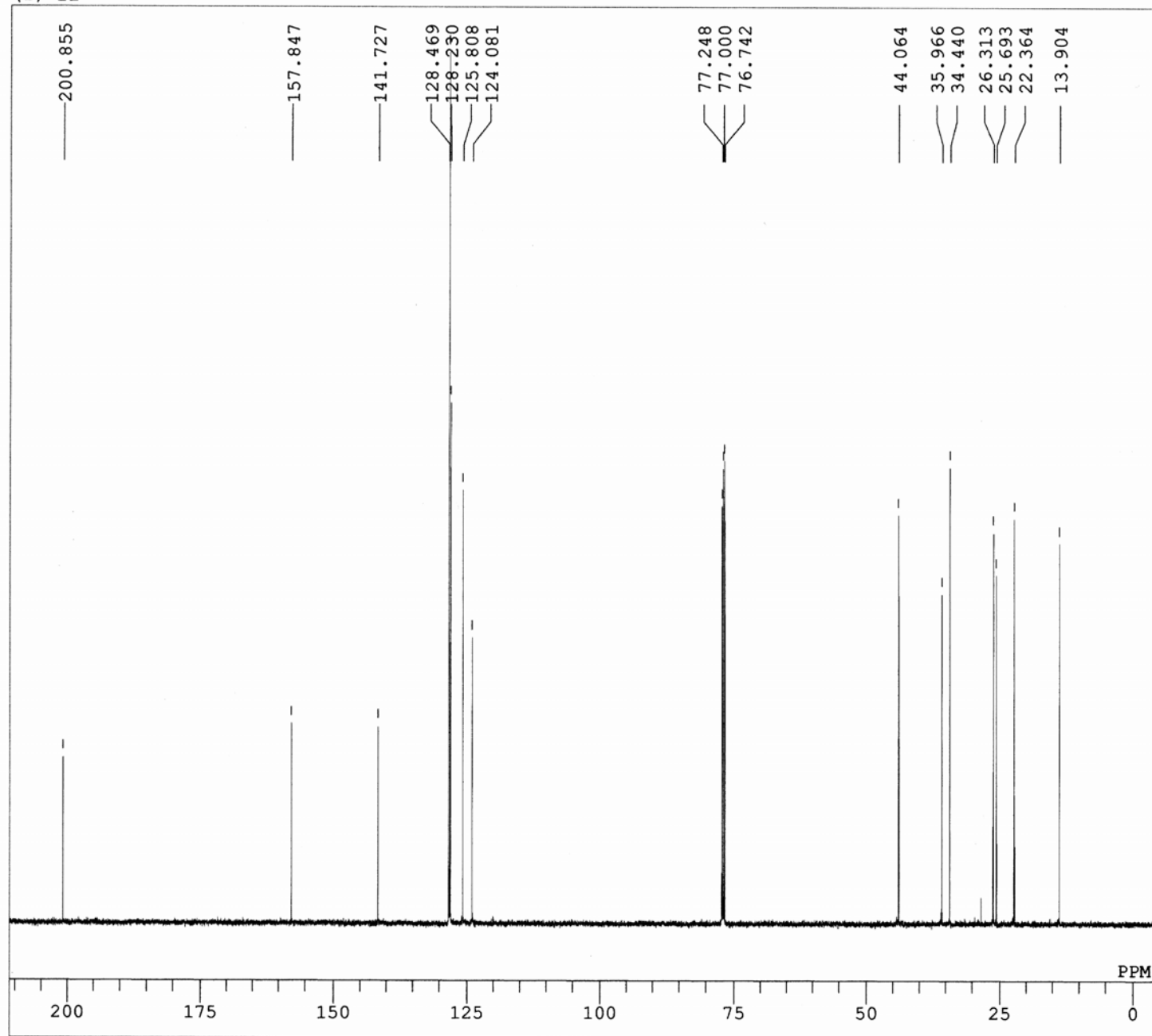
E:\0300-\Yyy0397-21NON_E7.als
Yyy0397-2



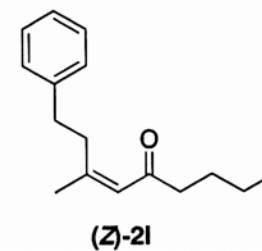
DFILE E:\0300-\Yyy0397-21NON_E7.als
 COMNT Yyy0397-2
 DATIM Thu Jul 12 21:15:21 2007
 OBNUC 1H
 EXMOD SINGL
 OBFRQ 499.10 MHz
 OBSET 0.00 KHz
 OBFIN 125250.00 Hz
 POINT 16384
 FREQU 9980.04 Hz
 SCANS 8
 ACQTM 1.6417 sec
 PD 2.0000 sec
 PW1 5.50 usec
 IRNUC 1H
 CTEMP -204.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 25



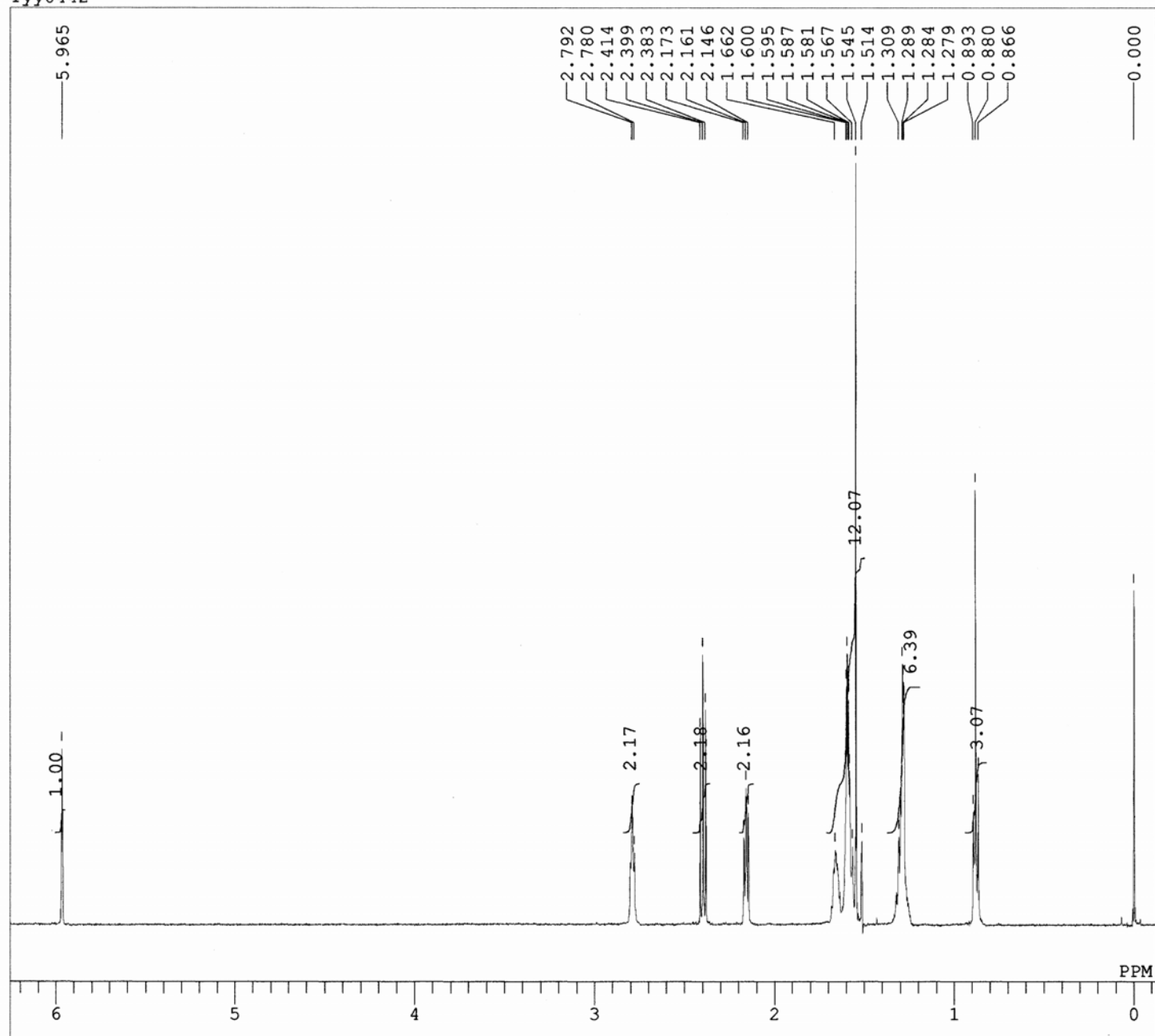
(Z)-21



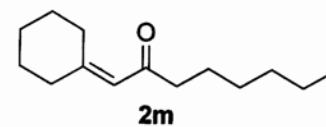
DFILE E:\M.Egi\21 (Z).1
COMNT (Z)-21
DATIM 15-11-2007 16:43:22
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 565
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 19.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



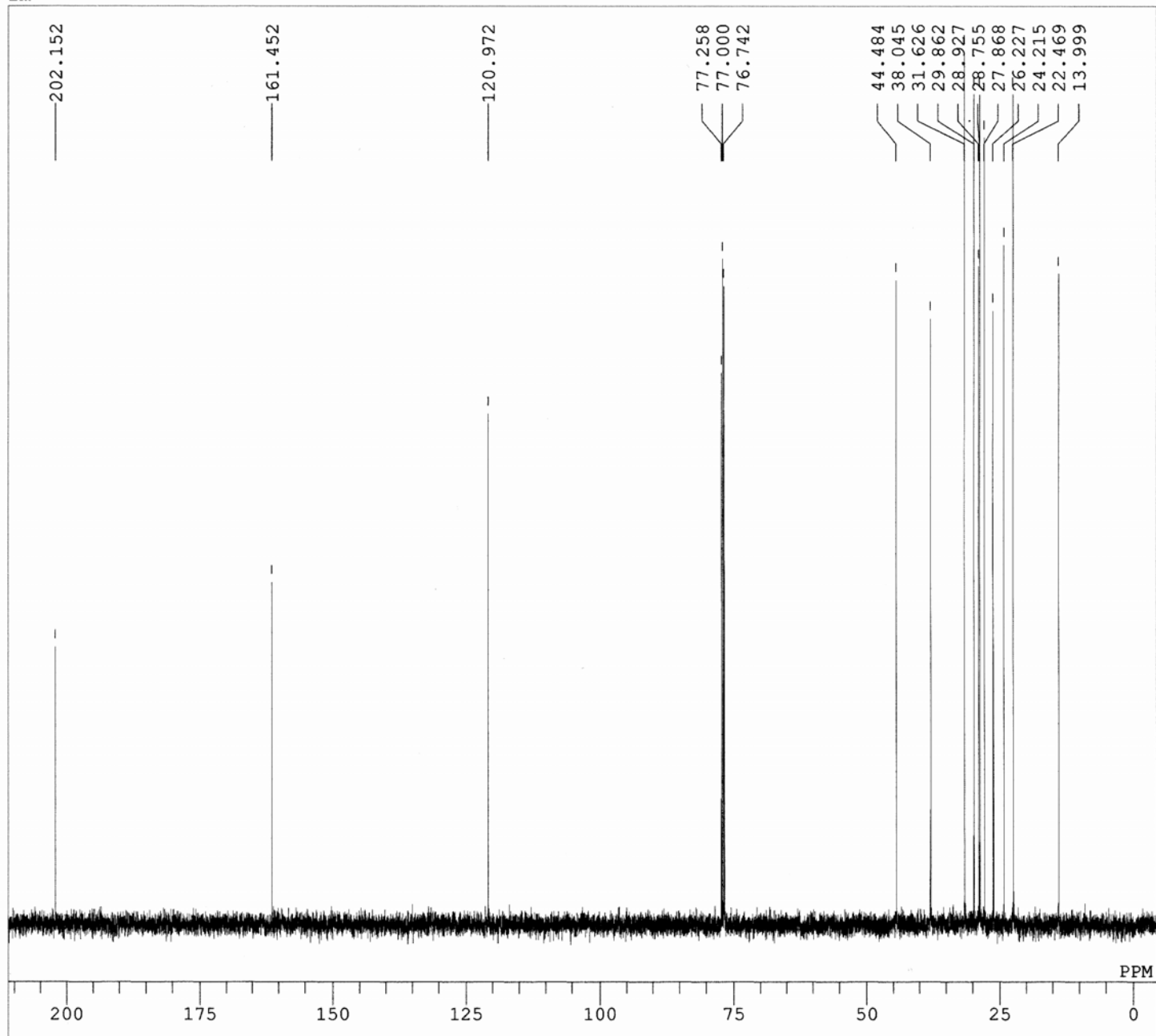
E:\3OH\Yyy04421NON_E1.als
Yyy0442



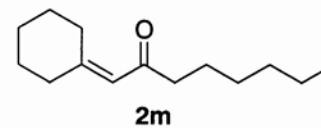
DFILE E:\3OH\Yyy04421NON_E1.als
COMNT Yyy0442
DATIM Thu Aug 30 17:22:49 2007
OBNUC 1H
EXMOD SINGL
OBFRQ 499.10 MHz
OBSET 0.00 KHz
OBFIN 125250.00 Hz
POINT 16384
FREQU 9980.04 Hz
SCANS 8
ACQTM 1.6417 sec
PD 2.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP -204.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.00 Hz
RGAIN 24



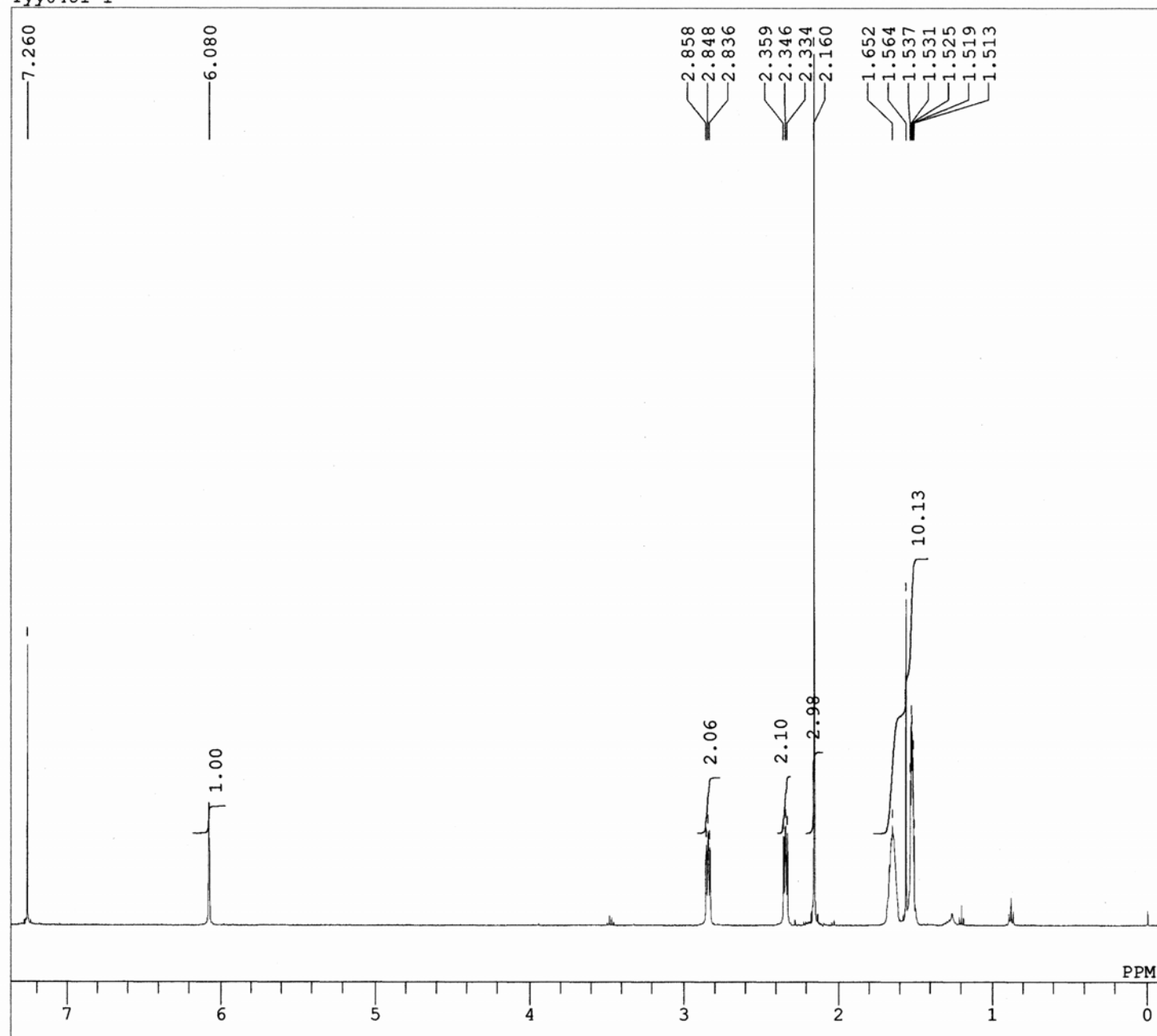
2m



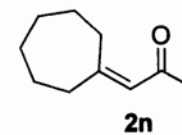
DFILE E:\M.Egi\2m.1
COMNT 2m
DATIM 20-10-2007 11:07:47
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 62
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



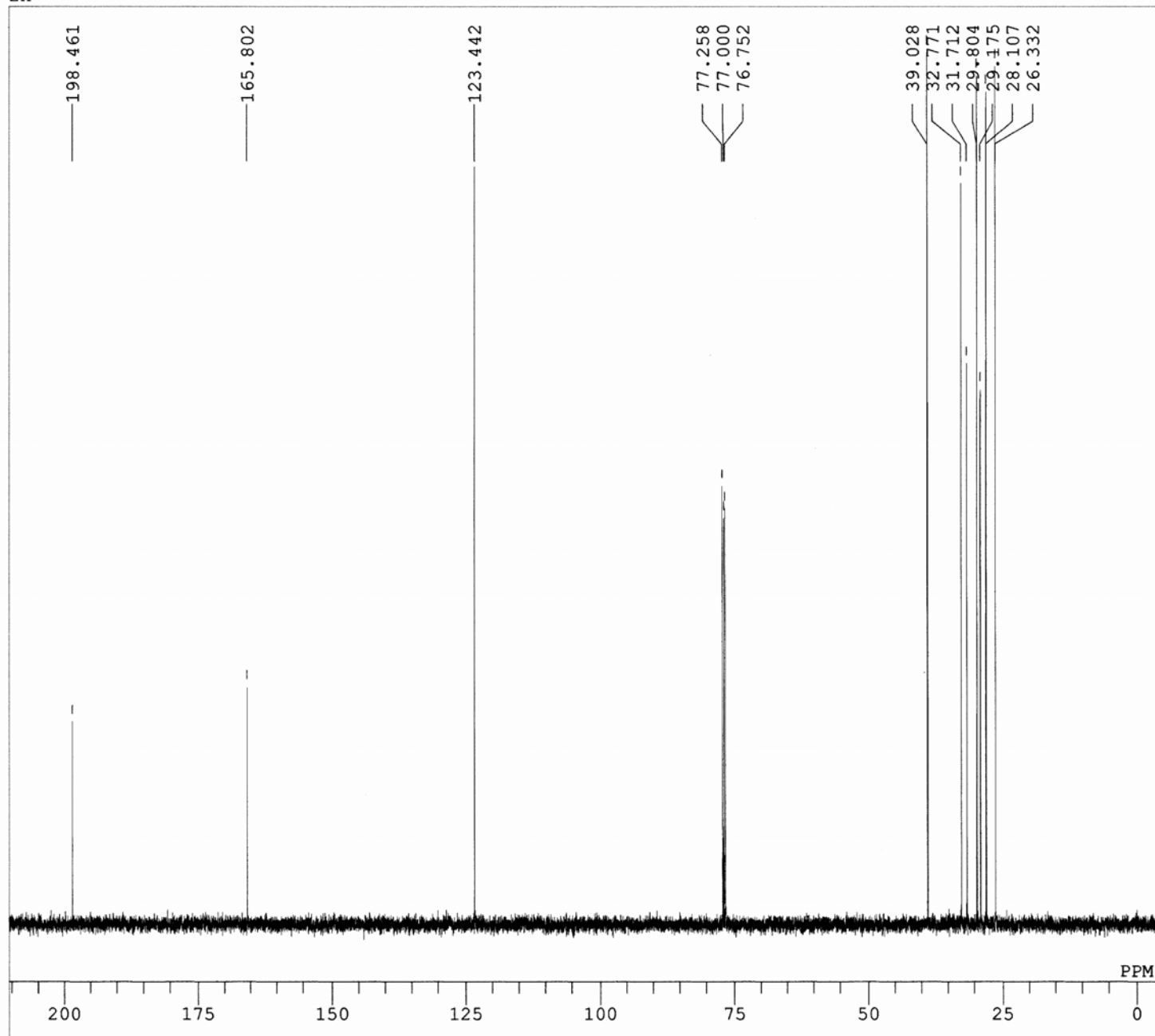
E:\3OH\Yyy0481-11NON_E1.als
Yyy0481-1



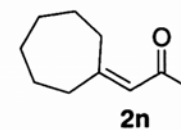
DFILE E:\3OH\Yyy0481-11NON_E1.als
COMNT Yyy0481-1
DATIM Mon Oct 22 20:39:51 2007
OBNUC 1H
EXMOD SINGL
OBFRQ 499.10 MHz
OBSET 0.00 KHz
OBFIN 125250.00 Hz
POINT 16384
FREQU 9980.04 Hz
SCANS 8
ACQTM 1.6417 sec
PD 2.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP -204.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 23



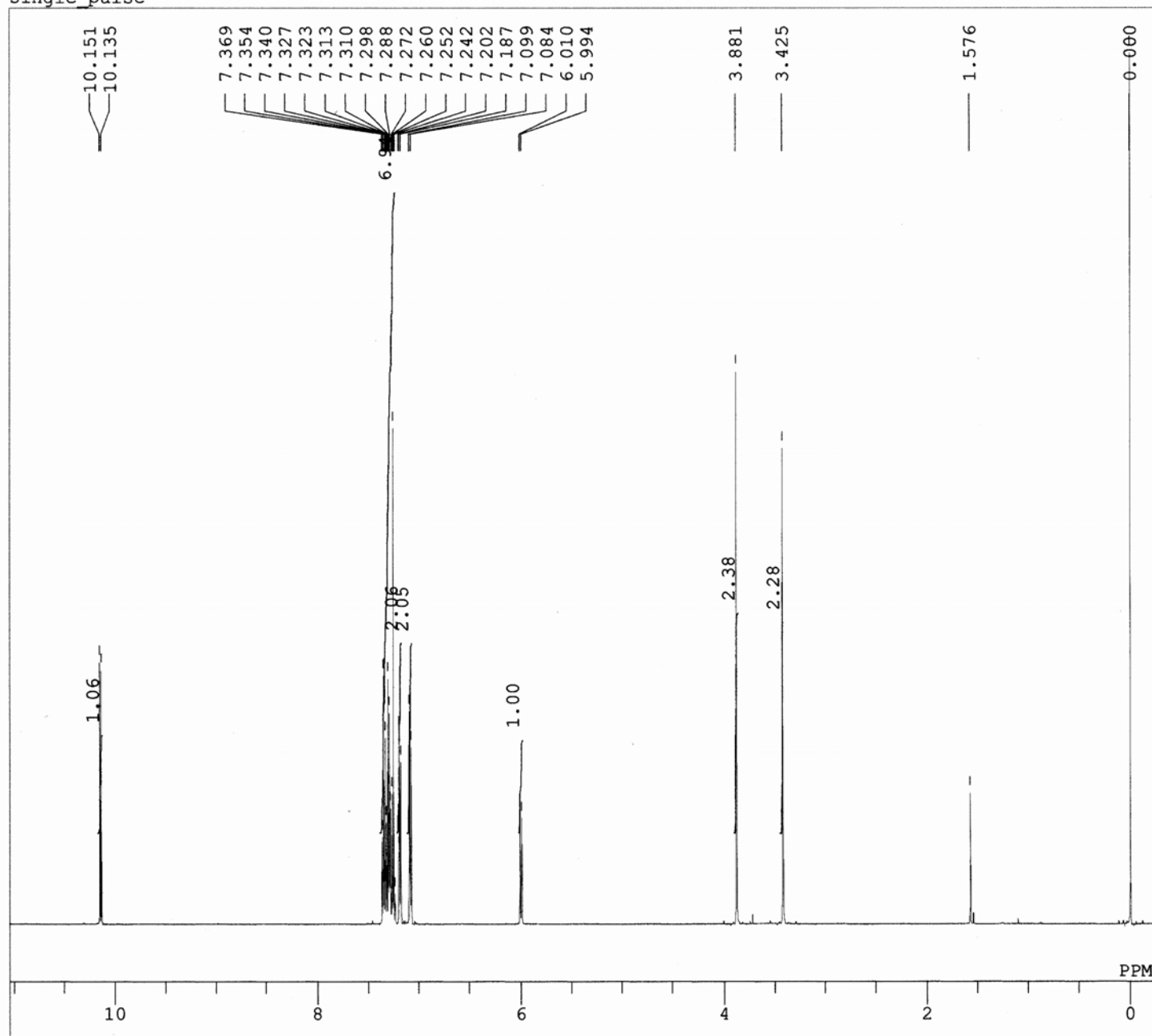
2n



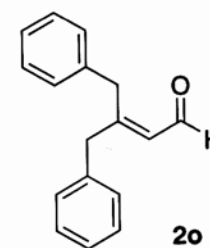
DFILE E:\M.Egi\2n.1
COMNT 2n
DATIM 09-11-2007 14:35:14
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 57
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



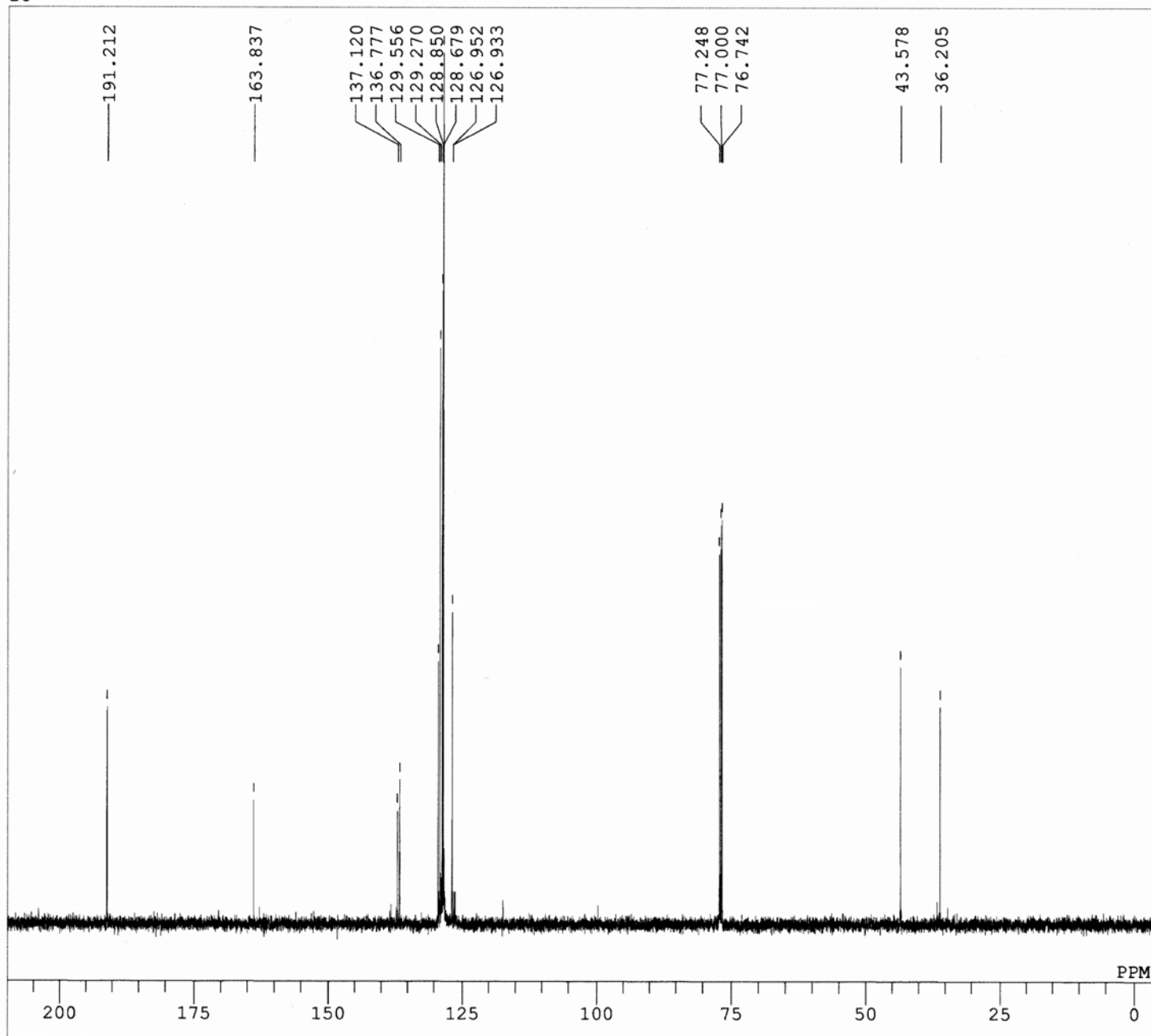
single_pulse



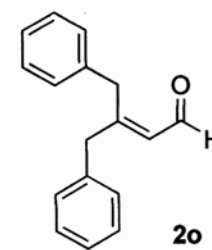
DFILE E:\NMR\aldehyde\2o\Yyy-2o.als
 COMNT single_pulse
 DATIM 28-01-2008 17:57:53
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.39 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 1.5000 sec
 PW1 6.00 usec
 IRNUC 1H
 CTEMP 16.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 50



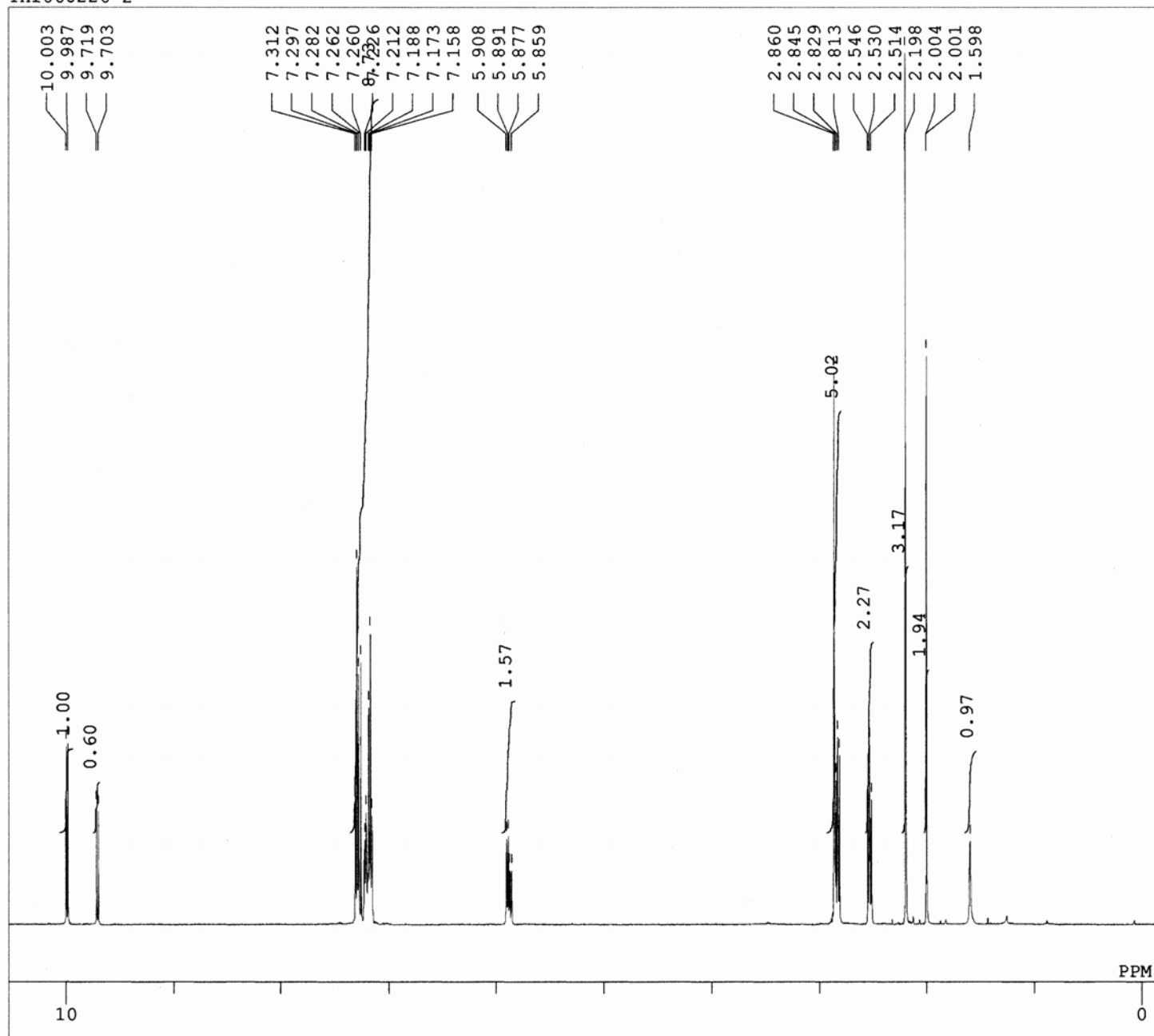
2o



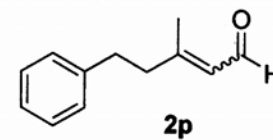
DFILE E:\M.Egi\2o.1
COMNT 2o
DATIM 04-10-2007 14:32:57
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 61
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 50



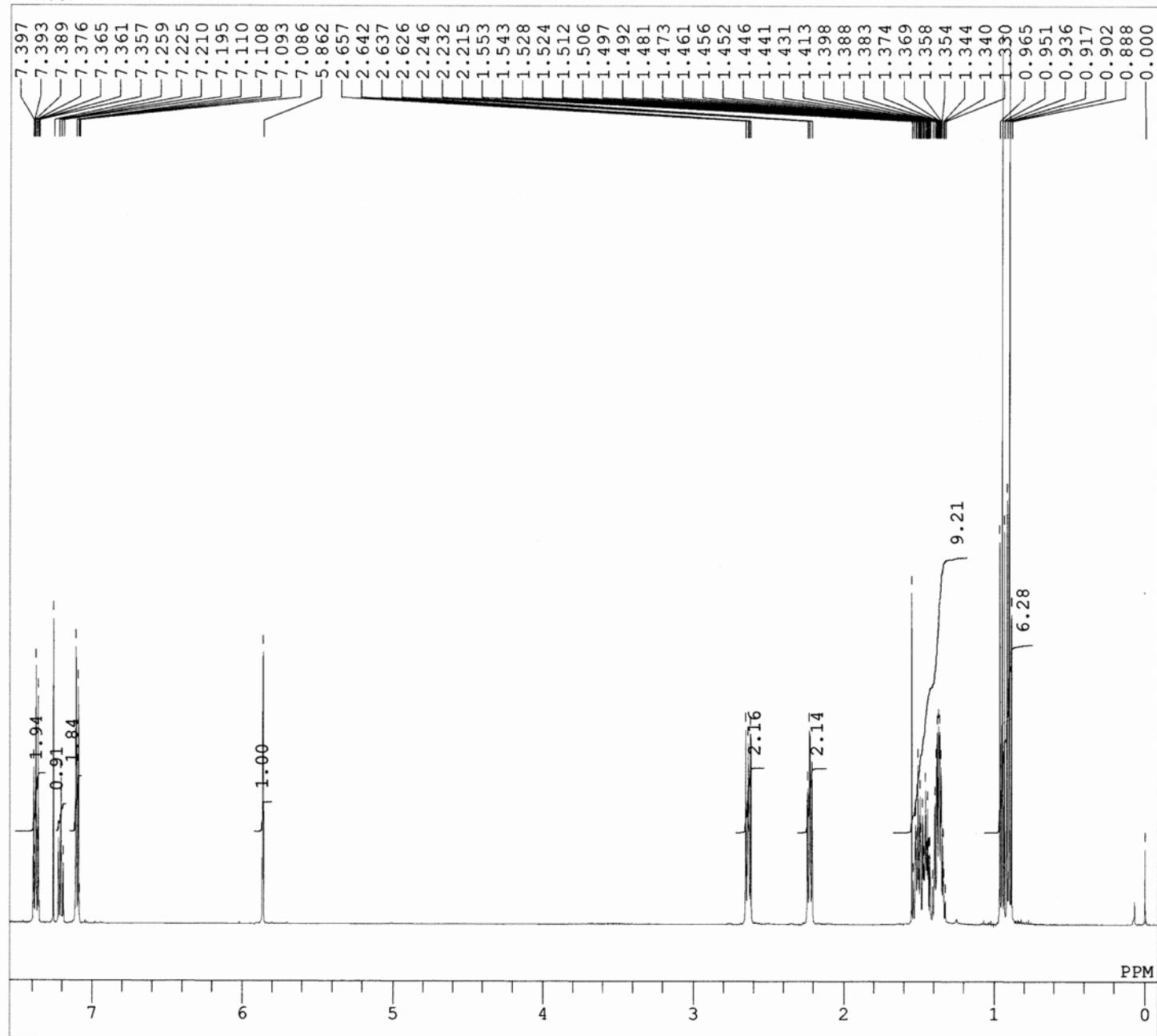
F:\060221-060230\060226\Ynf060226-2.als
Ynf060226-2



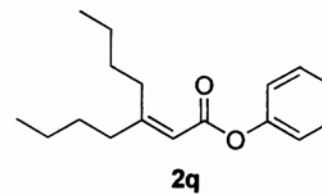
DFILE F:\060221-060230\060226\Ynf060226-2
COMNT Ynf060226-2
DATIM 03-09-2007 16:46:23
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.39 Hz
SCANS 16
ACQTM 1.7459 sec
PD 1.5000 sec
PW1 6.00 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.00 Hz
RGAIN 50



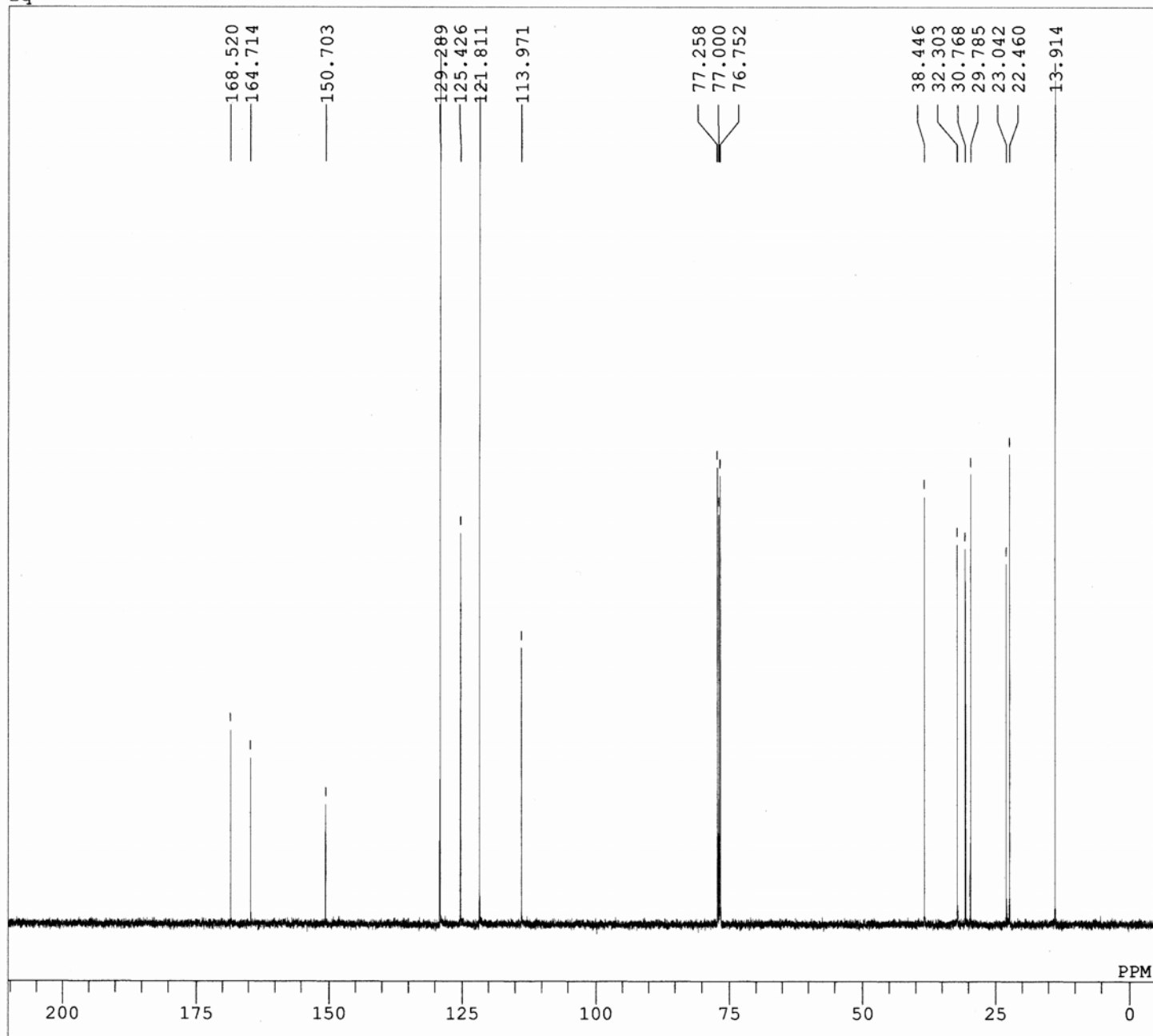
E:\ester type\Yka0052.als
Yka0052



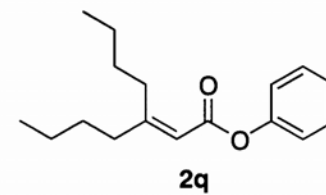
DFILE E:\ester type\Yka0052.als
COMNT Yka0052
DATIM 29-09-2007 18:00:23
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.39 Hz
SCANS 8
ACQTM 1.7459 sec
PD 1.5000 sec
PW1 6.00 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 48



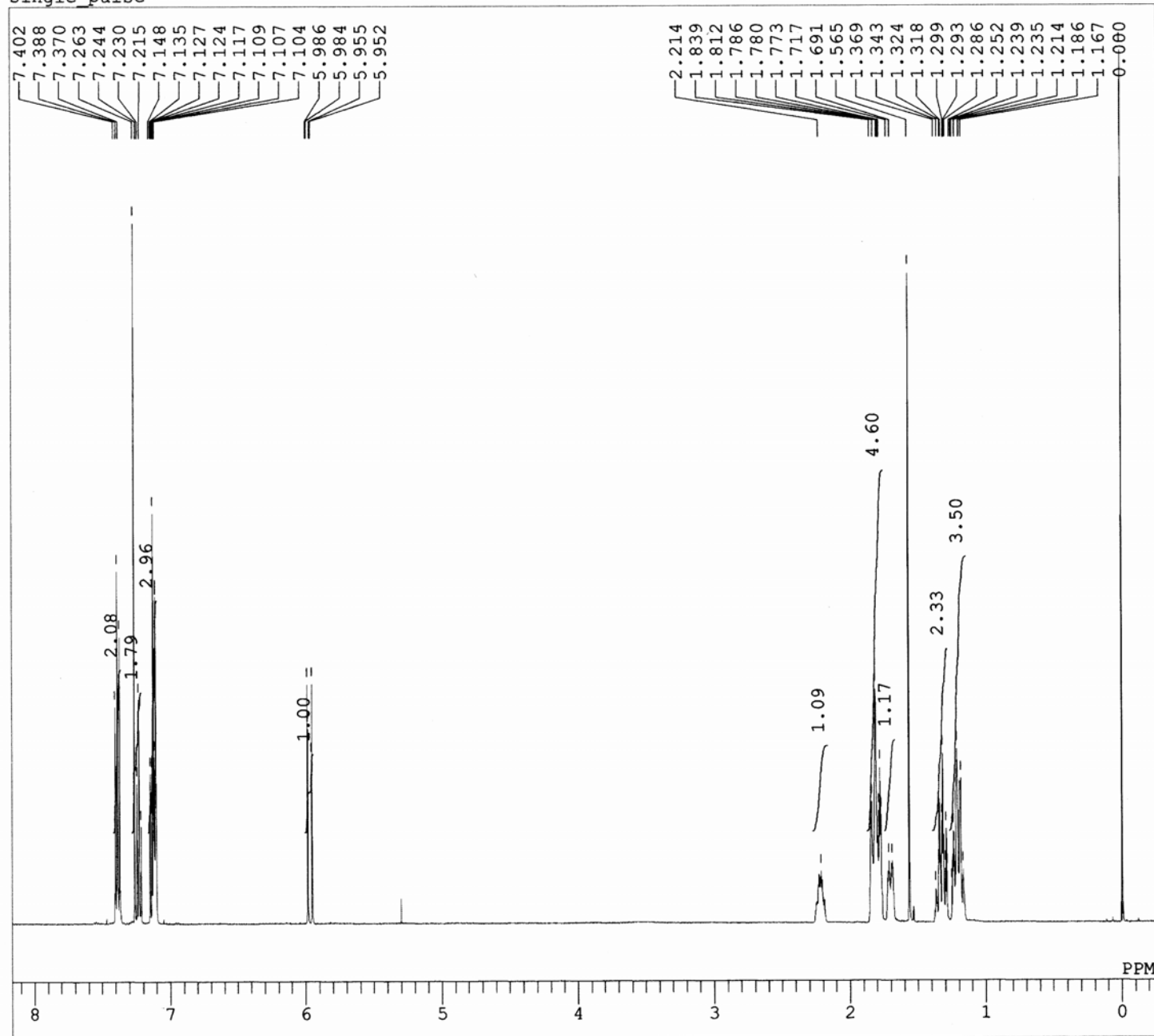
2q



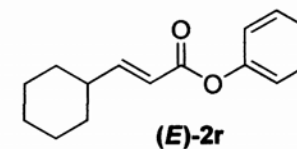
DFILE E:\M.Egi\2q.1
COMNT 2q
DATIM 01-10-2007 15:48:17
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 244
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



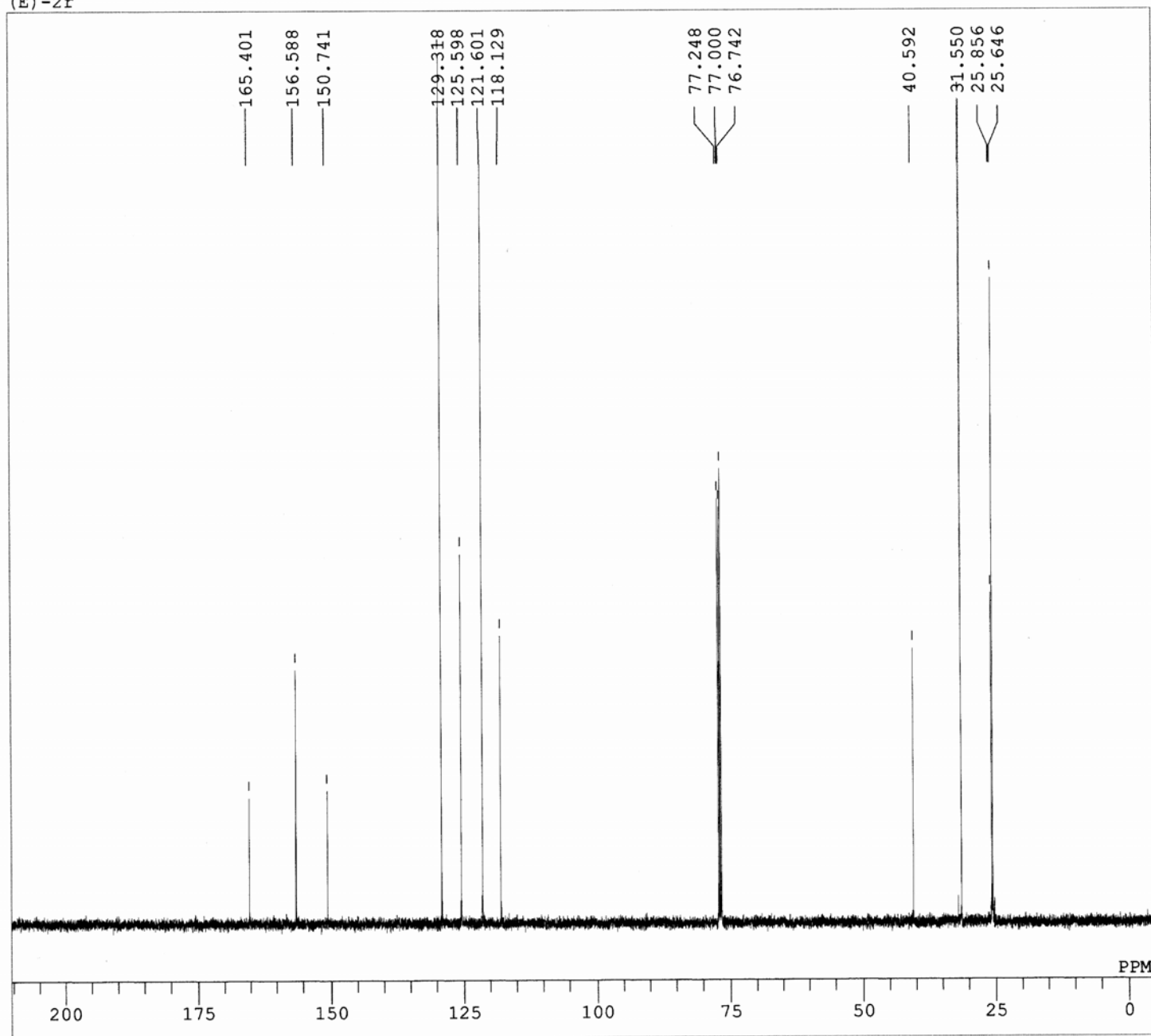
single_pulse



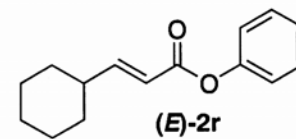
DFILE F:\NMR (ŽRĚŮ)\ester type\2r\E-2r
 COMNT single_pulse
 DATIM 26-01-2008 13:30:07
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.39 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 1.5000 sec
 PW1 6.00 usec
 IRNUC 1H
 CTEMP 16.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 50



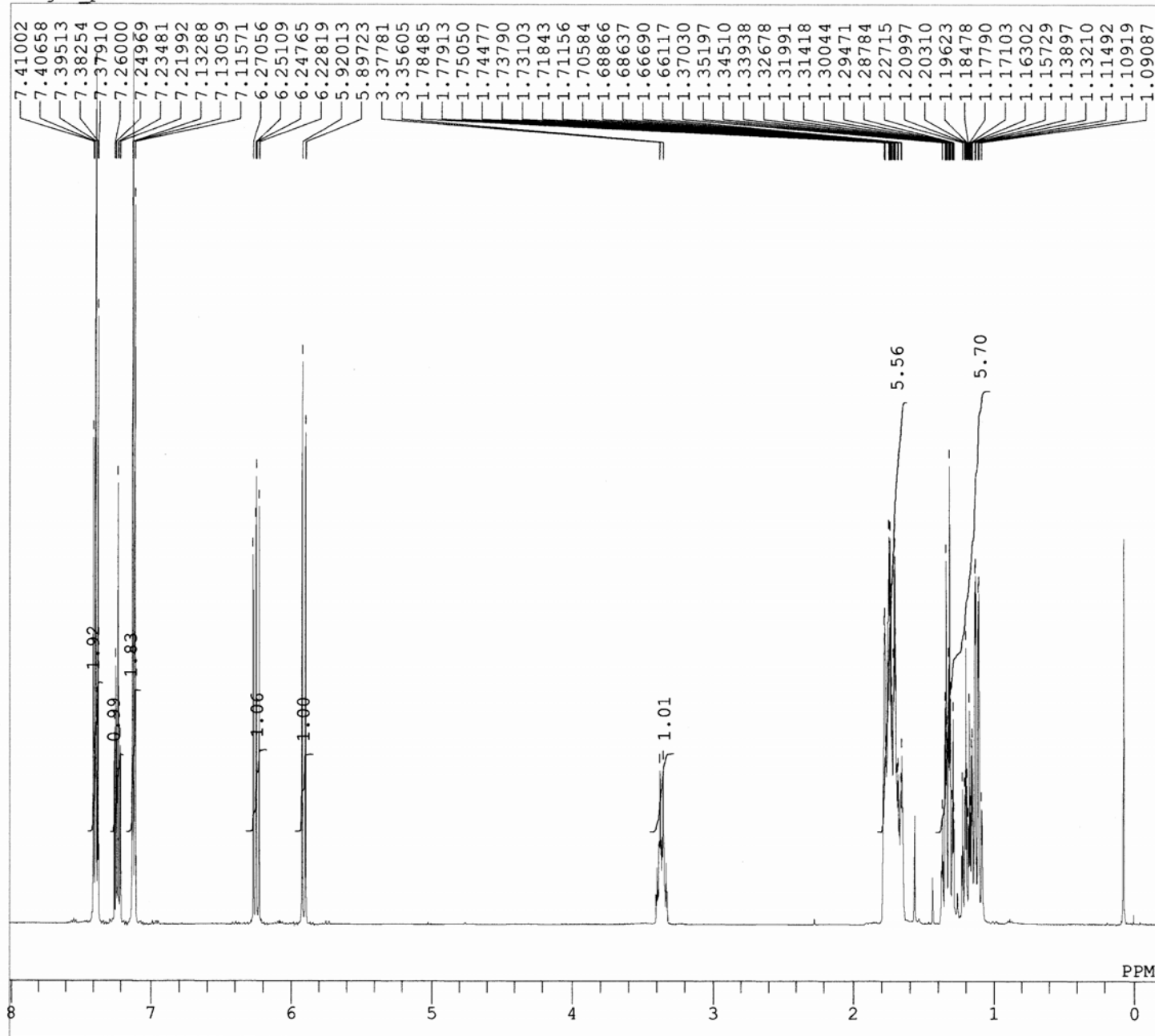
(E)-2r



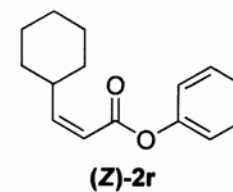
DFILE E:\M.Egi\2r (E).1
COMNT (E)-2r
DATIM 25-10-2007 16:21:57
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 128
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



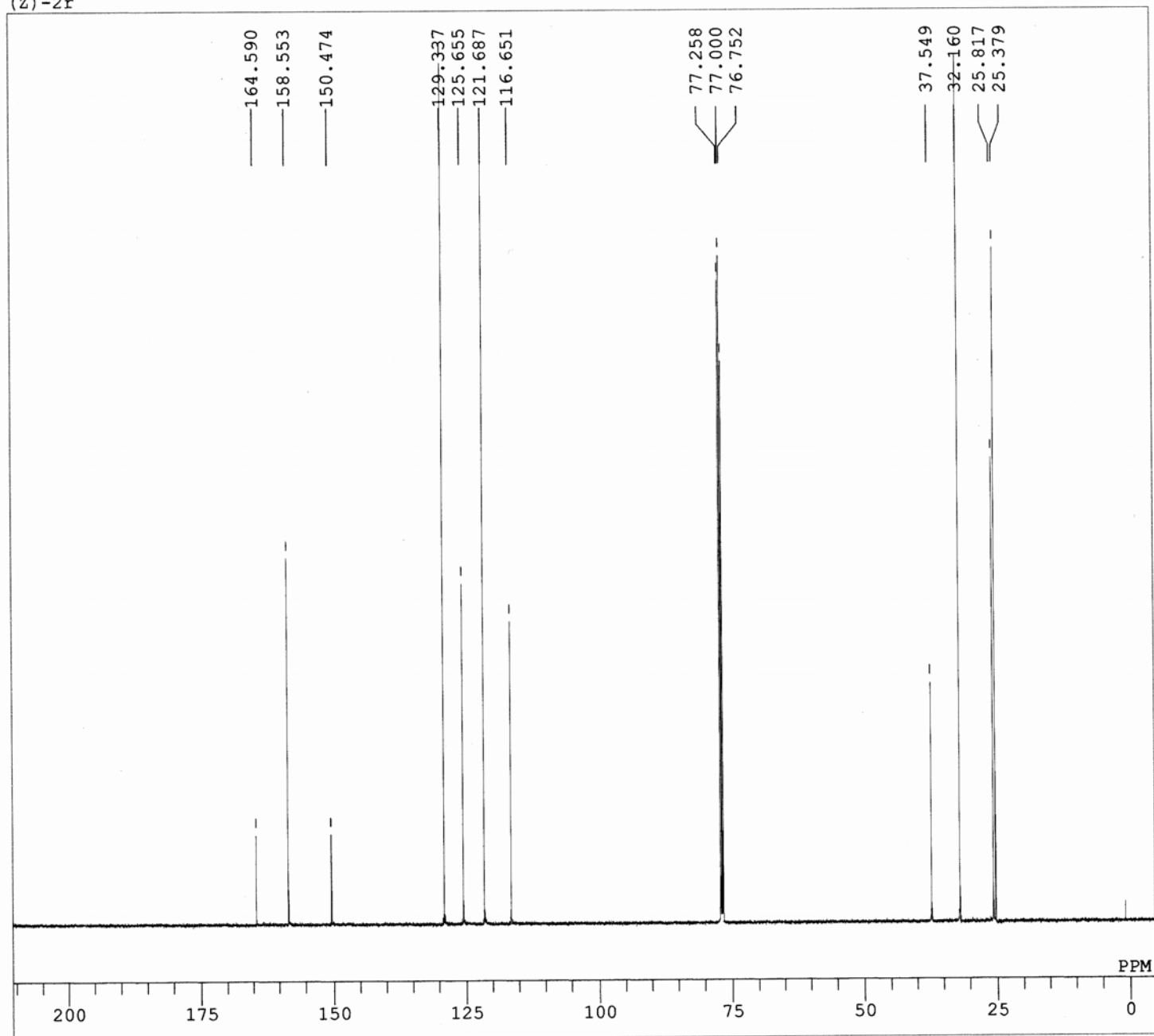
single_pulse



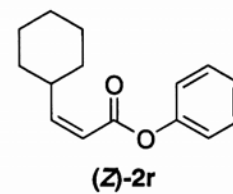
DFILE F:\NMR (ZrE0)\ester type\2r\Z-2r
 COMNT single_pulse
 DATIM 21-01-2008 13:16:37
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.39 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 1.5000 sec
 PW1 6.00 usec
 IRNUC 1H
 CTEMP 16.4 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 40



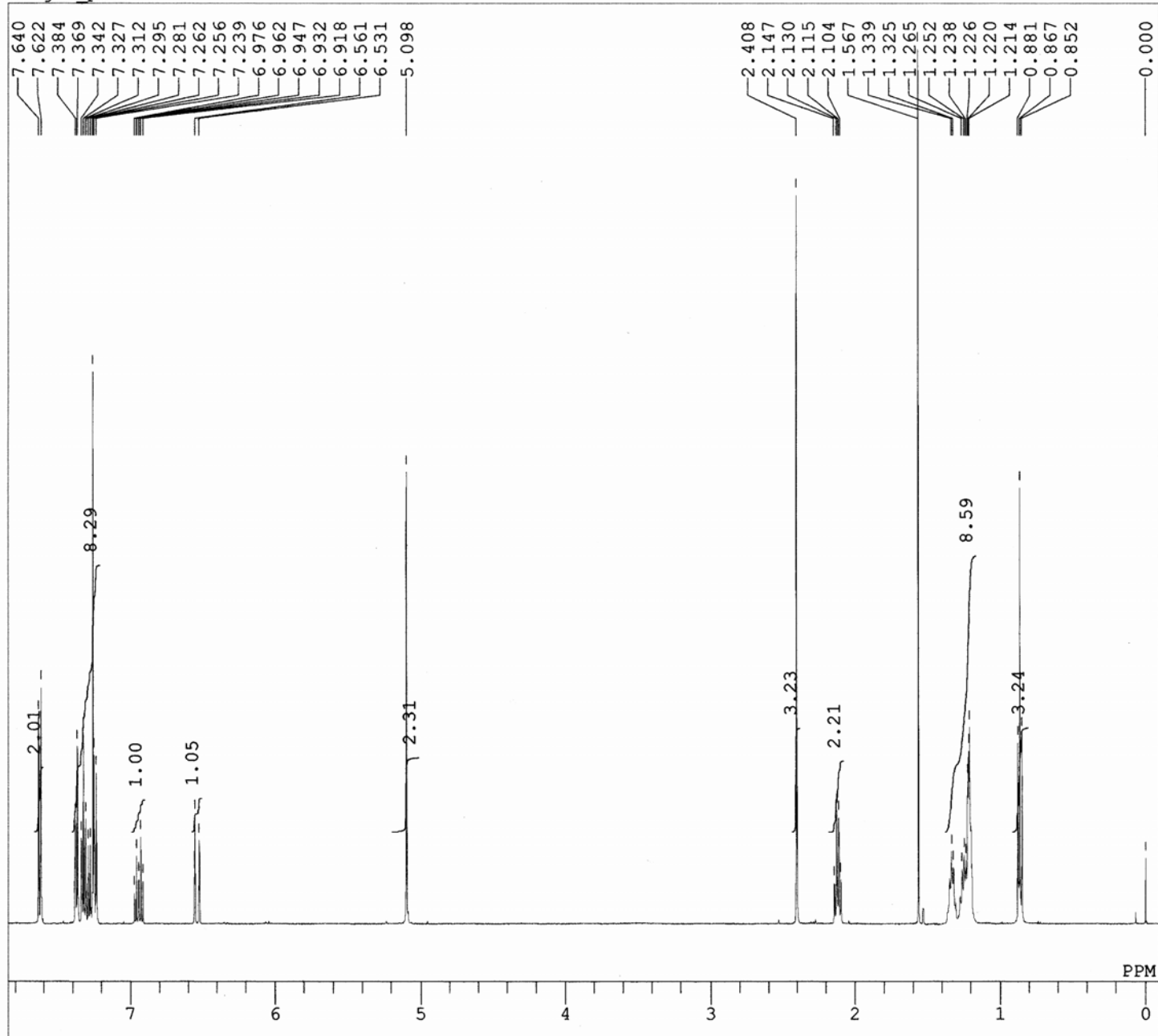
(Z)-2r



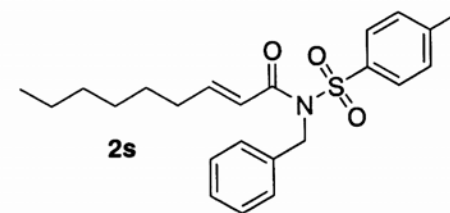
DFILE E:\M.Egi\2r (Z).1
COMNT (Z)-2r
DATIM 21-01-2008 15:40:13
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 2962
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 16.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60



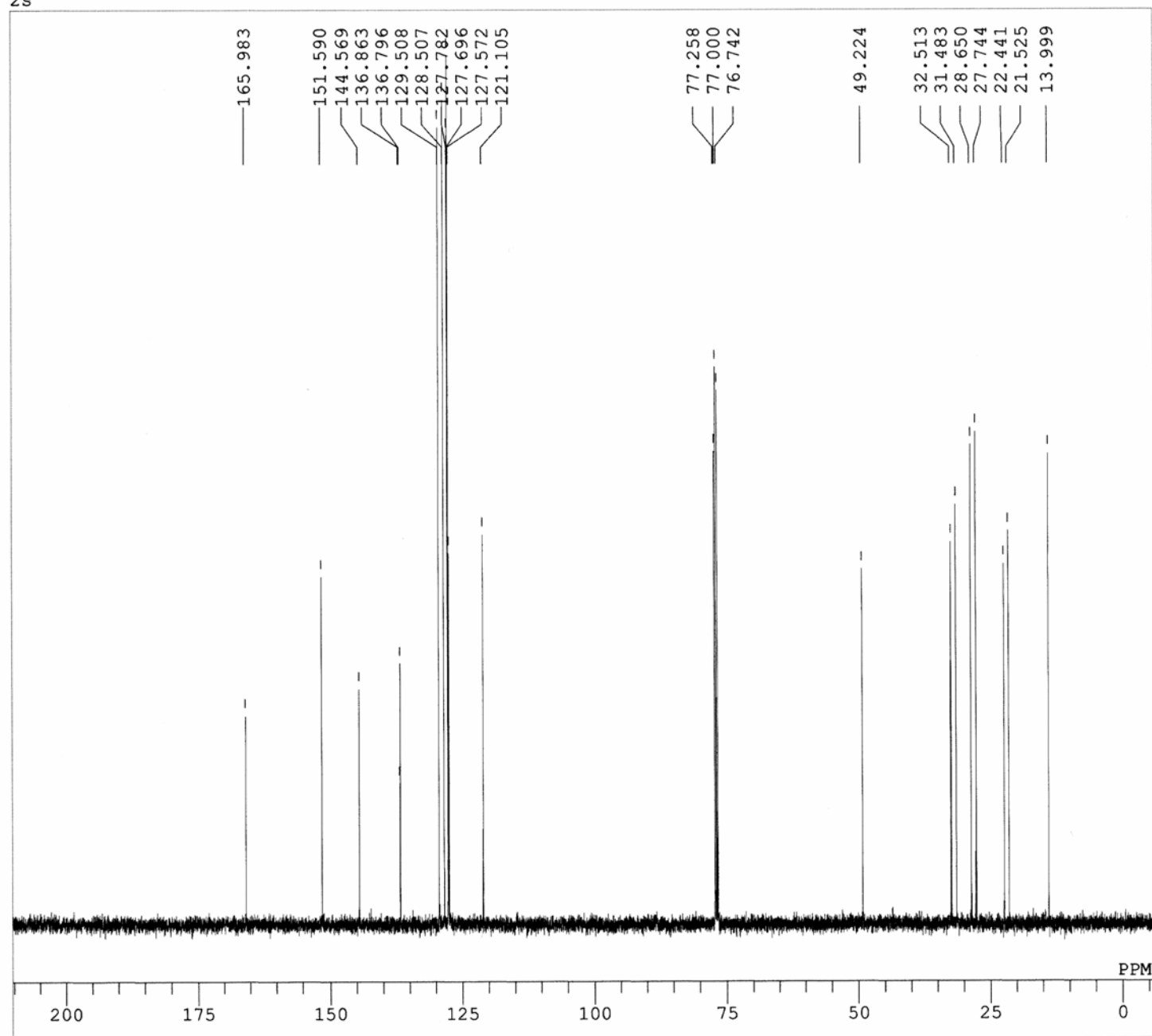
single_pulse



DFILE E:\NMR\amide type\2t\Yyy0472-1
 COMNT single_pulse
 DATIM 06-10-2007 17:09:59
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.39 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 1.5000 sec
 PW1 6.00 usec
 IRNUC 1H
 CTEMP 20.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 50



2s



DFILE E:\M.Egi\2s.1
COMNT 2s
DATIM 22-10-2007 16:12:08
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 40961
FREQU 49135.97 Hz
SCANS 88
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.00 Hz
RGAIN 60

