Supporting Information

Chemoselective Transformations of Aromatic Methoxymethyl Ethers Using Trialkylsilyl Triflate and 2,2'-Bipyridyl

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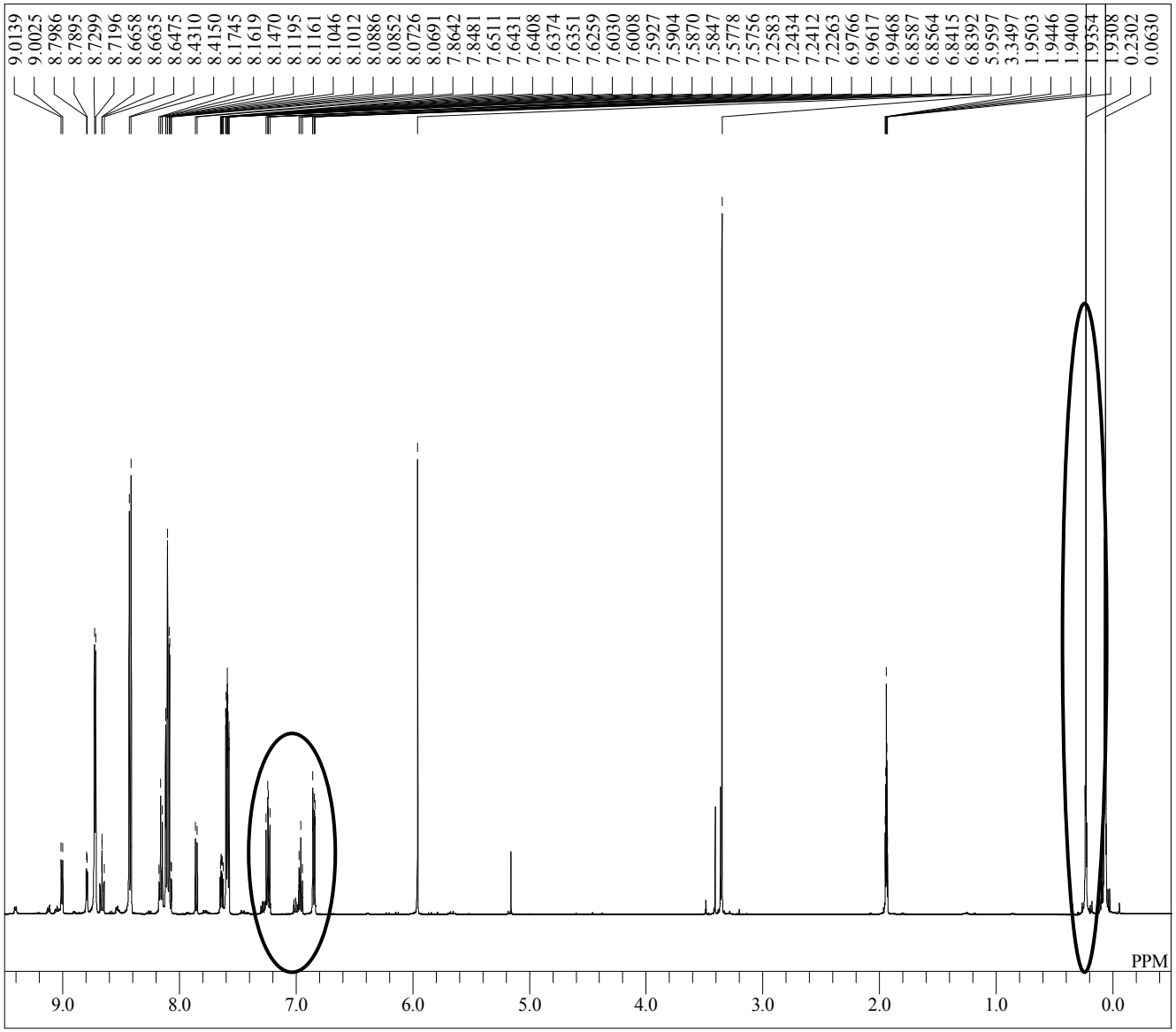

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OBNUC	1H
EXMOD	proton.jxp
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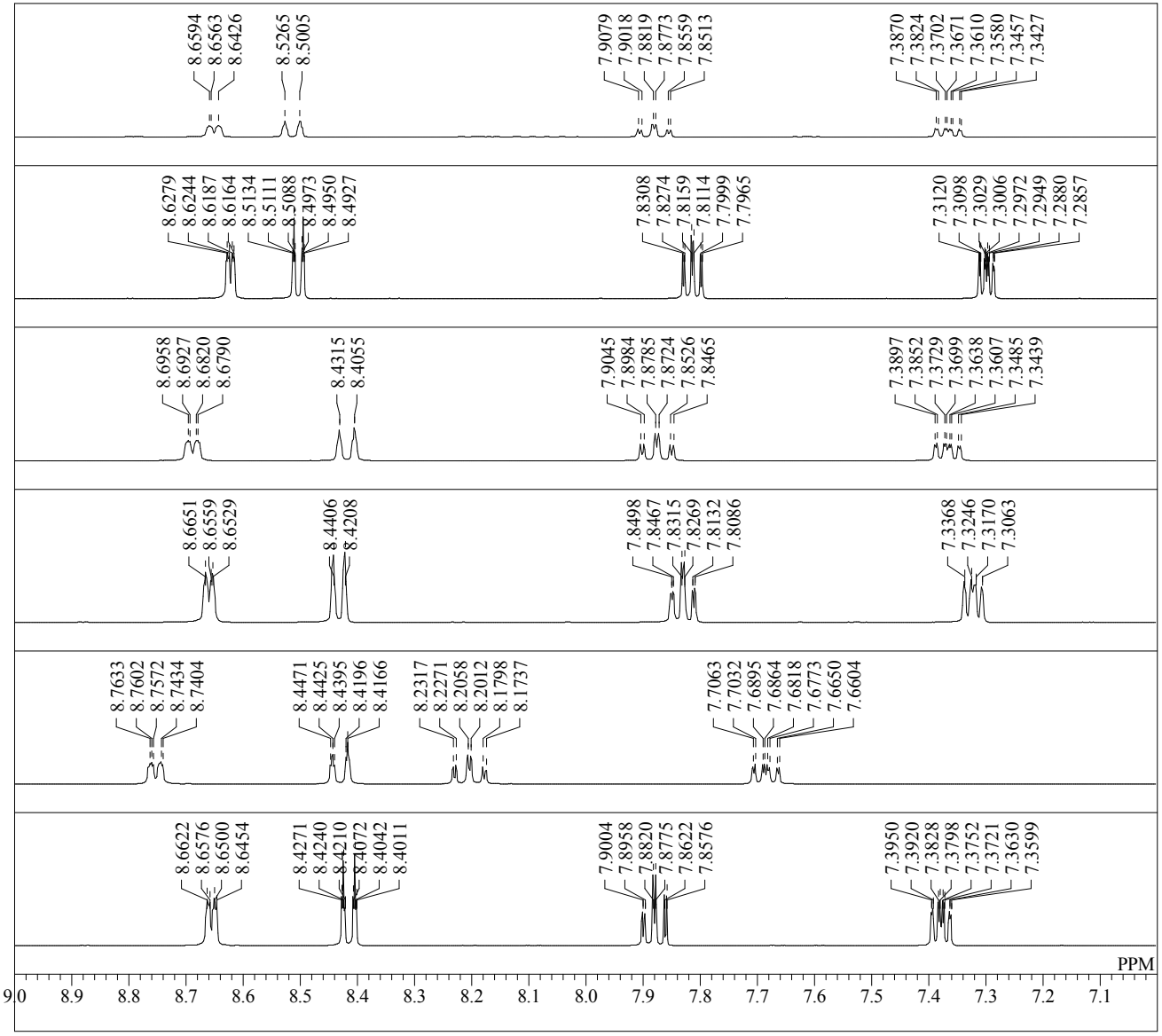
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	16
ACQTM	1.7459 sec
PD	2.0000 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	23.6 c
SLVNT	CD3CN
EXREF	1.94 ppm
BF	0.12 Hz
RGAIN	30

Reference 3, NMR spectroscopy in CD_3CN. The peak of enclosed by the circle is that of TMS ether of phenol.

Figure S1



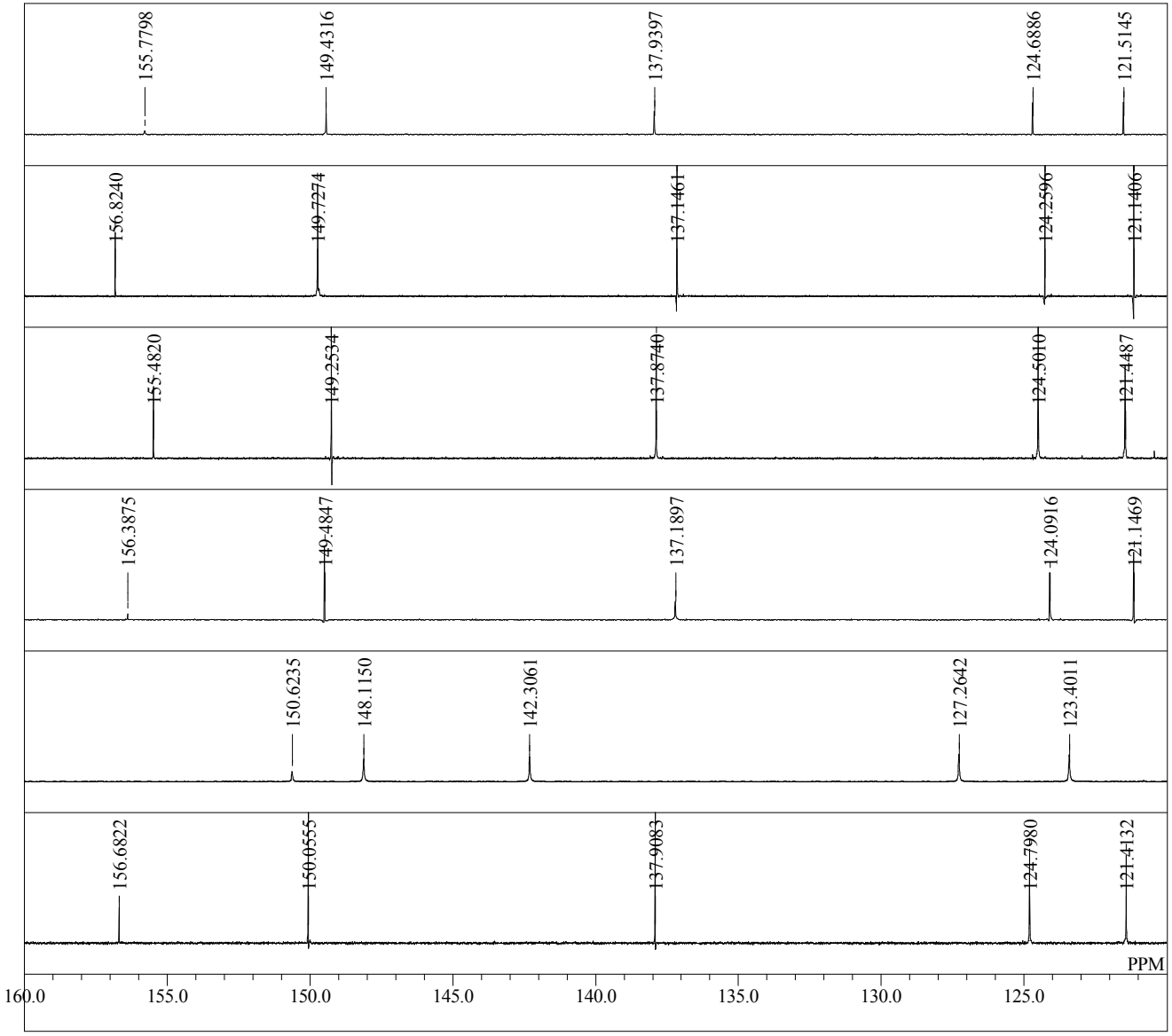
DFILE	yanagihara NMRex CD3CN 2,2_-bipyridy
COMNT	single_pulse
DATIM	2019-01-28 21:21:34
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	8000.00 Hz
SCANS	16
ACQTM	1.6384 sec
PD	2.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	18.8 c
SLVNT	CD3CN
EXREF	1.94 ppm
BF	0.12 Hz
RGAIN	42

In order from the top,

- 2,2’-bipyridyl and TMSOTf in THF-d8
- 2,2’-bipyridyl only in THF-d8
- 2,2’-bipyridyl and TMSOTf in CD_2Cl_2
- 2,2’-bipyridyl only in CD_2Cl_2
- 2,2’-bipyrisyl and TMSOTf in CD_3CN
- 2,2’-bipyridyl only in CD3CN

Remarkable chemical shift was observed only in CD_3CN.

Figure S2



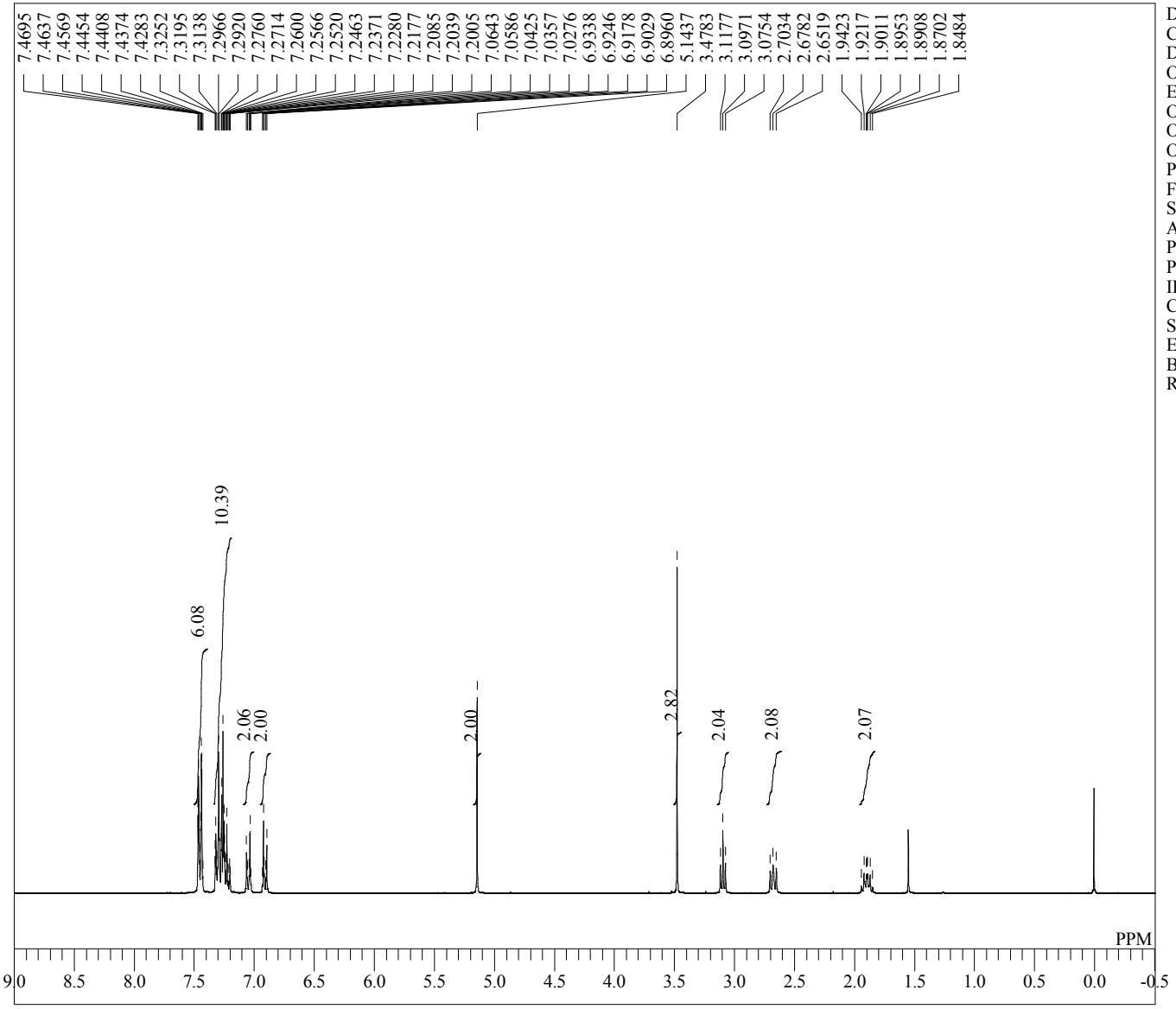
DFILE	yanagihara NMRex 2,2_-bipyrisyl CD3CN
COMNT	single pulse decoupled gated NOE
DATIM	2019-02-03 17:18:32
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	119
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CD3CN
EXREF	118.20 ppm
BF	0.12 Hz
RGAIN	60

In order from the top,

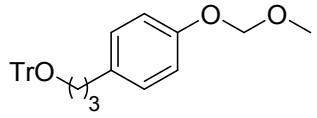
- 2,2'-bipyridyl and TMSOTf in THF-d8
- 2,2'-bipyridyl only in THF-d8
- 2,2'-bipyridyl and TMSOTf in CD_2Cl_2
- 2,2'-bipyridyl only in CD_2Cl_2
- 2,2'-bipyrisyl and TMSOTf in CD_3CN
- 2,2'-bipyridyl only in CD3CN

Remarkable chemical shift was observed only in CD_3CN.

Figure S3

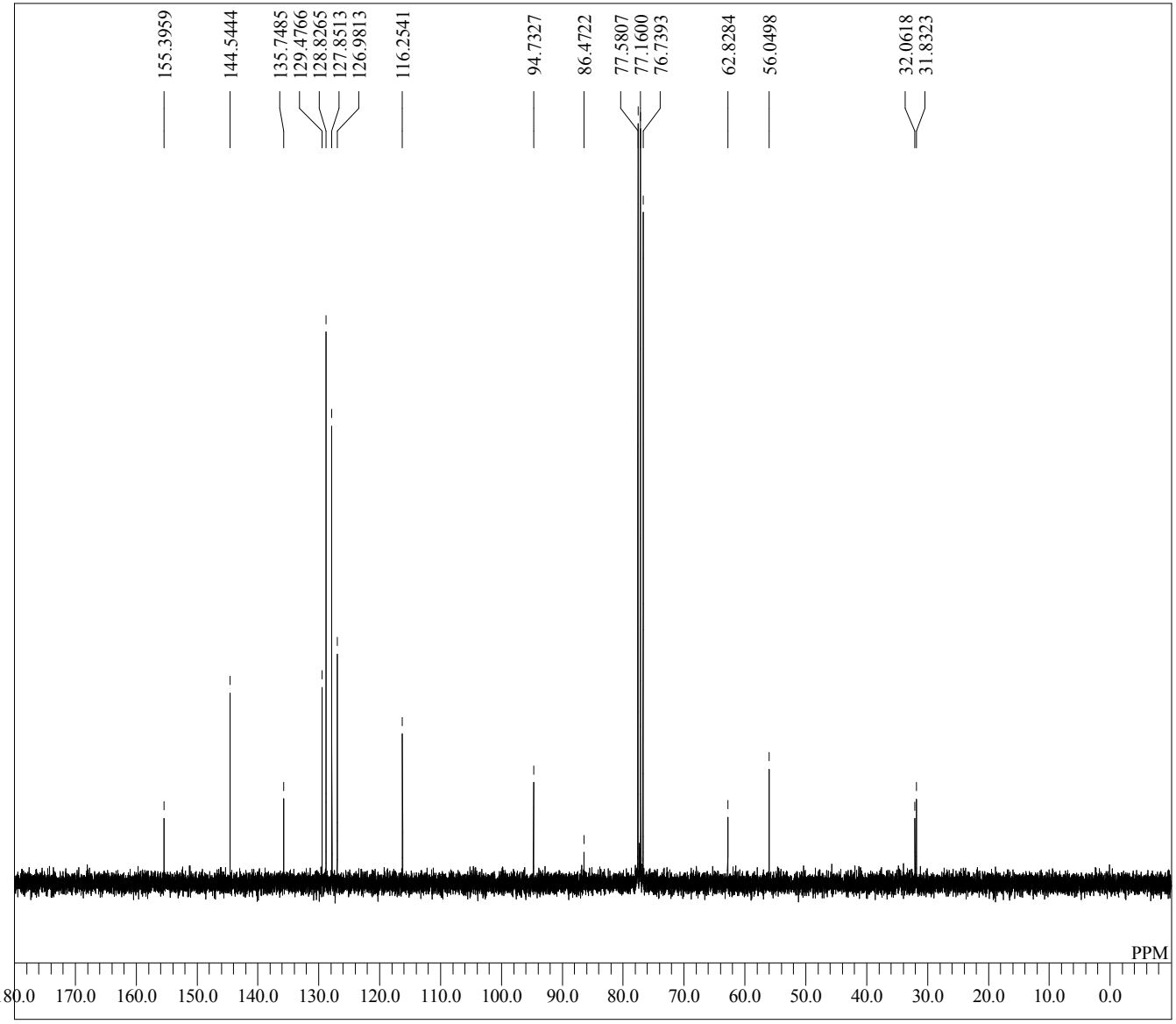


DFILE	yanagihara MOM Tr 1H_proton-1-1.als
COMNT	single_pulse
DATIM	2018-03-20 13:50:41
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	300.53 MHz
OBSET	1.15 KHz
OBFIN	8.57 Hz
POINT	13107
FREQU	4508.57 Hz
SCANS	16
ACQTM	2.9072 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.8 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	40

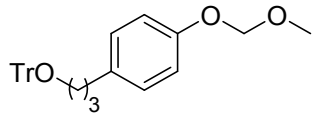


1g

Figure S4

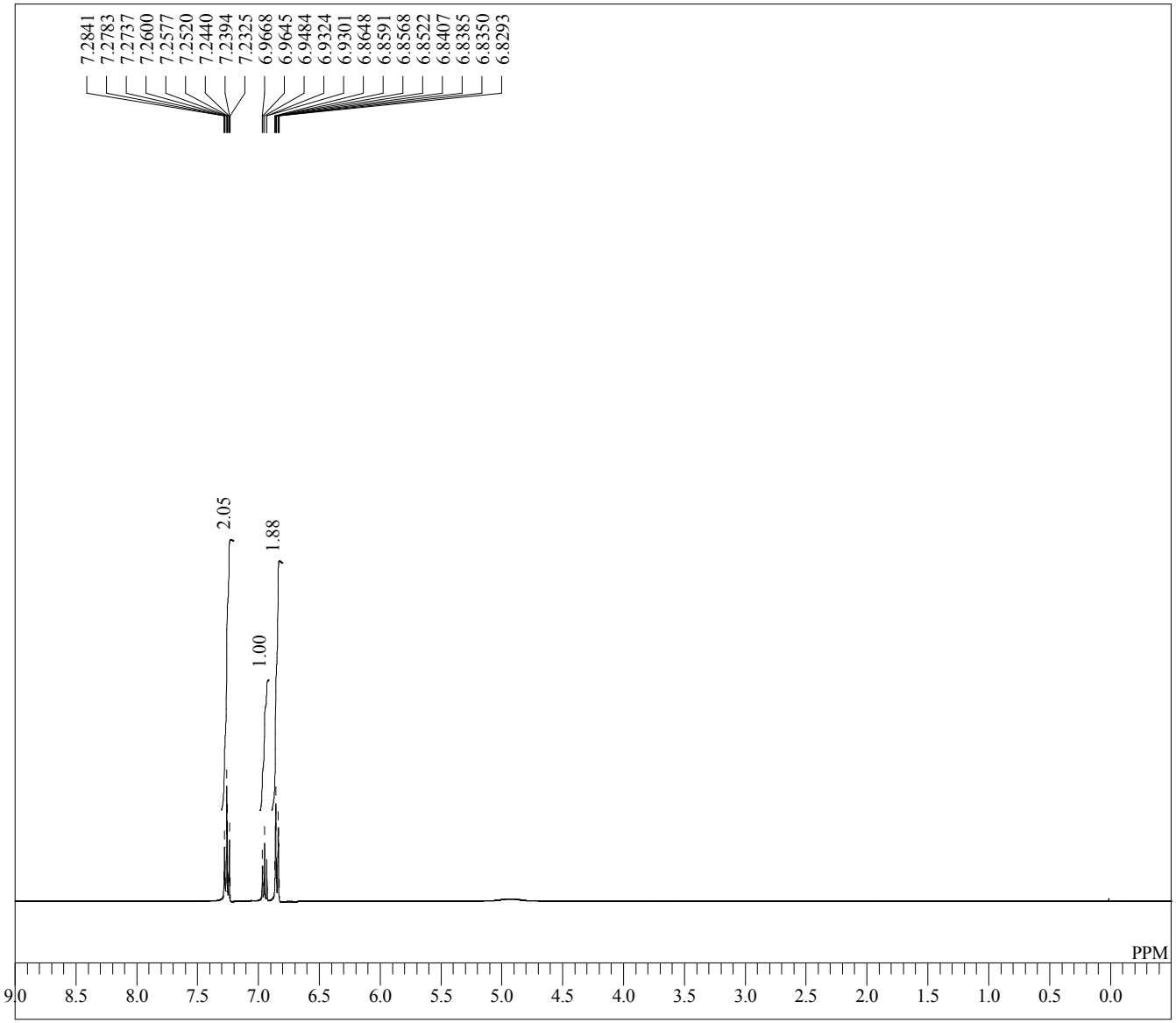


DFILE	yanagihara MOM Tr 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-03-20 13:54:12
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	75.57 MHz
OBSET	5.79 KHz
OBFIN	1.08 Hz
POINT	26214
FREQU	18939.39 Hz
SCANS	394
ACQTM	1.3841 sec
PD	2.5000 sec
PW1	3.73 usec
IRNUC	1H
CTEMP	20.0 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

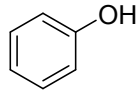


1g

Figure S5

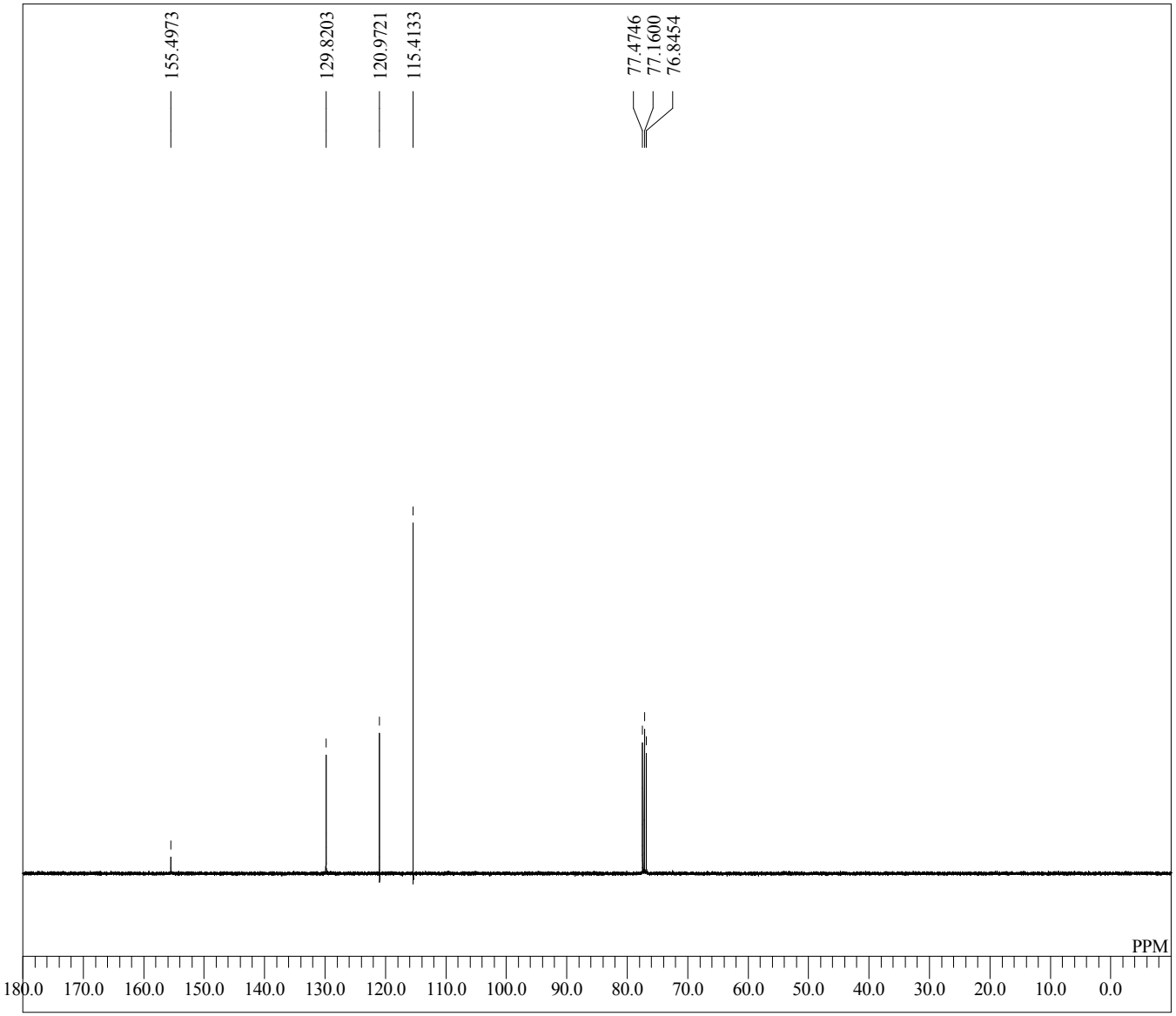


DFILE	yanagihara OH no 1H_proton-1-1.als
COMNT	single_pulse
DATIM	2018-05-15 21:34:57
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	42



2a

Figure S6



DFILE	yanagihara OH no 13C_carbon-1-1.als
COMNT	single pulse decoupled gated NOE
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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	297
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

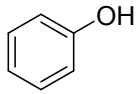

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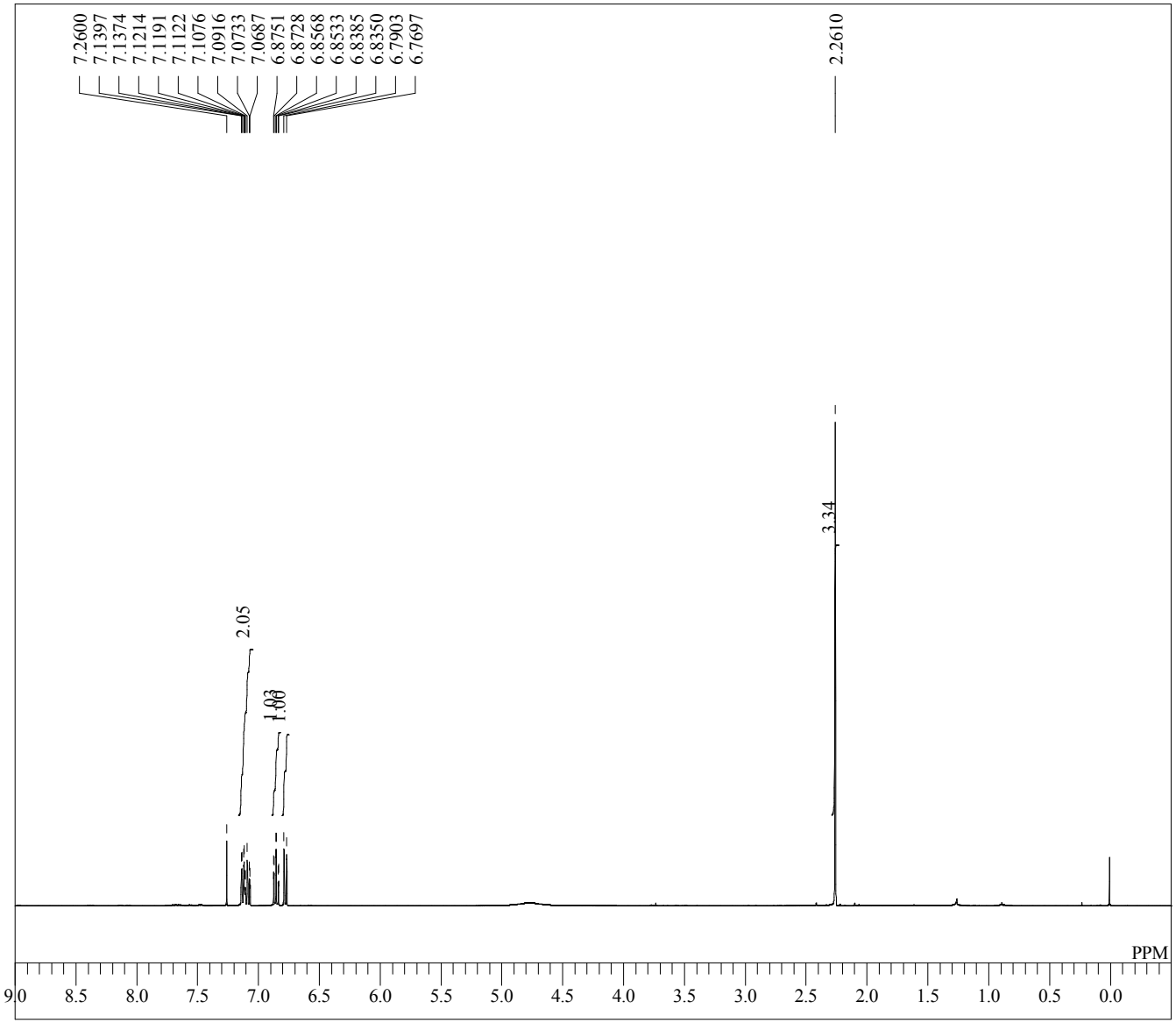
Figure S7



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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	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.2 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

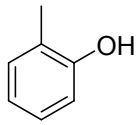

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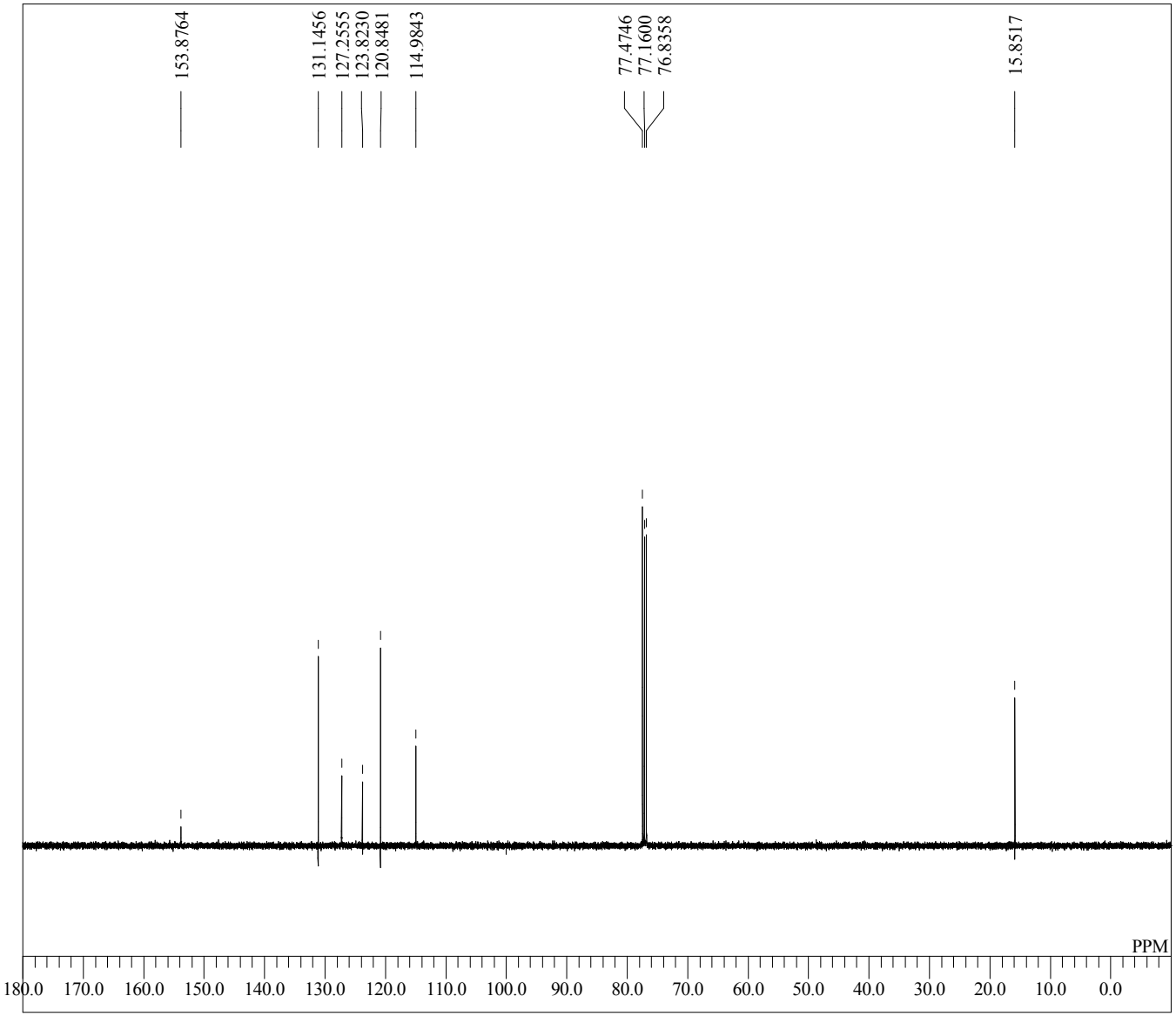
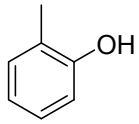
Figure S8

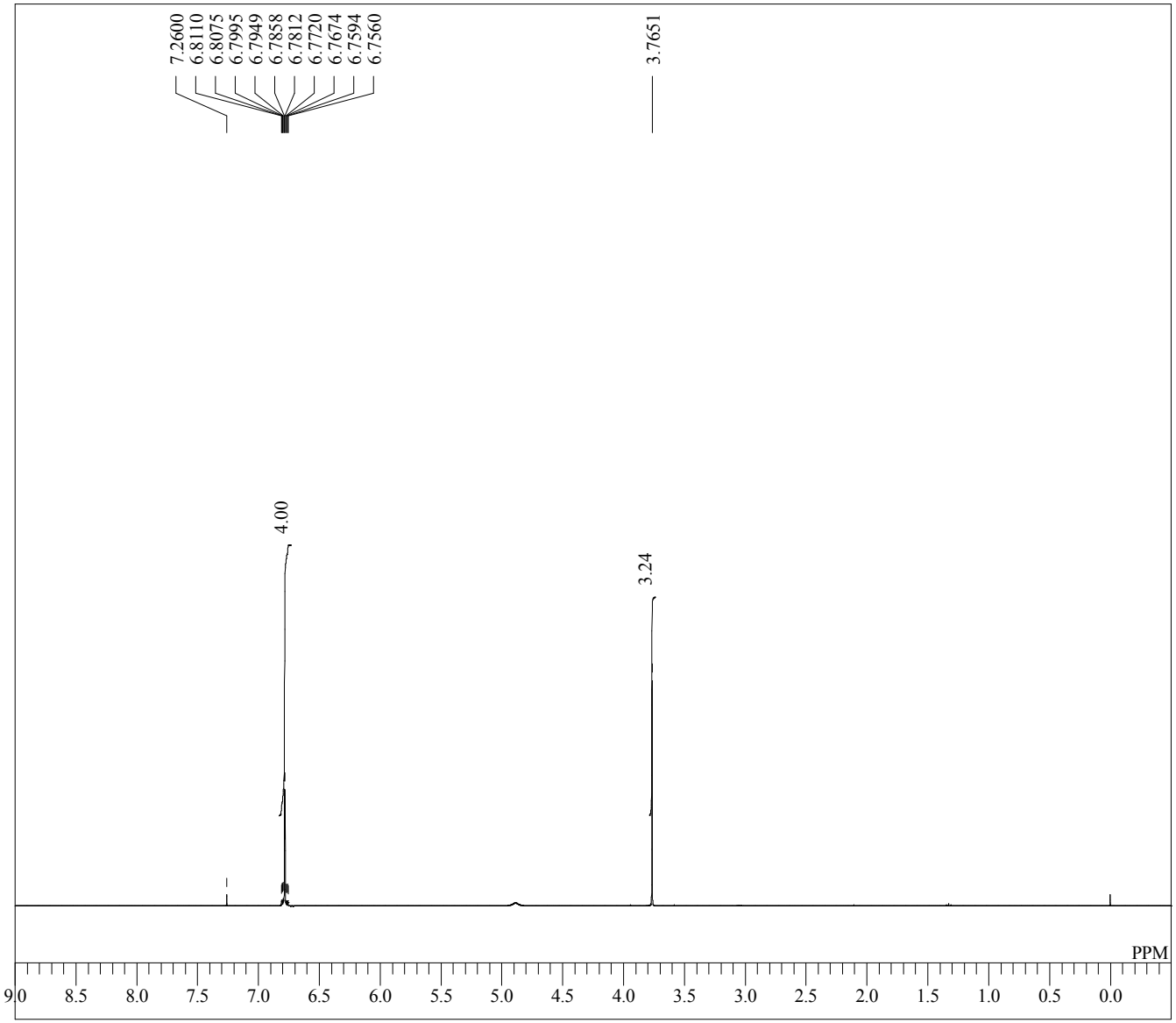


DFILE	yanagihara OH Me 13C_carbon-1-1.al
COMNT	single pulse decoupled gated NOE
DATIM	2018-05-16 10:30:15
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	325
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60



2b

Figure S9



DFILE	yanagihara OH OMe 1H_proton-1-1.al
COMNT	single_pulse
DATIM	2018-05-15 22:02:57
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.3 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	42

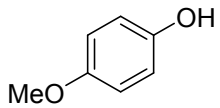


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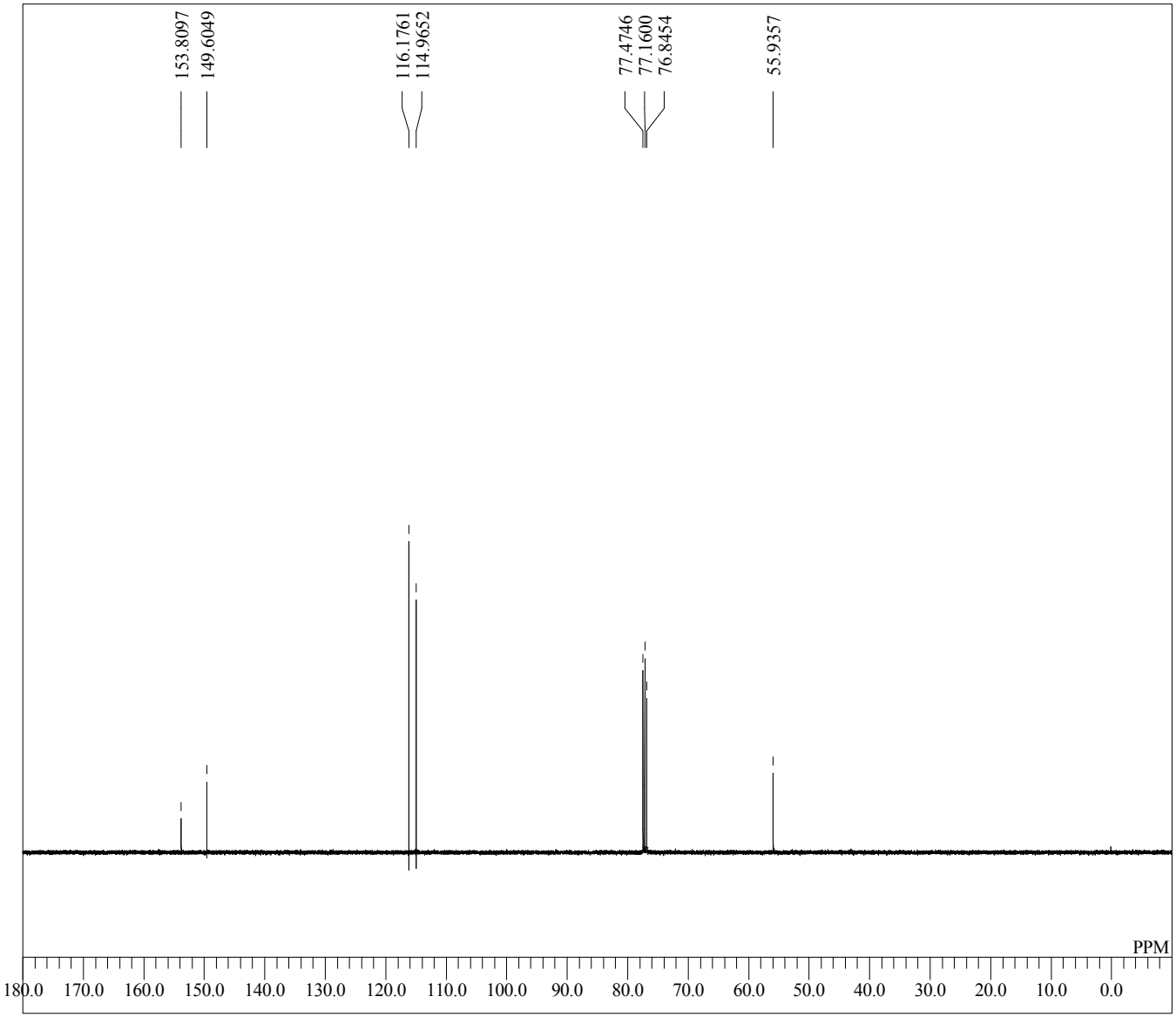
Figure S10



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COMNT	single pulse decoupled gated NOE
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OBNUC	13C
EXMOD	carbon.jxp
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OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	343
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

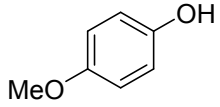

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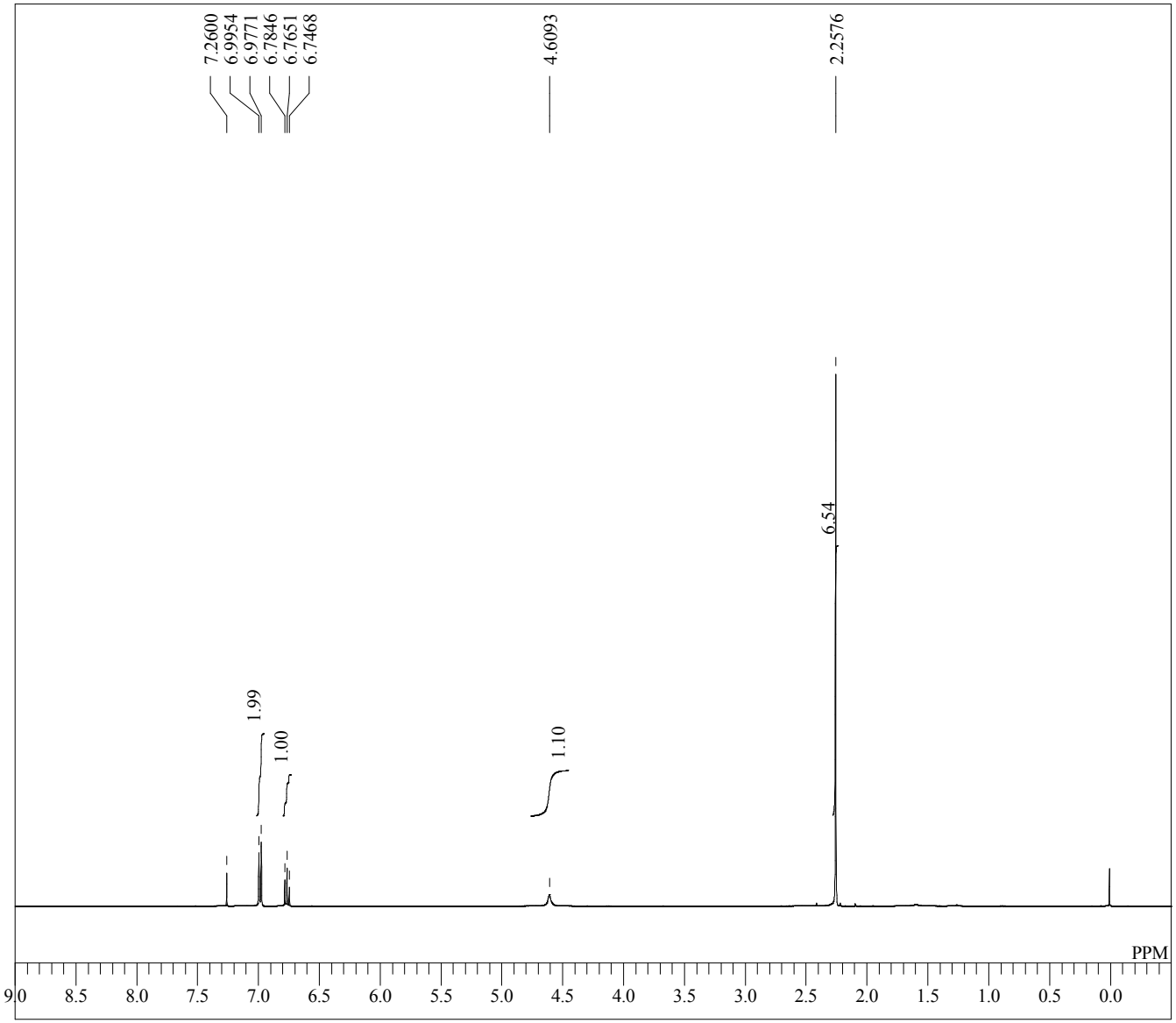
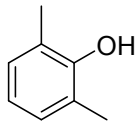
Figure S11

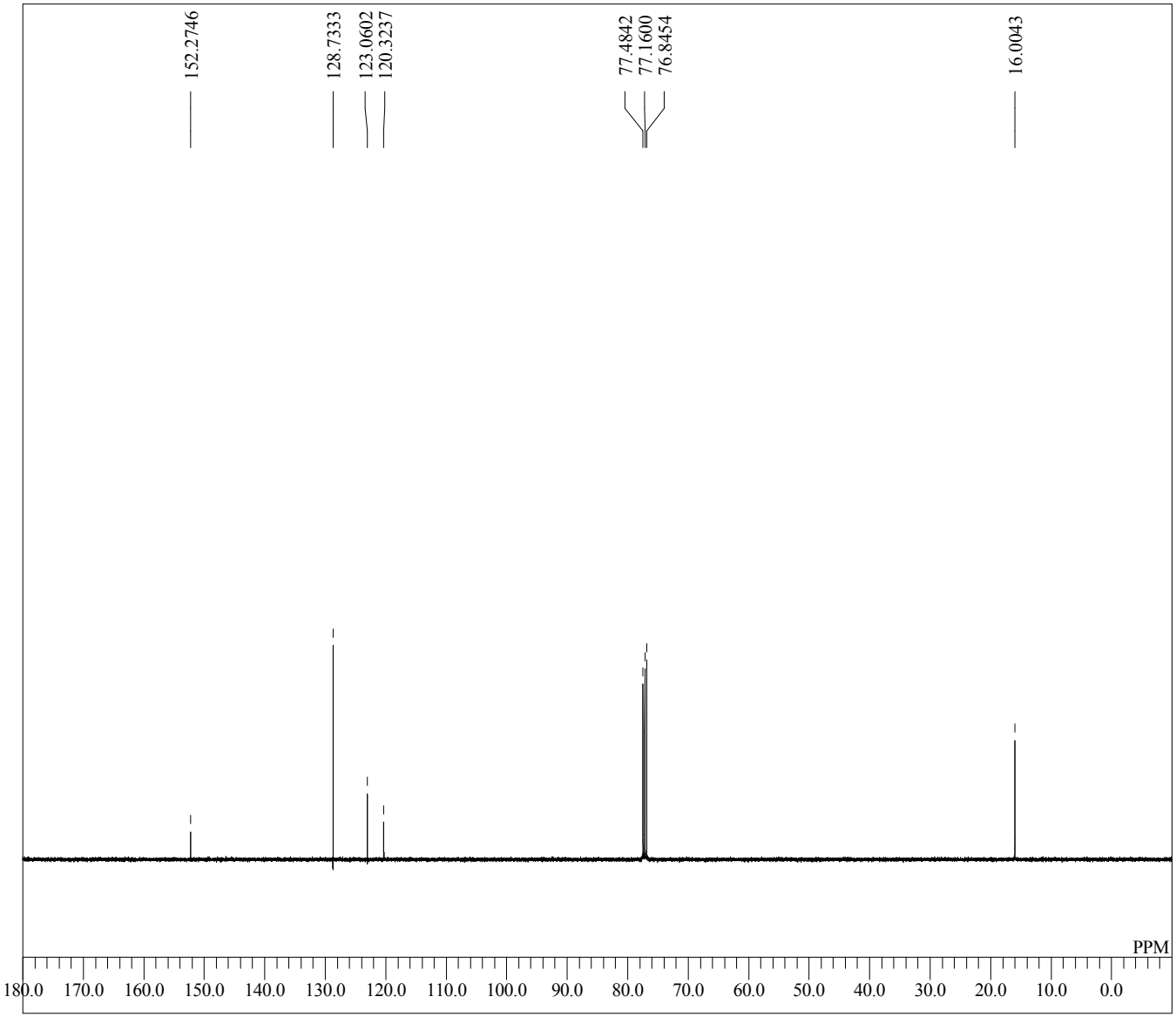


DFILE	yanagihara OH diMe 1H_proton-1-1.a
COMNT	single_pulse
DATIM	2018-05-16 10:52:17
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

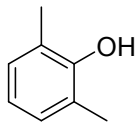


2d

Figure S12

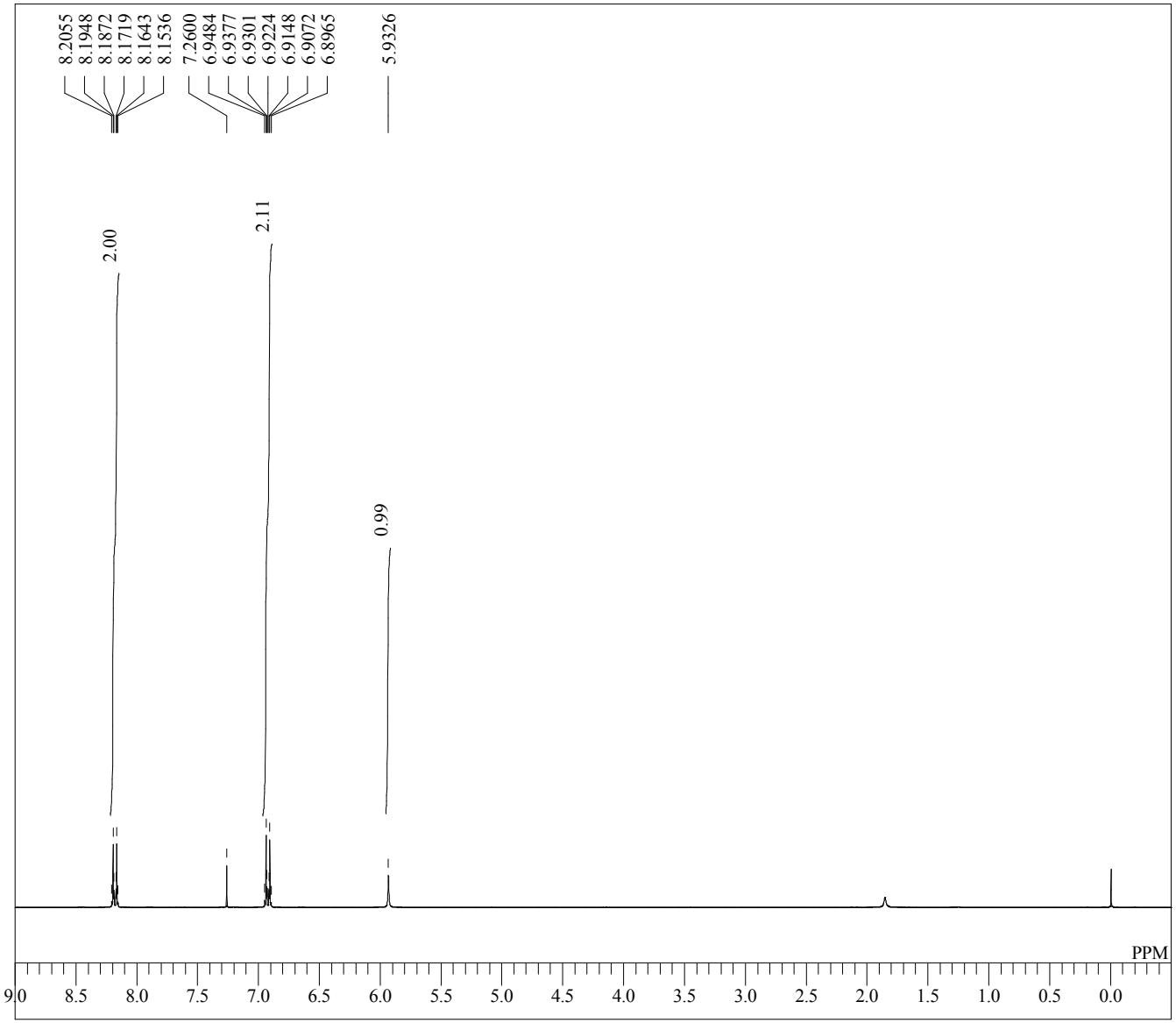


DFILE	yanagihara OH diMe 13C_carbon-1-1.
COMNT	single pulse decoupled gated NOE
DATIM	2018-05-16 10:55:40
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	528
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.4 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

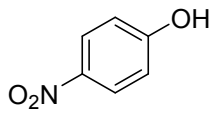


2d

Figure S13

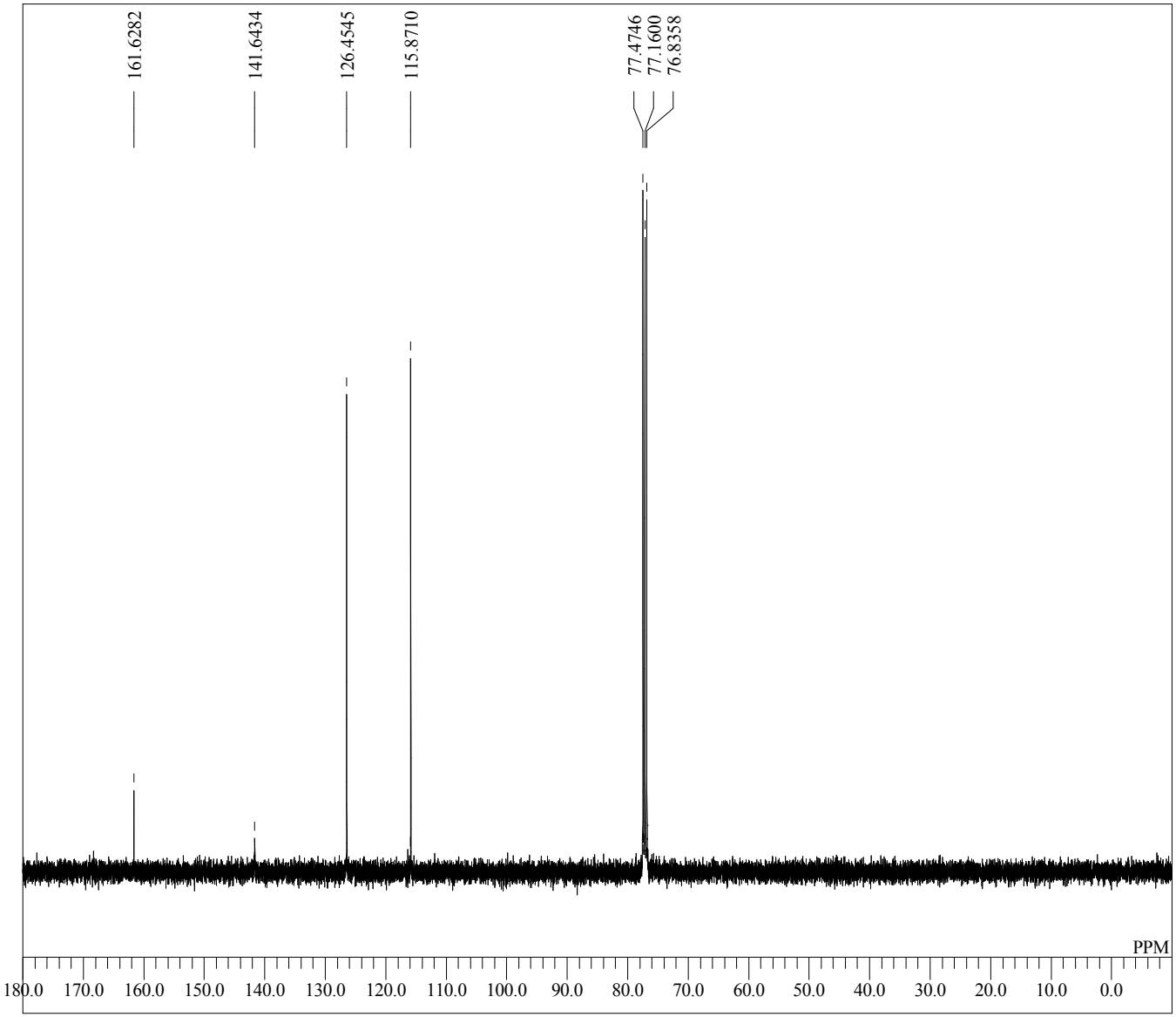


DFILE	yanagihara OH NO2 1H_proton-1-1.al
COMNT	single_pulse
DATIM	2018-05-22 10:33:53
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	300.53 MHz
OBSET	1.15 KHz
OBFIN	8.57 Hz
POINT	13107
FREQU	6016.85 Hz
SCANS	16
ACQTM	2.1784 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.6 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	40



2e

Figure S14



DFILE	yanagihara OH NO2 13C_carbon-1-1.a
COMNT	single pulse decoupled gated NOE
DATIM	2018-05-23 10:27:05
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	448
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.4 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

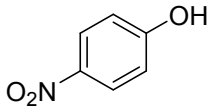


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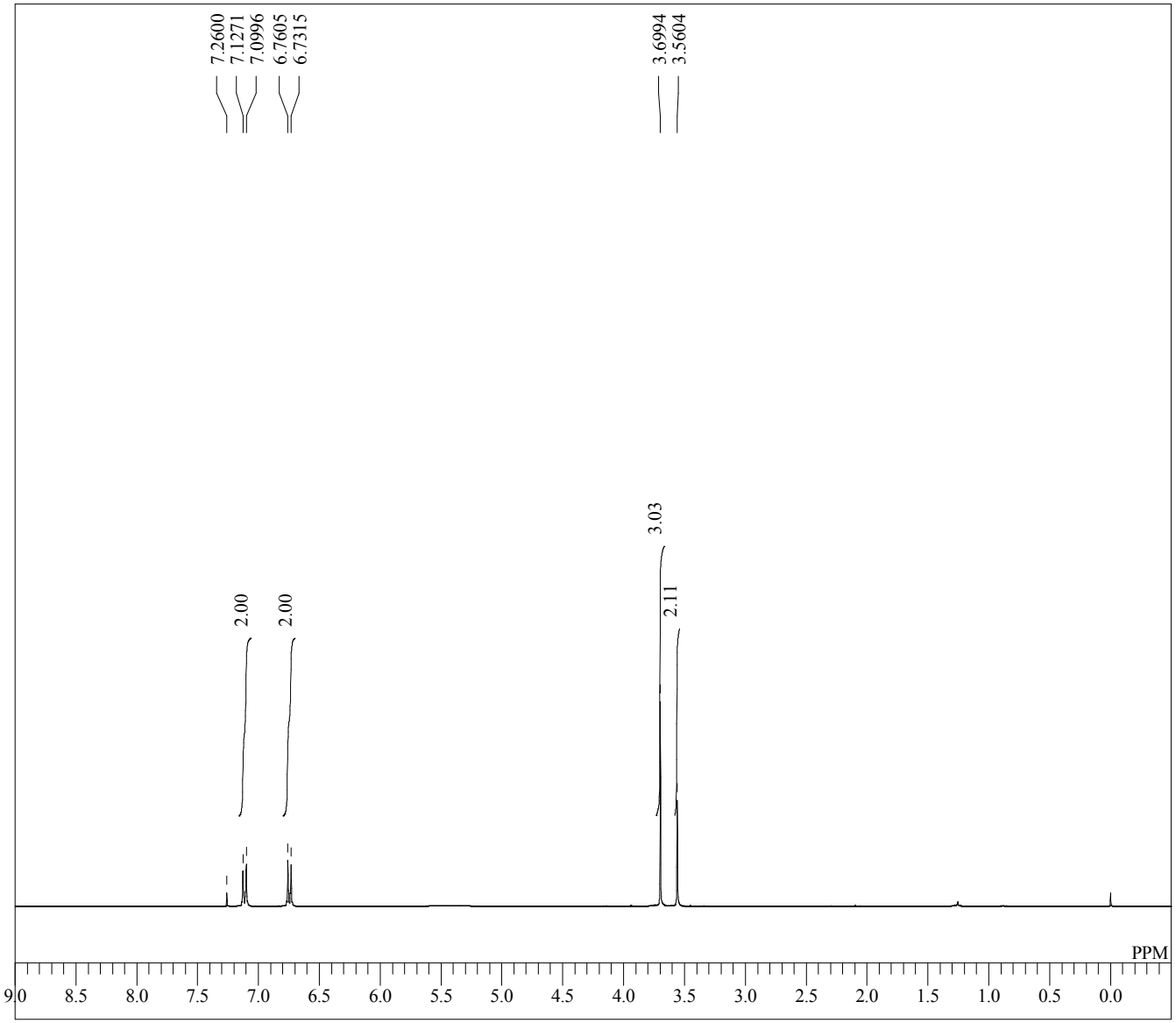
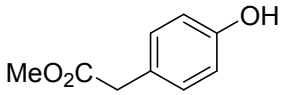
Figure S15

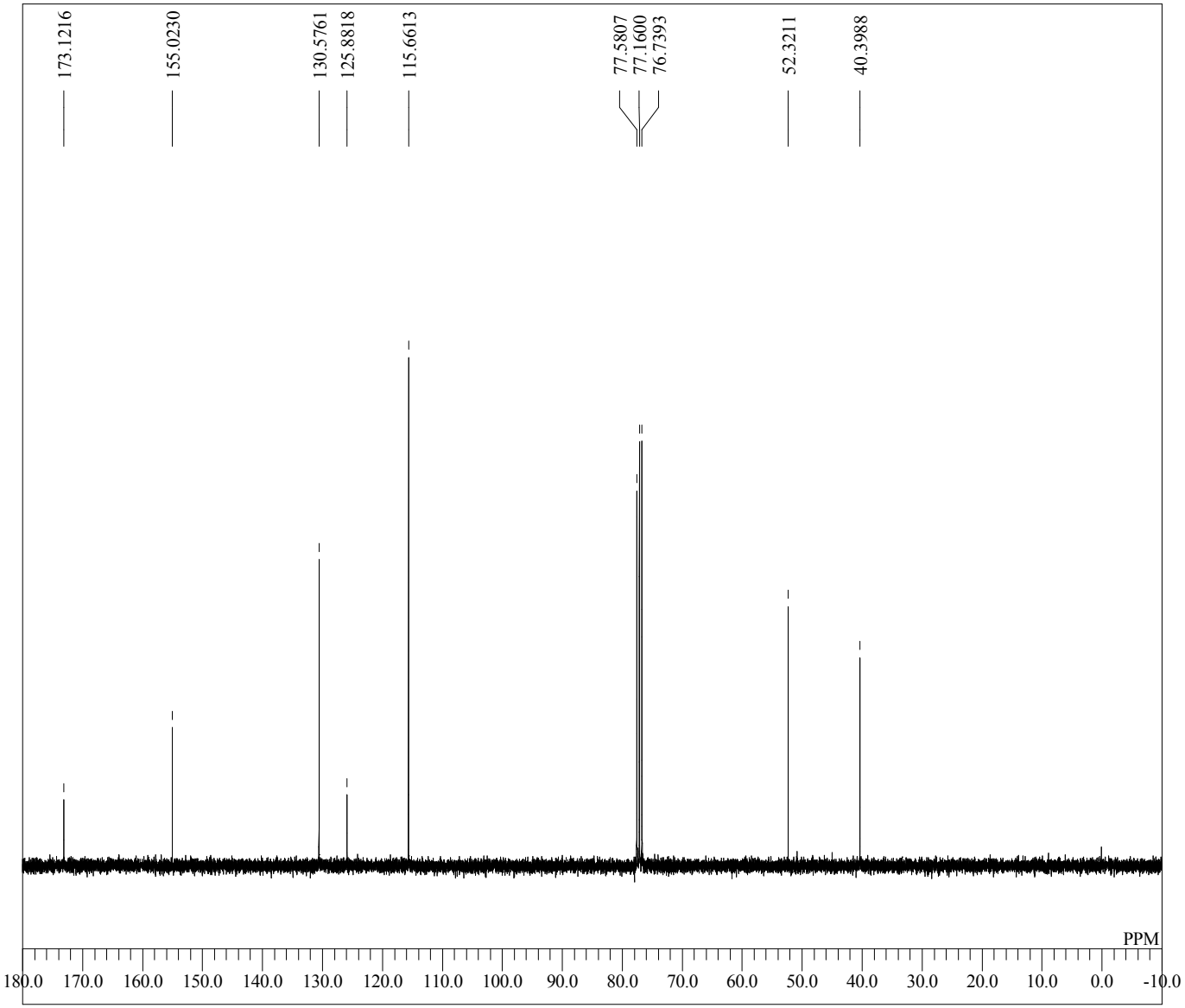


DFILE	yanagihara OH ester 1H_proton-1-1.al
COMNT	single_pulse
DATIM	2018-05-21 18:38:10
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	300.53 MHz
OBSET	1.15 KHz
OBFIN	8.57 Hz
POINT	13107
FREQU	6016.85 Hz
SCANS	16
ACQTM	2.1784 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	36

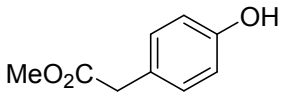


2f

Figure S16

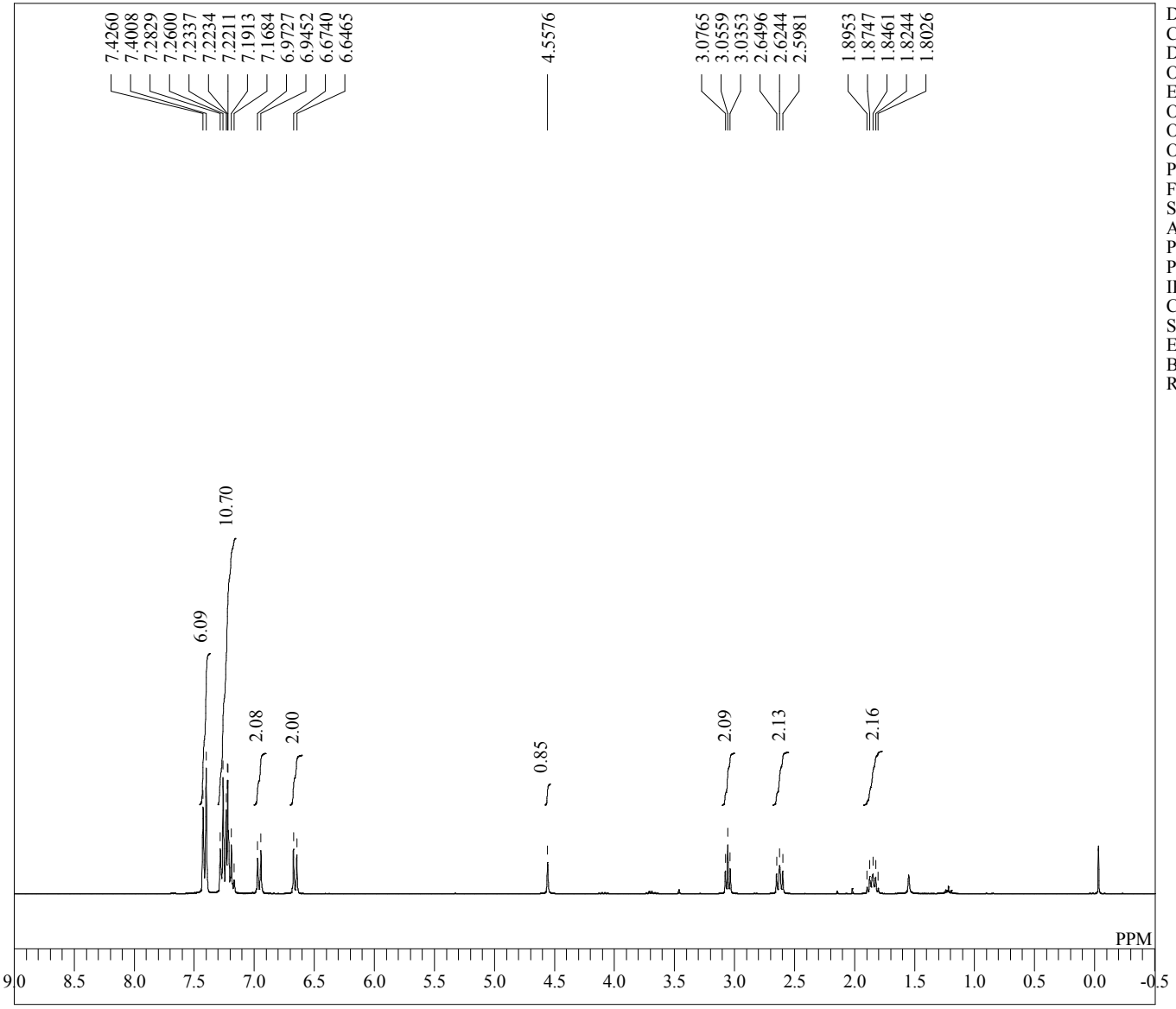


DFILE	yanagihara OH ester 13C_Carbon-1-1.
COMNT	single pulse decoupled gated NOE
DATIM	2018-05-21 18:44:16
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	75.57 MHz
OBSET	5.79 KHz
OBFIN	1.08 Hz
POINT	26214
FREQU	18939.39 Hz
SCANS	353
ACQTM	1.3841 sec
PD	2.5000 sec
PW1	3.73 usec
IRNUC	1H
CTEMP	20.0 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

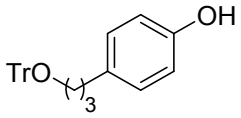


2f

Figure S17

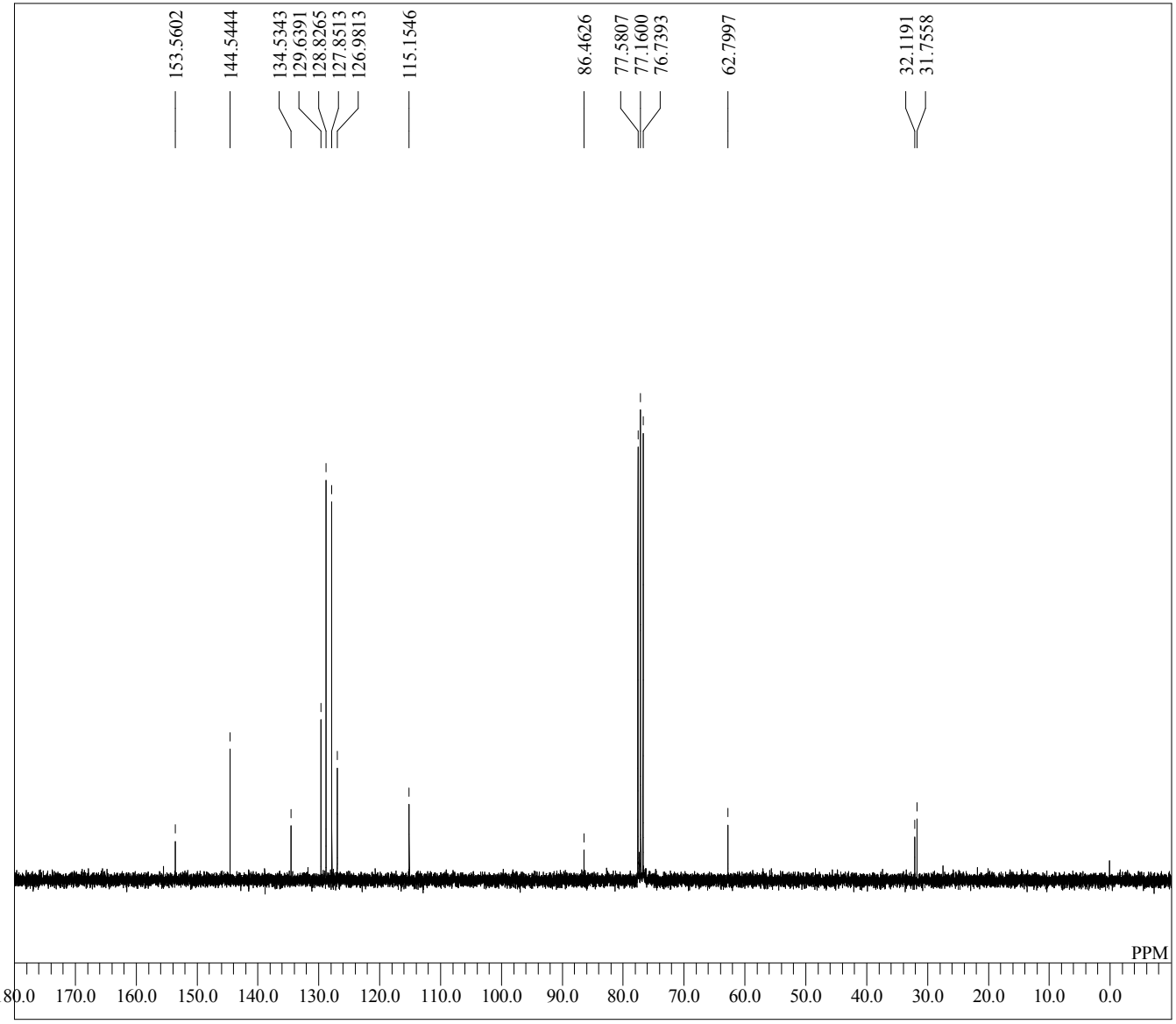


DFILE yanagihara OH Tr 1H_proton-1-1.als
COMNT single_pulse
DATIM 2018-03-20 17:17:40
OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 13107
FREQU 4508.57 Hz
SCANS 16
ACQTM 2.9072 sec
PD 1.0000 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 19.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 40

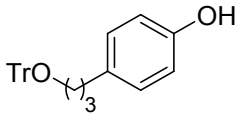


2g

Figure S18

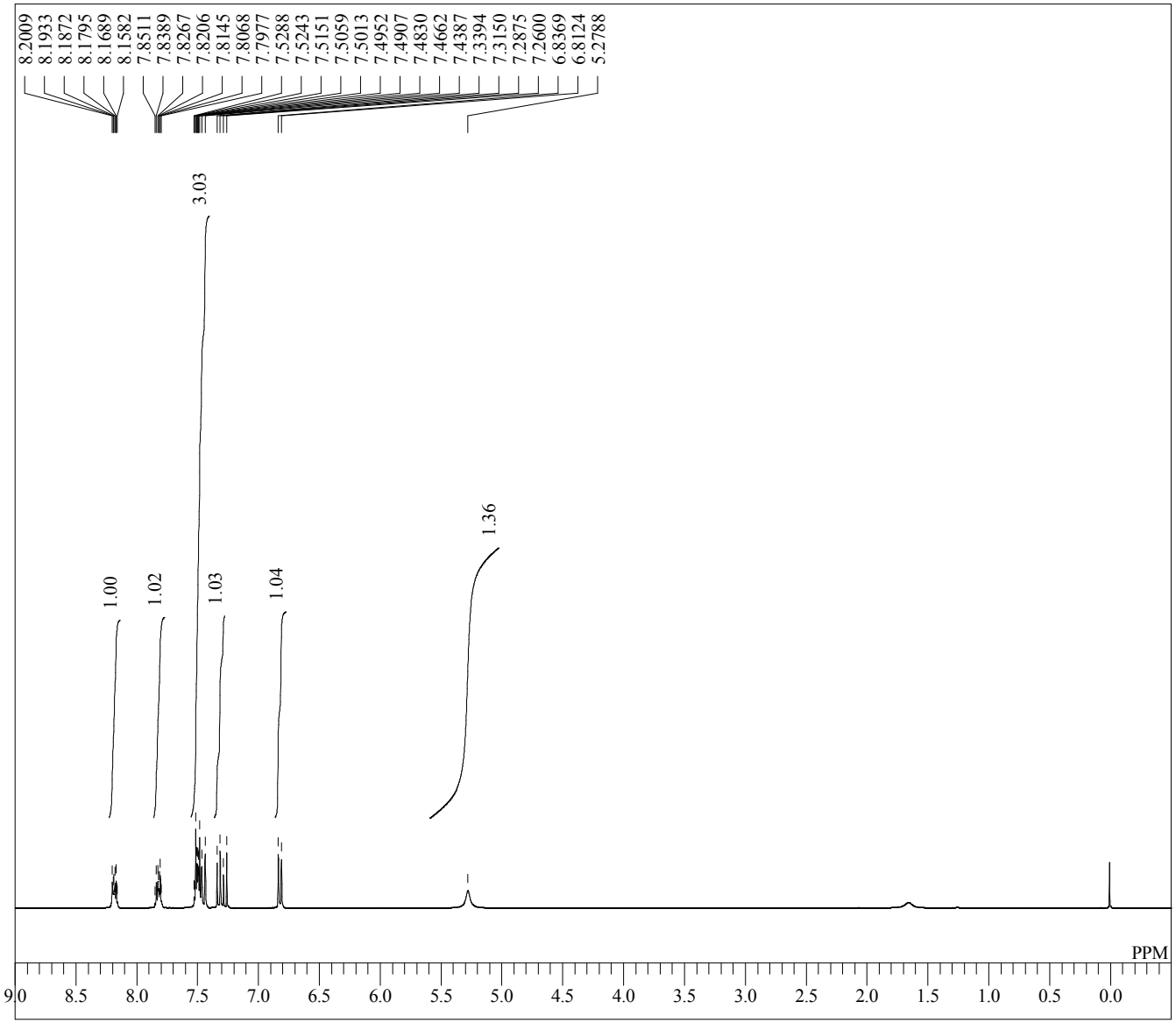


DFILE	yanagihara OH Tr 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-03-20 17:56:04
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	75.57 MHz
OBSET	5.79 KHz
OBFIN	1.08 Hz
POINT	26214
FREQU	18939.39 Hz
SCANS	349
ACQTM	1.3841 sec
PD	2.5000 sec
PW1	3.73 usec
IRNUC	1H
CTEMP	19.9 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

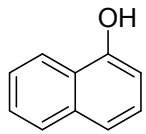


2g

Figure S19

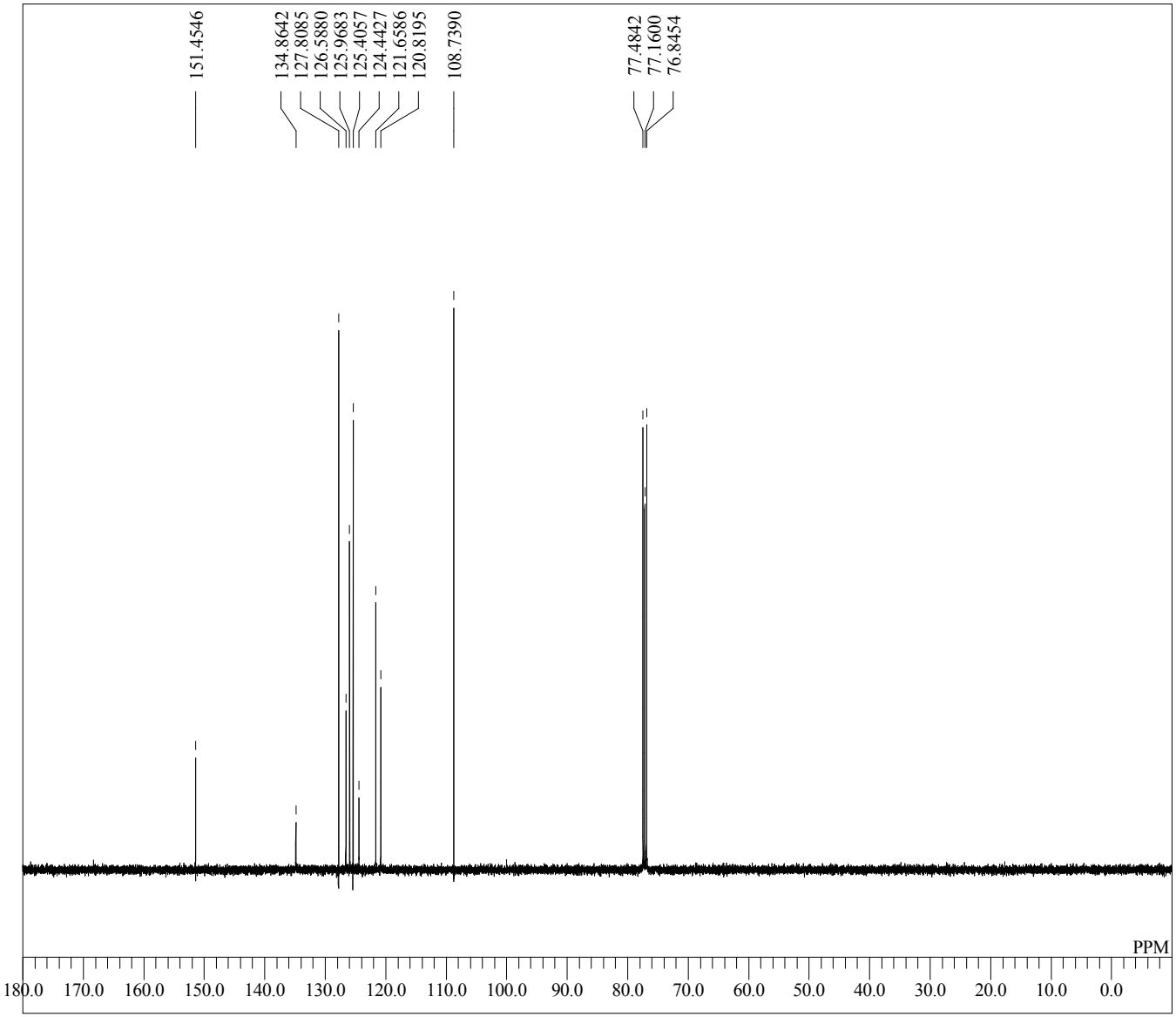


DFILE	yanagihara OH Np 1H_proton-1-1.als
COMNT	single_pulse
DATIM	2018-05-22 11:02:09
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	300.53 MHz
OBSET	1.15 KHz
OBFIN	8.57 Hz
POINT	13107
FREQU	6016.85 Hz
SCANS	16
ACQTM	2.1784 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.8 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	40

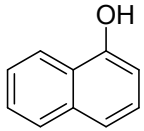


2h

Figure S20

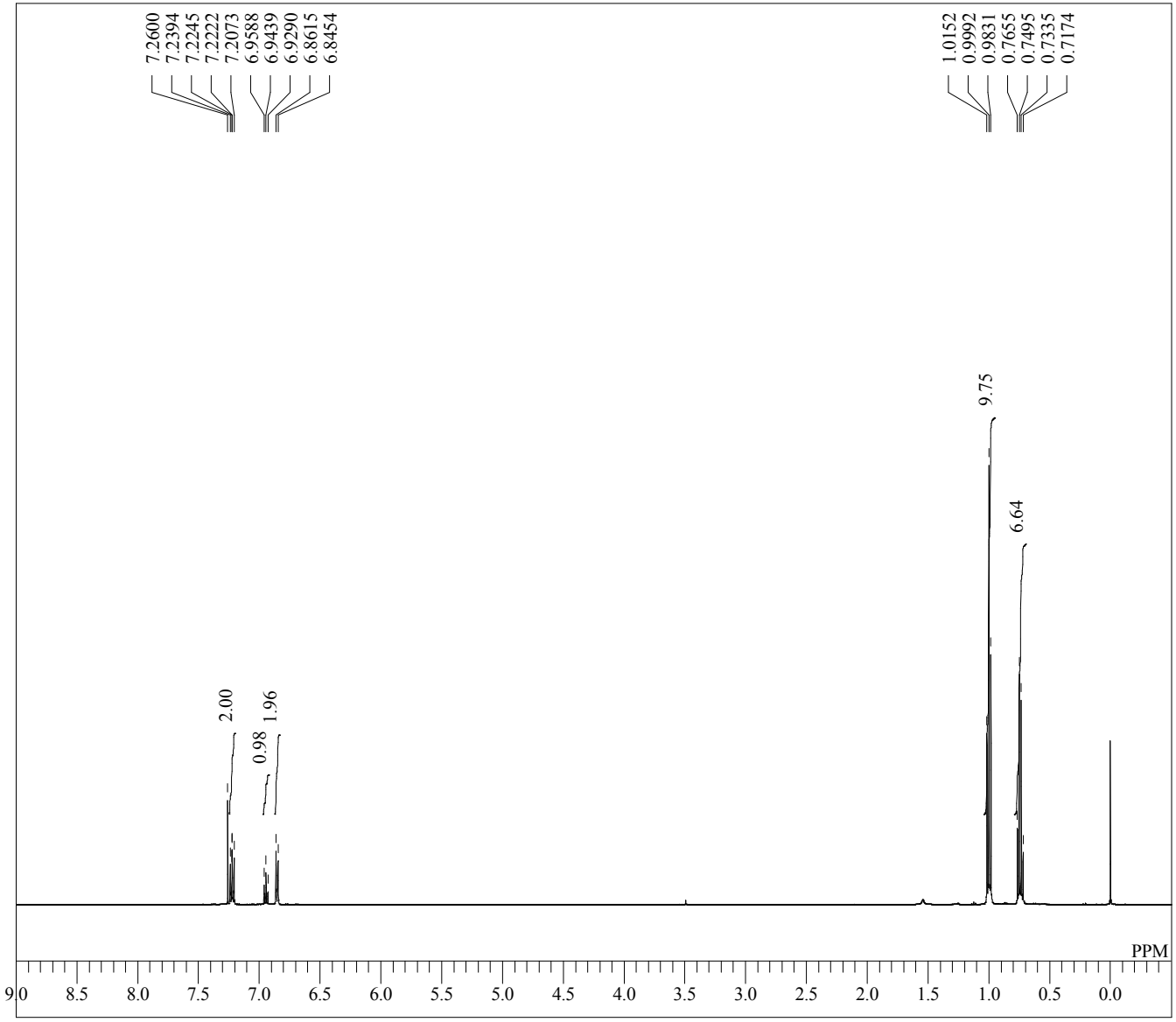


DFILE	yanagihara OH Np 13C_carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-05-23 10:56:41
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	341
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.3 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

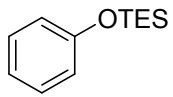


2h

Figure S21

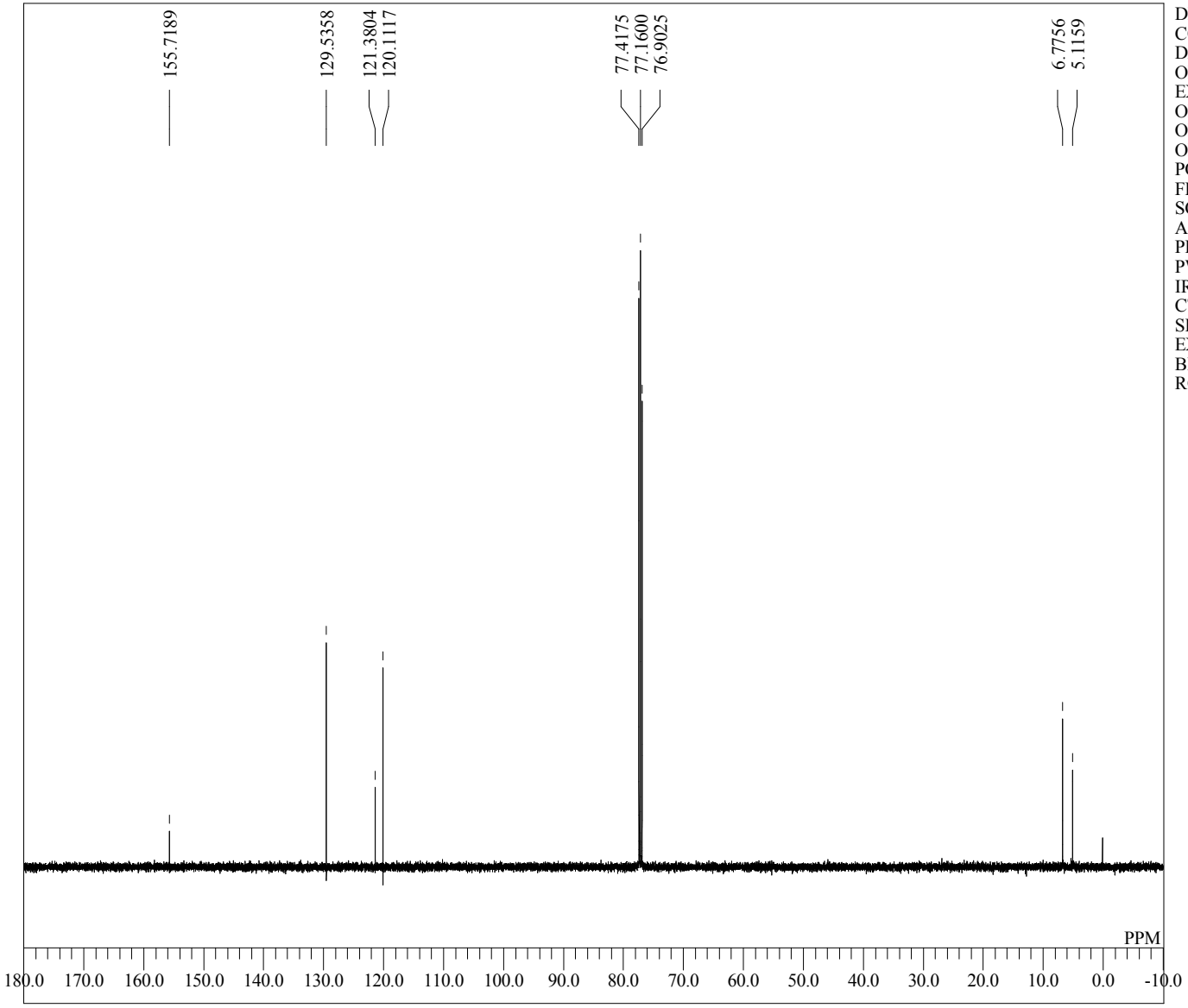


DFILE	yanagihara TES OH 1H_proton-1-1.als
COMNT	single_pulse
DATIM	04-04-2018 15:08:36
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	16
ACQTM	1.7459 sec
PD	2.5000 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	19.2 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

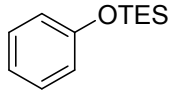


3a

Figure S22

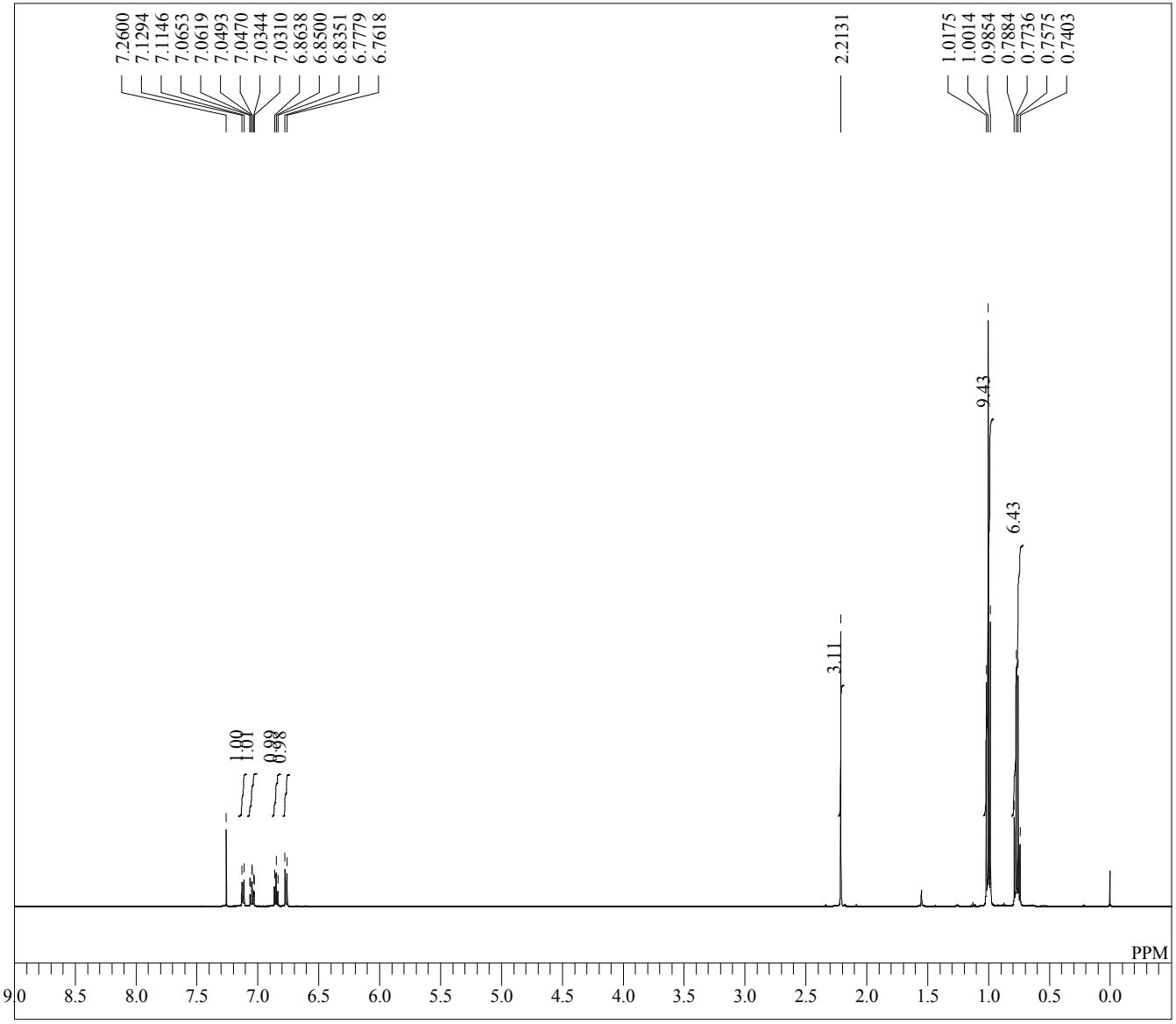


DFILE	yanagihara TES OH 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	04-04-2018 15:12:34
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	457
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.93 usec
IRNUC	1H
CTEMP	19.6 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60



3a

Figure S23



DFILE	yanagihara TES Me 1H_proton-1-1.als
COMNT	single_pulse
DATIM	2018-04-04 17:39:16
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	16
ACQTM	1.7459 sec
PD	2.5000 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	40

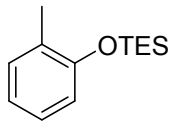


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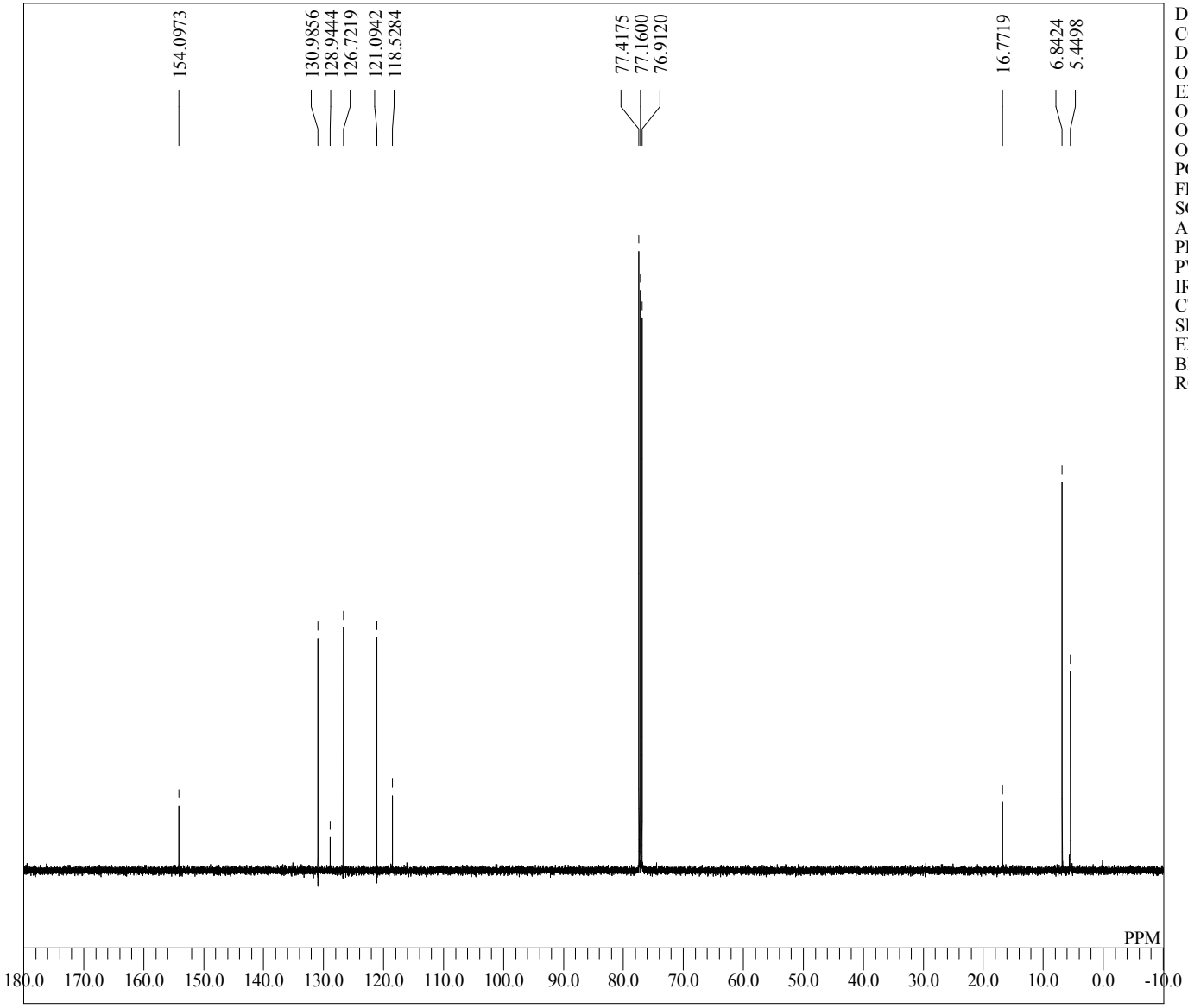
Figure S24



DFILE	yanagihara TES Me 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-04 17:43:22
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	618
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.93 usec
IRNUC	1H
CTEMP	19.9 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

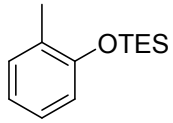


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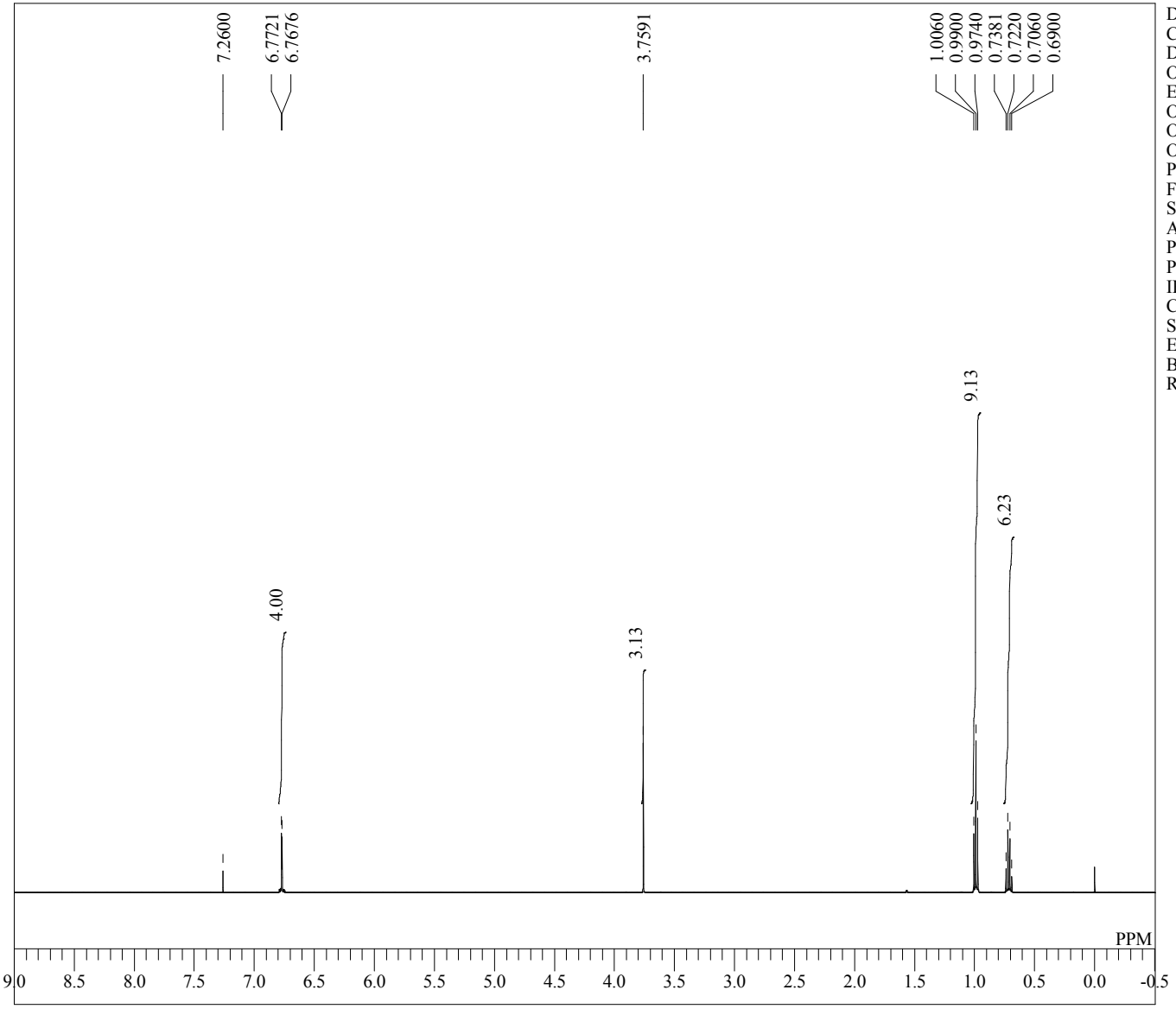
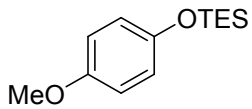
Figure S25

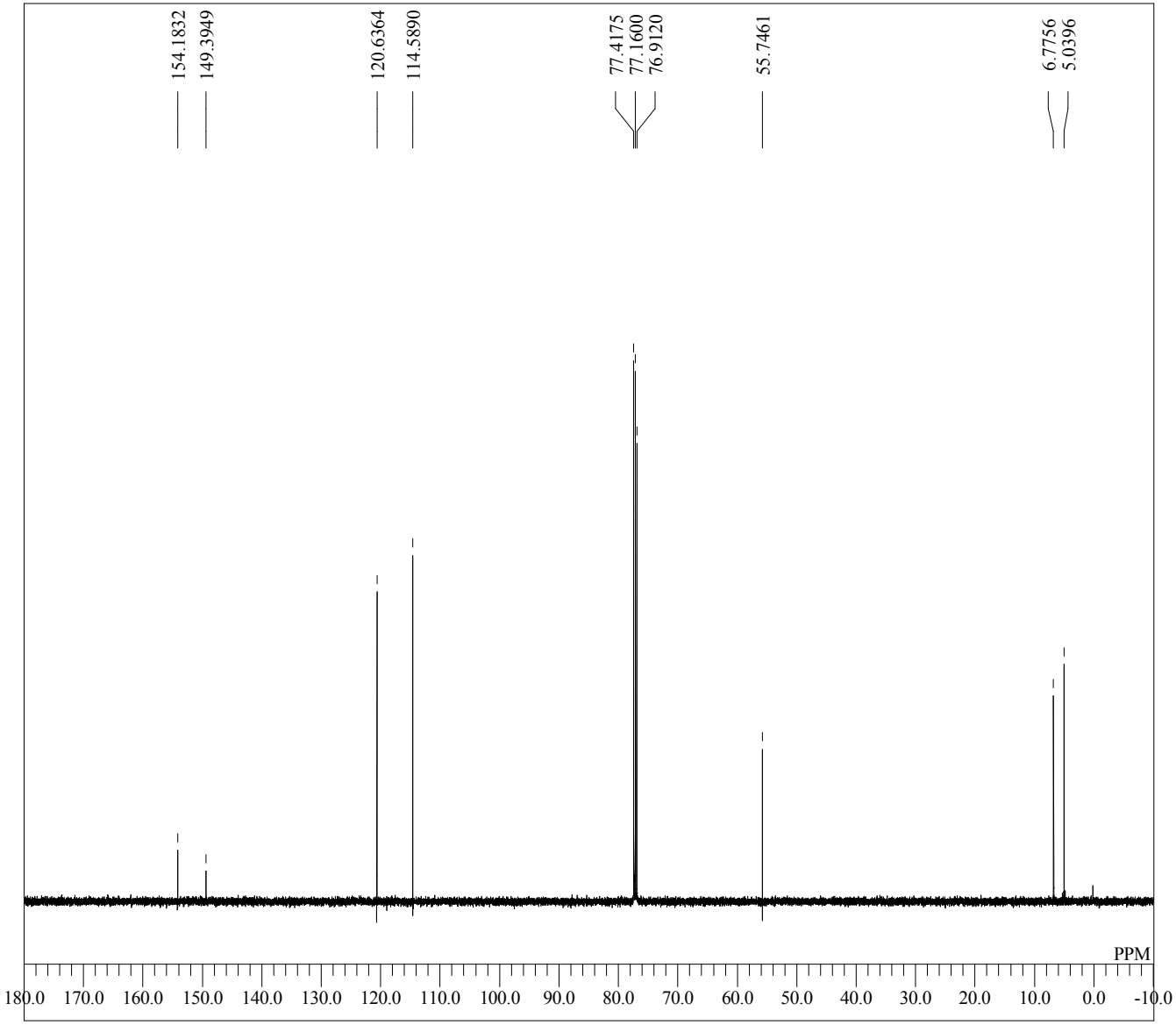


DFILE yanagihara TES OMe 1H_proton-1-1.als
COMNT single_pulse
DATIM 04-04-2018 20:00:51
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 16
ACQTM 1.7459 sec
PD 2.5000 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 40



3c

Figure S26



DFILE	yanagihara TES OMe 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	04-04-2018 20:04:57
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	431
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.93 usec
IRNUC	1H
CTEMP	20.1 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

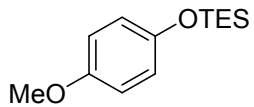


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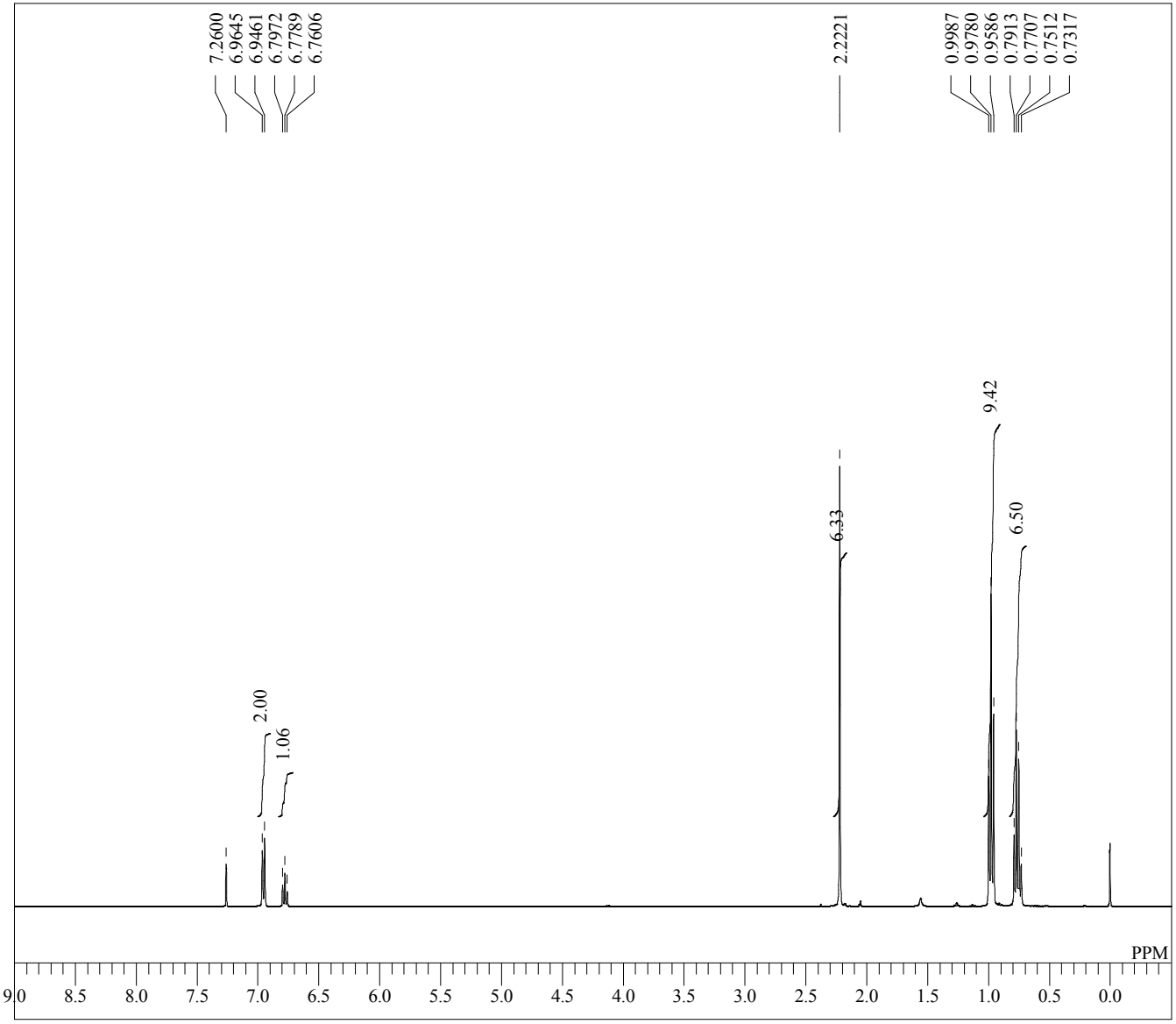
Figure S27



DFILE	yanagihara ex293 pure_proton-1-1.als
COMNT	single_pulse
DATIM	2018-02-14 21:35:33
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	6.40 usec
IRNUC	1H
CTEMP	19.6 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	34

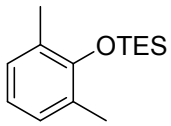


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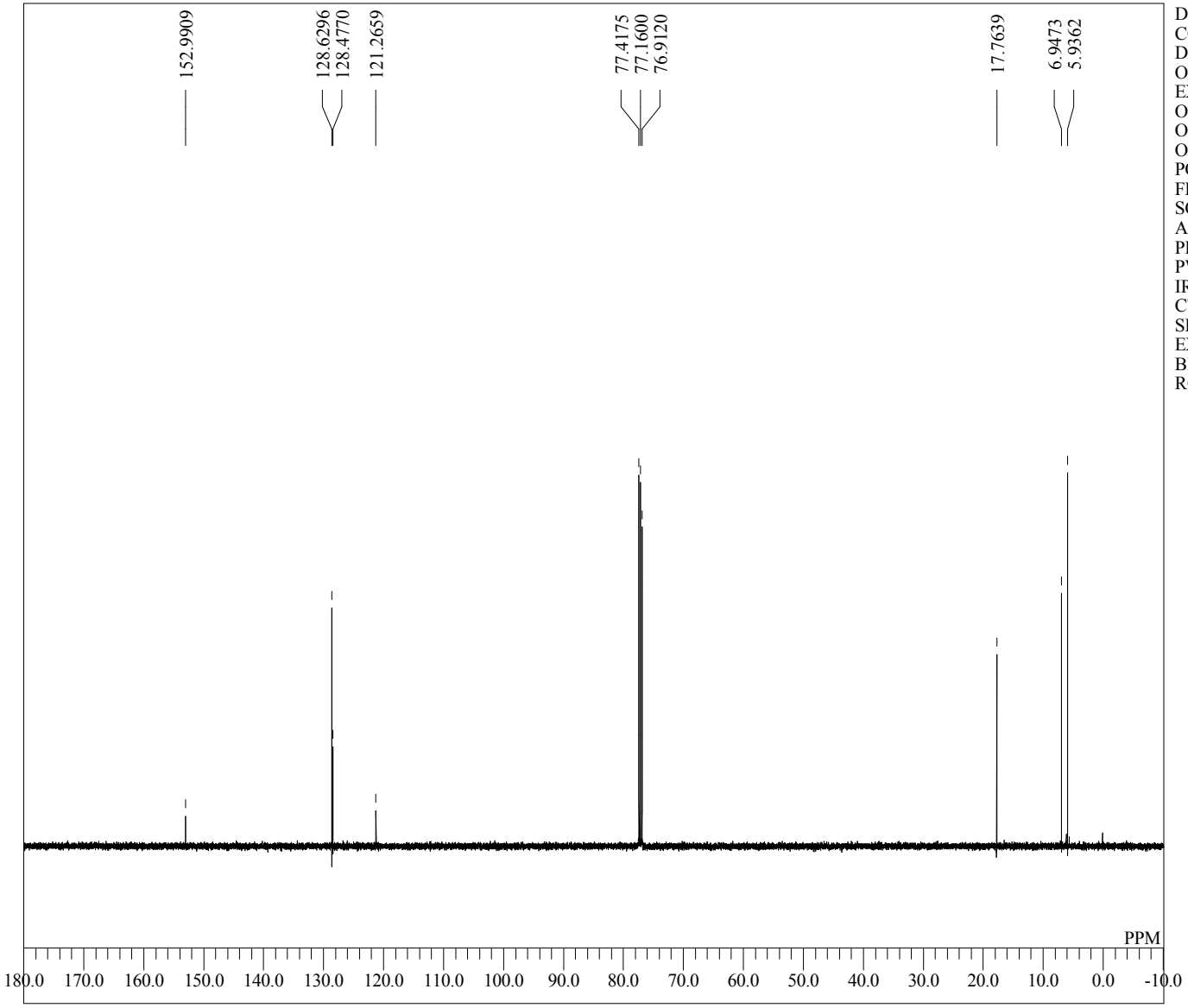
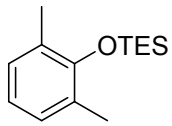
Figure S28

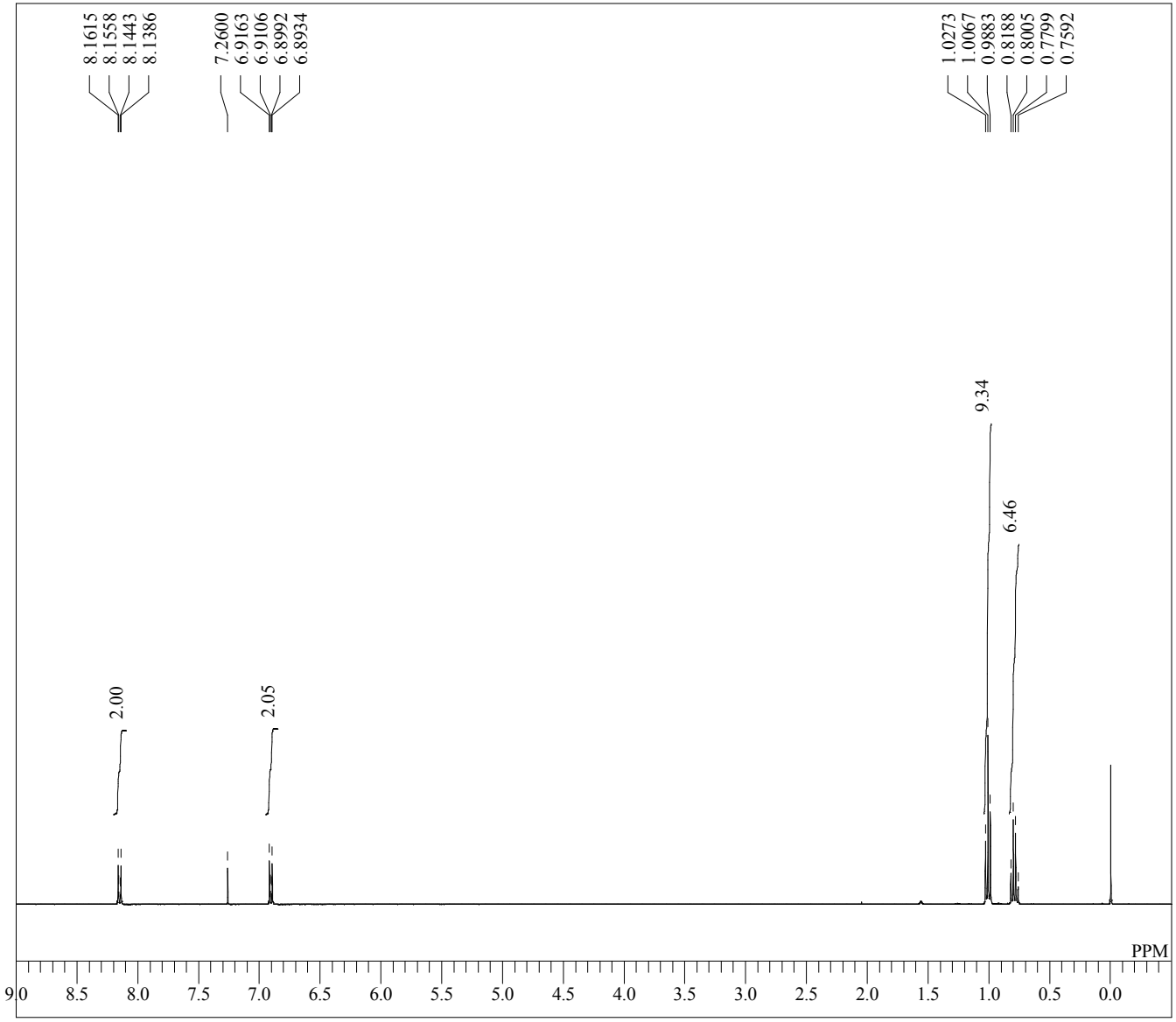


DFILE	yanagihara TES diMe 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-05 22:08:15
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	302
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.93 usec
IRNUC	1H
CTEMP	20.8 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

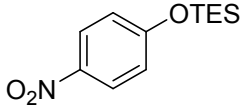


3d

Figure S29

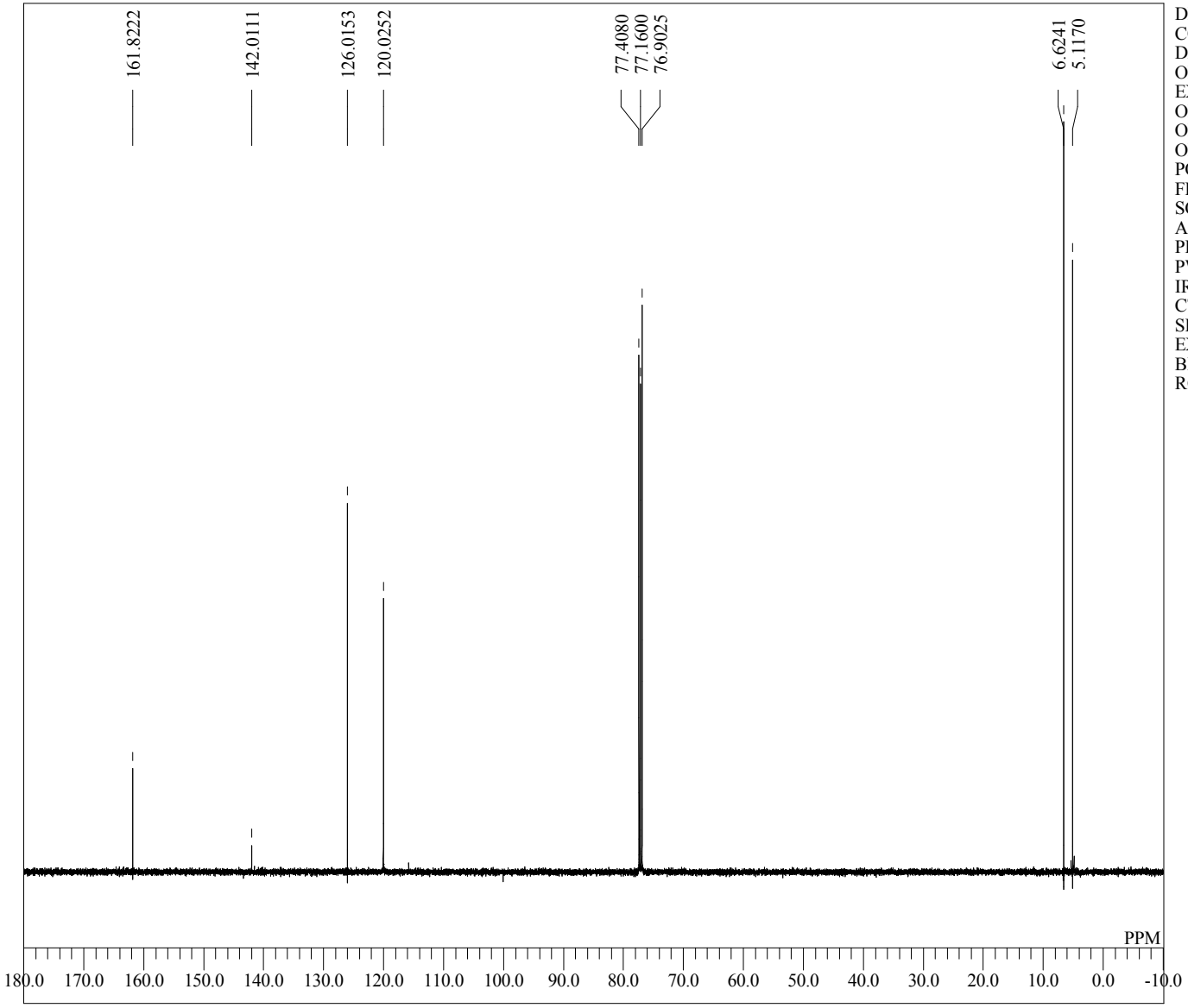


DFILE	yanagihara ex303 pure_proton-1-1.als
COMNT	single_pulse
DATIM	2018-02-27 16:09:56
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.4 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

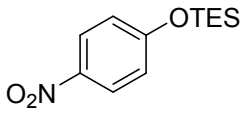


3e

Figure S30

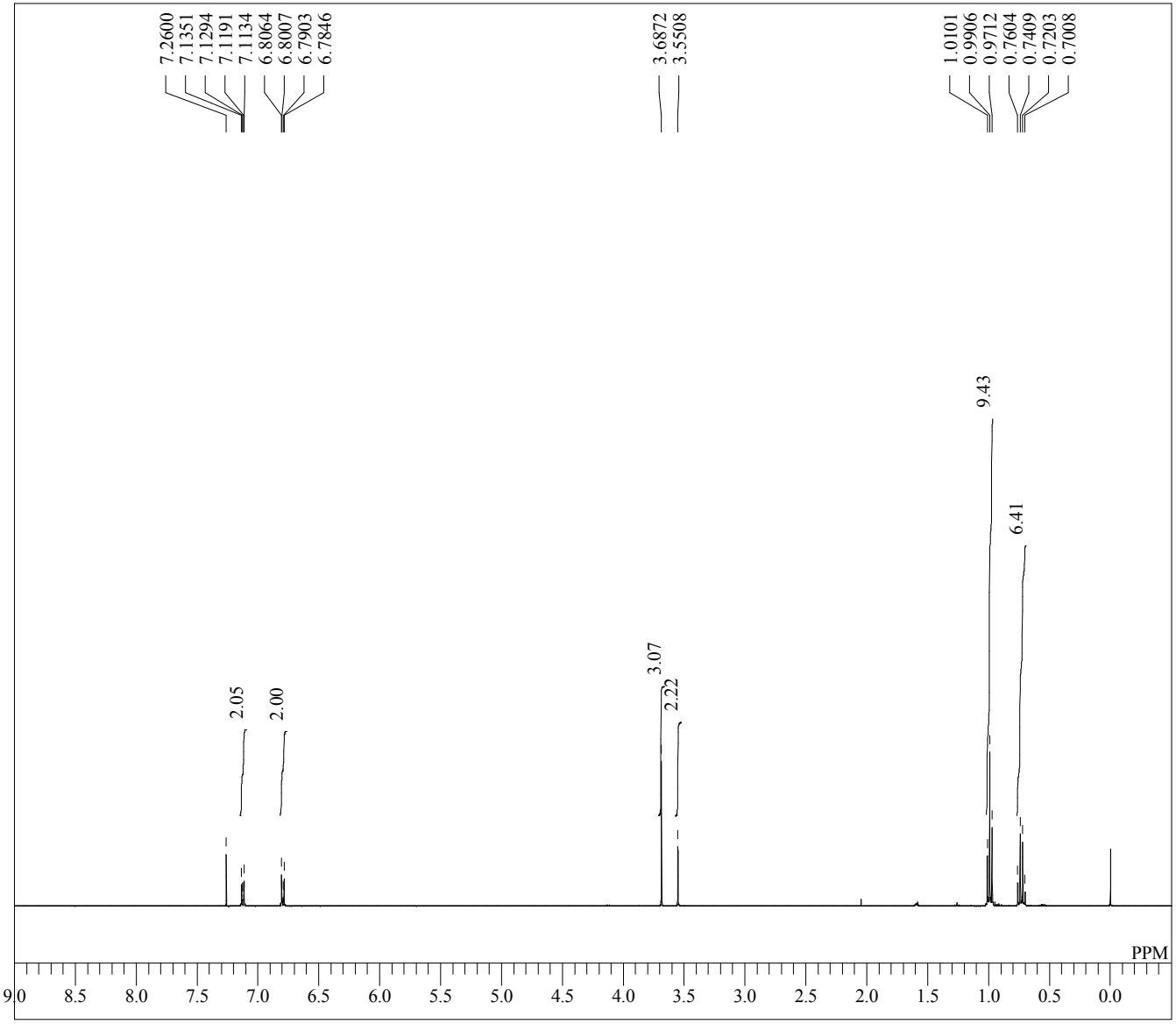


DFILE	yanagihara TES NO2 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-09 21:35:34
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	32767
FREQU	39308.18 Hz
SCANS	681
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.93 usec
IRNUC	1H
CTEMP	20.7 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

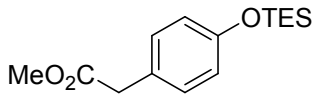


3e

Figure S31

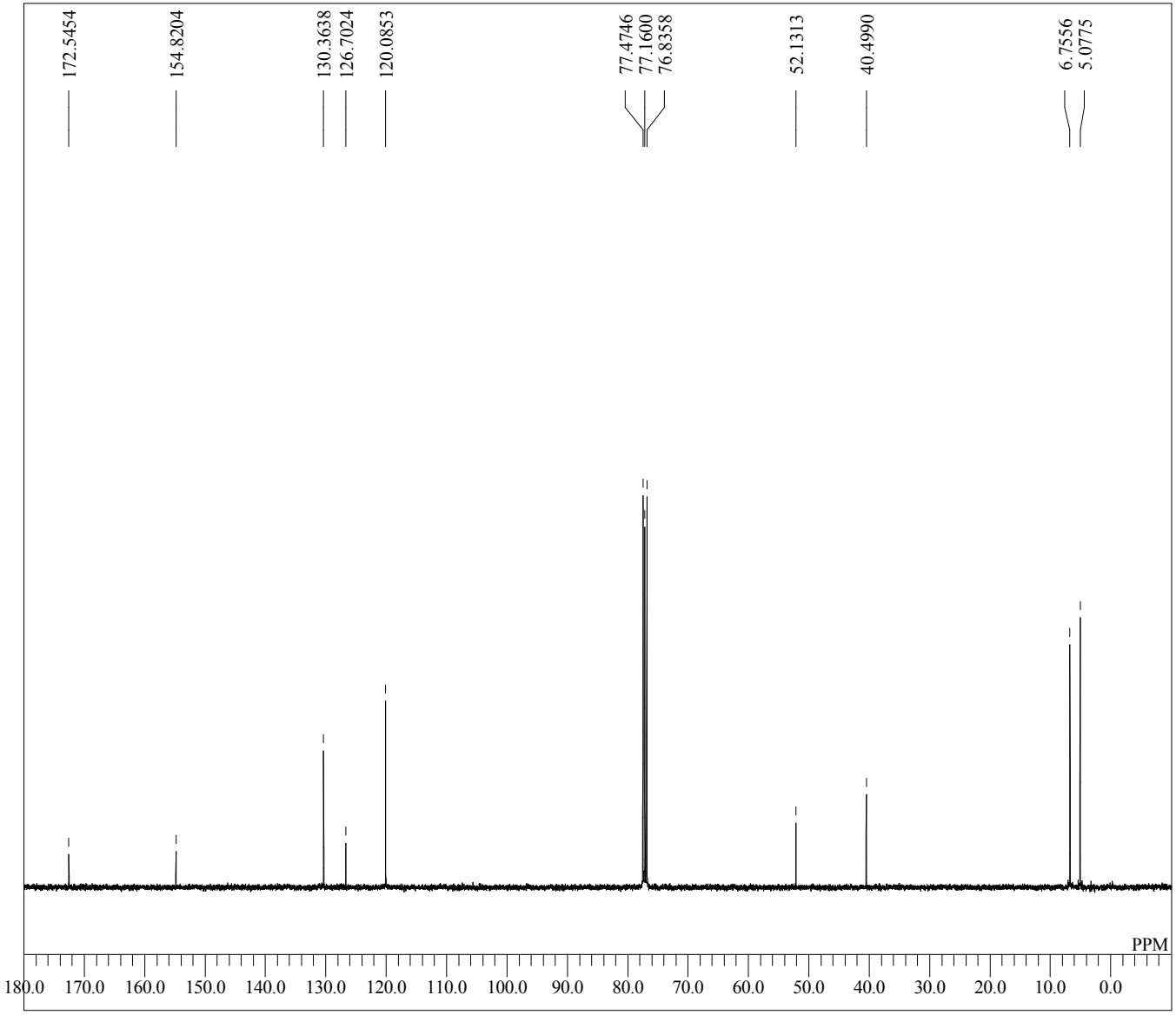


DFILE	yanagihara ex305 pure_proton-1-1.als
COMNT	single_pulse
DATIM	2018-03-12 16:43:34
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

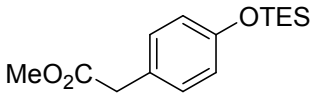


3f

Figure S32

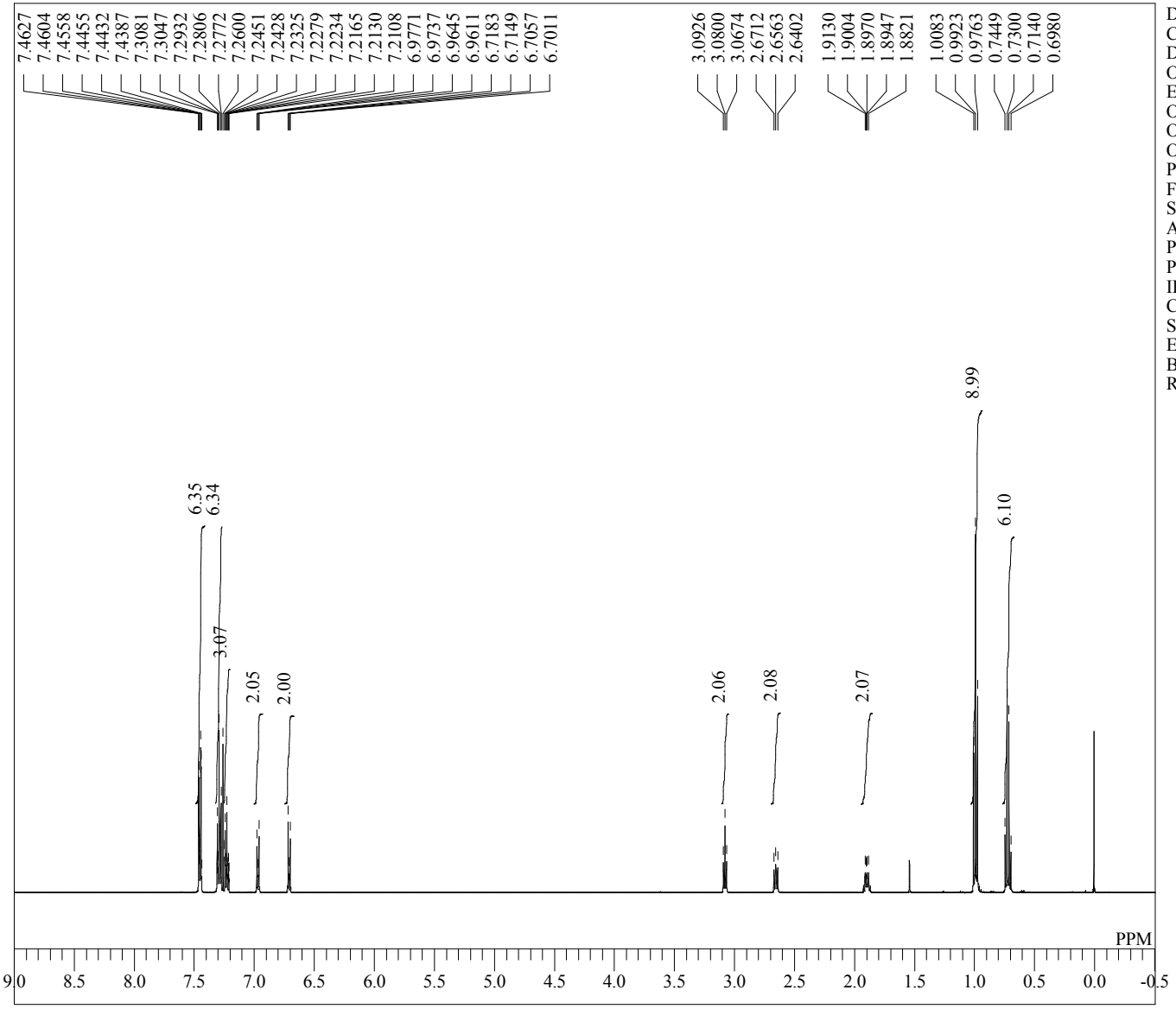


DFILE	yanagihara TES ester 13C_carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-09 20:19:51
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	358
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	1.20 Hz
RGAIN	60

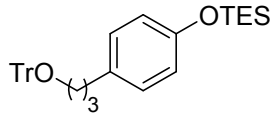


3f

Figure S33

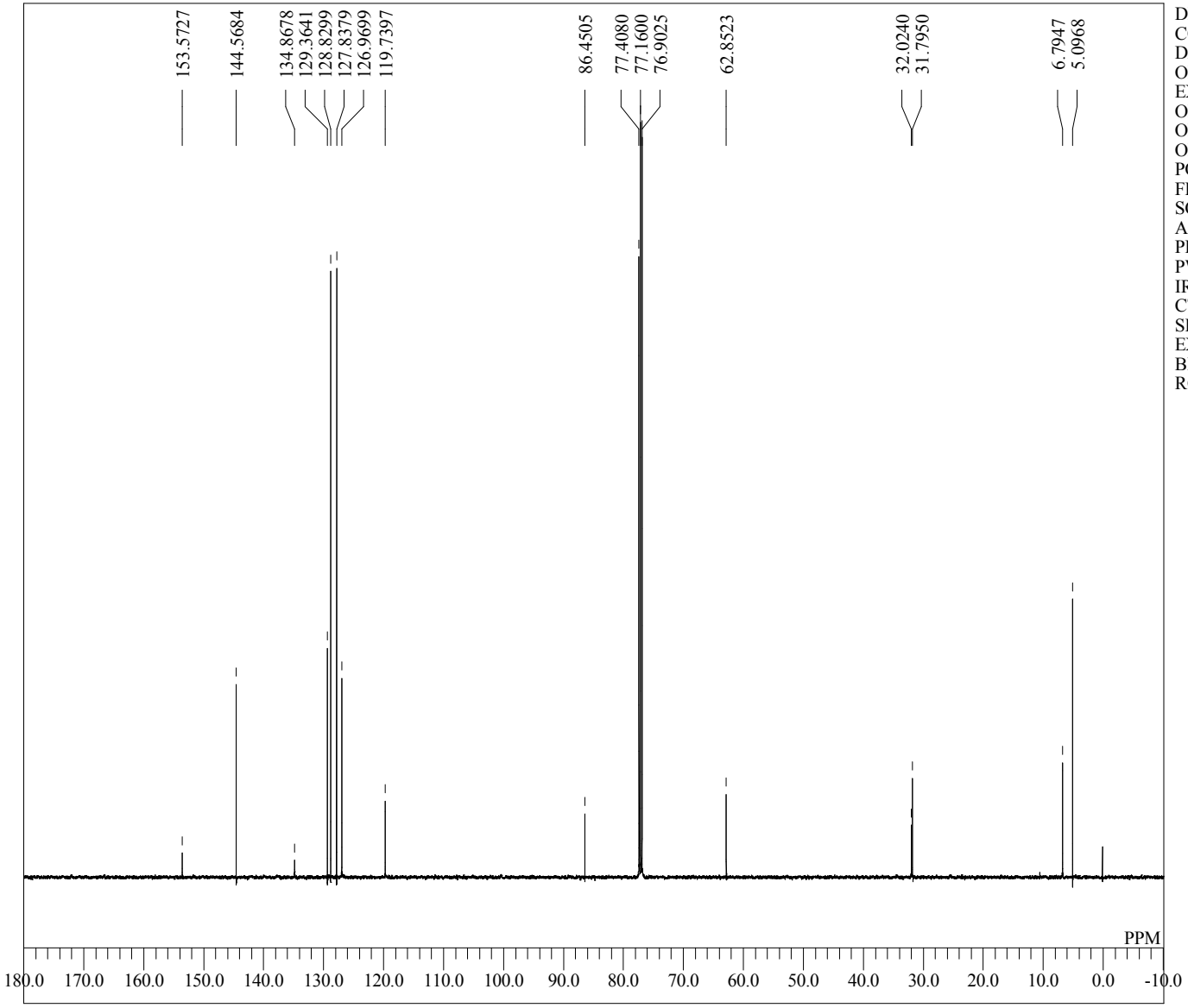


DFILE	yanagihara TES Tr 1H_proton-1-1.als
COMNT	single_pulse
DATIM	2018-04-04 21:11:53
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	16
ACQTM	1.7459 sec
PD	2.5000 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	19.9 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	40

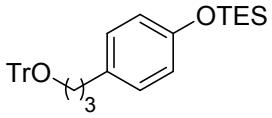


3g

Figure S34

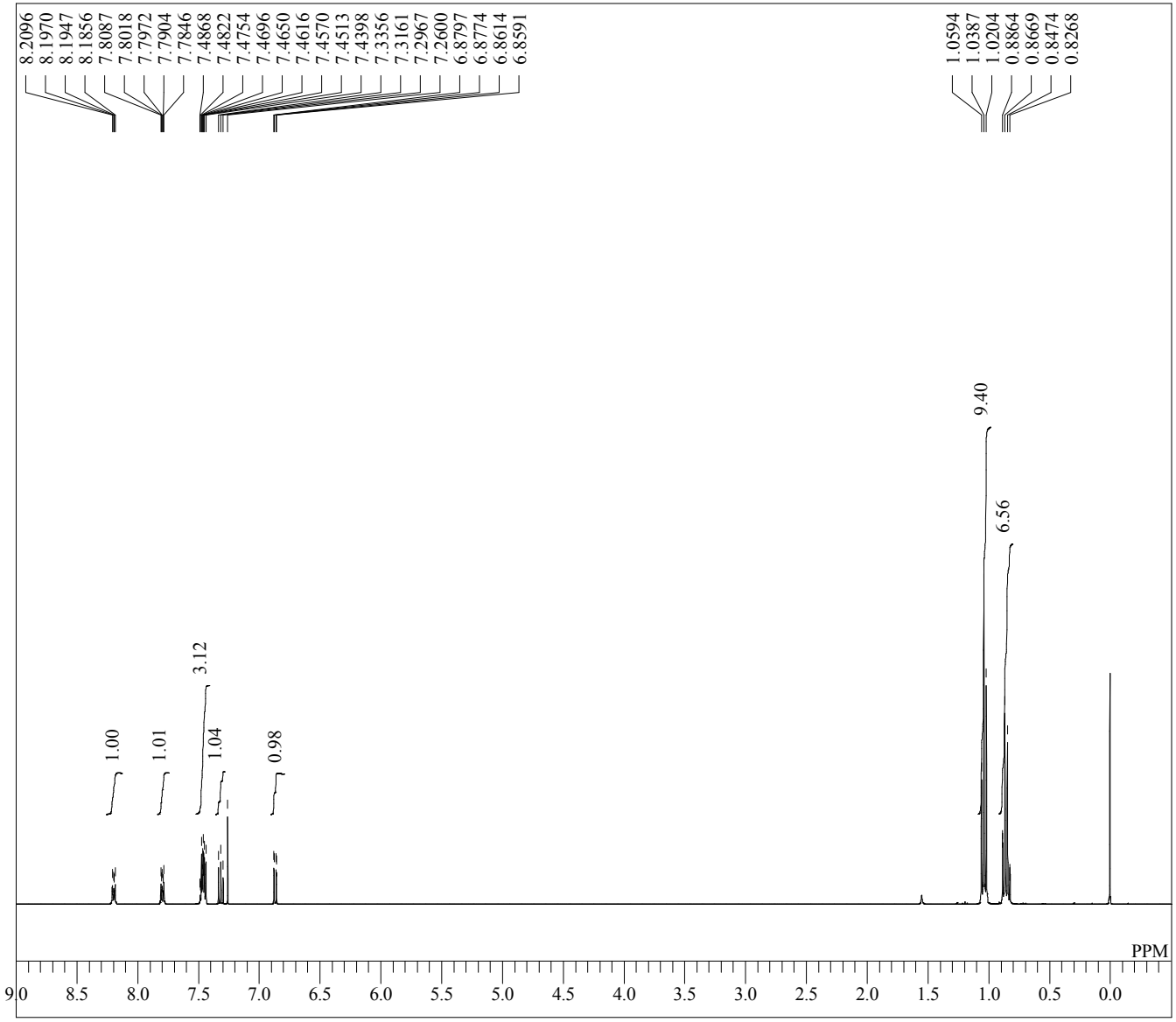


DFILE	yanagihara TES Tr 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-04 21:17:06
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	369
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.93 usec
IRNUC	1H
CTEMP	20.1 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	50

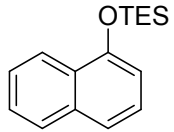


3g

Figure S35

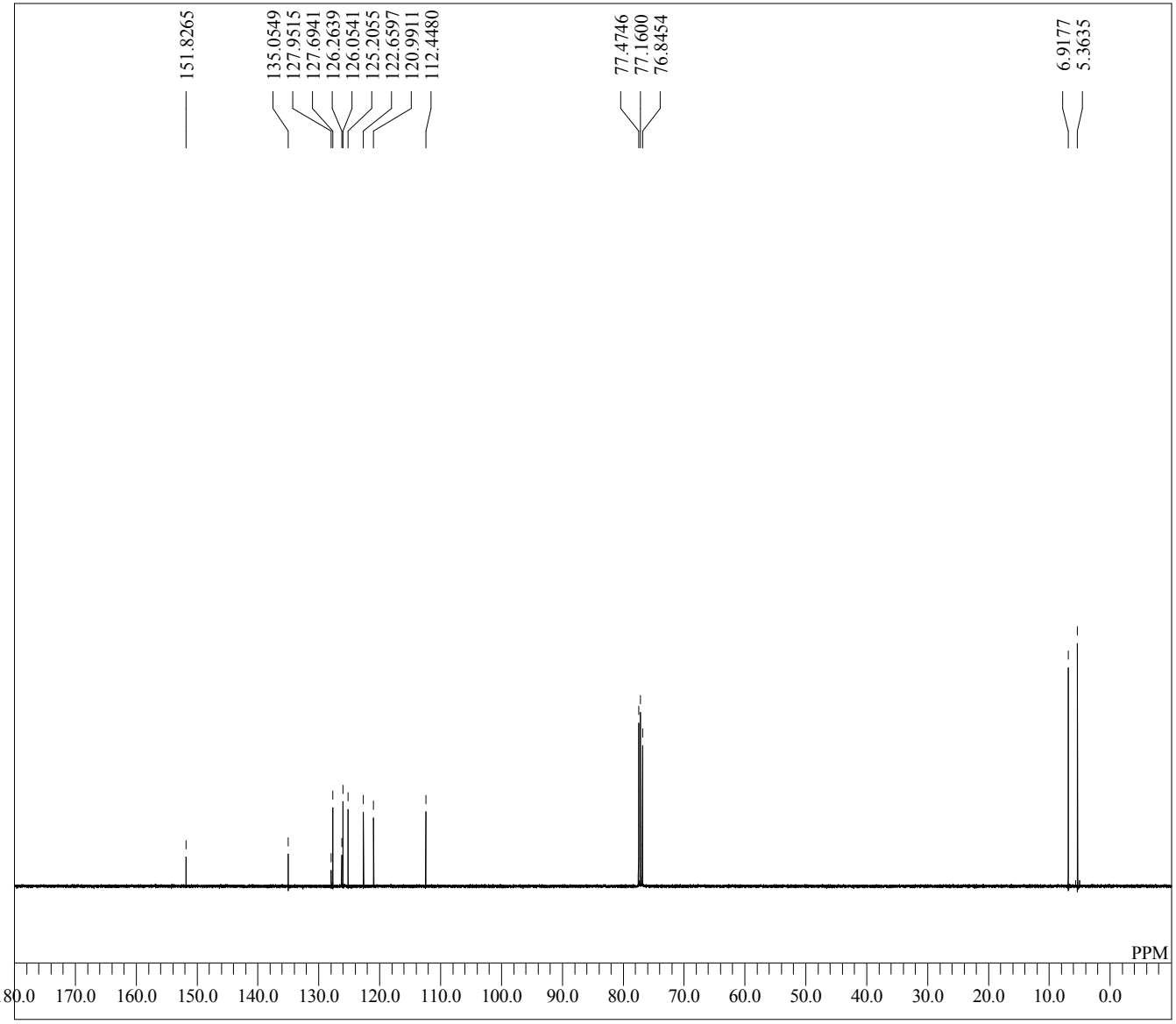


DFILE	yanagihara ex302 pure_proton-1-1.als
COMNT	single_pulse
DATIM	26-02-2018 21:47:17
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	1.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

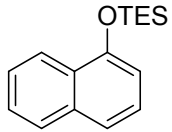


3h

Figure S36

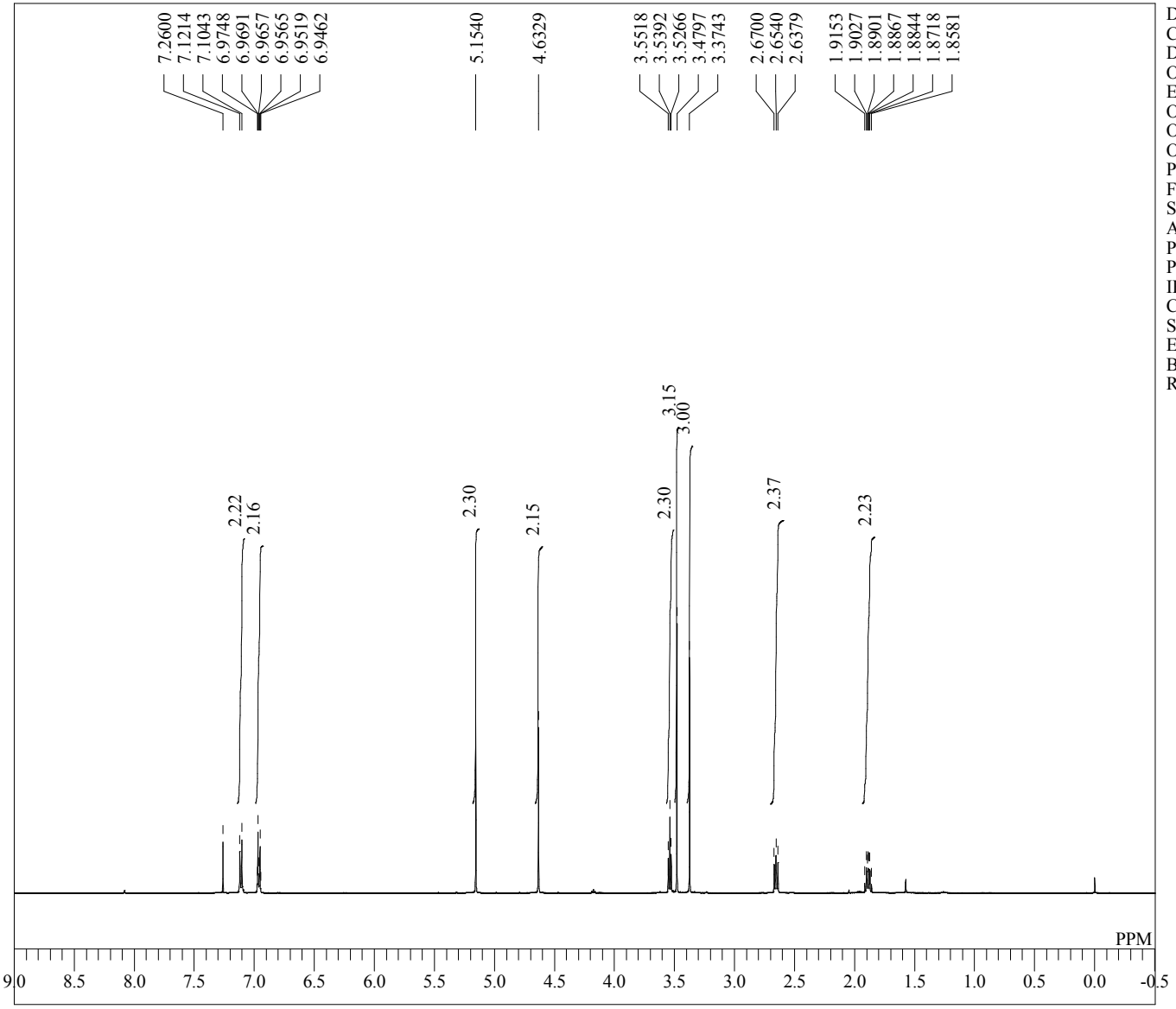


DFILE	yanagihara TES Np_carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-10 17:02:29
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	519
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

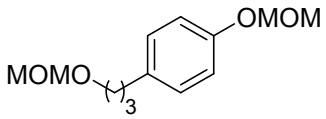


3h

Figure S37

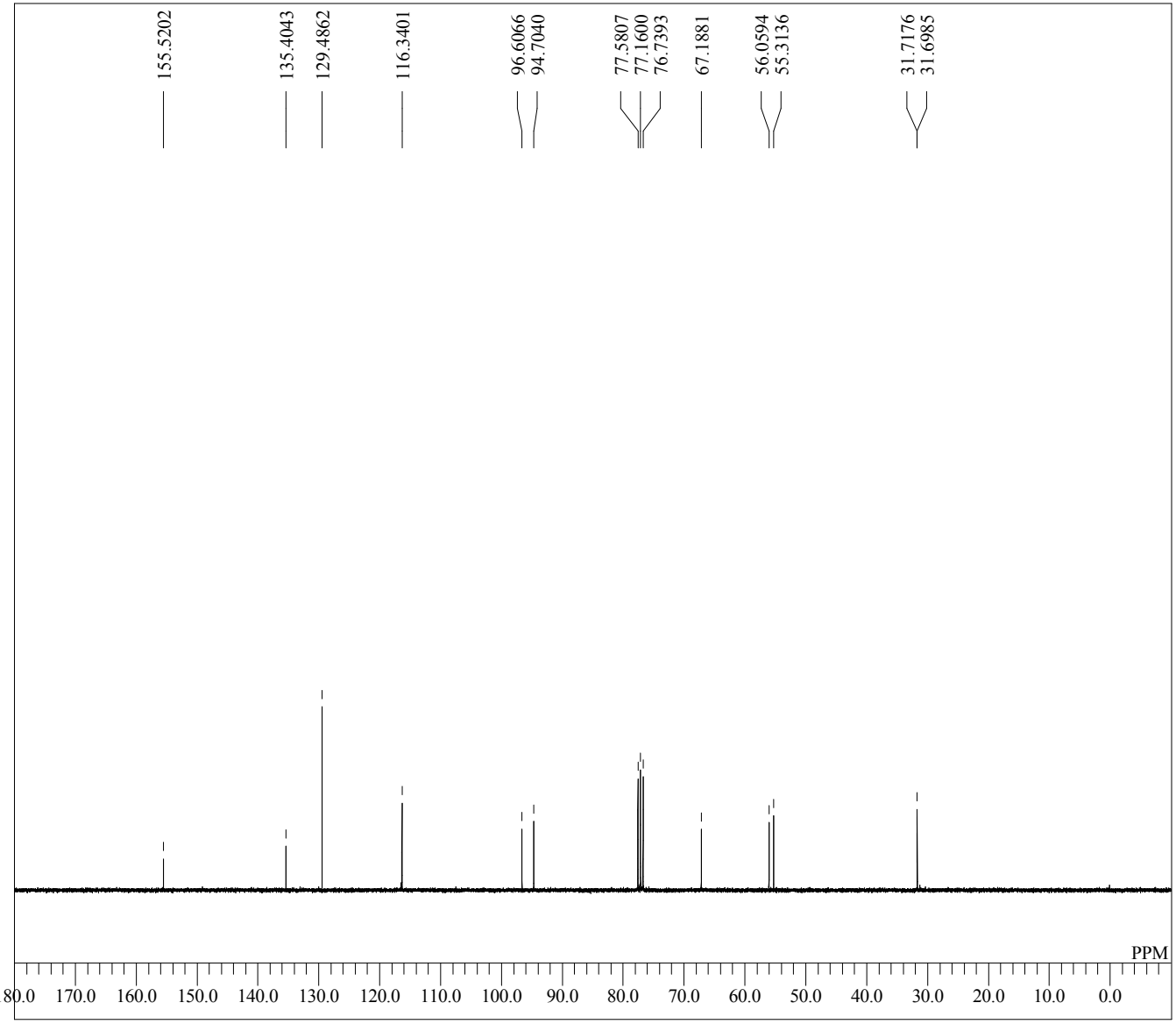


DFILE	yanagihara ex260 pure_proton-1-1.als
COMNT	single_pulse
DATIM	2018-01-09 13:10:12
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	16
ACQTM	1.7459 sec
PD	2.0000 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	19.9 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	44

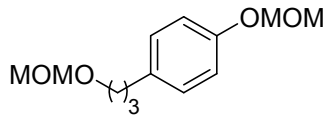


4

Figure S38

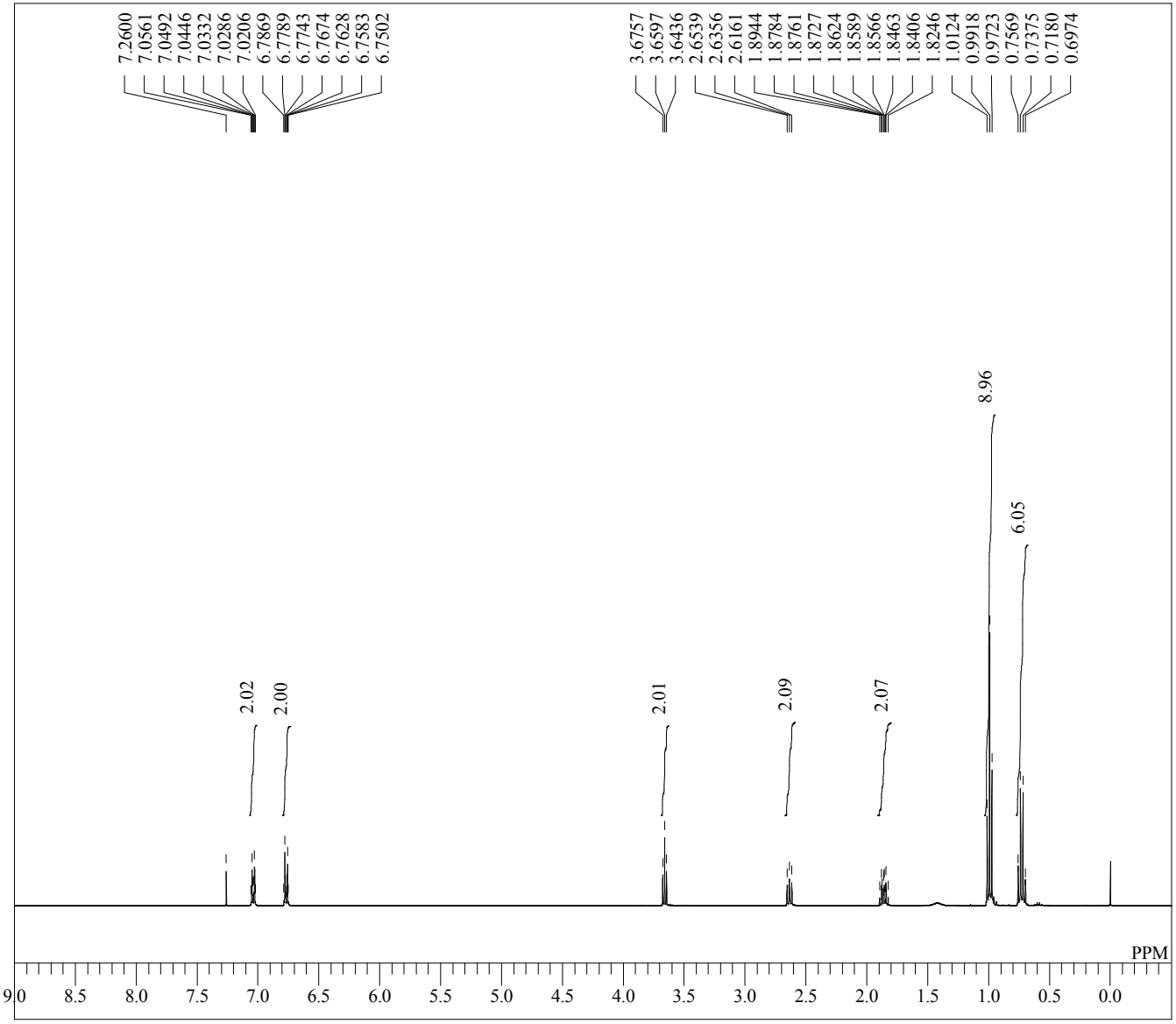


DFILE	yanagihara MOM MOM 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-10 17:44:47
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	75.57 MHz
OBSET	5.79 KHz
OBFIN	1.08 Hz
POINT	26214
FREQU	18939.39 Hz
SCANS	368
ACQTM	1.3841 sec
PD	2.5000 sec
PW1	3.73 usec
IRNUC	1H
CTEMP	19.8 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

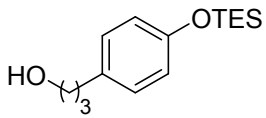


4

Figure S39

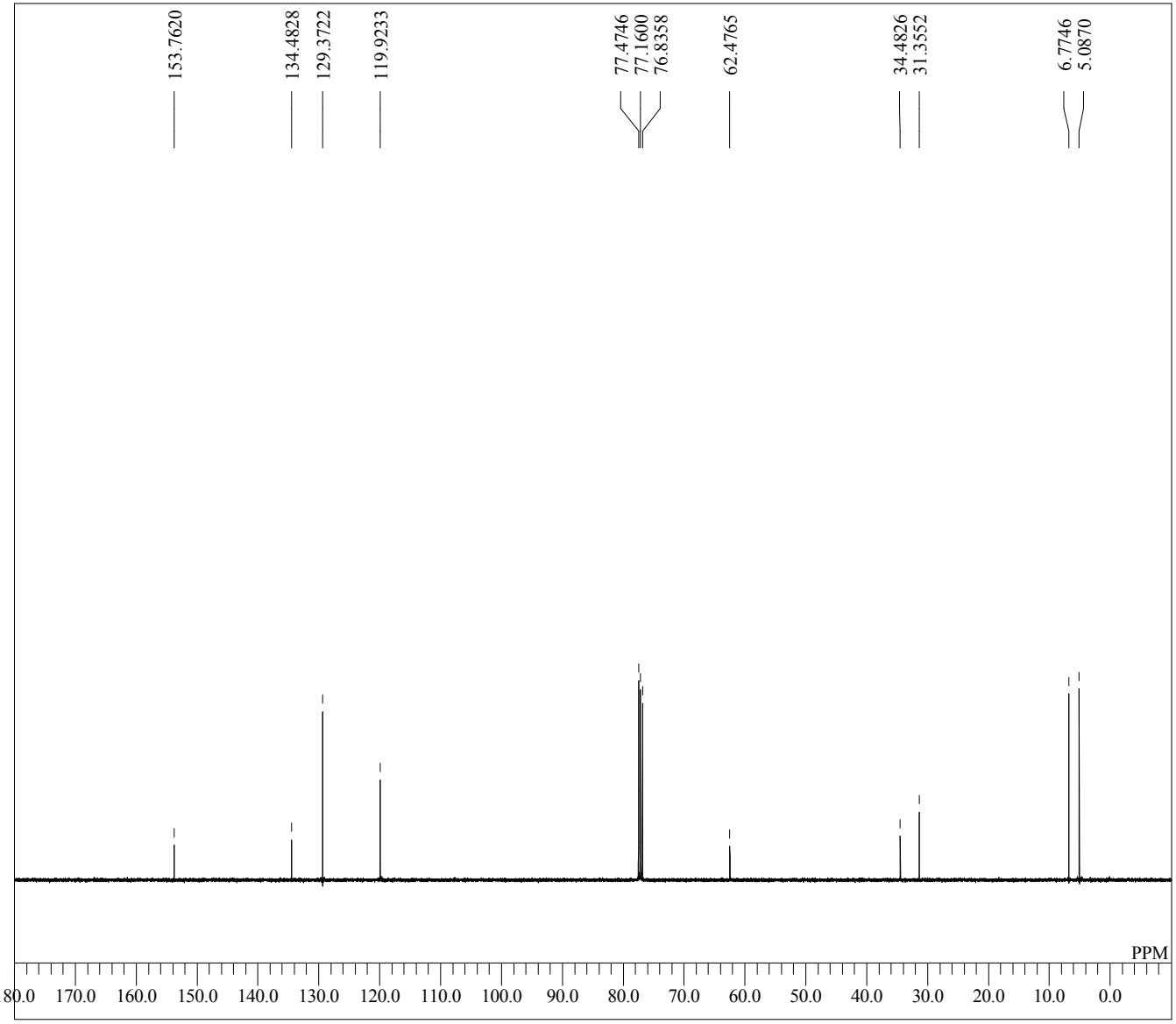


DFILE	yanagihara TES OH 1H_proton-1-1.als
COMNT	single_pulse
DATIM	2018-04-10 19:53:16
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	2.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.2 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	38

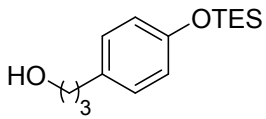


5a

Figure S40

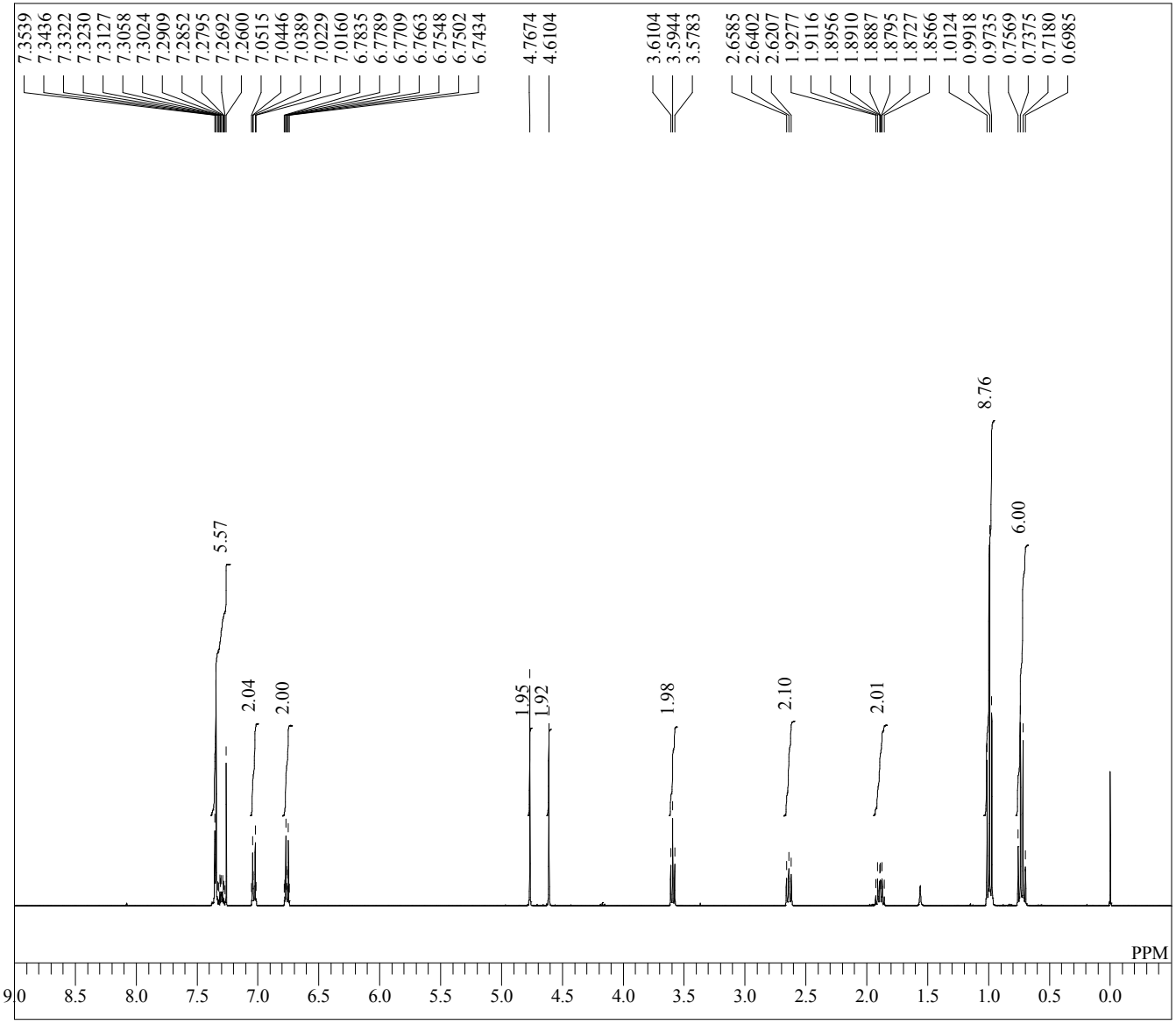


DFILE	yanagihara TES OH 13C_carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-10 19:57:05
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	524
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60

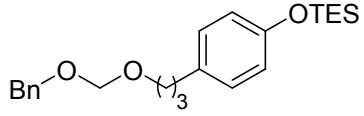


5a

Figure S41

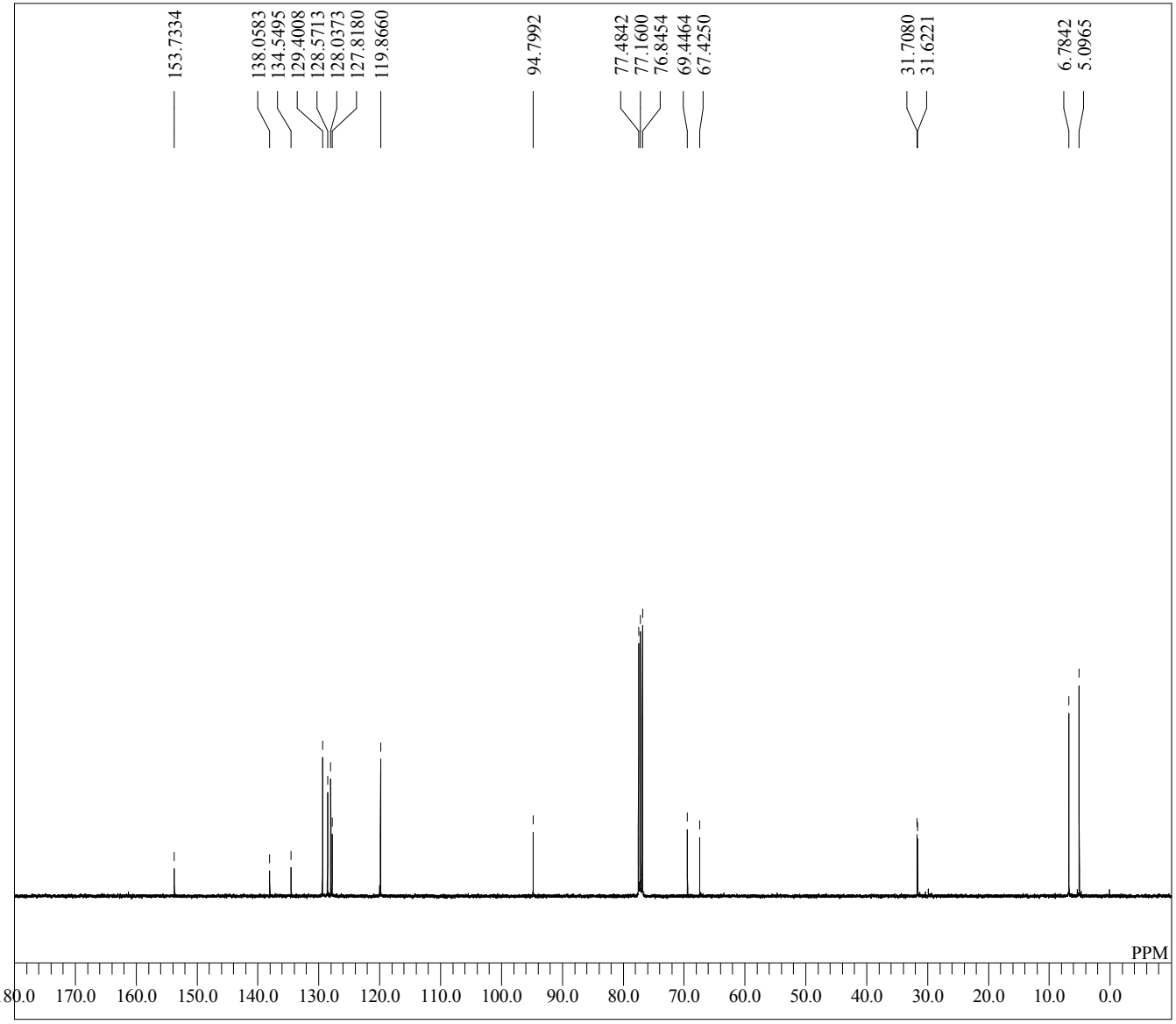


DFILE	yanagihara TES BOM 4_proton-1-1.als
COMNT	single_pulse
DATIM	12-04-2018 19:35:06
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	13107
FREQU	6002.40 Hz
SCANS	16
ACQTM	2.1837 sec
PD	2.0000 sec
PW1	7.25 usec
IRNUC	1H
CTEMP	19.3 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	46

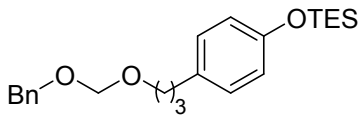


5b

Figure S42

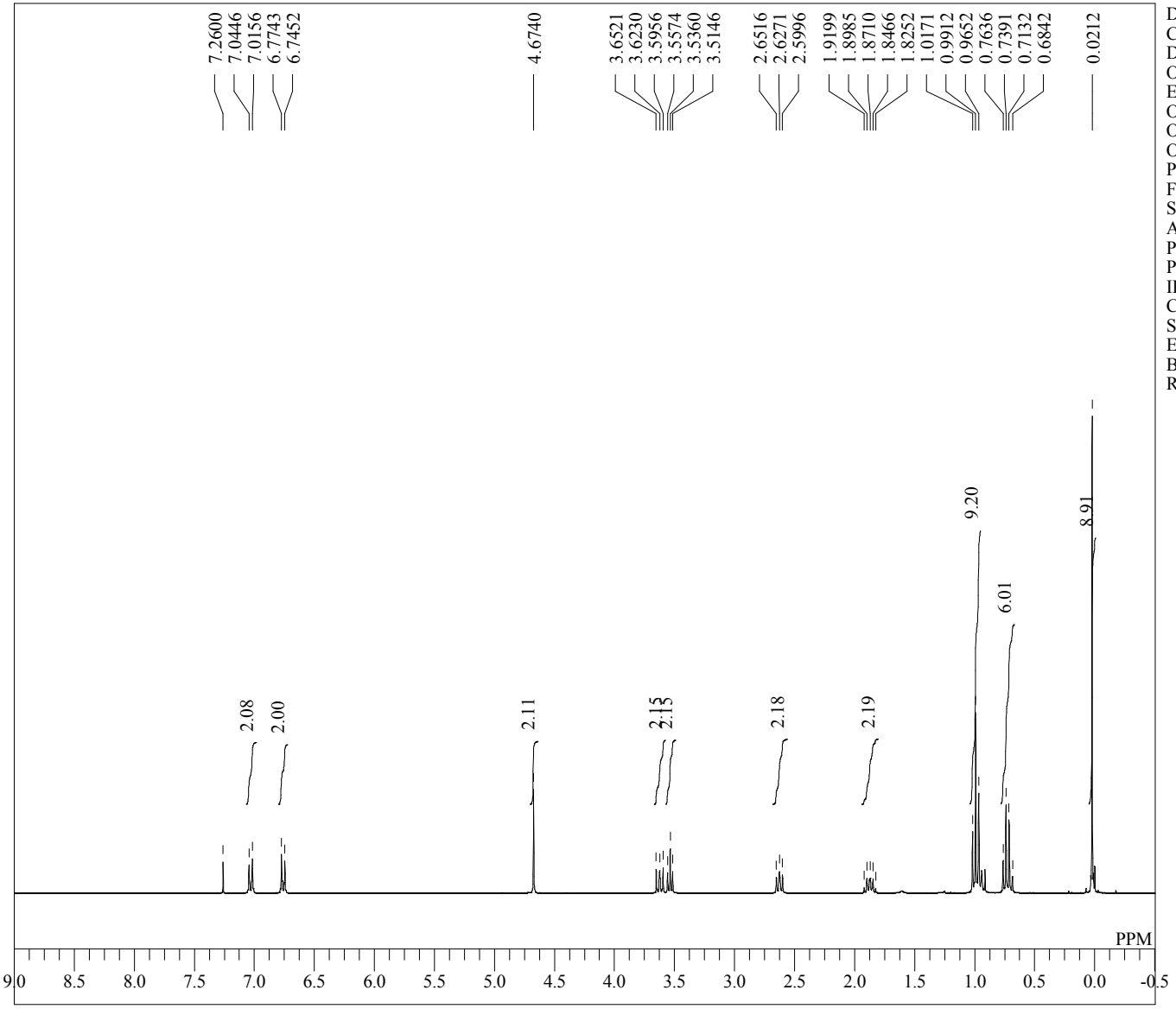


DFILE	yanagihara TES BOM 13C_carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-10 21:26:05
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	26214
FREQU	25125.63 Hz
SCANS	533
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	19.6 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	1.20 Hz
RGAIN	60

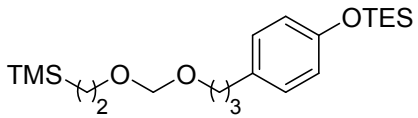


5b

Figure S43

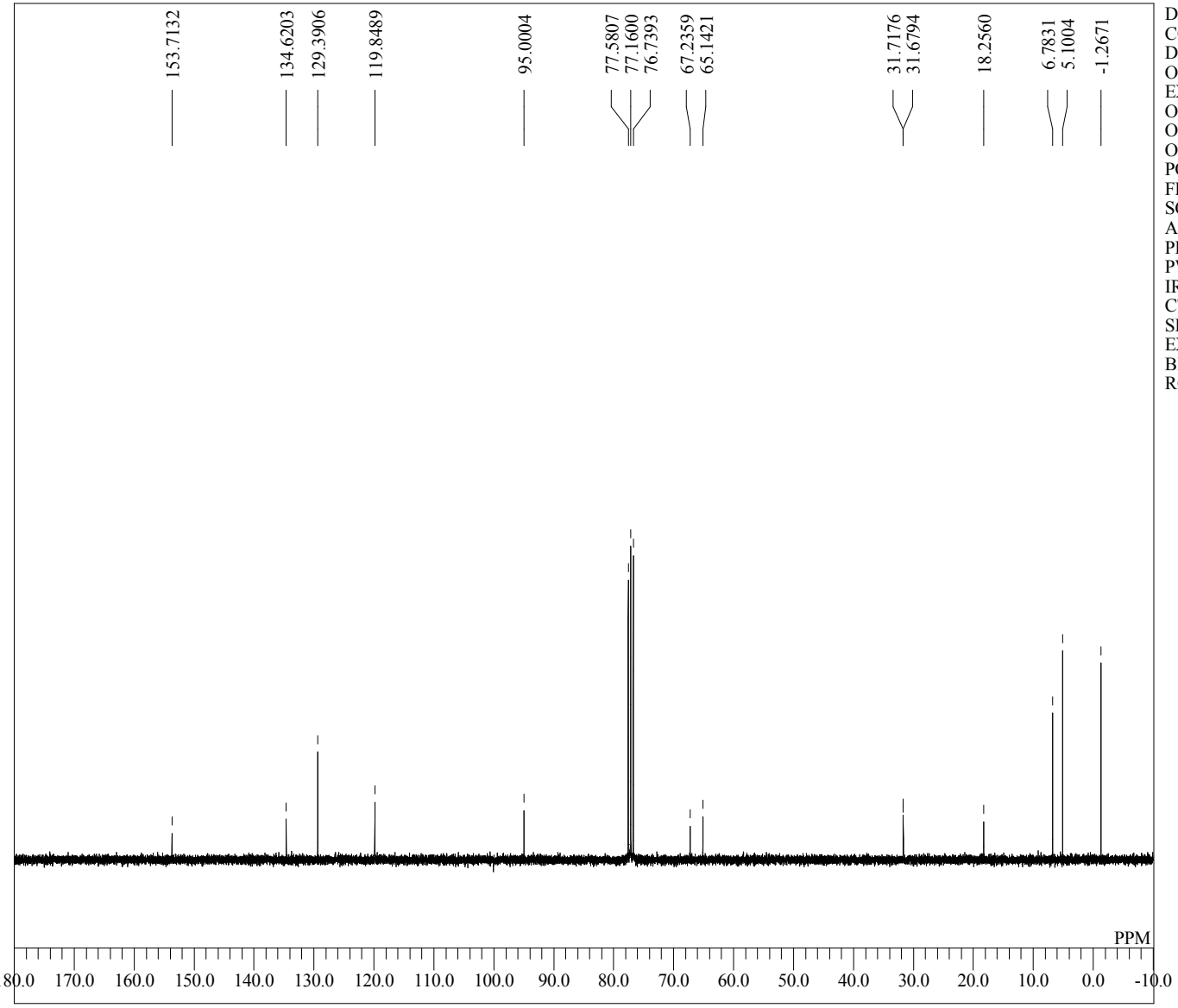


DFILE	yanagihara TES SEM_proton-1-1.als
COMNT	single_pulse
DATIM	2018-04-13 19:30:54
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	300.53 MHz
OBSET	1.15 KHz
OBFIN	8.57 Hz
POINT	13107
FREQU	6016.85 Hz
SCANS	16
ACQTM	2.1784 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	7.26 ppm
BF	0.12 Hz
RGAIN	36

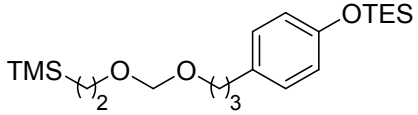


5c

Figure S44



DFILE	yanagihaera TES SEM 13C_Carbon-1-1.als
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-13 19:37:49
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	75.57 MHz
OBSET	5.79 KHz
OBFIN	1.08 Hz
POINT	26214
FREQU	18939.39 Hz
SCANS	374
ACQTM	1.3841 sec
PD	2.5000 sec
PW1	3.73 usec
IRNUC	1H
CTEMP	19.8 c
SLVNT	CDCL3
EXREF	77.16 ppm
BF	0.12 Hz
RGAIN	60



5c

Figure S45