

Supporting Information

Synthesis and Shuttling Behavior of [2]Rotaxanes with a Pyrrole Moiety

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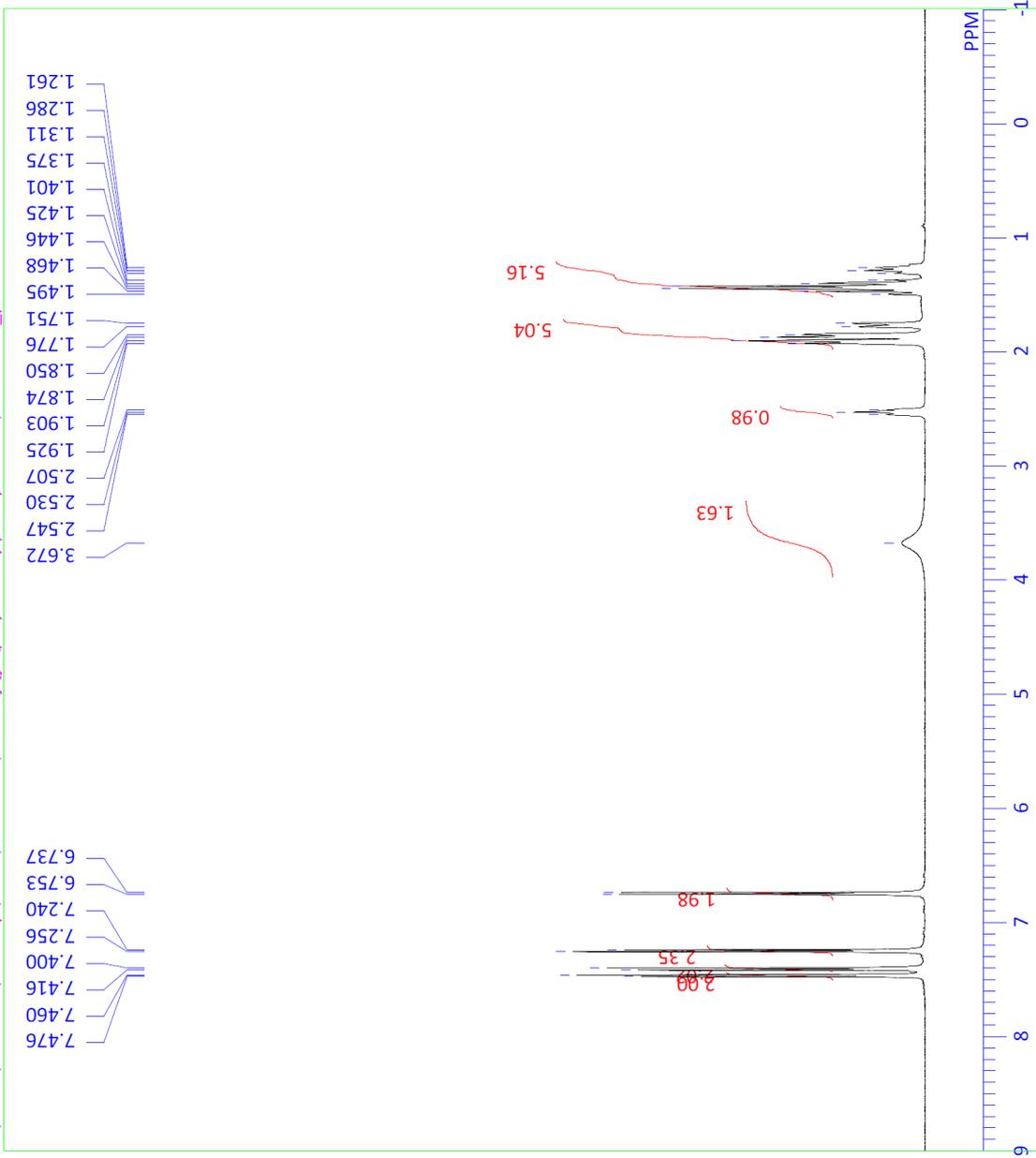
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[‡] Faculty of Pharmaceutical Sciences, Toho University, 2-2-1 Miyama, Funabashi, Chiba 274-8510, Japan

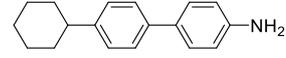
[§] Research Center for Medical and Dental Sciences, Tokyo Medical and Dental University, 1-5-45 Yushima, Bunkyo-ku, Tokyo 113-8510, Japan

¹ H and ¹³ C NMR spectra	S2-29
VT ¹ H NMR studies	S30-37
Evidence for the solvation of 7	S38

C:\Users\ssaitolab\Desktop\NMR\matsuoka\%>>1•jff\p-cyclohexylphenylamine\YM-3-95-3_proton.als



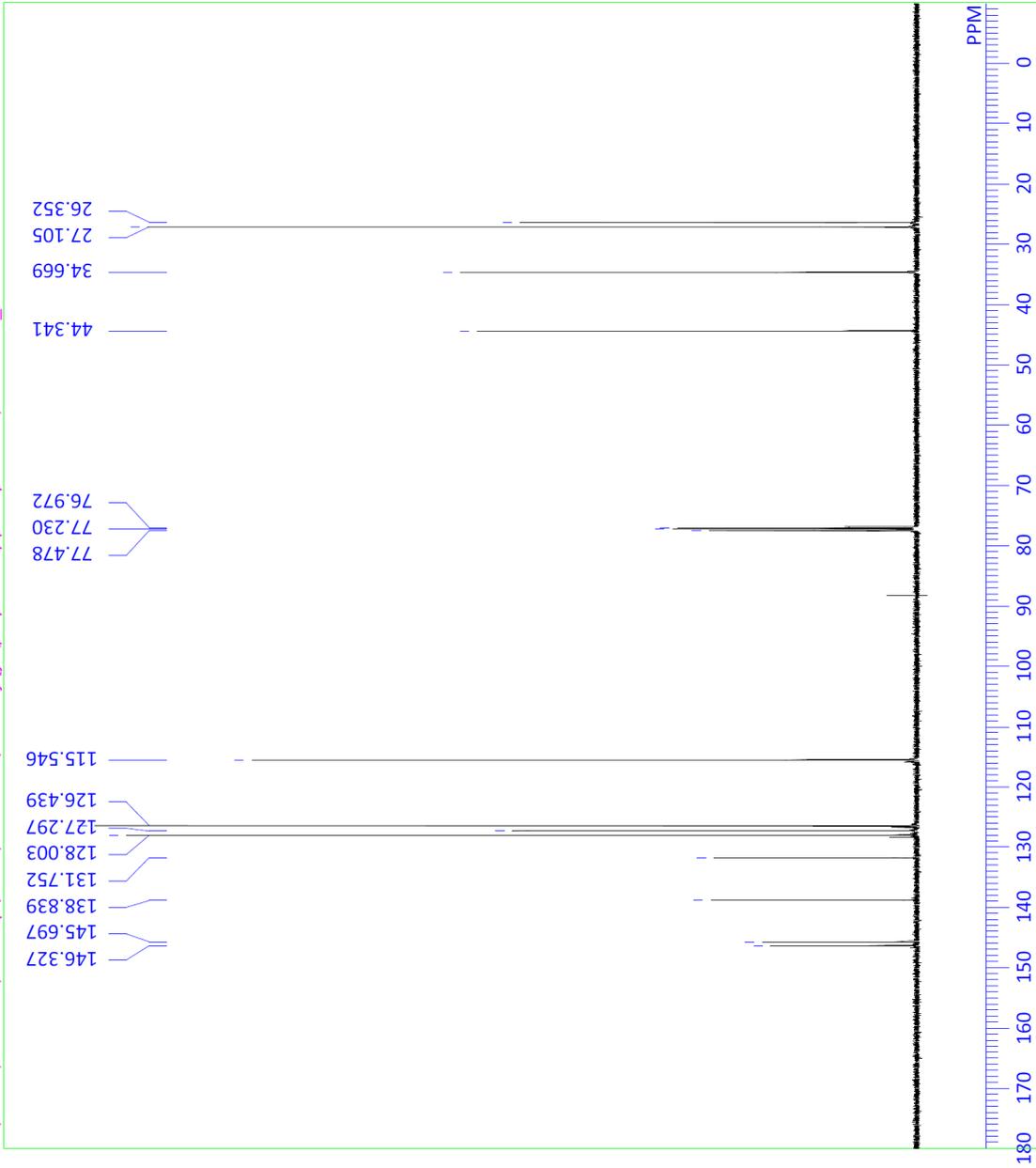
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 3.71 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 38



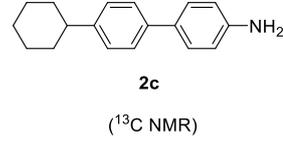
2c

(¹H NMR)

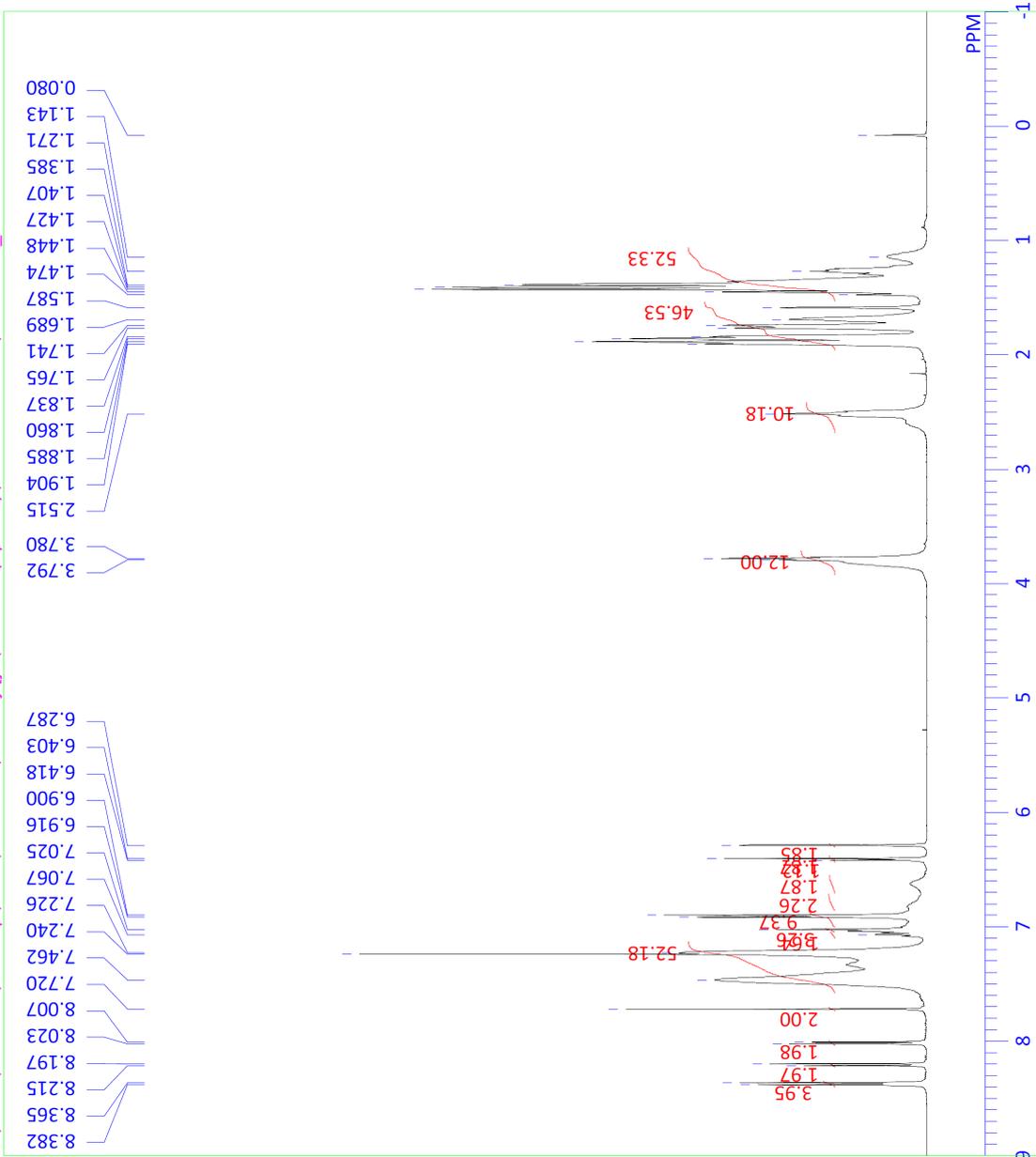
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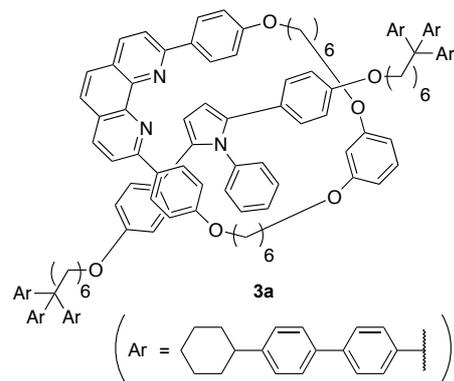
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EXMOD carbon:ixp
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OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31.446.54 Hz
SCANS 1024
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.58 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 20



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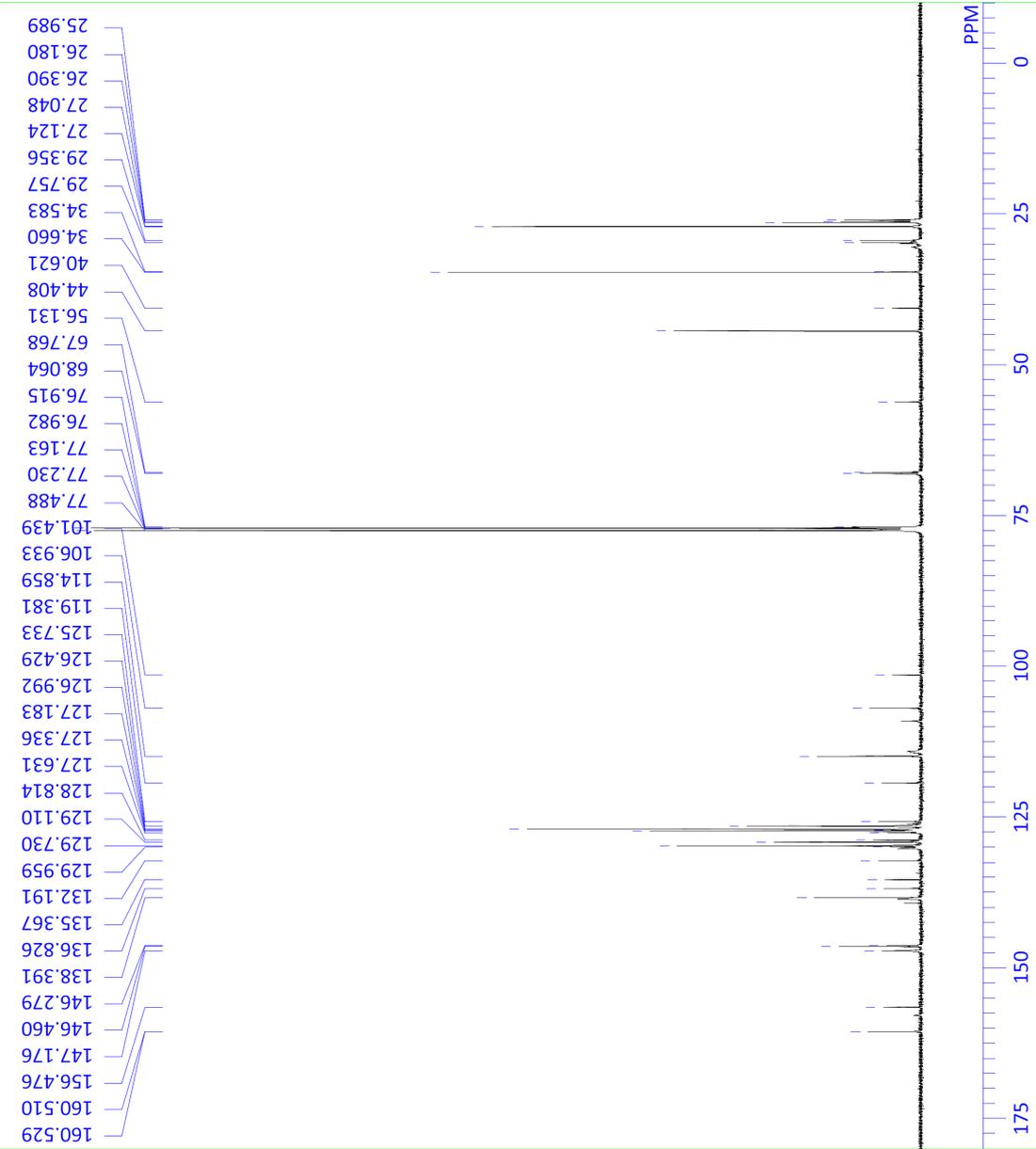


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 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.51 Hz
 SCANS 8
 ACQTM 1.7459 sec
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 PW1 3.71 usec
 IRNUC 1H
 CTEMP 21.6 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 28

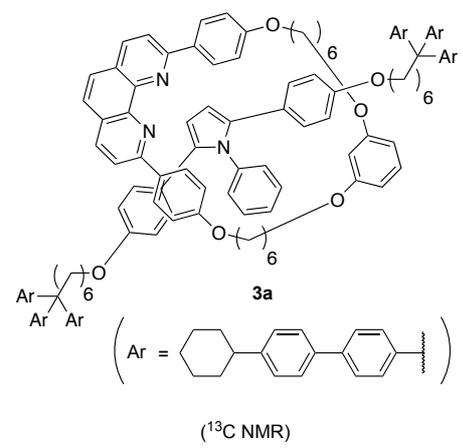


(¹H NMR)

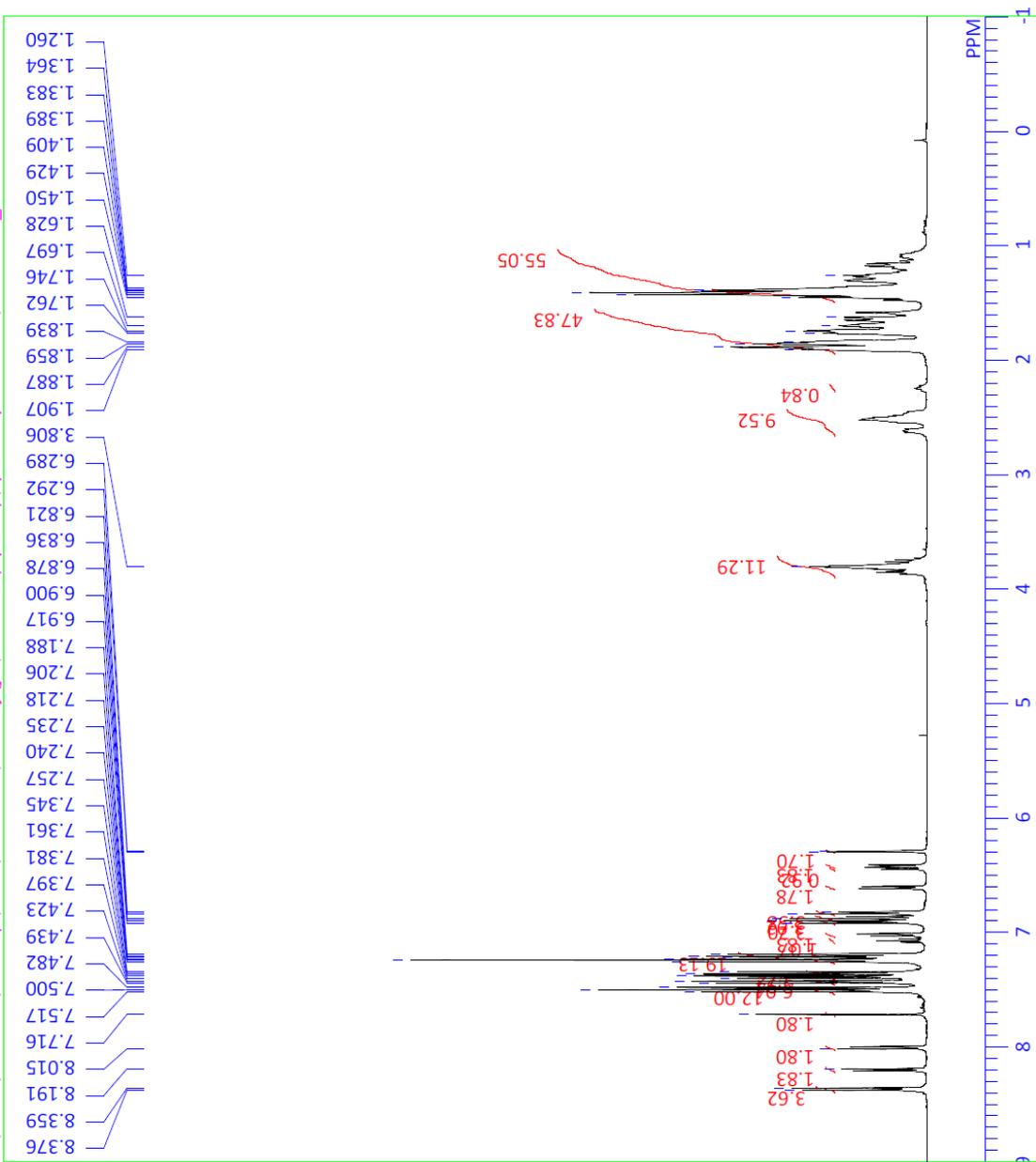
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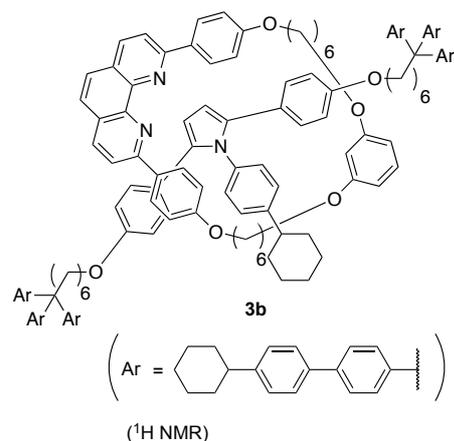
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 EXMOD carbon.ixp
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 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 14940
 ACQTM 0.0000 sec
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 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 50



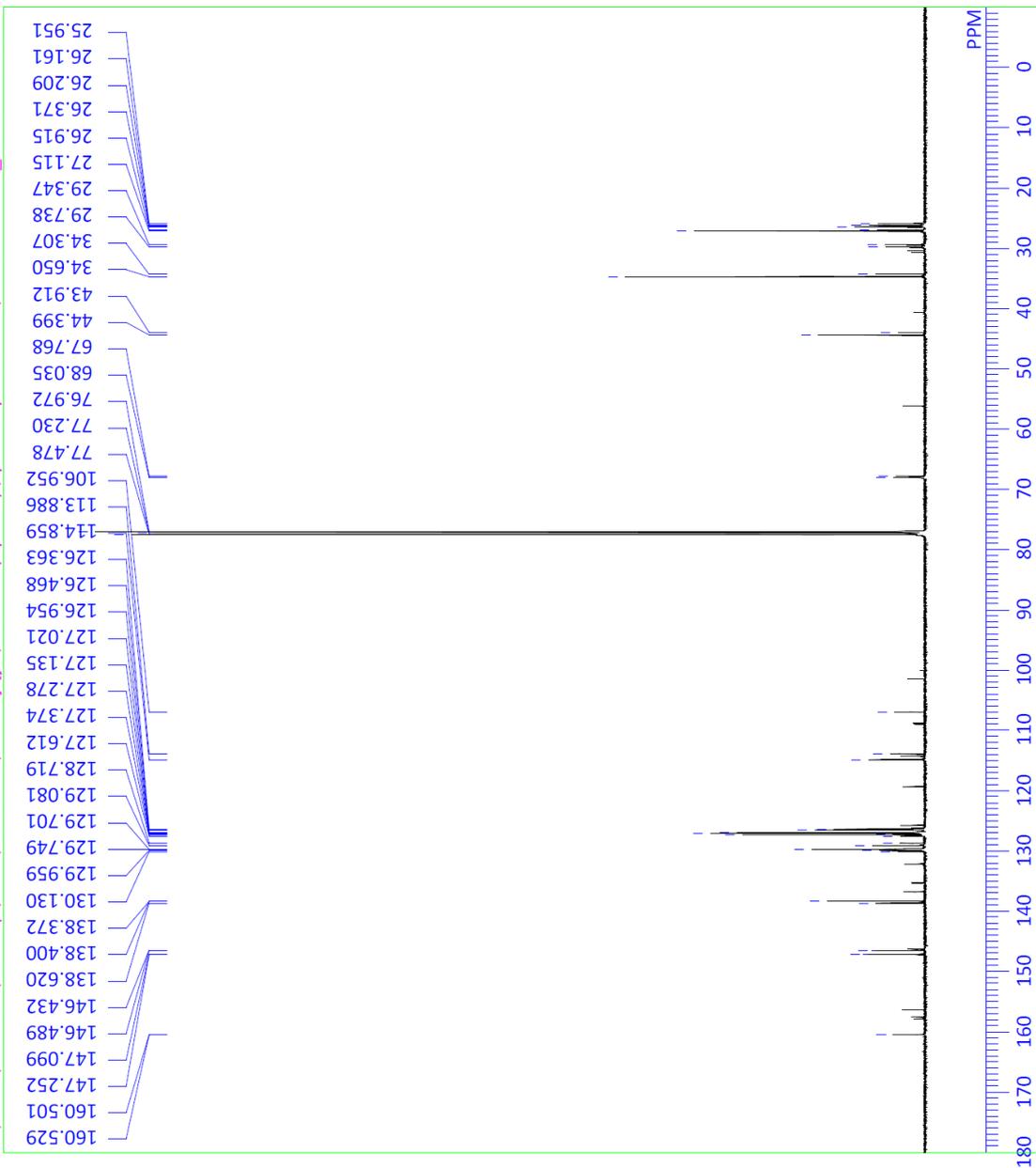
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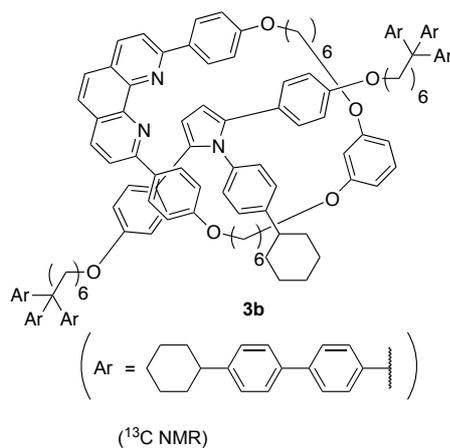
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 EXMOD proton.jxp
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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.51 Hz
 SCANS 8
 ACQTIM 1.7459 sec
 PD 5.0000 sec
 PW1 3.45 usec
 IRNUC 1H
 CTEMP 22.6 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 32



C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00±:ffj\rotaxane (Pyrrole)\cyclohexyl rotaxane\YM-3-11-2-13C_Carbon1-1.als



DFILE YM-3-11-2-13C_Carbon1-1.als
 COMMENT single pulse decoupled gated NOE
 DATIM 2014-10-28 22:03:06
 OBNUC 13C
 EXMOD carbon:ixp
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31.446.54 Hz
 SCANS 15022
 ACQTM 0.0000 sec
 PD 2.0000 sec
 PW1 3.44 usec
 IRNUC 1H
 CTEMP 22.3 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 50

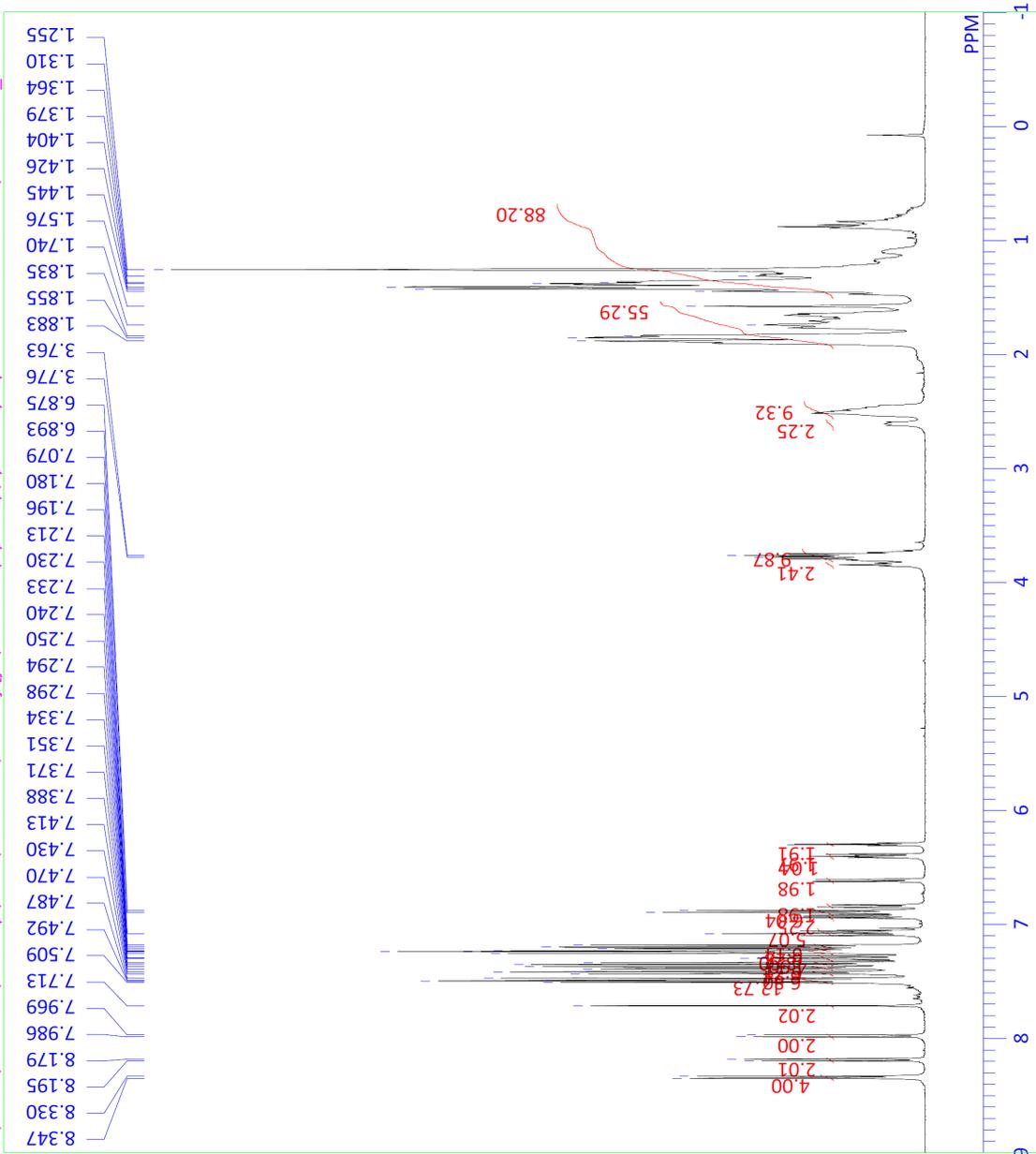
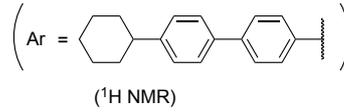
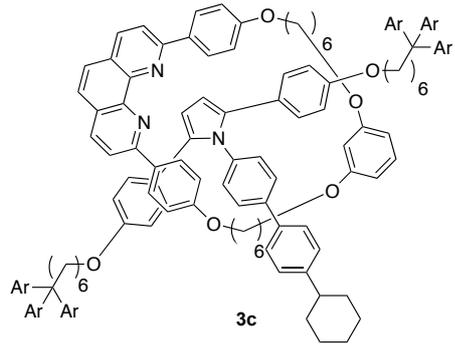


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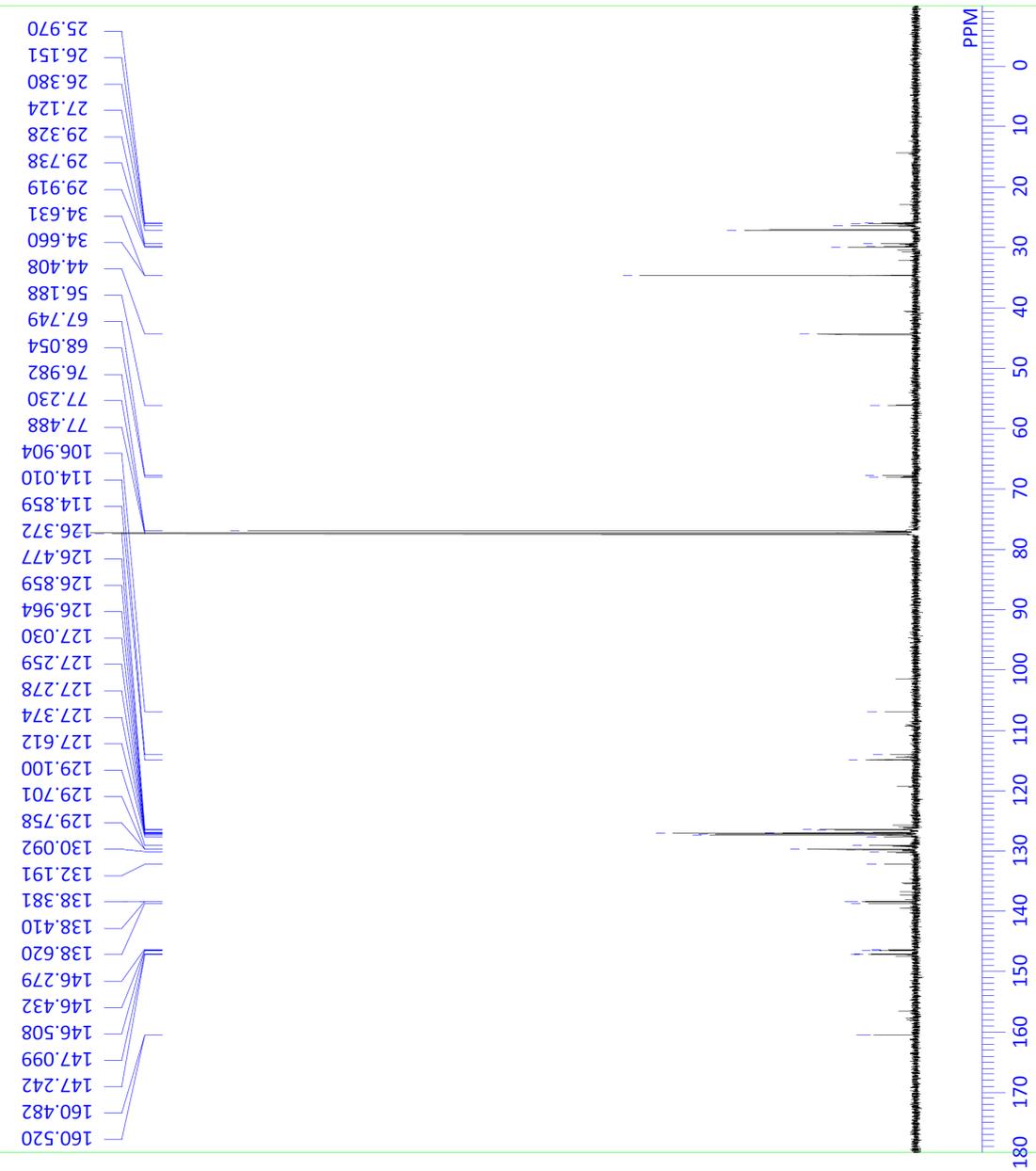
YM-3-13-5_Proton-1-1.als
 single_pulse
 2014-10-22 14:32:21

DFILE
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 DATIM
 OBNUC
 EXMOD
 OBFREQ
 OBSET
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 POINT
 FREQU
 SCANS
 ACQTIM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

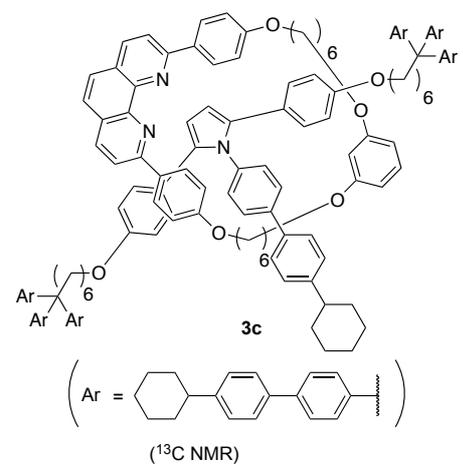
1H
 proton.jp
 500.16 MHz
 2.41 KHz
 6.01 Hz
 13107
 7507.51 Hz
 8
 1.7459 sec
 5.0000 sec
 3.45 usec
 1H
 23.0 c
 CDCL3
 7.24 ppm
 0.12 Hz
 30



C:\Users\ssaitolab\Desktop\NMR\matsuoka\%001\jffj\rotaxane (Pyrrole)\cyclohexylbiphenylamine rotaxane\YM-3-13-5_Carbon-1-1.als

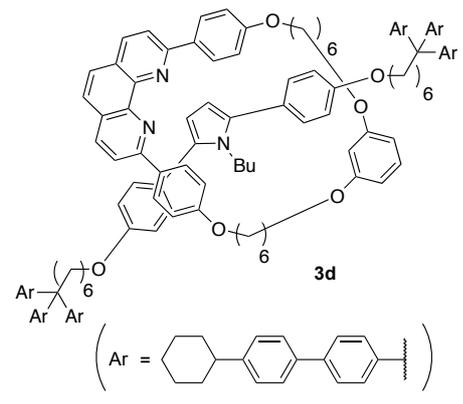


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 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 1300
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.44 usec
 IRNUC 1H
 CTEMP 22.6 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 50

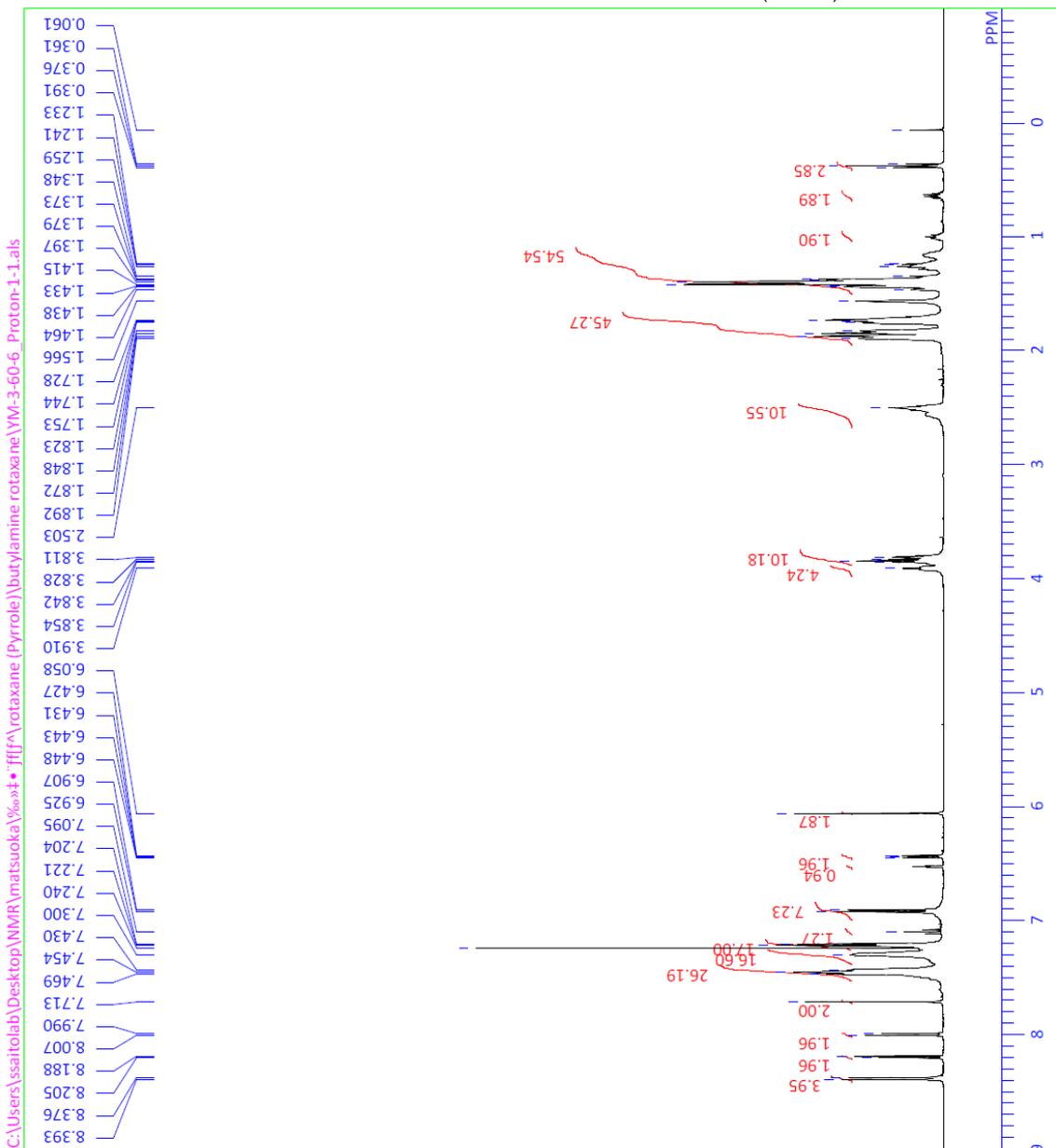


YM-3-60-6_Proton-1-1.als
 single_pulse
 2015-01-21 22:00:03
 1H
 proton:jpg
 500.16 MHz
 2.41 KHz
 6.01 Hz
 13107
 7507.51 Hz
 8
 1.7459 sec
 5.0000 sec
 3.71 usec
 1H
 20.9 c
 CDCl3
 7.24 ppm
 0.12 Hz
 38

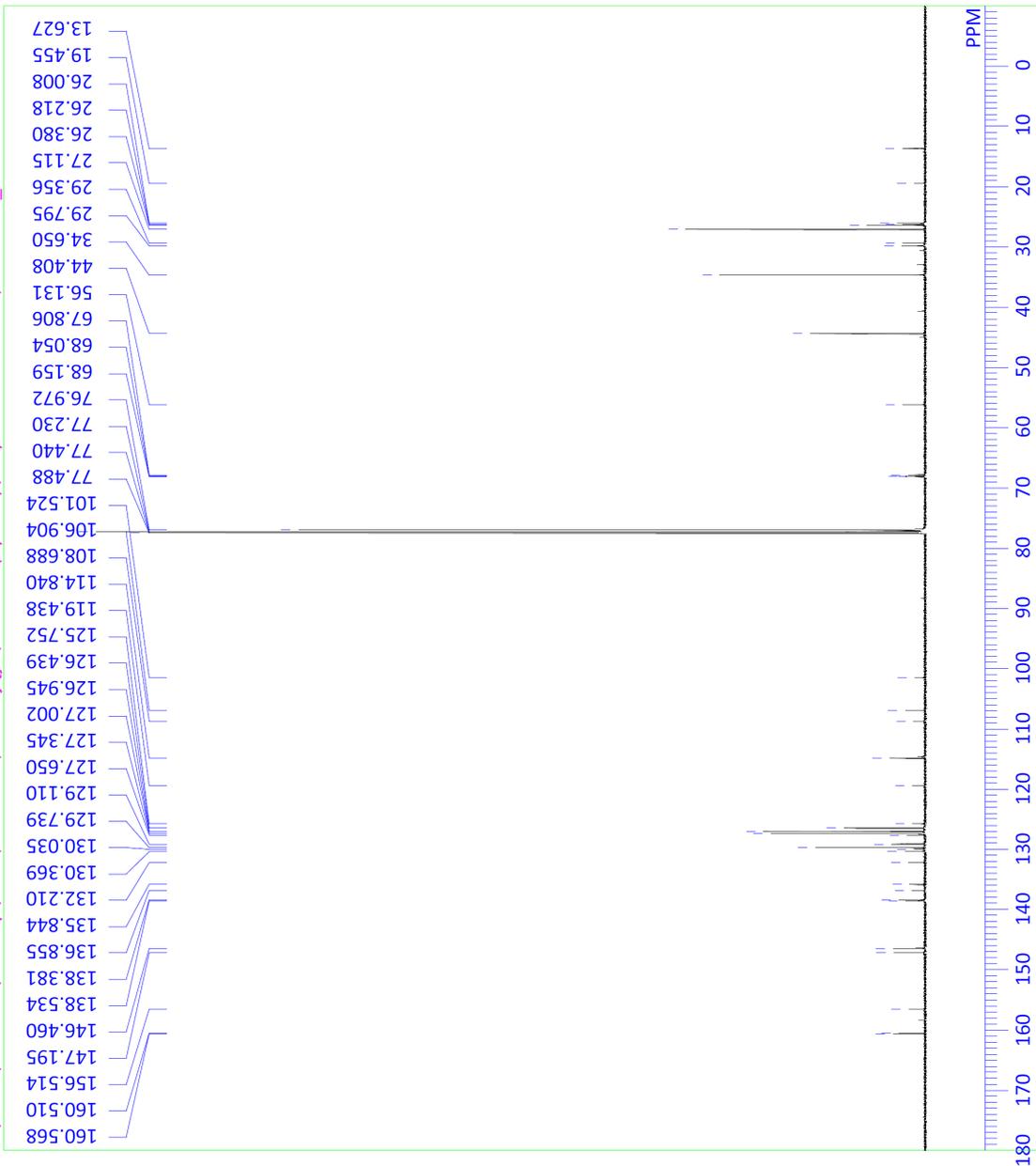
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 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN



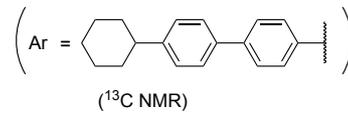
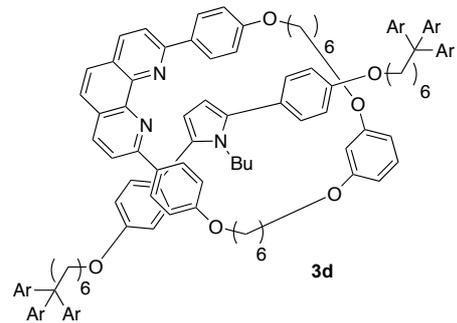
(¹H NMR)



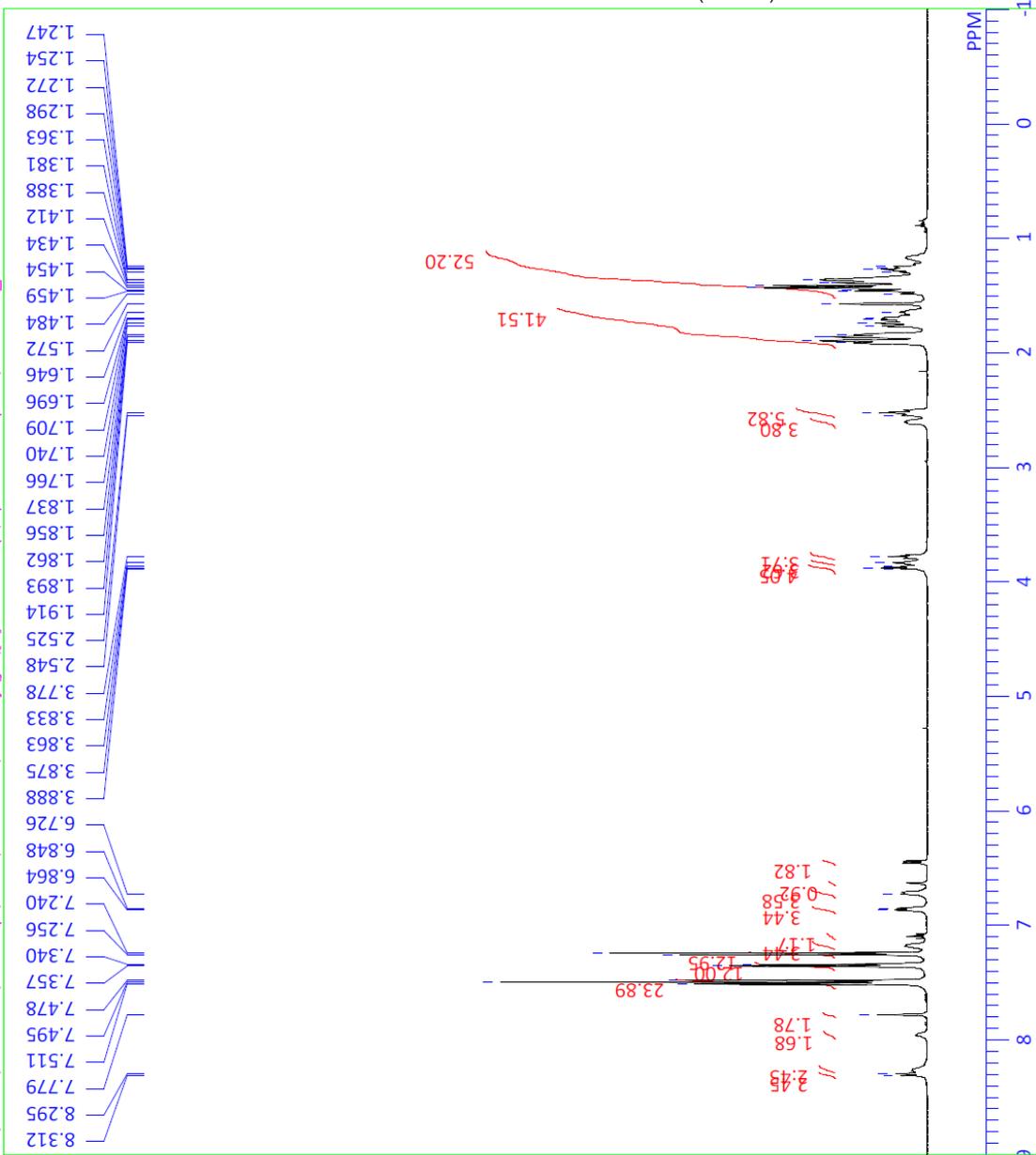
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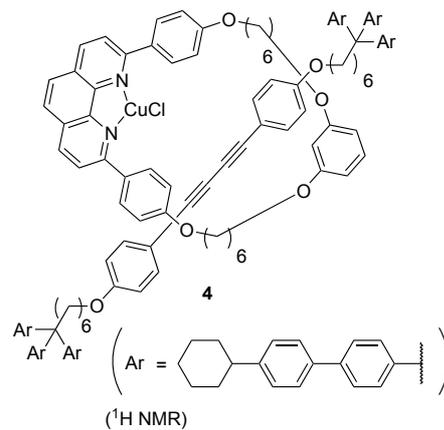
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EXMOD carbon:ixp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 15020
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.58 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 20



C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00*%*ffif\2]rotaxane (6,6) CuCl-complex\YM-4-7-2_Proton-1-1.als

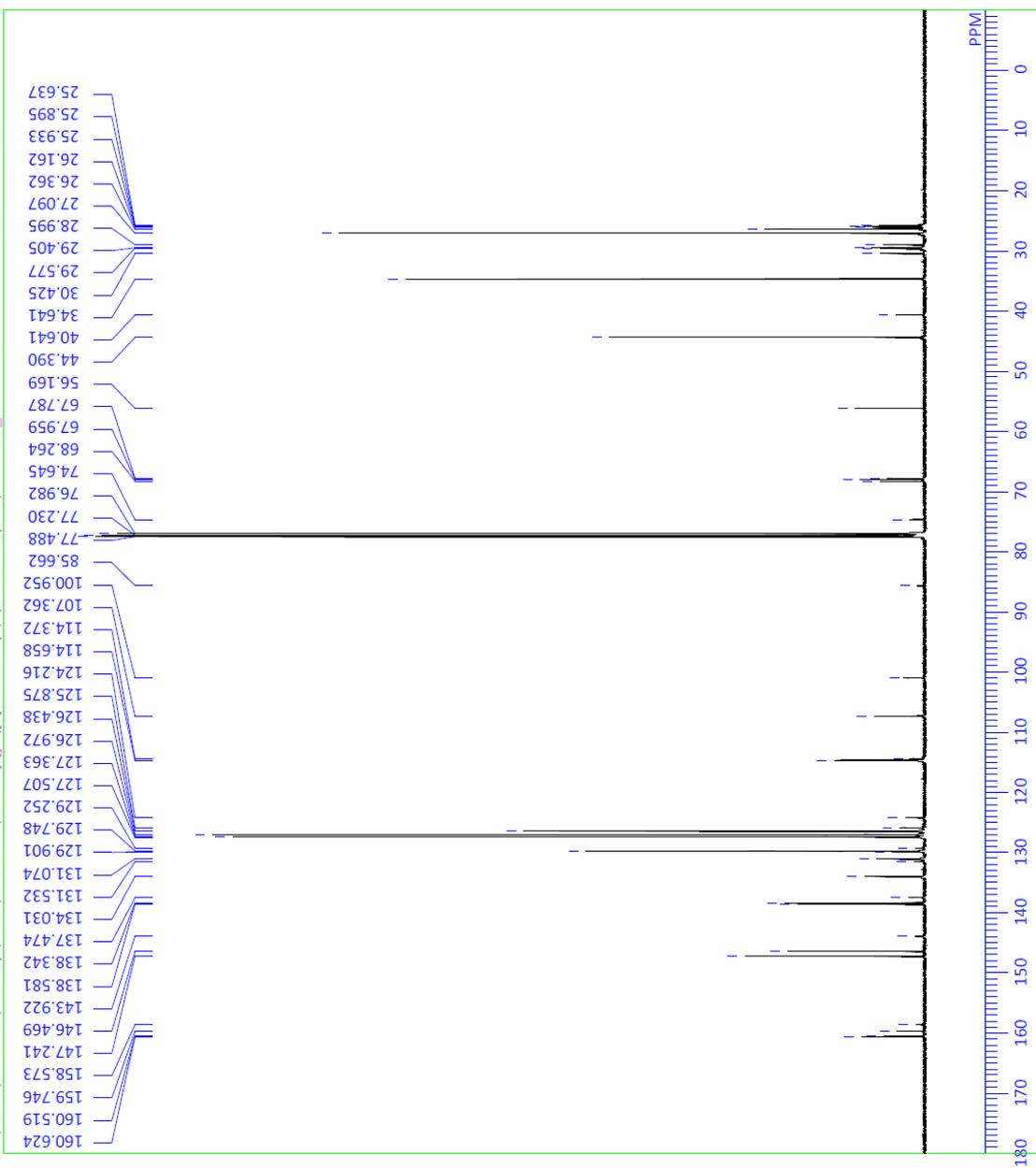
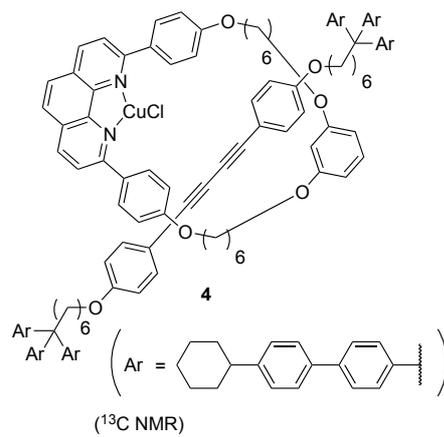


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 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.51 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 3.71 usec
 IRNUC 1H
 CTEMP 24.1 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 46



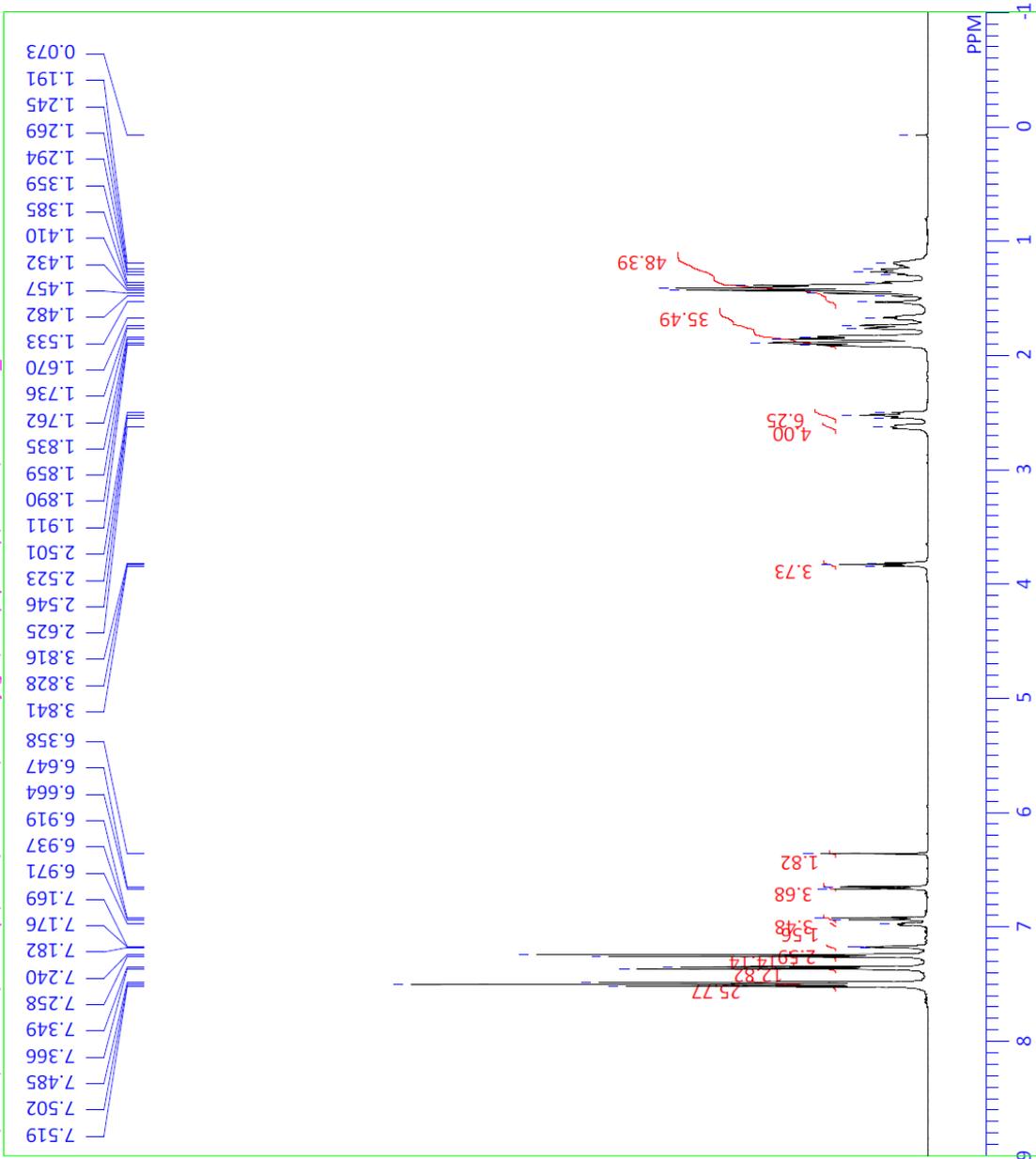
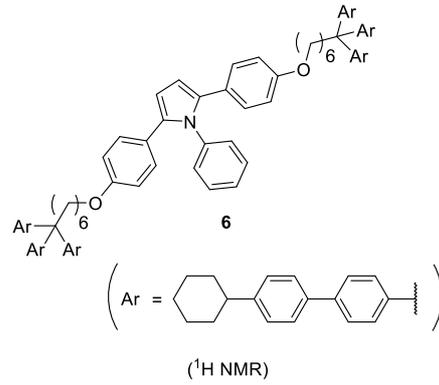
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 OBFIN 4.21 Hz
 POINT 32767
 FREQU 39308.18 Hz
 SCANS 15006
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.58 usec
 IRNUC 1H
 CTEMP 24.0 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 20



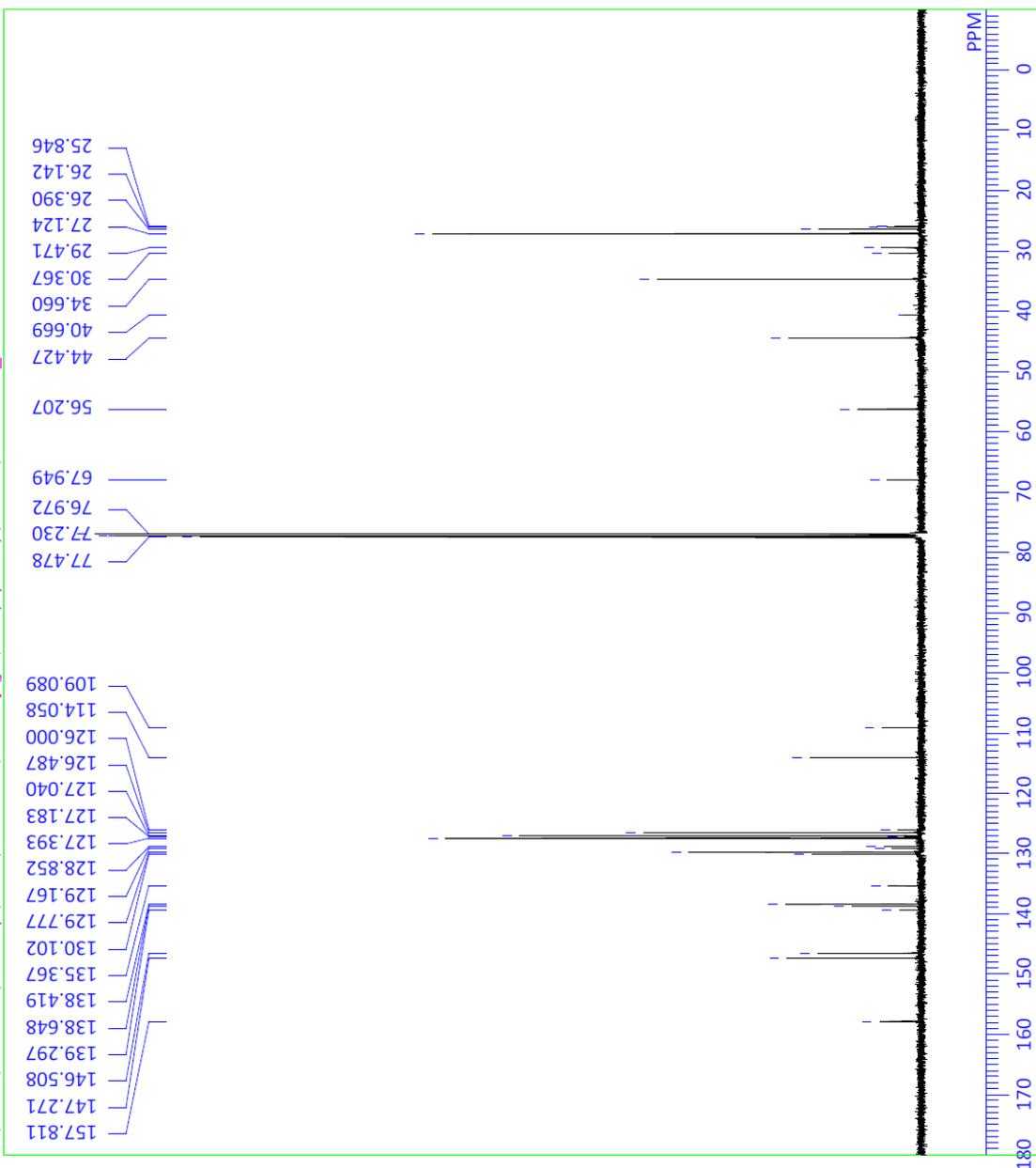
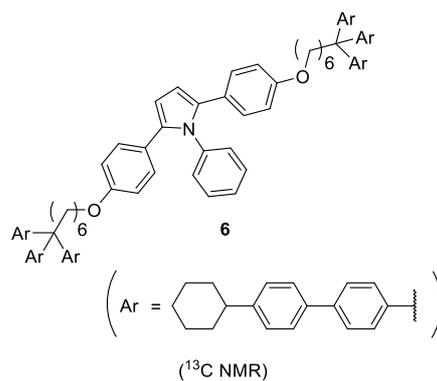
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 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.51 Hz
 SCANS 8
 ACQTIM 1.7459 sec
 PD 5.0000 sec
 PW1 3.71 usec
 IRNUC 1H
 CTEMP 23.7 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 36

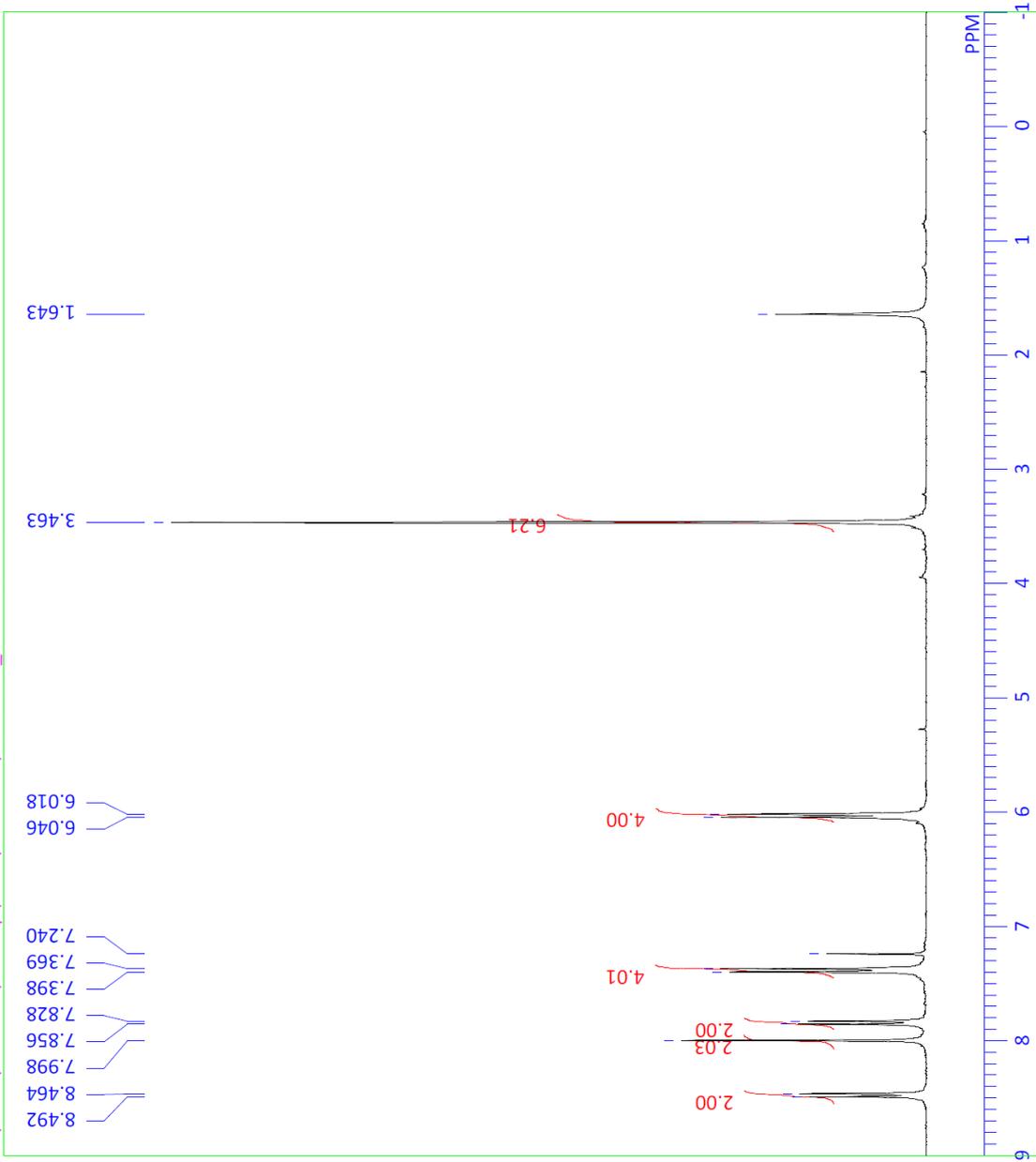


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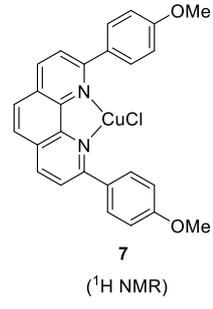
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 EXMOD carbon.jpg
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 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 1585
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.58 usec
 IRNUC 1H
 CTEMP 23.7 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 20



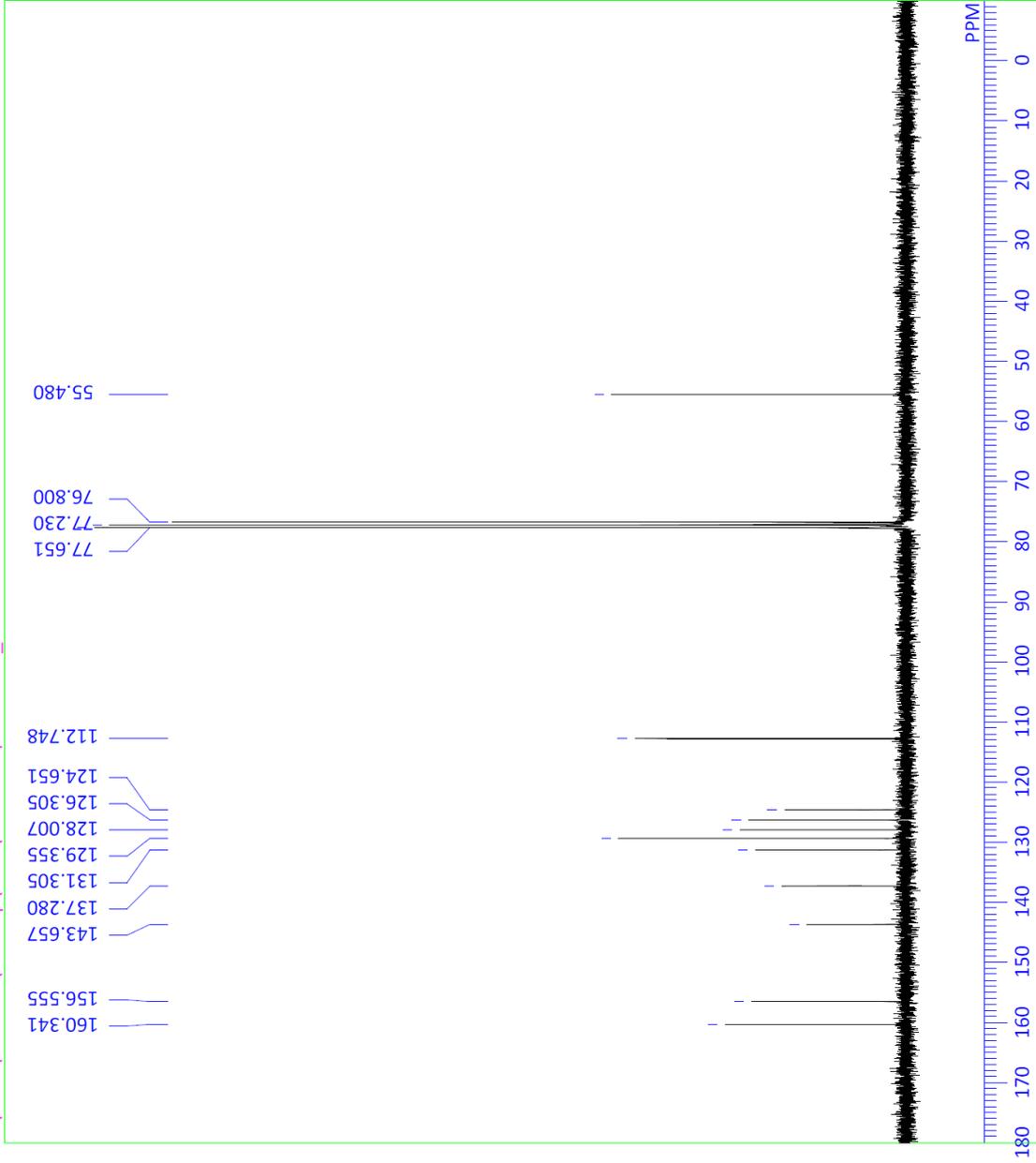
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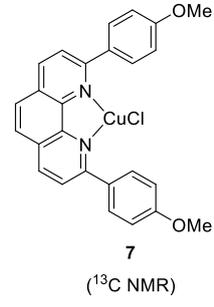
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OBNUC 1H
EXMOD proton.jxp
OBFRQ 300.53 MHz
OBSET 1.15 KHz
OBFIN 8.57 Hz
POINT 16384
FREQU 5635.71 Hz
SCANS 8
ACQTM 2.9072 sec
PD 5.0000 sec
PW1 5.10 usec
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 40



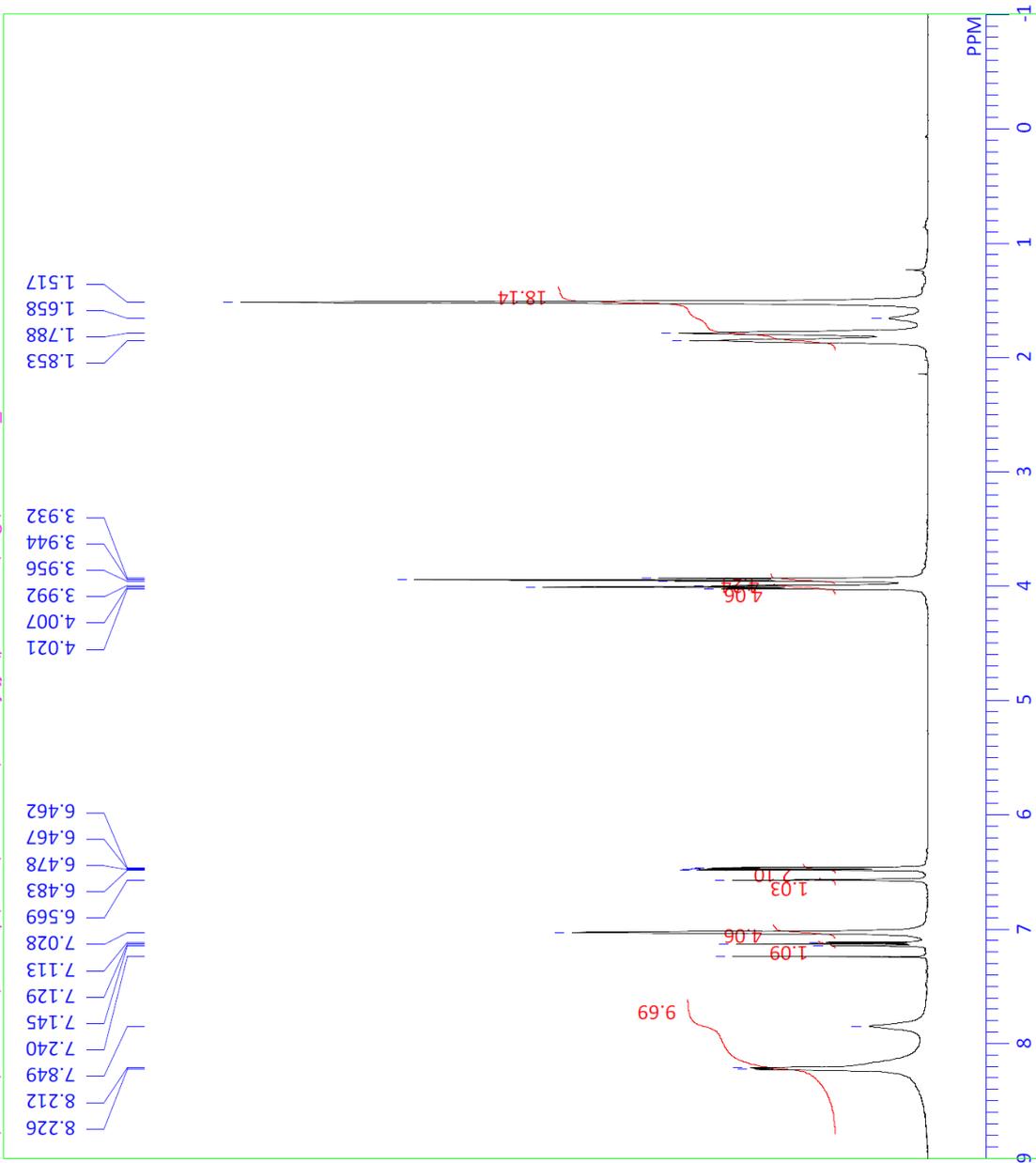
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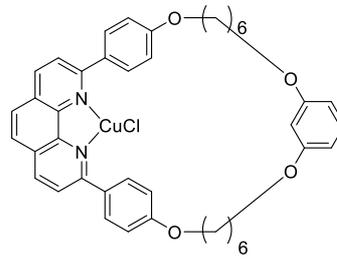
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OBNUC 13C
EXMOD carbon.jxp
OBFRQ 75.57 MHz
OBSET 5.79 KHz
OBFIN 1.08 Hz
POINT 32767
FREQU 23674.24 Hz
SCANS 868
ACQTM 1.3841 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 23.9 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 50



C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00#*ffjf\phen-CuCl\ring\YM-4-47-3_Proton-2-1.als

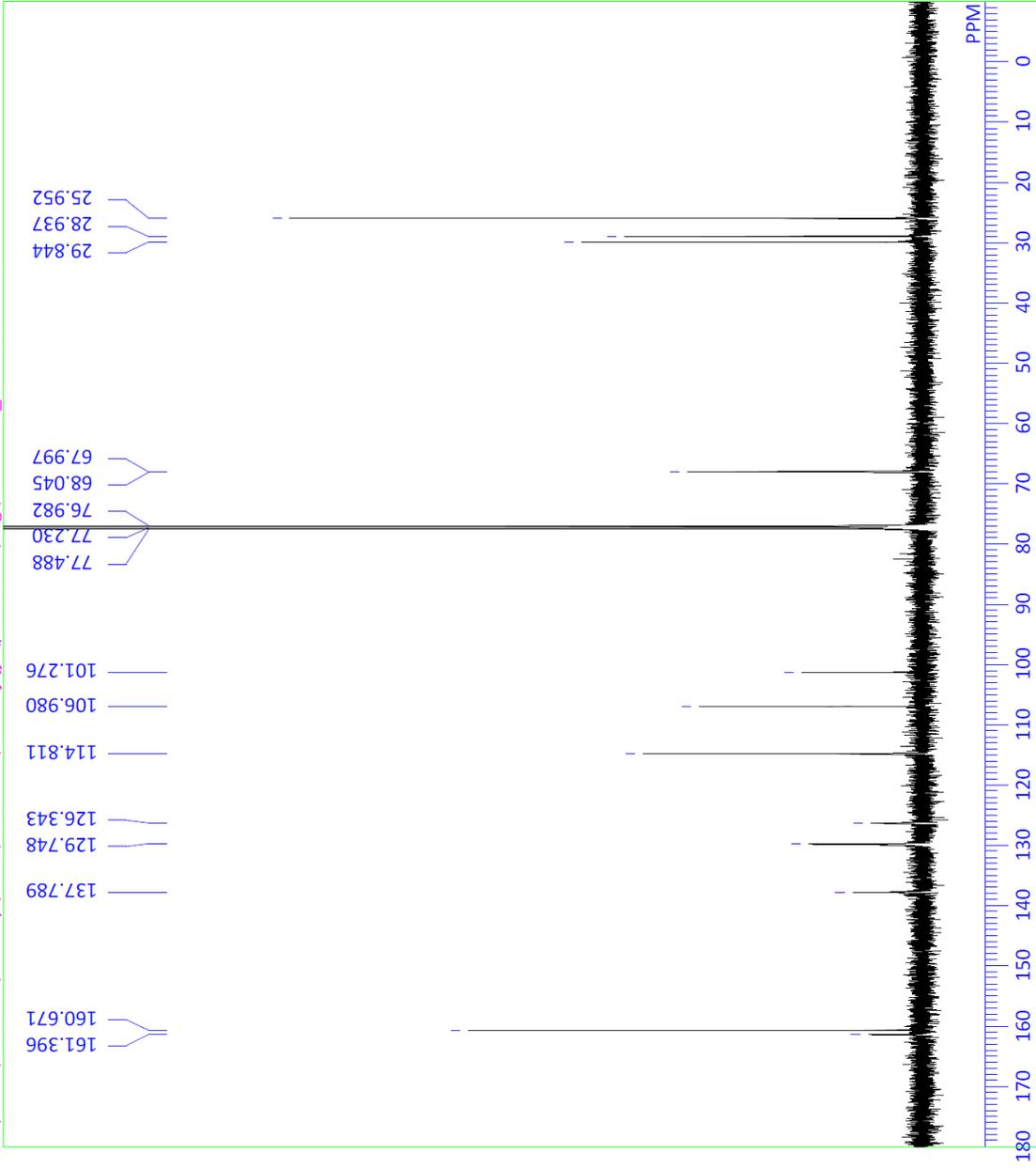


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 DATIM 2015-11-18 15:06:47
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 EXMOD proton.jxp
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTIM 1.7459 sec
 PD 5.0000 sec
 PW1 3.52 usec
 IRNUC 1H
 CTEMP 24.1 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 36



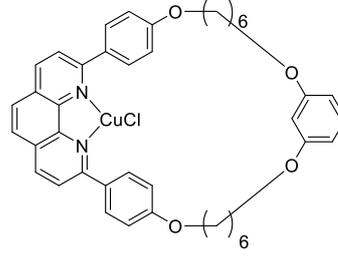
8
(¹H NMR)

C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00»†•:ffj^\phen-CuCl\ring\YM-4-47-4_Carbon-1-1.als



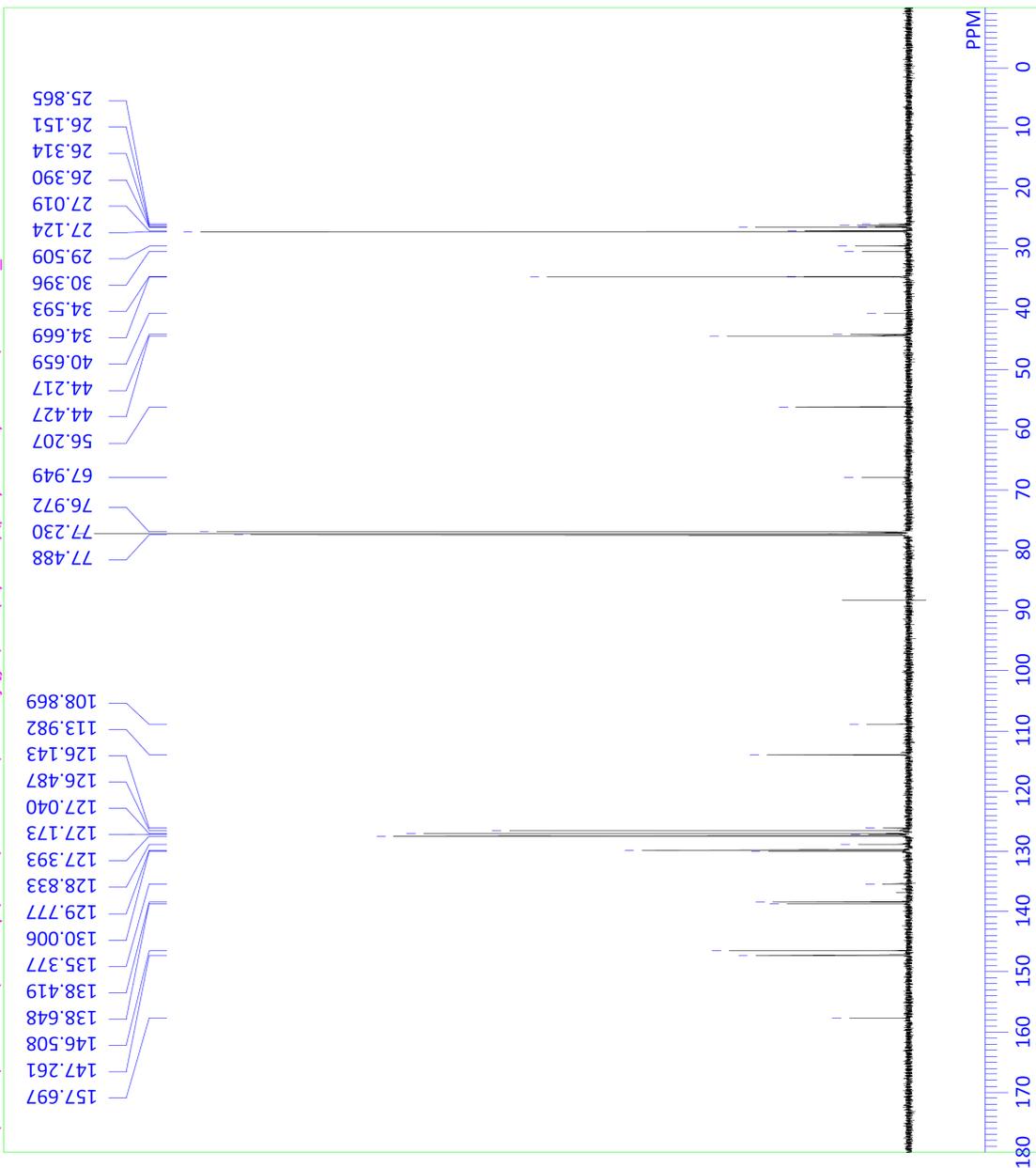
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COMINT single pulse decoupled gated NOE
DATIM 2015-11-18 18:03:08
OBNUC 13C

EXMOD carbon:ixp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32767
FREQU 39308.18 Hz
SCANS 1362
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.74 usec
IRNUC 1H
CTEMP 24.3 c
SLVNT CDCL3
EXREF 77.23 ppm
BF 0.12 Hz
RGAIN 24

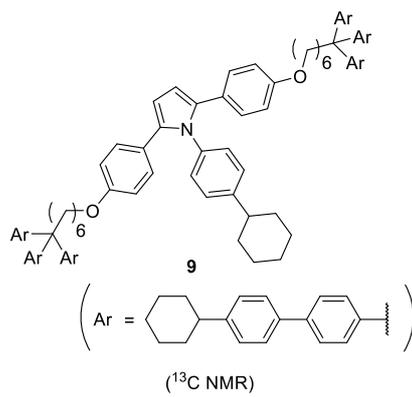


8
(¹³C NMR)

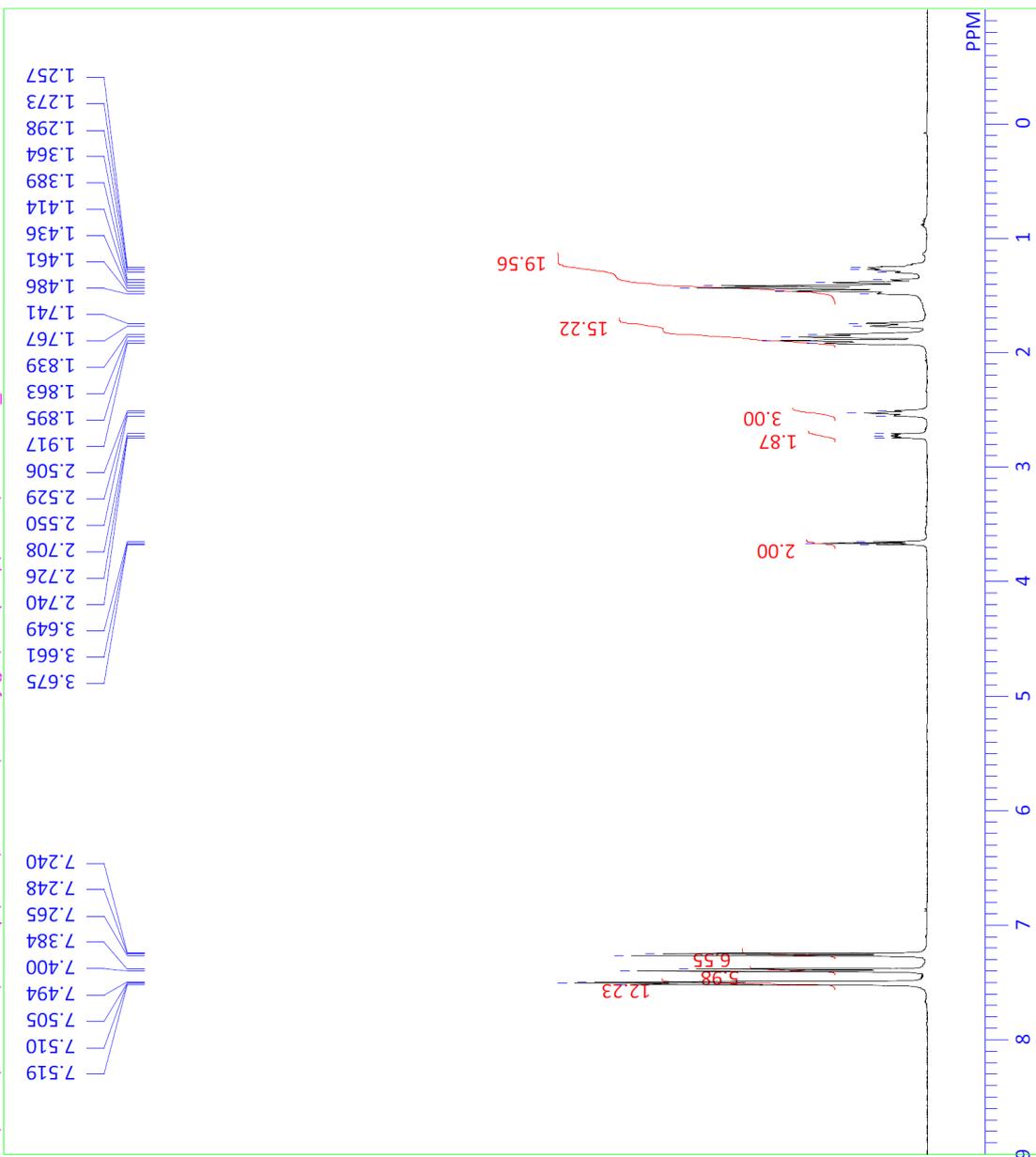
C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00»1•:ffj\axle (Pyrrole)\p-cyclohexylamine\YM-4-3-3_Carbon-1-1.als



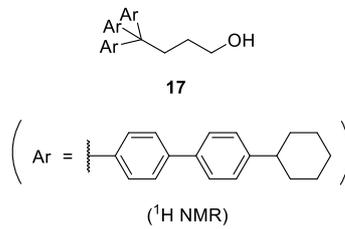
DFILE YM-4-3-3_Carbon-1-1.als
 COMNT single pulse decoupled gated NOE
 DATIM 2015-06-02 17:53:10
 OBNUC 13C
 EXMOD carbon:ixp
 OBFRC 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31.446.54 Hz
 SCANS 1528
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.58 usec
 IRNUC 1H
 CTEMP 23.7 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 18



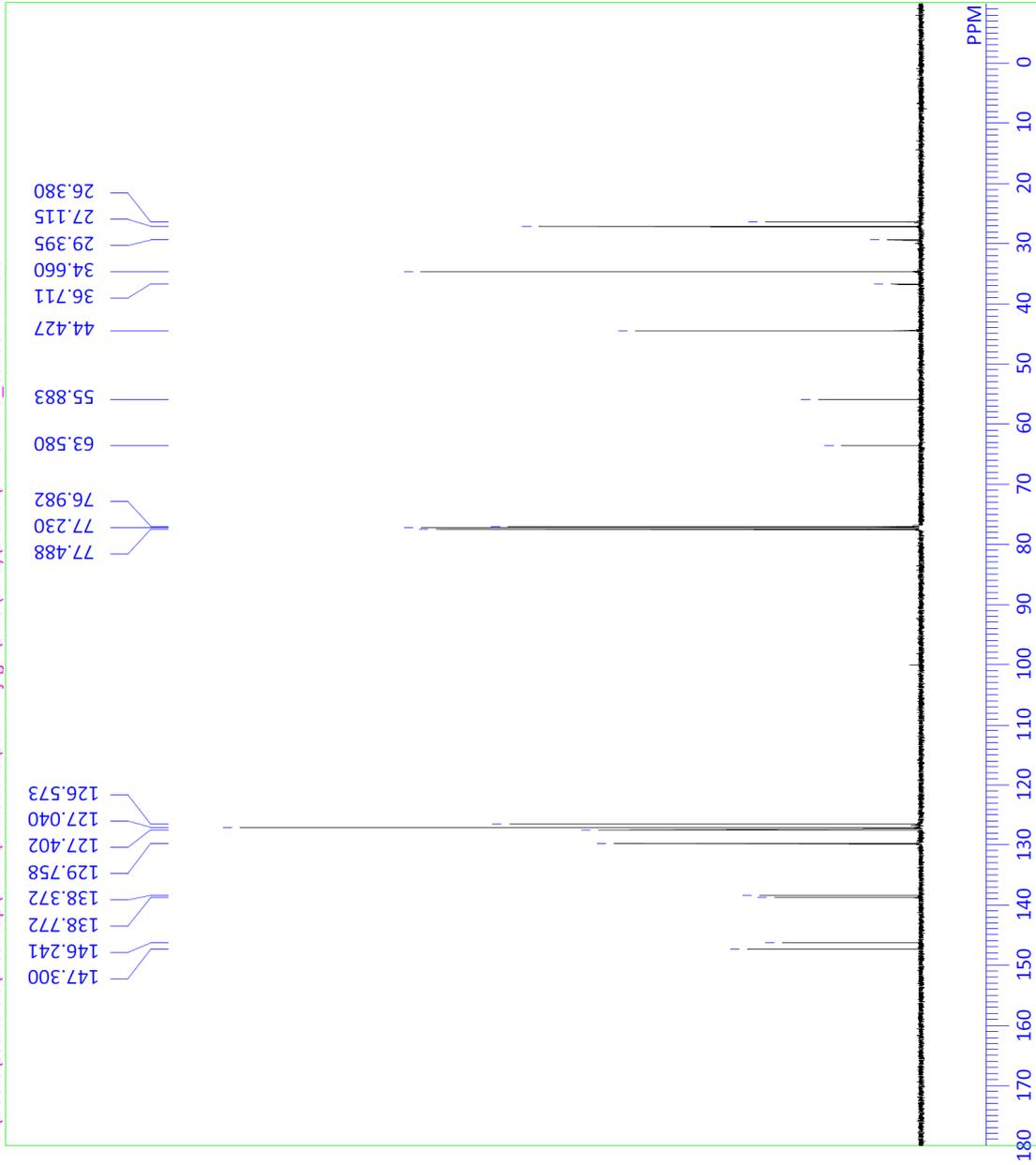
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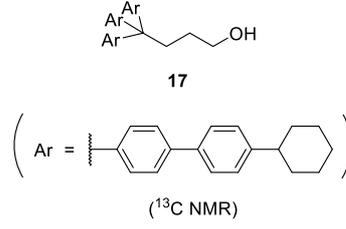
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EXMOD proton.jpg
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 3.71 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 26



C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00#1::ffj\axle (n=3)\alcho\YM-3-41-3_Carbon-2-1.als

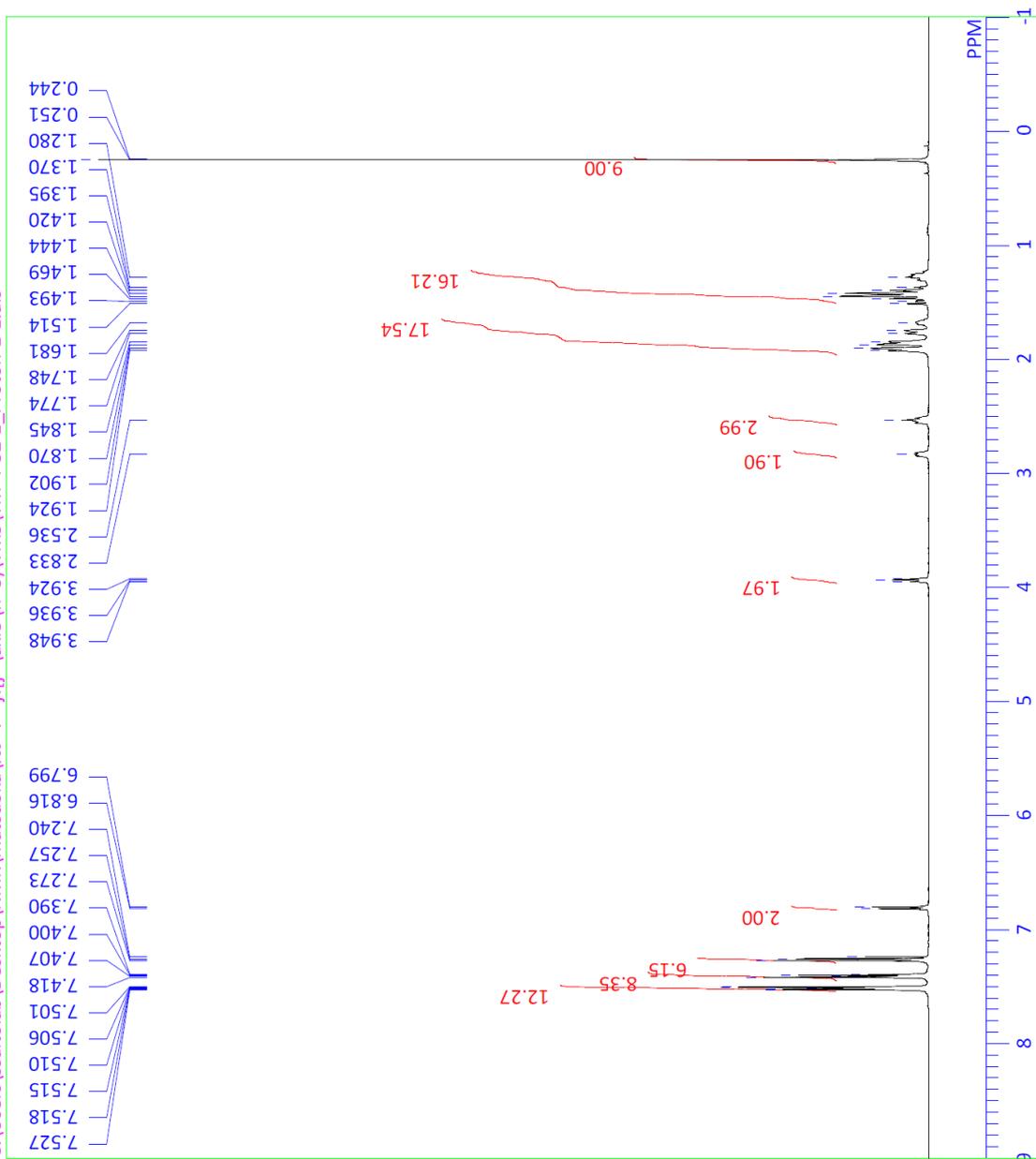
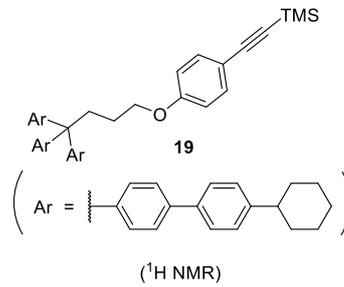


DFILE YM-3-41-3_Carbon-2-1.als
 COMNT single pulse decoupled gated NOE
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 EXMOD carbon:ixp
 OBFRC 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31.446.54 Hz
 SCANS 1437
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.58 usec
 IRNUC 1H
 CTEMP 23.4 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 24

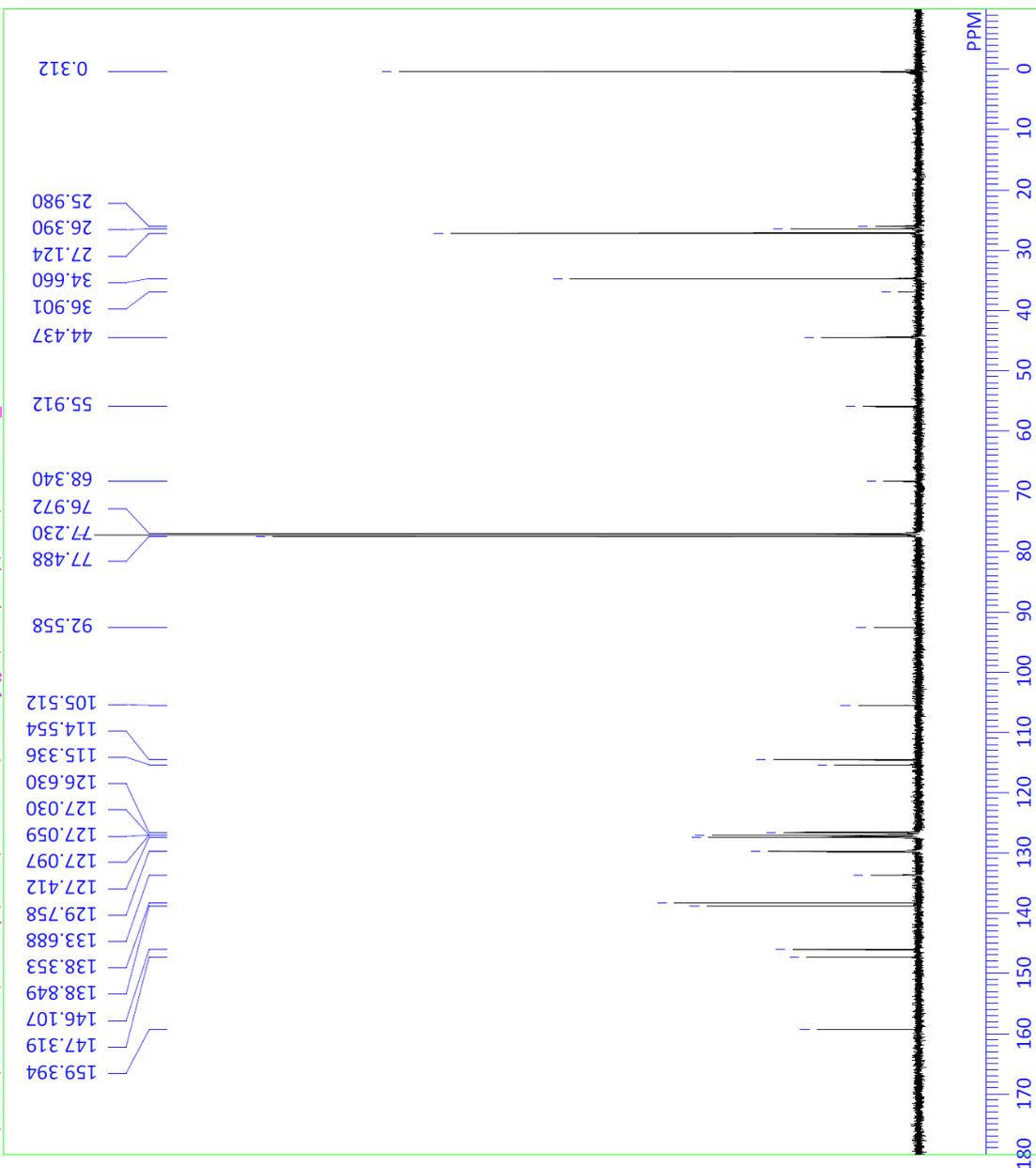


C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00#••ffjfv\axle (n=3)\TMS\YM-4-52-1_Proton-1-1.als

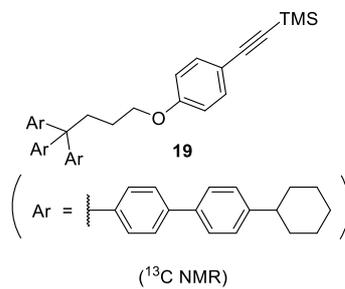
DFILE YM-4-52-1_Proton-1-1.als
 COMNT single_pulse
 DATIM 2015-11-18 15:14:49
 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 3.52 usec
 IRNUC 1H
 CTEMP 24.1 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 34



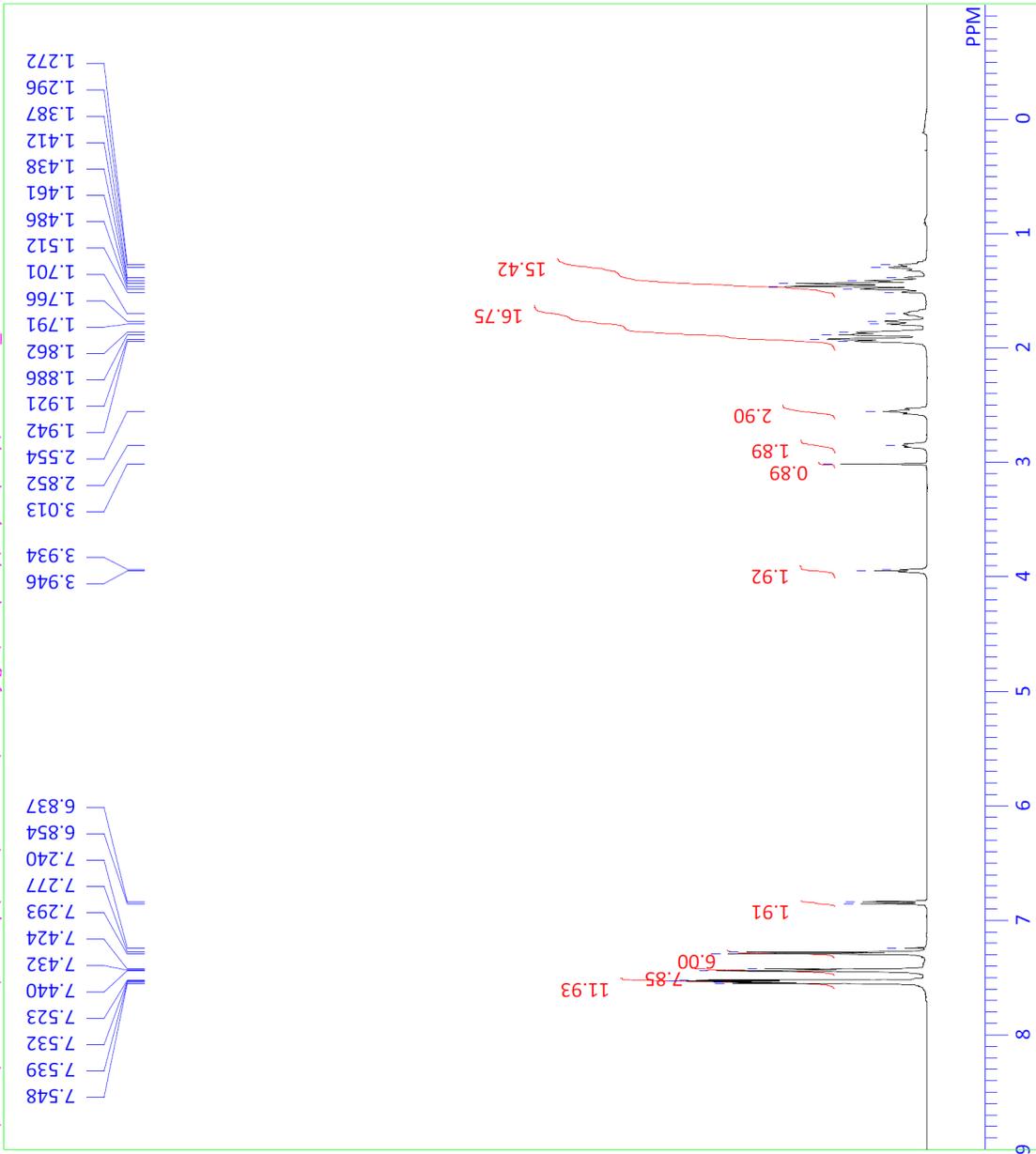
C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00»1•:jfj\axle (n=3)\TMS\YM-4-52-1_Carbon-1-1.als



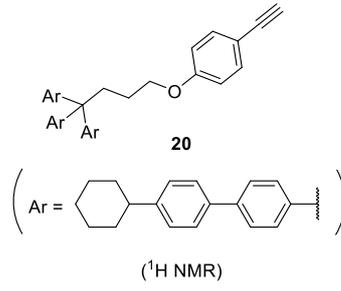
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 EXMOD carbon:jpg
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31.446.54 Hz
 SCANS 1200
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.74 usec
 IRNUC 1H
 CTEMP 24.1 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 24



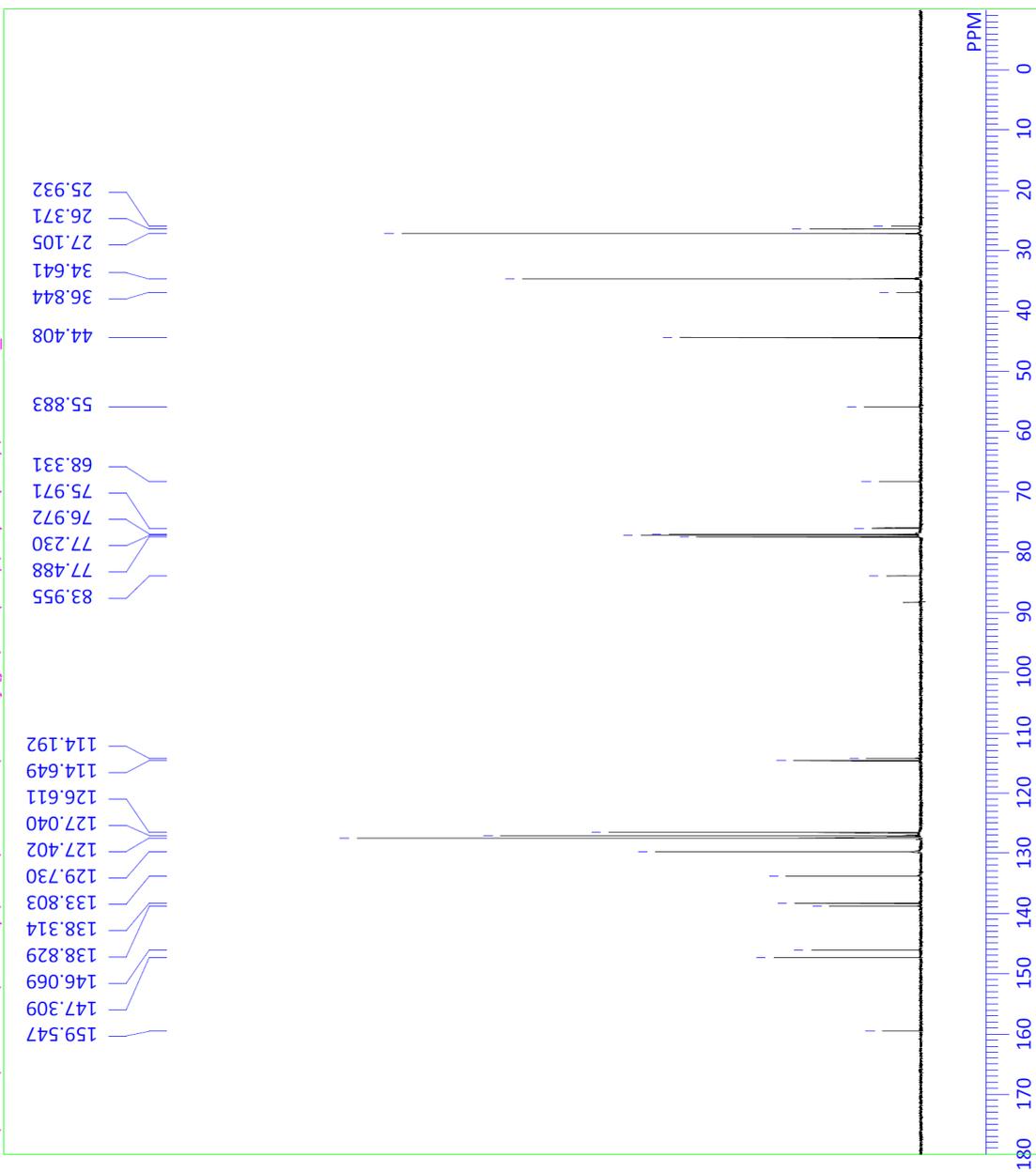
C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00#••ffjfv\axle (n=3)\alkyne (n=3)\YM-3-49-4_Proton-1-1.als



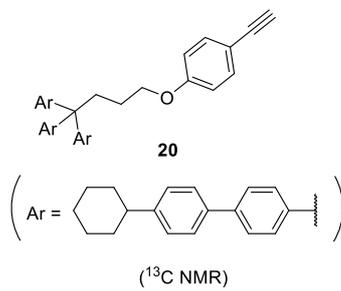
DFIL YM-3-49-4_Proton-1-1.als
 COMNT single_pulse
 DATIM 2015-02-20 13:34:53
 OBNUC 1H
 EXMOD proton.jxp
 OBFRC 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.51 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 3.71 usec
 IRNUC 1H
 CTEMP 20.8 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 26



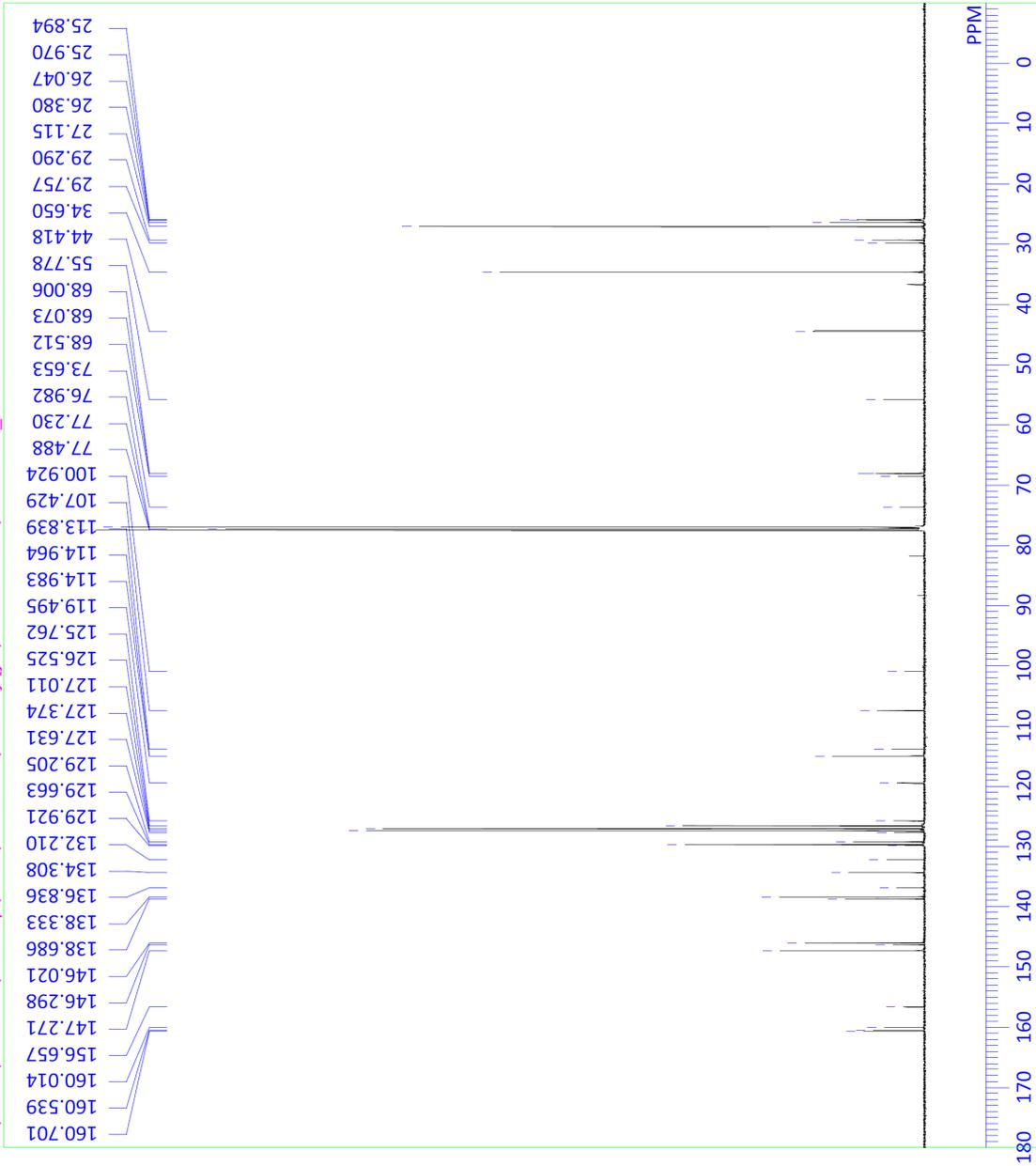
C:\Users\ssaitolab\Desktop\NMR\matsuoka\%00#1•ffjf\axle (n=3)\alkyne (n=3)\YM-3-49-4_Carbon-1-1.als



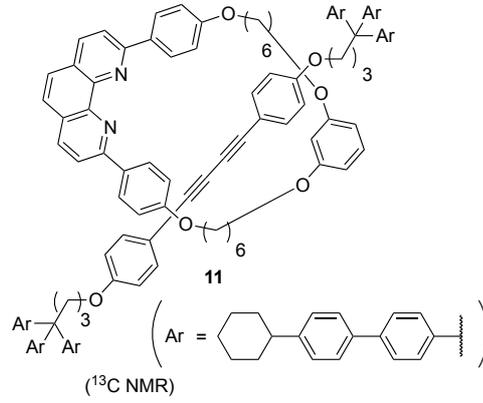
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 OBNUC 13C
 EXMOD carbon:ixp
 OBFRC 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31.446.54 Hz
 SCANS 1445
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.58 usec
 IRNUC 1H
 CTEMP 21.1 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 18



C:\Users\ssaitolab\Desktop\NMR\matsuoka\%001•jfjfn=3 rotaxane\YM-3-51-1_Carbon-1-1.als



DFILE YM-3-51-1_Carbon-1-1.als
 COMINT single pulse decoupled gated NOE
 DATIM 2015-01-13 22:01:37
 OBNUC 13C
 EXMOD carbon:ixp
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 15028
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.58 usec
 IRNUC 1H
 CTEMP 20.1 c
 SLVNT CDCL3
 EXREF 77.23 ppm
 BF 0.12 Hz
 RGAIN 18



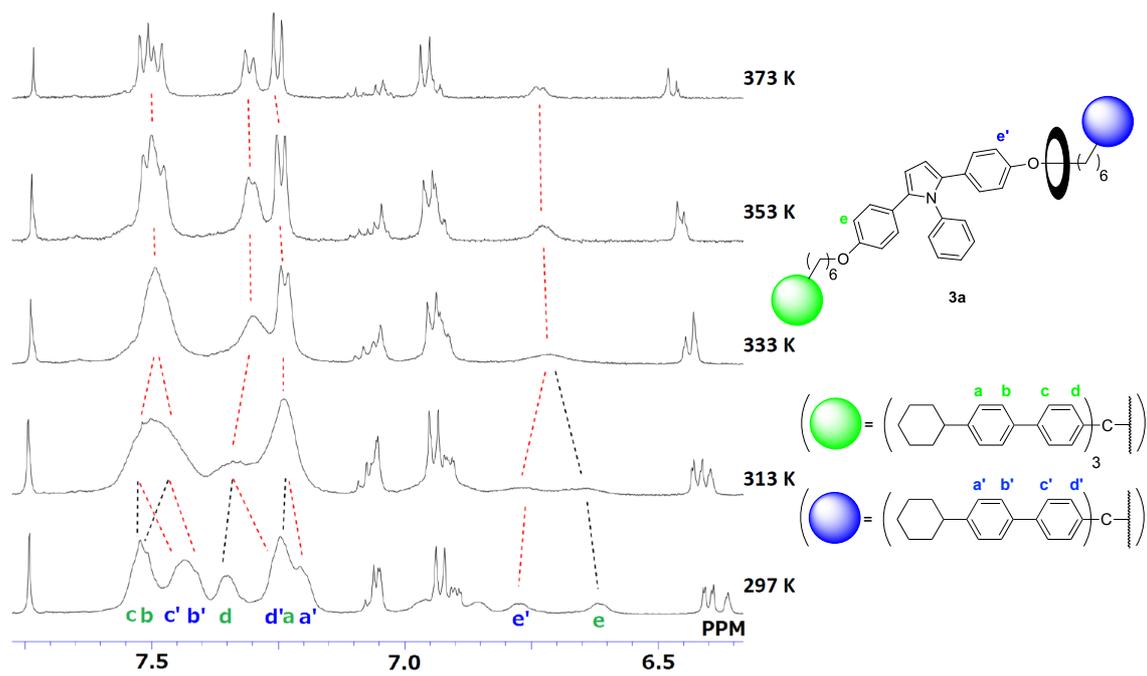


Figure S1. Partial VT ^1H NMR of **3a** (500 MHz, $(\text{CDCl}_2)_2$)

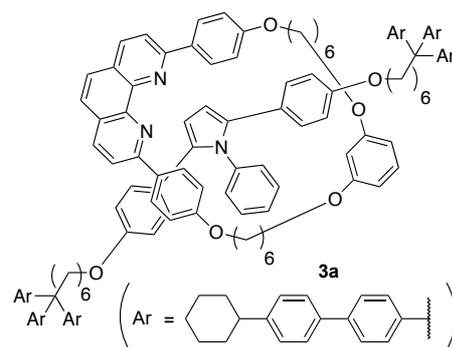
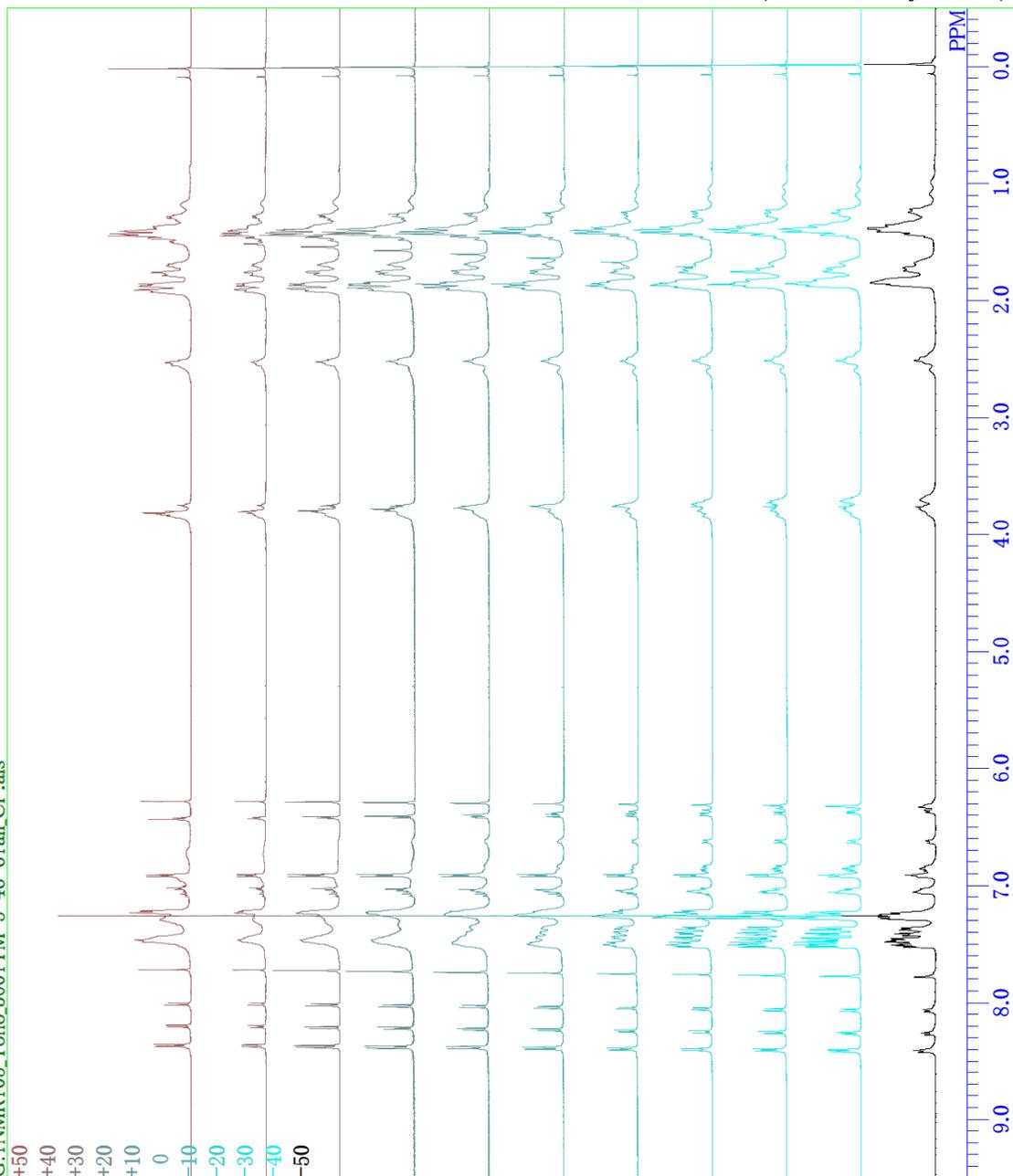
G:\NMR\05_Toho_500\YM-3-46-6\ail_CF.als

+50
+40
+30
+20
+10
0
-10
-20
-30
-40
-50

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

ail_CF.als
YM-3-46-6
2015-02-02 10:54:33
1H

proton.jp
500.16 MHz
2.41 KHz
6.01 Hz
26214
7507.51 Hz
3.4918 sec
3.5082 sec
3.44 usec
1H
-49.9 c
CDCL3
7.26 ppm
0.12 Hz
28



(VT ¹H NMR, CDCl₃, 223-323K)

C:\Rigaku\kikkawa\NMR\YM-3-60-6\YM-3-60-6 ALL_TCE.als

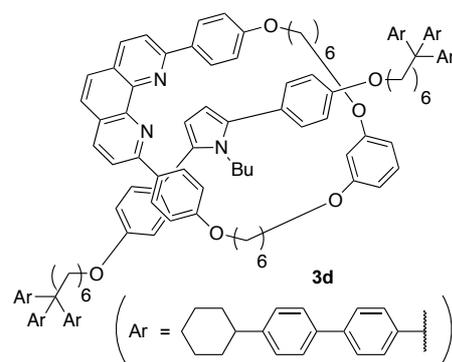
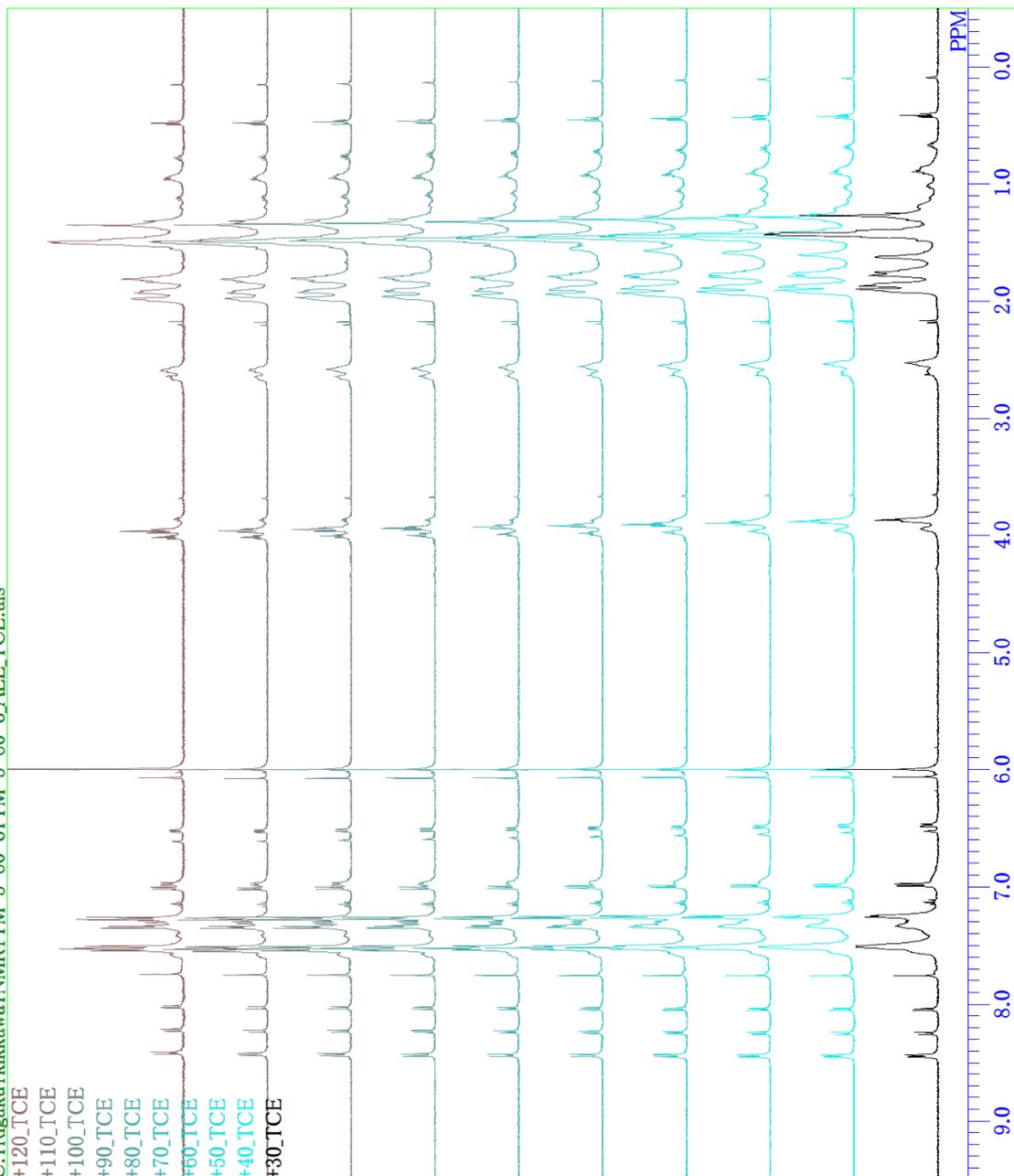
+120_TCE
+110_TCE
+100_TCE
+90_TCE
+80_TCE
+70_TCE
+60_TCE
+50_TCE
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+30_TCE

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

YM-3-60-6_ALL_TCE.als
+30_TCE
2015-02-26 20:49:56
1H

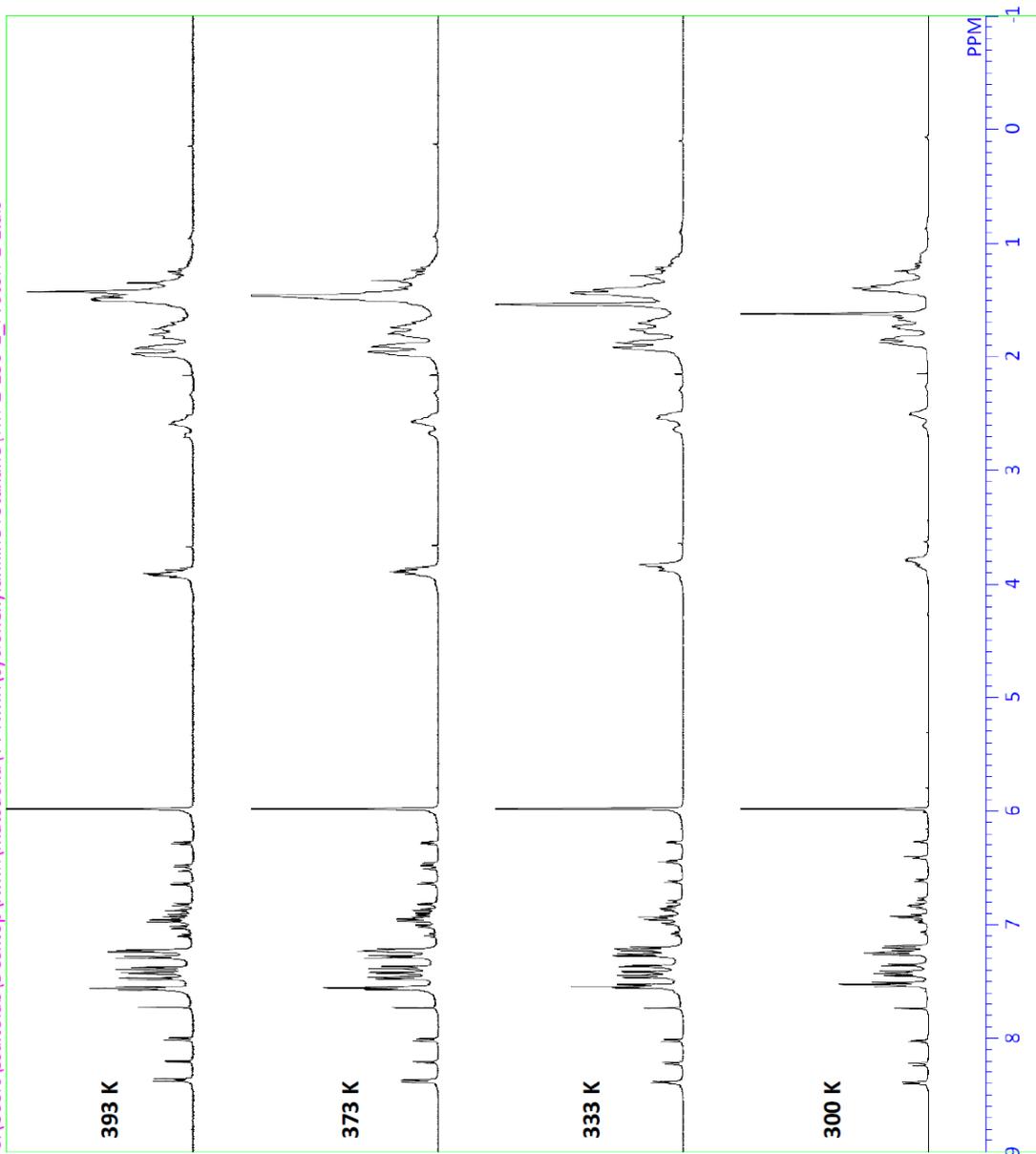
single_pulse.exp
499.22 MHz
8.25 KHz
0.33 Hz
16384
7490.64 Hz
2.1873 sec
4.0000 sec
6.42 usec

30.1 c
C2D2CL4
6.00 ppm
0.12 Hz
16

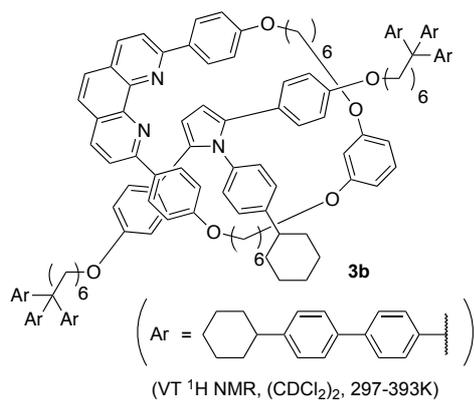


(VT ¹H NMR, (CDCl₂)₂, 303-393K)

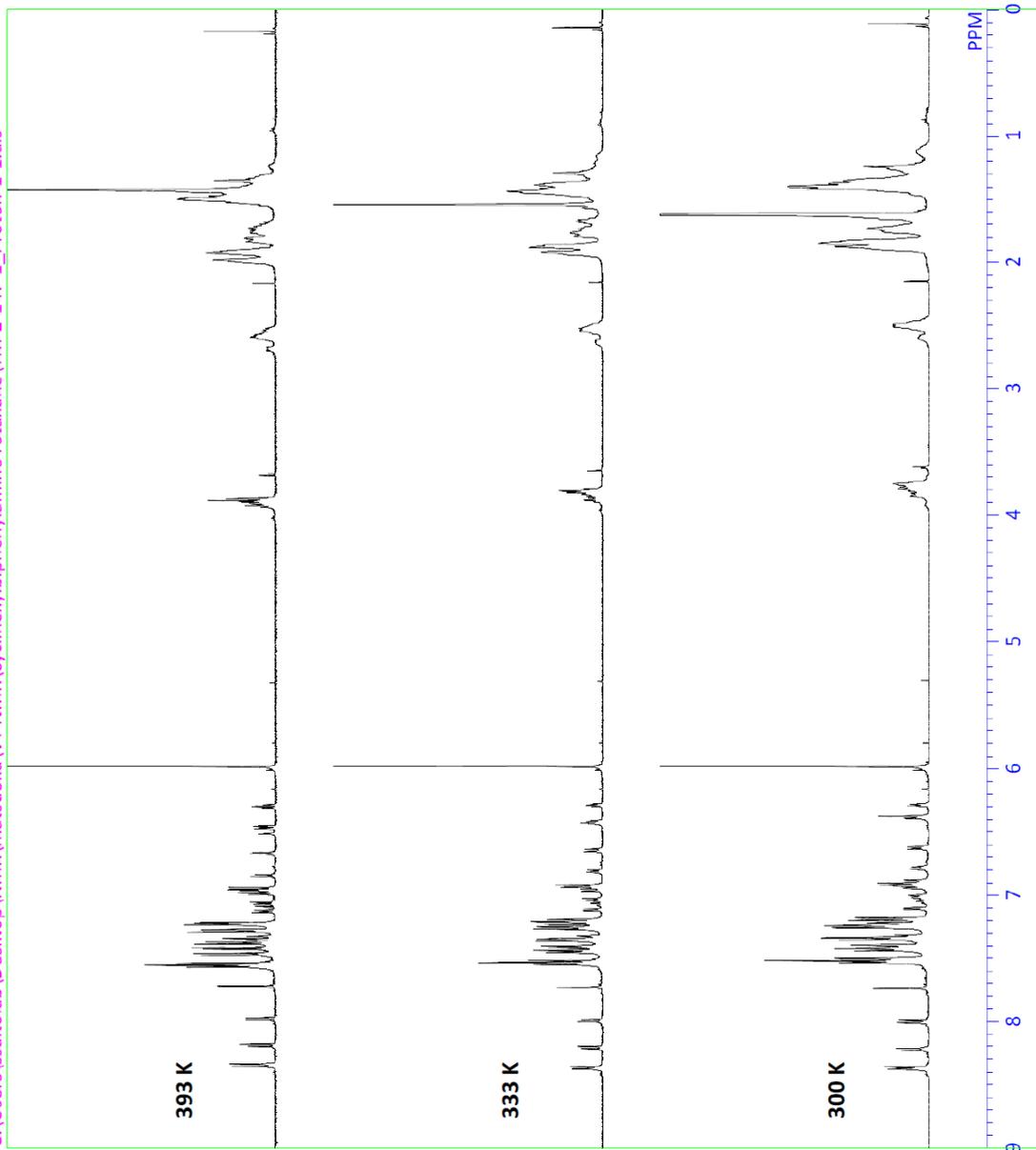
C:\Users\ssaitolab\Desktop\NMR\matsuoka\VT NMR\cyclohexylamine rotaxane\YM-2-150-1_Proton-1-1.als



DFILE YM-2-150-1_Proton-1-1.als
 COMNT single_pulse
 DATIM 2014-09-03 10:28:59
 OBNUC 1H
 EXMOD proton.jxp
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 13107
 FREQU 7507.51 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 3.45 usec
 IRNUC 1H
 CTEMP 24.6 c
 SLVNT C2D2CL4
 EXREF 5.98 ppm
 BF 0.12 Hz
 RGAIN 40

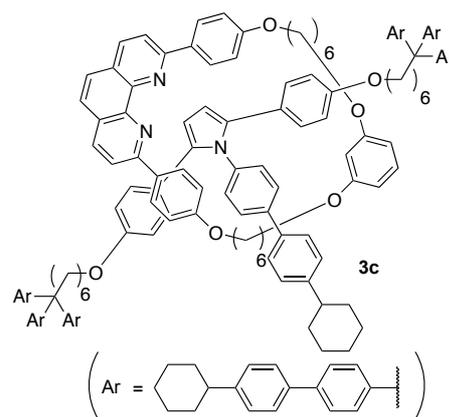


C:\Users\ssaito\lab\Desktop\NMR\matsuoka\VT NMR\cyclihexylbiphenylamine rotaxane\YM-2_147-1_Proton-1-1.als



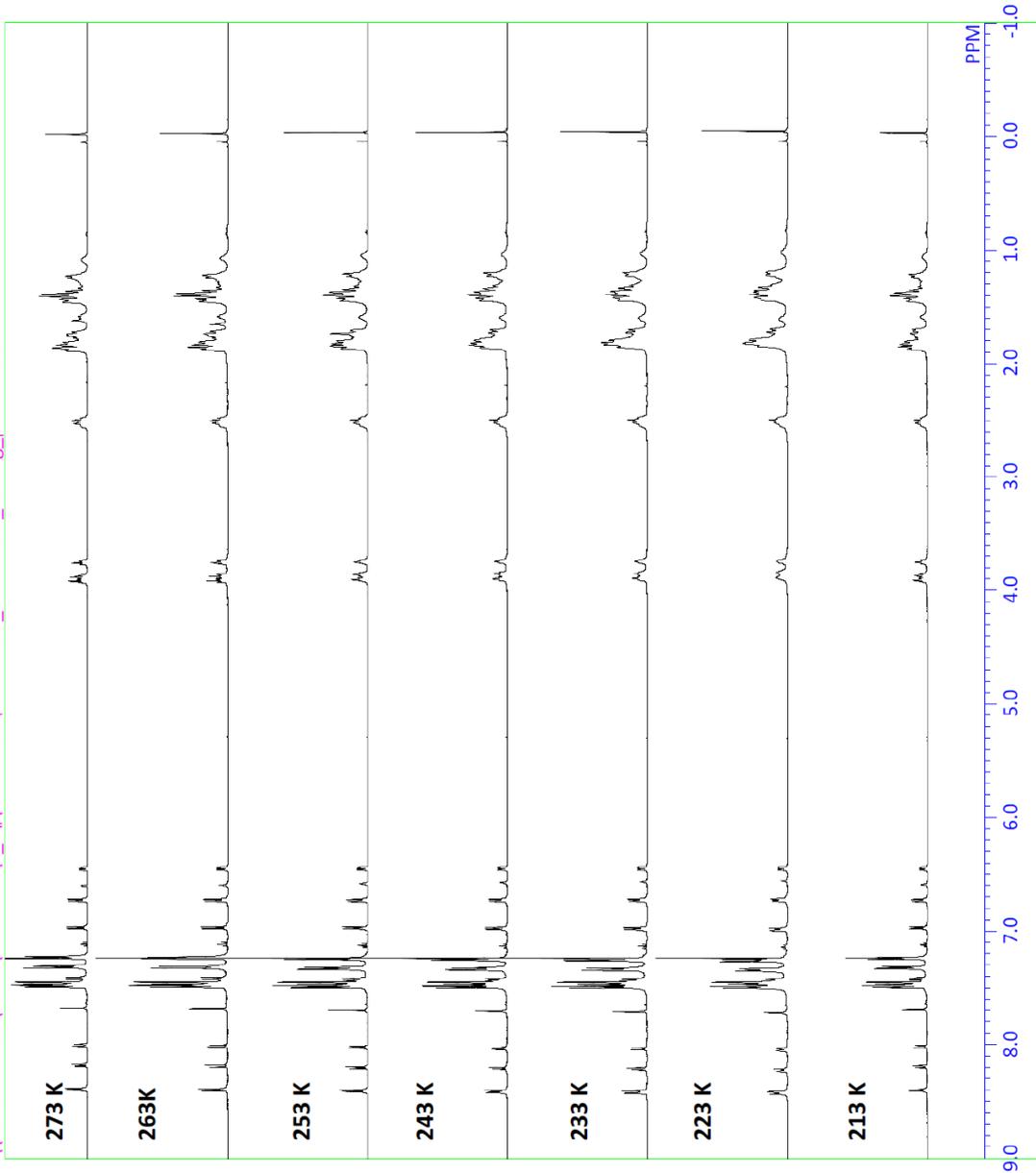
DM-2-147-1_Proton-1-1.als
single_pulse
2014-08-28 10:29:32
1H
proton.jxp
500.16 MHz
2.41 KHz
6.01 Hz
13107
7507.51 Hz
8
1.7459 sec
5.0000 sec
3.45 usec
1H
23.6 c
C2D2CL4
5.98 ppm
0.12 Hz
42

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFREQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

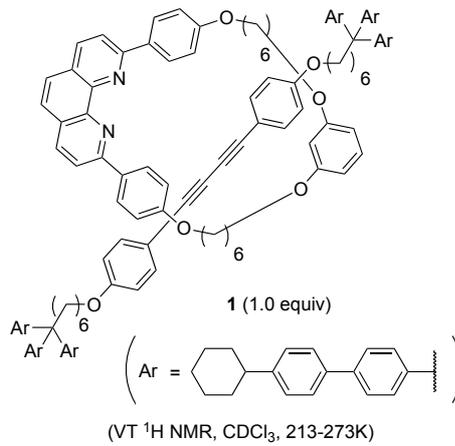


(VT ^1H NMR, $(\text{CDCl}_2)_2$, 297-393K)

\\SLAB-SHARED\share\yatsuoka\...\\YM-3-42-1\YM-3-42-1_YM-3-42-1_-10deg_proton-2-1.als



DFILE YM-3-42-1_YM-3-42-1_-10deg_proton
COMNT -10
DATIM 2015-02-02 15:33:06
OBNUC 1H
EXMOD proton.jpg
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 16
ACQTM 3.4918 sec
PD 3.5082 sec
PW1 3.44 usec
IRNUC 1H
CTEMP -10.0 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 26



Evidence for the solvation of 7

YM-4-46-3.als
 1H
 300.01 MHz
 1.85 KHz
 2.70 Hz
 32768
 6172.84 Hz
 8
 0.0000 sec
 0.0000 sec
 10.00 usec
 0.0 c
 7.24 ppm
 0.12 Hz
 0
 DFIL
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

