

Supporting Information

Faulknerynes A -C from a Bahamian Sponge *Diplastrella* sp. Stereo-Assignment and Critical Evaluation of two Exciton Coupled CD Methods

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Experimental Section

General Experimental Procedures.

Optical rotations were measured using a digital polarimeter using quartz cells of 1 cm or 5 cm pathlength. UV spectra were measured on a double-beam UV-vis spectrometer in 1 cm matched quartz cells. CD spectra were measured with a spectropolarimeter using spectroscopic grade solvents and a 2 mm quartz cell with 50 nm/min scan rate and 1 nm slit. IR spectra were measured using an FTIR spectrometer equipped with a ZnSe ATR plate. LR ESI mass spectra were obtained on a single quad mass spectrometer coupled to an UHPLC. ^1H , ^{13}C , and 2D NMR spectra were recorded at 600 MHz ($\{^{13}\text{C}/^{15}\text{N}\}^1\text{H}$, 1.7 mm microcryoprobe, or at 500 MHz ($\{^{13}\text{C}\}^1\text{H}$ 5 mm cryoprobe or $\{^{13}\text{C}\}^1\text{H}$ 5 mm cryoprobe), or a 400 MHz spectrometer ($\{^{13}\text{C}\}^1\text{H}$ 5 mm room temperature probe) in CD_3OD or CDCl_3 using solvent signals as internal standards [δ_{H} CHD_2OH 3.31 ppm; δ_{C} 49.00 ppm; CHCl_3 , δ_{C} 7.24 ppm; δ_{C} 77.0 ppm). HPLC was carried out using a dual-pump preparative HPLC with a high-dynamic range UV detector operating at 220 nm or a refractive index detector using HPLC grade solvents. TLC was performed on silica gel coated 0.25 mm aluminum backed plates and visualization by vanillin- H_2SO_4 -EtOH, phosphomolybdic acid or aqueous ceric ammonium nitrate. Anhydrous solvents were prepared by passage through a commercial alumina cartridges under Ar.

Table S1. NMR data (CDCl₃) for faulknerynes B (**4b**) and C (**4c**)

4b				4c			
no.	δ_{C} , mult. ^a	δ_{H} , mult. (<i>J</i> in Hz) ^b	COSY ^b	δ_{C} , mult. ^a	δ_{H} , mult. (<i>J</i> in Hz) ^b	COSY ^b	
1	66.1, CH	3.72, dd (11.3, 6.7)	H2	66.3, CH	3.69, dd (11.4, 6.3)	H2	
2	66.1, CH <i>d</i>	3.78, br 4.58, m	H2 H1	66.3, CH 63.6, CH <i>d</i>	3.74, dd (11.4, 3.8) 4.50, dd (6.2, 3.7)	H2 H1, H7	
3	<i>d</i>			<i>d</i>			
4	<i>d</i>			<i>d</i>			
5	<i>d</i>			<i>d</i>			
6	<i>d</i>			<i>d</i>			
7	<i>d</i>	5.50, d (11.0)	H8, H9	18.9, CH ₂	2.30, m	H2	
8	<i>d</i>	6.11, dt (10.9, 7.4)	H7, H9	27.5 ^c , CH ₂	1.57 ^c , m		
9	30.2, CH ₂	2.33, m (7.1)	H7, H8, H10	27.4 ^c , CH ₂	1.55 ^c , m		
10	27.7, CH ₂ ^c	1.53, m	H9	29.8, CH ₂	2.29, m	H10, H11	
11	27.6, CH ₂ ^c	1.55, m	H12	<i>d</i>	5.93, dt (10.8, 7.5)	H10, H12	
12	18.9, CH ₂	2.28, td (6.8, 1.9)	H11, H15	109.2, CH <i>d</i>	5.55, d (10.9)	H10, H11, H15	
13	<i>d</i>			<i>d</i>			
14	<i>d</i>			<i>d</i>			
15	<i>d</i>	6.19, dt (14.0)	H12, H16	117.4, CH	6.34, dd (14.0, 2.2)	H12, H16	
16	<i>d</i>	6.59, d (14.0)	H15	117.6, CH	6.66, d (14.0)	H15	

^a δ_{C} are measured by gHSQC exp. in 600 Hz. ^b600 MHz ^cPeaks may be interchanged within a column. ^dNot detected

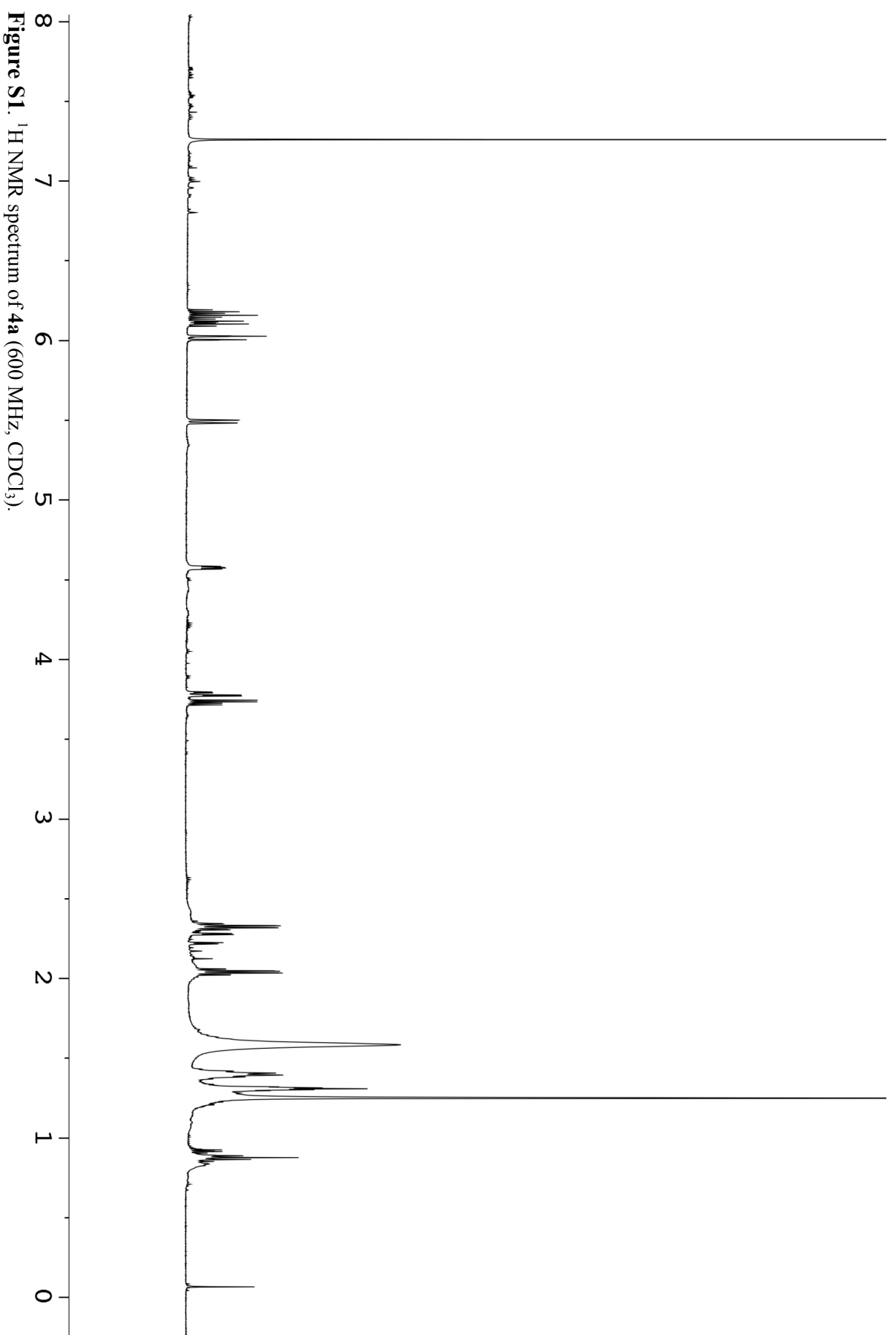


Figure S1. ^1H NMR spectrum of **4a** (600 MHz, CDCl_3).

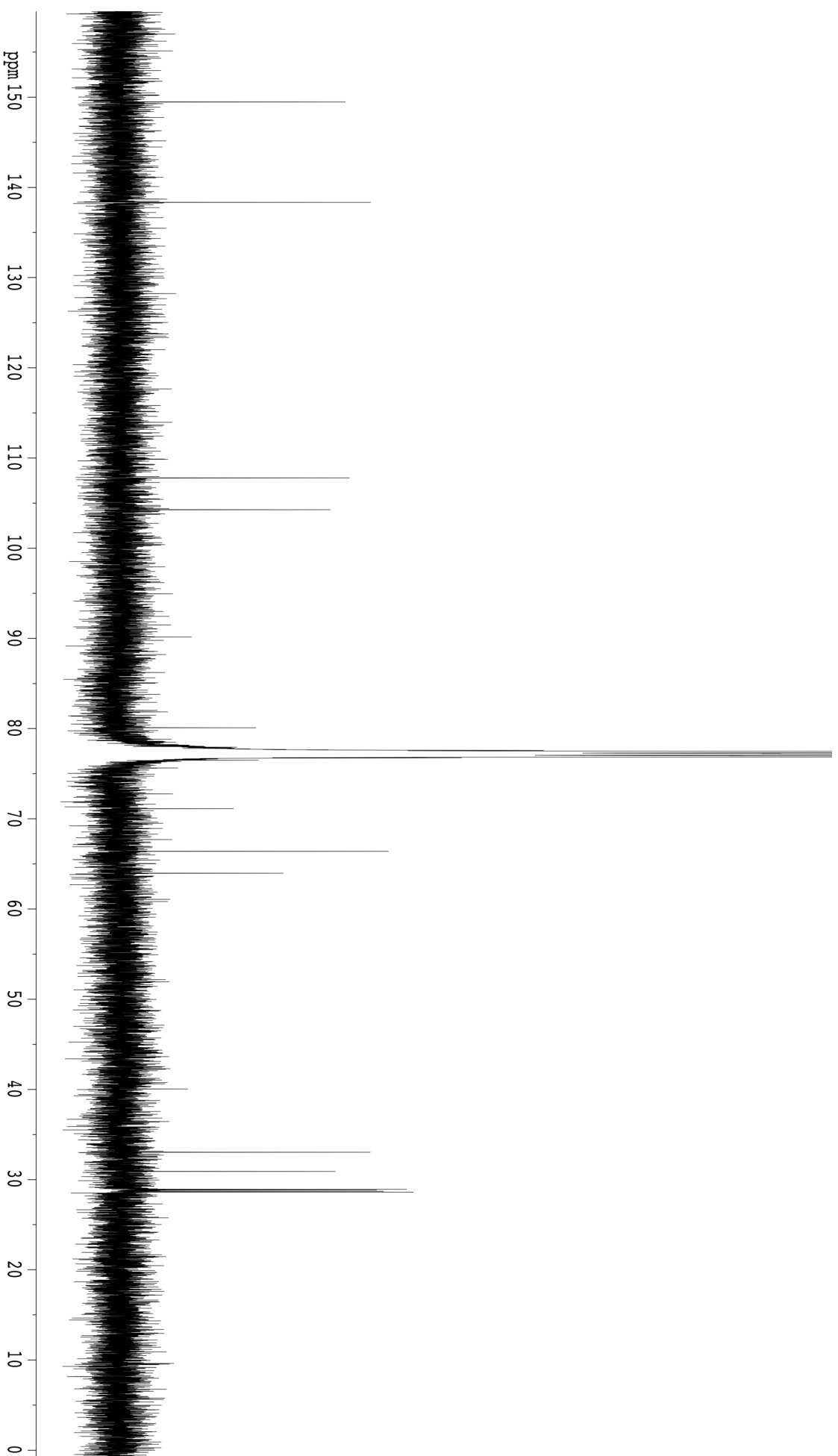


Figure S2. ^{13}C NMR spectrum of **4a** (125 MHz, CDCl_3).

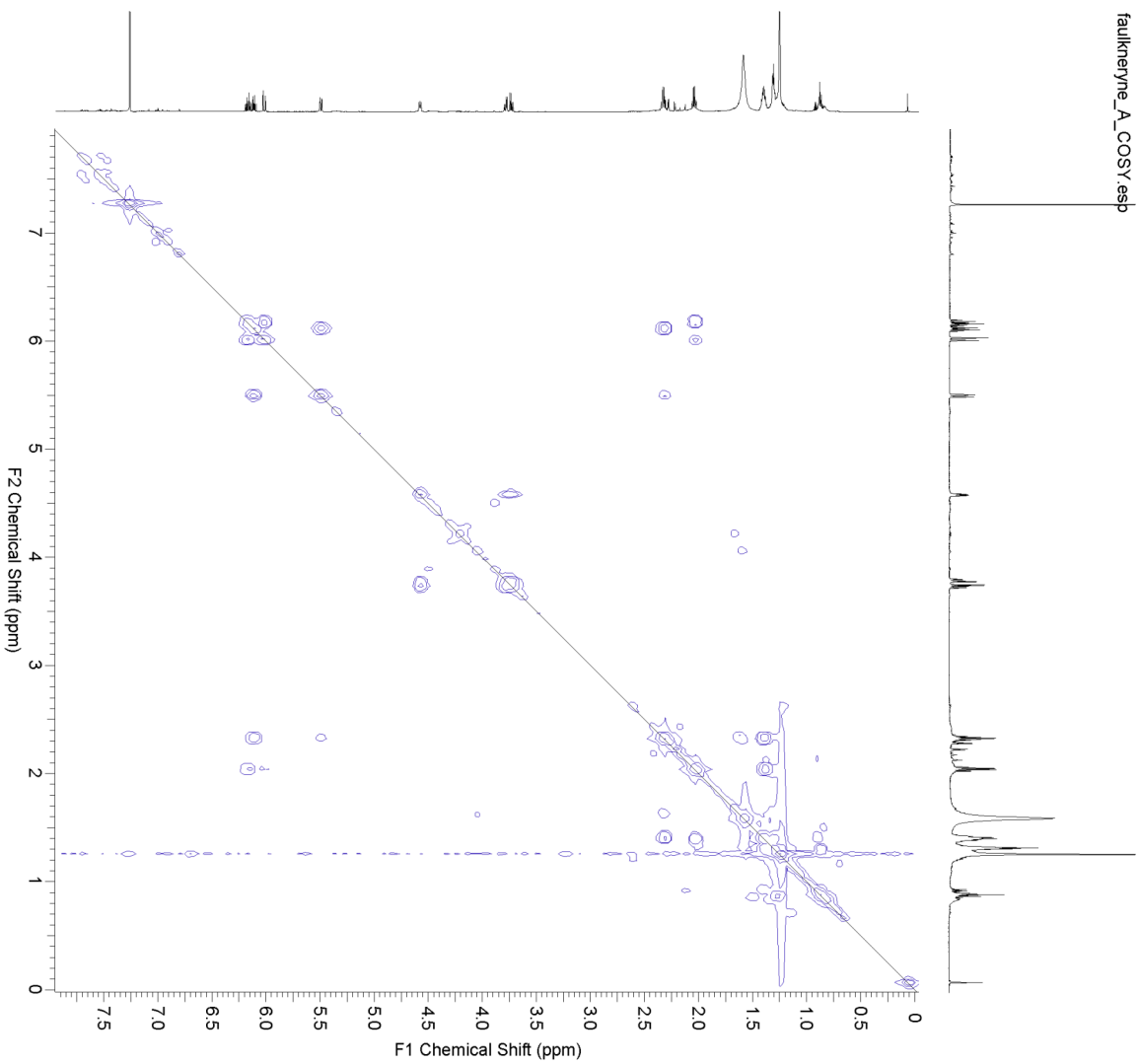


Figure S3. COSY spectrum of **4a** (600 MHz, CDCl₃).

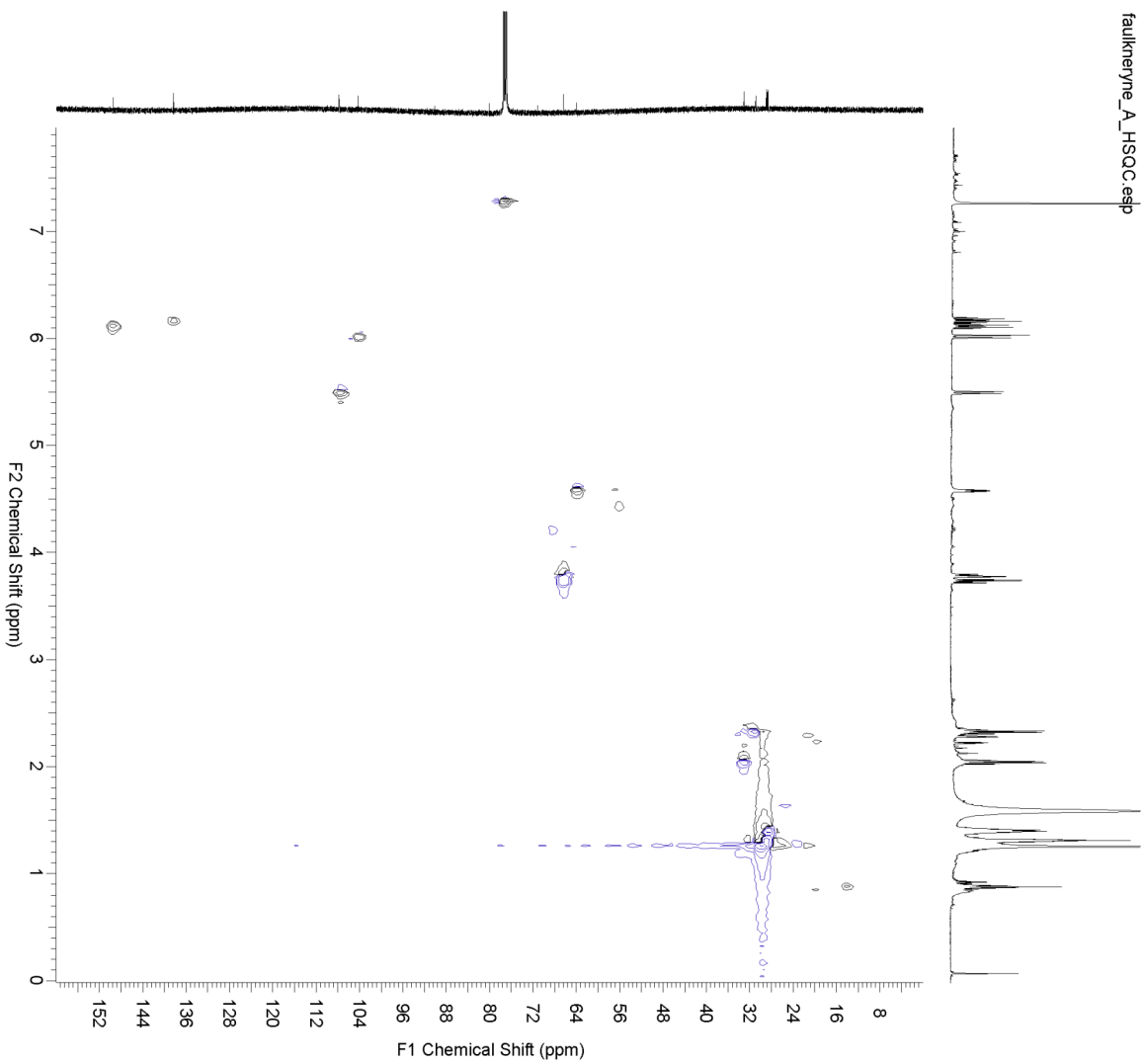


Figure S4. gHSQC spectrum of **4a** (600 MHz, CDCl₃).

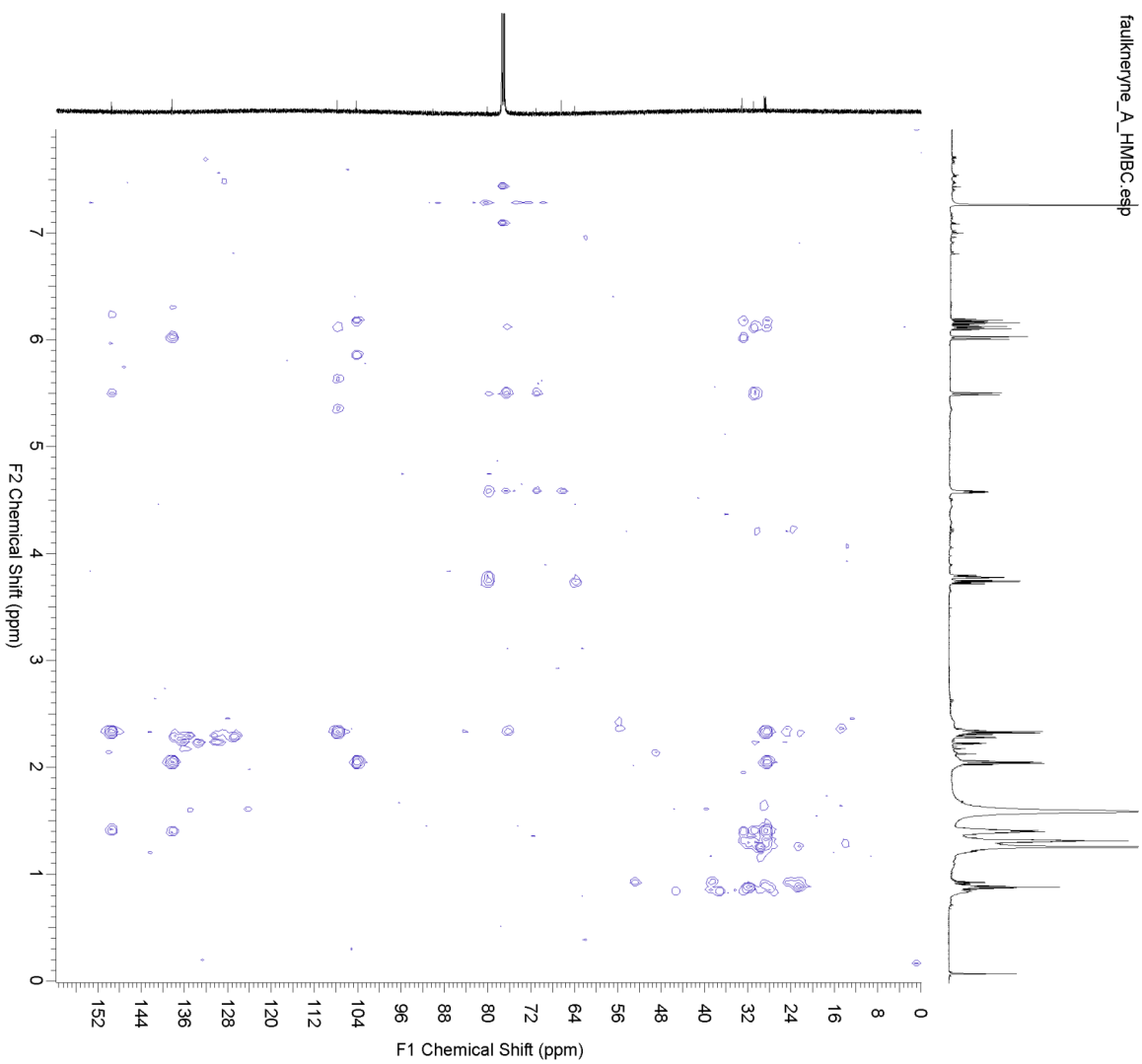


Figure S5. gHMBC spectrum of **4a** (600 MHz, CDCl_3 , $^nJ_{\text{CH}} = 8 \text{ Hz}$)

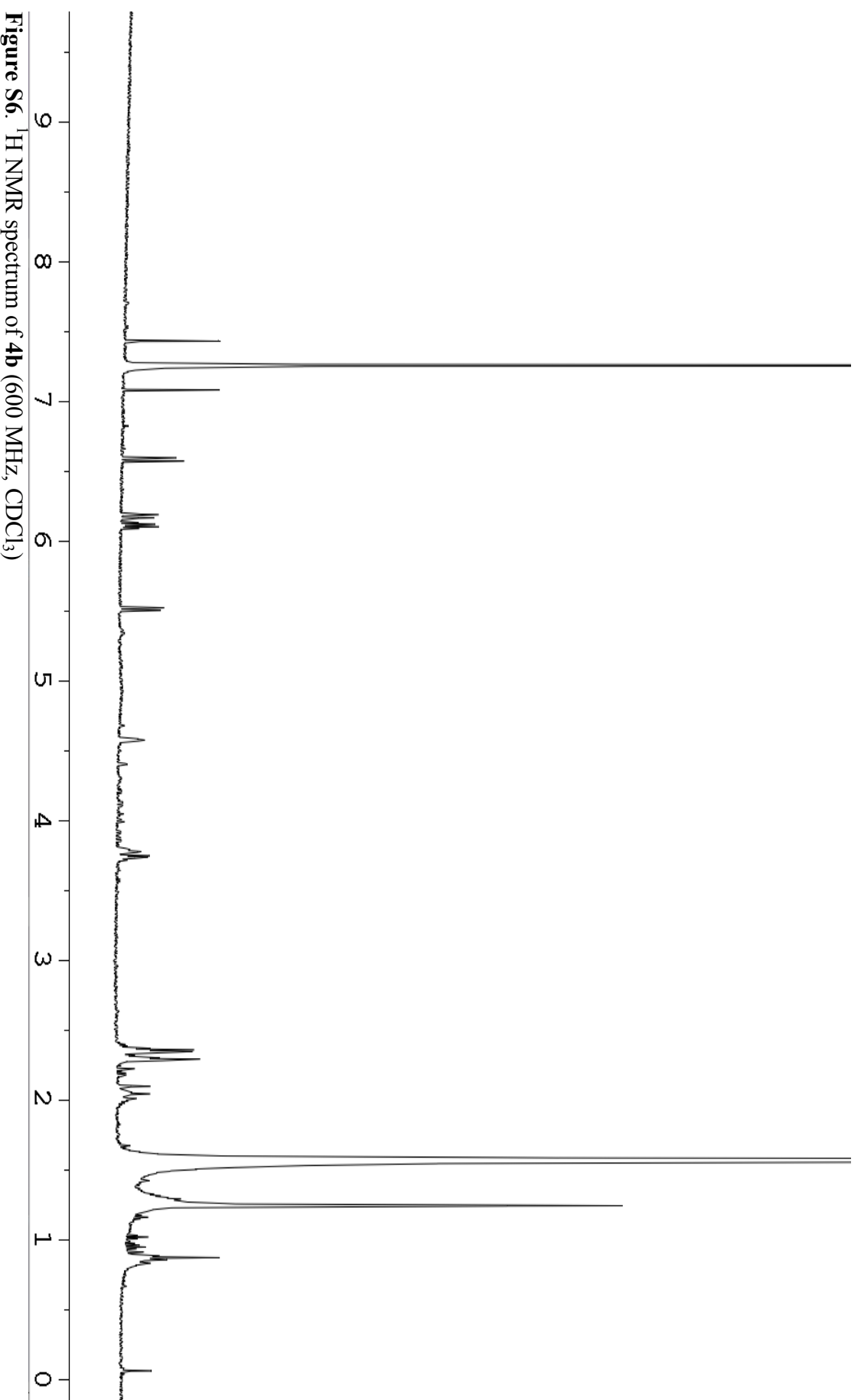


Figure S6. ^1H NMR spectrum of **4b** (600 MHz, CDCl_3)

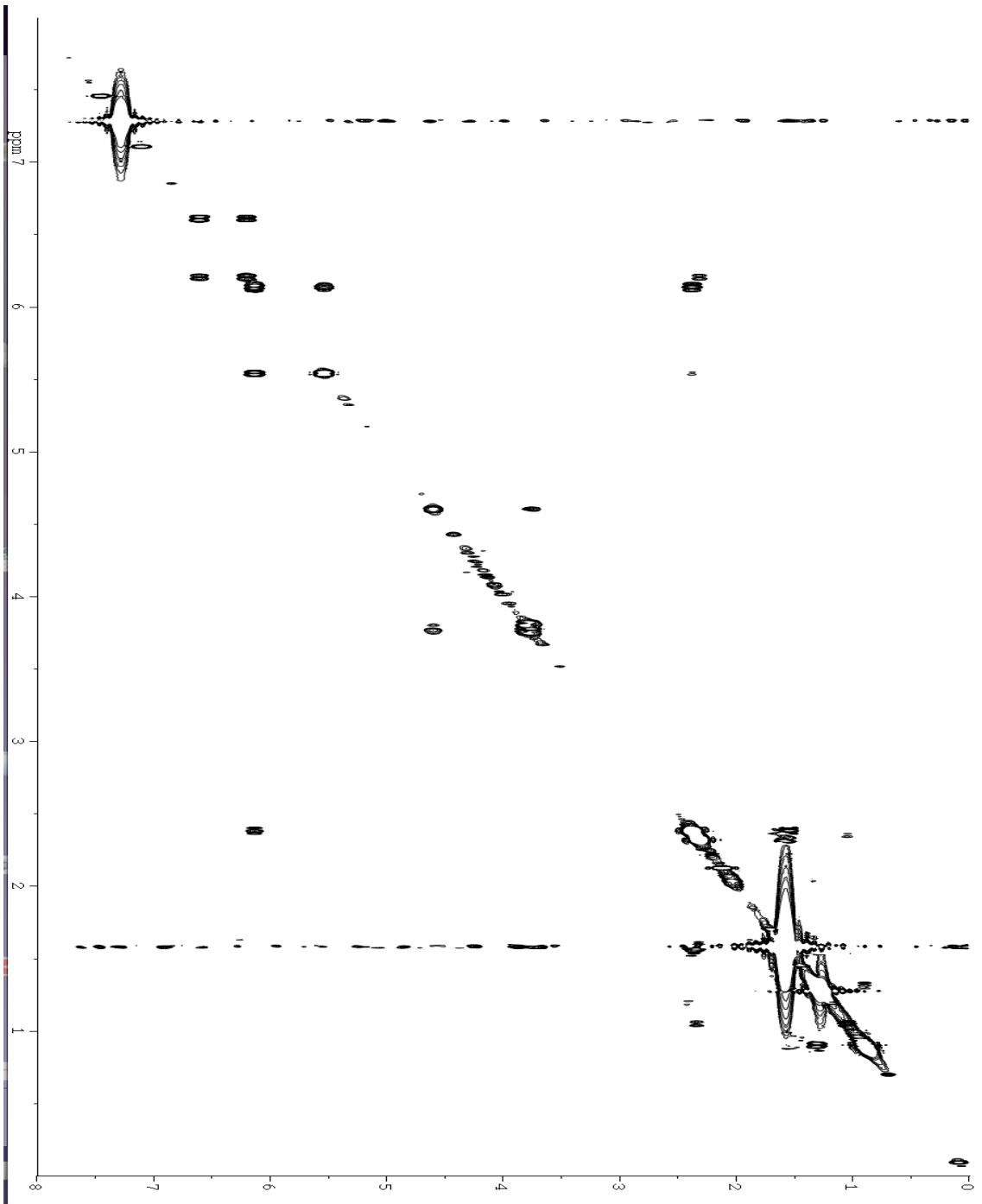


Figure S7. COSY NMR spectrum of **4b** (600 MHz, CDCl₃)

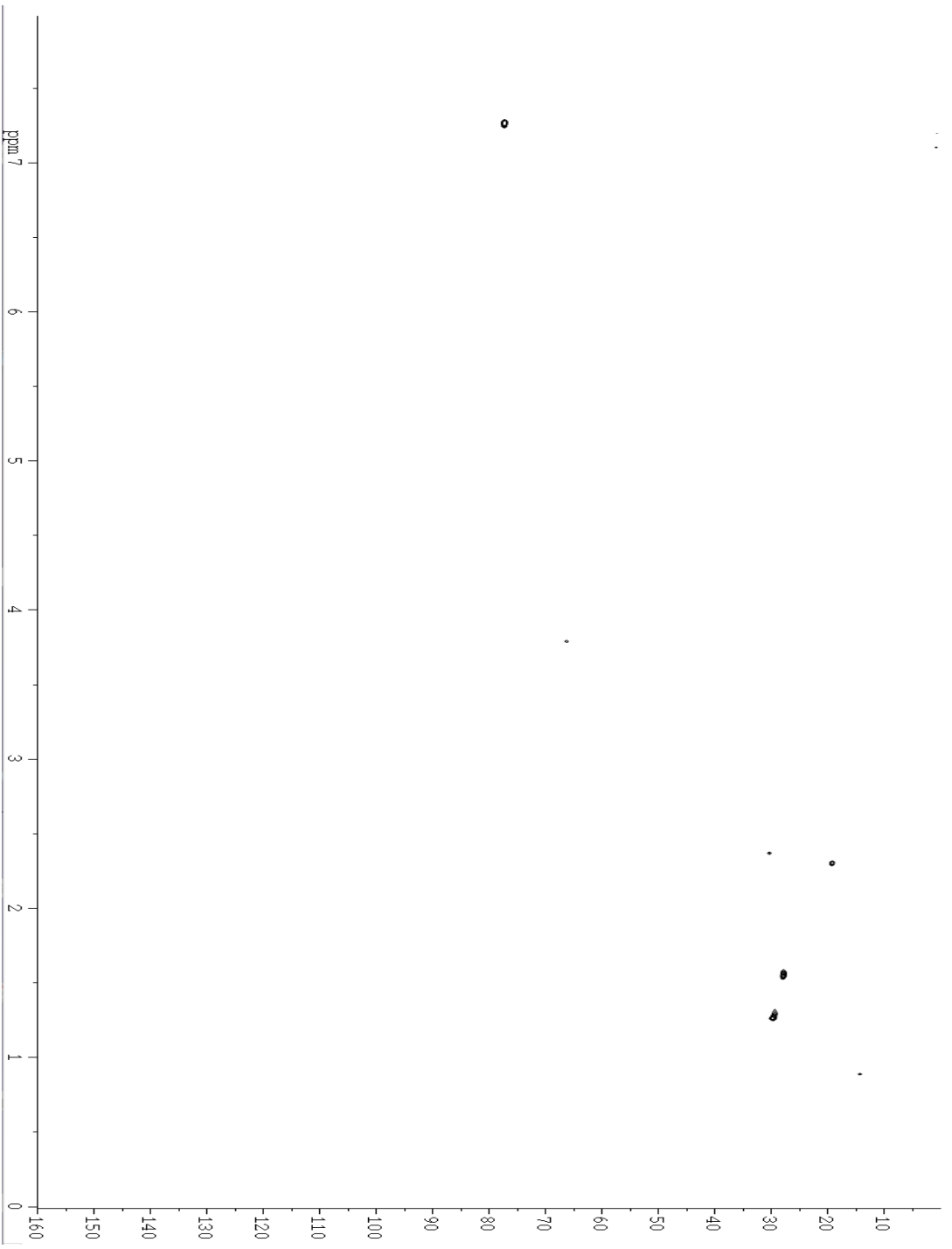


Figure S8. gHSQC spectrum of **4b** (600 MHz, CDCl₃)

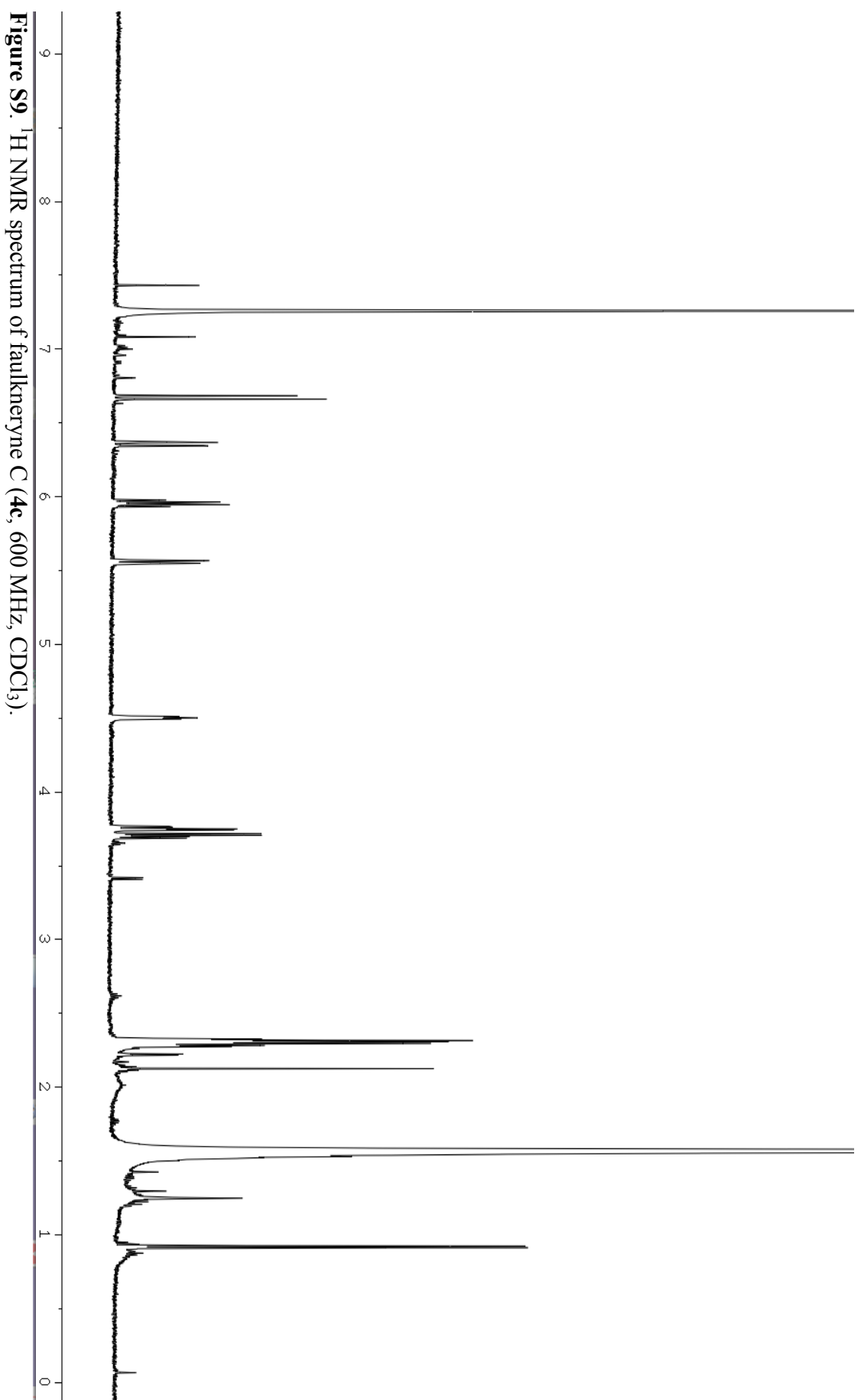


Figure S9. ^1H NMR spectrum of faulkneryne C (**4c**, 600 MHz, CDCl_3).

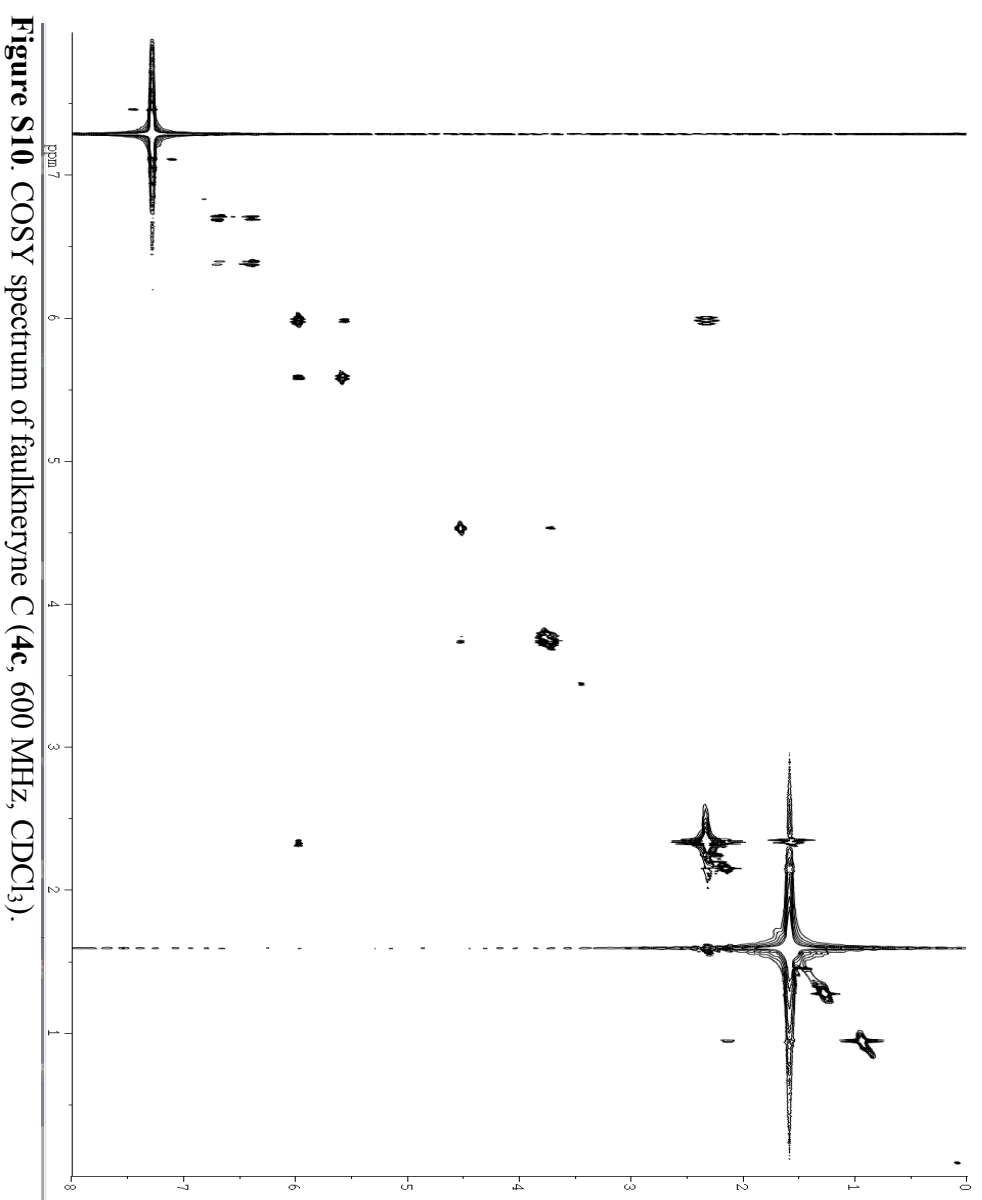


Figure S10. COSY spectrum of faulkneryne C (**4c**, 600 MHz, CDCl₃).

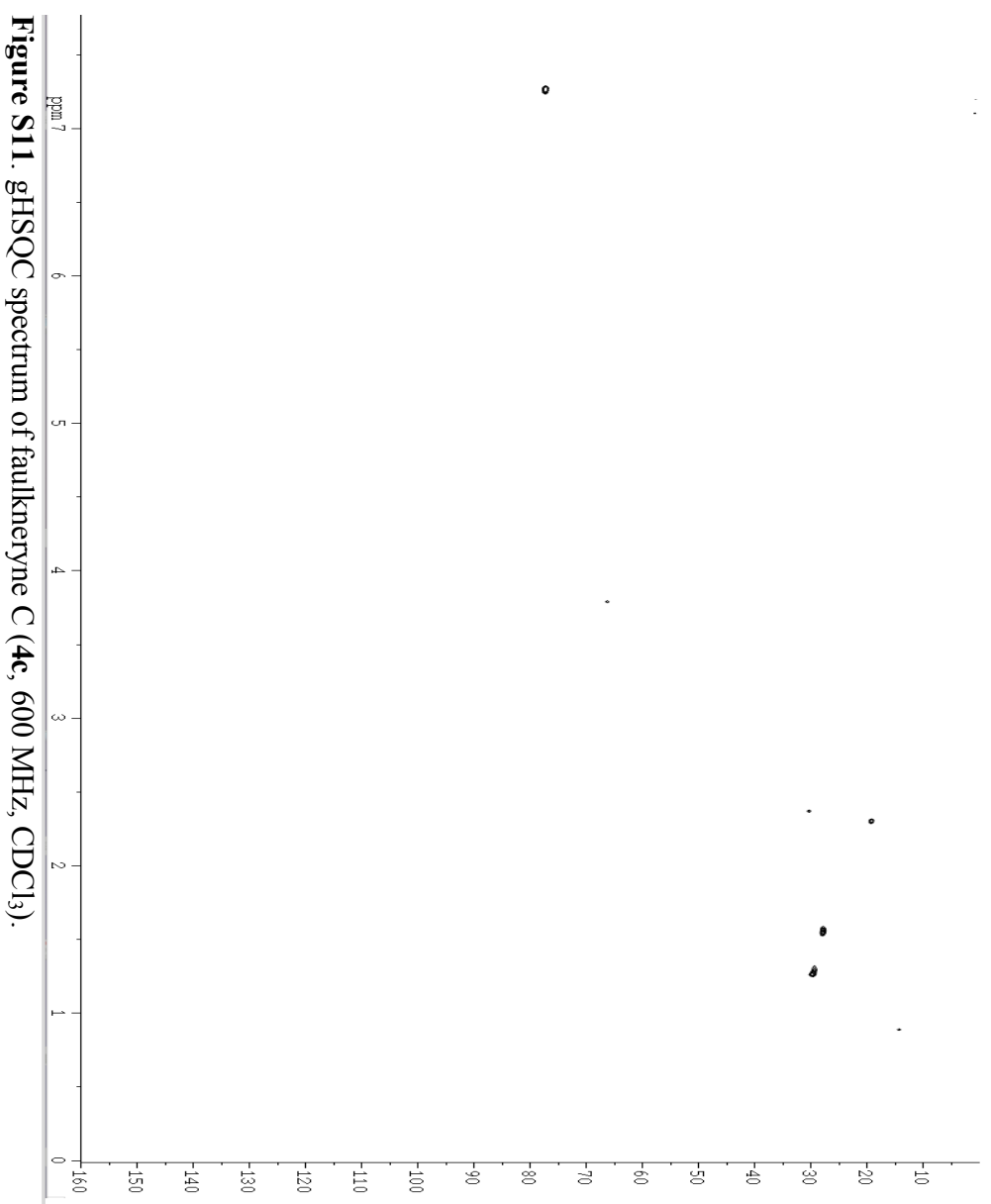


Figure S11. gHSQC spectrum of faulkneryne C (**4c**, 600 MHz, CDCl₃).

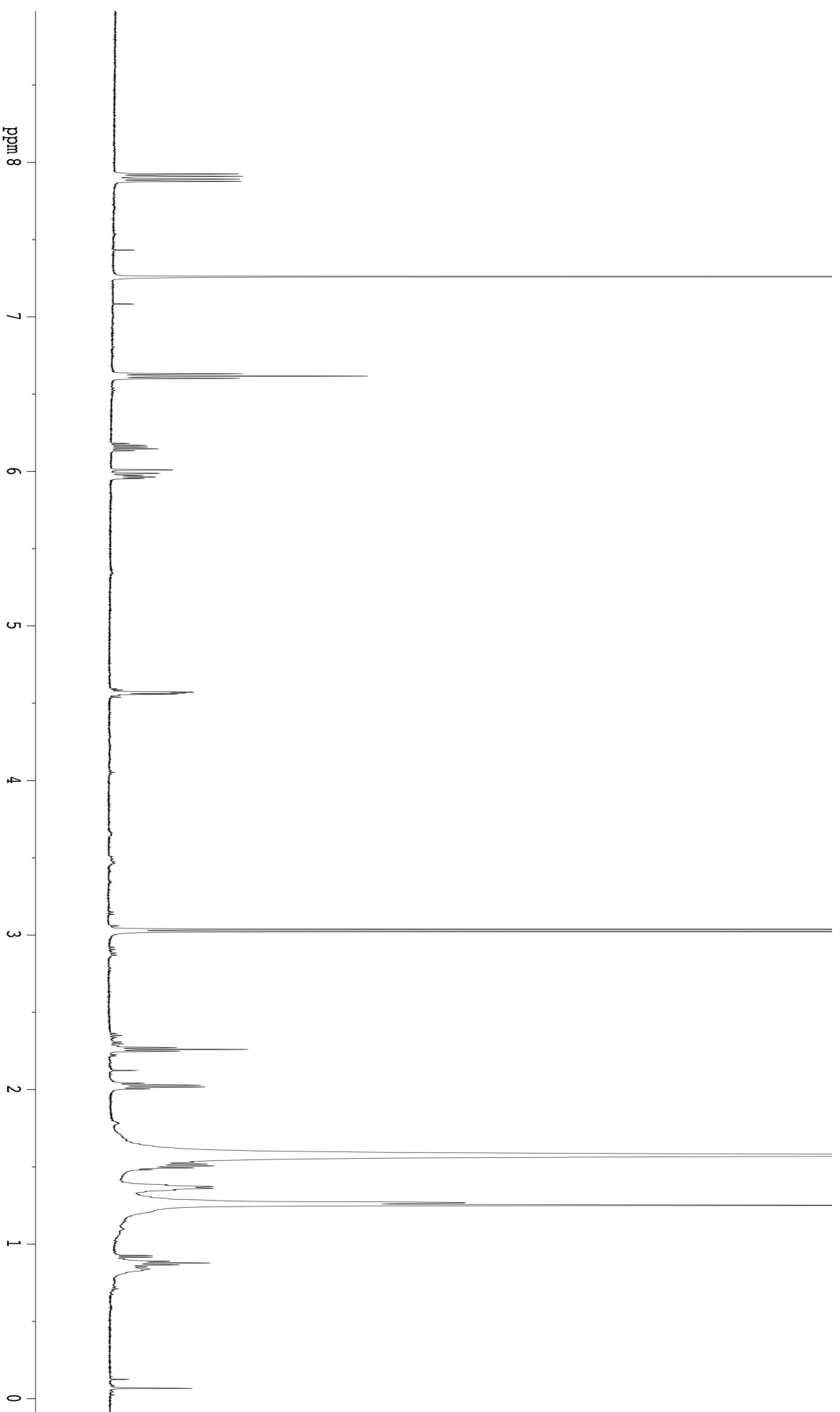


Figure S12. ^1H NMR spectrum of **5** (600 MHz, CDCl_3)

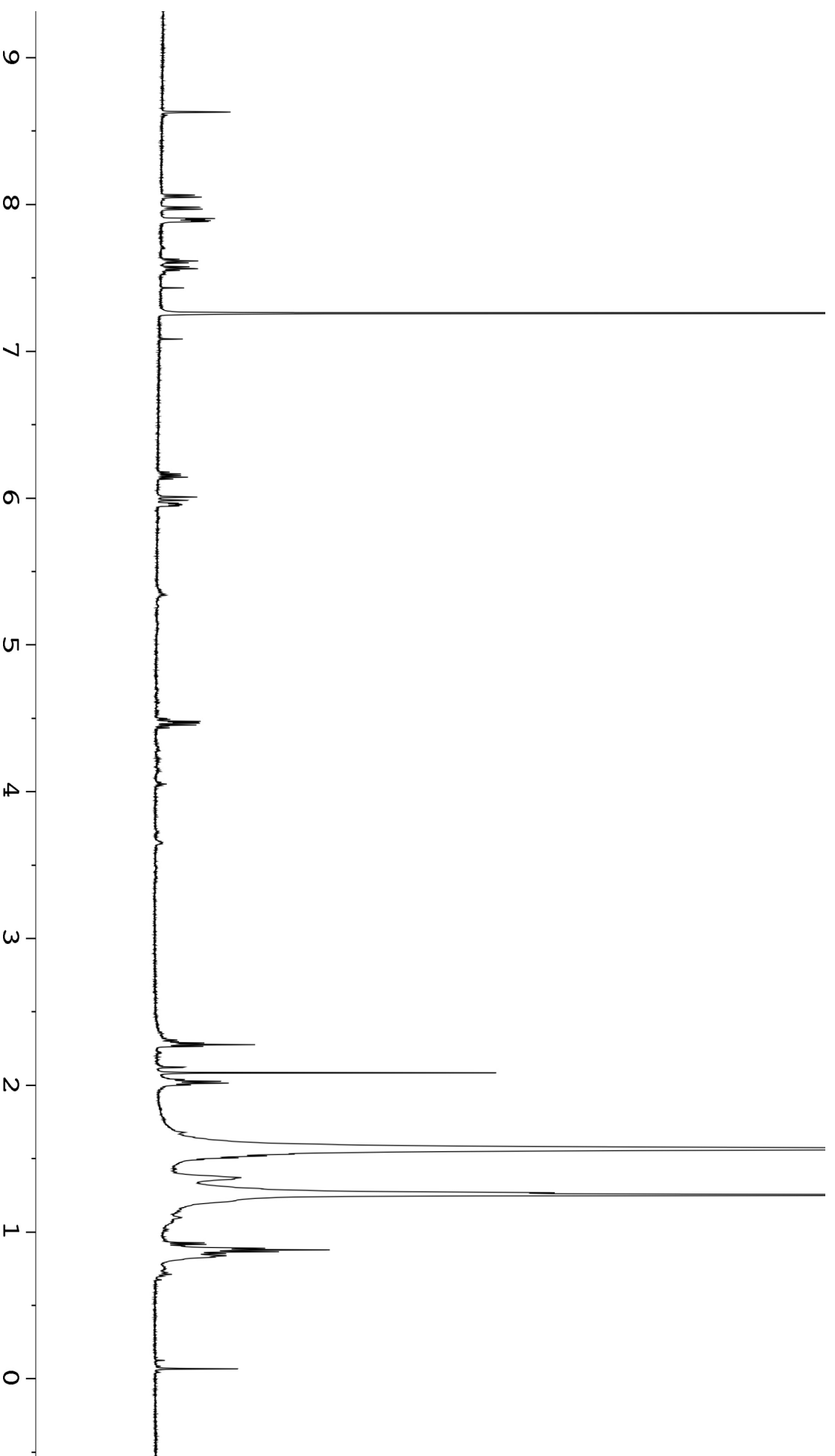


Figure S13. ^1H NMR spectrum of **6** (600 MHz, CDCl_3)

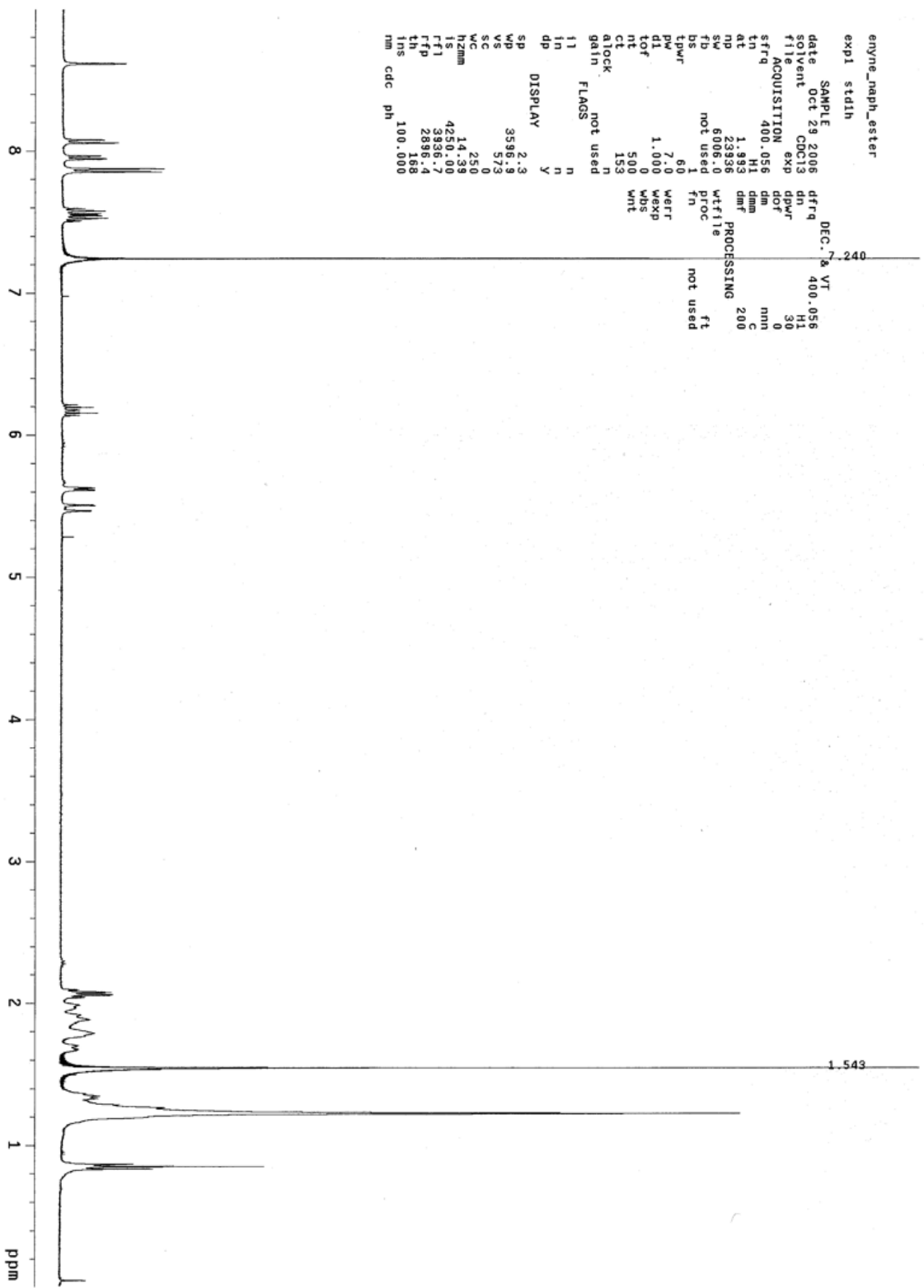


Figure S14. ¹H NMR spectrum of 7 (400 MHz, CDCl₃)

```

BM_55
exp3 stah
SAMPLE Nov 20 2006 DEC. & VT 400.125
SOLVENT CDCl3 dn H1
FILE ACQUISITION exp dppw H1
SFRQ 400.125 ddt 30
IN H1 dnm mmc
AT 1.993 dmf PROCESSING 200
NP 2396 wtfile
SW 6005.0 proc
FB not used fr not used
BS 1
TPWR 55
PW 7.0 wepp
DI 1.000 wexp
TOF 0 wbs
NT 64 wnt
CT 11
CLOCK
GAIN not used
FLAG not used
I1 n
IN n
DP y
DISPLAY 0.9
SP 3596.9
VS 70
SC 0
WC 250
N2mm 14.250
F1 500.131
RF 3882.4
TF 2896.9
TH 20
INS cdc ph 100.000

```

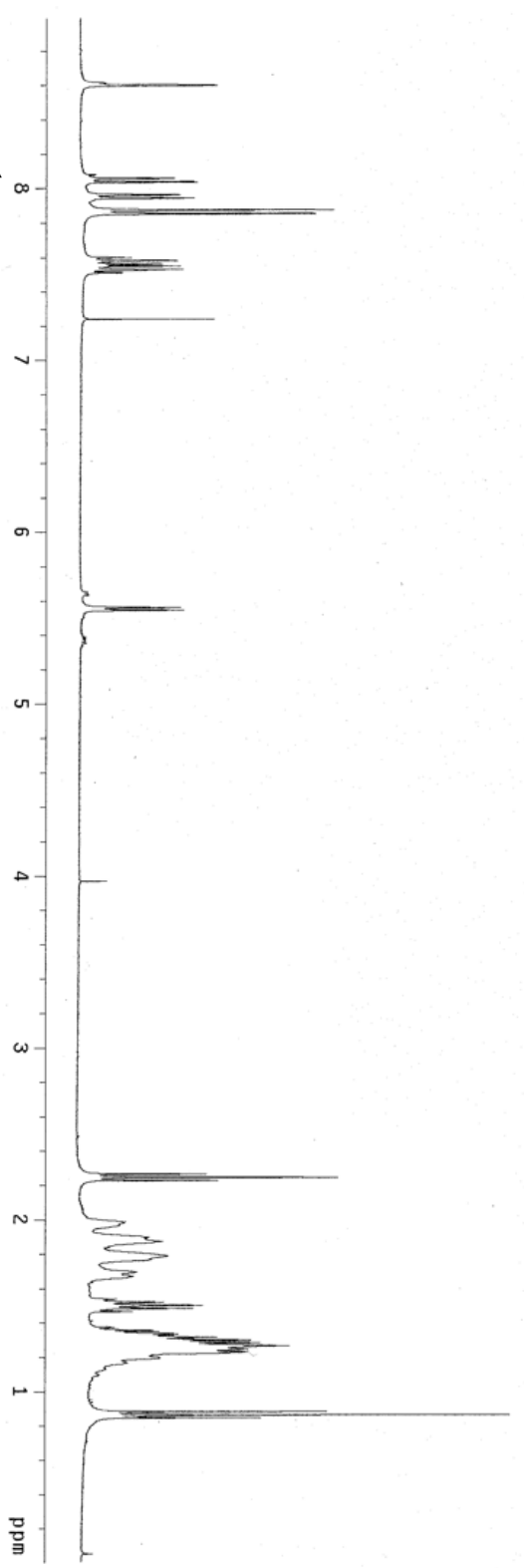


Figure S15. ¹H NMR spectrum of **8** (400 MHz, CDCl₃)

BM.55.13C
 exp2 std13c
 SAMPLE DEC. & VT
 date Nov 20 2006 dfrq 400.125
 solvent CDCl3 d1 38
 file exp dmpr 38
 ACQUISITION exp dof 0
 tn C13 dmf yyy
 at 1.199 dmf
 np 59968 PROCESSING 9700
 sw 25000.0 1b wt11e 1.00
 fb 13800 wt11e
 bs 18 proc not used
 tprvr 39 fn
 d1 1.500 weft
 tof 10000 wexp
 nt 1120 wds
 ct 1120 wnt
 alock not used
 gain not used
 flags
 l1 n
 ln n
 dp y
 DISPLAY
 sp -23.5
 wp 20156.9
 vs 57
 sc 0
 wc 250
 hzmm 80.63
 fs 500.00
 rfi 10744.5
 rfp 7747.1
 hfe 100.60
 nm no ph

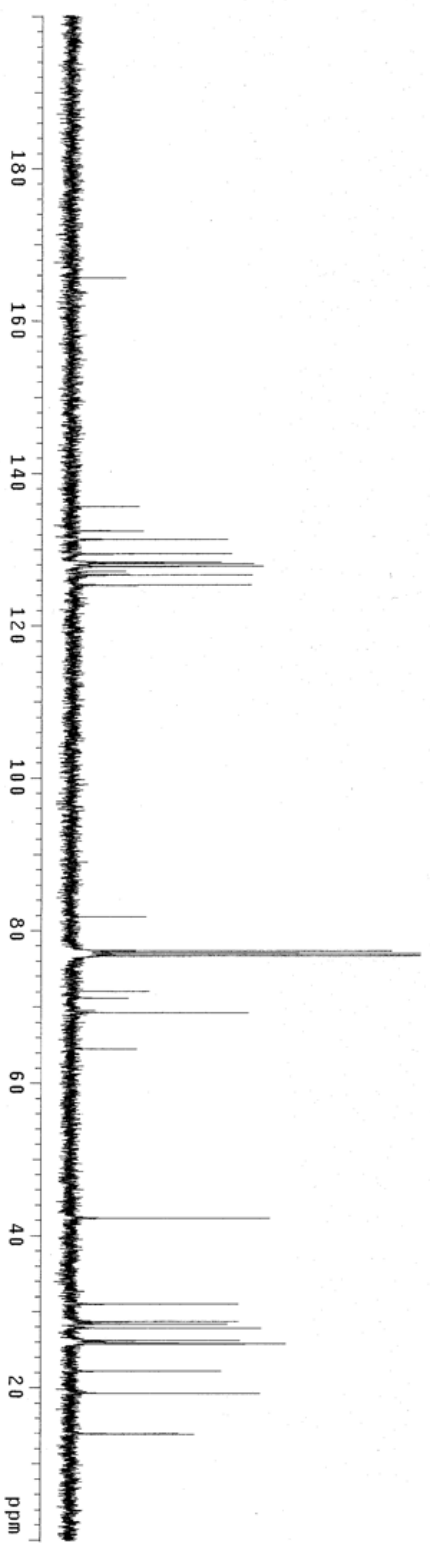


Figure S16. ¹³C NMR spectrum of **8** (400 MHz, CDCl₃)

```

exp2 std1h
SAMPLE      DEC. & VT
date        Aug 23 2006      dfrq      400.125
solvent     Aug 23 CDC13     dn         H1
file        ACQUISITION     exp         30
sfrq        400.125         dof        0
tn          1.993           dm         0
at          23936           dmf        nnn
np          6006.0          dm         c
sw          not used        wtfile     PROCESsing
fb          not used        proc       200
bs          1               fn         ft
tpwr        55              not used
pw          7.0             weirr
d1          1.000           wbs
tof         0               wnt
nt         16
ct         16
alock      not used
galn       not used
flags      not used
11         n
1n         n
dp         Y
DISPLAY   -985.2
SP         6005.4
WP         147
WC         1
SC         0
hzcmm     250
is         500.00
rf1        3882.4
rfp        2898.9
th         80
ins        100.000
nm cdc ph

```

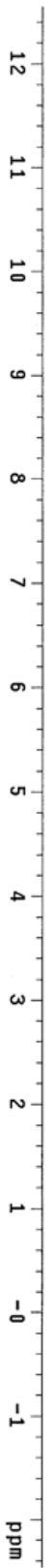


Figure S17. ¹H NMR spectrum of **13** (400 MHz, CDCl₃)

```

13C OBSERVE
exp1 std13c
SAMPLE DEC. & VT
date Aug 23 2006 dfreq 400.125
solvent CDCl3 dn H1
file exp dpwr 38
ACQUISITION dof 0
sfrq 100.621 dm YYY
tn C13 dnm W
dt 1.113 dmf 9700
np 5188 lb PROCESSING
fb 25080 1p 1.00
f2 13800 wifile
bs 16 proc not used
tpwr 58 fn
pw 8.7 werr
d1 1.000 wexp
tof 0 wds
nt 1000 wts
ct 112 wnt
a1ock not used
gain not used
FLAGS not used
f1 n
f2 n
f3 n
f4 n
f5 n
f6 n
f7 n
f8 n
f9 n
f10 n
f11 n
f12 n
f13 n
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f87 n
f88 n
f89 n
f90 n
f91 n
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f94 n
f95 n
f96 n
f97 n
f98 n
f99 n
f100 n
nm no ph 100.000

```

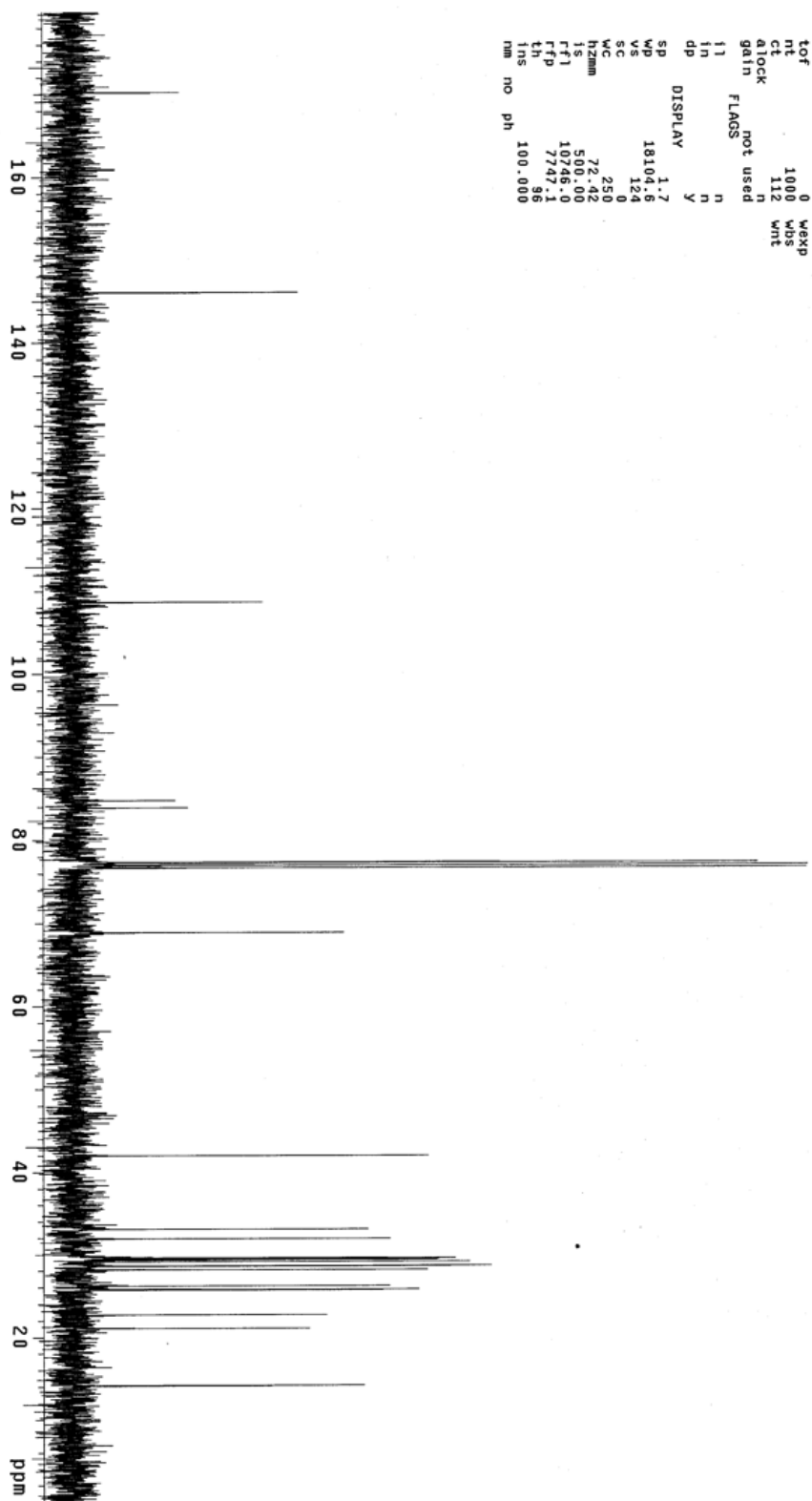


Figure S18. ¹³C NMR spectrum of **13** (400 MHz, CDCl₃)

```

BM.34.082306
exp2 std1h
SAMPLE DEC. & VT
date Aug 23 2006 dfreq 400.056
solvent CDCl3 dn H1
file ACQUISITION exp dpwr 43
ACQUISITION exp dof 0
sfrq 400.056 dm mn
tn H1 dmm c
at 1.995 dmf PROCESSING 9300
np 23936 1b
sw 5996.8 Wtfile 0.30
fb 3400 1b
bs 1 fn
tpwr 61 fn not used
pw 7.0 werr
d1 1.000 wexp
lof 0 wds
nt 300 wnt
cl 42
atlock not used
gain n
flags not used
ll n
ln n
dp DISPLAY y
sp -2.1
wp 3199.1
vs 141
sc 0
wc 250
hzmm 12.80
is 590.00
f1 3932.9
f1p 2896.4
th 91
ins 100.000
nm cdc ph

```

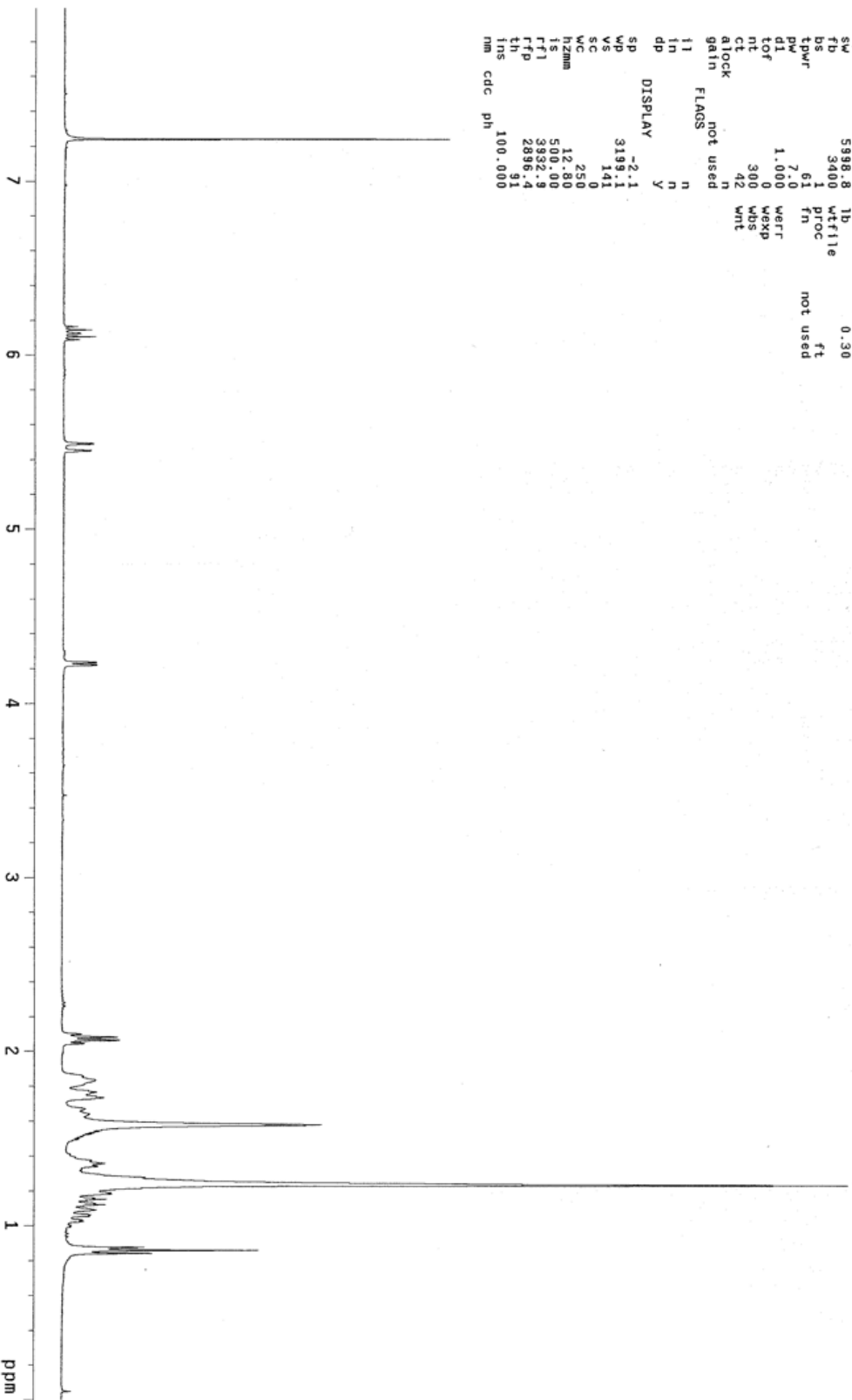


Figure S19. ¹H NMR spectrum of **14** (400 MHz, CDCl₃)

```

BM.34.13C
exp2 std13c
SAMPLE      DEC. & VT
date Aug 24 2006      dfrq 400.125
solvent CDCl3        dm 34
F1 ACQUISITION exp  dm 34
SFRQ 100.621      dof 0
tn C13           dmf yyy
at 1.199         dm 9700
np 59968         lb 1.00
sw 25000.0       wffile
fb 13800         proc not used
tpwr 16          fn
pw 8.7           wefr
d1 1.000         wexp
tof 100000       wds
nt 13424         wnt
ct atlock        not used
gain not used
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f2 n
f3 n
f4 n
f5 n
f6 n
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f8 n
f9 n
f10 n
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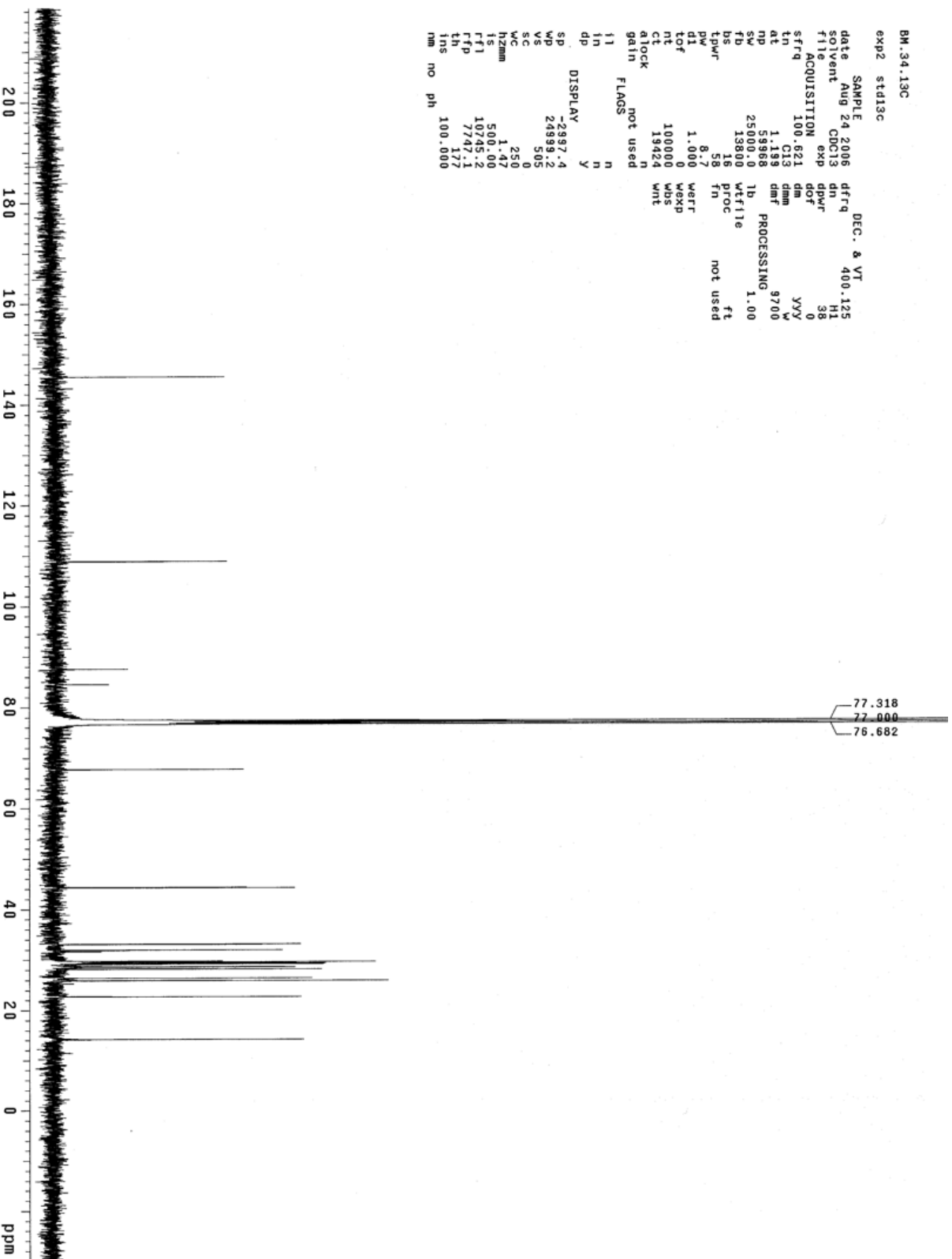


Figure S20. ¹³C NMR spectrum of **14** (400 MHz, CDCl₃)

```

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solvent CDCl3     dn    H1
file ACQUISITION exp  dpwr 30
sfrq 400.056      dm    mn
ln H1             dnm    mn
at 1.883          dmf    200
sp 2.883          wtfile
sb 608.9          proc
fb not used      ft
bs not used      fn
lpwr 60          werr 7.0
pw 7.0           wexp 1.000
d1 1.000         wbs
tof 0            wnt
nt 100          gain
ct 13           alock not used
gain not used   flags
11 n
1n n
dp y            DISPLAY
SP -1038.2
WP 6005.7
VC 100
WC 250
hzmm 0.35
IS 500.00
FFI 3935.9
FFP 2896.4
th 20
ins 100.000
nm cdc ph

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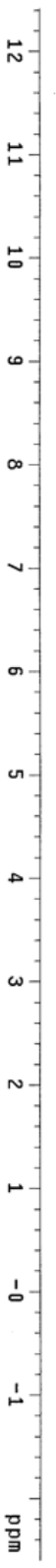


Figure S21. ¹H NMR spectrum of 15 (400 MHz, CDCl₃)


```

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f1 file exp dpmr 0
ACQUISITION dm dof 0
sfrq 100.603 dm
tn C13 dmm v
at 1.189 dmf 8500
mp 59968 lb PROCESSING 1.00
sw 25000.0 wtf1le
fd 13800 proc ft
ds 18 fn not used
lpwr 55
pw 87
tm 1.500 weff
tof 7128 wexp
nr 7128 wbs
ct 7128 wnt
atlock n
gain not used
flags
ii n
in n
dp y
DISPLAY
sp -3014.0
wp 24993.2
vs 136
vc 250
wcc 100.00
hzmm 500.00
is 3014.8
rf1 0
rfp 0
th 20
ins 100.000
nm no ph

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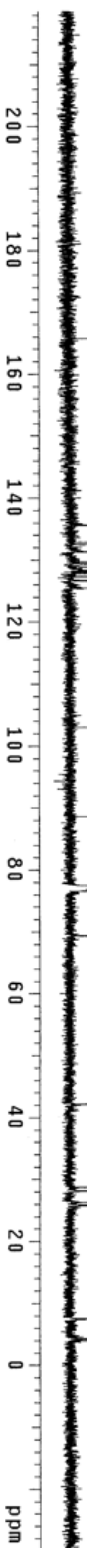


Figure S22. ¹³C NMR spectrum of **15** (400 MHz, CDCl₃)