Ring Contraction During the 6π-Electrocyclisation of Naphthopyran Valence Tautomers

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SUPPLEMENTARY DATA

Contents

Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Table 1. Crystal data and structure refinement for *cis*-sulfoxide (**4**) (CCDC670085)

Empirical formula	$C_{25}H_{16}O_2S$	
Formula weight	380.44	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.1939(5) Å	α = 90°
	b = 14.0344(4) Å	β = 101.498(2)°
	c = 11.7187(5) Å	γ = 90°
Volume	1804.06(12) Å^3	
Z	4	
Density (calculated)	1.401 Mg / m^3	
Absorption coefficient	0.198 mm^{-1}	
F(000)	792	
Crystal	Shard; Colourless	
Crystal size	0.08 × 0.07 × 0.04 mm^3	
θ range for data collection	3.16 – 27.48°	
Index ranges	$-14 \le h \le 14$, $-18 \le k \le 16$, $-15 \le l \le 15$	
Reflections collected	21913	
Independent reflections	4135 [R_{int} = 0.0999]	
Completeness to θ = 27.48°	99.8 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9921 and 0.9843	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4135 / 0 / 253	
Goodness-of-fit on F^2	1.065	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0671, $wR2$ = 0.1124	
R indices (all data)	$R1$ = 0.1094, $wR2$ = 0.1255	
Largest diff. peak and hole	0.369 and –0.361 e Å^{-3}	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SADABS Version 2.10.* (G. M. Sheldrick (2003)) Bruker AXS Inc., Madison, Wisconsin, USA. S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565).

Special details: All hydrogen atoms were fixed.

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	4114(2)	2467(2)	6498(2)	20(1)	1
C2	5268(2)	2753(2)	6096(2)	21(1)	1
C3	5607(2)	3661(2)	6108(2)	21(1)	1
C4	4823(2)	4400(2)	6429(2)	19(1)	1
C5	3648(2)	4143(2)	6477(2)	20(1)	1
C6	2779(2)	4800(2)	6691(2)	23(1)	1
C7	3101(3)	5738(2)	6871(2)	25(1)	1
C8	4296(2)	6051(2)	6851(2)	22(1)	1
C9	4636(3)	7021(2)	7044(2)	23(1)	1
C10	5781(3)	7320(2)	7014(2)	25(1)	1
C11	6651(2)	6655(2)	6798(2)	24(1)	1
C12	6361(2)	5713(2)	6612(2)	21(1)	1
C13	5173(2)	5380(2)	6632(2)	19(1)	1
C14	3514(2)	1595(2)	5840(2)	19(1)	1
C15	4061(2)	703(2)	6082(2)	20(1)	1
C16	3557(3)	−118(2)	5534(2)	25(1)	1
C17	2478(3)	−58(2)	4719(2)	28(1)	1
C18	1918(3)	819(2)	4477(2)	29(1)	1
C19	2423(3)	1639(2)	5037(2)	24(1)	1
C20	4408(2)	2223(2)	7804(2)	18(1)	1
C21	5012(2)	1374(2)	8158(2)	19(1)	1
C22	5271(2)	1088(2)	9312(2)	23(1)	1
C23	4896(3)	1657(2)	10145(2)	25(1)	1
C24	4288(3)	2501(2)	9811(2)	26(1)	1
C25	4041(2)	2786(2)	8648(2)	22(1)	1
O1	3233(2)	3218(1)	6290(2)	21(1)	1
O11	5563(2)	−384(1)	7593(2)	30(1)	1
S1	5476(1)	599(1)	7105(1)	22(1)	1

Table 3a. Bond lengths [Å].

C1–O1	1.432(3)
C1–C2	1.515(4)
C1–C14	1.529(3)
C1–C20	1.538(3)
C2–C3	1.329(3)
C2–H2	0.9500
C3–C4	1.455(4)
C3–H3	0.9500
C4–C5	1.376(4)
C4–C13	1.437(3)
C5–O1	1.382(3)
C5–C6	1.399(4)
C6–C7	1.370(4)
C6–H6	0.9500
C7–C8	1.413(4)
C7–H7	0.9500
C8–C9	1.419(3)
C8–C13	1.421(4)
C9–C10	1.356(4)
C9–H9	0.9500
C10–C11	1.408(4)
C10–H10	0.9500
C11–C12	1.369(3)
C11–H11	0.9500
C12–C13	1.413(4)
C12–H12	0.9500
C14–C19	1.386(4)
C14–C15	1.398(3)
C15–C16	1.383(4)
C15–S1	1.792(3)
C16–C17	1.385(4)
C16–H16	0.9500
C17–C18	1.385(4)
C17–H17	0.9500
C18–C19	1.388(4)
C18–H18	0.9500
C19–H19	0.9500
C20–C25	1.390(4)
C20–C21	1.391(3)
C21–C22	1.385(4)
C21–S1	1.798(3)
C22–C23	1.390(4)
C22–H22	0.9500
C23–C24	1.382(4)
C23–H23	0.9500
C24–C25	1.395(4)
C24–H24	0.9500
C25–H25	0.9500
O11–S1	1.4884(18)

Table 3b Bond angles [°].

O1–C1–C2	110.7(2)
O1–C1–C14	106.6(2)
C2–C1–C14	111.8(2)
O1–C1–C20	109.7(2)
C2–C1–C20	110.0(2)
C14–C1–C20	108.02(19)
C3–C2–C1	120.7(2)
C3–C2–H2	119.7
C1–C2–H2	119.7
C2–C3–C4	120.0(3)
C2–C3–H3	120.0
C4–C3–H3	120.0
C5–C4–C13	118.4(2)
C5–C4–C3	117.1(2)
C13–C4–C3	124.5(2)
C4–C5–O1	122.3(2)
C4–C5–C6	122.6(2)
O1–C5–C6	115.1(2)
C7–C6–C5	119.3(3)
C7–C6–H6	120.3
C5–C6–H6	120.3
C6–C7–C8	121.2(2)
C6–C7–H7	119.4
C8–C7–H7	119.4
C7–C8–C9	121.4(2)
C7–C8–C13	119.2(2)
C9–C8–C13	119.5(2)
C10–C9–C8	121.2(3)
C10–C9–H9	119.4
C8–C9–H9	119.4
C9–C10–C11	119.4(2)
C9–C10–H10	120.3
C11–C10–H10	120.3
C12–C11–C10	121.2(3)
C12–C11–H11	119.4
C10–C11–H11	119.4
C11–C12–C13	120.8(2)
C11–C12–H12	119.6
C13–C12–H12	119.6
C12–C13–C8	118.0(2)
C12–C13–C4	122.7(2)
C8–C13–C4	119.3(2)
C19–C14–C15	117.9(2)
C19–C14–C1	123.1(2)
C15–C14–C1	119.0(2)
C16–C15–C14	122.0(2)
C16–C15–S1	117.9(2)
C14–C15–S1	120.09(19)
C15–C16–C17	119.3(2)
C15–C16–H16	120.4
C17–C16–H16	120.4
C16–C17–C18	119.5(2)
C16–C17–H17	120.3
C18–C17–H17	120.3
C17–C18–C19	121.0(3)
C17–C18–H18	119.5
C19–C18–H18	119.5
C14–C19–C18	120.3(2)
C14–C19–H19	119.8
C18–C19–H19	119.8

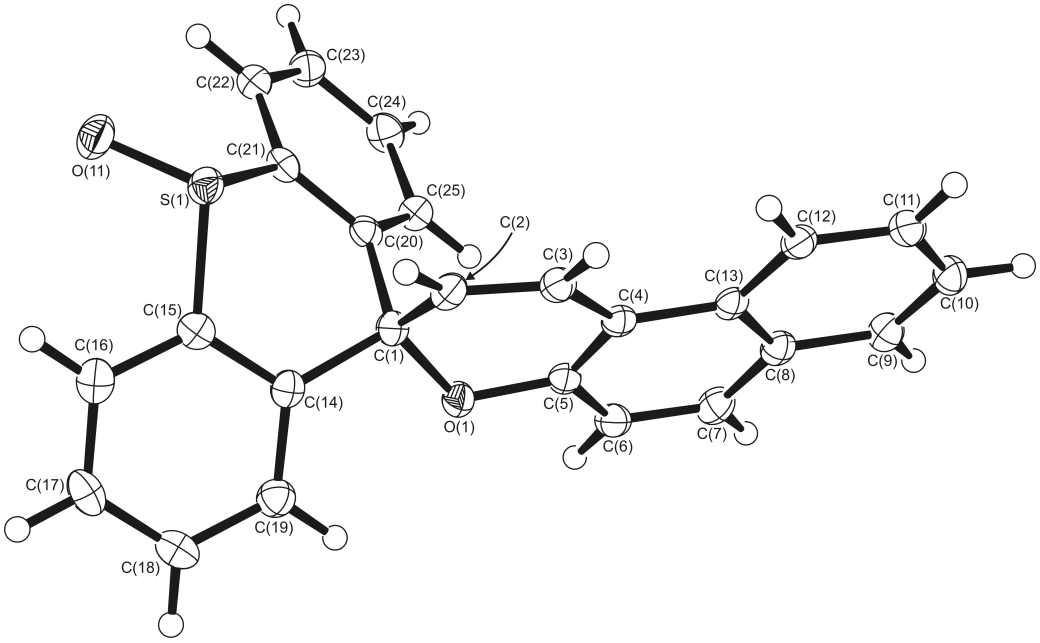
C25–C20–C21	118.0(2)
C25–C20–C1	123.1(2)
C21–C20–C1	118.8(2)
C22–C21–C20	122.3(2)
C22–C21–S1	117.45(19)
C20–C21–S1	120.24(19)
C21–C22–C23	119.0(2)
C21–C22–H22	120.5
C23–C22–H22	120.5
C24–C23–C22	119.6(2)
C24–C23–H23	120.2
C22–C23–H23	120.2
C23–C24–C25	120.9(3)
C23–C24–H24	119.6
C25–C24–H24	119.6
C20–C25–C24	120.2(2)
C20–C25–H25	119.9
C24–C25–H25	119.9
C5–O1–C1	117.80(19)
O11–S1–C15	108.29(12)
O11–S1–C21	107.64(11)
C15–S1–C21	94.15(12)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	21(1)	17(1)	21(1)	−2(1)	3(1)	1(1)
C2	25(2)	19(1)	19(1)	1(1)	5(1)	4(1)
C3	21(1)	21(1)	20(1)	2(1)	3(1)	1(1)
C4	22(1)	20(1)	14(1)	2(1)	2(1)	1(1)
C5	26(2)	18(1)	13(1)	0(1)	0(1)	−1(1)
C6	21(1)	25(1)	22(1)	1(1)	2(1)	0(1)
C7	27(2)	23(1)	25(1)	1(1)	6(1)	7(1)
C8	28(2)	21(1)	16(1)	2(1)	4(1)	1(1)
C9	29(2)	20(1)	21(1)	−2(1)	7(1)	3(1)
C10	34(2)	18(1)	22(1)	−2(1)	2(1)	−2(1)
C11	22(2)	25(1)	23(1)	3(1)	2(1)	−3(1)
C12	20(1)	21(1)	21(1)	3(1)	3(1)	2(1)
C13	27(2)	19(1)	11(1)	2(1)	2(1)	1(1)
C14	22(1)	19(1)	19(1)	1(1)	7(1)	0(1)
C15	21(1)	23(1)	18(1)	−1(1)	7(1)	−1(1)
C16	31(2)	23(1)	25(2)	−1(1)	11(1)	−1(1)
C17	32(2)	26(1)	27(2)	−10(1)	8(1)	−7(1)
C18	27(2)	33(2)	24(2)	−6(1)	1(1)	−4(1)
C19	26(2)	24(1)	23(1)	0(1)	5(1)	1(1)
C20	16(1)	20(1)	19(1)	0(1)	3(1)	−4(1)
C21	17(1)	20(1)	21(1)	−4(1)	4(1)	−3(1)
C22	22(2)	22(1)	23(1)	1(1)	2(1)	−2(1)
C23	31(2)	25(1)	19(1)	1(1)	4(1)	−1(1)
C24	31(2)	27(1)	21(1)	−5(1)	8(1)	−2(1)
C25	23(2)	21(1)	23(1)	1(1)	3(1)	0(1)
O1	21(1)	17(1)	25(1)	−1(1)	3(1)	1(1)
O11	41(1)	20(1)	27(1)	1(1)	5(1)	6(1)
S1	24(1)	20(1)	22(1)	−1(1)	4(1)	2(1)

Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H2	5754	2279	5831	25	1
H3	6362	3828	5908	25	1
H6	1974	4598	6711	27	1
H7	2511	6185	7013	30	1
H9	4051	7468	7198	28	1
H10	5994	7973	7136	30	1
H11	7455	6864	6782	28	1
H12	6964	5278	6469	25	1
H16	3946	–716	5714	30	1
H17	2125	–614	4328	33	1
H18	1176	861	3919	34	1
H19	2020	2233	4870	29	1
H22	5699	510	9530	27	1
H23	5055	1468	10939	30	1
H24	4036	2891	10382	31	1
H25	3620	3367	8431	27	1



View of *cis*-sulfoxide **4**. Ellipsoid probability: 50%.

Table 1. Crystal data and structure refinement for *trans*-sulfoxide (**5**) (CCDC670086).

Empirical formula	$C_{25}H_{16}O_2S$	
Formula weight	380.44	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.3454(2) Å	α = 90°
	b = 13.4896(2) Å	β = 96.3650(10)°
	c = 11.5736(3) Å	γ = 90°
Volume	1760.36(6) Å^3	
Z	4	
Density (calculated)	1.435 Mg / m^3	
Absorption coefficient	0.203 mm^{-1}	
F(000)	792	
Crystal	Prism; colourless	
Crystal size	0.30 × 0.30 × 0.20 mm^3	
θ range for data collection	3.02 – 27.49°	
Index ranges	$-14 \le h \le 14$, $-17 \le k \le 17$, $-15 \le l \le 14$	
Reflections collected	22230	
Independent reflections	4007 [R_{int} = 0.0303]	
Completeness to θ = 27.49°	99.3 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9605 and 0.9415	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4007 / 0 / 253	
Goodness-of-fit on F^2	1.059	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0364, $wR2$ = 0.0930	
R indices (all data)	$R1$ = 0.0389, $wR2$ = 0.0948	
Largest diff. peak and hole	0.360 and –0.470 e Å^{-3}	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SORTAV* (R. H. Blessing, Acta Cryst. A**51** (1995) 33–37; R. H. Blessing, J. Appl. Cryst. **30** (1997) 421–426). S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	5513(1)	1475(1)	6909(1)	15(1)	1
C2	5210(1)	1135(1)	5784(1)	18(1)	1
C3	5611(1)	1646(1)	4859(1)	19(1)	1
C4	6267(1)	2506(1)	5074(1)	20(1)	1
C5	6560(1)	2849(1)	6207(1)	18(1)	1
C6	6199(1)	2327(1)	7146(1)	14(1)	1
C7	6323(1)	851(1)	9013(1)	16(1)	1
C8	6645(1)	13(1)	9670(1)	21(1)	1
C9	7680(1)	41(1)	10439(1)	25(1)	1
C10	8375(1)	886(1)	10527(1)	24(1)	1
C11	8032(1)	1725(1)	9870(1)	21(1)	1
C12	6989(1)	1722(1)	9110(1)	16(1)	1
C13	6527(1)	2632(1)	8418(1)	15(1)	1
C14	7338(1)	3515(1)	8544(1)	17(1)	1
C15	6893(1)	4429(1)	8559(1)	17(1)	1
C16	5612(1)	4584(1)	8508(1)	15(1)	1
C17	4924(1)	3764(1)	8680(1)	14(1)	1
C18	3689(1)	3830(1)	8715(1)	17(1)	1
C19	3143(1)	4731(1)	8569(1)	18(1)	1
C20	3799(1)	5602(1)	8391(1)	16(1)	1
C21	3244(1)	6547(1)	8265(1)	20(1)	1
C22	3891(1)	7387(1)	8129(1)	21(1)	1
C23	5126(1)	7320(1)	8101(1)	21(1)	1
C24	5689(1)	6418(1)	8201(1)	19(1)	1
C25	5052(1)	5533(1)	8357(1)	15(1)	1
O1	4823(1)	–265(1)	7646(1)	24(1)	1
O2	5414(1)	2842(1)	8899(1)	16(1)	1
S1	4966(1)	781(1)	8059(1)	16(1)	1

Table 3a. Bond lengths [Å].

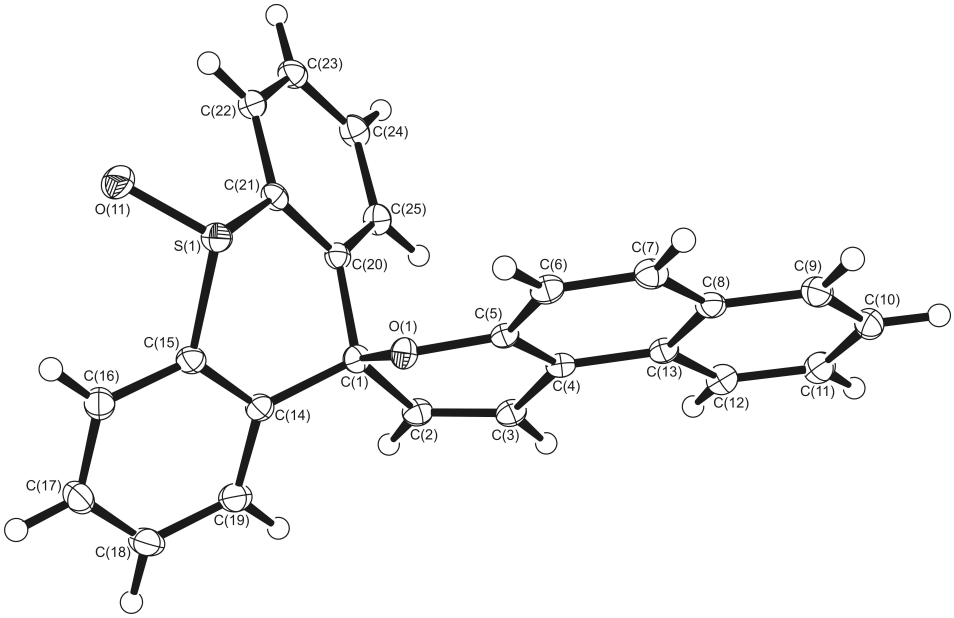
C1–C2	1.3880(18)
C1–C6	1.3974(18)
C1–S1	1.7932(13)
C2–C3	1.3919(19)
C3–C4	1.386(2)
C4–C5	1.3954(19)
C5–C6	1.3947(18)
C6–C13	1.5337(17)
C7–C8	1.3887(18)
C7–C12	1.3954(18)
C7–S1	1.7947(13)
C8–C9	1.393(2)
C9–C10	1.384(2)
C10–C11	1.395(2)
C11–C12	1.3939(18)
C12–C13	1.5260(18)
C13–O2	1.4632(14)
C13–C14	1.5024(17)
C14–C15	1.3336(19)
C15–C16	1.4620(17)
C16–C17	1.3817(18)
C16–C25	1.4320(18)
C17–O2	1.3738(15)
C17–C18	1.4085(17)
C18–C19	1.3670(19)
C19–C20	1.4179(19)
C20–C21	1.4212(18)
C20–C25	1.4298(18)
C21–C22	1.370(2)
C22–C23	1.408(2)
C23–C24	1.3737(19)
C24–C25	1.4169(18)
O1–S1	1.4930(10)

Table 3b. Bond angles [°].

C2–C1–C6	122.06(12)
C2–C1–S1	116.94(10)
C6–C1–S1	120.99(10)
C1–C2–C3	119.33(12)
C4–C3–C2	119.44(12)
C3–C4–C5	120.87(12)
C6–C5–C4	120.36(12)
C5–C6–C1	117.88(12)
C5–C6–C13	123.48(12)
C1–C6–C13	118.64(11)
C8–C7–C12	122.28(12)
C8–C7–S1	116.73(10)
C12–C7–S1	120.96(10)
C7–C8–C9	118.70(13)
C10–C9–C8	120.16(13)
C9–C10–C11	120.41(13)
C12–C11–C10	120.51(13)
C11–C12–C7	117.90(12)
C11–C12–C13	123.18(12)
C7–C12–C13	118.88(11)
O2–C13–C14	110.73(10)
O2–C13–C12	102.55(10)
C14–C13–C12	114.55(11)
O2–C13–C6	106.85(10)
C14–C13–C6	112.73(10)
C12–C13–C6	108.71(10)
C15–C14–C13	120.41(11)
C14–C15–C16	120.48(12)
C17–C16–C25	118.88(12)
C17–C16–C15	117.08(12)
C25–C16–C15	123.94(12)
O2–C17–C16	121.80(11)
O2–C17–C18	115.82(11)
C16–C17–C18	122.27(12)
C19–C18–C17	119.41(12)
C18–C19–C20	121.16(12)
C19–C20–C21	121.62(12)
C19–C20–C25	119.30(12)
C21–C20–C25	119.07(12)
C22–C21–C20	121.15(12)
C21–C22–C23	119.78(13)
C24–C23–C22	120.67(13)
C23–C24–C25	121.18(12)
C24–C25–C20	118.14(12)
C24–C25–C16	122.87(12)
C20–C25–C16	118.98(12)
C17–O2–C13	117.02(10)
O1–S1–C1	106.89(6)
O1–S1–C7	107.57(6)
C1–S1–C7	94.87(6)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement
factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	13(1)	16(1)	15(1)	1(1)	2(1)	2(1)
C2	17(1)	17(1)	19(1)	−1(1)	0(1)	2(1)
C3	21(1)	22(1)	15(1)	−1(1)	1(1)	5(1)
C4	23(1)	22(1)	17(1)	4(1)	6(1)	3(1)
C5	19(1)	17(1)	19(1)	1(1)	4(1)	0(1)
C6	14(1)	15(1)	15(1)	−1(1)	2(1)	2(1)
C7	18(1)	18(1)	13(1)	−1(1)	2(1)	2(1)
C8	29(1)	18(1)	15(1)	0(1)	3(1)	3(1)
C9	34(1)	23(1)	16(1)	2(1)	0(1)	9(1)
C10	24(1)	30(1)	18(1)	–2(1)	–4(1)	7(1)
C11	20(1)	24(1)	18(1)	−3(1)	0(1)	1(1)
C12	17(1)	17(1)	13(1)	–2(1)	2(1)	2(1)
C13	14(1)	16(1)	16(1)	−1(1)	3(1)	1(1)
C14	14(1)	19(1)	18(1)	−1(1)	2(1)	–2(1)
C15	15(1)	19(1)	17(1)	–2(1)	2(1)	–3(1)
C16	15(1)	17(1)	12(1)	−1(1)	1(1)	–1(1)
C17	16(1)	16(1)	11(1)	–2(1)	1(1)	0(1)
C18	16(1)	19(1)	15(1)	−1(1)	2(1)	–4(1)
C19	14(1)	22(1)	18(1)	–2(1)	2(1)	–1(1)
C20	17(1)	19(1)	12(1)	−1(1)	0(1)	1(1)
C21	20(1)	22(1)	17(1)	−1(1)	1(1)	4(1)
C22	28(1)	18(1)	16(1)	1(1)	1(1)	5(1)
C23	28(1)	17(1)	18(1)	1(1)	3(1)	–2(1)
C24	20(1)	19(1)	18(1)	0(1)	3(1)	–2(1)
C25	17(1)	17(1)	12(1)	−1(1)	2(1)	–1(1)
O1	30(1)	17(1)	23(1)	1(1)	−1(1)	–7(1)
O2	15(1)	15(1)	18(1)	0(1)	4(1)	1(1)
S1	17(1)	17(1)	16(1)	2(1)	2(1)	–3(1)



View of *trans*-sulfoxide **5**. Ellipsoid probability: 50%.

Table 1. Crystal data and structure refinement for compound (**6**) (CCDC661552)

Formula	$C_{25}H_{16}O_3S$	
Formula weight	396.44	
Size	0.31 x 0.20 x 0.08 mm	
Crystal morphology	Pale brown plate	
Temperature	150(2) K	
Wavelength	0.71073 Å [Mo-K_α]	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.97170(10) Å	$\alpha = 90°$
	b = 20.6854(3) Å	$\beta = 101.1430(7)°$
	c = 11.1804(2) Å	$\gamma = 90°$
Volume	1808.87(5) Å^3	
Z	4	
Density (calculated)	1.456 Mg/m^3	
Absorption coefficient	0.205 mm^{-1}	
F(000)	824	
Data collection range	$2.71 \le \theta \le 26°$	
Index ranges	$-9 \le h \le 9$, $-25 \le k \le 25$, $-13 \le l \le 13$	
Reflections collected	34563	
Independent reflections	3553 [R(int) = 0.084]	
Observed reflections	3006 [$I > 2\sigma(I)$]	
Absorption correction	none	
Refinement method	Full	
Data / restraints / parameters	3553 / 0 / 262	
Goodness of fit	1.058	
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0396, wR_2 = 0.1011	
R indices (all data)	R_1 = 0.0483, wR_2 = 0.1084	
Largest diff. peak and hole	0.298 and -0.545e.Å^{-3}	

Table 2. Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^4) with standard uncertainties (s.u.s) in parentheses. U_{eq} is defined as $^1/_3$ of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(2)	489(2)	1308.2(8)	5886.9(15)	235(3)
C(3)	-433(2)	772.3(8)	6141.0(16)	274(4)
C(4)	-1040(2)	756.0(9)	7224.0(17)	319(4)
C(5)	-707(2)	1267.5(9)	8030.5(17)	332(4)
C(6)	225(2)	1799.2(9)	7769.5(16)	303(4)
C(7)	838(2)	1830.7(8)	6685.2(15)	250(4)
C(8)	1929(2)	2404.6(8)	6435.3(15)	249(4)
C(9)	3376(2)	2207.3(8)	5800.9(15)	247(3)
C(10)	4977(2)	2494.9(8)	6130.7(16)	290(4)
C(11)	6332(2)	2295.7(9)	5605.3(16)	310(4)
C(12)	6118(2)	1807.4(9)	4735.7(16)	302(4)
C(13)	4538(2)	1513.4(8)	4391.9(15)	269(4)
C(14)	3188(2)	1720.4(8)	4923.1(15)	237(3)
C(81)	899(2)	2947.9(8)	5757.9(15)	252(4)
C(83)	-906(2)	3763.2(8)	5669.5(15)	258(4)
C(84)	-2032(2)	4223.3(8)	5989.9(16)	299(4)
C(85)	-2557(2)	4702.6(8)	5160.9(16)	313(4)
C(86)	-2008(2)	4735.5(8)	4019.2(16)	292(4)
C(87)	-2518(2)	5248.6(9)	3187.9(17)	340(4)
C(88)	-1984(2)	5275.0(9)	2098.5(17)	363(4)
C(89)	-918(2)	4791.8(9)	1777.1(17)	353(4)
C(90)	-399(2)	4283.9(9)	2553.5(16)	310(4)
C(91)	-911(2)	4247.8(8)	3694.4(15)	269(4)
C(92)	-360(2)	3751.9(8)	4570.6(15)	258(4)
C(93)	800(2)	3213.6(8)	4643.3(16)	265(4)
O(1)	37.2(15)	1737.4(6)	3664.9(11)	317(3)
O(2)	1478.9(16)	687.0(6)	4082.9(11)	319(3)
O(82)	-145.4(14)	3272.4(5)	6417.5(10)	263(3)
S(1)	1195.2(5)	1330.79(19)	4492.4(4)	243.5(14)

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3). The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2)	230(8)	229(8)	245(8)	16(6)	44(6)	22(6)
C(3)	256(8)	229(8)	330(9)	22(7)	43(7)	8(6)
C(4)	324(9)	258(9)	400(10)	72(8)	132(8)	12(7)
C(5)	382(10)	320(10)	328(9)	68(8)	154(8)	64(8)
C(6)	370(10)	254(9)	298(9)	3(7)	96(7)	54(7)
C(7)	253(8)	218(8)	272(8)	27(6)	35(7)	33(6)
C(8)	280(8)	213(8)	249(8)	-20(6)	41(7)	-3(6)
C(9)	269(8)	213(8)	251(8)	28(6)	27(7)	10(6)
C(10)	301(9)	251(9)	295(9)	-16(7)	4(7)	-29(7)
C(11)	238(8)	301(9)	370(10)	38(8)	8(7)	-25(7)
C(12)	271(9)	286(9)	356(9)	45(7)	83(7)	34(7)
C(13)	300(8)	236(8)	279(9)	19(7)	72(7)	14(7)
C(14)	244(8)	215(8)	243(8)	23(6)	25(6)	-10(6)
C(81)	252(8)	200(8)	310(9)	-40(7)	70(7)	-15(6)
C(83)	270(8)	208(8)	289(9)	0(7)	36(7)	-26(6)
C(84)	297(9)	293(9)	312(9)	-23(7)	69(7)	15(7)
C(85)	279(9)	256(9)	389(10)	-29(8)	30(7)	35(7)
C(86)	254(8)	252(9)	339(9)	-11(7)	-19(7)	-31(7)
C(87)	303(9)	248(9)	427(10)	9(8)	-32(8)	-6(7)
C(88)	369(10)	294(10)	377(10)	83(8)	-51(8)	-66(8)
C(89)	385(10)	347(10)	308(9)	28(8)	17(8)	-101(8)
C(90)	327(9)	278(9)	314(9)	-2(7)	31(7)	-49(7)
C(91)	259(8)	234(8)	297(9)	-19(7)	12(7)	-60(7)
C(92)	254(8)	216(8)	294(9)	-25(7)	30(7)	-39(6)
C(93)	291(8)	214(8)	301(9)	-12(7)	83(7)	-11(7)
O(1)	302(6)	353(7)	278(6)	37(5)	12(5)	-18(5)
O(2)	382(7)	243(6)	351(7)	-80(5)	118(5)	-57(5)
O(82)	297(6)	215(6)	280(6)	-4(5)	66(5)	15(5)
S(1)	260(2)	230(2)	239(2)	-14.9(16)	44.4(16)	-30.7(15)

Table 4. Hydrogen atom co-ordinates (x 10^3) and isotropic displacement parameters (Å^2 x 10^2) with s.u.s in parentheses.

	x	y	z	U_{eq}
H(3)	-646.	422.	5582.	33.
H(4)	-1680.	395.	7410.	38.
H(5)	-1121.	1255.	8772.	40.
H(6)	447.	2145.	8337.	36.
H(8)	2479.	2582.	7249.	30.
H(10)	5144.	2831.	6721.	35.
H(11)	7418.	2496.	5843.	37.
H(12)	7052.	1676.	4379.	36.
H(13)	4377.	1176.	3804.	32.
H(84)	-2410.	4203.	6744.	36.
H(85)	-3313.	5025.	5350.	38.
H(87)	-3241.	5579.	3391.	41.
H(88)	-2338.	5623.	1554.	44.
H(89)	-552.	4816.	1019.	42.
H(90)	307.	3955.	2322.	37.
H(93)	1384.	3073.	4026.	32.

Table 5. Interatomic distances (Å) with s.u.s in parentheses.

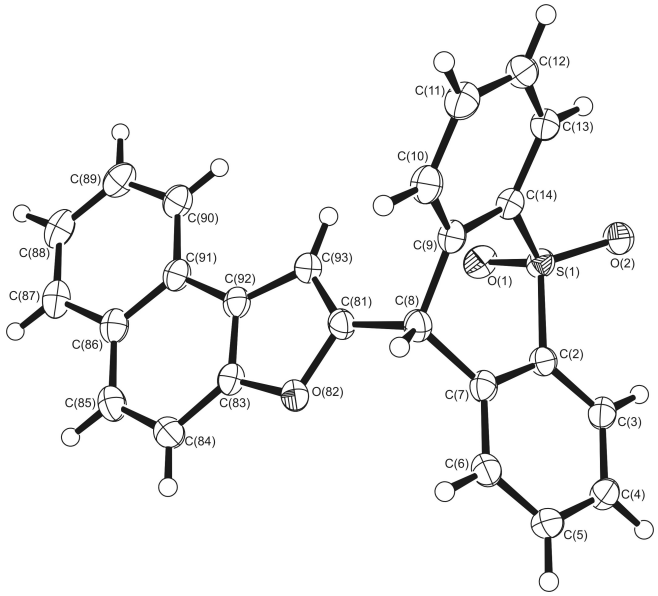
C(2)-C(3)	1.389(2)	C(2)-C(7)	1.395(2)
C(2)-S(1)	1.7578(16)	C(3)-C(4)	1.388(2)
C(4)-C(5)	1.382(3)	C(5)-C(6)	1.389(3)
C(6)-C(7)	1.394(2)	C(7)-C(8)	1.529(2)
C(8)-C(81)	1.507(2)	C(8)-C(9)	1.522(2)
C(9)-C(10)	1.392(2)	C(9)-C(14)	1.394(2)
C(10)-C(11)	1.388(2)	C(11)-C(12)	1.390(3)
C(12)-C(13)	1.384(2)	C(13)-C(14)	1.393(2)
C(14)-S(1)	1.7635(16)	C(81)-C(93)	1.350(2)
C(81)-O(82)	1.3871(19)	C(83)-O(82)	1.379(2)
C(83)-C(92)	1.380(2)	C(83)-C(84)	1.401(2)
C(84)-C(85)	1.367(2)	C(85)-C(86)	1.429(2)
C(86)-C(87)	1.418(2)	C(86)-C(91)	1.427(2)
C(87)-C(88)	1.367(3)	C(88)-C(89)	1.403(3)
C(89)-C(90)	1.375(3)	C(90)-C(91)	1.414(2)
C(91)-C(92)	1.428(2)	C(92)-C(93)	1.440(2)
O(1)-S(1)	1.4441(12)	O(2)-S(1)	1.4402(12)

Table 6. Angles between interatomic vectors (°) with s.u.s in parentheses.

C(3)-C(2)-C(7)	122.38(15)	C(3)-C(2)-S(1)	118.38(13)
C(7)-C(2)-S(1)	119.22(12)	C(4)-C(3)-C(2)	119.00(16)
C(5)-C(4)-C(3)	119.68(16)	C(4)-C(5)-C(6)	120.79(16)
C(5)-C(6)-C(7)	120.76(17)	C(6)-C(7)-C(2)	117.38(15)
C(6)-C(7)-C(8)	120.19(15)	C(2)-C(7)-C(8)	122.35(14)
C(81)-C(8)-C(9)	110.76(13)	C(81)-C(8)-C(7)	113.38(13)
C(9)-C(8)-C(7)	112.70(13)	C(10)-C(9)-C(14)	117.62(15)
C(10)-C(9)-C(8)	120.04(15)	C(14)-C(9)-C(8)	122.28(15)
C(11)-C(10)-C(9)	120.64(16)	C(10)-C(11)-C(12)	120.76(16)
C(13)-C(12)-C(11)	119.73(16)	C(12)-C(13)-C(14)	118.86(16)
C(13)-C(14)-C(9)	122.38(15)	C(13)-C(14)-S(1)	118.20(13)
C(9)-C(14)-S(1)	119.40(12)	C(93)-C(81)-O(82)	111.09(15)
C(93)-C(81)-C(8)	134.12(15)	O(82)-C(81)-C(8)	114.74(13)
O(82)-C(83)-C(92)	110.49(14)	O(82)-C(83)-C(84)	124.97(15)
C(92)-C(83)-C(84)	124.51(16)	C(85)-C(84)-C(83)	116.54(16)
C(84)-C(85)-C(86)	122.27(16)	C(87)-C(86)-C(91)	118.33(16)
C(87)-C(86)-C(85)	121.53(16)	C(91)-C(86)-C(85)	120.14(15)
C(88)-C(87)-C(86)	121.01(17)	C(87)-C(88)-C(89)	120.53(17)
C(90)-C(89)-C(88)	120.39(17)	C(89)-C(90)-C(91)	120.39(17)
C(90)-C(91)-C(86)	119.34(16)	C(90)-C(91)-C(92)	123.54(16)
C(86)-C(91)-C(92)	117.11(15)	C(83)-C(92)-C(91)	119.37(15)
C(83)-C(92)-C(93)	105.80(15)	C(91)-C(92)-C(93)	134.70(16)
C(81)-C(93)-C(92)	106.79(15)	C(83)-O(82)-C(81)	105.80(12)
O(2)-S(1)-O(1)	117.08(8)	O(2)-S(1)-C(2)	110.75(7)
O(1)-S(1)-C(2)	108.00(7)	O(2)-S(1)-C(14)	108.71(8)
O(1)-S(1)-C(14)	109.84(7)	C(2)-S(1)-C(14)	101.31(8)

Table 7. Torsion angles (°) with s.u.s in parentheses.

C(7)-C(2)-C(3)-C(4)	0.4(2)	S(1)-C(2)-C(3)-C(4)	-178.25(13)
C(2)-C(3)-C(4)-C(5)	-0.5(3)	C(3)-C(4)-C(5)-C(6)	0.1(3)
C(4)-C(5)-C(6)-C(7)	0.4(3)	C(5)-C(6)-C(7)-C(2)	-0.4(2)
C(5)-C(6)-C(7)-C(8)	-177.28(16)	C(3)-C(2)-C(7)-C(6)	0.1(2)
S(1)-C(2)-C(7)-C(6)	178.71(12)	C(3)-C(2)-C(7)-C(8)	176.84(15)
S(1)-C(2)-C(7)-C(8)	-4.5(2)	C(6)-C(7)-C(8)-C(81)	-91.71(18)
C(2)-C(7)-C(8)-C(81)	91.61(18)	C(6)-C(7)-C(8)-C(9)	141.46(16)
C(2)-C(7)-C(8)-C(9)	-35.2(2)	C(81)-C(8)-C(9)-C(10)	91.41(18)
C(7)-C(8)-C(9)-C(10)	-140.38(16)	C(81)-C(8)-C(9)-C(14)	-91.58(18)
C(7)-C(8)-C(9)-C(14)	36.6(2)	C(14)-C(9)-C(10)-C(11)	-0.5(2)
C(8)-C(9)-C(10)-C(11)	176.60(15)	C(9)-C(10)-C(11)-C(12)	0.3(3)
C(10)-C(11)-C(12)-C(13)	-0.3(3)	C(11)-C(12)-C(13)-C(14)	0.6(2)
C(12)-C(13)-C(14)-C(9)	-0.9(2)	C(12)-C(13)-C(14)-S(1)	-178.95(13)
C(10)-C(9)-C(14)-C(13)	0.8(2)	C(8)-C(9)-C(14)-C(13)	-176.23(15)
C(10)-C(9)-C(14)-S(1)	178.91(12)	C(8)-C(9)-C(14)-S(1)	1.8(2)
C(9)-C(8)-C(81)-C(93)	13.2(3)	C(7)-C(8)-C(81)-C(93)	-114.6(2)
C(9)-C(8)-C(81)-O(82)	-163.87(13)	C(7)-C(8)-C(81)-O(82)	68.28(18)
O(82)-C(83)-C(84)-C(85)	175.23(15)	C(92)-C(83)-C(84)-C(85)	-2.6(3)
C(83)-C(84)-C(85)-C(86)	0.5(3)	C(84)-C(85)-C(86)-C(87)	-177.77(16)
C(84)-C(85)-C(86)-C(91)	1.8(3)	C(91)-C(86)-C(87)-C(88)	0.4(2)
C(85)-C(86)-C(87)-C(88)	179.99(16)	C(86)-C(87)-C(88)-C(89)	0.1(3)
C(87)-C(88)-C(89)-C(90)	0.2(3)	C(88)-C(89)-C(90)-C(91)	-1.1(3)
C(89)-C(90)-C(91)-C(86)	1.6(2)	C(89)-C(90)-C(91)-C(92)	-177.00(16)
C(87)-C(86)-C(91)-C(90)	-1.3(2)	C(85)-C(86)-C(91)-C(90)	179.17(15)
C(87)-C(86)-C(91)-C(92)	177.42(15)	C(85)-C(86)-C(91)-C(92)	-2.2(2)
O(82)-C(83)-C(92)-C(91)	-175.90(14)	C(84)-C(83)-C(92)-C(91)	2.2(3)
O(82)-C(83)-C(92)-C(93)	0.63(18)	C(84)-C(83)-C(92)-C(93)	178.69(16)
C(90)-C(91)-C(92)-C(83)	178.90(15)	C(86)-C(91)-C(92)-C(83)	0.3(2)
C(90)-C(91)-C(92)-C(93)	3.6(3)	C(86)-C(91)-C(92)-C(93)	-175.02(17)
O(82)-C(81)-C(93)-C(92)	0.89(19)	C(8)-C(81)-C(93)-C(92)	-176.26(17)
C(83)-C(92)-C(93)-C(81)	-0.91(18)	C(91)-C(92)-C(93)-C(81)	174.83(18)
C(92)-C(83)-O(82)-C(81)	-0.11(17)	C(84)-C(83)-O(82)-C(81)	-178.16(16)
C(93)-C(81)-O(82)-C(83)	-0.50(18)	C(8)-C(81)-O(82)-C(83)	177.24(13)
C(3)-C(2)-S(1)-O(2)	-29.02(15)	C(7)-C(2)-S(1)-O(2)	152.29(13)
C(3)-C(2)-S(1)-O(1)	100.39(14)	C(7)-C(2)-S(1)-O(1)	-78.30(14)
C(3)-C(2)-S(1)-C(14)	-144.21(13)	C(7)-C(2)-S(1)-C(14)	37.10(14)
C(13)-C(14)-S(1)-O(2)	25.58(15)	C(9)-C(14)-S(1)-O(2)	-152.56(13)
C(13)-C(14)-S(1)-O(1)	-103.70(14)	C(9)-C(14)-S(1)-O(1)	78.16(14)
C(13)-C(14)-S(1)-C(2)	142.28(13)	C(9)-C(14)-S(1)-C(2)	-35.86(14)



View of compound **6**. Ellipsoid probability: 50%.

Table 1. Crystal data and structure refinement for *trans*-sulfoxide (**11**) (CCDC663292)

Formula	$C_{25}H_{16}O_2S$	
Formula weight	380.44	
Size	0.29 x 0.26 x 0.21 mm	
Crystal morphology	Pale brown fragment	
Temperature	150K	
Wavelength	0.71073 Å [Mo-K_α]	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	*a* = 19.3719(8) Å	α = 90°
	b = 11.5100(5) Å	β = 99.926(2)°
	c = 16.4409(6) Å	γ = 90°
Volume	3611.0(3) Å^3	
Z	8	
Density (calculated)	1.4 Mg/m^3	
Absorption coefficient	0.198 mm^{-1}	
F(000)	1584	
Data collection range	$2.32 \le \theta \le 28.3°$	
Index ranges	$-25 \le h \le 25$, $-15 \le k \le 15$, $-18 \le l \le 21$	
Reflections collected	29976	
Independent reflections	4465 [*R*(int) = 0.0437]	
Observed reflections	3671 [$I > 2\sigma(I)$]	
Absorption correction	none	
Refinement method	Full	
Data / restraints / parameters	4465 / 0 / 253	
Goodness of fit	1.025	
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0370, wR_2 = 0.0875	
R indices (all data)	R_1 = 0.0486, wR_2 = 0.0936	
Largest diff. peak and hole	0.309 and -0.541e.Å^{-3}	

Table 2. Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^4) with standard uncertainties (s.u.s) in parentheses. U_{eq} is defined as $^1/_3$ of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
S(1)	40111.4(18)	63846(3)	14996(2)	207.8(10)
O(15)	40050(5)	39201(8)	21656(6)	189(2)
C(2)	38939(7)	63744(12)	25552(8)	205(3)
C(16)	40353(7)	27615(11)	19756(8)	184(3)
O(1)	39697(6)	76173(9)	12188(7)	332(3)
C(7)	35791(7)	54362(12)	28826(8)	205(3)
C(17)	45482(7)	24407(11)	15004(8)	197(3)
C(9)	29334(7)	47862(11)	15067(8)	190(3)
C(14)	31891(7)	57117(11)	10960(8)	183(3)
C(25)	36162(7)	19587(12)	22749(9)	244(3)
C(18)	49577(7)	32629(12)	11557(9)	221(3)
C(8)	33418(7)	43876(11)	23385(8)	197(3)
C(27)	29510(7)	35077(13)	27616(9)	260(3)
C(26)	30882(8)	23829(13)	27307(10)	284(3)
C(10)	23252(7)	42396(13)	11221(9)	258(3)
C(3)	41629(8)	73144(13)	30391(9)	267(3)
C(24)	37233(9)	7643(13)	21263(10)	315(4)
C(13)	28409(7)	61113(12)	3411(9)	223(3)
C(6)	35218(8)	54808(14)	37137(9)	297(3)
C(22)	46405(8)	12325(12)	13615(9)	258(3)
C(12)	22276(8)	55646(13)	-261(9)	268(3)
C(11)	19785(8)	46257(14)	3570(10)	301(3)
C(19)	54298(8)	29004(14)	6784(9)	284(3)
C(21)	51530(9)	9032(14)	8865(10)	339(4)
C(23)	42216(9)	4093(12)	16907(10)	319(4)
C(5)	37853(9)	64183(16)	42012(10)	360(4)
C(20)	55291(9)	17107(15)	5468(10)	347(4)
C(4)	41113(9)	73225(15)	38698(10)	333(4)

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3). The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	237.0(18)	189.5(16)	206.2(18)	5.8(13)	64.5(13)	-34.5(13)
O(15)	167(4)	151(4)	260(5)	15(4)	66(4)	8(3)
C(2)	198(6)	216(6)	202(7)	-13(5)	34(5)	51(5)
C(16)	206(6)	155(6)	172(6)	22(5)	-21(5)	-1(5)
O(1)	482(7)	211(5)	296(6)	53(4)	44(5)	-92(5)
C(7)	200(6)	233(7)	185(7)	8(5)	40(5)	55(5)
C(17)	218(6)	181(6)	169(6)	-16(5)	-34(5)	14(5)
C(9)	184(6)	191(6)	207(7)	3(5)	63(5)	29(5)
C(14)	190(6)	182(6)	189(6)	-24(5)	67(5)	19(5)
C(25)	250(7)	213(7)	246(7)	55(6)	-22(6)	-56(5)
C(18)	214(7)	232(6)	211(7)	-30(5)	19(5)	11(5)
C(8)	178(6)	205(6)	218(7)	38(5)	67(5)	16(5)
C(27)	199(7)	321(8)	274(8)	94(6)	79(6)	-14(6)
C(26)	239(7)	312(8)	295(8)	128(6)	32(6)	-85(6)
C(10)	212(7)	279(7)	287(8)	28(6)	54(6)	-26(6)
C(3)	251(7)	245(7)	291(8)	-55(6)	3(6)	32(6)
C(24)	383(9)	196(7)	324(8)	62(6)	-59(7)	-103(6)
C(13)	264(7)	226(7)	194(7)	15(5)	85(5)	45(5)
C(6)	312(8)	383(9)	206(7)	44(6)	69(6)	55(6)
C(22)	340(8)	206(7)	183(7)	-47(5)	-78(6)	42(6)
C(12)	255(7)	350(8)	193(7)	9(6)	18(6)	58(6)
C(11)	218(7)	380(9)	288(8)	-11(7)	-2(6)	-28(6)
C(19)	268(7)	361(8)	225(7)	-35(6)	48(6)	35(6)
C(21)	485(10)	276(8)	220(8)	-88(6)	-37(7)	141(7)
C(23)	465(9)	154(6)	286(8)	-28(6)	-85(7)	-13(6)
C(5)	399(9)	494(10)	180(7)	-46(7)	31(6)	123(8)
C(20)	382(9)	424(9)	228(8)	-74(7)	37(7)	153(7)
C(4)	340(8)	358(8)	273(8)	-125(7)	-26(6)	80(7)

Table 4. Hydrogen atom co-ordinates (x 10^3) and isotropic displacement parameters ($Å^2$ x 10^2) with s.u.s in parentheses.

	x	y	z	U_{eq}
H(18)	4905.	4068.	1256.	27.
H(27)	2599.	3764.	3057.	31.
H(26)	2838.	1847.	3010.	34.
H(10)	2144.	3598.	1382.	31.
H(3)	4379.	7942.	2804.	32.
H(24)	3441.	200.	2335.	38.
H(13)	3020.	6752.	78.	27.
H(6)	3300.	4862.	3951.	36.
H(12)	1980.	5836.	-540.	32.
H(11)	1566.	4238.	96.	36.
H(19)	5692.	3458.	434.	34.
H(21)	5236.	102.	804.	41.
H(23)	4289.	-397.	1607.	38.
H(5)	3741.	6437.	4767.	43.
H(20)	5861.	1469.	218.	42.
H(4)	4301.	7952.	4210.	40.

Table 5. Interatomic distances (Å) with s.u.s in parentheses.

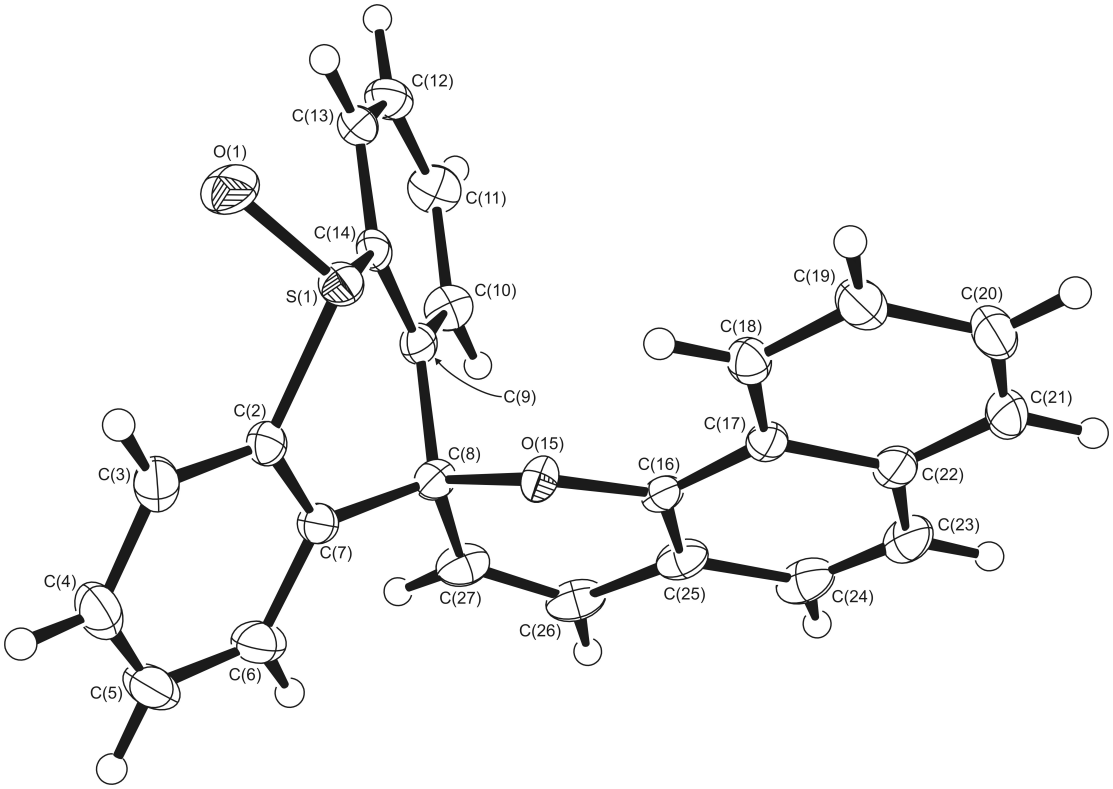
S(1)-O(1)	1.4900(11)	S(1)-C(2)	1.7887(14)
S(1)-C(14)	1.7922(14)	O(15)-C(16)	1.3731(15)
O(15)-C(8)	1.4652(16)	C(2)-C(3)	1.3900(19)
C(2)-C(7)	1.393(2)	C(16)-C(25)	1.3758(19)
C(16)-C(17)	1.415(2)	C(7)-C(6)	1.391(2)
C(7)-C(8)	1.5253(19)	C(17)-C(18)	1.415(2)
C(17)-C(22)	1.4255(18)	C(9)-C(10)	1.3881(19)
C(9)-C(14)	1.3969(19)	C(9)-C(8)	1.5276(18)
C(14)-C(13)	1.3851(19)	C(25)-C(24)	1.418(2)
C(25)-C(26)	1.453(2)	C(18)-C(19)	1.369(2)
C(8)-C(27)	1.5049(19)	C(27)-C(26)	1.324(2)
C(10)-C(11)	1.393(2)	C(3)-C(4)	1.387(2)
C(24)-C(23)	1.360(3)	C(13)-C(12)	1.387(2)
C(6)-C(5)	1.388(2)	C(22)-C(23)	1.415(2)
C(22)-C(21)	1.416(2)	C(12)-C(11)	1.379(2)
C(19)-C(20)	1.405(2)	C(21)-C(20)	1.359(3)
C(5)-C(4)	1.377(3)		

Table 6. Angles between interatomic vectors (°) with s.u.s in parentheses.

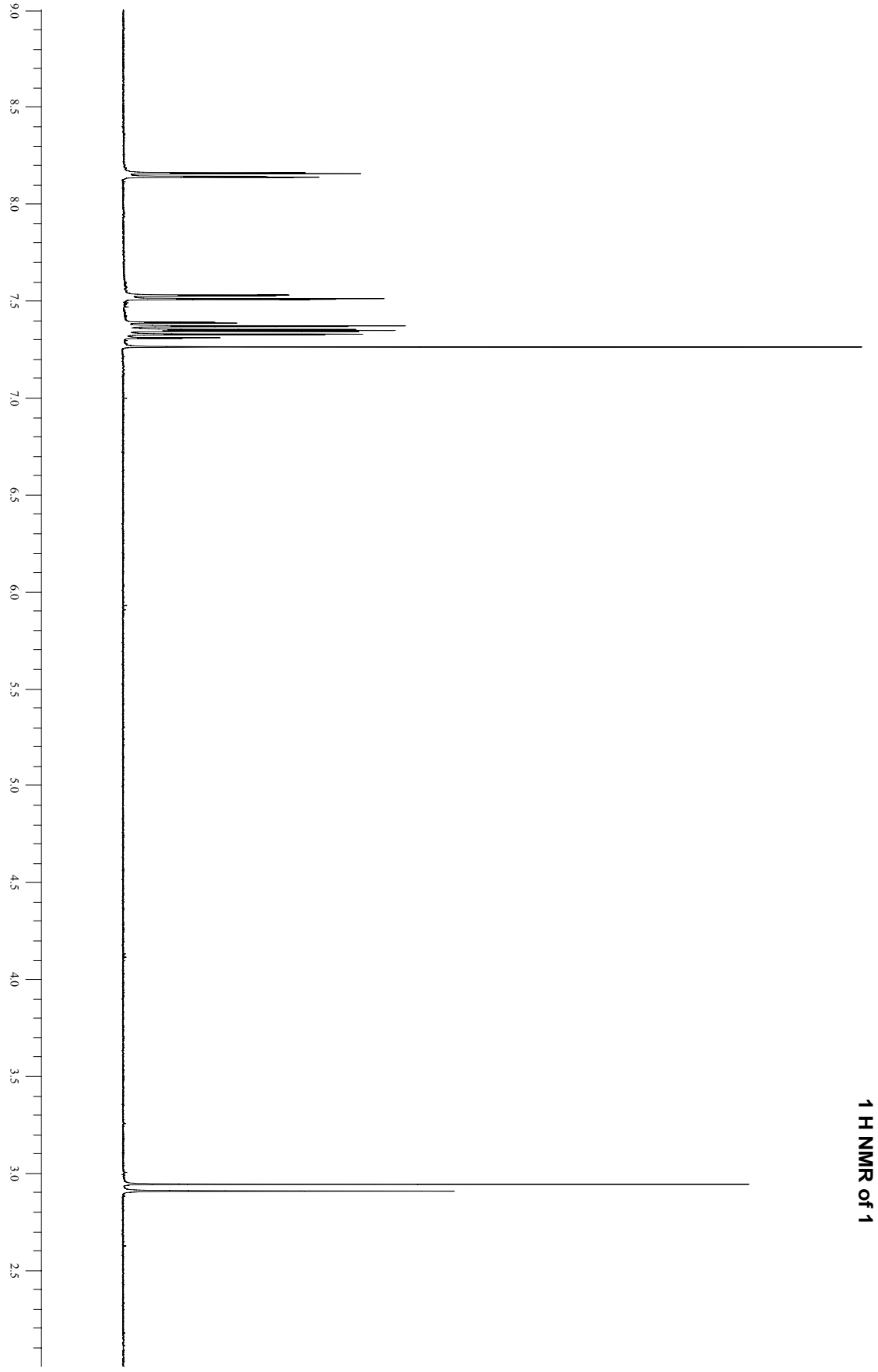
O(1)-S(1)-C(2)	107.33(6)	O(1)-S(1)-C(14)	107.45(6)
C(2)-S(1)-C(14)	95.92(6)	C(16)-O(15)-C(8)	118.30(10)
C(3)-C(2)-C(7)	121.88(14)	C(3)-C(2)-S(1)	116.90(11)
C(7)-C(2)-S(1)	121.14(10)	O(15)-C(16)-C(25)	121.33(13)
O(15)-C(16)-C(17)	116.15(11)	C(25)-C(16)-C(17)	122.42(13)
C(6)-C(7)-C(2)	117.74(13)	C(6)-C(7)-C(8)	122.57(13)
C(2)-C(7)-C(8)	119.63(12)	C(16)-C(17)-C(18)	122.84(12)
C(16)-C(17)-C(22)	117.56(13)	C(18)-C(17)-C(22)	119.60(13)
C(10)-C(9)-C(14)	117.99(12)	C(10)-C(9)-C(8)	122.66(12)
C(14)-C(9)-C(8)	119.31(12)	C(13)-C(14)-C(9)	121.86(13)
C(13)-C(14)-S(1)	116.92(10)	C(9)-C(14)-S(1)	121.14(10)
C(16)-C(25)-C(24)	118.47(15)	C(16)-C(25)-C(26)	118.04(13)
C(24)-C(25)-C(26)	123.49(14)	C(19)-C(18)-C(17)	120.13(14)
O(15)-C(8)-C(27)	111.74(11)	O(15)-C(8)-C(7)	102.64(10)
C(27)-C(8)-C(7)	112.72(12)	O(15)-C(8)-C(9)	105.83(10)
C(27)-C(8)-C(9)	113.06(11)	C(7)-C(8)-C(9)	110.16(11)
C(26)-C(27)-C(8)	121.32(14)	C(27)-C(26)-C(25)	120.81(13)
C(9)-C(10)-C(11)	120.41(14)	C(4)-C(3)-C(2)	119.03(15)
C(23)-C(24)-C(25)	121.35(14)	C(14)-C(13)-C(12)	119.18(13)
C(5)-C(6)-C(7)	120.81(15)	C(23)-C(22)-C(21)	122.32(14)
C(23)-C(22)-C(17)	119.74(14)	C(21)-C(22)-C(17)	117.95(14)
C(11)-C(12)-C(13)	119.84(13)	C(12)-C(11)-C(10)	120.68(14)
C(18)-C(19)-C(20)	120.54(15)	C(20)-C(21)-C(22)	121.32(14)
C(24)-C(23)-C(22)	120.42(13)	C(4)-C(5)-C(6)	120.47(15)
C(21)-C(20)-C(19)	120.40(15)	C(5)-C(4)-C(3)	120.03(15)

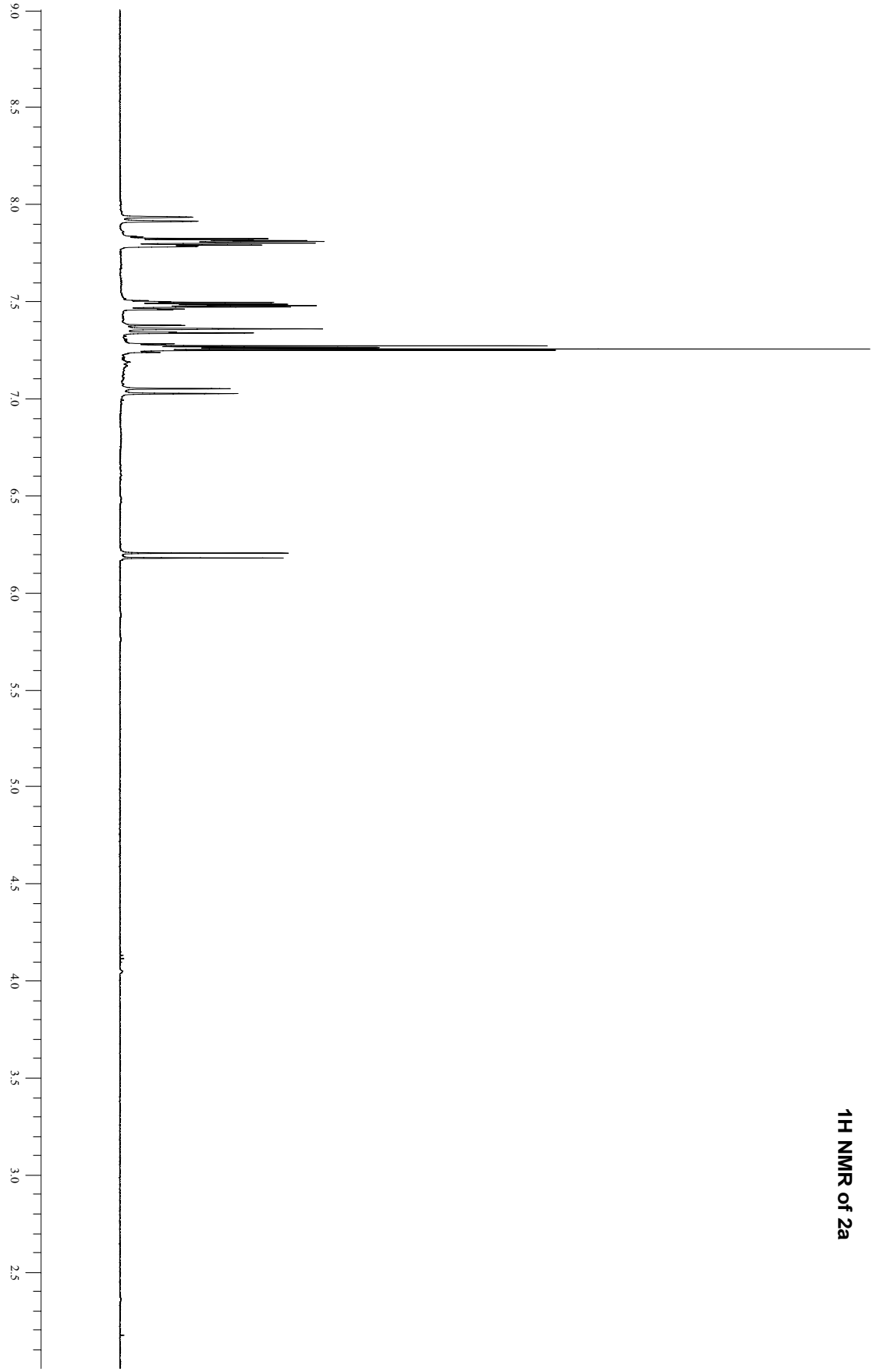
Table 7. Torsion angles (°) with s.u.s in parentheses.

O(1)-S(1)-C(2)-C(3)	-34.24(12)	C(14)-S(1)-C(2)-C(3)	-144.62(11)
O(1)-S(1)-C(2)-C(7)	148.95(11)	C(14)-S(1)-C(2)-C(7)	38.58(12)
C(8)-O(15)-C(16)-C(25)	-28.59(17)	C(8)-O(15)-C(16)-C(17)	155.09(11)
C(3)-C(2)-C(7)-C(6)	1.9(2)	S(1)-C(2)-C(7)-C(6)	178.50(10)
C(3)-C(2)-C(7)-C(8)	-175.47(12)	S(1)-C(2)-C(7)-C(8)	1.17(17)
O(15)-C(16)-C(17)-C(18)	-6.94(18)	C(25)-C(16)-C(17)-C(18)	176.79(13)
O(15)-C(16)-C(17)-C(22)	173.95(11)	C(25)-C(16)-C(17)-C(22)	-2.32(19)
C(10)-C(9)-C(14)-C(13)	2.3(2)	C(8)-C(9)-C(14)-C(13)	-179.92(12)
C(10)-C(9)-C(14)-S(1)	-174.31(10)	C(8)-C(9)-C(14)-S(1)	3.51(17)
O(1)-S(1)-C(14)-C(13)	31.97(12)	C(2)-S(1)-C(14)-C(13)	142.25(11)
O(1)-S(1)-C(14)-C(9)	-151.30(11)	C(2)-S(1)-C(14)-C(9)	-41.03(12)
O(15)-C(16)-C(25)-C(24)	-173.61(12)	C(17)-C(16)-C(25)-C(24)	2.5(2)
O(15)-C(16)-C(25)-C(26)	6.13(19)	C(17)-C(16)-C(25)-C(26)	-177.78(12)
C(16)-C(17)-C(18)-C(19)	-177.82(13)	C(22)-C(17)-C(18)-C(19)	1.3(2)
C(16)-O(15)-C(8)-C(27)	33.83(16)	C(16)-O(15)-C(8)-C(7)	154.86(10)
C(16)-O(15)-C(8)-C(9)	-89.63(13)	C(6)-C(7)-C(8)-O(15)	-111.96(14)
C(2)-C(7)-C(8)-O(15)	65.23(14)	C(6)-C(7)-C(8)-C(27)	8.39(18)
C(2)-C(7)-C(8)-C(27)	-174.41(12)	C(6)-C(7)-C(8)-C(9)	135.69(13)
C(2)-C(7)-C(8)-C(9)	-47.11(16)	C(10)-C(9)-C(8)-O(15)	111.86(14)
C(14)-C(9)-C(8)-O(15)	-65.85(15)	C(10)-C(9)-C(8)-C(27)	-10.76(19)
C(14)-C(9)-C(8)-C(27)	171.53(12)	C(10)-C(9)-C(8)-C(7)	-137.87(13)
C(14)-C(9)-C(8)-C(7)	44.41(16)	O(15)-C(8)-C(27)-C(26)	-19.60(19)
C(7)-C(8)-C(27)-C(26)	-134.58(14)	C(9)-C(8)-C(27)-C(26)	99.67(16)
C(8)-C(27)-C(26)-C(25)	-0.9(2)	C(16)-C(25)-C(26)-C(27)	8.9(2)
C(24)-C(25)-C(26)-C(27)	-171.36(14)	C(14)-C(9)-C(10)-C(11)	-1.2(2)
C(8)-C(9)-C(10)-C(11)	-178.95(13)	C(7)-C(2)-C(3)-C(4)	-0.5(2)
S(1)-C(2)-C(3)-C(4)	-177.30(11)	C(16)-C(25)-C(24)-C(23)	-0.7(2)
C(26)-C(25)-C(24)-C(23)	179.52(14)	C(9)-C(14)-C(13)-C(12)	-1.2(2)
S(1)-C(14)-C(13)-C(12)	175.47(10)	C(2)-C(7)-C(6)-C(5)	-1.5(2)
C(8)-C(7)-C(6)-C(5)	175.76(14)	C(16)-C(17)-C(22)-C(23)	0.47(19)
C(18)-C(17)-C(22)-C(23)	-178.67(12)	C(16)-C(17)-C(22)-C(21)	-179.99(12)
C(18)-C(17)-C(22)-C(21)	0.87(19)	C(14)-C(13)-C(12)-C(11)	-0.9(2)
C(13)-C(12)-C(11)-C(10)	1.9(2)	C(9)-C(10)-C(11)-C(12)	-0.8(2)
C(17)-C(18)-C(19)-C(20)	-2.0(2)	C(23)-C(22)-C(21)-C(20)	177.18(14)
C(17)-C(22)-C(21)-C(20)	-2.3(2)	C(25)-C(24)-C(23)-C(22)	-1.0(2)
C(21)-C(22)-C(23)-C(24)	-178.36(14)	C(17)-C(22)-C(23)-C(24)	1.2(2)
C(7)-C(6)-C(5)-C(4)	-0.2(2)	C(22)-C(21)-C(20)-C(19)	1.7(2)
C(18)-C(19)-C(20)-C(21)	0.6(2)	C(6)-C(5)-C(4)-C(3)	1.6(2)
C(2)-C(3)-C(4)-C(5)	-1.2(2)		

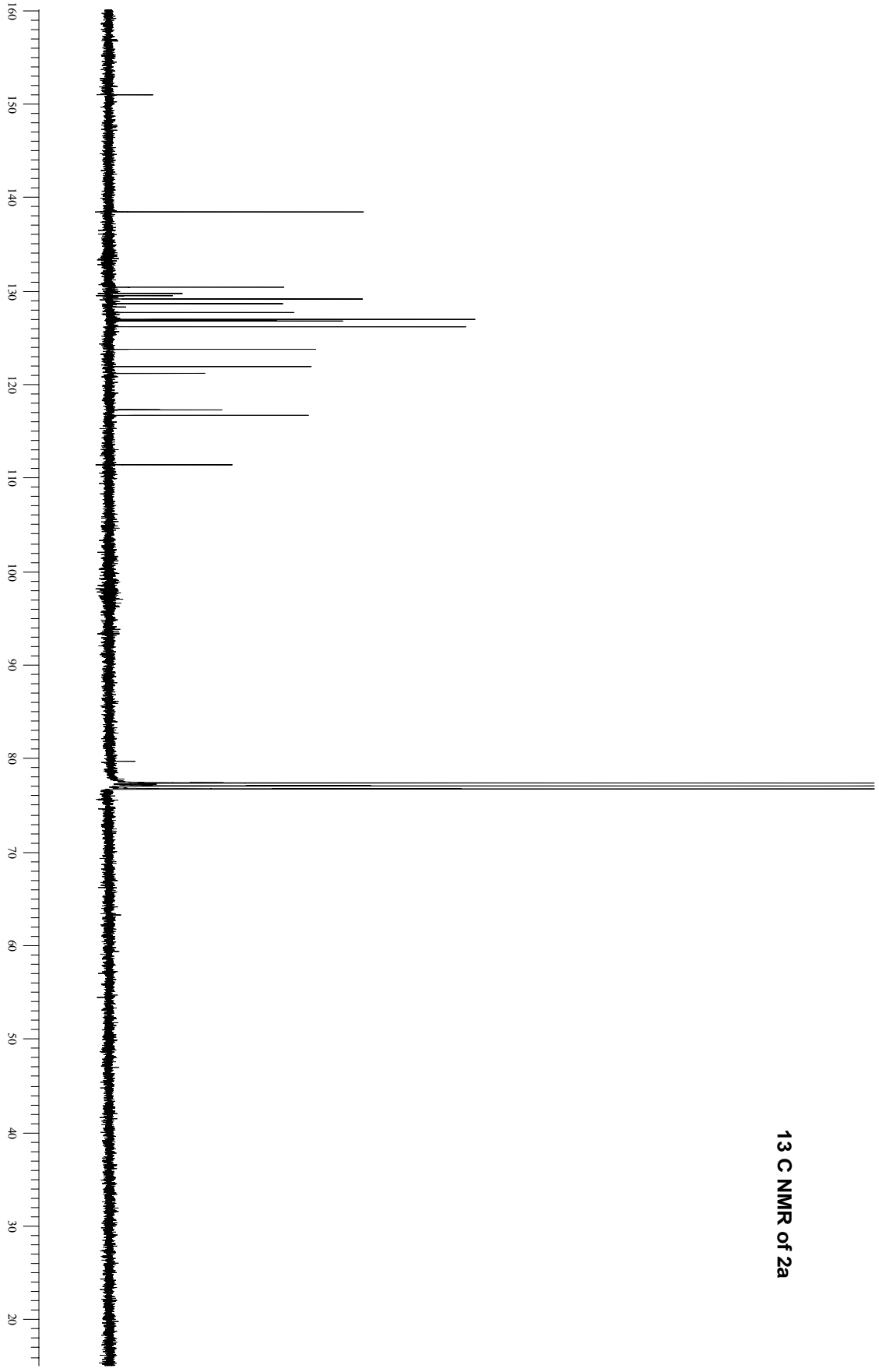


View of *trans*-sulfoxide (**11**). Ellipsoid probability: 50%.

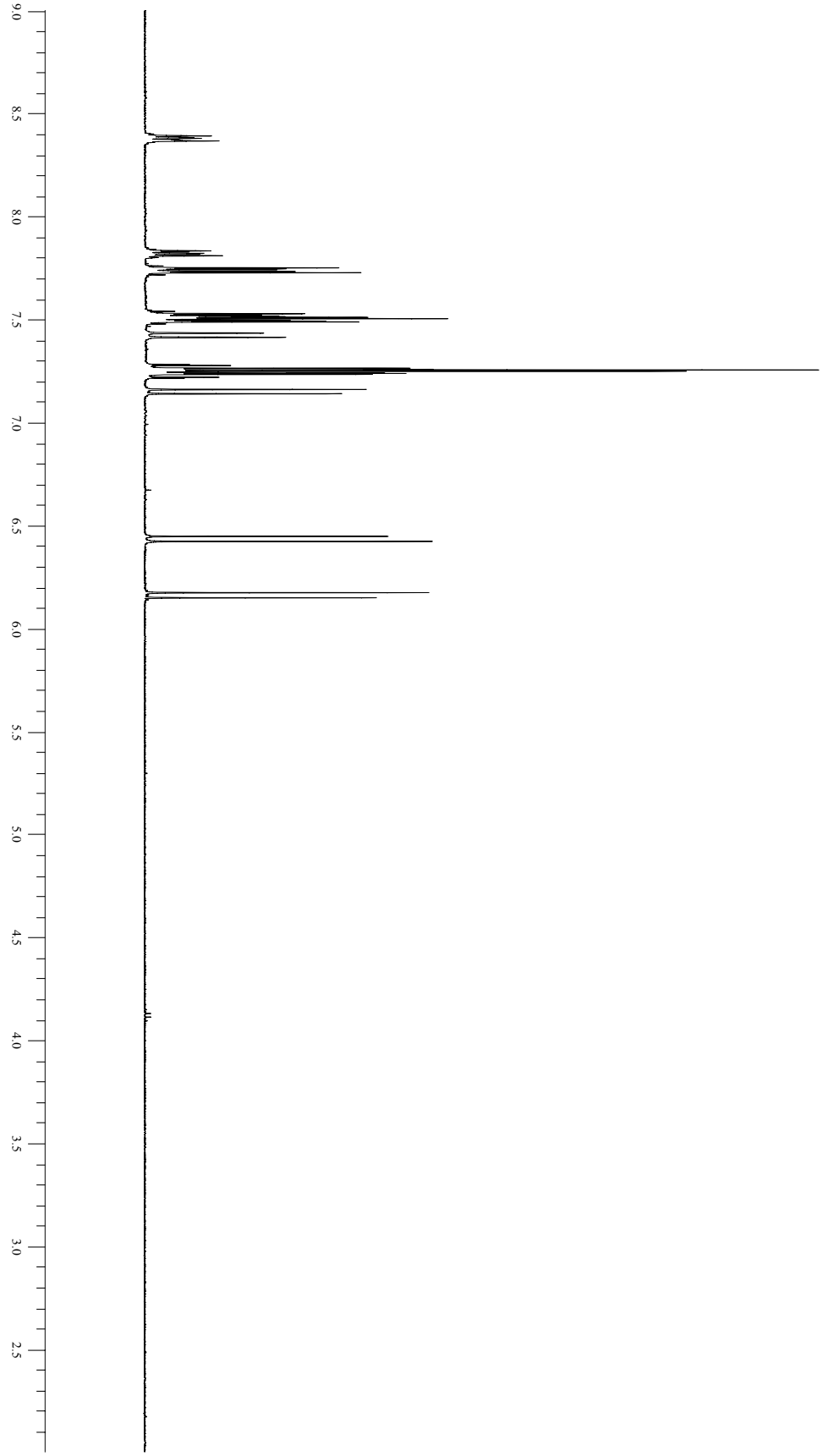




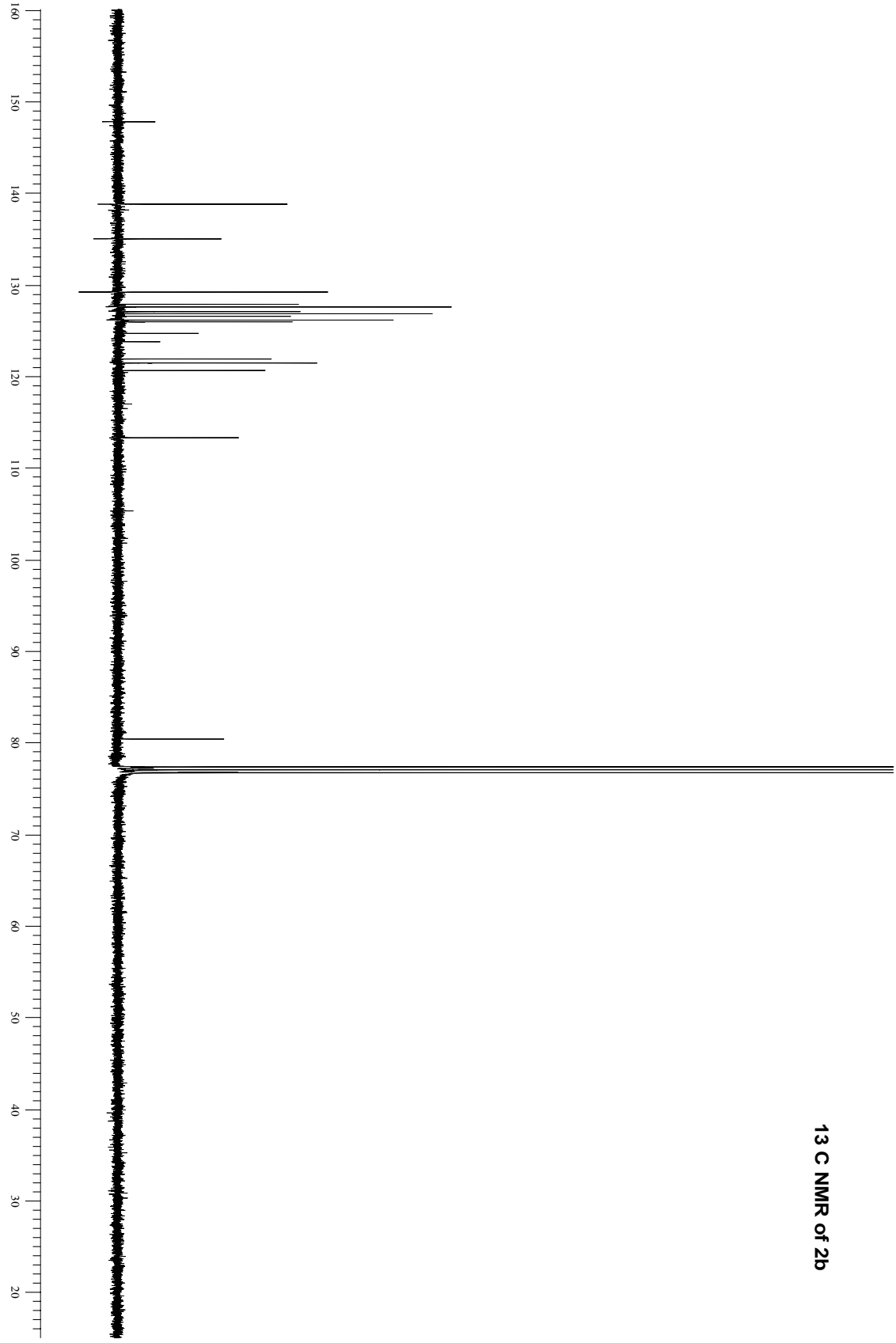
1H NMR of 2a



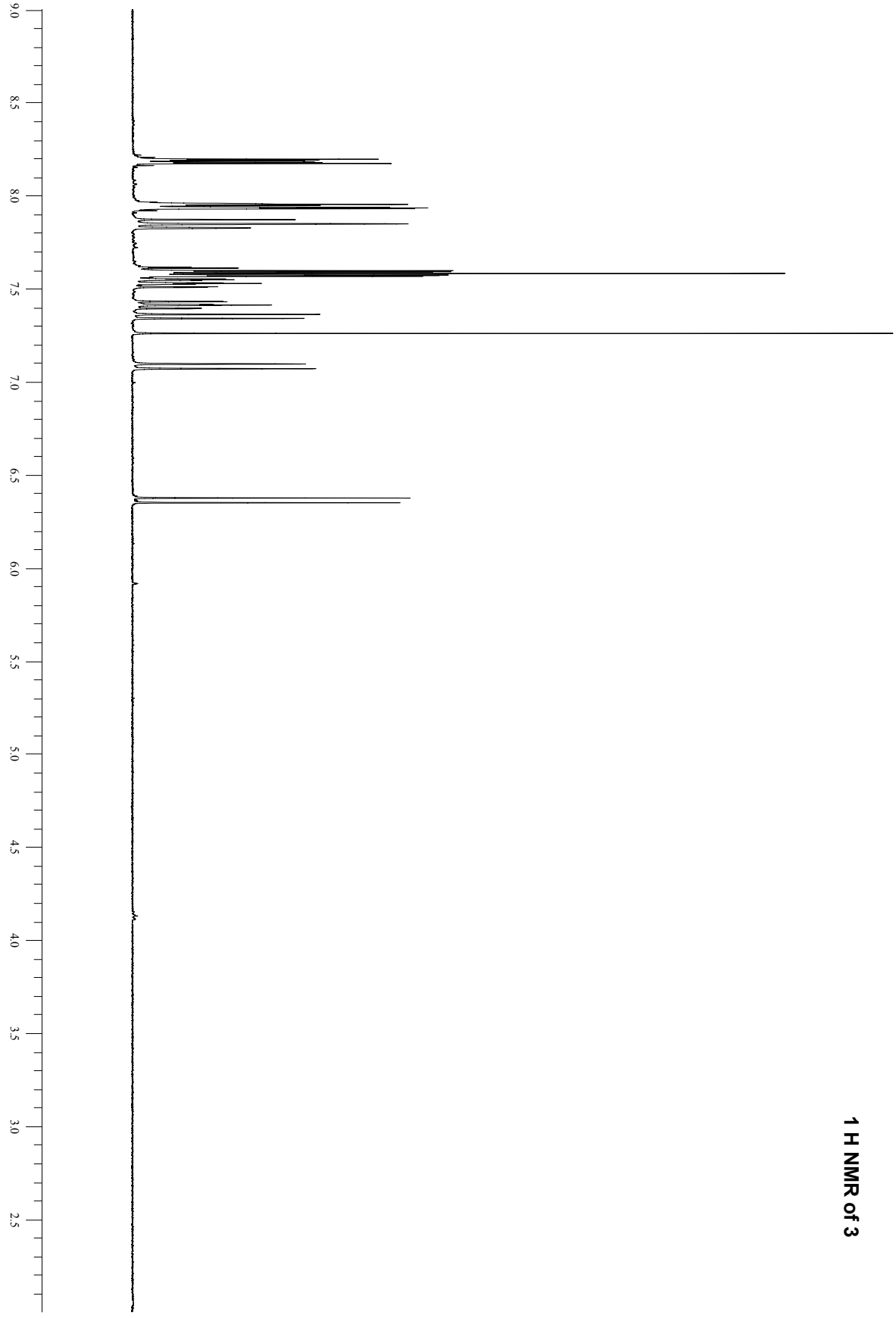
13 C NMR of 2a



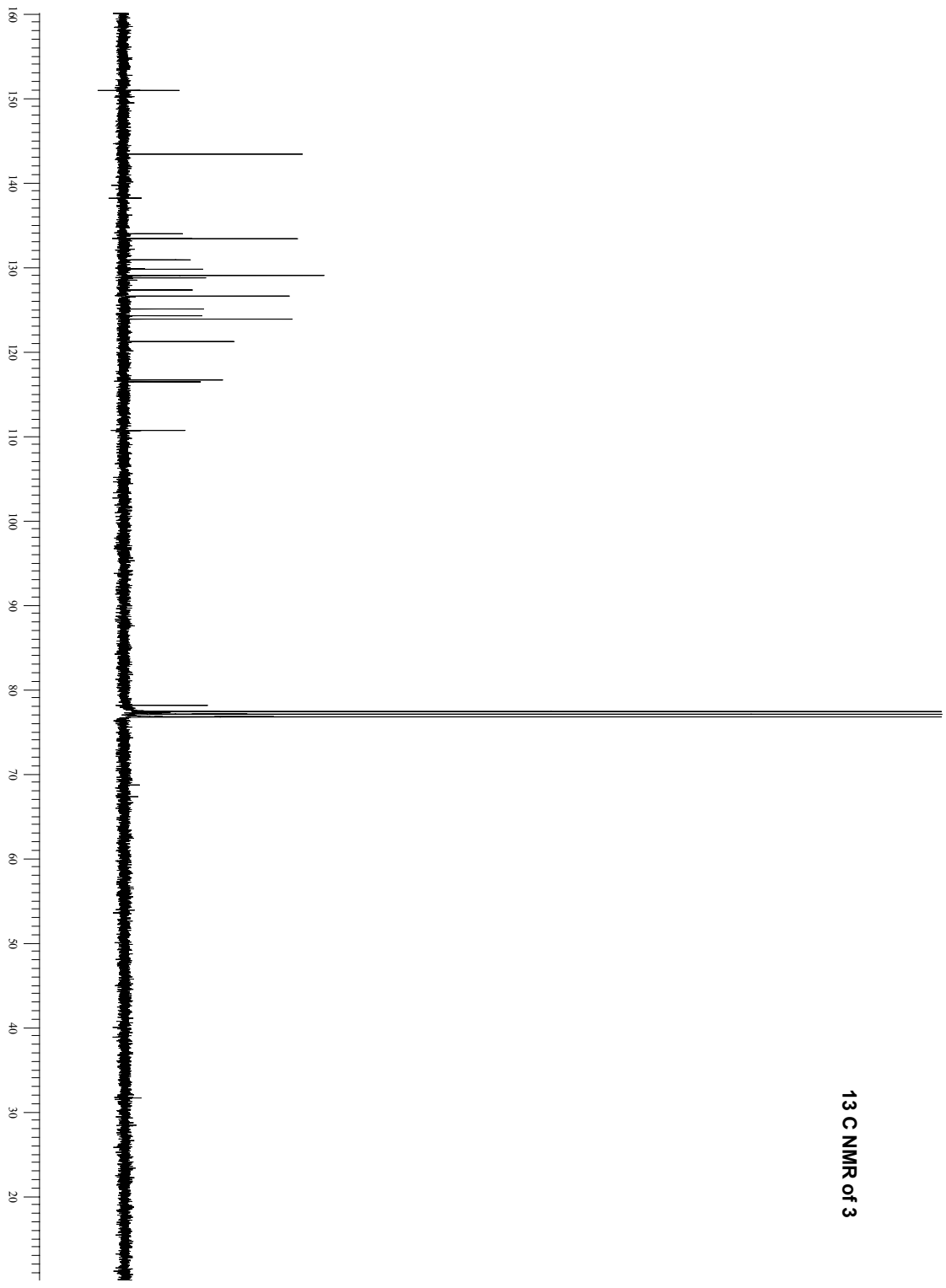
1H NMR of 2b

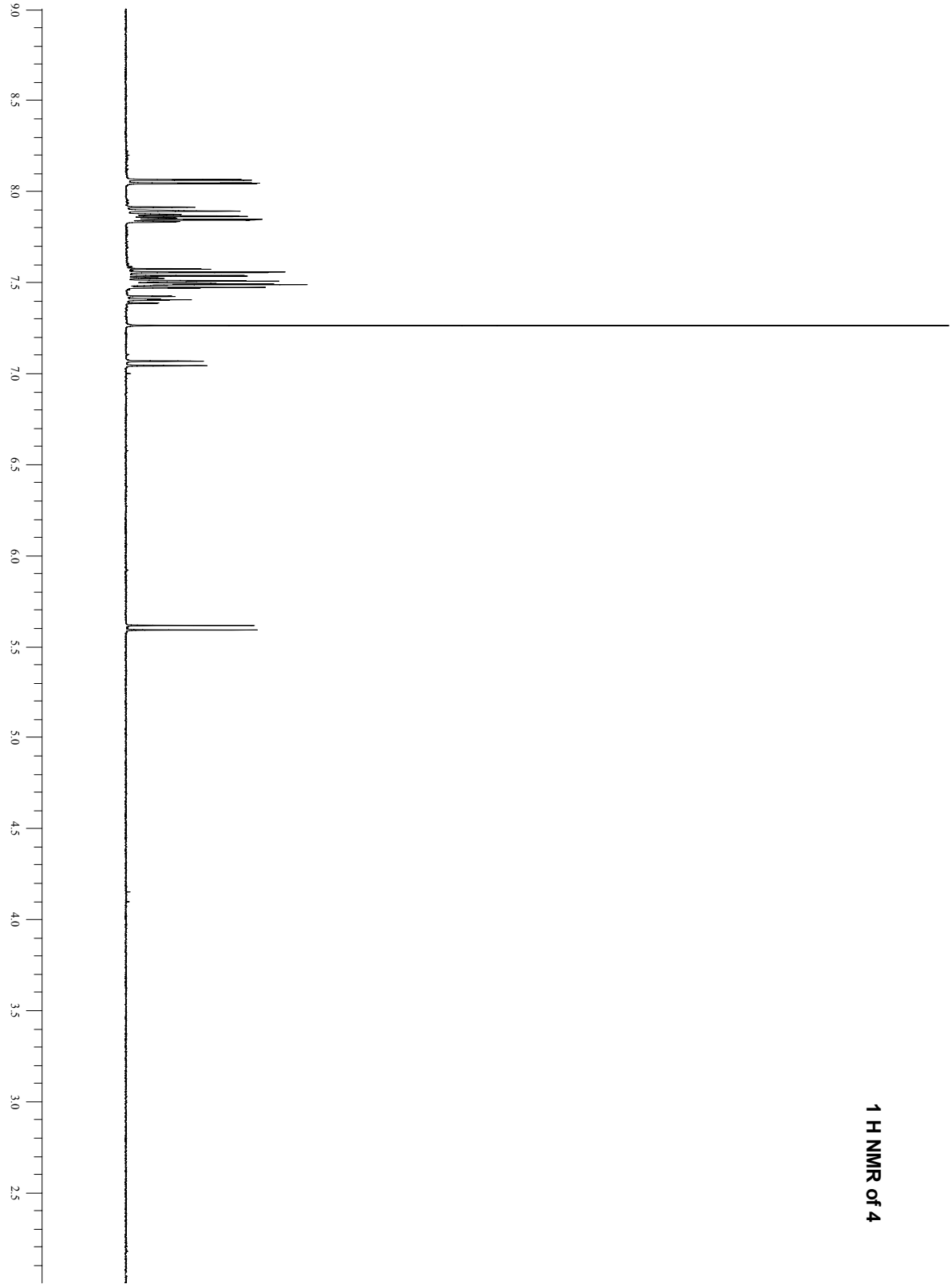


13 C NMR of 2b

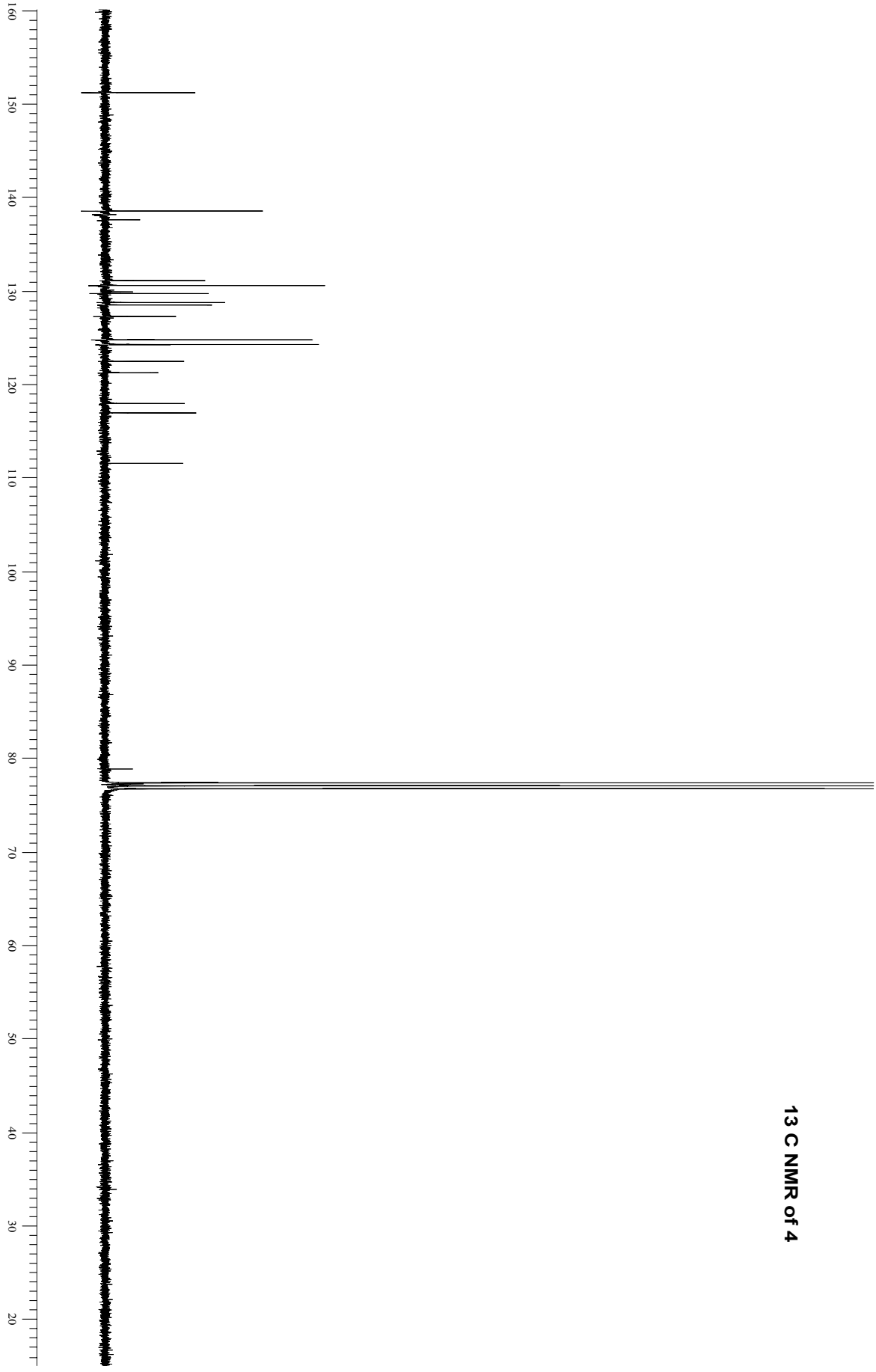


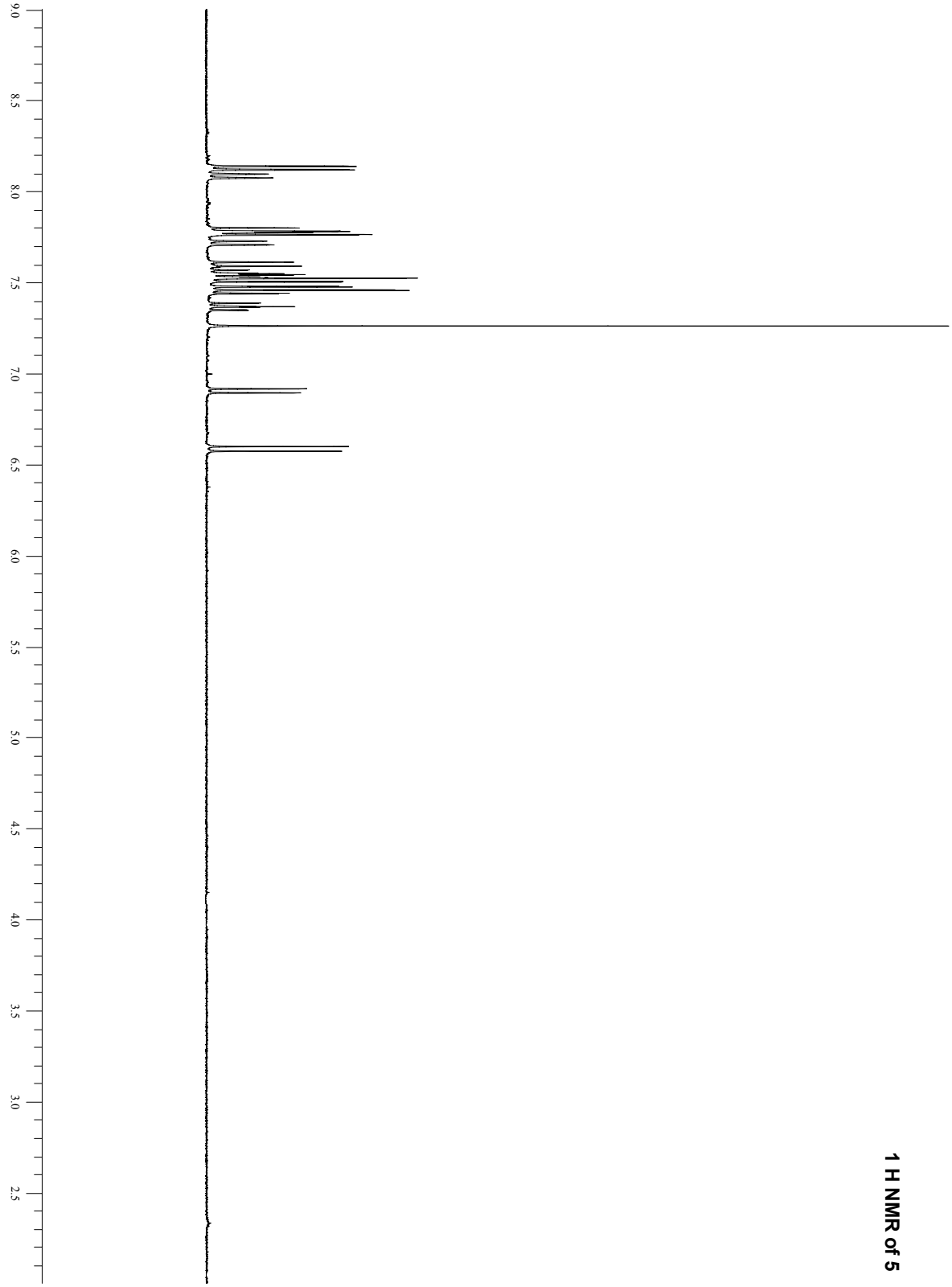
1 H NMR of 3



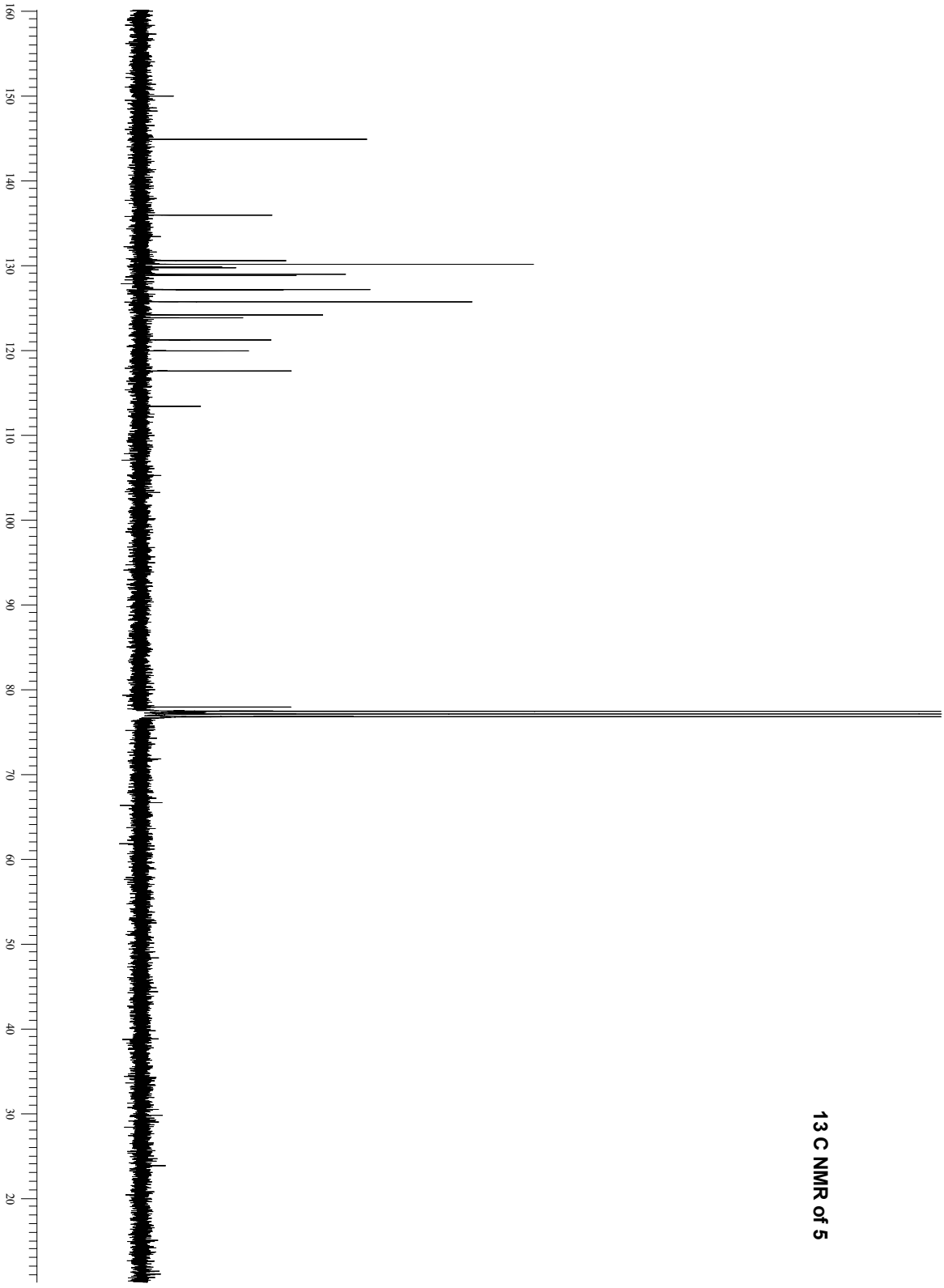


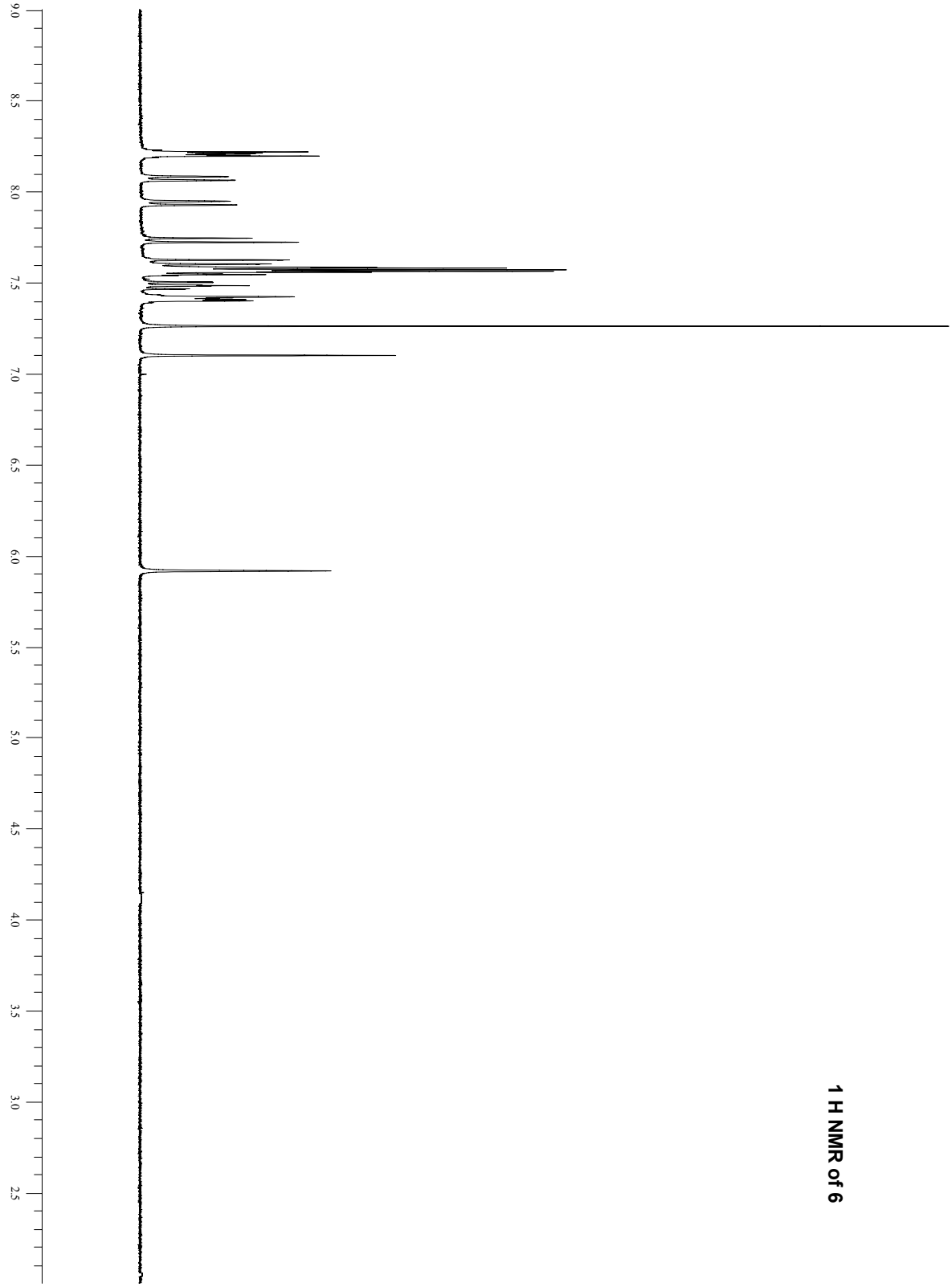
1 H NMR of 4



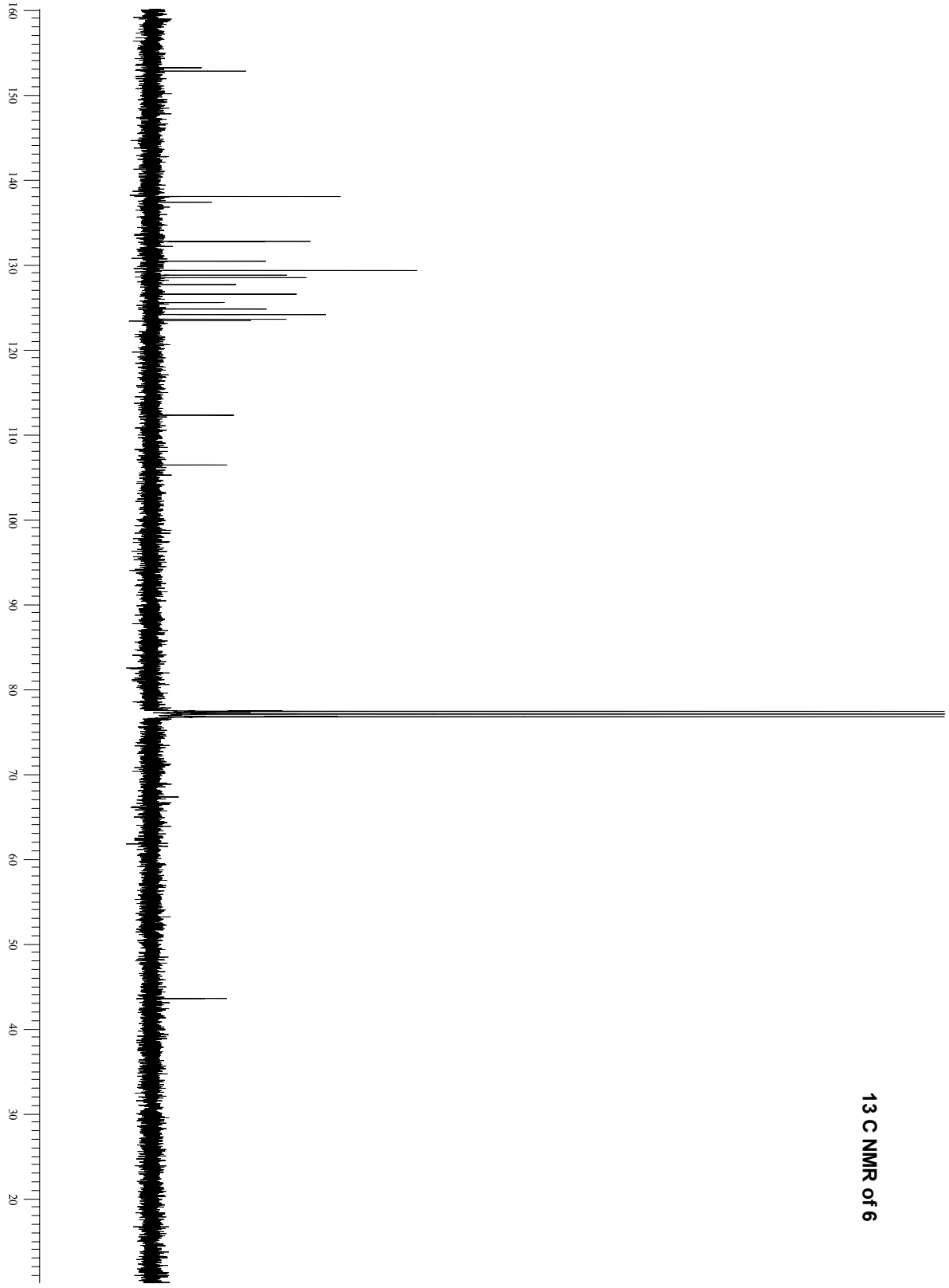


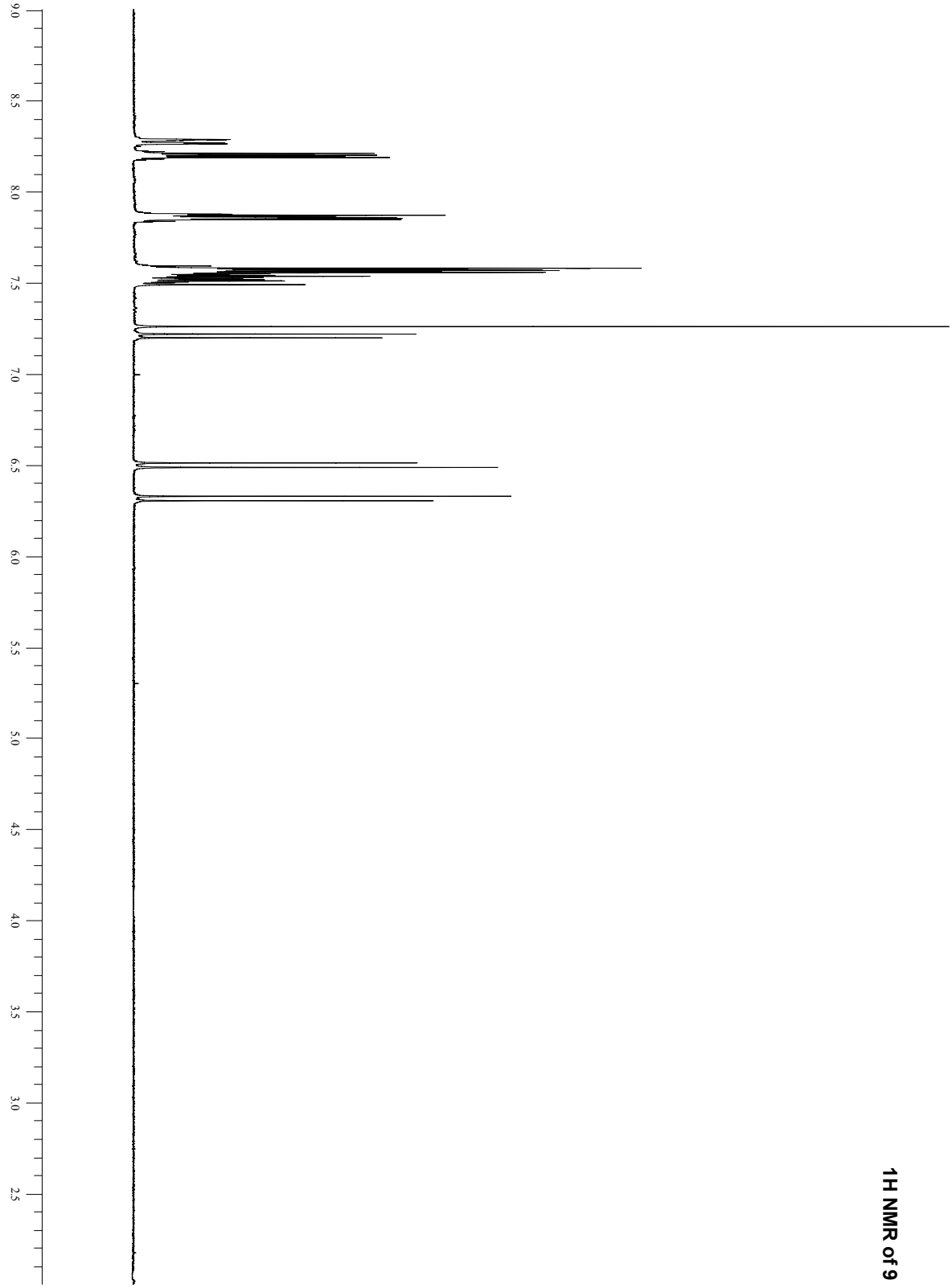
1 H NMR of 5

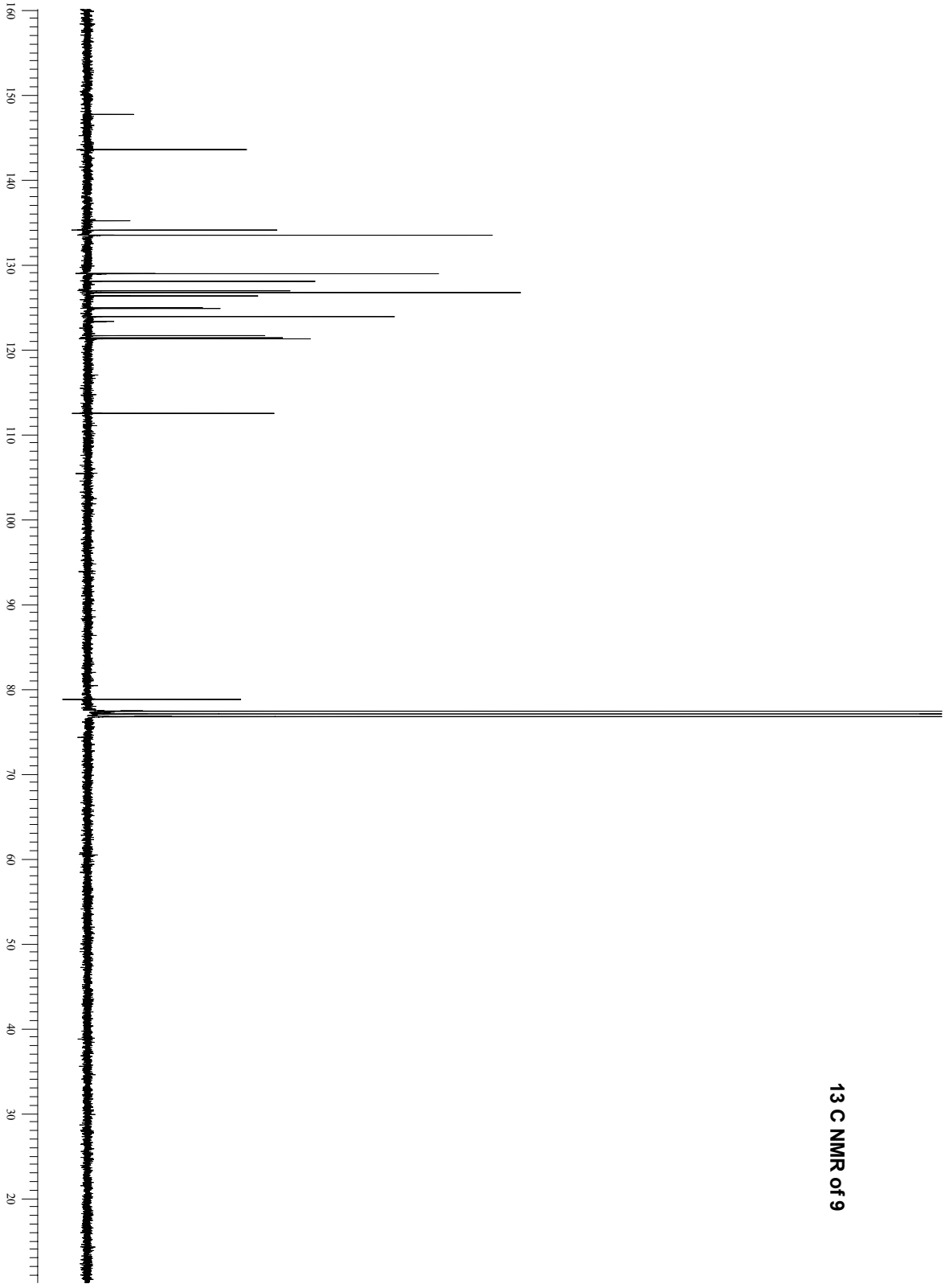


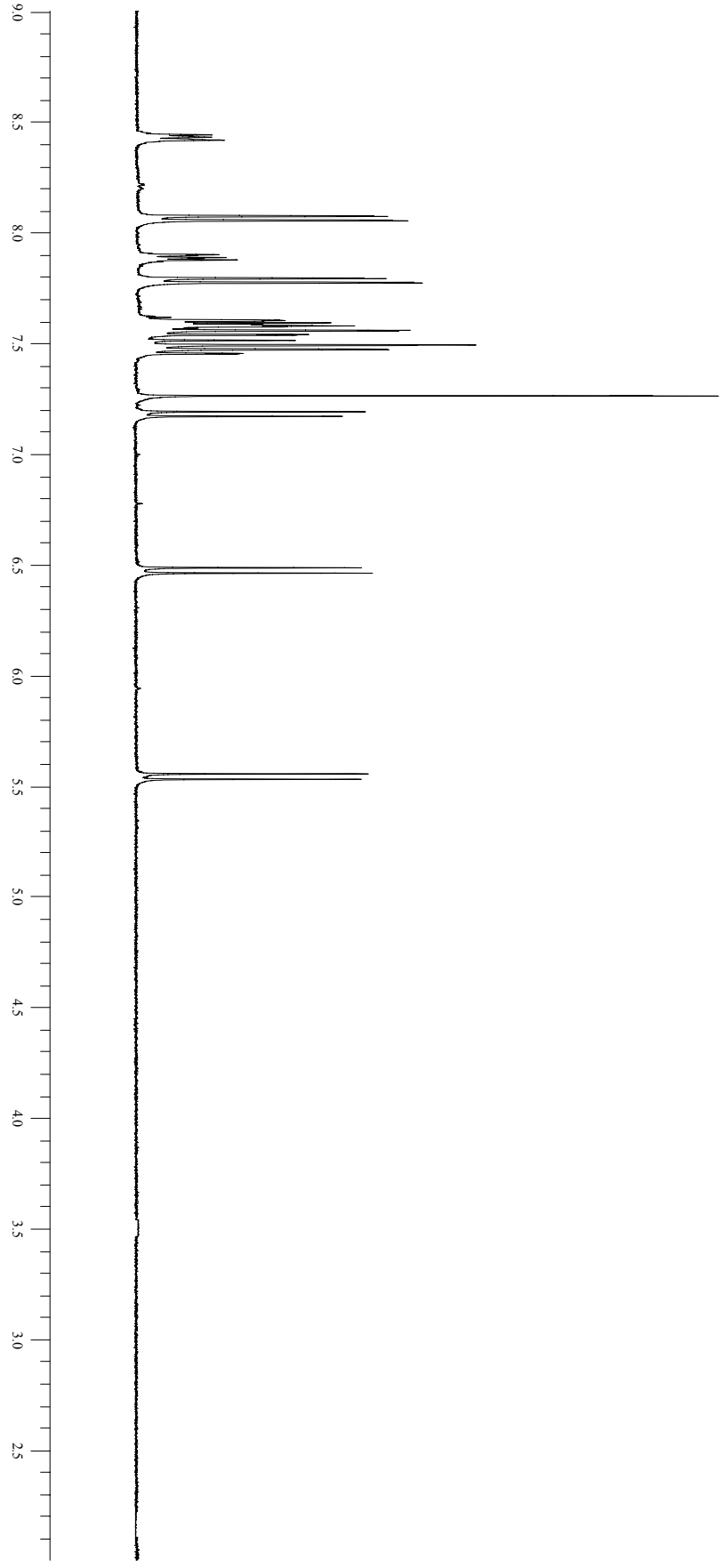


1 H NMR of 6

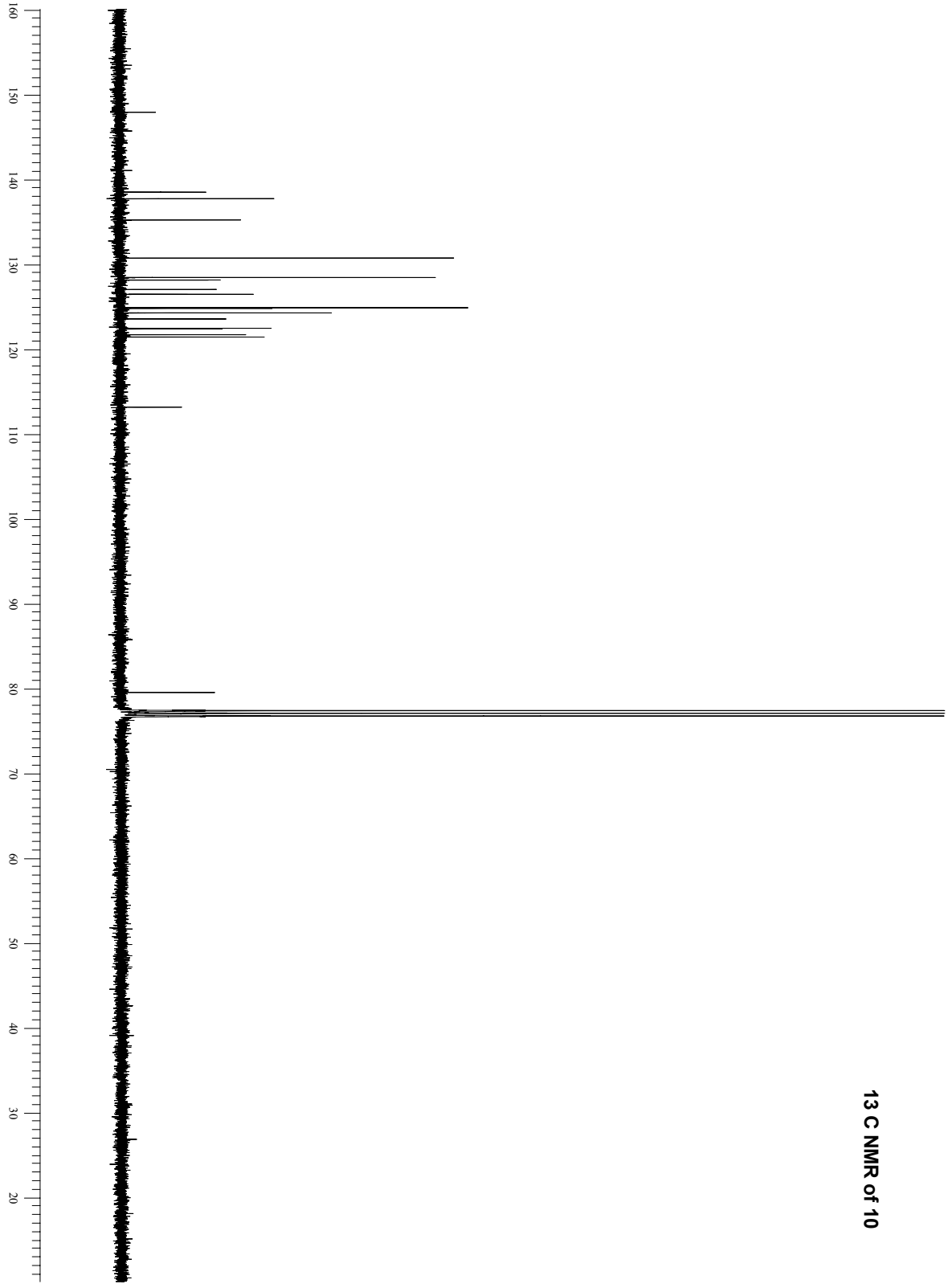


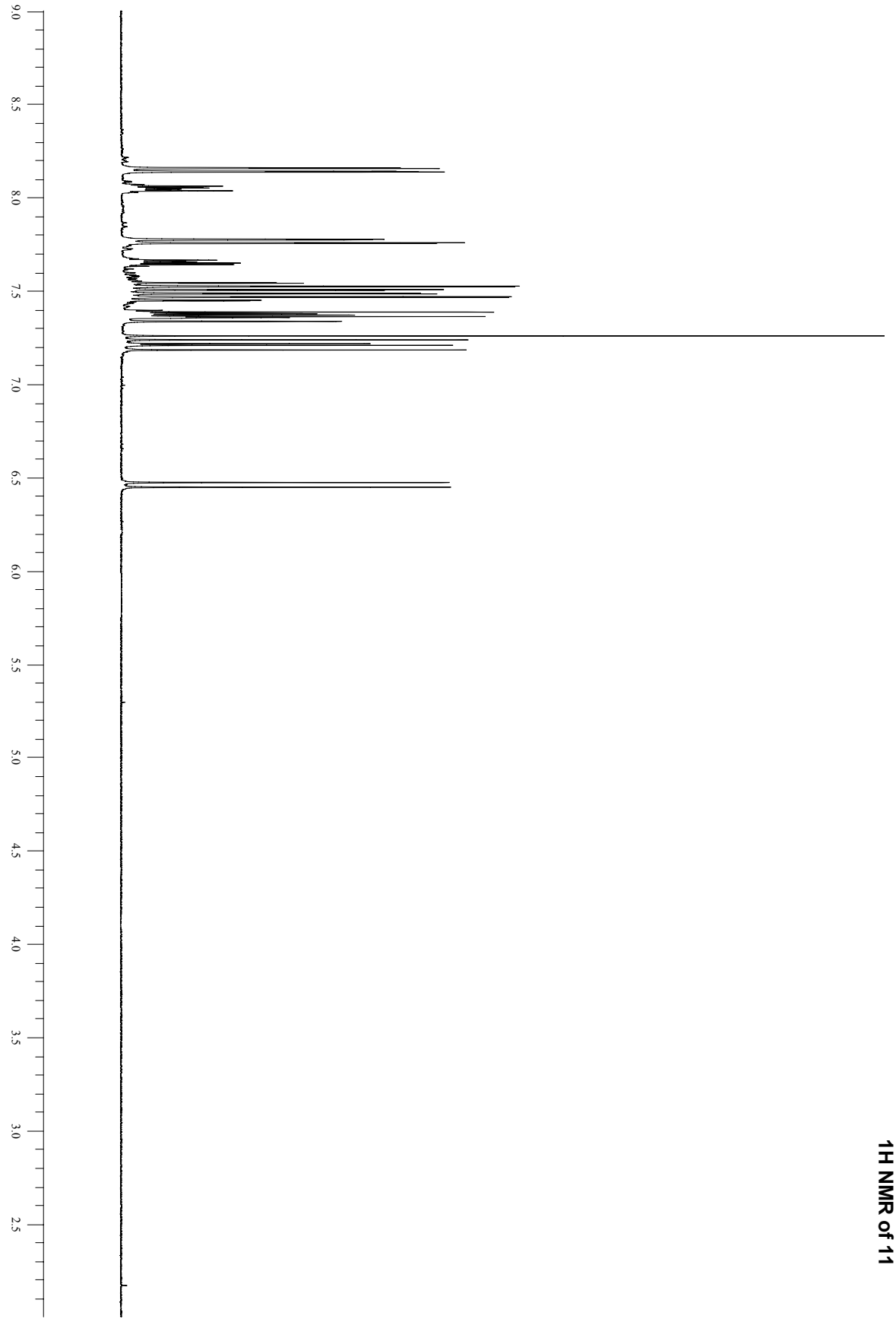




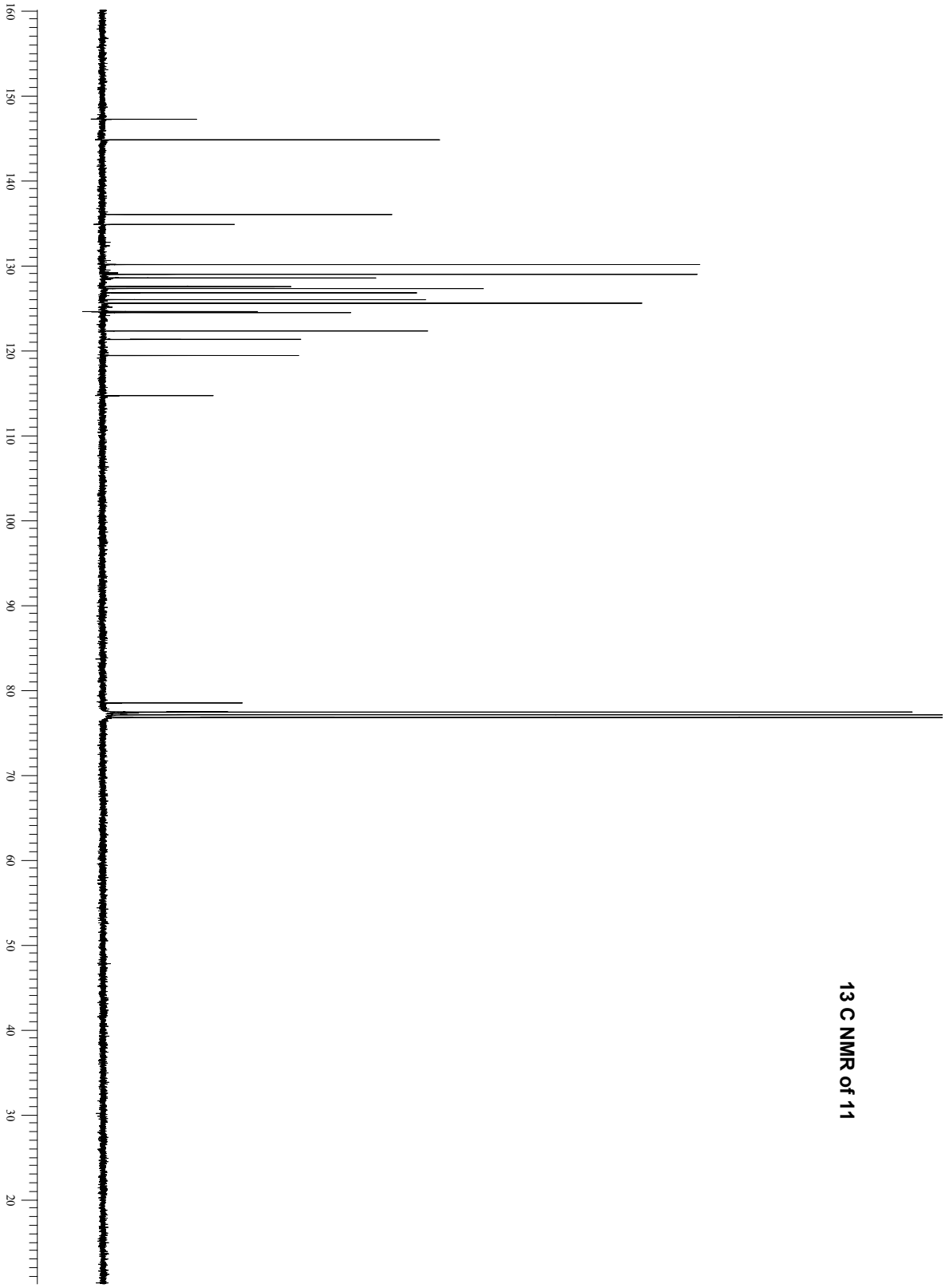


1 H NMR of 10

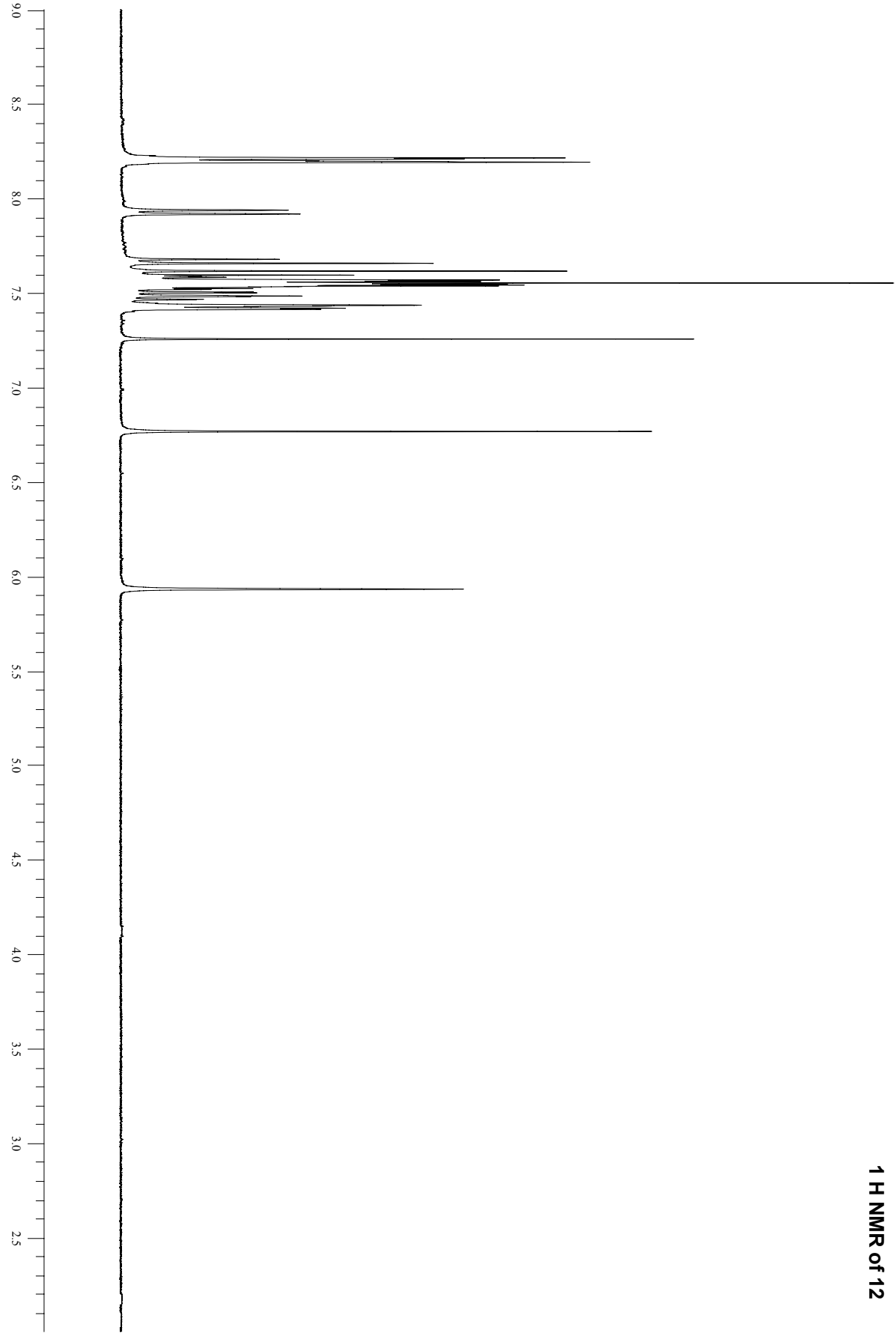




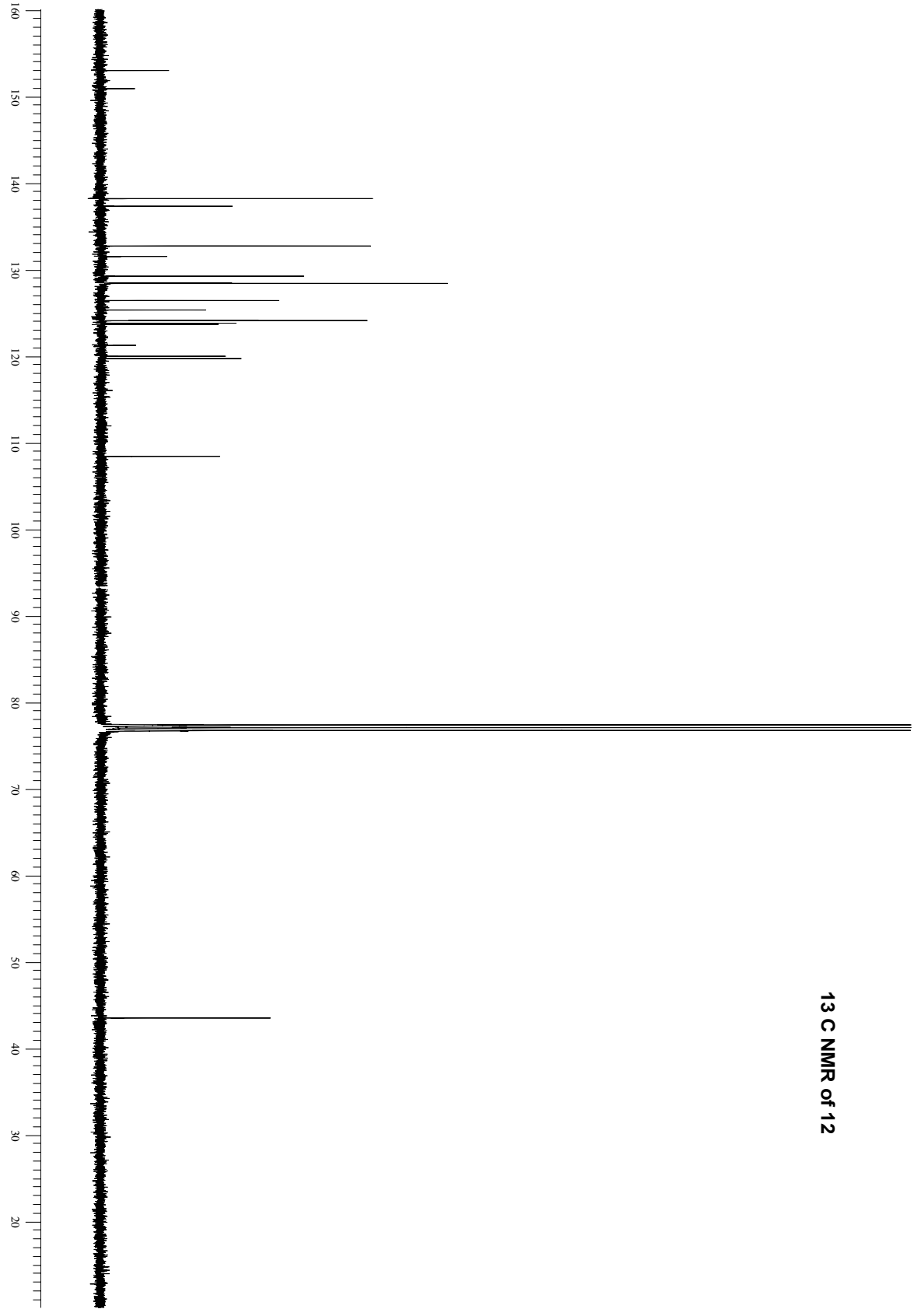
1H NMR of 11

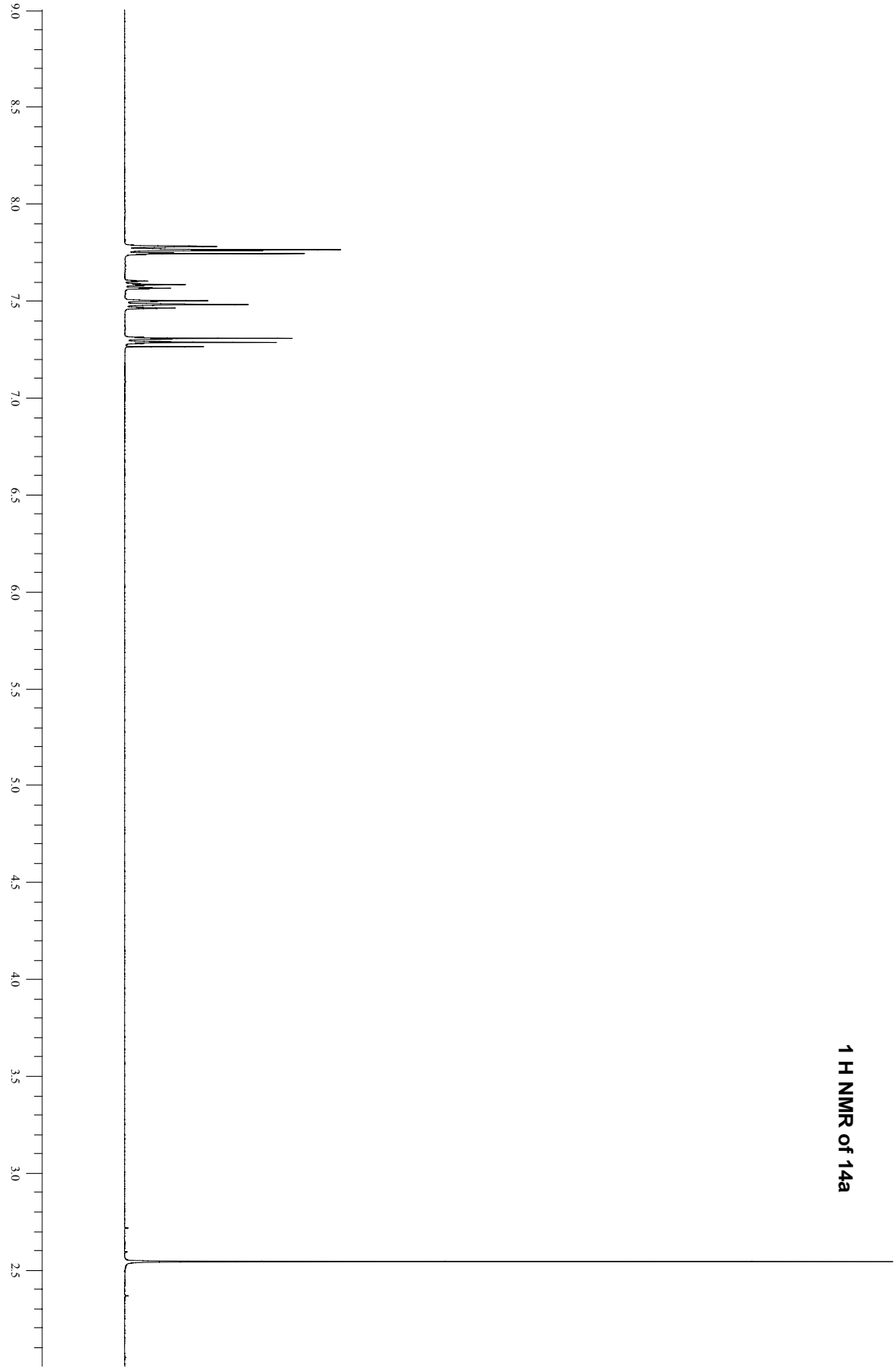


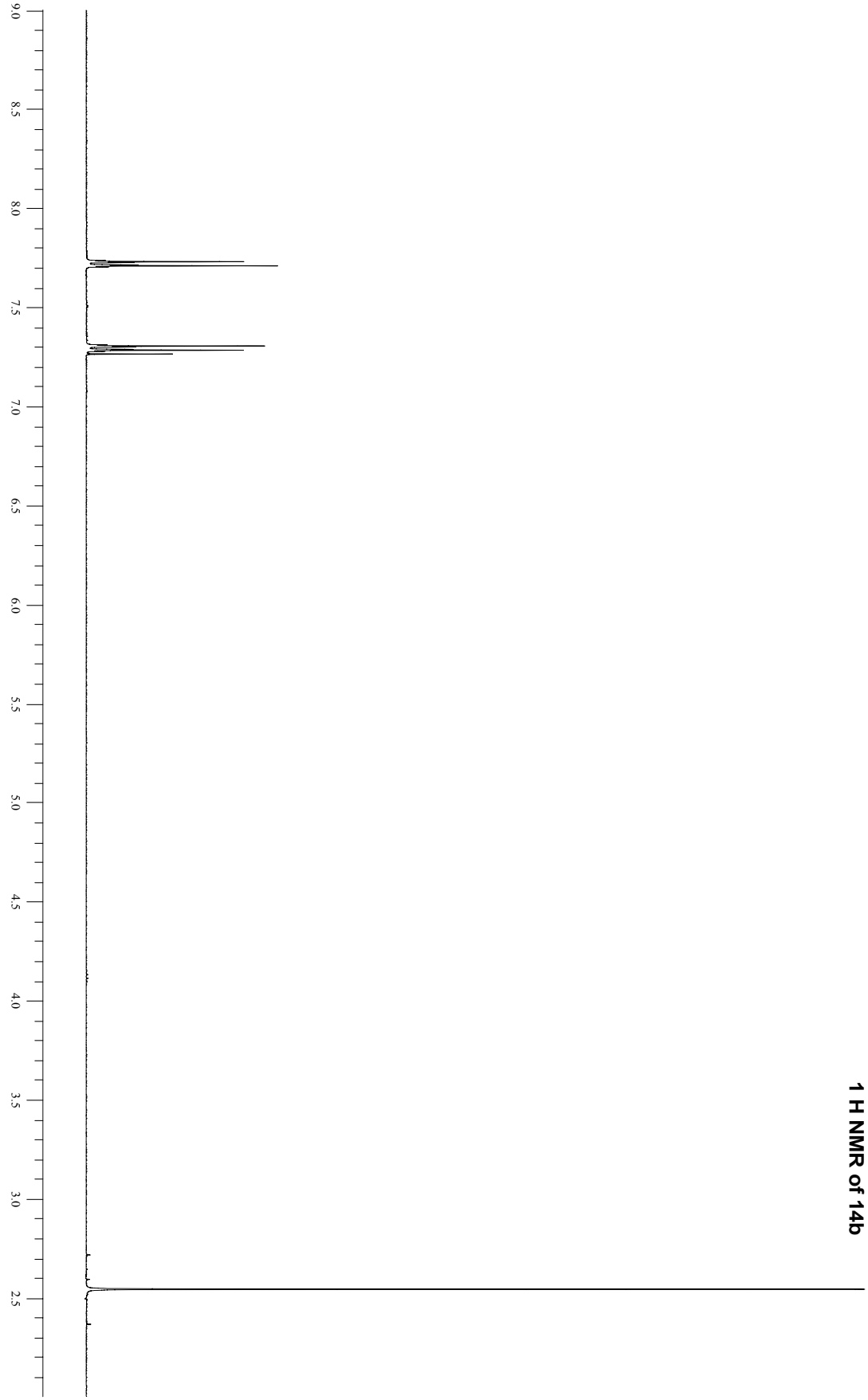
13 C NMR of 11

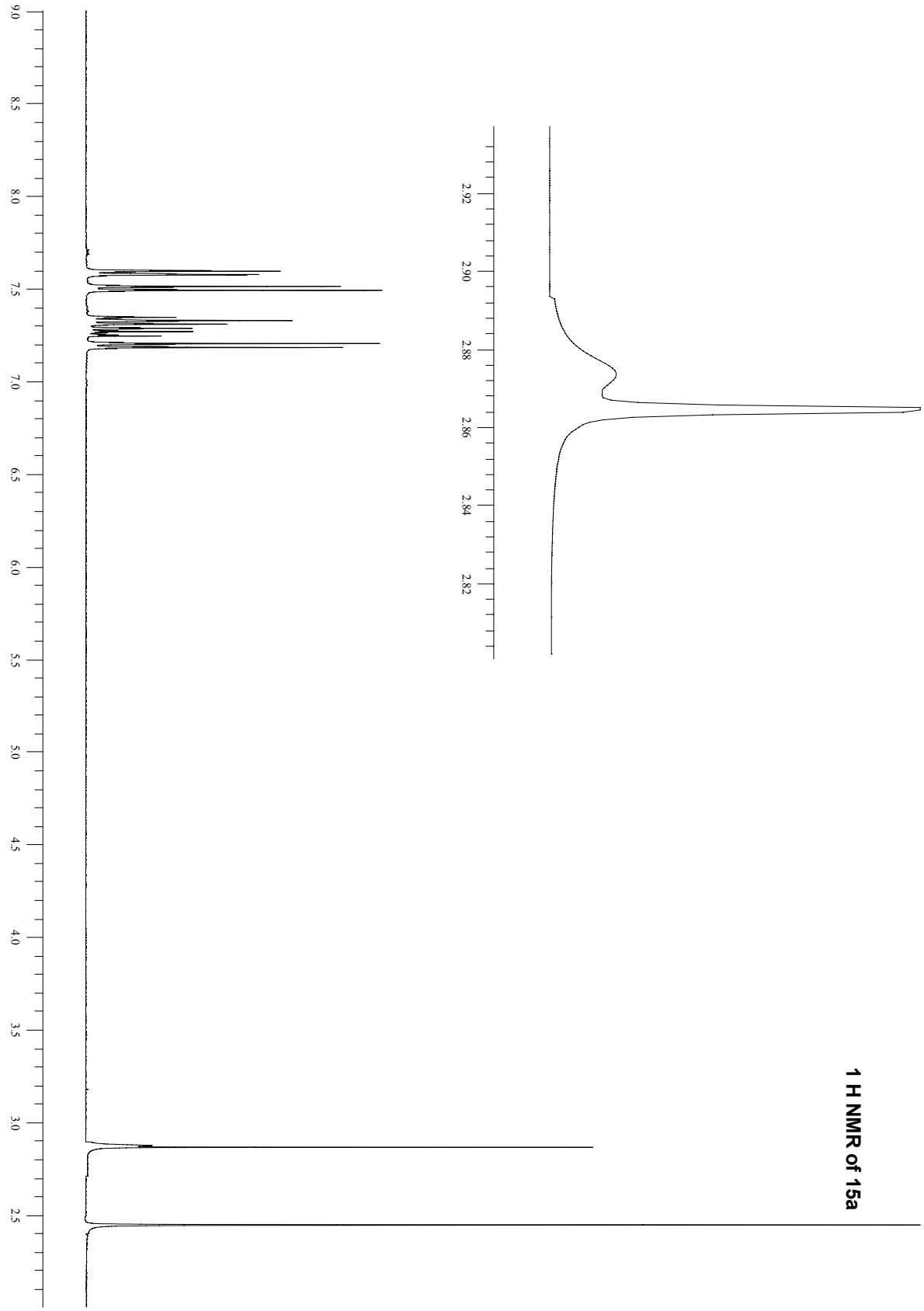


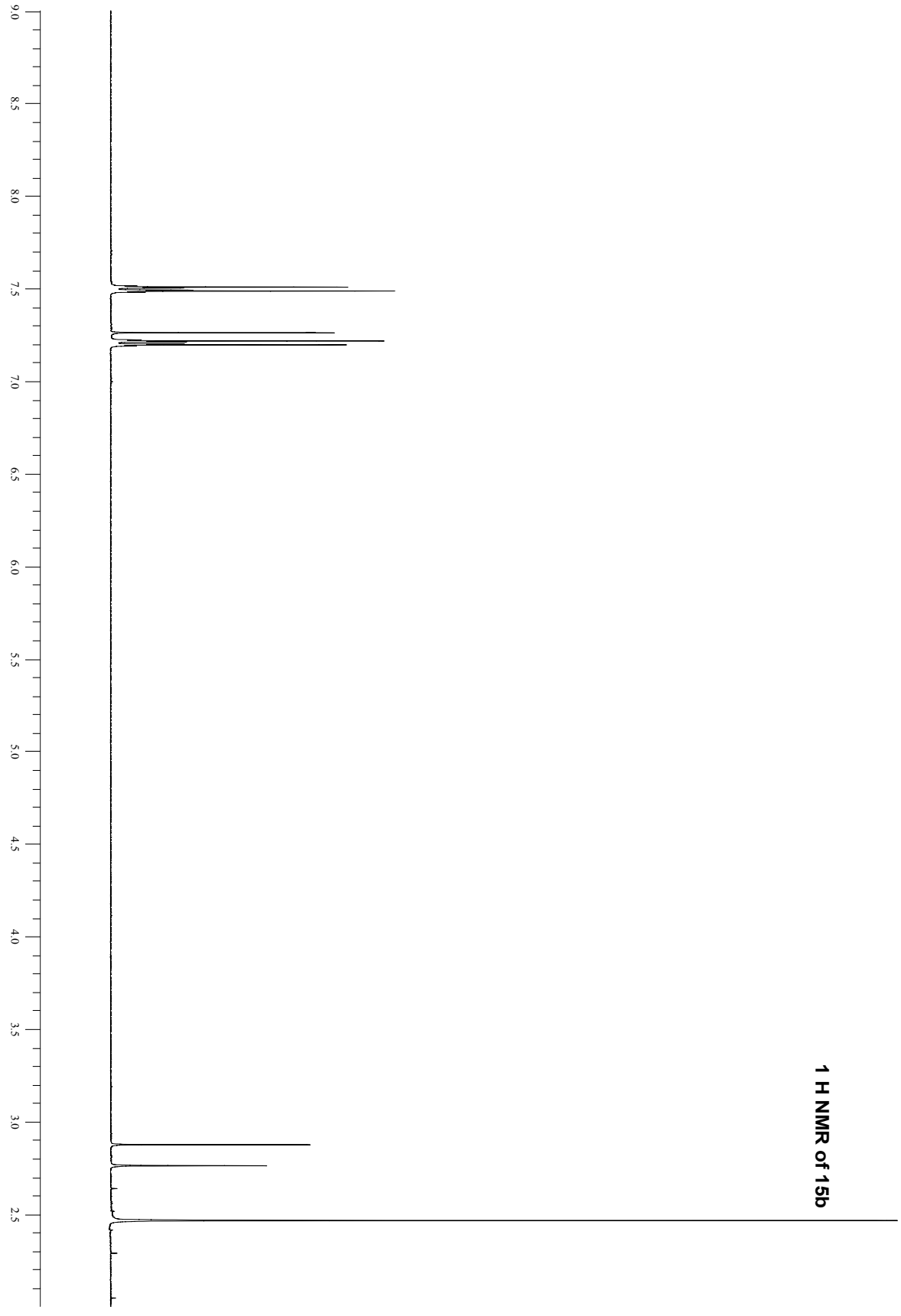
1 H NMR of 12

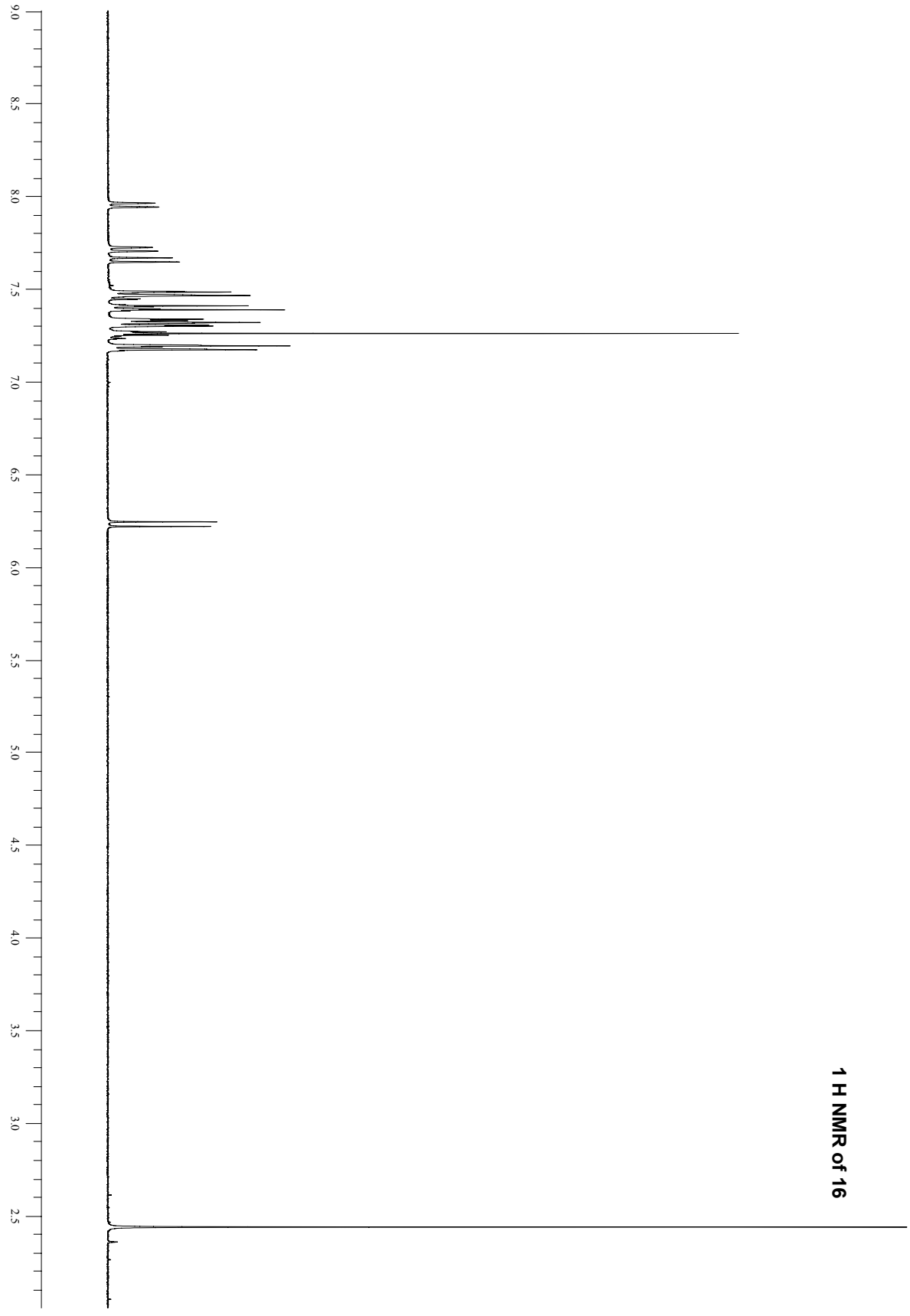


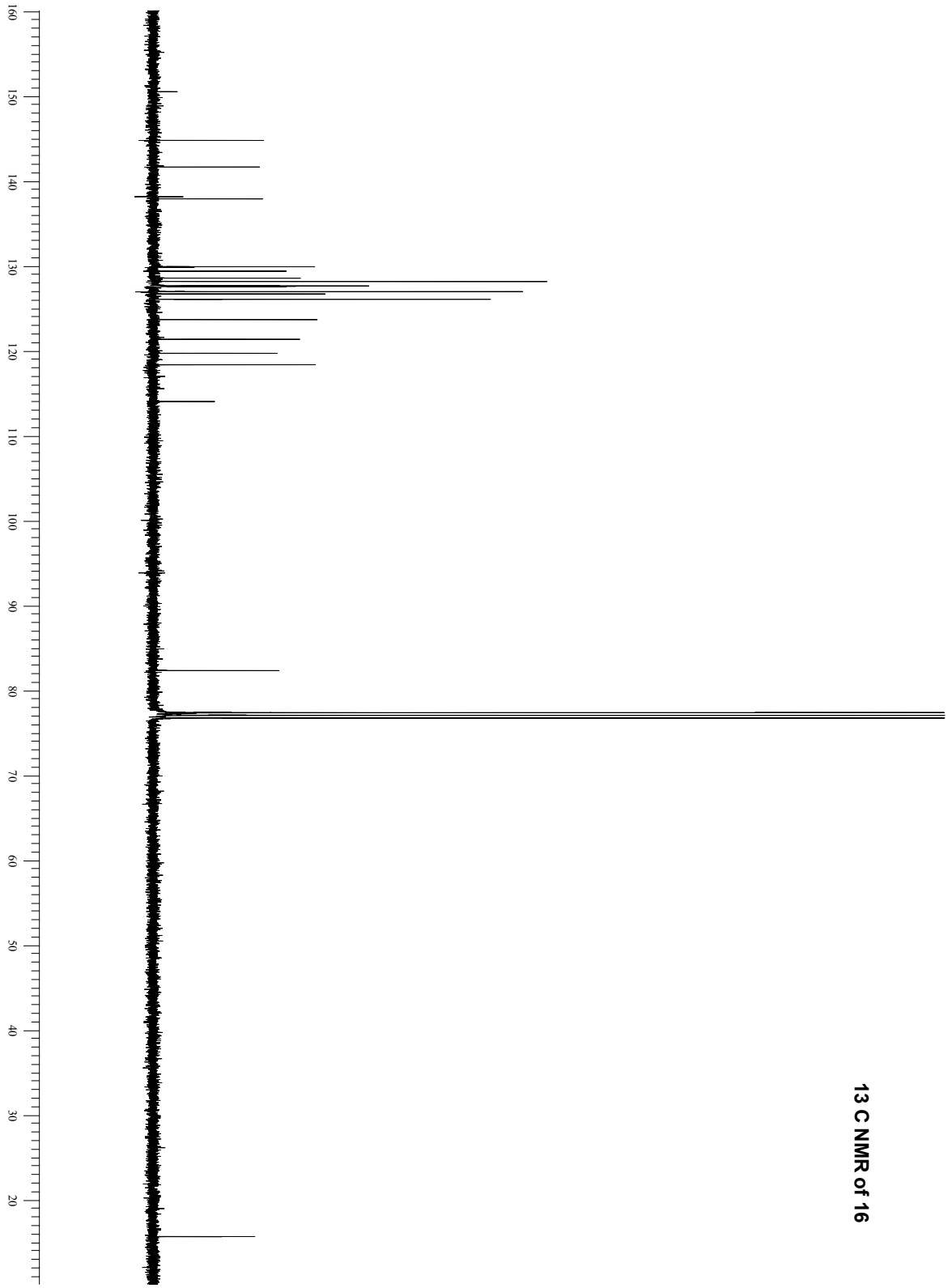




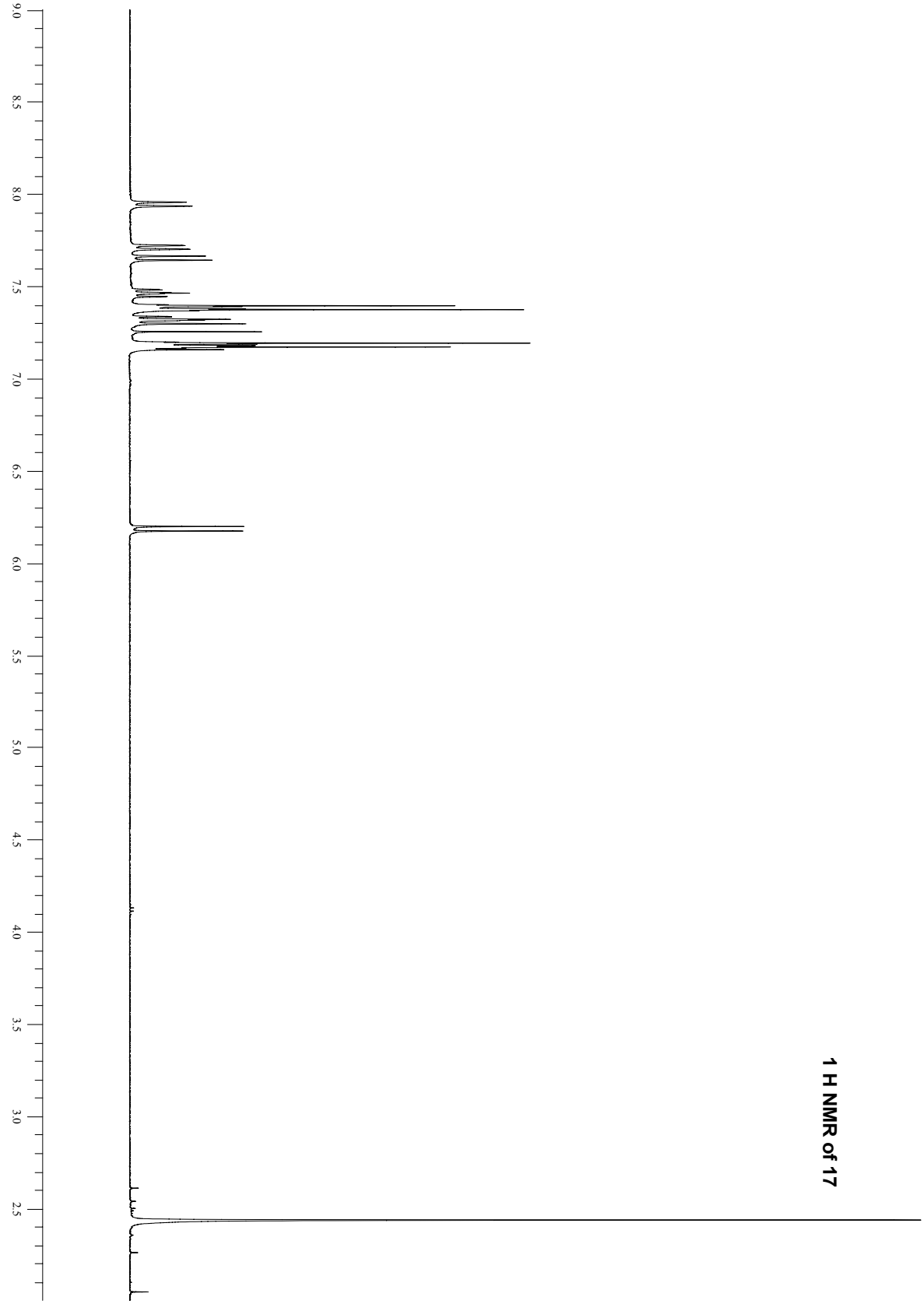


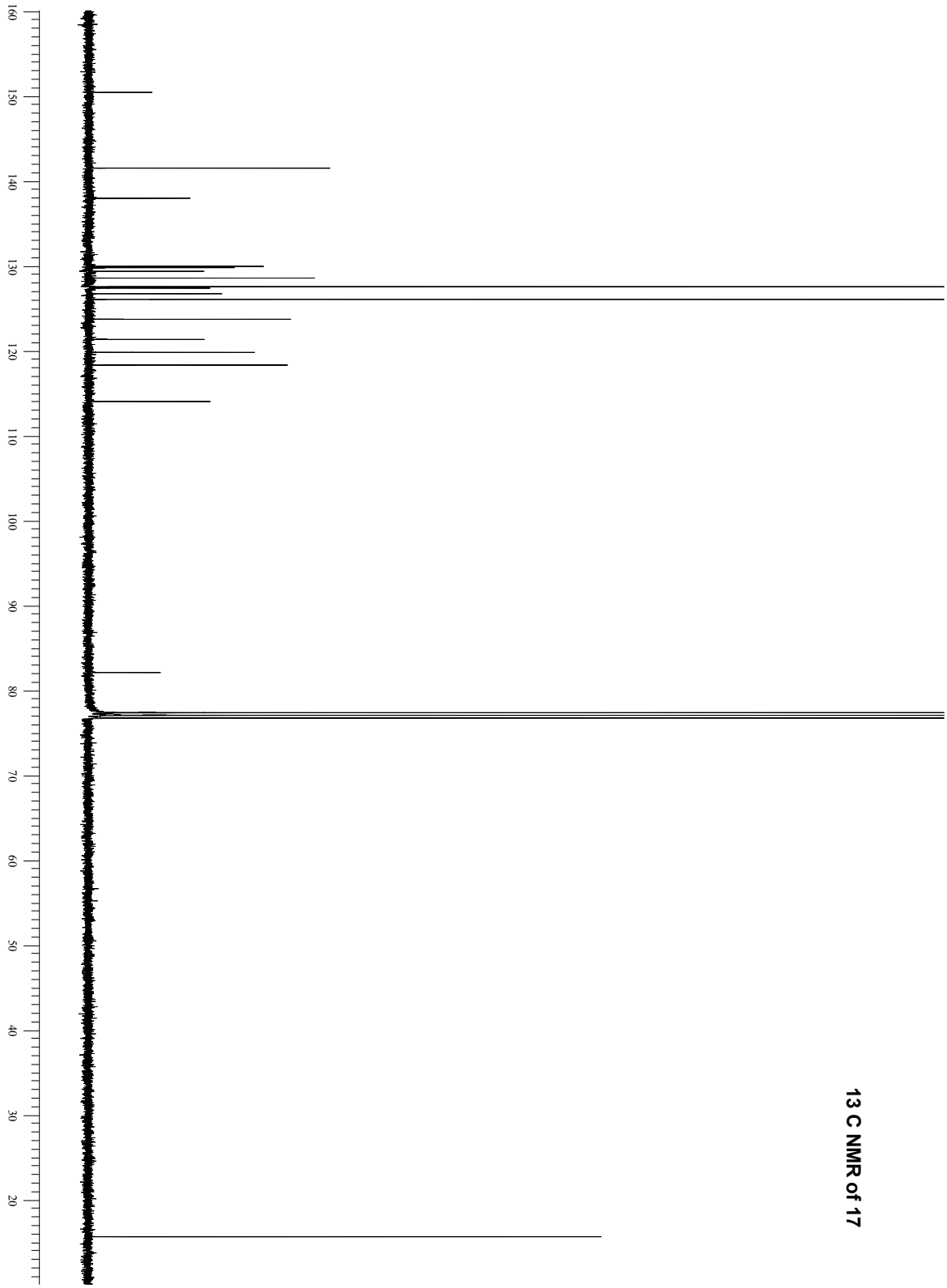


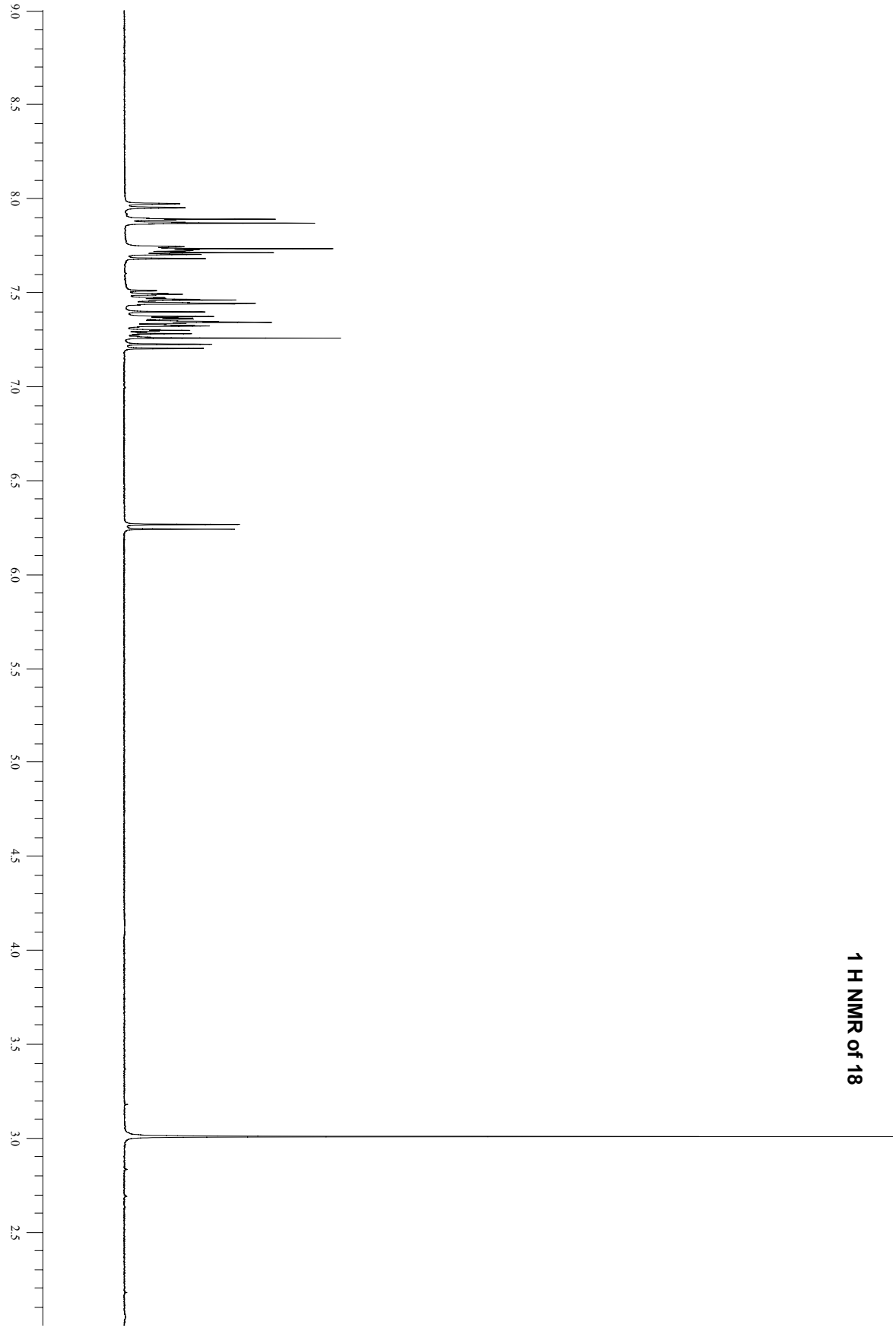


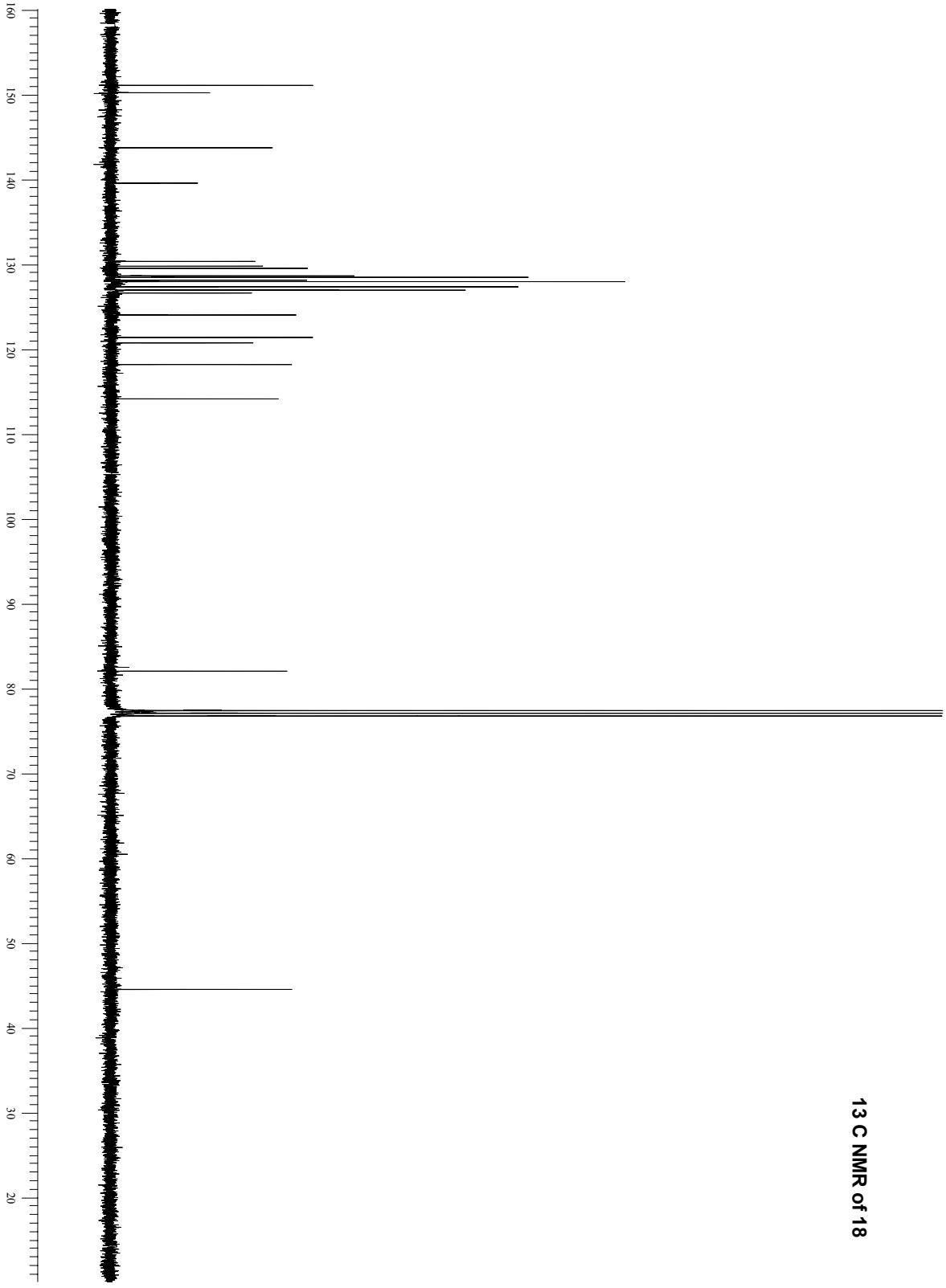


13 C NMR of 16

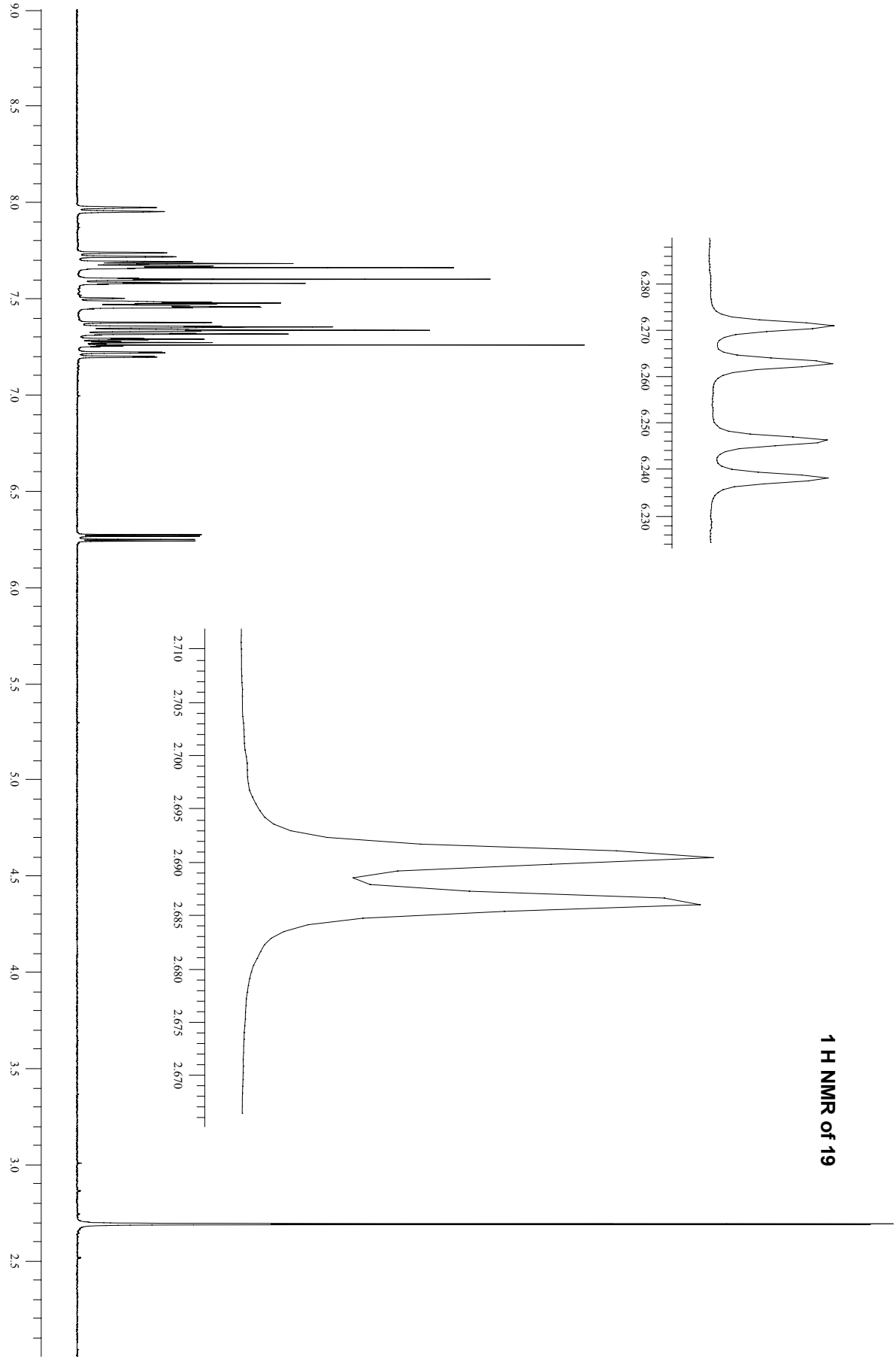


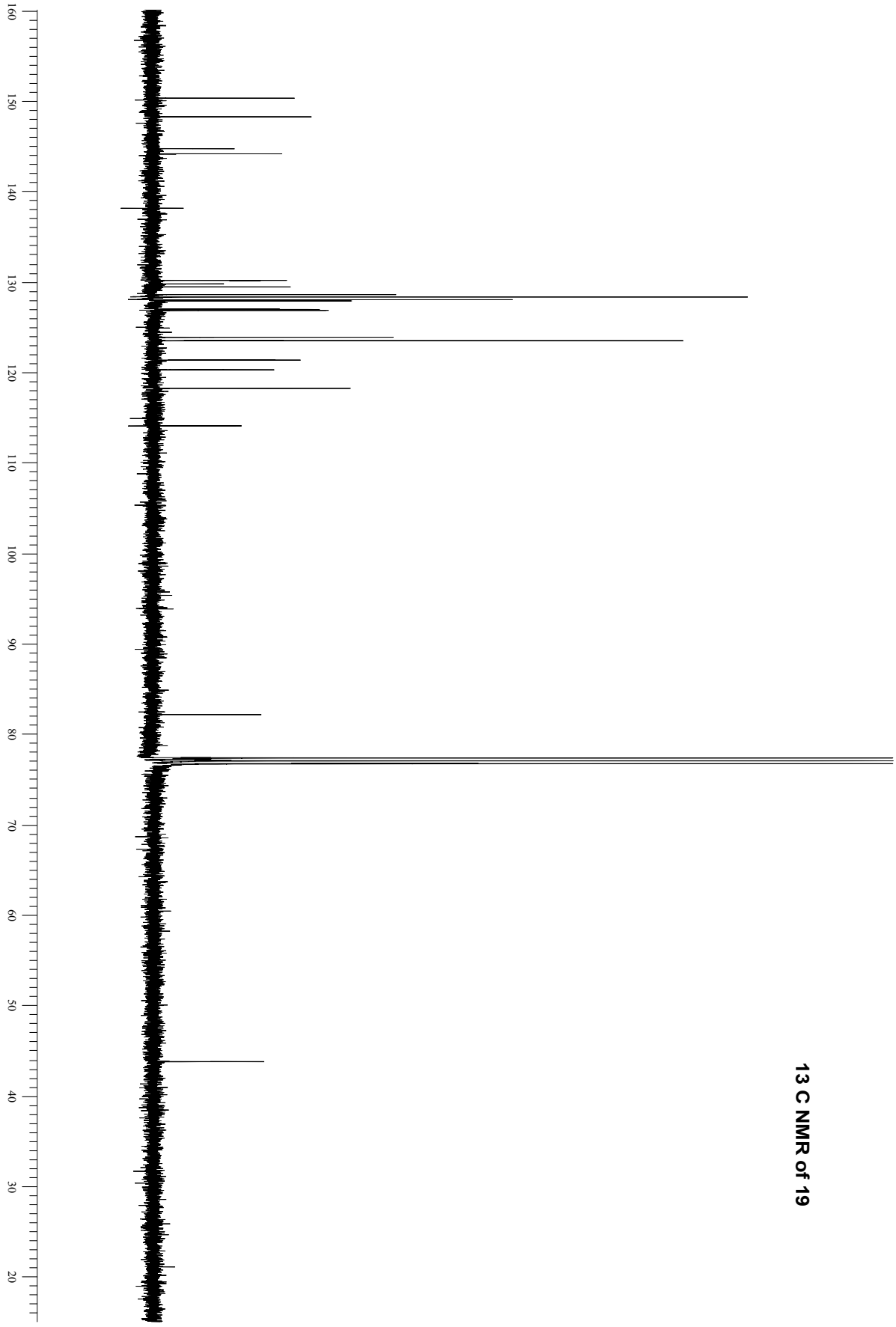


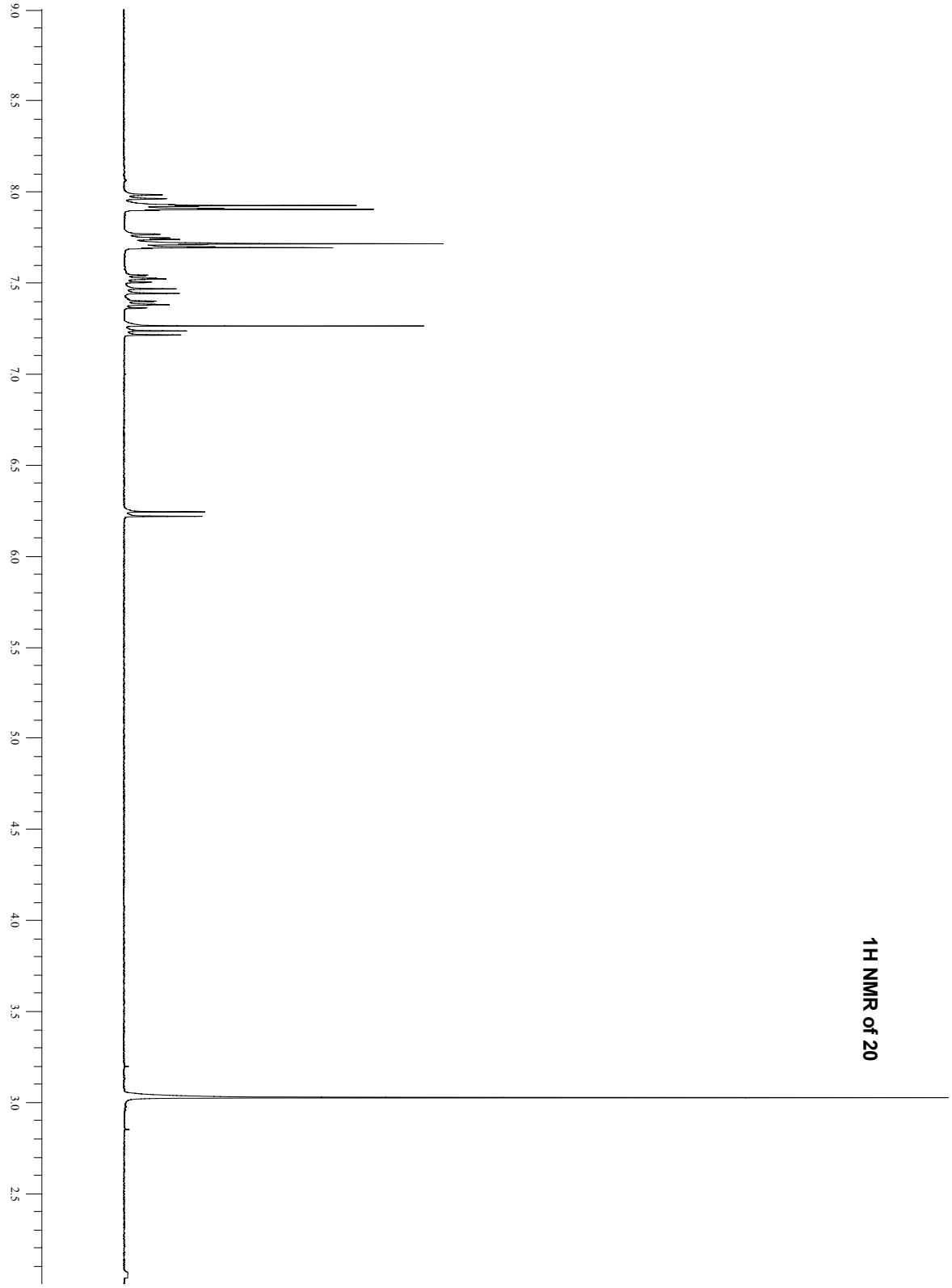


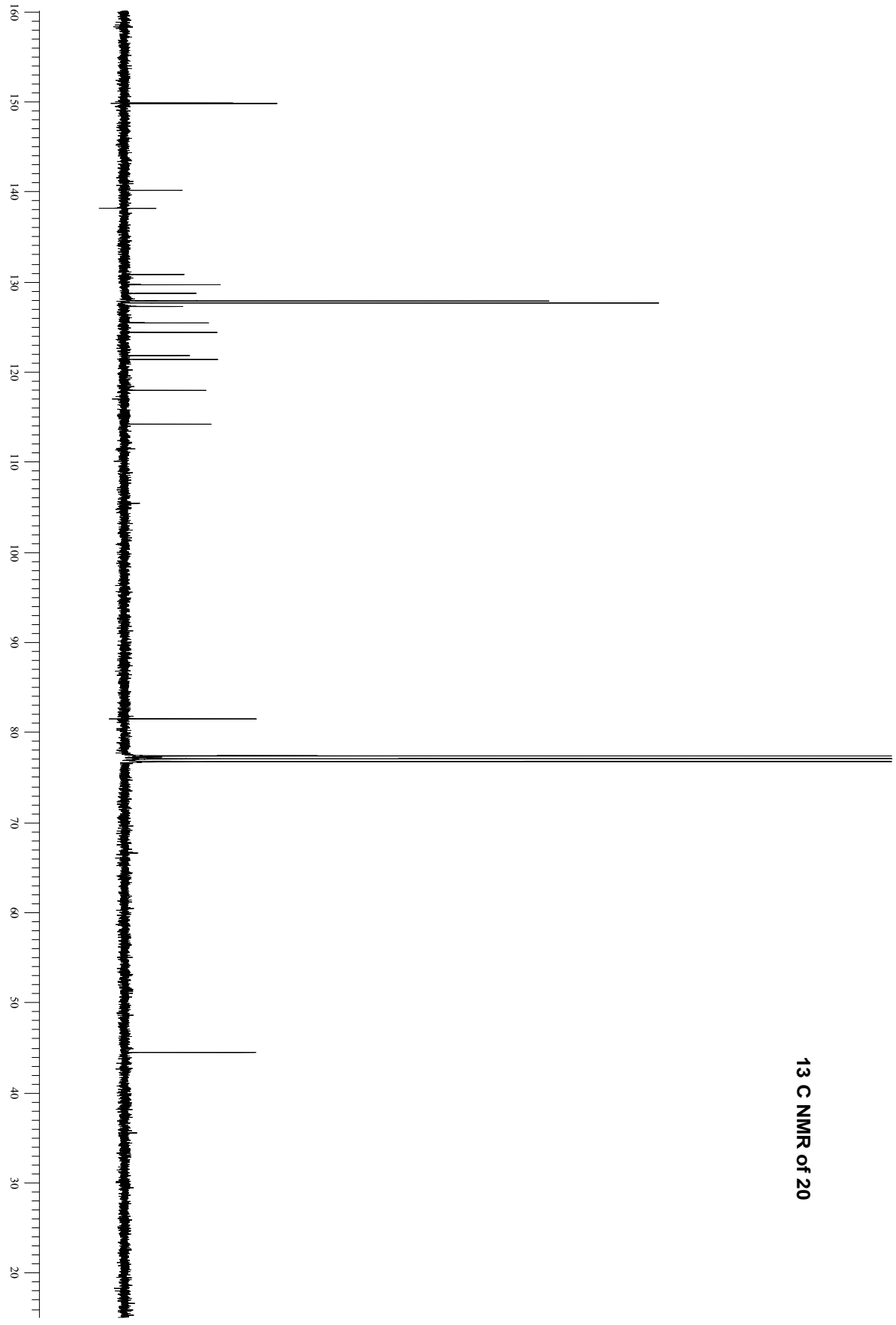


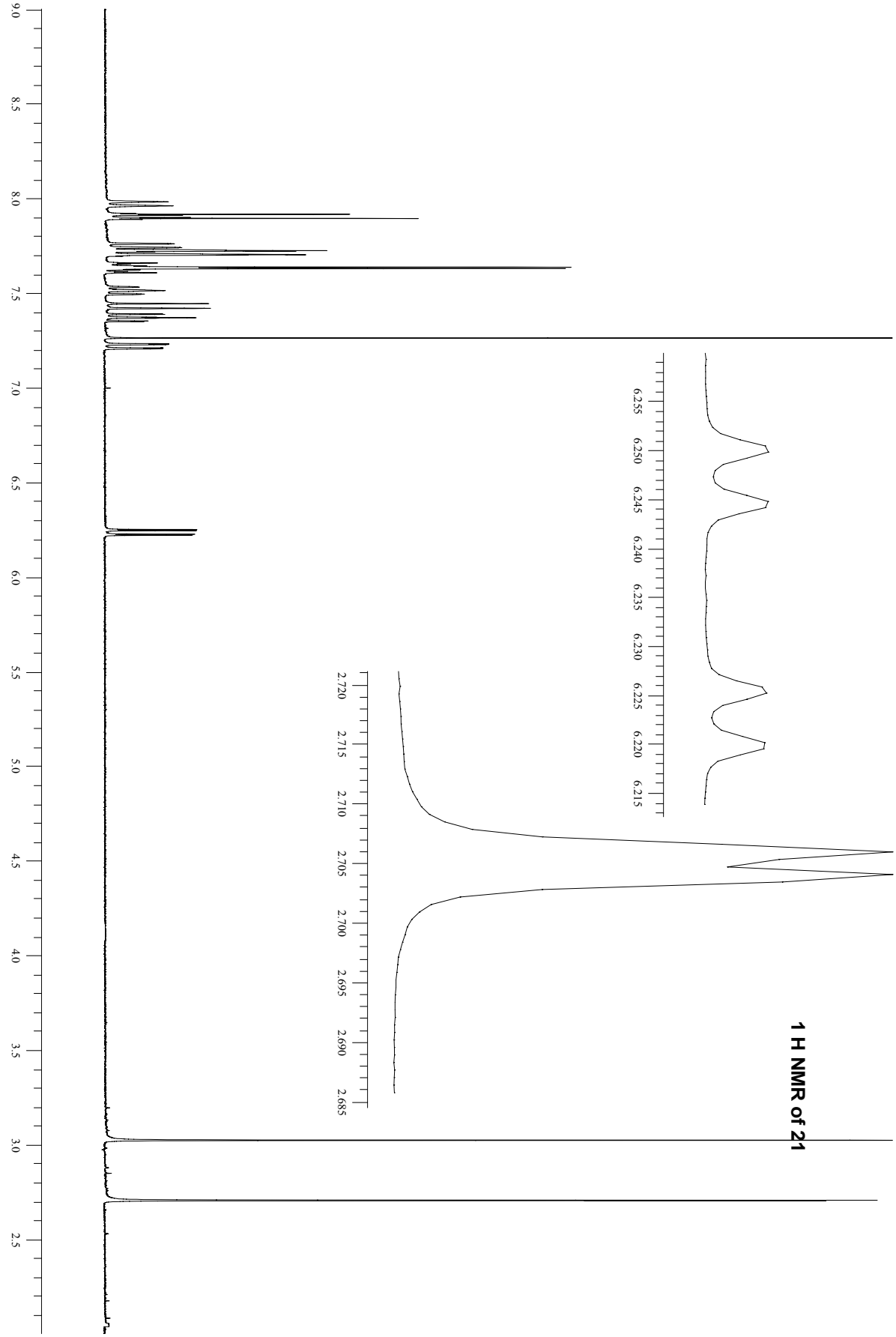
13 C NMR of 18

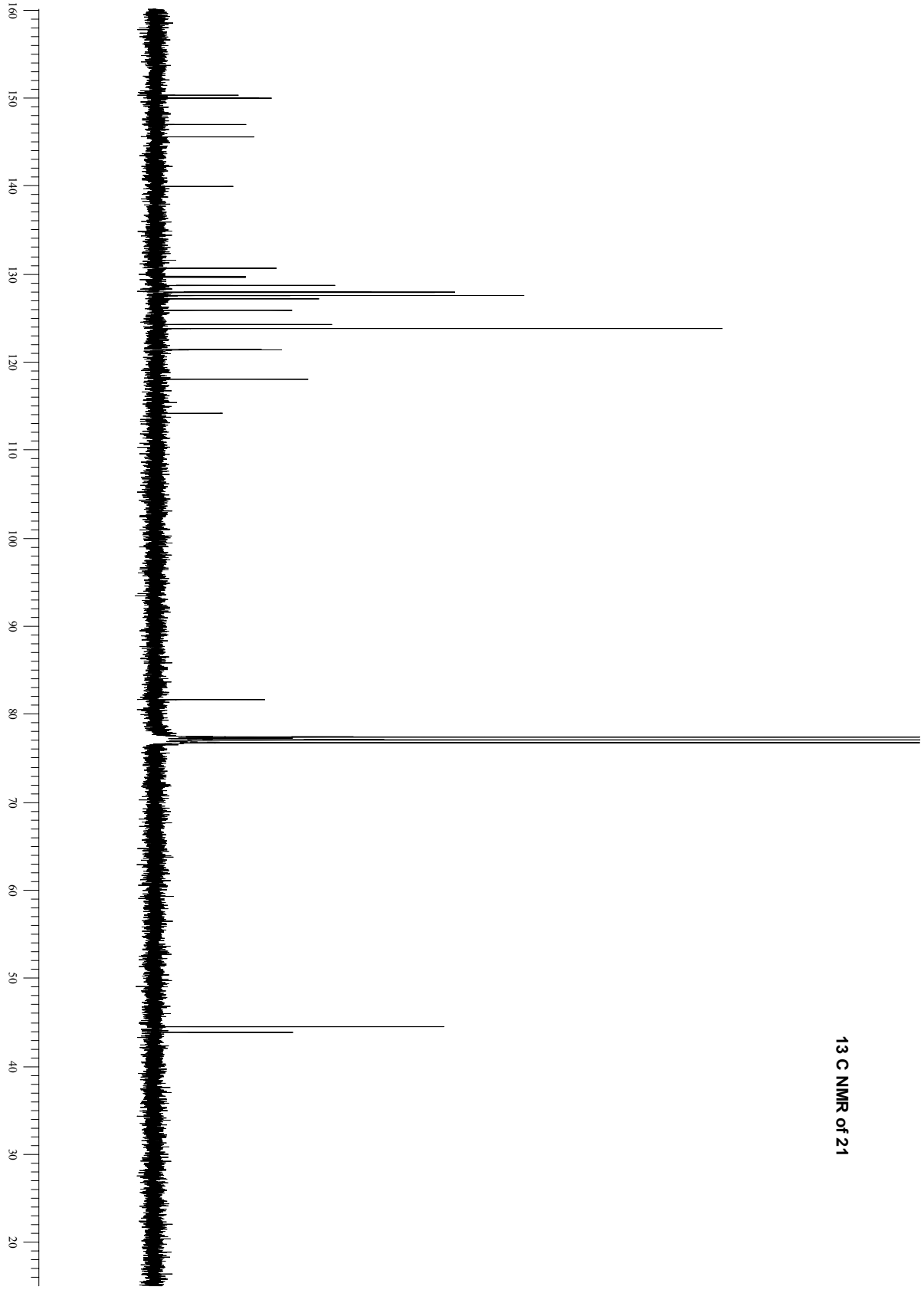


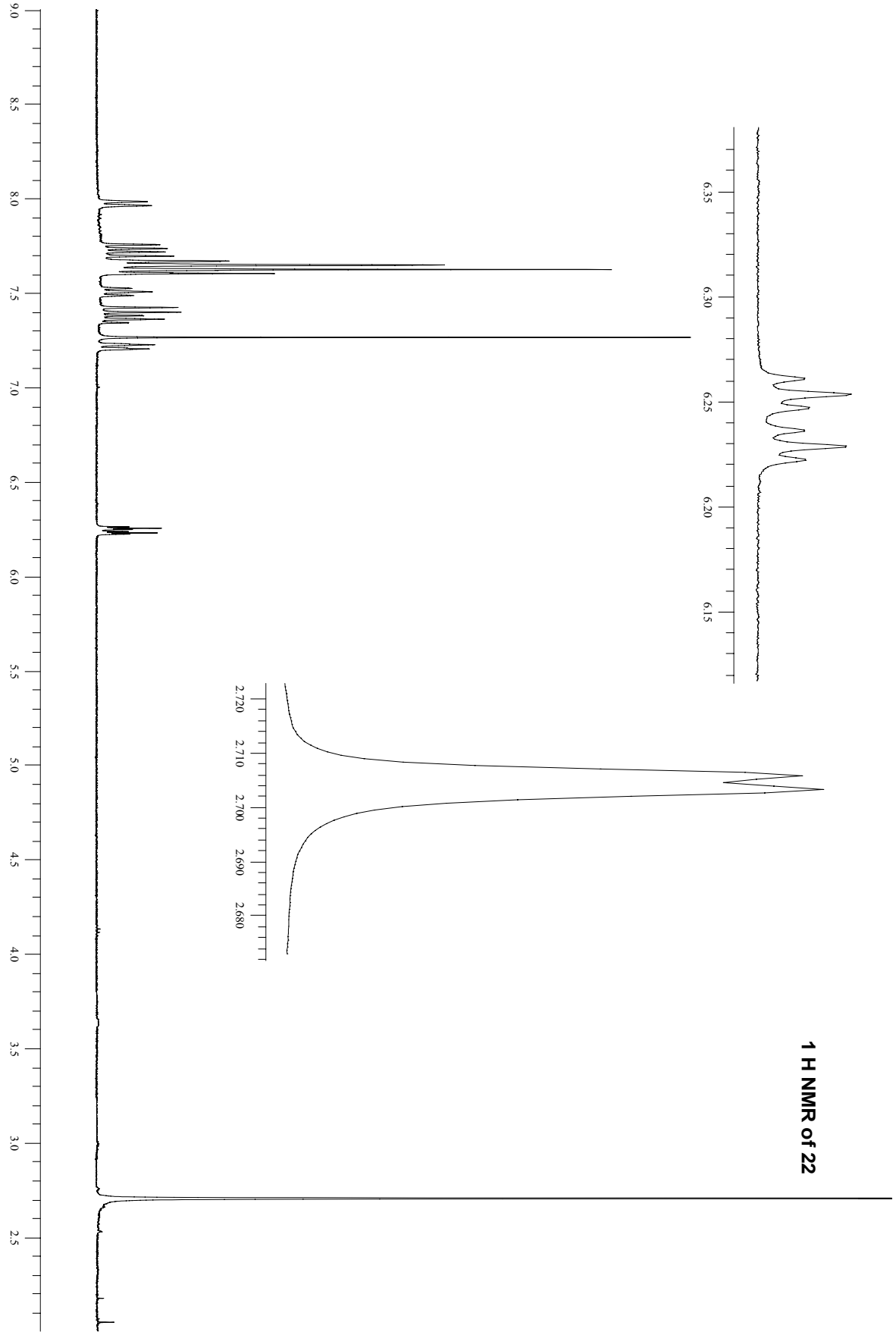


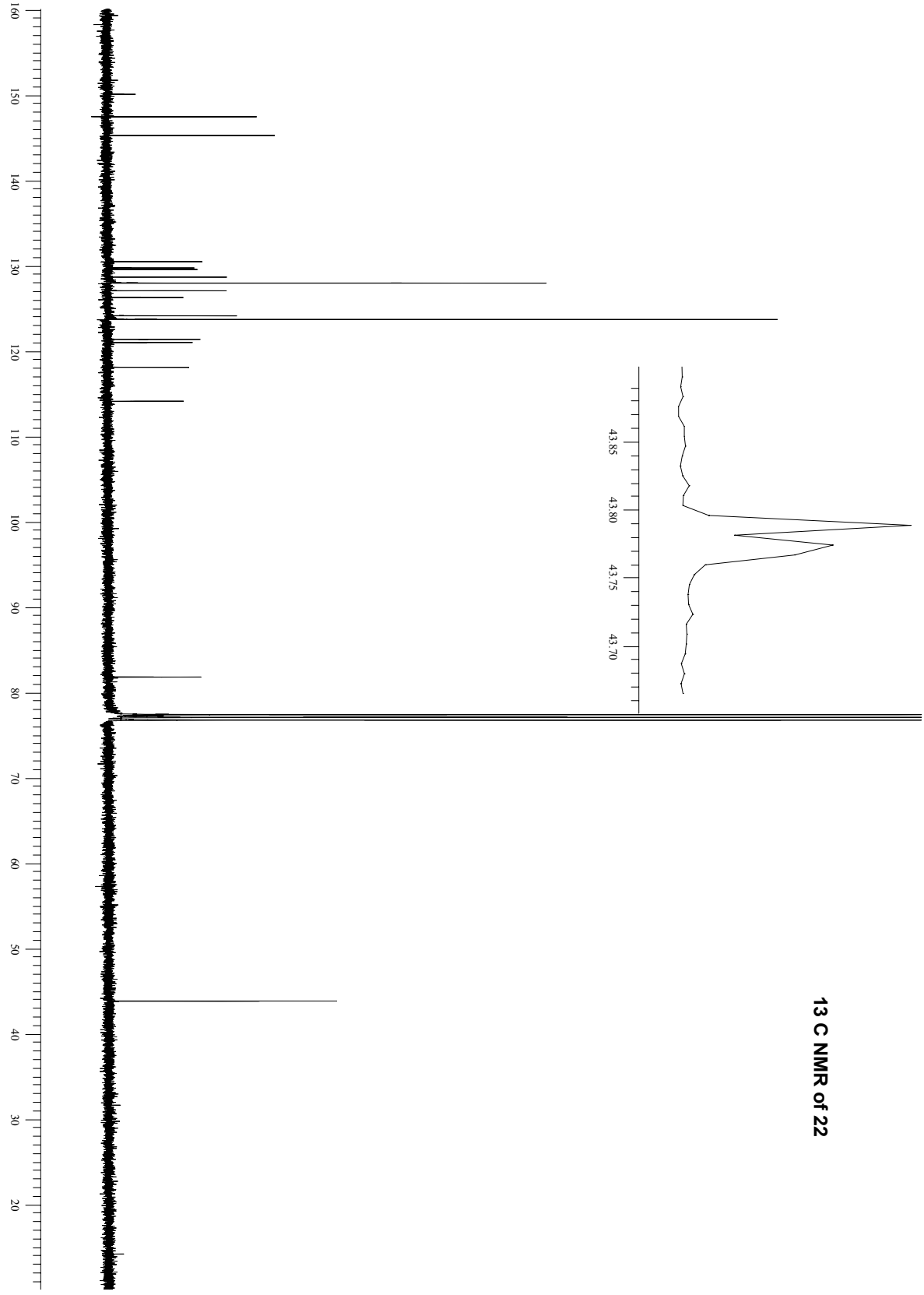












13 C NMR of 22