S1886Z : Oct 23 09:20:32 1998

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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G T O T H E P A P E R

Dinuclear and Trinuclear Zn(II) Calix[4]arene Complexes as Models for Hydrolytic Metalloenzymes. Synthesis and Catalytic Activity in Phosphate Diester Transesterification.

b y

Peter Molenveld, Wendy M.G. Stikvoort, Huub Kooijman, Anthony L. Spek, Johan F.J. Engbersen, and David Reinhoudt

C o m p o u n d (1)Zn(CH3COO)2.H2O

C o n t e n t s
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Table S1 - Crystal Data and Details of the Structure Determination for: S1886Z

Crystal Data

Empirical Formula			C15 H25 N3 O4 Zn, H2 O
Formula Weight			394.79
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	9.0875(15)	16.725(3)	14.255(2)
alpha, beta, gamma [deg]	90	120.11(8)	90
V [Ang**3]			1874.2(16)
Z			4
D(calc) [g/cm**3]			1.399
F(000)			832
Mu(MoKa) [/mm]			1.3
Crystal Size [mm]			0.2 x 0.2 x 0.3

Data Collection

Temperature (K)			150
Radiation [Angstrom]	MoKa (graphite monochromator)		0.71073
Theta Min-Max [Deg]			1.5, 28.5
Refined mosaicity (deg)			0.785(2)
Dataset	-12: 12 ; -22: 21 ; -19: 19		
Total X-ray exposure time (h)			8
Tot., Uniq. Data, R(int)		26707,	4293, 0.046
Completeness at Sin(Theta)/Labda=0.6 (%)		99.9	(-3 refl)

No absorption correction applied

Refinement

Npar	230
wR2, R1, S	0.0831, 0.0344 [for 3610 I > 2 sigma(I)], 1.025
w [sigma**2(F)+(0.0405P)**2+1.36P]**-1, P=(Max(Fo**2,0)+2Fc**2)/3	
Max. and Av. Shift/Error	-0.001, 0.000
Min. and Max. resd. dens. [e/Ang^3]	-0.61, 0.31

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: S1886Z

Atom	x	y	z	U(eq) [Ang^2]
Zn15	0.43561(3)	0.30773(1)	0.25852(2)	0.0187(1)
O16	0.30130(17)	0.21563(8)	0.17332(11)	0.0243(4)
O18	0.13763(19)	0.22010(9)	0.24837(13)	0.0320(5)
O20	0.63906(17)	0.30554(8)	0.24076(11)	0.0244(4)
O21	0.68013(19)	0.42712(9)	0.31224(13)	0.0339(5)
N1	0.37320(19)	0.37931(9)	0.34914(12)	0.0185(4)
N8	0.5636(2)	0.24576(9)	0.42413(13)	0.0227(5)
N12	0.2777(2)	0.40788(10)	0.13981(13)	0.0222(5)
C2	0.3127(2)	0.45293(11)	0.31442(15)	0.0190(5)
C3	0.2702(2)	0.50304(11)	0.37433(16)	0.0219(5)
C4	0.2935(2)	0.47601(12)	0.47280(16)	0.0242(6)
C5	0.3577(2)	0.39988(12)	0.50853(16)	0.0234(5)
C6	0.3957(2)	0.35256(11)	0.44399(15)	0.0198(5)
C7	0.4566(3)	0.26745(12)	0.47142(16)	0.0244(6)
C9	0.5775(3)	0.15851(12)	0.41989(19)	0.0336(7)
C10	0.7347(3)	0.28013(13)	0.49041(17)	0.0294(6)
C11	0.3023(3)	0.47761(11)	0.20966(16)	0.0225(6)
C13	0.0988(3)	0.38139(13)	0.08592(17)	0.0300(6)
C14	0.3220(3)	0.42975(13)	0.05686(18)	0.0325(7)
C17	0.1843(2)	0.18774(11)	0.18959(17)	0.0231(5)
C19	0.1053(3)	0.11023(13)	0.1324(2)	0.0340(7)
C21	0.7231(2)	0.37164(12)	0.27467(16)	0.0250(6)
C22	0.8809(3)	0.37851(15)	0.2655(2)	0.0424(8)
O23	-0.1261(3)	0.16802(11)	0.29011(16)	0.0422(6)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: S1886Z

Atom	x	y	z	U(iso) [Ang^2]
H3	0.22590	0.55490	0.34850	0.0260
H4	0.26570	0.50940	0.51550	0.0290
H5	0.37520	0.38060	0.57610	0.0280
H7A	0.52320	0.26100	0.55120	0.0290
H7B	0.35750	0.23110	0.44300	0.0290
H9A	0.63070	0.13660	0.49350	0.0500
H9B	0.64730	0.14530	0.38740	0.0500
H9C	0.46380	0.13540	0.37590	0.0500
H10A	0.72650	0.33860	0.49010	0.0440
H10B	0.80640	0.26430	0.46030	0.0440
H10C	0.78500	0.26050	0.56500	0.0440
H11A	0.20640	0.51530	0.17060	0.0270
H11B	0.40840	0.50570	0.22570	0.0270
H13A	0.07030	0.36470	0.14080	0.0450
H13B	0.08280	0.33630	0.03780	0.0450
H13C	0.02440	0.42560	0.04340	0.0450
H14A	0.25070	0.47460	0.01360	0.0490
H14B	0.30280	0.38380	0.00940	0.0490
H14C	0.44200	0.44550	0.09240	0.0490
H19A	0.01160	0.09600	0.14450	0.0510
H19B	0.19130	0.06780	0.16100	0.0510
H19C	0.06170	0.11650	0.05440	0.0510
H22A	0.90760	0.43510	0.26380	0.0630
H22B	0.86130	0.35240	0.19860	0.0630
H22C	0.97640	0.35250	0.32800	0.0630
H23A	-0.188(4)	0.2051(19)	0.275(3)	0.053(10)

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: S1886Z

Atom	x	y	z	U(iso) [Ang^2]
H23B	-0.042(5)	0.182(2)	0.280(3)	0.0800

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: S1886Z

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zn15	0.0203(1)	0.0158(1)	0.0243(1)	-0.0028(1)	0.0143(1)	-0.0012(1)
O16	0.0230(7)	0.0210(7)	0.0321(7)	-0.0058(6)	0.0162(6)	-0.0056(5)
O18	0.0305(8)	0.0331(8)	0.0406(9)	-0.0082(7)	0.0240(7)	-0.0048(6)
O20	0.0220(7)	0.0246(7)	0.0304(7)	-0.0070(6)	0.0160(6)	-0.0053(5)
O21	0.0347(8)	0.0304(8)	0.0445(9)	-0.0136(7)	0.0257(7)	-0.0070(7)
N1	0.0197(7)	0.0158(7)	0.0238(8)	-0.0013(6)	0.0137(6)	-0.0005(6)
N8	0.0263(8)	0.0177(8)	0.0249(8)	0.0013(6)	0.0134(7)	0.0035(6)
N12	0.0280(8)	0.0198(8)	0.0235(8)	0.0011(6)	0.0164(7)	0.0018(7)
C2	0.0188(8)	0.0156(8)	0.0252(9)	0.0000(7)	0.0130(8)	-0.0004(7)
C3	0.0203(9)	0.0180(9)	0.0294(10)	-0.0016(7)	0.0140(8)	0.0005(7)
C4	0.0237(9)	0.0255(10)	0.0286(10)	-0.0067(8)	0.0170(8)	-0.0020(8)
C5	0.0234(9)	0.0266(10)	0.0242(9)	-0.0003(8)	0.0150(8)	-0.0012(8)
C6	0.0194(9)	0.0202(9)	0.0223(9)	0.0002(7)	0.0124(7)	-0.0019(7)
C7	0.0304(10)	0.0219(10)	0.0241(10)	0.0043(8)	0.0160(8)	0.0024(8)
C9	0.0438(13)	0.0191(10)	0.0379(12)	0.0030(9)	0.0206(10)	0.0071(9)
C10	0.0252(10)	0.0304(11)	0.0274(10)	0.0011(9)	0.0093(9)	0.0037(9)
C11	0.0298(10)	0.0152(9)	0.0270(10)	0.0032(7)	0.0176(9)	0.0035(7)
C13	0.0268(10)	0.0294(11)	0.0299(11)	0.0017(8)	0.0113(9)	0.0040(8)
C14	0.0498(13)	0.0286(11)	0.0310(11)	0.0052(9)	0.0291(10)	0.0061(10)
C17	0.0182(9)	0.0201(9)	0.0303(10)	-0.0002(8)	0.0116(8)	0.0008(7)
C19	0.0287(11)	0.0250(10)	0.0546(14)	-0.0091(10)	0.0257(11)	-0.0078(9)
C21	0.0240(9)	0.0267(10)	0.0269(10)	-0.0058(8)	0.0147(8)	-0.0054(8)
C22	0.0347(12)	0.0433(14)	0.0621(16)	-0.0205(12)	0.0340(12)	-0.0165(11)
O23	0.0491(11)	0.0303(9)	0.0611(12)	0.0038(8)	0.0380(10)	0.0004(8)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: S1886Z

Zn15	-O16	1.9623(14)	C21	-C22	1.508(4)
Zn15	-O20	1.9883(18)	C3	-H3	0.9493
Zn15	-N1	2.0392(17)	C4	-H4	0.9489
Zn15	-N8	2.2903(16)	C5	-H5	0.9504
Zn15	-N12	2.3004(17)	C7	-H7B	0.9893
O16	-C17	1.284(3)	C7	-H7A	0.9903
O18	-C17	1.238(3)	C9	-H9B	0.9800
O20	-C21	1.292(2)	C9	-H9A	0.9798
O21	-C21	1.229(3)	C9	-H9C	0.9799
O23	-H23A	0.79(4)	C10	-H10B	0.9795
O23	-H23B	0.88(5)	C10	-H10A	0.9806
N1	-C2	1.338(2)	C10	-H10C	0.9796
N1	-C6	1.339(2)	C11	-H11A	0.9900
N8	-C7	1.480(3)	C11	-H11B	0.9907
N8	-C10	1.472(3)	C13	-H13B	0.9800
N8	-C9	1.469(3)	C13	-H13A	0.9799
N12	-C13	1.475(3)	C13	-H13C	0.9798
N12	-C11	1.476(3)	C14	-H14B	0.9800
N12	-C14	1.474(3)	C14	-H14A	0.9808
C2	-C11	1.506(3)	C14	-H14C	0.9803
C2	-C3	1.383(3)	C19	-H19B	0.9803
C3	-C4	1.386(3)	C19	-H19C	0.9810
C4	-C5	1.387(3)	C19	-H19A	0.9792
C5	-C6	1.382(3)	C22	-H22C	0.9800
C6	-C7	1.506(3)	C22	-H22A	0.9804
C17	-C19	1.508(3)	C22	-H22B	0.9805

Table S6 - Bond Angles (Degrees)
for: S1886Z

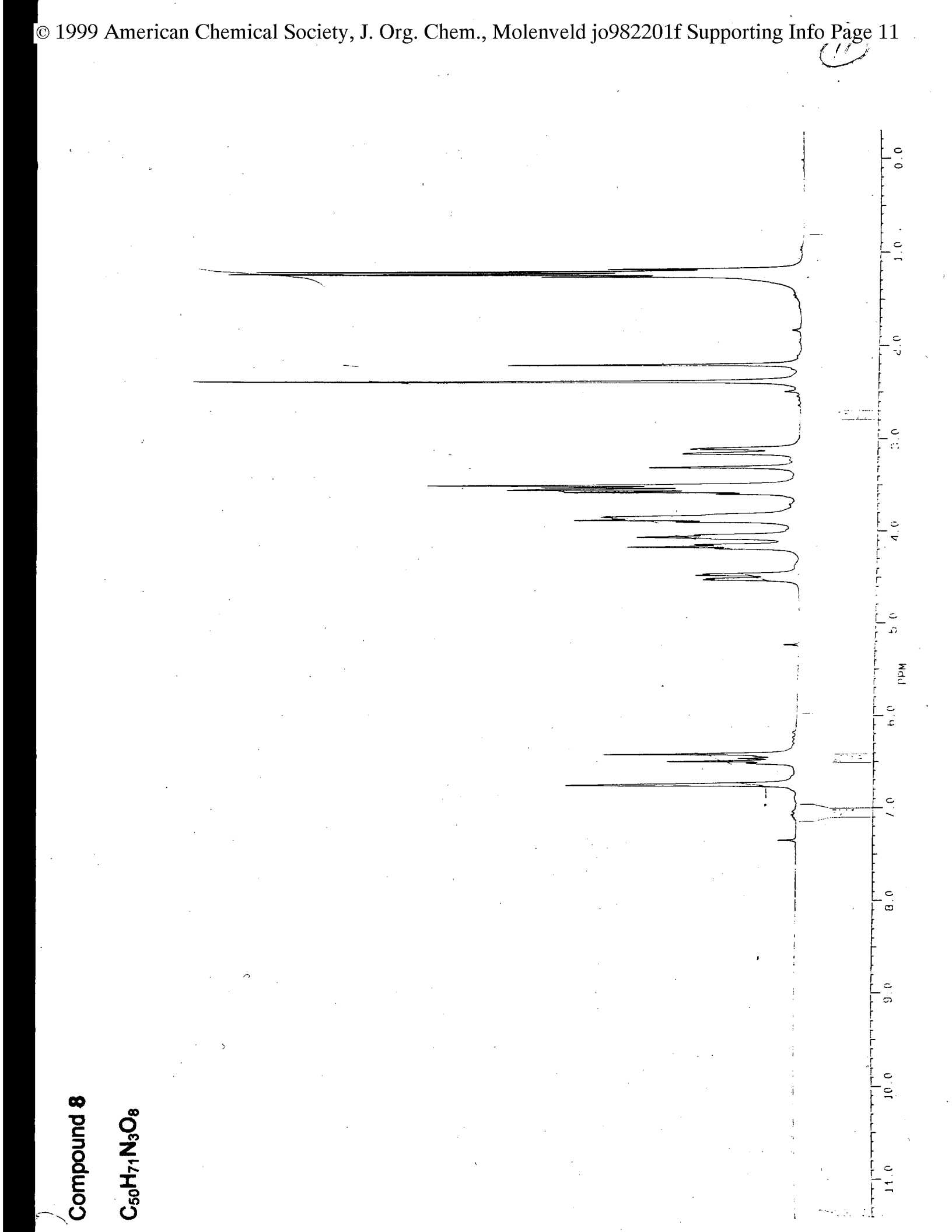
O16	-Zn15	-O20	103.66(10)	N1	-C2	-C11	115.39(19)
O16	-Zn15	-N1	124.65(11)	C3	-C2	-C11	123.25(19)
O16	-Zn15	-N8	96.85(10)	N1	-C2	-C3	121.30(19)
O16	-Zn15	-N12	98.71(10)	C2	-C3	-C4	118.67(19)
O20	-Zn15	-N1	131.56(10)	C3	-C4	-C5	119.6(2)
O20	-Zn15	-N8	95.69(10)	C4	-C5	-C6	118.7(2)
O20	-Zn15	-N12	101.33(10)	N1	-C6	-C7	115.34(19)
N1	-Zn15	-N8	76.79(10)	C5	-C6	-C7	123.4(2)
N1	-Zn15	-N12	76.67(10)	N1	-C6	-C5	121.21(19)
N8	-Zn15	-N12	153.46(10)	N8	-C7	-C6	110.69(19)
Zn15	-O16	-C17	119.18(15)	N12	-C11	-C2	111.43(17)
Zn15	-O20	-C21	110.46(15)	O16	-C17	-O18	124.0(2)
H23A	-O23	-H23B	108(4)	O16	-C17	-C19	115.3(2)
Zn15	-N1	-C6	119.57(15)	O18	-C17	-C19	120.7(2)
C2	-N1	-C6	120.48(19)	O20	-C21	-O21	123.5(2)
Zn15	-N1	-C2	119.94(15)	O20	-C21	-C22	116.2(2)
Zn15	-N8	-C9	114.64(15)	O21	-C21	-C22	120.3(2)
Zn15	-N8	-C10	108.15(15)	C4	-C3	-H3	120.69
Zn15	-N8	-C7	104.40(14)	C2	-C3	-H3	120.65
C7	-N8	-C10	109.62(18)	C3	-C4	-H4	120.20
C9	-N8	-C10	109.2(2)	C5	-C4	-H4	120.21
C7	-N8	-C9	110.6(2)	C4	-C5	-H5	120.63
Zn15	-N12	-C11	104.57(14)	C6	-C5	-H5	120.64
Zn15	-N12	-C13	106.39(15)	N8	-C7	-H7B	109.51
C11	-N12	-C13	110.1(2)	C6	-C7	-H7A	109.54
C11	-N12	-C14	109.59(19)	C6	-C7	-H7B	109.51
Zn15	-N12	-C14	116.76(17)	H7A	-C7	-H7B	108.04
C13	-N12	-C14	109.27(19)	N8	-C7	-H7A	109.50

Table S6 - Bond Angles (Degrees) (continued)
for: S1886Z

N8	-C9	-H9B	109.44	H13B	-C13	-H13C	109.49
N8	-C9	-H9C	109.48	N12	-C13	-H13C	109.49
N8	-C9	-H9A	109.51	N12	-C14	-H14B	109.49
H9A	-C9	-H9C	109.46	N12	-C14	-H14C	109.44
H9B	-C9	-H9C	109.47	N12	-C14	-H14A	109.52
H9A	-C9	-H9B	109.46	H14A	-C14	-H14C	109.40
N8	-C10	-H10A	109.46	H14B	-C14	-H14C	109.52
N8	-C10	-H10C	109.47	H14A	-C14	-H14B	109.45
H10A	-C10	-H10B	109.47	C17	-C19	-H19A	109.51
N8	-C10	-H10B	109.50	C17	-C19	-H19B	109.48
H10B	-C10	-H10C	109.53	H19A	-C19	-H19B	109.46
H10A	-C10	-H10C	109.40	H19A	-C19	-H19C	109.46
N12	-C11	-H11B	109.33	C17	-C19	-H19C	109.45
C2	-C11	-H11A	109.38	H19B	-C19	-H19C	109.46
C2	-C11	-H11B	109.36	C21	-C22	-H22B	109.49
H11A	-C11	-H11B	107.94	C21	-C22	-H22C	109.53
N12	-C11	-H11A	109.33	C21	-C22	-H22A	109.48
N12	-C13	-H13A	109.47	H22A	-C22	-H22C	109.50
N12	-C13	-H13B	109.47	H22B	-C22	-H22C	109.42
H13A	-C13	-H13B	109.50	H22A	-C22	-H22B	109.41
H13A	-C13	-H13C	109.40				

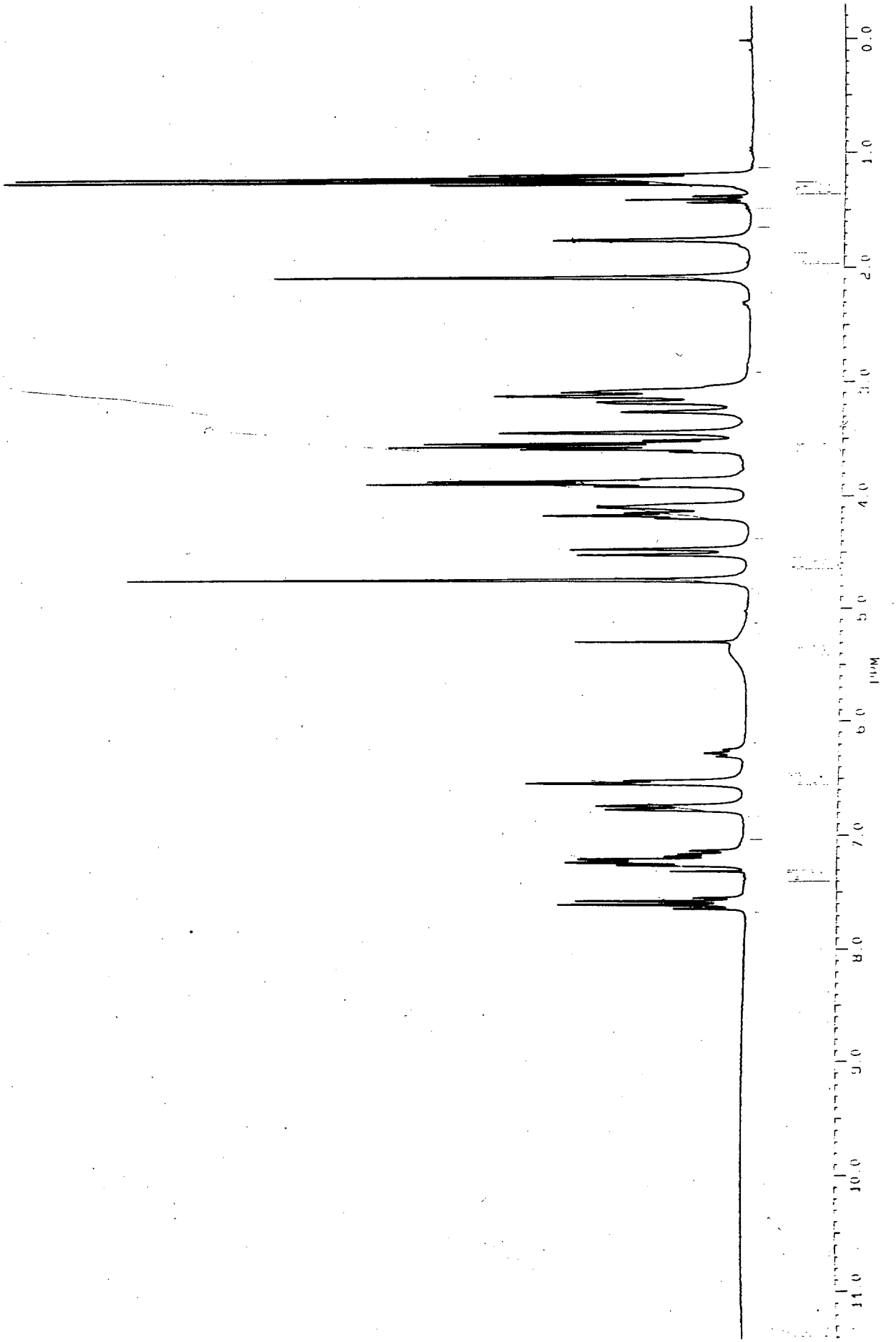
Table S7 - Hydrogen Bonds (Angstrom, Deg)
for: S1886Z

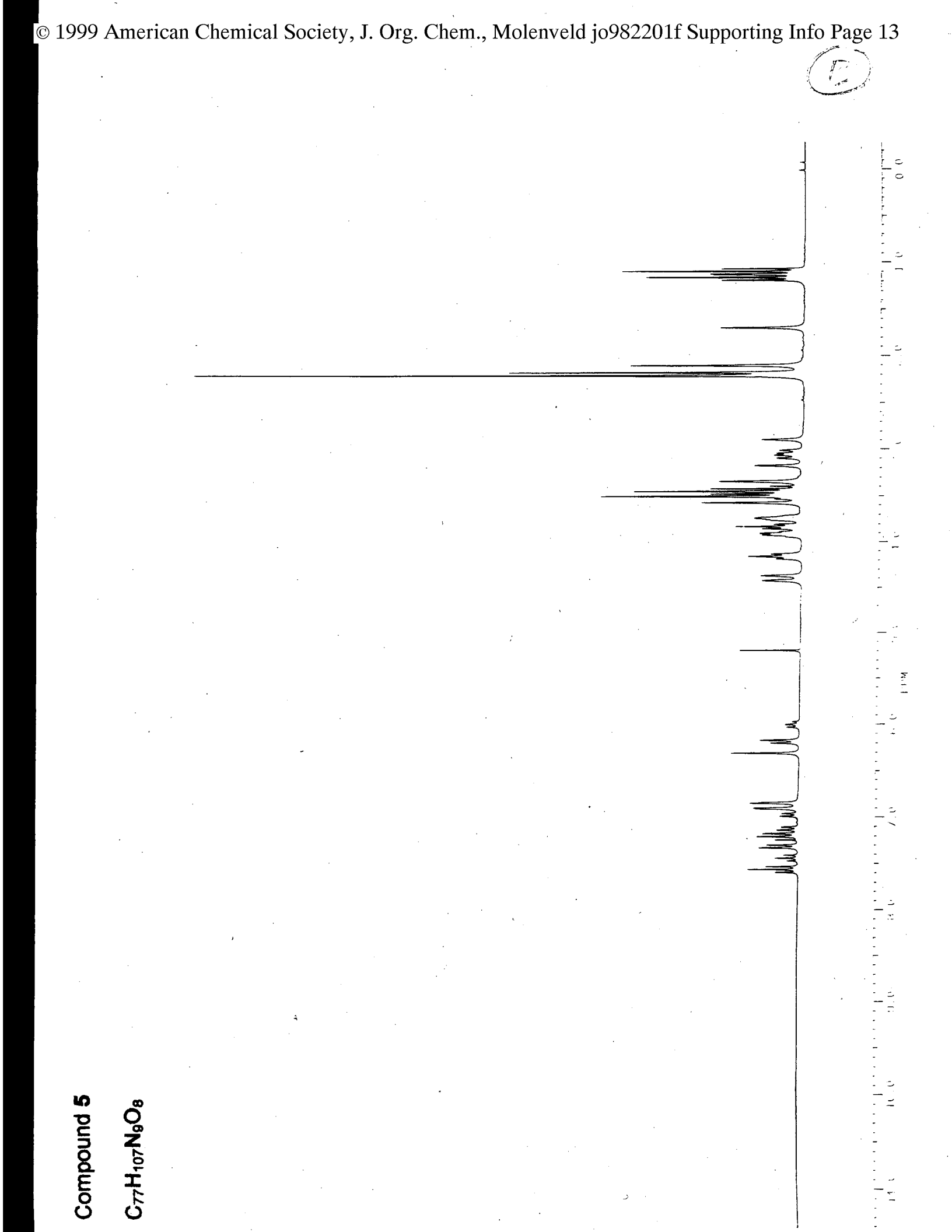
D	--	H	..	A	D-H	H .. A	D .. A	D--H .. A
O23	--	H23A	..	O20[x-1,y,z]	0.79(4)	2.18(4)	2.972(3)	177(4)
O23	--	H23B	..	O18	0.88(5)	2.00(5)	2.879(3)	176(3)

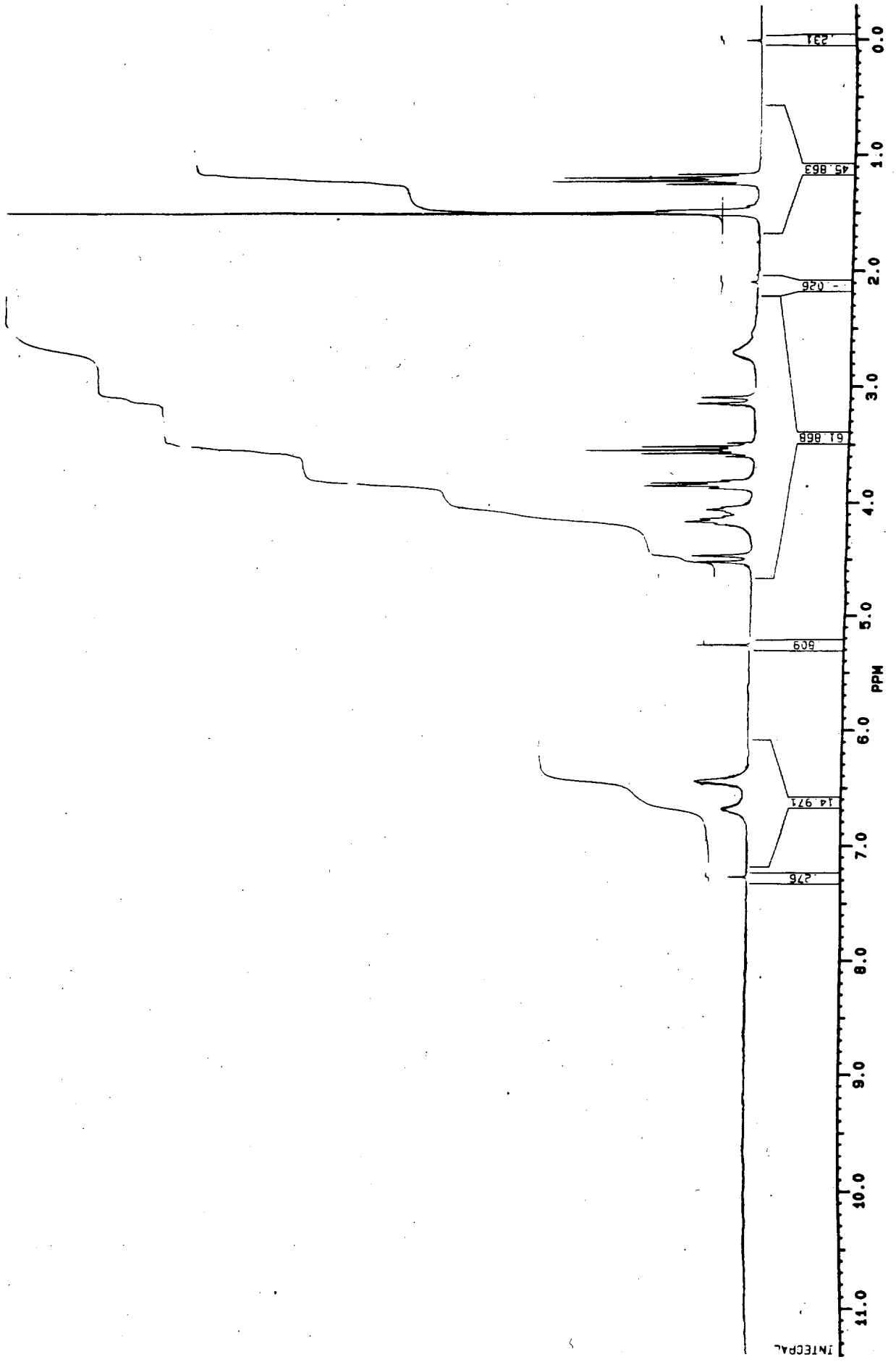


Compound 9

$C_{71}H_{92}N_8O_{11}$

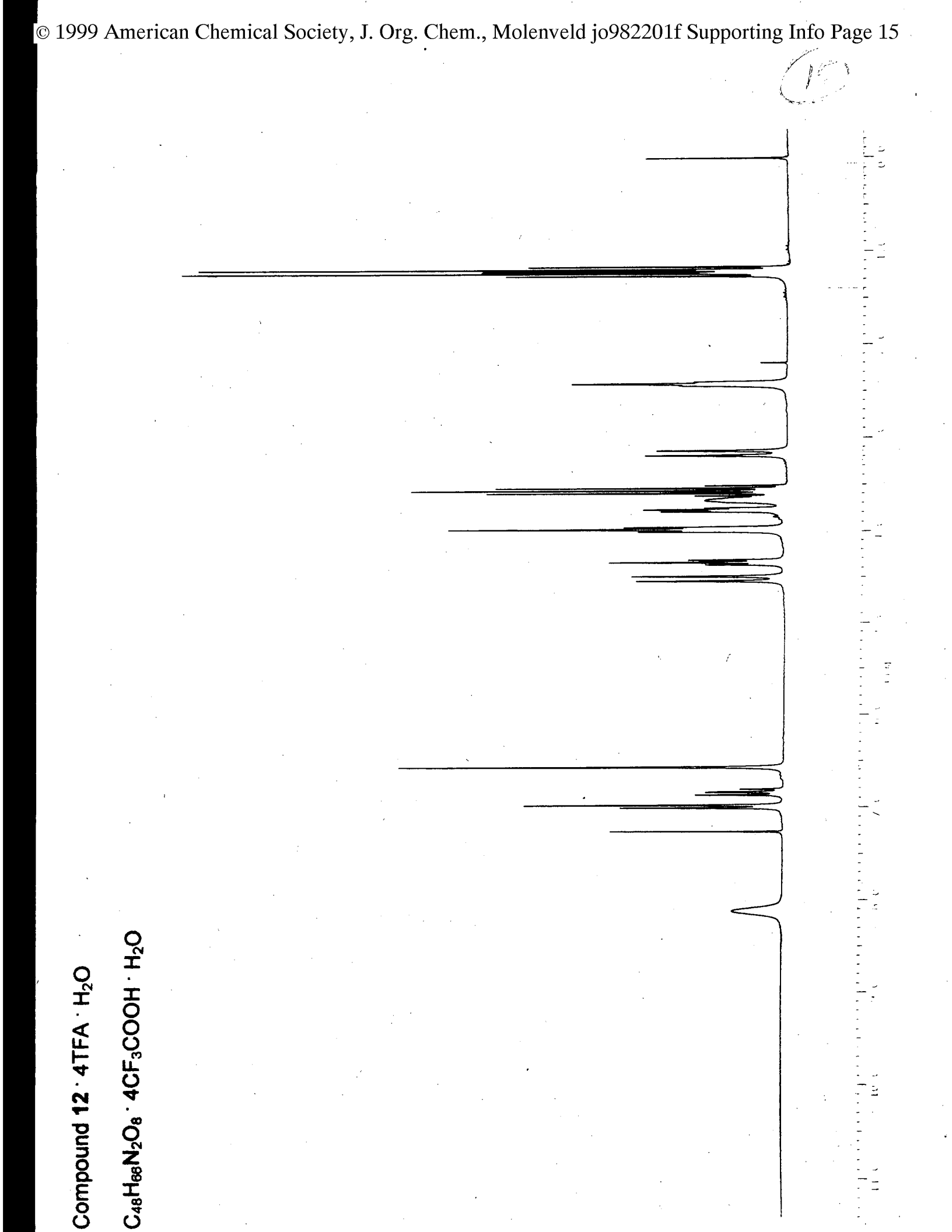






Compound 11

$C_{58}H_{82}N_2O_{12}$

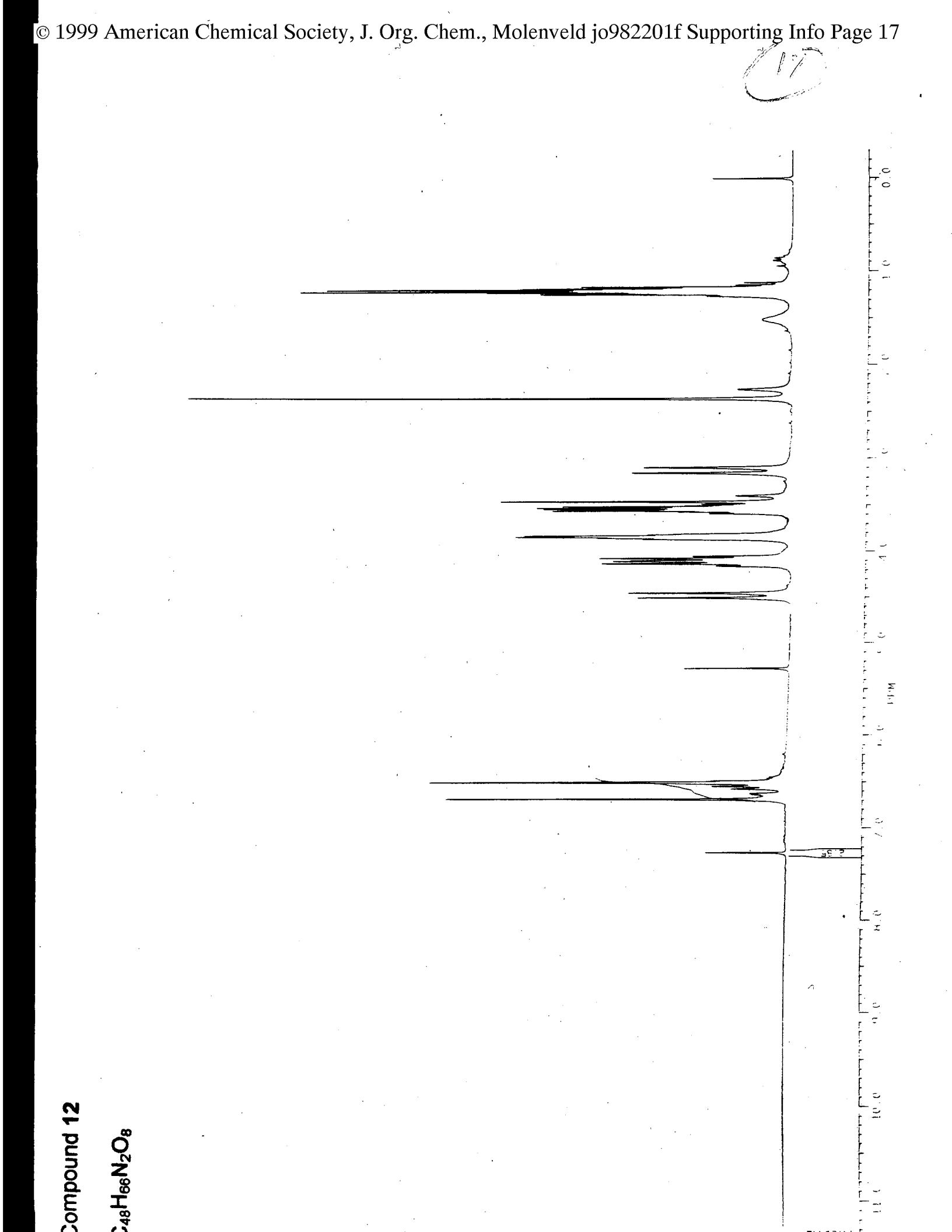


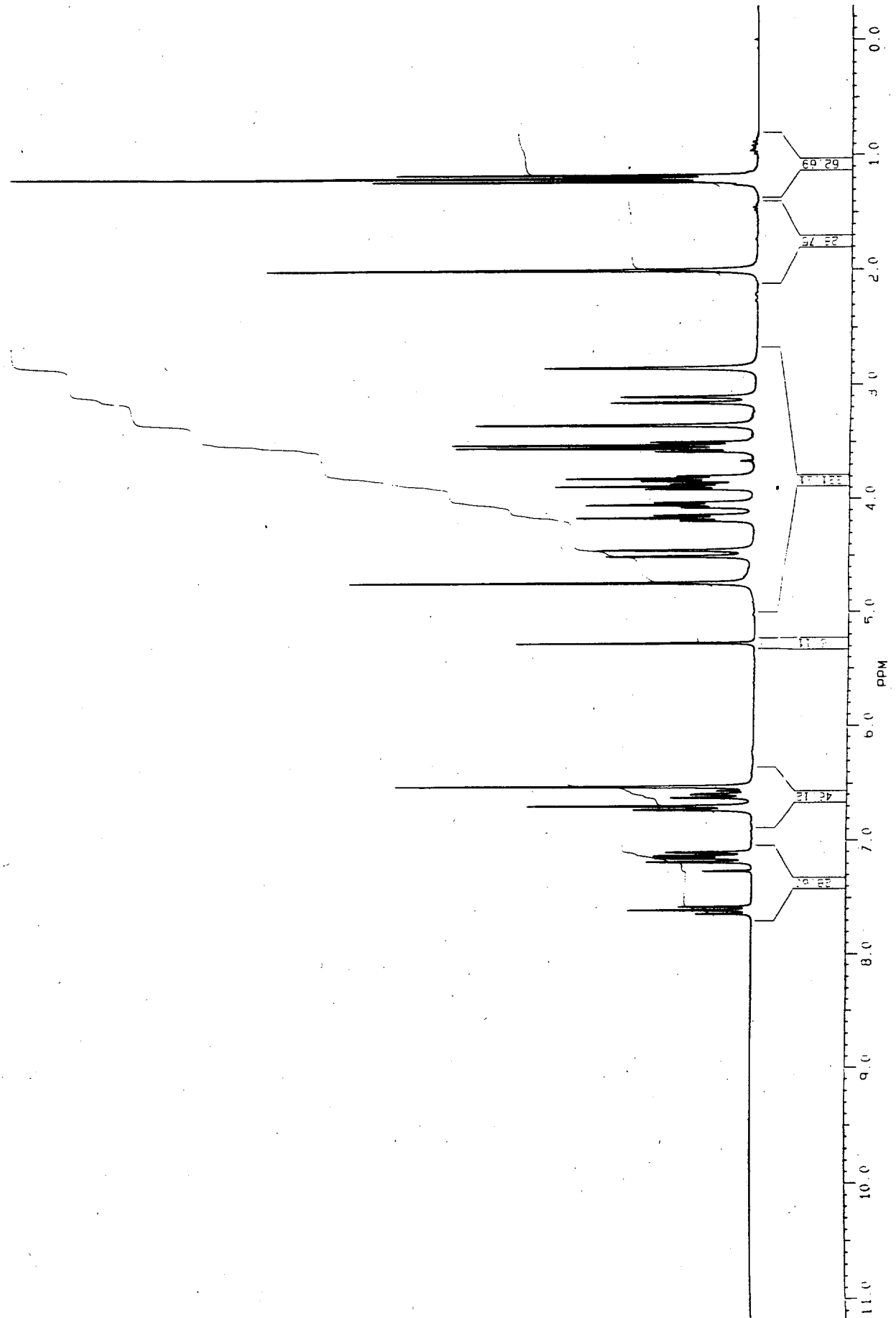
Compound **12** · 4TFA · H_2O

$C_{48}H_{68}N_2O_8 \cdot 4CF_3COOH \cdot H_2O$

Compound **12** · 4TFA · H_2O
(continued)

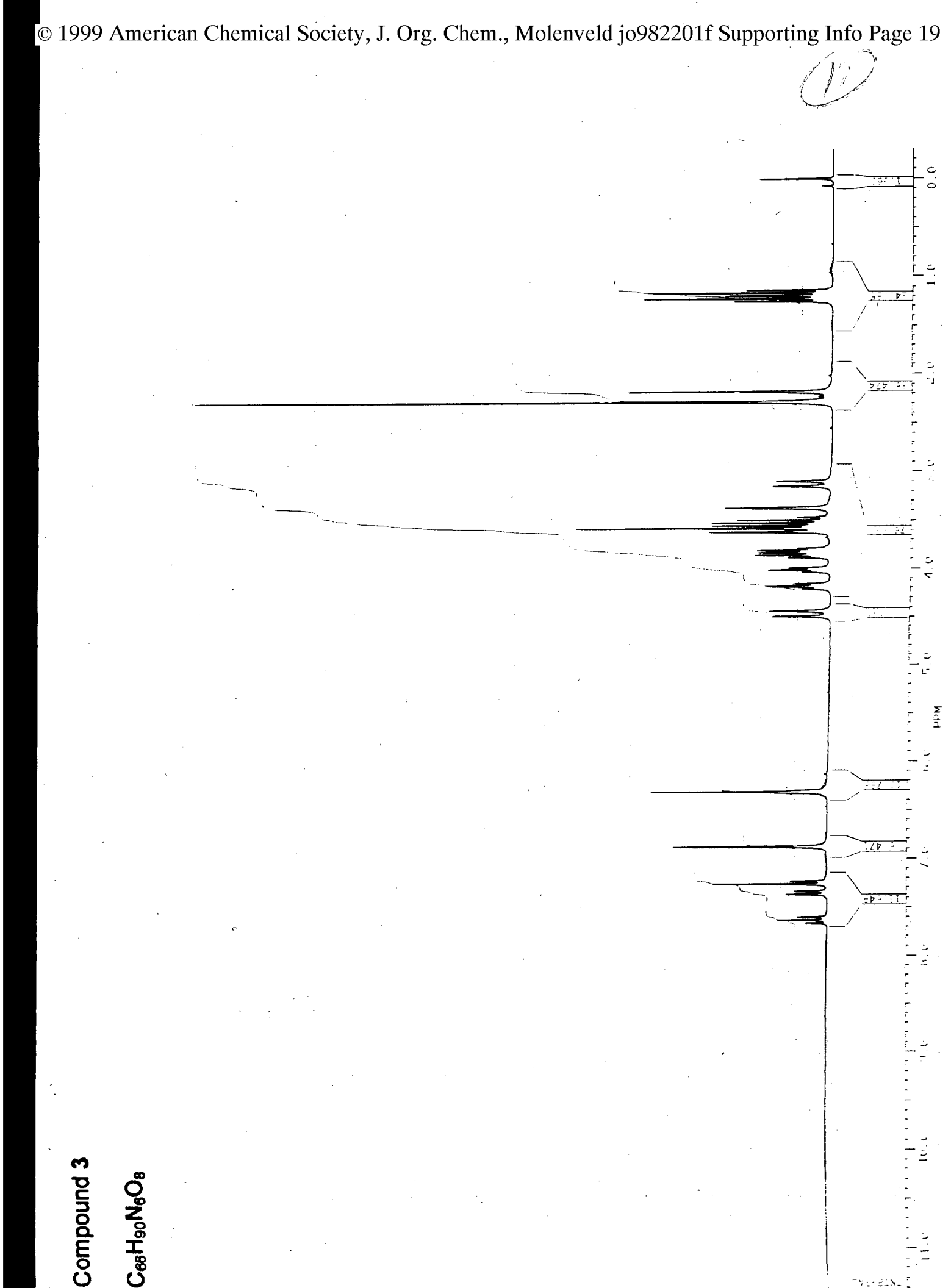
$C_{48}H_{66}N_2O_8 \cdot 4CF_3COOH \cdot H_2O$





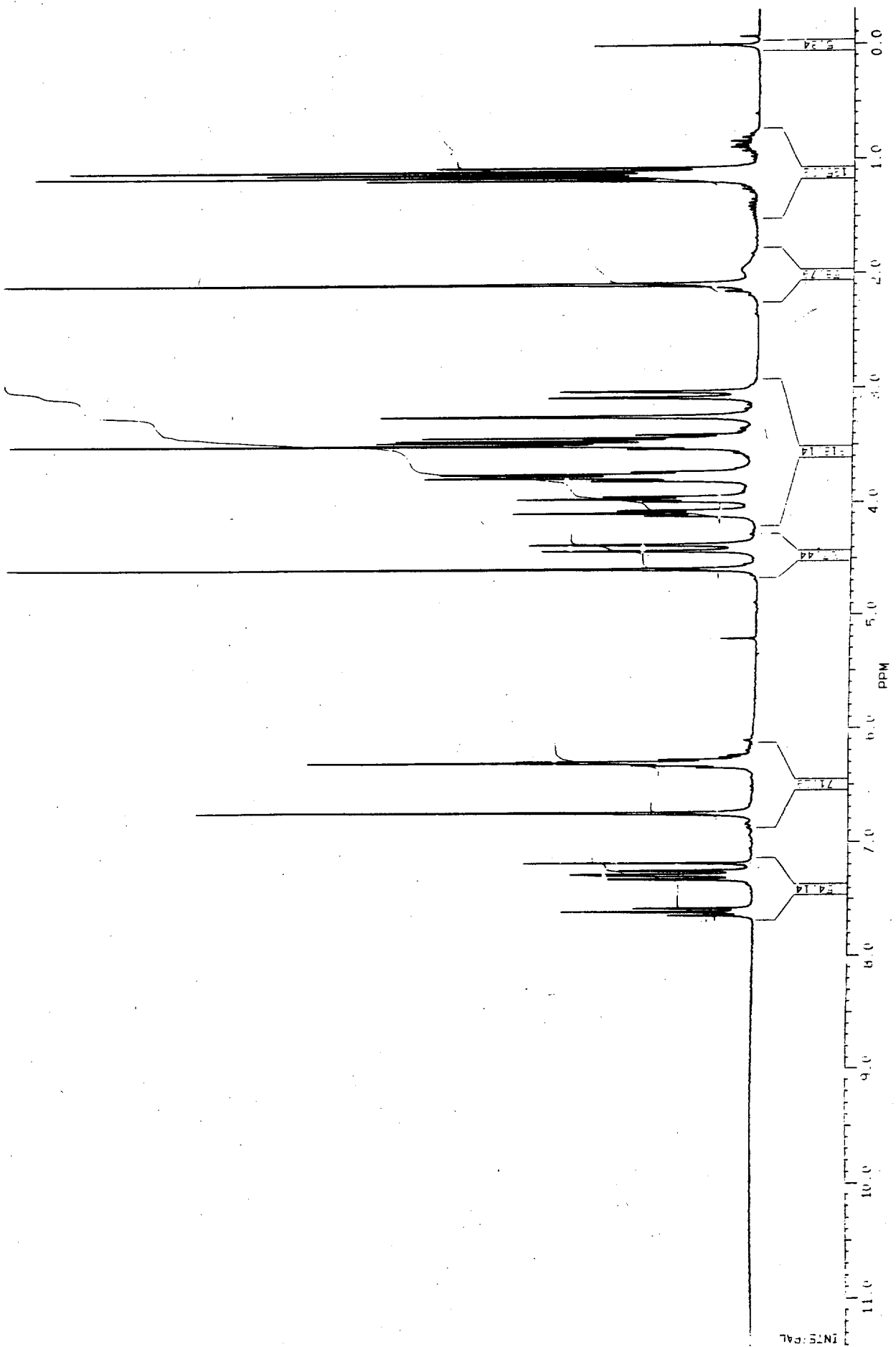
Compound 13

$C_{62}H_{80}N_4O_{10}$



Compound 3

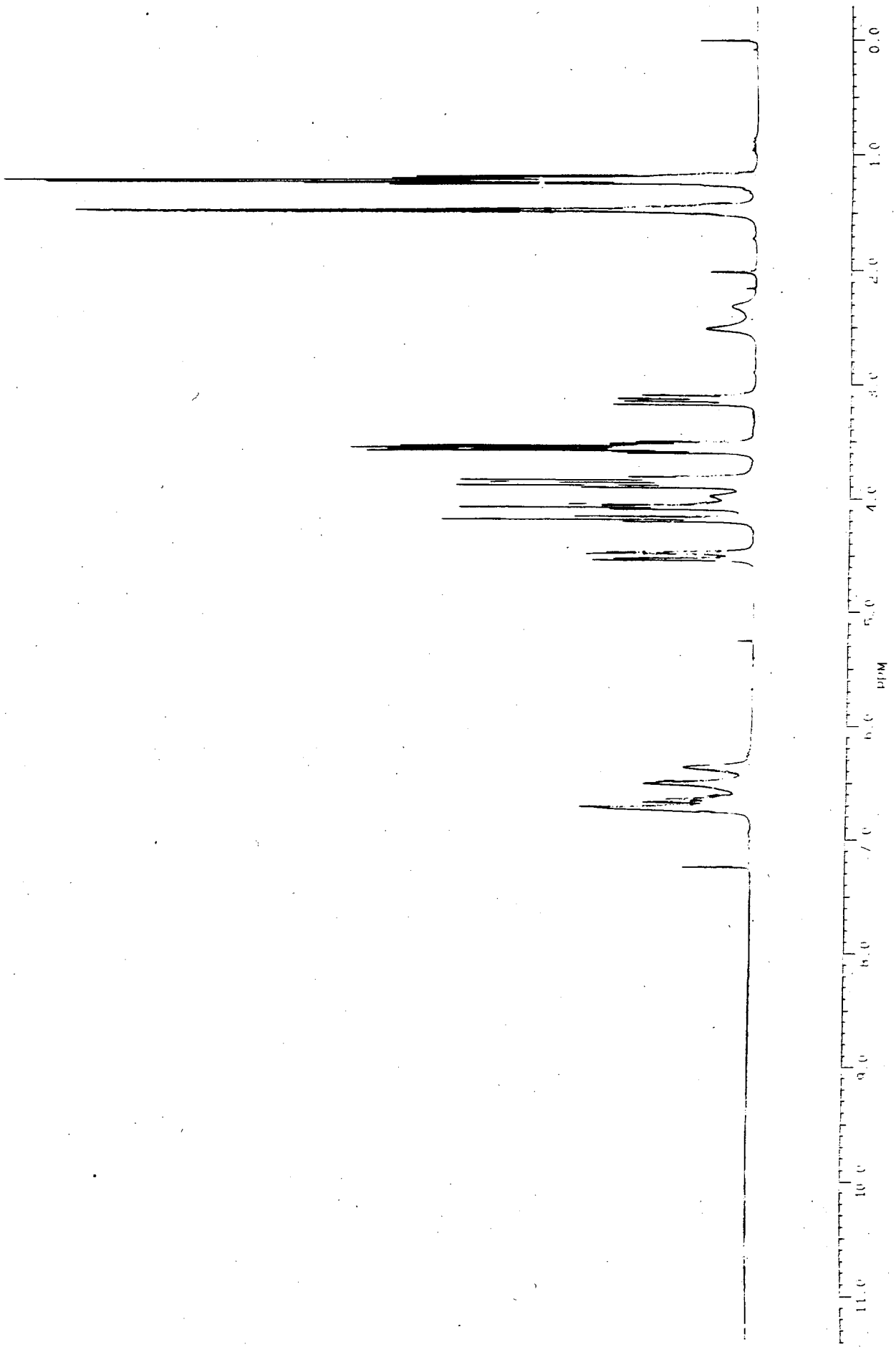
$C_{66}H_{90}N_6O_8$



Compound 14

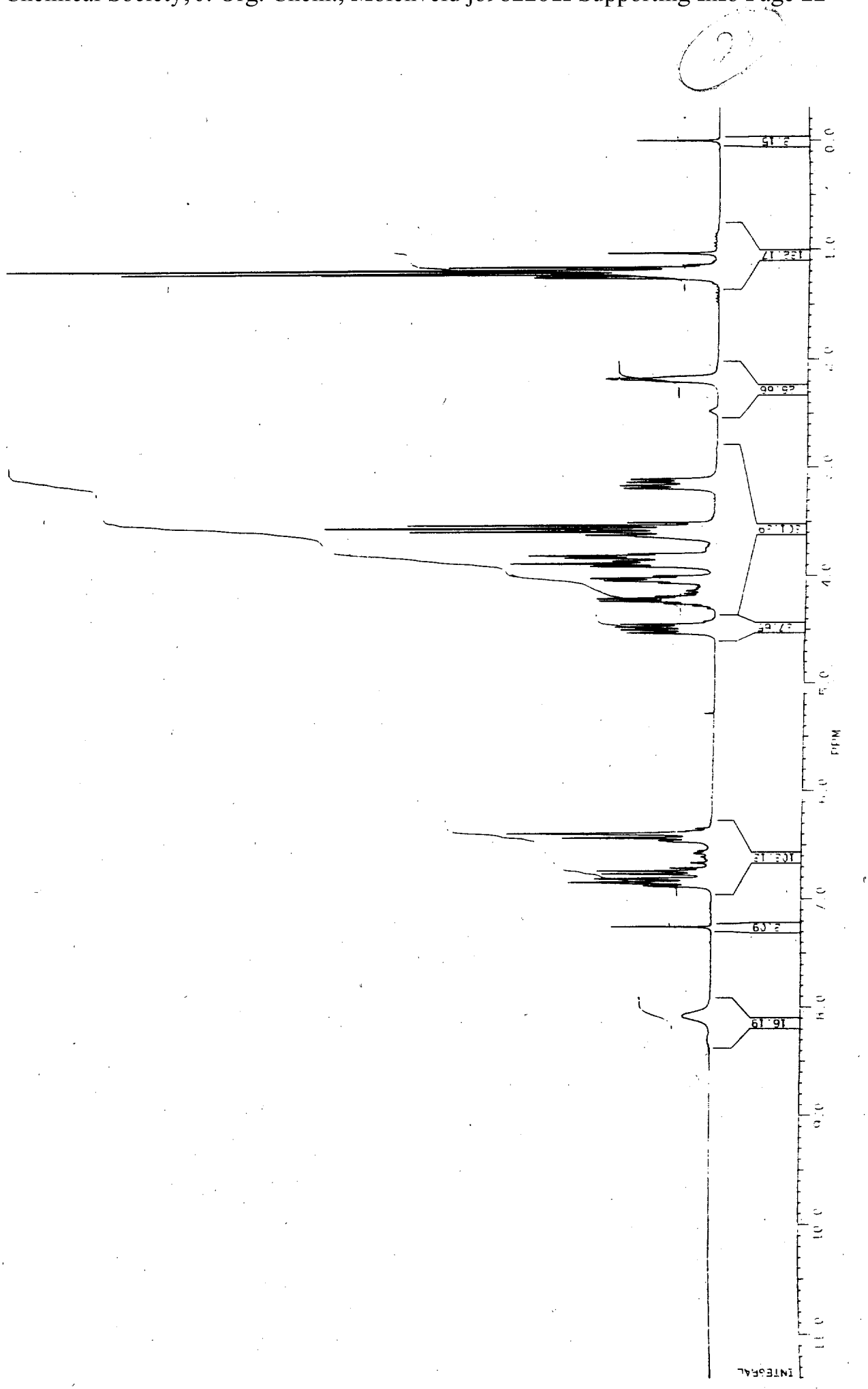
$C_{62}H_{78}N_4O_8Cl_2$

21



Compound 15

$C_{51}H_{69}NO_{10}$

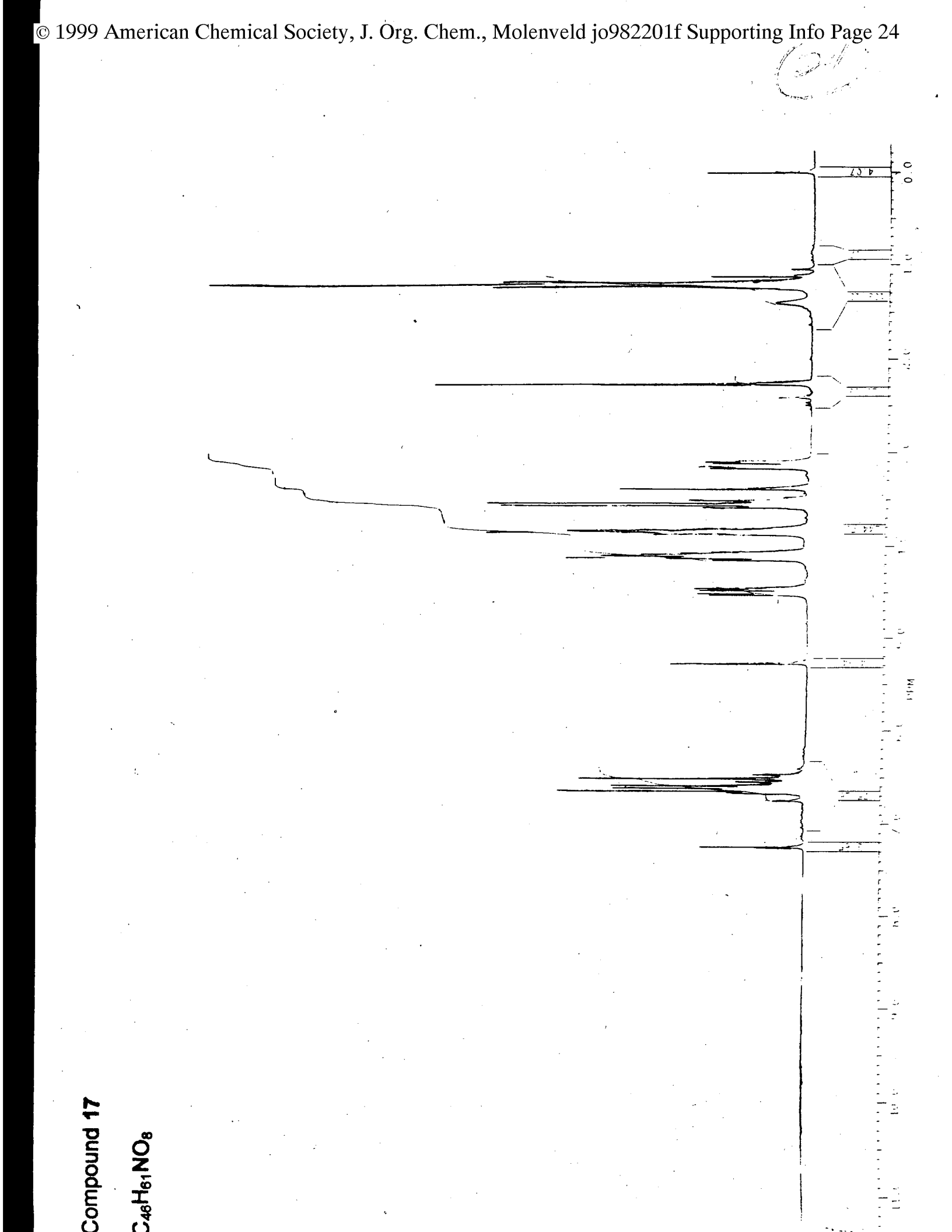


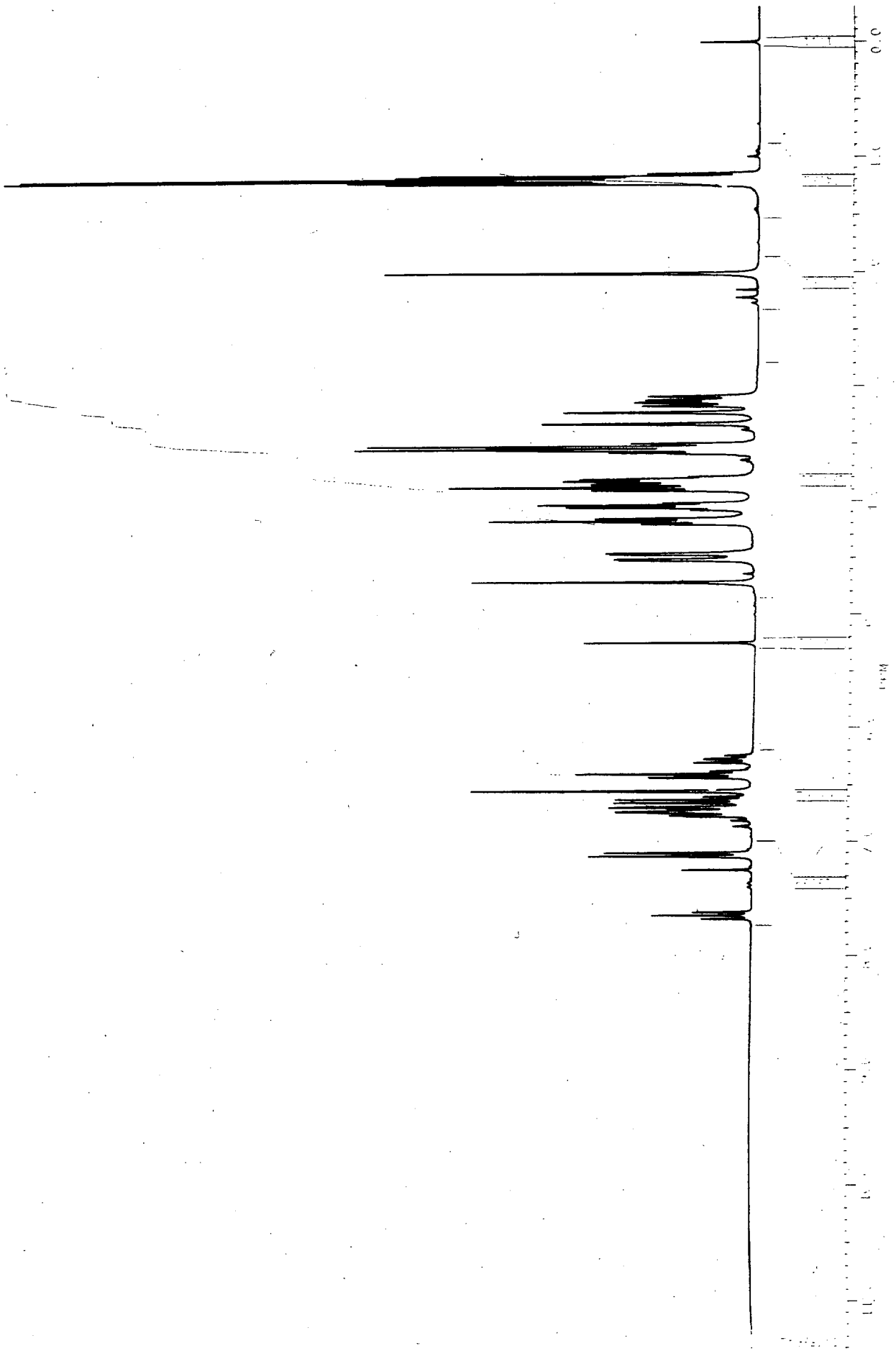
Compound **17** · 3TFA

$C_{46}H_{81}NO_8 \cdot 3CF_3COOH$

Compound 17 · 3TFA (continued)

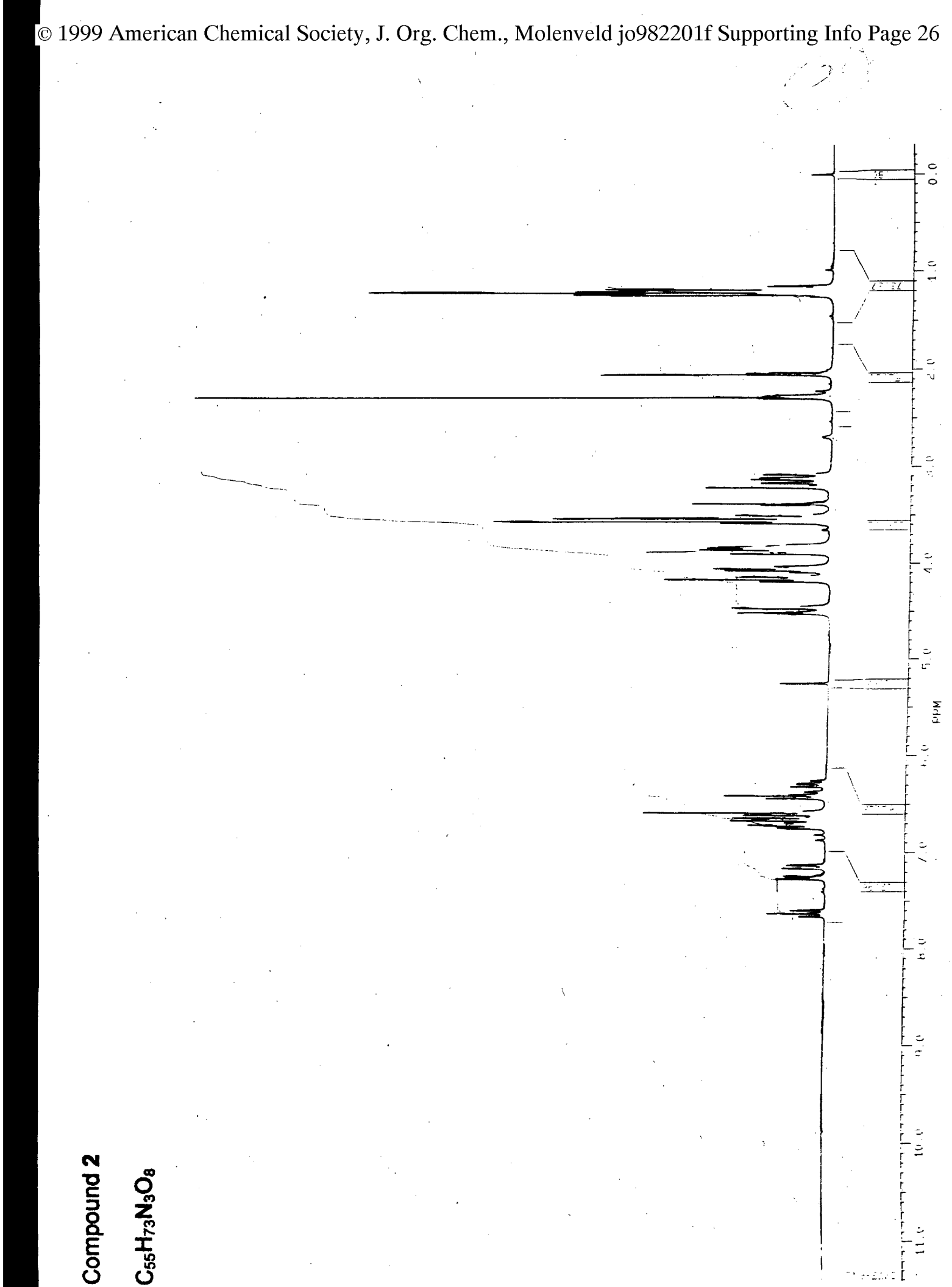
$C_{46}H_{61}NO_8 \cdot 3CF_3COOH$

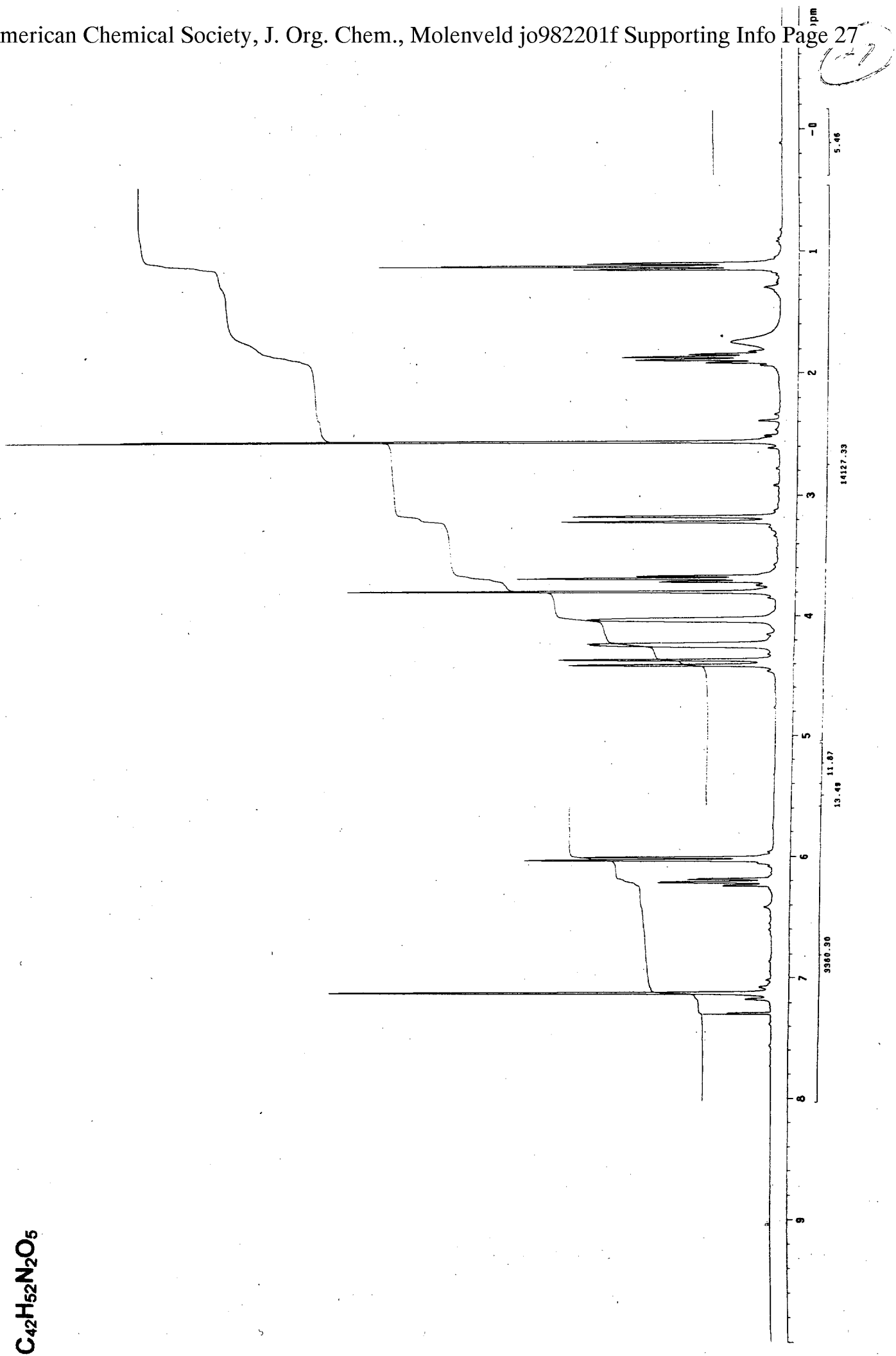




Compound 18

$C_{53}H_{88}N_2O_9$





Compound 19

$C_{42}H_{52}N_2O_5$