JOC The Journal of Organic Chemistry

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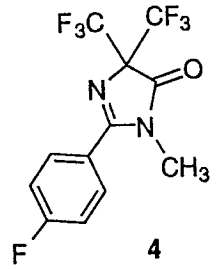


ACS Publications

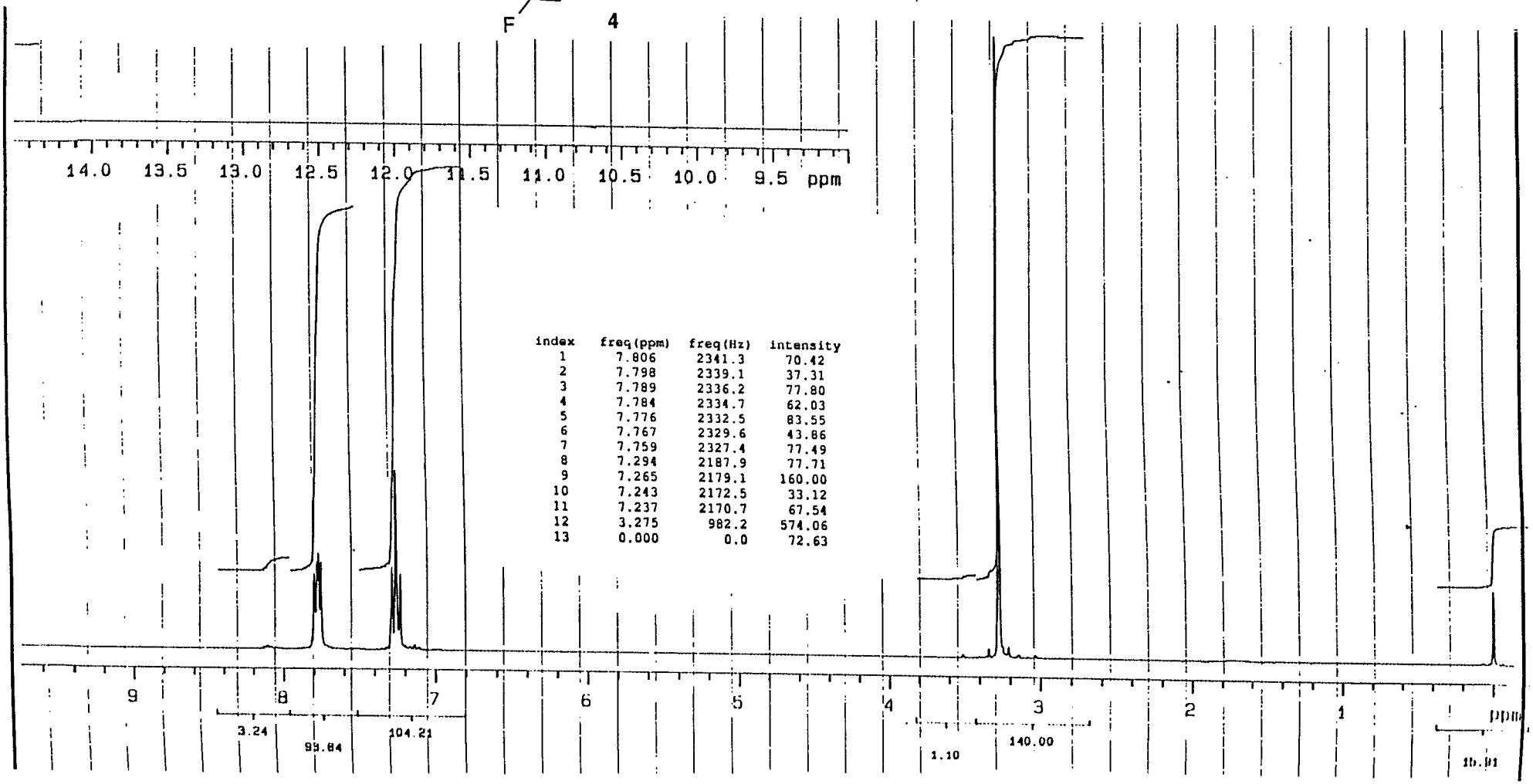
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^{1}H-NMR Spectrum of **4** (300 MHz, $CDCl_3$, TMS)



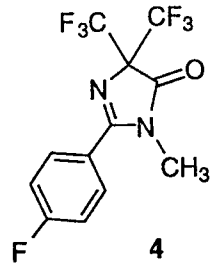
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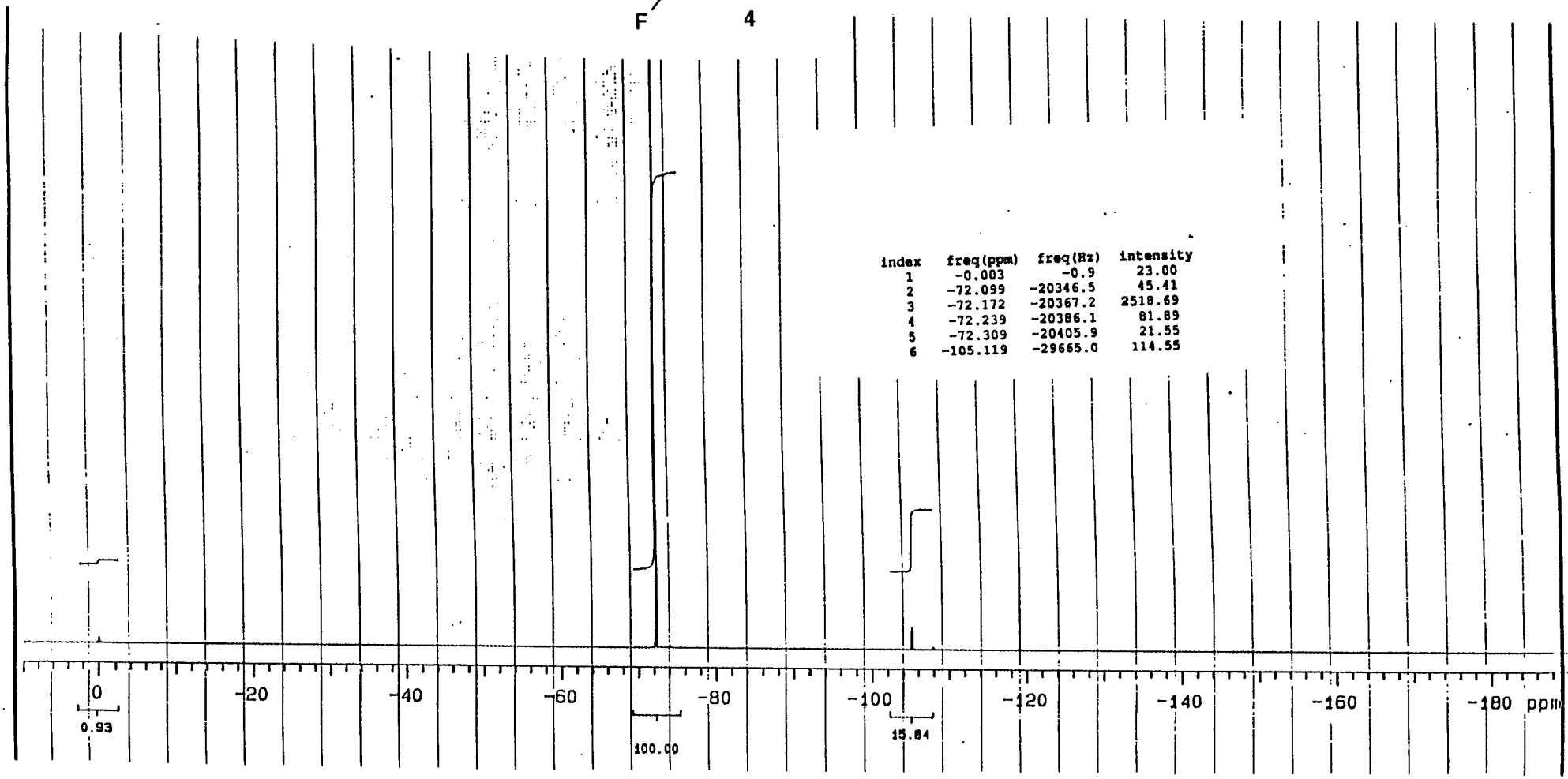
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5	7.776	2332.5	83.55
6	7.767	2329.6	43.86
7	7.759	2327.4	77.49
8	7.294	2187.9	77.71
9	7.265	2179.1	160.00
10	7.243	2172.5	33.12
11	7.237	2170.7	67.54
12	3.275	982.2	574.06
13	0.000	0.0	72.63

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^{19}F-NMR Spectrum of **4** (300 MHz, $CDCl_3$, $CFCl_3$)

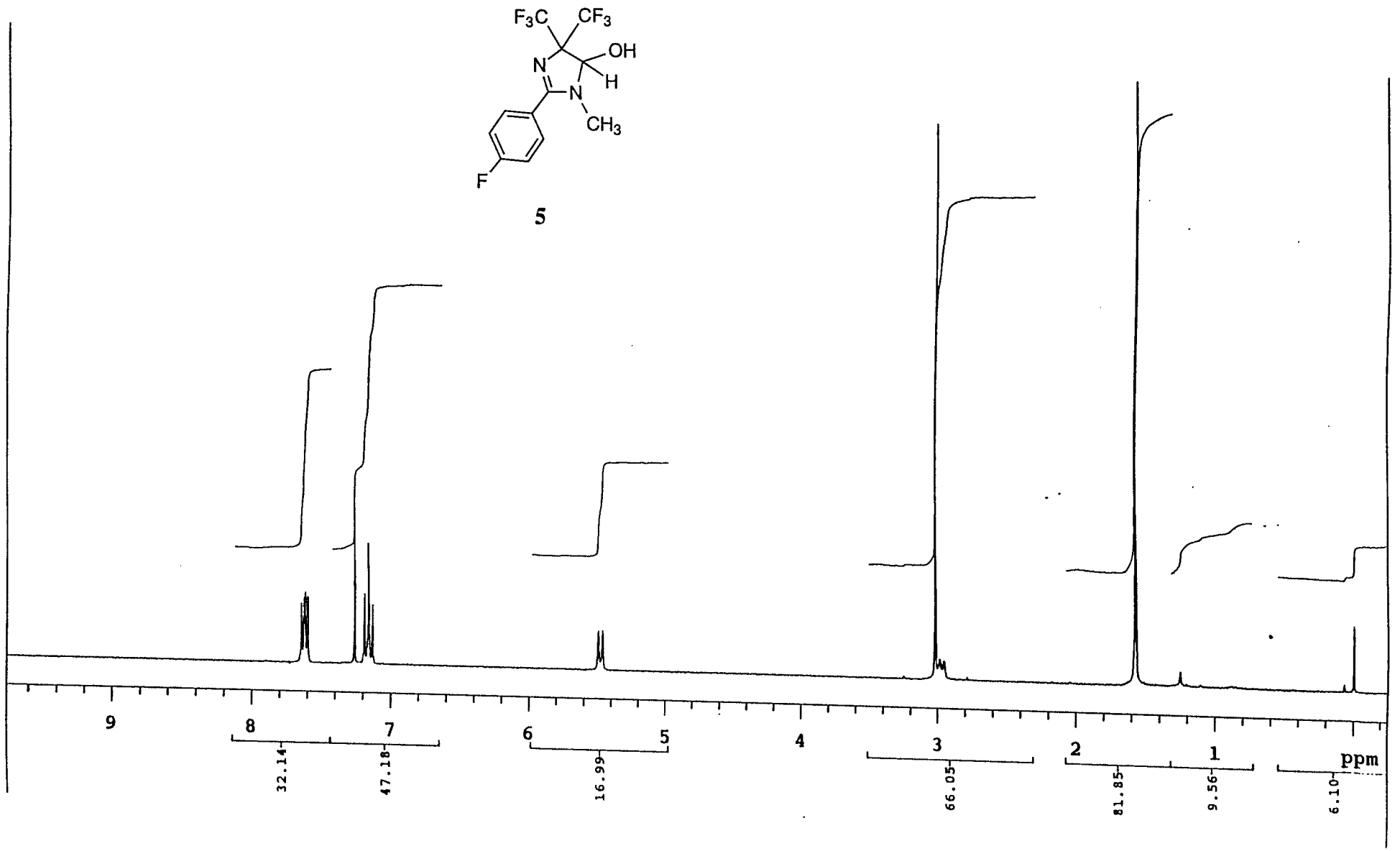


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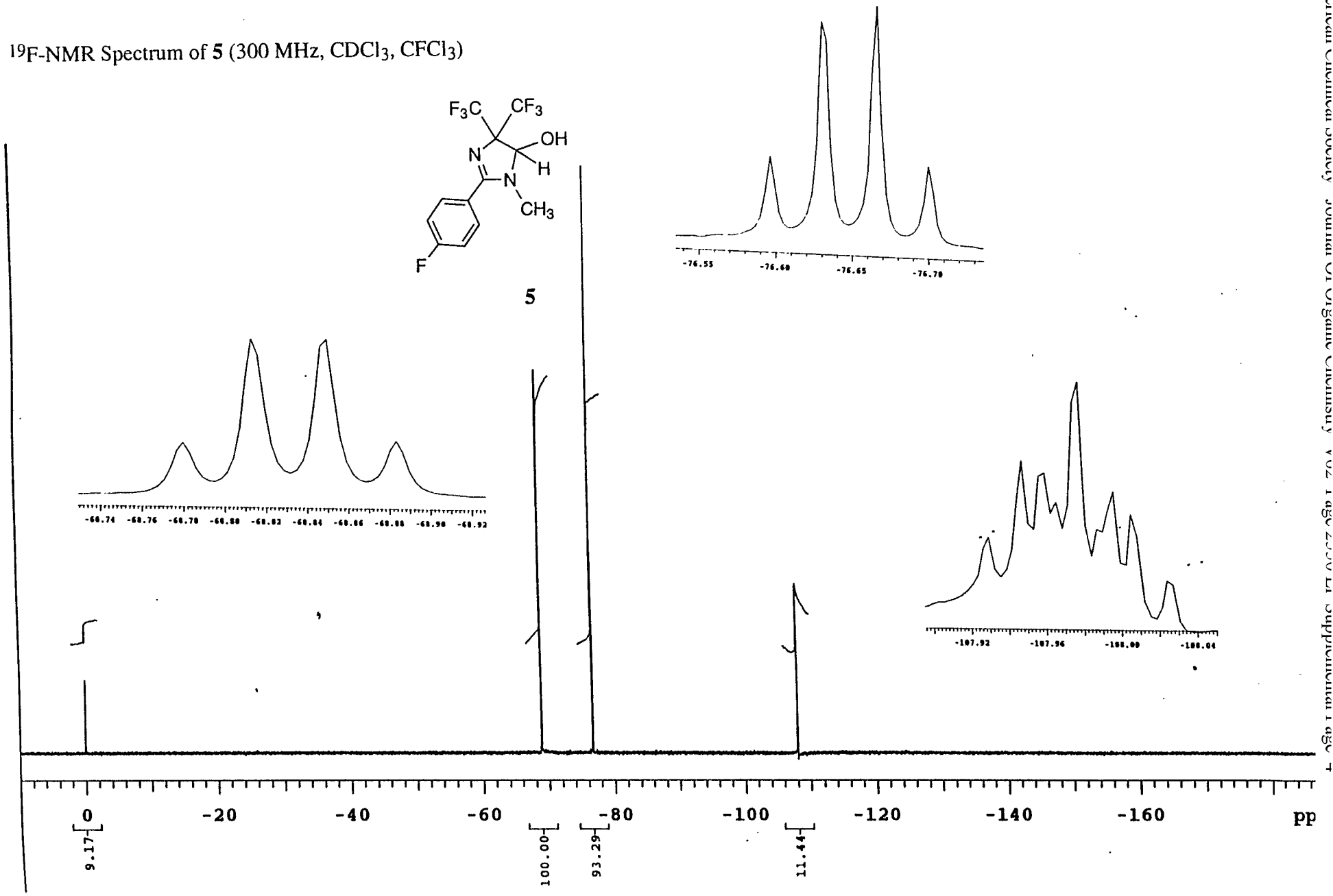
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^{1}H-NMR Spectrum of **5** (300 MHz, $CDCl_3$, TMS)



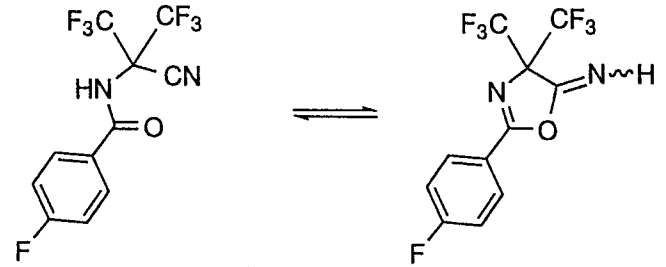
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^{19}F-NMR Spectrum of **5** (300 MHz, $CDCl_3$, $CFCl_3$)

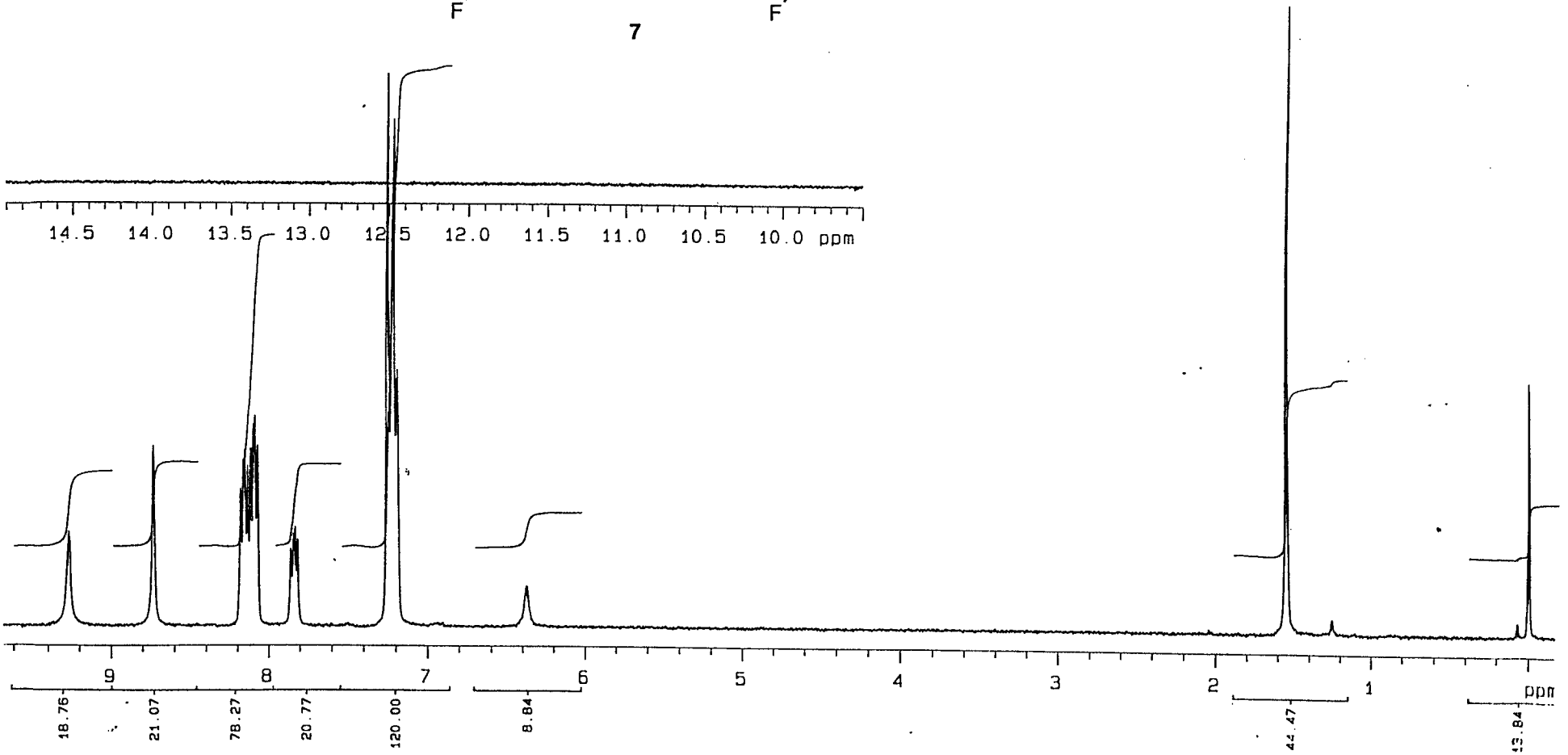


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^{1}H-NMR Spectrum of **7** (300 MHz, $CDCl_3$, TMS)

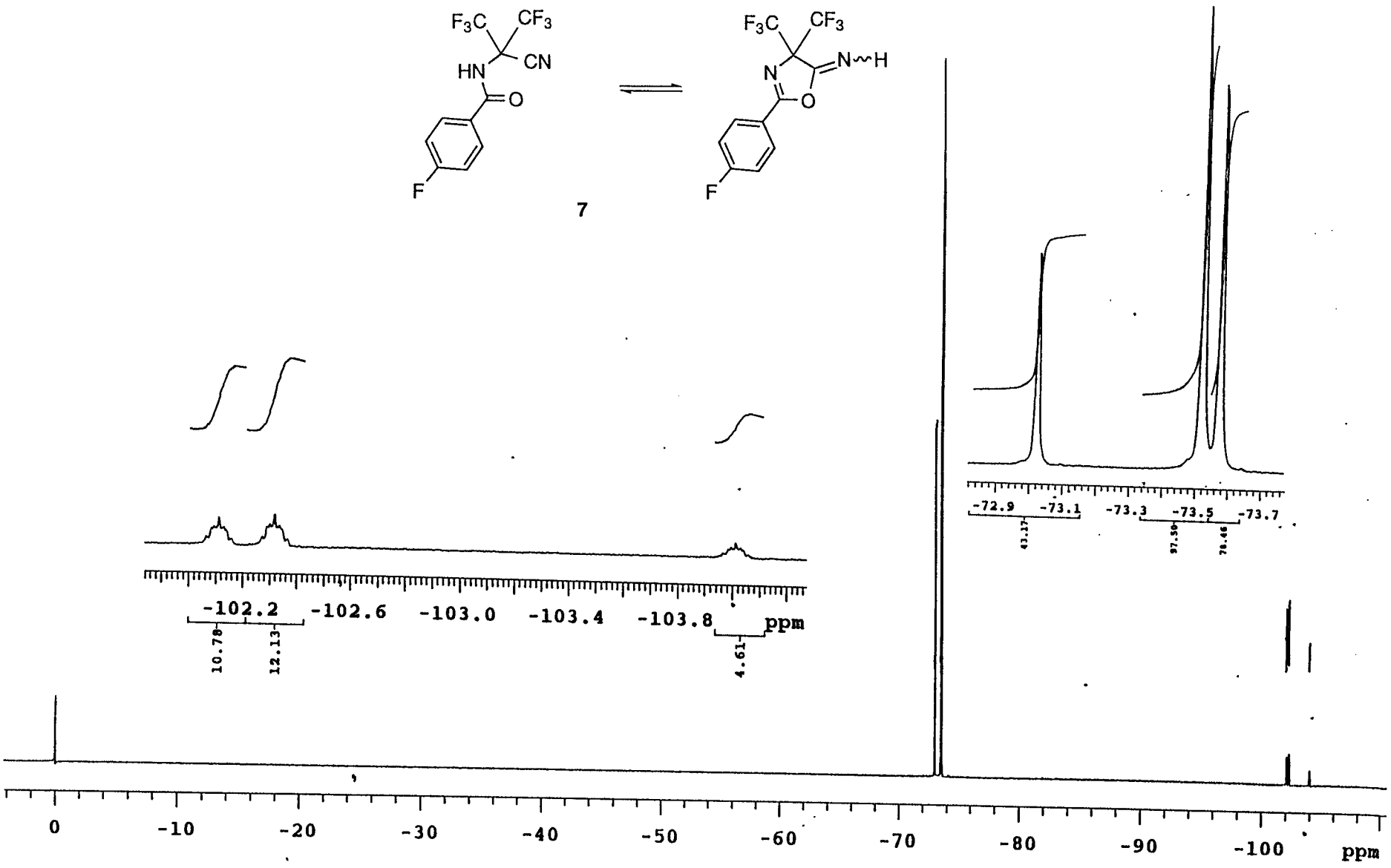


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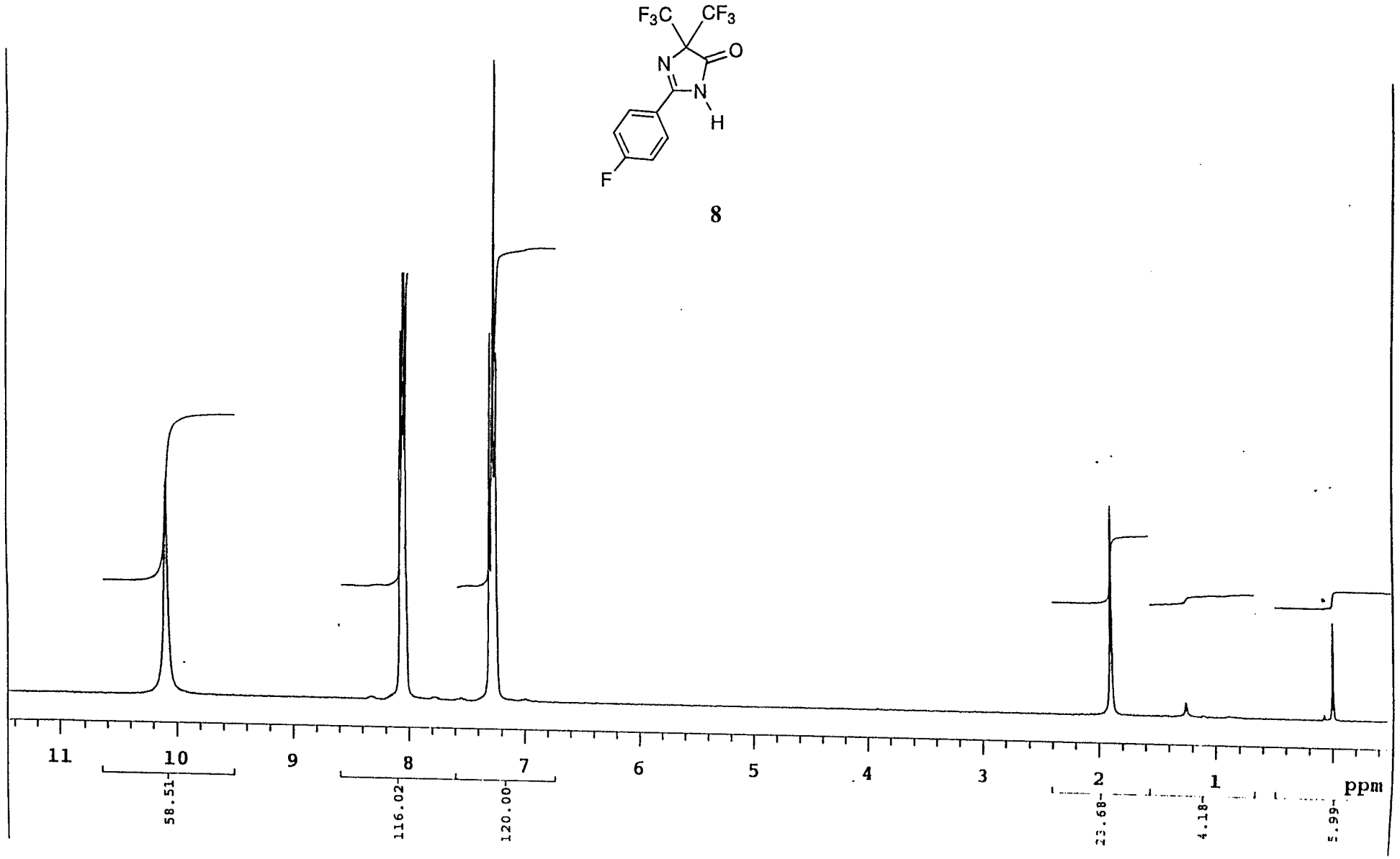
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^{19}F-NMR Spectrum of **7** (300 MHz, $CDCl_3$, $CFCl_3$)



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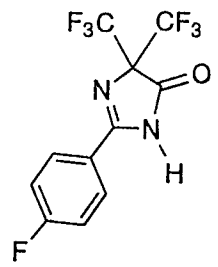
^{1}H-NMR Spectrum of **8** (300 MHz, $CDCl_3$, TMS)



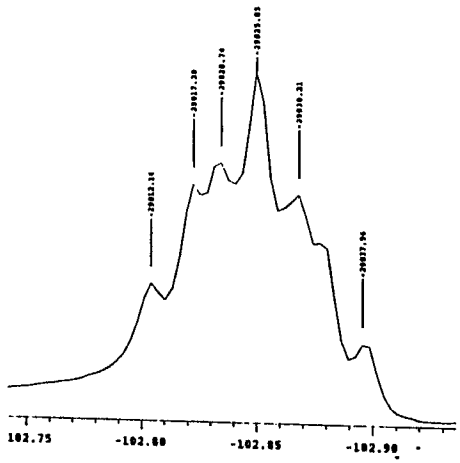
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^{19}F-NMR Spectrum of **8** (300 MHz, $CDCl_3$, $CFCl_3$)



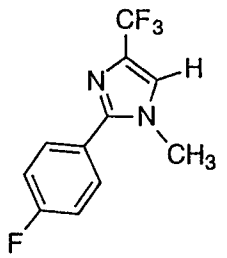
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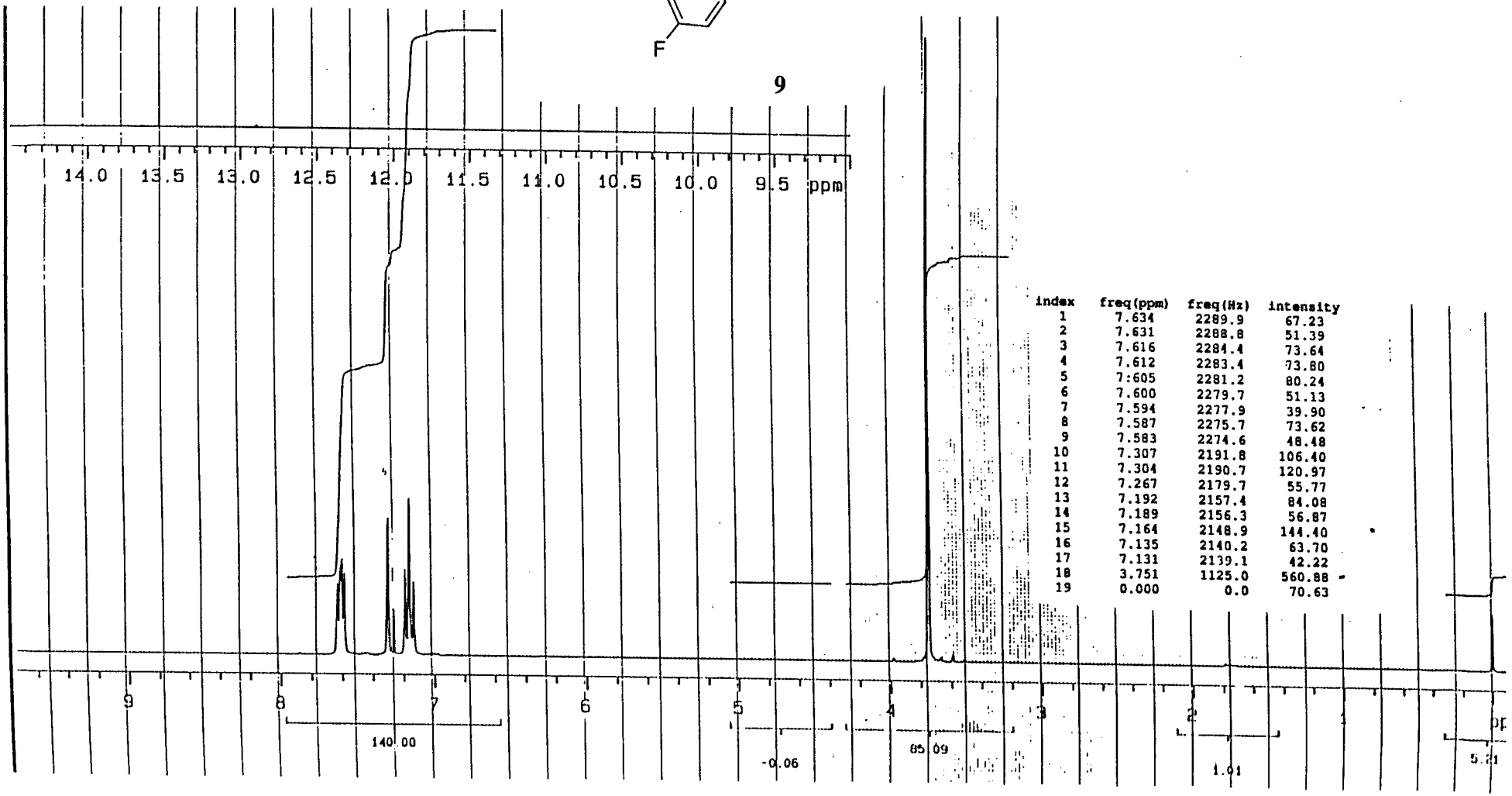
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^{1}H-NMR Spectrum of **9** (300 MHz, $CDCl_3$, TMS)



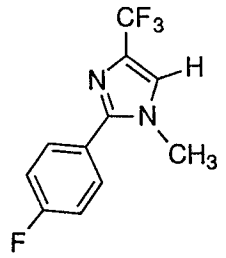
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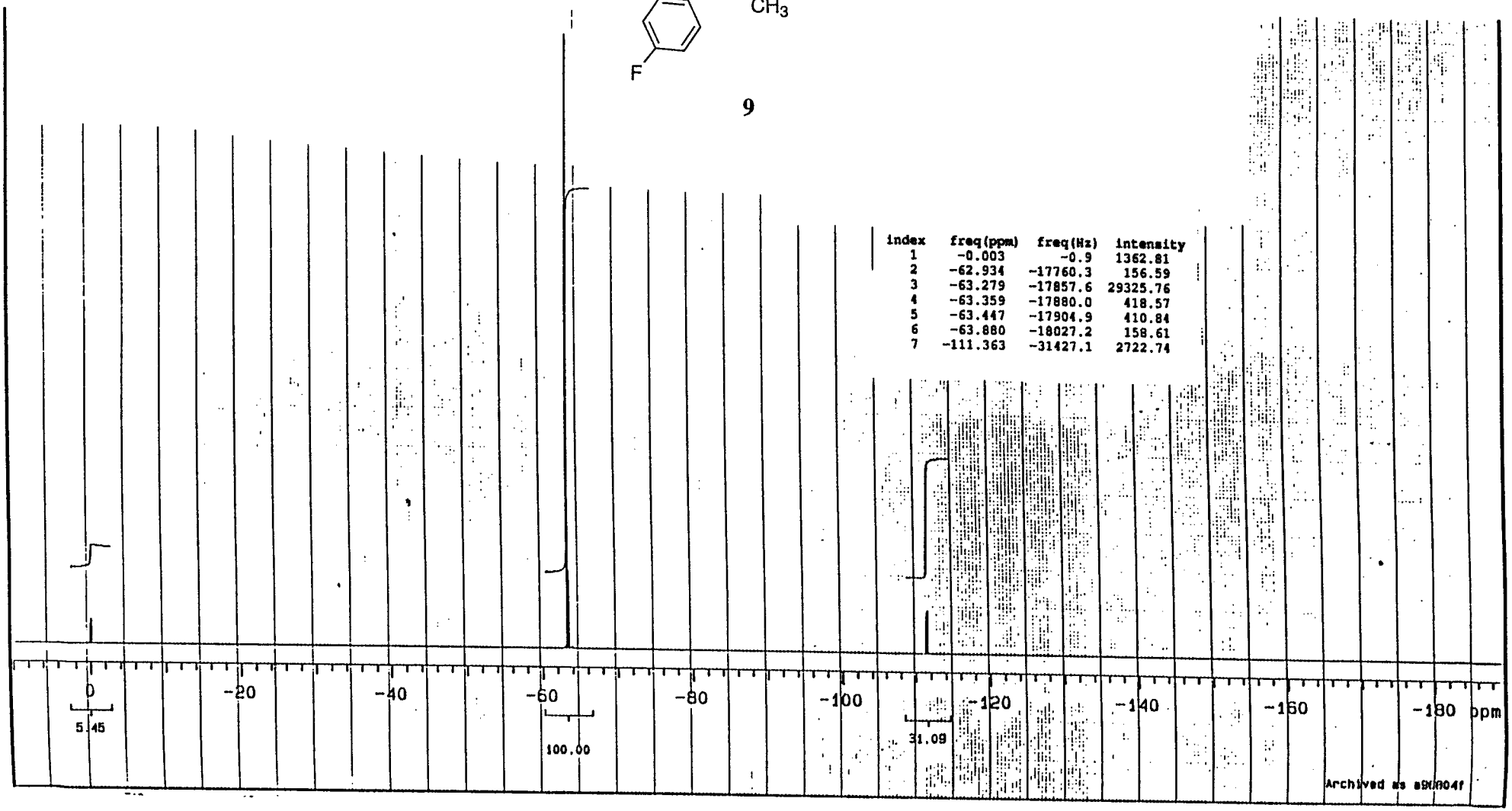
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6	7.600	2279.7	51.13
7	7.594	2277.9	39.90
8	7.587	2275.7	73.62
9	7.583	2274.6	48.48
10	7.307	2191.8	106.40
11	7.304	2190.7	120.97
12	7.267	2179.7	55.77
13	7.192	2157.4	84.08
14	7.189	2156.3	56.87
15	7.164	2148.9	144.40
16	7.135	2140.2	63.70
17	7.131	2139.1	42.22
18	3.751	1125.0	560.88
19	0.000	0.0	70.63

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^{19}F-NMR Spectrum of **9** (300 MHz, $CDCl_3$, $CFCl_3$)

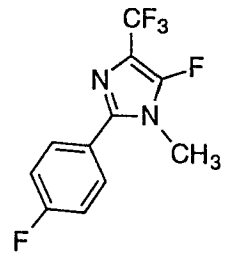


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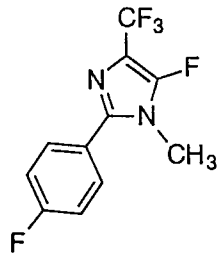
^{1}H-NMR Spectrum of **10** (300 MHz, $CDCl_3$, TMS)



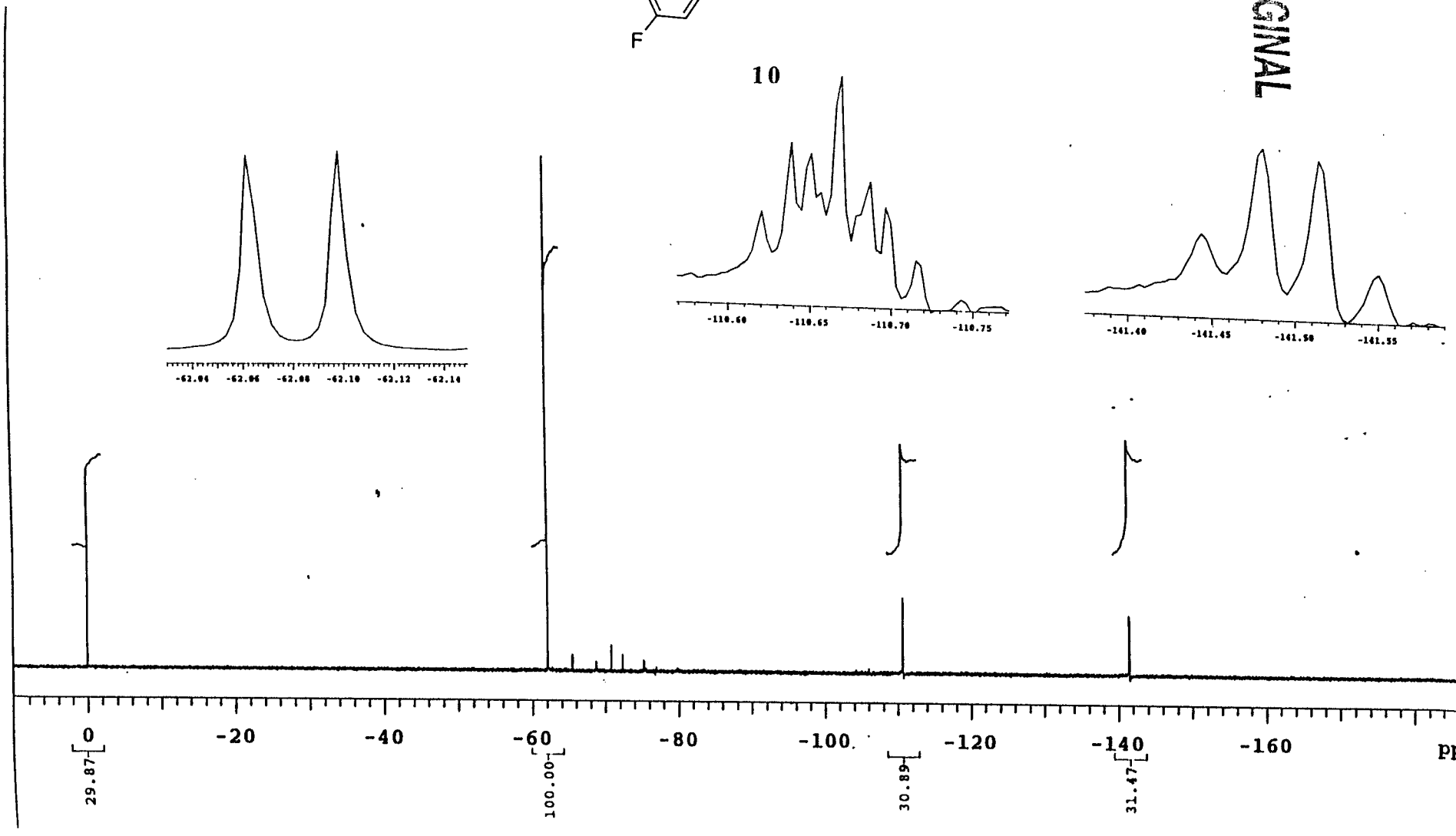
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^{19}F-NMR Spectrum of **10** (300 MHz, $CDCl_3$, $CFCl_3$)



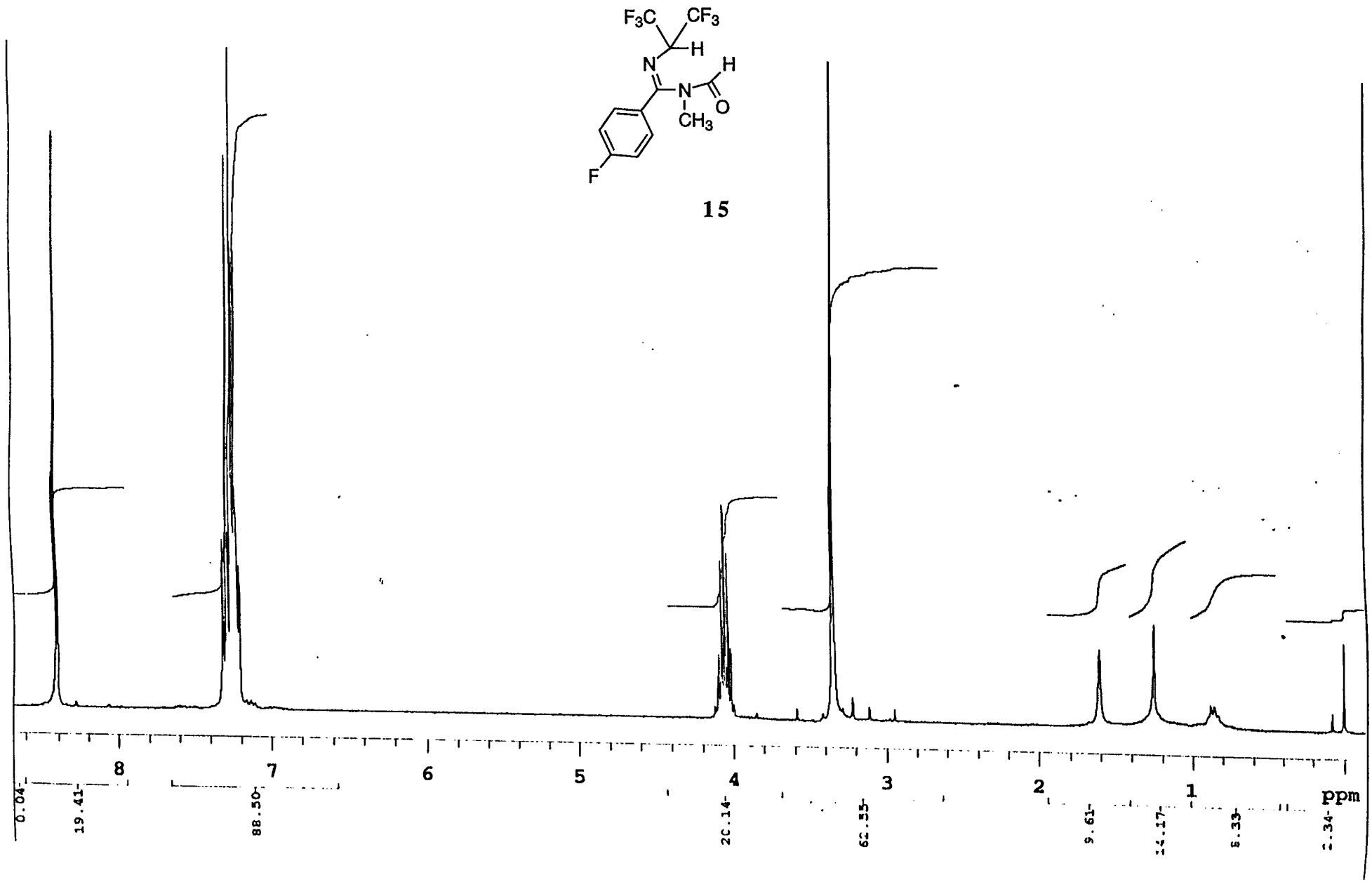
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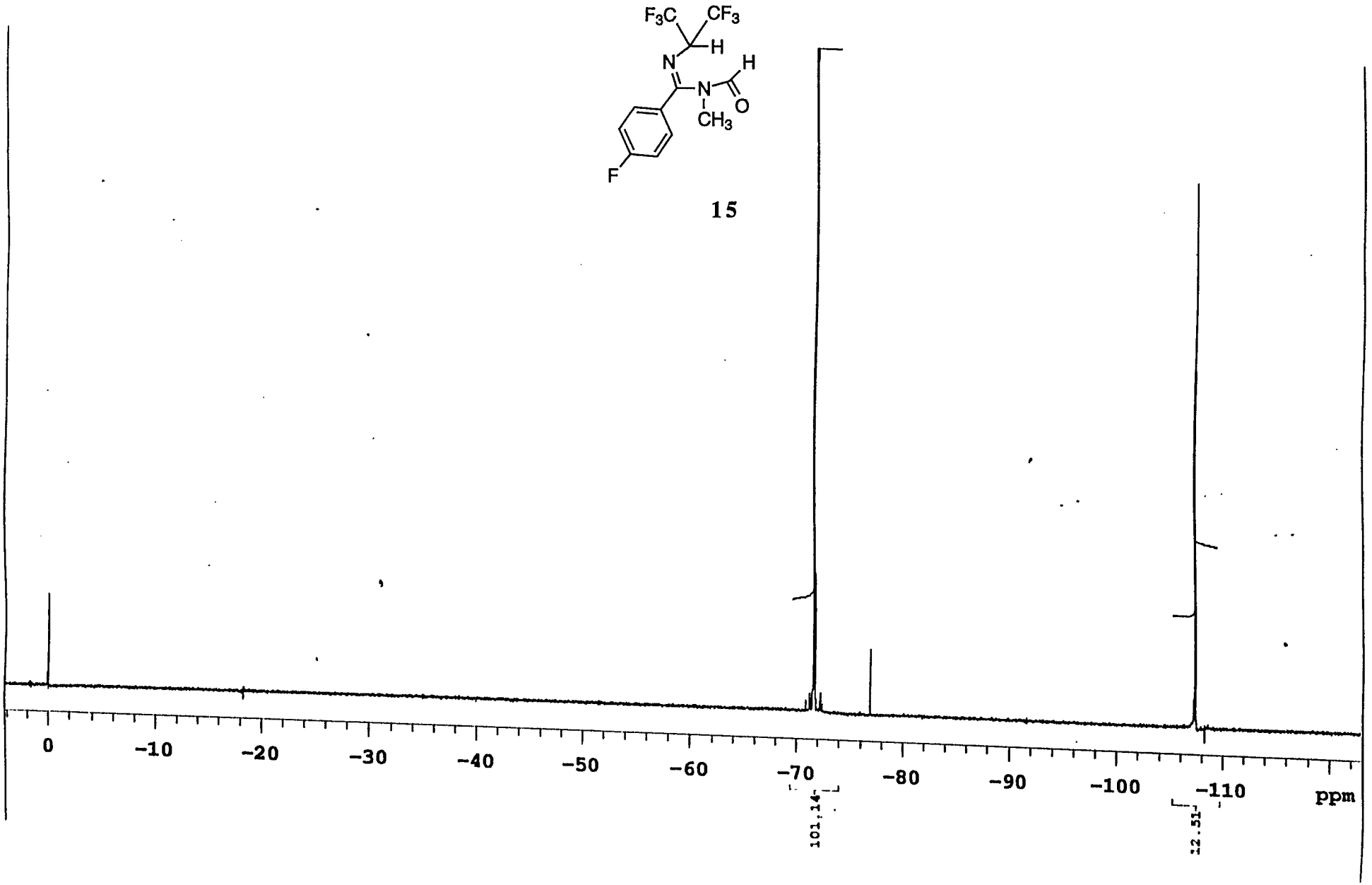
^{1}H-NMR Spectrum of **15** (300 MHz, $CDCl_3$, TMS)



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15

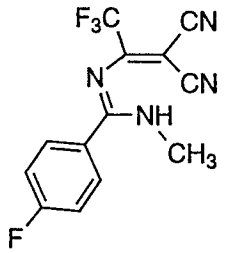
^{19}F-NMR Spectrum of **15** (300 MHz, $CDCl_3$, $CFCl_3$)



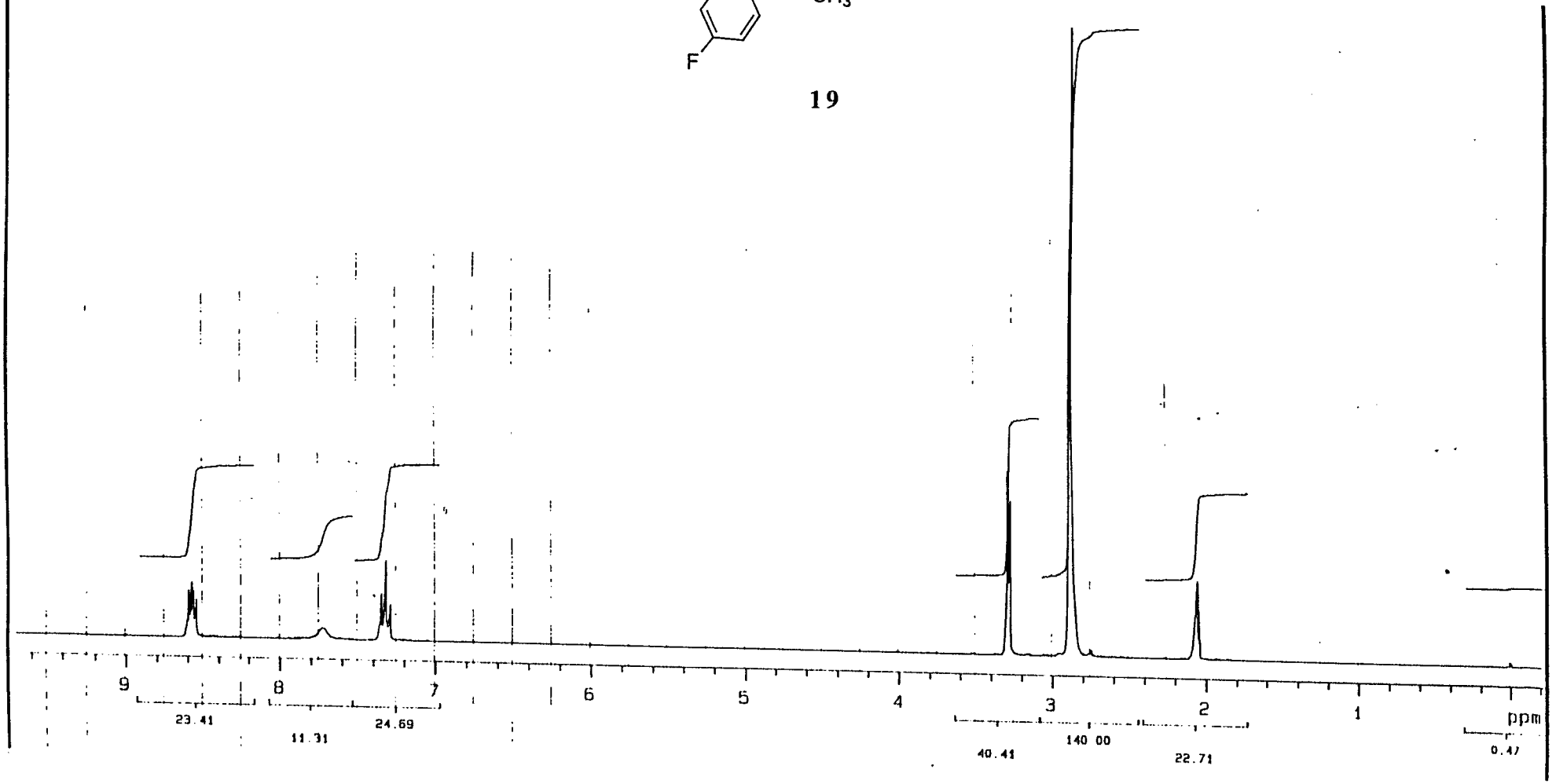
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^{1}H-NMR Spectrum of **19** (300 MHz, $CDCl_3$, TMS)

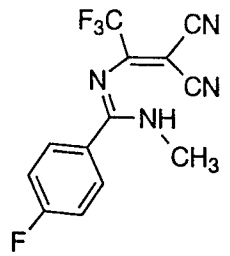


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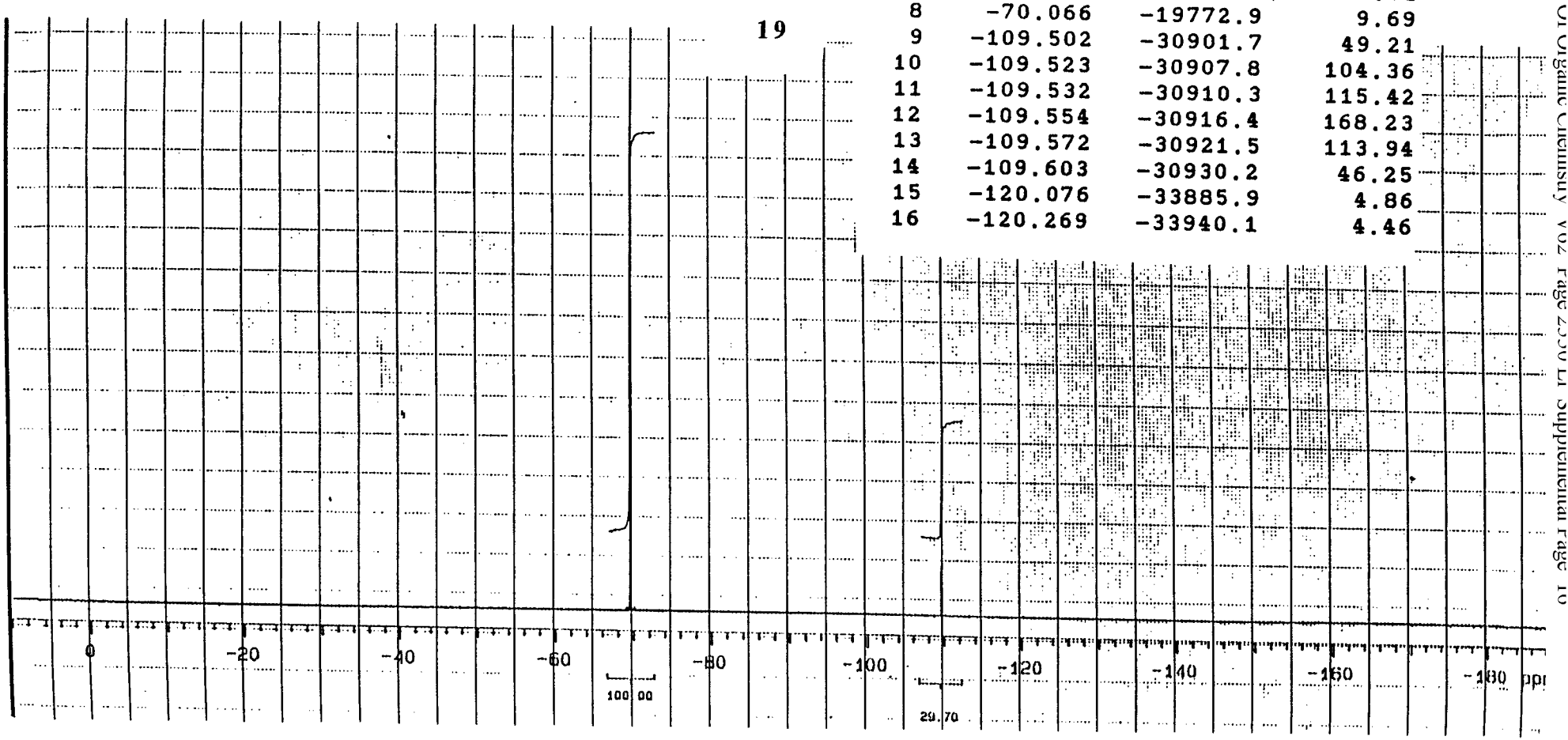
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^{19}F-NMR Spectrum of **19** (300 MHz, $CDCl_3$, $CFCl_3$)



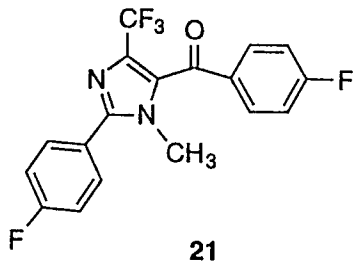
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5	-69.450	-19599.0	1688.60
6	-69.517	-19617.9	28.52
7	-69.587	-19637.7	23.54
8	-70.066	-19772.9	9.69
9	-109.502	-30901.7	49.21
10	-109.523	-30907.8	104.36
11	-109.532	-30910.3	115.42
12	-109.554	-30916.4	168.23
13	-109.572	-30921.5	113.94
14	-109.603	-30930.2	46.25
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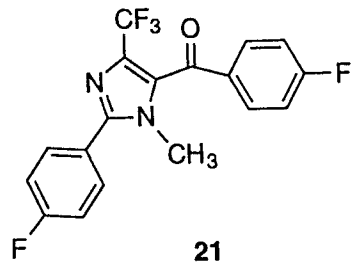
^{1}H-NMR Spectrum of **21** (300 MHz, $CDCl_3$, TMS)



21

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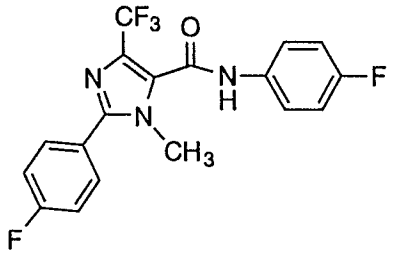
^{19}F-NMR Spectrum of **21** (300 MHz, $CDCl_3$, $CFCl_3$)



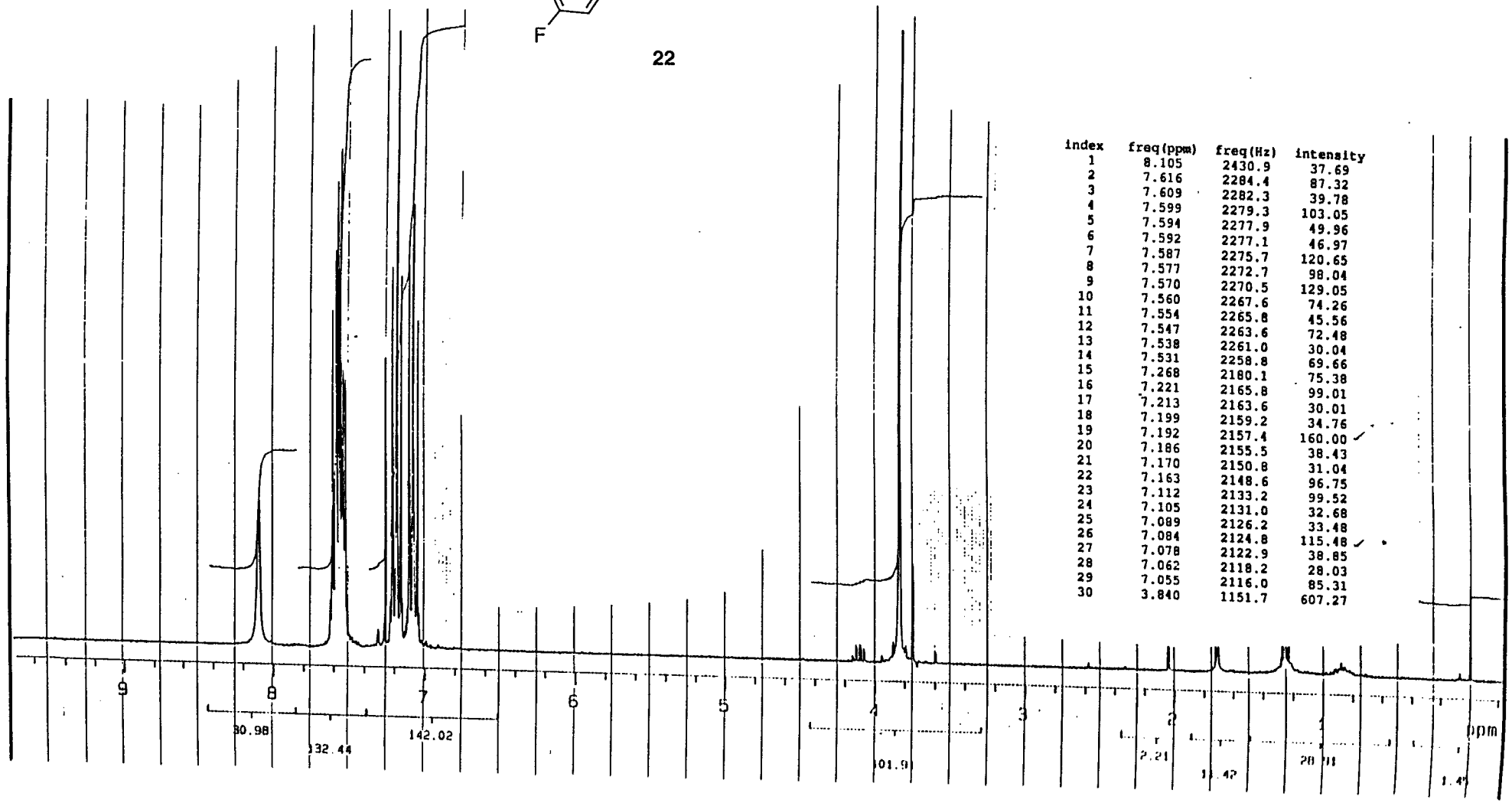
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^{1}H-NMR Spectrum of **22** (300 MHz, $CDCl_3$, TMS)



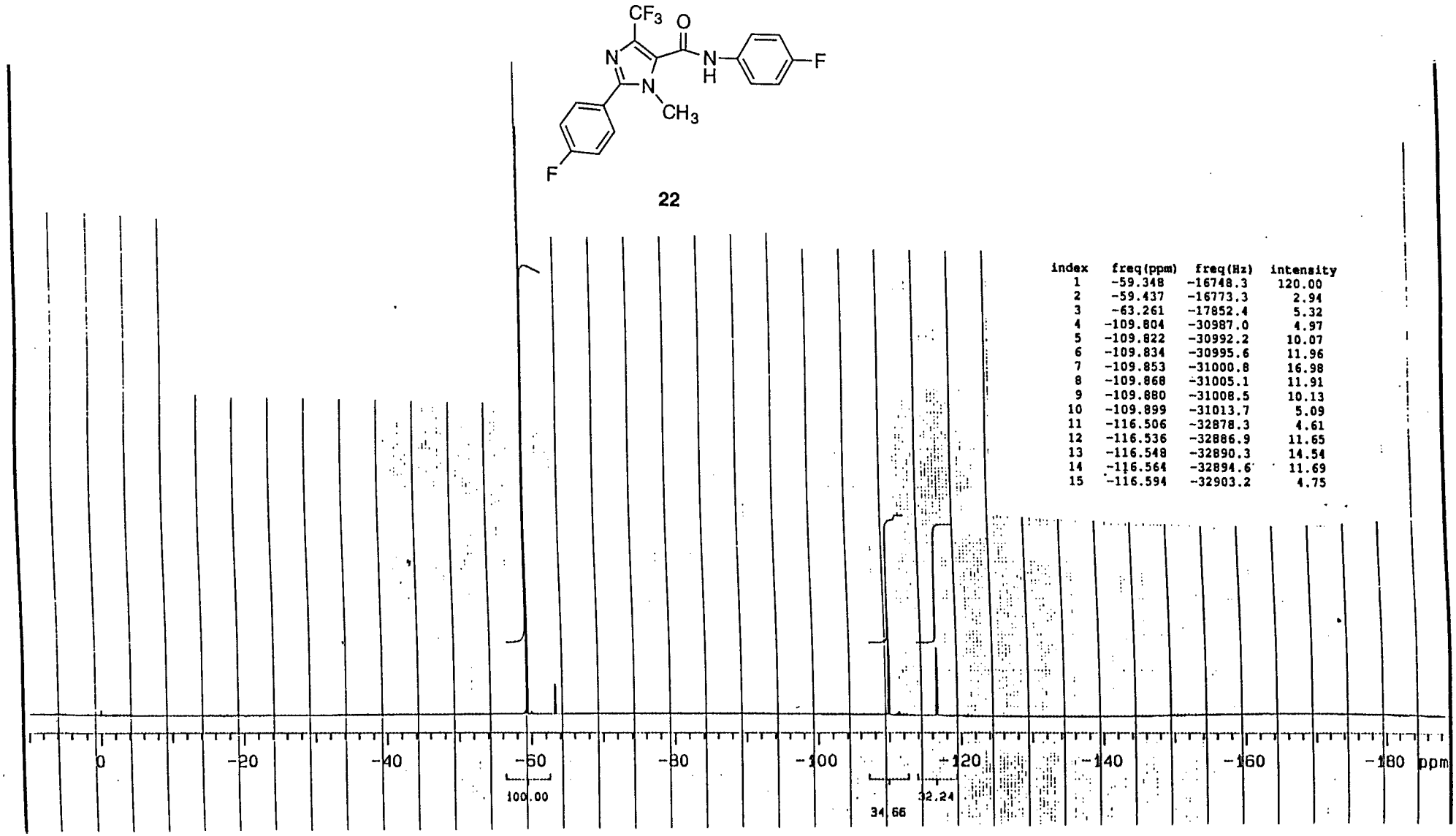
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4	7.599	2279.3	103.05
5	7.594	2277.9	49.96
6	7.592	2277.1	46.97
7	7.587	2275.7	120.65
8	7.577	2272.7	98.04
9	7.570	2270.5	129.05
10	7.560	2267.6	74.26
11	7.554	2265.8	45.56
12	7.547	2263.6	72.48
13	7.538	2261.0	30.04
14	7.531	2258.8	69.66
15	7.268	2180.1	75.38
16	7.221	2165.8	99.01
17	7.213	2163.6	30.01
18	7.199	2159.2	34.76
19	7.192	2157.4	160.00 ✓
20	7.186	2155.5	38.43
21	7.170	2150.8	31.04
22	7.163	2148.6	96.75
23	7.112	2133.2	99.52
24	7.105	2131.0	32.68
25	7.089	2126.2	33.48
26	7.084	2124.8	115.48 ✓
27	7.078	2122.9	38.85
28	7.062	2118.2	28.03
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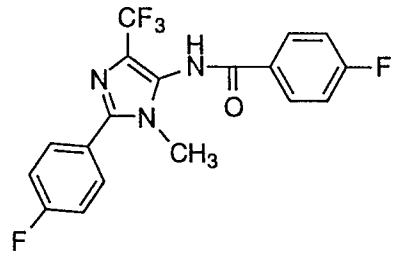
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^{19}F-NMR Spectrum of **22** (300 MHz, $CDCl_3$, $CFCl_3$)

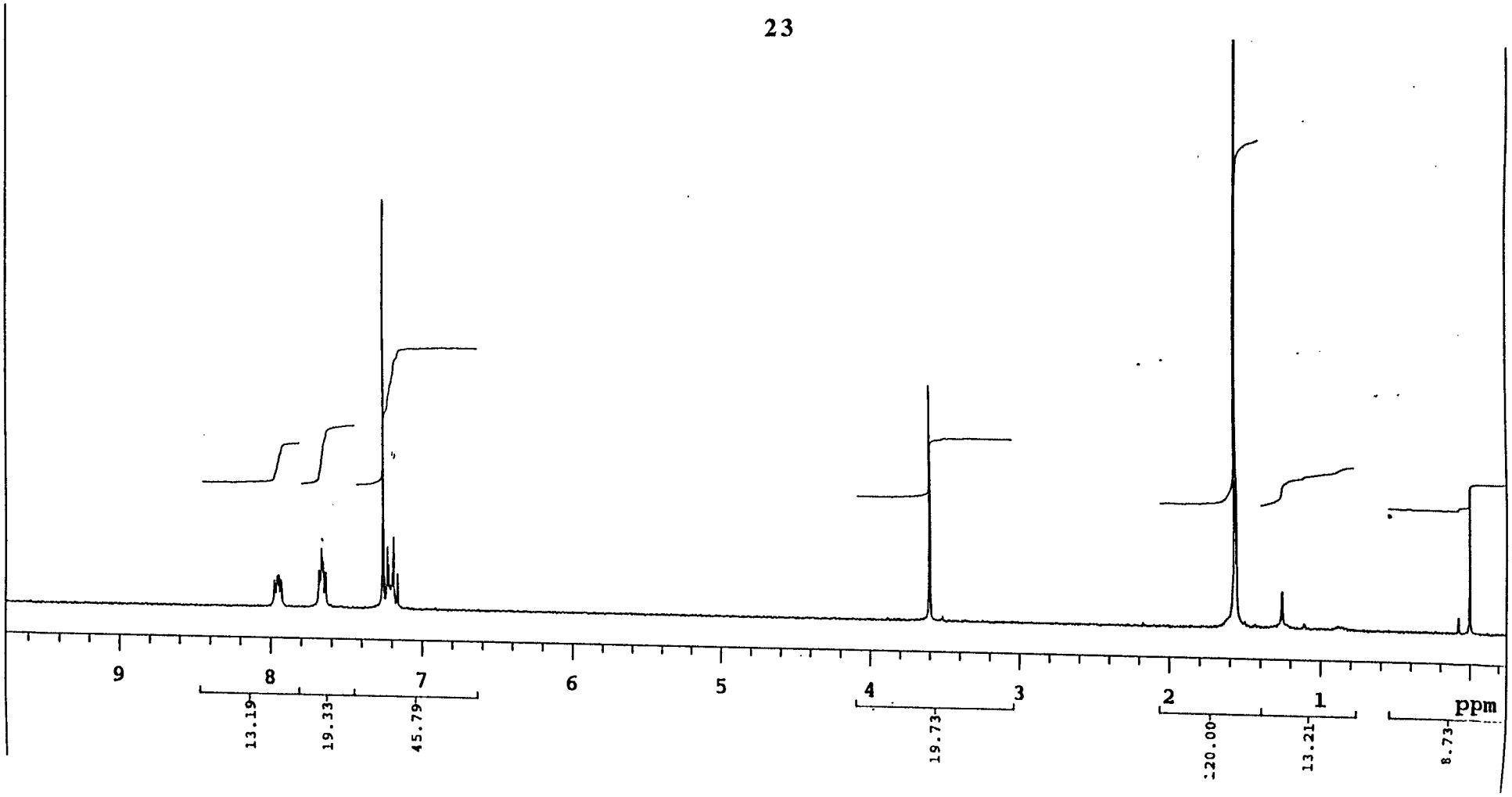


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^{1}H-NMR Spectrum of **23** (300 MHz, $CDCl_3$, TMS)

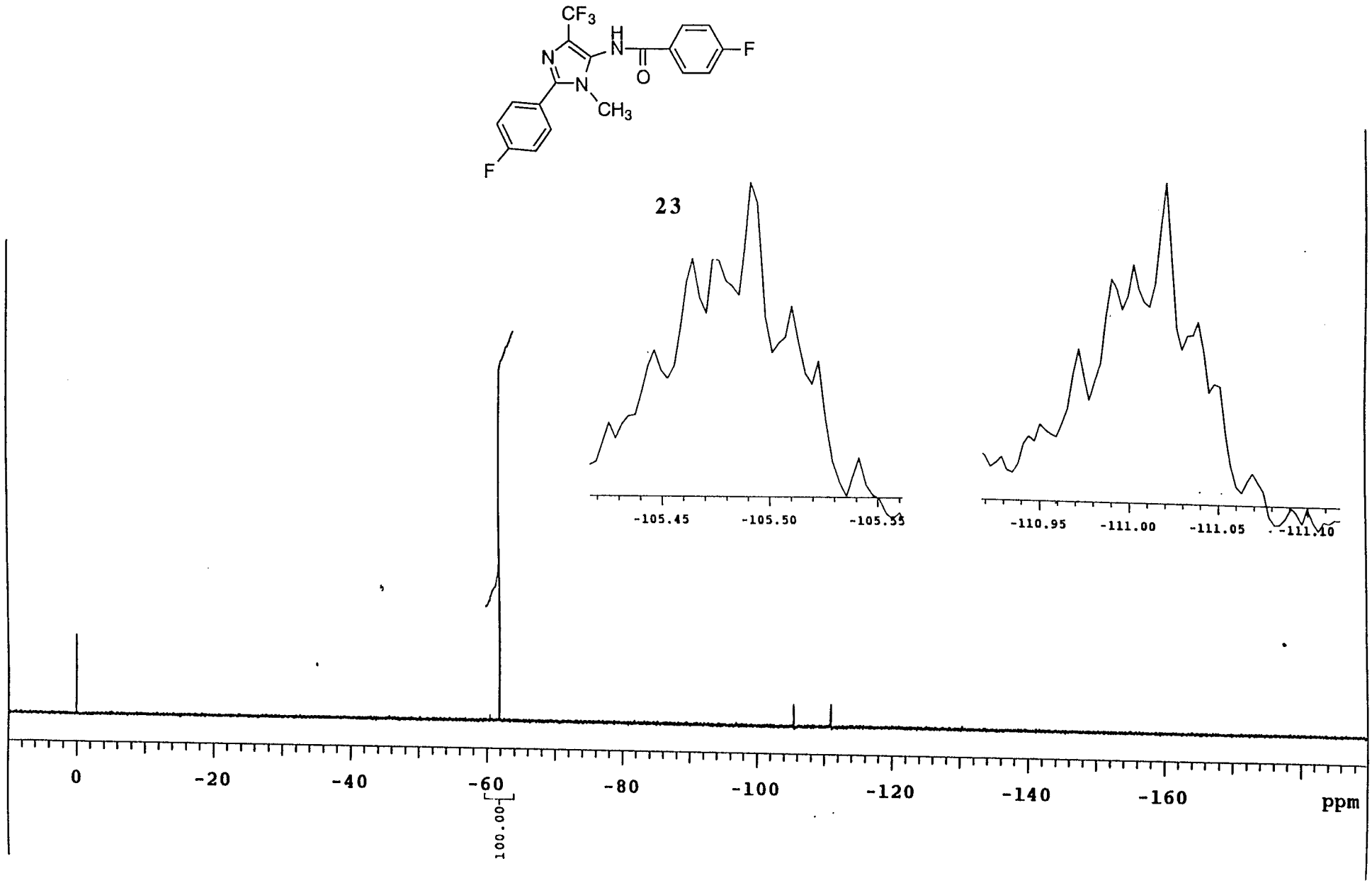


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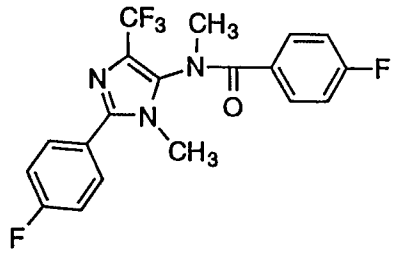
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^{19}F-NMR Spectrum of **23** (300 MHz, $CDCl_3$, $CFCl_3$)

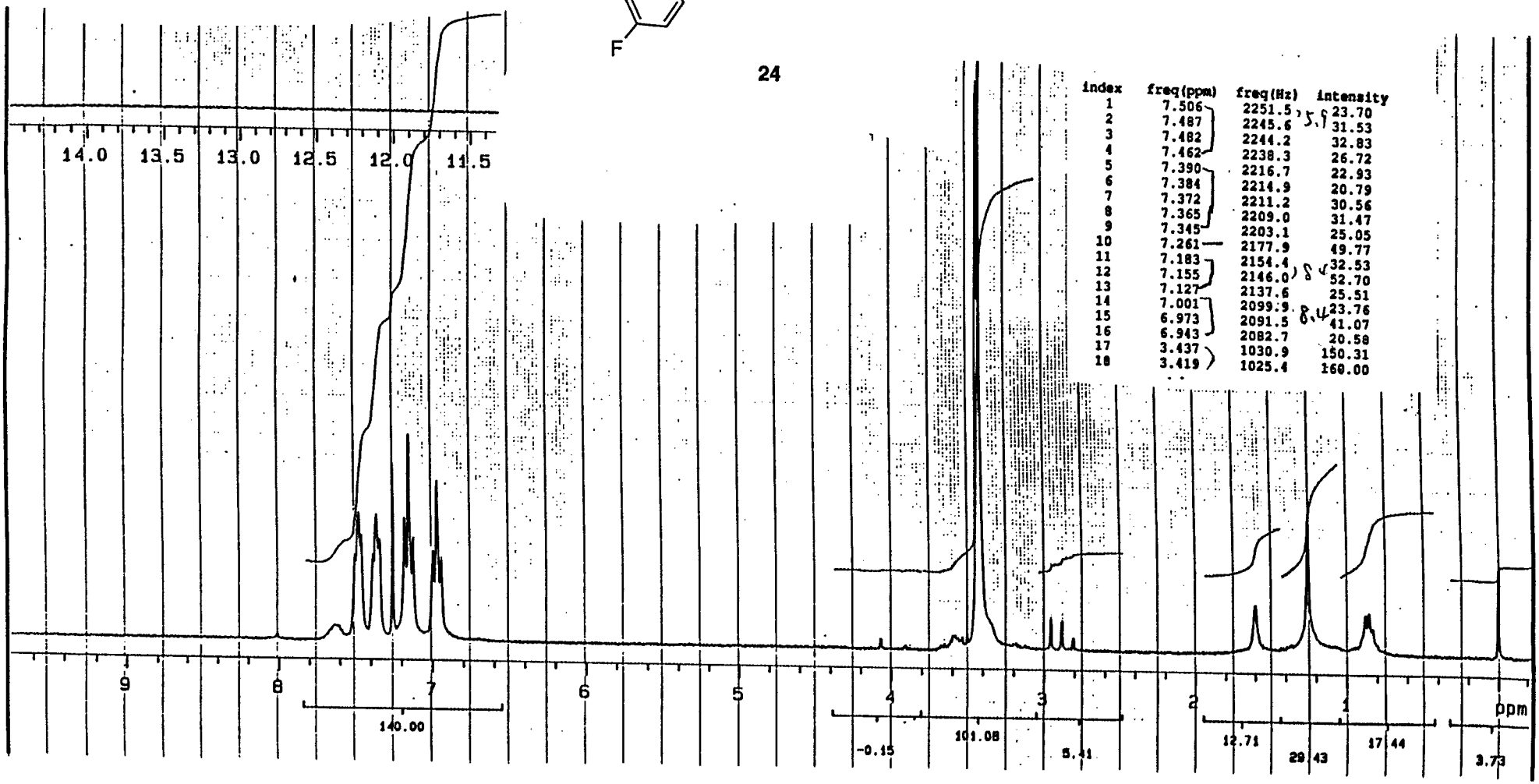


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^{1}H-NMR Spectrum of **24** (300 MHz, $CDCl_3$, TMS)

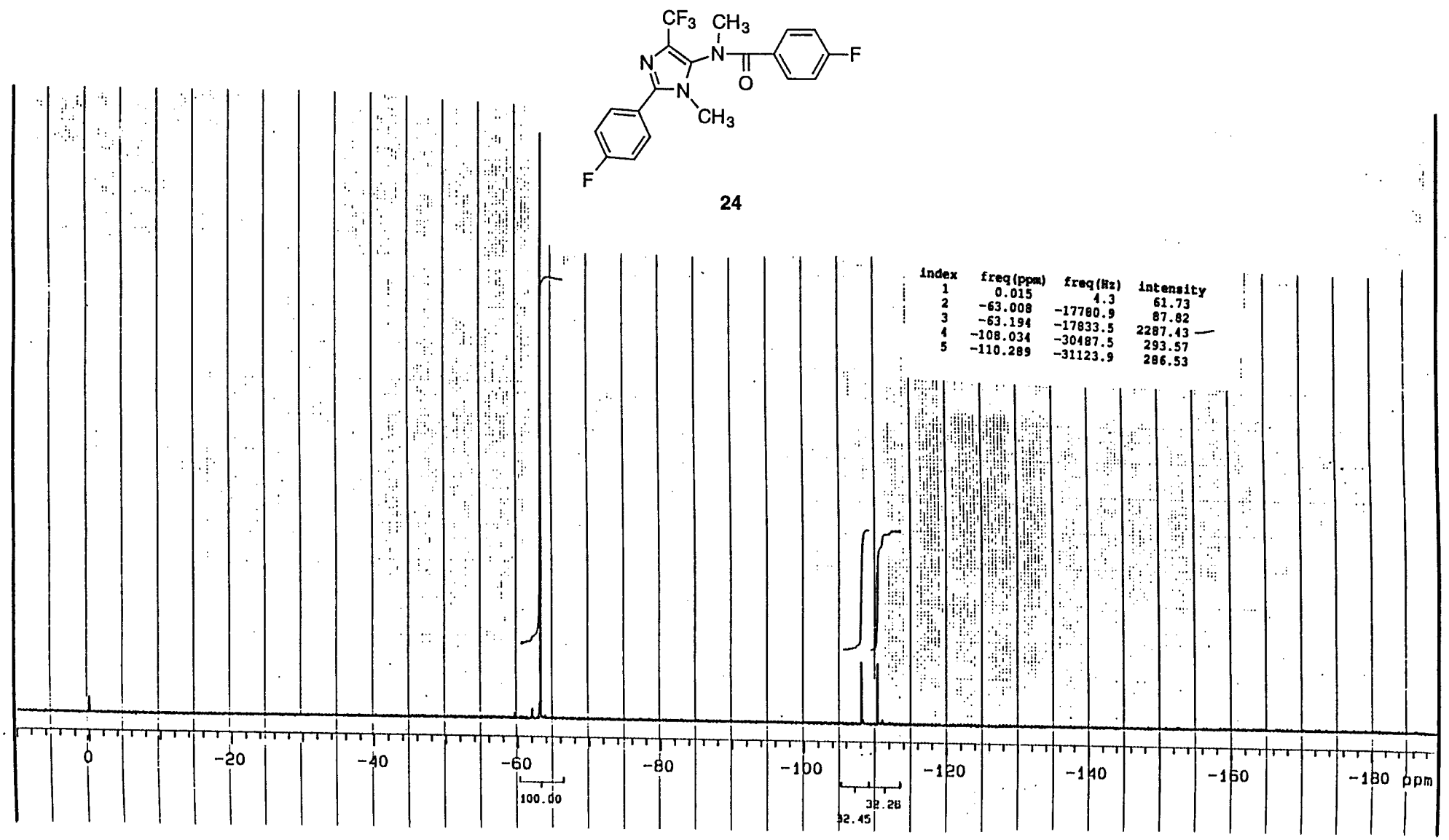


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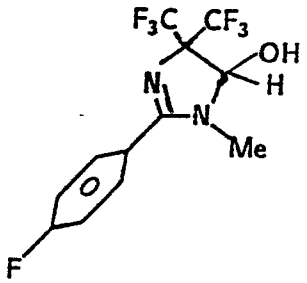
^{19}F-NMR Spectrum of **24** (300 MHz, $CDCl_3$, $CFCl_3$)



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X-ray crystal structure of 5



CRYSTAL DATA: $F_7ON_2C_{12}H_9$, from MeOH/EtOAc/hexane, colorless, trapezoidal block, ~0.29 x 0.12 x 0.45mm, monoclinic, $P2_1/c$ (No. 14), a = 7.690(3), b = 11.509(6), c = 14.858(6)Å, β = 91.31(2)°, from 25 reflections, T = -70°C, V = 1314.7Å^3, Z = 4, FW = 330.22, Dc = 1.668g/cc, μ(Mo) = 1.68cm^{-1},

DATA COLLECTION AND TREATMENT: Enraf-Nonius CAD4 diffractometer, MoKα radiation, 2261 data collected, $2.7° < 2\theta < 48.0°$, maximum h,k,l = 8 13 16, data octants = +++, -++, ω scan method, scan width = 1.20-1.90°ω, scan speed = 1.80-6.70°/min, typical half-height peak width = 0.20°ω, 2 standards collected 14 times, 5% fluctuation, 6.5% variation in azimuthal scan, no absorption correction, 1380 unique reflections with $I \geq 3.0\sigma(I)$,

SOLUTION AND REFINEMENT: Structure solved by direct methods (MULTAN). [The asymmetric unit consists of one molecule in a general position. Hydrogen atoms were idealized with C-H=.95Å and refined. The Me-hydrogens were idealized in orientations taken from a difference map. Due to the disorder of the hydroxyl group (Fig 3), the C2-hydrogen was omitted] refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, weights $\propto [\sigma^2(I)+0.0009I^2]^{-1/2}$, refined anisotropic: all non-hydrogen atoms, fixed atoms: H , 208 parameters, data/parameter ratio = 6.63, final R = 0.040, Rw = 0.044, error of fit = 1.53, max Δ/σ = 0.02, [the disordered OH was refined in two positions with atom multiplicities determined by refinement (.16/.84) Only the OH-hydrogen from the major component was included in the refinement], largest residual density = 0.22e/Å^3, near O2

RESULTS: This analysis confirms the structure of BPN4796-56, as part of a series of ACAT inhibitors (anti-atheroschlerotic agents), to determine the possibility of intramolecular hydrogen bonding between the CF3 and OH groups. The analysis shows that in the crystal, a strong intermolecular hydrogen bond predominates between the hydroxyl and the imidazole nitrogen, forming infinite chains along the y-axis (Fig. 4).

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TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
F(1)	10855(3)	-534(2)	5978(1)	4.0(1)'
F(2)	10575(3)	1311(2)	5899(1)	3.6(1)'
F(3)	8347(3)	251(2)	6115(1)	3.6(1)'
F(4)	13324(2)	-44(2)	7276(1)	3.8(1)'
F(5)	12664(2)	1758(2)	7336(1)	3.7(1)'
F(6)	12395(3)	690(2)	8503(1)	3.5(1)'
F(27)	4384(3)	3835(2)	10486(2)	5.1(1)'
O(2)	10867(3)	-1443(2)	8104(2)	2.3(1)'
O(2')	8839(20)	-1300(15)	7309(10)	2.6(5)'
N(1)	8609(3)	-183(2)	8519(2)	2.6(1)'
N(2)	9257(3)	1394(2)	7699(2)	2.3(1)'
C(1)	10292(4)	444(3)	7344(2)	2.1(1)'
C(2)	9614(5)	-694(3)	7789(2)	2.4(1)'
C(3)	8395(4)	964(3)	8360(2)	2.1(1)'
C(4)	10034(5)	372(3)	6325(2)	2.6(1)'
C(5)	12193(5)	695(3)	7610(2)	2.8(1)'
C(7)	7431(5)	-927(3)	9017(3)	4.3(1)'
C(21)	7280(4)	1692(3)	8929(2)	2.2(1)'
C(22)	6117(4)	2463(3)	8532(2)	2.8(1)'
C(23)	5113(5)	3186(3)	9055(3)	3.4(1)'
C(24)	5328(4)	3121(3)	9966(3)	3.1(1)'
C(25)	6479(5)	2387(3)	10382(2)	3.1(1)'
C(26)	7458(4)	1658(3)	9859(2)	2.8(1)'
H(2)	10620	-2294	7712	10.5
H(7)	6885	-555	9495	6.2
H(7')	7917	-1655	9076	9.2
H(7')	6663	-1278	8582	7.6
H(22)	6051	2498	7903	1.6
H(23)	4206	3674	8757	4.7
H(25)	6608	2382	11007	3.8
H(26)	8244	1184	10156	2.4

TABLE II. Anisotropic Thermal Parameters (Angs X 1000)
exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
F(1)	73(2)	46(1)	35(1)	20(1)	2(1)	-14(1)
F(2)	60(1)	43(1)	32(1)	-6(1)	7(1)	8(1)
F(3)	45(1)	52(1)	38(1)	-3(1)	-9(1)	2(1)
F(4)	35(1)	51(1)	59(1)	5(1)	8(1)	-6(1)
F(5)	48(1)	38(1)	53(1)	-17(1)	1(1)	5(1)
F(6)	49(1)	49(1)	34(1)	-10(1)	-7(1)	0(1)
F(27)	62(2)	62(2)	70(2)	12(1)	34(1)	-14(1)
O(2)	39(2)	18(1)	29(1)	5(1)	-1(1)	2(1)
O(2')	32(10)	38(11)	30(10)	-13(8)	-2(8)	6(8)
N(1)	44(2)	20(2)	36(2)	-3(1)	14(1)	2(1)
N(2)	38(2)	19(2)	30(2)	2(1)	7(1)	1(1)
C(1)	33(2)	20(2)	28(2)	0(2)	4(1)	-2(1)
C(2)	39(2)	24(2)	29(2)	-2(2)	7(2)	-4(2)
C(3)	31(2)	24(2)	26(2)	-2(2)	2(1)	-3(1)
C(4)	42(2)	23(2)	33(2)	3(2)	1(2)	-1(2)

TABLE II. Anisotropic Thermal Parameters (Angs X 1000) (continued)

C(5)	42(2)	31(2)	33(2)	-6(2)	2(2)	-1(2)
C(7)	71(3)	29(2)	66(3)	-9(2)	38(2)	0(2)
C(21)	28(2)	23(2)	32(2)	-5(2)	7(2)	-1(1)
C(22)	35(2)	37(2)	34(2)	-1(2)	6(2)	-1(2)
C(23)	34(2)	41(2)	52(3)	4(2)	7(2)	2(2)
C(24)	32(2)	32(2)	53(2)	0(2)	20(2)	-10(2)
C(25)	44(2)	45(2)	32(2)	-3(2)	12(2)	-6(2)
C(26)	37(2)	35(2)	35(2)	1(2)	5(2)	1(2)

TABLE III. Interatomic Distances (A)

F(1)-C(4)	1.328 (4)	N(2)-C(1)	1.459 (4)
F(2)-C(4)	1.325 (4)	N(2)-C(3)	1.295 (4)
F(3)-C(4)	1.335 (4)	C(1)-C(2)	1.563 (4)
F(4)-C(5)	1.321 (4)	C(1)-C(4)	1.524 (4)
F(5)-C(5)	1.342 (4)	C(1)-C(5)	1.533 (5)
F(6)-C(5)	1.332 (4)	C(3)-C(21)	1.478 (4)
F(27)-C(24)	1.350 (4)	C(21)-C(22)	1.383 (5)
O(2)-O(2')	1.941 (16)	C(21)-C(26)	1.385 (5)
O(2)-C(2)	1.367 (4)	C(22)-C(23)	1.385 (5)
O(2')-C(2)	1.153 (16)	C(23)-C(24)	1.362 (5)
N(1)-C(2)	1.469 (4)	C(24)-C(25)	1.362 (5)
N(1)-C(3)	1.350 (4)	C(25)-C(26)	1.378 (5)
N(1)-C(7)	1.460 (4)		

TABLE IV. Intramolecular Angles (Deg)

O(2')-O(2)-C(2)	35.8 (5)	O(2')-C(2)-N(1)	115.2 (8)
O(2)-O(2')-C(2)	43.8 (6)	O(2)-C(2)-C(1)	115.7 (3)
C(2)-N(1)-C(3)	109.1 (3)	O(2')-C(2)-C(1)	114.6 (8)
C(2)-N(1)-C(7)	118.8 (3)	N(1)-C(3)-N(2)	116.3 (3)
C(3)-N(1)-C(7)	126.0 (3)	N(2)-C(1)-C(2)	106.5 (2)
C(1)-N(2)-C(3)	106.3 (3)	N(2)-C(1)-C(4)	109.9 (3)
F(1)-C(4)-F(2)	107.3 (3)	N(2)-C(1)-C(5)	106.9 (3)
F(1)-C(4)-F(3)	107.1 (3)	N(1)-C(2)-C(1)	99.4 (2)
F(2)-C(4)-F(3)	106.7 (3)	N(1)-C(3)-C(21)	121.6 (3)
F(4)-C(5)-F(5)	106.8 (3)	N(2)-C(3)-C(21)	122.1 (3)
F(4)-C(5)-F(6)	108.0 (3)	C(2)-C(1)-C(4)	109.8 (3)
F(5)-C(5)-F(6)	106.3 (3)	C(2)-C(1)-C(5)	112.0 (3)
F(1)-C(4)-C(1)	112.1 (3)	C(4)-C(1)-C(5)	111.6 (3)
F(2)-C(4)-C(1)	113.3 (3)	C(3)-C(21)-C(22)	119.8 (3)
F(3)-C(4)-C(1)	110.0 (3)	C(3)-C(21)-C(26)	120.7 (3)
F(4)-C(5)-C(1)	114.4 (3)	C(22)-C(21)-C(26)	119.4 (3)
F(5)-C(5)-C(1)	110.8 (3)	C(21)-C(22)-C(23)	120.6 (3)
F(6)-C(5)-C(1)	110.2 (3)	C(22)-C(23)-C(24)	117.9 (3)
F(27)-C(24)-C(23)	118.7 (3)	C(23)-C(24)-C(25)	123.2 (3)
F(27)-C(24)-C(25)	118.1 (3)	C(24)-C(25)-C(26)	118.6 (3)
O(2)-C(2)-O(2')	100.4 (9)	C(21)-C(26)-C(25)	120.2 (3)
O(2)-C(2)-N(1)	112.2 (3)		

TABLE V. Intramolecular Non-Bonding Distances (A)

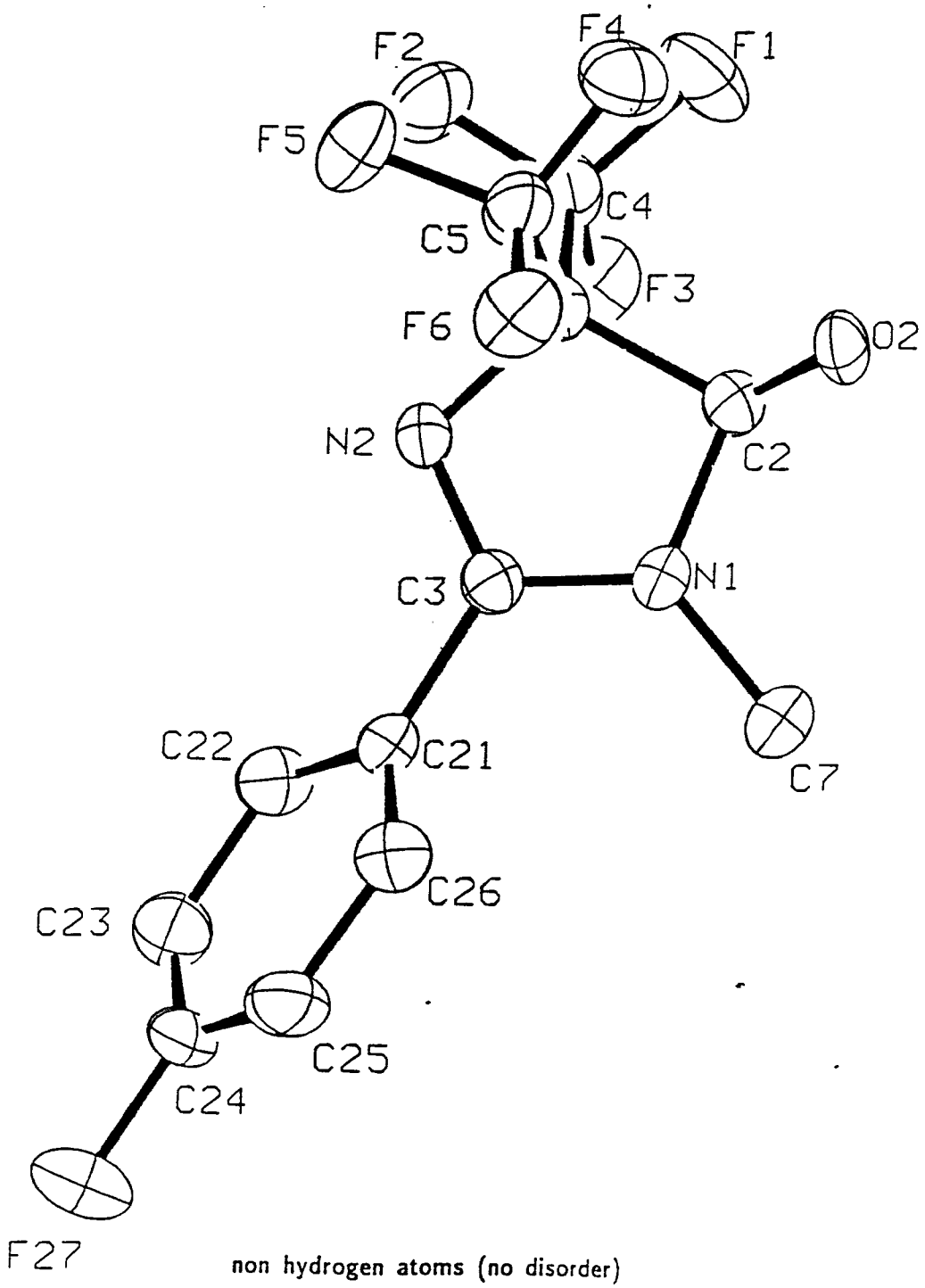
F(1)...F(4)	2.735 (3)
F(1)...F(5)	3.583 (3)
F(2)...F(4)	3.300 (3)
F(2)...F(5)	2.692 (3)
F(3)...N(1)	3.608 (4)
F(6)...N(1)	3.080 (3)
F(3)...C(3)	3.435 (4)
F(5)...C(3)	3.762 (4)
F(6)...C(3)	3.095 (4)
C(7)...C(26)	3.228 (5)

TABLE VI. Intermolecular Distances (A)

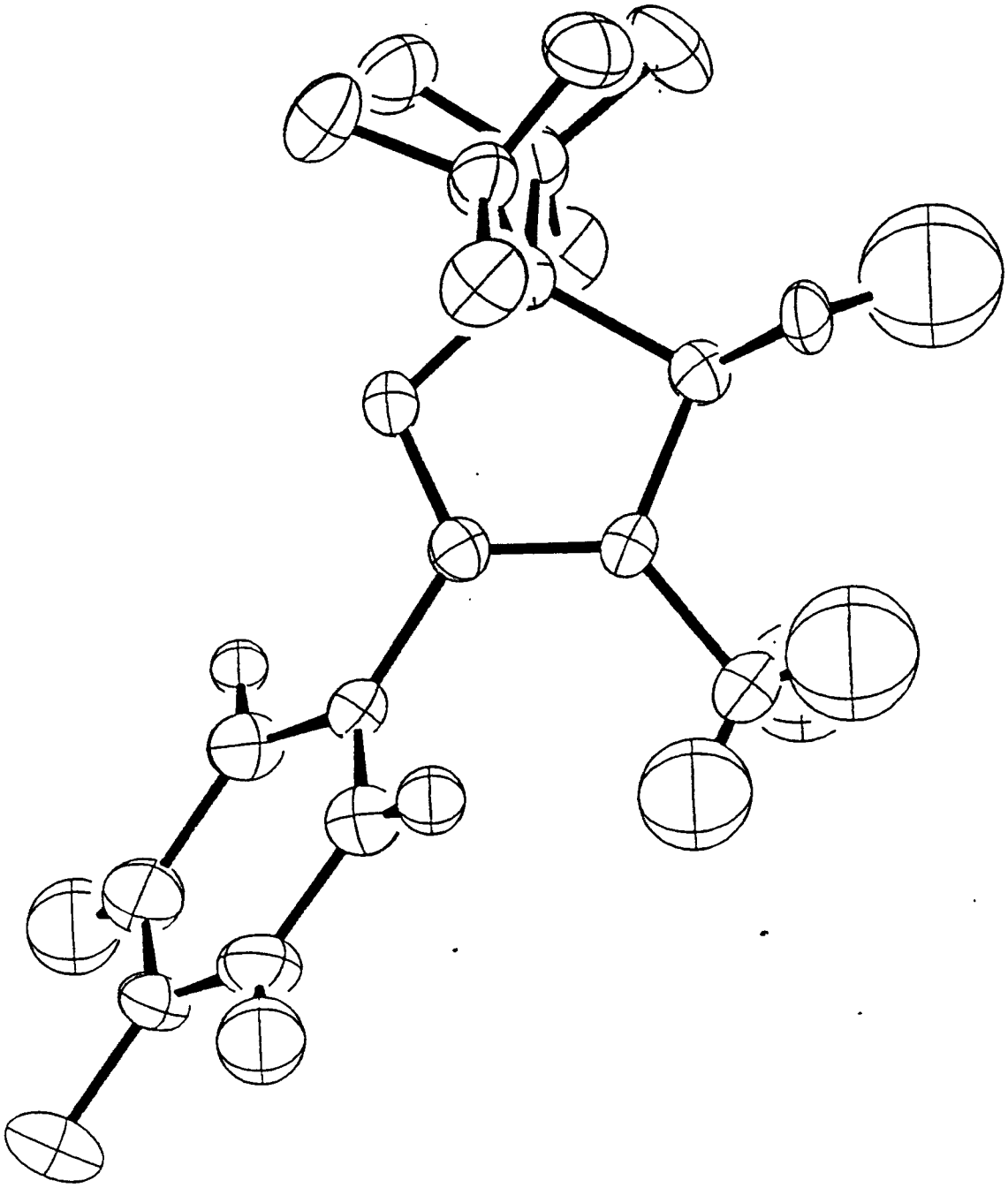
F(1)...F(1)a	3.391 (4)
F(1)...F(2)a	3.106 (3)
F(1)...F(3)a	3.199 (3)
F(2)...F(27)c	3.011 (3)
F(3)...F(27)e	3.337 (3)
F(4)...F(27)c	3.127 (3)
F(5)...F(27)c	3.153 (3)
F(27)...F(27)g	3.199 (5)
F(1)...C(22)b	3.346 (4)
F(3)...C(25)e	3.251 (4)
F(4)...C(22)b	3.143 (4)
F(4)...C(23)b	3.101 (4)
F(5)...C(7)d	3.337 (4)
F(5)...C(22)f	3.264 (4)
O(2)...N(2)b	2.762 (4)
O(2')...N(2)b	3.031 (17)
O(2)...C(25)h	3.193 (5)
O(2)...C(26)h	3.272 (5)
N(2)...H(2)d	1.632

Symmetry Operation Codes

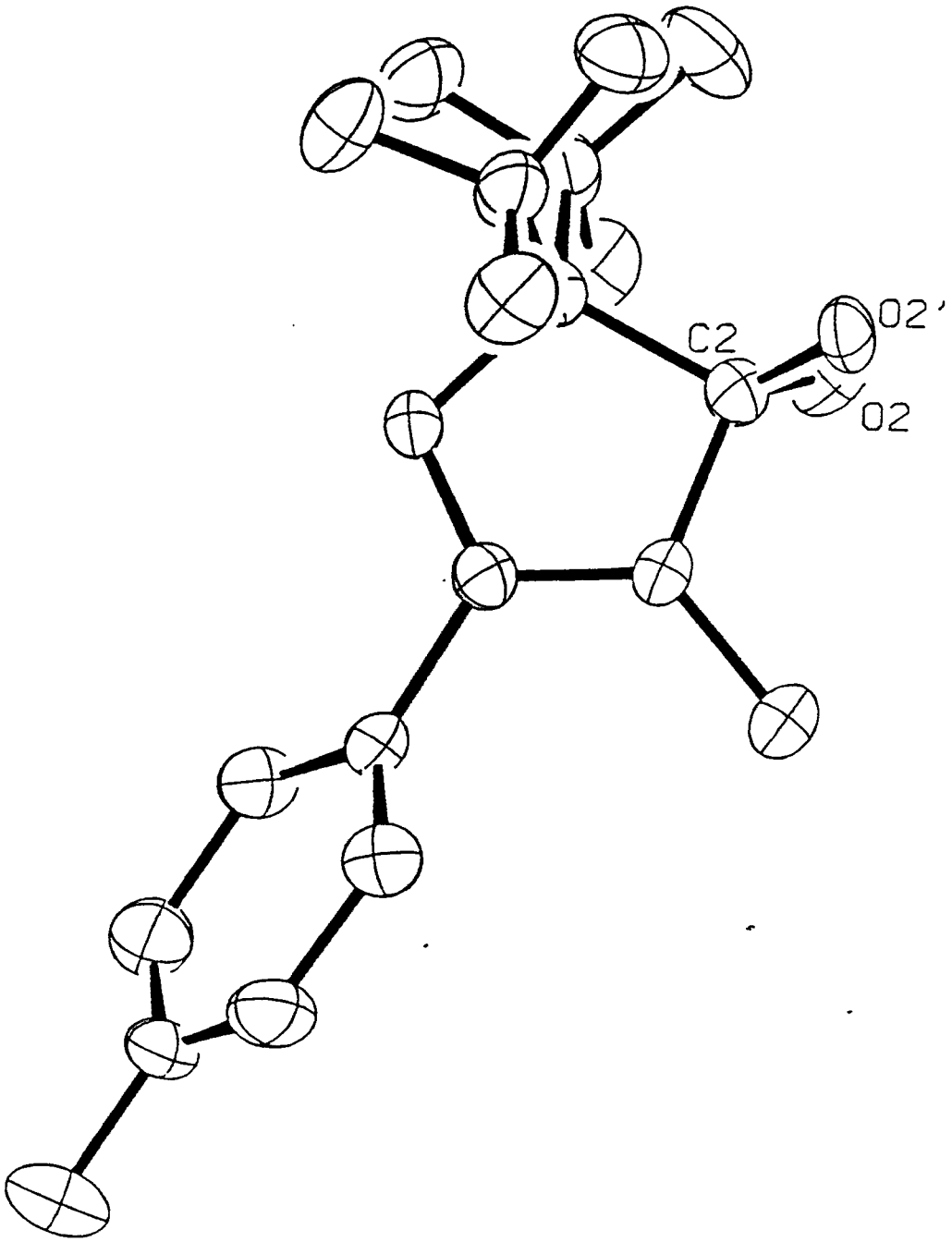
a	2-X,-Y,1-Z
b	2-X,-1/2+Y,3/2-Z
c	1+X,1/2-Y,-1/2+Z
d	2-X,1/2+Y,3/2-Z
e	X,1/2-Y,-1/2+Z
f	1+X,Y,Z
g	1-X,1-Y,2-Z
h	2-X,-Y,2-Z



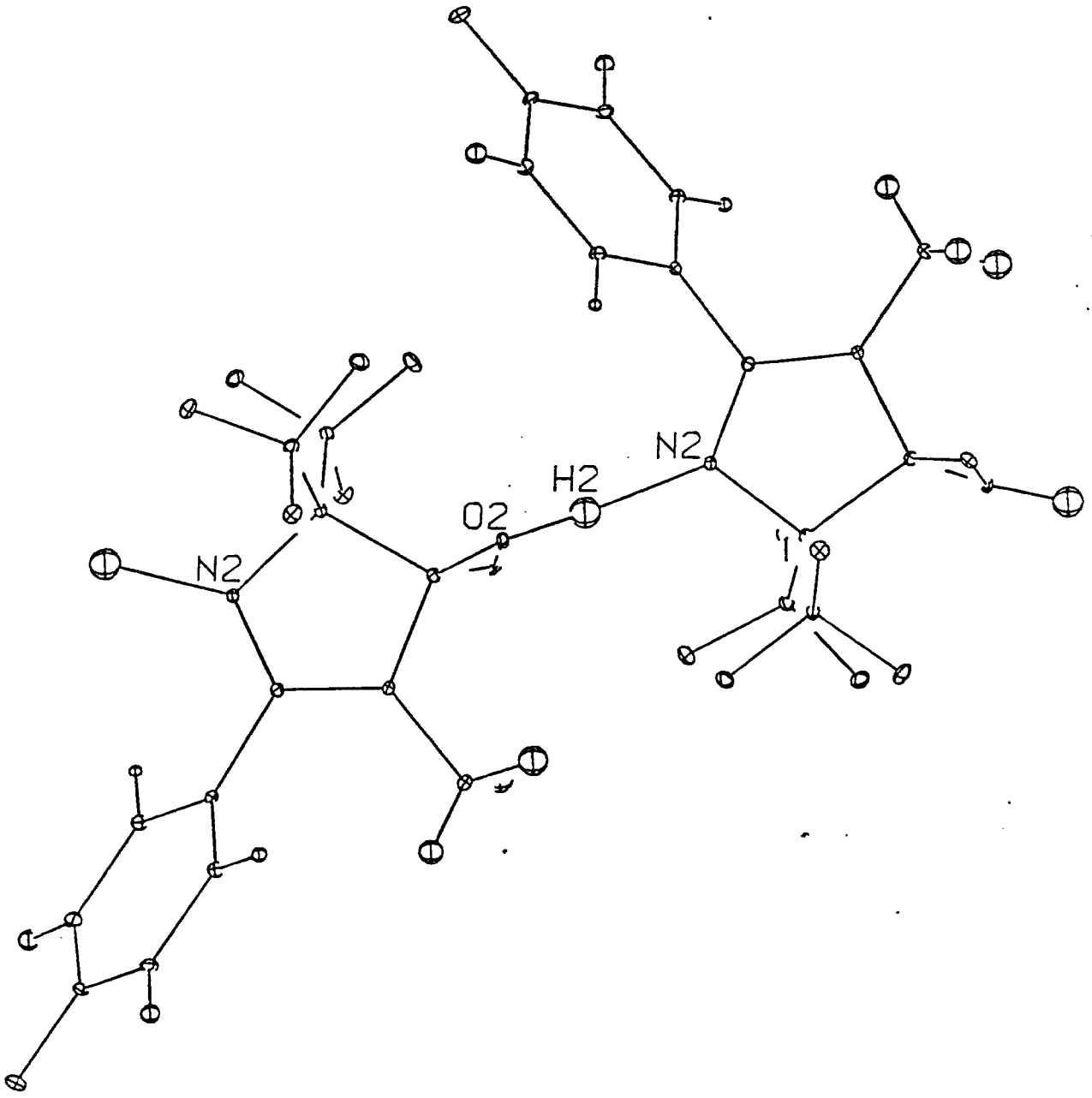
non hydrogen atoms (no disorder)



with hydrogen atoms



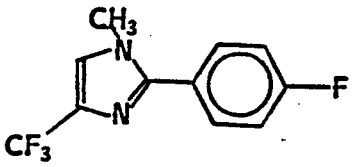
showing the O2 disorder



O-H...N hydrogen bonding

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X-ray crystal structure of **9**



CRYSTAL DATA: $F_4N_2C_{11}H_8$, from hexane/ether, colorless, parallelopiped, ~0.27 x 0.11 x 0.50mm, monoclinic, $P2_1/m$ (No. 11), a = 7.128(3), b = 6.806(1), c = 10.917(4)Å, β = 104.50(2)°, from 25 reflections, T = -70°C, V = 512.8Å^3, Z = 2, FW = 244.20, Dc = 1.581g/cc, μ(Mo) = 1.40cm^{-1}.

DATA COLLECTION AND TREATMENT: Enraf-Nonius CAD4 diffractometer, MoKα radiation, 1336 data collected, $3.9° < 2\theta < 55.0°$, maximum h,k,l = 9 8 14, data octants = +++, -++, ω scan method, scan width = 1.20-2.50°ω, scan speed = 1.80-5.00°/min, typical half-height peak width = 0.22°ω, 2 standards collected 10 times, 2% fluctuation, 9.7% variation in azimuthal scan, no absorption correction, 813 unique reflections with $I \geq 3.0\sigma(I)$.

SOLUTION AND REFINEMENT: Structure solved by direct methods (SHELXS). [The asymmetric unit consists of half a molecule lying on the mirror plane. Hydrogen atoms were taken from a difference map and refined], refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, weights $\propto [\sigma^2(I)+0.0009I^2]^{-1/2}$, refined anisotropic: all non-hydrogen atoms, isotropic: H , 122 parameters, data/parameter ratio = 6.66, final R = 0.042, Rw = 0.045, error of fit = 1.69, max Δ/σ = 0.05, largest residual density = 0.26e/Å^3, near C4

RESULTS: This analysis confirms the structure of 2-(4-fluorophenyl)-4-trifluoromethyl-1-N-methyl-imidazole as part of a study of ACAT inhibitors (cardiovascular). The structure is seen to be planar by crystallographic symmetry, similar to a previous analysis (91290)

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
F(37)	4355(3)	2500	-143(2)	5.3(1)'
F(41)	10185(2)	4060(2)	8107(1)	4.7(1)'
F(42)	8590(3)	2500	9226(2)	5.9(1)'
N(1)	4366(3)	2500	5867(2)	2.1(1)'
N(3)	7458(3)	2500	5827(2)	2.4(1)'
C(2)	5645(4)	2500	5121(2)	2.0(1)'
C(4)	7298(4)	2500	7045(3)	2.4(1)'
C(5)	5422(4)	2500	7093(3)	2.4(1)'
C(11)	2226(4)	2500	5516(3)	3.1(1)'
C(31)	5200(4)	2500	3728(3)	2.0(1)'
C(32)	6768(5)	2500	3175(3)	3.1(1)'
C(33)	6492(5)	2500	1876(3)	3.9(1)'
C(34)	4641(5)	2500	1133(3)	3.2(1)'
C(35)	3066(5)	2500	1624(3)	3.5(1)'
C(36)	3357(4)	2500	2926(3)	3.0(1)'
C(44)	9040(5)	2500	8119(3)	3.5(1)'
H(5)	4835(41)	2500	7775(28)	2.8(7)
H(11)	1809(50)	2500	6269(34)	4.0(8)
H(11')	1775(31)	1310(34)	4999(21)	3.9(6)
H(32)	8016(48)	2500	3700(30)	3.2(7)
H(33)	7618(49)	2500	1556(32)	4.2(8)
H(35)	1784(54)	2500	1070(34)	4.8(9)
H(36)	2239(46)	2500	3244(29)	3.3(7)

TABLE II. Anisotropic Thermal Parameters (Angs X 1000)
exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
F(37)	71.1(15)	110.8(21)	20.2(10)	0.0	10.8(10)	0.0
F(41)	40.3(8)	76.5(12)	53.2(9)	-15.2(8)	-3.9(6)	-8.9(8)
F(42)	45.6(12)	156.7(27)	20.7(10)	0.0	3.5(9)	0.0
N(1)	21.9(11)	33.1(16)	24.4(12)	0.0	6.9(9)	0.0
N(3)	25.0(13)	42.1(17)	22.1(12)	0.0	5.0(10)	0.0
C(2)	23(1)	28(2)	26(2)	0	9(1)	0
C(4)	27(2)	38(2)	23(1)	0	4(1)	0
C(5)	33(2)	39(2)	23(1)	0	12(1)	0
C(11)	23(2)	65(3)	32(2)	0	11(1)	0
C(31)	26(1)	30(2)	21(1)	0	7(1)	0
C(32)	29(2)	64(3)	27(2)	0	8(1)	0
C(33)	40(2)	79(3)	33(2)	0	17(2)	0
C(34)	52(2)	51(2)	18(2)	0	8(1)	0
C(35)	36(2)	66(3)	26(2)	0	0(1)	0
C(36)	26(2)	63(3)	24(2)	0	6(1)	0
C(44)	35(2)	67(3)	29(2)	0	6(1)	0

TABLE III. Interatomic Distances (A)

F(37)-C(34)	1.356 (3)	C(31)-C(36)	1.384 (4)
F(41)-C(44)	1.341 (2)	C(32)-C(33)	1.382 (4)
F(42)-C(44)	1.325 (4)	C(33)-C(34)	1.365 (5)
N(1)-C(2)	1.366 (3)	C(34)-C(35)	1.360 (5)
N(1)-C(5)	1.362 (4)	C(35)-C(36)	1.385 (4)
N(1)-C(11)	1.477 (4)	C(5)-H(5)	0.940 (29)
N(3)-C(2)	1.329 (3)	C(11)-H(11)	0.941 (36)
N(3)-C(4)	1.362 (4)	C(11)-H(11')	0.994 (23)
C(2)-C(31)	1.474 (4)	C(32)-H(32)	0.929 (32)
C(4)-C(5)	1.351 (4)	C(33)-H(33)	0.952 (34)
C(4)-C(44)	1.480 (4)	C(35)-H(35)	0.961 (37)
C(31)-C(32)	1.397 (4)	C(36)-H(36)	0.946 (31)

TABLE IV. Intramolecular Angles (Deg)

C(2)-N(1)-C(5)	107.4 (2)	C(2)-C(31)-C(32)	117.2 (2)
C(2)-N(1)-C(11)	130.2 (2)	C(2)-C(31)-C(36)	125.3 (2)
C(5)-N(1)-C(11)	122.4 (2)	C(32)-C(31)-C(36)	117.6 (3)
C(2)-N(3)-C(4)	105.0 (2)	C(31)-C(32)-C(33)	121.3 (3)
F(41)-C(44)-F(41)a	104.7 (3)	C(32)-C(33)-C(34)	118.6 (3)
F(41)-C(44)-F(42)	107.2 (2)	C(33)-C(34)-C(35)	122.4 (3)
F(37)-C(34)-C(33)	119.0 (3)	C(34)-C(35)-C(36)	118.6 (3)
F(37)-C(34)-C(35)	118.6 (3)	C(31)-C(36)-C(35)	121.6 (3)
F(41)-C(44)-C(4)	112.6 (2)	C(4)-C(5)-H(5)	132 (2)
F(42)-C(44)-C(4)	112.1 (3)	C(31)-C(32)-H(32)	119 (2)
N(1)-C(2)-N(3)	110.6 (2)	C(33)-C(32)-H(32)	120 (2)
N(1)-C(2)-C(31)	127.7 (2)	C(32)-C(33)-H(33)	117 (2)
N(3)-C(2)-C(31)	121.7 (2)	C(34)-C(33)-H(33)	124 (2)
N(3)-C(4)-C(5)	111.3 (2)	C(34)-C(35)-H(35)	120 (2)
N(3)-C(4)-C(44)	121.0 (3)	C(36)-C(35)-H(35)	121 (2)
N(1)-C(5)-C(4)	105.7 (3)	C(31)-C(36)-H(36)	121 (2)
N(1)-C(5)-H(5)	122 (2)	C(35)-C(36)-H(36)	117 (2)
N(1)-C(11)-H(11)	108 (2)	H(11)-C(11)-H(11')	112 (2)
N(1)-C(11)-H(11')	108 (1)	H(11')-C(11)-H(11')a	109 (3)
C(5)-C(4)-C(44)	127.7 (3)		

TABLE V. Intramolecular Non-Bonding Distances (A)

C(11)...C(36)	3.128 (5)

TABLE VI. Intermolecular Distances (A)

F(37)...F(41)b	3.282 (3)
F(37)...F(42)c	3.260 (3)
F(37)...C(5)c	3.291 (4)
F(41)...C(33)d	3.327 (3)
F(41)...C(35)e	3.359 (3)

Symmetry Operation Codes

a	X,1/2-Y,Z
b	-1+X,Y,-1+Z
c	X,Y,-1+Z
d	2-X,1/2+Y,1-Z
e	1-X,1/2+Y,1-Z

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