Supporting Information

Copper-Catalyzed Synthesis of Trifluoromethyl-Substituted Isoxazolines

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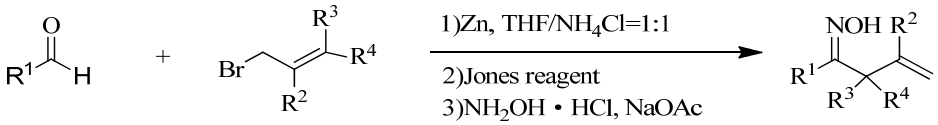
1. General remarks

Column chromatography was carried out on silica gel and analytical TLC was performed with silica gel GF254 plates. NMR spectra were recorded in $CDCl_3$ at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR) and 376 MHz (^{19}F NMR). IR spectra were recorded on a FT-IR spectrometer and only major peaks are reported in cm^{-1}. Data collections for crystal structure were performed at room temperature (293 K) using Mo*K*α radiation on a Bruker APEXII diffractometer. All trifluoromethylation products were further characterized by high resolution mass spectra (HRMS); copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. DMF were dried by $MgSO_4$ and distilled under reduced pressure before used.

2. General procedure for the synthesis of ketoximes

Procedure for the synthesis of ketoxime 1a-1h, 1j-1n:

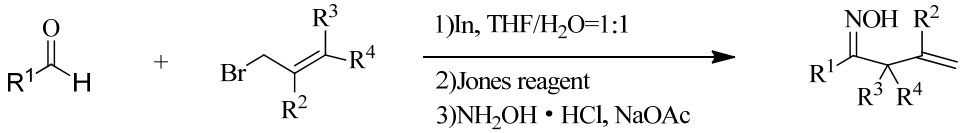


1) Aldehyde (1.0 equiv) was dissolved in anhydrous THF. A sample was taken out for analysis and allylbromide (2.0 equiv) was added. Another sample was taken out for analysis and saturated aqueous NH_4Cl was added. Portions of activated zinc dust (2.0 equiv) were added slowly on at 0℃ and the resulting suspension was stirred overnight at this temperature. The THF layer was separated from the aqueous layer, which was extracted with diethyl ether for 3 times. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in *vacuo*. The crude product was directly used in the next step without further purification.[1]

2) A solution of the homoallylic alcohol (1.0 equiv) in diethyl ether was stirred at 0℃ while Jones reagent (2.0-4.0 equiv) was added dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 1 h. The diethyl ether layer was then separated from the aqueous layer, which was extracted with diethyl ether for 3 times. The combined diethyl ether layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in *vacuo*. The crude product was directly used in the next step withoutfurther purification.[2]

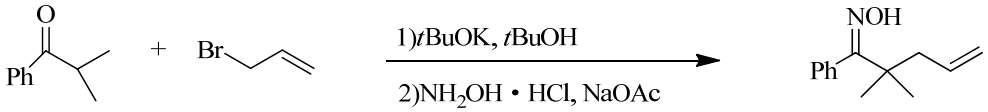
3) To a solution of hydroxylamine hydrochloride (5.0 equiv) in water was added a solution of sodium acetate (7.0 equiv) in ethanol. The mixture was stirred at room temperature while the *β,γ*-unsaturated ketone (1.0 equiv) was added as a solution in ethanol. The mixture was stirred overnight and concentrated in *vacuo.* Then, the mixture was extracted with ethyl acetate 3 times and the combined extracts were washed with water and brine, dried (Mg_2SO_4), filtered, and concentrated in *vacuo*. The crude material was purified by flash chromatography on silica gel to afford the *β,γ*-unsaturated oxime.[2]

Procedure for the synthesis of ketoxime 1i, and 1o-1q:



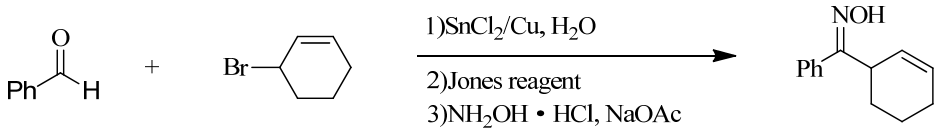
1)A round bottomed flask charged with a solution of the 3-bromo-2-methylprop-1-ene (1.1 equiv) or its analogue and indium (1.1 equiv) in THF/H_2O (1:1) was kept at room temperature with stirring. The aldehyde (1.0 equiv) was added to the solution and the resulting suspension was stirred for 10-24 h. Saturated ammonium chloride or 1 N hydrochloride solution was added at 0℃. The THF layer was separated from the aqueous layer, which was extracted with diethyl ether for 3 times. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in *vacuo*. The crude product was directly used in the next step without further purification.[3]
Steps 2) and 3) are same as above-mentioned.

Procedure for the synthesis of ketoxime 1r:



1)A mixture of isobutyrophenone (1.0 equiv), allyl bromide (1.1 equiv) and potassium *t*-butoxide (1.1 equiv) in *t*-butyl alcohol was heated at reflux for 2.5 h under a nitrogen atmosphere. Afterwards *t*-butanol was removed by distillation and the crude mixture was extracted with ethyl acetate 3 times and the combined extracts were washed with water and brine, dried (Mg_2SO_4), filtered, and concentrated in *vacuo*. The crude material was purified by flash chromatography on silica gel to afford the ketoxime **1s**.[5]
Steps 2) is the same as above-mentioned.

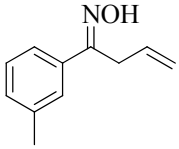
Procedure for the synthesis of ketoxime 1s:



1)Cyclohex-2-en-1-yl(phenyl)methanol were prepared through the reaction $SnCl_2$•H_2O, copper powder, benzaldehyde and primary 3-bromocyclohex-1-ene in water at the room temperature according to the literature procedure.[6]
Steps 2) and 3) are same as above-mentioned.

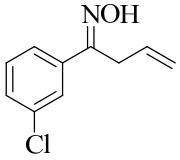
3. Characterization data

1-(*m*-tolyl)but-3-en-1-one oxime 1d



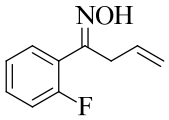
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 9.96(s, 1H), 7.44-7.41 (m, 2H), 7.27-7.14 (m, 2H), 5.97-5.90 (m, 1H), 5.19-5.08 (m, 2H), 3.58 (d, *J* = 5.6 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 156.9, 138.1, 135.5, 132.1, 130.0, 128.4, 127.0, 123.5, 117.0, 31.2, 21.4.

1-(3-chlorophenyl)but-3-en-1-one oxime 1g



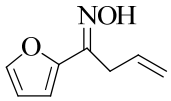
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 9.16 (d, *J* = 19.6 Hz, 1H), 7.62-7.61 (m, 1H), 7.52-7.49 (m, 1H), 7.36-7.25 (m, 2H), 5.97-5.87 (m, 1H), 5.19-5.11 (m, 2H), 3.58-3.55 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.9, 137.3, 134.6, 131.6, 129.8, 129.3, 126.5, 124.5, 117.4, 30.9.

1-(2-fluorophenyl)but-3-en-1-one oxime 1h



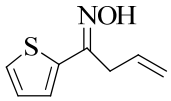
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 10.24 (s, 1H), 7.45-7.41 (m, 1H), 7.35-7.30 (m, 1H), 7.22-7.05 (m, 2H), 5.88-5.78 (m, 1H), 5.14-5.03 (m, 2H), 3.57 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 160.2 (d, *J* = 249.0 Hz), 154.9 (d, *J* = 2.0 Hz), 131.5, 130.7 (d, *J* = 8.0 Hz), 129.9 (d, *J* = 3.0 Hz), 124.2 (d, *J* = 4.0 Hz), 123.9 (d, *J* = 12.0 Hz), 117.6, 116.2 (d, *J* = 22.0 Hz), 32.8 (d, *J* = 3.0 Hz).

1-(furan-2-yl)but-3-en-1-one oxime 1l



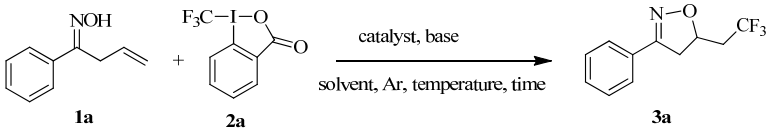
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 9.50 (s, 1H), 7.48-7.46(m, 2H), 6.55-6.54 (m, 1H), 6.04-5.97 (m, 1H), 5.23-5.11 (m, 2H), 3.45 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 146.0, 145.3, 142.6, 133.6, 118.4, 117.4, 112.1, 35.8.

1-(thiophen-2-yl)but-3-en-1-one oxime 1m



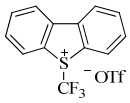
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 9.25 (s, 1H), 7.28 (d, *J* = 4.4 Hz 2H), 7.02 (t, *J* = 4.4 Hz 1H), 5.99-5.92 (m, 1H), 5.24-5.11 (m, 2H), 3.60 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 152.7, 139.1, 131.7, 127.2, 126.9, 126.8, 117.4, 31.3.

4. Table S1. Optimization of the reaction conditions [a]



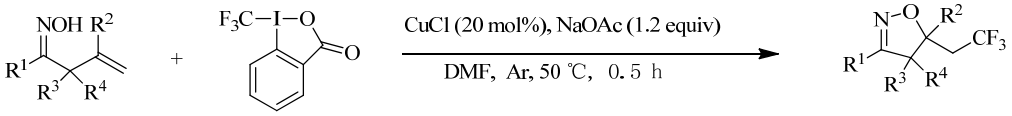
Entry	Catalyst (mol %)	Base (equiv)	Temperature (℃)	Time (h)	Solvent	Yield (%)[b]
1	CuCl (20)	KF (1.2)	50	0.5	DMF	65
2[c]	CuCl (20)	KF (1.2)	50	0.5	DMF	0
3[d]	CuCl (20)	KF (1.2)	50	0.5	DMF	0
4[e]	—	KF (1.2)	50	0.5	DMF	0
5	$Cu(OTf)_2$ (20)	KF (1.2)	50	0.5	DMF	18
6	$Cu(OAc)_2$ (20)	KF (1.2)	50	0.5	DMF	40
7	$[Cu(OTf)_2]\cdot C_6H_6$ (20)	KF (1.2)	50	0.5	DMF	10
8	$CuCl_2$ (20)	KF (1.2)	50	0.5	DMF	59
9	$Cu(CH_3CN)_4F_6$	KF (1.2)	50	0.5	DMF	18
10	CuI (20)	KF (1.2)	50	0.5	DMF	62
11	CuBr (20)	KF (1.2)	50	0.5	DMF	61
12	CuCl (20)	K_3PO_4 (1.2)	50	0.5	DMF	73
13	CuCl (20)	K_2CO_3 (1.2)	50	0.5	DMF	70
14	CuCl (20)	Cs_2CO_3 (1.2)	50	0.5	DMF	59
15	CuCl (20)	t-BuOK (1.2)	50	0.5	DMF	59
16	CuCl (20)	Et_3N (1.2)	50	0.5	DMF	69
17	**CuCl (20)**	**NaOAc (1.2)**	**50**	**0.5**	**DMF**	**79**
18	CuCl (10)	NaOAc (1.2)	50	0.5	DMF	66
19	CuCl (50)	NaOAc (1.2)	50	0.5	DMF	77
20	CuCl (100)	NaOAc (1.2)	50	0.5	DMF	77
21	CuCl (20)	NaOAc (1.0)	50	0.5	DMF	75
22	CuCl (20)	NaOAc (1.5)	50	0.5	DMF	79
23	CuCl (20)	NaOAc (2.0)	50	0.5	DMF	78
24	CuCl (20)	NaOAc (3.0)	50	0.5	DMF	76
25	CuCl (20)	NaOAc (1.2)	50	1.0	DMF	77
26	CuCl (20)	NaOAc (1.2)	50	2.0	DMF	78
27	CuCl (20)	NaOAc (1.2)	50	5.0	DMF	78
28	CuCl (20)	NaOAc (1.2)	40	0.5	DMF	74
29	CuCl (20)	NaOAc (1.2)	60	0.5	DMF	78
30	CuCl (20)	NaOAc (1.2)	80	0.5	DMF	79
31	CuCl (20)	NaOAc (1.2)	50	0.5	CH_3CN	42
32	CuCl (20)	NaOAc (1.2)	50	0.5	THF	30
33	CuCl (20)	NaOAc (1.2)	50	0.5	NMP	70
34	CuCl (20)	NaOAc (1.2)	50	0.5	DMSO	69
35	CuCl (20)	NaOAc (1.2)	50	0.5	DMAC	67
36	CuCl (20)	NaOAc (1.2)	50	0.5	toluene	trace
37	CuCl (20)	NaOAc (1.2)	50	0.5	1,4-dioxane	20

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), copper catalyst, base, solvent (3 mL), temperature , time, under argon. [b] Isolated yield. [c] $TMSCF_3$ was used. [d] Umemoto reagent **2b** was used. [e] Without CuCl.



2b

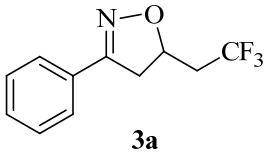
5. General experimental procedure



1 **2a** **3**

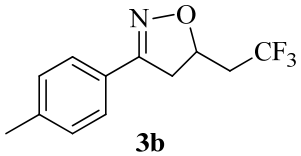
DMF (3 mL) was added to ketoxime **1** (0.2 mmol, 1.0 equiv) , *Togni*-reagent **2a** (0.3 mmol, 1.5 equiv), NaOAc (0.24 mmol, 1.2 equiv) and CuCl (0.04mmol, 0.2 equiv) under Argon. The mixture was stirred for 0.5 hours at 50 ℃ and extracted with ethyl acetate. The combined organic layers were washed with saturated brine, dried over Na_2SO_4, concentrated in *vacuo* and purified by flash column chromatography (silica gel) to afford the product **3**.

6. Characterization data of 3a-3q, and 3s



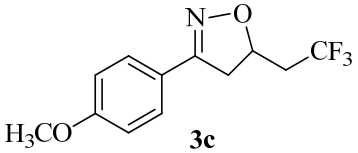
3a

3-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3a: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.68-7.66 (m, 2H), 7.43-7.39 (m, 3H), 5.01-4.97 (m, 1H), 3.60-3.53 (m, 1H), 3.20-3.14 (m, 1H), 2.77-2.69 (m, 1H), 2.48-2.40 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 156.6, 130.4, 128.9, 128.8, 126.7, 125.2 (q, J = 275.0 Hz, CF_3), 74.7 (d, J = 3.0 Hz), 40.4, 39.1 (q, J = 27.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.82 (s, 3F). IR (neat, cm^{-1}): 3395, 2923, 2361, 1384, 1076, 767, 672. HRMS (ESI) Calcd for $C_{11}H_{10}F_3NO$: M+H = 230.0787. Found: 230.0784.



3b

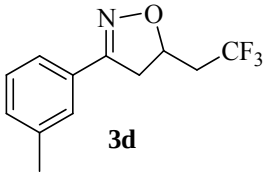
3-(p-tolyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3b: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.56 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 5.00-4.92 (m, 1H), 3.57-3.50 (m, 1H), 3.17-3.10 (m, 1H), 2.75-2.67 (m, 1H), 2.47-2.39 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 156.5, 140.7, 129.4, 126.6, 126.0, 125.3 (q, J = 275.0 Hz, CF_3), 74.6 (d, J = 3.0 Hz), 40.5, 39.3 (q, J = 28.0 Hz, CH_2CF_3), 21.4 . ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.85 (s, 3F). IR (neat, cm^{-1}): 3437, 2931, 2360, 1407, 1279, 1150, 823, 661. HRMS (ESI) Calcd for $C_{12}H_{12}F_3NO$: M+H = 244.0944. Found: 244.0947.



3c

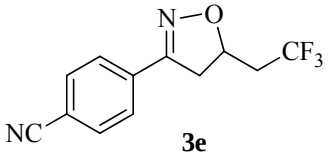
3-(4-methoxyphenyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3c: Solid, ^{1}H

NMR (400 MHz, $CDCl_3$) δ ppm 7.60 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.99-4.91 (m, 1H), 3.84 (s, 3H), 3.56-3.50 (m, 1H), 3.16-3.10 (m, 1H), 2.75-2.67 (m, 1H), 2.47-2.39 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.3, 156.1, 128.3, 128.1, 125.3 (q, *J* = 275.0 Hz, CF_3), 114.2, 74.5, 55.3, 40.6, 39.1 (q, *J* = 27.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.84 (s, 3F). IR (neat, cm^{-1}): 3438, 2924, 1516, 1256, 1118, 1040, 838, 658 . HRMS (ESI) Calcd for $C_{12}H_{12}F_3NO_2$: M+H = 260.0893. Found: 260.0890.



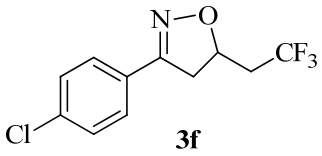
3d

3-(m-tolyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3d: Solid, ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.50-7.43 (m, 2H), 7.32-7.23 (m, 2H), 5.00-4.92 (m, 1H), 3.57-3.50 (m, 1H), 3.17-3.11 (m, 1H), 2.75-2.67 (m, 1H), 2.46-2.38 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 156.7, 138.5, 131.2, 128.8, 128.7, 127.3, 125.3 (q, *J* = 275.0 Hz, CF_3), 123.9, 74.7 (d, *J* = 3.0 Hz), 40.5, 39.1 (q, *J* = 28.0 Hz, CH_2CF_3), 21.3. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.83 (s, 3F). IR (neat, cm^{-1}): 3396, 2924, 2361, 1385, 1255, 1113, 912, 792. HRMS (ESI) Calcd for $C_{12}H_{12}F_3NO$: M+H = 244.0944. Found: 244.0941.



3e

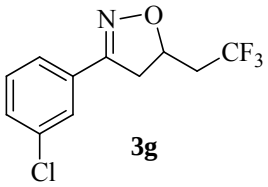
4-(5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazol-3-yl)benzonitrile 3e: Solid, ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.78-7.70 (m, 2H), 5.10-5.02 (m, 1H), 3.61-3.54 (m, 1H), 3.20-3.14 (m, 1H), 2.79-2.71 (m, 1H), 2.52-2.44 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.3, 133.2, 132.5, 127.1, 125.0 (q, *J* = 275.0 Hz, CF_3), 118.1, 113.7, 75.7 (d, *J* = 3.0 Hz), 39.7, 39.0 (q, *J* = 28.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.81 (s, 3F). IR (neat, cm^{-1}): 3439, 2922, 2361, 1388, 1253, 1114, 915, 837. HRMS (ESI) Calcd for $C_{12}H_9F_3N_2O$: M+H = 255.0740. Found: 255.0743.



3f

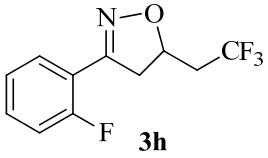
3-(4-chlorophenyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3f: Solid, ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.60 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.8 Hz, 2H), 5.04-4.96 (m, 1H), 3.57-3.51 (m, 1H), 3.17-3.11 (m, 1H), 2.77-2.67 (m, 1H), 2.52-2.41 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.7, 136.5, 129.1, 127.9, 127.4, 125.2 (q, *J* = 275.0 Hz, CF_3), 75.07, 40.3, 39.0 (q, *J* = 28.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.84 (s, 3F). IR (neat, cm^{-1}): 3437, 2950, 1403, 1247,

1156, 1077, 819, 654. HRMS (ESI) Calcd for $C_{11}H_9ClF_3NO$: M+H = 264.0398. Found: 264.0402.



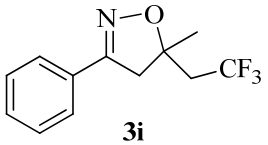
3g

3-(3-chlorophenyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3g: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.64 (s, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.41-7.33 (m, 2H), 5.05-4.97 (m, 1H), 3.57-3.50 (m, 1H), 3.17-3.10 (m, 1H), 2.77-2.66 (m, 1H), 2.49-2.41 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 125.5, 134.8, 130.7, 130.4, 130.1, 126.7, 125.2 (q, *J* =275.0 Hz, CF_3), 124.8, 75.1 (d, *J* = 3.0 Hz), 40.1, 39.0 (q, *J* = 28.0 Hz, CH_2CF_3). IR (neat, cm^{-1}): 2921, 1774, 1490, 1383, 1283, 1067. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.83 (s, 3F). IR (neat, cm^{-1}): 3439, 2927, 1562, 1431, 1255, 1150, 915, 787. HRMS (ESI) Calcd for $C_{11}H_9ClF_3NO$: M+H = 264.0398. Found: 264.0401.



3h

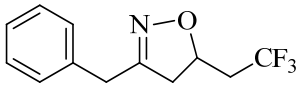
3-(2-fluorophenyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3h: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.85 (d, *J* = 7.6 Hz, 1H), 7.42-7.39 (m, 1H), 7.21-7.10 (m, 2H), 5.03-4.95 (m, 1H), 3.69-3.61 (m, 1H), 3.28-3.72 (m, 1H) , 2.75-2.66 (m, 1H), 2.49-2.40 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 160.3 (d, *J* = 251.0 Hz,) 153.4 (d, *J* = 3.0 Hz, CF), 132.1 (d, *J* = 9.0 Hz), 129.0, 125.2 (q, *J* = 275.0 Hz, CF_3), 124.6 (d, *J* = 3.0 Hz), 117.1 (d, *J* = 9.0 Hz), 116.4 (d, *J* = 22.0 Hz), 75.0 (t, *J* = 3.0 Hz), 42.1 (d, *J* = 7.0 Hz), 39.2 (q, *J* = 28.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.89 (s, 3F). IR (neat, cm^{-1}): 3419, 2924, 1594, 1455, 1254, 1114, 824, 762. HRMS (APCI) Calcd for $C_{11}H_9F_4NO$: M+H = 248.0693. Found: 248.0697.



3i

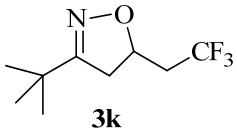
5-methyl-3-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3i: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.65 (t, *J* = 3.6 Hz, 2H), 7.40 (d, *J* = 3.6 Hz, 3H), 3.39 (d, *J* = 16.8 Hz, 1H), 3.18-3.10 (m, 1H), 2.68-2.57 (m, 2H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 156.5, 130.2, 128.7, 128.6, 126.5, 125.2 (q, *J* = 276.0 Hz, CF_3), 83.2 (d, *J* = 2.0 Hz), 45.6, 42.8 (q, *J* = 27.0 Hz, CH_2CF_3), 25.5 (d, *J* = 1.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ -61.33 (s, 3F). IR (neat, cm^{-1}): 3396, 2925, 1597, 1365, 1259, 1157, 918, 759. HRMS (ESI) Calcd for $C_{12}H_{12}F_3NO$: M+H = 244.0944.

Found: 244.0941.



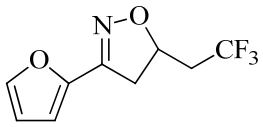
3j

3-benzyl-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3j: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.35-7.22 (m, 5H), 4.80-4.72 (m, 1H), 3.69 (s, 2H), 3.04-2.98 (m, 1H), 2.63-2.51 (m, 2H), 2.32-2.22 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 158.0, 135.2, 128.9, 128.7, 127.2, 125.2 (q, J = 275.0 Hz, CF_3), 74.0, 41.7, 38.9 (q, J = 28.0 Hz, CH_2CF_3), 33.9. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.98 (s, 3F). IR (neat, cm^{-1}): 3438, 2920, 1388, 1254, 1143, 855, 702. HRMS (ESI) Calcd for $C_{12}H_{12}F_3NO$: M+H = 244.0944. Found: 244.0941.



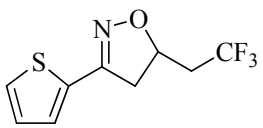
3k

3-(tert-butyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3k: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 4.81-4.74 (m, 1H), 3.19-3.12 (m, 1H), 2.79-2.73 (m, 1H), 2.66-2.55 (m, 1H), 2.38-2.27 (m, 1H), 1.22 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 166.1, 125.3 (q, J = 275.0 Hz, CF_3), 74.0 (d, J = 3.0 Hz), 39.74, 38.8 (q, J = 27.0 Hz, CH_2CF_3), 33.0, 28.0. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.86 (s, 3F). IR (neat, cm^{-1}): 3439, 2920, 1624, 1384, 1067, 772, 548. HRMS (ESI) Calcd for $C_9H_{14}F_3NO$: M+H = 210.1100. Found: 210.1096.



3l

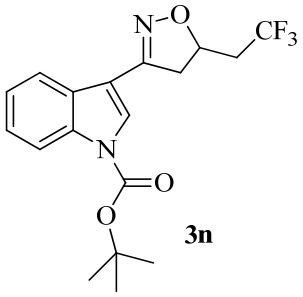
3-(furan-2-yl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3l: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.54 (s, 1H), 6.76 (d, J = 3.2 Hz, 1H), 6.52 (s, 1H), 4.99-4.92 (m, 1H), 3.56-3.50 (m, 1H), 3.17-3.11 (m, 1H), 2.76-2.67 (m, 1H), 2.47-2.39 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 148.8, 144.7, 144.2, 125.1 (q, J = 275.0 Hz, CF_3), 112.3, 111.8, 74.6, 40.3, 38.9 (q, J = 28.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, CDCl3): δ -63.87 (s, 3F). IR (neat, cm^{-1}): 3389, 2923, 1695, 1384, 1252, 1043, 763, 586. HRMS (APCI) Calcd for $C_9H_8F_3NO_2$: M+H = 220.0580. Found: 220.0586.



3m

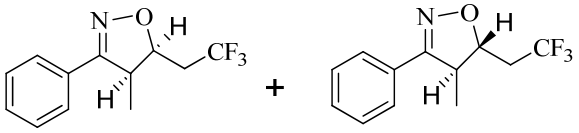
3-(thiophen-2-yl)-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3m: Solid, ^{1}H

NMR (400 MHz, $CDCl_3$) δ ppm 7.42 (d, *J* = 4.8 Hz, 1H), 7.22 (d, *J* = 3.2 Hz, 1H), 7.09-7.06 (m, 1H), 5.01-4.94 (m, 1H), 3.60-3.53 (m, 1H), 3.20-3.14 (m, 1H), 2.76-2.68 (m, 1H), 2.48-2.40 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 152.3, 131.3, 128.8, 128.7, 127.3, 125.2 (q, *J* = 275.0 Hz, CF_3), 75.0 (d, *J* = 3.0 Hz), 41.2, 38.9 (q, *J* = 28.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.83 (s, 3F). IR (neat, cm^{-1}): 3438, 2921, 2361, 1434, 1258, 1121, 810, 719. HRMS (ESI) Calcd for $C_9H_8F_3NOS$: M+H = 236.0351. Found: 236.0355.



3n

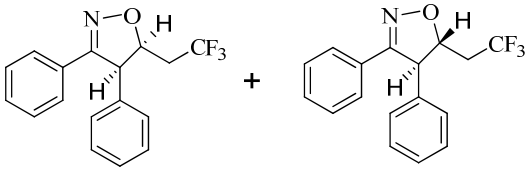
tert-butyl-3-(5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazol-3-yl)-1H-indole-1-carboxylate 3n: Solid, ^1H NMR (400 MHz, $CDCl_3$) δ ppm 8.22 (d, *J* = 7.6 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.73 (s, 1H), 7.43-7.33 (m, 1H), 7.27 (s, 1H), 5.00-4.92 (m, 1H), 3.62-3.56 (m, 1H), 3.23-3.17 (m, 1H), 2.81-2.69 (m, 1H), 2.53-2.39 (m, 1H), 1.71 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 152.2, 149.3, 135.8, 127.0, 126.9, 125.7, 125.4 (q, *J* = 275.0 Hz, CF_3), 123.9, 123.0, 115.1, 111.3, 84.9, 73.7, 41.4, 39.1 (q, *J* = 28.0 Hz, CH_2CF_3), 28.2. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.81 (s, 3F) IR (neat, cm^{-1}): 3428, 2980. 1736, 1627, 1371, 1251, 1155, 891, 754. HRMS (APCI) Calcd for $C_{18}H_{19}F_3N_2O_3$: M+H = 369.1421. Found: 369.1426.



cis-**3o**
Major

trans-**3o**
Minor

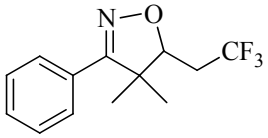
4-methyl-3-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3o: Solid, d.r.(*cis*:*trans*) = 3.3:1, ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.73-7.67 (m, 2.8H), 7.44-7.42 (m, 4.2 H), 4.76-4.74 (m, 0.3H), 4.64-4.60 (m, 1.0H), 3.65-3.62 (m, 0.3H), 3.58-3.52 (m, 1.0H), 2.65-2.55 (m, 1.6H), 2.41-2.33 (m, 1.0H), 1.37 (s, 3.1H), 1.35 (s, 0.9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.9, 160.4, 130.4, 130.3, 128.9, 128.9, 128.3, 128.1, 127.0, 127.0, 125.6 (q, *J* = 275.0 Hz, CF_3), 125.4 (q, *J* = 275.0 Hz, CF_3), 81.8 (d, *J* = 3.0Hz), 78.0 (d, *J* = 3.0Hz), 47.7, 43.7, 38.5 (q, *J* = 27.0 Hz, CH_2CF_3), 32.9 (q, *J* = 29.0 Hz, CH_2CF_3), 17.5, 11.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.31 (s, 3F), δ -64.34 (s, 3F). IR (neat, cm^{-1}): 3394, 2924, 1651, 1384, 1255, 1077, 769, 699. HRMS (ESI) Calcd for $C_{12}H_{12}F_3NO$: M+H = 244.0944. Found: 244.0940.



cis-**3p**
Major

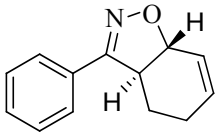
trans-**3p**
Minor

3,4-diphenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3p: Solid, d.r.(*cis*:*trans*) = 3.4:1, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.61-7.59 (m, 2.6H), 7.37-7.16 (m, 10.3H), 5.02-4.99 (m, 0.3H), 4.83-4.79 (m, 1.0H), 4.67-4.65 (m, 0.3H), 4.56-4.55 (m, 1.0H), 2.73-2.56 (m, 1.0H), 2.54-2.48 (m, 1.0H), 2.28-2.24 (m, 0.3H), 2.22-2.12 (m, 0.3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 160.7, 158.0, 137.7, 132.9, 130.2, 130.2, 129.4, 129.4, 129.2, 128.7, 128.5, 128.2, 128.1, 127.4, 127.3, 127.3, 127.2, 127.1, 125.6 (q, J = 275.0 Hz, CF_3), 125.3 (q, J = 275.0 Hz, CF_3), 83.6 (d, J = 3.0 Hz), 79.1 (d, J = 3.0 Hz), 59.7, 56.8, 38.8 (q, J = 27.0 Hz, CH_2CF_3), 34.0 (q, J = 29.0 Hz, CH_2CF_3). ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.88 (s, 3F), δ -64.23 (s, 3F). IR (neat, cm^{-1}): 3435, 2922, 1597, 1385, 1255, 1126, 770, 696. HRMS (ESI) Calcd for $C_{17}H_{14}F_3NO$: M+H = 306.1100. Found: 306.1097.



3q

4,4-dimethyl-3-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydroisoxazole 3q: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.65-7.62 (m, 2H), 7.44-7.39 (m, 3H), 4.41-4.38 (m, 1H), 2.63-2.55 (m, 1H), 2.45-2.37 (m, 1H), 1.41 (s, 3H), 1.25 (s, 3H),. ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 164.9, 130.0, 128.8, 128.7, 127.4, 125.9 (q, J = 275.0 Hz, CF_3), 83.9 (d, J = 3.0 Hz), 51.5, 33.2 (q, J = 29.0 Hz, CH_2CF_3), 23.3, 19.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.72 (s, 3F). IR (neat, cm^{-1}): 3395, 2923, 1654, 1403, 1257, 1120, 903, 694. HRMS (ESI) Calcd for $C_{13}H_{14}F_3NO$: M+H = 258.1100. Found: 258.1103.



3s

3-phenyl-3a,4,5,7a-tetrahydrobenzo[d]isoxazole 3s: Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.73-7.71 (m, 2H), 7.42-7.41 (m, 3H), 6.20-6.17 (m, 1H), 6.05-6.03 (m, 1H), 4.84-4.82 (m, 1H), 3.54-3.48 (m, 1H), 2.14-2.09 (m, 1H), 2.03-1.97 (m, 2H), 1.58-1.51 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.1, 133.1, 129.9, 129.2, 128.8, 126.9, 122.4, 76.7, 44.1, 23.0, 22.4. HRMS (ESI) Calcd for $C_{13}H_{13}NO$: M+H = 200.1070. Found: 200.1067.

7. References:

[1] J. H. Dam, P. Fristrup and R. Madsen, *J. Org. Chem*., 2008, **73**, 3228.

[2] D. Jiang, J. Peng and Y. Chen, *Org. Lett.*, 2008, **10**, 1695.

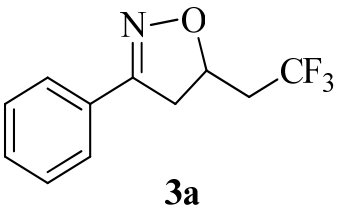
[3] M.-K. Zhu, J.-F. Zhao and T.-P. Loh, *J. Am. Chem. Soc.* 2010, **132**, 6284.

[4] F. Miege, C. Meyer and J. Cossy, *Angew. Chem. Int. Ed*., 2011, **123**, 6054.

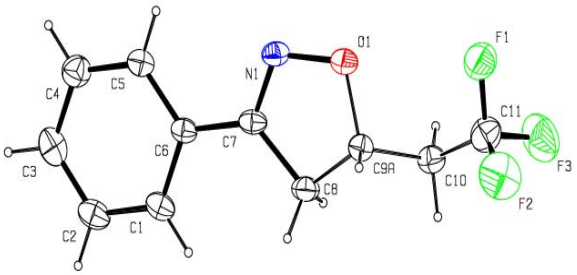
[5] H. M. Barentsen, A. B. Sieval and J. Corenelisse, *Tetrahedron,* 1995, **51**, 7495.

[6] X.-H. Tan, C.-Z. Tao, Y.-Q. Hou, L. Luo, L. Liu and Q.-X. Guo, *Chinese J. Chem.,* 2005, **23**, 237.

8. Crystallographic data of 3a



3a



structure of 3a

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alpha=90 beta=102.331(12) gamma=90

Temperature: 293 K

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Hall group	-P 2yab	-P 2yab
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Sum formula	C11 H10 F3 N O	C11 H10 F3 N O
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Dx,g cm-3	1.425	1.425
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Mu (mm-1)	0.127	0.127
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F000'	944.70	
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Tmin,Tmax	0.967,0.974	
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Correction method= Not given

Data completeness= 0.998 Theta(max)= 25.680

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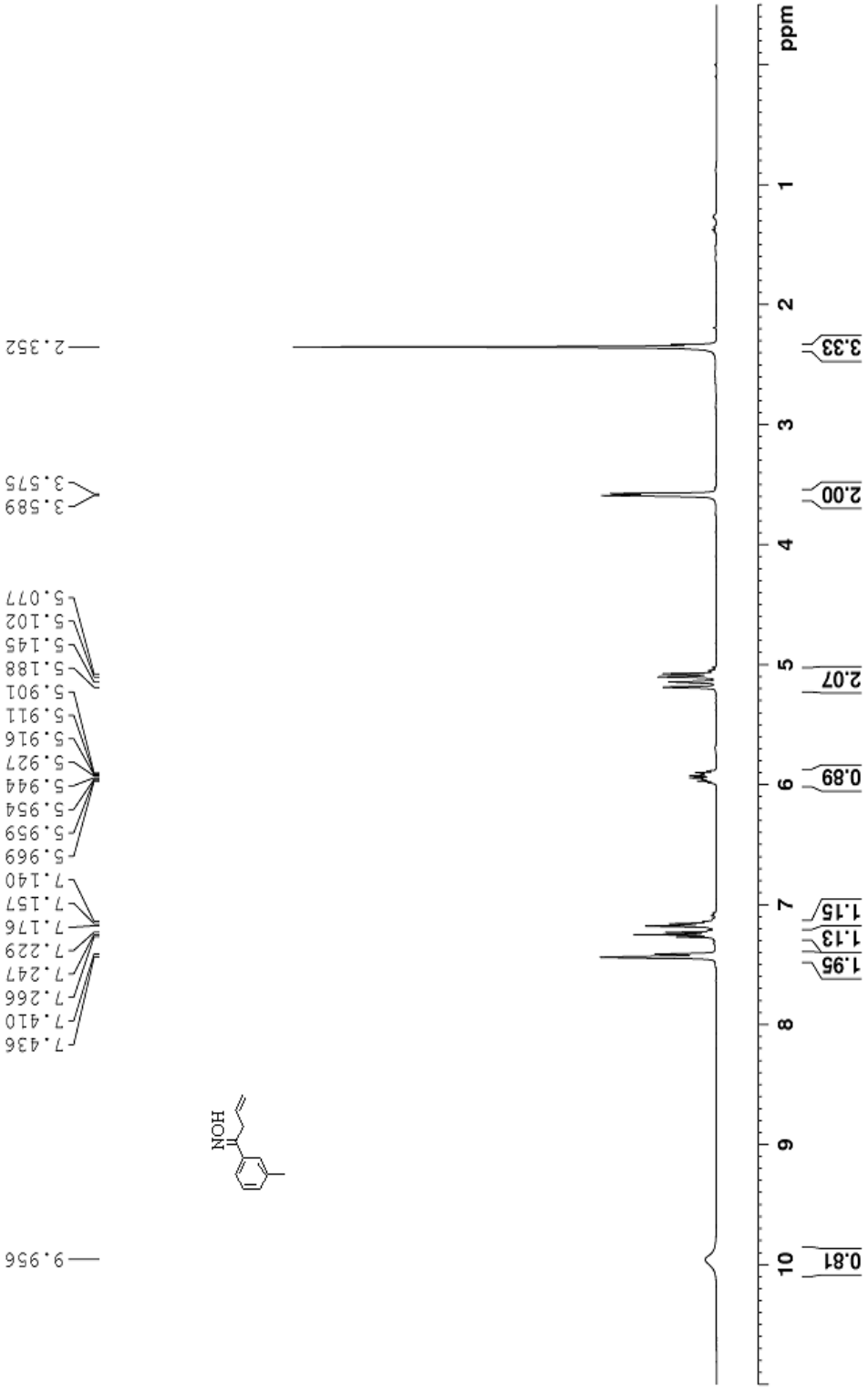
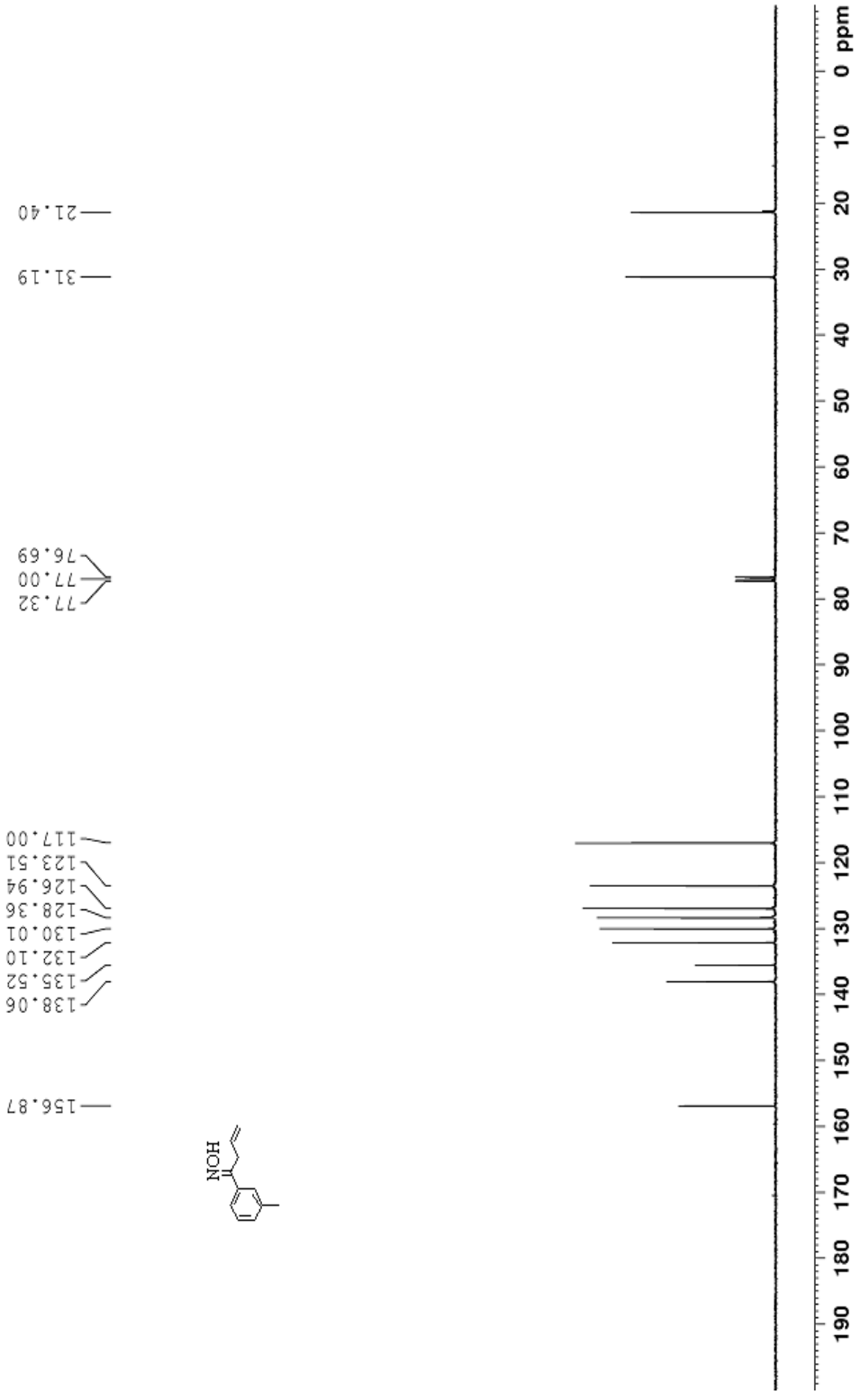
9. ^{1}H NMR and ^{13}C NMR spectra for substrates 1d, 1g, 1h, 1l, 1m

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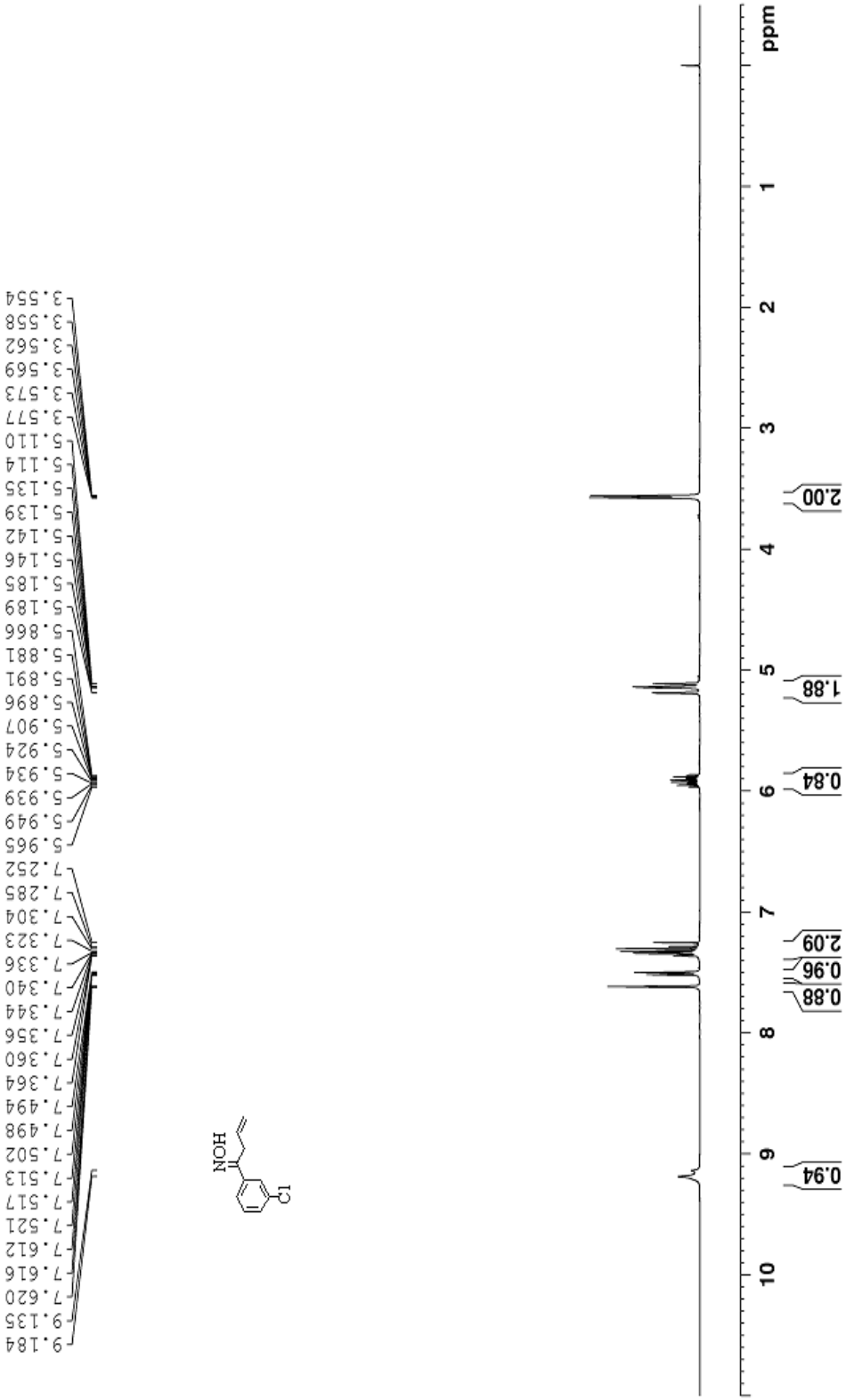
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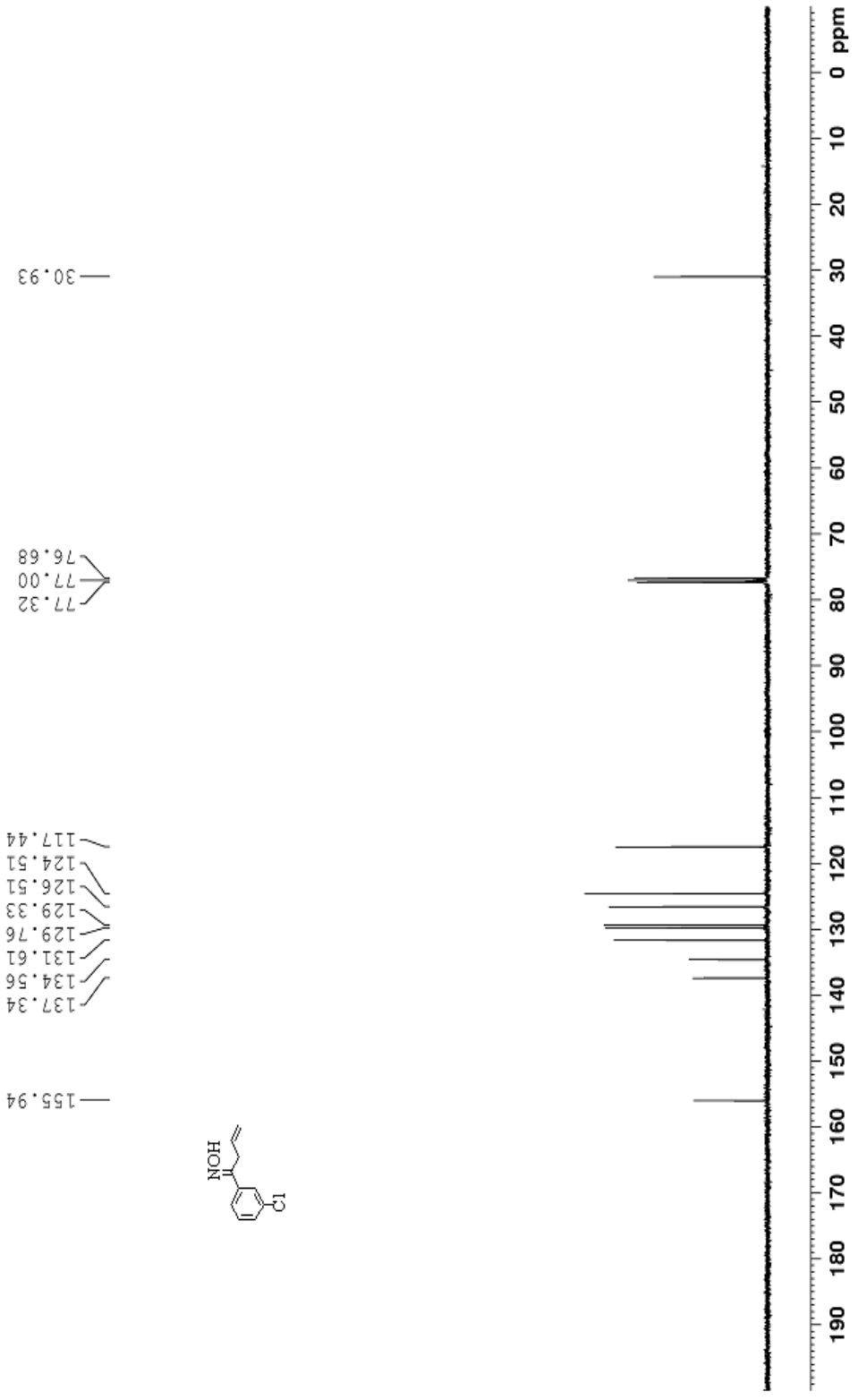
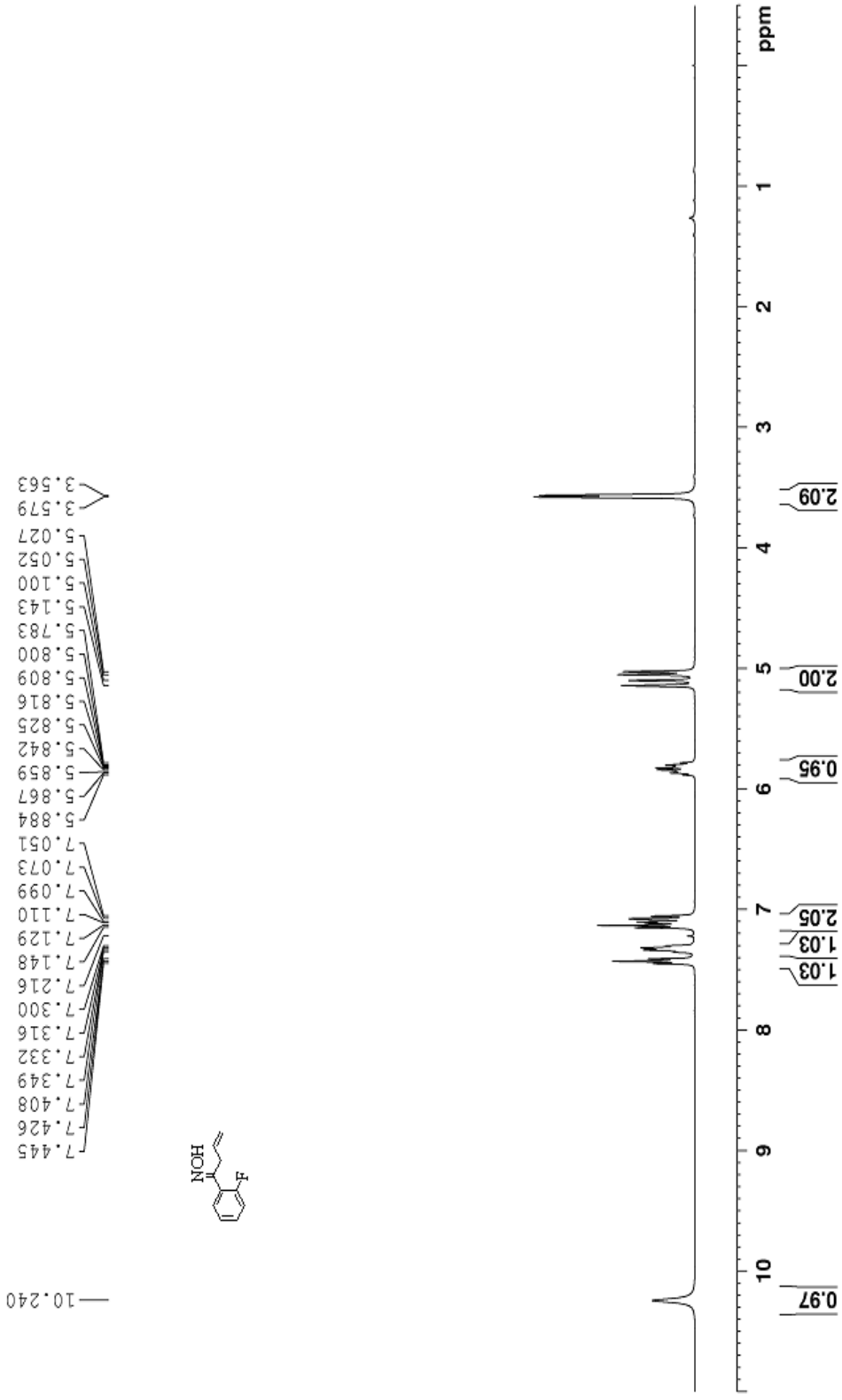
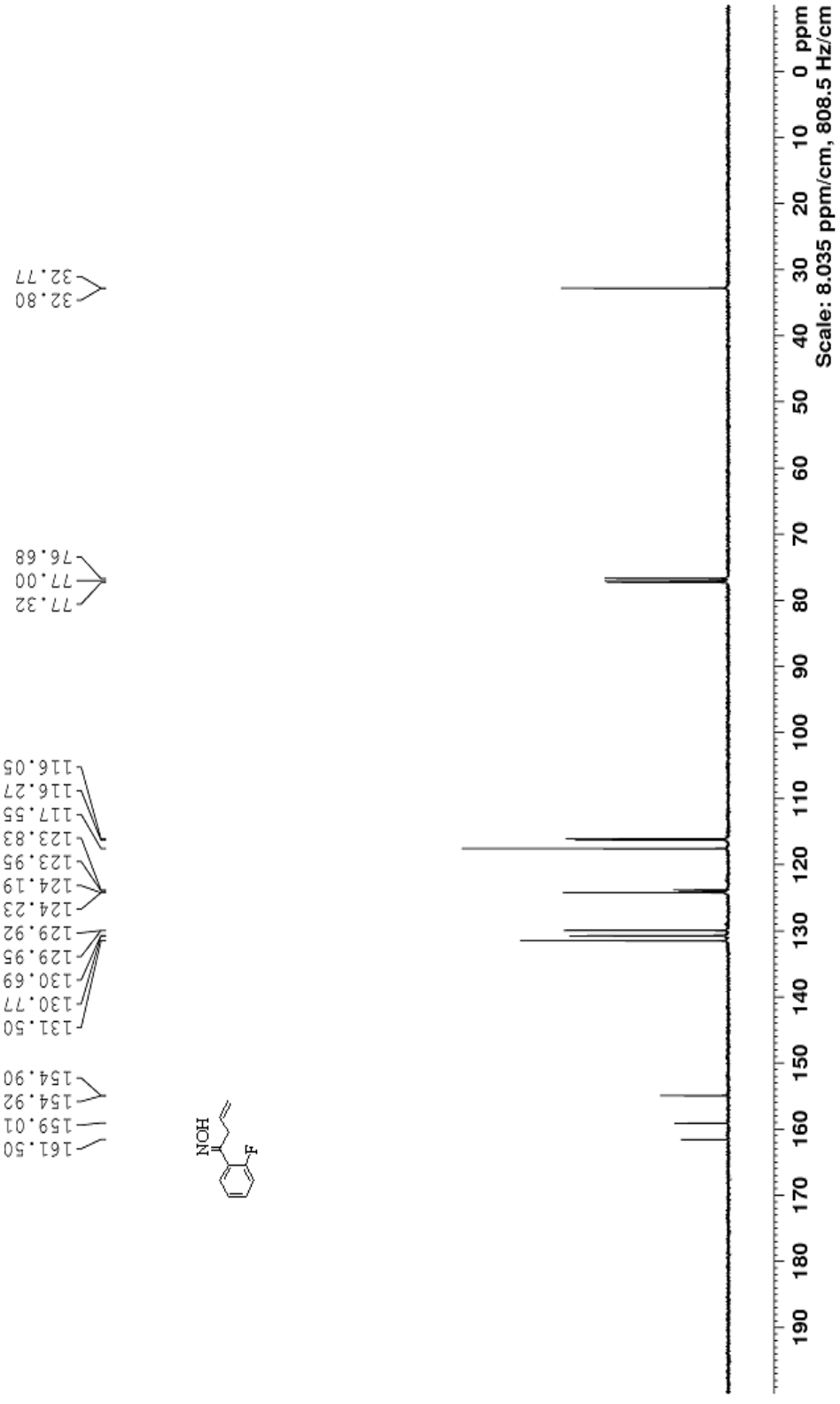
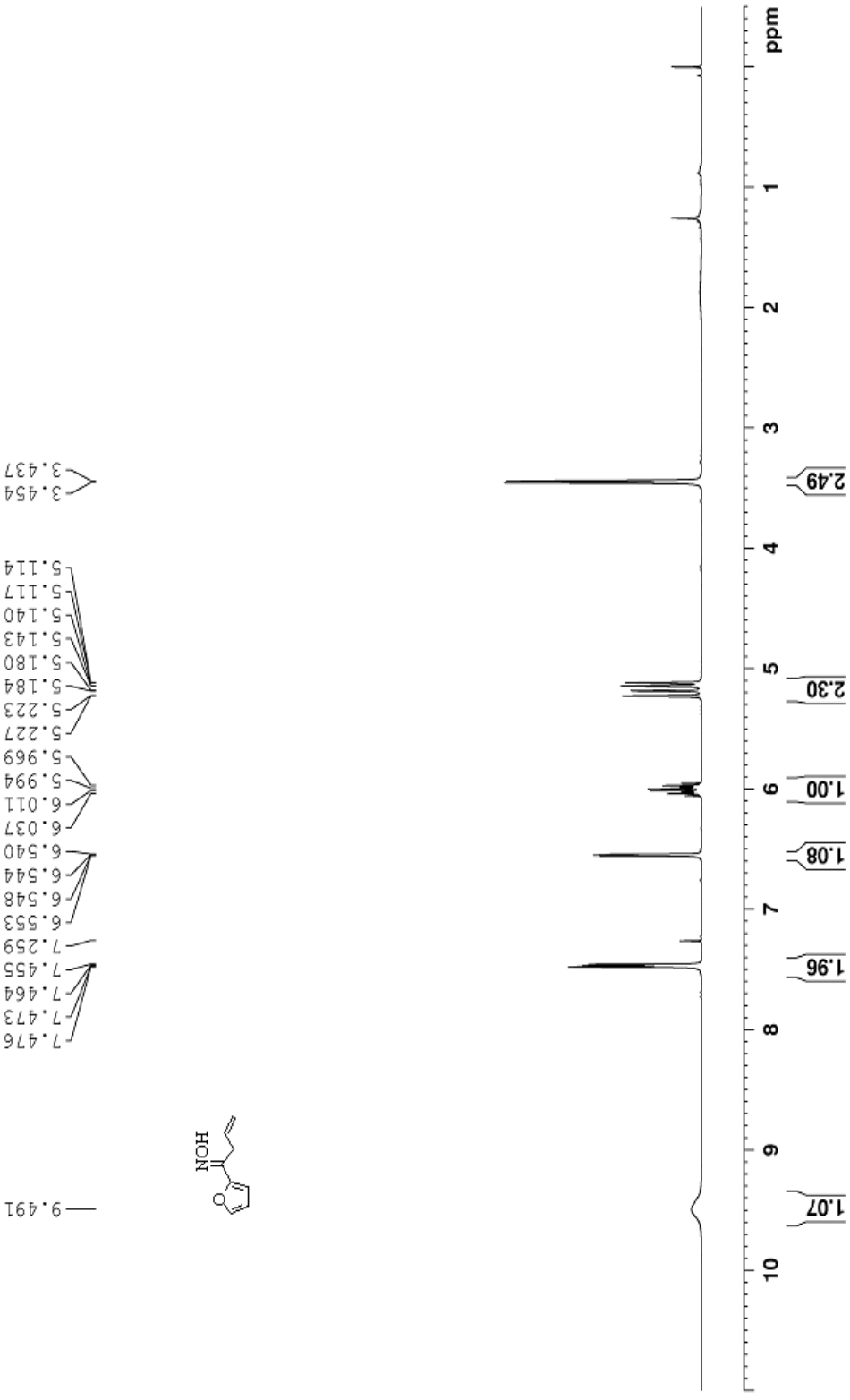
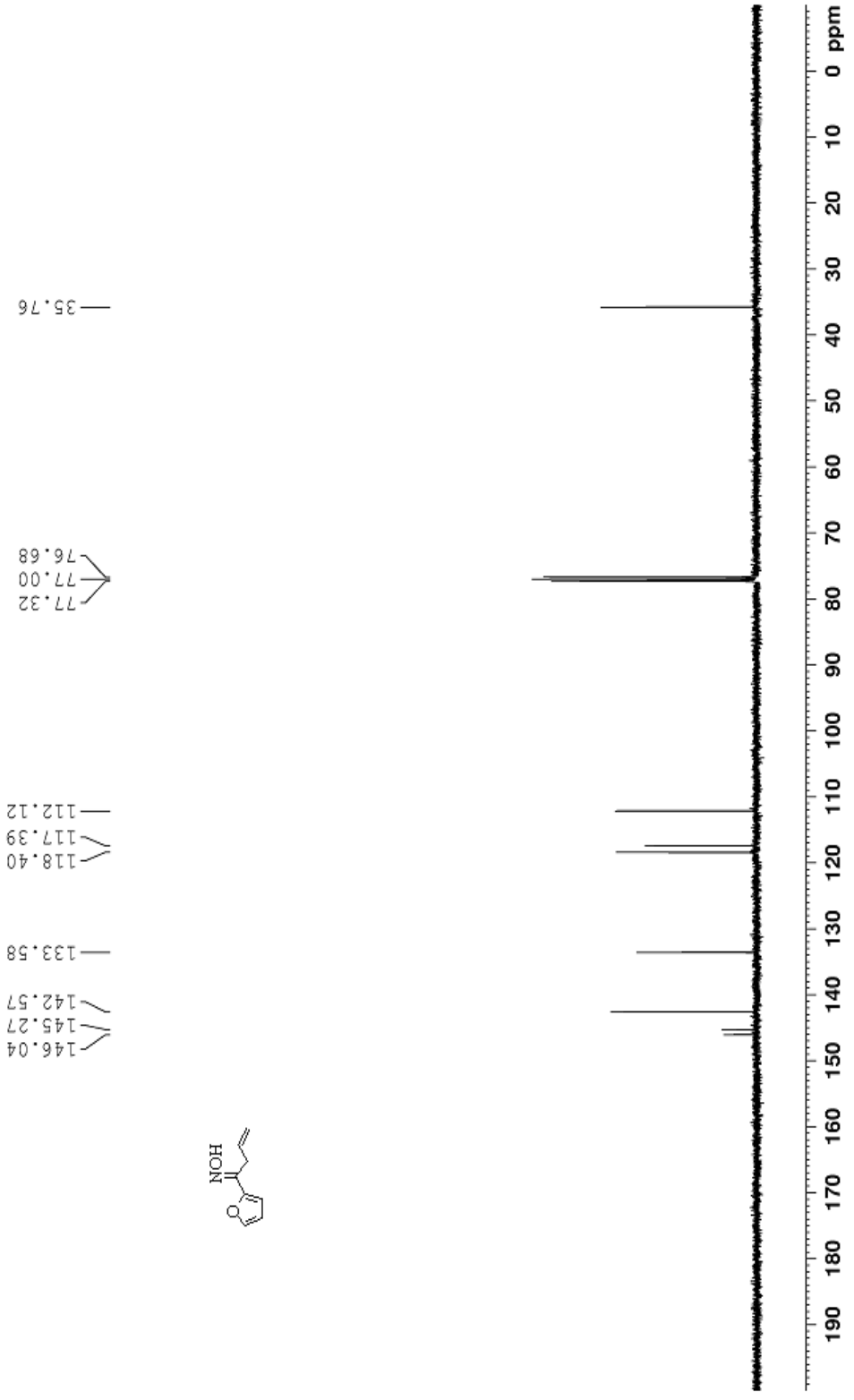
7.252
7.285
7.304
7.323
7.336
7.340
7.344
7.356
7.360
7.364
7.494
7.498
7.502
7.513
7.517
7.521
7.612
7.616
7.620
9.135
9.184
NOH
Cl
ppm
0.94
0.88
0.96
2.09
0.84
1.88
2.00

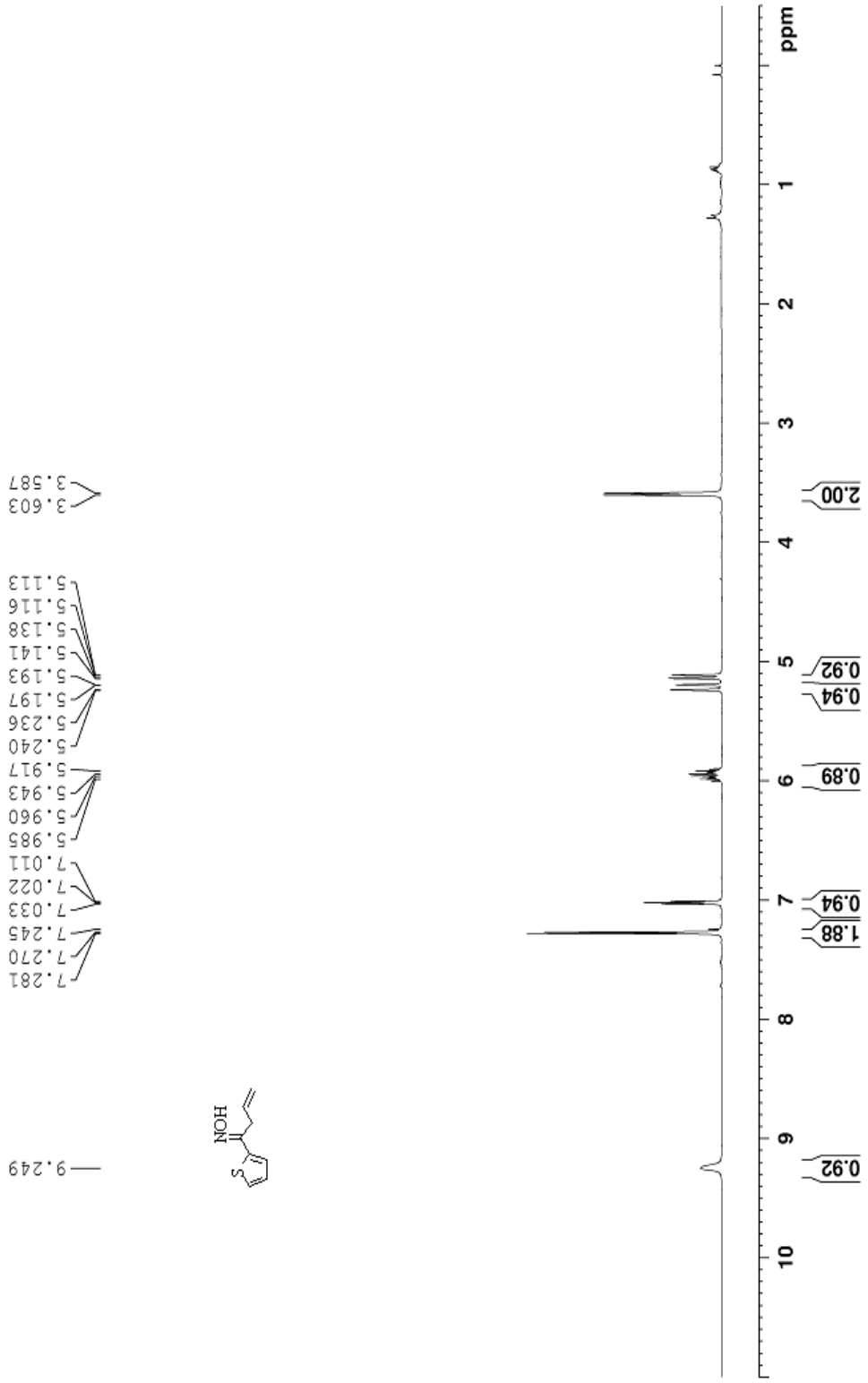

30.93
76.68
77.00
77.32
117.44
124.51
126.51
129.33
129.76
131.61
134.56
137.34
155.94
NOH
Cl
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

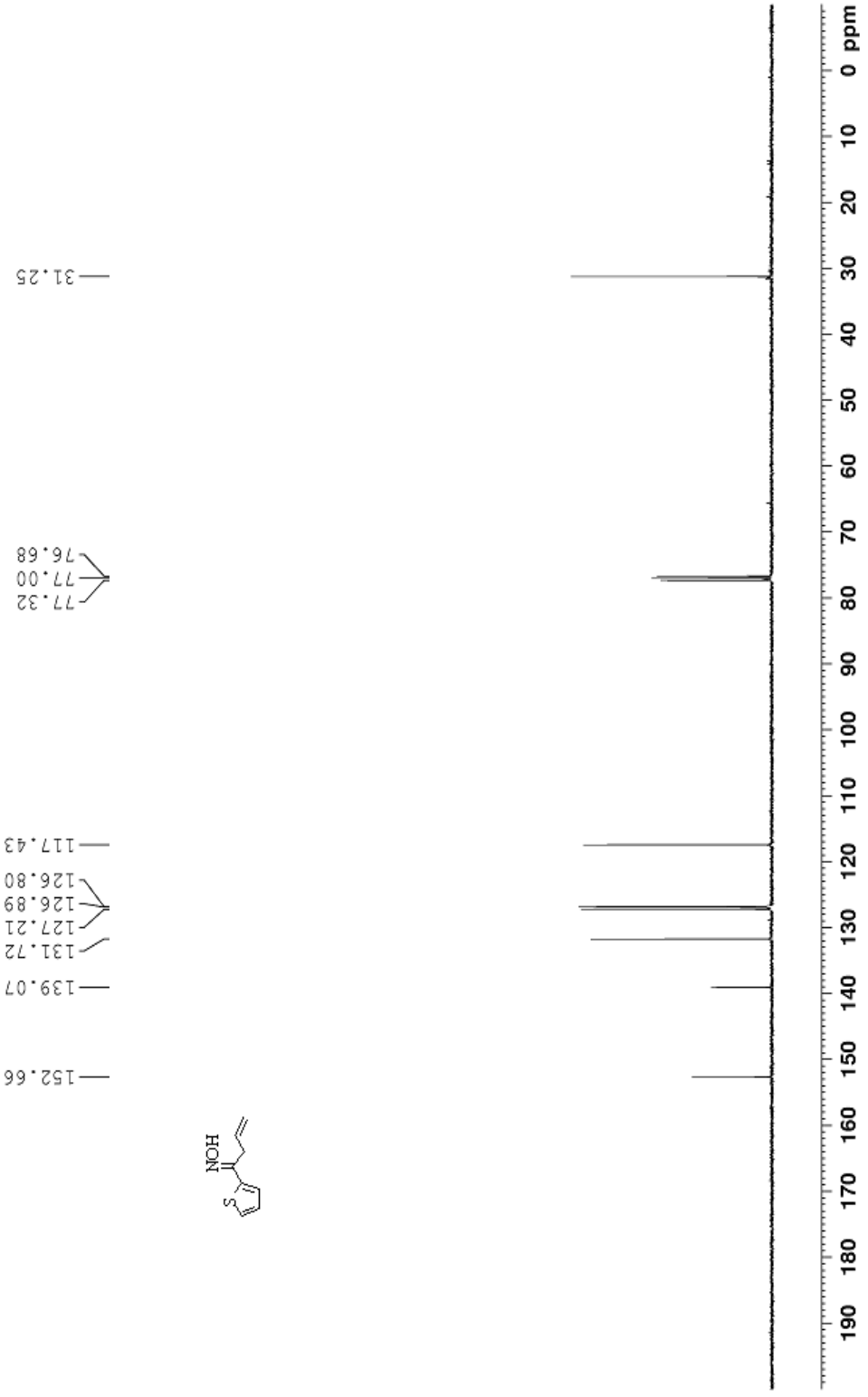

10.240
7.445
7.426
7.408
7.349
7.332
7.316
7.300
7.216
7.148
7.129
7.110
7.099
7.073
7.051
5.884
5.867
5.859
5.842
5.825
5.816
5.809
5.800
5.783
5.143
5.100
5.052
5.027
3.579
3.563
HON
F
ppm
0.97
2.09
2.00
0.95
2.05
1.03
1.03


32.77
32.80
76.68
77.00
77.32
116.05
116.27
117.55
123.83
123.95
124.19
124.23
129.92
129.95
130.69
130.77
131.50
154.90
154.92
159.01
161.50
NOH
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm
Scale: 8.035 ppm/cm, 808.5 Hz/cm

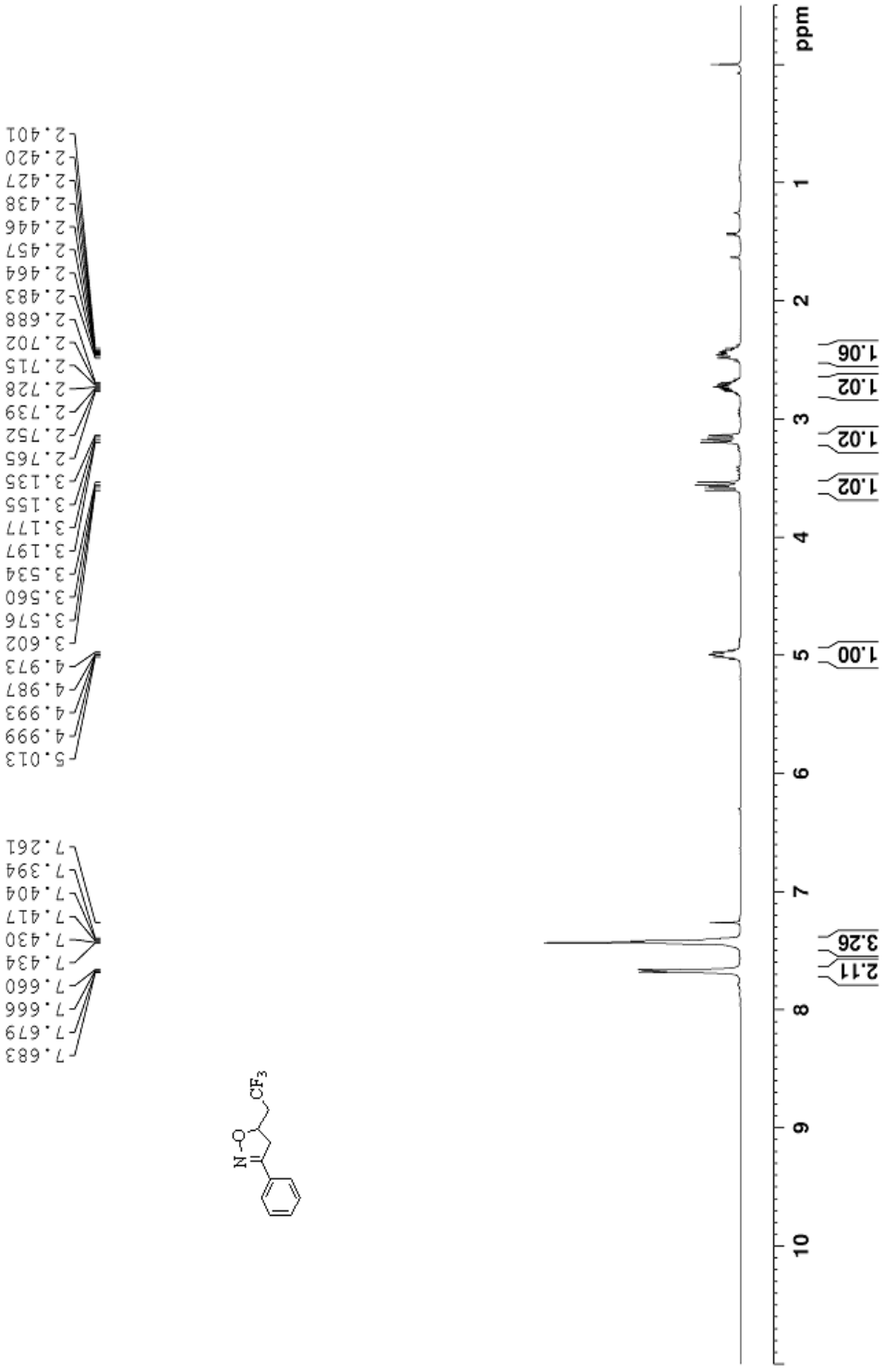

9.491
7.476
7.473
7.464
7.455
7.259
6.553
6.548
6.544
6.540
6.037
6.011
5.994
5.969
5.227
5.223
5.184
5.180
5.143
5.140
5.117
5.114
3.454
3.437
HON
ppm
1
2
3
4
5
6
7
8
9
10
1.07
1.96
1.08
1.00
2.30
2.49

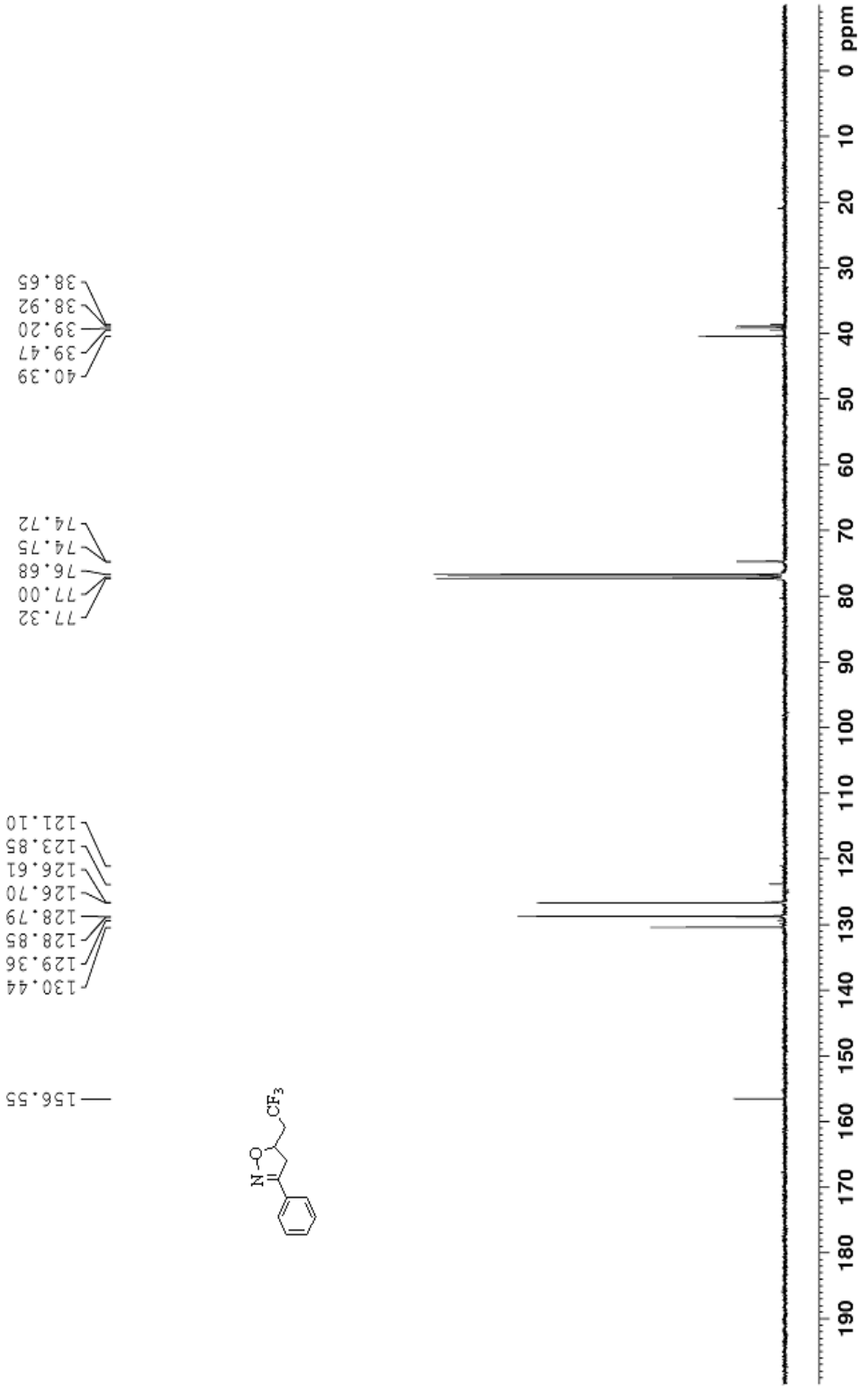

146.04
145.27
142.57
133.58
118.40
117.39
112.12
77.32
77.00
76.68
35.76
NOH
O
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190


ppm
1
2
3
4
5
6
7
8
9
10
0.92
1.88
0.94
0.89
0.94
0.92
2.00
NOH
S
9.249
7.281
7.270
7.245
7.033
7.022
7.011
5.985
5.960
5.943
5.917
5.240
5.236
5.197
5.193
5.141
5.138
5.116
5.113
3.603
3.587

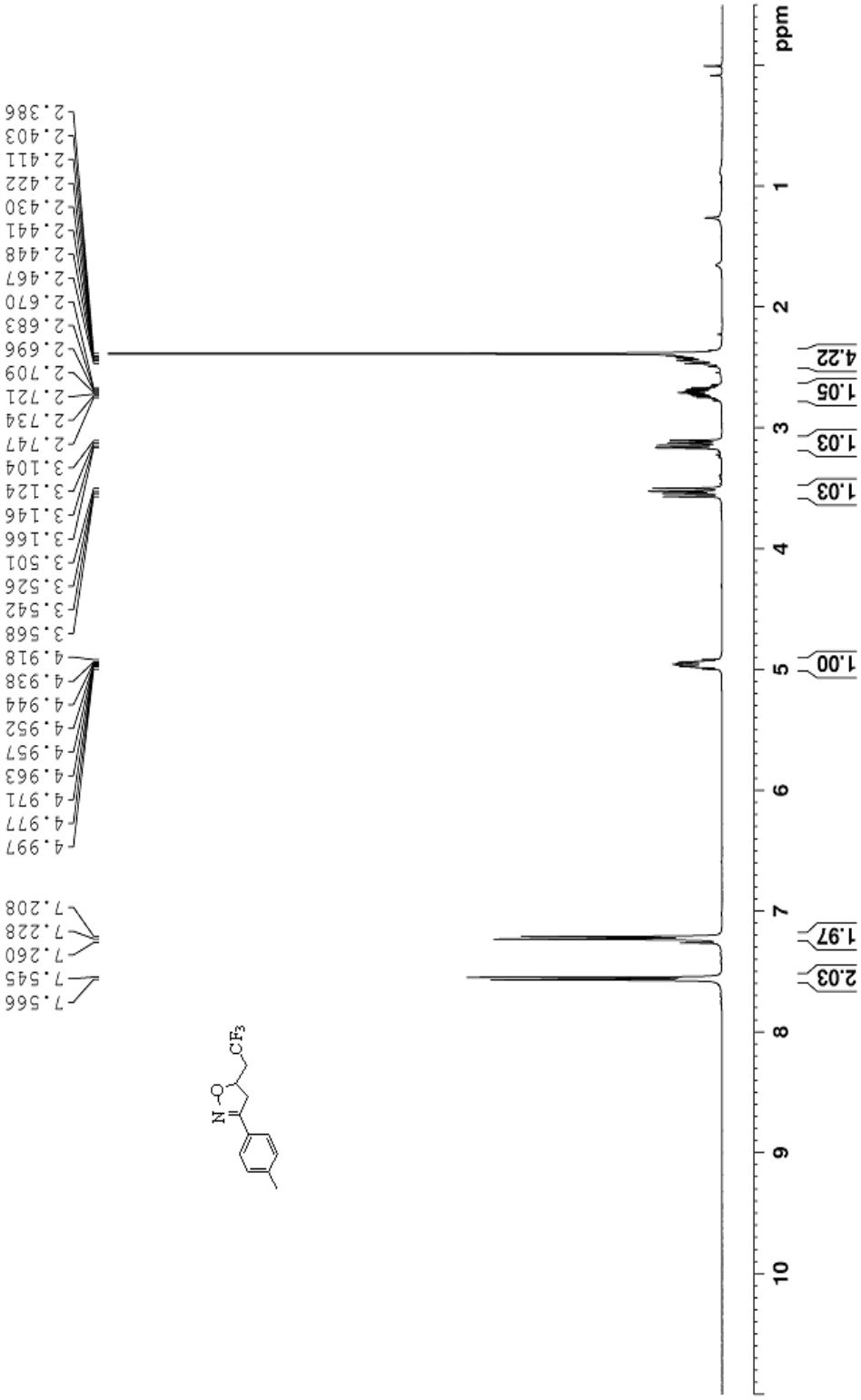

31.25
76.68
77.00
77.32
117.43
126.80
126.89
127.21
131.72
139.07
152.66
NOH
S
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

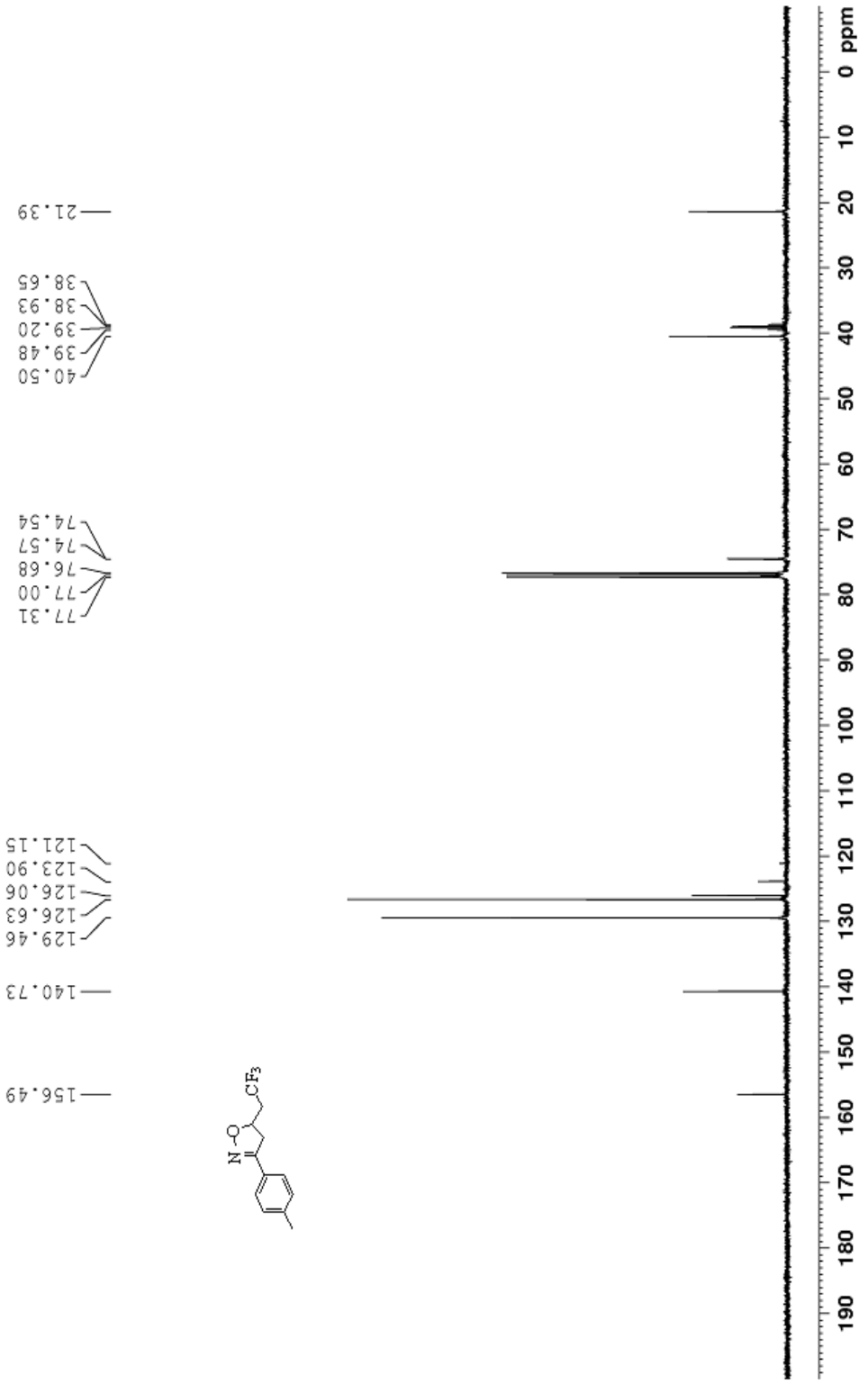
10. ^{1}H NMR、^{13}C NMR、^{19}F NMR spectra and 1D-NOESY for products 3a-3q, and 3s

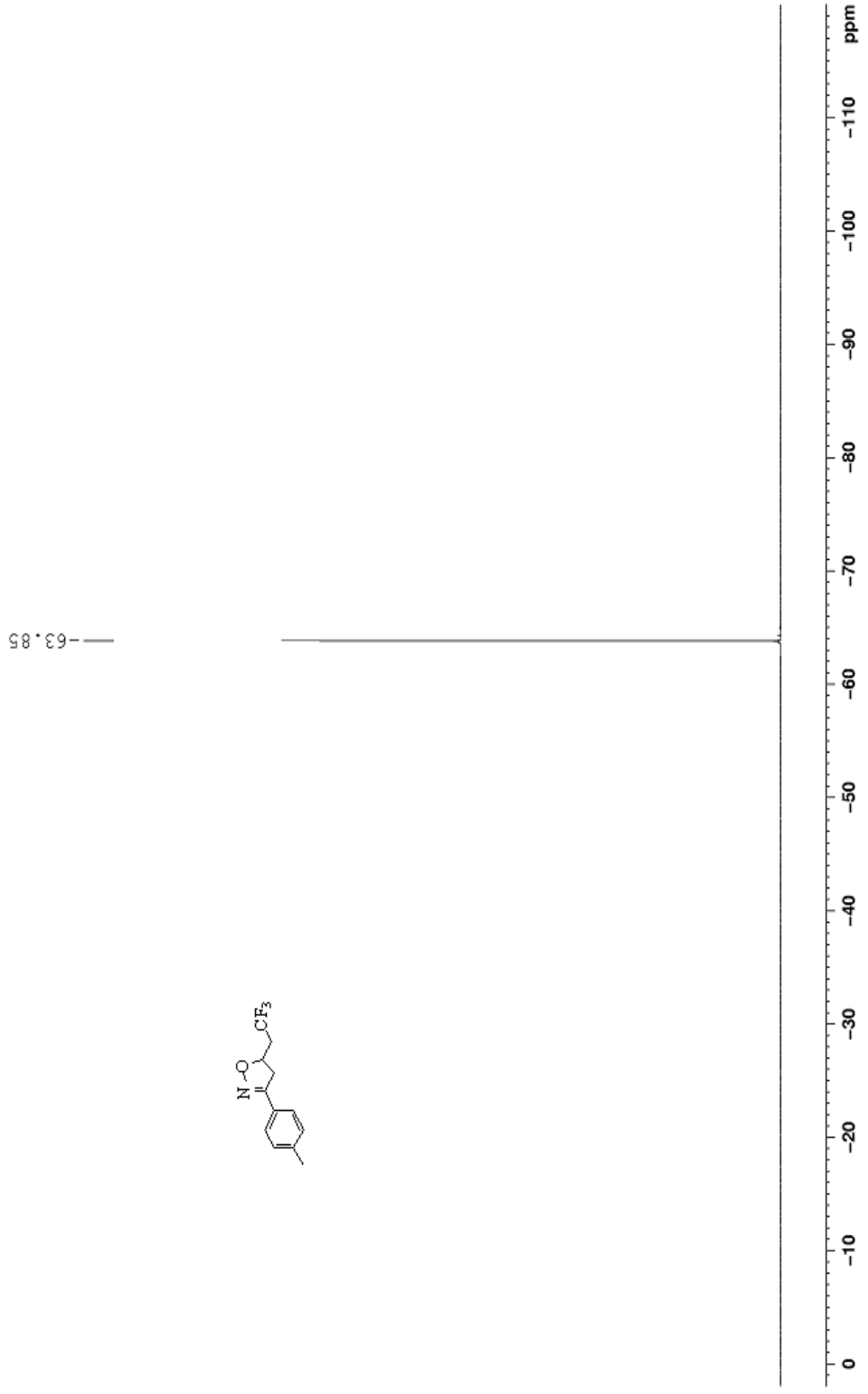


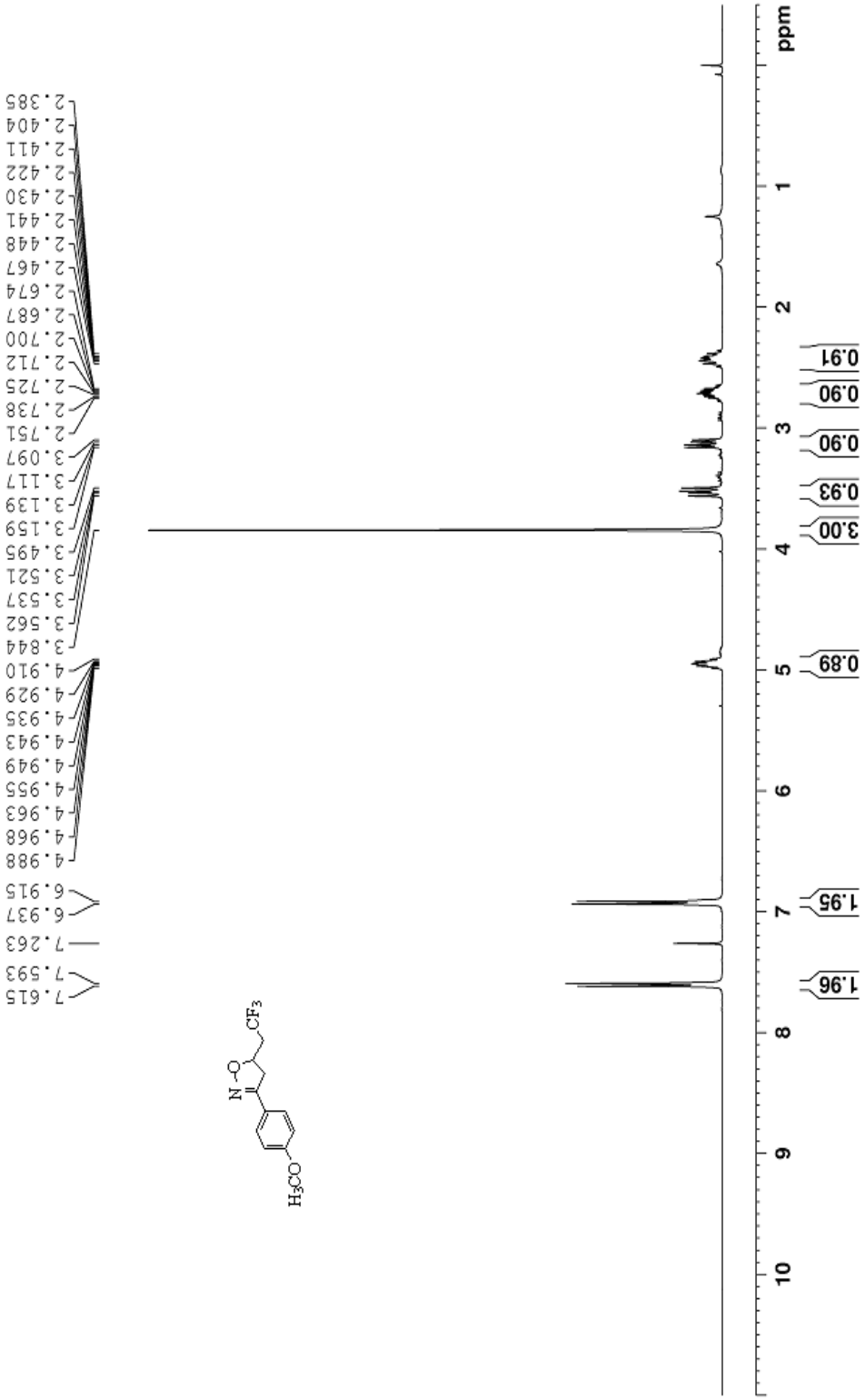

156.55
130.44
129.36
128.85
128.79
126.70
126.61
123.85
121.10
77.32
77.00
76.68
74.75
74.72
40.39
39.47
39.20
38.92
38.65
CF3
N
O
0 ppm

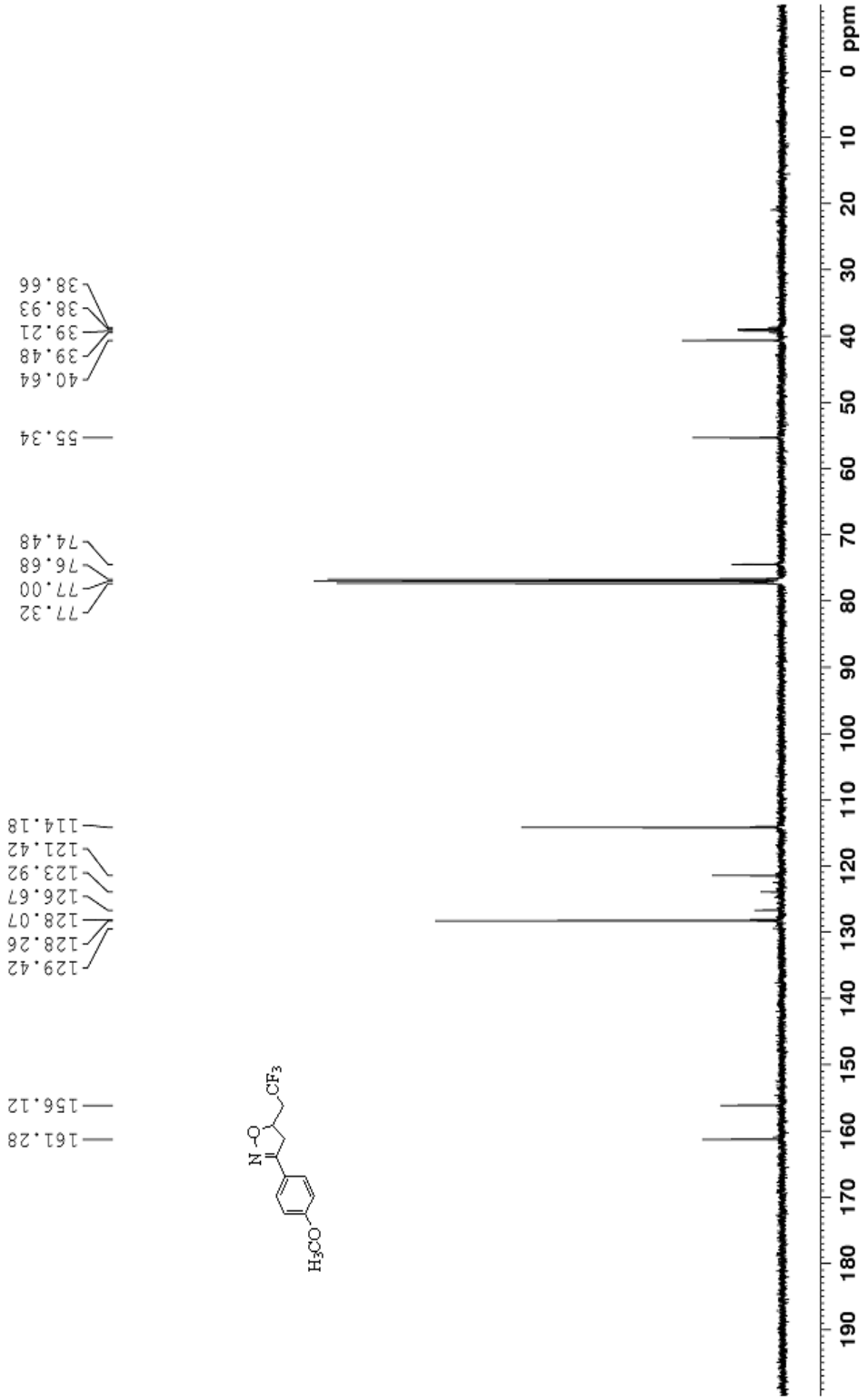

-63.82
CF3
N
O
ppm
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110

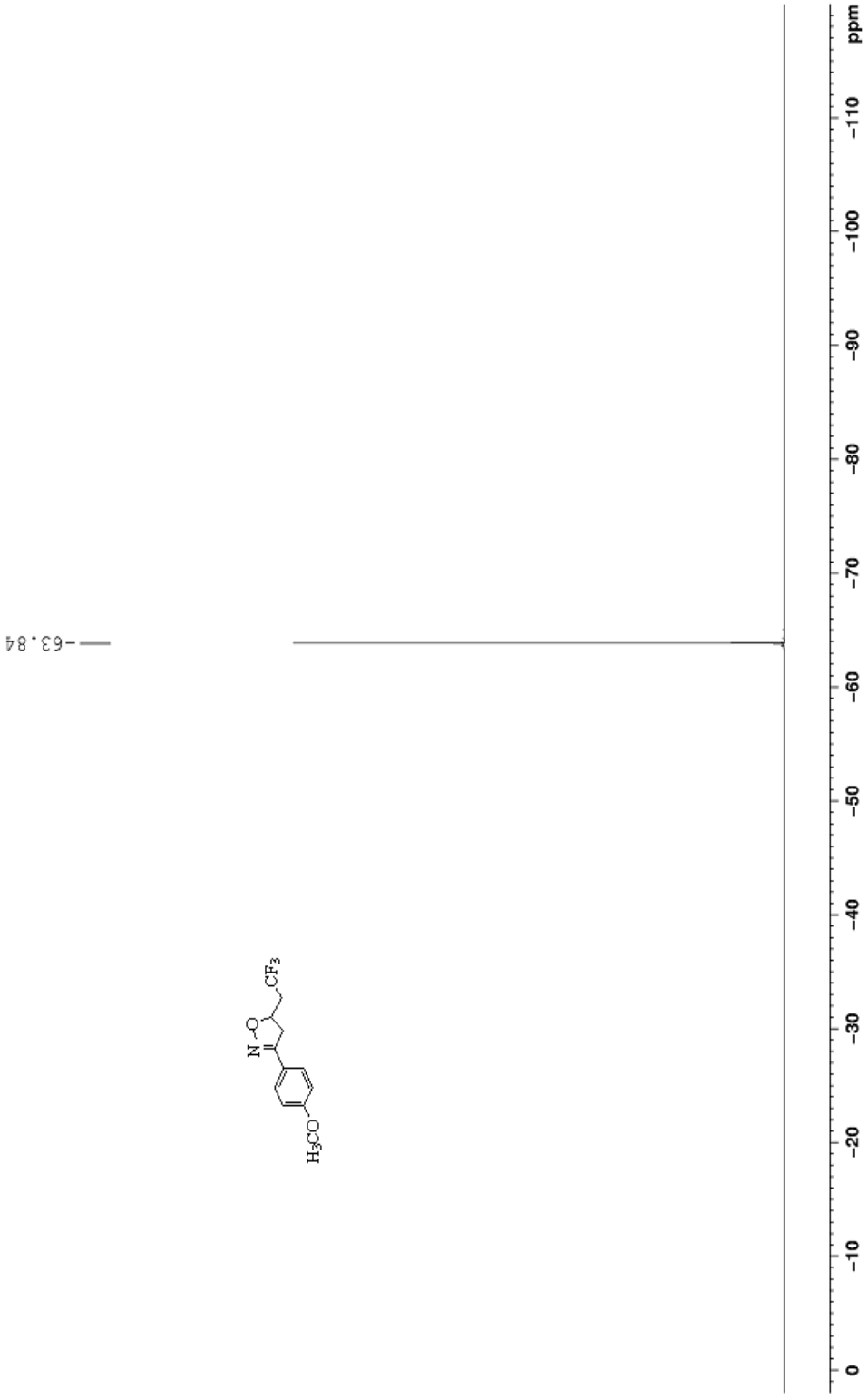

ppm
1
2
3
4
5
6
7
8
9
10
4.22
1.05
1.03
1.03
1.00
1.97
2.03
2.386
2.403
2.411
2.422
2.430
2.441
2.448
2.467
2.670
2.683
2.696
2.709
2.721
2.734
2.747
3.104
3.124
3.146
3.166
3.501
3.526
3.542
3.568
4.918
4.938
4.944
4.952
4.957
4.963
4.971
4.977
4.997
7.208
7.228
7.260
7.545
7.566
CF3
O
N

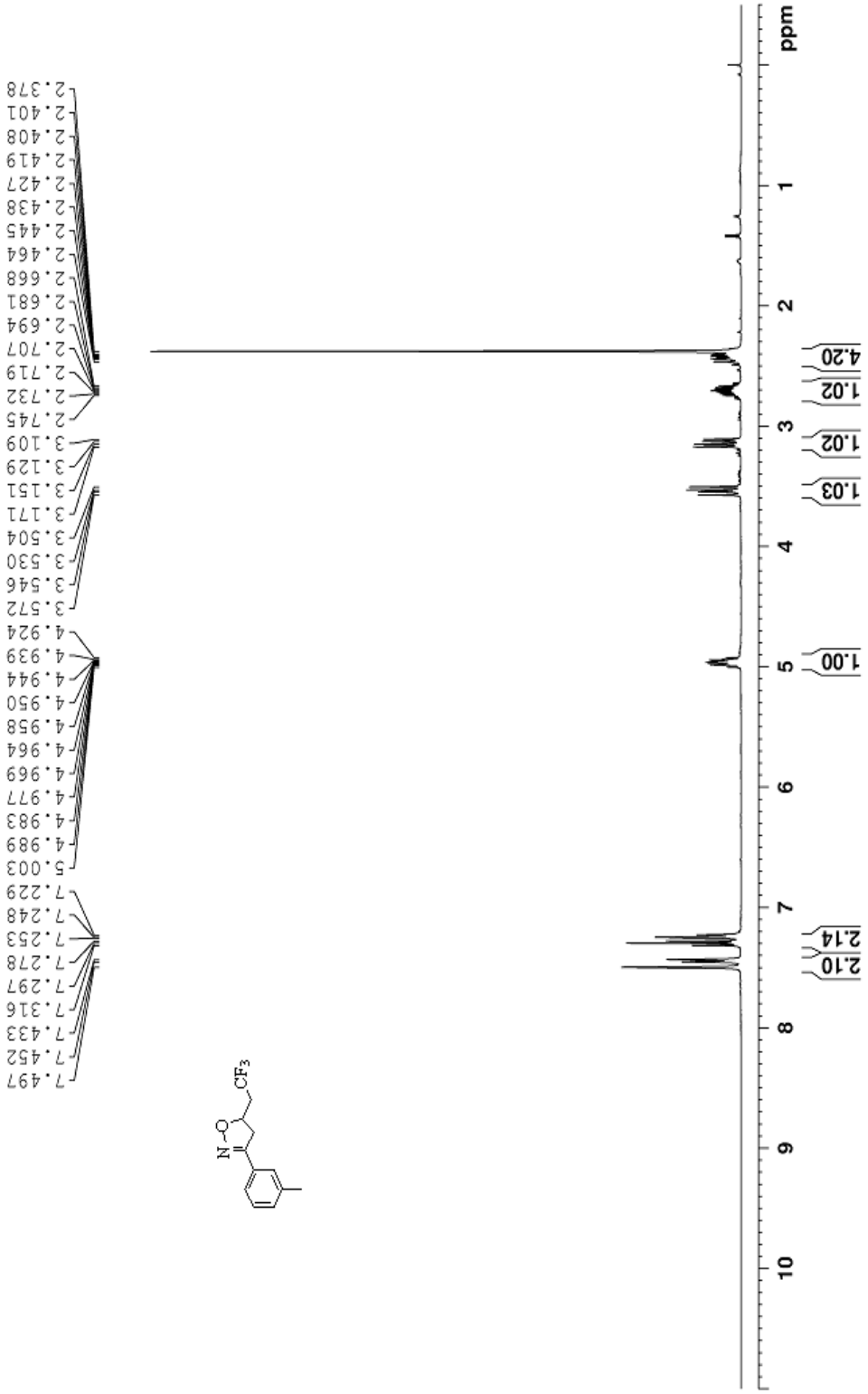

21.39
38.65
38.93
39.20
39.48
40.50
74.54
74.57
76.68
77.00
77.31
121.15
123.90
126.06
126.63
129.46
140.73
156.49
CF3
N
O
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

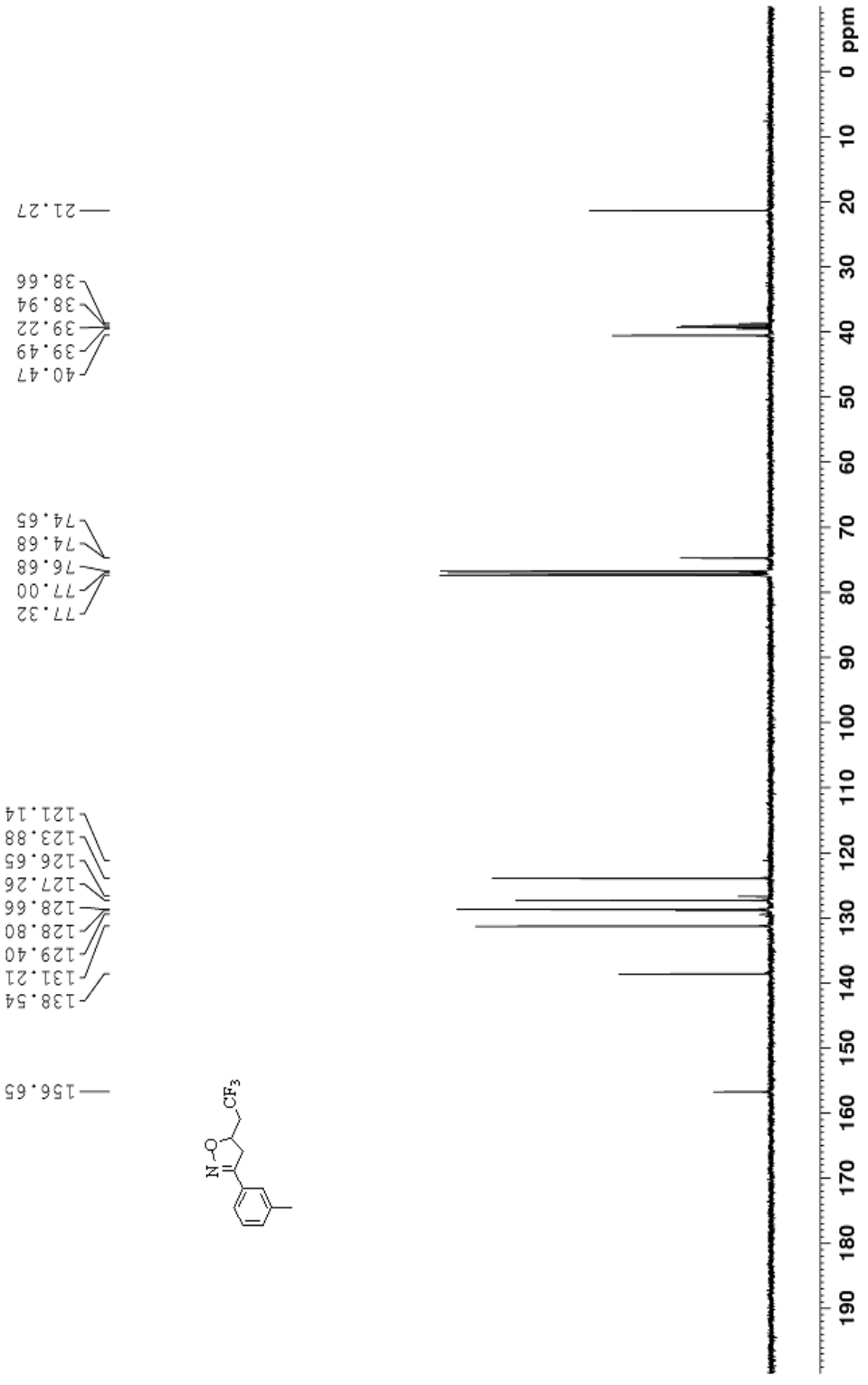

-63.85
ppm
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
CF3
N
O

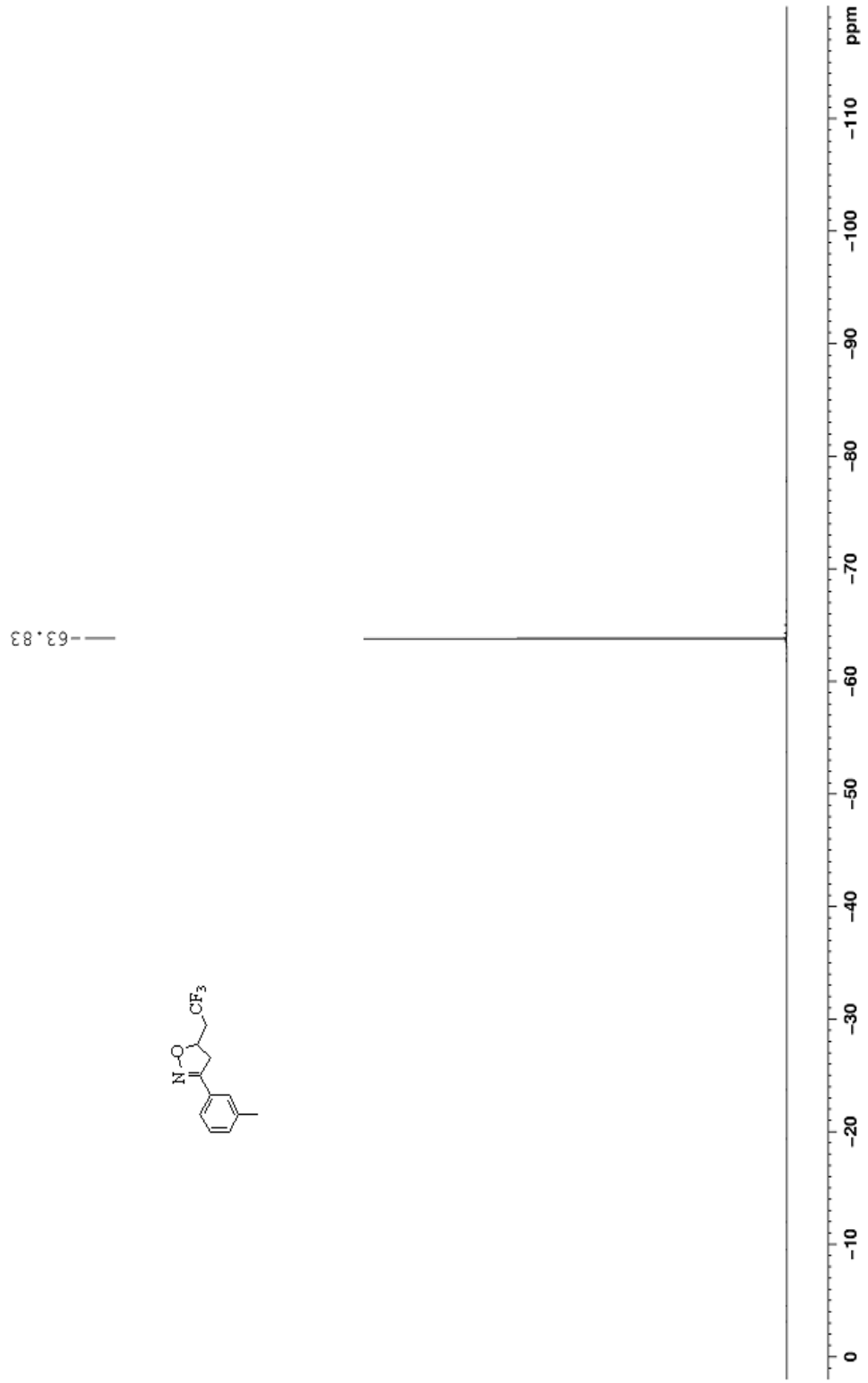

7.615
7.593
7.263
6.937
6.915
4.988
4.968
4.963
4.955
4.949
4.943
4.935
4.929
4.910
3.844
3.562
3.537
3.521
3.495
3.159
3.139
3.117
3.097
2.751
2.738
2.725
2.712
2.700
2.687
2.674
2.467
2.448
2.441
2.430
2.422
2.411
2.404
2.385
ppm
1.96
1.95
0.89
3.00
0.93
0.90
0.90
0.91
N
O
CF3
H3CO

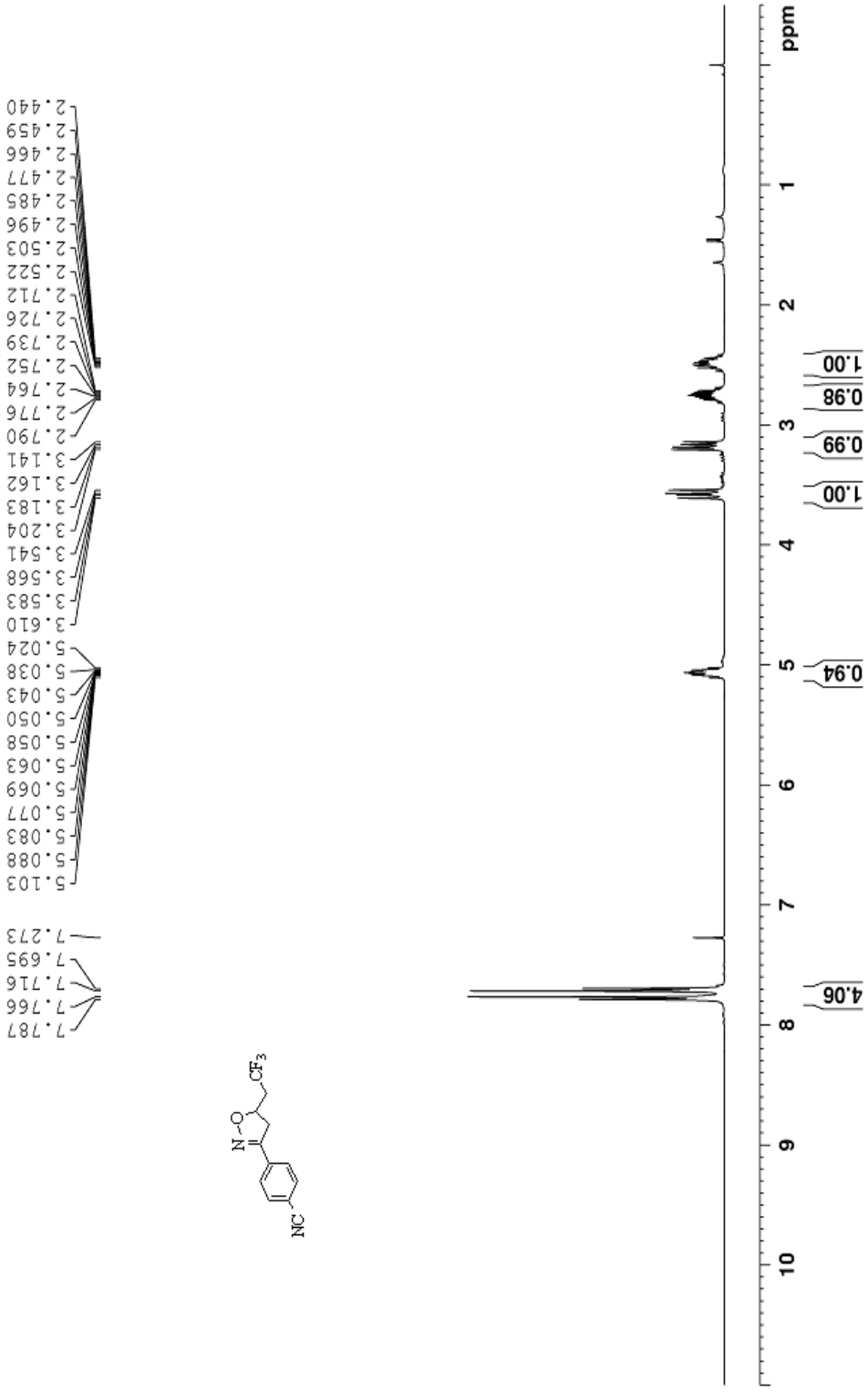

38.66
38.93
39.21
39.48
40.64
55.34
74.48
76.68
77.00
77.32
114.18
121.42
123.92
126.67
128.07
128.26
129.42
156.12
161.28
CF3
O
N
H3CO
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

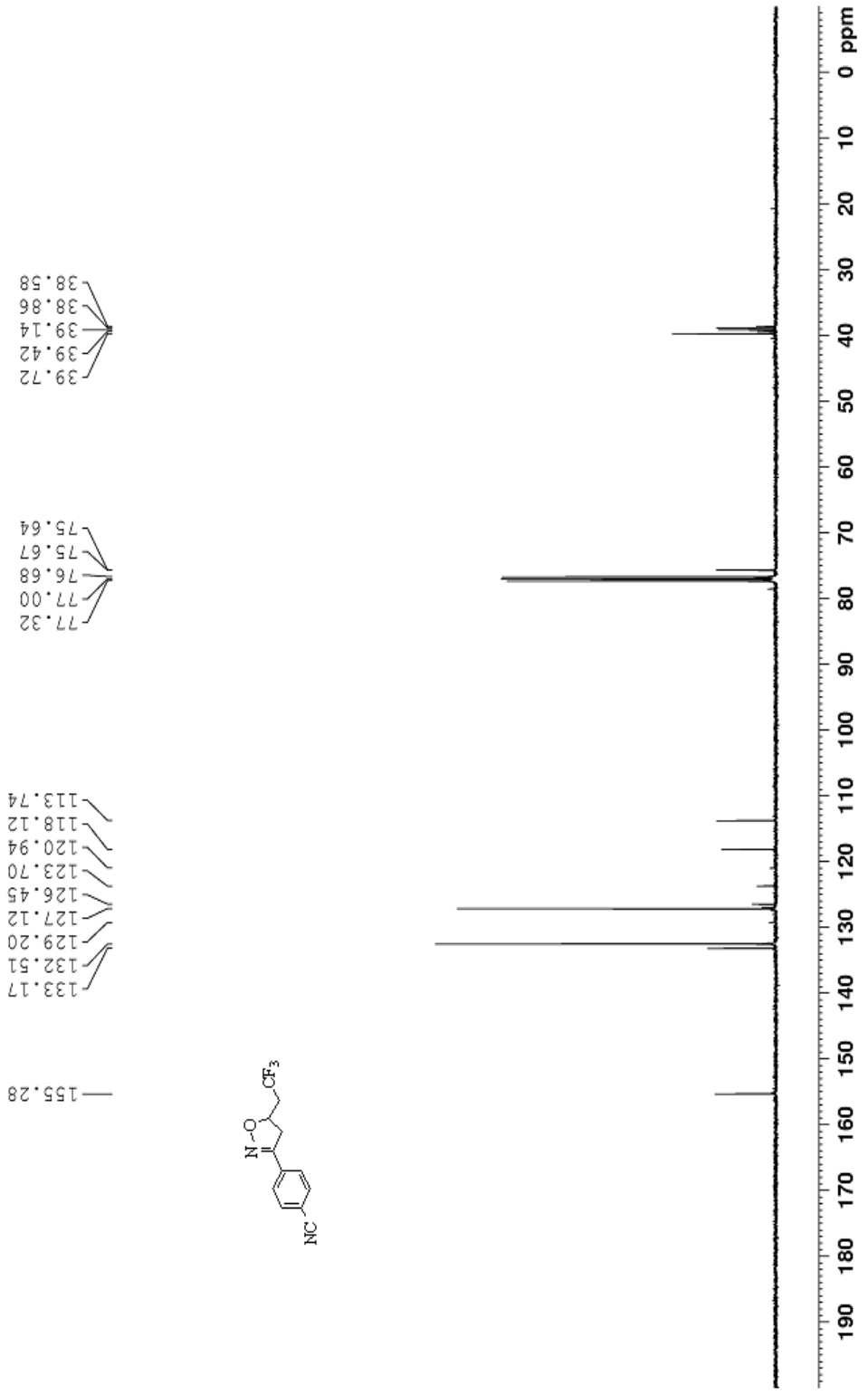

-63.84
CF3
N
O
H3CO
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm

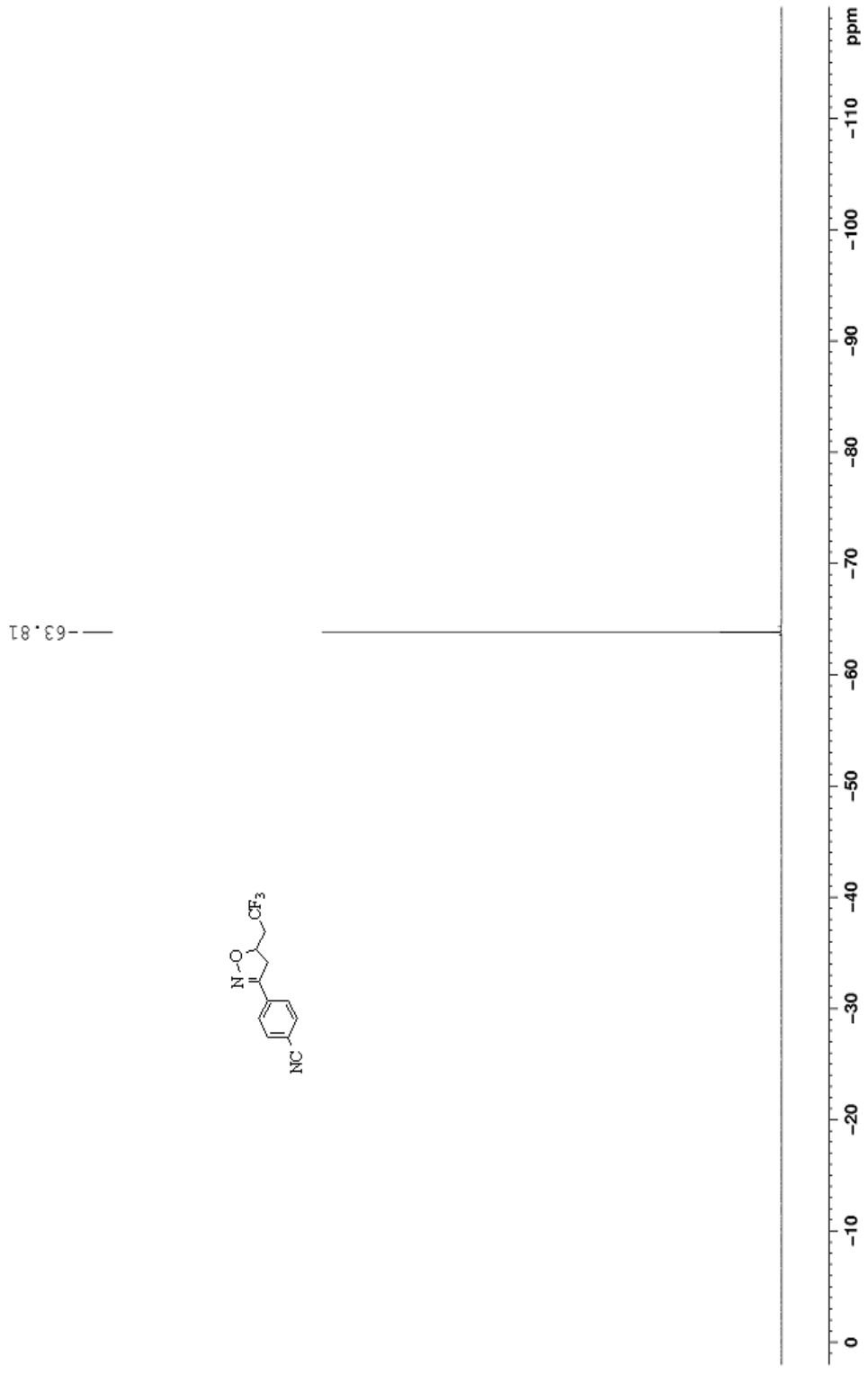

ppm
1
2
3
4
5
6
7
8
9
10
4.20
1.02
1.02
1.03
1.00
2.14
2.10
2.378
2.401
2.408
2.419
2.427
2.438
2.445
2.464
2.668
2.681
2.694
2.707
2.719
2.732
2.745
3.109
3.129
3.151
3.171
3.504
3.530
3.546
3.572
4.924
4.939
4.944
4.950
4.958
4.964
4.969
4.977
4.983
4.989
5.003
7.229
7.248
7.253
7.278
7.297
7.316
7.433
7.452
7.497
CF3
N
O

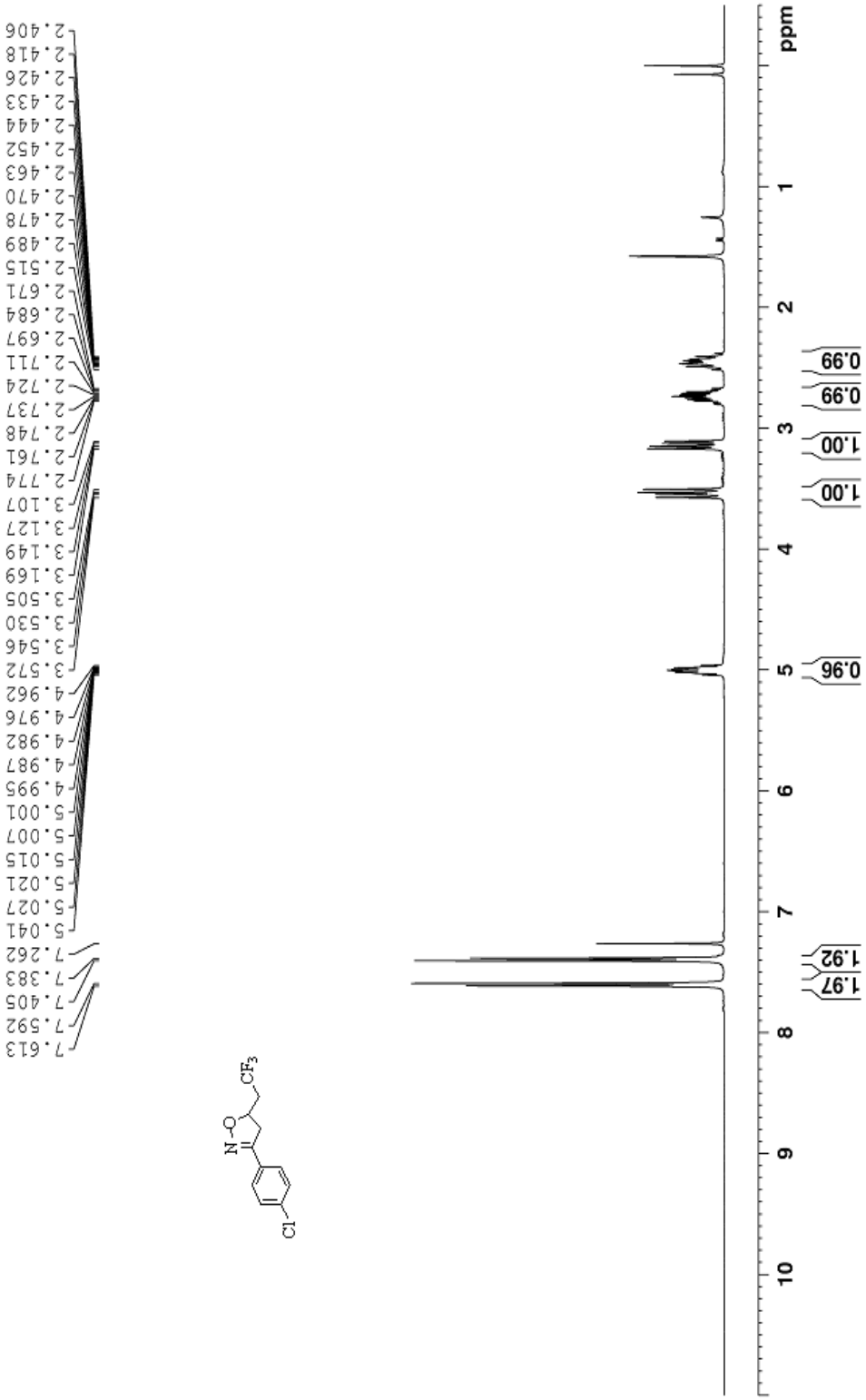

21.27
38.66
38.94
39.22
39.49
40.47
74.65
74.68
76.68
77.00
77.32
121.14
123.88
126.65
127.26
128.66
128.80
129.40
131.21
138.54
156.65
CF3
N
O
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

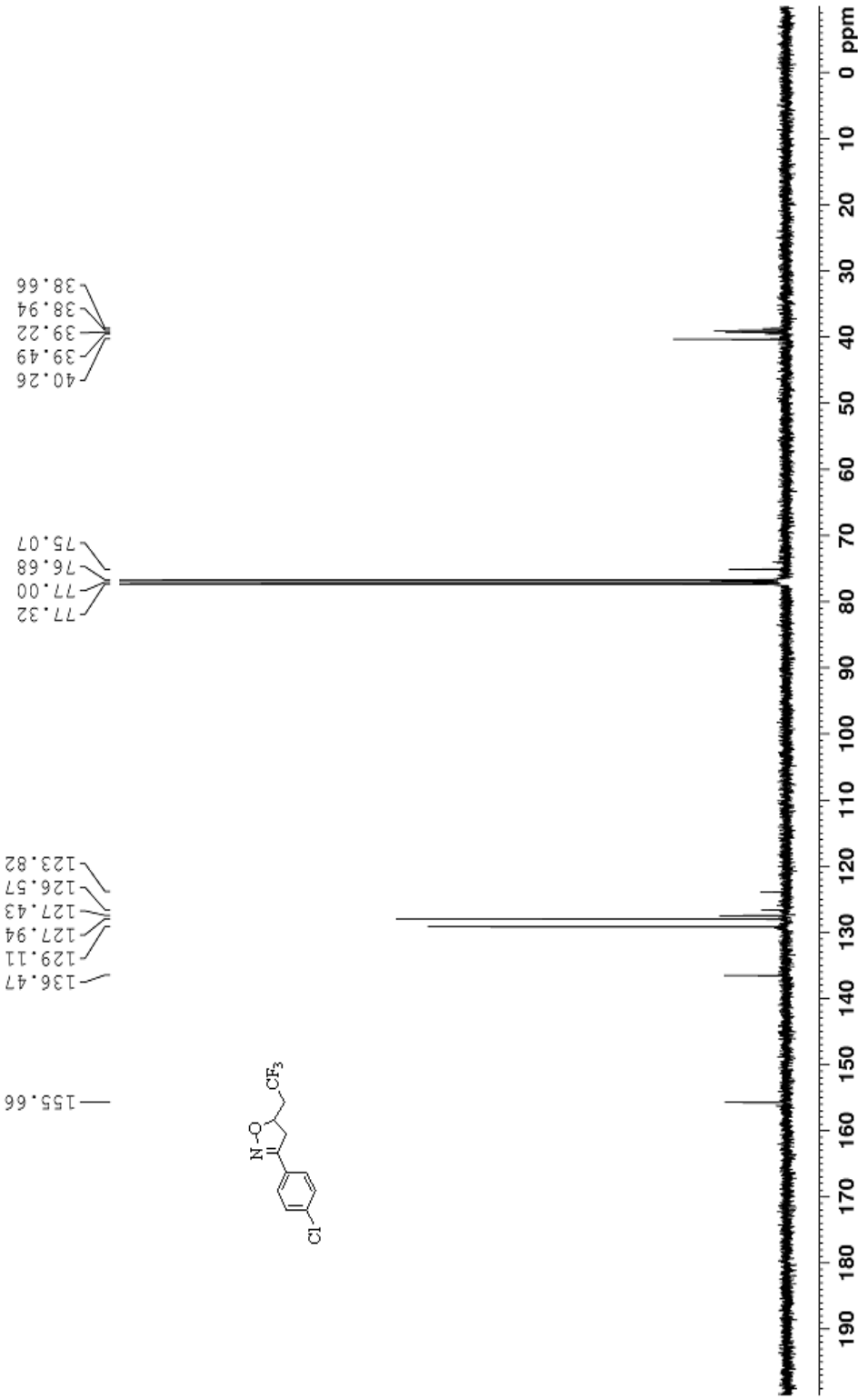

-63.83
CF3
N
O
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm

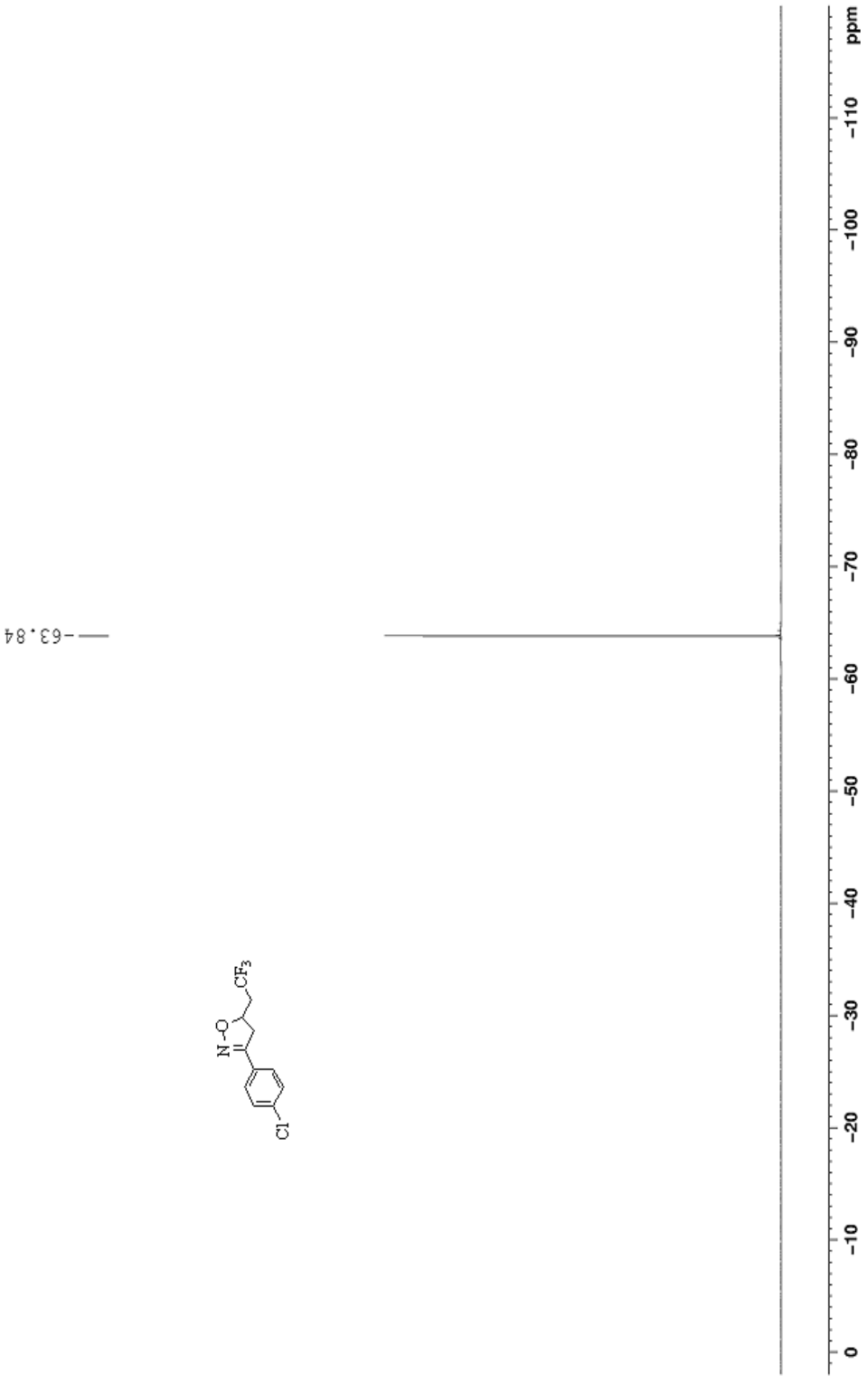

7.787
7.766
7.716
7.695
7.273
5.103
5.088
5.083
5.077
5.069
5.063
5.058
5.050
5.043
5.038
5.024
3.610
3.583
3.568
3.541
3.204
3.183
3.162
3.141
2.790
2.776
2.764
2.752
2.739
2.726
2.712
2.522
2.503
2.496
2.485
2.477
2.466
2.459
2.440
CF3
O
N
NC
ppm
1
2
3
4
5
6
7
8
9
10
4.06
0.94
1.00
0.99
0.98
1.00

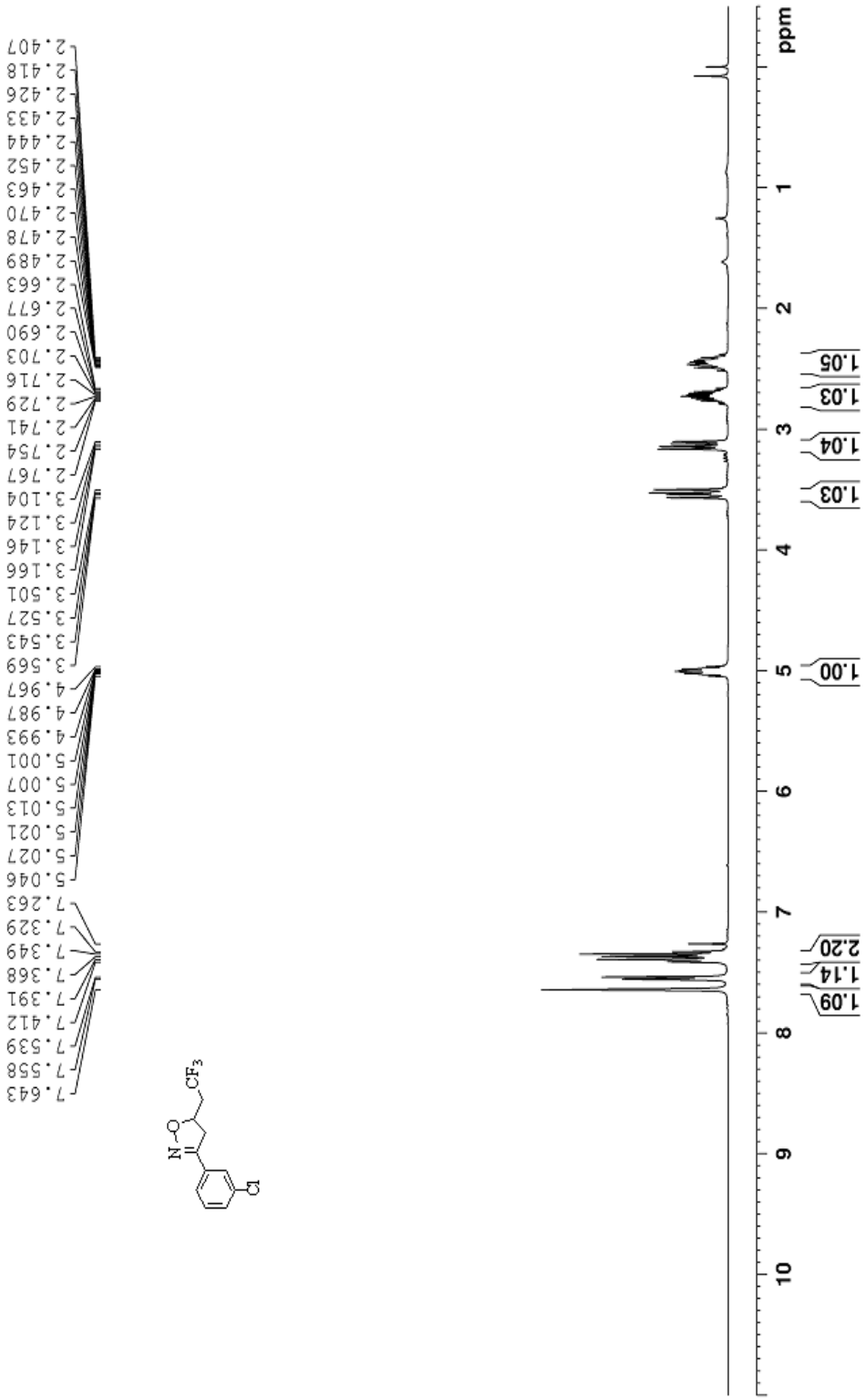

155.28
133.17
132.51
129.20
127.12
126.45
123.70
120.94
118.12
113.74
77.32
77.00
76.68
75.67
75.64
39.72
39.42
39.14
38.86
38.58
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
CF3
N
O
NC

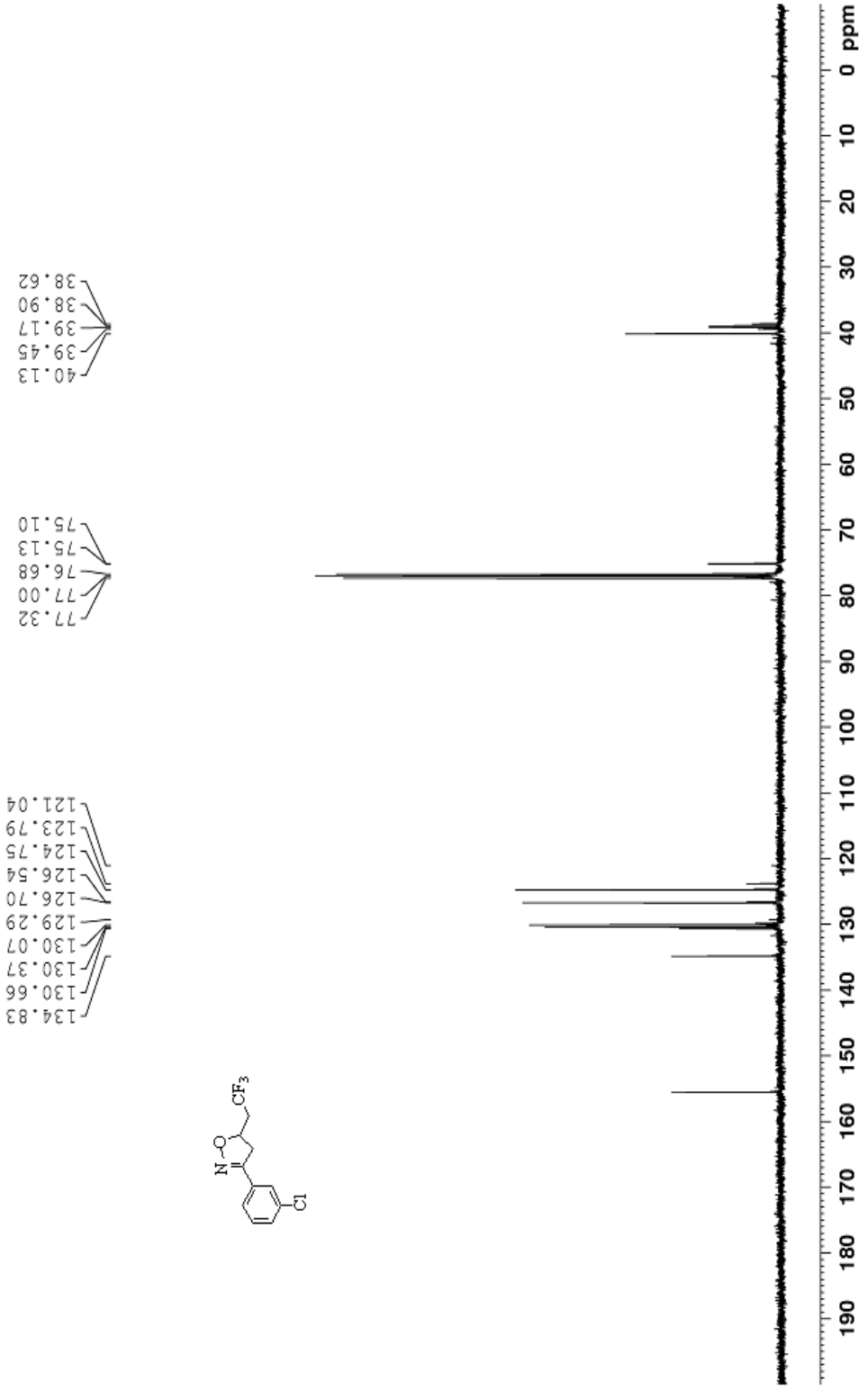

-63.81
ppm
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
CF3
O
N
NC

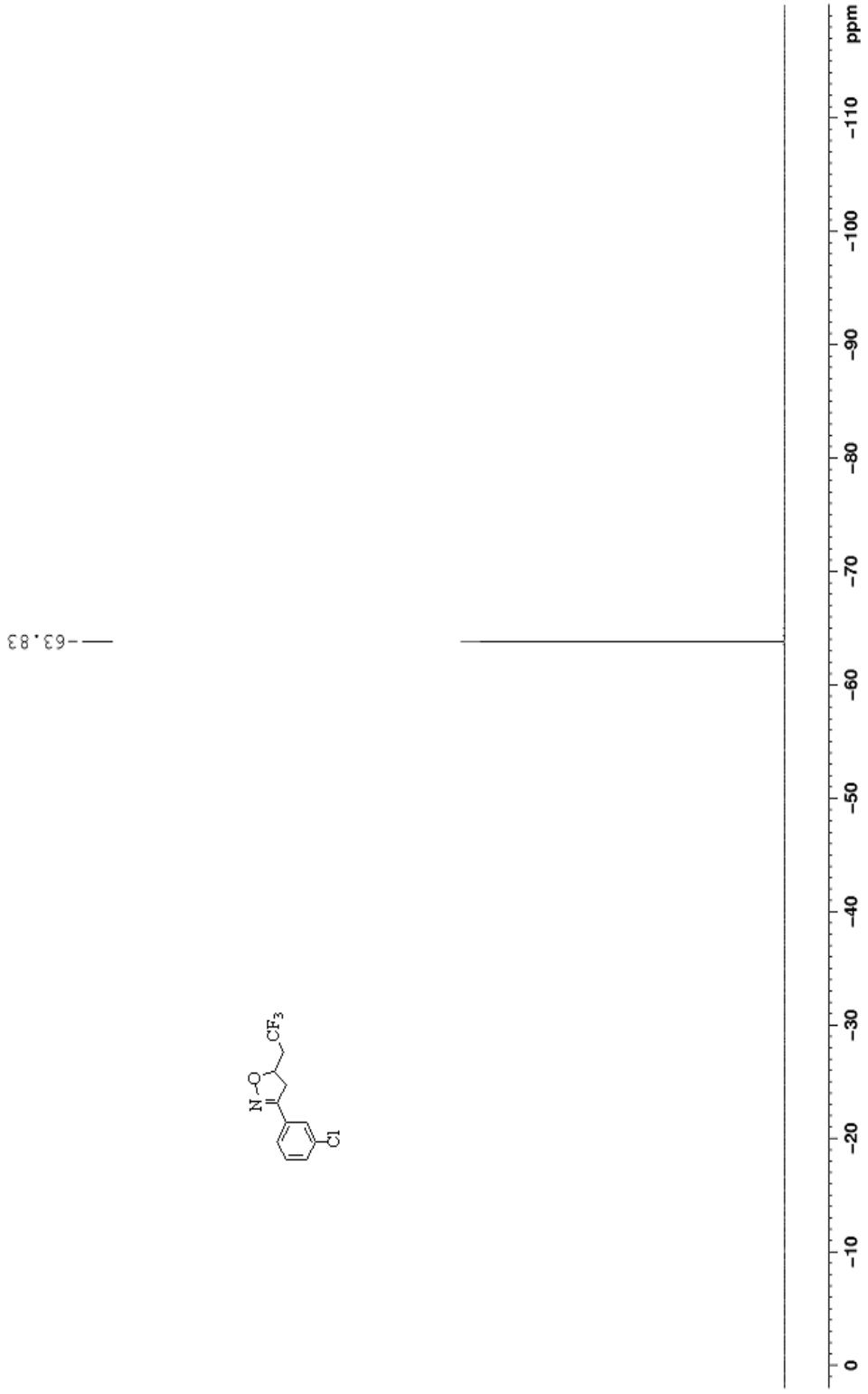

2.406
2.418
2.426
2.433
2.444
2.452
2.463
2.470
2.478
2.489
2.515
2.671
2.684
2.697
2.711
2.724
2.737
2.748
2.761
2.774
3.107
3.127
3.149
3.169
3.505
3.530
3.546
3.572
4.962
4.976
4.982
4.987
4.995
5.001
5.007
5.015
5.021
5.027
5.041
7.262
7.383
7.405
7.592
7.613
CF3
N
O
Cl
ppm
1
2
3
4
5
6
7
8
9
10
0.96
1.00
1.00
0.99
0.99
1.92
1.97

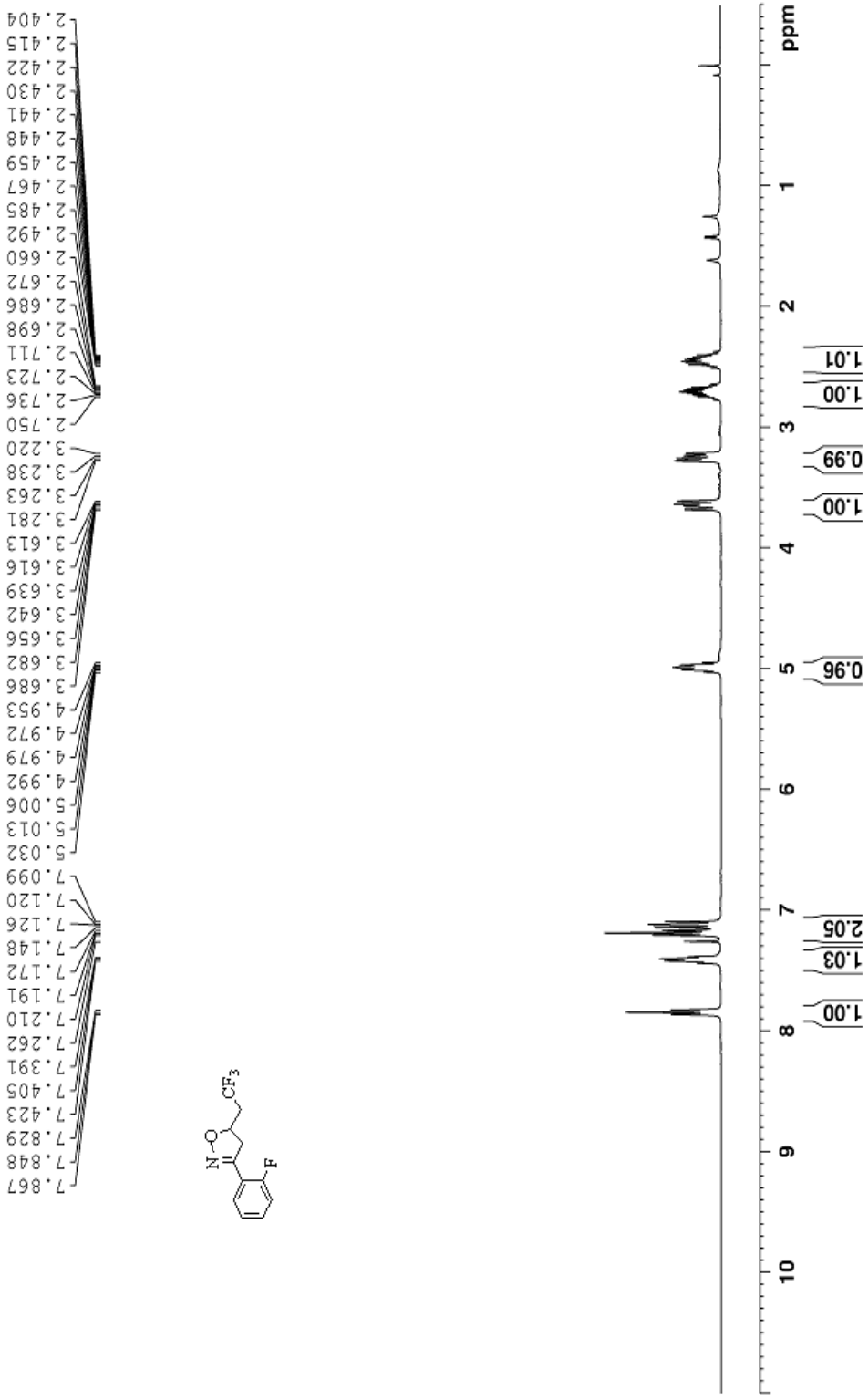

155.66
136.47
129.11
127.94
127.43
126.57
123.82
77.32
77.00
76.68
75.07
40.26
39.49
39.22
38.94
38.66
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
CF3
N
O
Cl


-63.84
CF3
N-O
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm


2.407
2.418
2.426
2.433
2.444
2.452
2.463
2.470
2.478
2.489
2.663
2.677
2.690
2.703
2.716
2.729
2.741
2.754
2.767
3.104
3.124
3.146
3.166
3.501
3.527
3.543
3.569
4.967
4.987
4.993
5.001
5.007
5.013
5.021
5.027
5.046
7.263
7.329
7.349
7.368
7.391
7.412
7.539
7.558
7.643
CF3
N
O
Cl
ppm
1
2
3
4
5
6
7
8
9
10
1.05
1.03
1.04
1.03
1.00
2.20
1.14
1.09


38.62
38.90
39.17
39.45
40.13
75.10
75.13
76.68
77.00
77.32
121.04
123.79
124.75
126.54
126.70
129.29
130.07
130.37
130.66
134.83
CF3
N
O
Cl
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190


-63.83
CF3
N
O
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm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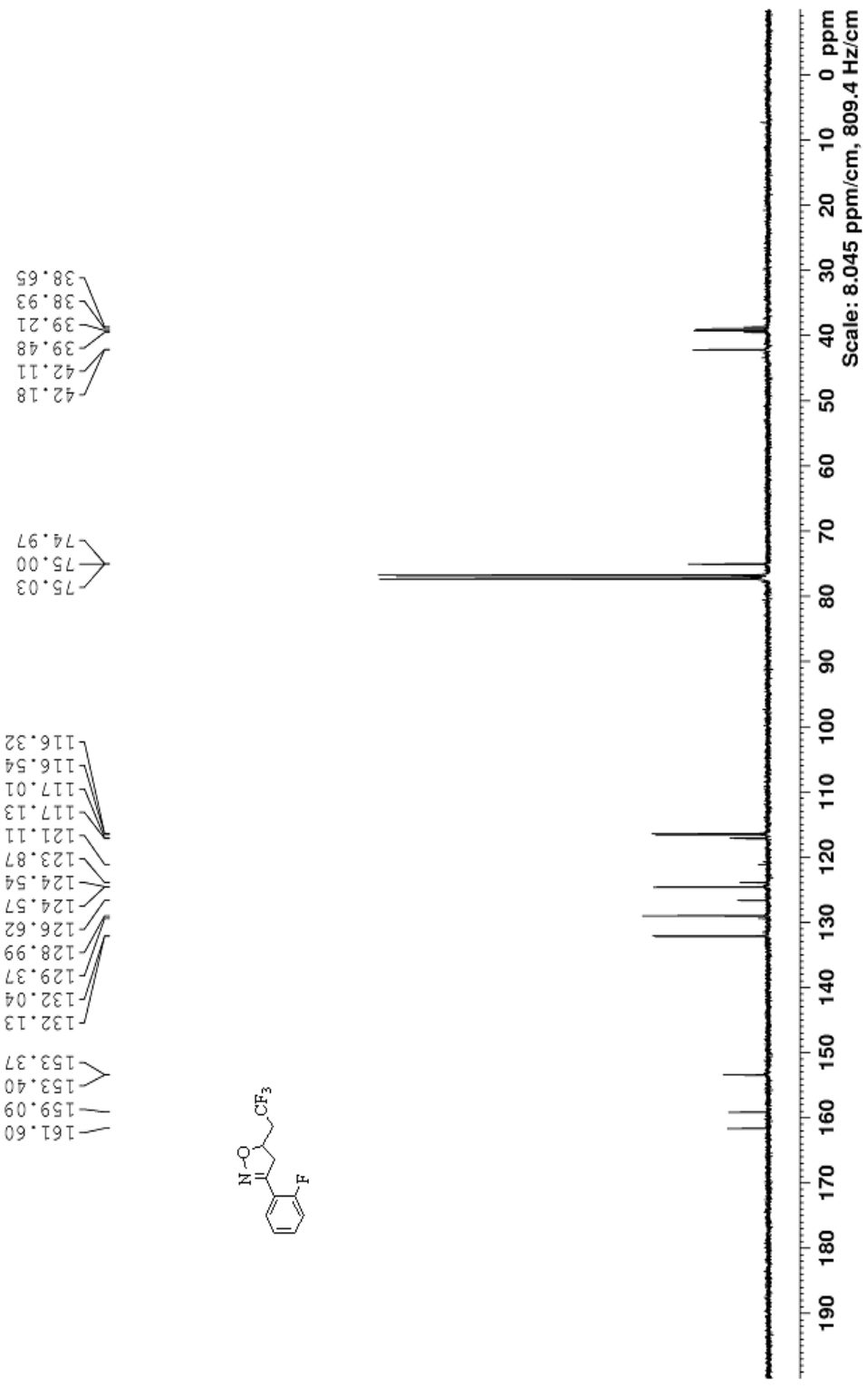
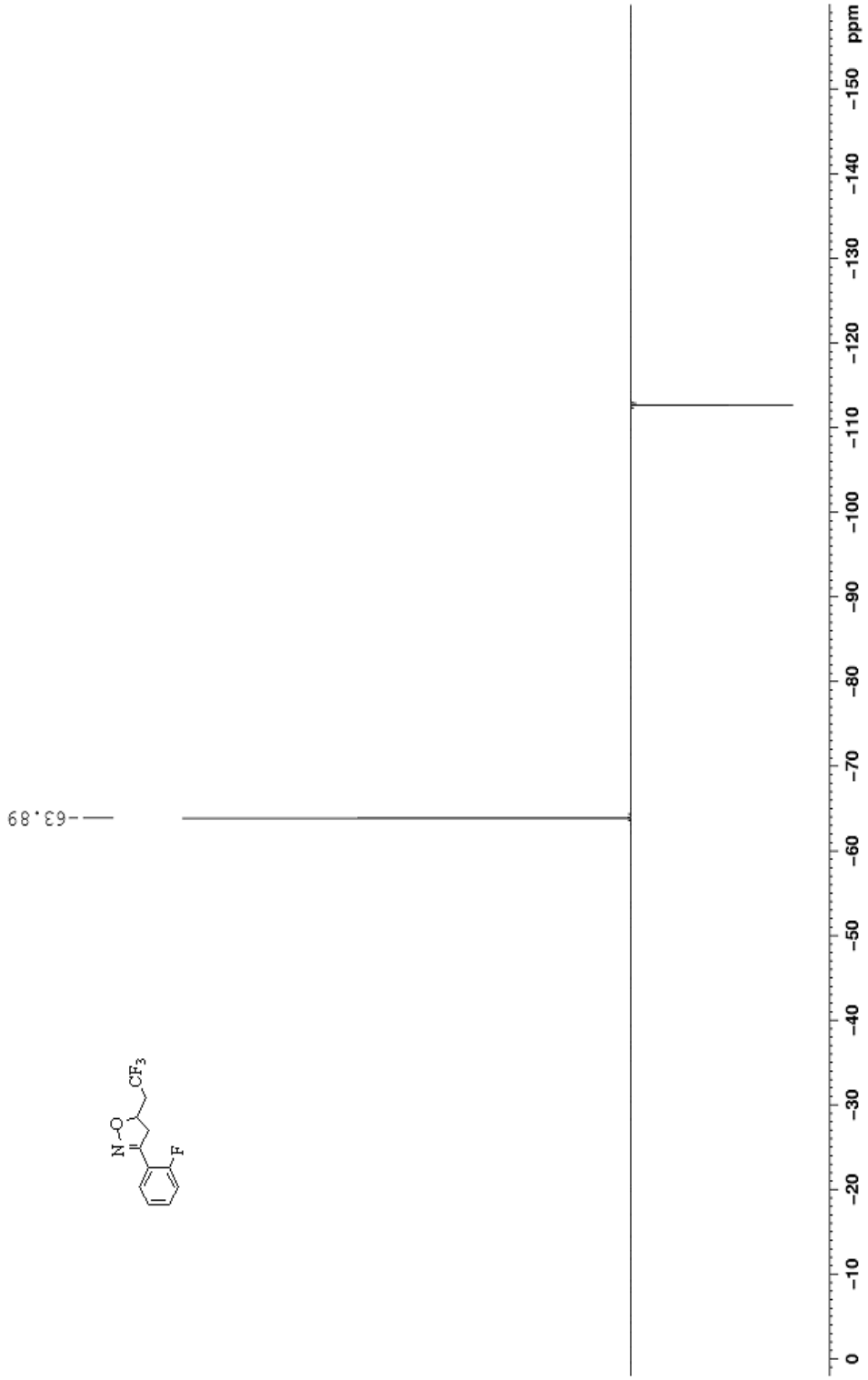
2.415
2.422
2.430
2.441
2.448
2.459
2.467
2.485
2.492
2.660
2.672
2.686
2.698
2.711
2.723
2.736
2.750
3.220
3.238
3.263
3.281
3.613
3.616
3.639
3.642
3.656
3.682
3.686
4.953
4.972
4.979
4.992
5.006
5.013
5.032
7.099
7.120
7.126
7.148
7.172
7.191
7.210
7.262
7.391
7.405
7.423
7.829
7.848
7.867
CF3
N
O
F
ppm
1.00
1.03
2.05
1.00
0.96
1.00
0.99
1.00
1.01


38.65
38.93
39.21
39.48
42.11
42.18
74.97
75.00
75.03
116.32
116.54
117.01
117.13
121.11
123.87
124.54
124.57
126.62
128.99
129.37
132.04
132.13
153.37
153.40
159.09
161.60
CF3
N
O
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Scale: 8.045 ppm/cm, 809.4 Hz/cm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ppm
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-10
-20
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-40
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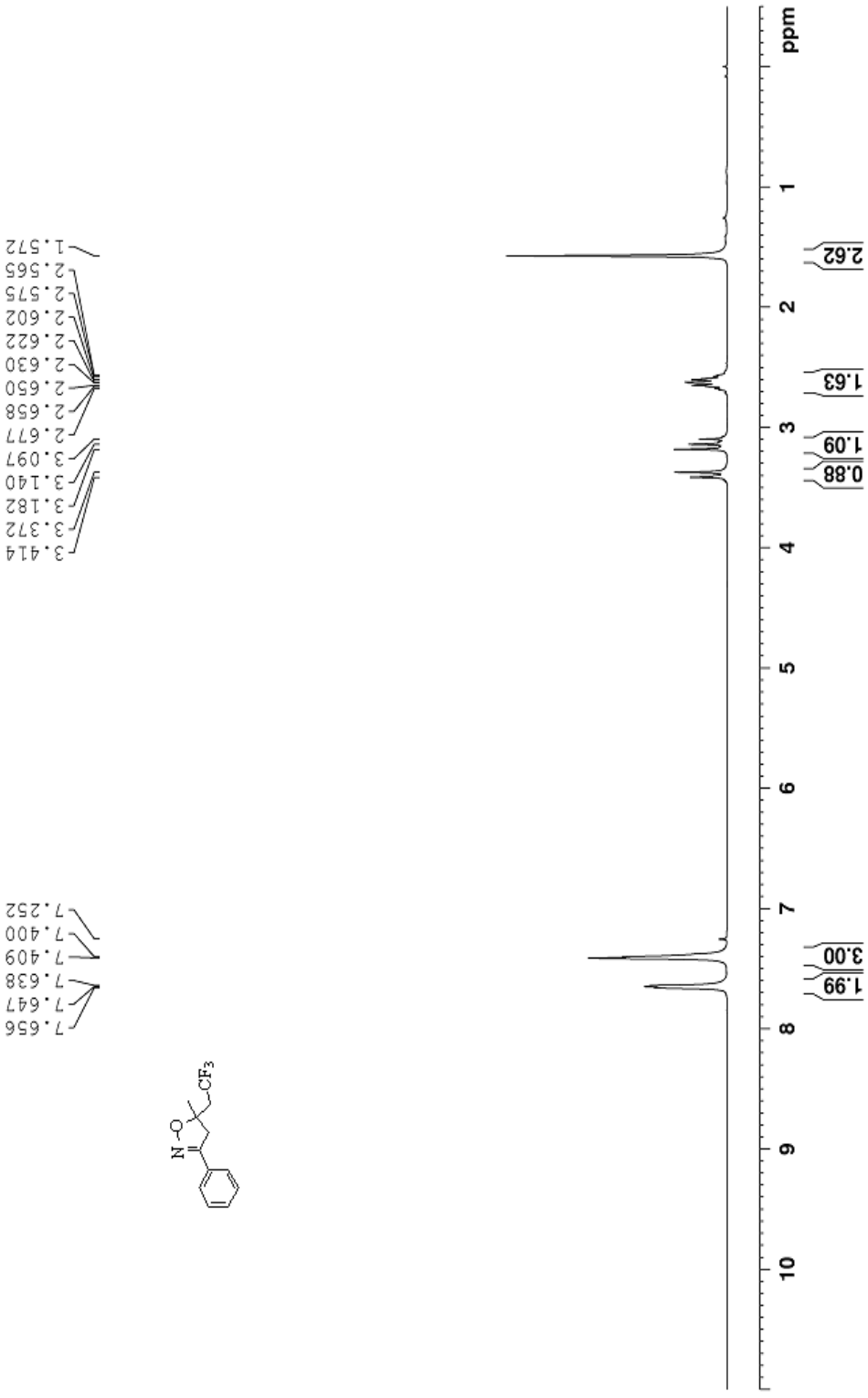
-70
-80
-90
-100
-110
-120
-130
-140
-150
CF3
N
O
F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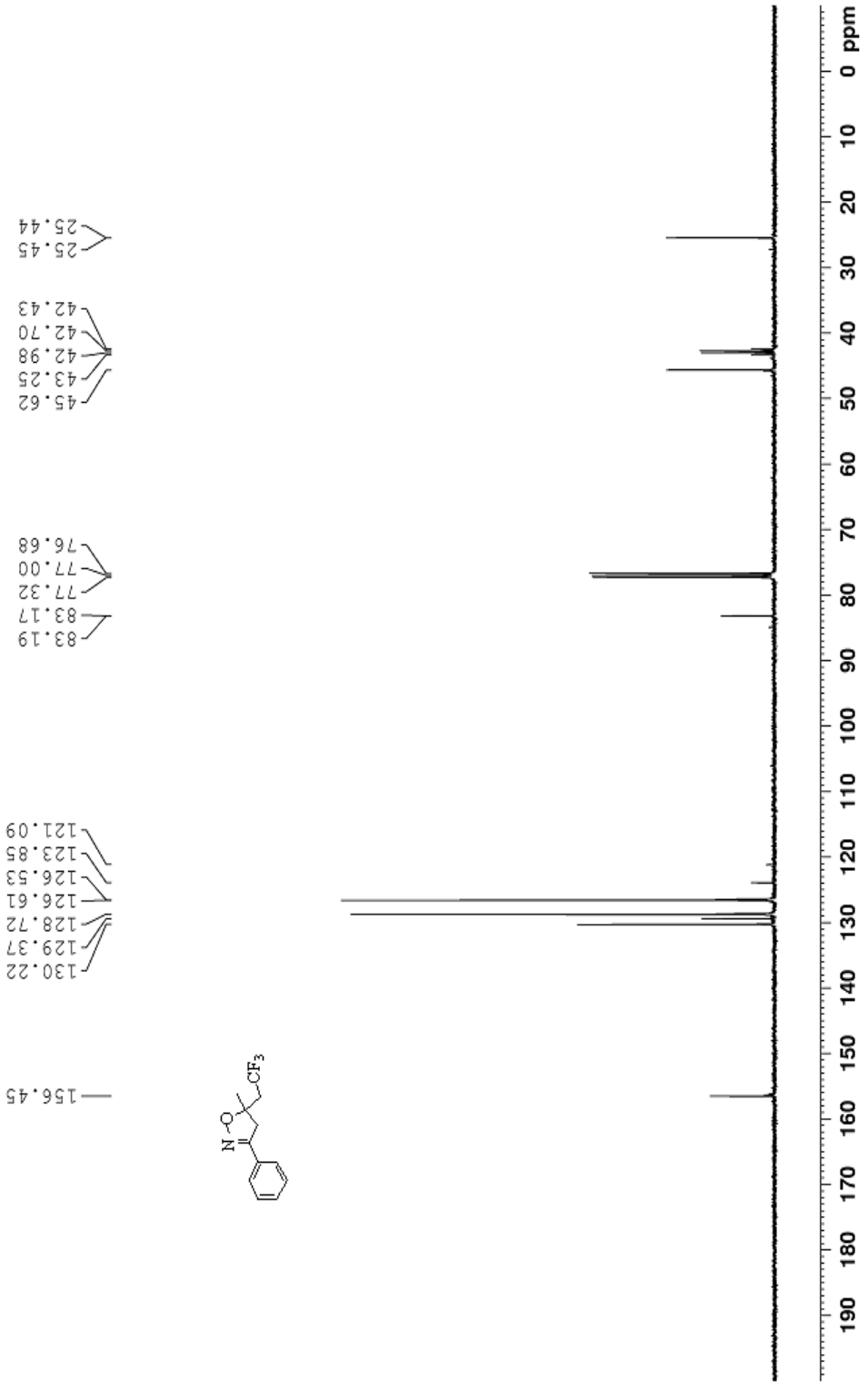
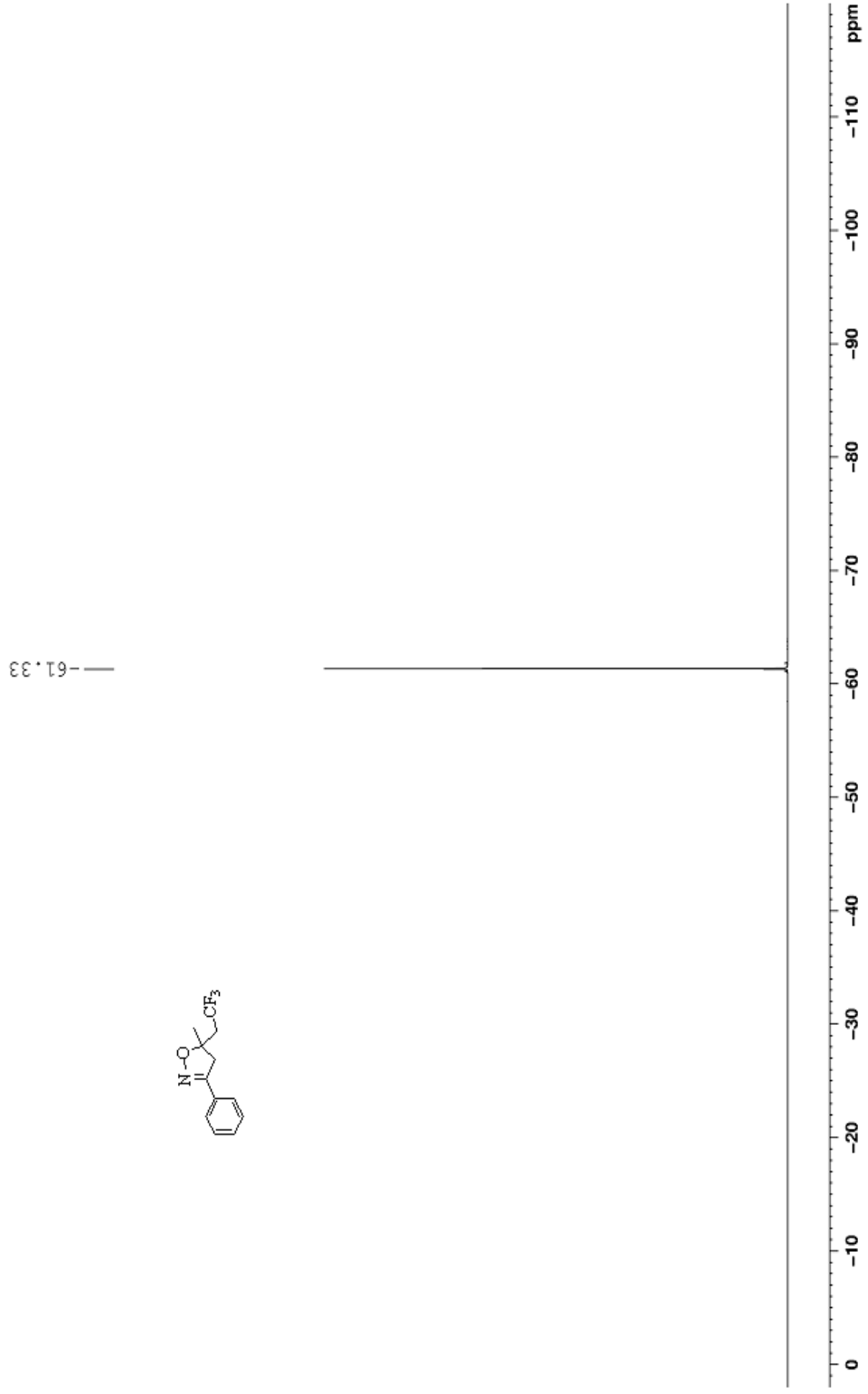
2.565
2.575
2.602
2.622
2.630
2.650
2.658
2.677
3.097
3.140
3.182
3.372
3.414
7.252
7.400
7.409
7.638
7.647
7.656
F3C
O
N
ppm
1
2
3
4
5
6
7
8
9
10
2.62
1.63
1.09
0.88
3.00
1.99


25.44
25.45
42.43
42.70
42.98
43.25
45.62
76.68
77.00
77.32
83.17
83.19
121.09
123.85
126.53
126.61
128.72
129.37
130.22
156.45
CF3
N
O
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190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ppm
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-40
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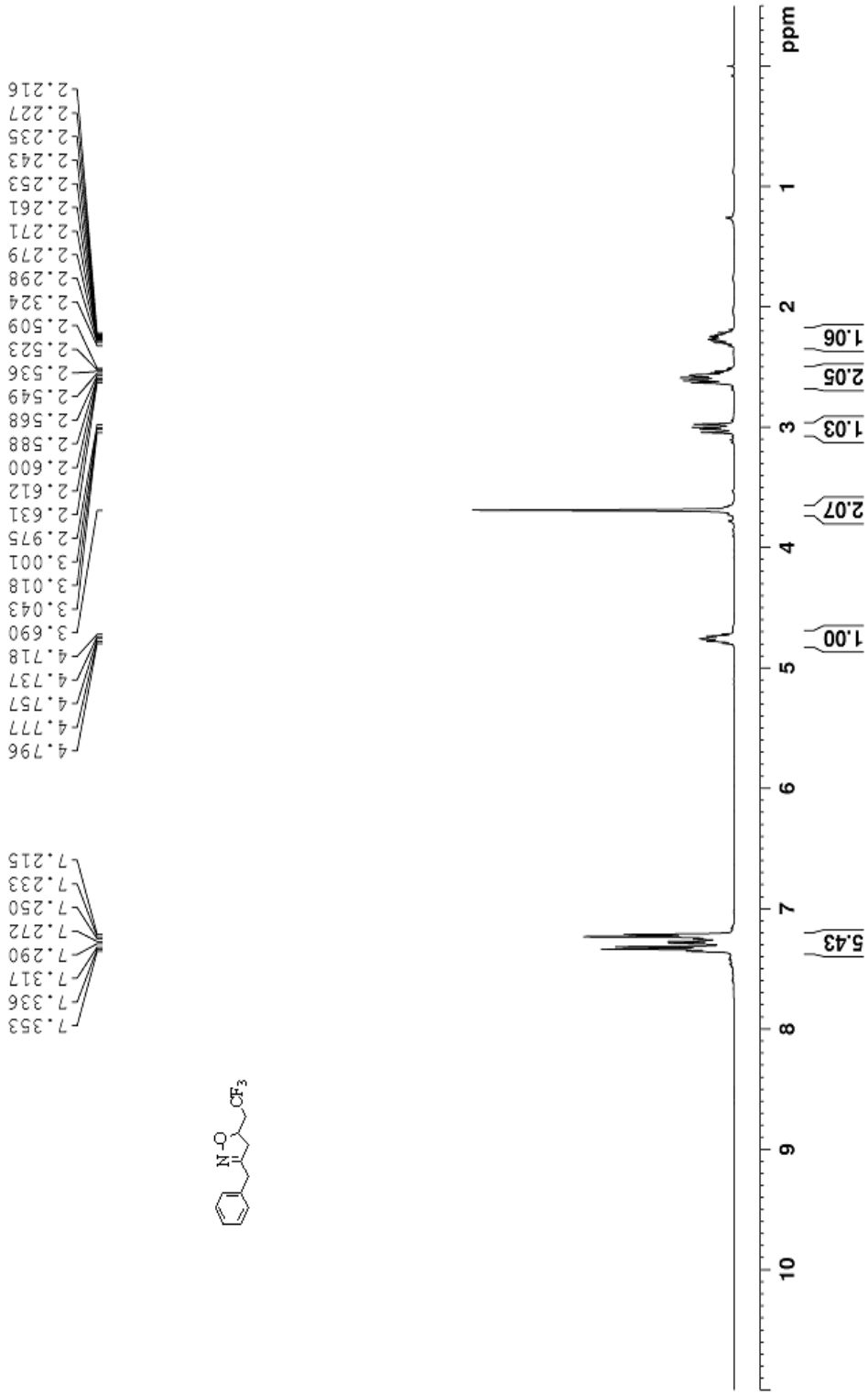
-60
-70
-80
-90
-100
-110
CF3
N
O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7.290
7.272
7.250
7.233
7.215
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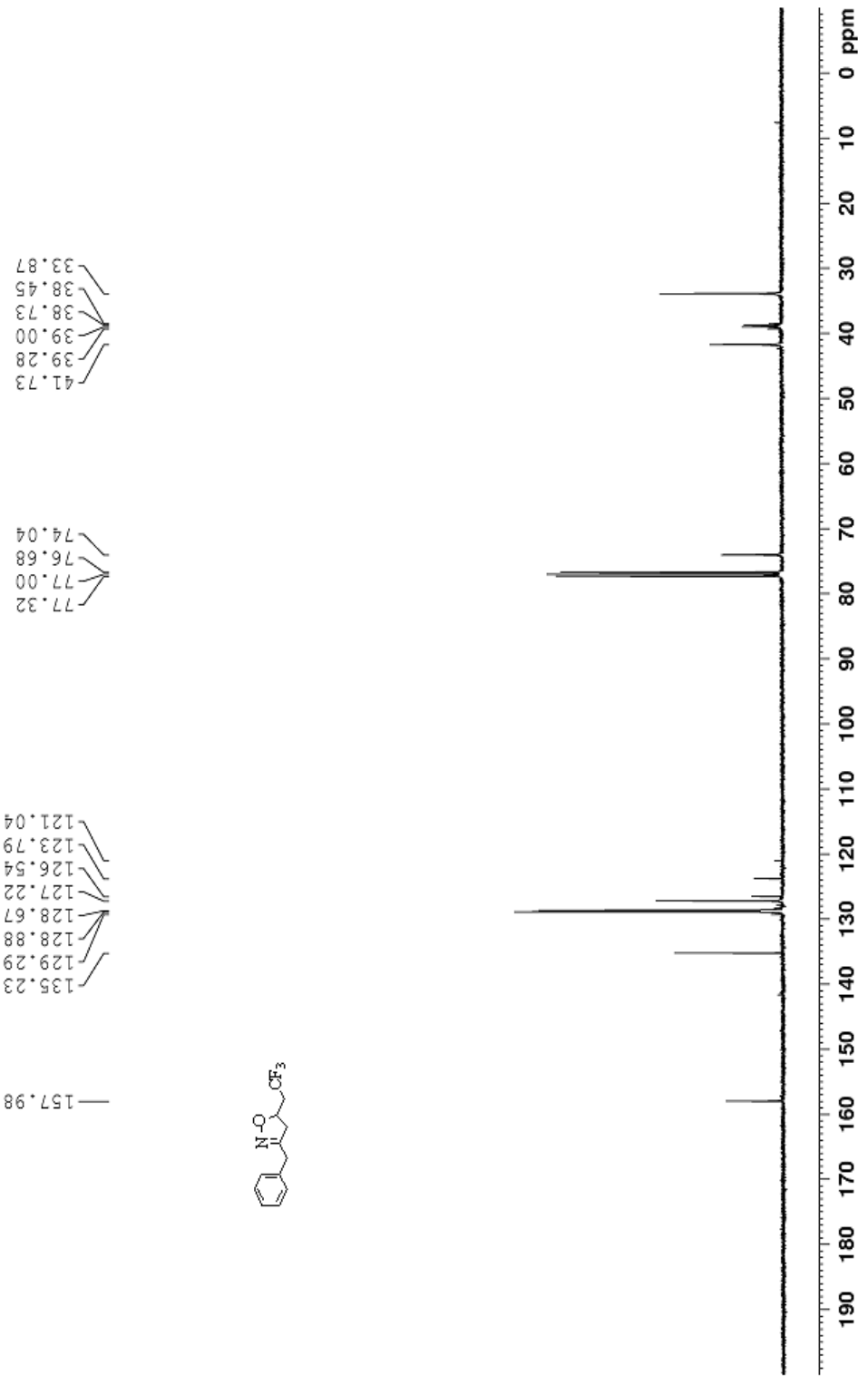
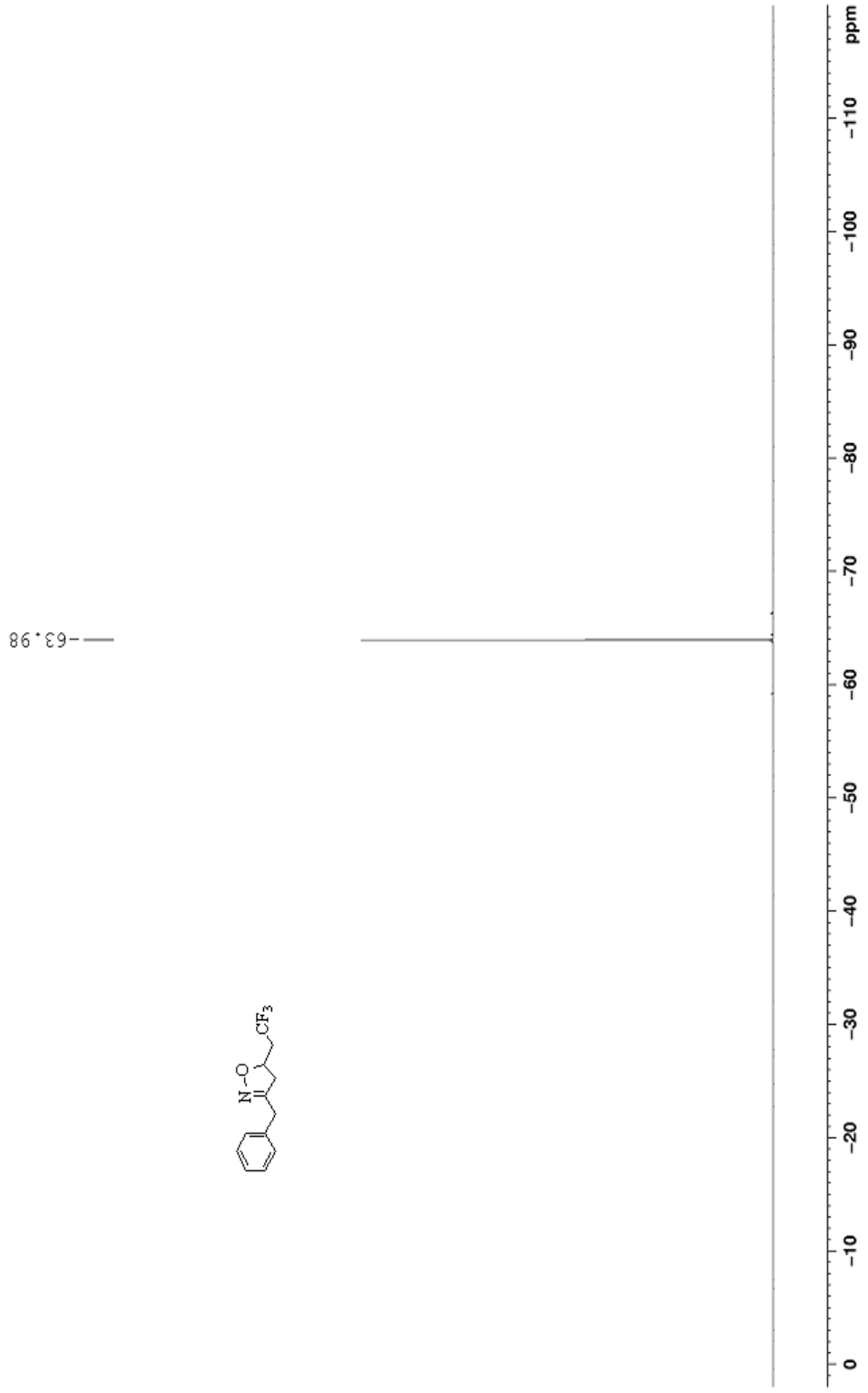
4.777
4.757
4.737
4.718
3.690
3.043
3.018
3.001
2.975
2.631
2.612
2.600
2.588
2.568
2.549
2.536
2.523
2.509
2.324
2.298
2.279
2.271
2.261
2.253
2.243
2.235
2.227
2.216
N
O
CF3
ppm
1
2
3
4
5
6
7
8
9
10
5.43
1.00
2.07
1.03
2.05
1.06


157.98
135.23
129.29
128.88
128.67
127.22
126.54
123.79
121.04
77.32
77.00
76.68
74.04
41.73
39.28
39.00
38.73
38.45
33.87
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190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CF3
N
O
ppm
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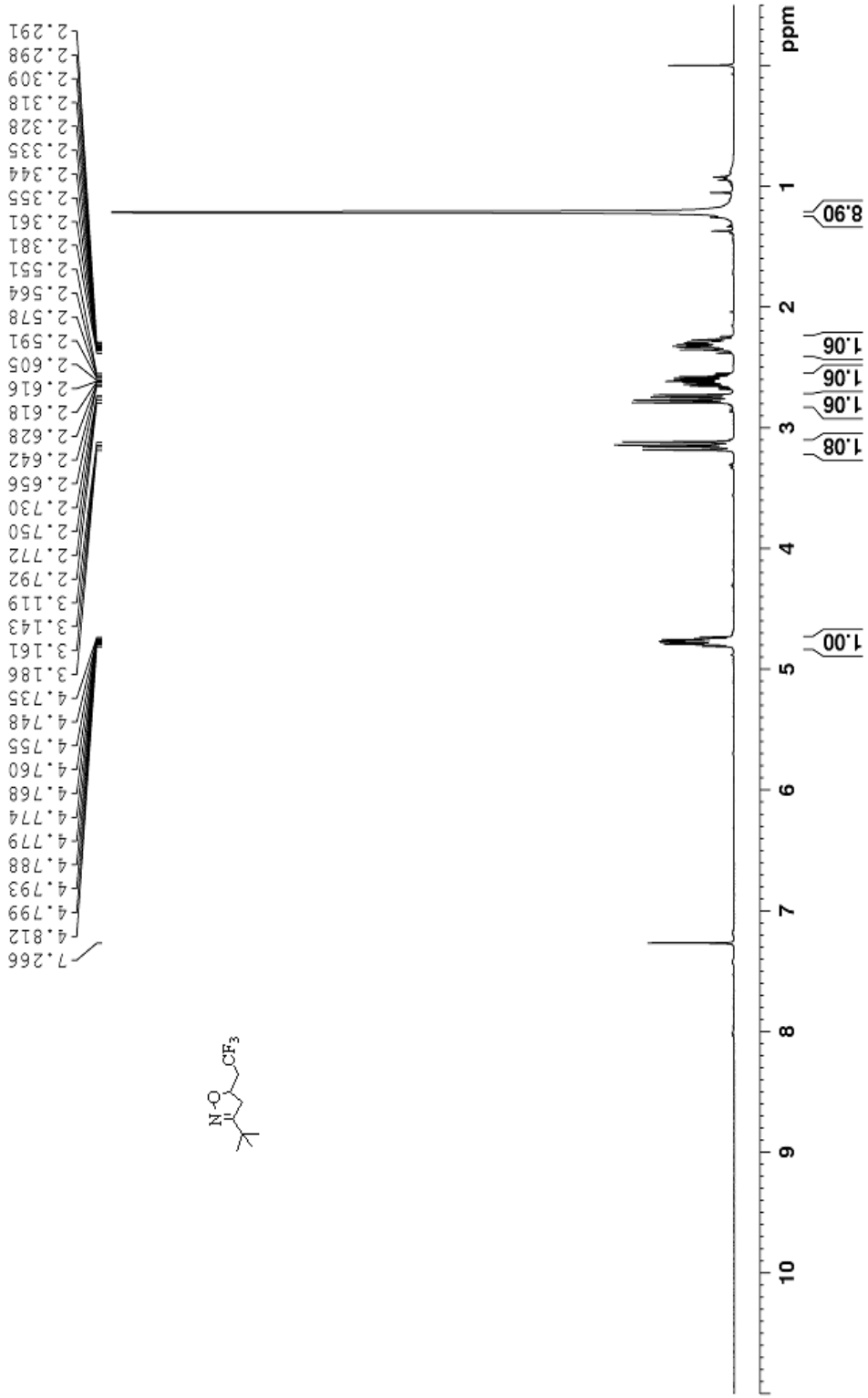
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110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2.309
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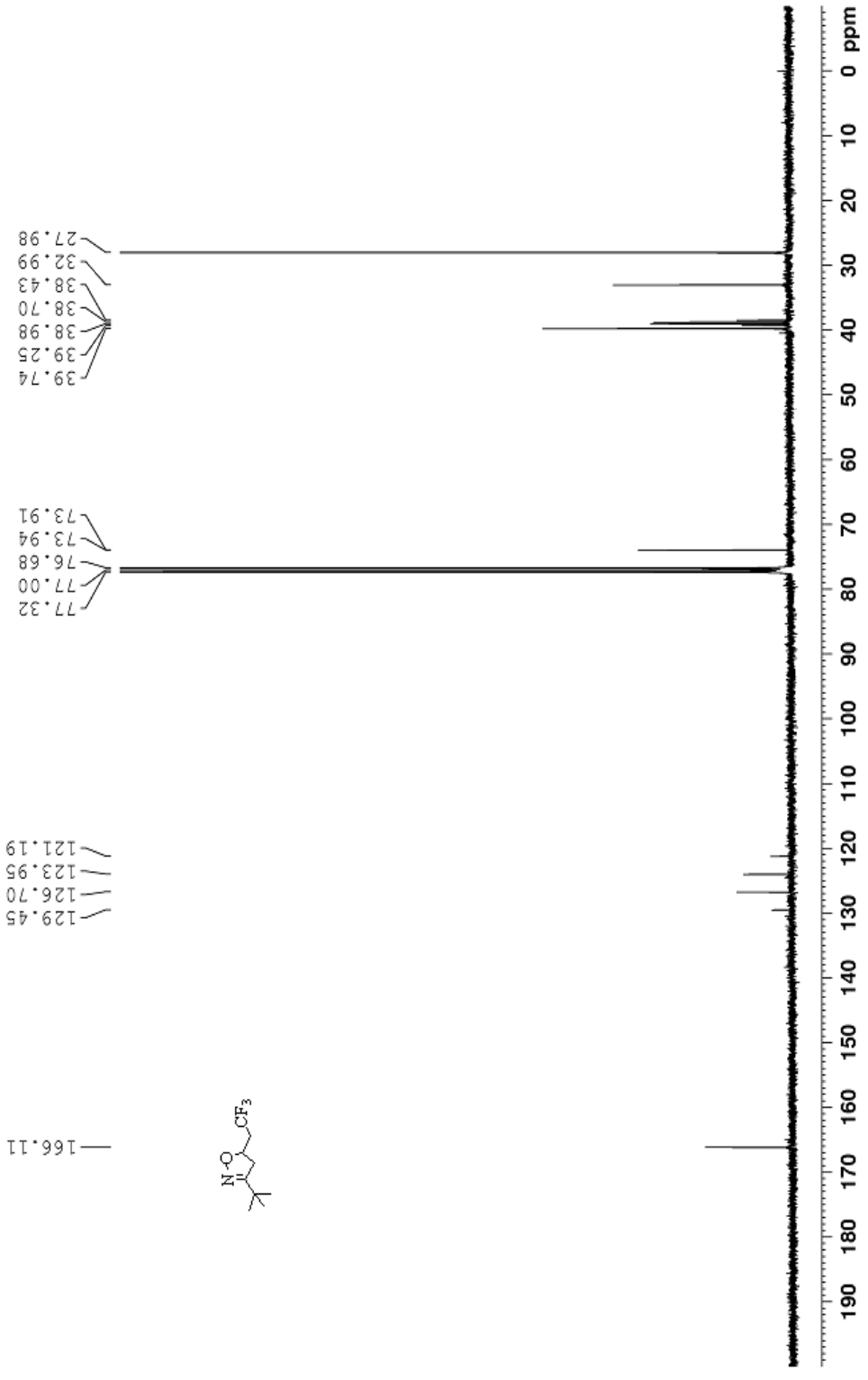
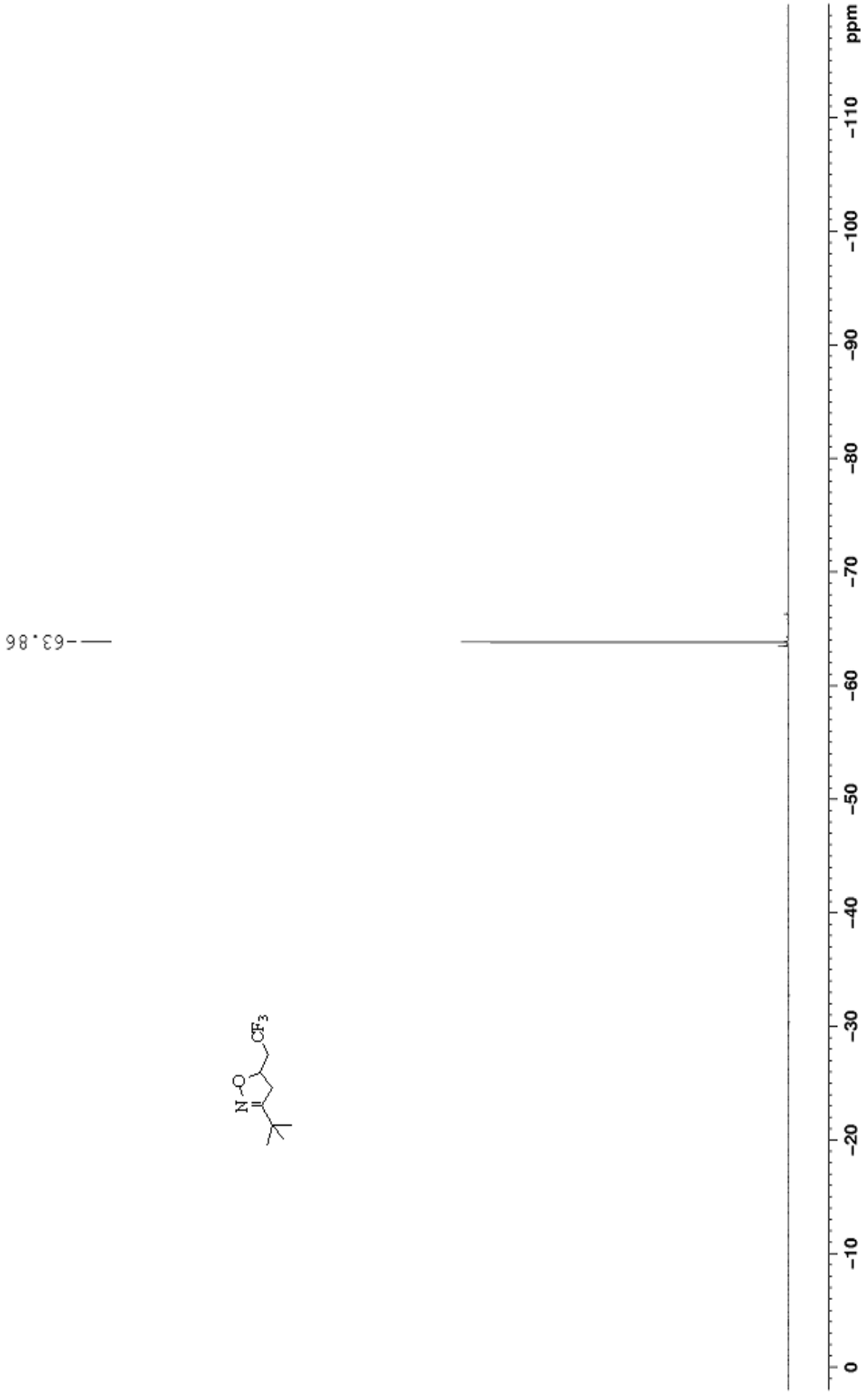
2.328
2.335
2.344
2.355
2.361
2.381
2.551
2.564
2.578
2.591
2.605
2.616
2.618
2.628
2.642
2.656
2.730
2.750
2.772
2.792
3.119
3.143
3.161
3.186
4.735
4.748
4.755
4.760
4.768
4.774
4.779
4.788
4.793
4.799
4.812
7.266
8.90
1.06
1.06
1.06
1.08
1.00
ppm
1
2
3
4
5
6
7
8
9
10
N
O
CF3


27.98
32.99
38.43
38.70
38.98
39.25
39.74
73.91
73.94
76.68
77.00
77.32
121.19
123.95
126.70
129.45
166.11
CF3
N
O
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190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CF3
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O
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-40
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-60
-70
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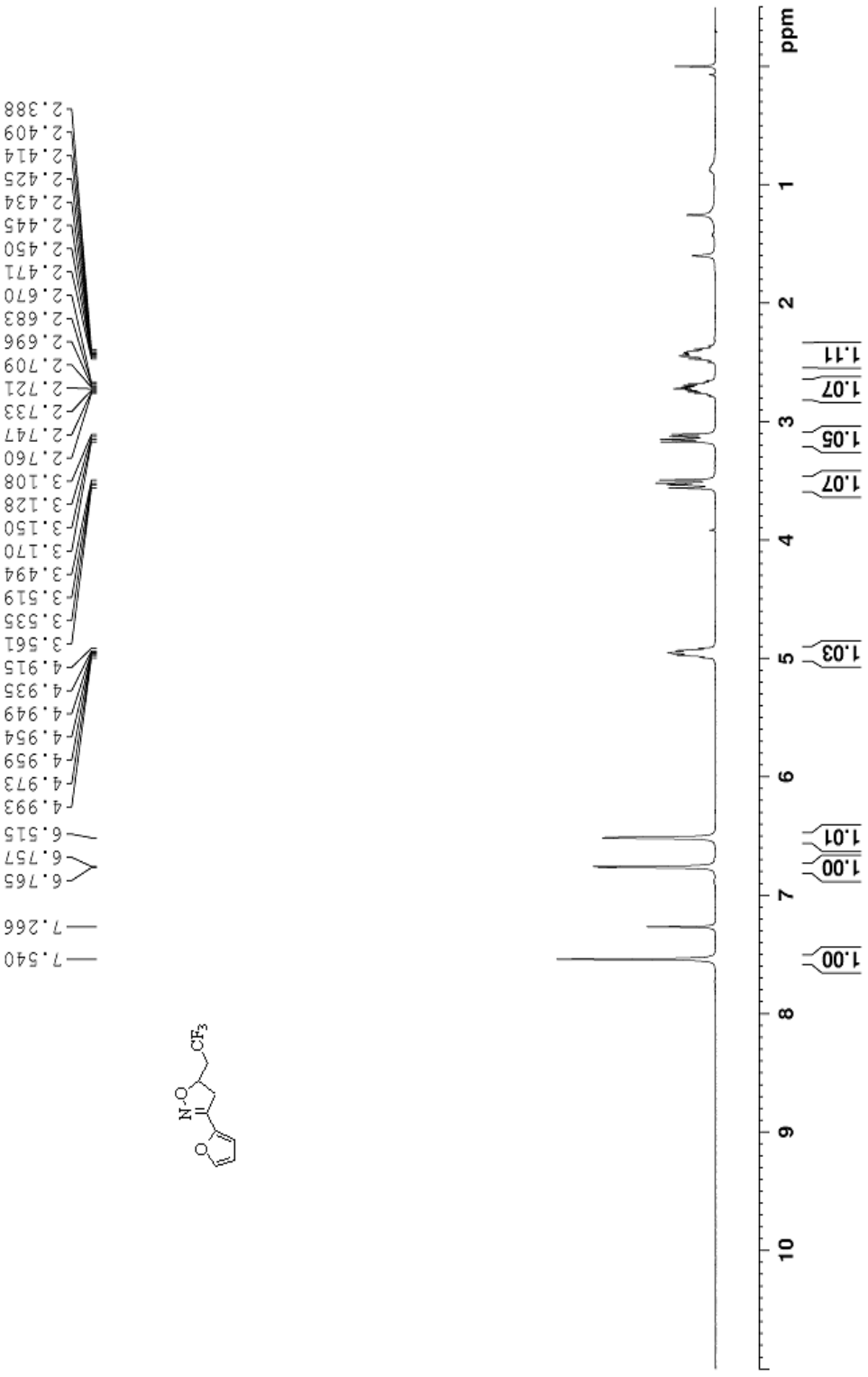
-100
-110
ppm


2.388
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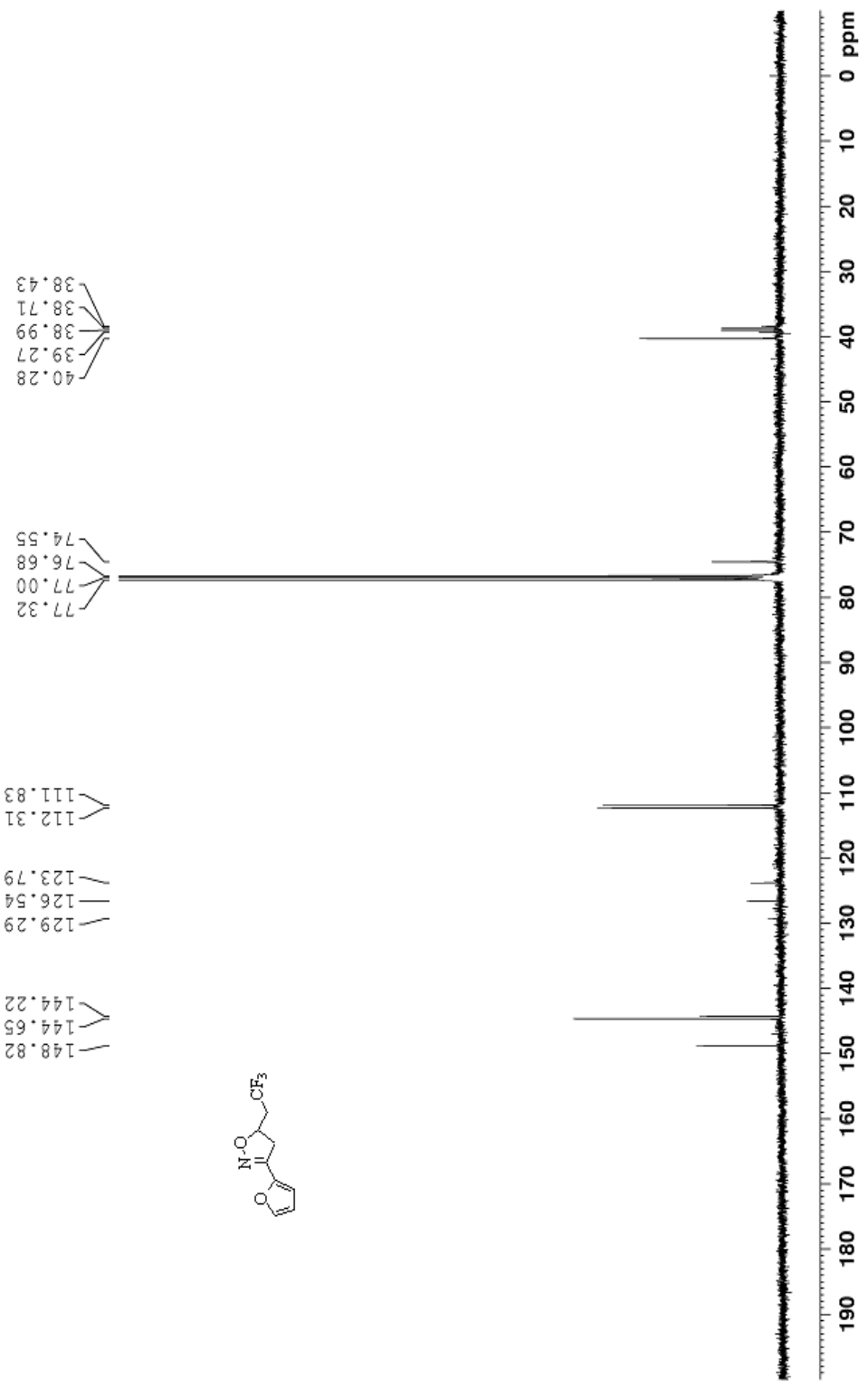
2.414
2.425
2.434
2.445
2.450
2.471
2.670
2.683
2.696
2.709
2.721
2.733
2.747
2.760
3.108
3.128
3.150
3.170
3.494
3.519
3.535
3.561
4.915
4.935
4.949
4.954
4.959
4.973
4.993
6.515
6.757
6.765
7.266
7.540
CF3
N
O
O
ppm
1.00
1.01
1.00
1.03
1.07
1.05
1.07
1.11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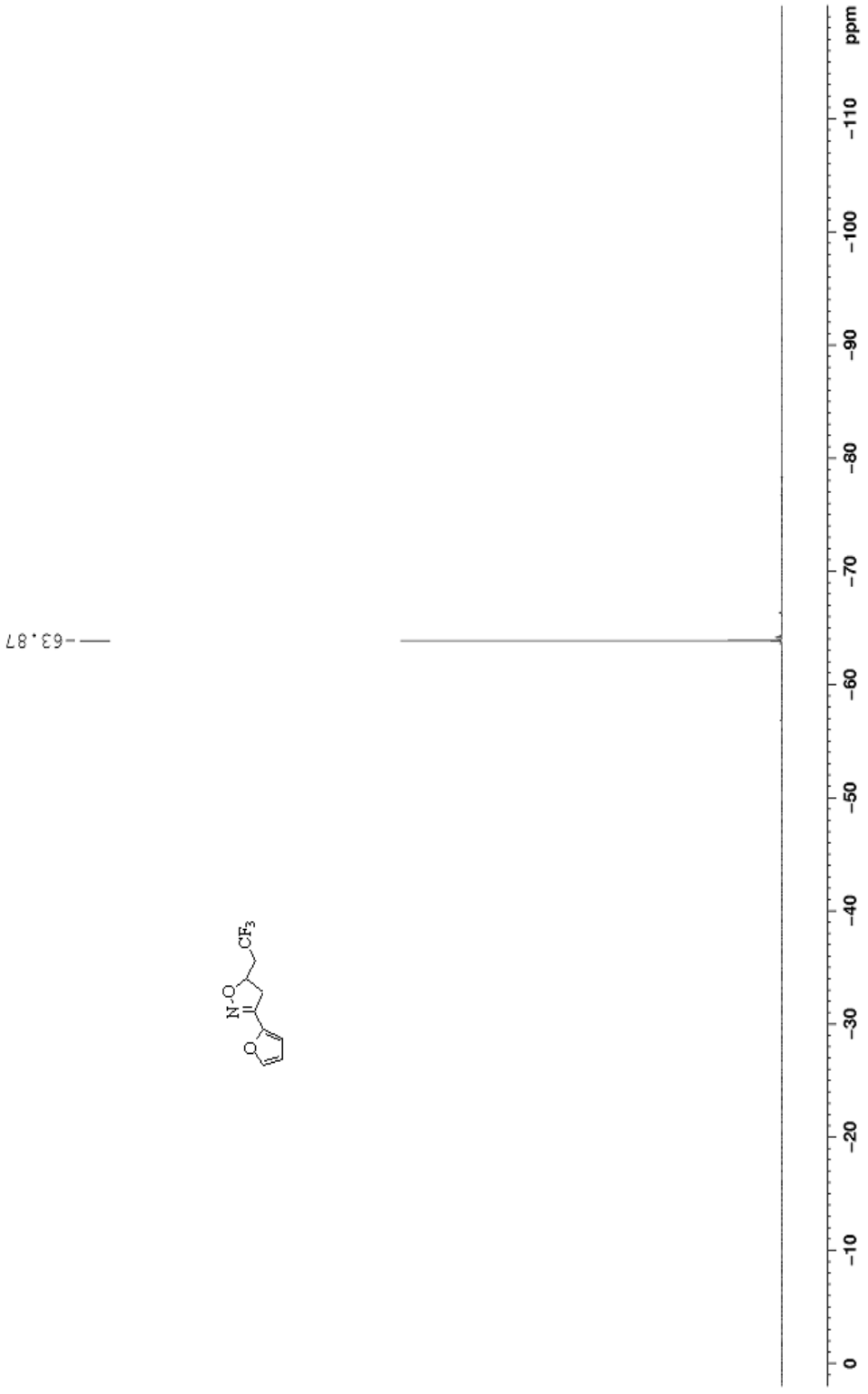
38.71
38.99
39.27
40.28
74.55
76.68
77.00
77.32
111.83
112.31
123.79
126.54
129.29
144.22
144.65
148.82
CF3
N
O
O
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190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CF3
N
O
O
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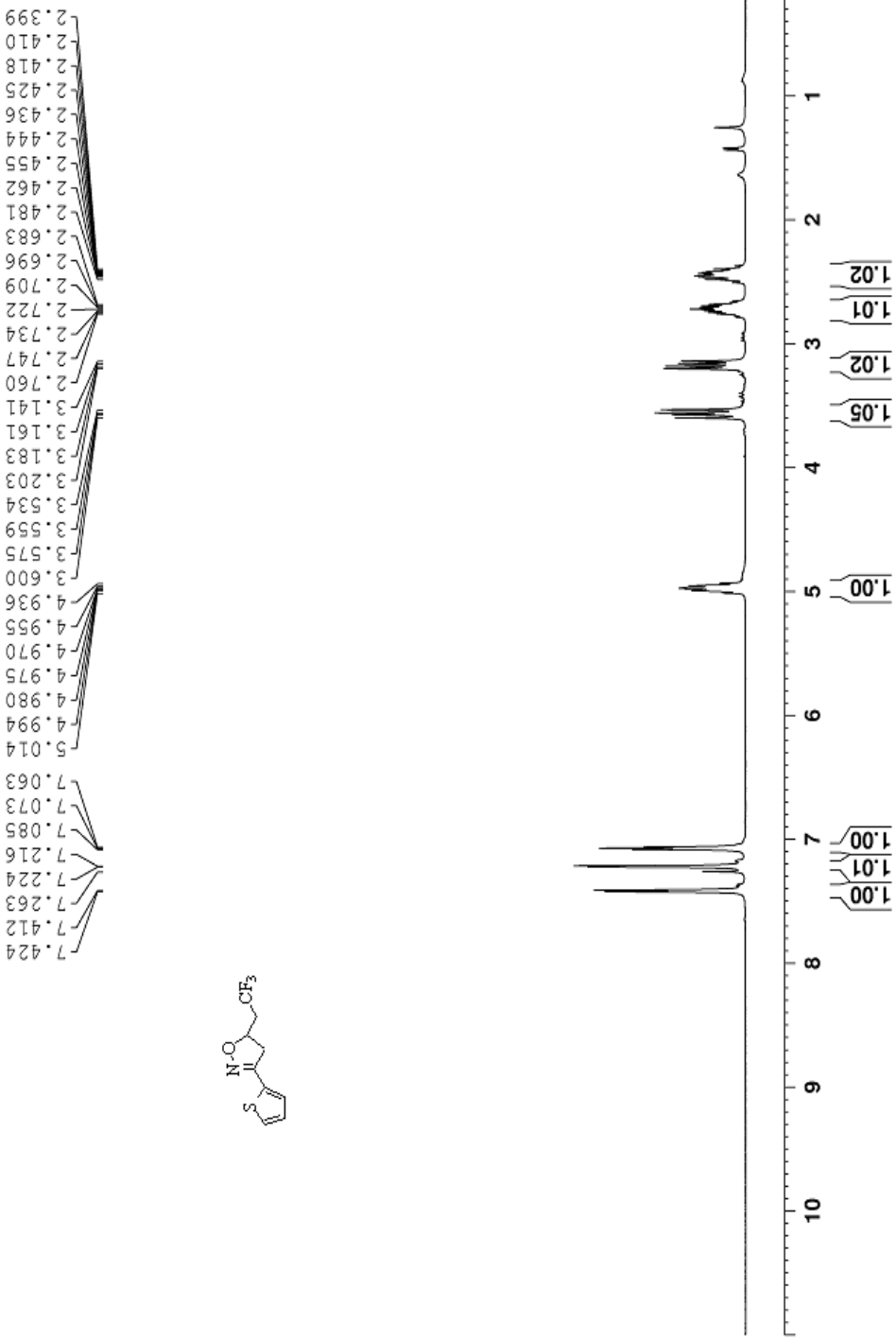
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm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7.412
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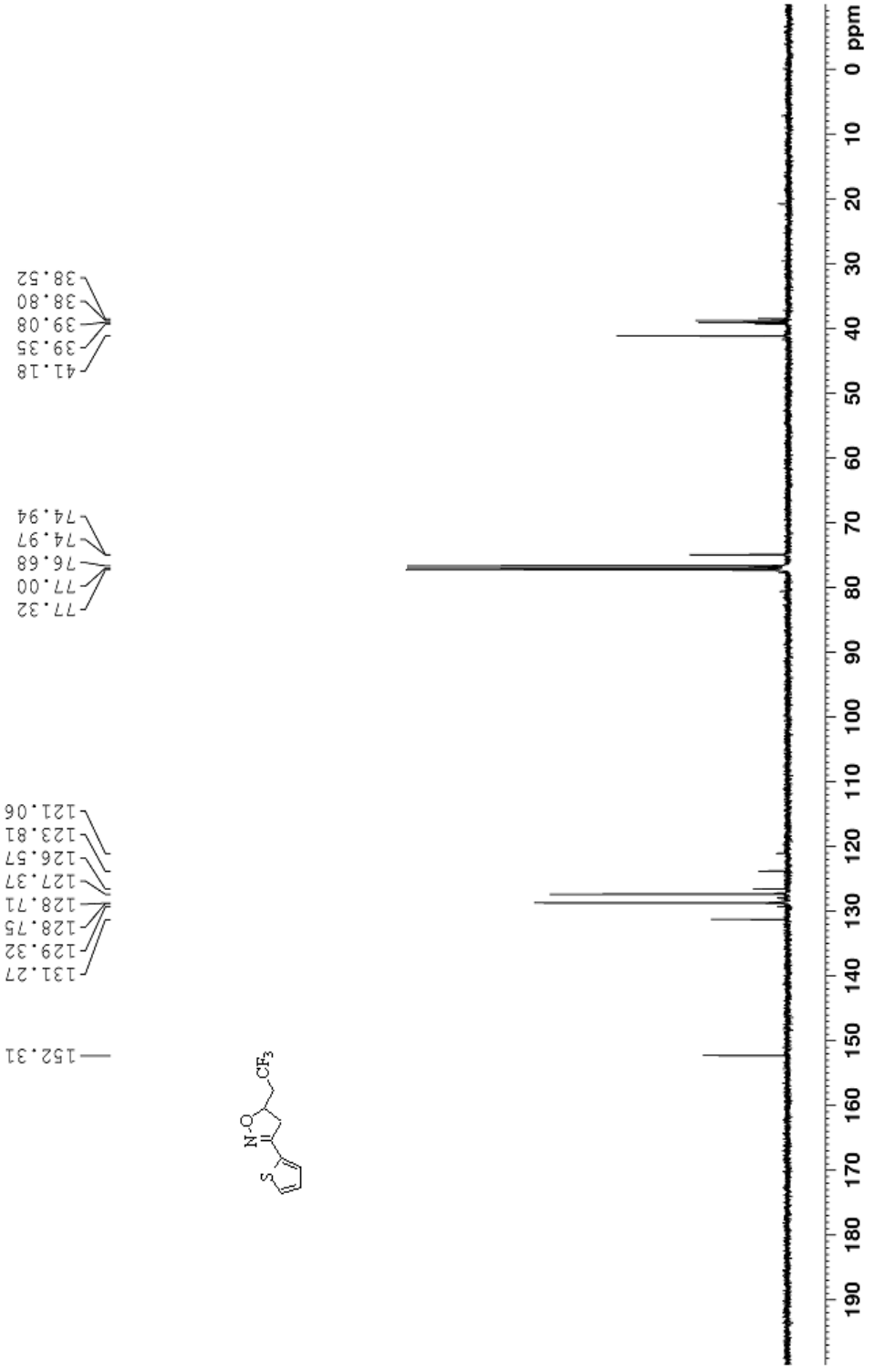
7.224
7.216
7.085
7.073
7.063
5.014
4.994
4.980
4.975
4.970
4.955
4.936
3.600
3.575
3.559
3.534
3.203
3.183
3.161
3.141
2.760
2.747
2.734
2.722
2.709
2.696
2.683
2.481
2.462
2.455
2.444
2.436
2.425
2.418
2.410
2.399
CF3
N
O
S
ppm
1
2
3
4
5
6
7
8
9
10
1.00
1.01
1.00
1.02
1.01
1.02
1.05
1.00


38.52
38.80
39.08
39.35
41.18
74.94
74.97
76.68
77.00
77.32
121.06
123.81
126.57
127.37
128.71
128.75
129.32
131.27
152.31
CF3
N
O
S
0 ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
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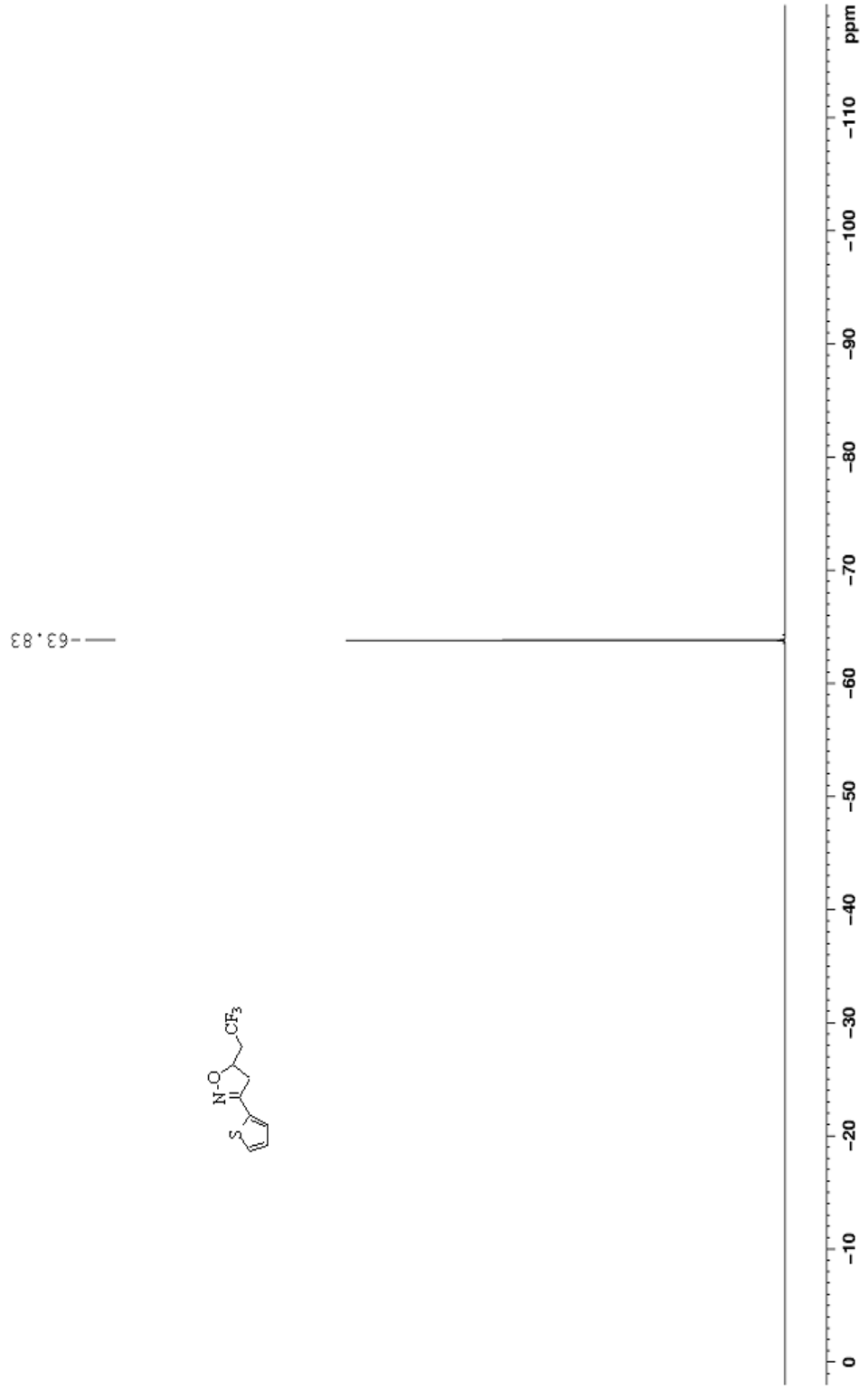
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CF3
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O
S
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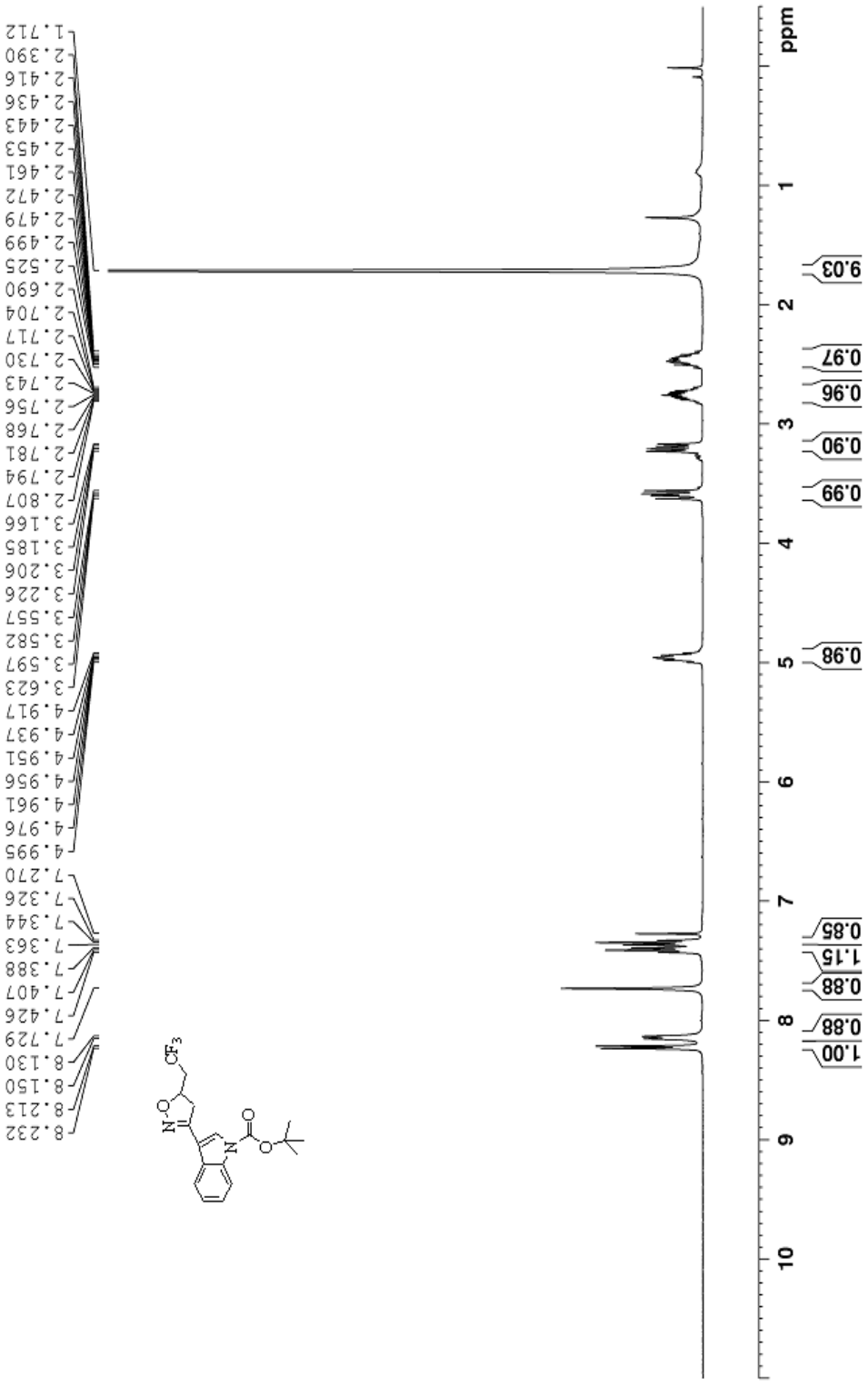
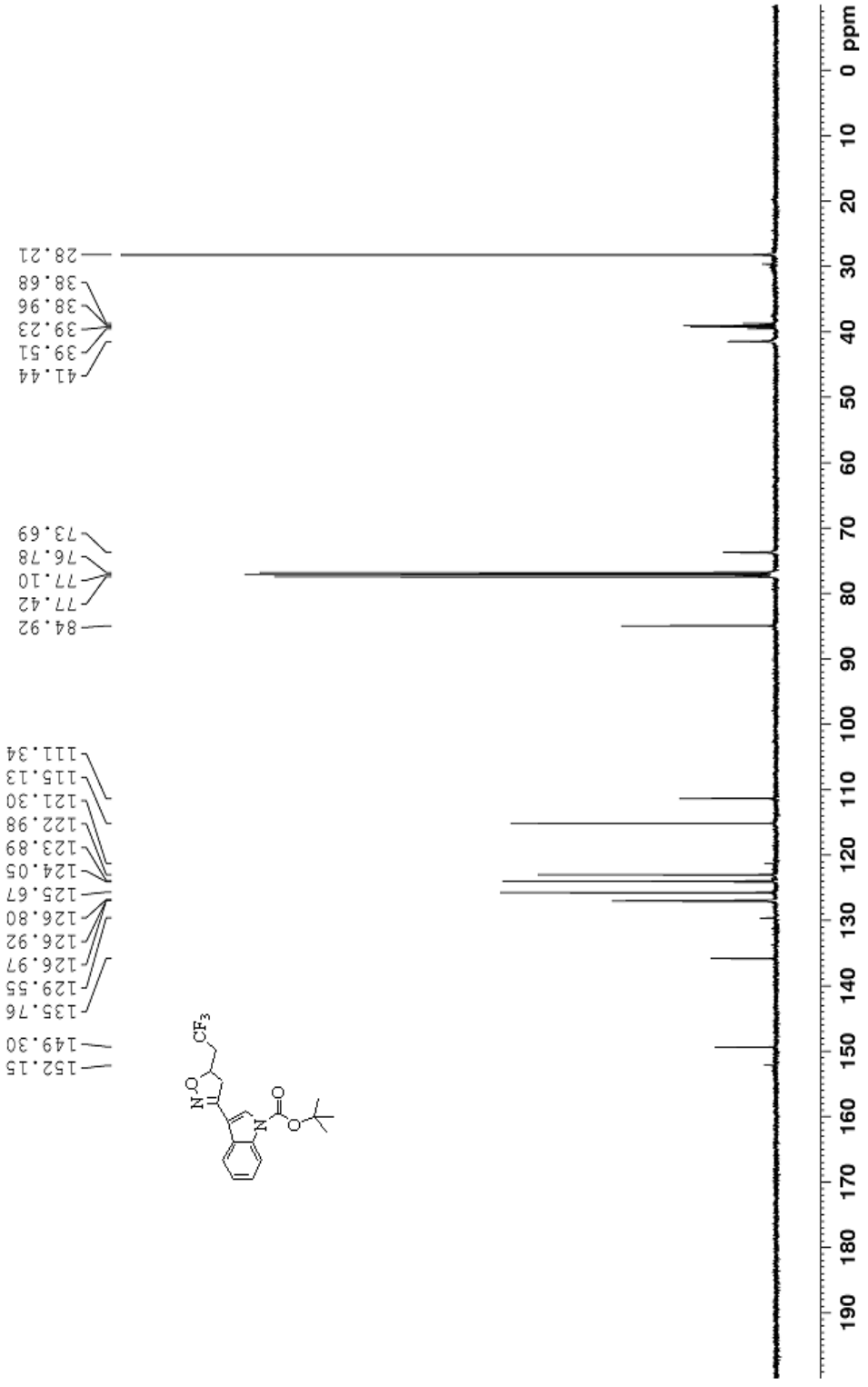
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm


ppm
9.03
0.97
0.96
0.90
0.99
0.98
0.85
1.15
0.88
0.88
1.00
CF3
N
O
N
O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38.68
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39.23
39.51
41.44
73.69
76.78
77.10
77.42
84.92
111.34
115.13
121.30
122.98
123.89
124.05
125.67
126.80
126.92
126.97
129.55
135.76
149.30
152.15
CF3
O
N
O
N
O
O
0 ppm
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20
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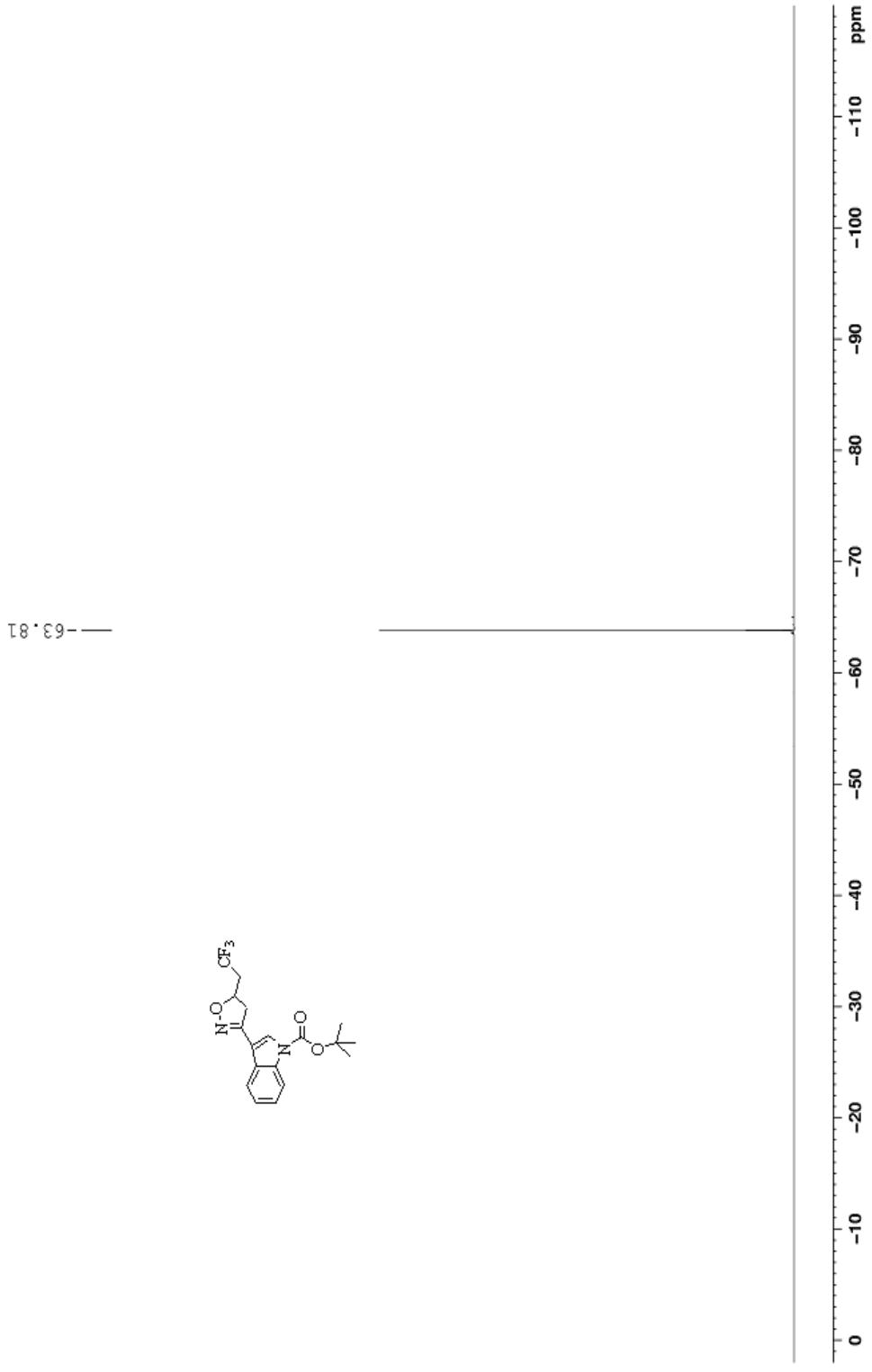
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190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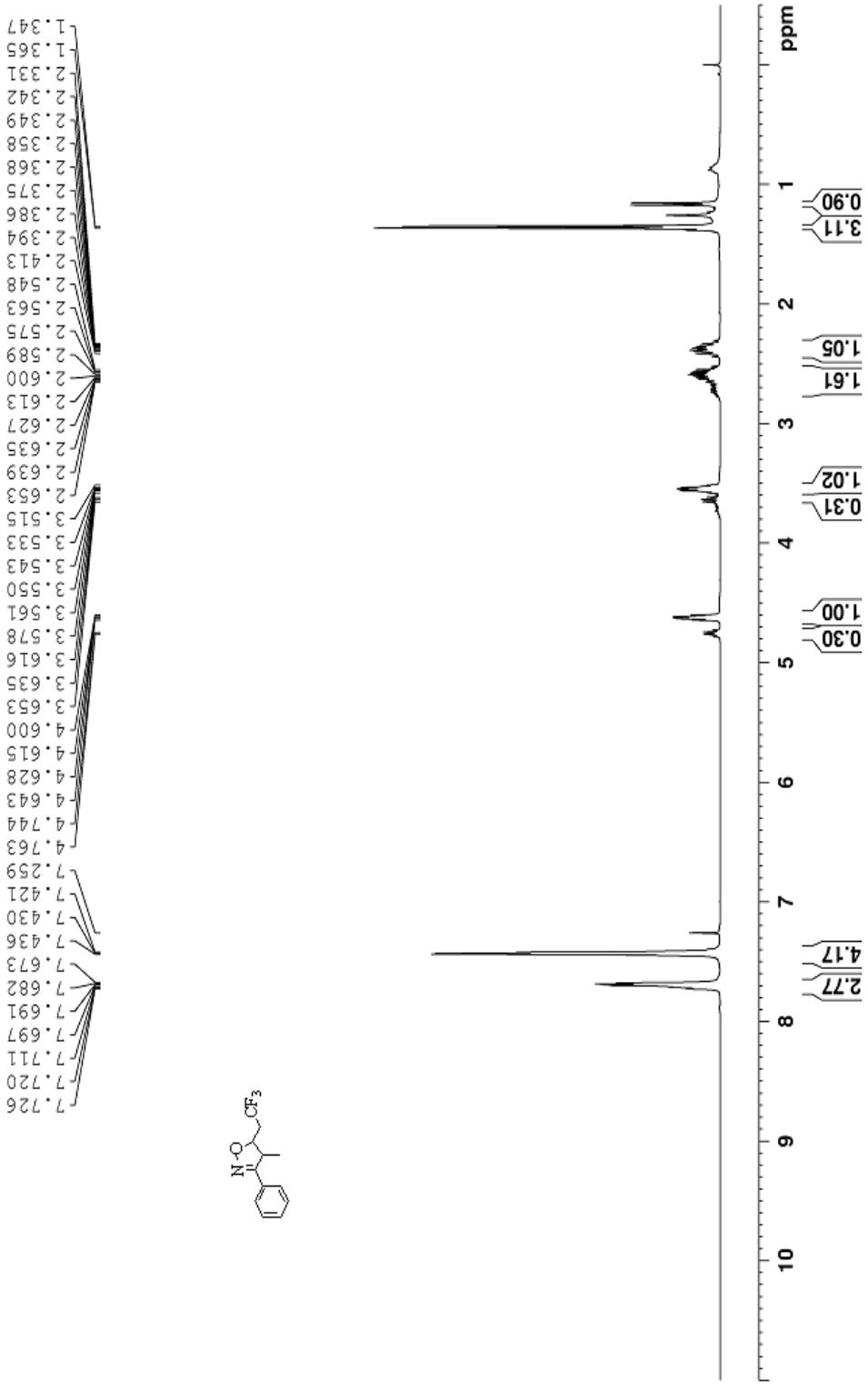
ppm
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
CF3
O
N
O
O
N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2.358
2.368
2.375
2.386
2.394
2.413
2.548
2.563
2.575
2.589
2.600
2.613
2.627
2.635
2.639
2.653
3.515
3.533
3.543
3.550
3.561
3.578
3.616
3.635
3.653
4.600
4.615
4.628
4.643
4.744
4.763
7.259
7.421
7.430
7.436
7.673
7.682
7.691
7.697
7.711
7.720
7.726
CF3
ppm
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3.11
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1.05
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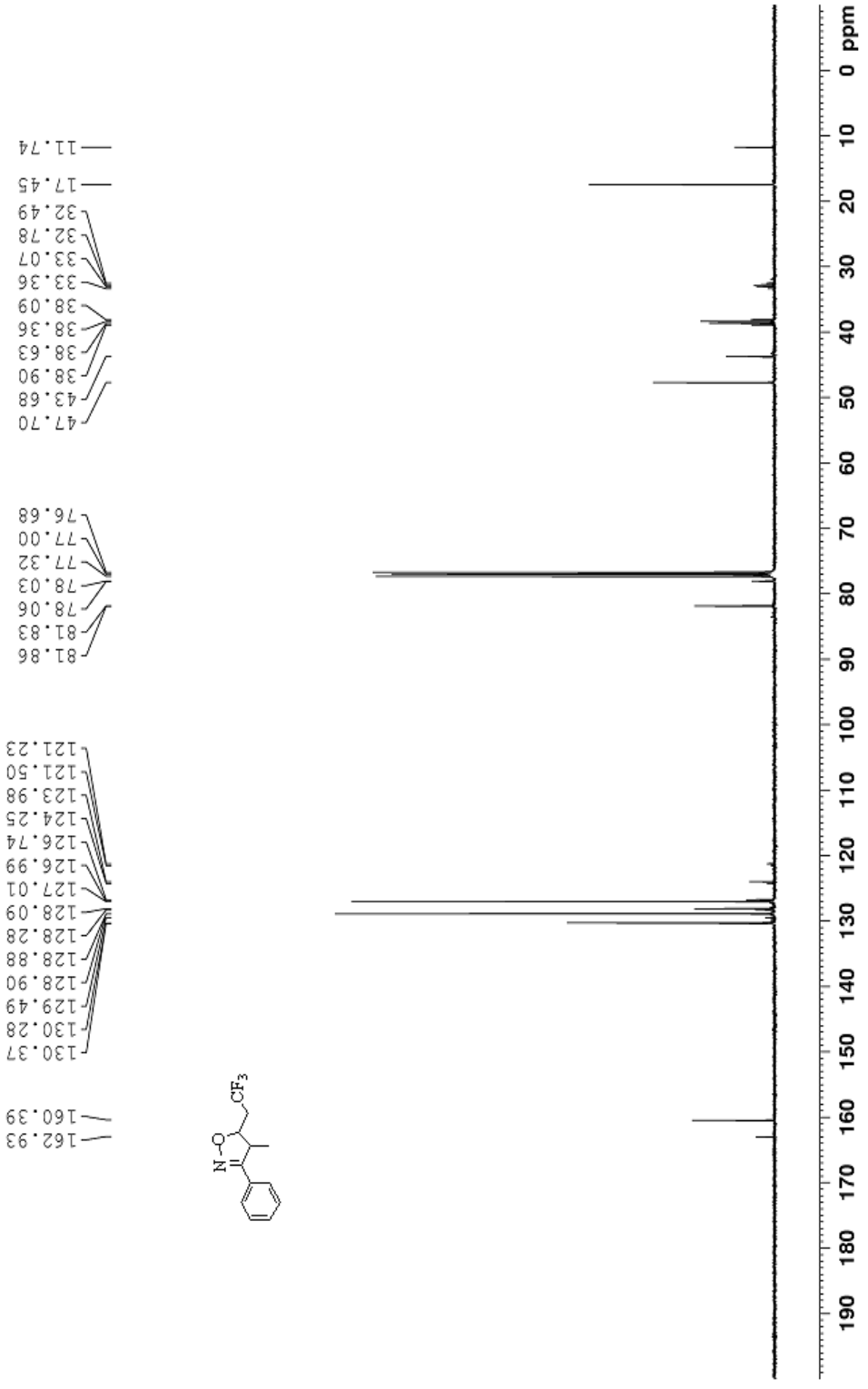
1.02
0.30
1.00
2.77
4.17


11.74
17.45
32.49
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33.07
33.36
38.09
38.36
38.63
38.90
43.68
47.70
76.68
77.00
77.32
78.03
78.06
81.83
81.86
121.23
121.50
123.98
124.25
126.74
126.99
127.01
128.09
128.28
128.88
128.90
129.49
130.28
130.37
160.39
162.93
CF3
N
O
0 ppm
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20
30
40
50
60
70
80
90
100
110
120
130
140
150
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170
180
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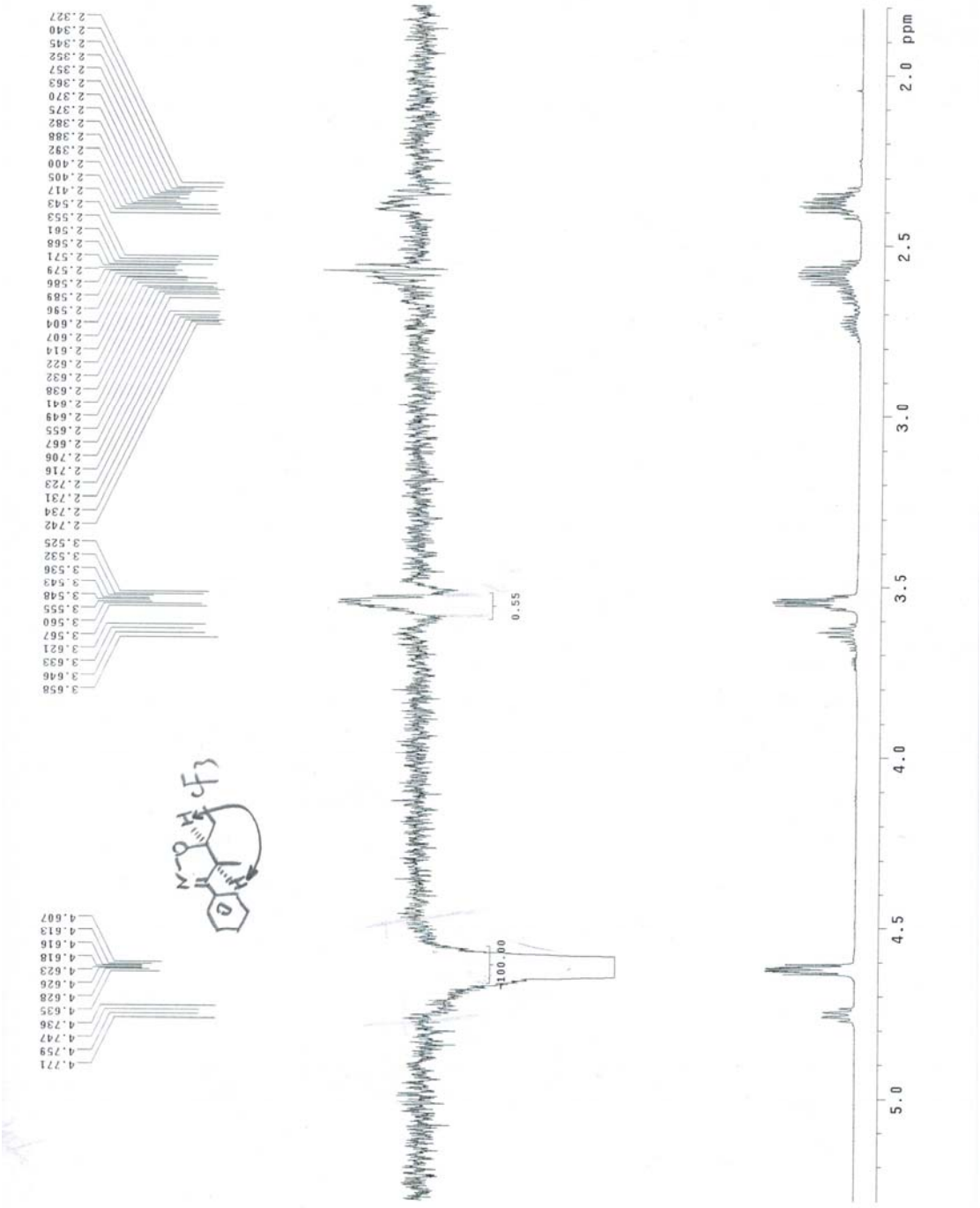
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2.352
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2.363
2.370
2.375
2.382
2.388
2.392
2.400
2.405
2.417
2.543
2.553
2.561
2.568
2.571
2.579
2.586
2.589
2.596
2.604
2.607
2.614
2.622
2.632
2.638
2.641
2.649
2.655
2.667
2.706
2.716
2.723
2.731
2.734
2.742
3.525
3.532
3.536
3.543
3.548
3.555
3.560
3.567
3.621
3.633
3.646
3.658
4.607
4.613
4.616
4.618
4.623
4.626
4.628
4.635
4.736
4.747
4.759
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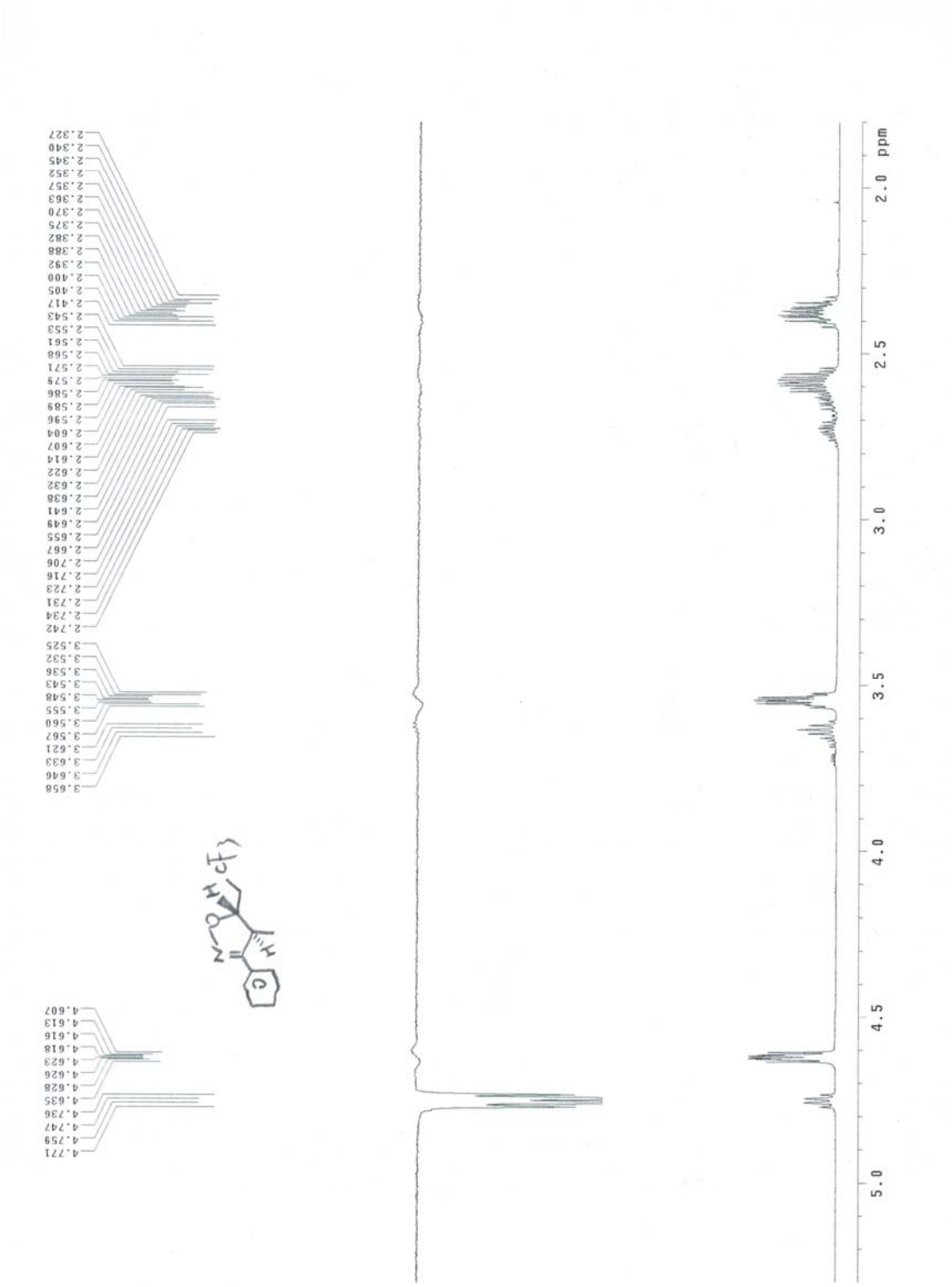
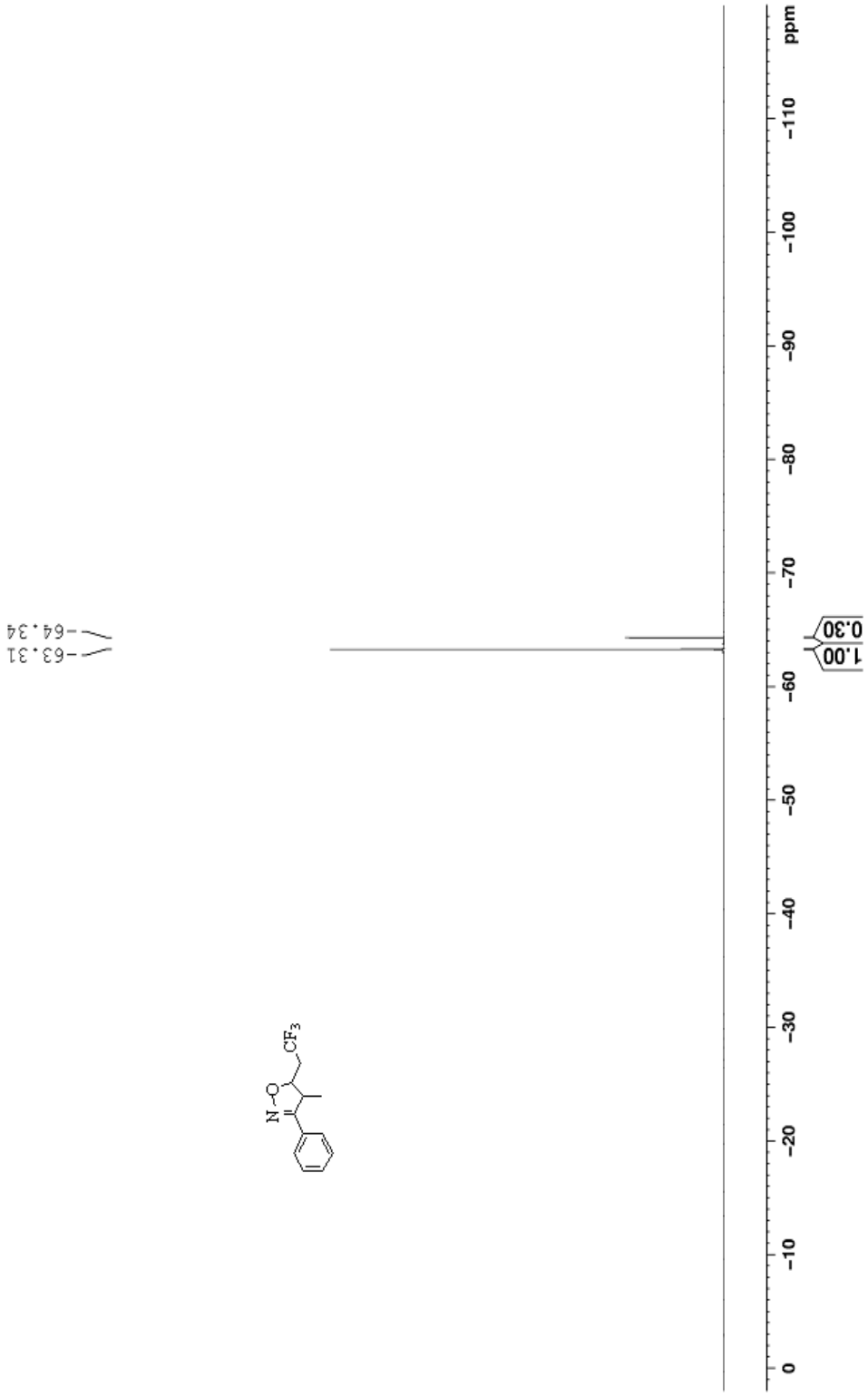
0.55
100.00
5.0
4.5
4.0
3.5
3.0
2.5
2.0 ppm


2.327
2.340
2.345
2.352
2.357
2.363
2.370
2.375
2.382
2.388
2.392
2.400
2.405
2.417
2.543
2.553
2.561
2.568
2.571
2.579
2.586
2.589
2.596
2.604
2.607
2.614
2.622
2.632
2.638
2.641
2.649
2.655
2.667
2.706
2.716
2.723
2.731
2.734
2.742
3.525
3.532
3.536
3.543
3.548
3.555
3.560
3.567
3.621
3.633
3.646
3.658
4.607
4.613
4.616
4.618
4.623
4.626
4.628
4.635
4.736
4.747
4.759
4.771
2.0 ppm
2.5
3.0
3.5
4.0
4.5
5.0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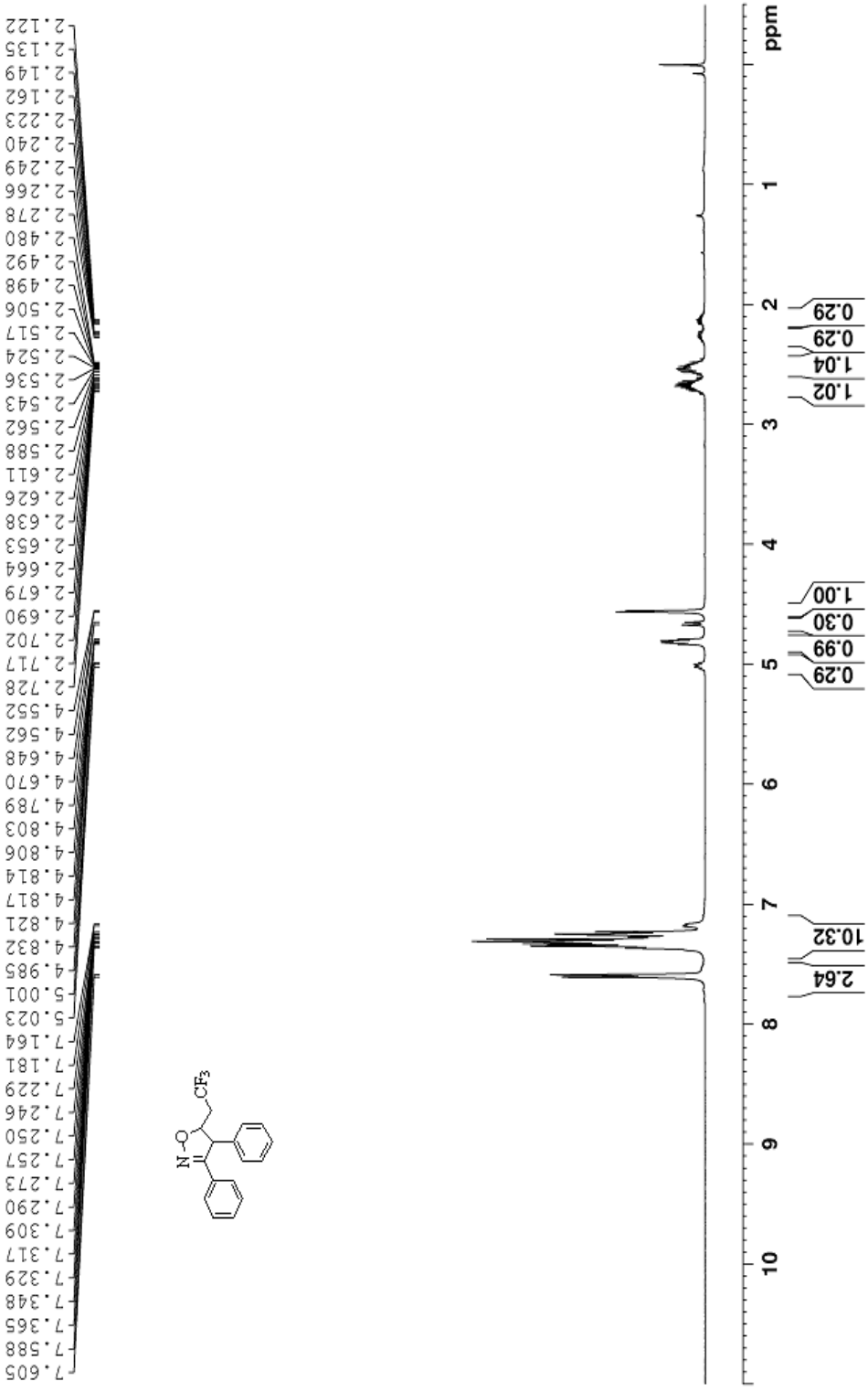
ppm
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
CF3
O
N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7.290
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7.246
7.229
7.181
7.164
5.023
5.001
4.985
4.832
4.821
4.817
4.814
4.806
4.803
4.789
4.670
4.648
4.562
4.552
2.728
2.717
2.702
2.690
2.679
2.664
2.653
2.638
2.626
2.611
2.588
2.562
2.543
2.536
2.524
2.517
2.506
2.498
2.492
2.480
2.278
2.266
2.249
2.240
2.223
2.162
2.149
2.135
2.122
CF3
N
O
ppm
1
2
3
4
5
6
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0.29
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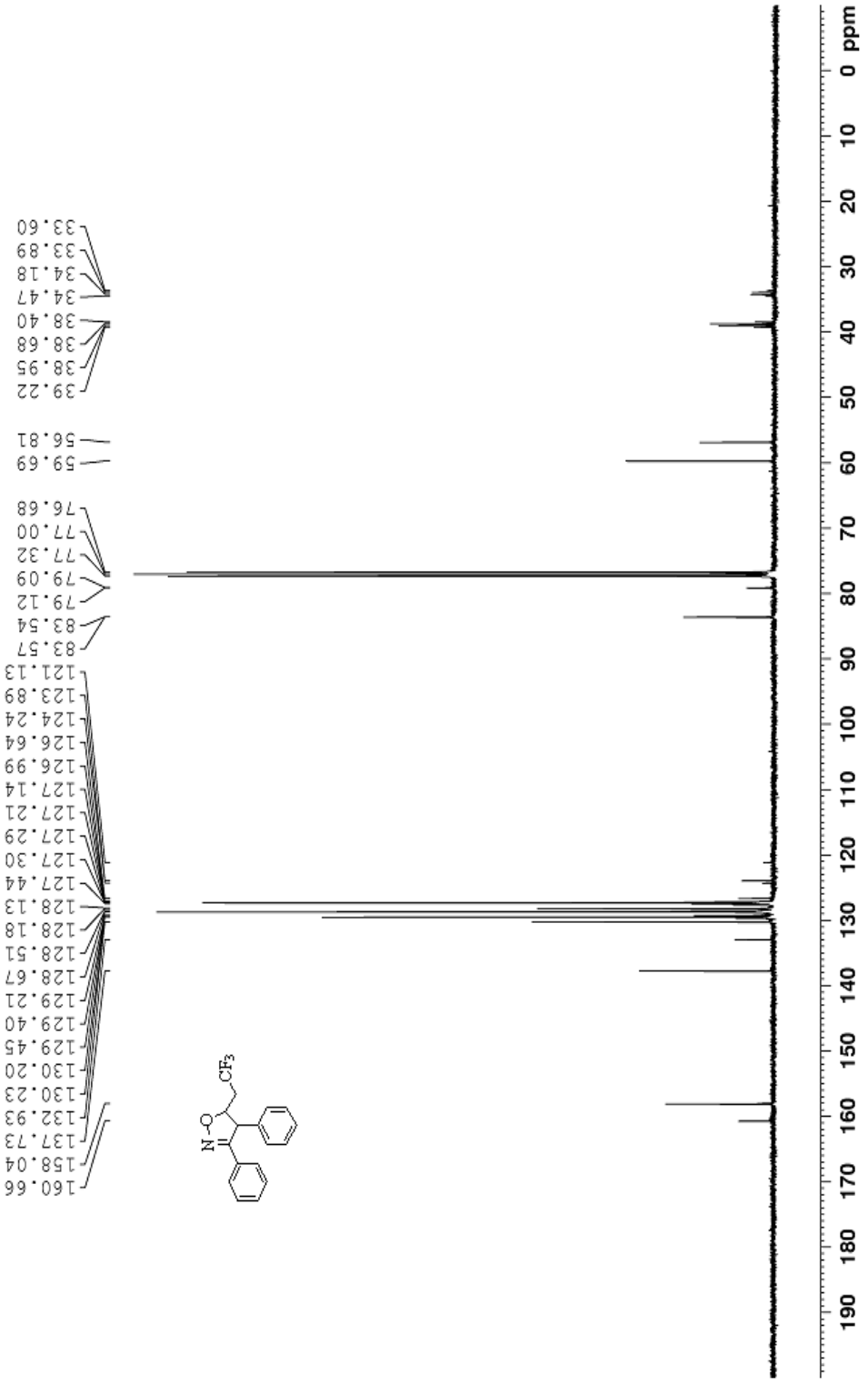

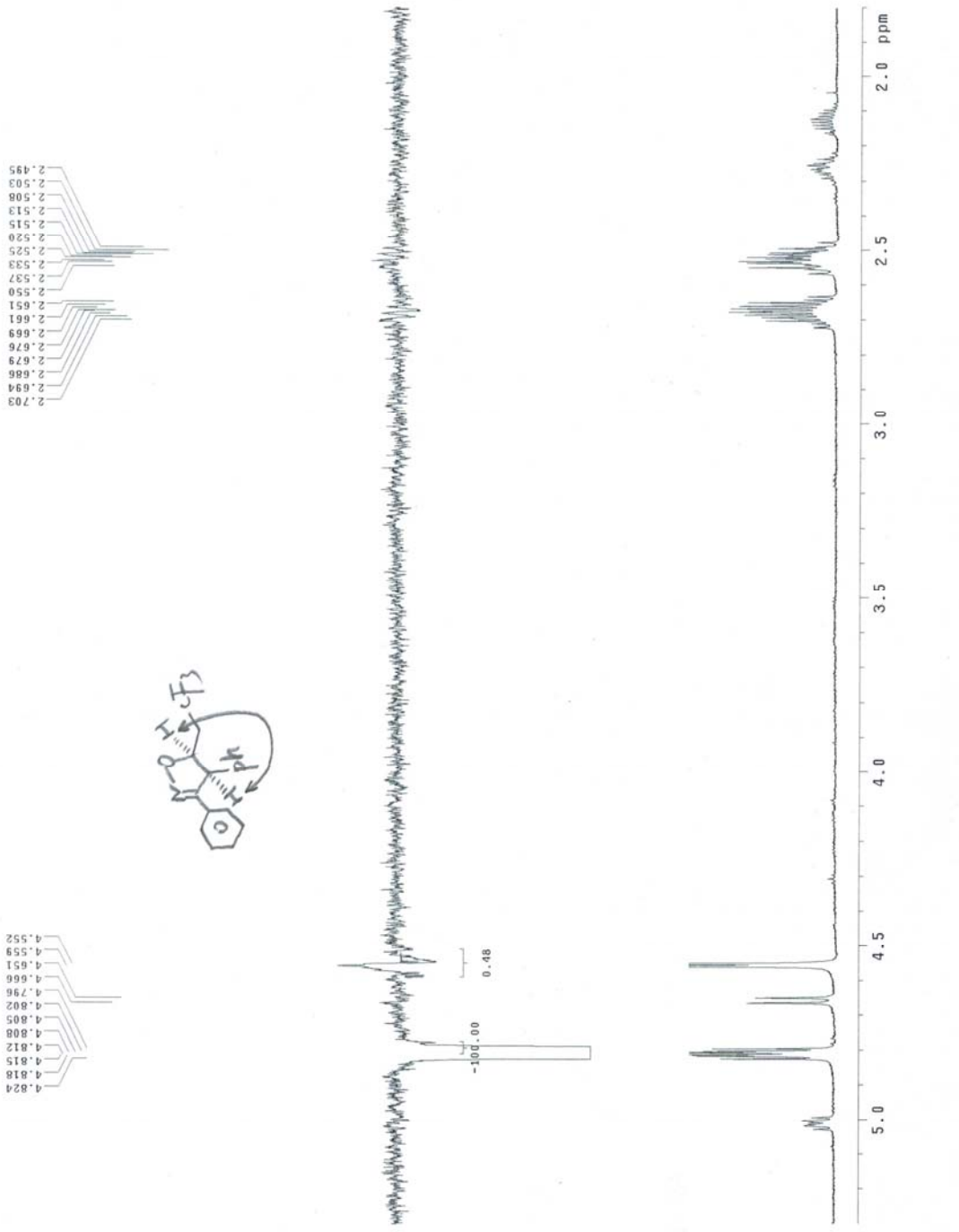
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2.503
2.508
2.513
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2.520
2.525
2.533
2.537
2.550
2.651
2.661
2.669
2.676
2.679
2.686
2.694
2.703
4.552
4.559
4.651
4.666
4.796
4.802
4.805
4.808
4.812
4.815
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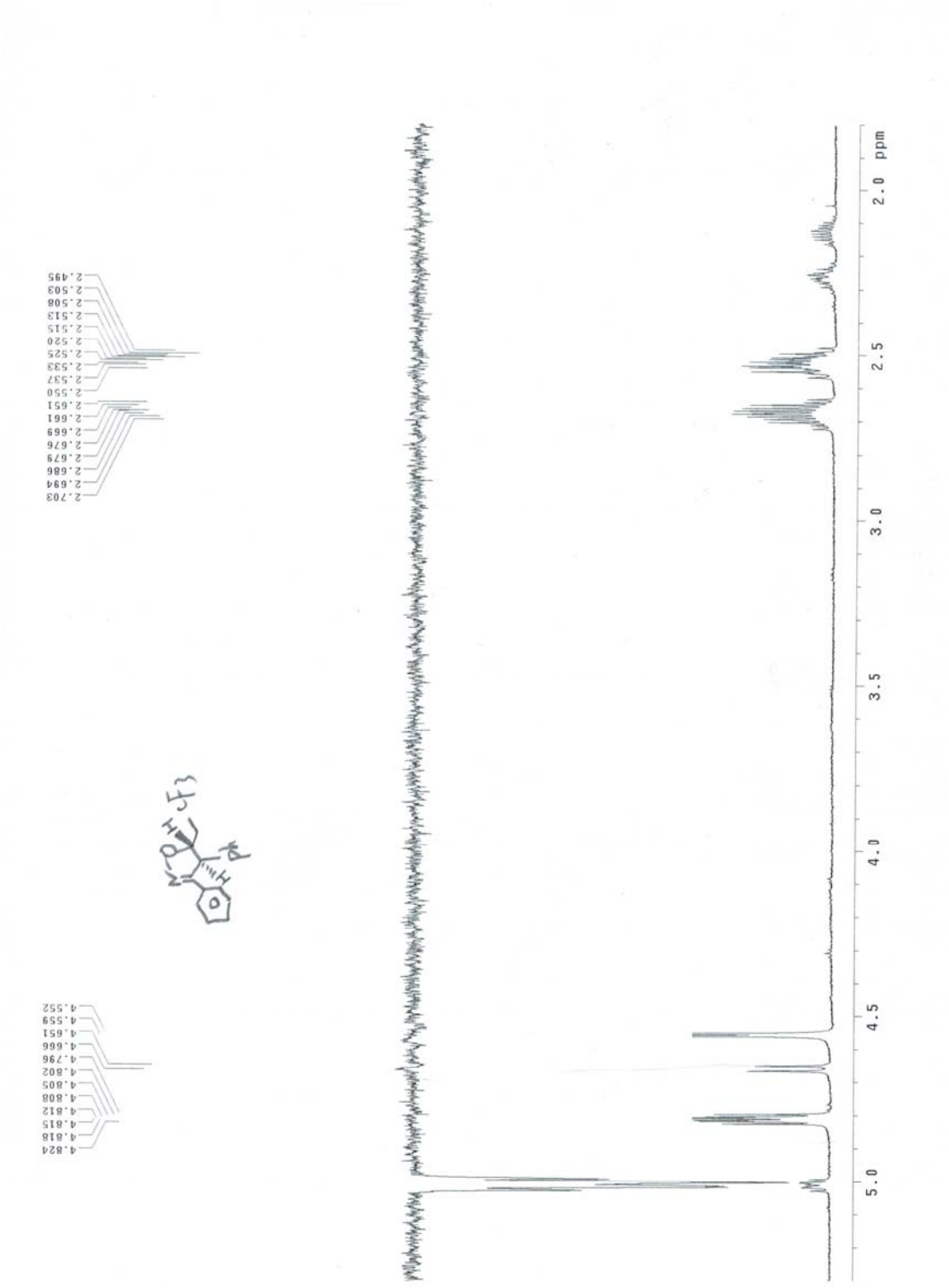
4.824
0.48
100.00
5.0
4.5
4.0
3.5
3.0
2.5
2.0 ppm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2.533
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2.651
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2.669
2.676
2.679
2.686
2.694
2.703
4.552
4.559
4.651
4.666
4.796
4.802
4.805
4.808
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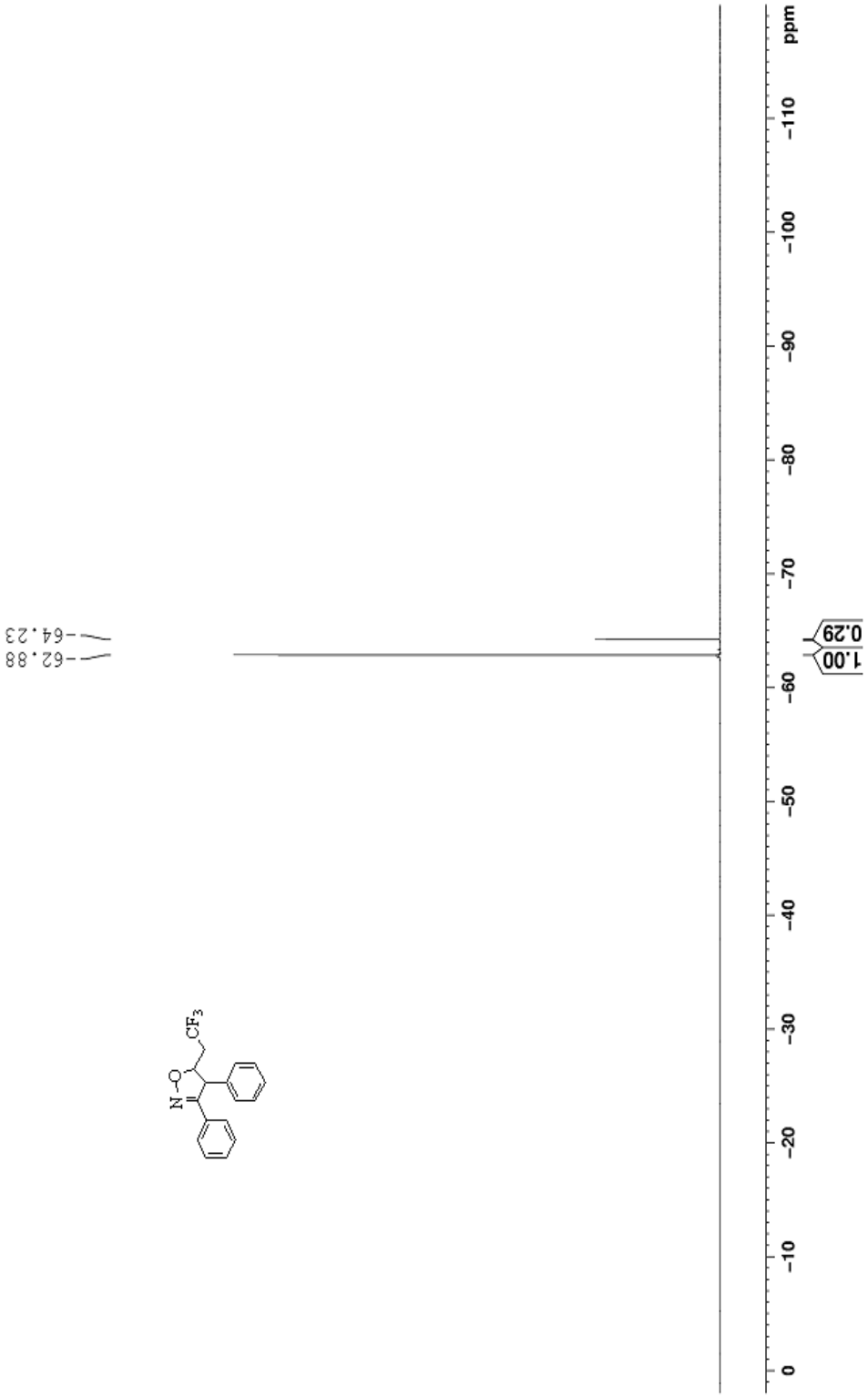
4.818
4.824
5.0
4.5
4.0
3.5
3.0
2.5
2.0 ppm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-90
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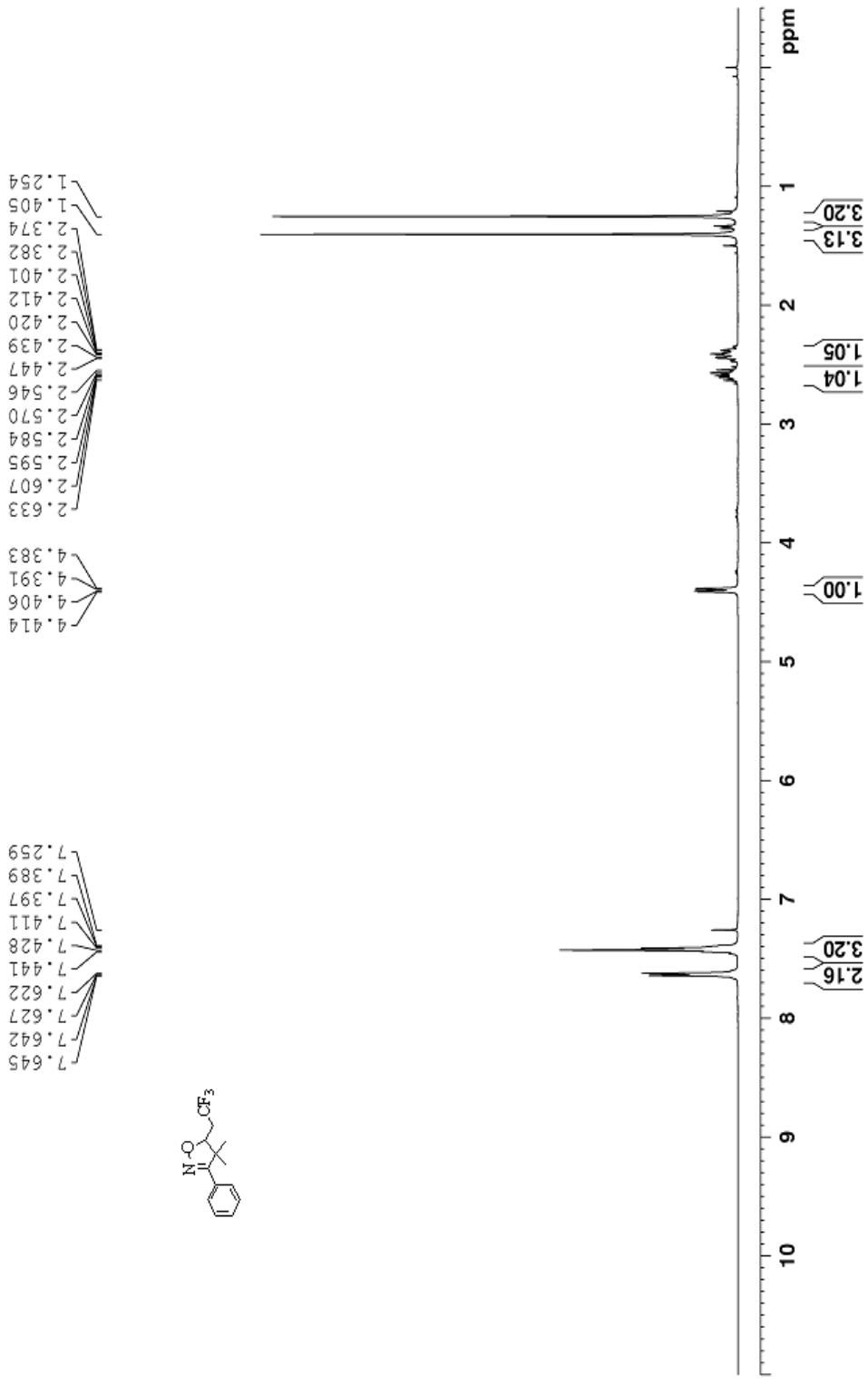
-110
CF3
N
O


ppm
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2
3
4
5
6
7
8
9
10
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3.13
1.05
1.04
1.00
3.20
2.16
1.254
1.405
2.374
2.382
2.401
2.412
2.420
2.439
2.447
2.546
2.570
2.584
2.595
2.607
2.633
4.383
4.391
4.406
4.414
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7.627
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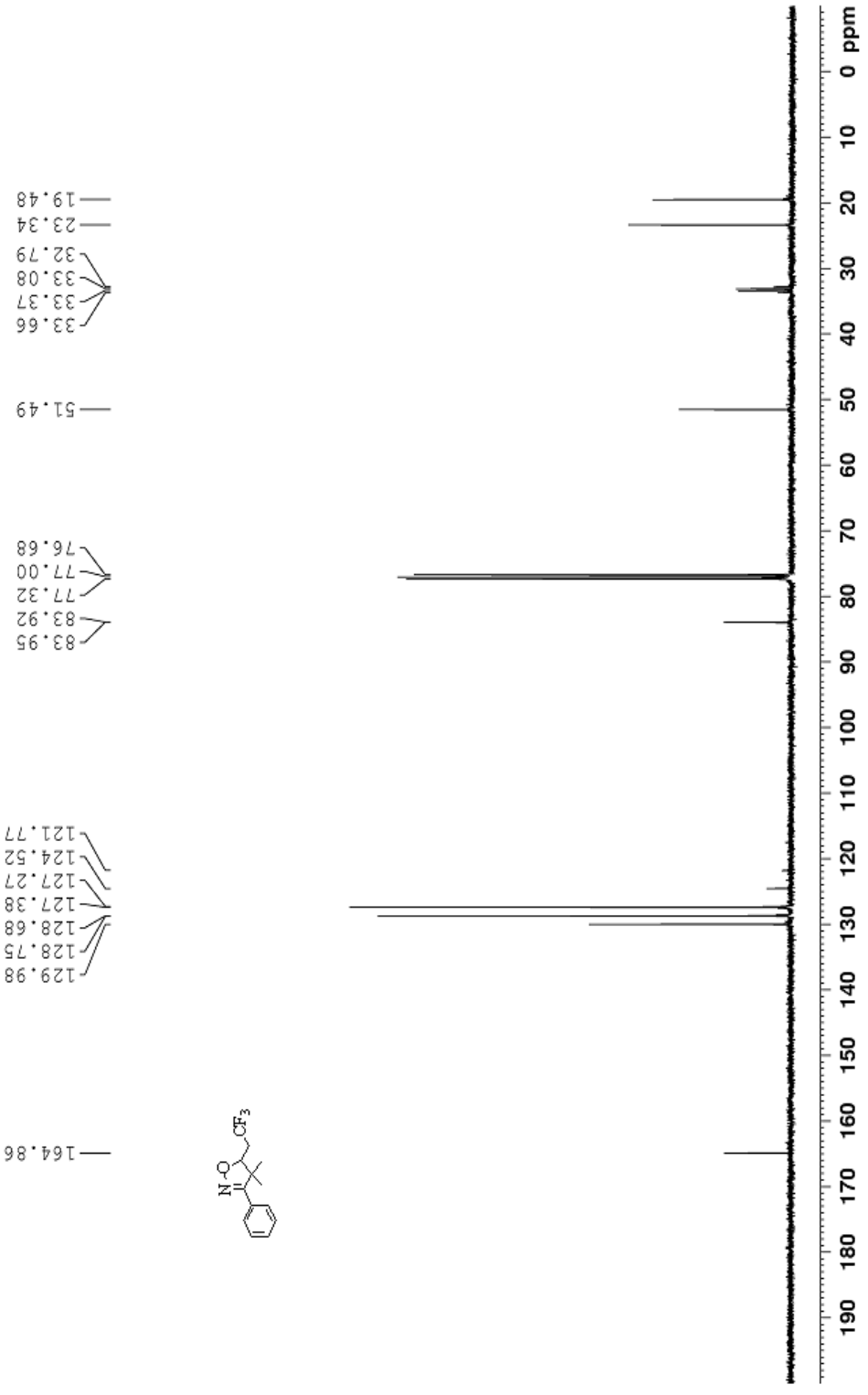
7.645
CF3
N
O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51.49
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77.00
77.32
83.92
83.95
121.77
124.52
127.27
127.38
128.68
128.75
129.98
164.86
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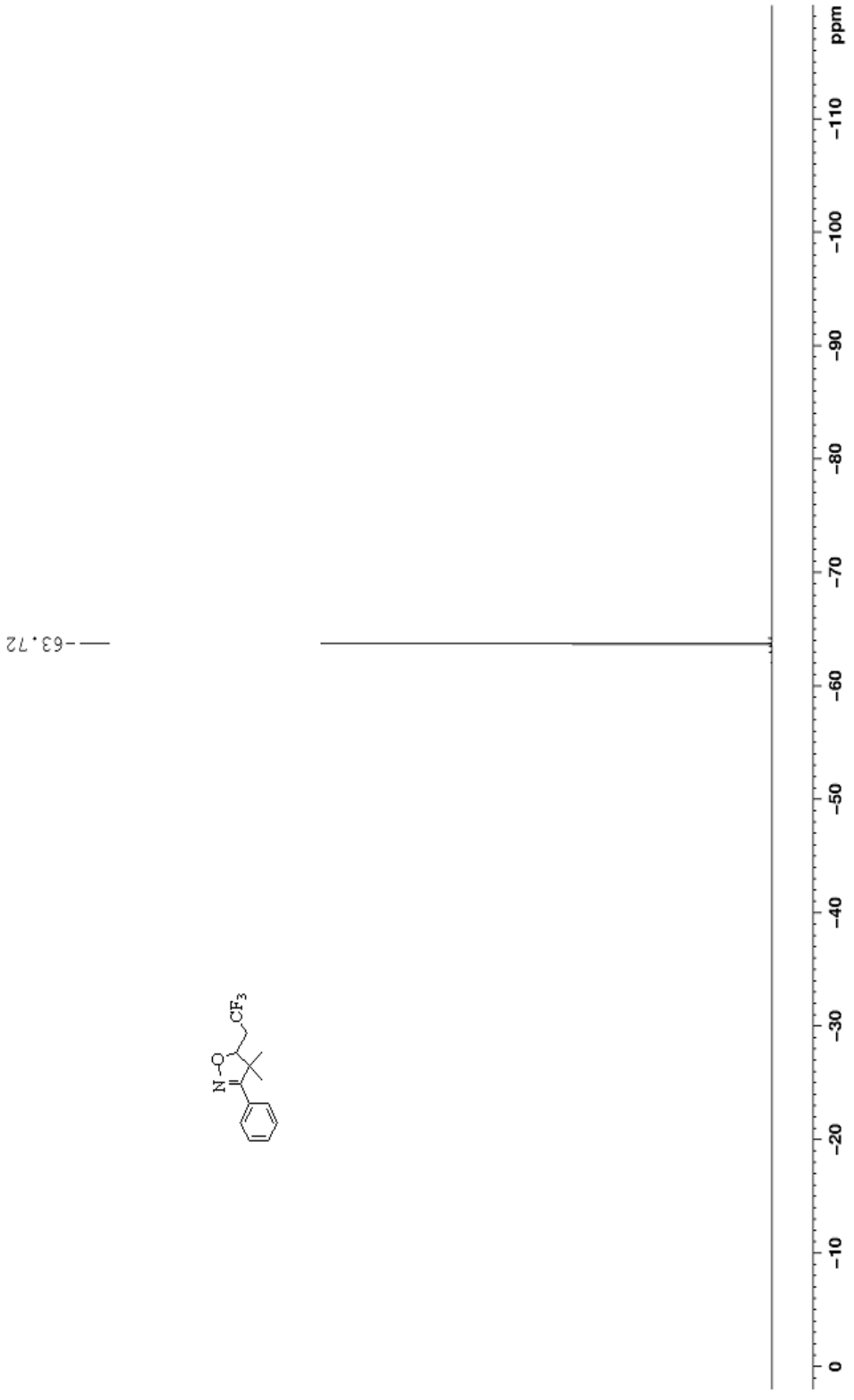
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190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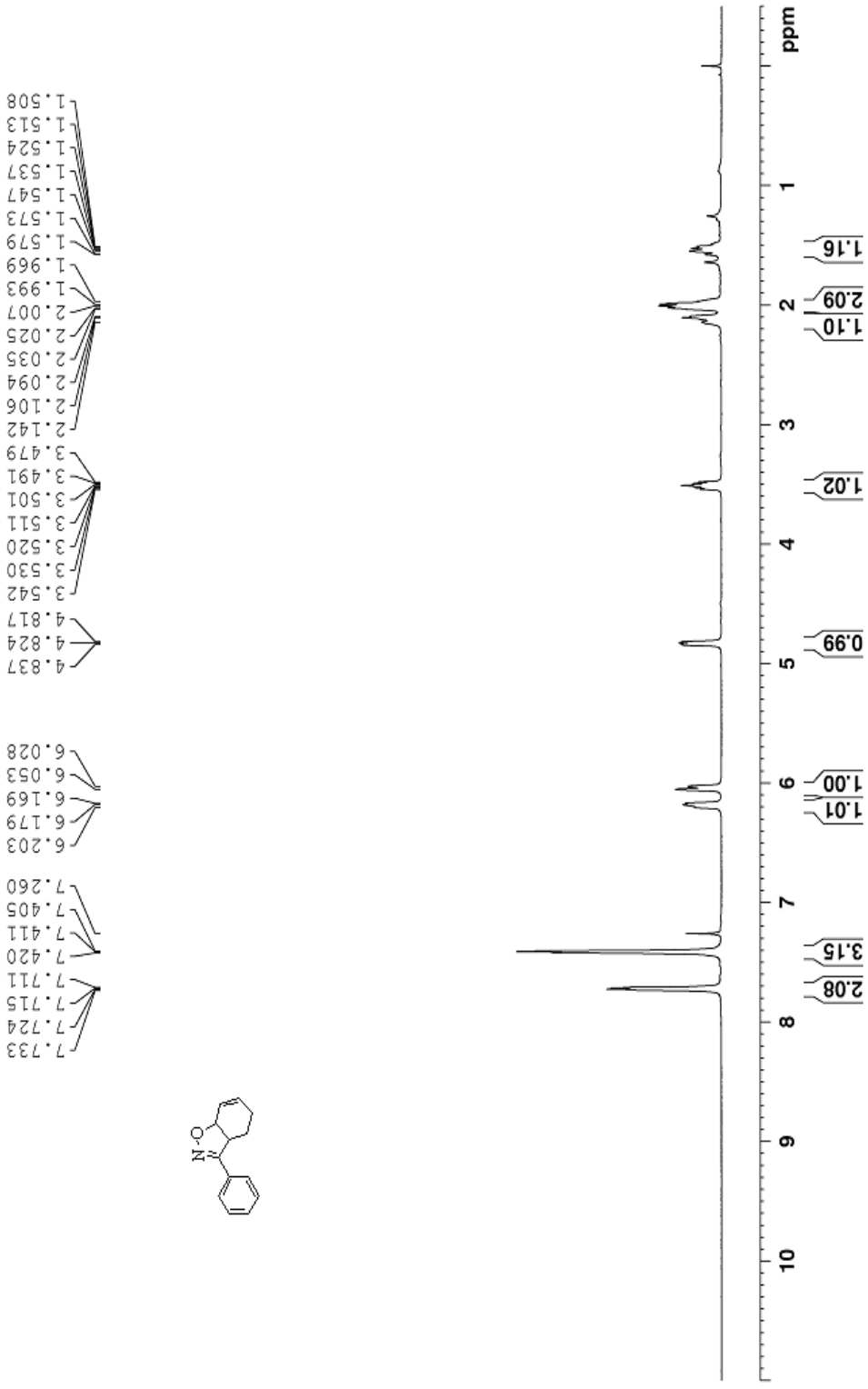
-110
ppm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1.524
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1.573
1.579
1.969
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2.025
2.035
2.094
2.106
2.142
3.479
3.491
3.501
3.511
3.520
3.530
3.542
4.817
4.824
4.837
6.028
6.053
6.169
6.179
6.203
7.260
7.405
7.411
7.420
7.711
7.715
7.724
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ppm
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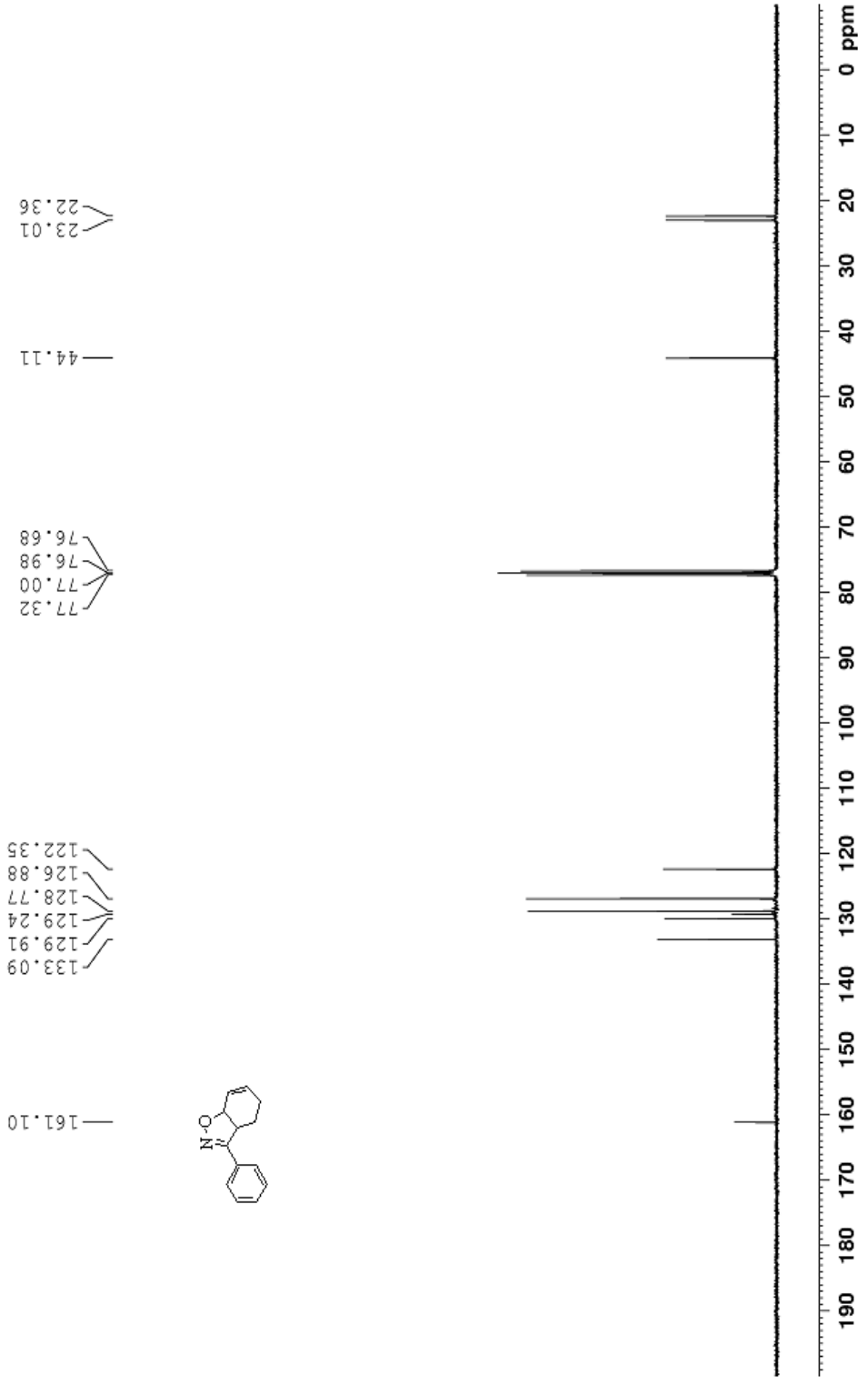
1.10
1.02
0.99
1.00
1.01
3.15
2.08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76.98
77.00
77.32
122.35
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128.77
129.24
129.91
133.09
161.10
0 ppm
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40
50
60
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80
90
100
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120
130
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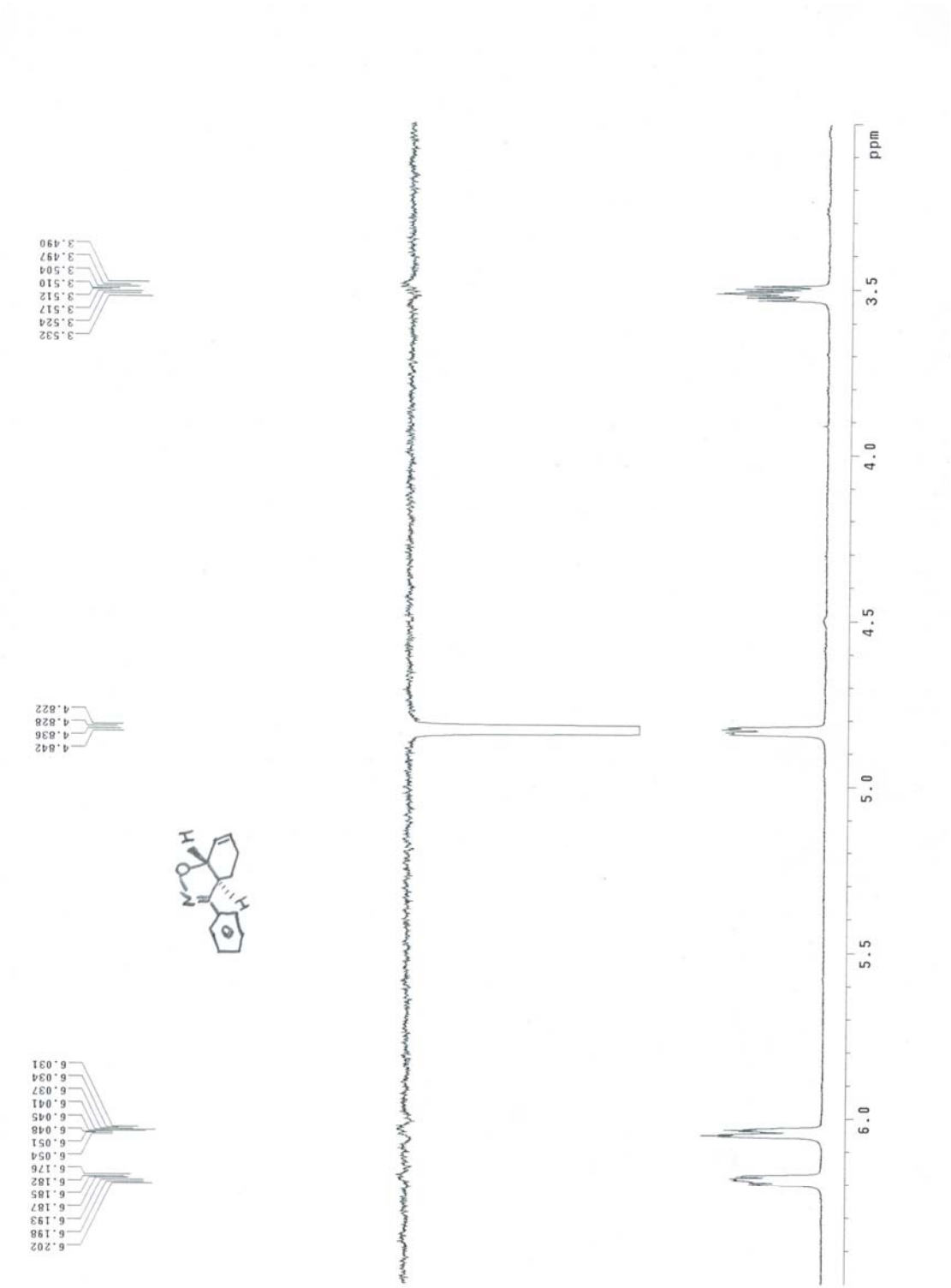
170
180
190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3.497
3.504
3.510
3.512
3.517
3.524
3.532
4.822
4.828
4.836
4.842
6.031
6.034
6.037
6.041
6.045
6.048
6.051
6.054
6.176
6.182
6.185
6.187
6.193
6.198
6.202
ppm
3.5
4.0
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5.0
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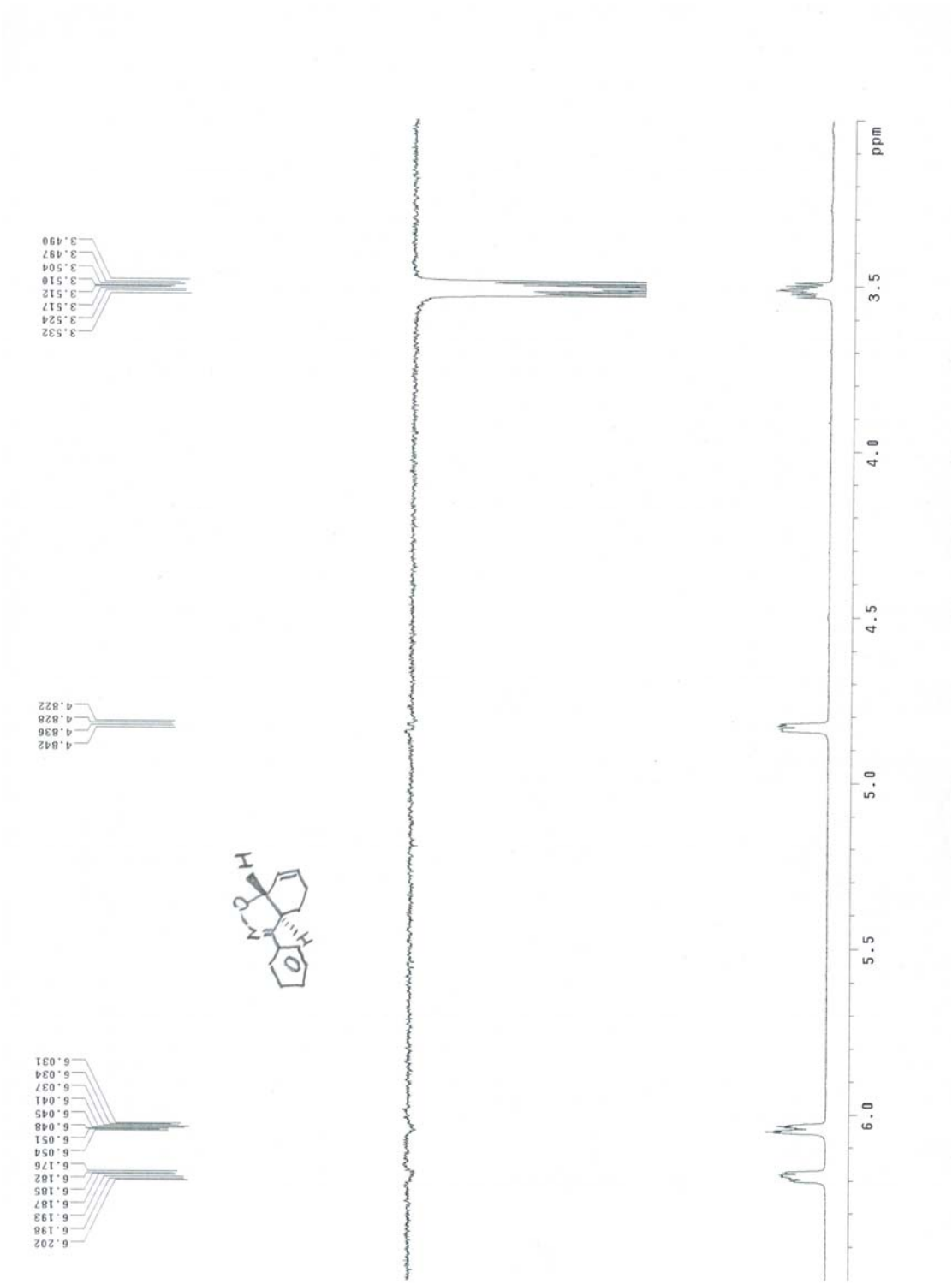
6.0


3.490
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6.031
6.034
6.037
6.041
6.045
6.048
6.051
6.054
6.176
6.182
6.185
6.187
6.193
6.198
6.202
H
O
N
H
O
ppm
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5.5
5.0
4.5
4.0
3.5