Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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SUPPORTING INFORMATION

Synthesis and biological evaluation of the first pentafluorosulfanyl analogs of mefloquine

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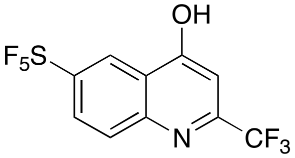
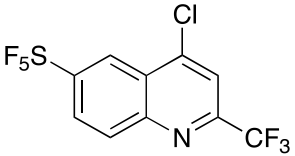
General Information.

Reactions were monitored by TLC analysis (pre-coated silica gel 60 F_{254} plates, 250 μm layer thickness) and visualization was accomplished with a 254 nm UV light and by staining with a PMA solution (5 g of phosphomolybdic acid in 100 mL of 95% EtOH), *p*-anisaldehyde solution (2.5 mL of *p*-anisaldehyde, 2 mL of AcOH, and 3.5 mL of conc. H_2SO_4 in 100 mL of 95% EtOH), Vaughn's reagent (4.8 g of $(NH_4)_6Mo_7O_{24}$•4 H_2O and 0.2 g of $Ce(SO_4)_2$ in 100 mL of a 3.5 N H_2SO_4 solution) or a $KMnO_4$ solution (1.5 g of $KMnO_4$ and 1.5 g of K_2CO_3 in 100 mL of a 0.1% NaOH solution). Flash chromatography on SiO_2 was used to purify the crude reaction mixtures. ^{1}H spectra were obtained at 300 MHz in $CDCl_3$ unless otherwise noted. Chemical shifts were reported in parts per million with the residual solvent peak used as an internal standard. ^{1}H NMR spectra were obtained and are tabulated as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qu=quintet, m = multiplet), number of protons, and coupling constant(s). ^{13}C NMR spectra were recorded at 75 or 150 MHz using a proton-decoupled pulse sequence and are tabulated by observed peak. ^{19}F NMR spectra were recorded at 282 MHz using a proton-decoupled pulse sequence in the presence of fluorobenzene as an internal standard.



6a

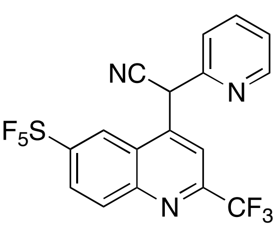
4-Hydroxy-6-pentafluorosulfanyl-2-(trifluoromethyl)quinoline (6a). A solution of 4-aminophenylsulfur pentafluoride (110 mg, 0.502 mmol) in polyphosphoric acid (7.0 mL) at 110 °C was treated with ethyl 4,4,4-trifluoroacetoacetate (1.5 mL, 10.0 mmol) and heated up to reflux at 150 °C for 3 h. The reaction mixture was quenched with 5% NaOH solution (30 mL), extracted with EtOAc (2x), washed with brine, dried ($MgSO_4$) and concentrated. The brown residue was purified by chromatography on SiO_2 (25% EtOAc/Hexanes) to yield **6a** (76.4 mg, 44%) as a beige solid: Mp 252.0 °C (dec.); IR 3200-3000 (br), 2337, 1580, 1208, 1142, 822, 777 cm $^{-1}$; ^{1}H NMR (acetone-d_6) δ 8.68 (d, 1 H, *J* = 2.4 Hz), 8.23 (dd, 1 H, *J* =2.7, 9.3 Hz), 8.09 (d, 1 H, *J* = 9.3 Hz), 7.03 (s, 1 H); ^{13}C NMR (acetone-d_6) δ 170.7, 151.4 (qu, *J* = 18.0 Hz), 146.7, 135.1, 129.5 (appt, *J* = 4.5 Hz), 127.0, 123.5 (appt, *J* = 5.3 Hz), 122.0 (q, *J* = 272.3 Hz), 117.3, 105.5; ^{19}F NMR δ 85.2 (qu, *J* = 145.5 Hz), 64.6 (d, *J* = 145.5 Hz), -67.0; HRMS (TOF-ESI) *m/z* calcd for $C_{10}H_6F_8NOS$ 340.0042, found 340.0032.



7a

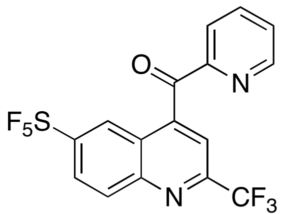
4-Chloro-6-pentafluorosulfanyl-2-(trifluoromethyl)quinoline (7a). After addition of preheated (60 °C) phosphorus oxychloride (108 mg, 0.701 mmol) to **6a** (23.8 mg, 0.0702 mmol), the reaction mixture was warmed to 110 °C and stirred at this temperature for 1.5 h. The conversion was monitored by TLC (10% EtOAc/Hexanes) and the solution was cooled down to room temperature upon the disappearance of the starting material, quenched with ice water (3.0 mL), extracted with Et_2O, washed with sat. $NaHCO_3$ solution and brine, dried ($MgSO_4$) and concentrated. The yellow residue was purified by chromatography on SiO_2 (5% EtOAc/Hexanes) to provide **7a** (19.3 mg, 77%) as a beige solid: Mp 107.9-109.0 °C; IR 2922, 1343, 1202, 1135, 1100, 833, 818, 768 cm^{-1}; ^{1}H

NMR δ 8.75 (d, 1 H, *J* = 2.4 Hz), 8.37 (d, 1 H, *J* = 9.3 Hz), 8.22 (dd, 1 H, *J* = 2.4, 9.3 Hz), 7.96 (s, 1 H); ^{13}C NMR δ 154.1 (qu, *J* = 18.0 Hz), 150.6 (q, *J* = 36.0 Hz), 148.3, 146.5, 132.0, 128.5 (appt, *J* = 4.5 Hz), 126.5, 123.4 (qu, *J* = 5.3 Hz), 120.8 (q, *J* = 273.8 Hz), 118.9 (appd, *J* = 2.3 Hz); ^{19}F NMR δ 82.0 (qu, *J* = 149.3 Hz), 63.3 (d, *J* = 149.7 Hz), -67.9; EI-MS *m/z* 357 (M, 100), 249 (55), 180 (70), 84 (75); HRMS (EI) *m/z* calcd for $C_{10}H_4NF_8SCl$ 356.9625, found 356.9622.



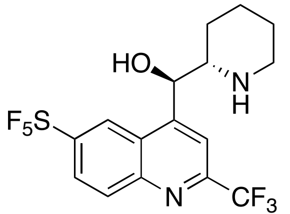
8a

α-(2-Pyridyl)-6-pentafluorosulfanyl-(2-trifluoromethyl)-4-quinolylacetonitrile (8a). A cooled (0 - 5 °C) suspension of sodium hydride (11.9 mg, 0.494 mmol) in toluene (1.2 mL) and DMF (0.60 mL) was treated under Ar with a solution of 2-pyridylacetonitrile (27 μL, 0.247 mmol) in toluene (0.60 mL) and DMF (0.15 mL) over 5 min. The resulting yellow-brown colored suspension was stirred for 1 h at the same temperature. A solution of **7a** (58.9 mg, 0.165 mmol) in toluene (1.2 mL) and DMF (0.50 mL) was added drop by drop to the suspension over 5 min. After 0.5 h, the reaction mixture was quenched with ice water (10 mL), extracted with EtOAc, washed with water (3x) and brine, dried ($MgSO_4$) and concentrated. The orange residue was purified by chromatography on SiO_2 (25% EtOAc/Hexanes) to provide **8a** (62.0 mg, 86%) as a light orange solid: Mp 113.5-115.5 °C; IR 2251, 1187, 1141, 1109, 820 cm^{-1}; ^{1}H NMR δ 8.87 (d, 1 H, *J* = 2.1 Hz), 8.60 (appd, 1 H, *J* = 4.8 Hz), 8.37 (d, 1 H, *J* = 9.3 Hz), 8.18 (s, 1 H), 8.16 (dd, 1 H, *J* = 2.1, 9.3 Hz), 7.78 (ddd, 1 H, *J* = 1.5, 7.5, 7.8 Hz), 7.53 (d, 1 H, *J* = 7.8 Hz), 7.32 (appdd, 1 H, *J* = 4.8, 7.5 Hz), 6.09 (s, 1 H); ^{13}C NMR δ 153.6 (qu, *J* = 18.8 Hz), 152.8, 150.8 (q, *J* = 35.3 Hz), 150.5, 148.1, 144.6, 138.4, 132.3, 127.9 (appt, *J* = 3.8 Hz), 125.4, 124.3, 123.4 (appt, *J* = 5.3 Hz), 122.6, 121.0 (q, *J* = 273.8 Hz), 117.7 (d, *J* = 2.3 Hz), 117.2, 43.3; ^{19}F NMR δ 82.2 (qu, *J* = 149.2 Hz), 63.2 (d, *J* = 148.3 Hz), -67.8; EI-MS *m/z* 439 (M, 100), 311 (40), 78 (22); HRMS (EI) *m/z* calcd for $C_{17}H_9N_3F_8S$ 439.0389, found 439.0385.



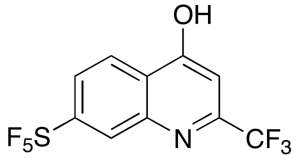
9a

2-Pyridyl-6-pentafluorosulfanyl-(2-trifluoromethyl)-4-quinolylketone (9a). A suspension of **8a** (60.0 mg, 0.137 mmol) in acetic acid (0.24 mL) was treated dropwise with H_2O_2 (53 μL, 0.683 mmol) at room temperature. The reaction mixture was placed in a preheated (75 °C) oil bath until the color turned to light yellow. The mixture was quenched with ice water (3.0 mL), extracted with Et_2O, washed with sat. $NaHCO_3$ solution and brine, dried ($MgSO_4$) and concentrated. The yellow residue was purified by chromatography on SiO_2 (16% EtOAc/Hexanes) to provide **9a** (49.6 mg, 85%) as a white solid: Mp 122.0-124.0 °C; IR 1683, 1182, 1133, 1105, 835, 820, 768, 764 cm^{-1}; ^{1}H NMR δ 8.65 (ddd, 1 H, *J* = 0.9, 1.5, 4.8 Hz), 8.46-8.41 (m, 2 H), 8.39 (s, 1 H), 8.18 (dd, 1 H, *J* = 2.4, 9.6 Hz), 8.06 (ddd, 1 H, *J* = 1.8, 7.8, 7.8 Hz), 8.01 (s, 1 H), 7.62 (ddd, 1 H, *J* = 0.9, 4.5, 7.5 Hz); ^{13}C NMR δ 193.5, 153.8 (qu, *J* = 18.0 Hz), 152.8, 149.9 (q, *J* = 36.0 Hz), 149.7, 148.0, 147.1, 137.9, 131.7, 128.5, 127.7 (appt, *J* = 4.5 Hz), 125.3, 124.8 (appt, *J* = 5.3 Hz), 124.7, 121.2 (q, *J* = 273.8 Hz), 118.9 (d, *J* = 1.5 Hz); ^{19}F NMR δ 82.4 (qu, *J* = 151.9 Hz), 62.6 (d, *J* = 151.1 Hz), -67.8; EI-MS *m/z* 428 (M, 30), 399 (40), 273 (100), 78 (80); HRMS (EI) *m/z* calcd for $C_{16}H_8N_2OF_8S$ 428.0230, found 428.0210.



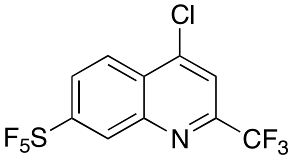
2

α-(2-Piperidyl)-6-pentafluorosulfanyl-(2-trifluoromethyl)-4-quinolinemethanol (2). A solution of **9a** (20.0 mg, 0.0467 mmol) in conc. hydrochloric acid (58.0 μL, 0.233 mmol) and abs EtOH (0.56 mL) was treated with platinum oxide (4.2 mg, 0.0187 mmol). The reaction mixture was purged with hydrogen twice and hydrogenated under balloon pressure. After 2 h, there was no alcohol intermediate left by TLC analysis (10% MeOH/DCM). The mixture was filtered through florisil, concentrated, and extracted with Et_2O. The combined organic layers were washed with sat $NaHCO_3$ solution and brine, dried ($MgSO_4$) and concentrated. The black residue was purified by chromatography on SiO_2 (5% NEt_3 in EtOAc then 5% NEt_3 and 5% MeOH in EtOAc). The crude product was recrystallized from MeOH to get pure **9a** (8.5 mg, 42%) as a white solid and a dr 20:1: Mp 198 °C (dec.); IR 3000-2900 (br), 1368, 1258, 1139, 1105, 835, 822, 798 cm^{-1}; ^1H NMR (acetone-d_6, 600 MHz) δ 9.01 (d, 1 H, *J* = 2.4 Hz), 8.38 (d, 1 H, *J* = 9.0 Hz), 8.31 (dd, 1 H, *J* = 2.4, 9.0 Hz), 8.16 (s, 1 H), 5.54 (d, 1 H, *J* = 4.8 Hz), 3.04 (ddd, 1 H, *J* = 2.4, 5.4, 7.8 Hz), 2.97 (bd, 1 H, *J* = 8.4 Hz), 2.54 (dt, 1 H, *J* = 2.4, 12.0 Hz), 1.76-1.71 (m, 1 H), 1.58-1.53 (m, 1 H), 1.51-1.46 (m, 1 H), 1.35-1.20 (m, 4 H); ^{13}C NMR (acetone-d_6, 600 MHz) δ 155.5, 153.0 (qu, *J* = 18.0 Hz), 150.6 (q, *J* = 34.5 Hz), 148.7, 132.7, 127.6 (appt, *J* = 4.5 Hz), 127.2, 124.9 (appt, *J* = 4.5 Hz), 122.6 (q, *J* = 273.0 Hz), 117.5 (d, *J* = 1.5 Hz), 74.2, 62.6, 47.7, 28.0, 27.0, 25.2; ^{19}F NMR δ 84.7 (qu, *J* = 152.2 Hz), 64.5 (d, *J* = 149.5 Hz), -66.8; HRMS (ESI) *m/z* calcd for $C_{16}H_{17}N_2OF_8S$ 437.0928, found 437.0893.



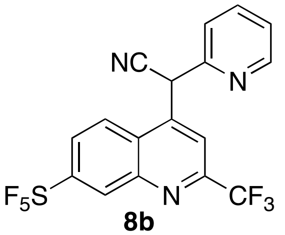
6b

4-Hydroxy-7-pentafluorosulfanyl-2-(triflurometh yl)quinoline (6b). A solution of 3-aminophenylsulfur pentafluoride (110 mg, 0.502 mmol) in polyphosphoric acid (2.0 mL) at 110 °C was treated with ethyl 4,4,4-trifluoroacetoacetate (1.5 mL, 10.0 mmol) and the mixture was heated up to 150 °C to reflux for 4 h. The reaction mixture was quenched with 5% NaOH solution (30 mL), extracted with EtOAc (2x), washed with brine, dried ($MgSO_4$) and concentrated. The crude brown residue was purified by chromatography on SiO_2 (25% EtOAc/Hexanes) to yield **6b** (128 mg, 75%) as a beige solid: Mp 261.2-262.2 °C; IR 3200-3000 (br), 1580, 1277, 1198, 1157, 839, 820 cm^{-1}; ^1H NMR (acetone-d_6) δ 8.48 (d, 1 H, *J* = 2.4 Hz), 8.47 (d, 1 H, *J* = 9.0 Hz), 8.05 (dd, 1 H, *J* = 2.4, 9.0 Hz), 7.27 (s, 1 H); ^{13}C NMR (acetone-d_6) δ 165.8, 156.0 (qu, *J* = 18.0 Hz), 149.9 (q, *J* = 35.3 Hz), 147.5, 127.2, 125.5, 124.6, 124.0 (appt, *J* = 4.5 Hz), 122.5 (q, *J* = 272.3 Hz), 104.1; ^{19}F NMR δ 84.3 (qu, *J* = 151.4 Hz), 64.0 (d, *J* = 151.4 Hz), -67.0; EI-MS *m/z* 339 (M, 40), 231 (15), 137 (30), 95 (30), 81 (100); HRMS (EI) *m/z* calcd for $C_{10}H_5NOF_8S$ 338.9964, found 338.9953.



7b

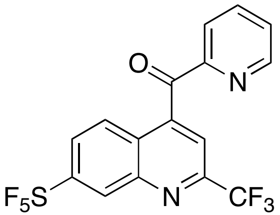
4-Chloro-7-pentafluorosulfanyl-2-(trifluromethyl)quinoline (7b). After addition of preheated (60 °C) phosphorus oxychloride (306 mg, 1.99 mmol) to **6b** (135 mg, 0.399 mmol), the reaction mixture was warmed to 110 °C and stirred at this temperature for 0.5 h. The conversion was monitored by TLC (10% EtOAc/Hexanes) and the solution was cooled down to room temperature after the disappearance of the starting material, quenched with ice water (3.0 mL), and extracted with Et_2O. The combined organic layers were washed with sat. $NaHCO_3$ solution and brine, dried ($MgSO_4$) and concentrated. The yellow residue was purified by chromatography on SiO_2 (5% EtOAc/Hexanes) to provide **7b** (112 mg, 78%) as a beige solid: Mp 94.8-96.8 °C; IR 1558, 1433, 1336, 1206, 1150, 1105, 1079, 835, 816 cm^{-1}; ^{1}H NMR δ 8.74 (d, 1 H, *J* = 2.1 Hz), 8.42 (d, 1 H, *J* = 9.3 Hz), 8.12 (dd, 1 H, *J* = 2.1, 9.3 Hz), 7.97 (s, 1 H); ^{13}C NMR δ 155.7 (qu, *J* = 18.8 Hz), 149.9 (q, *J* = 36.0 Hz), 147.1, 145.1, 129.5 (appt, *J* = 5.3 Hz), 128.4, 126.4 (qu, *J* = 4.5 Hz), 125.5, 120.8 (q, *J* = 274.5 Hz), 119.6 (appd, *J* = 2.3 Hz); ^{19}F NMR δ 81.8 (qu, *J* = 149.5 Hz), 63.1 (d, *J* = 149.5 Hz), -67.8; EI-MS *m/z* 357 (M, 50), 249 (25), 180 (25), 117 (30), 84 (100); HRMS (EI) *m/z* calcd for $C_{10}H_4NF_8SCl$ 356.9625, found 356.9630.



8b

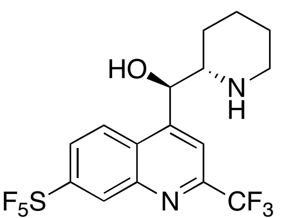
α-(2-Pyridyl)-7-pentafluorosulfanyl-(2-trifluoromethyl)-4-quinolylacetonitrile (8b).

A cooled (0 – 5 °C) suspension of sodium hydride (19.9 mg, 0.830 mmol) in toluene (2.0 mL) and DMF (1.0 mL) was treated under Ar with a solution of 2-pyridylacetonitrile (46 μL, 0.415 mmol) in toluene (1.0 mL) and DMF (0.25 mL) over 5 min. The resulting yellow-brown colored suspension was stirred for 1 h at the same temperature. A solution of **7b** (98.9 mg, 0.277 mmol) in toluene (2.0 mL) and DMF (1.0 mL) was added drop by drop to the suspension over 5 min. After 0.5 h, the reaction mixture was quenched with ice water (10 mL), extracted with EtOAc, washed with water (3x) and brine, dried ($MgSO_4$) and concentrated. The orange residue was purified by chromatography on SiO_2 (25% EtOAc/Hexanes) to provide **8b** (111 mg, 92%) as an orange foam: IR 2249, 1588, 1435, 1366, 1258, 1187, 1142, 1111, 1085, 839, 811 cm^{-1}; ^{1}H NMR δ 8.73 (d, 1 H, *J* = 2.1 Hz), 8.60 (ddd, 1 H, *J* = 0.9, 1.5, 4.8 Hz), 8.35 (d, 1 H, *J* = 9.3 Hz), 8.14 (s, 1 H), 8.03 (dd, 1 H, *J* = 2.4, 9.6 Hz), 7.79 (ddd, 1 H, *J* = 1.8, 7.8, 7.8 Hz), 7.49 (d, 1 H, *J* = 7.8 Hz), 7.33 (ddd, 1 H, *J* = 0.9, 4.8, 7.8 Hz), 6.08 (s, 1 H); ^{13}C NMR δ 155.0 (qu, *J* = 18.8 Hz), 152.7, 150.6, 150.1 (q, *J* = 36.0 Hz), 147.0, 143.1, 138.4, 129.9 (appt, *J* = 4.5 Hz), 127.5, 126.2 (appt, *J* = 4.5 Hz), 125.0, 124.3, 126.6, 121.0 (q, *J* = 274.5 Hz), 118.9 (d, *J* = 2.3 Hz), 117.3, 43.0; ^{19}F NMR δ 81.8 (qu, *J* = 152.3 Hz), 63.0 (d, *J* = 152.3 Hz), -67.6; EI-MS *m/z* 439 (M, 35), 412 (10), 119 (30), 91 (100), 84 (60); HRMS (EI) *m/z* calcd for $C_{17}H_9N_3F_8S$ 439.0389, found 439.0380.



9b

2-Pyridyl-7-pentafluorosulfanyl-(2-trifluoromethyl)-4-quinolylketone (9b). To a suspension of **8b** (109 mg, 0.248 mmol) in acetic acid (0.43 mL) was added H_2O_2 (98 μL, 1.24 mmol) dropwise at room temperature. The reaction mixture was placed in a preheated (75 °C) oil bath until the color turned to light yellow. The mixture was quenched with ice water (10 ml), extracted with Et_2O, washed with sat. $NaHCO_3$ solution and brine, dried ($MgSO_4$) and concentrated. The yellow residue was purified by chromatography on SiO_2 (16% EtOAc/Hexanes) to provide **9b** (98.0 mg, 92%) as a white solid: Mp 99.5-101.1 °C; IR 1687, 1437, 1189, 1135, 1105, 826, 813, 801 cm^{-1}; ^{1}H NMR δ 8.78 (d, 1 H, *J* = 2.1 Hz), 8.64 (ddd, 1 H, *J* = 0.9, 1.5, 4.8 Hz), 8.38 (appd, 1 H, *J* = 7.2 Hz), 8.07 (d, 1 H, *J* = 9.6 Hz), 8.01 (dd, 1 H, *J* = 1.8, 7.8 Hz), 8.00 (s, 1 H), 7.99 (ddd, 1 H, *J* = 2.4, 9.3, 9.3 Hz), 7.61 (ddd, 1 H, *J* = 1.2, 4.8, 7.8 Hz); ^{13}C NMR δ 193.8, 154.9 (qu, *J* = 18.8 Hz), 152.9, 149.8, 149.2 (q, *J* = 36.0 Hz), 146.9, 146.2, 137.8, 129.4 (appt, *J* = 4.5 Hz), 128.5, 127.3, 126.7, 126.0 (appt, *J* = 4.5 Hz), 124.5, 121.2 (q, *J* = 273.4 Hz), 119.3 (d, *J* = 2.3 Hz); ^{19}F NMR δ 82.2 (qu, *J* = 152.3 Hz), 63.1 (d, *J* = 152.3 Hz), -67.6; EI-MS *m/z* 428 (M, 100), 399 (95), 331 (35), 301 (40), 119 (50), 99 (50); HRMS (EI) *m/z* calcd for $C_{16}H_8N_2OF_8S$ 428.0230, found 428.0231.

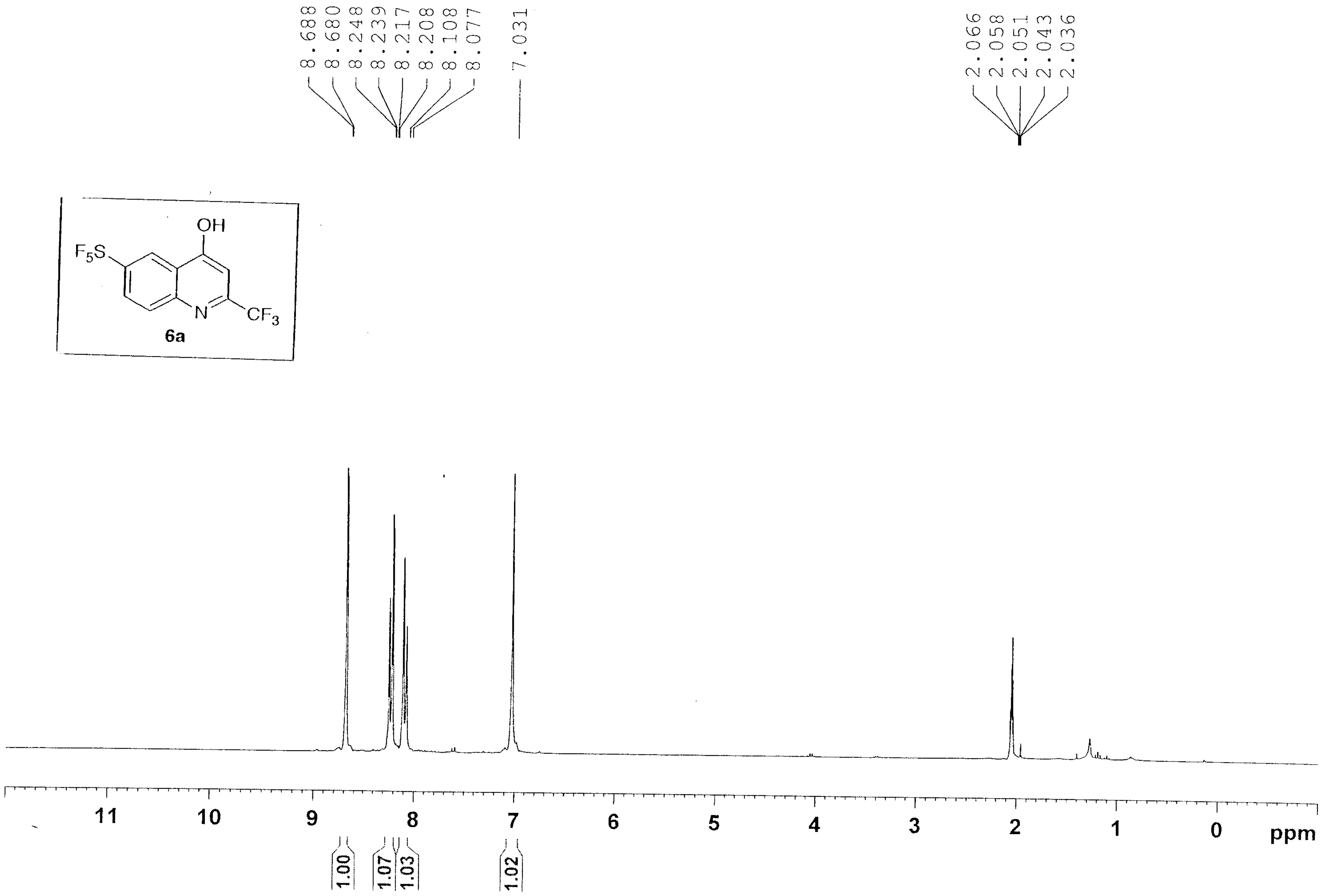


3

α-(2-Piperidyl)-7-pentafluorosulfanyl-(2-trifluoromethyl)-4-quinolinemethanol (3)

A solution of **9b** (70.5 mg, 0.165 mmol) in acetic acid (0.57 mL, 9.88 mmol) and abs EtOH (1.1 mL) was treated with platinum oxide (15.0 mg, 0.0658 mmol). The reaction mixture was purged with hydrogen twice and hydrogenated under balloon pressure. After 4 h, there was no alcohol intermediate detected by TLC (10% MeOH/DCM). The solution was filtered through florisil, concentrated, and extracted with Et_2O. The combined organic layers were washed with sat. $NaHCO_3$ solution and brine, dried ($MgSO_4$) and concentrated. The black residue was purified by chromatography on SiO_2 (5% NEt_3 in EtOAc then 5% NEt_3 and 5% MeOH in EtOAc). The crude product was recrystallized from MeOH to get 33.1 mg (46%) of product as a white solid with a dr 20:1: Mp 179.2-180.2 °C; IR 3000-2900 (br), 1442, 1366, 1256, 1182, 1139, 1109, 1083, 932, 848, 816 cm^{-1}; ^{1}H NMR (acetone-d$_6$, 600MHz) δ 8.66 (d, 1 H, *J* = 2.4 Hz), 8.64 (d, 1 H, *J* = 9.6 Hz), 8.20 (s, 1 H), 8.17 (dd, 1 H, *J* = 2.4, 9.6 Hz), 5.54 (d, 1 H, *J* = 4.8 Hz), 3.04 (ddd, 1 H, *J* = 3.0, 4.8, 10.8 Hz), 2.97 (dm, 1 H, *J* = 12.0 Hz), 2.55 (dt, 1 H, *J* = 2.4, 12.0 Hz), 1.74-1.69 (m, 1 H), 1.50-1.42 (m, 2 H), 1.36-1.27 (m, 2 H), 1.22 (tq, 1 H, *J* = 3.6, 12.6 Hz); ^{13}C NMR (acetone-d$_6$, 600 MHz) δ 154.9 (qu, *J* = 18.0 Hz), 154.2, 150.0

(q, *J* = 34.5 Hz), 147.1, 129.7 (appt, *J* = 4.5 Hz), 129.3, 127.3, 125.3 (appt, *J* = 4.5 Hz), 122.6 (q, *J* = 273.0 Hz), 118.1 (d, *J* = 1.5 Hz), 73.4, 62.2, 47.6, 27.4, 27.0, 25.1; ^{19}F NMR δ 84.2 (qu, *J* = 149.5 Hz), 64.1 (d, *J* = 149.5 Hz), -66.7; HRMS (ESI) *m/z* calcd for $C_{16}H_{17}N_2OF_8S$ 437.0928, found 437.0948.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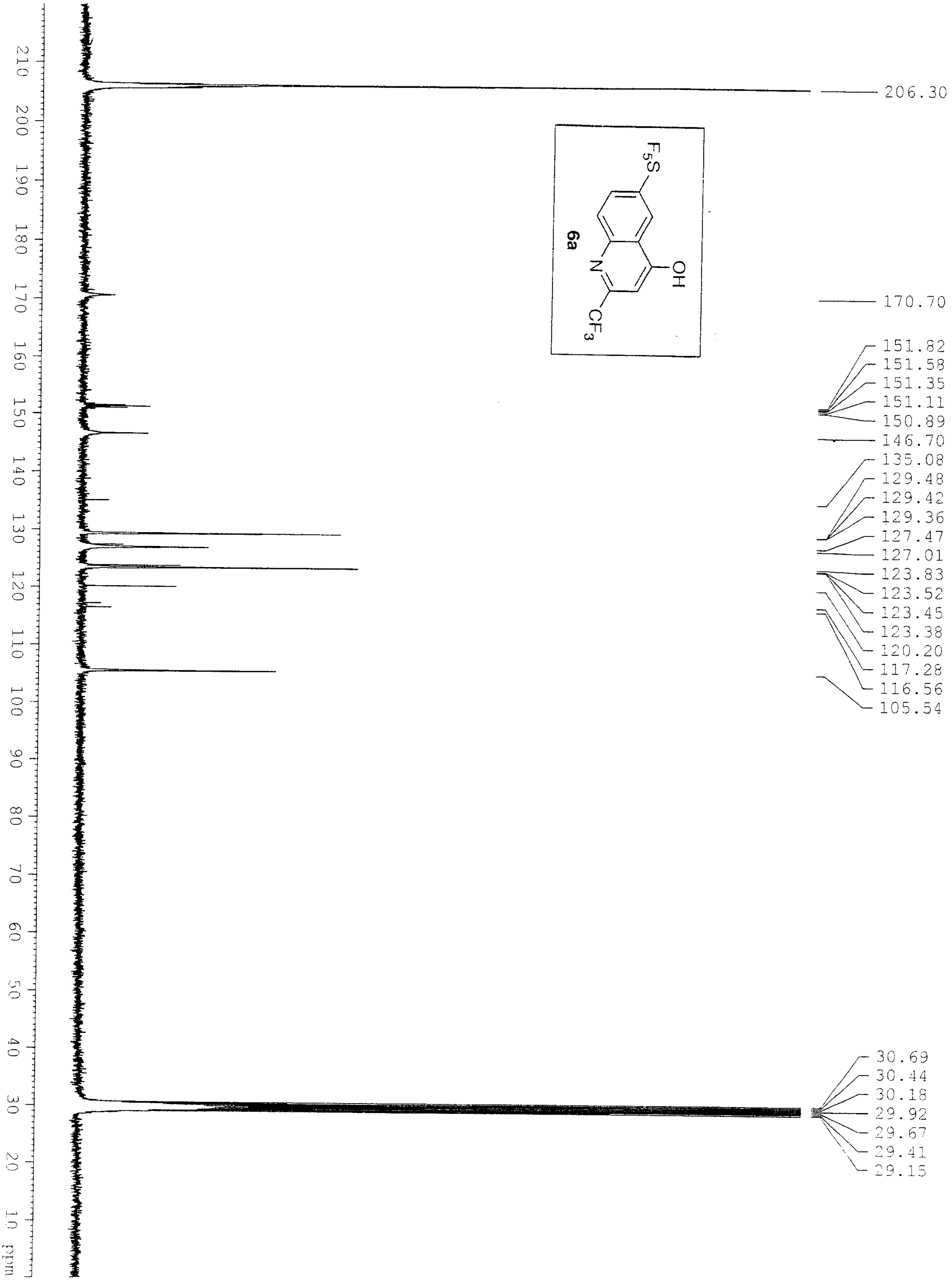
2.058
2.051
2.043
2.036
OH
F5S
N
CF3
6a
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.07
1.03
1.02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146.70
135.08
129.48
129.42
129.36
127.47
127.01
123.83
123.52
123.45
123.38
120.20
117.28
116.56
105.54
30.69
30.44
30.18
29.92
29.67
29.41
29.15
F5S
OH
N
CF3
6a
210
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90
80
70
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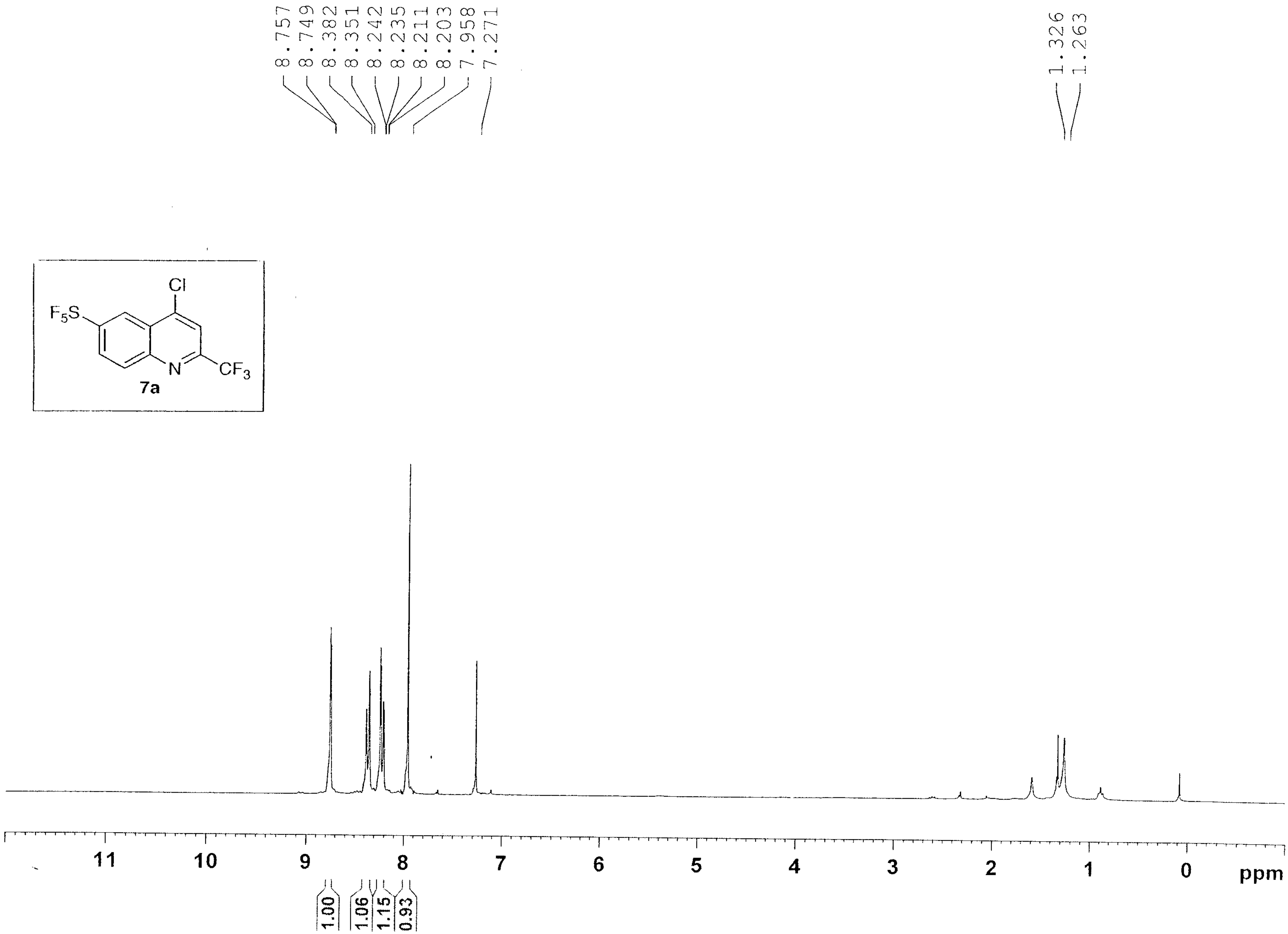
50
40
30
20
10
ppm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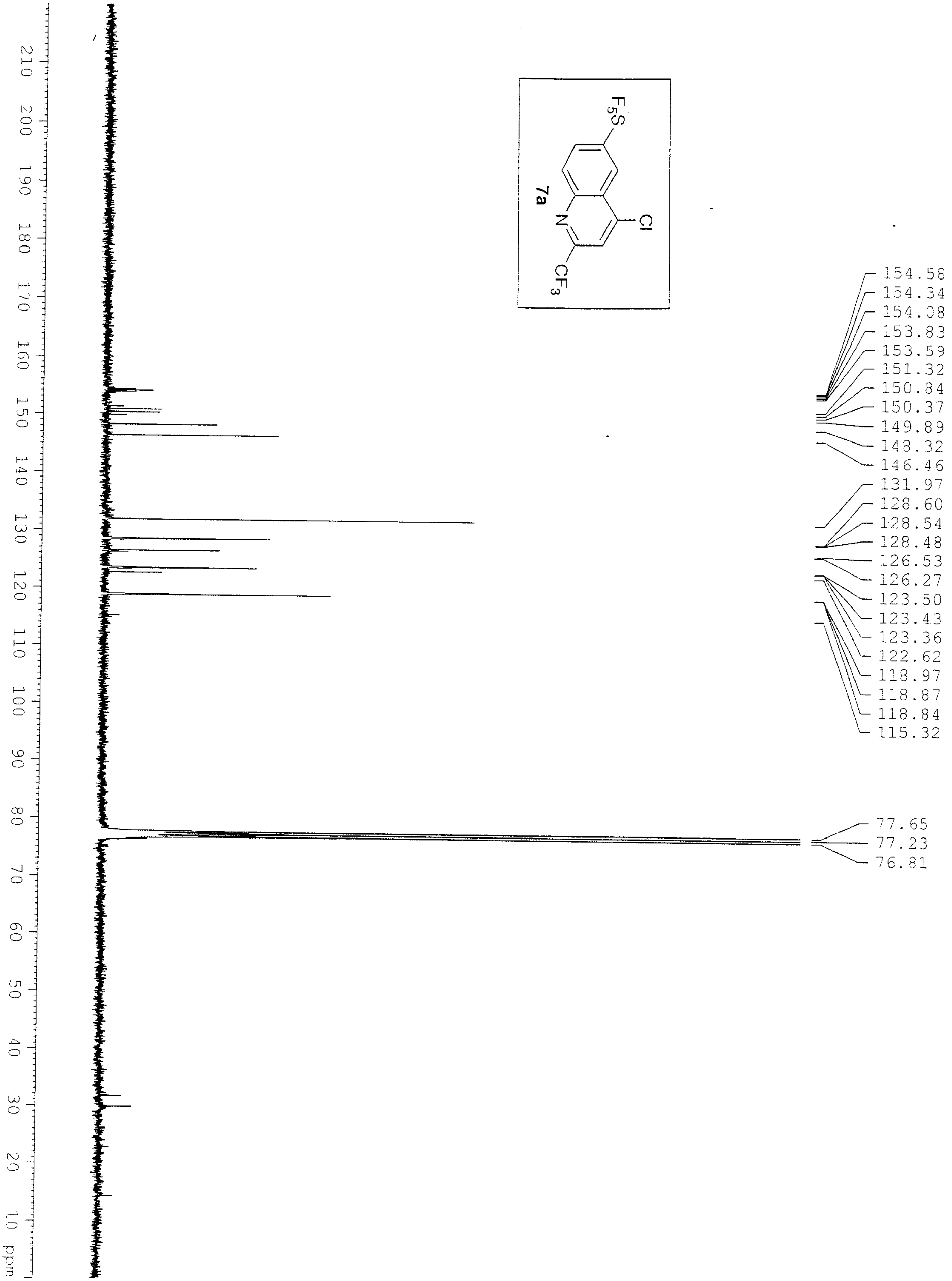
Cl
F_5S
N
CF_3
7a
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.06
1.15
0.93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CF3
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149.89
148.32
146.46
131.97
128.60
128.54
128.48
126.53
126.27
123.50
123.43
123.36
122.62
118.97
118.87
118.84
115.32
77.65
77.23
76.81
210
200
190
180
170
160
150
140
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120
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100
90
80
70
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50
40
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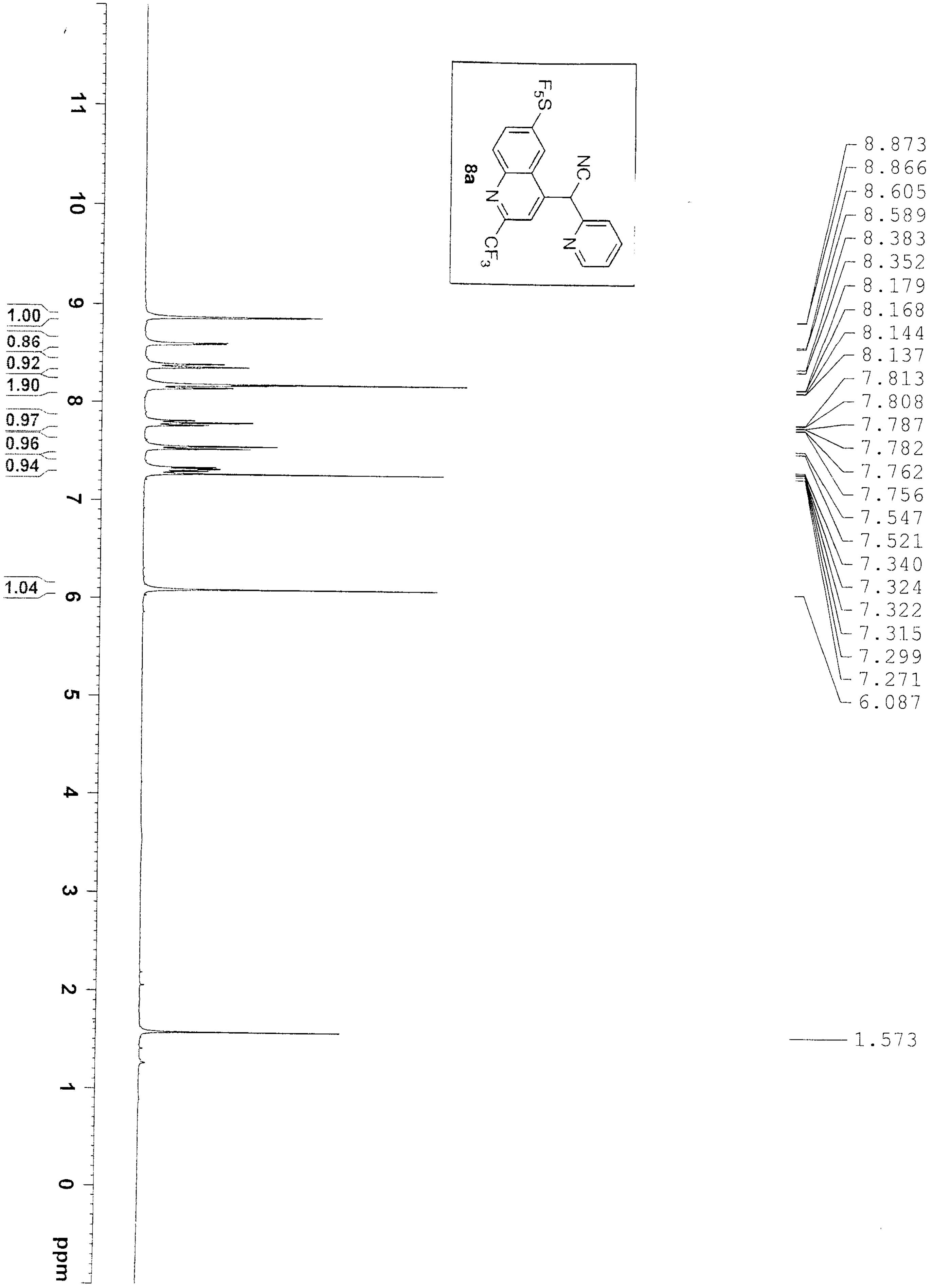
20
10 ppm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CF3
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10
9
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0.92
1.90
0.97
0.96
0.94
1.04
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8.866
8.605
8.589
8.383
8.352
8.179
8.168
8.144
8.137
7.813
7.808
7.787
7.782
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7.322
7.315
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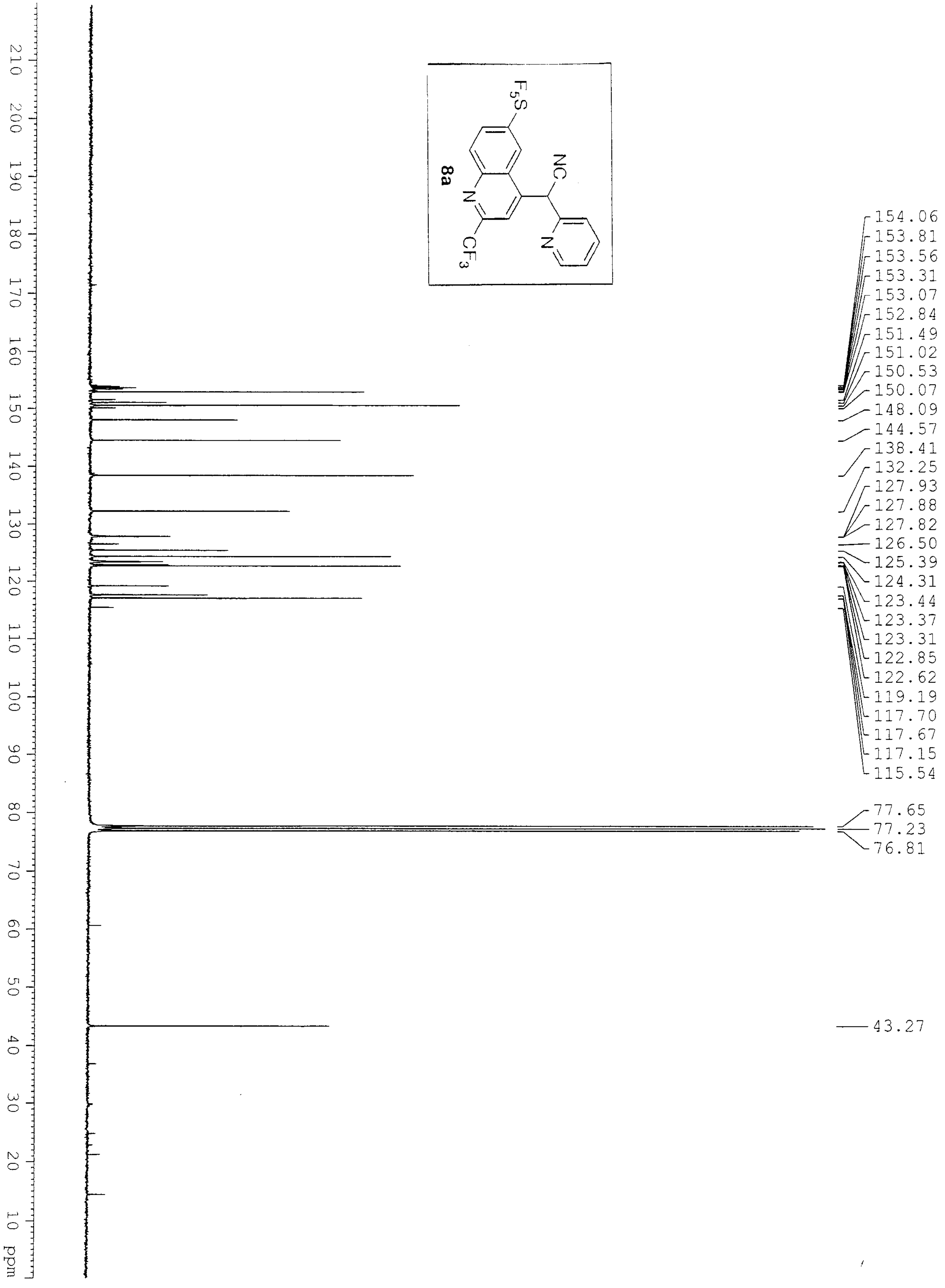
1.573



210
200
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180
170
160
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130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
F5S
NC
N
N
CF3
8a
154.06
153.81
153.56
153.31
153.07
152.84
151.49
151.02
150.53
150.07
148.09
144.57
138.41
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127.93
127.88
127.82
126.50
125.39
124.31
123.44
123.37
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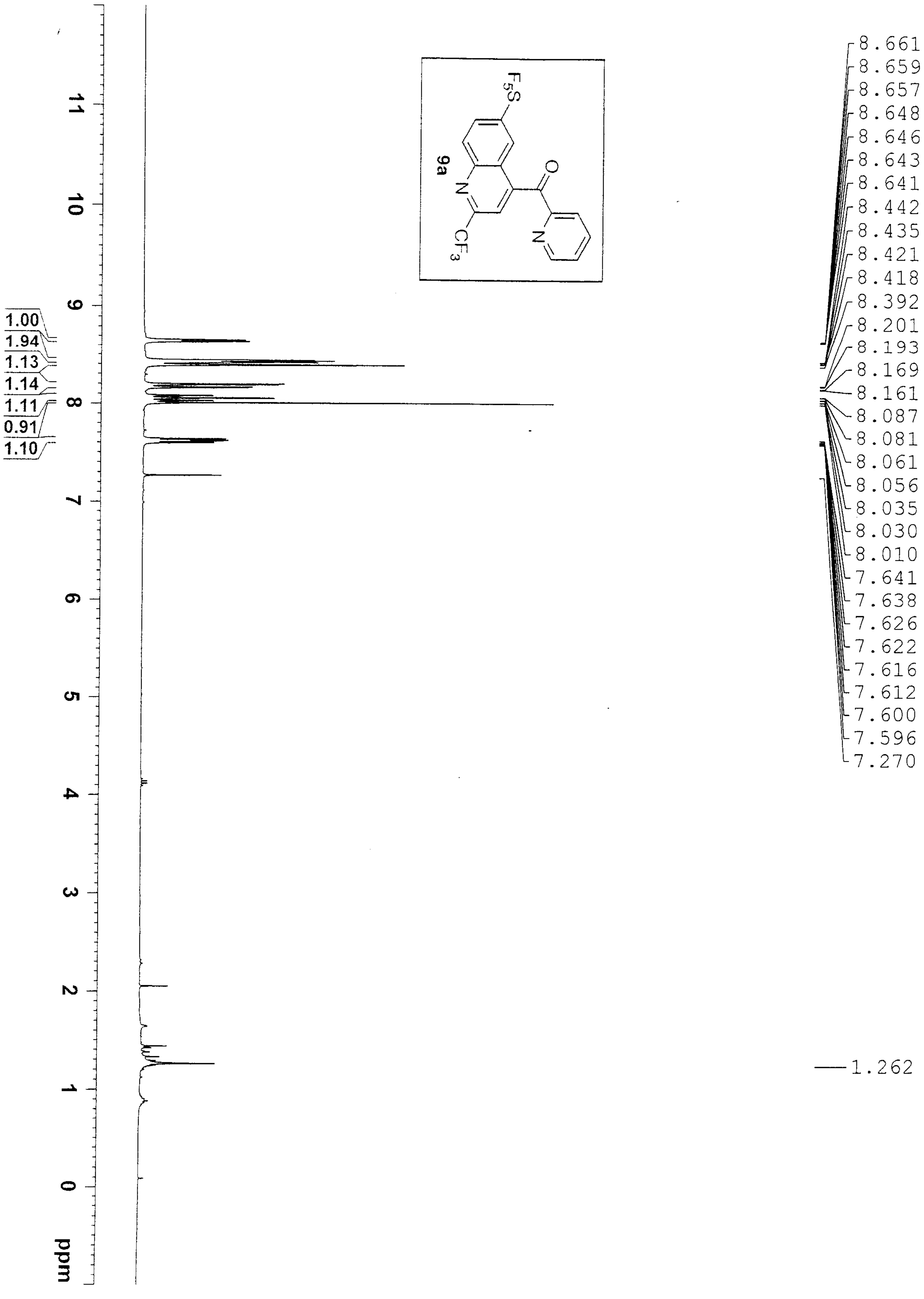
76.81
43.27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8.657
8.648
8.646
8.643
8.641
8.442
8.435
8.421
8.418
8.392
8.201
8.193
8.169
8.161
8.087
8.081
8.061
8.056
8.035
8.030
8.010
7.641
7.638
7.626
7.622
7.616
7.612
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6
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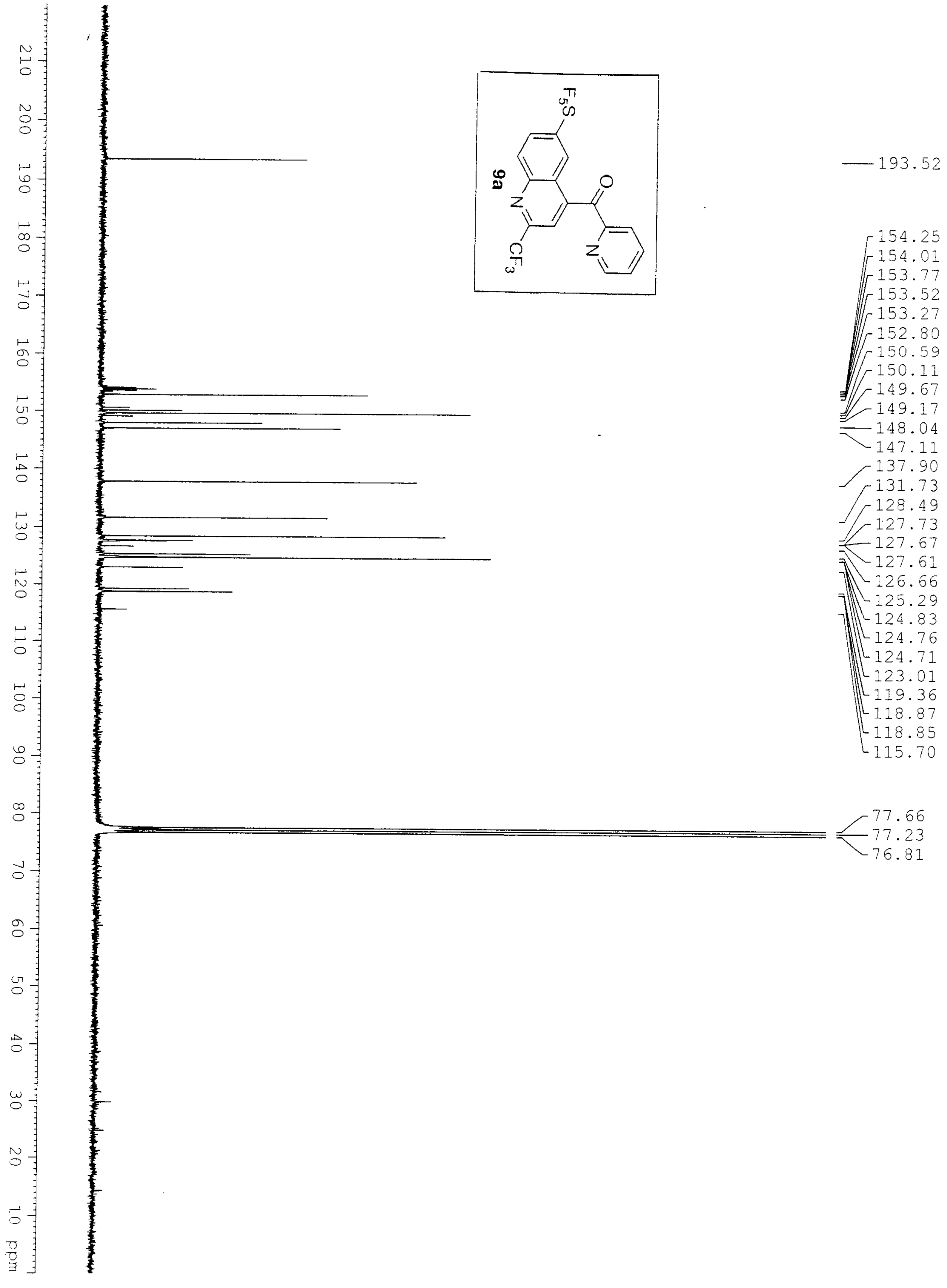
ppm



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N
CF3
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153.27
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150.59
150.11
149.67
149.17
148.04
147.11
137.90
131.73
128.49
127.73
127.67
127.61
126.66
125.29
124.83
124.76
124.71
123.01
119.36
118.87
118.85
115.70
77.66
77.23
76.81
210
200
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150
140
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70
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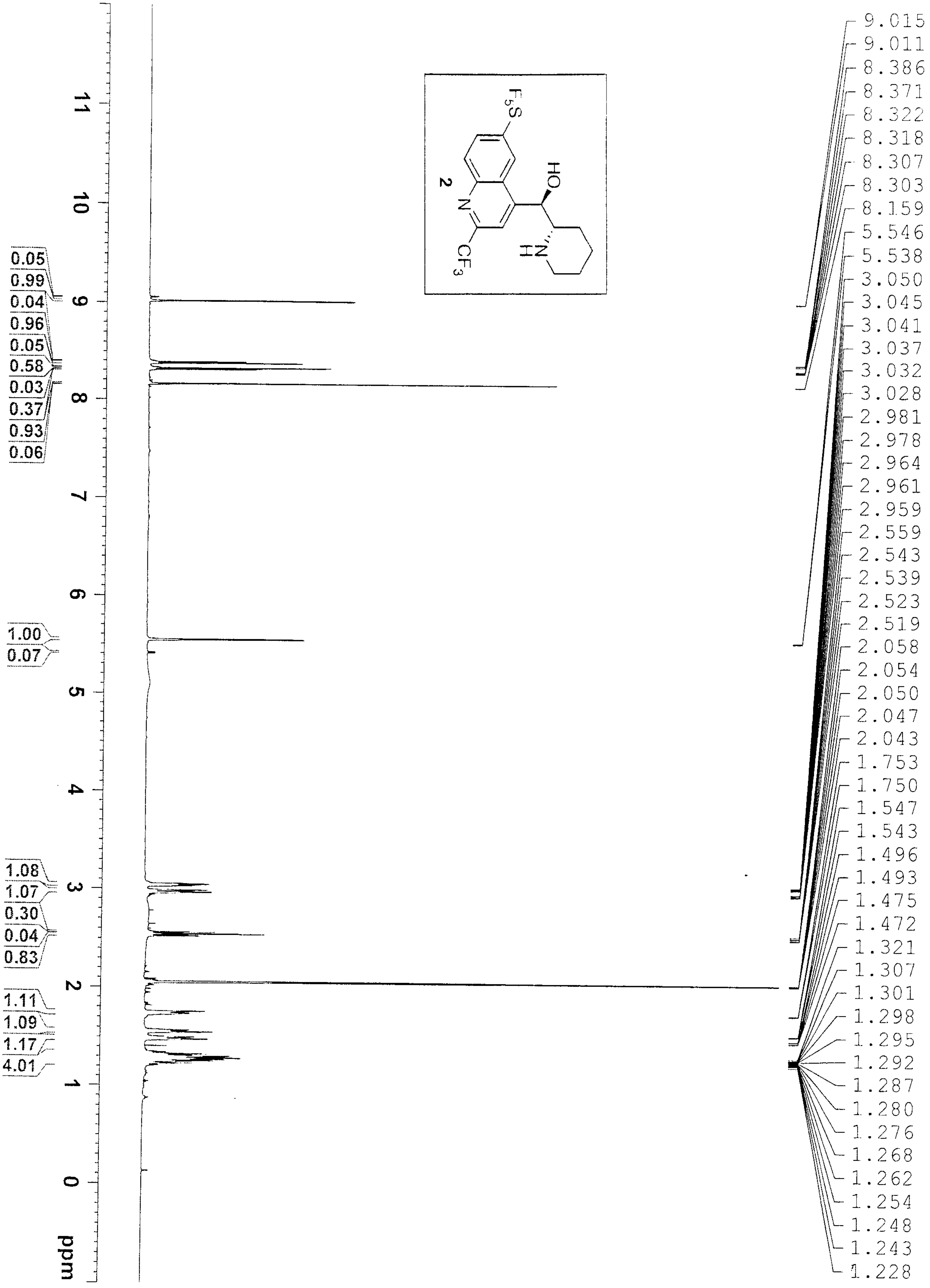
30
20
10
ppm



2
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HO
N
H
CF3
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9.011
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8.371
8.322
8.318
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8.303
8.159
5.546
5.538
3.050
3.045
3.041
3.037
3.032
3.028
2.981
2.978
2.964
2.961
2.959
2.559
2.543
2.539
2.523
2.519
2.058
2.054
2.050
2.047
2.043
1.753
1.750
1.547
1.543
1.496
1.493
1.475
1.472
1.321
1.307
1.301
1.298
1.295
1.292
1.287
1.280
1.276
1.268
1.262
1.254
1.248
1.243
1.228
0.05
0.99
0.04
0.96
0.05
0.58
0.03
0.37
0.93
0.06
1.00
0.07
1.08
1.07
0.30
0.04
0.83
1.11
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1.17
4.01
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8
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6
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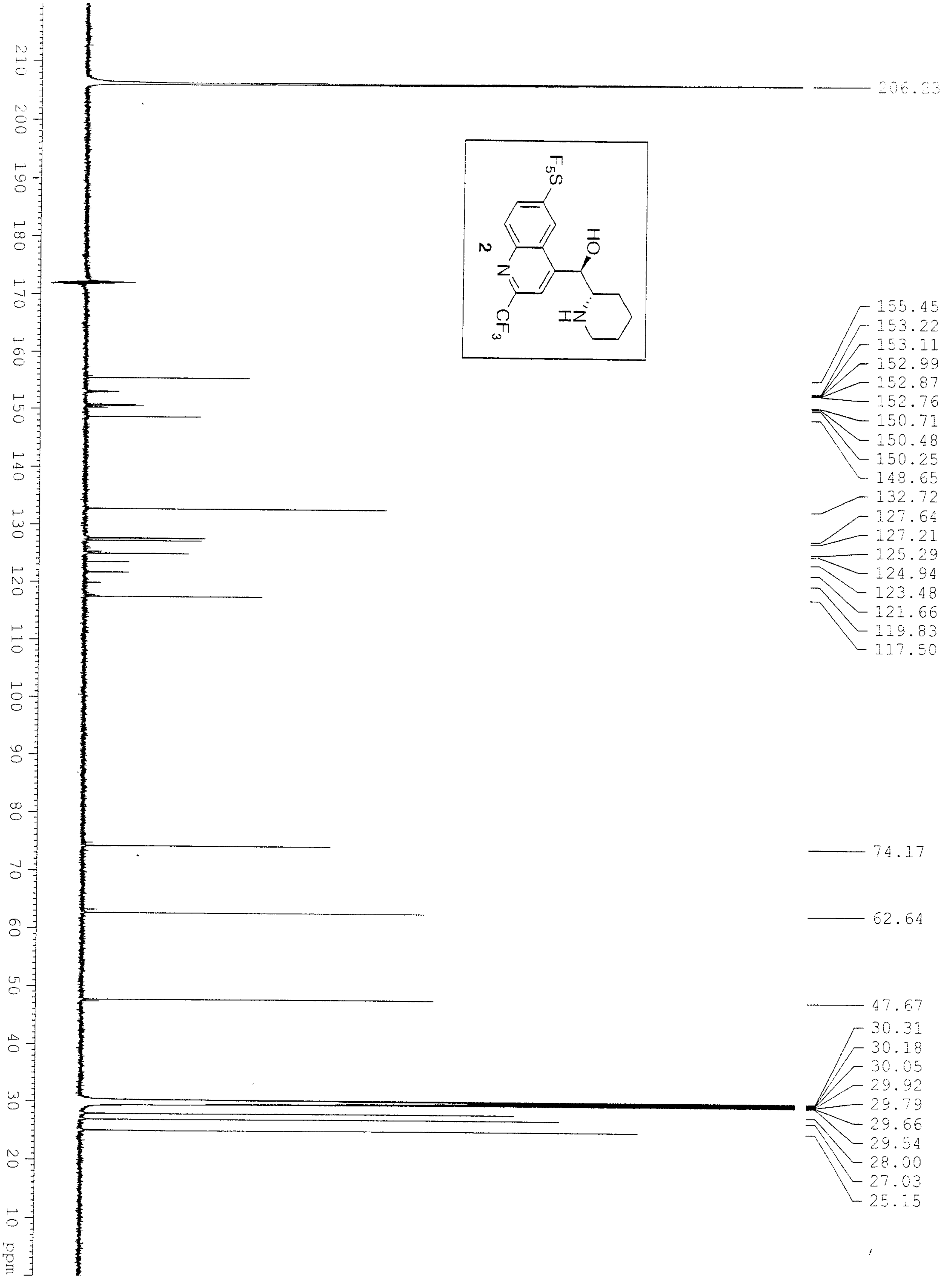
ppm



2
F5S
HO
N
H
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
206.23
155.45
153.22
153.11
152.99
152.87
152.76
150.71
150.48
150.25
148.65
132.72
127.64
127.21
125.29
124.94
123.48
121.66
119.83
117.50
74.17
62.64
47.67
30.31
30.18
30.05
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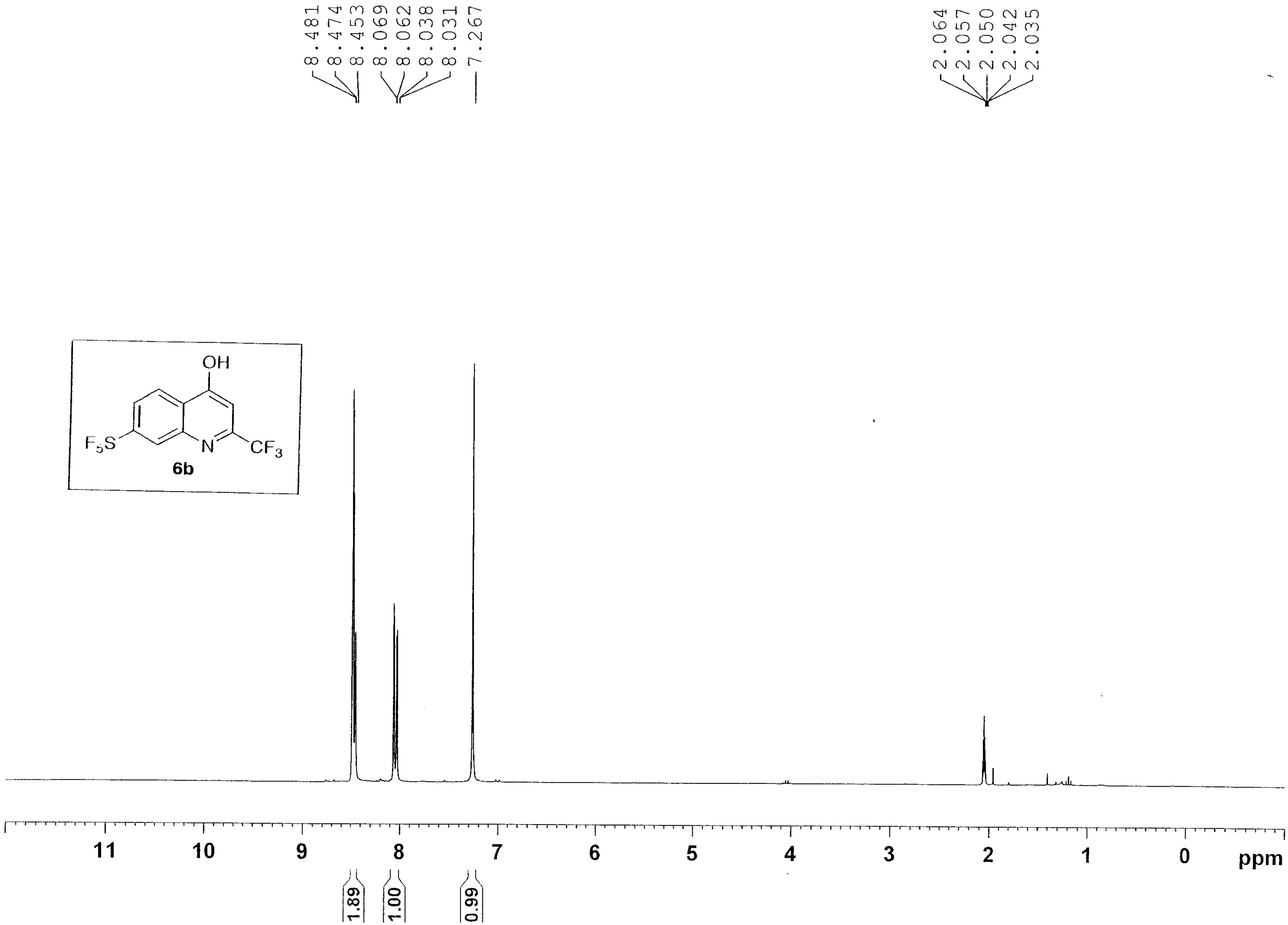
29.66
29.54
28.00
27.03
25.15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2.035
OH
F_5S
N
CF_3
6b
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10
9
8
7
6
5
4
3
2
1
0
ppm
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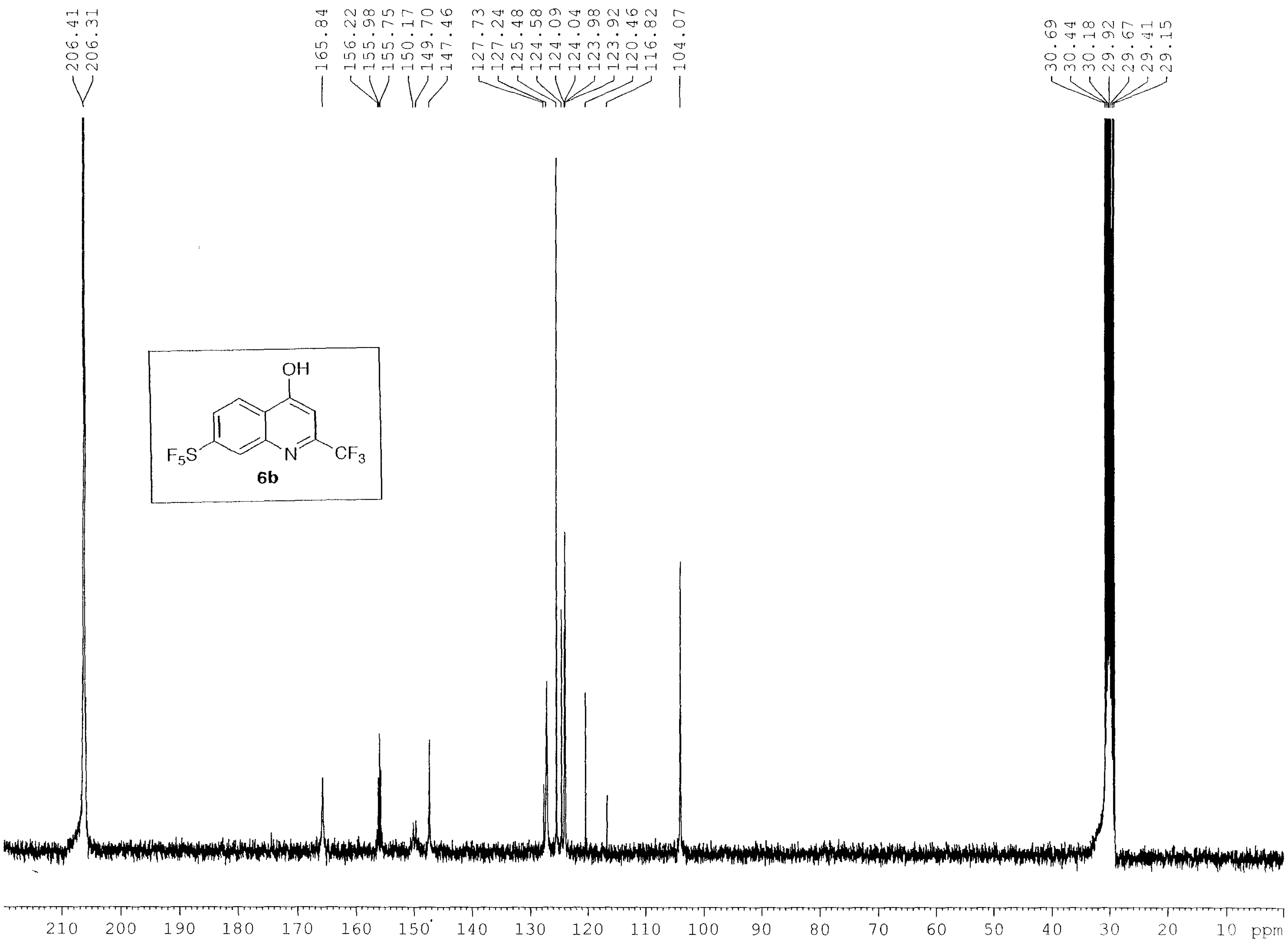
1.00
0.99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124.58
124.09
124.04
123.98
123.92
120.46
116.82
104.07
30.69
30.44
30.18
29.92
29.67
29.41
29.15
OH
F_5S
N
CF_3
6b
210
200
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180
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160
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140
130
120
110
100
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70
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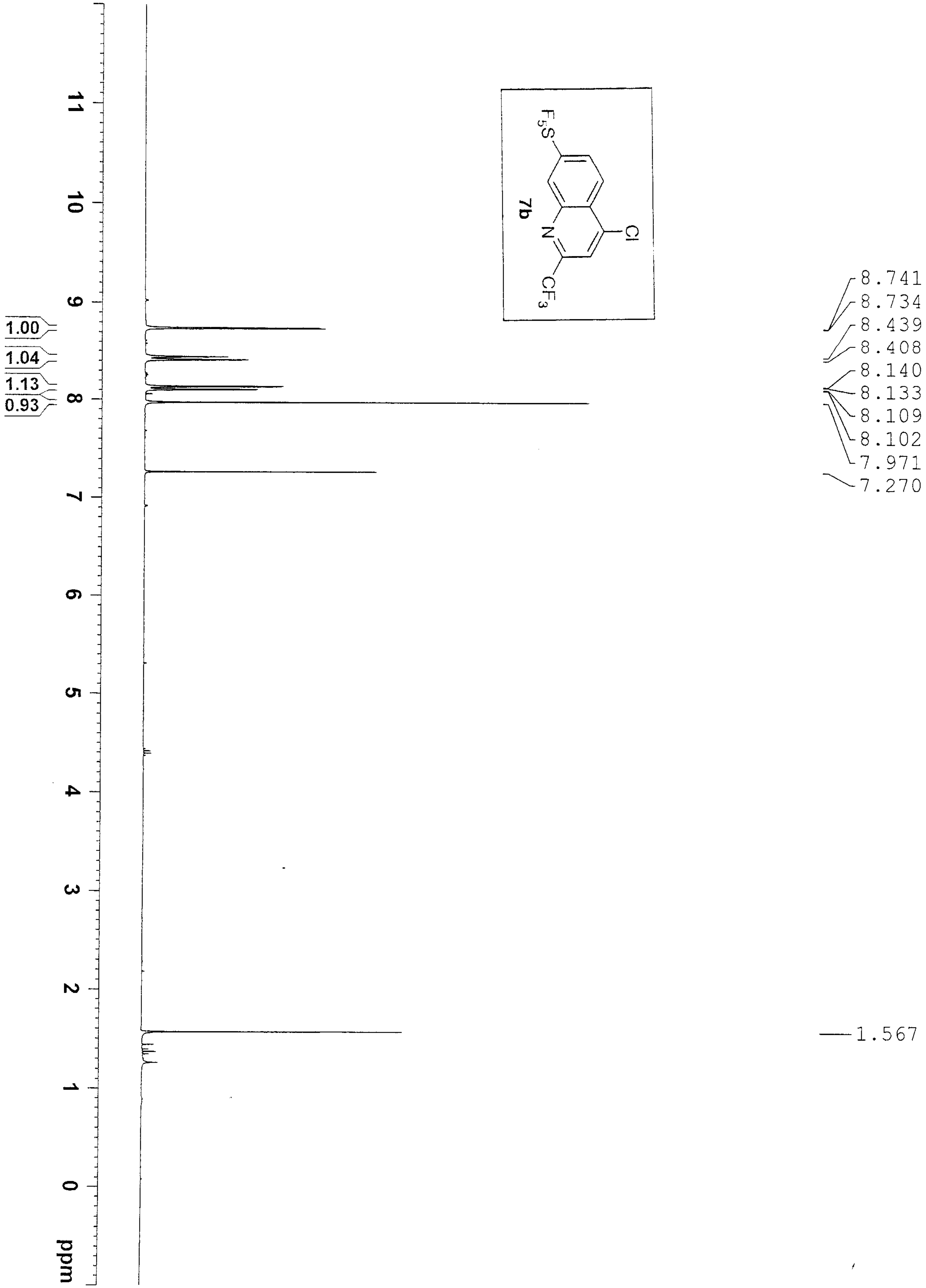
50
40
30
20
10
ppm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F5S
Cl
N
CF3
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8.408
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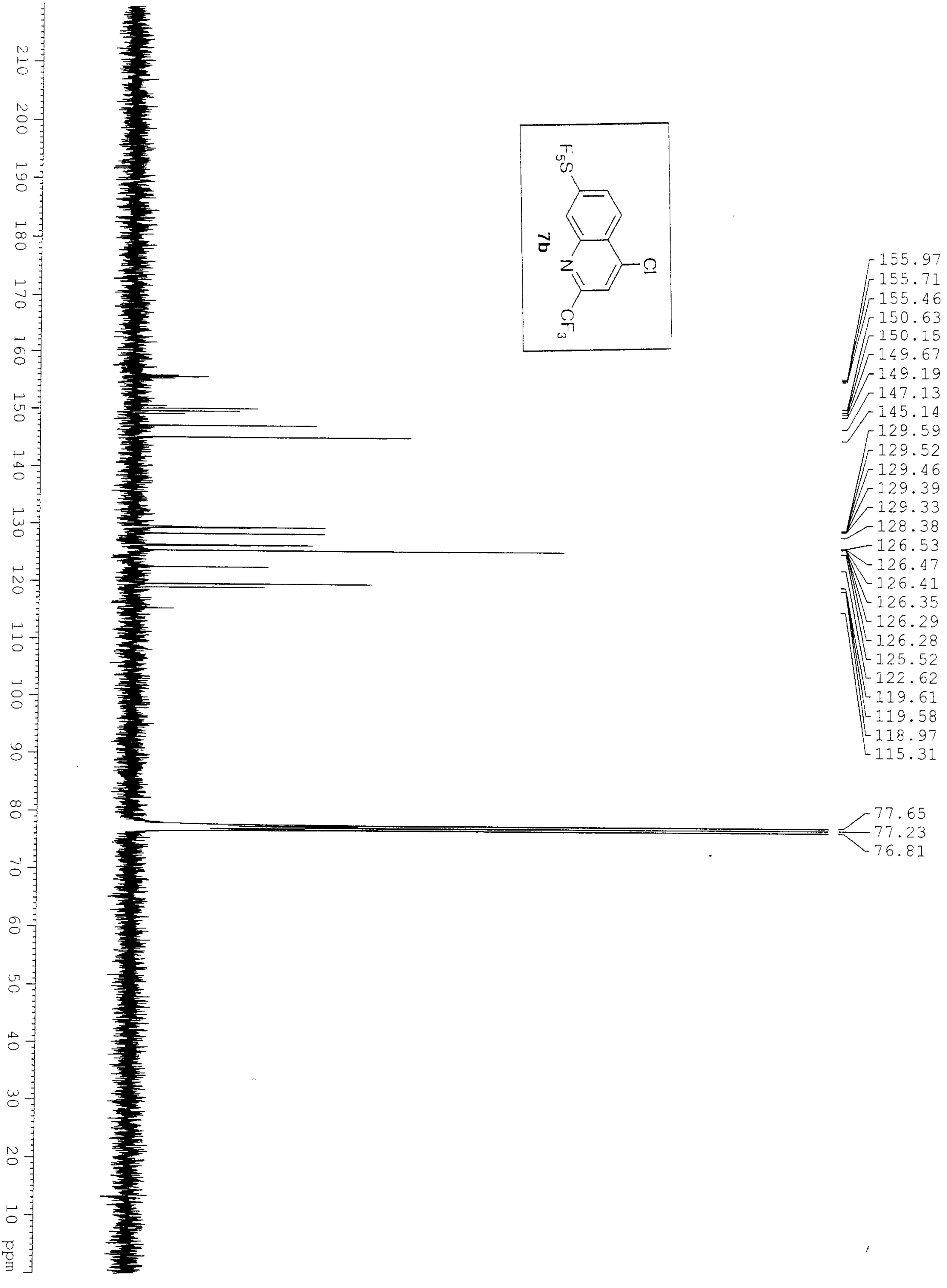
8.133
8.109
8.102
7.971
7.270
1.567
1.00
1.04
1.13
0.93
11
10
9
8
7
6
5
4
3
2
1
0
ppm


7b
F5S
Cl
N
CF3
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150.63
150.15
149.67
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145.14
129.59
129.52
129.46
129.39
129.33
128.38
126.53
126.47
126.41
126.35
126.29
126.28
125.52
122.62
119.61
119.58
118.97
115.31
77.65
77.23
76.81
210
200
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180
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150
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120
110
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10
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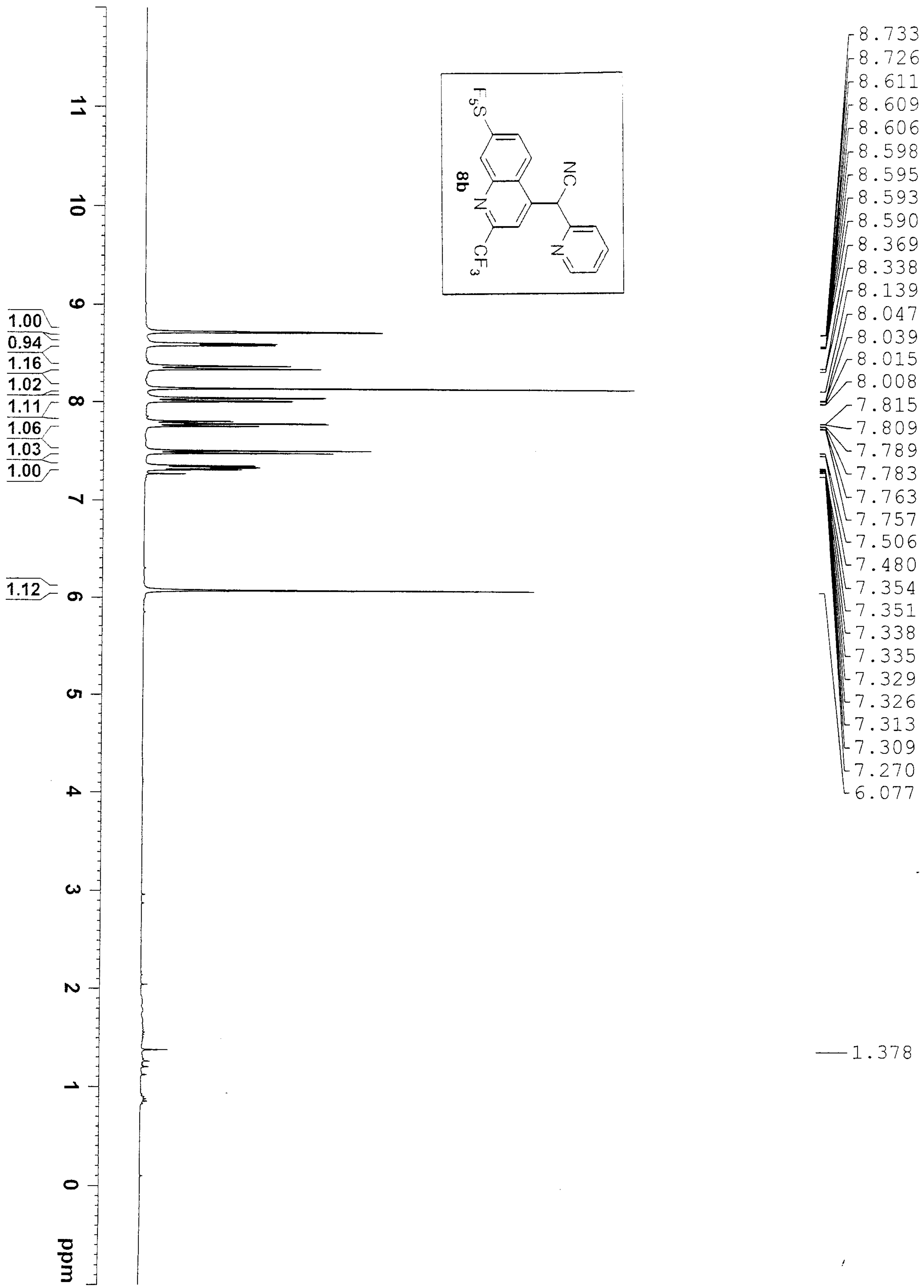
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8.590
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8.139
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8.039
8.015
8.008
7.815
7.809
7.789
7.783
7.763
7.757
7.506
7.480
7.354
7.351
7.338
7.335
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7.326
7.313
7.309
7.270
6.077
1.378
1.00
0.94
1.16
1.02
1.11
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6
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4
3
2
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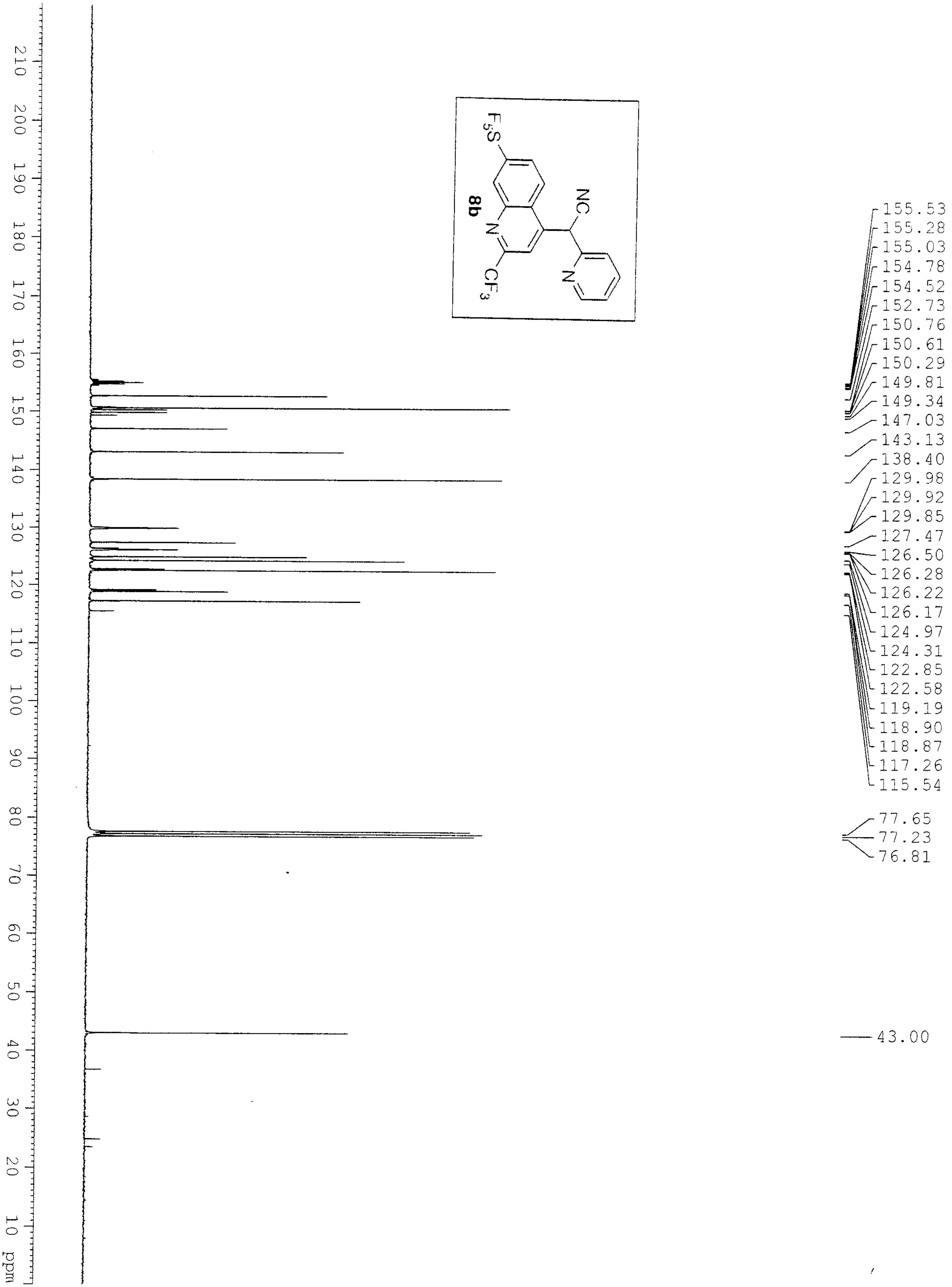
0
ppm



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147.03
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124.31
122.85
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118.87
117.26
115.54
77.65
77.23
76.81
43.00
210
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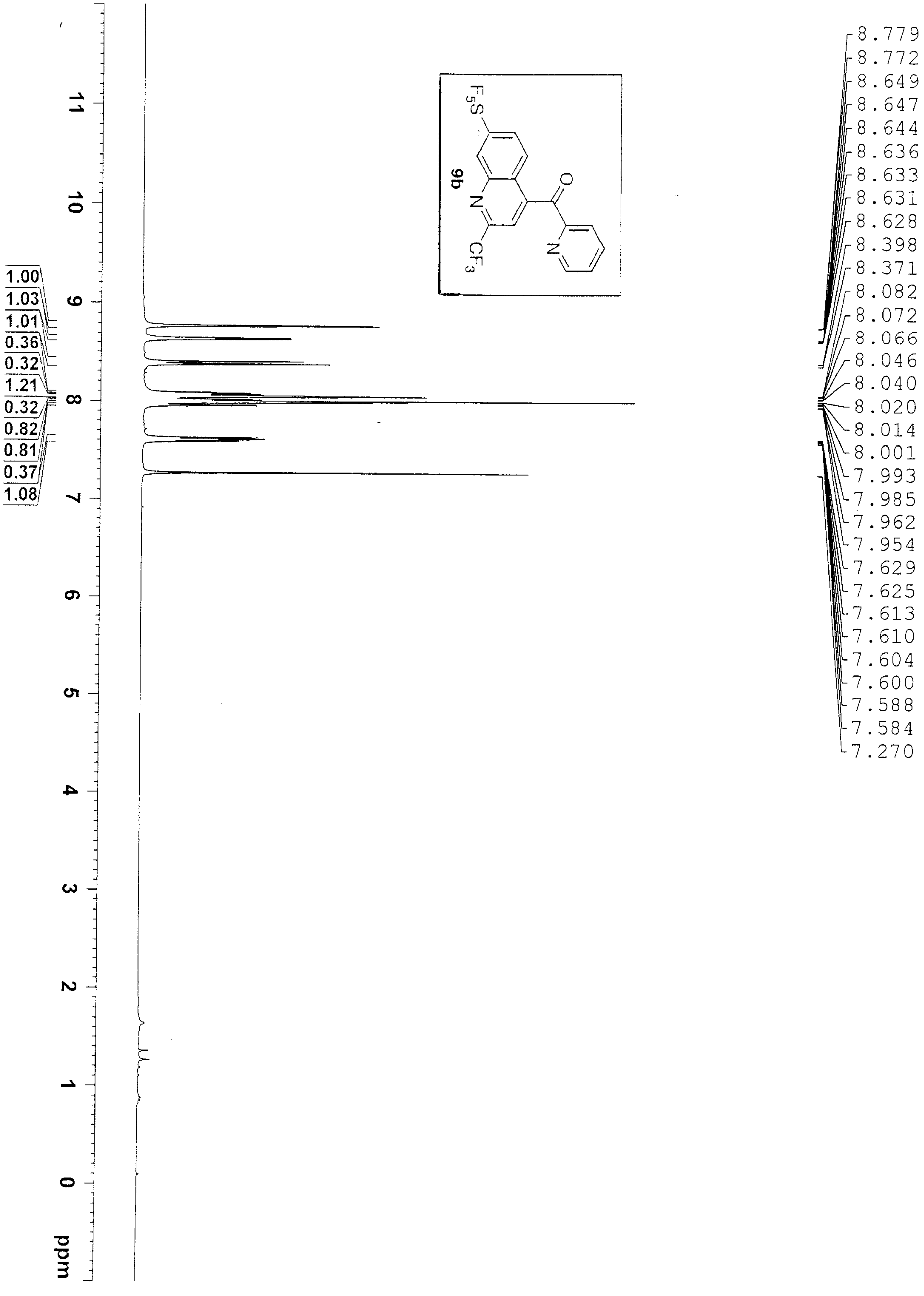
40
30
20
10
ppm



9b
F5S
N
CF3
O
N
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8.647
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8.636
8.633
8.631
8.628
8.398
8.371
8.082
8.072
8.066
8.046
8.040
8.020
8.014
8.001
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7.985
7.962
7.954
7.629
7.625
7.613
7.610
7.604
7.600
7.588
7.584
7.270
1.00
1.03
1.01
0.36
0.32
1.21
0.32
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1.08
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6
5
4
3
2
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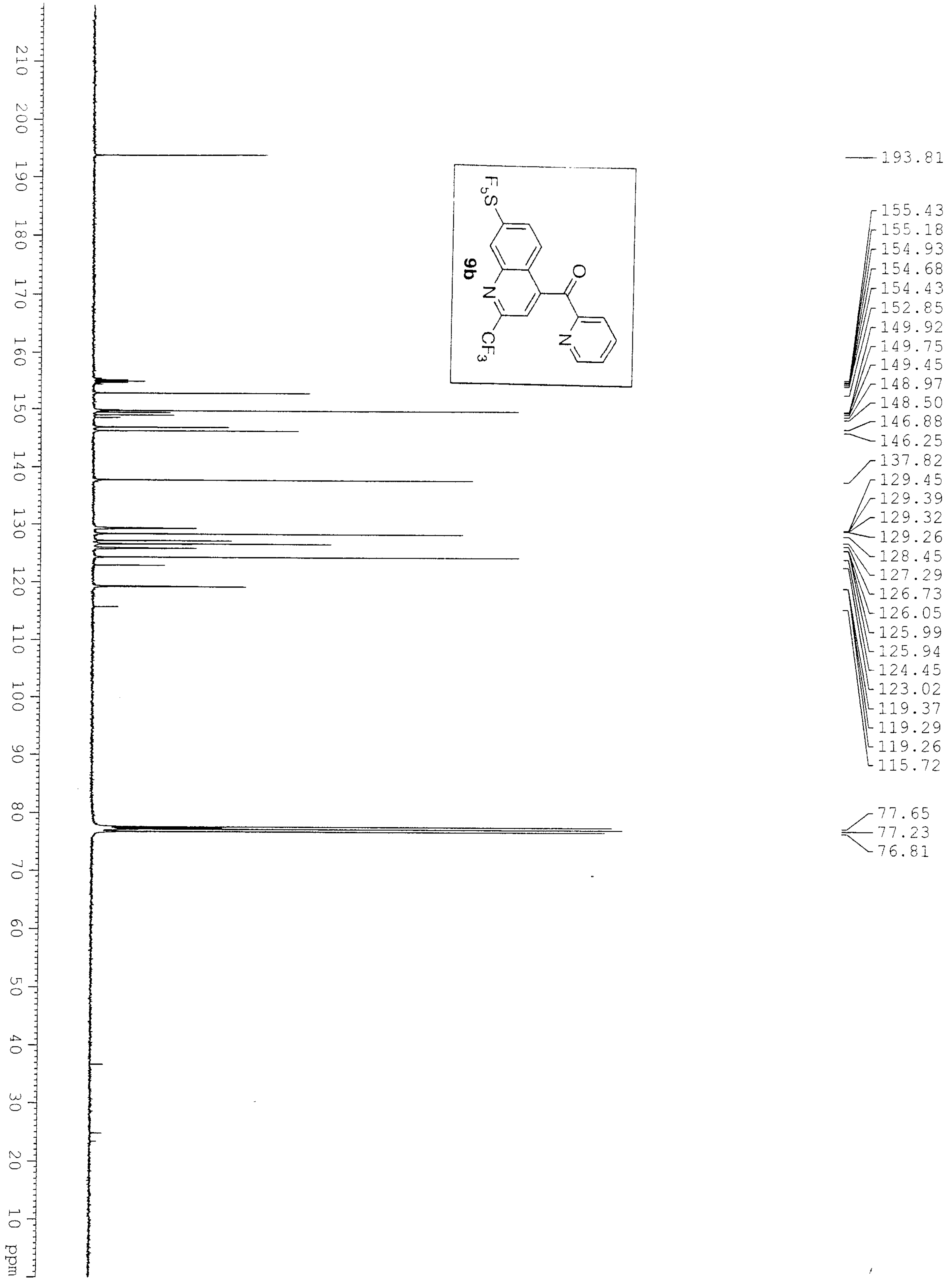
0
ppm



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154.43
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149.92
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146.88
146.25
137.82
129.45
129.39
129.32
129.26
128.45
127.29
126.73
126.05
125.99
125.94
124.45
123.02
119.37
119.29
119.26
115.72
77.65
77.23
76.81
F5S
N
CF3
O
N
9b
210
200
190
180
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70
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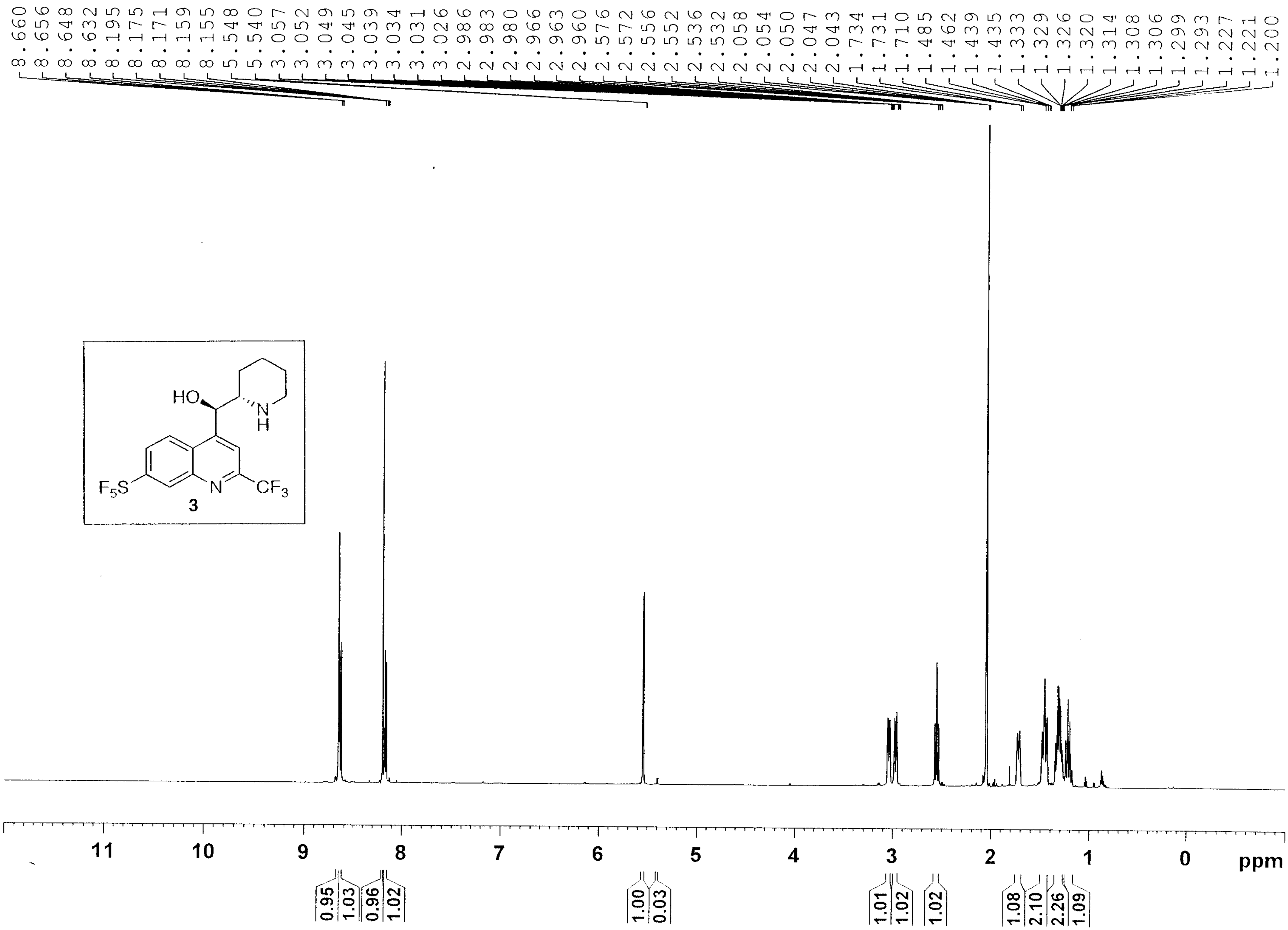
40
30
20
10
ppm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3.052
3.049
3.045
3.039
3.034
3.031
3.026
2.986
2.983
2.980
2.966
2.963
2.960
2.576
2.572
2.556
2.552
2.536
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2.058
2.054
2.050
2.047
2.043
1.734
1.731
1.710
1.485
1.462
1.439
1.435
1.333
1.329
1.326
1.320
1.314
1.308
1.306
1.299
1.293
1.227
1.221
1.200
HO
N
H
F5S
N
CF3
3
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
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0.96
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1.00
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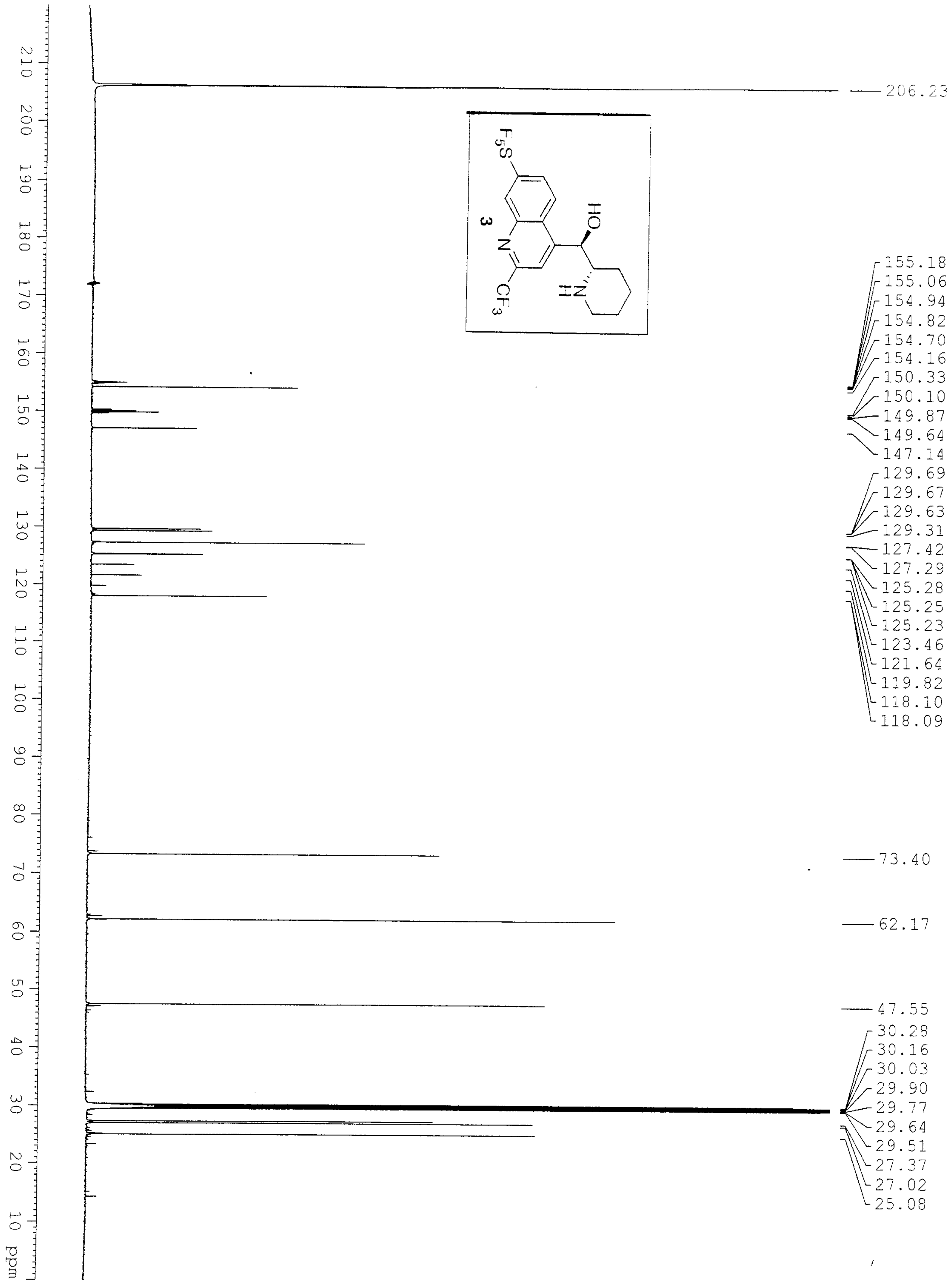
1.01
1.02
1.02
1.08
2.10
2.26
1.09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170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm
206.23
155.18
155.06
154.94
154.82
154.70
154.16
150.33
150.10
149.87
149.64
147.14
129.69
129.67
129.63
129.31
127.42
127.29
125.28
125.25
125.23
123.46
121.64
119.82
118.10
118.09
73.40
62.17
47.55
30.28
30.16
30.03
29.90
29.77
29.64
29.51
27.37
27.02
25.08
F5S
HO
N
CF3
NH
3