Supporting Information

for

Nickel-Catalyzed Decarbonylation of *N*-Acylated *N*-Heteroarenes

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CONTENTS

I. General Information.

^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer (JEOL, Tokyo, Japan) or VARIAN UNITY INOVA-600 spectrometer in $CDCl_3$ with tetramethylsilane as an internal reference standard. NMR data have been reported as follows: chemical shift (δ) in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), coupling constant (*J*) in Hz, and integration. Infrared spectra (IR) were obtained on a JASCO FT/IR-4000 spectrometer, and the absorptions have been reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra were obtained on a Shimadzu GCMS-QP 5000 or GCMS-QP 2010 instrument with an ionization voltage of 70 eV. High resolution mass spectra (HRMS) were obtained on a JEOL JMS-T100LP AccuTOF LC-plus in direct analysis real time (DART) method using PEG as the internal standard. Analytical gas chromatography (GC) was carried out on Shimadzu GC-2014, equipped with a flame ionization detector. Melting points were determined using a Yamato melting point apparatus. Column chromatography was performed over SiO_2 (Silycycle Silica Flash F60 (230-400 mesh)) and NH Silica (Silica Gel 60 (spherical) NH_2 (40–50 μm)). Some of the compounds were purified by LC-908 HPLC (GPC). Data collection for X-ray crystal analysis were performed on a Rigaku / XtaLAB Pro P200 Hybrid Photon Counting diffractometer (Mo-Kα, λ = 0.71075 Å for **6a** and Cu-Kα, λ = 1.54184 Å for **6f**). The structure was solved with direct methods and refined with full-matrix least squares.

II. Materials.

Toluene (for Organic Synth.) was purchased from Wako Chemicals and used as received. $Ni(cod)_2$ was purchased from Strem Chemicals and used as received. PCy_3 (Sigma-Aldrich), dcype (Sigma-Aldrich), IPr·HCl (TCI), IMes·HCl (TCI), ICy·HCl (TCI) PPh_3 (TCI), and $Ni(CO)_2$(dcype) (Kanto Chemical) were purchased from commercial suppliers and used as received. $IMes^{Me}$·HCl[1] was prepared according to the literature procedures. 4-[(Benzyloxy)carbonyl]benzoic acid **S1** [CAS: 18520-63-3][2] was prepared according to the literature procedure. 4-(Morpholine-4-carbonyl)benzoic acid **S4** [CAS: 160816-43-3][2] was prepared according to the literature procedure. 2-(5-Methoxy-1*H*-indol-3-yl)-*N*,*N*-bis(phenylmethyl)ethanamine **S6** [CAS: 300834-81-5][3] was prepared according to the literature procedure. *N*-Acylated *N*-heteroarenes **7a** [CAS: 62573-86-8],[4] and **7c** [CAS: 28997-

[1] Kinuta, H.; Tobisu, M; Chatani, N. *J. Am. Chem. Soc.* **2015**, *137*, 159.
[2] Simpson, F. P.; Mandle, R. J.; Moore, J. N.; Goodby, J. W. *J. Mater. Chem. C,* **2017**, *5*, 5102.
[3] Xu, Y-C.; Schaus, J. M.; Walker, C.; Krushinski, J.; Adham, N.; Zgombick, J. M.; Liang, S. X.; Lohlman, D. T.; Audia, J. E. *J. Med. Chem.* **1999**, *42*, 526.
[4] Zhao, J.; Li, P.; Xia, C.; Li, F. *Chem. Commun.* **2014**, *50*, 4751.

00-4],[5] were prepared according to the literature procedure. 1*H*-Benzimidazole-2-*d* **S19** [CAS: 61233-51-0][6] was prepared according to the literature procedures.

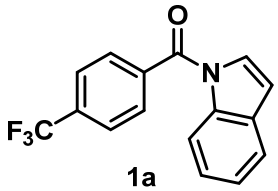
III. Synthesis of Starting Materials.

General Procedure I: Synthesis of amides from acid halides. Aroyl chloride (20 mmol) was partially added to a solution of indole (20 mmol, 1equiv), Et_3N (1 equiv) and *N*,*N*-dimethyl-4-aminopyridine (0.4 mmol) in 20 mL of CH_2Cl_2 at 0 °C. After addition was complete, the reaction mixture was stirred at room temperature for 12 h. The reaction was quenched by the addition of H_2O, and the resulting mixture was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried ($MgSO_4$), and concentrated to give a residue, which was purified by recrystallization or column chromatography to give the desired *N*-acylpyrrole derivative.

General Procedure II: Synthesis of amides from carboxylic acids. *N*,*N*-dimethylformamide (0.2 mL) was added to a solution of carboxylic acid (20 mmol) and oxalyl chloride (40 mmol, 2 equiv) in 200 mL of CH_2Cl_2 at 0 °C. After gas evolution ceased, the mixture was allowed to gradually warm to room temperature and was then stirred until the starting carboxylic acid disappeared by TLC. The solution was concentrated to give an aroyl chloride, which was used in the next step without further purification. The aroyl chloride was partially added to a solution of indole (20 mmol, 1 equiv), Et_3N (1 equiv) and *N*,*N*-dimethyl-4-aminopyridine (0.4 mmol) in 20 mL of CH_2Cl_2 at 0 °C. After the addition was complete, the reaction mixture was stirred at room temperature for 12 h. The reaction was quenched by the addition of H_2O, and the resulting mixture was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried ($MgSO_4$), and concentrated to give a residue, which was purified by recrystallization or column chromatography to give the desired *N*-acylpyrrole derivative.

(1*H*-Indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (1a) [CAS: 1018967-38-8].[7]

[5] Ovian, J. M.; Kelly, C. B.; Pistritto, V. A.; Leadbeater, N. E. *Org. Lett.* **2017**, *19*, 1286.
[6] Gröll, B.; Schnürch, M.; Mihovilovic, M. D. *J. Org. Chem.* **2012**, *77*, 4432.
[7] Wang, L.; Neumann, H.; Spannenberg, A.; Beller, M. *Chem. Eur. J*. **2018**, *24*, 2164.



1a

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride (50 mmol scale).

White solid (7.4g, 51%). Mp 132.9–133.1 °C. R_f 0.34 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.65 (d, *J* = 3.7 Hz, 1H), 7.19 (d, *J* = 3.7 Hz, 1H), 7.35 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.40 (dd, *J* = 7.3, 8.0 Hz, 1H), 7.62 (d, *J* = 7.3 Hz, 1H), 7.87–7.80 (m, 4H), 8.41 (d, *J* = 8.2 Hz, 1H).

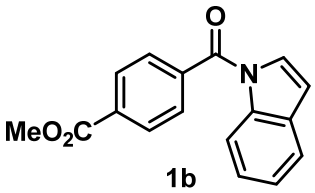
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 109.5, 116.4, 121.1, 123.5 (q, J_{CF} = 272.6 Hz), 124.4, 125.3, 125.7 (q, J_{CF} = 4.1 Hz), 127.0, 129.4, 130.7, 133.5 (q, J_{CF} = 33.2 Hz), 135.9, 137.9, 167.3.

IR (ATR): 1679 s, 1542 w, 1452 w, 1407 w, 1328 m, 1205 m, 1170 s, 1128 s, 1068 m, 854 m, 769 w, 727 m.

MS, *m/z* (relative intensity, %): 290 (10), 289 (M^+, 54), 173 (100), 145 (52).

HRMS Calcd for $C_{16}H_{11}F_3NO$ ([M+H^+]): 290.0793. Found: 290.0792.

Methyl 4-(1*H*-indole-1-carbonyl)benzoate (1b).



1b

The general procedure I was followed using methyl 4-(chloroformyl)benzoate.

White solid (4.3 g, 77%). Mp 167.5–167.8 °C. R_f 0.11 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.98 (s, 3H), 6.64 (d, *J* = 3.7 Hz, 1H), 7.21 (d, *J* = 3.7 Hz, 1H), 7.33 (dd, *J* = 7.4, 8.2 Hz, 1H), 7.40 (dd, *J* = 7.4, 8.2 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 2H), 8.20 (d, *J* = 8.3 Hz, 2H), 8.40 (d, *J* = 8.2 Hz, 1H).

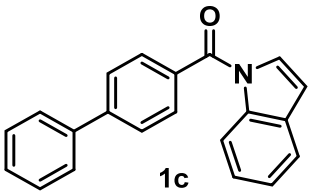
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 52.6, 109.3, 116.4, 121.0, 124.2, 125.2, 127.1, 129.0, 129.8, 130.7, 132.9, 135.9, 138.5, 166.1, 167.8.

IR (ATR): 1720 m, 1679 s, 1448 m, 1378 w, 1347 s, 1278 s, 1209 m, 1109 m, 1018 w, 887 w, 769 s, 728 m.

MS, *m/z* (relative intensity, %): 279 (M^+, 35), 164 (10), 163 (100), 135 (22), 103 (14).

HRMS Calcd for $C_{17}H_{14}NO_3$ ([M+H$^+$]): 280.0974. Found: 280.0978.

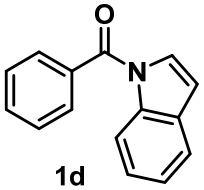
[1,1'-Biphenyl]-4-yl(1*H*-indol-1-yl)methanone (1c) [CAS 1018967-39-9].



1c

The general procedure I was followed using 4-phenylbenzoyl chloride. Spectroscopic data were consistent with those reported in the literature.[8]

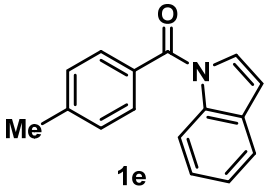
(1*H*-Indol-1-yl)(phenyl)methanone (1d) [CAS 1496-76-0].



1d

The general procedure I was followed using benzoyl chloride. Spectroscopic data were consistent with those reported in the literature.[9]

(1*H*-Indol-1-yl)(p-tolyl)methanone (1e) [CAS 69888-36-4].

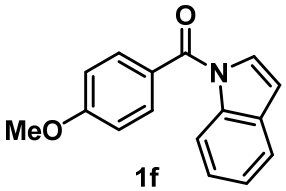


1e

The general procedure I was followed using *p*-toluoyl chloride. Spectroscopic data were consistent with those reported in the literature.[10]

(1*H*-Indol-1-yl)(4-methoxyphenyl)methanone (1f) [CAS 52498-87-0].

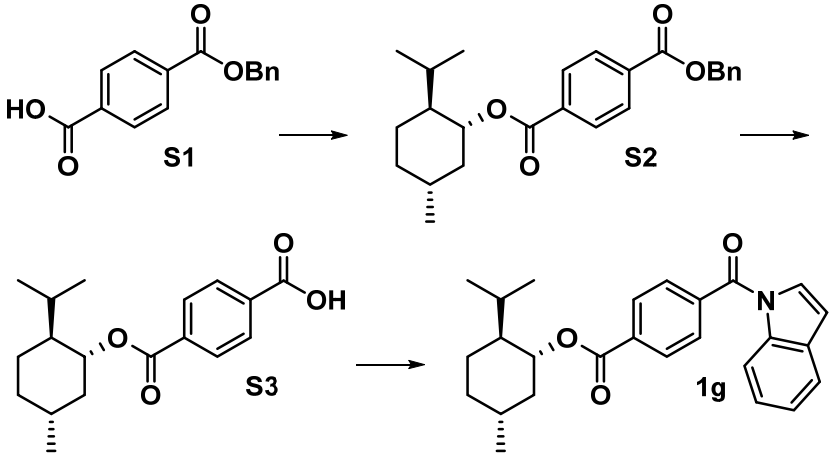
[8] Abid, M.; De Paolis, O.; Török, B. *Synlett* **2008**, *3*, 410.
[9] Umehara, A.; Ueda, H.; Tokuyama, H. *J. Org. Chem.* **2016**, *81*, 11444.
[10] Aggarwal, R.; Benedetti, F.; Berti, F.; Buchini, S.; Colombatti, A.; Dinon, F.; Galasso, V.; Norbedo, S. *Chem. Eur. J.* **2003**, *9*, 3132.



1f

The general procedure I was followed using 4-methoxybenzoyl chloride. Spectroscopic data were consistent with those reported in the literature.[11]

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-(1*H*-indole-1-carbonyl)benzoate (1g).



N,*N*-dimethylformamide (50 μL) was added to a solution of 4-[(benzyloxy)carbonyl]benzoic acid (**S1**) (10 mmol) and oxalyl chloride (25 mmol, 2.5 equiv) in 30 mL of CH_2Cl_2 at 0 °C. After gas evolution ceased, the mixture was allowed to be gradually warm to room temperature and was then stirred until the starting carboxylic acid was disappeared by TLC. The solution was concentrated to give an aroyl chloride, which was used in the next step without further purification. The aroyl chloride was partially added to a solution of (-)-menthol (10 mmol, 1 equiv), Et_3N (1 equiv) and *N*,*N*-dimethyl-4-aminopyridine (0.2 mmol) in 20 mL of CH_2Cl_2 at 0 °C. After addition was completed, the reaction mixture was stirred at room temperature for 12 hours. The reaction was quenched by the addition of H_2O, and the resulting mixture was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried ($MgSO_4$), and concentrated to give a residue, which was purified by column chromatography to give **S2** as a colorless oil.

Colorless oil (3.42 g, 87%). R_f 0.43 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 0.81 (d, *J* = 6.8 Hz, 3H), 0.93–0.96 (m, 7H), 1.09–1.21 (m, 2H),

[11] Wu, X. F.; Oschatz, S.; Sharif, M.; Langer, P. *Synthesis*, **2015** *47*, 2641.

1.52–1.64 (m, 2H), 1.72–1.78 (m, 2H), 1.91–2.02 (m, 1H), 2.10–2.15 (m, 1H), 4.96 (td, *J* = 10.8, 4.4 Hz, 1H), 5.39 (s, 2H), 7.34–7.44 (m, 3H), 7.46–7.49 (m, 2H), 8.10–8.16 (m, 4H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 16.6, 20.9, 22.2, 23.9, 26.9, 31.8, 34.6, 41.2, 47.6, 67.6, 75.7, 128.6, 128.7, 128.9, 129.80, 129.85, 134.1, 135.2, 136.3, 165.4, 165.9.

IR (KBr, cm^{-1}): 3421 w, 3066 w, 3034 w, 2955 s, 2870 m, 1951 w, 1716 s, 1610 w, 1577 w, 1504 m, 1456 m, 1408 m, 1374 m, 1268 s, 1180 m, 1118 s, 1101 s, 1038 m, 1018 s, 982 m, 960 m, 915 m, 875 m, 846 m, 795 w, 731 s, 696 m.

HRMS Calcd for $C_{25}H_{31}O_4$ ([M+H$^+$]): 395.2217. Found: 395.2222.

To a stirred solution of benzyl ester **S2** (2.5 g, 6.3 mmol) in methanol (50 mL) was added 10% palladium on carbon (130 mg) slowly, in small portions. The mixture was then stirred vigorously under an atmosphere of hydrogen for 5 h, filtered through Celite® and the solvent was removed in vacuo to afford **S3** (1.9 g, 100%) as a white solid.

Mp 46.3–48.5 °C. R_f 0.46 (SiO_2, EtOAc/MeOH = 9/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 0.80 (d, *J* = 6.8 Hz, 3H), 0.92–0.95 (m, 7H), 1.09–1.21 (m, 2H), 1.51–1.63 (m, 2H), 1.73–1.78 (m, 2H), 1.91–2.02 (m, 1H), 2.10–2.15 (m, 1H), 4.96 (td, *J* = 10.8, 4.4 Hz, 1H), 8.13–8.21 (m, 4H), 12.62 (s, 1H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 16.6, 20.9, 22.2, 23.9, 26.9, 31.8, 34.6, 41.2, 47.6, 75.9, 129.9, 130.4, 133.1, 136.0, 165.4, 171.8.

IR (KBr, cm^{-1}): 3417 w, 2956 s, 2928 s, 2871 s, 2667 m, 2545 m, 2285 w, 1952 w, 1822 w, 1716 s, 1695 s, 1614 w, 1577 m, 1507 m, 1455 m, 1423 s, 1388 m, 1371 m, 1272 s, 1180 m, 1129 s, 1104 s, 1038 m, 1019 s, 982 m, 959 s, 916 m, 879 m, 876 m, 846 m, 797 m, 768 m, 731 s, 693 m, 674 w.

HRMS Calcd for $C_{18}H_{25}O_4$ ([M+H$^+$]): 305.1747. Found: 305.1741.

N,*N*-dimethylformamide (30 μL) was added to a solution of benzoic acid **S3** (1.8 g, 6.0 mmol) and oxalyl chloride (12 mmol, 2.0 equiv) in 18 mL of CH_2Cl_2 at 0 °C. After gas evolution ceased, the mixture was allowed to be gradually warm to room temperature and was then stirred until the starting carboxylic acid was disappeared by TLC. The solution was concentrated to give an aroyl chloride, which was used in the next step without further purification. The aroyl chloride was partially added to a solution of indole (6.0 mmol, 1 equiv), Et_3N (1 equiv) and *N*,*N*-dimethyl-4-aminopyridine (0.12 mmol) in 12 mL of CH_2Cl_2 at 0 °C. After addition was completed, the reaction mixture was stirred at room temperature for 12 hour. The reaction was quenched by the addition of H_2O, and the resulting mixture was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried ($MgSO_4$),

and concentrated to give a residue, which was purified by column chromatography on NH silica gel (hexane/CH_2Cl_2 = 1/1) to give **1g** as a colorless oil.

Colorless oil (1.46 g, 60%). R_f 0.66 (NH silica, hexane/CH_2Cl_2 = 1/1).

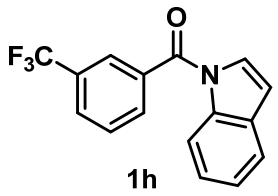
^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 0.82 (d, *J* = 6.8 Hz, 3H), 0.91–1.01 (m, 7H), 1.11–1.22 (m, 2H) , 1.53–1.64 (m, 2H), 1.73–1.79 (m, 2H), 1.93–2.04 (m, 1H), 2.12–2.17 (m, 1H), 4.98 (td, *J* = 10.9, 5.6 Hz, 1H), 6.66 (dd, *J* = 3.7, 0.8 Hz, 1H), 7.24 (d, *J* = 4.0 Hz, 1H), 7.31–7.41 (m, 2H), 7.63 (dq, *J* = 7.7, 0.7 Hz, 1H), 7.79 (dt, *J* = 8.4, 1.6 Hz, 2H), 8.18–8.21 (m, 2H), 8.40 (dd, *J* = 8.2, 1.2 Hz, 1H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 16.6, 20.9, 22.2, 23.9, 26.9, 31.8, 34.6, 41.2, 47.6, 75.8, 109.2, 116.6, 121.3, 124.4, 125.3, 127.7, 129.3, 130.0, 131.2, 134.1, 136.3, 138.6, 165.3, 168.2.

IR (KBr, cm^{-1}): 3416 w, 3363 w, 3150 m, 3120 m, 3053 m, 2955 s, 2870 s, 2722 w, 1942 w, 1713 s, 1692 s, 1606 m, 1585 m, 1572 m, 1536 s, 1504 s, 1451 s, 1405 s, 1381 s, 1343 s, 1275 s, 1244 s, 1206 s, 1186 s, 1152 s, 1117 s, 1108 s, 1065 s, 1038 m, 1018 s, 982 s, 959 s, 917 s, 891 s, 864 s, 843 s, 750 s, 733 s, 715 s.

HRMS Calcd for $C_{26}H_{30}NO_3$ ([M+H$^+$]): 404.2226. Found: 404.2220.

(1H-Indol-1-yl)(3-(trifluoromethyl)phenyl)methanone (1h) [CAS: 1792982-64-9].



1h

The general procedure I was followed using 3-(trifluoromethyl)benzoyl chloride.

White solid (4.2 g, 73%). Mp 85.0–85.3 °C. R_f 0.23 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.66 (d, *J* = 3.7 Hz, 1H), 7.20 (d, *J* = 3.7 Hz, 1H), 7.34 (dd, *J* = 7.0, 8.0 Hz, 1H), 7.42 (dd, *J* = 7.0, 7.8 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.69 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 8.02 (s, 1H), 8.41 (d, *J* = 8.0 Hz, 1H).

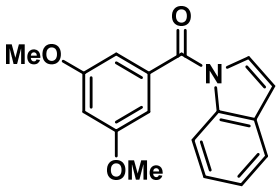
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 109.5, 116.4, 121.1, 123.4 (q, J_{CF} = 272.6 Hz), 124.3, 125.3, 126.0 (q, J_{CF} = 4.2 Hz), 126.9, 128.4, 129.3, 130.7, 131.3 (q, J_{CF} = 33.2 Hz), 132.3, 135.4, 135.9, 167.0.

IR (ATR): 2360 w, 1691 m, 1538 w, 1452 m, 1351 m, 1321 s, 1240 w, 1207 w, 1172 m, 1130 m, 1072 w, 902 w, 771 s, 703 m.

MS, *m/z* (relative intensity, %): 290 (12), 289 (M$^+$, 67), 173 (100), 145 (50).

HRMS Calcd for $C_{16}H_{11}F_3NO$ ([M+H$^+$]): 290.0793. Found: 290.0808.

(3,5-Dimethoxyphenyl)(1*H*-indol-1-yl)methanone (1i).



1i

The general procedure I was followed using 3,4-(dimethoxy)benzoyl chloride.

White solid (3.8 g, 68%). Mp 74.5–74.8 °C. R_f 0.31 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.83 (s, 6H), 6.61 (d, *J* = 3.8 Hz, 1H), 6.67 (t, *J* = 2.3 Hz, 1H), 6.85 (d, *J* = 2.3 Hz, 2H), 7.35–7.30 (m, 2H), 7.40 (dd, 7.3, 8.1 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 8.41 (d, *J* = 8.1 Hz, 1 H).

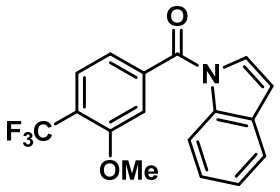
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 55.6, 103.9, 106.9, 108.6, 116.4, 120.9, 124.0, 124.9, 127.6, 130.8, 135.9, 136.3, 160.7, 168.4.

IR (ATR): 2939 w, 1687 m, 1595 m, 1527 w, 1450 m, 1331 s, 1201 m, 1157 m, 1124 m, 1065 m, 931 w, 847 w, 754 m, 688 w.

MS, *m/z* (relative intensity, %): 281 (M^+, 26), 166 (11), 165 (100), 137 (27), 122 (19), 107 (11), 77 (10).

HRMS Calcd for $C_{17}H_{16}NO_3$ ([M+H^+]): 282.1130. Found: 282.1135.

(1*H*-Indol-1-yl)(3-methoxy-4-(trifluoromethyl)phenyl)methanone (1j).



1j

The general procedure II was followed using 3-methoxy-4-(trifluoromethyl)benzoic acid (5 mmol scale).

Pale yellow solid (0.4 g, 26%). Mp 106.8–107.0 °C. R_f 0.2 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.97 (s, 3H), 6.66 (d, *J* = 3.7 Hz, 1H), 7.23 (d, *J* = 3.7 Hz, 1H), 7.37–7.31 (m, 3H), 7.34 (dd, *J* = 7.3, 7.6 Hz, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 8.42 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 56.2, 109.4, 112.3, 116.4, 120.2, 120.3 (q, J_{CF} = 273.6 Hz), 121.0,

121.6 (q, J_{CF} = 31.1 Hz), 124.4, 125.3, 127.0, 127.4 (q, J_{CF} = 5.2 Hz), 130.8, 135.8, 139.4, 157.7, 167.3.

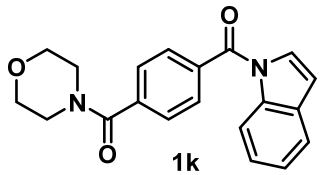
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.8 (s, 3F).

IR (ATR): 1690 m, 1617 w, 1581 w, 1536 w, 1508 w, 1452 m, 1412 m, 1380 w, 1343 s, 1315 s, 1275 w, 1232 m, 1206 m, 1176 m, 1127 m, 1073 w, 1042 m, 913 w, 879 w, 808 m, 769 m, 752 m.

MS, *m/z* (relative intensity, %): 319 (M^+, 43), 203 (100), 175 (21), 127 (21).

HRMS Calcd for $C_{17}H_{13}F_3NO_2$ ([M+H^+]): 320.0898. Found: 320.0916.

(4-(1*H*-Indole-1-carbonyl)phenyl)(morpholino)methanone (1k).



1k

The general procedure II was followed using 4-(morpholine-4-carbonyl)benzoic acid **S4** (15 mmol scale).

White solid (1.6 g, 22%). Mp 176.5–176.8 °C. R_f 0.08 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.46–3.82 (m, 8H), 6.64 (d, *J* = 3.8 Hz, 1H), 7.24 (d, *J* = 3.8 Hz, 1H), 7.33 (dd, *J* = 7.2, 7.6 Hz, 1H), 7.40 (dd, *J* = 7.2, 8.3 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 8.41 (d, *J* = 8.3 Hz, 1H).

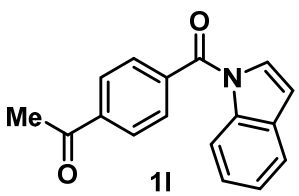
^{13}C NMR ($CDCl_3$, 150.92 MHz) δ: 42.5 (br), 48.1 (br), 66.8, 109.1, 116.3, 120.9, 124.2, 125.1, 127.1, 127.3, 129.3, 130.7, 135.9, 138.6, 167.7, 169.0.

IR (ATR): 2925 w, 1687 m, 1633 m, 1508 w, 1454 s, 1340 s, 1265 w, 1211 m, 1160 w, 1118 m, 1068 w, 1018 w, 889 w, 843 w, 746 m.

MS, *m/z* (relative intensity, %): 334 (M^+, 31), 219 (15), 218 (100), 105 (13), 104 (30), 103 (10), 76 (19).

HRMS Calcd for $C_{20}H_{19}N_2O_3$ ([M+H^+]): 335.1396. Found: 335.1395.

1-(4-(1*H*-Indole-1-carbonyl)phenyl)ethanone (1l).



1l

The general procedure II was followed using 4-acetylbenzoyl chloride (10 mmol scale).

Pale yellow solid (0.2 g, 5%). Mp 160.0–160.3 °C. R_f 0.2 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 2.69 (s, 3H), 6.66 (d, *J* = 3.7 Hz, 1H), 7.20 (d, *J* = 3.7 Hz, 1H), 7.33 (dd, *J* = 7.0, 7.3 Hz, 1H), 7.41 (dd, *J* = 7.0, 8.2 Hz, 1H), 7.61 (d, *J* = 7.3 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 2H), 8.10 (d, *J* = 7.8 Hz, 2H), 8.40 (d, *J* = 8.3 Hz, 1H).

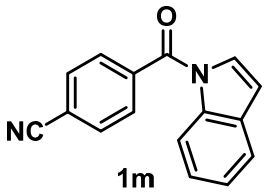
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 26.9, 109.3, 116.4, 121.0, 124.3, 125.2, 127.0, 128.4, 129.2, 130.7, 135.8, 138.5, 139.2, 167.7, 197.2.

IR (ATR): 1690 m, 1617 w, 1581 w, 1536 w, 1508 w, 1452 m, 1412 m, 1380 w, 1343 s, 1315 s, 1275 w, 1232 m, 1206 m, 1176 m, 1127 m, 1073 w, 1042 m, 913 w, 879 w, 808 m, 769 m, 752 m.

MS, *m/z* (relative intensity, %): 263 (M^+, 36), 148 (13), 147 (100), 119 (20), 91 (25), 76 (13), 43 (25).

HRMS Calcd for $C_{17}H_{14}NO_2$ ([M+H^+]): 264.1025. Found: 264.1027.

4-(1*H*-Indole-1-carbonyl)benzonitrile (1m).



1m

The general procedure I was followed using 4-cyanobenzoyl chloride.

White solid (2.7 g, 54%). Mp 117.1–117.4 °C. R_f 0.11 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.66 (d, *J* = 3.7 Hz, 1H), 7.14 (d, *J* = 3.7 Hz, 1H), 7.35 (dd, *J* = 7.3, 7.7 Hz, 1H), 7.40 (dd, *J* = 7.7, 8.3 Hz, 1H), 7.62 (d, *J* = 7.3 Hz, 1H), 7.84 (m, 4H), 8.38 (d, *J* = 8.3 Hz, 1H).

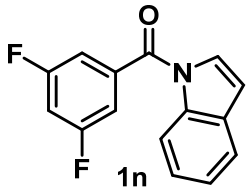
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 109.8, 115.4, 116.4, 117.7, 121.1, 124.5, 125.4, 126.6, 129.5, 130.7, 132.4, 135.8, 138.5, 166.7.

IR (ATR): 2360 w, 2233 w, 1689 m, 1536 w, 1450 w, 1378 w, 1342 m, 1211 w, 1066 w, 1018 w, 889 w, 848 w, 769 s.

MS, *m/z* (relative intensity, %): 246 (M^+, 35), 130 (100), 102 (46).

HRMS Calcd for $C_{16}H_{11}N_2O$ ([M+H^+]): 247.0871. Found: 247.0884.

(3,5-Difluorophenyl)(1*H*-indol-1-yl)methanone (1n).



1n

The general procedure I was followed using 3,5-difluorobenzoyl chloride.

Pale yellow solid (0.20 g, 4%). Mp 55.3–55.5 °C. R_f 0.31 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.67 (d, *J* = 3.7 Hz, 1H), 7.06 (tt, *J* = 2.3, 8.7 Hz, 1H), 7.23 (d, *J* = 3.7 Hz, 1H), 7.30–7.25 (m, 2H), 7.34 (dd, *J* = 7.3, 7.8 Hz, 1H), 7.40 (dd, *J* = 7.8, 8.2 Hz, 1H), 7.61 (d, *J* = 7.3 Hz, 1H), 8.40 (d, *J* = 8.2 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 107.4 (t, *J* = 25.9 Hz), 109.7, 112.3 (dd, *J* = 18.7 Hz), 116.4, 121.1, 124.5, 125.3, 126.7, 130.7 (t, *J* = 9.3 Hz), 135.8, 137.4, 162.7 (dd, *J* = 251.9 Hz), 165.9.

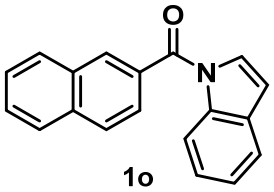
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –106.9 (s, 2F).

IR (ATR): 1691 m, 1595 m, 1537 w, 1452 m, 1381 m, 1350 s, 1205 m, 1124 m, 992 w, 878 w, 791 m, 754 m.

MS, *m/z* (relative intensity, %): 257 (M^+, 44), 141 (100), 113 (50), 63 (10).

HRMS Calcd for $C_{15}H_{10}F_2NO$ ([M+H^+]): 258.0730. Found: 258.0740.

(1*H*-Indol-1-yl)(naphthalen-2-yl)methanone (1o) [CAS: 74117-26-3].



1o

The general procedure I was followed using 2-naphthoyl chloride (27 mmol scale).

Pale pink solid (1.5 g, 20%). Mp 167.5–167.8 °C. R_f 0.11 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.64 (d, *J* = 3.6 Hz, 1H), 7.43–7.32 (m, 3H), 7.67–7.59 (m, 3H), 7.82 (d, *J* = 8.7 Hz, 1H), 8.01–7.94 (m, 3H), 8.25 (s, 1H), 8.44 (d, *J* = 8.2 Hz, 1H).

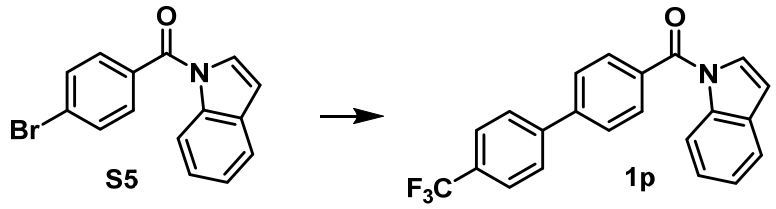
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 108.6, 116.4, 120.9, 123.9, 124.9, 125.3, 127.1, 127.7, 127.9, 128.2, 128.5, 129.0, 130.2, 130.7, 131.7, 132.2, 134.7, 136.0, 168.7.

IR (ATR): 3054 w, 1727 w, 1677 m, 1536 w, 1446 m, 1336 m, 1199 m, 1116 w, 1068 w, 1012 w, 960 w, 912 w, 800 w, 771 s.

MS, *m/z* (relative intensity, %): 271 (M^+, 33), 156 (12), 155 (100), 127 (70).

HRMS Calcd for $C_{19}H_{14}NO$ ([M+H$^+$]): 272.1075. Found: 272.1074.

(1*H*-Indol-1-yl)(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)methanone (1p).



The general procedure I was followed using 4-bromobenzoyl chloride to give (4-bromophenyl)(1*H*-indol-1-yl)methanone **S5**, which was purified by recrystallization with hexane/EtOAc (100m L/20 mL) (white solid, 3.2 g, 53%).

Mp 120.9–121.5 °C. R_f 0.36 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 6.66 (dd, *J* = 3.6, 0.4 Hz, 1H), 7.27 (d, *J* = 3.6 Hz, 1H), 7.30–7.40 (m, 2H), 7.60–7.65 (m, 3H), 7.70 (dt, *J* = 8.4, 2.0 Hz, 2H), 8.36 (dd, *J* = 8.0, 0.8 Hz, 1H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 109.1, 116.5 , 121.3, 124.4, 125.3, 126.9, 127.7, 131.1, 132.3, 132.7, 133.8, 136.4, 167.9.

^{19}F NMR (CD_2Cl_2, 376.17 MHz) δ: –62.4 (s, 3F).

IR (KBr): 3348 w, 3173 w, 3116 w, 3079 m, 3051 w, 3034 w, 1945 w, 1925 w, 1800 w, 1742 w, 1678 s, 1604 m, 1587 s, 1540 m, 1504 w, 1482 m, 1471 m, 1451 s, 1395 s, 1381 s, 1351 s, 1292 m, 1277 m, 1246 m, 1205 s, 1186 s, 1149 s, 1126 m, 1113 m, 1090 m, 1073 m, 1065 m, 1010 s, 971 w, 957 w, 944 m, 889 s, 872 s, 841 s, 769 s, 746 s, 732 s, 689 m.

HRMS Calcd for $C_{15}H_{11}NOBr$ ([M+H$^+$]): 300.0019. Found: 300.0011.

A dry three-necked flask was charged with (4-bromophenyl)(1*H*-indol-1-yl)methanone **S5** (1.5 g, 5 mmol), (4-(trifluoromethyl)phenyl)boronic acid (1.07 g, 5.6 mmol), 2M K_2CO_3 aq.(15 mL), $Pd(PPh_3)_4$ (18.8 mg, 0.015 mmol), and THF (50 mL) under a nitrogen atmosphere, and the resulting mixture was heated at reflux for 12 h. The mixture was then cooled to room temperature and treated with deionized water, and the resulting mixture was extracted with EtOAc. The combined extracts were then washed with brine, dried ($MgSO_4$) and concentrated to give a residue, which was purified by column chromatography (hexane/EtOAc = 10/1) to give **1p** as a white solid.

White solid (1.3 g, 37%). Mp 192.2–292.3 °C. R_f 0.26 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.66 (d, *J* = 3.6 Hz, 1H), 7.32–7.36 (m, 2H), 7.42 (dd, *J* = 7.4, 8.1 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 1 H), 7.71–7.75 (m, 6H), 7.86 (d, *J* = 8.5 Hz, 2H), 8.44 (d, *J* = 8.2 Hz,

1H).

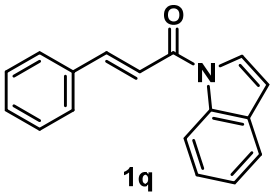
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 108.8, 116.4, 120.9, 124.1 (q, J_{CF} = 272.1 Hz), 124.1, 125.0, 126.0 (q, J_{CF} = 3.7 Hz), 127.4, 127.5, 127.6, 130.0, 130.3 (q, J_{CF} = 32.9 Hz), 130.8, 134.1, 136.0, 143.2, 143.3, 168.2.

IR (ATR): 3005 w, 2360 w, 1710 s, 1423 w, 1360 m, 1228 m, 1092 w, 899 w.

MS, *m/z* (relative intensity, %): 365 (M^+, 23), 249 (100), 250 (16), 201 (21), 152 (29).

HRMS Calcd for $C_{22}H_{15}F_3NO$ ([M+H^+]): 366.1106. Found: 366.1121.

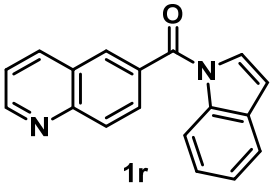
(*E*)-1-(1*H*-indol-1-yl)-3-phenylprop-2-en-1-one (1q) [CAS 201486-55-7].



1q

The general procedure I was followed using ciannamoyl chloride. Spectroscopic data were consistent with those reported in the literature.[12]

(1*H*-Indol-1-yl)(quinolin-6-yl)methanone (1r).



1r

The general procedure II was followed using quinoline-6-carboxylic acid (30 mmol scale).

White solid (1.1 g, 13%). Mp 129.0–129.5 °C. R_f 0.1 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.66 (d, *J* = 3.7 Hz, 1H), 7.36–7.31 (m, 2H), 7.41 (dd, *J* = 7.4, 7.8 Hz, 1H), 7.53 (dd, *J* = 4.1, 8.3 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 8.29–8.25 (m, 3H), 8.41 (d, *J* = 8.2 Hz, 1H), 9.06 (d, *J* = 4.1 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 109.1, 116.4, 121.1, 122.3, 124.1, 125.1, 127.36, 127.38, 128.9, 130.0, 130.2, 130.7, 132.5, 136.0, 137.0, 149.2, 152.5, 168.0.

IR (ATR): 1690 m, 1617 w, 1581 w, 1536 w, 1508 w, 1452 m, 1412 m, 1380 w, 1343 s, 1315 s, 1275

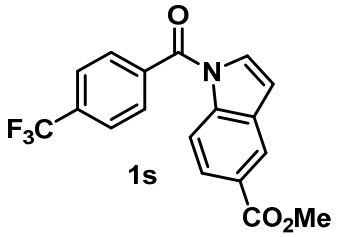
[12] Yang, Y.; Duan, X.-H.; Deng, J.-Y.; Jin, B.; Jia, H.-M.; Liu, B.-L. *Bioorg. Med. Chem. Lett.* **2011**, *21*, 5594.

w, 1232 m, 1206 m, 1176 m, 1127 m, 1073 w, 1042 m, 913 w, 879 w, 808 m, 769 m, 752 m.

MS, *m/z* (relative intensity, %): 272 (M^+, 37), 157 (11), 156 (100), 101 (18).

HRMS Calcd for $C_{18}H_{13}N_2O$ ([M+H^+]): 273.1028. Found: 273.1034.

Methyl 1-(4-(trifluoromethyl)benzoyl)-1*H*-indole-5-carboxylate (1s).



The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (5.4 g, 78%). Mp 142.9–143.2 °C. R_f 0.14 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.96 (s, 3H), 6.72 (d, *J* = 3.7 Hz, 1H), 7.27 (d, *J* = 3.7 Hz, 1H), 7.87–7.81 (m, 4H), 8.10 (d, *J* = 8.7 Hz, 1H), 8.35 (s, 1H), 8.44 (d, *J* = 8.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 52.2, 109.6, 116.1, 123.2, 123.4 (q, J_{CF} = 272.6 Hz), 125.8 (q, J_{CF} = 3.1 Hz), 126.2, 126.5, 128.1, 129.5, 130.5, 133.8 (q, J_{CF} = 33.2 Hz), 137.3, 138.5, 167.2, 167.3.

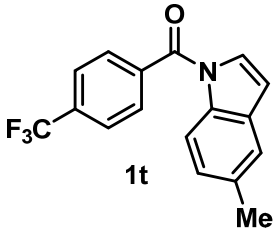
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –63.0 (s, 3F).

IR (ATR): 3127 w, 1697 m, 1609 w, 1580 w, 1536 w, 1469 w, 1440 m, 1407 w, 1376 m, 1348 w, 1320 s, 1284 w, 1235 m, 1176 s, 1106 s, 1063 m, 1016 w, 989 w, 908 w, 887 m, 852 m, 759 m, 727 w, 701 w, 670 w.

MS, *m/z* (relative intensity, %): 347 (M^+, 35), 173 (100), 145 (39).

HRMS Calcd for $C_{18}H_{13}F_3NO_3$ ([M+H^+]): 348.0848. Found: 348.0848.

(5-Methyl-1*H*-indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (1t).



The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride (18 mmol).

White solid (3.7 g, 67%). Mp 157.0–159.9 °C. R_f 0.34 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 2.48 (s, 3H), 6.58 (d, *J* = 3.5 Hz, 1H), 7.14 (d, *J* = 3.5 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.40 (s, 1H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.84 (d, *J* = 8.2 Hz, 2H), 8.28 (d, *J* = 8.4

Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 21.4, 109.3, 116.1, 121.0, 123.5 (q, J_{CF} = 272.6 Hz), 125.6 (q, J_{CF} = 3.1 Hz), 126.6, 127.0, 129.3, 131.0, 133.4 (q, J_{CF} = 32.1 Hz), 134.0, 138.0, 138.0, 167.1.

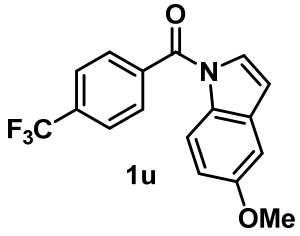
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.9 (s, 3F).

IR (ATR): 1675 w, 1467 w, 1407 w, 1375 w, 1323 m, 1215 w, 1191 w, 1163 w, 1128 m, 1110 w, 1073 w, 1017 w, 908 m, 888 w, 854 w, 814 w, 756 s, 687 w, 669 w.

MS, *m/z* (relative intensity, %): 303 (M^+, 49), 173 (100), 145 (45).

HRMS Calcd for $C_{17}H_{13}F_3NO$ ([M+H^+]): 304.0949. Found: 304.0945.

(5-Methoxy-1*H*-indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (1u).



The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

Pale yellow solid (4.9 g, 77%). Mp 139.5–140.0 °C. R_f 0.2 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.88 (s, 3H), 6.58 (d, *J* = 3.6 Hz, 1H), 7.01 (dd, *J* = 2.8, 8.7 Hz, 1H), 7.07 (d, *J* = 2.8 Hz, 1H), 7.14 (d, *J* = 3.6 Hz, 1H), 7.85–7.79 (m, 4H), 8.33 (d, *J* = 8.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 55.6, 103.7, 109.4, 113.6, 117.3, 123.5 (q, J_{CF} = 272.6 Hz), 125.6 (q, J_{CF} = 4.1 Hz), 127.6, 129.3, 130.5, 131.8, 133.2 (q, J_{CF} = 33.2 Hz), 137.9, 156.9, 166.9.

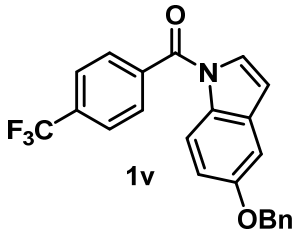
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.9 (s, 3F).

IR (ATR): 2965 w, 1676 m, 1613 m, 1588 w, 1540 w, 1476 m, 1440 m, 1406 m, 1380 m, 1321 m, 1275 m, 1200 m, 1187 m, 1164 s, 1131 s, 1110 m, 1074 m, 1027 m, 941 w, 911 w, 888 m, 853 m, 821 m, 796 w, 755 m, 726 m, 688 w.

MS, *m/z* (relative intensity, %): 320 (13), 319 (M^+, 67), 173 (100), 145 (40).

HRMS Calcd for $C_{17}H_{13}F_3NO_2$ ([M+H^+]): 320.0898. Found: 320.0886.

(5-(Benzyloxy)-1*H*-indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (1v).



The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (5.5 g, 69%). Mp 177.0–177.3 °C. R_f 0.2 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 5.15 (s, 2H), 6.57 (d, *J* = 3.7 Hz, 1H), 7.10 (d, *J* = 9.2 Hz, 1H), 7.15–7.14 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.41 (dd, *J* = 7.0, 7.6 Hz, 2H), 7.48 (d, *J* = 7.0 Hz, 2H), 7.85–7.79 (m, 4H), 8.34 (d, *J* = 9.2 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 70.5, 105.1, 109.4, 114.4, 117.3, 123.5 (q, J_{CF} = 272.6 Hz), 125.6 (q, J_{CF} = 3.1 Hz), 127.5, 127.6, 127.9, 128.6, 129.3, 130.7, 131.7, 133.3 (q, J_{CF} = 33.2 Hz), 137.0, 137.9, 156.1, 166.9.

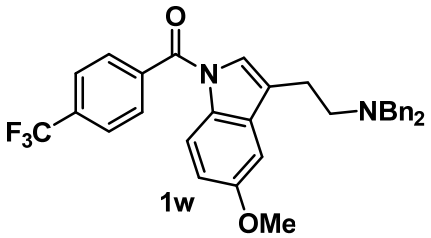
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.9 (s, 3F).

IR (ATR): 1673 s, 1586 w, 1538 w, 1454 w, 1406 w, 1383 m, 1334 w, 1272 w, 1193 m, 1156 m, 1138 m, 1114 s, 1078 m, 1017 w, 909 w, 889 w, 855 w, 815 w, 751 s, 727 m, 704 m.

MS, *m/z* (relative intensity, %): 395 (M^+, 27), 173 (37), 145 (18), 91 (100).

HRMS Calcd for $C_{23}H_{17}F_3NO_2$ ([M+H^+]): 396.1211. Found: 396.1210.

(3-(2-(Dibenzylamino)ethyl)-5-methoxy-1*H*-indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (1w).



The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride and 2-(5-methoxy-1*H*-indol-3-yl)-*N*,*N*-bis(phenylmethyl)ethanamine **S6**.

White solid (2.4 g, 44%). Mp 122.5–123.4 °C. R_f 0.23 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 2.72–2.78 (m, 2H), 2.81–2.86 (m, 2H), 3.62 (s, 4H), 3.75 (s, 3H), 6.77 (d, *J* = 2.4 Hz, 1H), 6.90 (s, 1H), 6.94 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.16–7.25 (m, 6H), 7.28–7.31 (m, 4H), 7.79 (s, 4H), 8.27 (d, *J* = 8.8 Hz, 1H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 23.2, 53.0, 55.9, 58.6, 102.1, 113.7, 117.6, 121.7, 124.1(q, J_{CF} =

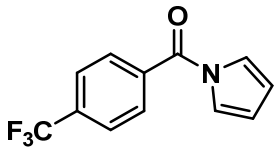
272.4 Hz), 125.0, 125.9 (qt, J_{CF} = 3.6 Hz), 127.1, 128.4, 128.9, 129.6, 131.0, 132.6, 133.1(q, J_{CF} = 32.6 Hz), 138.8, 140.1, 157.2, 166.8.

^{19}F NMR (CD_2Cl_2, 376.17 MHz) δ: –63.2 (s, 3F).

IR (KBr, cm^{-1}): 3069 m, 3031 m, 2963 m, 2838 m, 2807 m, 1934 w, 1859 w, 1804 w, 1747 w, 1734 w, 1681 s, 1620 m, 1601 s, 1576 m, 1514 m, 1496 m, 1477 s, 1451 s, 1439 s, 1389 s, 1325 s, 1265 s, 1227 s, 1209 s, 1173 s, 1117 s, 1065 s, 1029 s, 980 s, 930 s, 901 s, 849 s, 819 s, 778 s, 770 s, 747 s, 728 s, 698 s, 660 m.

HRMS Calcd for $C_{33}H_{30}F_3N_2O_2$ ([M+H$^+$]): 543.2259. Found: 543.2254.

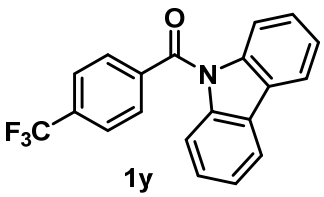
(1*H*-Pyrrol-1-yl)(4-(trifluoromethyl)phenyl)methanone (1x) [CAS 633313-82-3].



1x

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride. Spectroscopic data were consistent with those reported in the literature.[13]

(9*H*-Carbazol-9-yl)(4-(trifluoromethyl)phenyl)methanone (1y).



1y

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (5.42 g, 77%). Mp 143.5–143.7 °C. R_f 0.31 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.33–7.40 (m, 4H), 7.49 (d, J = 8.2 Hz, 2H), 7.80–7.86 (m, 4H), 8.02 (d, J = 7.8 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 115.7, 120.0, 123.5 (q, J_{CF} = 272.6 Hz), 123.9, 126.0 (q, J_{CF} = 3.1 Hz), 126.2, 127.0, 129.3, 133.8 (q, J_{CF} = 32.2 Hz), 138.8, 139.0, 168.1.

^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.8 (s, 3F).

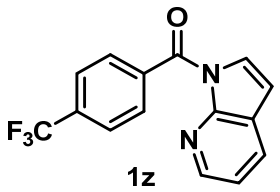
[13] Meng, G.; Szostak, R.; Szostak, M. *Org. Lett*. **2017**, *19*, 3596.

IR (ATR): 1678 m, 1585 w, 1513 w, 1478 w, 1443 m, 1408 w, 1360 w, 1302 s, 1214 w, 1169 m, 1128 s, 1075 m, 1064 m, 1018 w, 948 w, 873 w, 840 w, 753 s, 722 m, 700 w, 672 w.

MS, *m/z* (relative intensity, %): 339 (M^+, 44), 173 (100), 145 (41).

HRMS Calcd for $C_{20}H_{13}F_3NO$ ([M+H^+]): 340.0944. Found: 340.0945

(1*H*-Pyrrolo[2,3-b]pyridin-1-yl)(4-(trifluoromethyl)phenyl)methanone (1z).



1z

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (3.1 g, 53%). Mp 91.7–92.0 °C. R_f 0.2 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.68 (d, *J* = 4.1 Hz, 1H), 7.19 (dd, *J* = 4.6, 7.8 Hz, 1H), 7.74–7.77 (m, 3H), 7.89–7.93 (m, 3H), 8.23 (d, *J* = 4.6 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 106.6, 119.3, 123.3, 125.0 (q, J_{CF} = 272.6 Hz), 127.0, 127.7 (q, J_{CF} = 3.1 Hz), 129.4, 130.3, 133.8 (q, J_{CF} = 32.2 Hz), 137.4, 144.4, 148.0, 166.5.

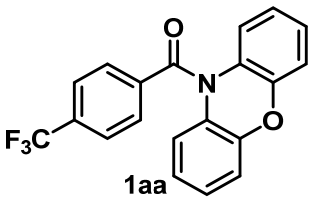
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.9 (s, 3F).

IR (ATR): 1687 s, 1583 w, 1531 w, 1409 s, 1330 w, 1268 m, 1160 m, 1112 s, 1068 m, 1018 w, 925 w, 852 w, 804 w, 771 m, 725 w, 692 w.

MS, *m/z* (relative intensity, %): 290 (M^+, 33), 289 (50), 263 (13), 262 (80), 173 (100).

HRMS Calcd for $C_{15}H_{10}F_3N_2O$ ([M+H^+]): 291.0745. Found: 291.0748.

(10*H*-Phenoxazin-10-yl)(4-(trifluoromethyl)phenyl)methanone (1aa).



1aa

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

Pale yellow solid (5.5 g, 77%). Mp 131.1–131.6 °C. R_f 0.2 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.94–6.99 (m, 2H), 7.15–7.17 (m, 4H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.55 (m, 4H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 116.8, 123.45, 123.53 (q, J_{CF} = 272.6 Hz), 124.6, 125.1 (q, J_{CF} = 3.1 Hz), 126.9, 129.2, 129.5, 132.2 (q, J_{CF} = 33.2 Hz), 138.5, 150.3, 166.7.

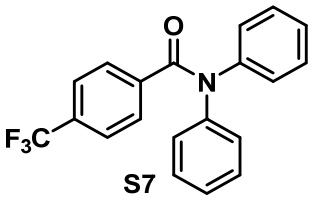
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.8 (s, 3F).

IR (ATR): 1668 m, 1579 w, 1481 m, 1409 w, 1321 s, 1272 m, 1170 w, 1128 m, 1087 w, 1066 w, 1020 w, 883 w, 842 w, 765 m, 669 w.

MS, *m/z* (relative intensity, %): 355 (M^+, 22), 182 (100), 173 (28), 145 (11).

HRMS Calcd for $C_{20}H_{13}F_3NO_2$ ([M+H^+]): 356.0898. Found: 356.0894.

_N_,_N_-Diphenyl-4-(trifluoromethyl)benzamide (S7) [CAS 77826-14-3].



S7

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (3.7 g, 54%). Mp 142.0–142.4 °C. R_f 0.1 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.15–7.23 (m, 6H), 7.29–7.33 (m, 4H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H).

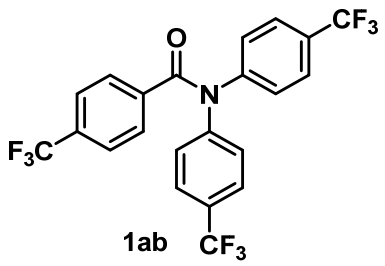
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 123.6 (q, J_{CF} = 272.6 Hz), 124.9 (q, J_{CF} = 4.2 Hz), 126.8, 127.4, 129.26, 129.34, 131.7 (q, J_{CF} = 32.1 Hz), 139.6, 143.2, 169.1.

IR (ATR): 2356 w, 1660 m, 1592 w, 1488 w, 1407 w, 1319 s, 1218 w, 1168 m, 1124 m, 1066 w, 1020 w, 840 w, 769 s, 696 m.

MS, *m/z* (relative intensity, %): 341 (M^+, 29), 248 (39), 173 (100), 167 (10), 145 (41).

HRMS Calcd for $C_{20}H_{15}F_3NO$ ([M+H^+]): 342.1100. Found: 342.1101.

4-(Trifluoromethyl)-_N_,_N_-bis(4-(trifluoromethyl)phenyl)benzamide (1ab).



1ab

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (685 mg, 18%). Mp 112.4–112.8 °C. R_f 0.14 (SiO_2, hexane/$CHCl_3$ = 1/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 7.27 (d, J = 8.4 Hz, 4H), 7.54–7.62 (m, 8H).

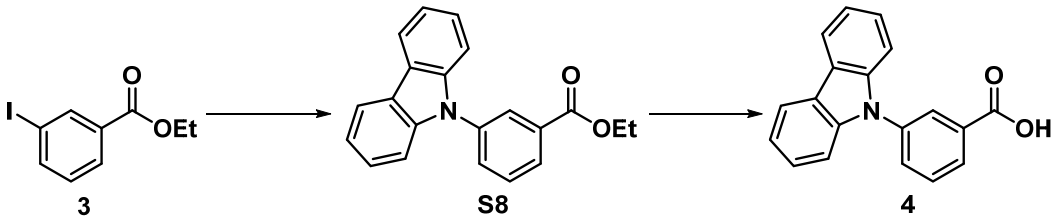
^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 124.0(q, J_{CF} = 272.6 Hz), 124.2(q, J_{CF} = 272.2 Hz), 125.7(qt, J_{CF} = 3.6 Hz), 126.9(qt, J_{CF} = 3.8 Hz), 128.1, 129.0(q, J_{CF} = 32.8 Hz), 129.9, 132.6(q, J_{CF} = 32.6 Hz) , 139.0, 146.4, 169.3.

^{19}F NMR (CD_2Cl_2, 376.17 MHz) δ: –61.4 (s, 6F), –60.8 (s, 3F).

IR (KBr, cm^{-1}): 3314 w, 3082 w, 2931 w, 2640 w, 1919 w, 1805 w, 1752 w, 1666 s, 1613 s, 1583 m, 1516 s, 1409 s, 1325 s, 1170 s, 1127 s, 1110 s, 1068 s, 1019 s, 963 m, 953 m, 876 m, 845 s, 770 s, 741 w, 722 w, 703 m, 656 m.

HRMS Calcd for $C_{22}H_{13}F_9NO$ ([M+H$^+$]):478.0848. Found: 478.0853.

3-(9*H*-Carbazol-9-yl)benzoic acid (4) [CAS: 19287-67-3].



A mixture of carbazole (4.68 g, 28.0 mmol), ethyl 3-iodobenzoate **3** (5.52 g, 20.0 mmol), CuI (762 mg, 4.0 mmol), Cs_2CO_3 (13.0 g, 40 mmol) in DMF (40 mL) was vigorously stirred at 120 °C under nitrogen atmosphere for 24 h. After cooling the mixture to ambient temperature, the reaction mixture was diluted with EtOAc (160 mL) and washed with H_2O (2×120 mL). The aqueous phase was extracted with EtOAc (2×120 mL), and the combined organic phases were dried over Na_2SO_4. After filtration and evaporation of the solvents in vacuo, the crude product was purified by column chromatography on silica gel (hexane/EtOAc = 9/1) to give **S8**[14] (3.00 g, 48%) as a white solid. White solid (3.00 mg, 48%). Mp 91.1–92.0 °C. R_f 0.37 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 1.41 (t, J = 7.1 Hz, 3H), 4.43 (q, J = 7.0 Hz, 2H), 7.30–7.34 (m, 2H), 7.39–7.46 (m, 4H), 7.70 (t, J = 7.8 Hz, 1H), 7.78 (dt, J = 7.9, 1.7 Hz, 1H), 8.17 (dd, J = 7.8, 0.9 Hz, 3H), 8.28 (t, J = 1.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 14.3, 61.4, 109.6, 120.2, 120.4, 123.5, 126.1, 128.2, 128.5, 130.0, 131.5, 132.6, 138.0, 140.7, 165.8.

IR (KBr, cm^{-1}): 3042 w, 2991 m, 1732 s, 1596 m, 1498 m, 1480 m, 1451 s, 1365 s, 1336 m, 1314 m, 1292 s, 1260 s, 1227 s, 1179 m, 1120 m, 1099 m, 1080 s, 1023 s, 1003 w, 920 m, 879 w, 750 s, 721 s, 690 s.

MS, *m/z* (relative intensity, %): 316(23), 315 (M$^+$, 100), 288(15), 287 (70), 242(23), 241 (42), 240(11),

[14] Swapna, K.; Murthy, S. N.; Nageswar, Y. V. D. *Eur. J. Org. Chem*. **2010**, *2010*, 6678.

135(11), 121 (39), 316 (21), 144 (11), 143 (10).

HRMS Calcd for $C_{21}H_{17}NO_2$ ([M^+]): 315.1259. Found: 312.1255.

Ethyl 3-(9*H*-carbazol-9-yl)benzoate **S8** (2.71 g, 8.6 mmol) in mixed solution of MeOH (25 mL), THF (25 mL), 1 M NaOH aq. (17.2 mL, 17.2 mmol) was stirred at 50 °C for 8 h. After cooling the mixture to ambient temperature, 1M HCl aq (17.2 mL, 17.2 mmol) was added to the reaction solution, and the precipitated solid was collected by filtration and dried to give **4**.

White solid (2.36 g, 96%). Mp 233.4–234.3 °C. R_f 0.71 (SiO_2, methanol/EtOAc = 1/1).

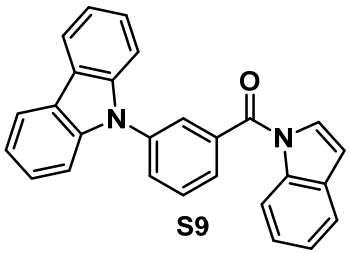
^{1}H NMR (CD_3OD, 399.78 MHz) δ: 4.85 (s, 1H), 7.25–7.28 (m, 2H), 7.34–7.42 (m, 4H), 7.73–7.81 (m, 2H), 8.13–8.16 (m, 3H), 8.18 (t, *J* = 1.8 Hz, 1H).

^{13}C NMR (CD_3OD, 100.53 MHz) δ: 110.5, 121.3, 121.4, 124.9, 127.3, 129.0, 129.7, 131.4, 132.5, 134.2, 139.4, 142.0, 168.9.

IR (KBr, cm^{-1}): 3042 m, 2827 m, 2679 m, 2575 m, 1683 s, 1586 s, 1492 s, 1463 s, 1450 s, 1362 s, 1307 s, 1229 s, 1166 m, 1149 m, 1119 m, 1084 w, 1002 m, 979 m, 939 m, 927 m, 815 w, 746 s, 722 s, 691 s, 669 m.

HRMS Calcd for $C_{19}H_{13}NO_2$ ([M^+]): 287.0946. Found: 287.0946.

(3-(9*H*-Carbazol-9-yl)phenyl)(1*H*-indol-1-yl)methanone (S9).



S9

DMF (30 μL) was added to a solution of (3 mmol) and oxalyl chloride (6 mmol, 2 equiv) in 30 mL of CH_2Cl_2 at 0 °C. After gas evolution **4** ceased, the mixture was allowed to be gradually warm to room temperature and was then stirred until the starting carboxylic acid was disappeared by TLC. The solution was concentrated to give an aroyl chloride, which was used in the next step without further purification. The aroyl chloride was partially added to a solution of indole (3 mmol, 1 equiv), Et_3N (1 equiv) and *N*,*N*-dimethyl-4-aminopyridine (0.06 mmol) in 40 mL of CH_2Cl_2 at 0 °C. After addition was completed, the reaction mixture was stirred at room temperature for 12 hour. The reaction was quenched by the addition of H_2O, and the resulting mixture was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried ($MgSO_4$), and concentrated to give a residue, which was purified by column chromatography and GPC to give a white solid.

White solid (712 mg, 60%). Mp 74.2–76.1 °C. R_f 0.69 (NH silica, hexane/CH_2Cl_2 = 1/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 6.69 (d, *J* = 3.7 Hz, 1H), 7.31–7.36 (m, 3H), 7.39–7.51 (m, 6H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.79–7.89 (m, 3H), 7.98 (t, *J* = 1.6 Hz, 1H), 8.17 (d, *J* = 7.8 Hz, 2H), 8.43 (d, *J* = 8.2 Hz, 1H).

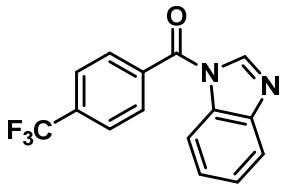
^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 119.2, 120.1, 126.8, 130.8, 130.9, 131.5, 133.9, 134.5, 135.4, 136.7, 137.8, 138.0, 138.4, 140.7, 140.9, 141.3, 146.5, 147.0, 148.5, 150.9, 177.9.

IR (KBr, cm^{-1}): 3055 w, 1687 s, 1597 m, 1584 m, 1535 m, 1495 s, 1477 m, 1451 s, 1378 s, 1362 s, 1337 s, 1230 s, 1206 s, 1150 m, 1123 w, 1067 w, 1016 w, 926 w, 889 m, 872 w, 809 w, 750 s, 724 s, 699 m.

MS, *m/z* (relative intensity, %): 387 (19), 386 (M^+, 57), 271 (13), 270 (57), 243 (17), 242 (100), 241 (71), 240 (11), 207 (22), 193 (15), 121 (15), 116 (11), 73 (20), 44 (11).

HRMS Calcd for $C_{27}H_{18}N_2O$ ([M^+]): 386.1419. Found: 386.1425.

(1*H*-Benzo[*d*]imidazol-1-yl)(4-(trifluoromethyl)phenyl)methanone (7b) [CAS: 1907216-47-0].



7b

The general procedure I was followed using 4-(trifluoromethyl)benzoyl chloride.

White solid (4.4 g, 75%). Mp 161.1–161.4 °C. R_f 0.49 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.43–7.49 (m, 2H), 7.83–7.88 (m, 3H), 7.93 (d, *J* = 8.1 Hz, 2H), 8.14 (s, 1H), 8.18–8.20 (m, 1H).

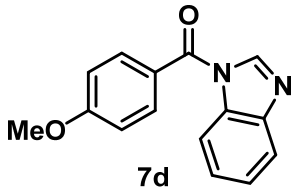
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 165.8, 144.0, 142.5, 136.1, 134.6 (q, J_{CF} = 33.2 Hz), 131.8, 129.8, 126.1 (q, J_{CF} = 4.2 Hz), 126.1, 125.7, 123.2 (q, J_{CF} = 272.6 Hz), 120.7, 115.5.

IR (ATR): 3101 w, 2360 w, 1697 m, 1606 w, 1514 w, 1452 w, 1410 w, 1369 w, 1327 m, 1198 m, 1167 m, 1130 m, 1066 w, 906 w, 852 w, 756 s.

MS, *m/z* (relative intensity, %): 290 (M^+, 46), 174 (14), 173 (100), 145 (89), 95 (16), 90 (10).

HRMS Calcd for $C_{15}H_{10}F_3N_2O$ ([M+H^+]): 291.0740. Found: 291.0747.

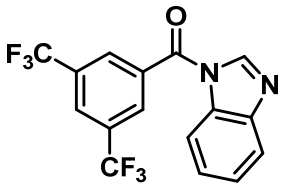
(1*H*-Benzo[*d*]imidazol-1-yl)(4-methoxyphenyl)methanone (7d) [CAS: 13361-55-2].



7d

The general procedure I was followed using 4-methoxybenzoyl chloride. Spectroscopic data were consistent with those reported in the literature.[15]

(1*H*-Benzo[*d*]imidazol-1-yl)(3,5-bis(trifluoromethyl)phenyl)methanone (7e) [CAS: 1899226-42-6].



7e

The general procedure I was followed using 3,5-bis(trifluoromethyl)benzoyl chloride (6 mmol scale). White solid (1.2 g, 55%). Mp 84.7–84.1 °C. *Rf* 0.66 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 8.27 (s, 2H), 8.21 (s, 1H), 8.21–8.16 (m, 1H), 8.10 (s, 1H), 7.87–7.85 (m, 1H), 7.52–7.46 (m, 2H).

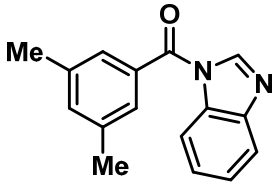
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 164.1, 144.1, 141.8, 134.9, 133.0 (q, J_{CF} = 34.2 Hz), 131.7, 129.4 (q, J_{CF} = 3.1 Hz), 126.5 (qt, J_{CF} = 3.1 Hz), 126.0, 122.5 (q, J_{CF} = 273.1 Hz), 120.9, 118.4, 115.4.

IR (ATR): 2360 w, 1707 m, 1512 w, 1452 w, 1396 w, 1356 m, 1284 s, 1180 s, 1142 s, 910 w, 771 s, 708 w.

MS, *m/z* (relative intensity, %): 358 (M^+, 33), 242 (10), 241 (100), 213 (48), 163 (10).

HRMS calcd for $C_{16}H_9F_6N_2O$ ([M+H^+]): 359.0614. Found: 359.0628.

(1*H*-Benzo[*d*]imidazol-1-yl)(3,5-dimethylphenyl)methanone (7f).



7f

[15] Ding, W.; Mai, S.; Song, Q. *Beilstein. J. Org. Chem.* **2015**, *11*, 2158.

The general procedure I was followed using 3,5-dimethylbenzoyl chloride.

White solid (1.7 g, 35%). Mp 197.4–197.8 °C. R_f 0.54 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 8.23 (s, 1H), 8.22–8.20 (m, 1H), 7.85–7.83 (m, 1H), 7.48–7.40 (m, 4H), 7.31 (s, 1H), 2.42 (s, 6H).

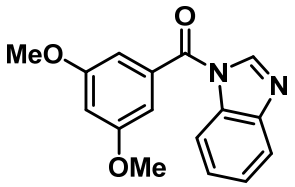
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 167.5, 144.1, 143.3, 138.9, 134.8, 132.8, 132.1, 127.2, 125.7, 125.2, 120.5, 115.5, 21.2.

IR (ATR): 2349 w, 1720 w, 1650 w, 1518 m, 1364 m, 1281 m, 1241 m, 1217 m, 1176 m, 1145 m, 1024 w, 912 w, 771 s, 709 m, 663 w.

MS, *m/z* (relative intensity, %): 250 (M^+, 18), 133 (100), 105 (34), 103 (10), 79 (17), 77 (17).

HRMS calcd for $C_{16}H_{15}N_2O$ ([M+H$^+$]): 251.1179. Found: 251.1186.

(1*H*-Benzo[*d*]imidazol-1-yl)(3,5-dimethoxyphenyl)methanone (7g) [CAS: 333347-97-0].



7g

The general procedure I was followed using 3,5-dimethoxybenzoyl chloride.

White solid (4.1 g, 73%). Mp 109.2–109.5 °C. R_f 0.36 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 8.27 (s, 1H), 8.23–8.20 (m, 1H), 7.85–7.83 (m, 1H), 7.49–7.42 (m, 2H), 6.89 (d, J = 2.3 Hz, 2H), 6.73 (d, J = 2.3 Hz, 1H), 2.29 (s, 6H).

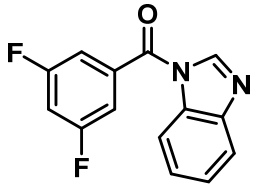
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 166.9, 161.1, 144.1, 143.1, 134.6, 132.1, 125.8, 125.3, 120.6, 115.5, 107.2, 105.1, 55.7.

IR (ATR): 2360 m, 1705 m, 1599 m, 1510 m, 1452 m, 1360 m, 1284 s, 1146 m, 1063 m, 771 s.

MS, *m/z* (relative intensity, %): 282 (M^+, 24), 165 (100), 137 (29), 122 (22), 107 (13), 77 (12).

HRMS calcd for $C_{16}H_{15}N_2O_3$ ([M+H$^+$]): 283.1077. Found: 283.1099.

(1*H*-Benzo[*d*]imidazol-1-yl)(3,5-difluorophenyl)methanone (7h) [CAS: 1789402-95-4].



7h

The general procedure I was followed using 3,5-difluorobenzoyl chloride.

White solid (3.4 g, 66%). Mp 125.0–125.3 °C. R_f 0.54 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 8.20–8.16 (m, 2H), 7.86–7.83 (m, 1H), 7.50–7.44 (m, 2H), 7.37-7.31 (m, 2H), 7.16 (tt, J = 2.3, 8.5 Hz, 1H).

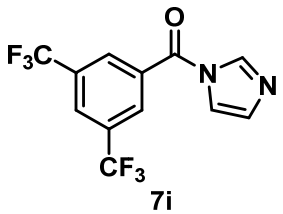
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 164.4 (t, J_{CF} = 3.0 Hz), 163.0 (dd, J_{CF} = 12.0, 253.5 Hz), 144.1, 142.2, 135.6 (t, J_{CF} = 8.8 Hz), 131.8, 126.2, 125.7, 120.8, 115.4, 112.72 (dd, J_{CF} = 8.3, 19.4 Hz), 108.7 (t, J_{CF} = 24.9 Hz).

IR (ATR): 3094 m, 1692 m, 1598 m, 1513 m, 1477 m, 1452 m, 1378 s, 1324 m, 1287 m, 1221 m, 1193 m, 1133 m, 1000 m, 978 m, 912 w, 869 m, 799 s, 772 s, 754 s, 678 w.

MS, *m/z* (relative intensity, %): 259 (10), 258 (M^+, 60), 142 (18), 141 (100), 113 (86), 90 (11), 63 (35).

HRMS calcd for $C_{14}H_9F_2N_2O$ ([M+H$^+$]): 259.0677. Found: 259.0703.

(3,5-bis(trifluoromethyl)phenyl)(1*H*-imidazol-1-yl)methanone (7i).



7i

The general procedure I was followed using 3,5-bis(trifluoromethyl)benzoyl chloride.

White solid (4.6 g, 75%). Mp 125.0–125.3 °C. R_f 0.66 (SiO_2, EtOAc).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 8.30 (s, 2H), 8.20 (s, 1H), 8.06 (s, 1H), 7.51 (t, J = 1.5 Hz, 1H), 7.24 (s, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 163.4, 137.7, 134.0, 133.1 (q, J_{CF} = 34.5 Hz), 132.1, 129.6 (q, J_{CF} = 3.6 Hz), 126.9 (qt, J_{CF} = 3.7 Hz), 122.4 (q, J_{CF} = 273.2 Hz), 117.7.

^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.9 (s, 6F).

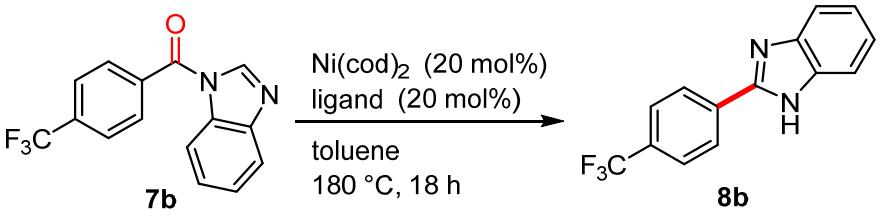
IR (ATR): 1720 m, 1621 w, 1472 w, 1397 m, 1365 m, 1281 s, 1242 m, 1175 m, 1137 s, 1024 m, 947 w, 911 m, 774 s, 710 m, 681 m.

MS, *m/z* (relative intensity, %): 308 (M^+, 13), 242 (13), 241 (100), 213 (76), 163 (21), 144 (11), 143 (10).

HRMS calcd for $C_{12}H_7F_6N_2O$ ([M+H$^+$]): 309.0457. Found: 309.0469.

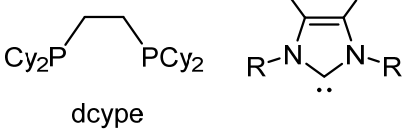
IV. Optimization Studies.

1,2-Migratory decarbonylation of *N*-acyl imidazoles.



entry	ligand	GC yields (%)[a]	
		9b	**7b**
1	PPh_3	0	0
2	PCy_3	0	58
3	dcype	77	0
4	dcypp	11	36
5	dcypb	0	57
6	dcypf	0	68
7	dppe	0	46
8[b]	ICy	0	35
9[b]	IMes	0	35
10[b]	$IMes^{Me}$	0	34
11[b]	IPr	0	78

[a] Determined by GC using undecane as an internal standard.
[b] Carbene was generated in situ from the corresponding imidazolium salt and NaO^{t}Bu (25 mol%) was used to generate carbene.



dcype

ICy (R = cyclohexyl, R' = H)
IMes (R = 2,4,6-$Me_3C_6H_2$, R' = H)
$IMes^{Me}$ (R = 2,4,6-$Me_3C_6H_2$, R' = Me)
IPr (R = 2,6-$^i Pr_2C_6H_3$, R' = H)

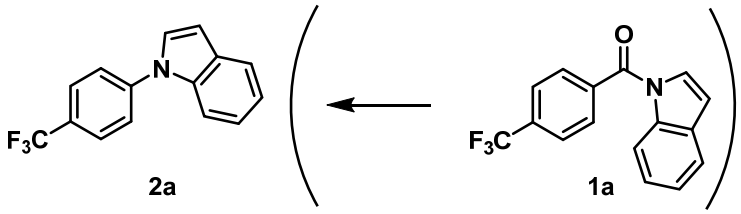
V. Typical Procedures.

Condition A: Procedure for the Ni/dcype-catalyzed decarbonylation of *N*-acylpyrrole derivatives. $Ni(cod)_2$ (13.8 mg, 0.050 mmol), dcype (21.1 mg, 0.050 mmol), *N*-acylpyrrole derivatives and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was then closed. The contents of the vial were then stirred at 180 °C for 18 h. The reaction was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel before being analyzed by GC. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel.

Condition B: Procedure for the Ni/PCy_3-mediated decarbonylation of *N*-acylpyrrole derivatives. $Ni(cod)_2$ (68.8 mg, 0.25 mmol), PCy_3 (70.1 mg, 0.25 mmol), *N*-acylpyrrole derivatives and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was then closed. The contents of the vial were then stirred at 80 °C for 18 h. The reaction was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel before being analyzed by GC. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel.

VI. Spectroscopic Data of Products.

1-(4-(Trifluoromethyl)phenyl)-1*H*-indole (2a) [CAS: 174621-55-7].



The typical procedure (Condition A) was followed using **1a** as the substrate.

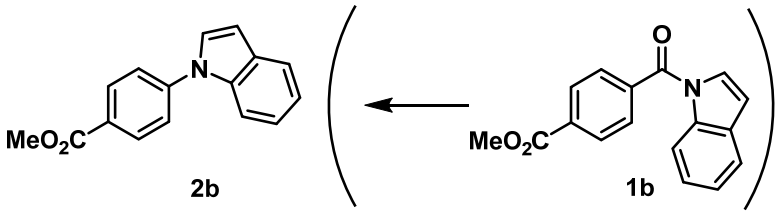
White solid (54.9 mg, 84%). R_f 0.57 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.76 (d, *J* = 3.2 Hz, 1H), 7.23 (dd, *J* = 6.9, 7.8 Hz, 1H), 7.29 (dd, *J* = 6.8, 8.2 Hz, 1H), 7.37 (d, *J* = 3.2 Hz, 1H), 7.61–7.66 (m, 3H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 104.9, 110.3, 121.0, 121.4, 122.9, 123.9, 124.0 (q, J_{CF} = 272.6 Hz), 126.9 (q, J_{CF} = 4.1 Hz), 127.4, 128.2 (q, J_{CF} = 28.0 Hz), 129.7, 135.5, 142.8.

HRMS Calcd for $C_{15}H_{11}F_3N$ ([M+H$^+$]): 262.0838. Found: 262.0839.

Methyl 4-(1*H*-indol-1-yl)benzoate (2b) [CAS: 212382-74-6].



The typical procedure (Condition A) was followed using **1b** as the substrate.

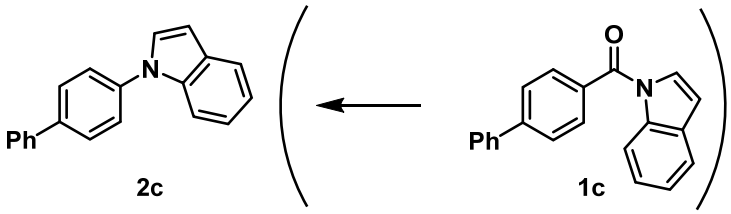
Colorless oil (53.4 mg, 85%). R_f 0.23 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.97 (s, 3H), 6.73 (d, *J* = 3.6 Hz, 1H), 7.21 (dd, *J* = 7.3, 7.8 Hz, 1H), 7.27 (dd, *J* = 7.3, 8.2 Hz, 1H), 7.38 (d, *J* = 3.6 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.64 (d, *J* = 8.2 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 8.20 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 52.2, 104.9, 110.5, 120.9, 121.4, 122.9, 123.2, 127.4, 127.6, 129.8, 131.2, 135.4, 143.7, 166.4.

HRMS Calcd for $C_{16}H_{14}NO_2$ ([M+H$^+$]): 252.1019. Found: 252.1017.

1-([1,1'-Biphenyl]-4-yl)-1*H*-indole (2c) [CAS: 174621-51-3].



The typical procedure (Conditions A and B) was followed using **1c** as the substrate.

White solid (30% GC yield for Condition A, 53.2 mg, 79% for Condition B).

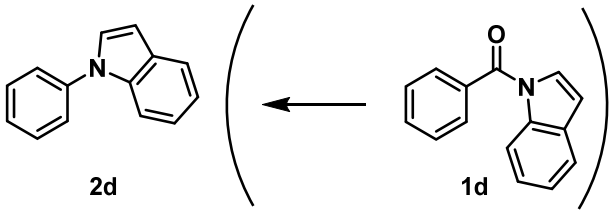
R_f 0.57 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.75 (d, *J* = 3.2 Hz, 1H), 7.22 (dd, *J* = 6.8, 7.3 Hz, 1H), 7.29 (dd, *J* = 7.3, 8.2 Hz, 1H), 7.39–7.44 (m, 2H), 7.49–7.54 (m, 2H), 7.59–7.62 (m, 2H), 7.66–7.70 (m, 3H), 7.34–7.78 (m, 3H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 103.7, 110.6, 120.4, 121.2, 122.4, 124.5, 127.0, 127.5, 127.8, 128.2, 128.9, 129.4, 135.8, 139.0, 139.3, 140.2.

HRMS Calcd for $C_{20}H_{16}N$ ([M+H$^+$]): 270.1277. Found: 270.1274.

1-Phenyl-1*H*-indole (2d) [CAS: 16096-33-6].



The typical procedure (Conditions A and B) was followed using **1d** as the substrate.

White solid (23% GC yield for Condition A, 34.3 mg, 71% for Condition B).

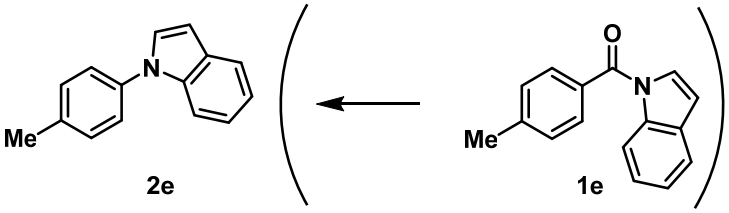
R_f 0.49 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.70 (d, *J* = 3.2 Hz, 1H), 7.19 (dd, *J* = 6.9, 7.3 Hz, 1H), 7.24 (dd, *J* = 7.3, 8.2 Hz, 1H), 7.39–7.35 (m, 2H), 7.52–7.54 (m, 4H), 7.59 (d, *J* = 6.8 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 103.5, 110.5, 120.3, 121.1, 122.3, 124.4, 126.4, 127.9, 129.3, 129.6, 135.8, 139.8.

HRMS Calcd for $C_{14}H_{12}N$ ([M+H$^+$]): 194.0964. Found: 194.0974.

1-(*p*-Tolyl)-1*H*-indole (2e) [CAS: 167283-32-1].



The typical procedure (Conditions A and B) was followed using **1e** as the substrate.

Colorless oil (18% GC yield for Condition A, 32.6 mg, 63% for Condition B).

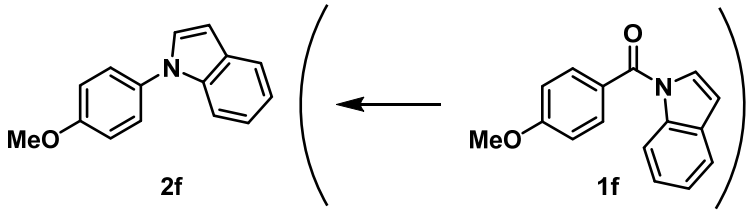
R_f 0.49 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 2.45 (s, 3H), 6.67 (d, *J* = 3.2 Hz, 1H), 7.17 (dd, *J* = 6.9, 7.8 Hz, 1H), 7.21 (dd, *J* = 6.9, 8.3 Hz, 1H), 7.33–7.31 (m, 3H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 21.0, 103.2, 110.5, 120.1, 121.0, 122.2, 124.3, 128.0, 129.1, 130.1, 136.0, 136.3, 137.3.

HRMS Calcd for $C_{15}H_{14}N$ ([M+H$^+$]): 208.1121. Found: 208.1122.

1-(4-Methoxyphenyl)-1*H*-indole (2f) [CAS: 93597-01-4].



The typical procedure (Conditions A and B) was followed using **1f** as the substrate.

The yield under condition A was determined to be 8% by GC. The yield under condition B was determined by NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard (14%). Isolated

yield under condition B was 12% (6.7 mg). The yield was increased to 33% GC yield when $Ni(cod)_2$ (100 mol%) and 3,4-bis(dicyclohexylphosphino)thiophene (100 mol%) were used as the catalyst at 180 °C.

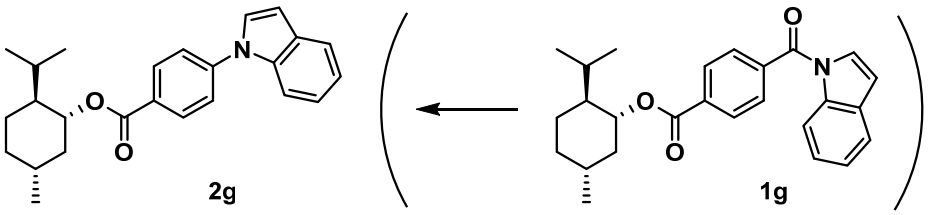
R_f 0.47 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.90 (s, 3H), 6.70 (dd, *J* = 3.2, 0.7 Hz, 1H), 7.04–7.08 (m, 2H), 7.18–7.27 (m, 2H), 7.32 (d, *J* = 3.2 Hz, 1H), 7.42–7.46 (m, 2H), 7.50 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.72–7.74 (m, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 55.5, 102.8, 110.3, 114.7, 120.0, 121.0, 122.1, 125.9, 128.2, 128.9, 132.8, 136.2, 158.2.

HRMS Calcd for $C_{15}H_{14}NO$ ([M+H$^+$]): 224.1070. Found: 224.1077.

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-(1*H*-indol-1-yl)benzoate (2g).



The typical procedure (Condition A) was followed using **1g** as the substrate.

Colorless oil (89.2 mg, 95%). R_f 0.71 (NH silica, hexane/CH_2Cl_2 = 1/1).

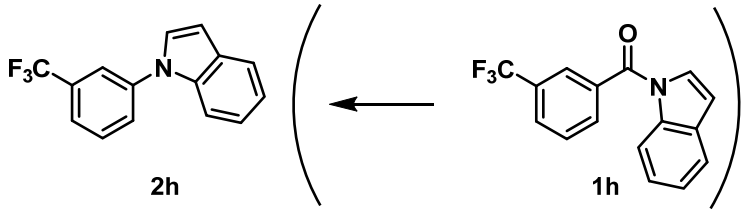
^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 0.83 (d, *J* = 6.8 Hz, 3H), 0.91–1.02 (m, 7H), 1.09–1.27 (m, 2H), 1.53–1.65 (m, 2H), 1.74–1.79 (m, 2H), 1.95–2.05 (m, 1H), 2.12–2.17 (m, 1H), 4.96 (td, *J* = 10.8, 4.0 Hz, 1H), 6.73 (dd, *J* = 3.3, 0.8 Hz, 1H), 7.17–7.27 (m, 2H), 7.42 (d, *J* = 3.2 Hz, 1H), 7.60–7.69 (m, 4H), 8.20 (dt, *J* = 8.8, 2.0 Hz, 2H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 16.6, 20.9, 22.2, 23.9, 26.9, 31.8, 34.6, 41.3, 47.6, 75.3, 104.9, 110.9, 121.2, 121.6, 123.1, 123.5, 127.9, 128.8, 130.1, 131.4, 135.8, 143.8, 165.5.

IR (KBr, cm^{-1}): 3400 w, 3053 m, 2954 s, 2925 s, 2868 s, 1928 w, 1712 s, 1604 s, 1519 s, 1455 s, 1335 s, 1311 s, 1274 s, 1236 s, 1211 s, 1175 s, 1117 s, 1099 s, 1038 m, 1014 s, 983 s, 954 s, 917 m, 883 m, 862 s, 775 s, 759 s, 741 s, 715 s, 700 s.

HRMS Calcd for $C_{25}H_{30}NO_2$ ([M+H$^+$]): 376.2271. Found: 376.2271.

1-(3-(Trifluoromethyl)phenyl)-1*H*-indole (2h) [CAS: 167283-36-5].



The typical procedure (Condition A) was followed using **1h** as the substrate.

Colorless oil (47.0 mg, 72%). R_f 0.4 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.74 (d, *J* = 3.2 Hz, 1H), 7.22 (dd, *J* = 6.9, 7.8 Hz, 1H), 7.28 (dd, *J* = 6.9, 7.4 Hz, 1H), 7.36 (d, *J* = 3.2 Hz, 1H), 7.56 (d, *J* = 3.2 Hz, 1H), 7.69–7.62 (m, 2H), 7.74−7.71 (m, 2H), 7.79 (s, 1H).

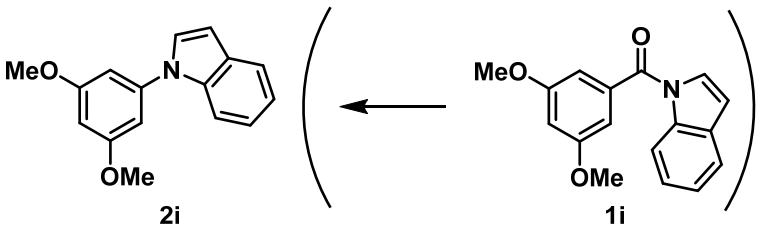
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 104.6, 110.1, 120.9, 121.0 (q, J_{CF} = 3.8 Hz), 121.4, 122.9, 123.0 (q, J_{CF} = 3.8 Hz), 123.7 (q, J_{CF} = 273.1 Hz), 127.3, 127.5, 129.5, 130.3, 132.4 (q, J_{CF} = 32.6 Hz), 135.6, 140.3.

IR (ATR): 3058 w, 1698 w, 1598 w, 1496 w, 1461 m, 1319 m, 1272 w, 1213 w, 1170 m, 1128 s, 1070 w, 975 w, 894 w, 800 w, 742 m, 703 m.

MS, *m/z* (relative intensity, %): 262.2 (17), 261.1 (M^+, 100), 165.1 (9), 90 (9), 89 (9).

HRMS Calcd for $C_{15}H_{11}F_3N$ ([M+H^+]): 262.0838. Found: 262.0840.

1-(3,5-Dimethoxyphenyl)-1*H*-indole (2i).



The typical procedure (Conditions A and B) was followed using **1i** as the substrate.

White solid (30.9 mg, 49% for Condition A, 43.8 mg, 69% for Condition B).

R_f 0.17 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.86 (s, 6H), 6.48 (t, *J* = 2.2 Hz, 1H), 6.68 (m, 3H), 7.18 (dd, 7.1, 7.7 Hz, 1H), 7.24 (dd, 7.1, 8.2 Hz, 1H), 7.35 (d, *J* = 3.4 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1 H), 7.69 (d, *J* = 7.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 55.5, 98.4, 102.7, 103.5, 110.8, 120.4, 121.1, 122.4, 127.9, 129.3, 135.7, 141.4, 161.4.

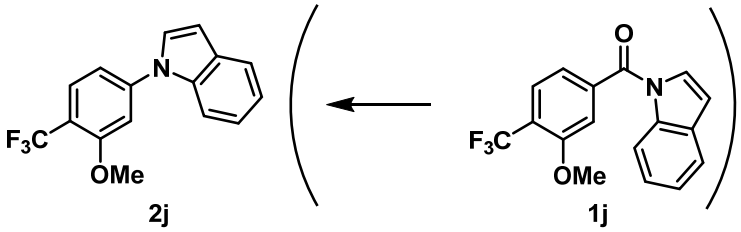
IR (ATR): 2937 w, 2360 w, 1716 w, 1601 s, 1516 m, 1459 m, 1321 m, 1275 m, 1211 s, 1157 m, 1128

m, 1061 w, 931 w, 839 w, 742 m, 690 w.

MS, *m/z* (relative intensity, %): 254 (18), 253 (M^+, 100), 224 (11), 167 (16).

HRMS Calcd for $C_{16}H_{16}NO_2$ ([M+H^+]): 254.1176. Found: 254.1166.

1-(3-Methoxy-4-(trifluoromethyl)phenyl)-1*H*-indole (2j).



The typical procedure (Conditions A and B) was followed using **1j** as the substrate.

White solid (64.8 mg, 89% for Condition A, 61.7 mg, 85% for Condition B).

Mp 80.3–80.5 °C. R_f 0.29 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 4.00 (s, 3H), 6.78 (d, J = 3.7 Hz, 1H), 7.18–7.20 (m, 2H), 7.26 (dd, J = 6.9, 7.8 Hz, 1H), 7.32 (dd, J = 6.9, 8.3 Hz, 1H), 7.40 (d, J = 3.7 Hz, 1H), 7.67 (d, J = 8.3 Hz, 1H), 7.74–7.77 (m, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 56.1, 104.7, 107.6, 110.4, 115.0, 116.4 (q, J_{CF} = 31.1 Hz), 120.9, 121.4, 122.9, 123.4 (q, J_{CF} = 272.6 Hz), 127.4, 128.4 (q, J_{CF} = 5.2 Hz), 129.7, 135.4, 144.2, 158.5.

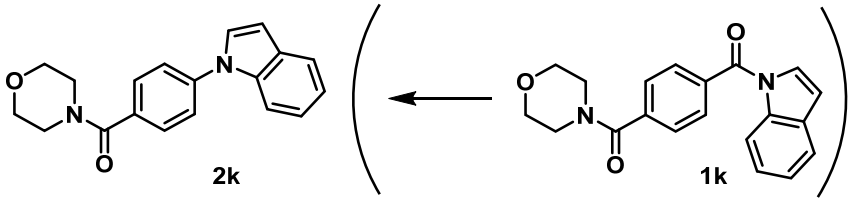
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.0 (s, 3F).

IR (ATR): 3016 w, 2937 w, 1612 m, 1517 m, 1459 m, 1423 w, 1313 s, 1261 m, 1216 m, 1122 s, 1072 w, 1043 m, 954 w, 850 w, 825 w, 746 s, 661 w.

MS, *m/z* (relative intensity, %): 292 (19), 291 (M^+, 100), 248 (22).

HRMS Calcd for $C_{16}H_{13}F_3NO$ ([M+H^+]): 292.0944. Found: 292.0966.

(4-(1*H*-Indol-1-yl)phenyl)(morpholino)methanone (2k).



The typical procedure (Condition A) was followed using **1k** as the substrate.

White solid (68.9 mg, 90%). Mp 123.6–124.1 °C. R_f 0.23 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.75 (m, 8H), 6.72 (d, J = 3.3 Hz, 1H), 7.20 (dd, J = 7.1, 7.6 Hz,

1H), 7.25 (dd, *J* = 7.1, 8.3 Hz, 1H), 7.34 (d, *J* = 3.3 Hz, 1H), 7.61–7.58 (m, 5H), 7.70 (d, *J* = 8.3 Hz, 1H).

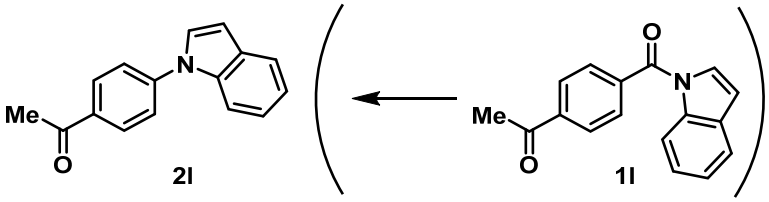
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 42.7 (br), 48.2 (br), 66.9, 104.4, 110.4, 120.7, 121.3, 122.7, 123.9, 127.5, 128.8, 129.5, 132.9, 135.5, 141.1, 169.6.

IR (ATR): 2966 w, 2918 w, 2856 w, 2360 w, 1712 m, 1629 s, 1517 m, 1454 s, 1429 s, 1338 m, 1277 m, 1068 w, 1016 m, 950 w, 891 w, 842 m, 744 m.

MS, *m/z* (relative intensity, %): 307 (12), 306 (M^+, 56), 221 (17), 220 (100), 192 (37), 191 (38), 110 (14), 96 (19).

HRMS Calcd for $C_{19}H_{19}N_2O_2$ ([M+H^+]): 307.1441. Found: 307.1442.

1-(4-(1*H*-Indol-1-yl)phenyl)ethanone (2l) [CAS: 25700-07-6].



The typical procedure (Conditions A and B) was followed using **1l** as the substrate.

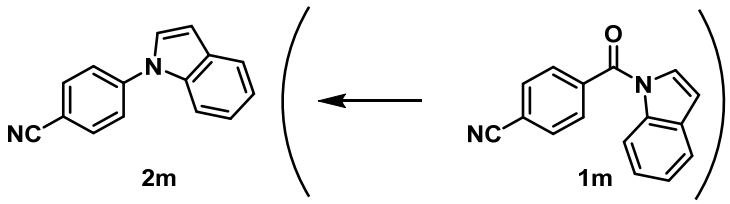
Colorless oil (33.1 mg, 56% for Condition A, 45.0 mg, 61% for Condition B). R_f 0.14 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 2.67 (s, 3H), 6.75 (d, *J* = 3.2 Hz, 1H), 7.22 (dd, *J* = 6.5, 7.6 Hz, 1H), 7.28 (dd, *J* = 6.5, 8.2 Hz, 1H), 7.39 (d, *J* = 3.2 Hz, 1H), 7.63 (d, *J* = 6.9 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 6.9 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 26.6, 105.0, 110.5, 121.0, 121.4, 122.9, 123.3, 127.3, 129.8, 130.0, 134.5, 135.3, 143.8, 196.8.

HRMS Calcd for $C_{16}H_{14}NO$ ([M+H^+]): 236.1070. Found: 236.1066.

4-(1*H*-Indol-1-yl)benzonitrile (2m) [CAS: 25699-92-7].



The typical procedure (Condition A) was followed using **1m** as the substrate and 1,3-

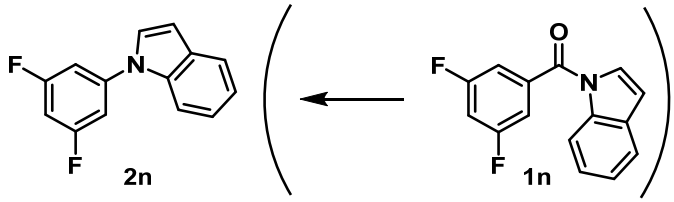
bis(dicyclohexylphosphino)propane as the ligand. Colorless oil (38.2 mg, 69%). R_f 0.28 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.76 (d, *J* = 3.2 Hz, 1H), 7.22 (dd, *J* = 7.3, 7.8 Hz, 1H), 7.28 (dd, *J* = 7.3, 8.7 Hz, 1H), 7.34 (d, *J* = 3.2 Hz, 1H), 7.61–7.66 (m, 3H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.79–7.83 (m, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 105.7, 109.2, 110.3, 118.4, 121.4, 121.6, 123.2, 123.8, 127.0, 129.9, 133.8, 135.2, 143.6.

HRMS Calcd for $C_{15}H_{11}N_2$ ([M+H$^+$]): 219.0917. Found: 219.0931.

1-(3,5-Difluorophenyl)-1*H*-indole (2n).



The typical procedure (Condition A) was followed using **1n** as the substrate.

Colorless oil (43.8 mg, 76%). R_f 0.6 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.73 (d, *J* = 3.2 Hz, 1H), 6.82 (tt, *J* = 2.3, 8.7 Hz, 1H), 7.12–7.07 (m, 2H), 7.24 (dd, *J* = 7.4, 7.8 Hz, 1H), 7.28–7.32 (m, 2H), 7.64 (*J* = 8.2 Hz, 1H), 7.70 (*J* = 7.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 101.6 (t, *J* = 24.9 Hz), 105.0, 107.0 (dd, *J* = 19.7 Hz), 110.3, 121.1, 121.4, 123.0, 127.3, 129.6, 135.2, 141.9 (t, *J* = 12.4 Hz), 163.5 (dd, *J* = 249.8 Hz).

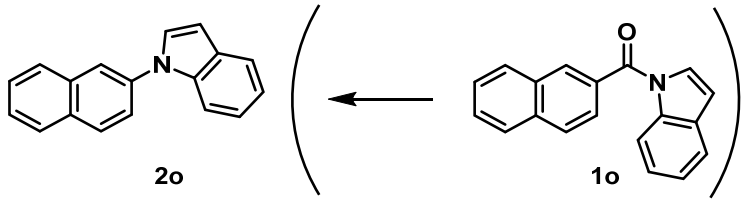
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –107.6 (s, 2F).

IR (ATR): 3091 w, 2360 m, 1614 s, 1521 m, 1481 s, 1357 w, 1305 w, 1270 m, 1203 m, 1120 m, 989 w, 848 w, 767 m, 742 m, 680 w.

MS, *m/z* (relative intensity, %): 230 (16), 229 (M$^+$, 100), 202 (22), 90 (18), 89 (16).

HRMS Calcd for $C_{14}H_{10}F_2N$ ([M+H$^+$]): 230.0776. Found: 230.0788.

1-(Naphthalen-2-yl)-1*H*-indole (2o) [CAS: 348111-49-9].



The typical procedure (Conditions A and B) was followed using **1o** as the substrate.

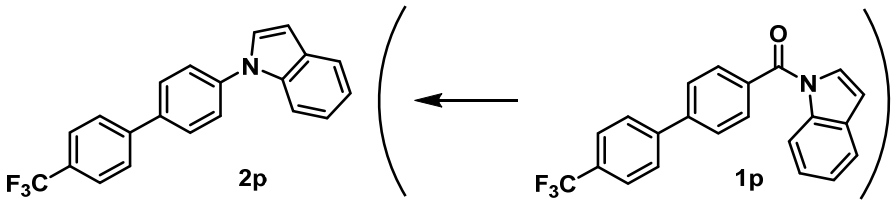
Colorless oil (35.9 mg, 59% for Condition A, 45.0 mg, 90% for Condition B). R_f 0.40 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.77 (d, *J* = 3.2 Hz, 1H), 7.21–7.30 (m, 2H), 7.47–7.49 (m, 1H), 7.60–7.53 (m, 2H), 7.67–7.71 (m, 2H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.90–7.96 (m, 3H), 8.01 (d, *J* = 8.7 Hz, 1H)

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 103.8, 110.5, 120.5, 121.2, 121.9, 122.4, 123.2, 126.0, 126.9, 127.7, 127.8, 128.1, 129.4, 129.6, 131.8, 133.8, 136.0, 137.3.

HRMS Calcd for $C_{18}H_{14}N$ ([M+H$^+$]): 244.1121. Found: 244.1135.

1-(4'-(Trifluoromethyl)-[1,1'-biphenyl]-4-yl)-1*H*-indole (2p).



The typical procedure (Conditions A and B) was followed using **1p** as the substrate.

White solid (60.1 mg, 71% for Condition A, 72.7 mg, 86% for Condition B). Mp 133.3–133.8 °C. R_f 0.23 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.74 (d, *J* = 3.3 Hz, 1H), 7.21 (dd, *J* = 6.9, 7.2 Hz, 1H), 7.27 (dd, *J* = 7.1, 8.2 Hz, 1H), 7.40 (d, *J* = 3.3 Hz, 1H), 7.66–7.62 (m, 3H), 7.79–7.72 (m, 7H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 104.1, 110.5, 120.6, 121.3, 122.6, 124.2 (q, J_{CF} = 272.2 Hz), 124.6, 125.9 (q, J_{CF} = 2.9 Hz), 127.3, 127.7, 128.4, 129.5, 129.6 (q, J_{CF} = 32.6 Hz), 135.7, 137.7, 139.8, 143.7.

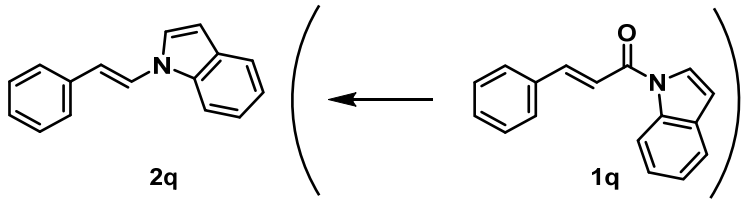
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.3 (s, 3F).

IR (ATR): 2942 w, 2865 w, 1713 m, 1616 w, 1526w, 1473 m, 1379 w, 1324 s, 1263 m, 1217 w, 1163 m, 1124 m, 1069 m, 1016 w, 958 w, 883 w, 848 w, 830 w, 803 w, 770 w, 743 w, 718 w, 696 w, 677 w.

MS, *m/z* (relative intensity, %): 338 (23), 337 (M$^+$, 100), 89 (13).

HRMS Calcd for $C_{21}H_{15}F_3N$ ([M+H$^+$]): 338.1151. Found: 338.1149.

(*E*)-1-Styryl-1*H*-indole (2q) [CAS: 405150-29-0].



The typical procedure (Condition A and B) was followed using **1q** as the substrate. Under condition A, no **2q** was formed and 77% of **1q** was remained unreacted.

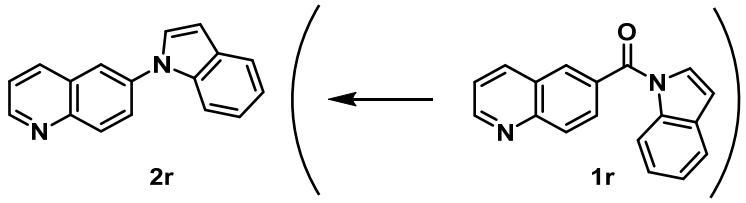
White solid (49.9 mg, 91% for Condition B). White solid (49.9 mg, 91%). R_f 0.34 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.74–6.70 (m, 2H), 7.22 (t, *J* = 7.4 Hz, 1H), 7.35–7.27 (m, 2H), 7.41 (dd, *J* = 7.4, 7.8 Hz, 2H), 7.48 (d, *J* = 7.8 Hz, 2H), 7.55 (d, *J* = 3.2 Hz, 1H), 7.59 (d, *J* = 8.2 Hz, 1H), 7.73–7.67 (m, 2H).

^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 105.6, 109.9, 114.1, 121.2, 121.5, 123.1, 123.8, 124.0, 125.9, 127.2, 129.1, 129.5, 136.0, 136.5.

HRMS Calcd for $C_{16}H_{14}N$ ([M+H$^+$]): 220.1121. Found: 220.1128.

6-(1*H*-Indol-1-yl)quinoline (2r).



The typical procedure (Condition A) was followed using **1r** as the substrate.

Colorless oil (56.8 mg, 69%). R_f 0.43 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.76 (d, *J* = 3.2 Hz, 1H), 7.22 (dd, *J* = 6.6, 7.6 Hz, 1H), 7.27 (dd, *J* = 6.6, 8.2 Hz, 1H), 7.44–7.49 (m, 2H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.90–7.94 (m, 2H), 8.20 (d, *J* = 6.9 Hz, 1H), 8.27 (d, *J* = 8.7 Hz, 1H), 8.96 (d, *J* = 4.1 Hz, 1H).

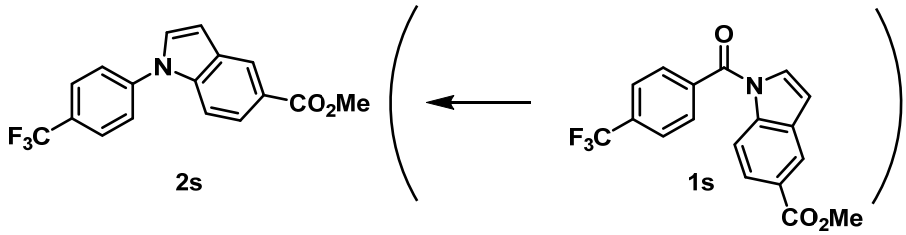
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 104.4, 110.3, 120.7, 121.2, 121.3, 121.9, 122.7, 126.6, 127.9, 128.7, 129.5, 131.1, 135.8, 137.8, 146.48, 146.49, 150.4.

IR (ATR): 3052 w, 2360 w, 1612 m, 1506 s, 1457 s, 1423 w, 1311 s, 1261 w, 1216 m, 1126 s, 1043 m, 883 w, 838 m, 765 s, 742 s.

MS, *m/z* (relative intensity, %): 245 (19), 244 (M^+, 100), 243 (31), 242 (11), 216 (13), 1221 (16), 108 (11).

HRMS Calcd for $C_{17}H_{13}N_2$ ([M+H^+]): 245.1073. Found: 245.1095.

Methyl 1-(4-(trifluoromethyl)phenyl)-1*H*-indole-5-carboxylate (2s) [CAS: 1373525-79-1].



The typical procedure (Condition A) was followed using **1s** as the substrate.

White solid (60.6 mg, 76%). Mp 141.8–142.1 °C. R_f 0.18 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.95 (s, 3H), 6.81 (d, *J* = 3.2 Hz, 1H), 7.41 (d, *J* = 3.2 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.95 (d, *J* = 8.8 Hz, 1H), 8.45 (s, 1H).

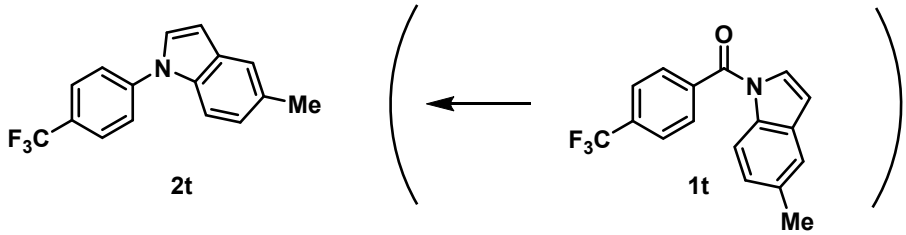
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 52.0, 105.96, 105.97, 110.0, 123.0, 123.8 (q, J_{CF} = 272.2 Hz), 124.2, 127.0 (q, J_{CF} = 3.8 Hz), 128.8 (q, J_{CF} = 15.3 Hz), 128.9, 129.2, 137.91, 137.92, 142.2, 167.7.

IR (ATR): 2951 w, 1712 m, 1610 m, 1526 w, 1475 w, 1436 w, 1377 w, 1359 w, 1324 s, 1272 m, 1228 m, 1198 m, 1166 m, 1123 mm, 1087 w, 1066 m, 1016 w, 987 w, 954 w, 909 w, 848 w, 754 m, 718 w, 667 w.

MS, *m/z* (relative intensity, %): 320 (17), 319 (M^+, 89), 289 (18), 288 (100), 260 (28), 240 (13), 191 (30), 144 (16).

HRMS Calcd for $C_{17}H_{13}F_3NO_2$ ([M+H^+]): 320.0893. Found: 320.0881.

5-Methyl-1-(4-(trifluoromethyl)phenyl)-1*H*-indole (2t).



The typical procedure (Condition A) was followed using **1t** as the substrate.

White solid (49.5 mg, 72%). Mp 60.5–60.9 °C. R_f 0.45 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 2.48 (s, 3H), 6.66 (d, *J* = 3.2 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 1H), 7.32

(d, J = 3.2 Hz, 1H), 7.49–7.52 (m, 2H), 7.62 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 21.3, 104.5, 110.0, 121.1, 123.6, 124.0, 124.5, 126.8, 127.4, 127.9, 130.0, 130.3, 133.8, 142.9.

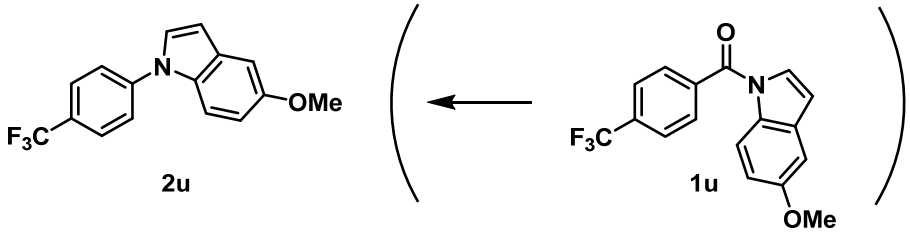
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.1 (s, 3F).

IR (ATR): 2941 w, 2865 w, 2156 w, 1712 w, 1616 w, 1525 w, 1473 m, 1451 w, 1378 w, 1323 s, 1260 m, 1218 w, 1162 m, 1122 m, 1066 m, 1015 w, 958 w, 913 w, 882 w, 846 w, 800 w, 770 w, 751 w, 717 w, 696 w, 677 w.

MS, *m/z* (relative intensity, %): 276 (17), 275 (M^+, 100), 274 (65), 77 (12).

HRMS Calcd for $C_{16}H_{13}F_3N$ ([M+H^+]): 276.0995. Found: 276.0987.

5-Methoxy-1-(4-(trifluoromethyl)phenyl)-1*H*-indole (2u).



The typical procedure (Condition A) was followed using **1u** as the substrate.

White solid (53.1 mg, 73%). Mp 84.8–85.1 °C. R_f 0.38 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.89 (s, 3H), 6.66 (d, J = 3.2 Hz, 1H), 6.92 (d, J = 2.3, 9.2 Hz, 1H), 7.15 (d, J = 2.3 Hz, 1H), 7.33 (d, J = 3.2 Hz, 1H), 7.51 (d, J = 9.2 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 55.8, 103.0, 104.6, 111.2, 112.9, 123.5, 124.0 (q, J_{CF} = 271.8 Hz), 126.9 (q, J_{CF} = 3.7 Hz), 127.7 (q, J_{CF} = 32.7 Hz), 127.8, 130.3, 130.5, 142.8, 154.9.

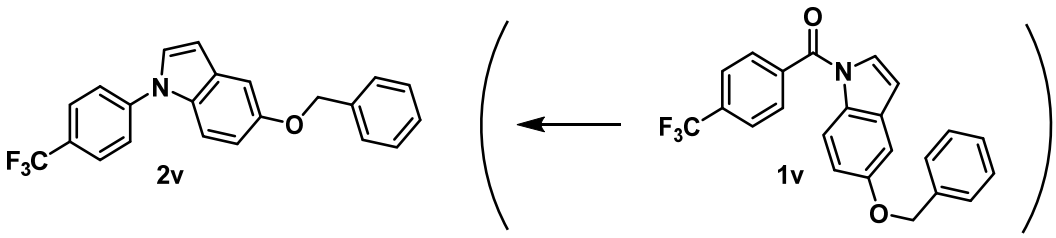
^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.1 (s, 3F).

IR (ATR): 2941 w, 1712 w, 1616 w, 1524 w, 1476 m, 1449 w, 1378 w, 1323 s, 1262 m, 1217 w, 1159 m, 1120 m, 1066 m, 1033 w, 1016 w, 957 w, 846 w, 803 w, 771 w, 754 w, 717 w.

MS, *m/z* (relative intensity, %): 292 (18), 291 (M^+, 100), 277 (12), 276 (70), 248 (42).

HRMS Calcd for $C_{16}H_{13}F_3NO$ ([M+H^+]): 292.0944. Found: 292.0937.

5-(Benzyloxy)-1-(4-(trifluoromethyl)phenyl)-1*H*-indole (2v) [CAS: 161460-21-5].



The typical procedure (Condition A) was followed using **1v** as the substrate.

White solid (69.8 mg, 76%). Mp 104.3–104.8 °C. R_f 0.34 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 5.15 (s, 2H), 6.65 (d, J = 3.2 Hz, 1H), 7.00 (dd, J = 2.8, 8.7 Hz, 1H), 7.23 (d, J = 2.8 Hz, 1H), 7.32–7.34 (m, 2H), 7.39–7.42 (m, 2H), 7.52–7.65 (m, 3H), 7.61 (d, J = 8.3 Hz, 2H), 7.77 (d, J = 8.3 Hz, 2H).

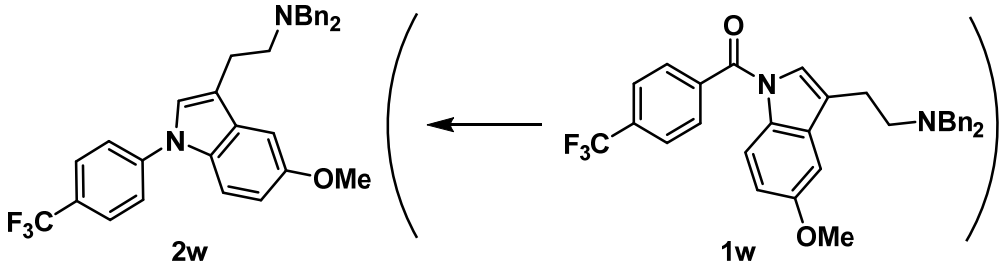
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 70.7, 104.5, 104.6, 111.2, 113.6, 123.5, 123.9 (q, J_{CF} = 272.6 Hz), 126.9 (q, J_{CF} = 3.1 Hz), 127.5, 127.8, 127.9 (q, J_{CF} = 32.1 Hz), 128.5, 128.6, 130.3, 130.7, 137.4, 142.8, 154.0.

IR (ATR): 3033 w, 2863 w, 1708 w, 1616 m, 1572 w, 1524 m, 1472 m, 1450 m, 1424 w, 1379 w, 1322 s, 1258 m, 1217 w, 1159 s, 1115 s, 1065 m, 1015 m, 957 w, 911 w, 845 m, 802 w, 737 m, 717 m, 697 m.

MS, *m/z* (relative intensity, %): 367 (M^+, 39), 277 (18), 276 (100), 248 (27), 91 (65).

HRMS Calcd for $C_{22}H_{17}F_3NO$ ([M+H^+]): 368.1257. Found: 368.1251.

_N_,_N_-Dibenzyl-2-(5-methoxy-1-(4-(trifluoromethyl)phenyl)-1_H_-indol-3-yl)ethan-1-amine (2w).



The typical procedure (Condition A) was followed using **1w** as the substrate.

Colorless oil (88.1 mg, 69%). R_f 0.29 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 2.84 (t, J = 7.2 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 3.71 (s, 4H), 3.74 (s, 3H), 6.83–6.86 (m, 2H), 7.11 (s, 1H), 7.20–7.24 (m, 2H), 7.28–7.31 (m, 4H), 7.41 (d, J = 7.2 Hz, 4H), 7.49 (dd, J = 8.2, 1.6 Hz, 1H), 7.57 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 23.0, 53.4, 55.8, 58.4, 101.0, 111.2, 112.8, 116.6, 123.0, 124.0 (q, J_{CF} = 271.7 Hz), 125.2, 126.8, 126.8 (qt, J_{CF} = 2.6 Hz), 127.1, 127.4, 128.2, 128.7, 130.3 (q, J_{CF} = 34.5

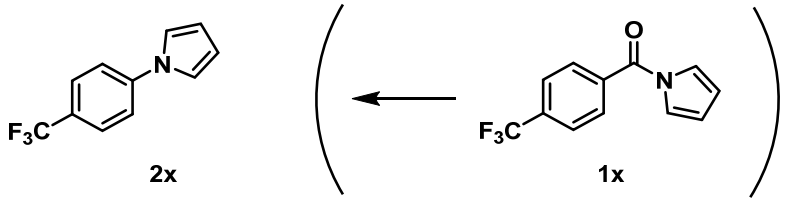
Hz), 139.8, 142.9, 154.5.

^{19}F NMR (CD_2Cl_2, 376.17 MHz) δ: –62.3 (s, 3F).

IR (KBr, cm^{-1}): 3061 m, 3028 m, 2930 m, 2832 m, 2798 m, 2714 w, 1616 s, 1524 s, 1480 s, 1452 s, 1390 m, 1325 s, 1255 s, 1213 m, 1166 s, 1122 s, 1067 s, 1030 m, 1014 m, 973 s, 952 s, 846 m, 790 m, 744 m, 699 m.

HRMS Calcd for $C_{32}H_{30}F_3N_2O$ ([M+H$^+$]): 515.2305. Found: 515.2310.

1-(4-(Trifluoromethyl)phenyl)-1*H*-pyrrole (2x) [CAS: 92636-38-9].



The typical procedure (Condition A) was followed using **1x** as the substrate.

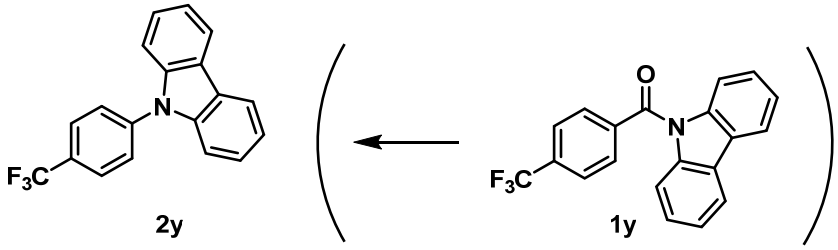
White solid (40.1 mg, 76%). R_f 0.40 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.39 (d, J = 3.7 Hz, 2H), 7.13 (d, J = 3.7 Hz, 2H), 7.49 (d, J = 8.8, 2H), 7.68 (d, J = 8.8 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 111.5, 119.1, 112.0, 124.0 (q, J_{CF} = 271.6 Hz), 126.9 (q, J_{CF} = 3.1 Hz), 127.4 (q, J_{CF} = 33.2 Hz), 143.2.

HRMS Calcd for $C_{11}H_9F_3N$ ([M+H$^+$]): 212.0682. Found: 212.0688.

9-(4-(Trifluoromethyl)phenyl)-9*H*-carbazole (2y) [CAS: 204066-03-5].



The typical procedure (Condition A) was followed using **1y** as the substrate.

White solid (69.3 mg, 89%). R_f 0.43 (SiO_2, hexane/EtOAc = 10/1).

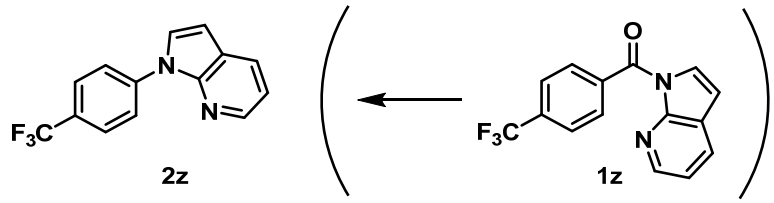
^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.31–7.34 (m, 2H), 7.41–7.45 (m, 4H), 7.73 (d, J = 8.2 Hz, 2H), 7.88 (d, J = 8.2 Hz, 2H), 8.15 (d, J = 8.9 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 109.5, 120.45, 120.56, 123.7, 123.9 (q, J_{CF} = 272.6 Hz), 126.2,

127.0, 127.1 (q, J_{CF} = 3.2 Hz), 129.1 (q, J_{CF} = 33.2 Hz), 140.3, 141.0.

HRMS Calcd for $C_{19}H_{13}F_3N$ ([M+H$^+$]): 312.0995. Found: 312.0991.

1-(4-(Trifluoromethyl)phenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (2z) [CAS: 1797430-69-3].



The typical procedure (Condition A) was followed using **1z** as the substrate and 1,3-bis(dicyclohexylphosphino)propane as the ligand.

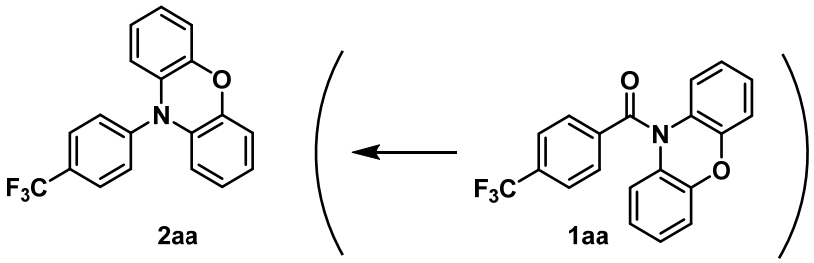
White solid (49.8 mg, 70%). R_f 0.34 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 6.69 (d, J = 3.7 Hz, 1H), 7.18 (dd, J = 4.8, 7.8 Hz, 1H), 7.55 (d, J = 3.7 Hz, 1H), 7.78 (d, J = 8.5 Hz, 2H), 7.97–8.00 (m, 3H), 8.39 (d, J = 4.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 102.9, 117.3, 121.9, 123.3, 124.0 (q, J_{CF} = 271.6 Hz), 126.6 (q, J_{CF} = 3.2 Hz), 127.0, 127.8 (q, J_{CF} = 33.2 Hz), 129.4, 141.4, 143.8, 137.4.

HRMS Calcd for $C_{14}H_{10}F_3N_2$ ([M+H$^+$]): 263.0791. Found: 263.0796.

10-(4-(Trifluoromethyl)phenyl)-10*H*-phenoxazine (2aa) [CAS: 58736-86-0].



The typical procedure (Condition A) was followed using **1aa** as the substrate.

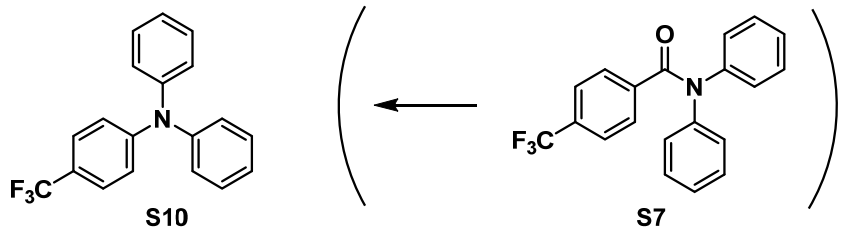
White solid (49.1 mg, 60%). R_f 0.54 (SiO_2, hexane/EtOAc = 20/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 5.90 (d, J = 7.8 Hz, 2H), 6.61 (dd, J = 7.3, 7.8 Hz, 2H), 6.67–6.74 (m, 4H), 7.51 (d, J = 8.0 Hz, 2H), 7.87 (d, J = 8.2 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 113.2, 115.7, 121.9, 123.3, 123.8 (q, J_{CF} = 272.6 Hz), 128.2 (q, J_{CF} = 4.1 Hz), 130.6 (q, J_{CF} = 32.1 Hz), 131.5, 133.7, 142.5, 143.9.

HRMS Calcd for $C_{19}H_{13}F_3NO$ ([M+H$^+$]): 328.0944. Found: 328.0944.

***N*,*N*-Diphenyl-4-(trifluoromethyl)aniline (S10) [CAS: 36809-32-2].**



The typical procedure (Conditions A or B) was followed using **S7** as the substrate.

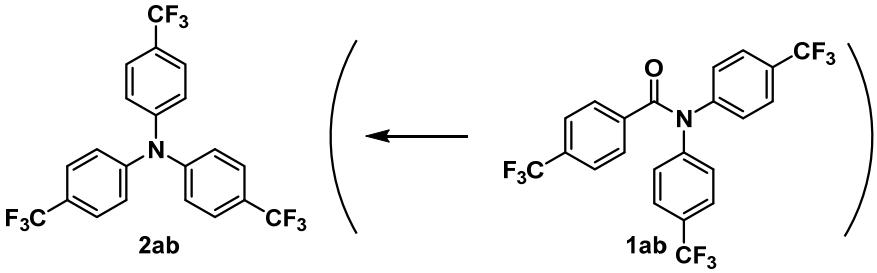
White solid (7.0 mg, 9% for Condition A, 7.6 mg, 10% for Condition B).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.05 (d, J = 8.3 Hz, 2H), 7.14–7.10 (m, 6H), 7.32–7.28 (m, 4H), 7.41 (d, J = 8.7 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ:121.0, 122.7 (q, J_{CF} = 33.2 Hz), 124.2, 123.3 (q, J_{CF} = 300.0 Hz), 125.4, 126.2 (q, J_{CF} = 4.1 Hz), 129.5, 146.8, 150.8.

HRMS Calcd for $C_{19}H_{15}F_3N$ ([M+H$^+$]): 314.1151. Found: 314.1149.

Tris(4-(trifluoromethyl)phenyl)amine (2ab) [CAS: 135761-41-0].



The modified condition A as specified below was used for substrate **1ab**, which gave the product **2ab** as a white solid. Isolated yield was 60% (55.0 mg) when $Ni(cod)_2$ (20 mol%) and dcype (20 mol%) were used as the catalyst for 48 h at 180 °C. Isolated yield was 60% (55.0 mg) when $Ni(cod)_2$ (100 mol%) and dcype (100 mol%) were used as the catalyst for 18 h at 180 °C.

White solid. R_f 0.26 (SiO_2, hexane/EtOAc = 9/1).

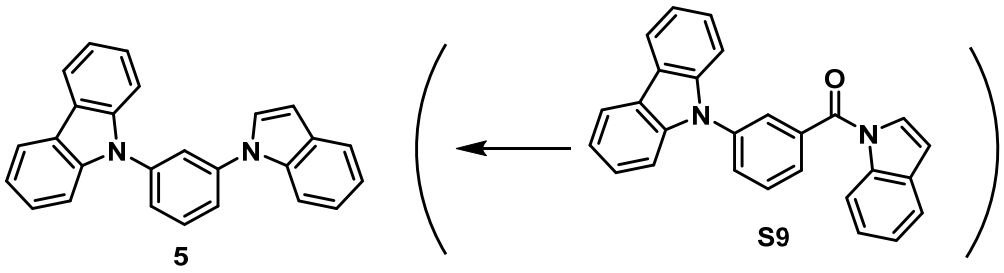
^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.55 (d, J = 8.4 Hz, 6H), 7.18 (d, J = 8.4 Hz, 6H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 149.4, 126.9(qt, J_{CF} = 3.8 Hz), 125.9(q, J_{CF} = 32.8 Hz), 124.1, 124.0(q, J_{CF} = 271.7 Hz).

MS, *m/z* (relative intensity, %): 359 (M$^+$, 20), 358 (100), 357 (M$^+$, 53), 344 (12), 343 (66), 118 (12), 116 (11), 91 (31), 77 (12), 65 (17).

HRMS Calcd for $C_{21}H_{13}F_9N$ ([M+H$^+$]): 450.0899. Found: 450.0899.

9-(3-(1*H*-Indol-1-yl)phenyl)-9*H*-carbazole (5) [CAS: 1688701-25-8].



The typical procedure (Condition A) was followed using **S9** as the substrate.

White solid (56.0 mg, 63%). Mp 164.4–166.7 °C. R_f 0.29 (NH silica, hexane/CH_2Cl_2 = 9/1).

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 6.72 (d, J = 4.1 Hz, 1H), 7.16 (td, J = 7.6, 0.9 Hz, 1H), 7.24 (td, J = 7.7, 1.0 Hz, 1H), 7.29–7.33 (m, 2H), 7.43–7.47 (m, 3H), 7.52 (s, 1H), 7.54 (s, 1H), 7.60 (dq, J = 7.8, 1.1 Hz, 1H), 7.66–7.69 (m, 3H), 7.76 (t, J = 2.0 Hz, 1H), 7.79 (t, J = 7.6 Hz, 1H), 8.17 (d, J = 7.8 Hz, 2H).

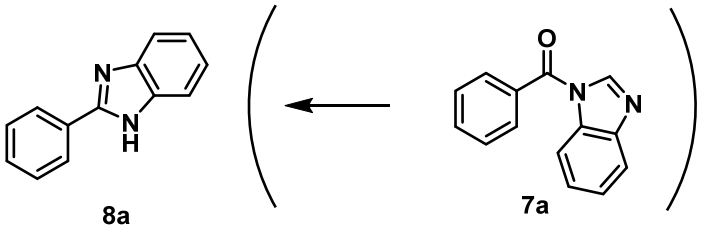
^{13}C NMR (CD_2Cl_2, 100.53 MHz) δ: 104.5, 110.1, 110.8, 120.6, 120.7, 121.0, 121.5, 122.7, 122.9, 123.3, 123.8, 125.1, 126.5, 128.2, 129.9, 131.4, 136.0, 139.3, 141.0, 141.7.

IR (KBr, cm^{-1}): 3054 w, 1601 s, 1576 w, 1516 m, 1497 s, 1475 m, 1451 s, 1333 s, 1318 m, 1229 s, 1213 m, 1174 w, 1166 w, 1153 w, 1134 w, 1120 w, 1016 w, 933 w, 902 w, 879 w, 849 w, 799 w, 748 s, 727 s, 700 m.

MS, *m/z* (relative intensity, %): 359 (29), 358 (M^+, 100), 357 (12), 241 (14), 179 (19).

HRMS Calcd for $C_{26}H_{18}N_2$ ([M^+]): 358.1465. Found: 358.1466.

2-Phenyl-1*H*-benzo[*d*]imidazole (8a) [CAS: 716-79-0].



The typical procedure (Condition A) was followed using **7a** as the substrate.

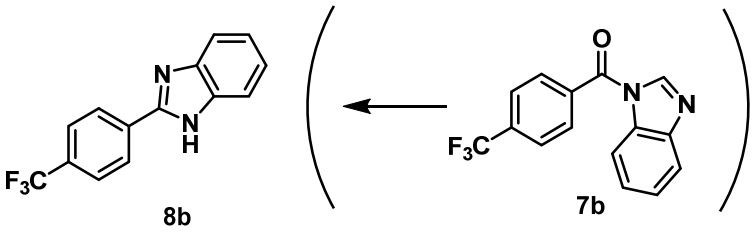
White solid (35.0 mg, 72%). R_f 0.40 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 7.18–7.21 (m, 2H), 7.48–7.57 (m, 4H), 7.66 (d, J = 7.0 Hz, 1H), 8.16–8.19 (m, 2H), 12.90 (s, 1H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 111.3, 118.9, 121.7, 122.5, 126.4, 129.0, 129.9, 130.2, 135.0, 143.8, 151.2.

HRMS Calcd for $C_{13}H_{11}N_2$ ([M+H^+]): 195.0917. Found: 195.0922.

2-(4-(Trifluoromethyl)phenyl)-1*H*-benzo[*d*]imidazole (8b) [CAS: 400073-79-2].



The typical procedure (Condition A) was followed using **7b** as the substrate. The ratio of *p*- and *m*-derivatives were determined by ^{1}H-NMR based on the literature data.[16]

White solid [50.5 mg, 77% (*p*:*m* = 52:1)]. R_f 0.51 (SiO_2, hexane/EtOAc = 1/1).

***p*-Isomer:**

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 7.14–7.31 (m, 2H), 7.57 (d, J = 6.9 Hz, 1H), 7.70 (d, J = 6.8 Hz, 1H), 7.92 (d, J = 8.2 Hz, 2H), 8.31 (d, J = 8.2 Hz, 2H), 13.16 (s, 1H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 122.6, 124.2 (q, J_{CF} = 272.2 Hz), 126.0 (q, J_{CF} = 3.8 Hz), 127.1, 129.6 (q, J_{CF} = 31.9 Hz), 133.9, 134.0, 134.0, 149.6.

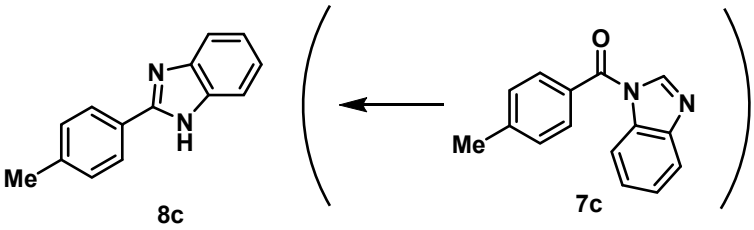
HRMS Calcd for $C_{14}H_{10}F_3N_2$ ([M+H$^+$]): 263.0791. Found: 263.0815.

***m*-Isomer:** This compound was identified based the following spectroscopic data.[15]

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 8.52 (s, 1H). Other peaks were overlapped with those of *p*-isomers.

MS, *m/z* (relative intensity, %): 263 (21), 262 (M$^+$, 100), 64 (18), 223 (18), 63 (16), 242 (13), 131 (13), 241 (12), 90 (12).

2-(*p*-Tolyl)-1*H*-benzo[*d*]imidazole (8c) [CAS: 120-03-6].



The typical procedure (Condition A) was followed using **7c** as the substrate. The ratio of *p*- and *m*-derivatives were determined by ^{1}H-NMR.[15]

White solid [25.5 mg, 49% (*p*:*m* = 9:1)]. R_f 0.46 (SiO_2, hexane/EtOAc = 1/1).

***p*-Isomer:**

[16] Marri, M. R.; Peraka, S.; Macharla, A. K.; Mameda, N.; Kodumari, S.; Nama, N. *Tetrahedron Lett.* **2014**, *55*, 6520.

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 2.37 (s, 3H), 7.22–7.16 (m, 2H), 7.35 (d, J = 8.2 Hz, 2H), 7.52 (d, J = 7.0 Hz, 1H), 7.65 (d, J = 7.0 Hz, 1H), 8.08 (d, J = 8.2 Hz, 2H), 12.85 (s, 1H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 21.0, 111.2, 118.7, 121.6, 122.3, 126.4, 127.5, 129.5, 135.0, 139.6, 143.8, 151.4.

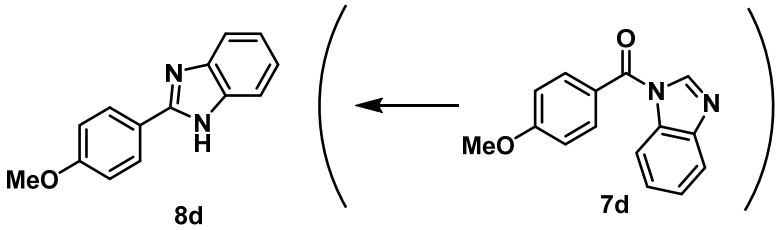
HRMS Calcd for $C_{14}H_{13}N_2$ ([M+H$^+$]): 209.1073. Found: 209.1100.

***m*-Isomer:** This compound was identified based the following spectroscopic data.[15]

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 7.97 (d, J = 7.6 Hz, 1H). Other peaks were overlapped with those of *p*-isomers.

MS, *m/z* (relative intensity, %): 209 (19), 208 (M$^+$, 100), 207 (42), 104 (14), 103 (16), 91 (11), 63 (11).

2-(*4*-Methoxyphenyl)-1*H*-benzo[*d*]imidazole (8d) [CAS: 2620-81-7].



The modified condition A as specified below was used for substrate **7d**, which gave the product **8d** as a white solid. Isolated yield was 70% (39.2 mg) when Ni(cod)$_2$ (40 mol%) and dcype (40 mol%) were used as the catalyst for 24 h at 180 °C. The ratio of *p*- and *m*- derivatives were determined by ^{1}H-NMR.[17] White solid [39.2 mg, 70% (*p*:*m* = 94:6)]. R_f 0.26 (NH silica, hexane/EtOAc = 1/1).

***p*-Isomer:**

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 3.83 (s, 3H), 7.10 (d, J = 8.8 Hz, 2H), 7.14–7.19 (m, 2H), 7.48 (d, J = 7.0 Hz, 1H), 7.61 (d, J = 7.0 Hz, 1H), 8.11 (d, J = 8.8 Hz, 2H), 12.75 (s, 1H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 55.4, 111.1, 114.4, 118.5, 121.5, 122.1, 122.7, 128.0, 135.0, 143.9, 151.4, 160.6.

HRMS Calcd for $C_{14}H_{13}N_2O$ ([M+H$^+$]): 225.1022. Found: 225.1021.

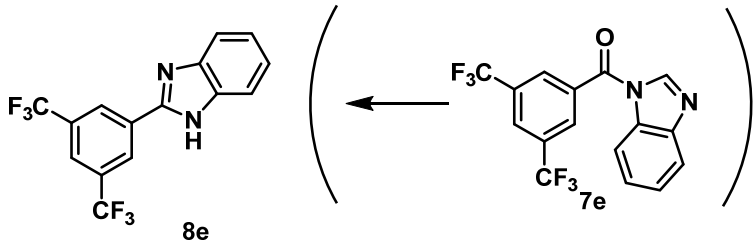
***m*-Isomer:** This compound was identified based the following spectroscopic data.[16]

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 12.9 (s, 1H). Other peaks were overlapped with those of *p*-isomers.

MS, *m/z* (relative intensity, %): 225 (15), 224 (M$^+$, 100), 223 (66), 195 (16), 194 (36), 193 (26), 112 (14), 90 (13), 77 (14), 64 (12), 63 (15).

[17] Das, K.; Mondal, A.; Srimani, D. *J. Org. Chem*. **2018**, *83*, 9553.

2-(3,5-Bis(trifluoromethyl)phenyl)-1*H*-benzo[*d*]imidazole (8e) [CAS: 1280585-62-7].



The typical procedure (Condition A) was followed using **7e** as the substrate.

White solid (64.4 mg, 78%). Mp 201.5–201.7 °C. R_f 0.66 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 13.34 (s, 1H), 8.79 (s, 2H), 8.20 (s, 1H), 7.77–7.55 (m, 2H), 7.27–7.25 (m, 2H).

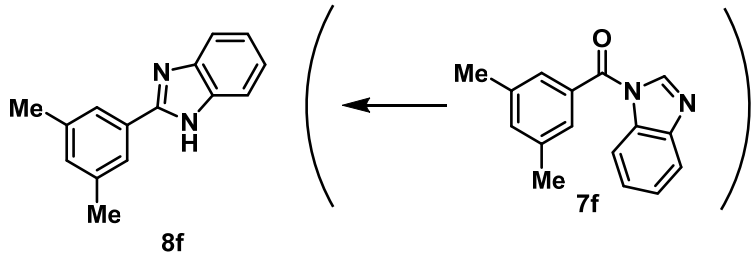
^{13}C NMR (Acetone-d_6, 100.53 MHz) δ: 149.2, 133.9, 132.7 (q, J_{CF} = 33.5 Hz), 127.5 (q, J_{CF} = 2.9 Hz), 124.3 (q, J_{CF} = 272.2 Hz), 124.0, 123.6 (qt, J_{CF} = 2.9 Hz), 116.4 (br).

IR (ATR): 3064 w, 1737 w, 1351 m, 1280 s, 1184 m, 1137 s, 902 w, 848 w, 746 w, 701 w.

MS, *m/z* (relative intensity, %): 331 (12), 330 (M^+, 100), 311 (12), 310 (17), 291 (26), 165 (15), 90 (19), 64 (24), 63 (19).

HRMS calcd for $C_{15}H_9F_6N_2$ ([M+H^+]): 331.0664. Found: 331.0703.

2-(3,5-Dimethylphenyl)-1*H*-benzo[*d*]imidazole (8f) [CAS: 1011735-85-5].



The typical procedure (Condition A) was followed using **7f** as the substrate.

Isolated yield was 70% (38.8 mg) when $Ni(cod)_2$ (40 mol%) and dcype (40 mol%) were used as the catalyst for 24 h at 180 °C.

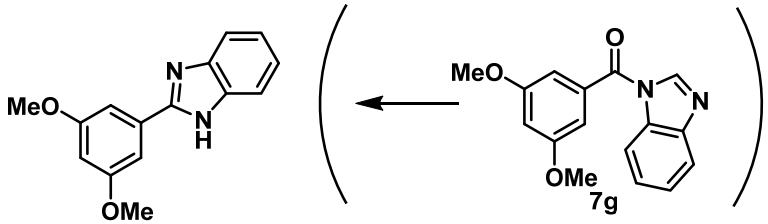
White solid (38.8 mg, 70%). R_f 0.47 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 12.83 (s, 1H), 7.81 (s, 2H), 7.64 (d, J = 7.2 Hz, 1H), 7.51 (d, J = 7.0 Hz, 1H), 7.22–7.16 (m, 2H), 7.13 (s, 1H), 2.37 (s, 6H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 151.4, 143.8, 138.0, 134.9, 131.3, 130.0, 124.2, 122.4, 121.6, 118.8, 111.3, 21.0.

HRMS calcd for $C_{15}H_{15}N_2$ ([M+H^+]): 223.1230. Found: 223.1246.

2-(3,5-Dimethoxyphenyl)-1*H*-benzo[*d*]imidazole (8g) [CAS: 393134-67-3].



The typical procedure (Condition A) was followed using **7g** as the substrate. Isolated yield was 60% (38.2 mg) when $Ni(cod)_2$ (40 mol%) and dcype (40 mol%) were used as the catalyst for 24 h at 180 °C.

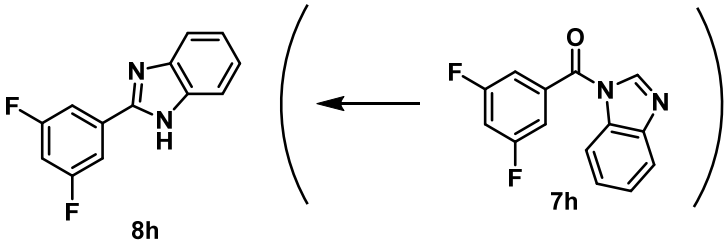
Pale yellow solid (38.2 mg, 60%). R_f 0.29 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 12.90 (s, 1H), 7.67 (d, J = 7.4 Hz, 1H), 7.53 (d, J = 7.4 Hz, 1H), 7.38 (d, J = 2.3 Hz, 2H), 7.25–7.17 (m, 2H), 6.62 (t, J = 2.3 Hz, 1H), 3.85 (s, 6H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 160.8, 151.0, 143.6, 134.9, 131.9, 122.7, 121.7, 118.9, 111.3, 104.2, 102.1, 55.5.

HRMS calcd for $C_{15}H_{15}N_2O_2$ ([M+H$^+$]): 255.1128. Found: 255.1146.

2-(3,5-Difluorophenyl)-1*H*-benzo[*d*]imidazole (8h) [CAS: 1094668-21-9].



The typical procedure (Condition A) was followed using **7h** as the substrate.

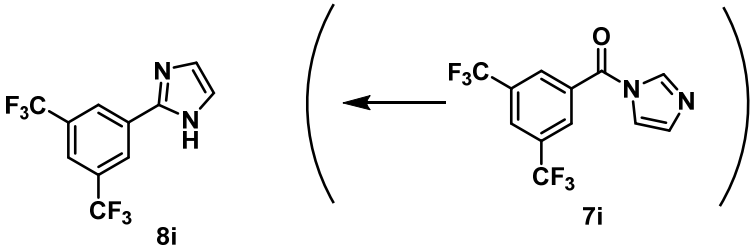
White solid (29.4 mg, 51%). R_f 0.57 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 10.36 (s, 1H), 7.84–7.82 (m, 1H), 7.61–7.48 (m, 3H), 7.34–7.29 (m, 2H), 6.89 (tt, J = 2.3, 8.7 Hz, 1H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 162.8 (dd, J_{CF} = 13.5, 245.3 Hz), 148.9 (t, J_{CF} = 2.8 Hz), 143.4, 135.0, 133.6 (t, J_{CF} = 10.5 Hz), 123.1, 122.5, 119.2, 111.8, 109.5 (dd, J_{CF} = 7.7, 20.1 Hz), 105.1 (t, J_{CF} = 25.9 Hz).

HRMS calcd for $C_{13}H_9F_2N_2$ ([M+H$^+$]): 231.0728. Found: 231.0744.

2-(3,5-Bis(trifluoromethyl)phenyl)-1*H*-imidazole (8i) [CAS: 1097069-74-3].



The typical procedure (Condition A) was followed using **7i** as the substrate. ^{13}C NMR spectrum of **8i** was recorded with ^{19}F decoupling.

White solid (32.9 g, 47%). Mp 162.2–163.0 °C. R_f 0.43 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 13.03 (s, 1H), 8.57 (s, 2H), 8.04 (s, 1H), 7.35–7.21 (m, 2H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 142.8, 133.0, 130.9, 129.9, 124.9, 123.3, 120.90, 119.5.

^{19}F NMR (DMSO-d_6, 376.17 MHz) δ: –61.5 (s, 6F).

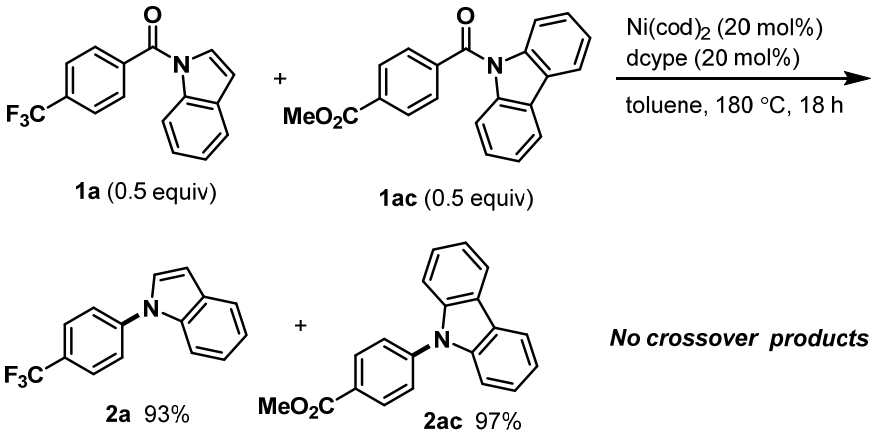
IR (ATR): 1718 m, 1481 w, 1417 m, 1347 m, 1282 s, 1180 m, 1135 s, 900 m.

MS, *m/z* (relative intensity, %): 281 (12), 280 (M^+, 100), 261 (17), 260 (28), 253 (18), 191 (10), 41 (23), 140 (20).

HRMS calcd for $C_{11}H_7F_6N_2$ ([M+H$^+$]): 281.0508. Found: 281.0508.

VII. Mechanistic Studies.

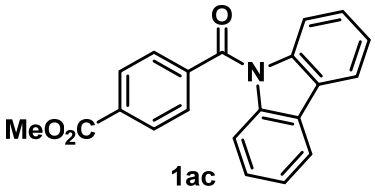
VII-1. Crossover experiments using indole amides (Scheme 4a).



$Ni(cod)_2$ (13.8 mg, 0.050 mmol), dcype (21.1 mg, 0.050 mmol), **1a** (36.2 mg, 0.125 mmol), **1ac** (41.2 mg, 0.125 mmol) and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed. The contents of the vial were then stirred at 180 °C for 18 h. The reaction

was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel before being analyzed by GC. As a result of GC analysis of the crude mixture, crossover products were not observed. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel to give **2a** (30.4 mg, 0.116 mmol) and **2ac** (36.5 mg, 0.121 mmol) as white solids.

Methyl 4-(9*H*-carbazole-9-carbonyl)benzoate (1ac).



1ac

The general procedure I was followed using methyl 4-(chloroformyl)benzoate.

White solid (3.4 g, 52%). Mp 139.7–139.9 °C. R_f 0.14 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 3.99 (s, 3H), 7.39–7.30 (m, 4H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.2 Hz, 2H), 8.01 (d, *J* = 8.2 Hz, 2H), 8.20 (d, *J* = 8.2 Hz, 2H).

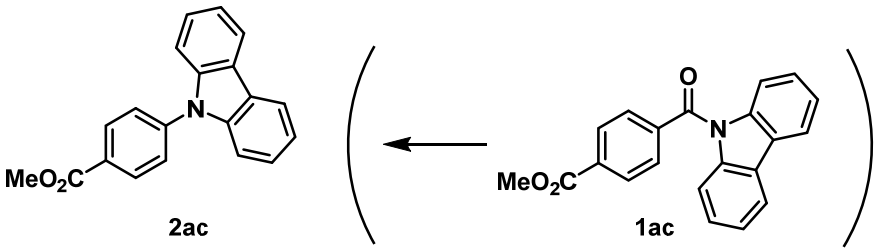
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 52.6, 115.8, 119.9, 123.8, 126.2, 126.9, 128.8, 130.1, 133.3, 138.8, 139.7, 166.1, 168.6.

IR (ATR): 2360 w, 1725 s, 1677 m, 1482 w, 1444 m, 1328 m, 1278 s, 1218 m, 1110 m, 1074 w, 1020 w, 948 w, 852 w, 821 w, 757 s, 723 m, 678 w.

MS, *m/z* (relative intensity, %): 329 (M^+, 36), 164 (10), 163 (100), 103 (12).

HRMS calcd for $C_{21}H_{16}NO_3$ ([M+H^+]): 330.1130. Found: 330.1134.

Methyl 4-(9*H*-carbazol-9-yl)benzoate (2ac) [CAS: 57103-16-9].



2ac **1ac**

The typical procedure (Condition A) was followed using **1ac** as the substrate.

White solid (70.8 mg, 94%). R_f 0.23 (SiO_2, hexane/EtOAc = 10/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 4.00 (s, 3H), 7.32 (dd, *J* = 6.9, 7.8 Hz, 2H), 7.43 (dd, *J* = 6.9, 8.2

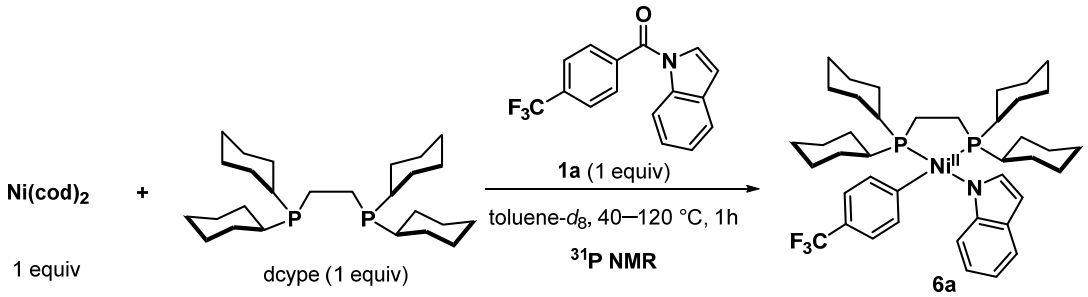
Hz, 2H), 7.47 (d, J = 8.2 Hz, 2H), 7.69 (d, J = 8.2 Hz, 2H), 8.16 (d, J = 7.8 Hz, 2H), 8.29 (d, J = 8.2 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 52.3, 109.7, 120.4, 120.5, 123.8, 126.2, 126.4, 128.6, 131.3, 140.2, 142.0, 166.4.

HRMS calcd for $C_{20}H_{15}NO_2$ ([M+H$^+$]): 302.1176. Found: 302.1172.

VII-2. Stoichiometric reactions (Scheme 4b).

NMR Studies.



$Ni(cod)_2$ (22.0 mg, 0.08 mmol), dcype (33.8 mg, 0.08 mmol), **1a** (23.1 mg, 0.08 mmol) and toluene-d_8 (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 1 h and transferred to a NMR tube equipped with a screw cap. The cap was closed, and then it was taken out of the glovebox. The contents were then heated at 40 °C for 1 h. The contents were cooled to room temperature, the reaction was monitored by ^{31}P NMR spectroscopy at room temperature. The same procedure was performed at 60, 80, 100 and120 ℃ (**Figure S1**).

During the course of the reaction, two new downfield peaks (**b:** δ = 63.0 and 59.9 ppm, J_{PP} = 56.6 Hz) appeared at 40 ℃ alongside the signal of the Ni(cod)(dcype) (**a :** δ = 60.3 ppm, s)[18] on ^{31}P NMR. The signal of the Ni(dcype)$(CO)_2$ (**d:** δ = 64.0 ppm)[19] started to appear at 60 ℃. Another two new downfield peaks (**6a**) (**c:** δ = 60.7 and 57.9 ppm, J_{PP} = 13.1 Hz) appeared at 80 ℃.

[18] Muto, K.; Yamaguchi, J.; Lei, A.; Itami, K. *J. Am. Chem. Soc*. **2013**, *135*, 16384.
[19] Amaike, K.; Muto, K.; Yamaguchi, J.; Itami, K. *J. Am. Chem. Soc*. **2012**, *134*, 13573.

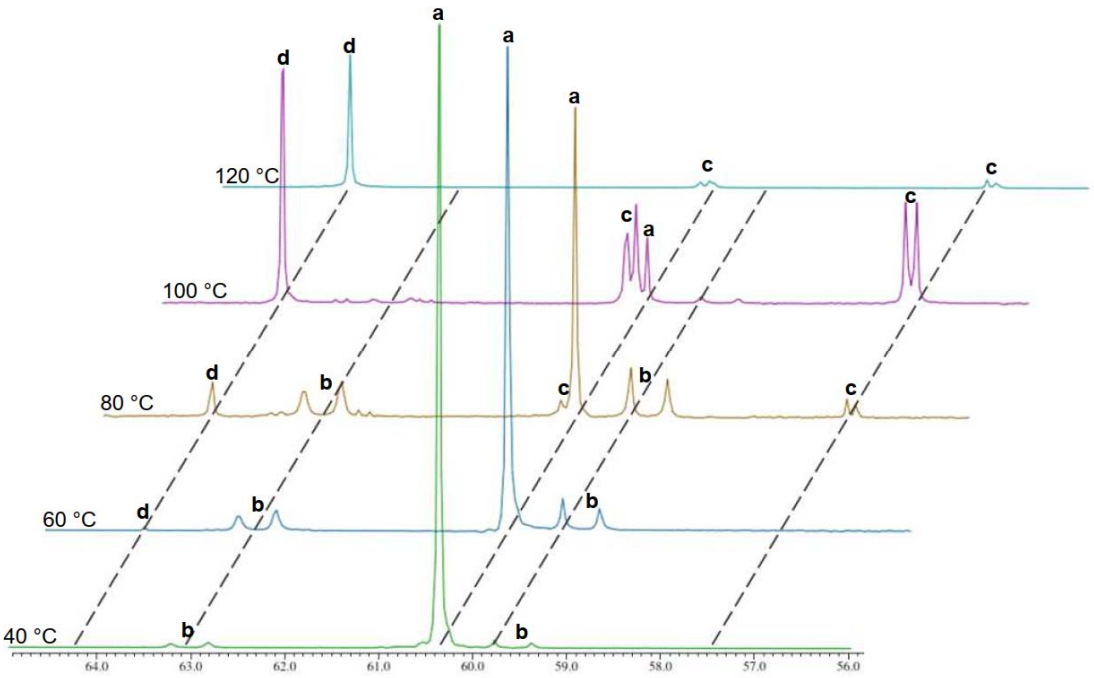
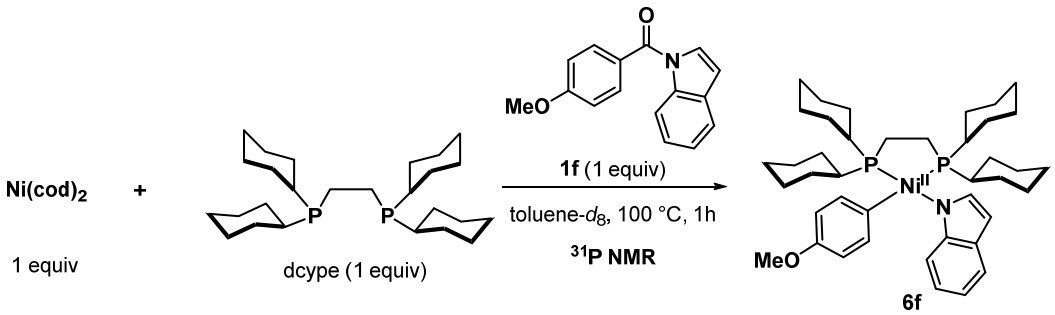


Figure S1



$Ni(cod)_2$ (22.0 mg, 0.08 mmol), dcype (33.8 mg, 0.08 mmol), **1f** (20.1 mg, 0.08 mmol) and toluene-d_8 (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 1 h and transferred to a NMR tube equipped with a screwed cap. The cap was closed, and then it was taken out of the glovebox. The contents were then heated at 100 °C for 1 h. The contents were cooled to room temperature, the reaction was monitored by ^{31}P NMR spectroscopy at room temperature. (**Figure S2**).

At 100 °C, resonances derived from the following three species were observed: δ = 60.3 ppm (s, **a**, [Ni(cod)(dcype)], δ = 60.2 ppm and 57.1 ppm (d, J = 13.2 Hz, **c'**, **6f**), δ = 64.0 ppm [s, **d**, $Ni(dcype)(CO)_2$].

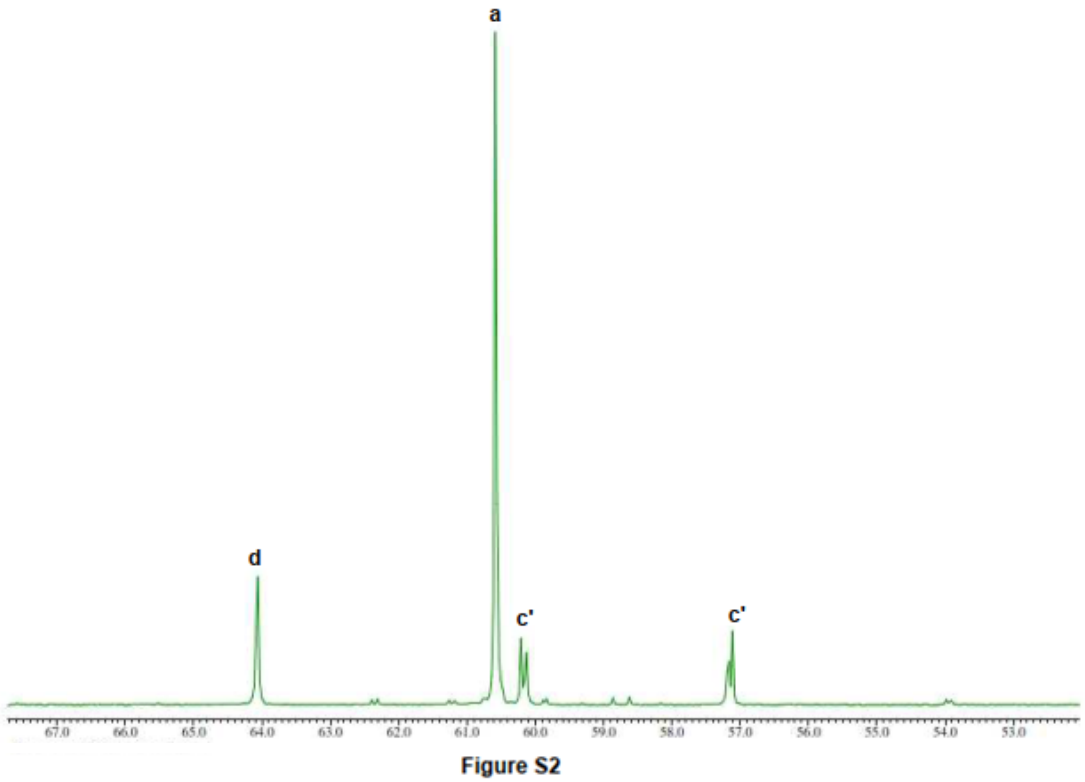
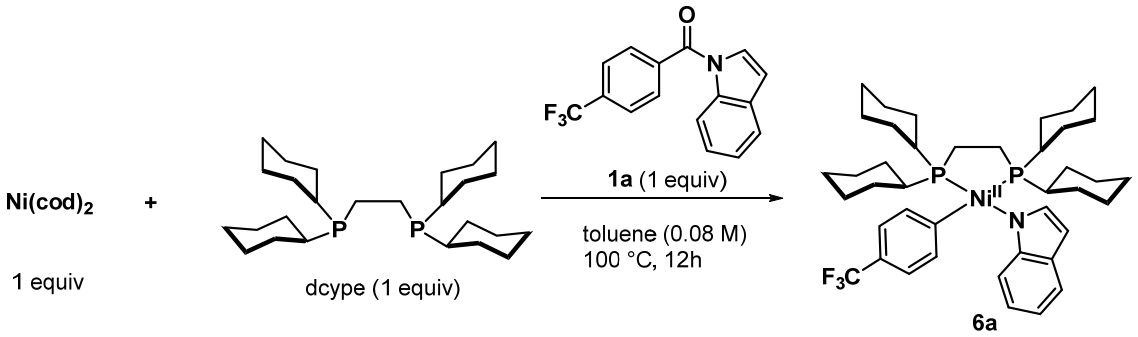


Figure S2

Complex 6a.



$Ni(cod)_2$ (66.0 mg, 0.24 mmol), dcype (101 mg, 0.24 mmol), **1a** (69.3 mg, 0.24 mmol) and toluene (3 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 1 h to give a homogeneous yellow solution, which was transferred to another vial without a stirrer bar. The cap was closed. The contents of the vial were then heated at 100 °C for 12 h without stirring. The reaction was cooled to room temperature, and the precipitated orange crystal was collected by filtration and dried in a glovebox filled with nitrogen.

Orange crystal (79.5 mg, 45%). Decomposition temperature 185.0 °C.

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 0.18–0.25 (m, 48H), 6.38 (d, J = 2.3 Hz, 1H), 6.71 (td, J = 7.3, 0.9 Hz, 1H), 6.87 (td, J = 7.4, 1.1 Hz, 1H) 7.05 (d, J = 7.8 Hz, 2H), 7.20 (d, J = 2.7 Hz, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.74 (t, J = 6.2 Hz, 2H), 7.79 (d, J = 8.2 Hz, 1H).

^{19}F NMR (CD_2Cl_2, 376.17 MHz) δ: –61.9 (s, 3F).

^{31}P NMR (CD_2Cl_2, 161.83 MHz) δ: 61.8 (d, J_{PP} = 17.5 Hz, 1P), 59.6 (d, J_{PP} = 17.5 Hz, 1P).

IR (KBr, cm^{-1}): 3047 w, 3005 w, 2926 s, 2851 s, 2666 m, 1580 s, 1445 s, 1415 m, 1319 s, 1293 s, 1265 m, 1212 m, 1182 m, 1159 s, 1110 s, 1068 s, 1008 s, 914 m, 888 m, 851 s, 819 s, 795 m, 742 s, 712 m, 674 m.

HRMS Calcd for $C_{41}H_{58}F_3NNiP_2$ ([M^+]): 741.3345. Found: 741.3353.

The structure of **6a** was unambiguously determined by X-ray crystallography.

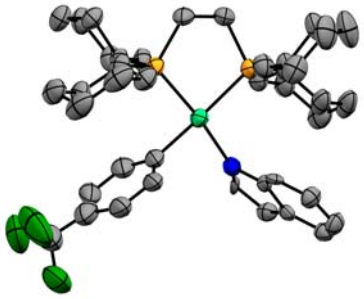
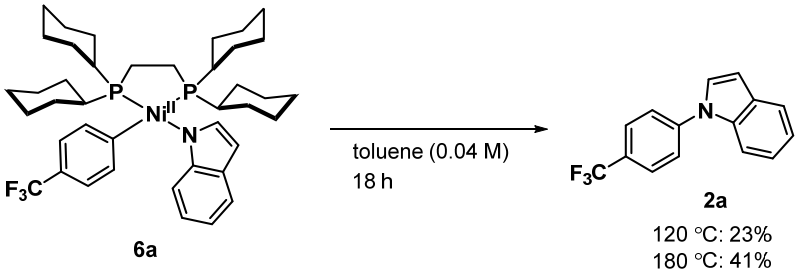


Figure S3 ORTEP drawing of **6a** with thermal ellipsoids set at the 50% probability level. All hydrogen atoms are omitted for the sake of clarity.[a]

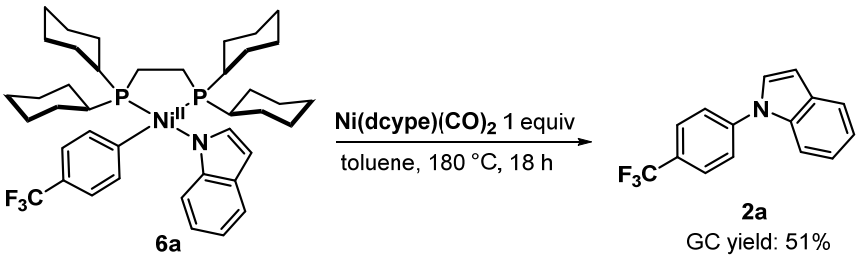
[a] Crystal data for **6a**, monoclinic, space group $P2_1/c$ (no. 14), a = 16.8932(6) Å, b = 36.2820(11) Å, c = 13.0079(5) Å, β = 103.787(4)°, V = 7743.1(5) Å^3, T = 123 K, Z = 4, R_1 (wR_2) = 0.0825 (0.2308) for 899 parameters and 19566 unique reflections. GOF = 1.050. CCDC 1901697.

Reductive elimination from 6a.



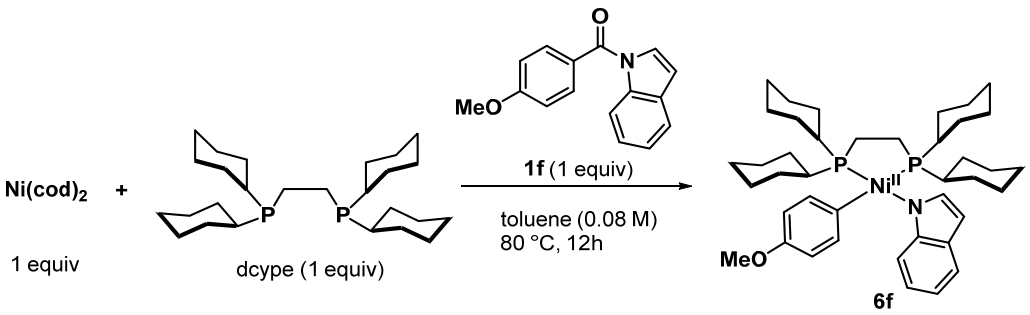
Complex **6a** (28.8 mg, 0.04 mmol) and toluene (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room

temperature for 3 min and the cap was closed, and then it was taken out of the glovebox. The contents of the vial were then heated at 120 °C (or 180 °C) for 18 h. The contents were cooled to room temperature, the product yield was determined by GC using undecane as an internal standard: 23% at 120 °C and 41% at 180 °C.



To investigate the possibility that CO accelerates the reductive elimination process, we examined the reductive elimination of **6a** in the presence of $Ni(CO)_2$(dcype), which is a potential CO source under the catalytic conditions used in this study. Complex **6a** (28.8 mg, 0.04 mmol) and $Ni(dcype)(CO)_2$ (20.8 mg, 0.04 mmol) toluene (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed, and then it was taken out of the glovebox. The contents of the vial were then stirred at 180 °C for 18 h. The contents were cooled to room temperature, the product yield was determined by GC using undecane as an internal standard. The yield of **2a** increased from 41% to 51%, indicating that CO can, in fact, promote the reductive elimination process under catalytic conditions.

Complex 6f.



$Ni(cod)_2$ (26.4 mg, 96 μmol), dcype (40.6 mg, 96 μmol), **1f** (24.1 mg, 96 μmol) and toluene (1.2 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 1 h to give a homogeneous yellow solution, which was transferred to an NMR tube equipped with a screw cap. The cap was closed. The contents were then heated at 80 °C for 12 h. The contents were cooled to room temperature, and the precipitated

orange crystal was collected by filtration and dried in a glovebox filled with nitrogen.

Orange crystal (35.2 mg, 52%). Decomposition temperature 180.0 °C.

^{1}H NMR (CD_2Cl_2, 399.78 MHz) δ: 2.30–3.60 (m, 48H), 5.16 (s, 3H), 7.92 (d, J = 2.4 Hz, 1H), 8.08 (d, J = 7.3 Hz, 2H), 8.25 (t, J = 7.3 Hz, 1H), 8.42 (t, J = 7.3 Hz, 1H), 8.81 (d, J = 7.3 Hz, 1H), 8.90 (d, J = 7.9 Hz, 1H), 8.97 (t, J = 5.8 Hz, 2H), 9.38 (d, J = 7.9 Hz, 1H).

^{31}P NMR (CD_2Cl_2, 161.83 MHz) δ: 62.6 (d, J_{PP} = 13.0 Hz, 1P), 60.3 (d, J_{PP} = 13.0 Hz, 1P).

IR (KBr, cm^{-1}): 3033 m, 2998 m, 2926 s, 2847 s, 2359 w, 1598 m, 1574 m, 1478 s, 1446 s, 1415 m, 1342 m, 1292 s, 1258 s, 1229 s, 1214 s, 1170 s, 1159 s, 1119 w, 1081 w, 1051 m, 1026 m, 1005 s, 914 w, 889 m, 852 s, 816 s, 741 s, 664 m.

HRMS Calcd for $C_{41}H_{61}NNiOP_2$ ([M^+]): 703.3576. Found: 703.3577.

The structure of **6f** was unambiguously determined by X-ray crystallography.

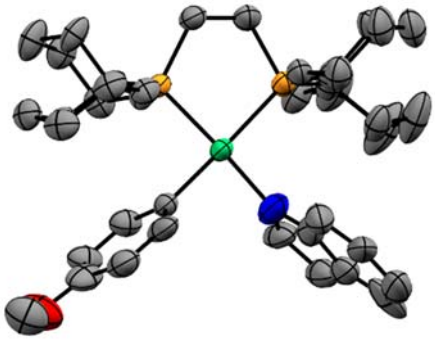
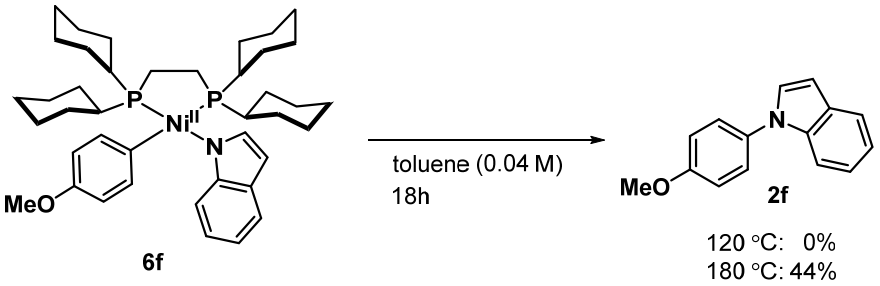


Figure S4 ORTEP drawing of **6f** with thermal ellipsoids set at the 50% probability level. All hydrogen atoms are omitted for the sake of clarity.[a]

[a]Crystal data for **6f**, monoclinic, space group $P2_1/c$ (no. 14), a = 13.2163(3) Å, b = 19.2858(3) Å, c = 17.1259(3) Å, β = 111.810(2) °, V = 4052.71(14) Å^3, T = 123 K, Z = 4, R_1 (wR_2) = 0.1119 (0.2828) for 415 parameters and 8146 unique reflections. GOF = 1.107. CCDC 1901702. The SQUEEZE subroutine of PLATON[20] was used because the refinement for the structure of solvent molecule was unsuccessful due to a significant disorder of chlorobenzene used as a solvent.

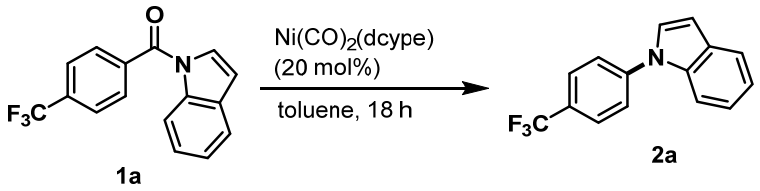
Reductive elimination from 6f.

[20] Spek, A. L. *Acta. Crystallogr. Sect. D* **2009**, *65*,148.



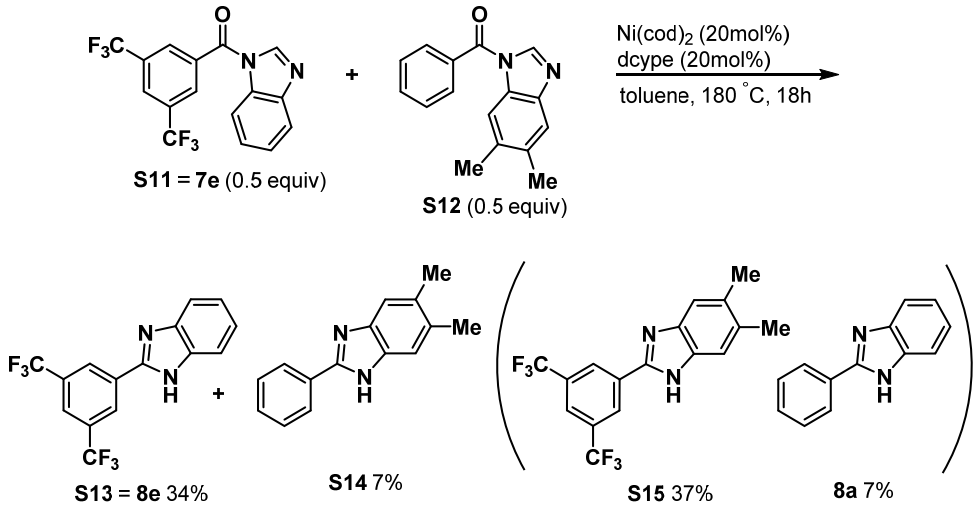
Complex **6f** (0.04 mmol) and toluene (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed, and then it was taken out of the glovebox. The contents of the vial were then stirred at 180 °C for 18 h. The contents were cooled to room temperature, the product yield was determined by GC using undecane as an internal standard: 0% at 120 °C and 44% at 180 °C. Therefore, the reductive elimination from **6f** requires higher temperature to occur than required for **6a**.

VII-3. Effect of CO ligand.



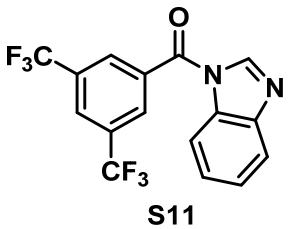
$Ni(CO)_2$(dcype) (0.050 mmol), **1a** (0.25 mmol) and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed. The contents of the vial were then stirred at 120 (or 180 °C) for 18 h. The contents were cooled to room temperature, the product yield was determined by GC using undecane as an internal standard: 1% at 120 °C and 73% at 180 °C.

VII-4. Crossover experiments using *N*-acylated benzimidazoles.



$Ni(cod)_2$ (13.8 mg, 0.050 mmol), dcype (21.1 mg, 0.050 mmol), **S11** (44.8 mg, 0.125 mmol), **S12** (31.3 mg, 0.125 mmol) and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was closed. The contents of the vial were then stirred at 180 °C for 18 h. The reaction was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography (hexane:EtOAc = 5:1→1:1) over silica gel to give two fractions. The first fraction contained **S13** and **S15** [R_f = 0.46 (hexane:EtOAc = 5:1), 30.8 mg]. The second fraction contained **S14** and **8a** [R_f = 0.09 (hexane:EtOAc = 5:1), 3.8 mg]. The yields for the four compounds were determined by ^{1}H-NMR using 1,1,2,2-tetrachloroethane as an internal standard by comparison with the spectroscopic data of the independently synthesized authentic compounds. The NMR yields of **S13**, **S14**, **S15** and **8a** were 34%, 7%, 37% and 7%, respectively.

(1*H*-Benzo[*d*]imidazol-1-yl)(3,5-bis(trifluoromethyl)phenyl)methanone (S11) [CAS: 1899226-42-6].



S11

The general procedure I was followed using 3,5-bis(trifluoromethyl)benzoyl chloride (6 mmol scale). White solid (1.2 g, 55%). Mp 84.7–84.1 °C. R_f 0.66 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.46–7.52 (m, 2H), 7.85–7.87 (m, 1H), 8.10 (s, 1H), 8.16–8.21 (m,

1H), 8.21 (s, 1H), 8.27 (s, 2H).

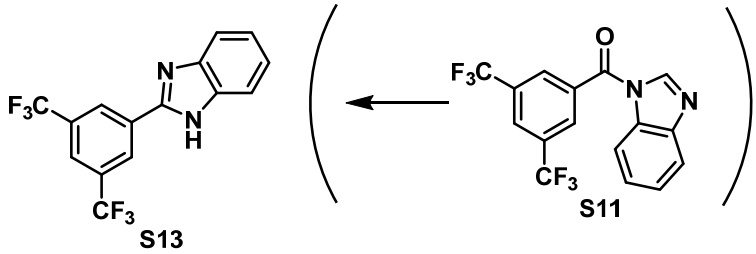
^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 115.4, 118.4, 120.9, 122.5 (q, J_{CF} = 273.1 Hz), 126.0, 126.5 (qt, J_{CF} = 3.1 Hz), 129.4 (q, J_{CF} = 3.1 Hz), 131.7, 133.0 (q, J_{CF} = 34.2 Hz), 134.9, 141.8, 144.1, 164.1.

IR (ATR): 2360 w, 1707 m, 1512 w, 1452 w, 1396 w, 1356 m, 1284 s, 1180 s, 1142 s, 910 w, 771 s, 708 w.

MS, *m/z* (relative intensity, %): 358 (M^+, 33), 242 (10), 241 (100), 213 (48), 163 (10).

HRMS Calcd for $C_{16}H_9F_6N_2O$ ([M+H^+]): 359.0614. Found: 359.0628.

2-(3,5-Bis(trifluoromethyl)phenyl)-1*H*-benzo[*d*]imidazole (S13) [CAS: 1280585-62-7].



The typical procedure (Condition A) was followed using **S11** as the substrate.

White solid (64.4 mg, 78%). Mp 201.5–201.7 °C. R_f 0.66 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO- d_6, 399.78 MHz) δ: 7.25–7.27 (m, 2H), 7.55‑7.77 (m, 2H), 8.20 (s, 1H), 8.79 (s, 2H), 13.34 (s, 1H).

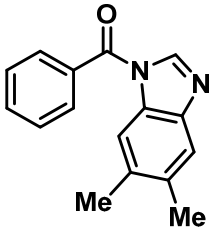
^{13}C NMR (Acetone-d_6, 100.53 MHz) δ: 116.4 (br), 123.6 (qt, J_{CF} = 2.9 Hz), 124.0, 124.3 (q, J_{CF} = 272.2 Hz), 127.5 (q, J_{CF} = 2.9 Hz), 132.7 (q, J_{CF} = 33.5 Hz), 133.9, 149.2.

IR (ATR): 3064 w, 1737 w, 1351 m, 1280 s, 1184 m, 1137 s, 902 w, 848 w, 746 w, 701 w.

MS, *m/z* (relative intensity, %): 331 (12), 330 (M^+, 100), 311 (12), 310 (17), 291 (26), 165 (15), 90 (19), 64 (24), 63 (19).

HRMS Calcd for $C_{15}H_9F_6N_2$ ([M+H^+]): 331.0664. Found: 331.0703.

(5,6-Dimethyl-1*H*-benzo[d]imidazol-1-yl)(phenyl)methanone (S12) [CAS 16109-46-9].

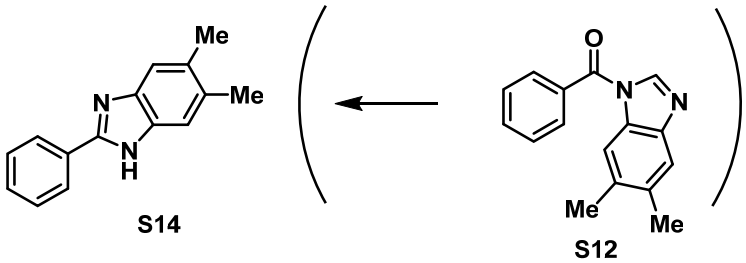


S12

The general procedure I was followed using benzoyl chloride. Spectroscopic data were consistent with

those reported in the literature.[21]

5,6-Dimethyl-2-phenyl-1*H*-benzo[*d*]imidazole (S14) [CAS: 14313-45-2].



The typical procedure (Condition A) was followed using **S12** as the substrate.

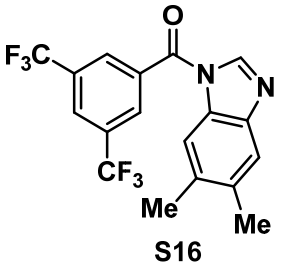
White solid (31.7 mg, 57%). R_f 0.40 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR (DMSO-d_6, 399.78 MHz) δ: 2.31 (s, 3H), 2.33 (s, 3H), 7.29 (s, 1H), 7.43–7.48 (m, 2H), 7.50–7.55 (m, 2H), 8.12–8.15 (m, 2H), 12.64 (s, 1H).

^{13}C NMR (DMSO-d_6, 100.53 MHz) δ: 20.0, 20.1, 111.3, 118.9, 126.2, 128.9, 129.5, 129.9, 130.5, 131.2, 133.5, 142.5, 150.3.

HRMS Calcd for $C_{15}H_{15}N_2$ ([M+H$^+$]): 223.1230. Found: 223.1240.

(3,5-Bis(trifluoromethyl)phenyl)(5,6-dimethyl-1*H*-benzo[d]imidazol-1-yl)methanone (**S16**).



The general procedure I was followed using 3,5-bis(trifluoromethyl)benzoyl chloride.

White solid (3.1 g, 40%). Mp 91.3–92.1 °C. R_f 0.71 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 2.41 (s, 3H), 2.42 (s, 3H), 7.60 (s, 1H), 7.95 (s, 1H), 7.98 (s, 1H), 8.19 (s, 1H), 8.25 (s, 2H).

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 20.4, 20.6, 115.6, 120.9, 122.5 (q, J_{CF} = 273.1 Hz), 126.4 (qt, J_{CF} = 2.8 Hz), 129.4 (q, J_{CF} = 2.8 Hz), 130.1, 132.9 (q, J_{CF} = 69.1 Hz), 135.2, 135.2, 135.9, 141.1 142.5, 164.0.

^{19}F NMR ($CDCl_3$, 376.17 MHz) δ: –62.8 (s, 6F).

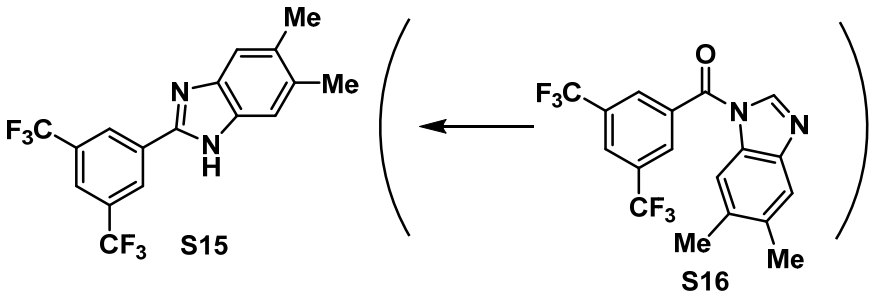
[21] Yu, L.; Wang, M.; Wang, L. *Tetrahedron* **2014**, *70*, 5391.

IR (KBr, cm^{-1}): 3055 m, 2954 w, 1752 m, 1709 s, 1624 m, 1515 s, 1471 s, 1397 s, 1356 s, 1301 s, 1280 s, 1190 s, 1174 s, 1133 s, 1111 s, 1025 m, 943 m, 908 s, 876 m, 850 m, 813 m, 760 m, 712 m, 681 s, 652 m.

MS, *m/z* (relative intensity, %): 386 (M^+, 37), 241 (100), 213 (42).

HRMS Calcd for $C_{18}H_{12}F_6N_2O$ ([M+H^+]): 387.0932. Found: 387.0930.

2-[3,5-Bis(trifluoromethyl)phenyl]-5,6-dimethyl-1*H*-benzimidazole (**S15**).



The typical procedure (Condition A) was followed using **S16** as the substrate.

White solid (58.4 mg, 65%). Mp 280.3–281.9 °C. R_f 0.26 (SiO_2, hexane/EtOAc = 9/1).

^{1}H NMR (acetone-d_6, 399.78 MHz) δ: 2.35 (s, 6H), 7.41 (s, 2H), 8.08 (s, 1H), 8.74 (s, 2H), 12.09 (s, 1H).

^{13}C NMR (acetone-d_6, 100.53 MHz) δ: 20.4, 112.5 (br), 120.7 (br), 123.1 (qt, J_{CF} = 3.7 Hz), 124.3 (q, J_{CF} = 272.2 Hz), 127.2 (q, J_{CF} = 2.8 Hz), 132.7 (br), 132.7 (q, J_{CF} = 33.5 Hz), 134.2, 148.3.

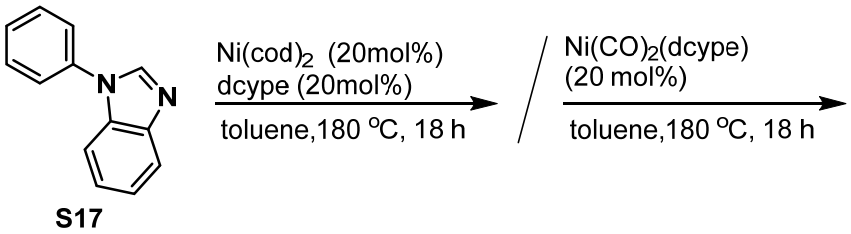
^{19}F NMR (acetone-d_6, 376.17 MHz) δ: –63.4 (s, 6F).

IR (KBr, cm^{-1}): 2924 m, 1818 w, 1718 w, 1623 m, 1588 m, 1537 w, 1476 m, 1449 s, 1432 m, 1402 s, 1376 s, 1341 s, 1325 s, 1283 s, 1233 m, 1171 s, 1135 s, 1024 m, 984 s, 901 s, 854 s, 722 m, 696 s, 683 s.

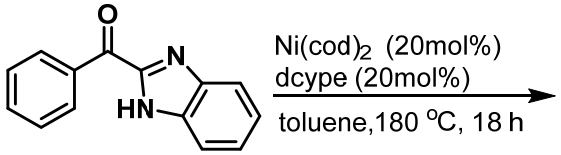
MS, *m/z* (relative intensity, %): 359 (M^+, 20), 358 (100), 357 (M^+, 53), 344 (12), 343 (66), 118 (12), 116 (11), 91 (31), 77 (12), 65 (17).

HRMS Calcd for $C_{17}H_{12}F_6N_2$ ([M+H^+]): 359.0983. Found: 359.0989.

VII-5. A control experiment using *N*-phenylbenzimidazole and 2-benzoylbenzimidazole.



S17

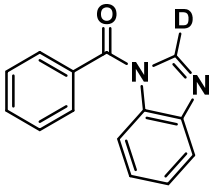


S18

The typical procedure (Condition A) was followed using *N*-phenylbenzimidazole (**S17**) or 2-benzoylbenzimidazole (**S18**) as the substrate. 2-Phenylbenzimidazole (**8a**) was not obtained under these conditions, suggesting that **S17** and **S18** are not involved as an intermediate of this 1,2-migratory decarbonylation.

VII-6. Labeling studies.

(1*H*-Benzo[*d*]imidazol-1-yl-2-d)(phenyl)methanone (7a-D)



7a-D

The general procedure I was followed using benzoyl chloride and 1*H*-benzimidazole-2-*d* **S19.**

White solid (3.1 g, 70%). Mp 89.7–90.1 °C. R_f 0.37 (SiO_2, hexane/EtOAc = 1/1).

^{1}H NMR ($CDCl_3$, 399.78 MHz) δ: 7.41–7.47 (m, 2H), 7.56–7.61 (m, 2H), 7.67–7.71 (m, 1H), 7.79–7.85 (m, 3H), 8.18–8.21 (m, 1H).

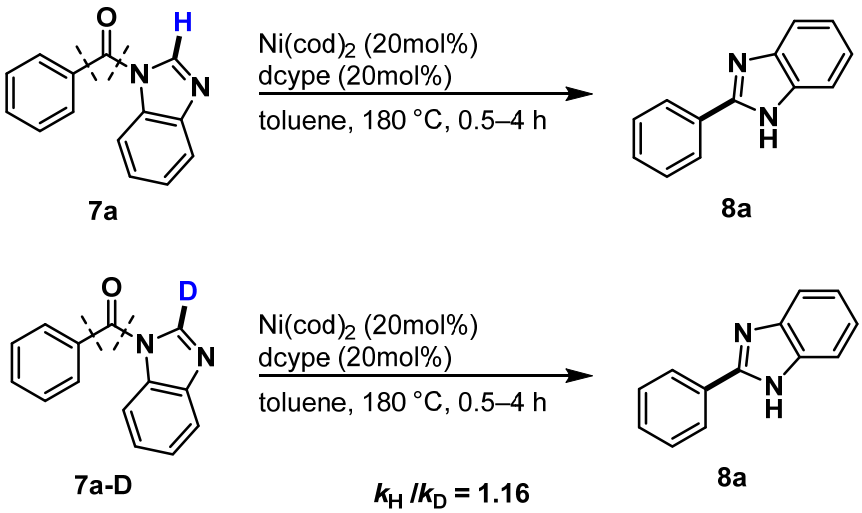
^{2}H NMR ($CHCl_3$, 61.37 MHz, internal atandard $CDCl_3$) δ: 8.25.

^{13}C NMR ($CDCl_3$, 100.53 MHz) δ: 115.4, 120.5, 125.2, 125.7, 129.0, 129.5, 132.1, 132.8, 133.2, 142.8 (t, J_{CD} = 31.7 Hz), 144.0, 167.0.

IR (KBr, cm^{-1}): 3117 w, 3058 w, 2328 w, 1908 w, 1800 w, 1772 w, 1699 s, 1601 m, 1488 m, 1467 s, 1447 s, 1353 s, 1293 m, 1259 s, 1238 m, 1179 s, 1146 m, 1095 m, 1077 m, 1031 m, 1002 m, 979 m, 940 m, 889 s, 856 m, 788 m, 753 s, 736 s, 720 s, 699 s.

MS, *m/z* (relative intensity, %): 223 (M^+, 16), 105 (100), 77 (58), 51 (15).

HRMS Calcd for $C_{14}H_{11}DN_2O$ ([M+H$^+$]): 224.0929. Found: 224.0934.



A typical procedure for kinetic studies.

$Ni(cod)_2$ (13.8 mg, 0.050 mmol), dcype (21.1 mg, 0.050 mmol), *N*-acylpyrrole derivatives (0.25 mmol) and toluene (1 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 3 min and the cap was then closed. The contents of the vial were then stirred at 180 °C. At the indicated times, the vial was rapidly cooled with running water. The crude mixture was filtered through a pad of silica gel before being analyzed by GC (**Table S1**, **Figure S5**). The progress of the reaction was monitored by GC. Dodecane was added as an internal standard. The k_H/k_D value was determined to be 1.16.

Table S1 Time dependence of ln[[**7a**]/[**7a**]$_0$] and ln[[**7a-D**]/[**7a-D**]$_0$].[a]

time / s	0	1800	3600	7200	10800	14400
ln[[**7a**]/[**7a**]$_0$]	0	-0.403	-0.631	-1.033	-1.191	-1.484
ln[[**7a-D**]/[**7a-D**]$_0$]	0	-0.228	-0.412	-0.799	-1.065	-1.163

[a] Average of two runs were used for ln[**7a**] and ln[**7a-D**].

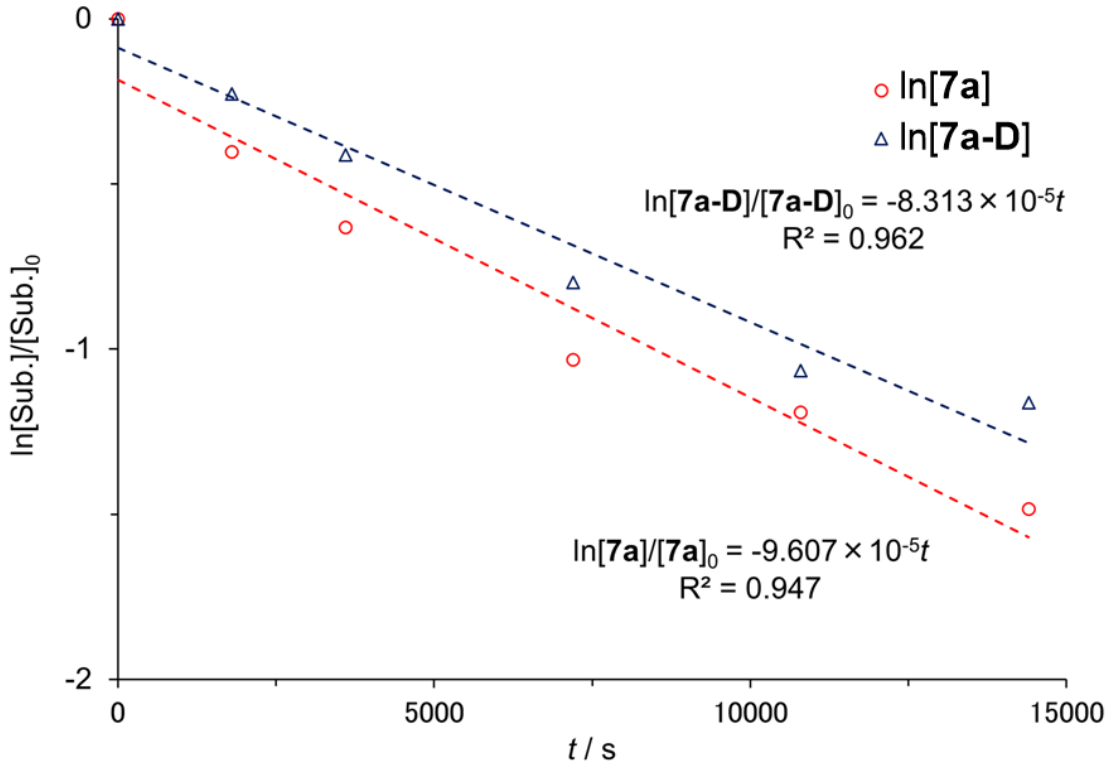
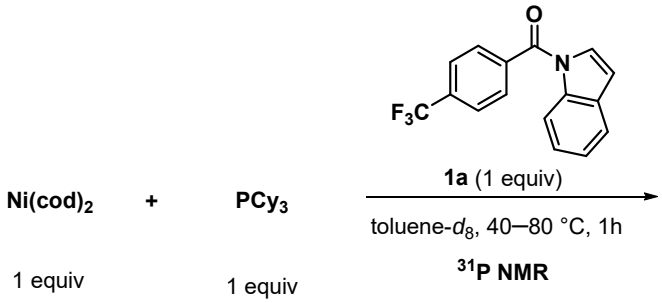


Figure S5 Time dependence of ln[**7a**]/[**7a**]$_0$. Reactions were performed using **7a** and **7a-D**. Average of two runs were plotted for both **7a** and (red circle) and **7a-D** (blue triangle). The linear regression fit to the data is also shown.

VII-7. NMR monitoring of the stoichiometric reaction of Ni(cod)$_2$, PCy$_3$ and 1a.



Ni(cod)$_2$ (22.0 mg, 0.08 mmol), PCy$_3$ (22.4 mg, 0.08 mmol), **1a** (23.1 mg, 0.08 mmol) and toluene-d_8 (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 1 h and transferred to a NMR tube equipped with a screw cap. The cap was closed, and then it was taken out of the glovebox. The contents were then heated at 40 °C for 1 h. The contents were cooled to room temperature, the reaction was monitored by ^{31}P NMR spectroscopy at room temperature. The same procedure was performed at 60 and 80 °C.

^{31}P NMR analysis of the solution revealed that new resonances appeared after 1 h stirring at rt (**a**: δ = 37.9 ppm, d, J = 35 Hz; δ = 33.1 ppm, d, J = 35 Hz) (see the chart below). As the temperature increased, these resonances decreased and additional new resonances (**b**: δ = 42.5 ppm, s; **c**: δ = 38.2 ppm, s; **d**: δ = 34.9 ppm, s) appeared in addition to the resonance assignable to [Ni(PCy$_3$)$_2$(CO)$_2$] (δ = 41.0 ppm, s). Unfortunately, however, we were unable to isolate these complexes at this stage. (**Figure S6**).

Ref. Ni(CO)(PCy$_3$)$_2$ δ 37.5,[22] Ni(CO)$_2$(PCy$_3$)$_2$ δ 41.0,[23] Ni(PCy$_3$)$_2$ δ 46.0,[2] Ni(CO)$_3$(PCy$_3$)$_3$ δ 45.0,[24] PCy$_3$-oxide δ 48.0.[25]

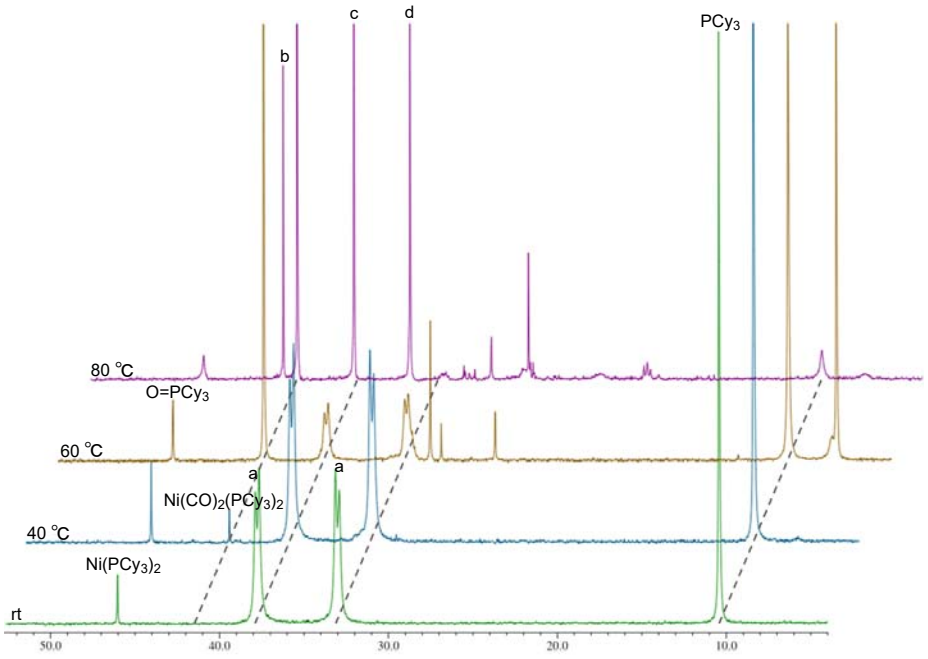
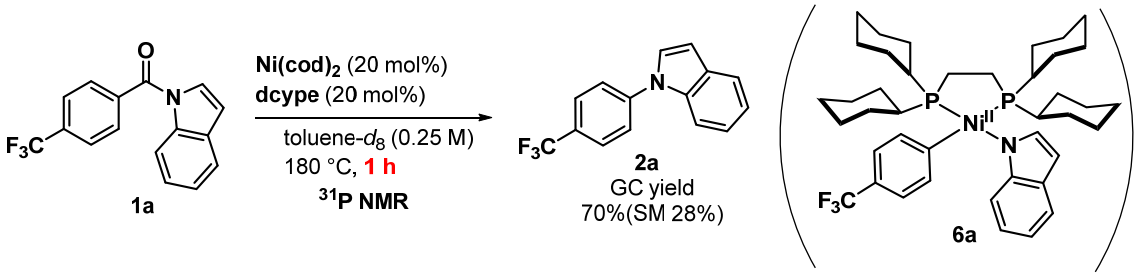


Figure S6

VII-8. NMR monitoring of the catalytic reaction of Ni(cod)$_2$, dcype and 1a.



[22] Cornella, J.; Gómez-Bengoa, E.; Martin, R. *J. Am. Chem. Soc.* **2013**, *135*, 1997.
[23] Xiao, L.-J.; Fu, X.-N.; Zhou, M.-J.; Xie, J.-H.; Wang, L.-X.; Xu, X.-F.; Zhou, Q.-L. *J. Am. Chem. Soc*. **2016**, *138*, 2957.
[24] Ohashi, M.; Taniguchi, T.; Ogoshi, S. *Organometallics* **2010**, *29*, 2386.
[25] Somerville, R.; Hale, L.; Gomez-Bengoa, E.; Bures, J.; Martin, R. *J. Am. Chem. Soc.* **2018**, *140*, 8771.

$Ni(cod)_2$ (13.8 mg, 0.05 mmol), dcype (21.1 mg, 0.05 mmol), **1a** (72.6 mg, 0.25 mmol) and toluene-d_8 (1.0 mL) were added to a 10 mL-sample vial with a Teflon-sealed screwcap in a glovebox filled with nitrogen. The resulting mixture was stirred at room temperature for 1 h and transferred to a NMR tube equipped with a screwed cap. The cap was closed, and then it was taken out of the glovebox. The contents were then heated at 180 °C for 1 h. The contents were cooled to room temperature, the reaction was monitored by ^{31}P NMR spectroscopy at room temperature. (**Figure S7)**. The product yield was determined to be 70% by GC using undecane as an internal standard. The results showed that complex **6a** is NOT a resting state of this catalytic reaction, but $Ni(CO)_2$(dcype) is.

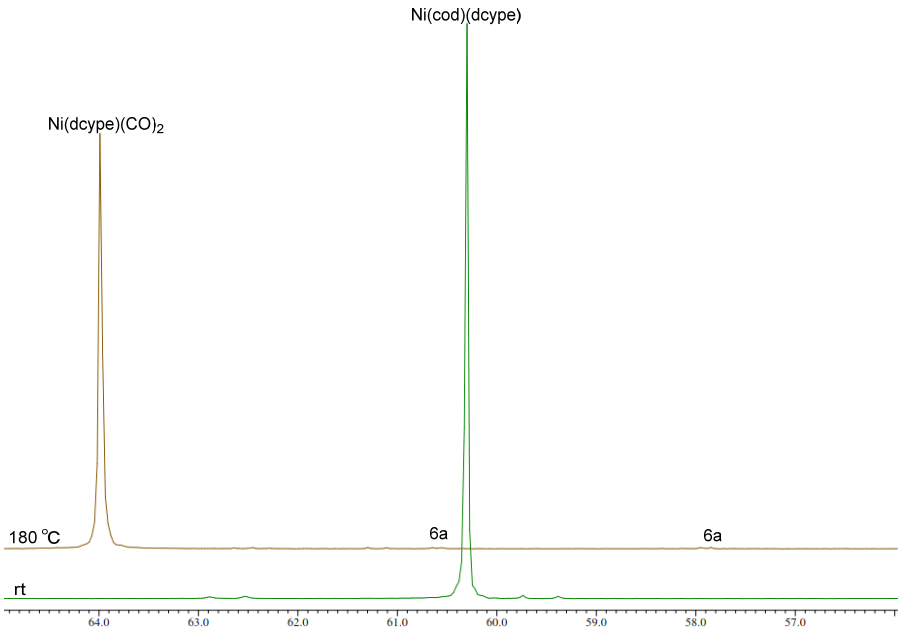
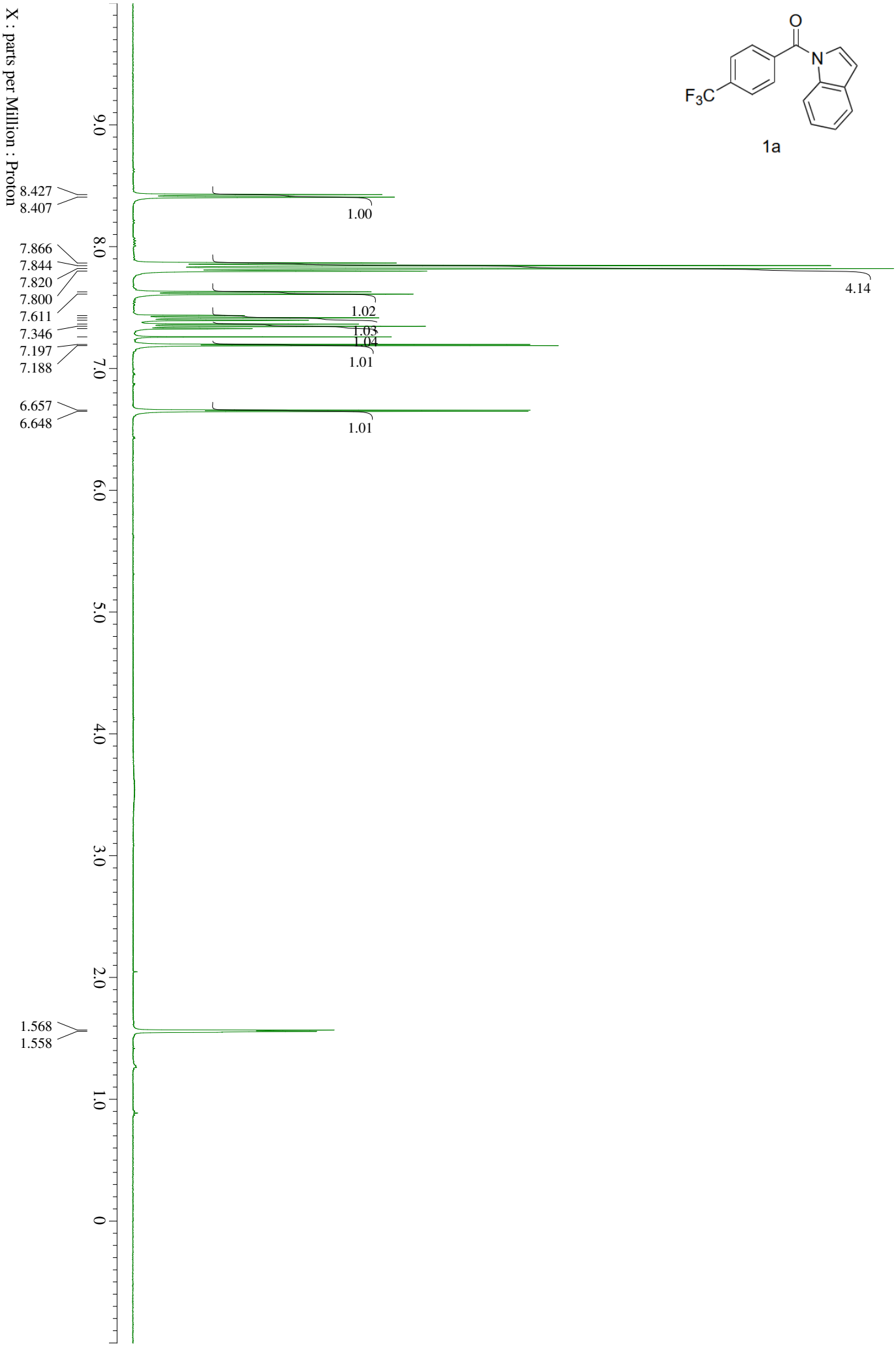


Figure S7


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.427
8.407
7.866
7.844
7.820
7.800
7.611
7.346
7.197
7.188
6.657
6.648
1.568
1.558
1.00
1.02
1.03
1.04
1.01
1.01
4.14
O
N
F3C
1a

X : parts per Million : aron13

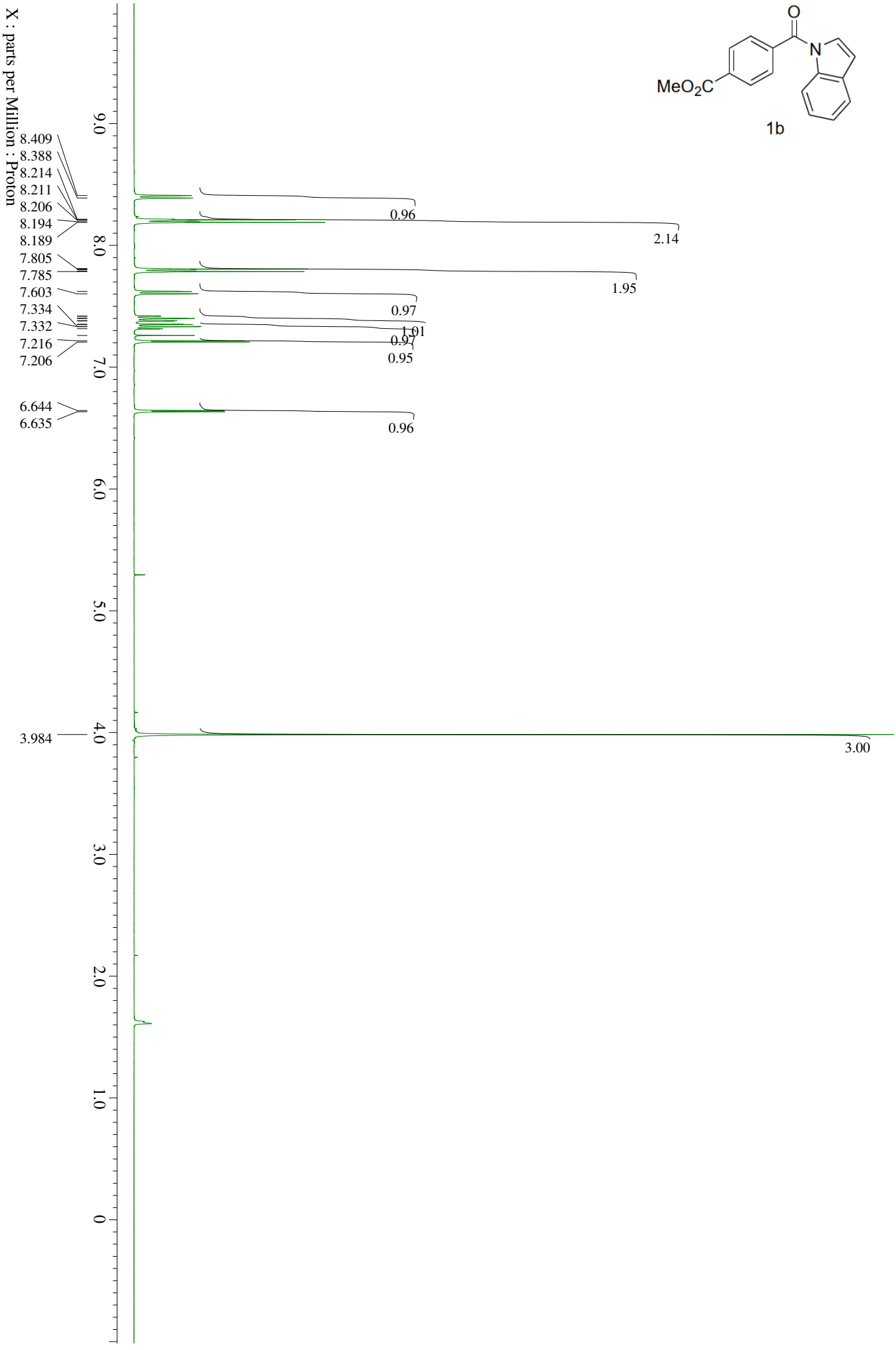
1a

167.270

137.933
135.881
133.952
133.633
133.303
132.973
130.745
129.364
127.559
126.951
125.713
125.672
125.290
124.847
124.373
122.135
121.052
119.423
116.443
109.472

77.320
77.000
76.691

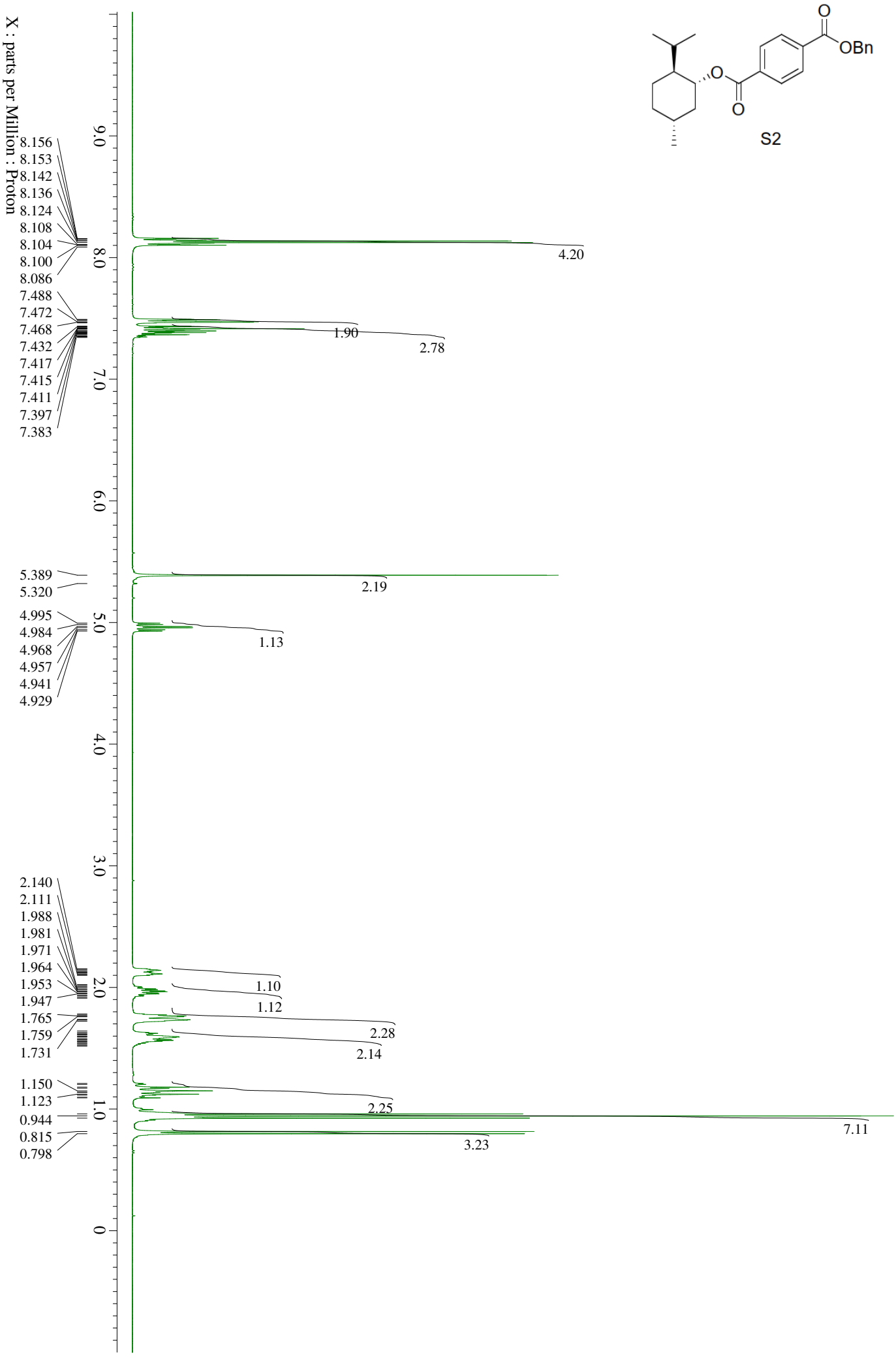
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

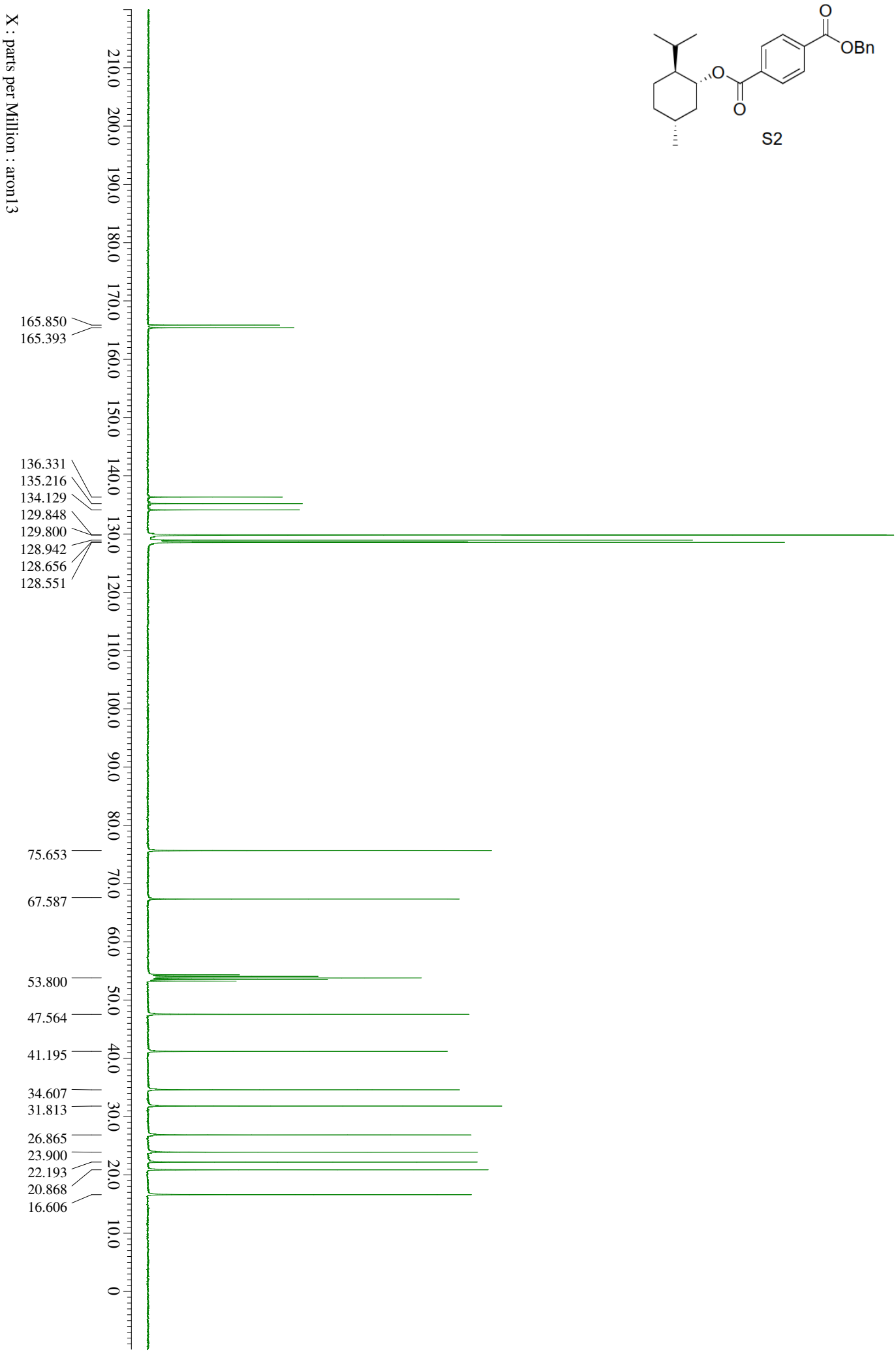

X : parts per Million : Proton
8.409
8.388
8.214
8.211
8.206
8.194
8.189
7.805
7.785
7.603
7.334
7.332
7.216
7.206
6.644
6.635
3.984
0.96
2.14
1.95
0.97
1.01
0.97
0.95
0.96
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
N
MeO2C
1b

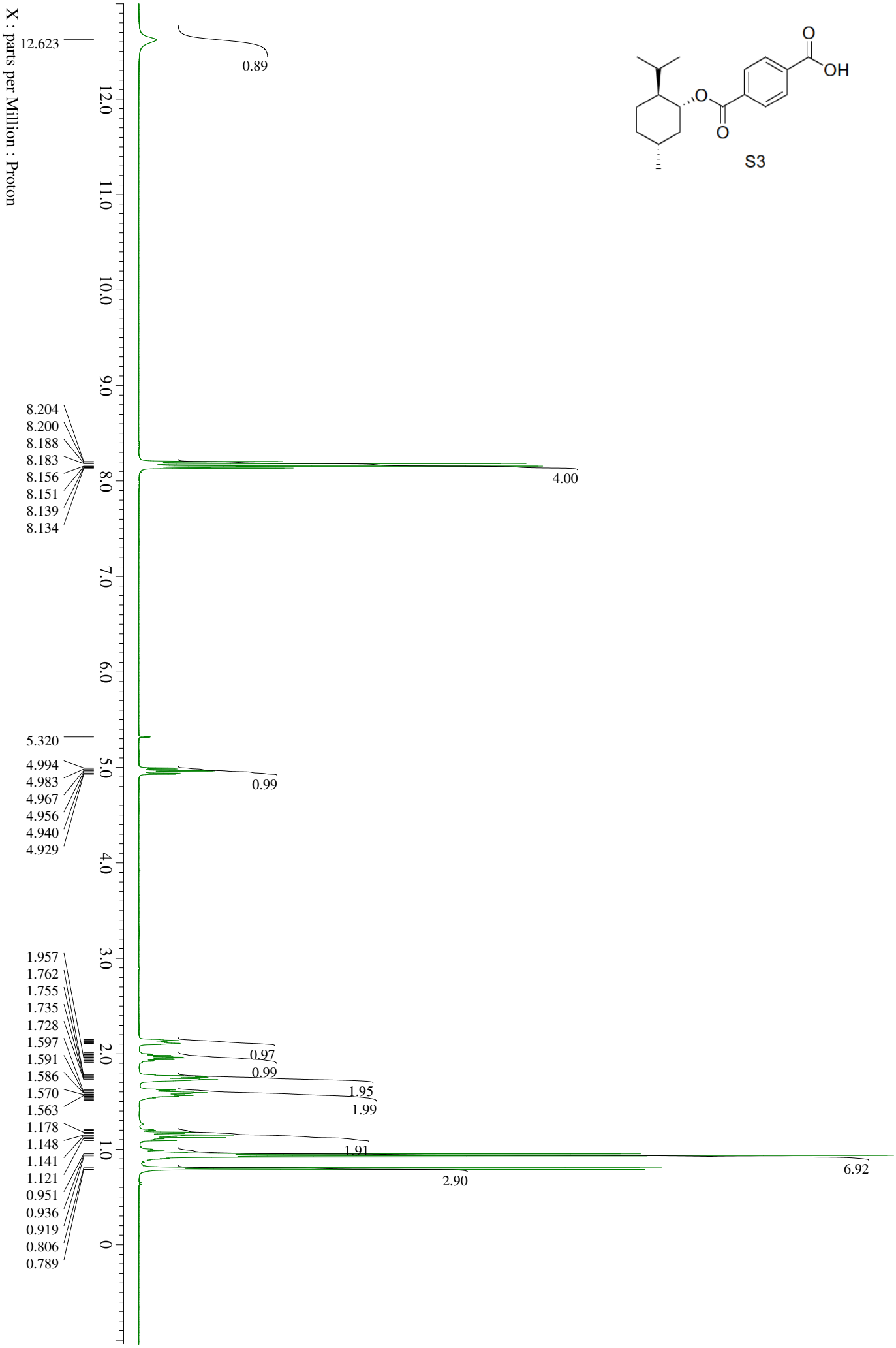
X : parts per Million : aron13

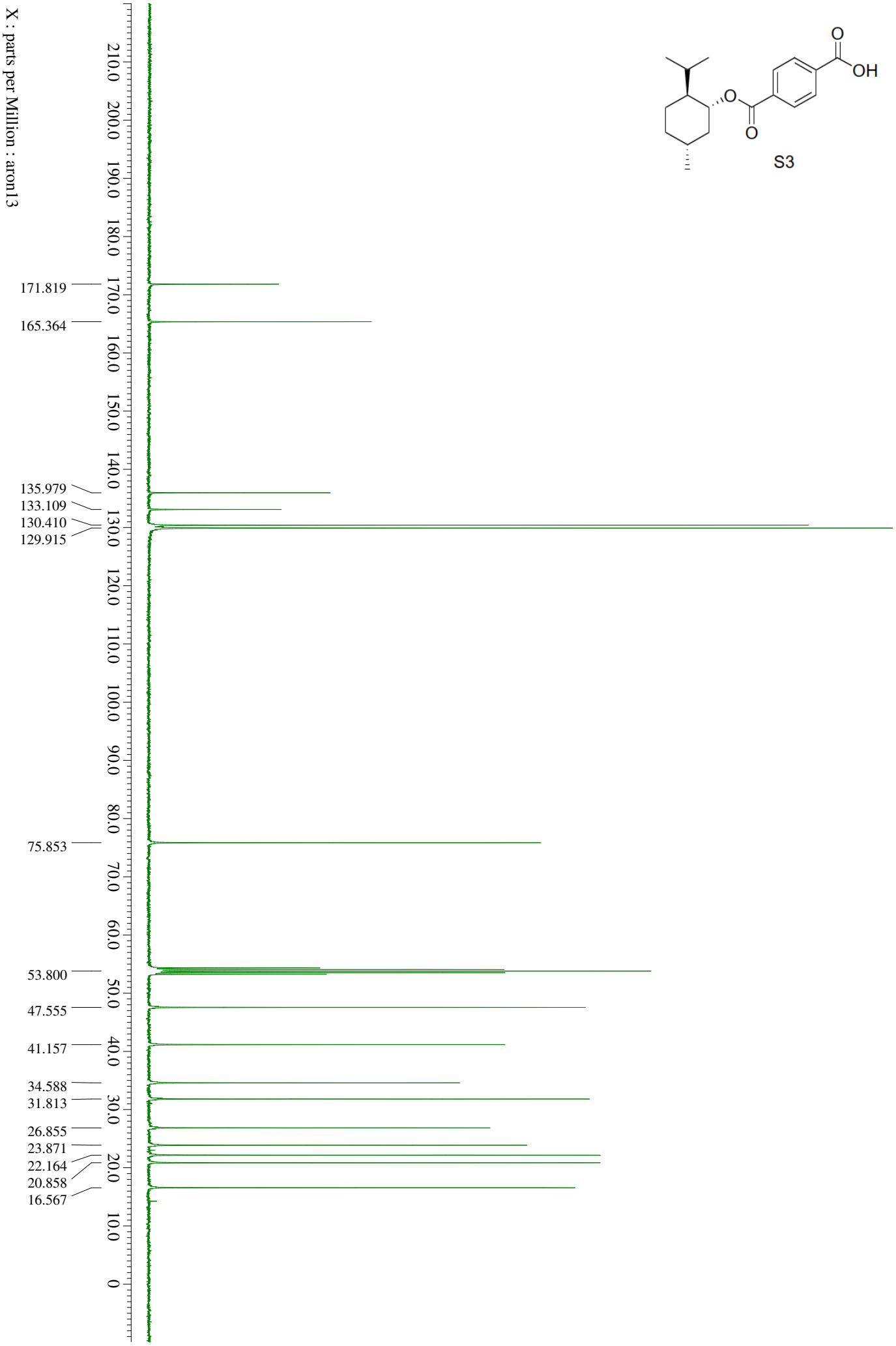
1b

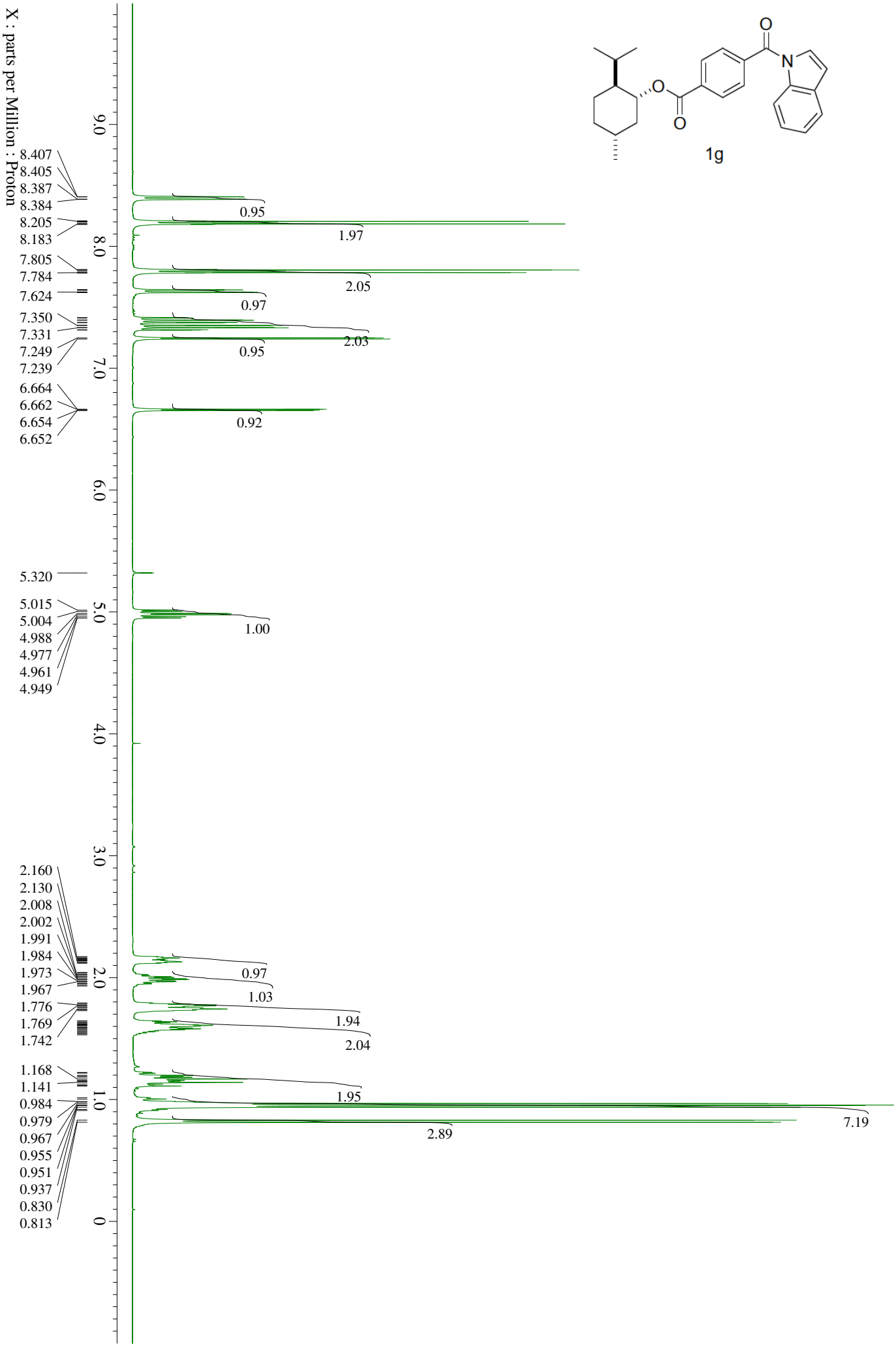
167.765
166.053
138.459
135.870
132.921
130.735
129.786
128.961
127.064
125.177
124.249
120.990
116.412
109.255
77.320
77.000
76.680
52.561

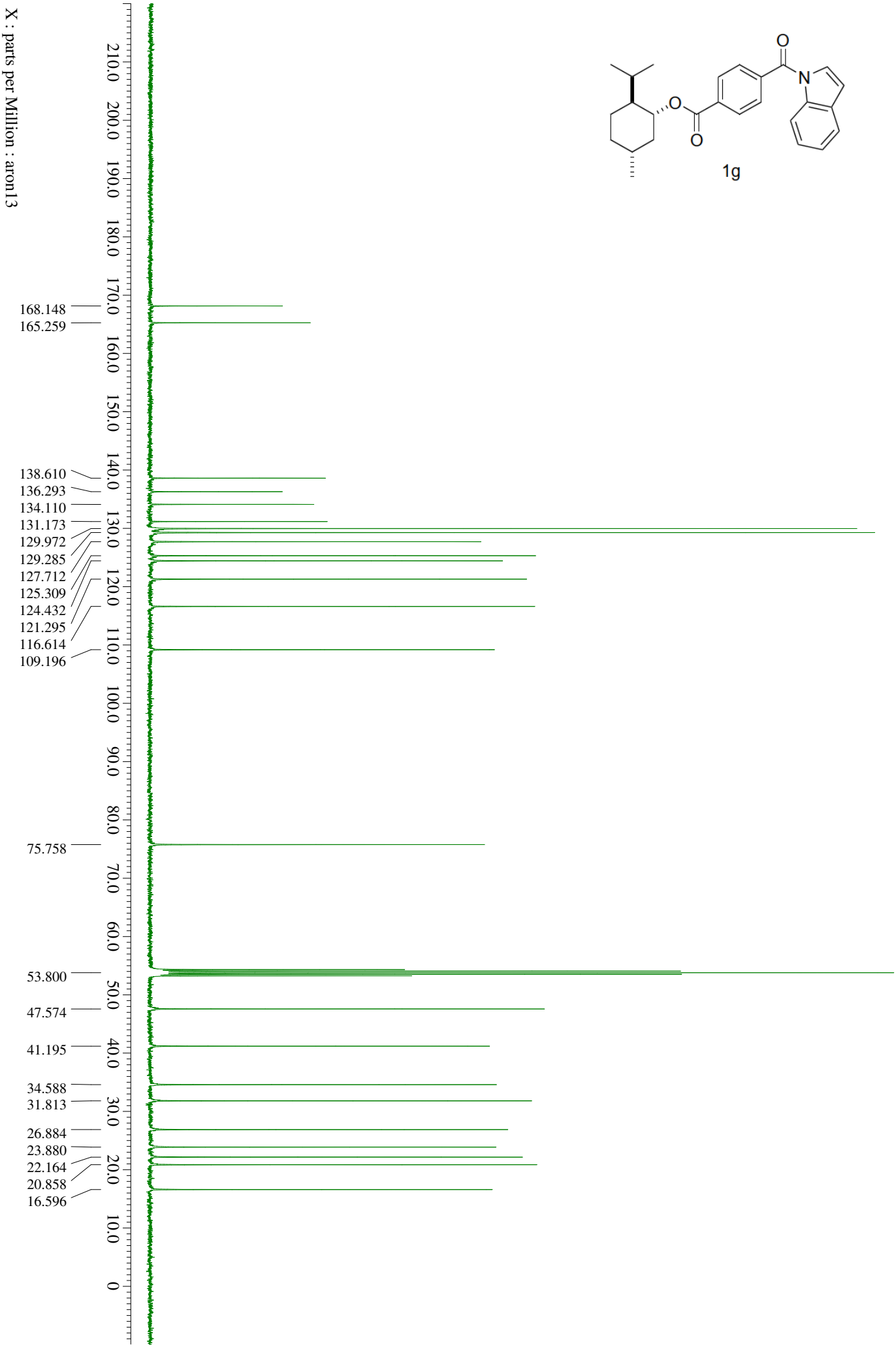

X : parts per Million : Proton
8.156
8.153
8.142
8.136
8.124
8.108
8.104
8.100
8.086
7.488
7.472
7.468
7.432
7.417
7.415
7.411
7.397
7.383
5.389
5.320
4.995
4.984
4.968
4.957
4.941
4.929
2.140
2.111
1.988
1.981
1.971
1.964
1.953
1.947
1.765
1.759
1.731
1.150
1.123
0.944
0.815
0.798
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
4.20
1.90
2.78
2.19
1.13
1.10
1.12
2.28
2.14
2.25
3.23
7.11
O
OBn
O
O
S2

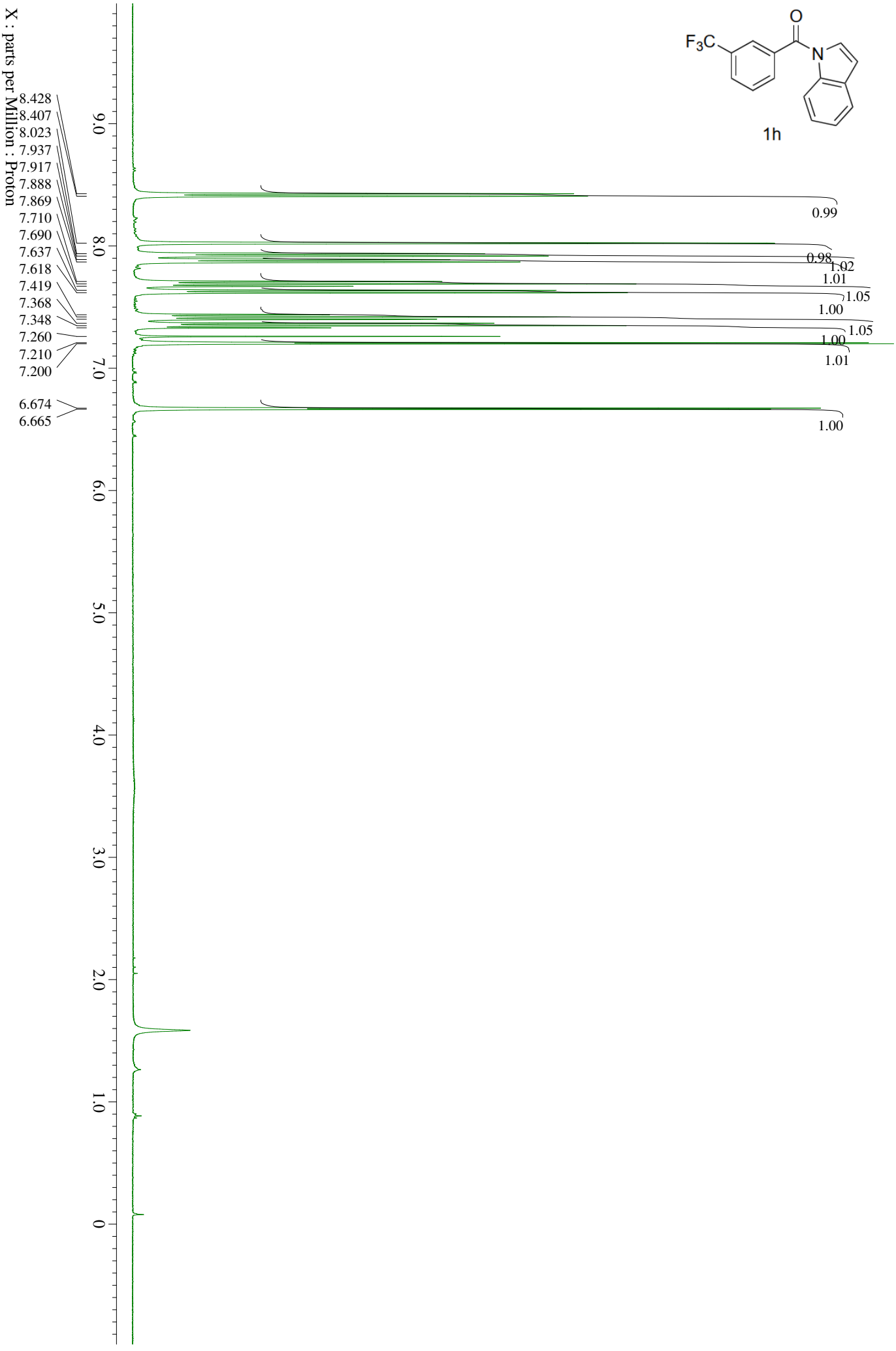

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
165.850
165.393
136.331
135.216
134.129
129.848
129.800
128.942
128.656
128.551
75.653
67.587
53.800
47.564
41.195
34.607
31.813
26.865
23.900
22.193
20.868
16.606
O
OBn
O
O
S2

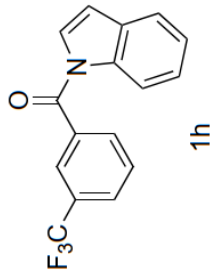

X : parts per Million : Proton
12.623
0.89
8.204
8.200
8.188
8.183
8.156
8.151
8.139
8.134
4.00
5.320
4.994
4.983
4.967
4.956
4.940
4.929
0.99
1.957
1.762
1.755
1.735
1.728
1.597
1.591
1.586
1.570
1.563
0.97
0.99
1.95
1.99
1.178
1.148
1.141
1.121
0.951
0.936
0.919
0.806
0.789
1.91
2.90
6.92
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
OH
O
O
S3


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.819
165.364
135.979
133.109
130.410
129.915
75.853
53.800
47.555
41.157
34.588
31.813
26.855
23.871
22.164
20.858
16.567
O
OH
O
O
S3


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.407
8.405
8.387
8.384
8.205
8.183
7.805
7.784
7.624
7.350
7.331
7.249
7.239
6.664
6.662
6.654
6.652
5.320
5.015
5.004
4.988
4.977
4.961
4.949
2.160
2.130
2.008
2.002
1.991
1.984
1.973
1.967
1.776
1.769
1.742
1.168
1.141
0.984
0.979
0.967
0.955
0.951
0.937
0.830
0.813
0.95
1.97
2.05
0.97
2.03
0.95
0.92
1.00
0.97
1.03
1.94
2.04
1.95
7.19
2.89
O
N
O
O
1g

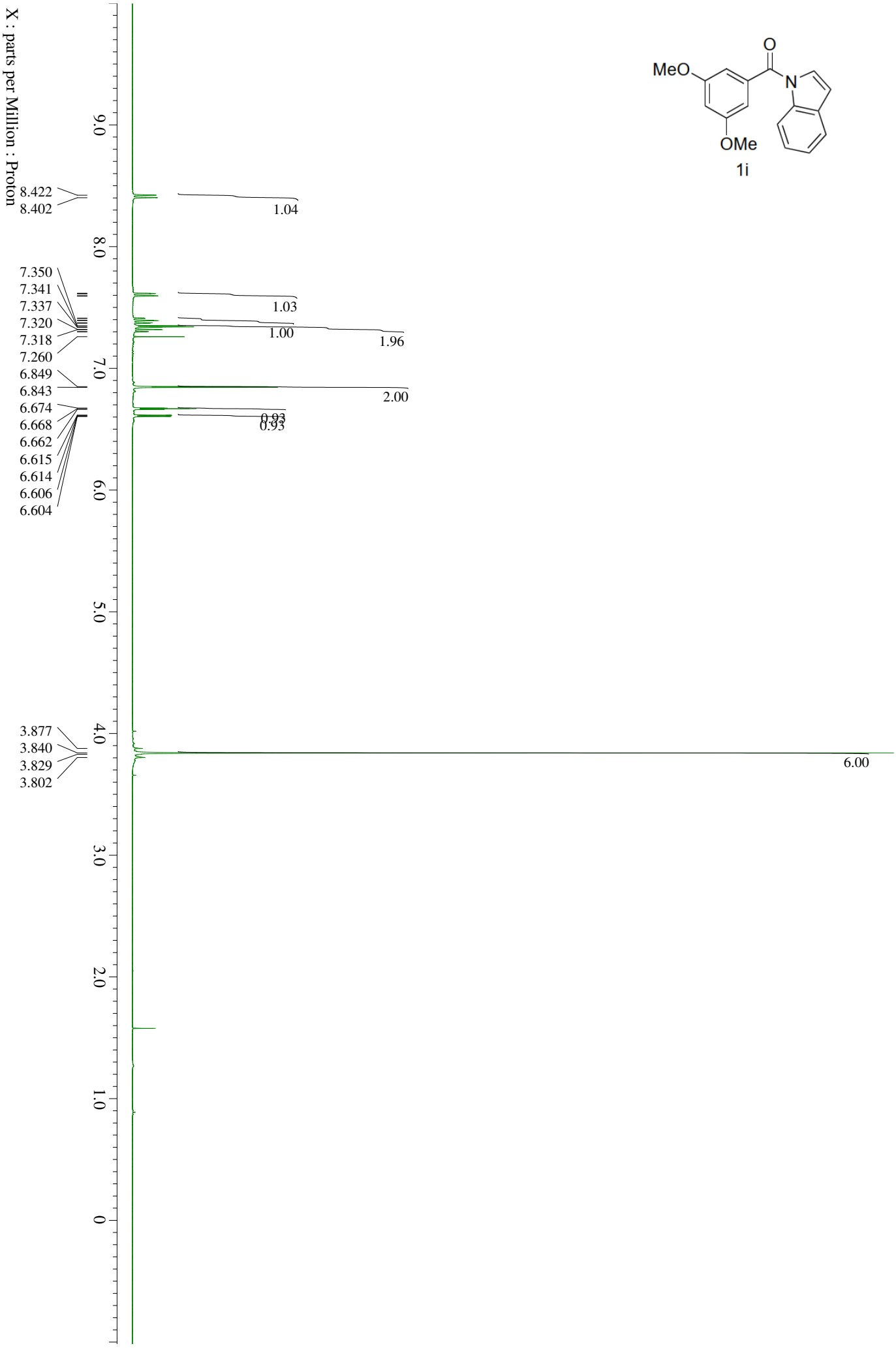

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.148
165.259
138.610
136.293
134.110
131.173
129.972
129.285
127.712
125.309
124.432
121.295
116.614
109.196
75.758
53.800
47.574
41.195
34.588
31.813
26.884
23.880
22.164
20.858
16.596
O
N
O
O
1g


X : parts per Million : Proton
8.428
8.407
8.023
7.937
7.917
7.888
7.869
7.710
7.690
7.637
7.618
7.419
7.368
7.348
7.260
7.210
7.200
6.674
6.665
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.99
0.98
1.02
1.01
1.05
1.00
1.05
1.00
1.01
1.00
O
F3C
N
1h



1h

X : parts per Million : aron13

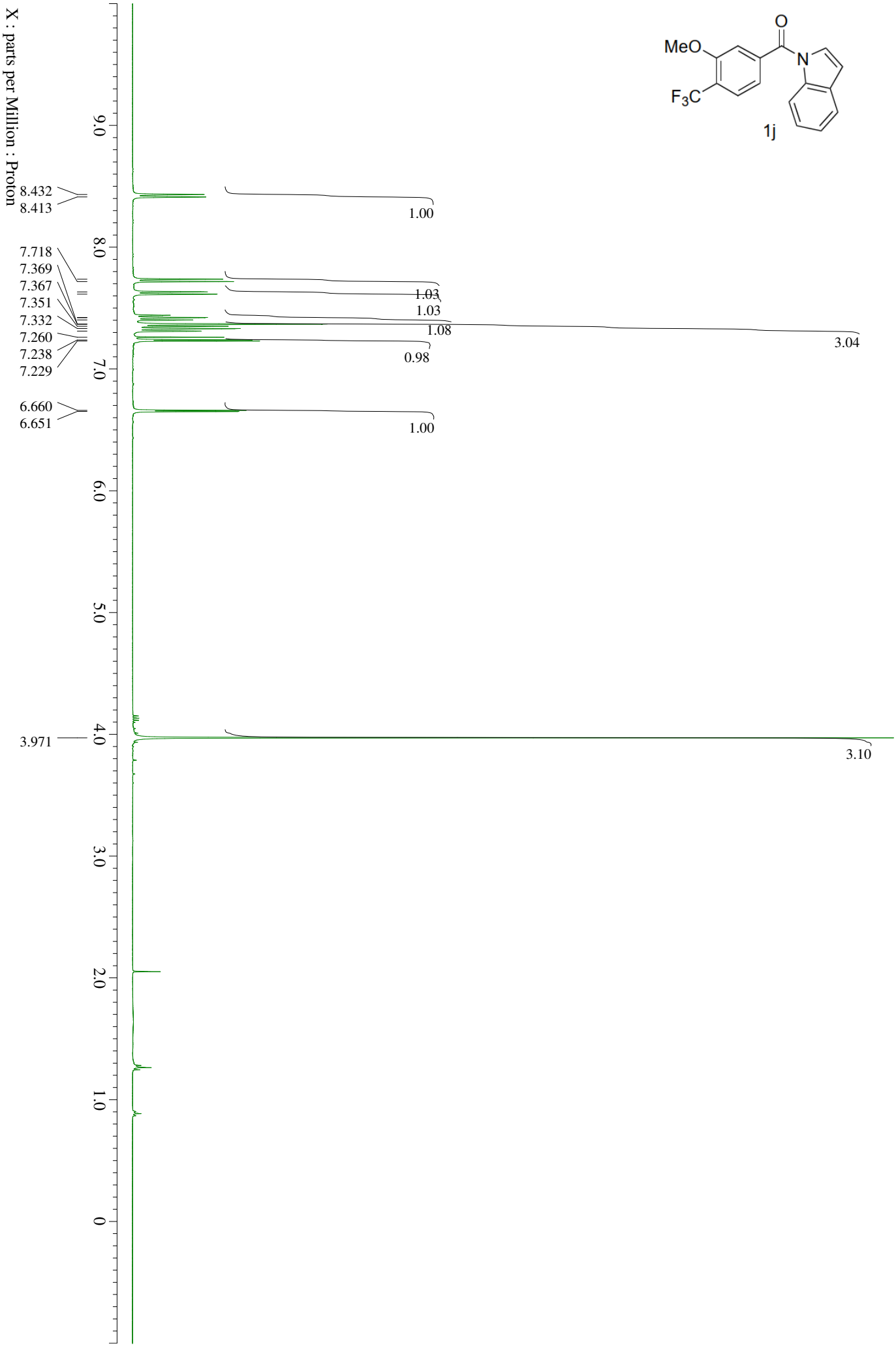

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.422
8.402
7.350
7.341
7.337
7.320
7.318
7.260
6.849
6.843
6.674
6.668
6.662
6.615
6.614
6.606
6.604
3.877
3.840
3.829
3.802
1.04
1.03
1.00
1.96
2.00
0.93
0.93
6.00
MeO
O
N
OMe
1i

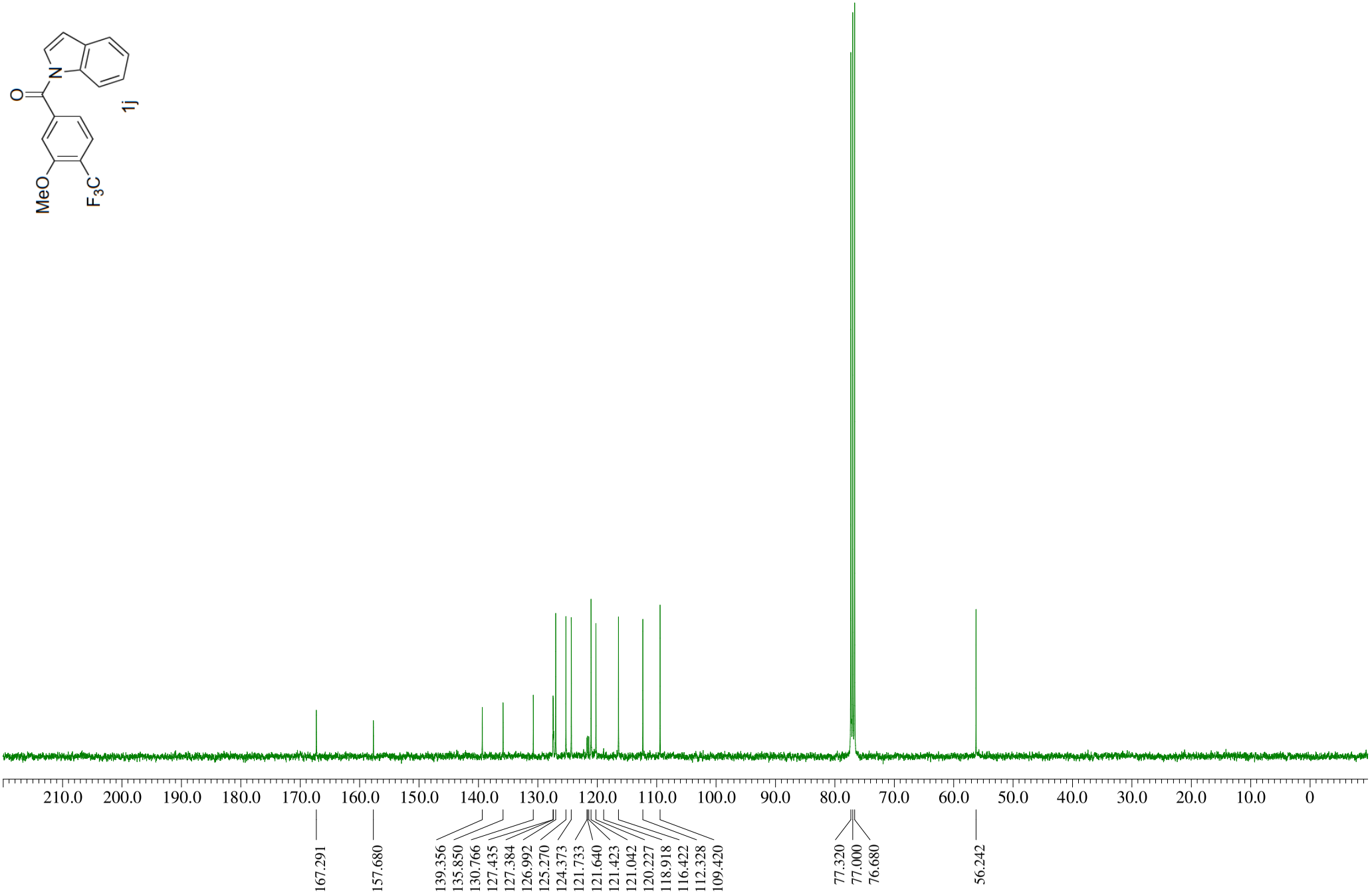
X : parts per Million : aron13

1i

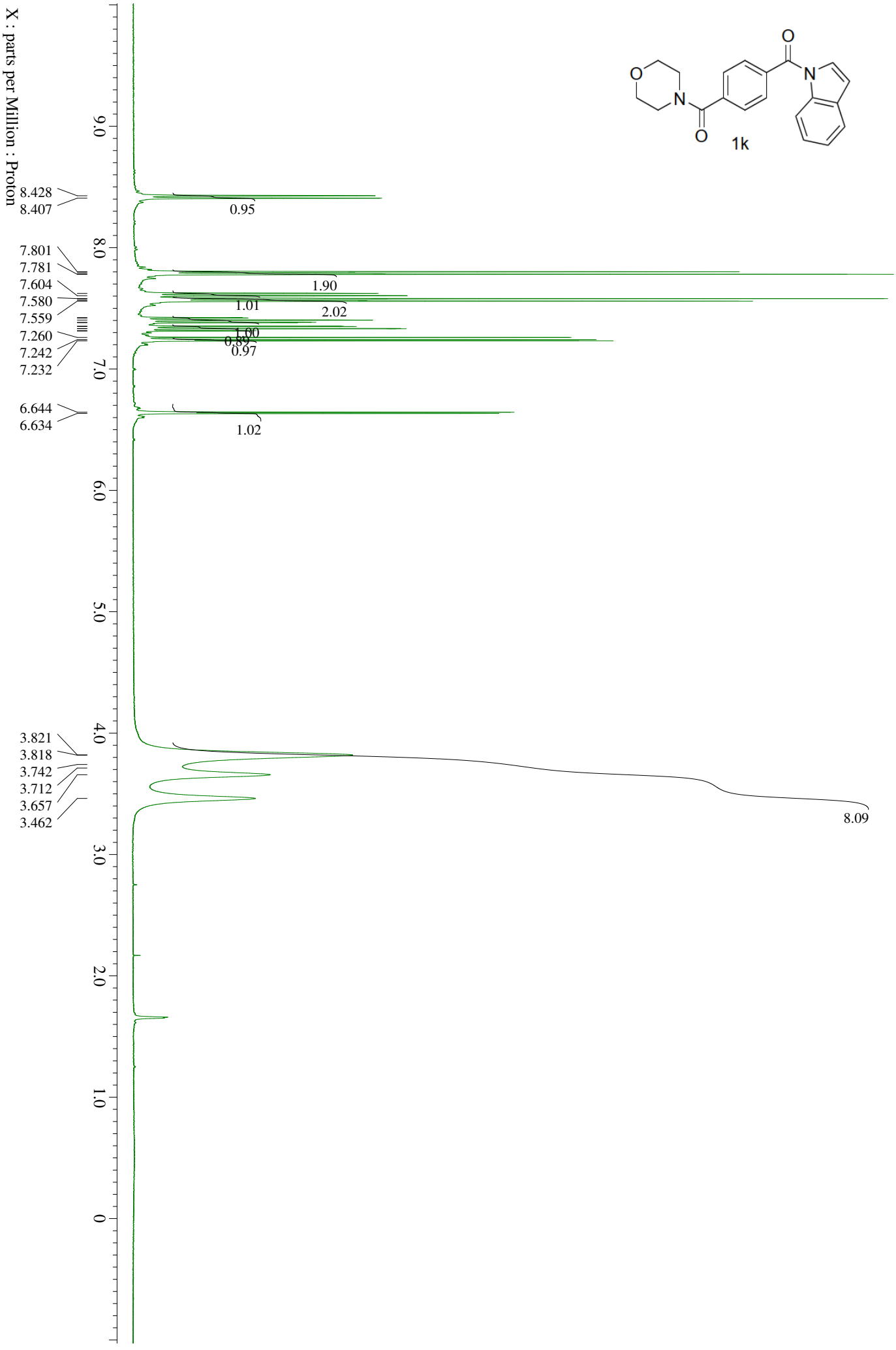
168.389
160.742
136.334
135.924
130.794
127.590
124.930
123.977
120.859
116.425
108.579
106.881
103.945
77.324
77.000
76.685
55.623

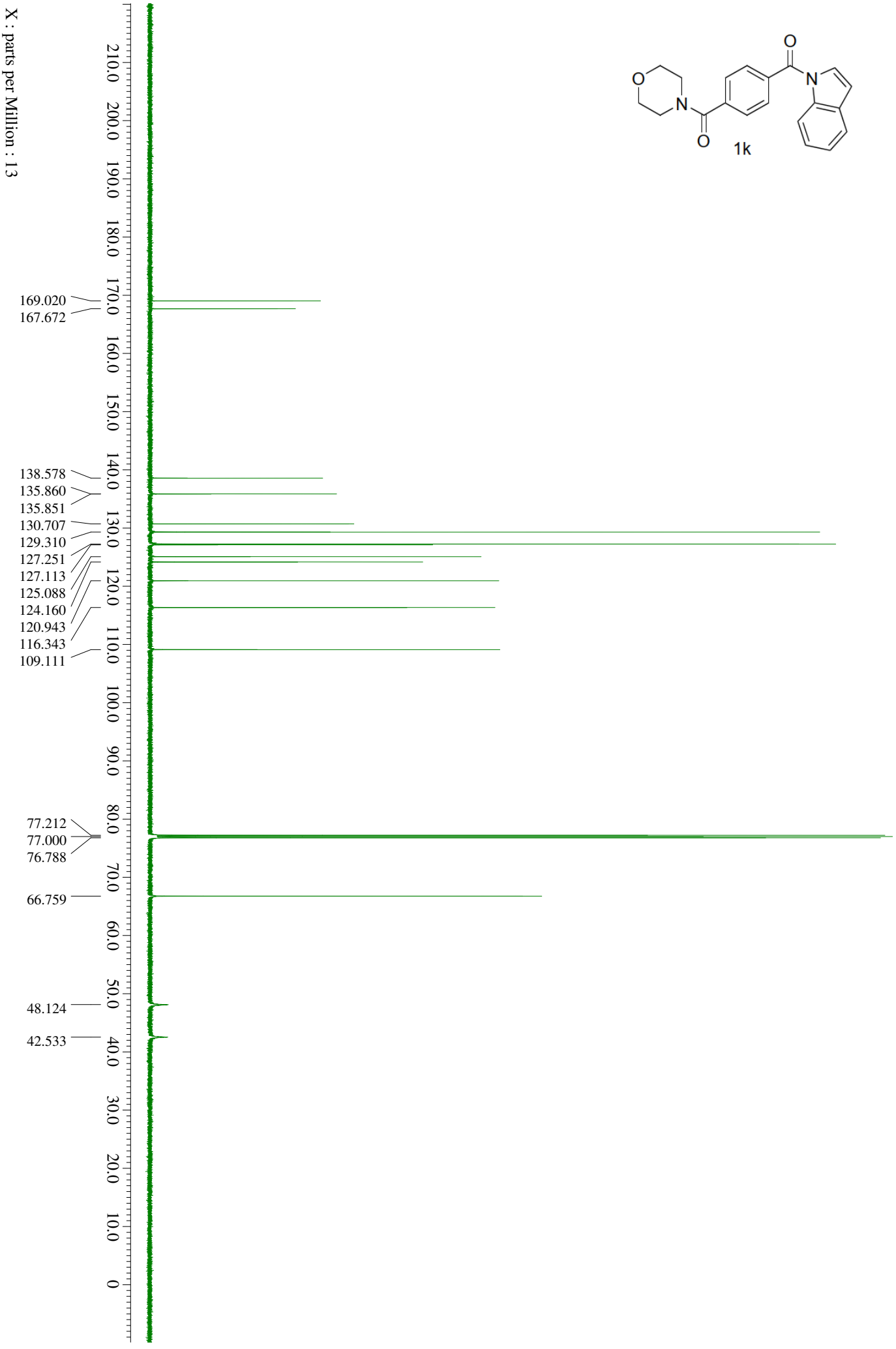
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

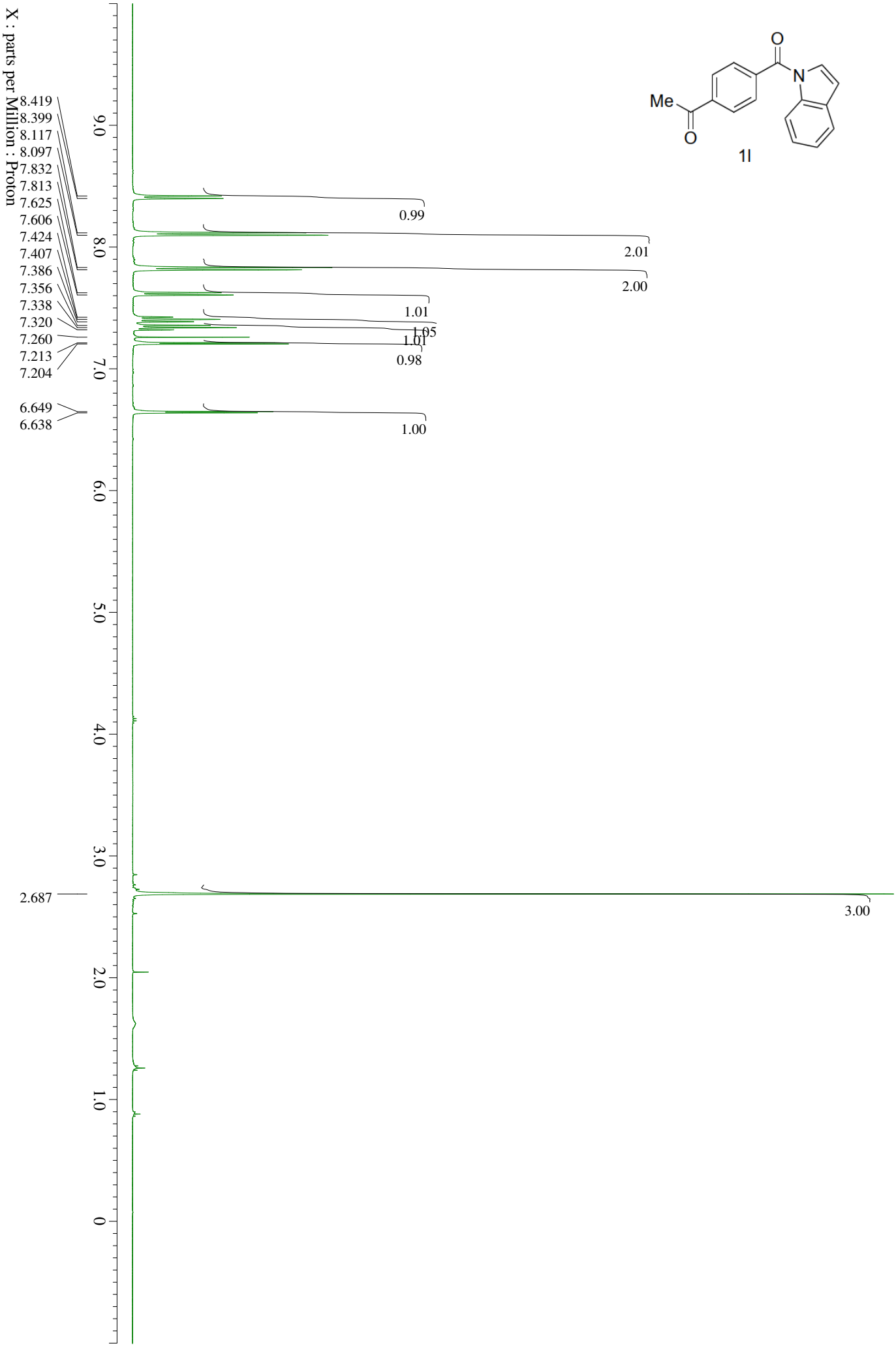

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.432
8.413
7.718
7.369
7.367
7.351
7.332
7.260
7.238
7.229
6.660
6.651
3.971
1.00
1.03
1.03
1.08
3.04
0.98
1.00
3.10
MeO
O
N
F3C
1j

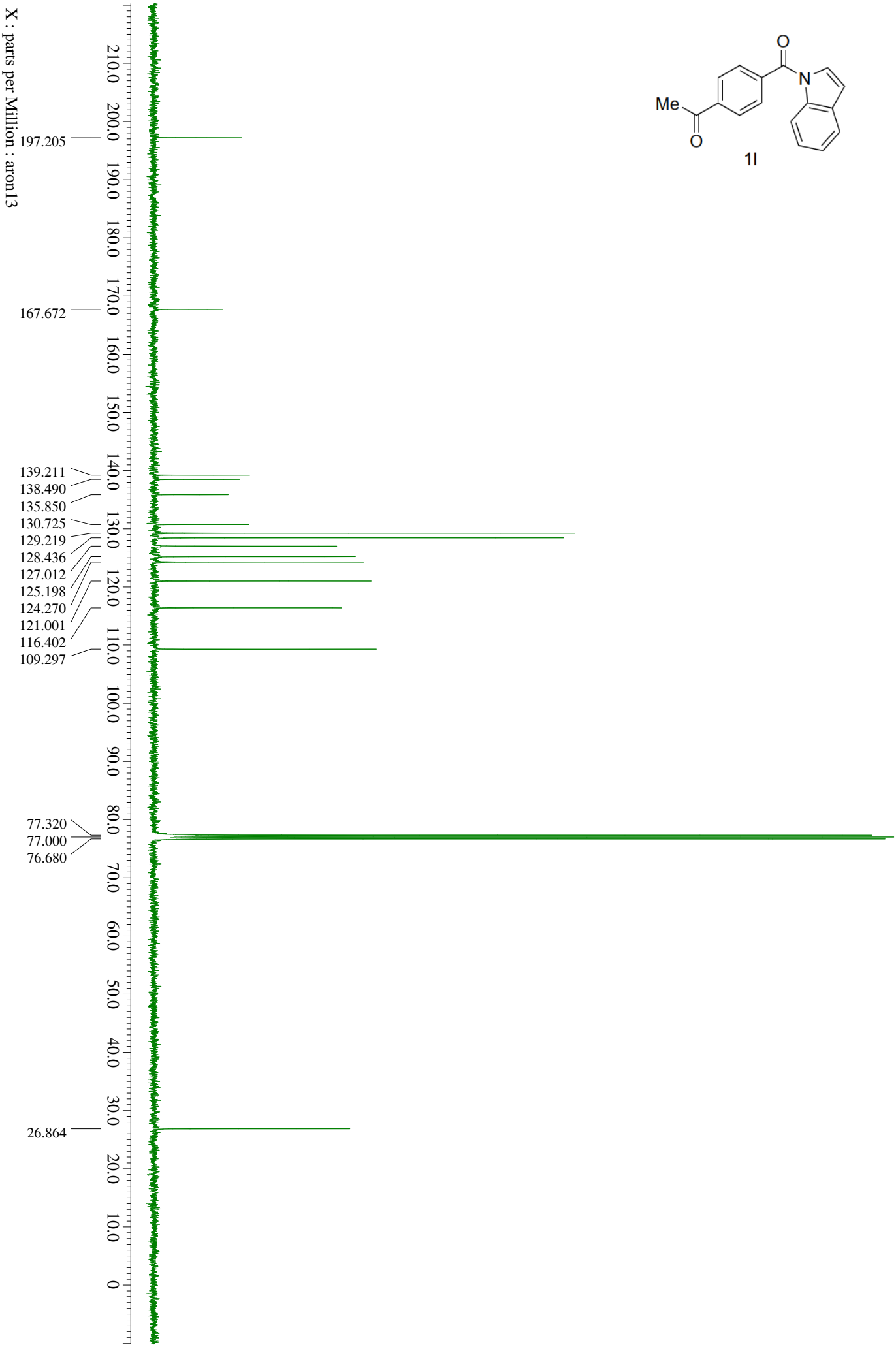


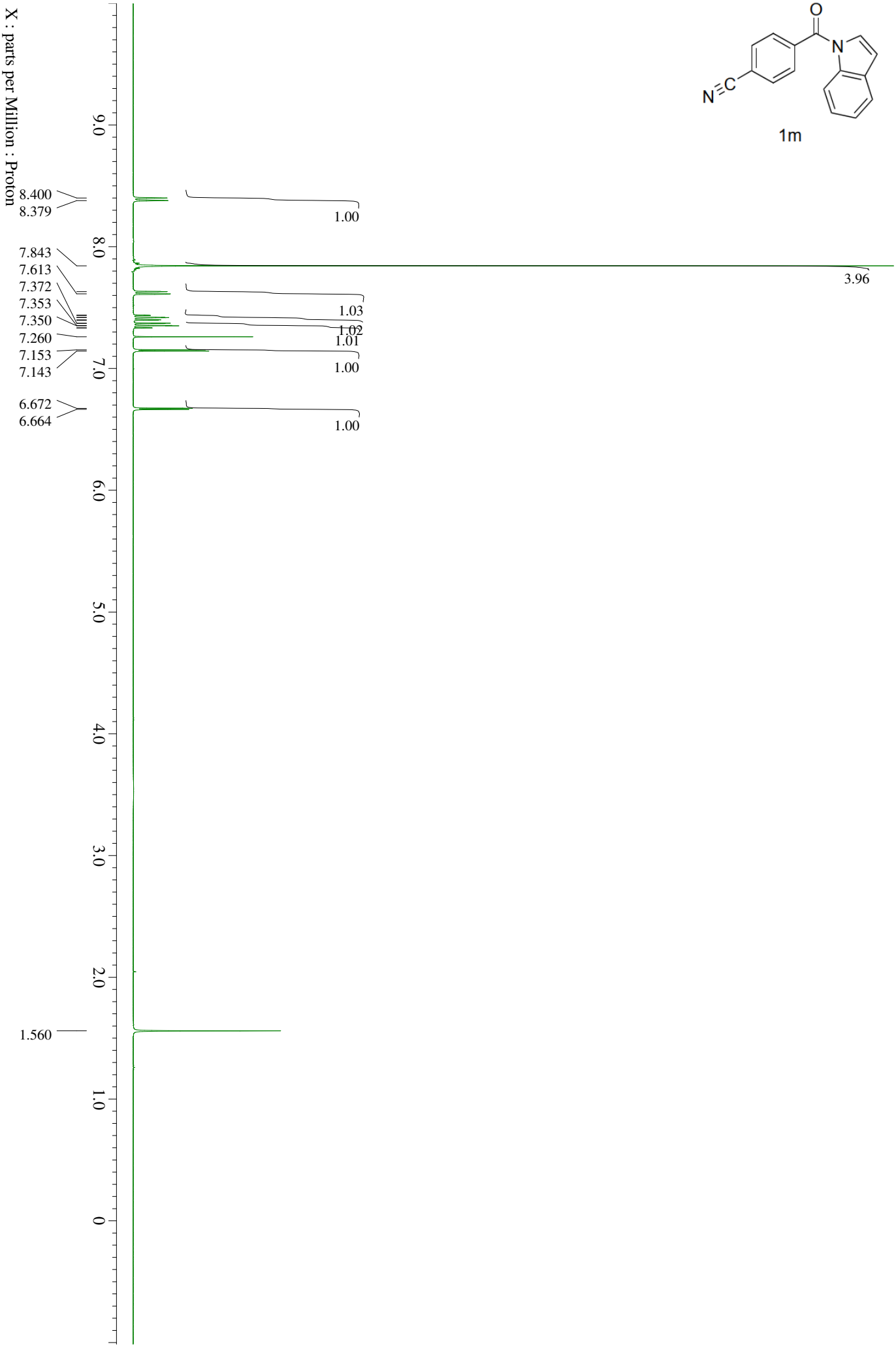
X : parts per Million : aron13


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.428
8.407
7.801
7.781
7.604
7.580
7.559
7.260
7.242
7.232
6.644
6.634
3.821
3.818
3.742
3.712
3.657
3.462
0.95
1.90
1.01
2.02
1.00
0.89
0.97
1.02
8.09
O
N
O
O
N
O
1k


X : parts per Million : 13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.020
167.672
138.578
135.860
135.851
130.707
129.310
127.251
127.113
125.088
124.160
120.943
116.343
109.111
77.212
77.000
76.788
66.759
48.124
42.533
O
N
O
O
N
1k


X : parts per Million : Proton
8.419
8.399
8.117
8.097
7.832
7.813
7.625
7.606
7.424
7.407
7.386
7.356
7.338
7.320
7.260
7.213
7.204
6.649
6.638
2.687
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.99
2.01
2.00
1.01
1.05
1.01
0.98
1.00
3.00
Me
O
O
N
1l

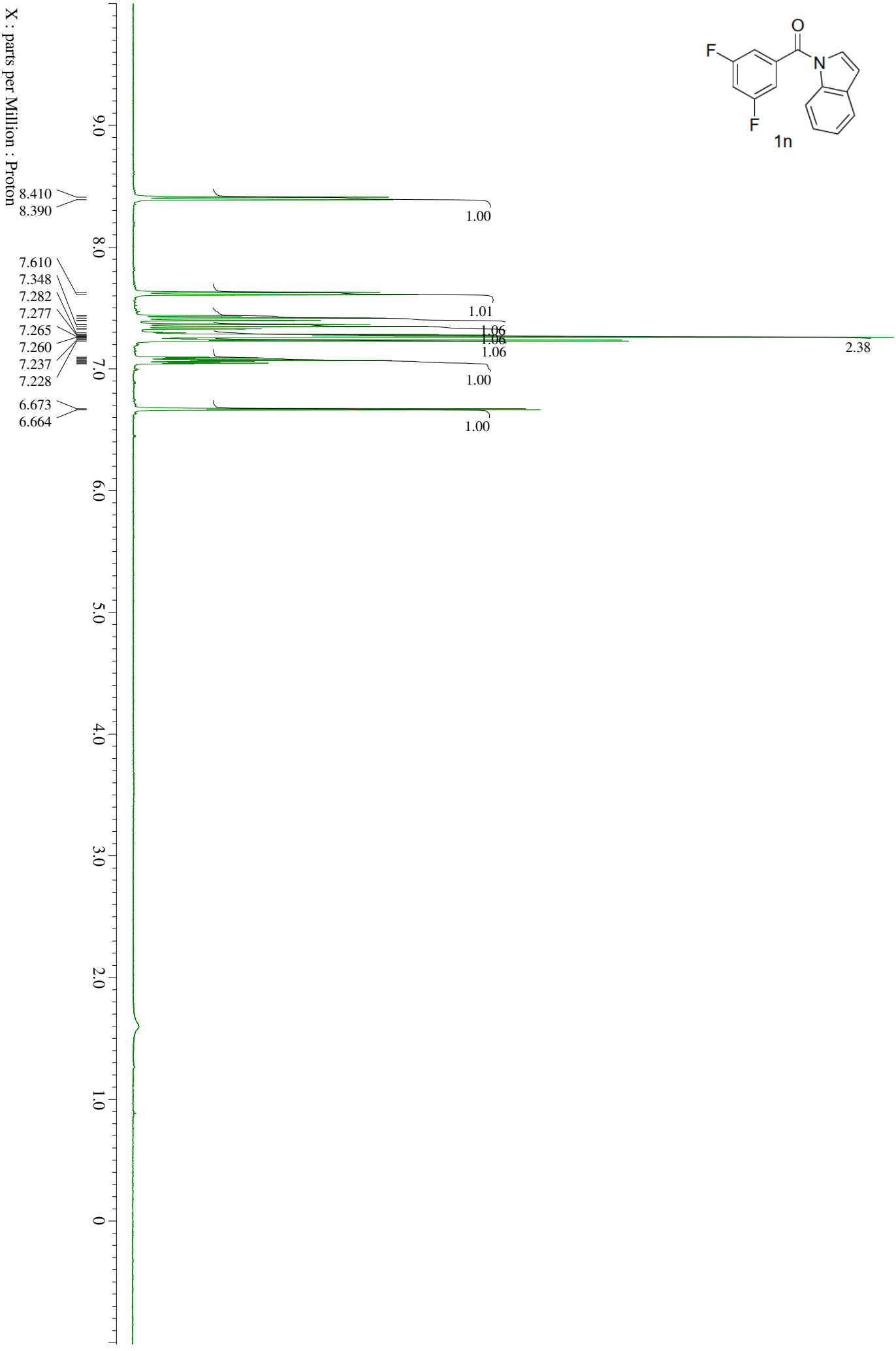

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.205
167.672
139.211
138.490
135.850
130.725
129.219
128.436
127.012
125.198
124.270
121.001
116.402
109.297
77.320
77.000
76.680
26.864
O
N
Me
O
1l

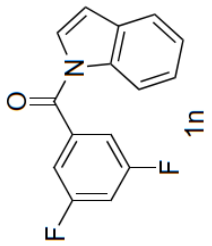

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.400
8.379
7.843
7.613
7.372
7.353
7.350
7.260
7.153
7.143
6.672
6.664
1.560
1.00
1.03
1.02
1.01
1.00
1.00
3.96
O
N
N≡C
1m

X : parts per Million : aron13

1m

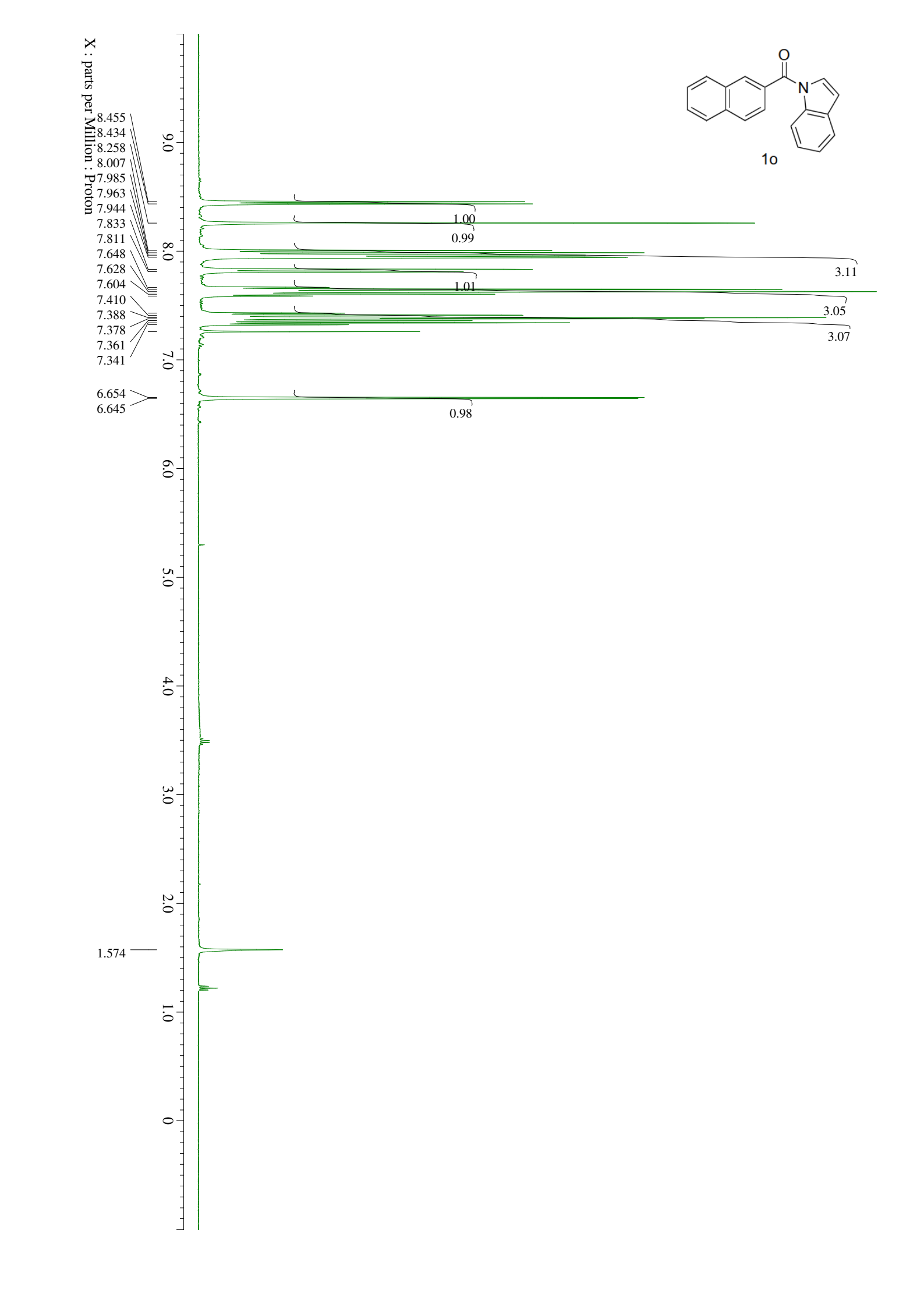
166.662
138.500
135.798
132.437
130.704
129.518
126.610
125.414
124.527
121.114
117.711
116.402
115.422
109.833
77.320
77.000
76.680

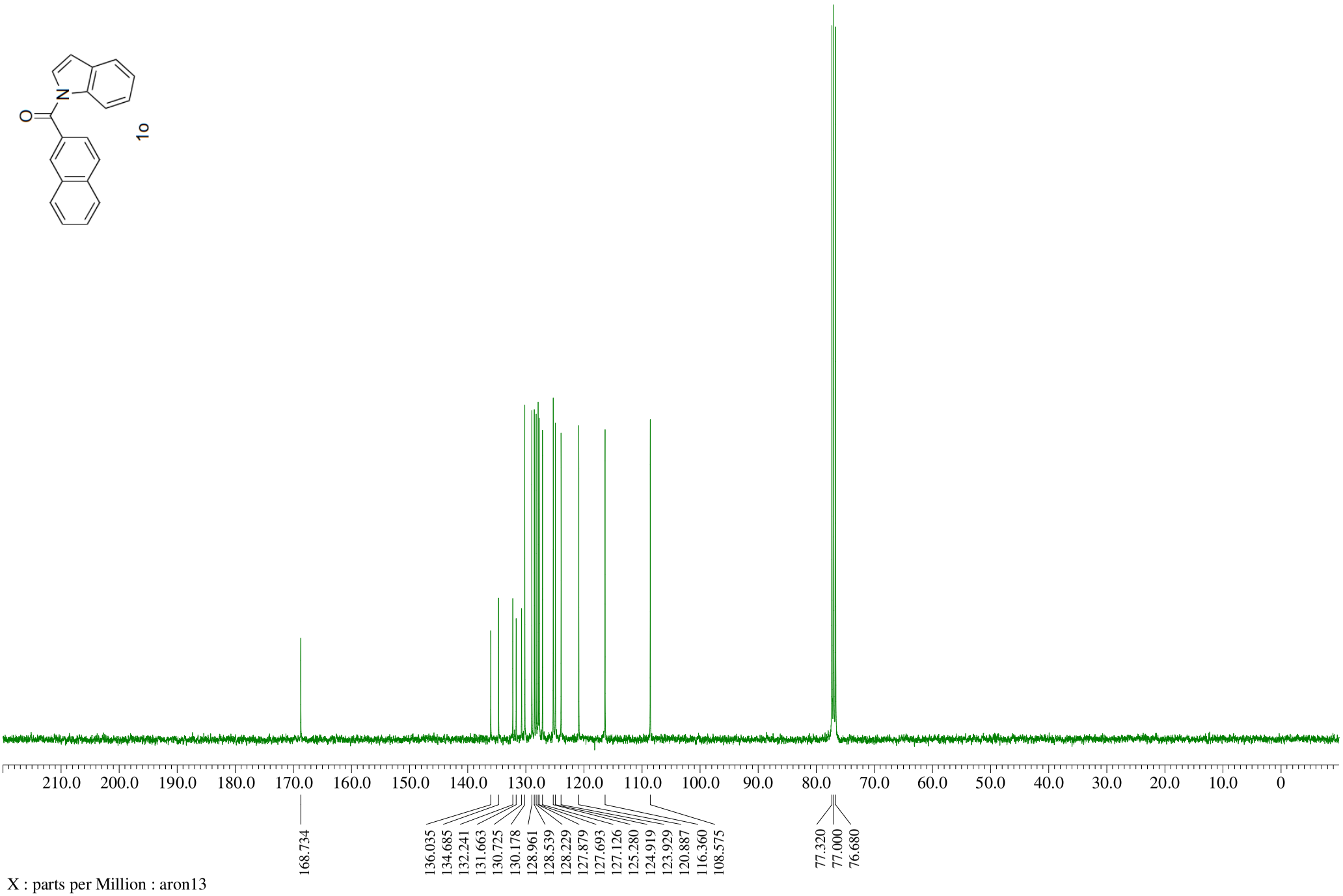

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.410
8.390
7.610
7.348
7.282
7.277
7.265
7.260
7.237
7.228
6.673
6.664
1.00
1.01
1.06
1.06
1.06
2.38
1.00
1.00
O
F
N
F
1n

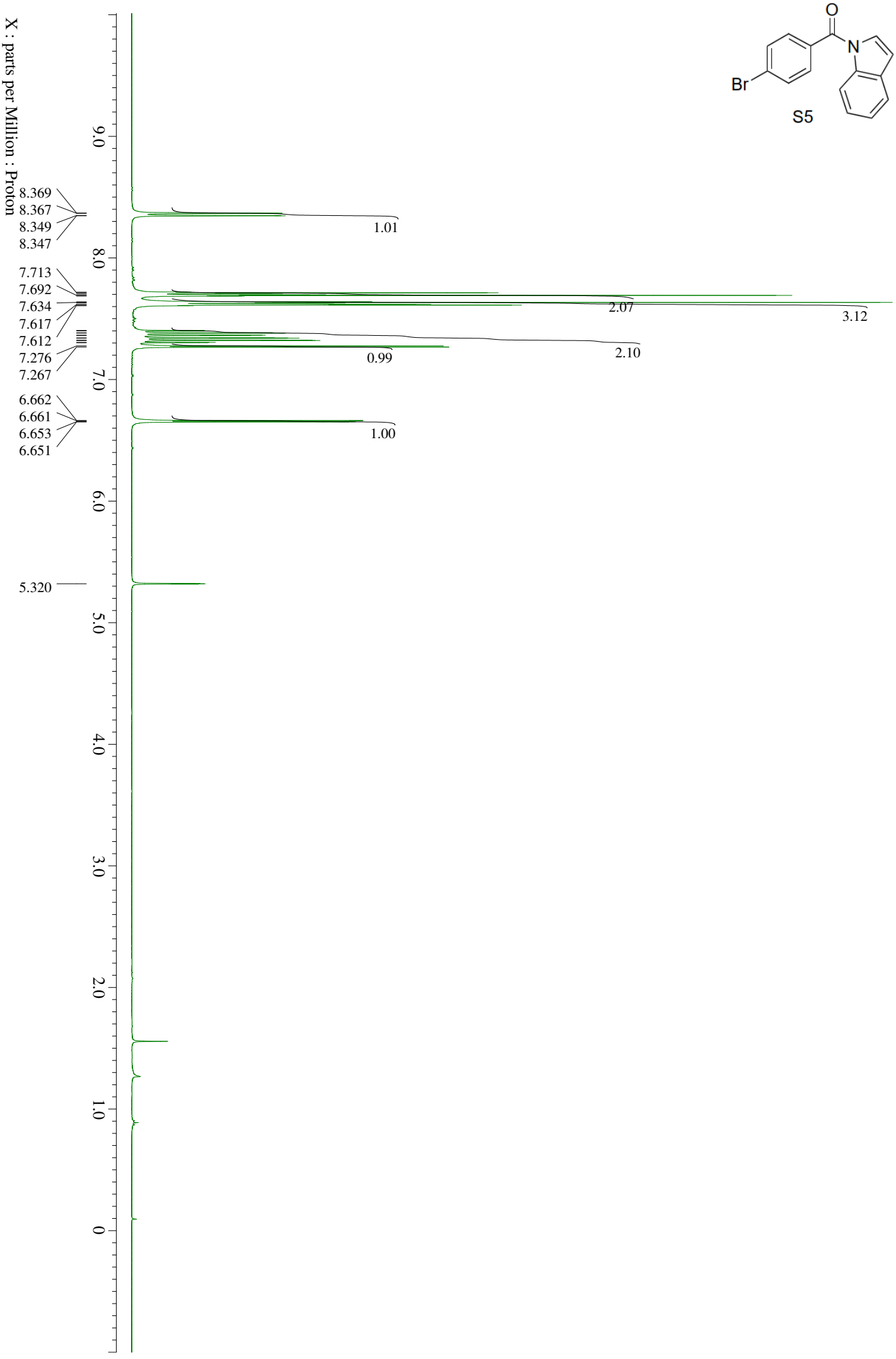


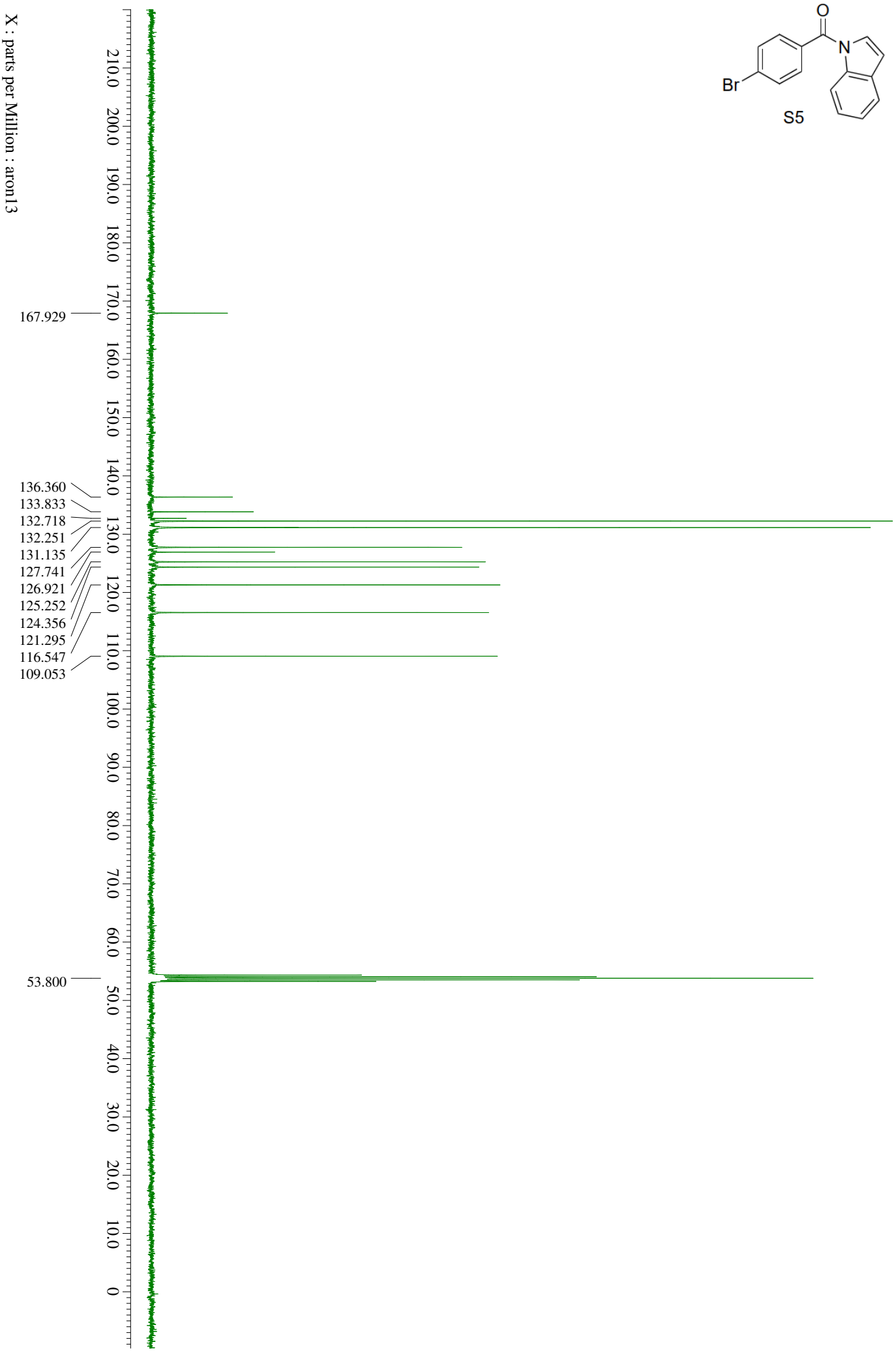
1n

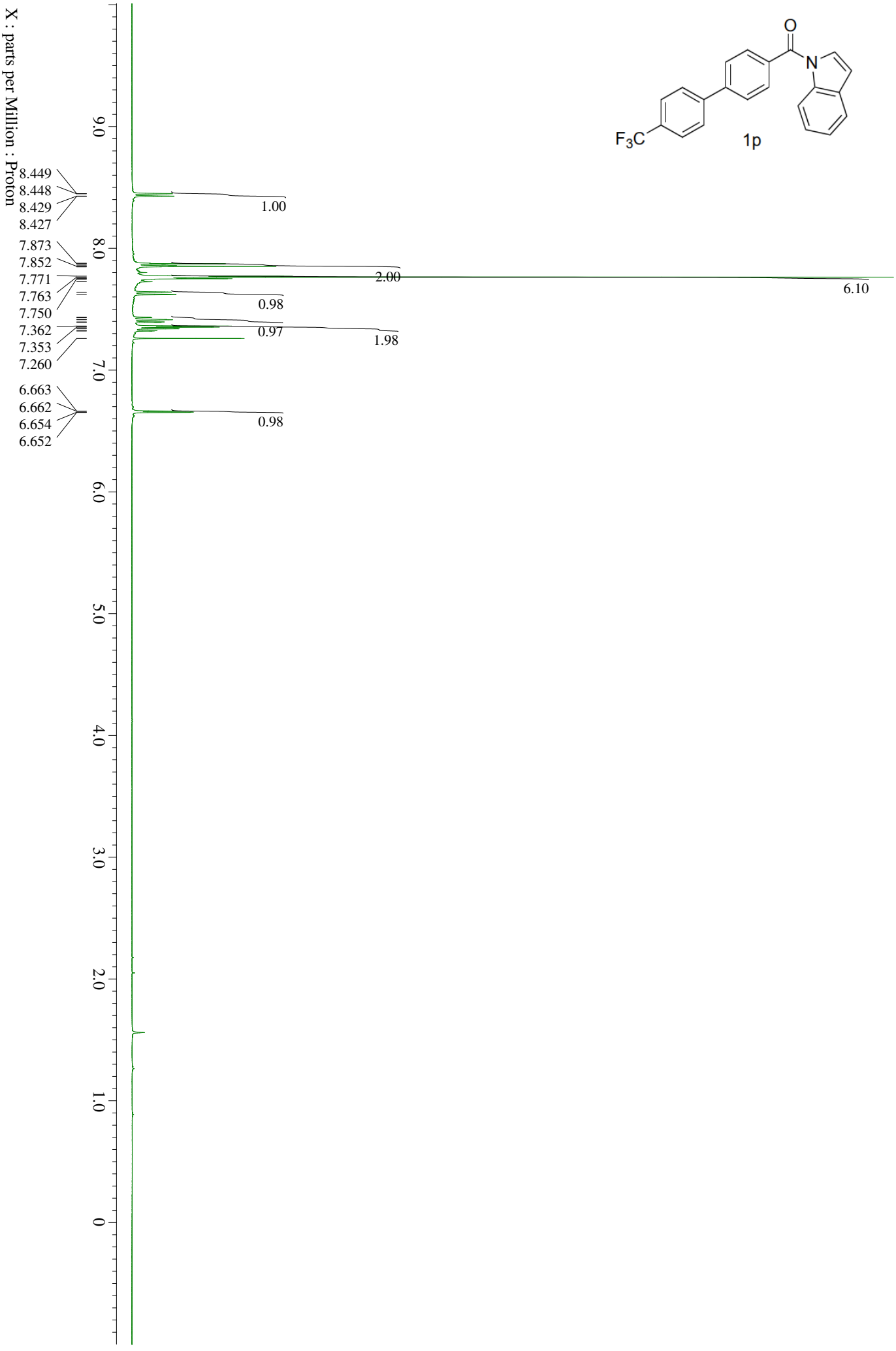
X : parts per Million : aron13

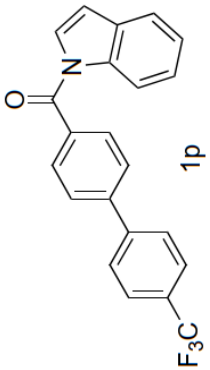

X : parts per Million : Proton
8.455
8.434
8.258
8.007
7.985
7.963
7.944
7.833
7.811
7.648
7.628
7.604
7.410
7.388
7.378
7.361
7.341
6.654
6.645
1.574
1.00
0.99
1.01
0.98
3.11
3.05
3.07
O
N
1o


O
N
1o
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.734
136.035
134.685
132.241
131.663
130.725
130.178
128.961
128.539
128.229
127.879
127.693
127.126
125.280
124.919
123.929
120.887
116.360
108.575
77.320
77.000
76.680
X : parts per Million : aron13


X : parts per Million : Proton
8.369
8.367
8.349
8.347
7.713
7.692
7.634
7.617
7.612
7.276
7.267
6.662
6.661
6.653
6.651
5.320
1.01
2.07
3.12
0.99
2.10
1.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
N
Br
S5

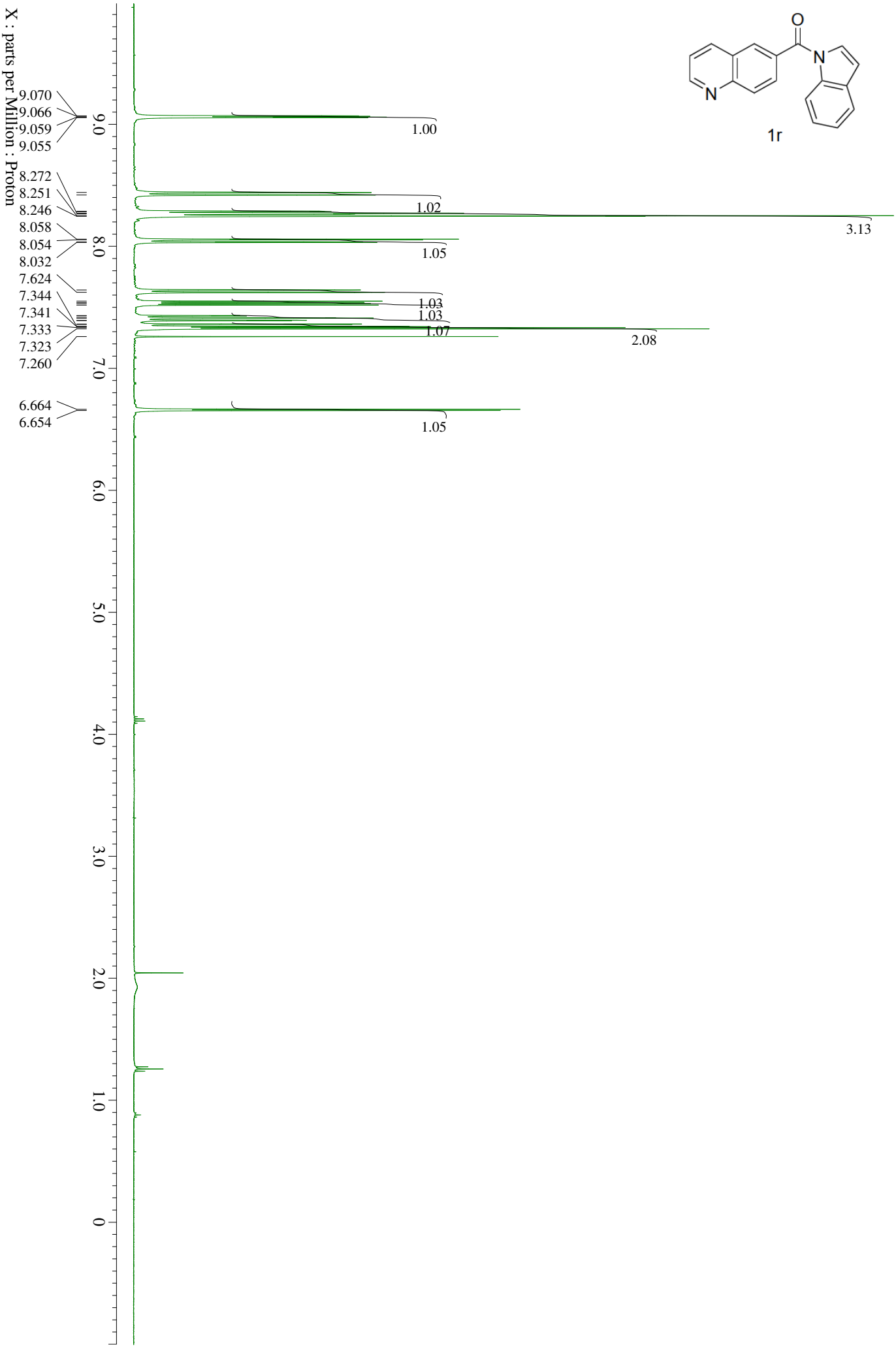

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
167.929
136.360
133.833
132.718
132.251
131.135
127.741
126.921
125.252
124.356
121.295
116.547
109.053
53.800
O
N
Br
S5


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.449
8.448
8.429
8.427
7.873
7.852
7.771
7.763
7.750
7.362
7.353
7.260
6.663
6.662
6.654
6.652
1.00
2.00
0.98
0.97
1.98
0.98
6.10
O
N
F3C
1p



1p

X : parts per Million : aron13

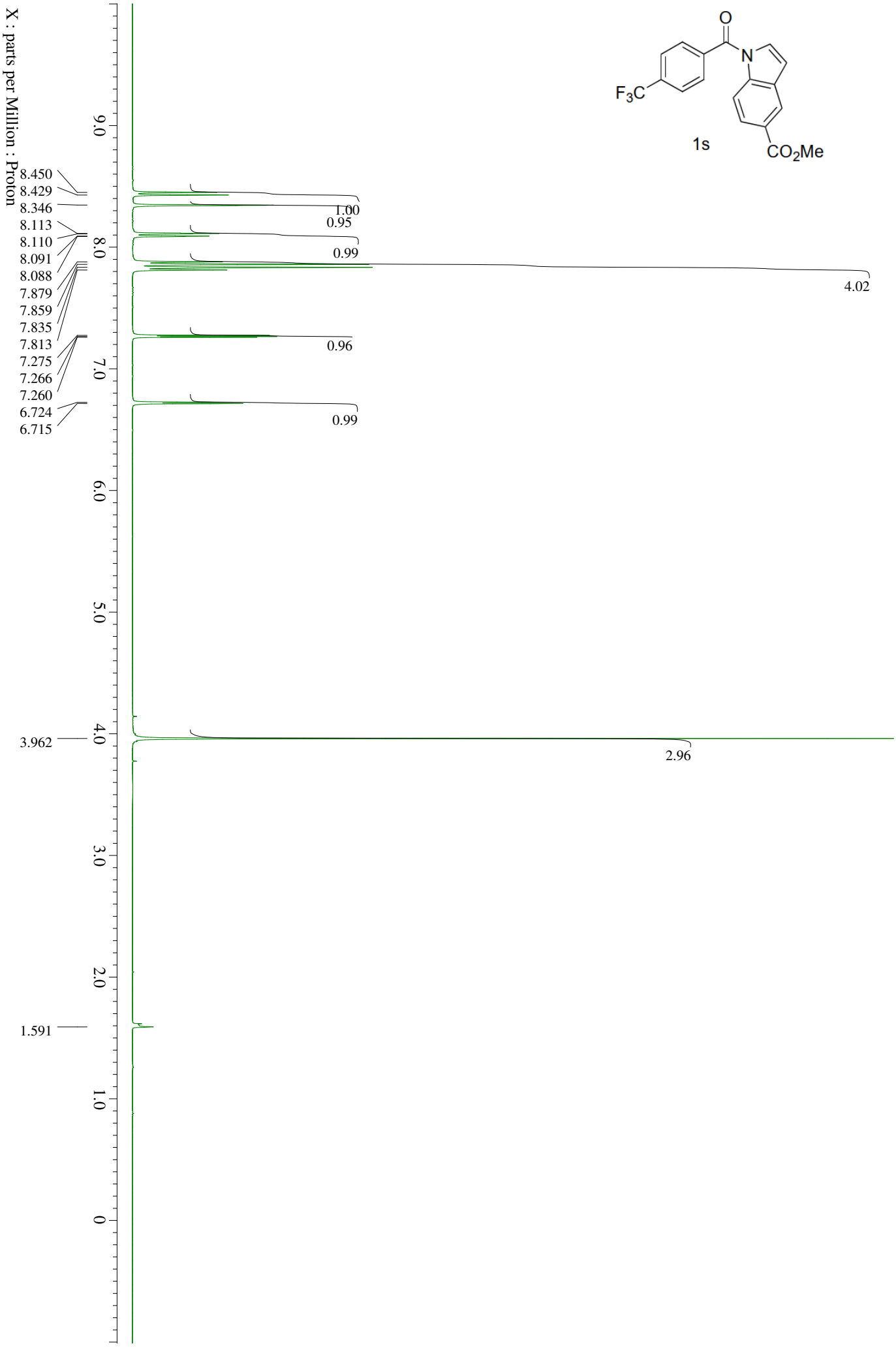

X : parts per Million : Proton
9.070
9.066
9.059
9.055
8.272
8.251
8.246
8.058
8.054
8.032
7.624
7.344
7.341
7.333
7.323
7.260
6.664
6.654
1.00
1.02
3.13
1.05
1.03
1.03
1.07
2.08
1.05
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
N
N
1r

X : parts per Million : aron13

1r

167.971
152.534
149.193
136.984
135.984
132.498
130.725
130.189
129.982
128.889
127.384
127.363
125.105
124.146
122.279
120.980
116.381
109.060
77.320
77.000
76.691

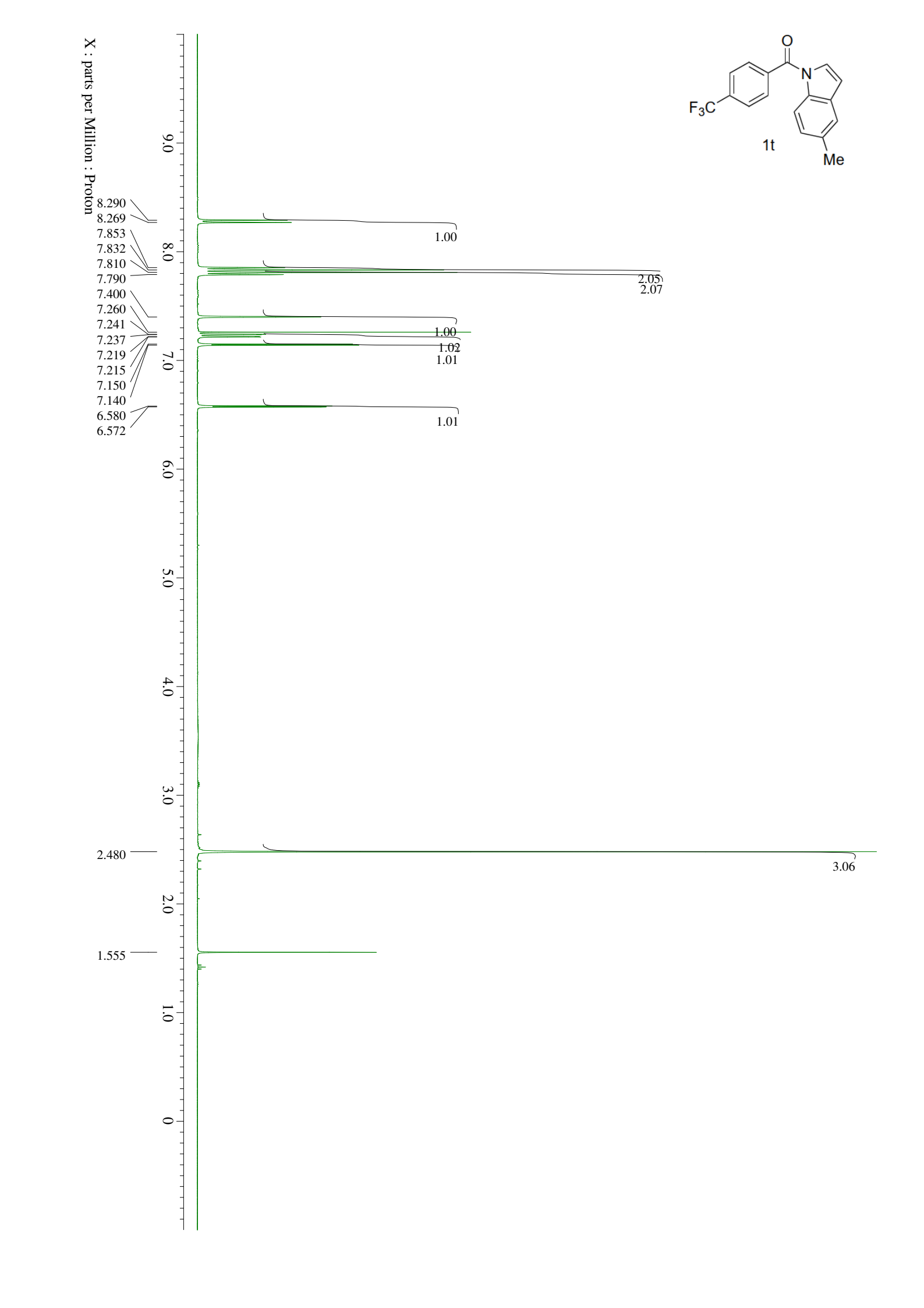
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.450
8.429
8.346
8.113
8.110
8.091
8.088
7.879
7.859
7.835
7.813
7.275
7.266
7.260
6.724
6.715
3.962
1.591
1.00
0.95
0.99
4.02
0.96
0.99
2.96
O
N
F3C
CO2Me
1s

X : parts per Million : aron13

1s

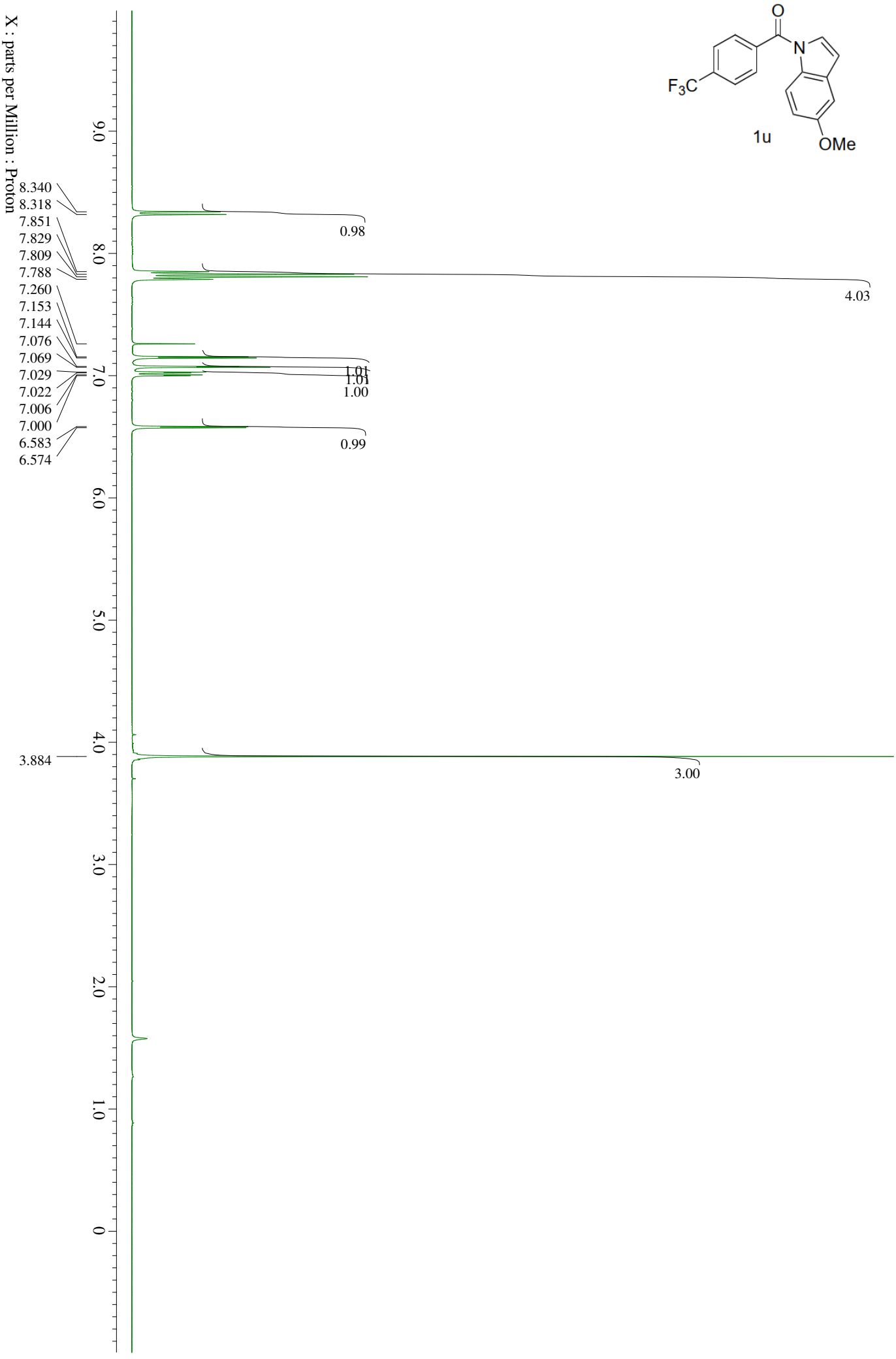
167.260
167.167
138.469
137.324
134.282
133.963
133.633
133.303
130.539
129.467
128.136
127.466
126.528
126.198
125.806
125.775
124.754
123.238
122.042
119.330
116.082
109.647
77.320
77.000
76.680
52.179

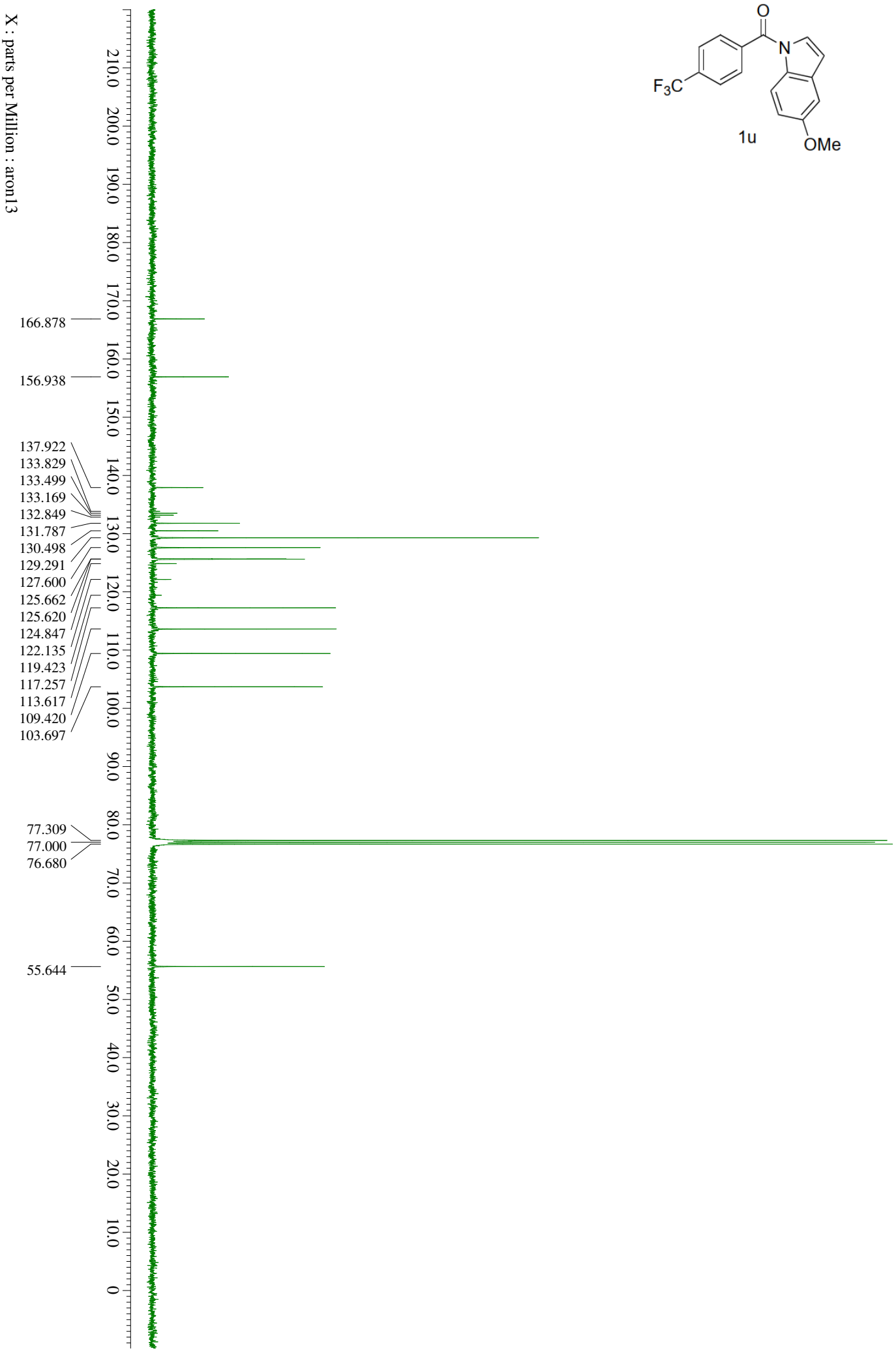

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.290
8.269
7.853
7.832
7.810
7.790
7.400
7.260
7.241
7.237
7.219
7.215
7.150
7.140
6.580
6.572
2.480
1.555
1.00
2.05
2.07
1.00
1.02
1.01
1.01
3.06
O
N
F3C
1t
Me

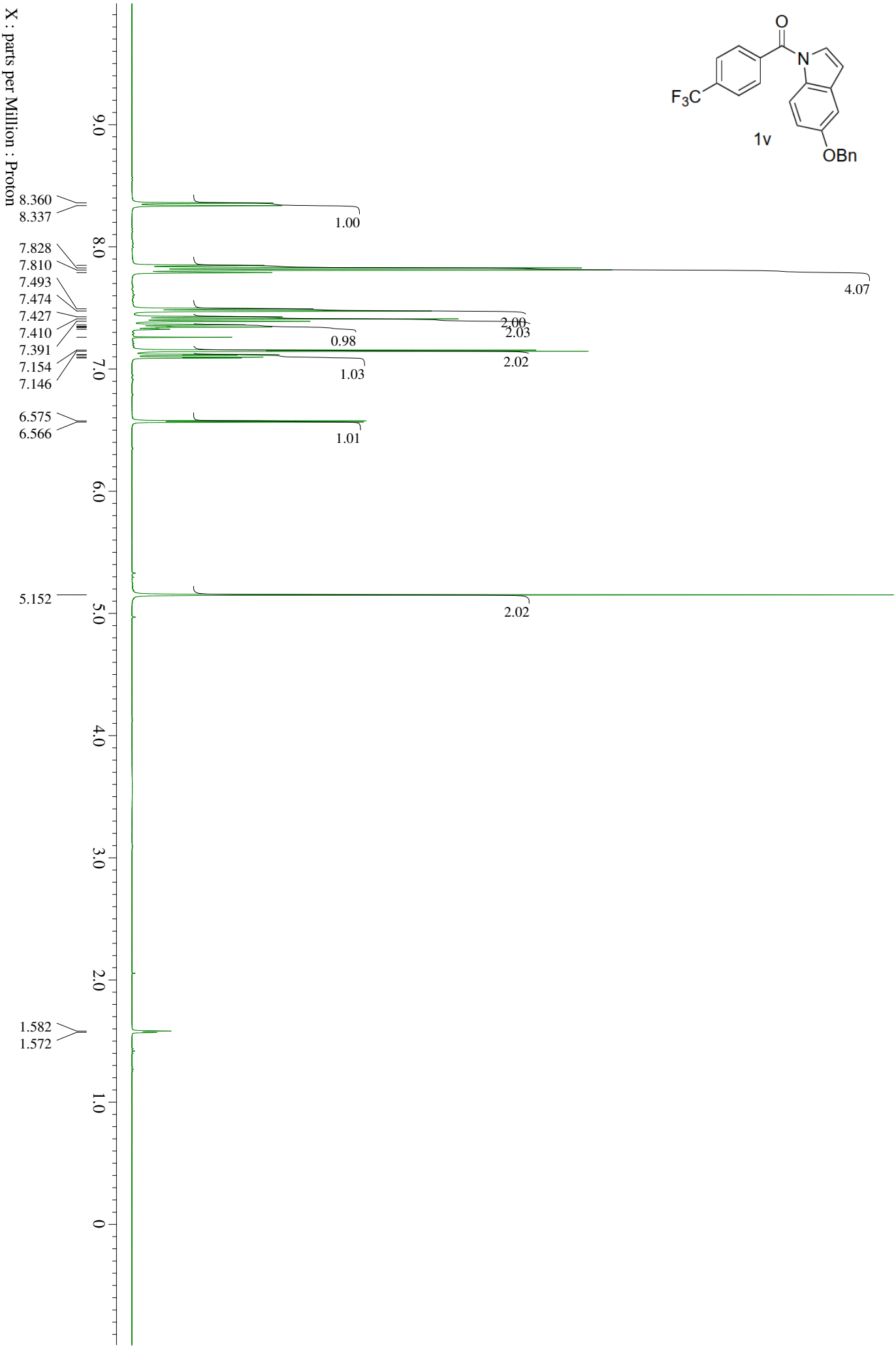
X : parts per Million : aron13

1t

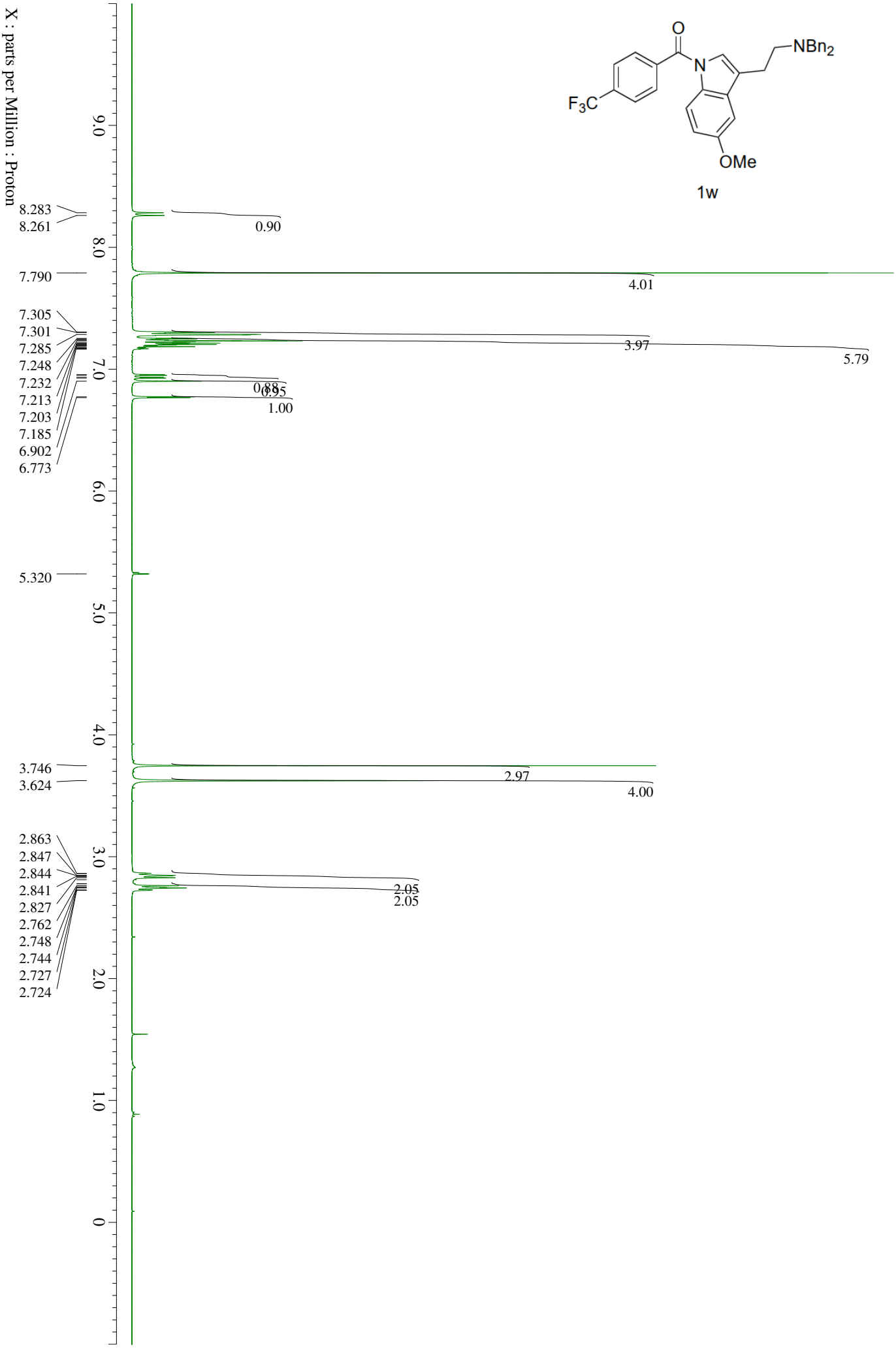
167.095
138.015
138.005
134.045
133.499
133.179
130.983
129.302
126.992
126.569
125.651
125.620
124.857
122.145
120.959
116.051
109.307
77.320
77.000
76.680
21.429

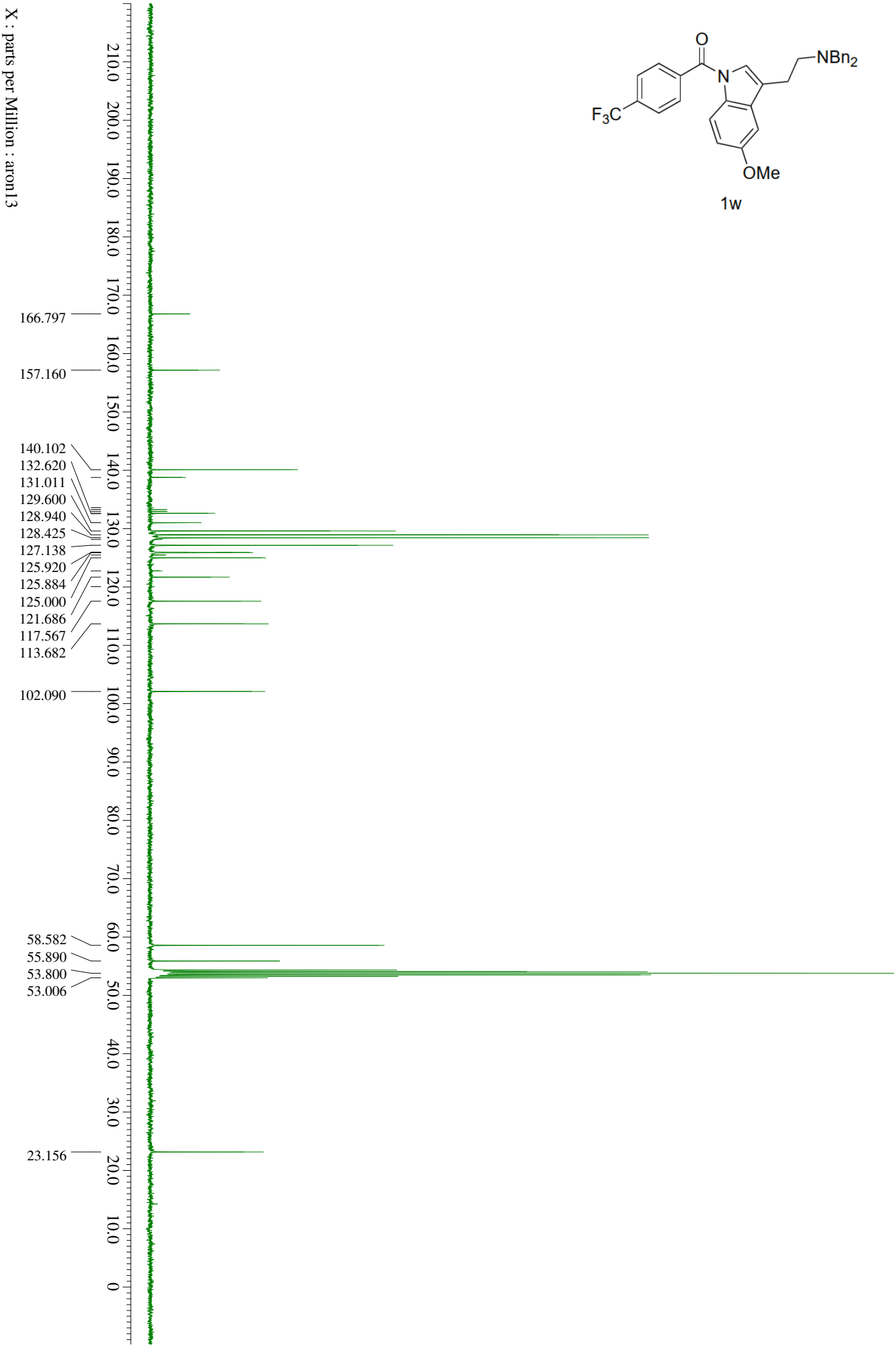

X : parts per Million : Proton
8.340
8.318
7.851
7.829
7.809
7.788
7.260
7.153
7.144
7.076
7.069
7.029
7.022
7.006
7.000
6.583
6.574
3.884
0.98
4.03
1.01
1.01
1.00
0.99
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
N
F3C
OMe
1u

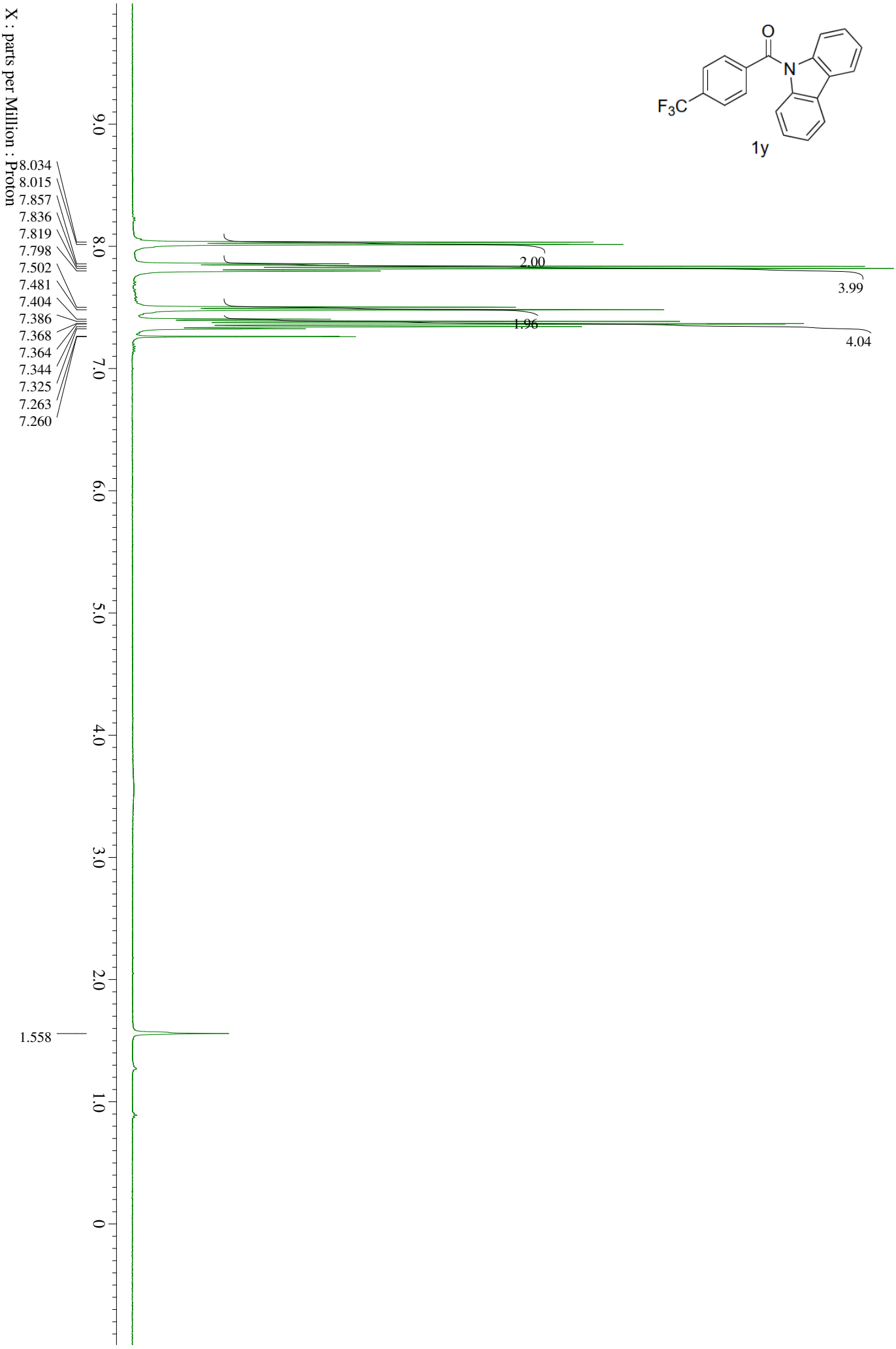

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.878
156.938
137.922
133.829
133.499
133.169
132.849
131.787
130.498
129.291
127.600
125.662
125.620
124.847
122.135
119.423
117.257
113.617
109.420
103.697
77.309
77.000
76.680
55.644
O
N
F3C
1u
OMe


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.360
8.337
7.828
7.810
7.493
7.474
7.427
7.410
7.391
7.154
7.146
6.575
6.566
5.152
1.582
1.572
1.00
4.07
2.00
2.03
0.98
2.02
1.03
1.01
2.02
O
N
F3C
1v
OBn

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.868
156.071
137.881
136.994
133.488
133.158
131.746
130.653
129.281
128.580
127.941
127.621
127.456
125.641
125.610
124.847
122.135
117.278
114.391
109.420
105.069
77.320
77.000
76.680
70.452
O
N
F3C
1v
OBn


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.283
8.261
7.790
7.305
7.301
7.285
7.248
7.232
7.213
7.203
7.185
6.902
6.773
5.320
3.746
3.624
2.863
2.847
2.844
2.841
2.827
2.762
2.748
2.744
2.727
2.724
0.90
4.01
3.97
5.79
0.88
0.95
1.00
2.97
4.00
2.05
2.05
O
N
NBn2
F3C
OMe
1w


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.797
157.160
140.102
132.620
131.011
129.600
128.940
128.425
127.138
125.920
125.884
125.000
121.686
117.567
113.682
102.090
58.582
55.890
53.800
53.006
23.156
O
N
NBn2
F3C
OMe
1w


X : parts per Million : Proton
8.034
8.015
7.857
7.836
7.819
7.798
7.502
7.481
7.404
7.386
7.368
7.364
7.344
7.325
7.263
7.260
1.558
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
3.99
1.96
4.04
O
N
F3C
1y

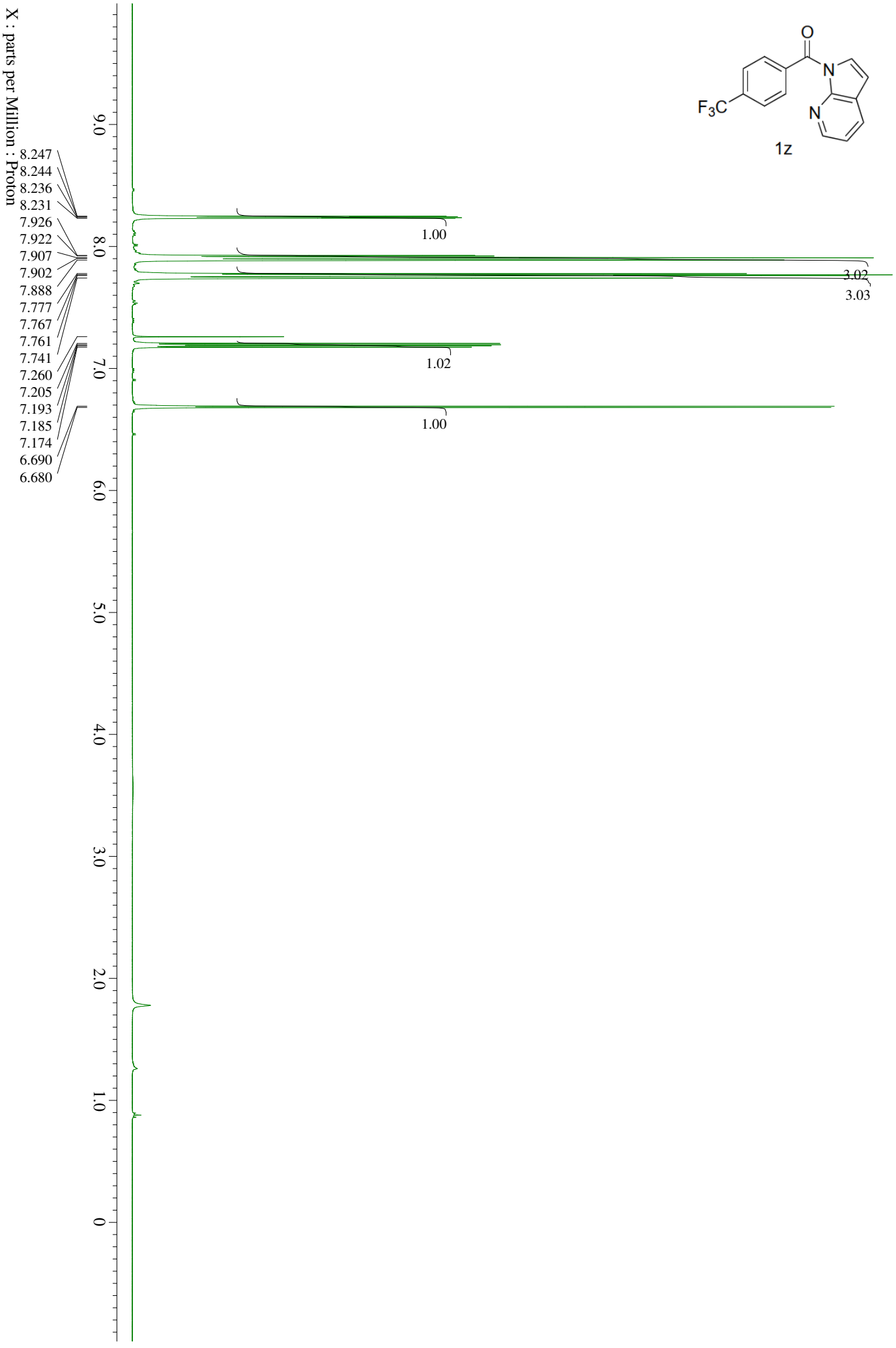
X : parts per Million : aron13

1y

168.074

139.036
138.768
134.313
133.983
133.653
133.323
129.333
127.580
126.961
126.198
126.002
125.971
124.868
123.867
122.156
119.980
115.711

77.309
77.000
76.680

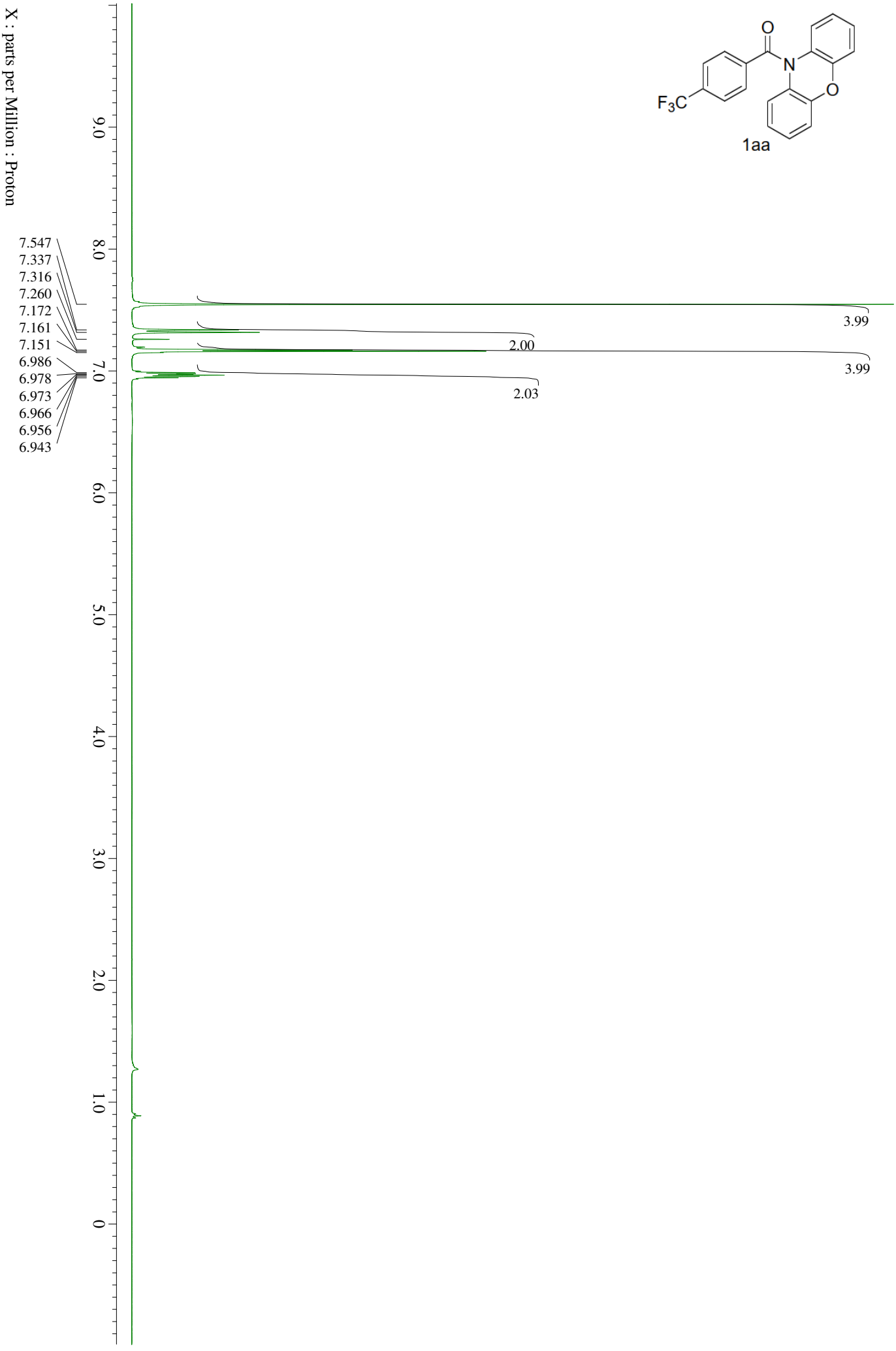

X : parts per Million : Proton
8.247
8.244
8.236
8.231
7.926
7.922
7.907
7.902
7.888
7.777
7.767
7.761
7.741
7.260
7.205
7.193
7.185
7.174
6.690
6.680
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
3.02
3.03
1.02
1.00
O
N
N
F3C
1z

X : parts per Million : aron13

1z

166.548
148.038
144.429
137.397
133.942
133.622
130.281
129.395
127.002
125.084
125.043
125.012
124.971
123.300
122.259
119.268
106.585
77.320
77.000
76.680

210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

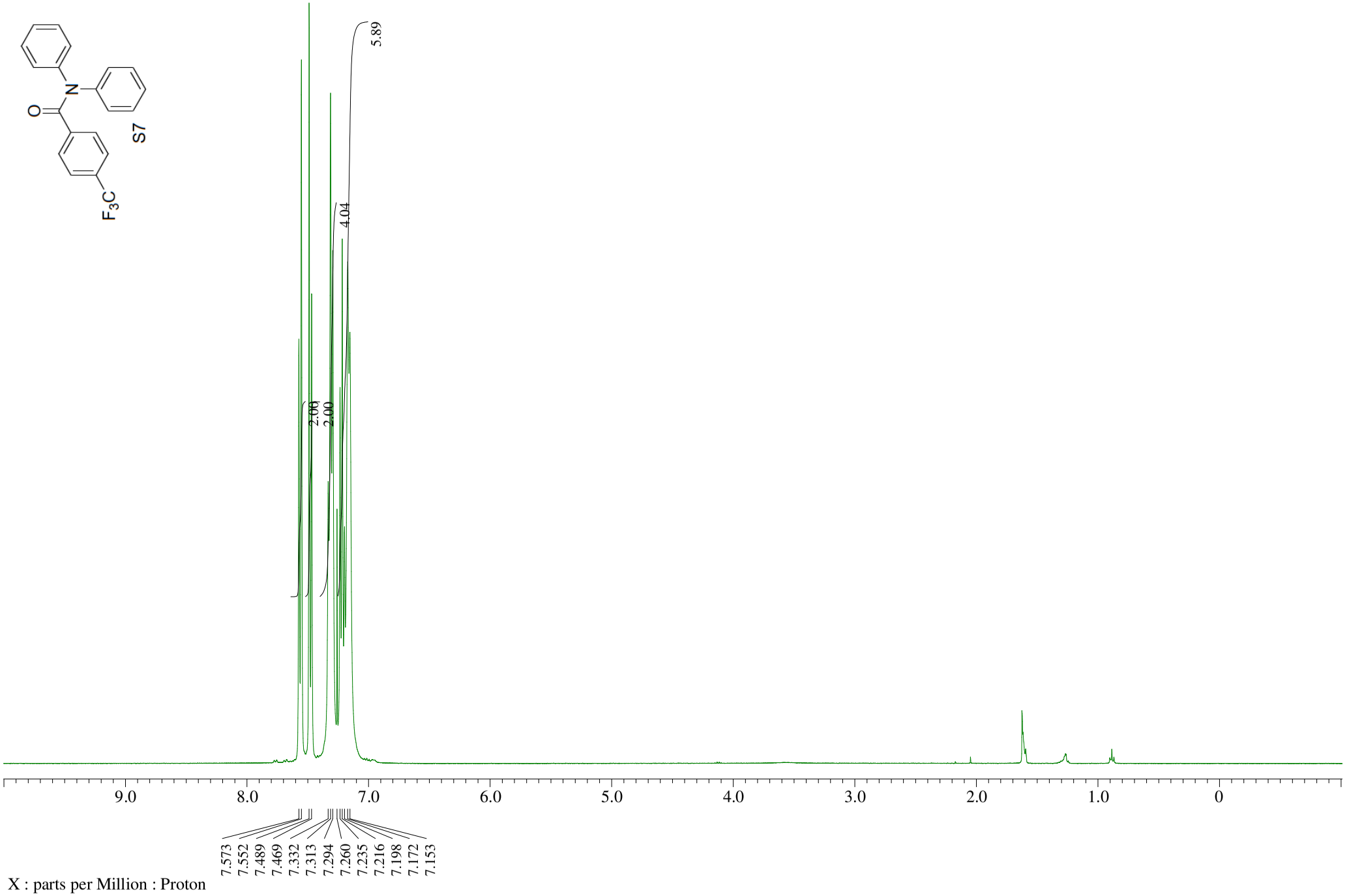

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.547
7.337
7.316
7.260
7.172
7.161
7.151
6.986
6.978
6.973
6.966
6.956
6.943
3.99
2.00
3.99
2.03
O
N
O
F3C
1aa

X : parts per Million : aron13

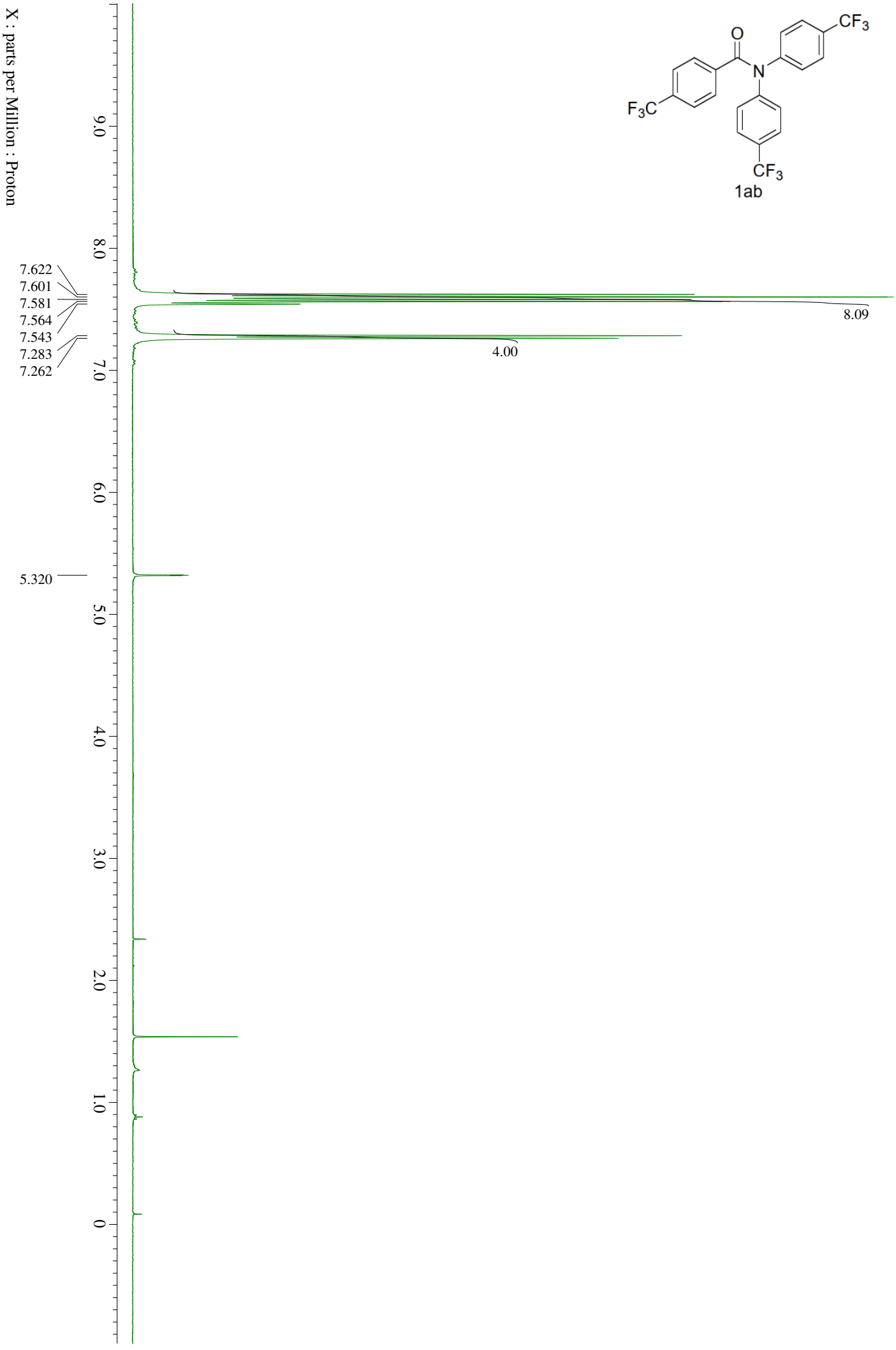
1aa

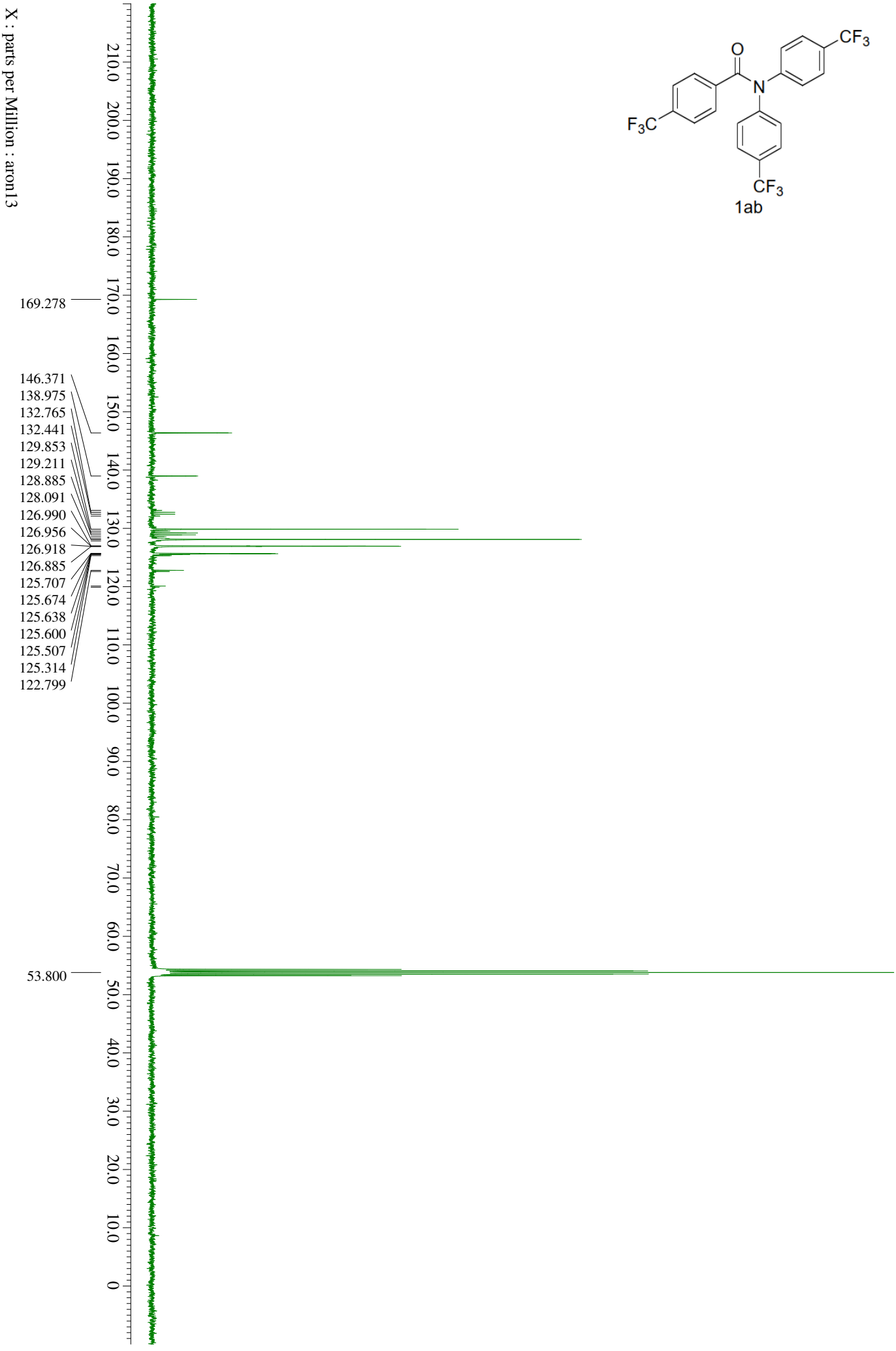
166.693
150.286
138.469
132.725
132.395
132.076
131.746
129.498
129.240
126.940
125.167
125.136
124.888
124.620
123.455
122.176
116.845
77.320
77.000
76.680

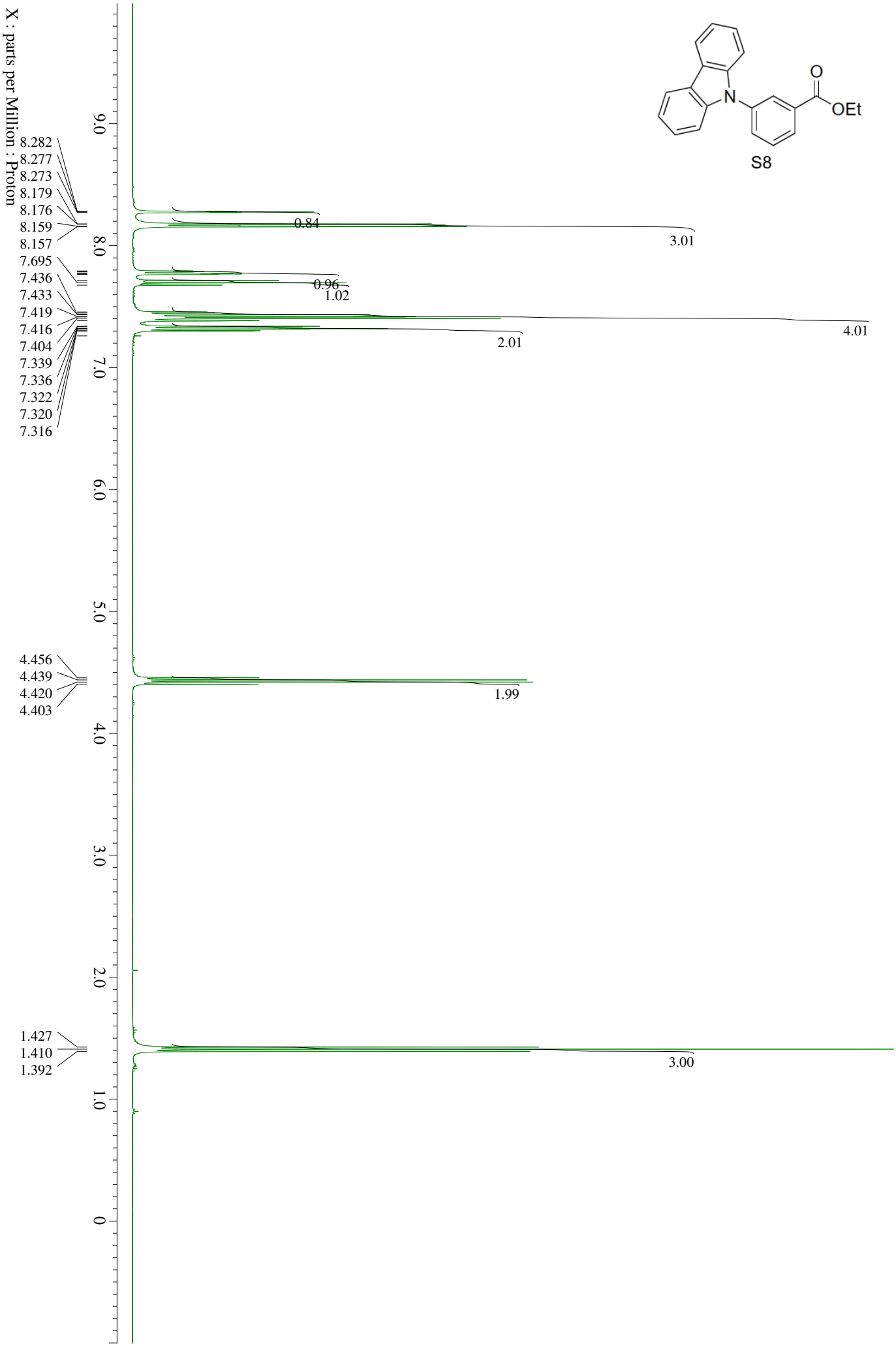
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

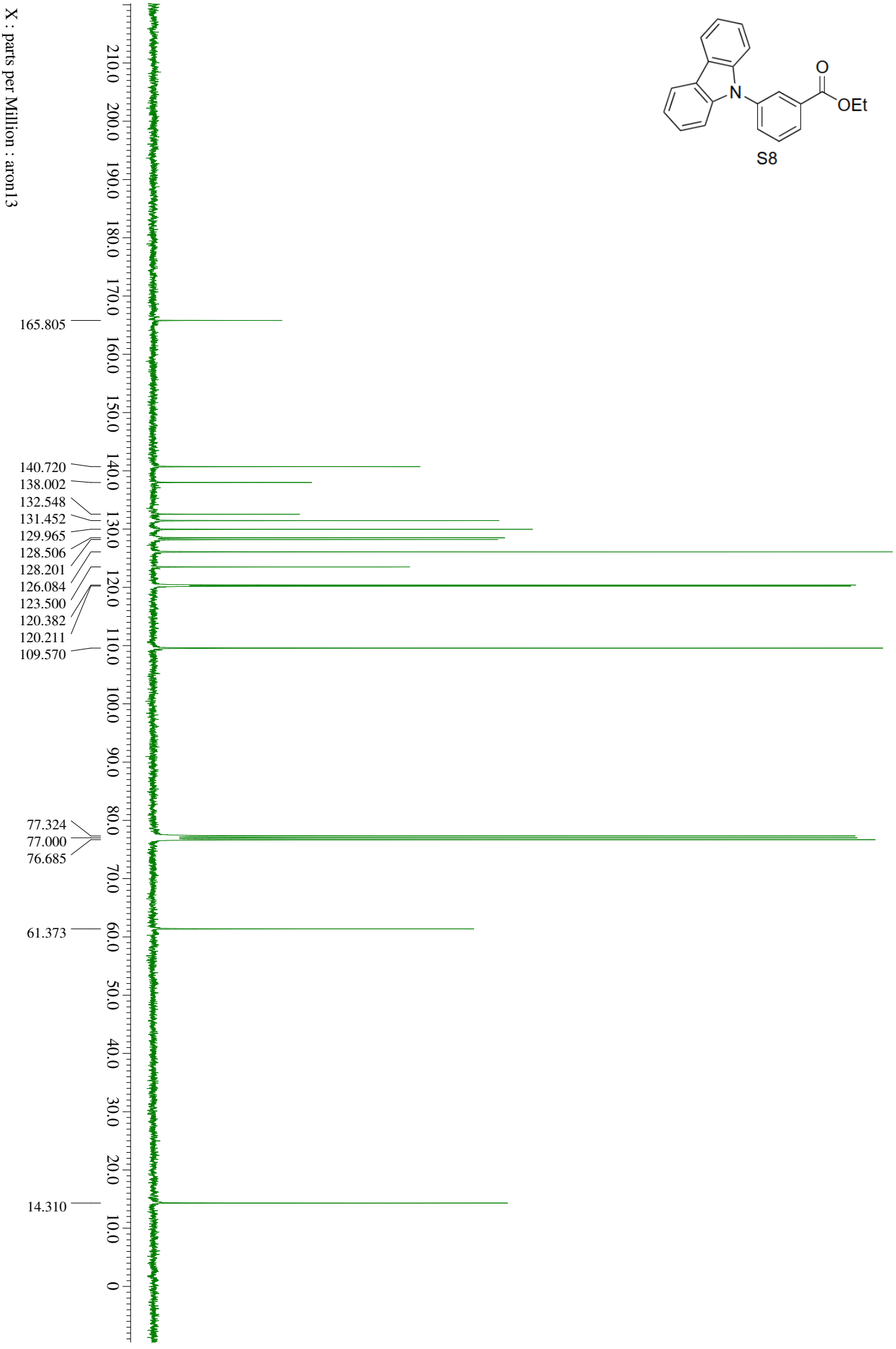

O
N
F3C
S7
5.89
4.04
2.00
2.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.573
7.552
7.489
7.469
7.332
7.313
7.294
7.260
7.235
7.216
7.198
7.172
7.153
X : parts per Million : Proton

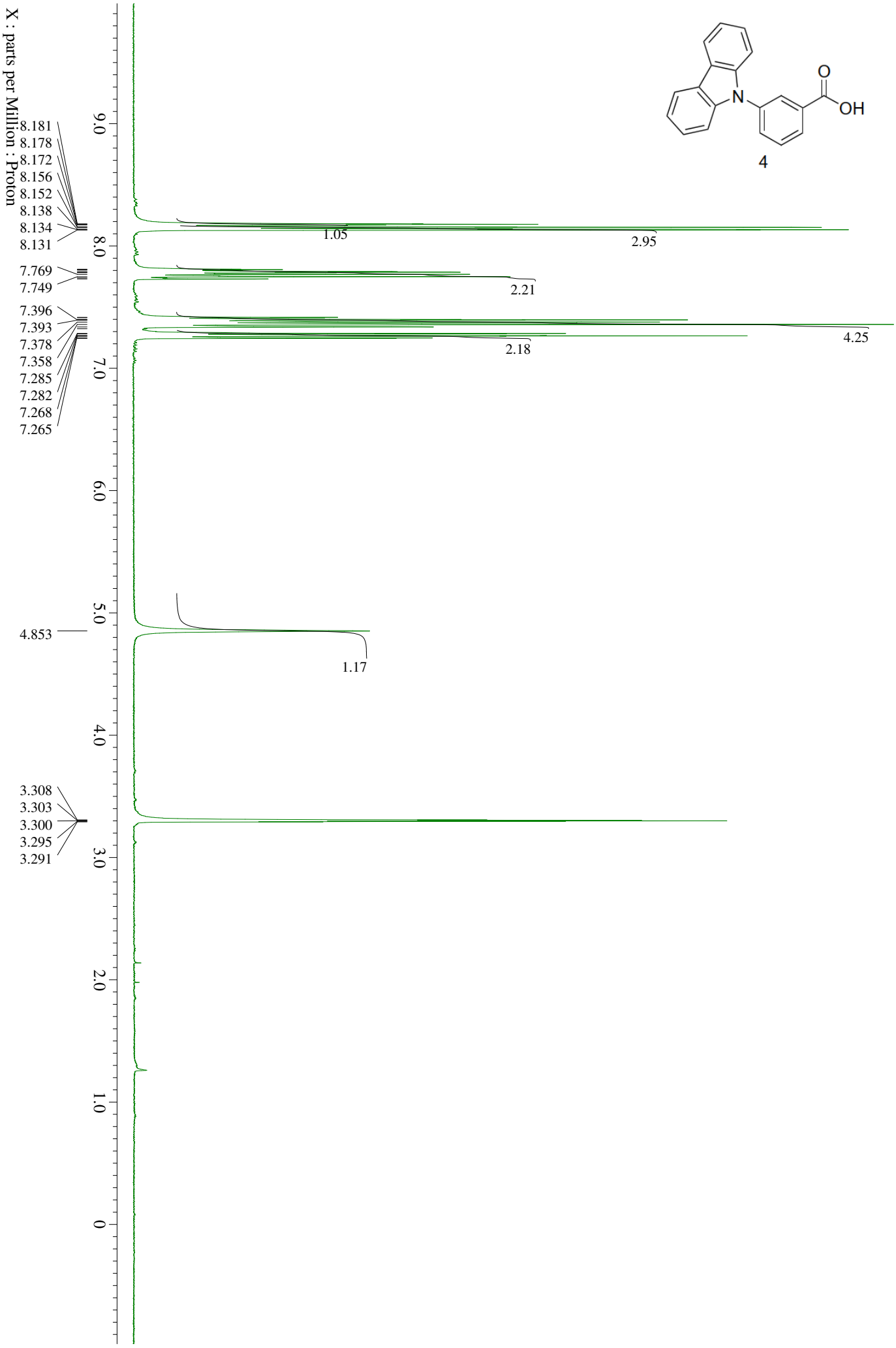
X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.075
143.212
139.614
132.158
131.828
131.508
131.178
129.343
129.260
127.373
126.775
124.909
124.868
122.217
119.505
77.309
77.000
76.680
O
N
F3C
S7


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.622
7.601
7.581
7.564
7.543
7.283
7.262
5.320
8.09
4.00
O
N
CF3
F3C
CF3
1ab


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.278
146.371
138.975
132.765
132.441
129.853
129.211
128.885
128.091
126.990
126.956
126.918
126.885
125.707
125.674
125.638
125.600
125.507
125.314
122.799
53.800
O
N
F3C
CF3
CF3
1ab


X : parts per Million : Proton
8.282
8.277
8.273
8.179
8.176
8.159
8.157
7.695
7.436
7.433
7.419
7.416
7.404
7.339
7.336
7.322
7.320
7.316
4.456
4.439
4.420
4.403
1.427
1.410
1.392
0.84
3.01
0.96
1.02
4.01
2.01
1.99
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
N
O
OEt
S8

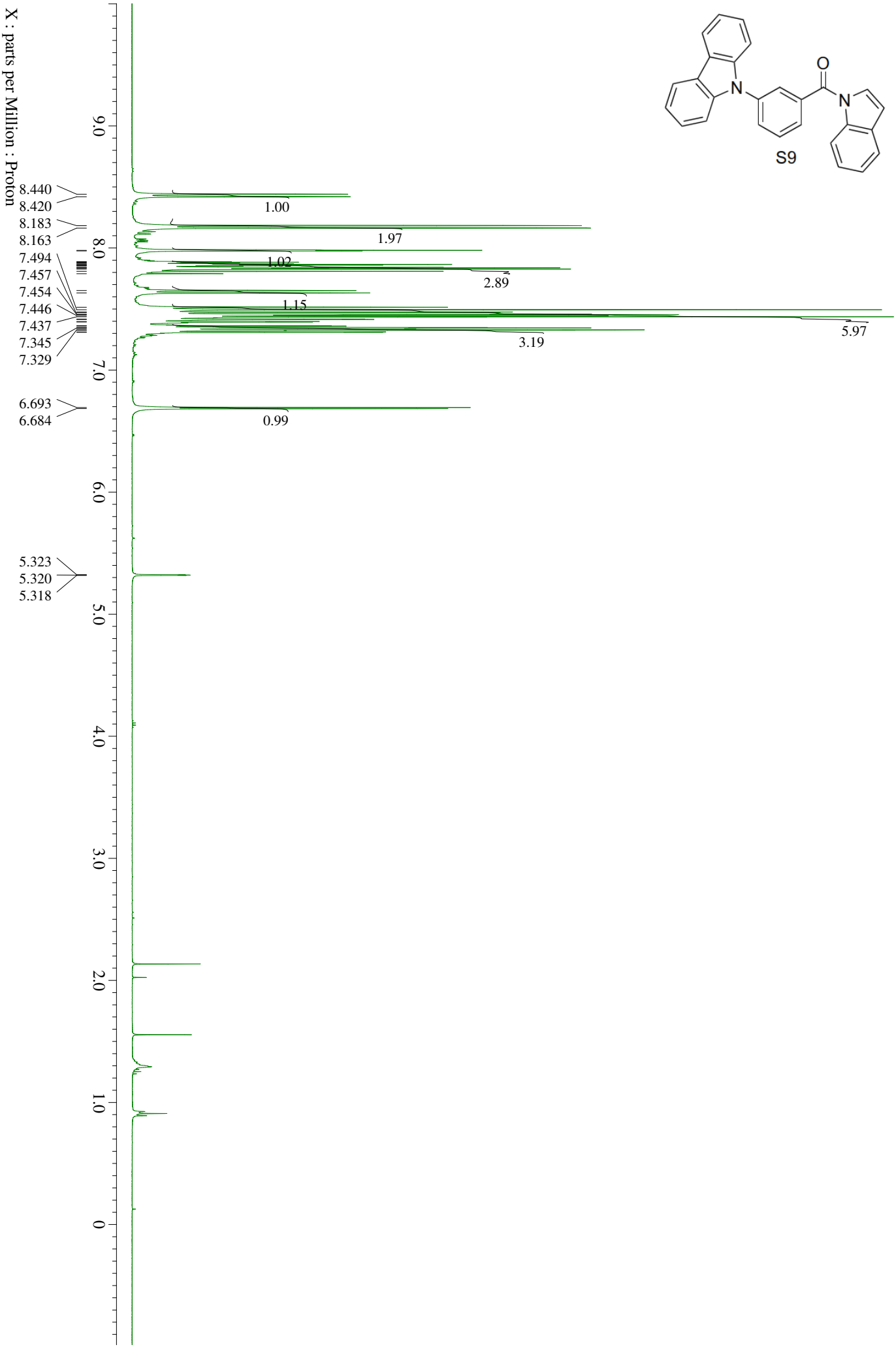

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
165.805
140.720
138.002
132.548
131.452
129.965
128.506
128.201
126.084
123.500
120.382
120.211
109.570
77.324
77.000
76.685
61.373
14.310
N
O
OEt
S8


X : parts per Million : Proton
8.181
8.178
8.172
8.156
8.152
8.138
8.134
8.131
7.769
7.749
7.396
7.393
7.378
7.358
7.285
7.282
7.268
7.265
4.853
3.308
3.303
3.300
3.295
3.291
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.05
2.95
2.21
4.25
2.18
1.17
O
N
OH
4

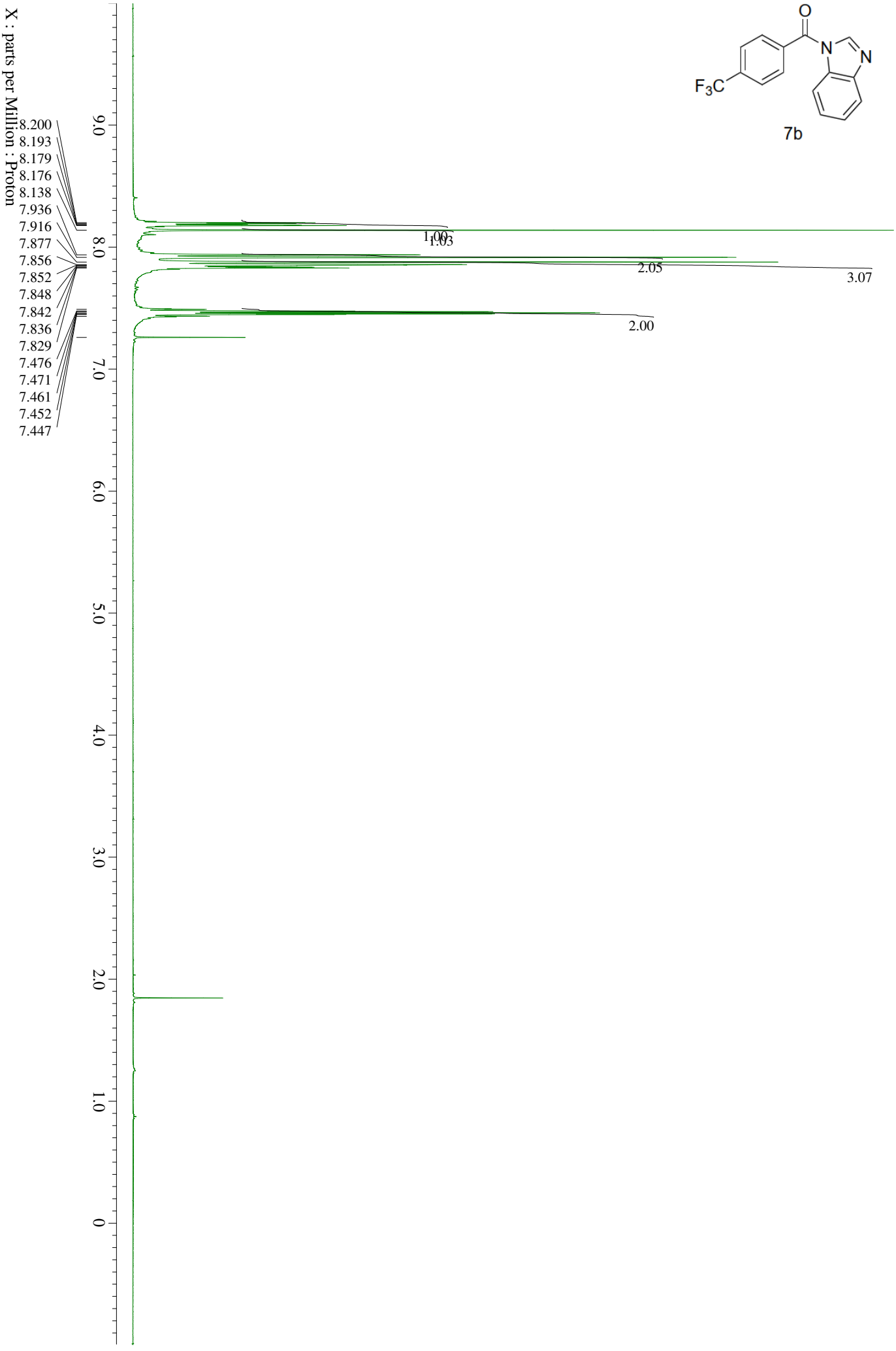
X : parts per Million : aron13

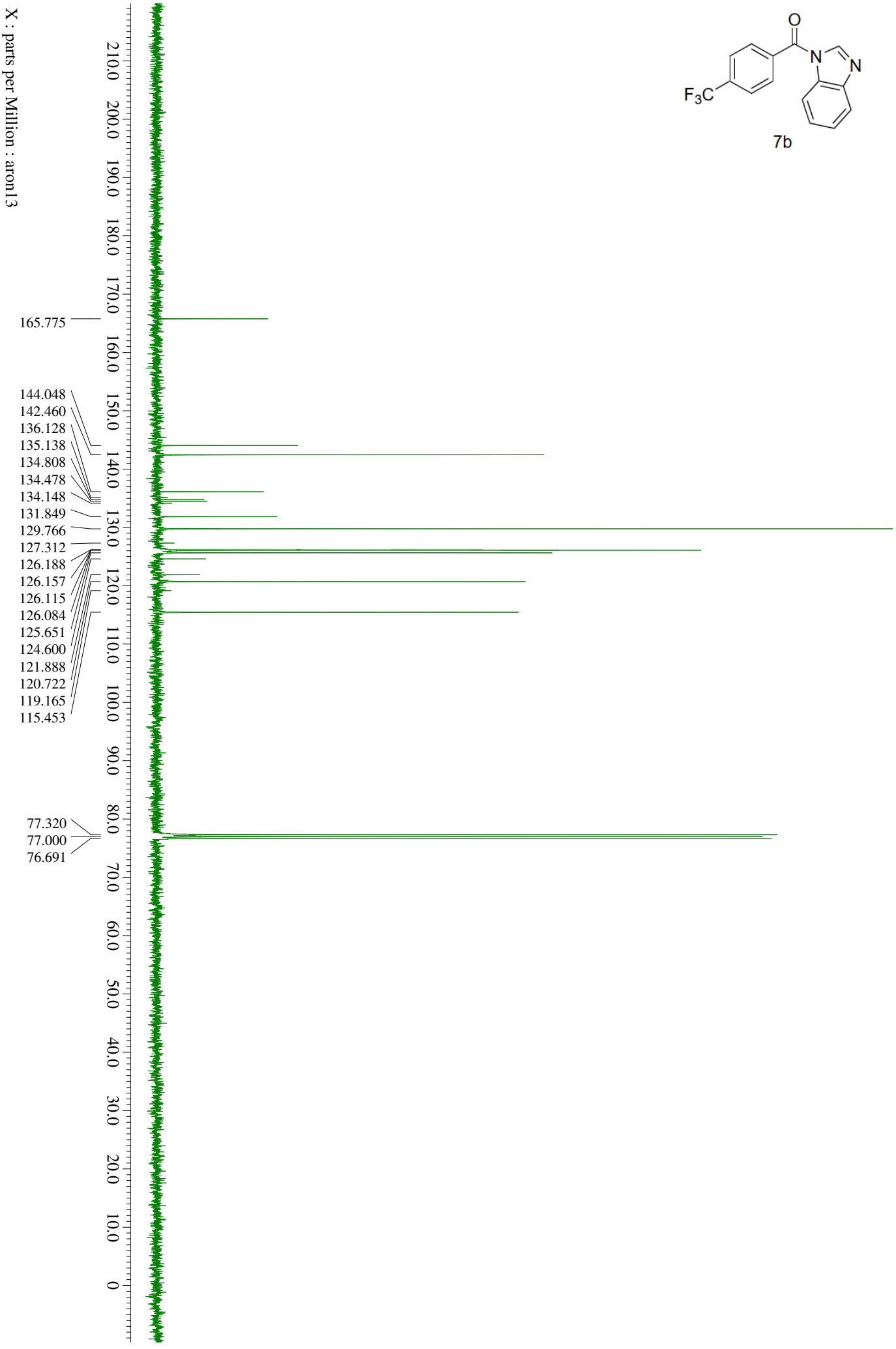
4

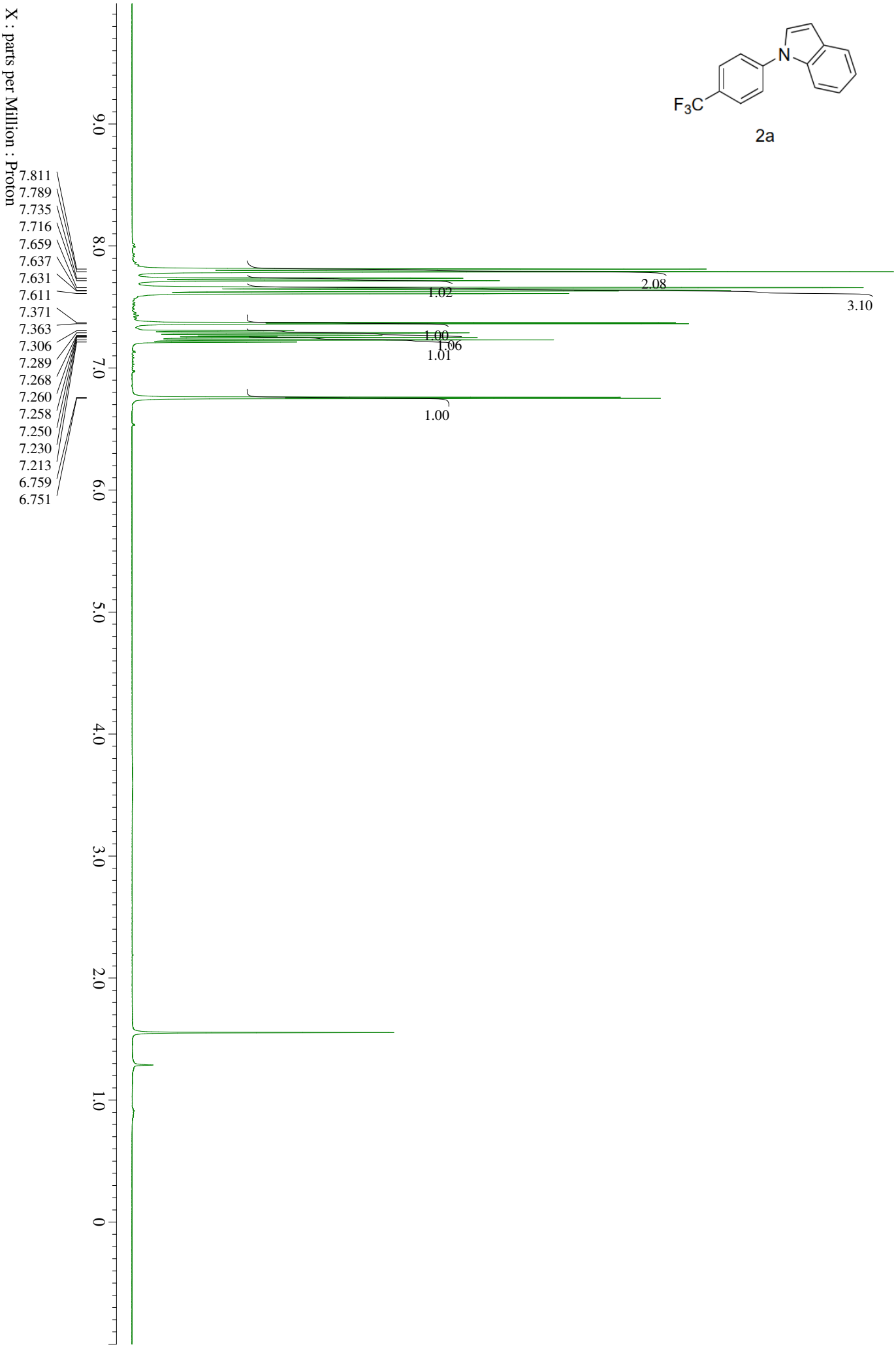
168.859
141.972
139.407
134.182
132.485
131.417
129.701
129.024
127.250
124.848
121.387
121.310
110.450
49.639
49.420
49.210
49.000
48.781
48.571
48.361


X : parts per Million : Proton
8.440
8.420
8.183
8.163
7.494
7.457
7.454
7.446
7.437
7.345
7.329
6.693
6.684
5.323
5.320
5.318
1.00
1.97
1.02
2.89
1.15
3.19
5.97
0.99
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
N
N
S9

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
177.875
150.939
148.536
146.982
146.467
141.290
140.851
140.689
138.353
138.039
137.829
136.685
135.426
134.540
133.939
131.488
130.916
130.840
126.750
120.085
119.208
54.267
54.038
53.800
53.571
53.333
O
N
N
S9


X : parts per Million : Proton
8.200
8.193
8.179
8.176
8.138
7.936
7.916
7.877
7.856
7.852
7.848
7.842
7.836
7.829
7.476
7.471
7.461
7.452
7.447
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
1.03
2.05
3.07
2.00
O
N
N
F3C
7b


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
165.775
144.048
142.460
136.128
135.138
134.808
134.478
134.148
131.849
129.766
127.312
126.188
126.157
126.115
126.084
125.651
124.600
121.888
120.722
119.165
115.453
77.320
77.000
76.691
O
N
N
F3C
7b


X : parts per Million : Proton
7.811
7.789
7.735
7.716
7.659
7.637
7.631
7.611
7.371
7.363
7.306
7.289
7.268
7.260
7.258
7.250
7.230
7.213
6.759
6.751
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.08
1.02
3.10
1.00
1.06
1.01
1.00
N
F3C
2a

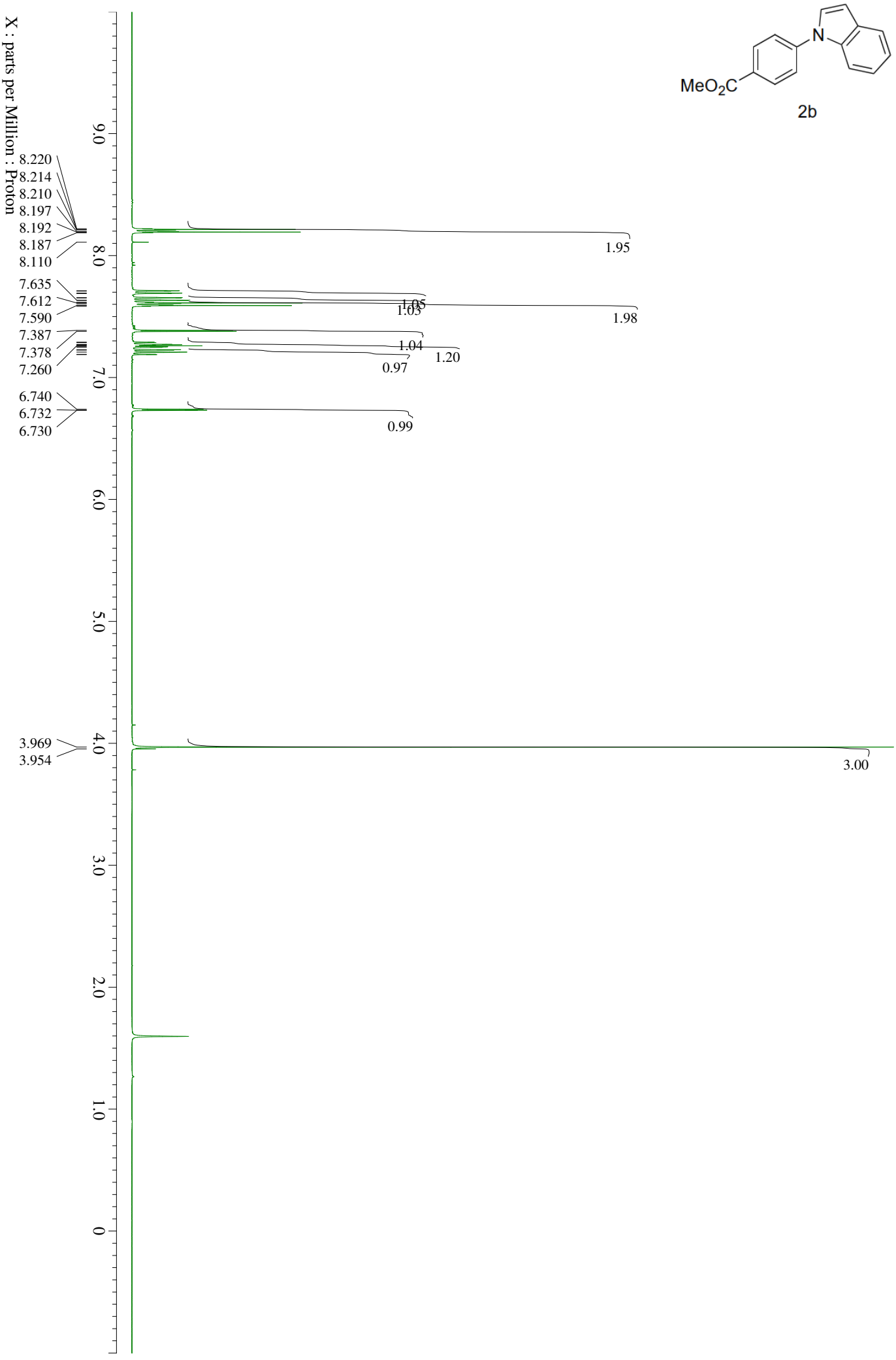
X : parts per Million : aron13

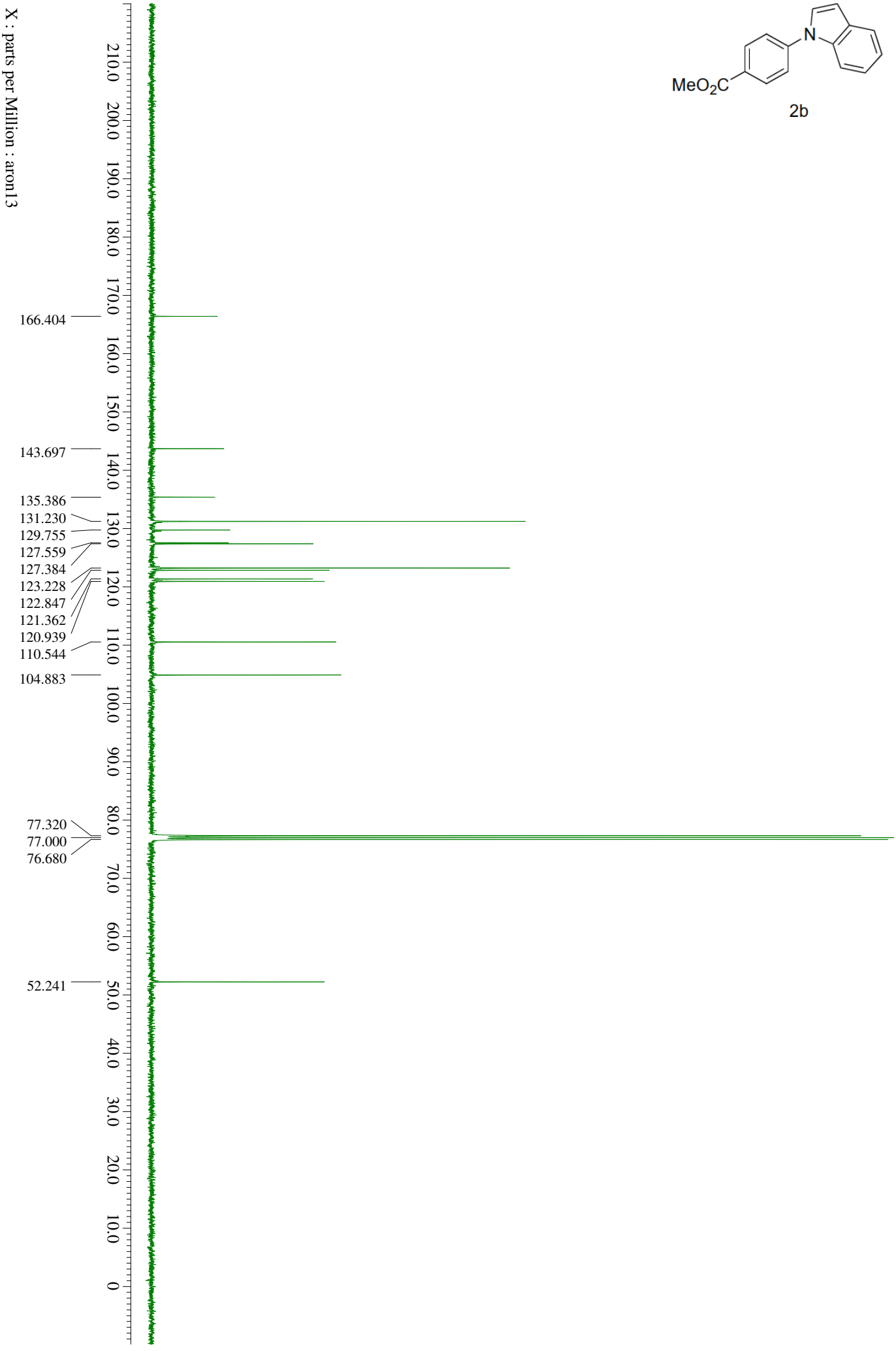
2a

142.779
135.458
129.683
128.611
128.291
128.013
127.961
127.394
126.920
126.878
125.311
123.898
122.908
122.609
121.413
120.980
119.897
110.318
104.894

77.320
77.000
76.691

210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0


X : parts per Million : Proton
8.220
8.214
8.210
8.197
8.192
8.187
8.110
7.635
7.612
7.590
7.387
7.378
7.260
6.740
6.732
6.730
3.969
3.954
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.95
1.03
1.05
1.98
1.04
0.97
1.20
0.99
3.00
MeO2C
N
2b


X : parts per Million : aron13
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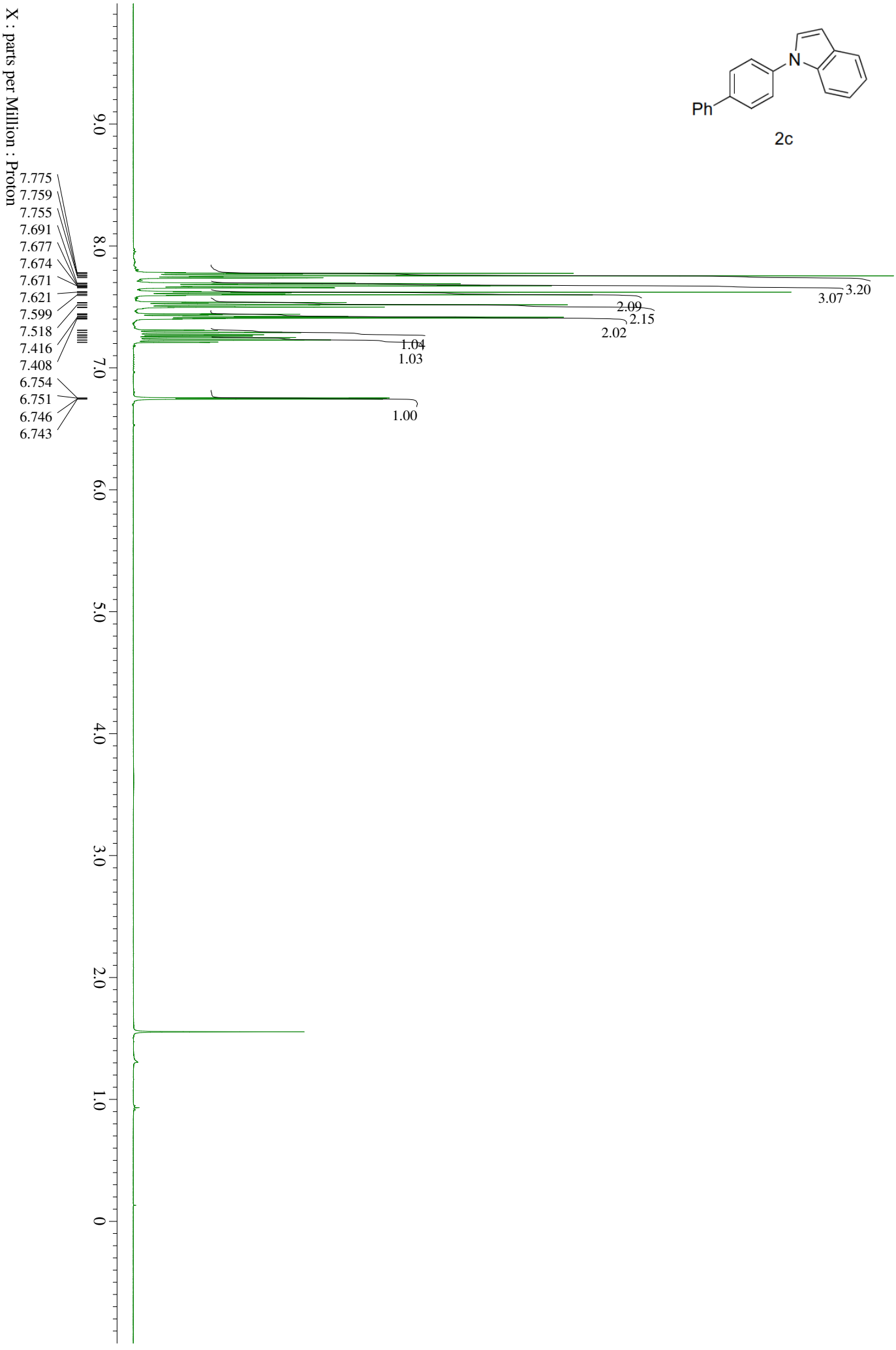
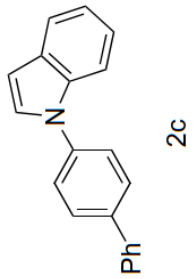
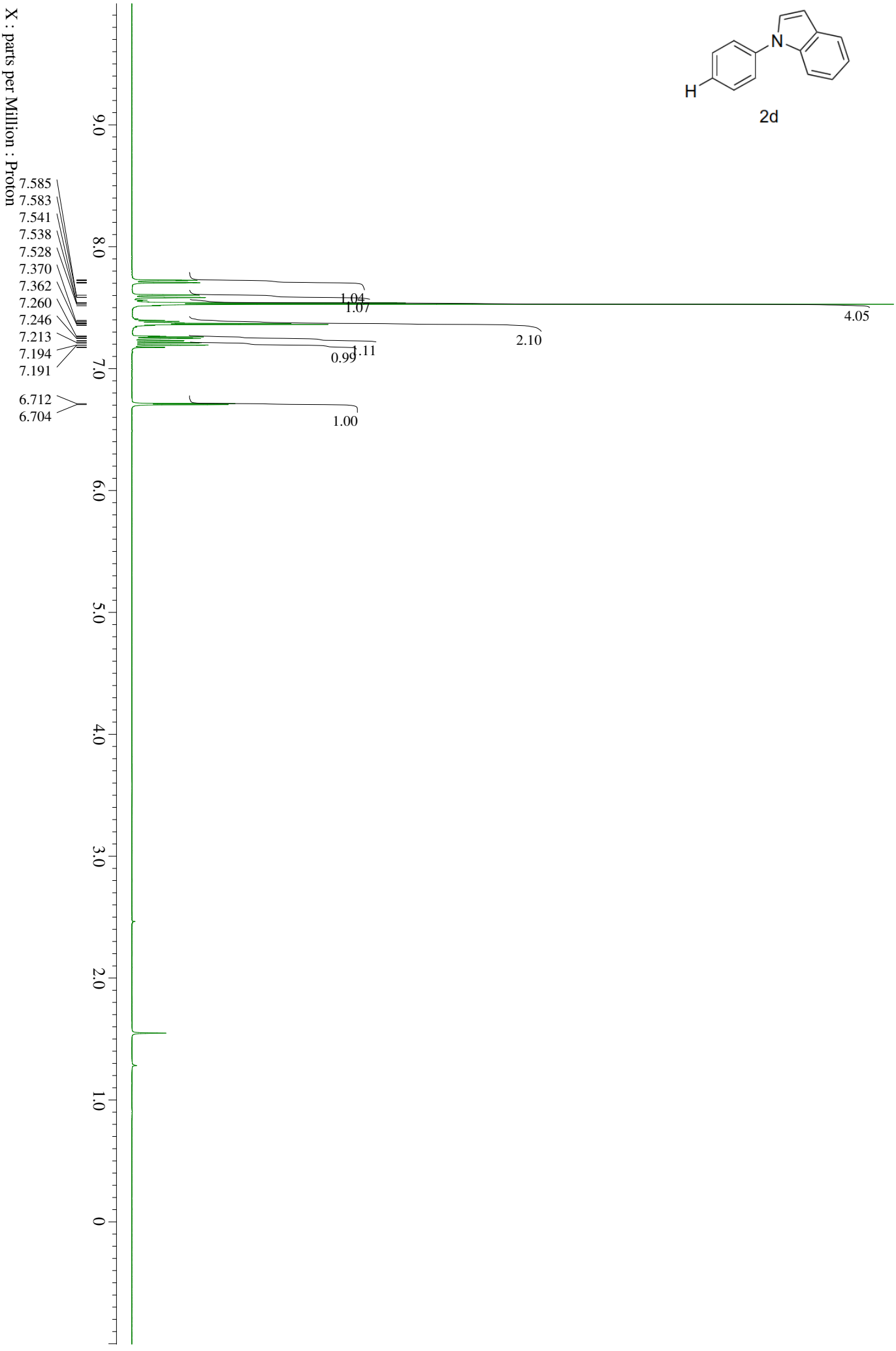
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.404
143.697
135.386
131.230
129.755
127.559
127.384
123.228
122.847
121.362
120.939
110.544
104.883
77.320
77.000
76.680
52.241
N
MeO2C
2b

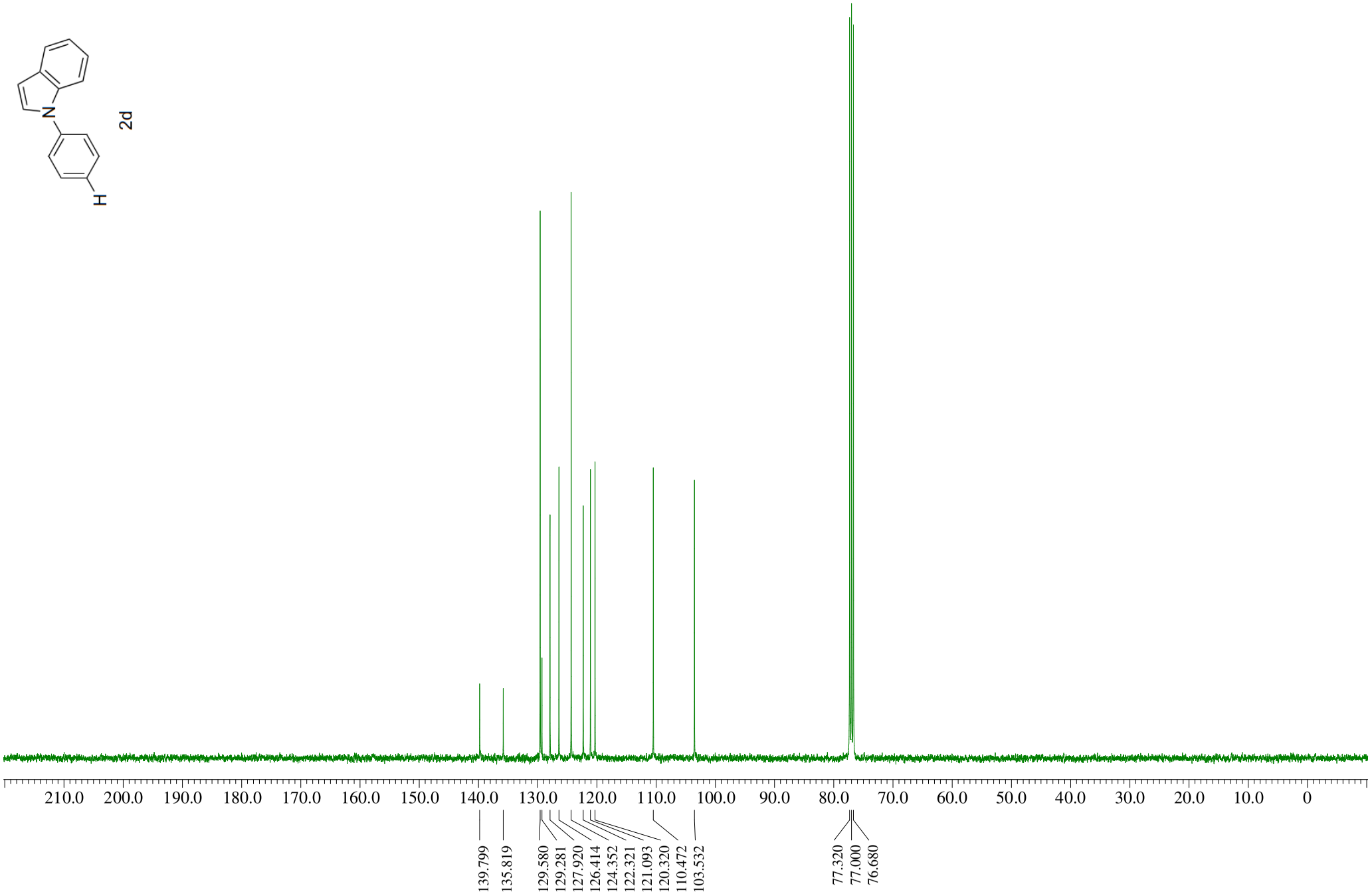

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.775
7.759
7.755
7.691
7.677
7.674
7.671
7.621
7.599
7.518
7.416
7.408
6.754
6.751
6.746
6.743
3.20
3.07
2.09
2.15
2.02
1.04
1.03
1.00
N
Ph
2c



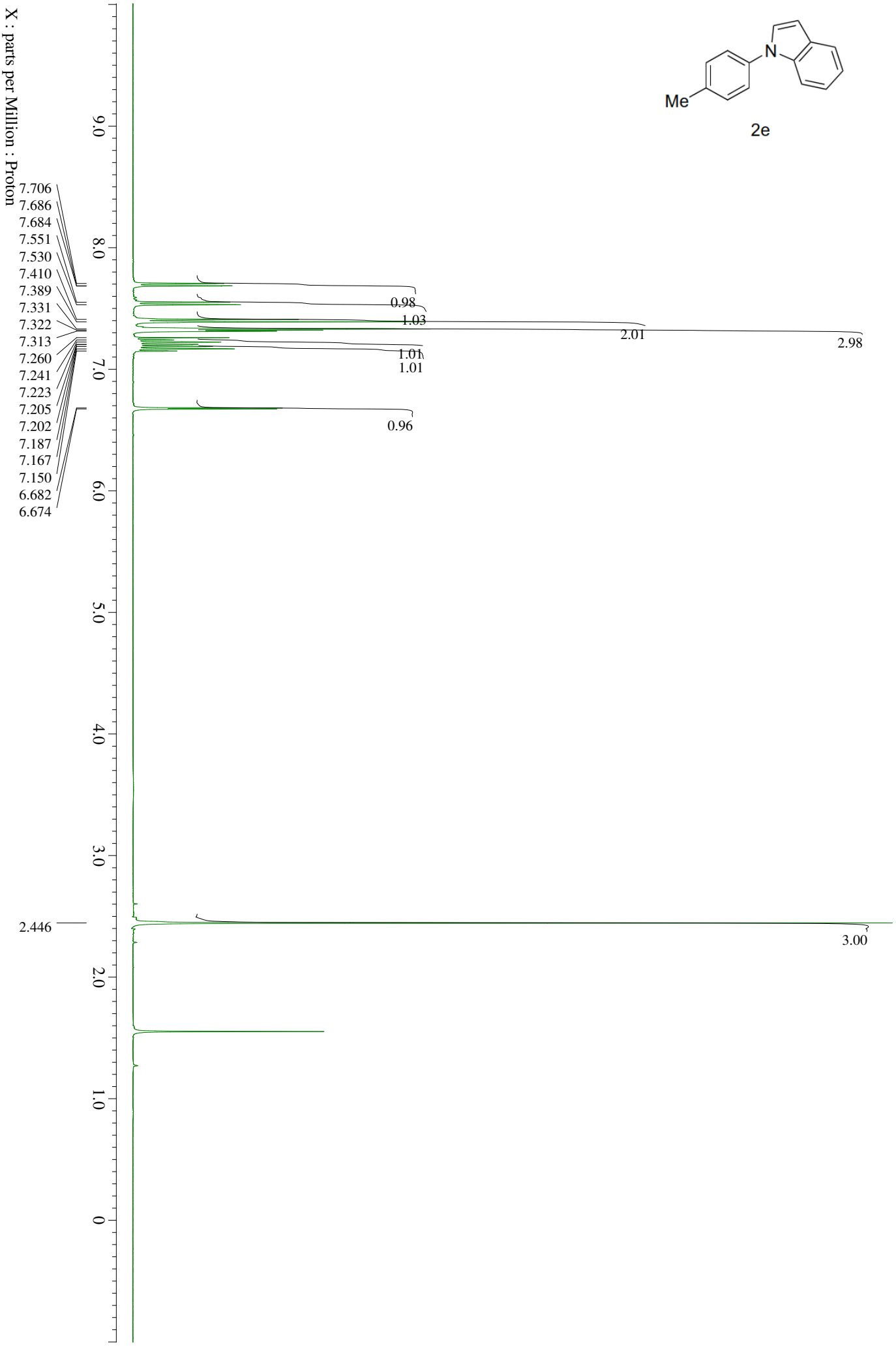
2c

X : parts per Million : aron13


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.585
7.583
7.541
7.538
7.528
7.370
7.362
7.260
7.246
7.213
7.194
7.191
6.712
6.704
1.04
1.07
4.05
2.10
0.99
1.11
1.00
N
H
2d

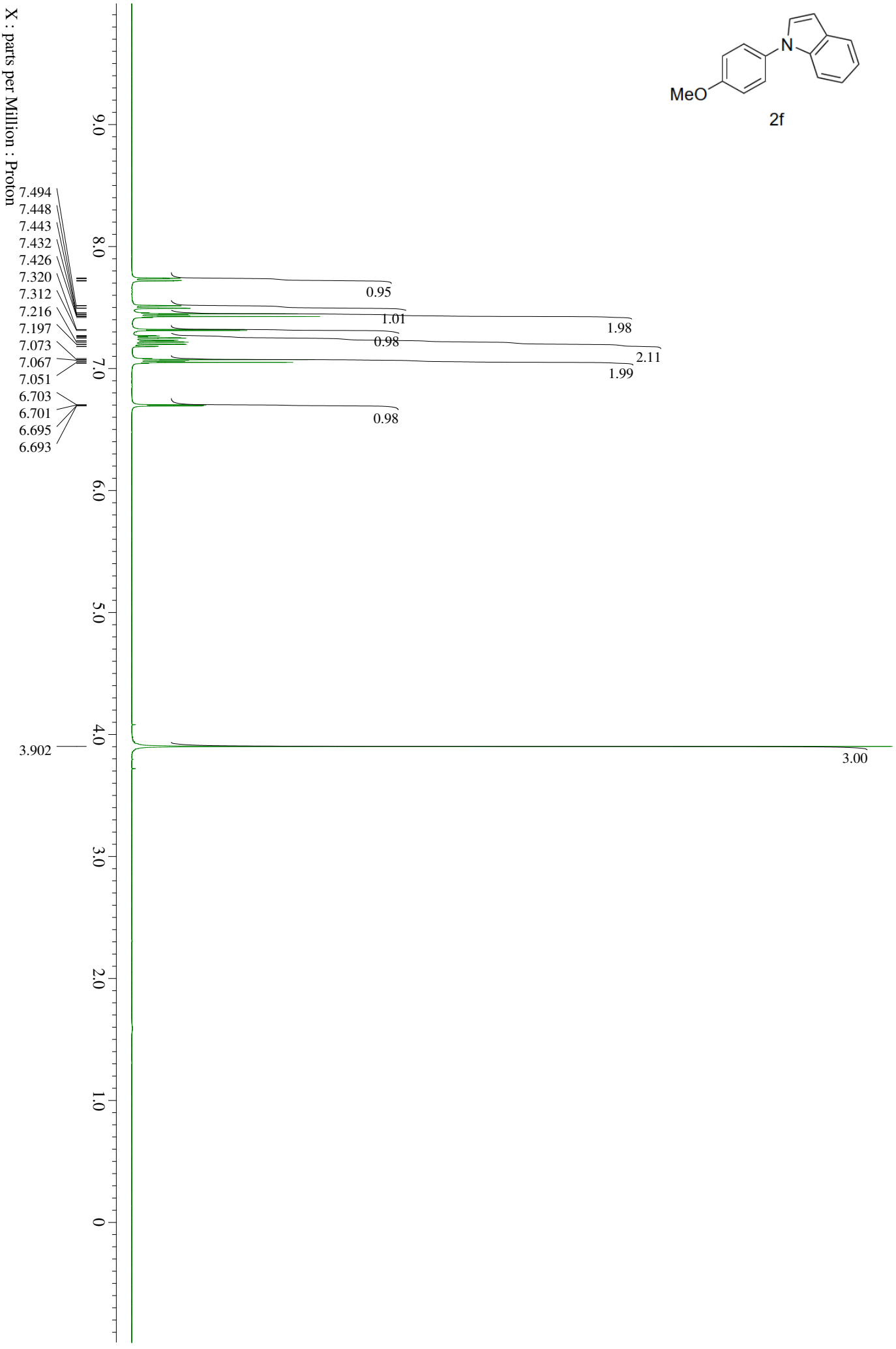


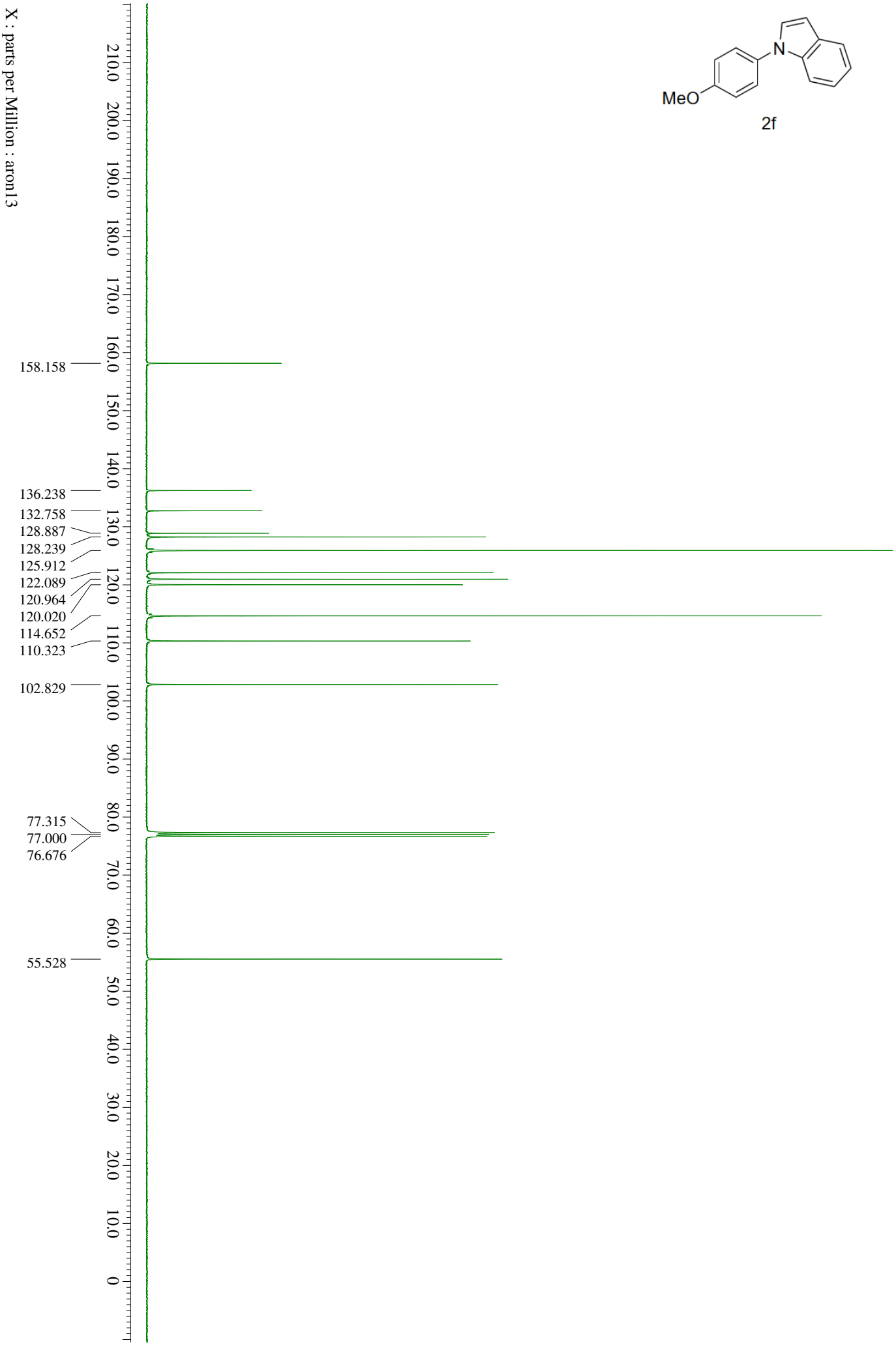
X : parts per Million : aron13

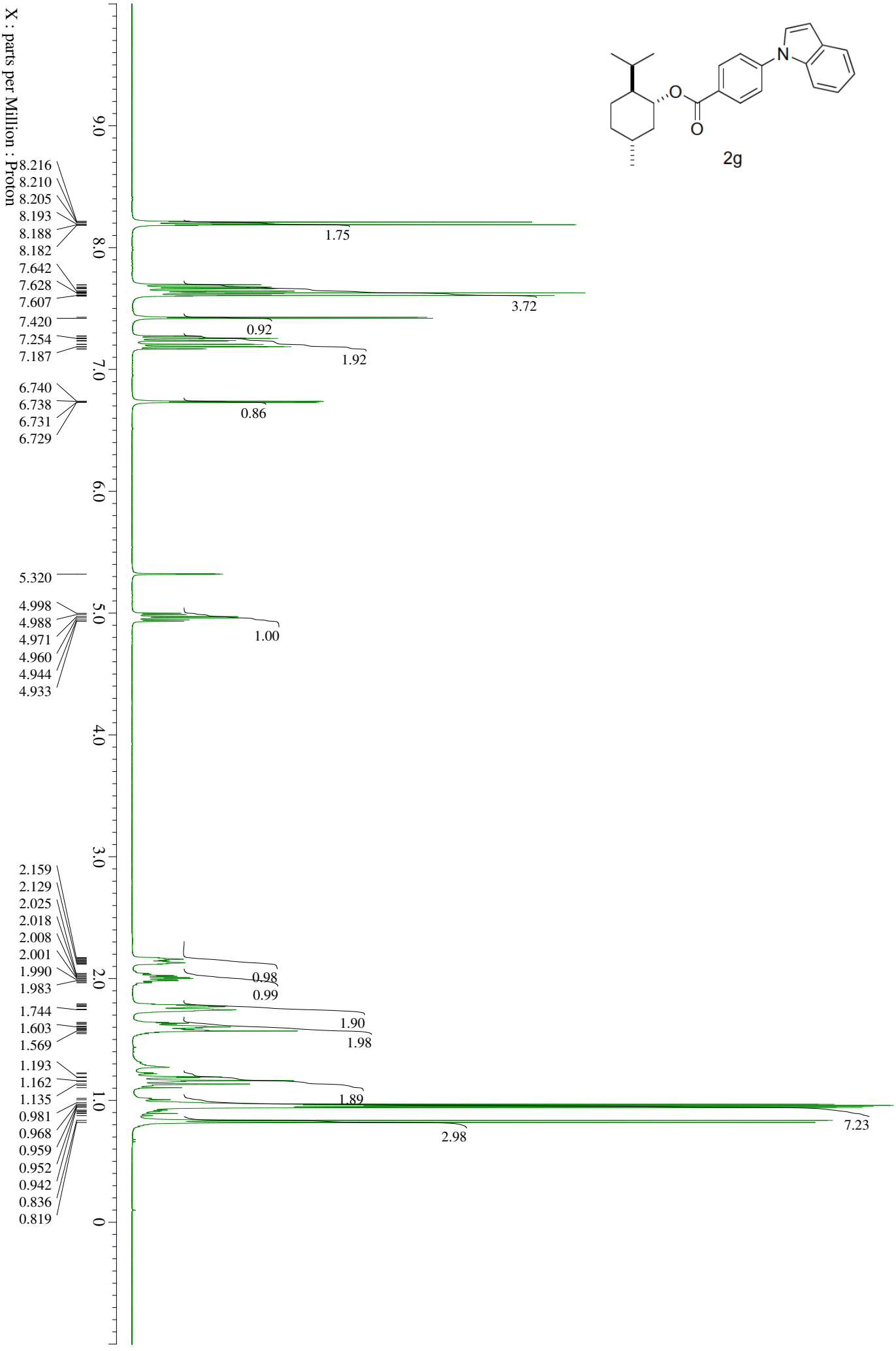

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.706
7.686
7.684
7.551
7.530
7.410
7.389
7.331
7.322
7.313
7.260
7.241
7.223
7.205
7.202
7.187
7.167
7.150
6.682
6.674
2.446
0.98
1.03
2.01
2.98
1.01
1.01
0.96
3.00
N
Me
2e

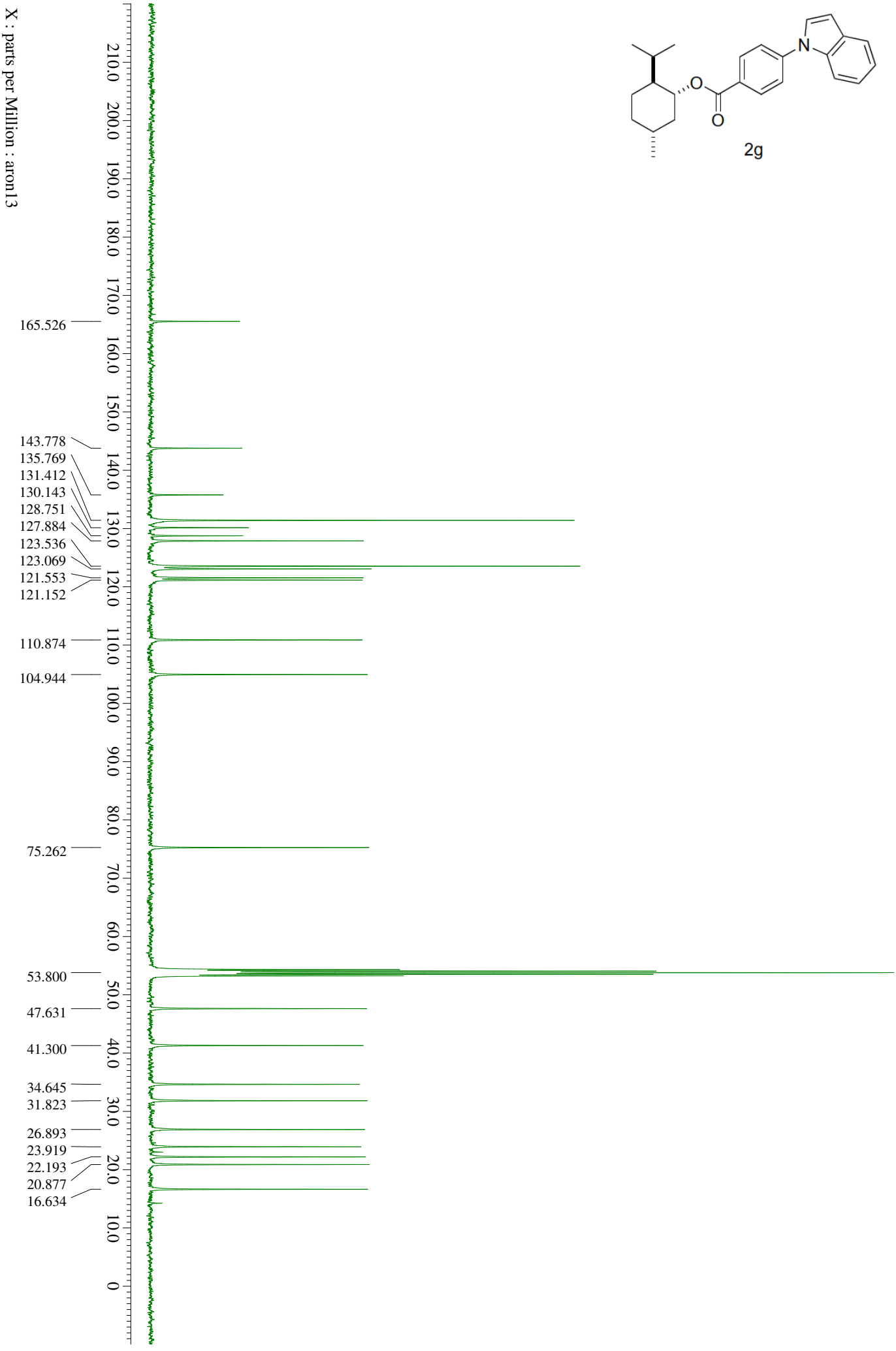
X : parts per Million : aron13

2e


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.494
7.448
7.443
7.432
7.426
7.320
7.312
7.216
7.197
7.073
7.067
7.051
6.703
6.701
6.695
6.693
3.902
0.95
1.01
0.98
1.98
2.11
1.99
0.98
3.00
MeO
N
2f


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
158.158
136.238
132.758
128.887
128.239
125.912
122.089
120.964
120.020
114.652
110.323
102.829
77.315
77.000
76.676
55.528
N
MeO
2f


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.216
8.210
8.205
8.193
8.188
8.182
7.642
7.628
7.607
7.420
7.254
7.187
6.740
6.738
6.731
6.729
5.320
4.998
4.988
4.971
4.960
4.944
4.933
2.159
2.129
2.025
2.018
2.008
2.001
1.990
1.983
1.744
1.603
1.569
1.193
1.162
1.135
0.981
0.968
0.959
0.952
0.942
0.836
0.819
1.75
3.72
0.92
1.92
0.86
1.00
0.98
0.99
1.90
1.98
1.89
2.98
7.23
O
O
N
2g


X : parts per Million : aron13
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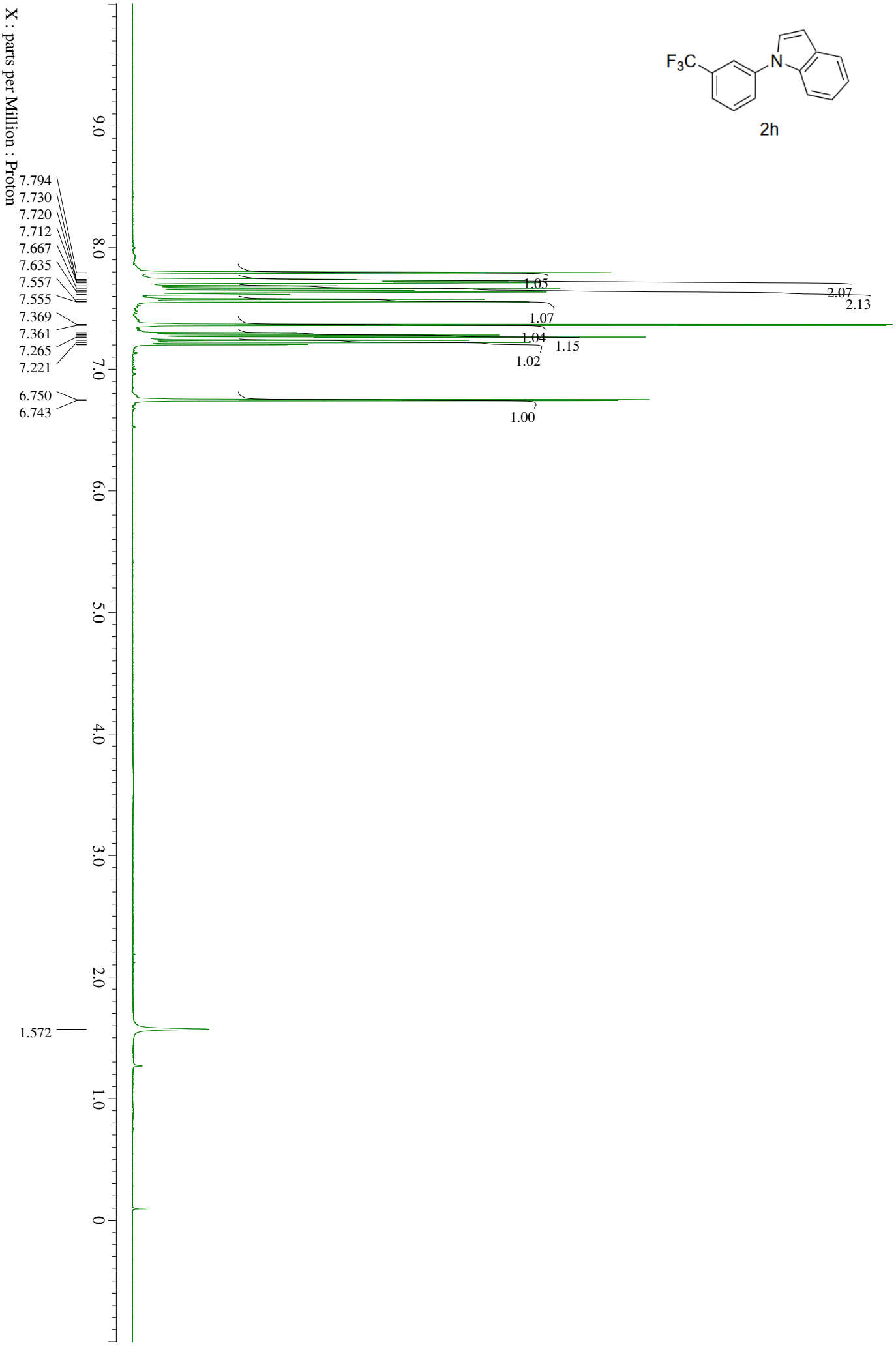
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
165.526
143.778
135.769
131.412
130.143
128.751
127.884
123.536
123.069
121.553
121.152
110.874
104.944
75.262
53.800
47.631
41.300
34.645
31.823
26.893
23.919
22.193
20.877
16.634
O
O
N
2g


X : parts per Million : Proton
9.0
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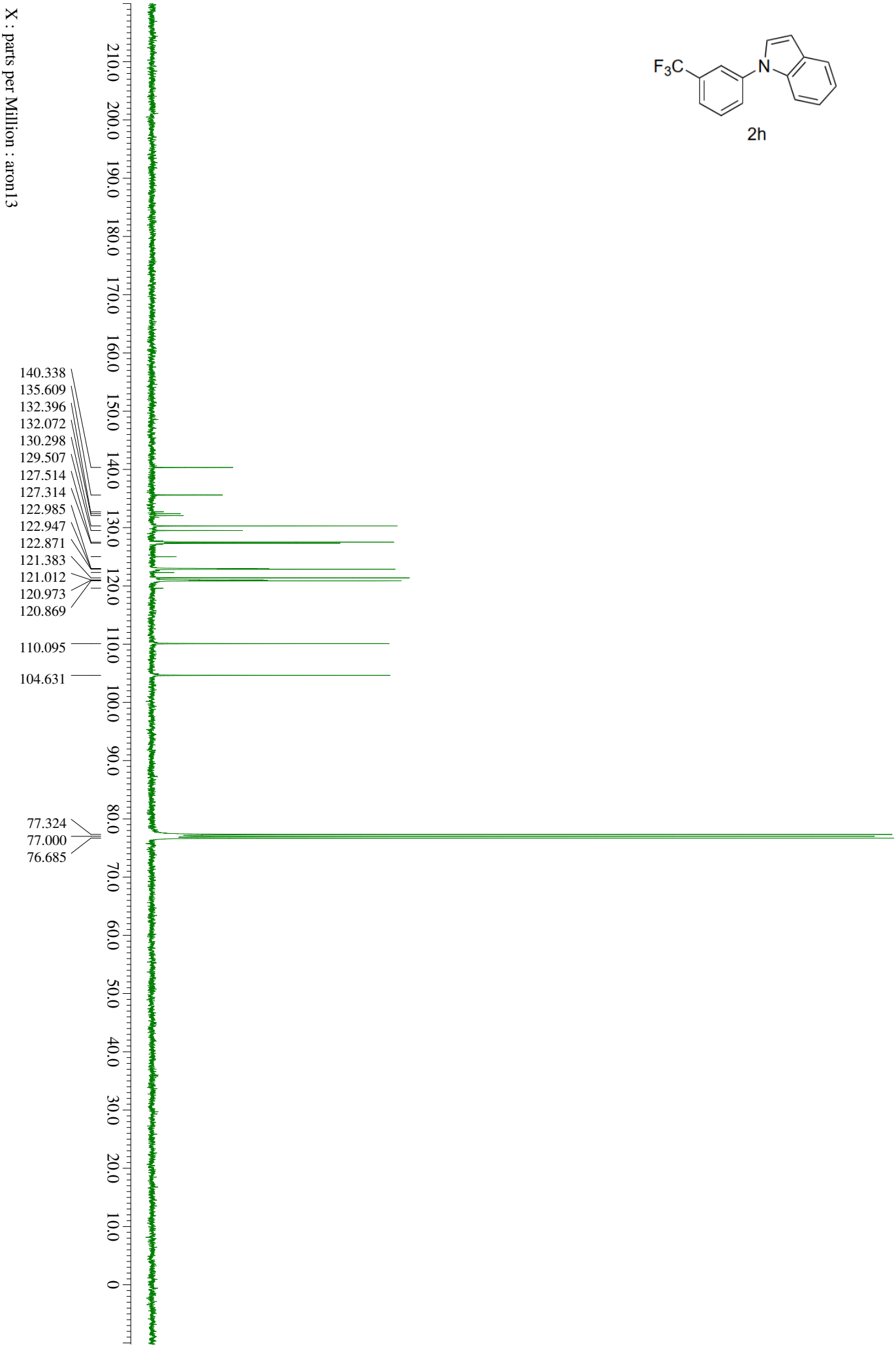
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.794
7.730
7.720
7.712
7.667
7.635
7.557
7.555
7.369
7.361
7.265
7.221
6.750
6.743
1.572
1.05
2.07
2.13
1.07
1.04
1.15
1.02
1.00
F3C
N
2h


X : parts per Million : aron13
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200.0
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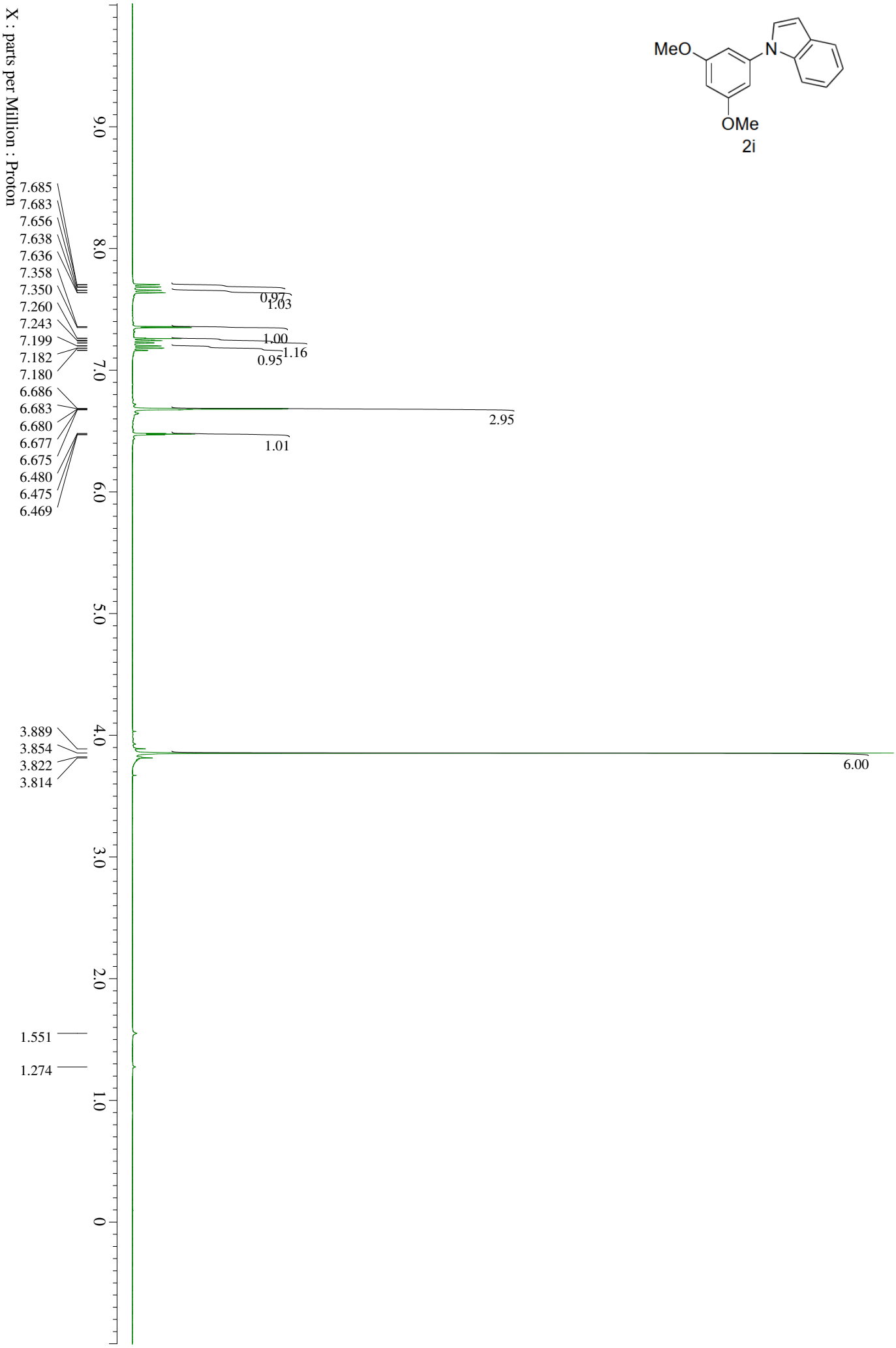
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
140.338
135.609
132.396
132.072
130.298
129.507
127.514
127.314
122.985
122.947
122.871
121.383
121.012
120.973
120.869
110.095
104.631
77.324
77.000
76.685
F3C
N
2h


X : parts per Million : Proton
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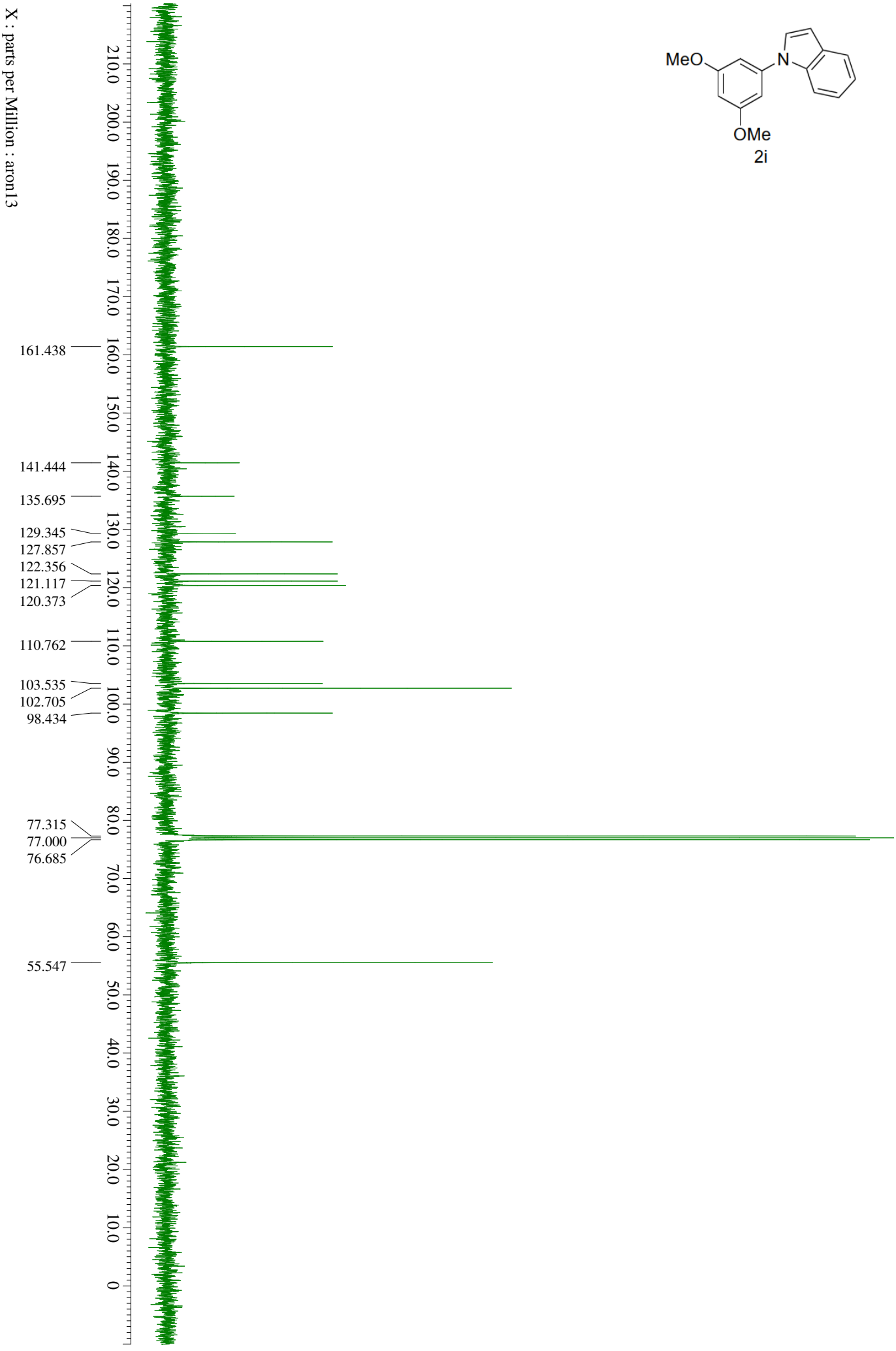
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.685
7.683
7.656
7.638
7.636
7.358
7.350
7.260
7.243
7.199
7.182
7.180
6.686
6.683
6.680
6.677
6.675
6.480
6.475
6.469
3.889
3.854
3.822
3.814
1.551
1.274
0.97
1.03
1.00
0.95
1.16
2.95
1.01
6.00
MeO
N
OMe
2i


X : parts per Million : aron13
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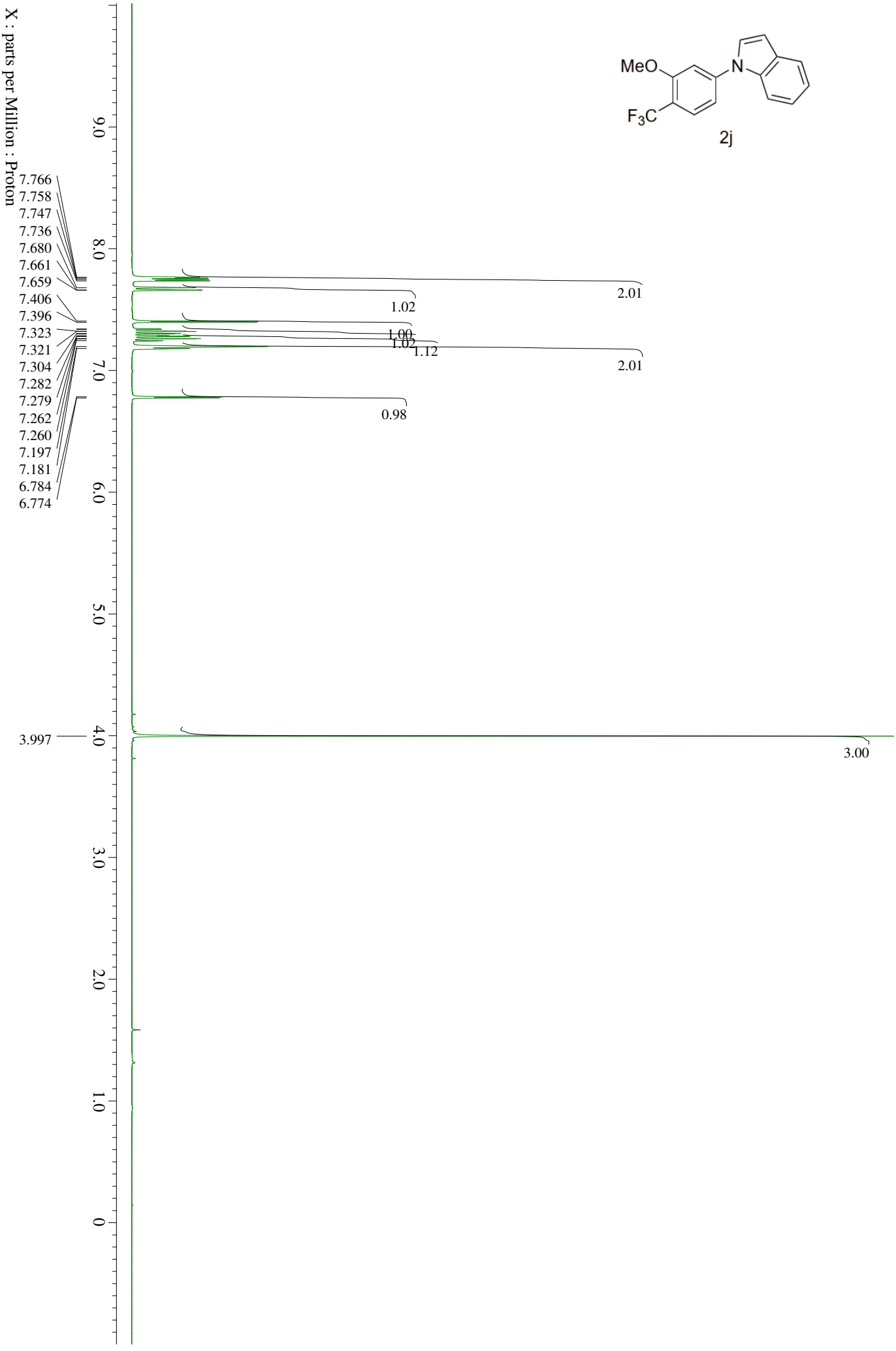
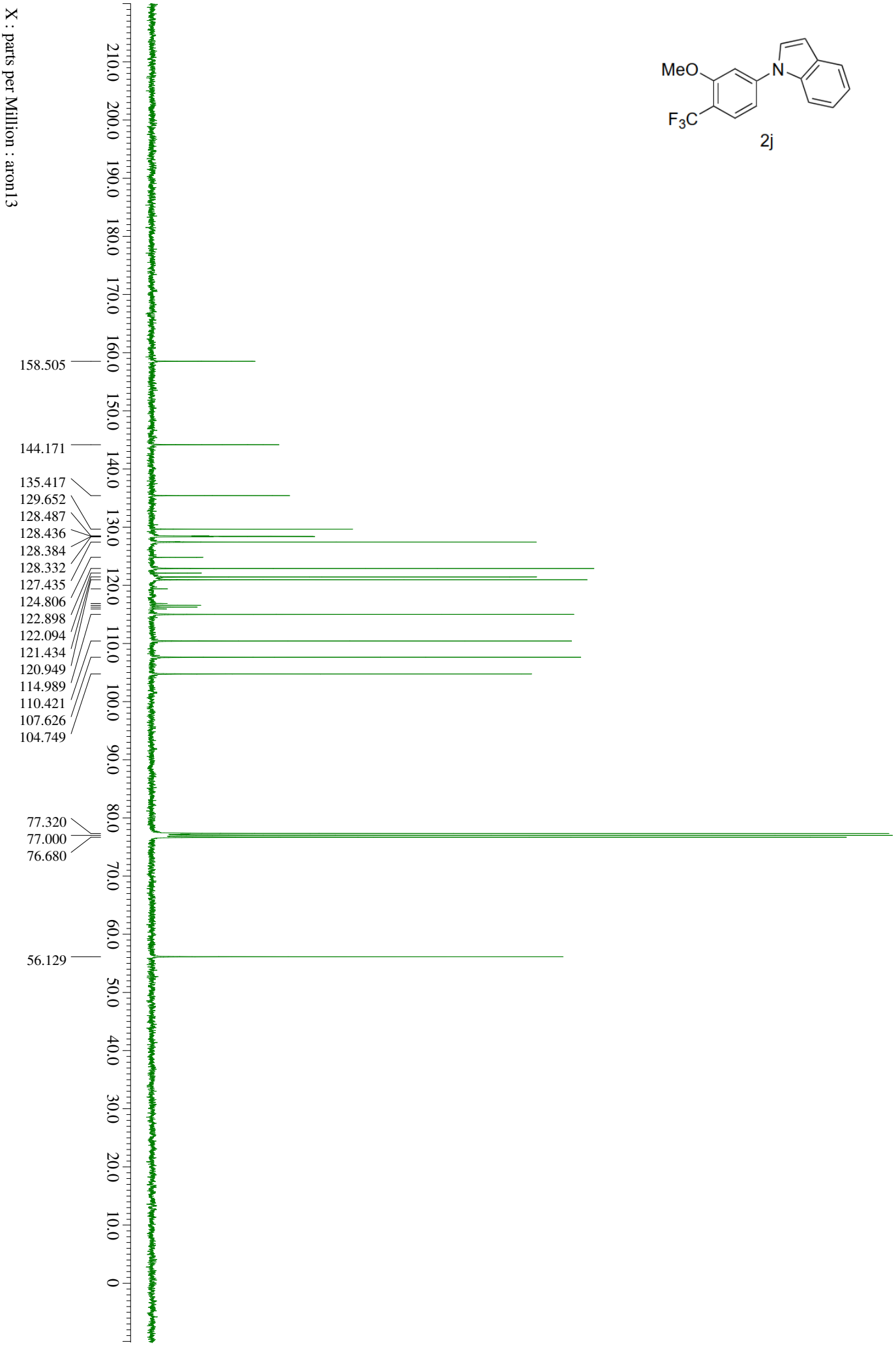
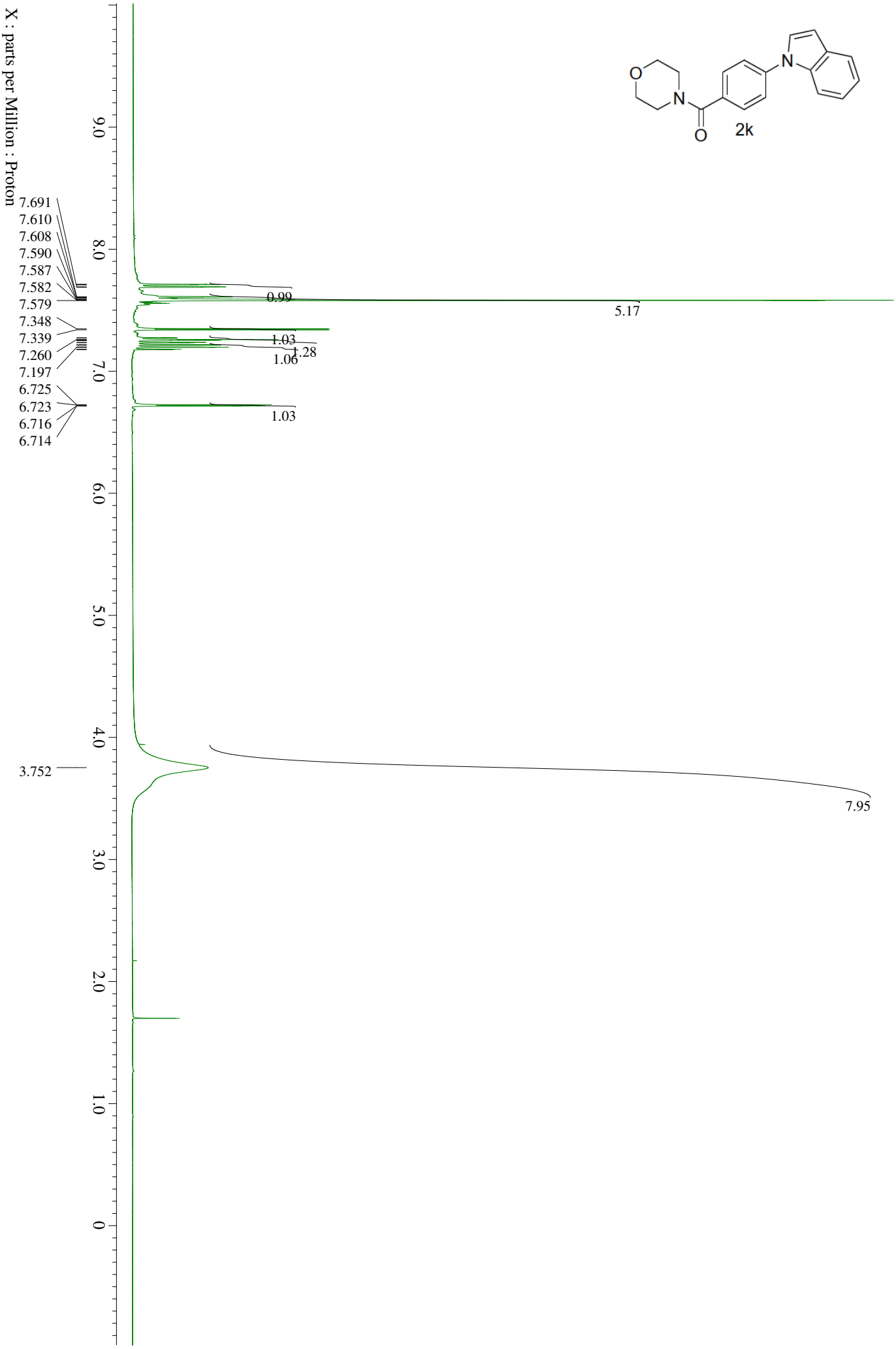
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.438
141.444
135.695
129.345
127.857
122.356
121.117
120.373
110.762
103.535
102.705
98.434
77.315
77.000
76.685
55.547
MeO
N
OMe
2i


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.766
7.758
7.747
7.736
7.680
7.661
7.659
7.406
7.396
7.323
7.321
7.304
7.282
7.279
7.262
7.260
7.197
7.181
6.784
6.774
3.997
2.01
1.02
1.00
1.02
1.12
2.01
0.98
3.00
MeO
N
F3C
2j

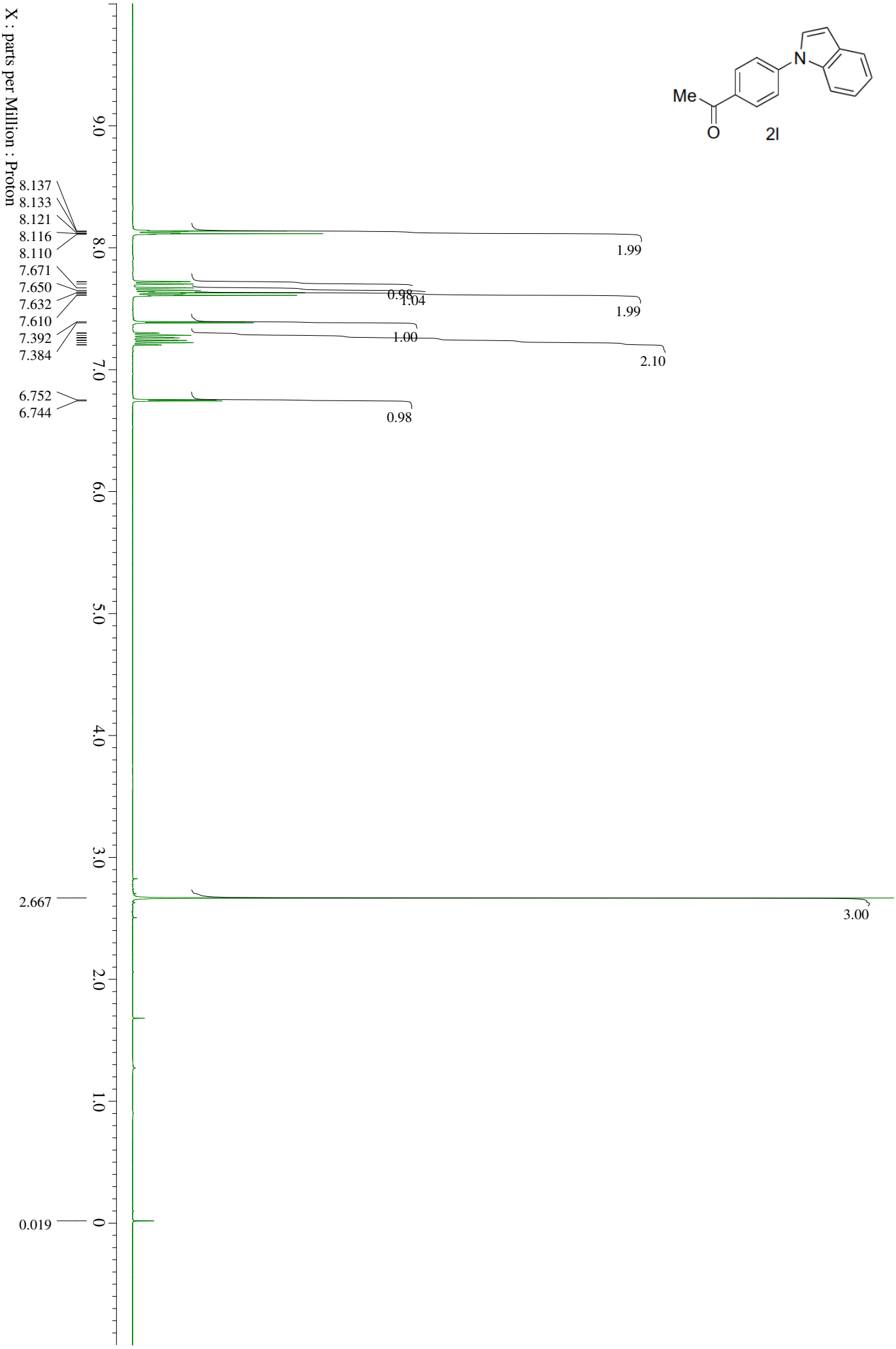

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
158.505
144.171
135.417
129.652
128.487
128.436
128.384
128.332
127.435
124.806
122.898
122.094
121.434
120.949
114.989
110.421
107.626
104.749
77.320
77.000
76.680
56.129
MeO
N
F3C
2j


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.691
7.610
7.608
7.590
7.587
7.582
7.579
7.348
7.339
7.260
7.197
6.725
6.723
6.716
6.714
3.752
0.99
1.03
1.06
1.28
1.03
5.17
7.95
O
N
O
N
2k

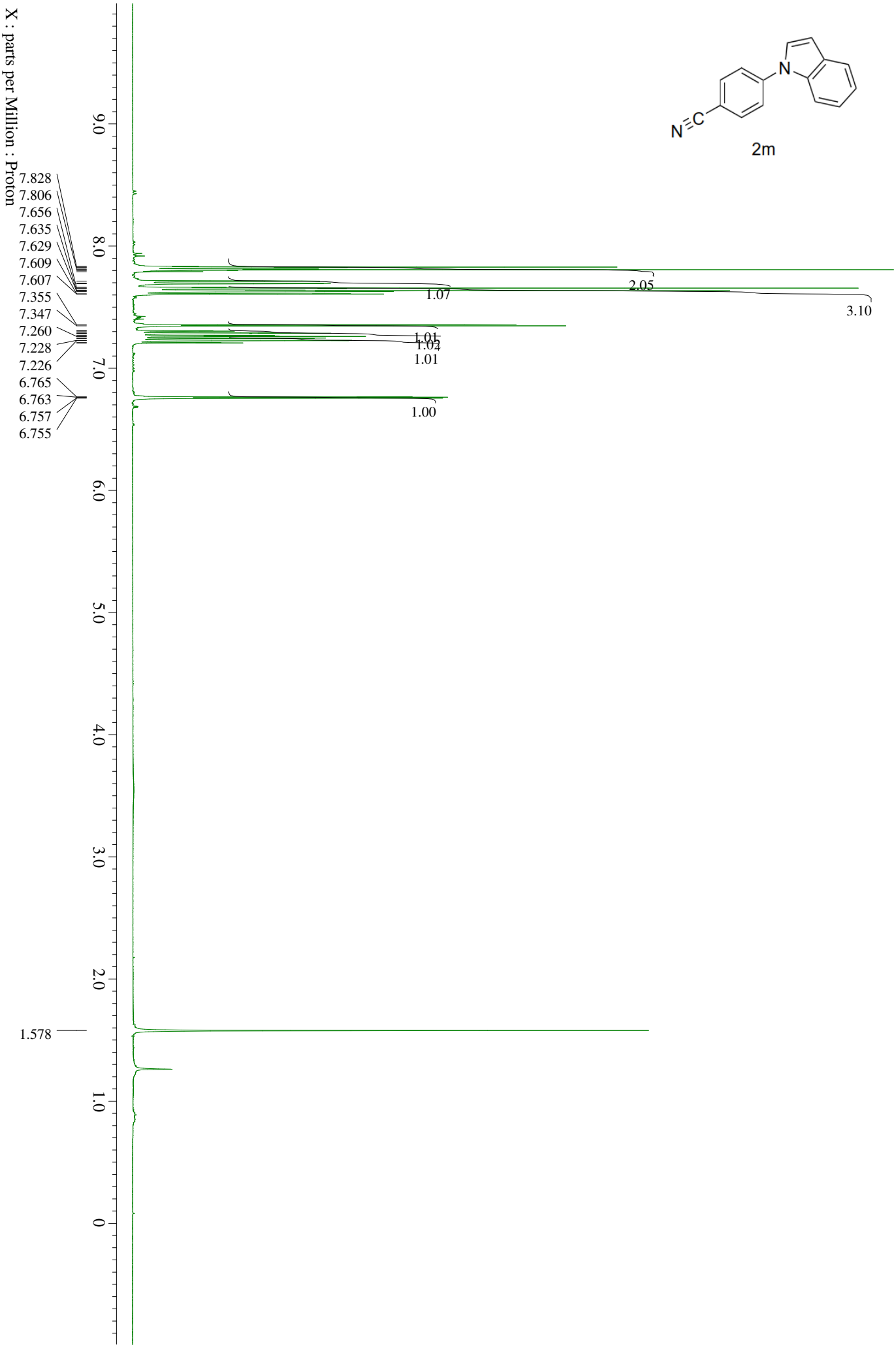
X : parts per Million : aron13

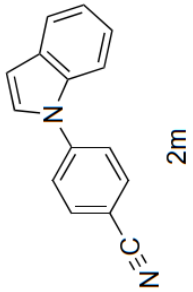
169.590
141.139
135.495
132.949
129.497
128.782
127.476
123.920
122.680
121.279
120.726
110.352
104.412
77.315
77.000
76.685
66.865
48.206
42.666

210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.137
8.133
8.121
8.116
8.110
7.671
7.650
7.632
7.610
7.392
7.384
6.752
6.744
2.667
0.019
1.99
0.98
1.04
1.99
1.00
2.10
0.98
3.00
Me
O
N
2l

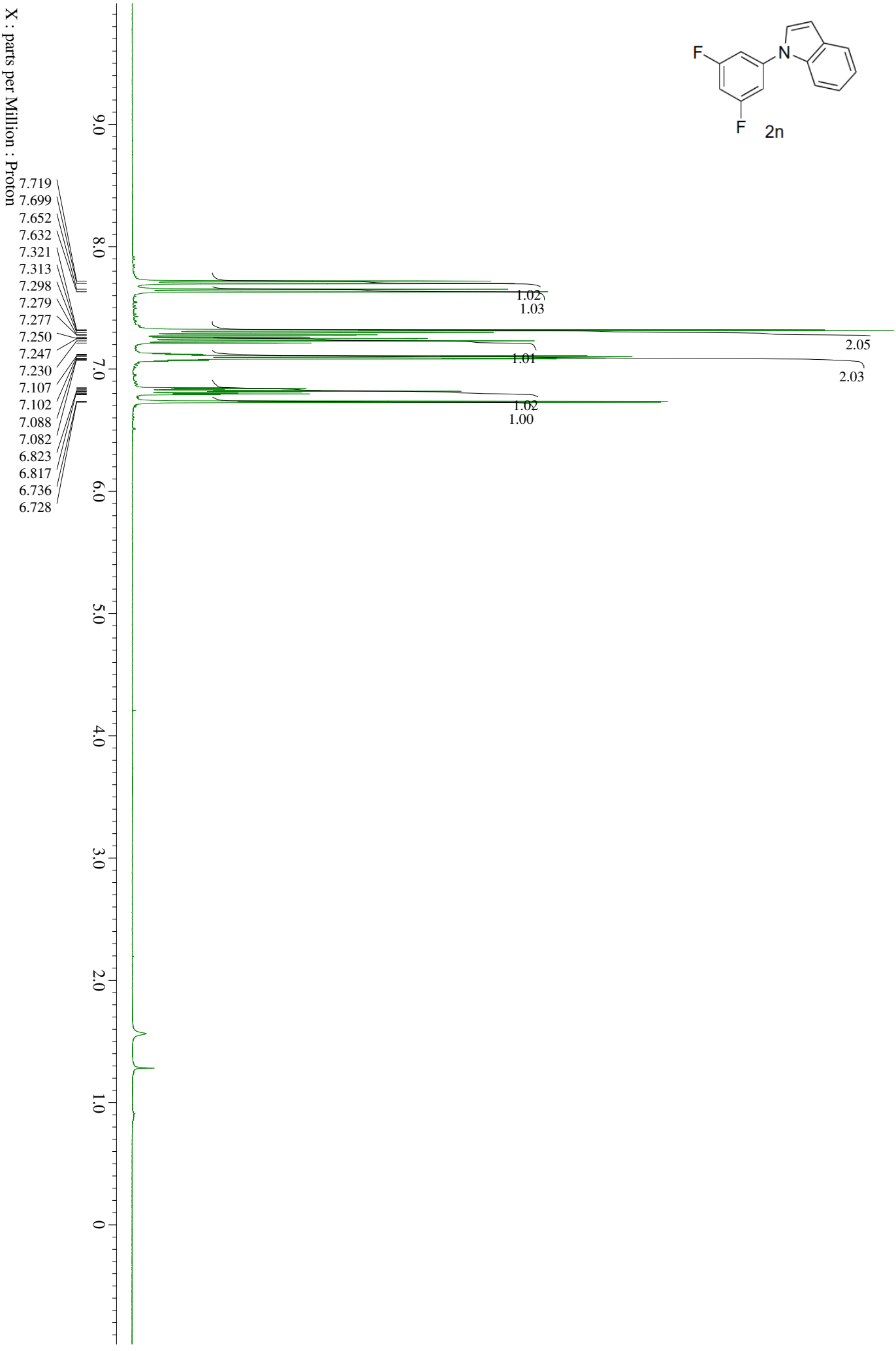
X : parts per Million : aron13
196.831
143.780
135.342
134.503
130.041
129.783
127.314
123.262
122.890
121.393
121.002
110.543
105.032
77.315
77.000
76.676
26.591
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
Me
O
N
2l


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.828
7.806
7.656
7.635
7.629
7.609
7.607
7.355
7.347
7.260
7.228
7.226
6.765
6.763
6.757
6.755
1.578
1.07
2.05
3.10
1.01
1.02
1.01
1.00
N
N≡C
2m

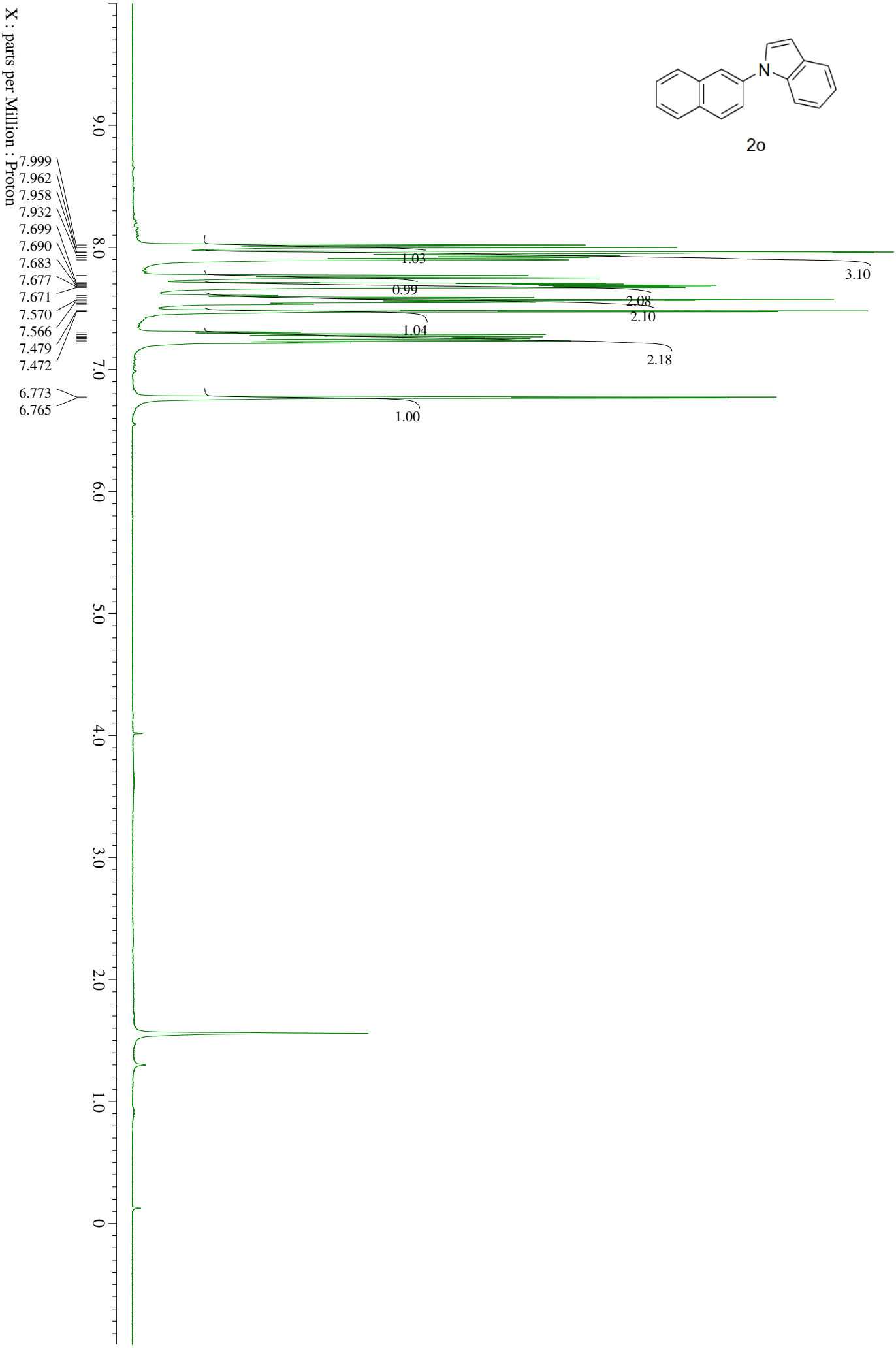


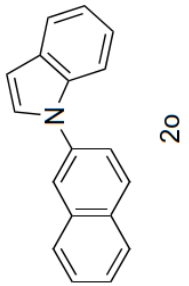
2m

X : parts per Million : aron13


X : parts per Million : Proton
7.719
7.699
7.652
7.632
7.321
7.313
7.298
7.279
7.277
7.250
7.247
7.230
7.107
7.102
7.088
7.082
6.823
6.817
6.736
6.728
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.02
1.03
2.05
1.01
2.03
1.02
1.00
F
N
F
2n

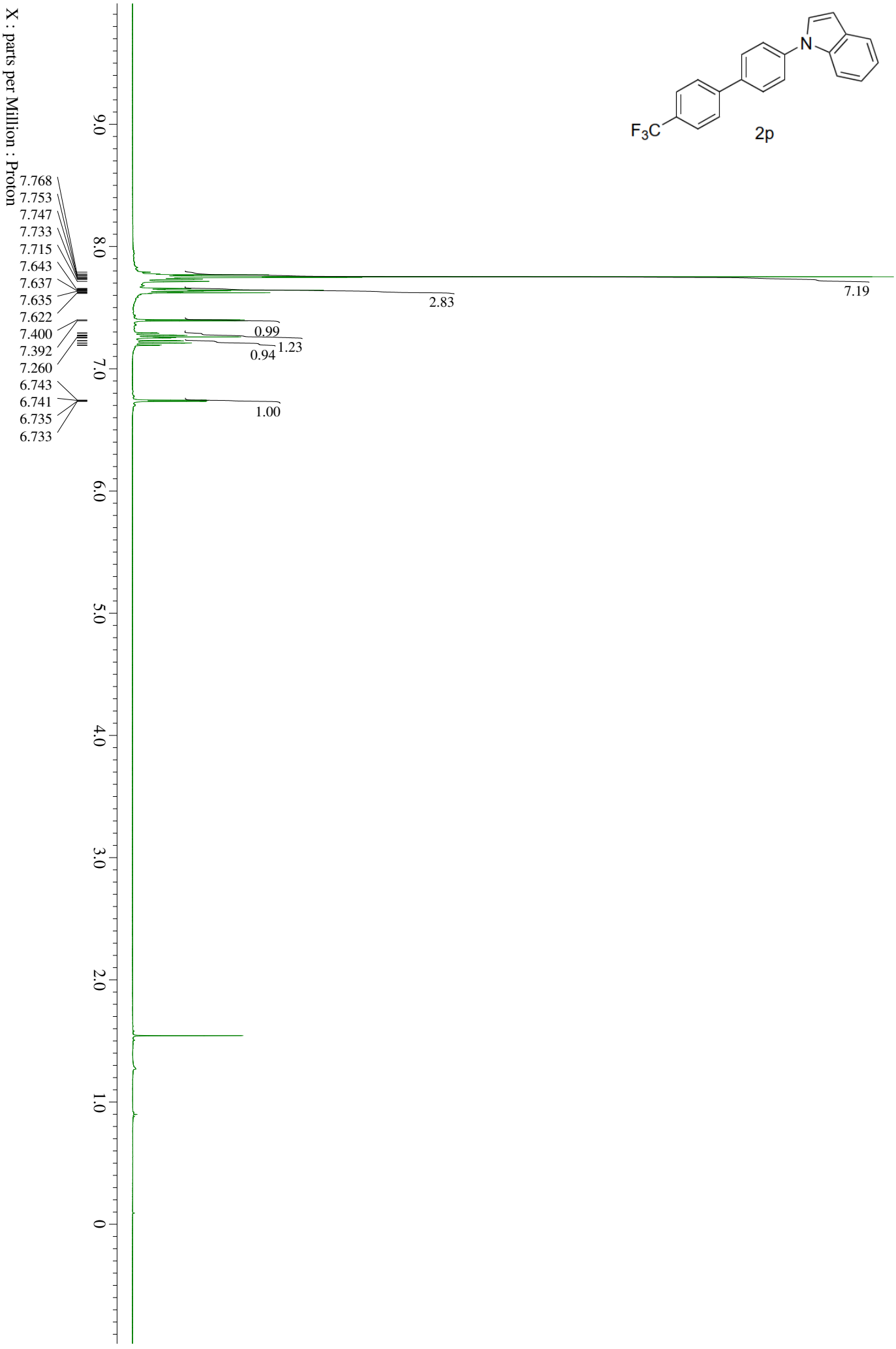
X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.775
164.630
162.289
162.145
142.037
141.913
141.789
135.241
129.632
127.250
123.022
121.423
121.073
110.328
107.183
107.100
106.987
106.904
104.997
101.852
101.604
101.346
77.309
77.000
76.680
F
N
F
2n

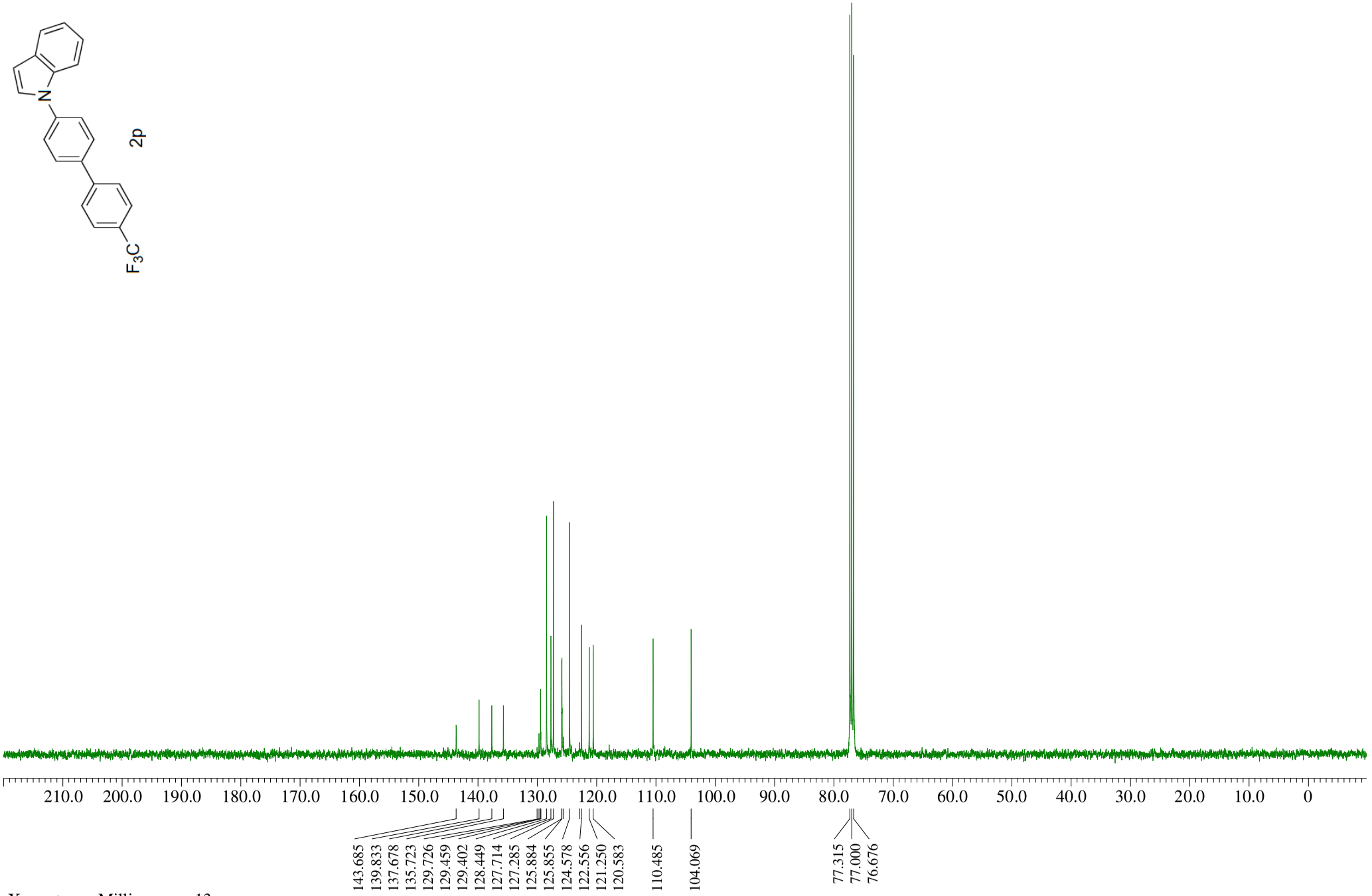

X : parts per Million : Proton
7.999
7.962
7.958
7.932
7.699
7.690
7.683
7.677
7.671
7.570
7.566
7.479
7.472
6.773
6.765
1.03
0.99
1.04
1.00
2.08
2.10
2.18
3.10
N
2o
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0



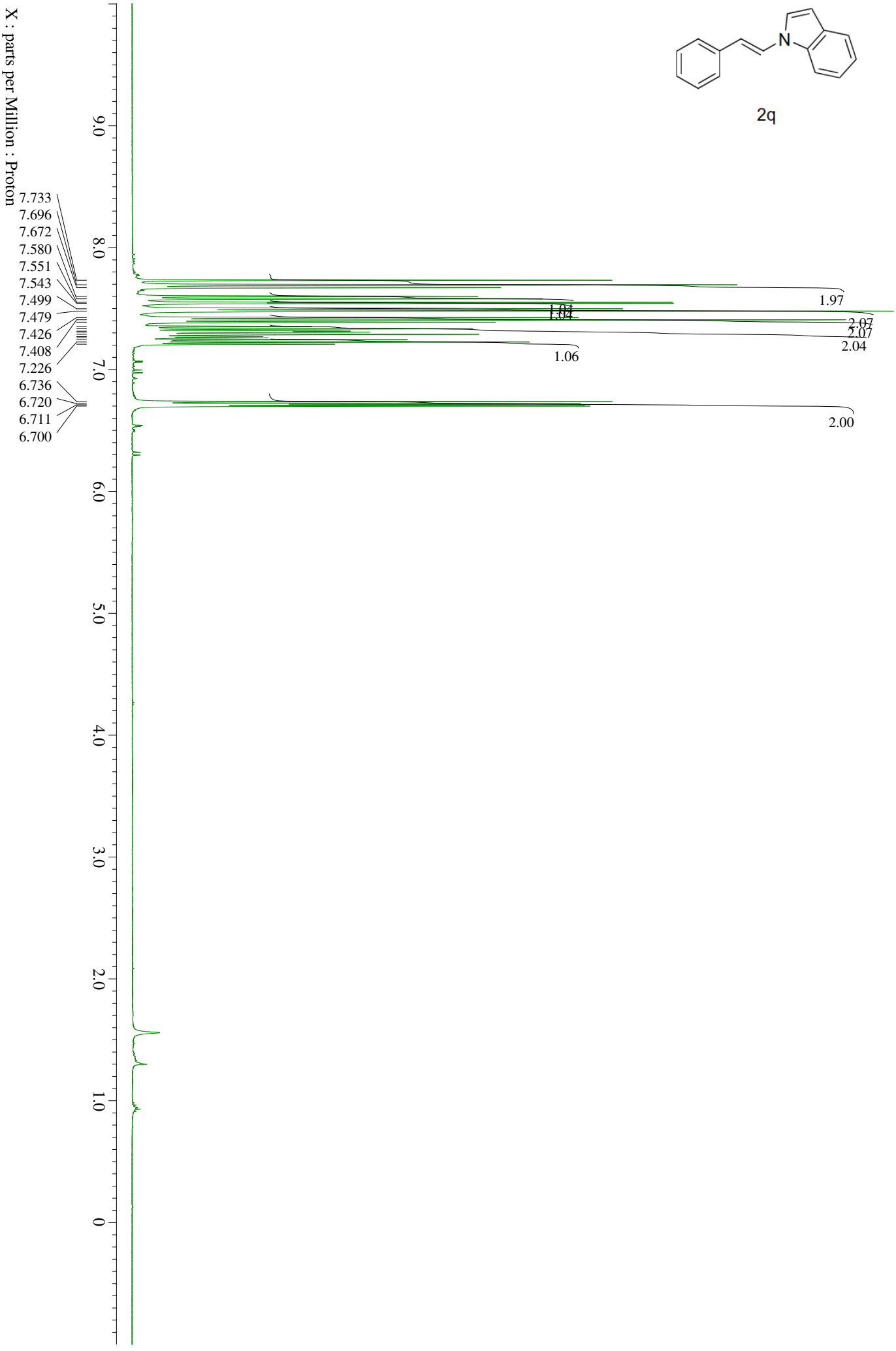
2o

X : parts per Million : aron13


X : parts per Million : Proton
7.768
7.753
7.747
7.733
7.715
7.643
7.637
7.635
7.622
7.400
7.392
7.260
6.743
6.741
6.735
6.733
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.83
7.19
0.99
1.23
0.94
1.00
N
F3C
2p

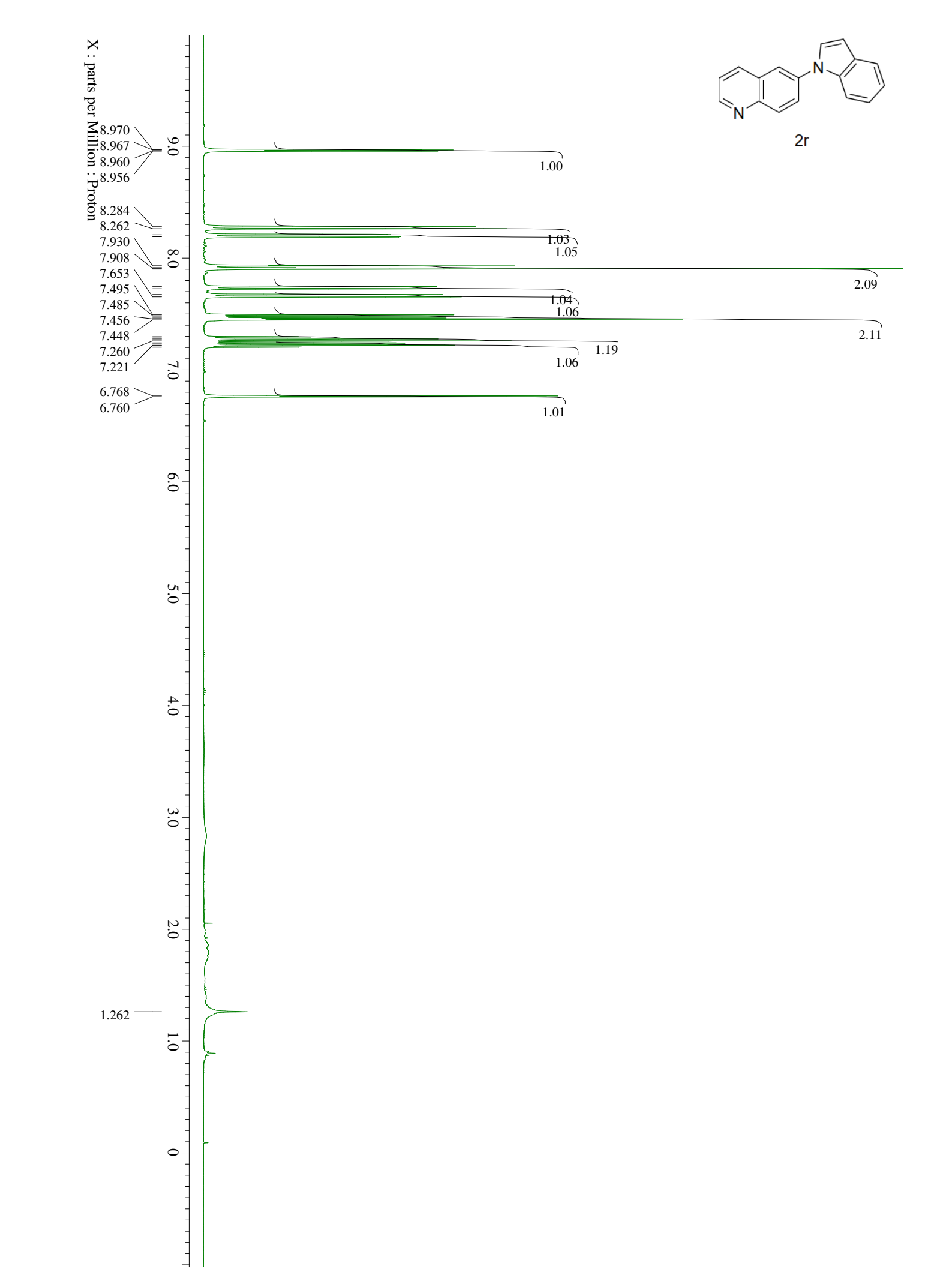


X : parts per Million : aron13


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.733
7.696
7.672
7.580
7.551
7.543
7.499
7.479
7.426
7.408
7.226
6.736
6.720
6.711
6.700
1.97
1.04
2.07
2.07
2.04
1.06
2.00
N
2q

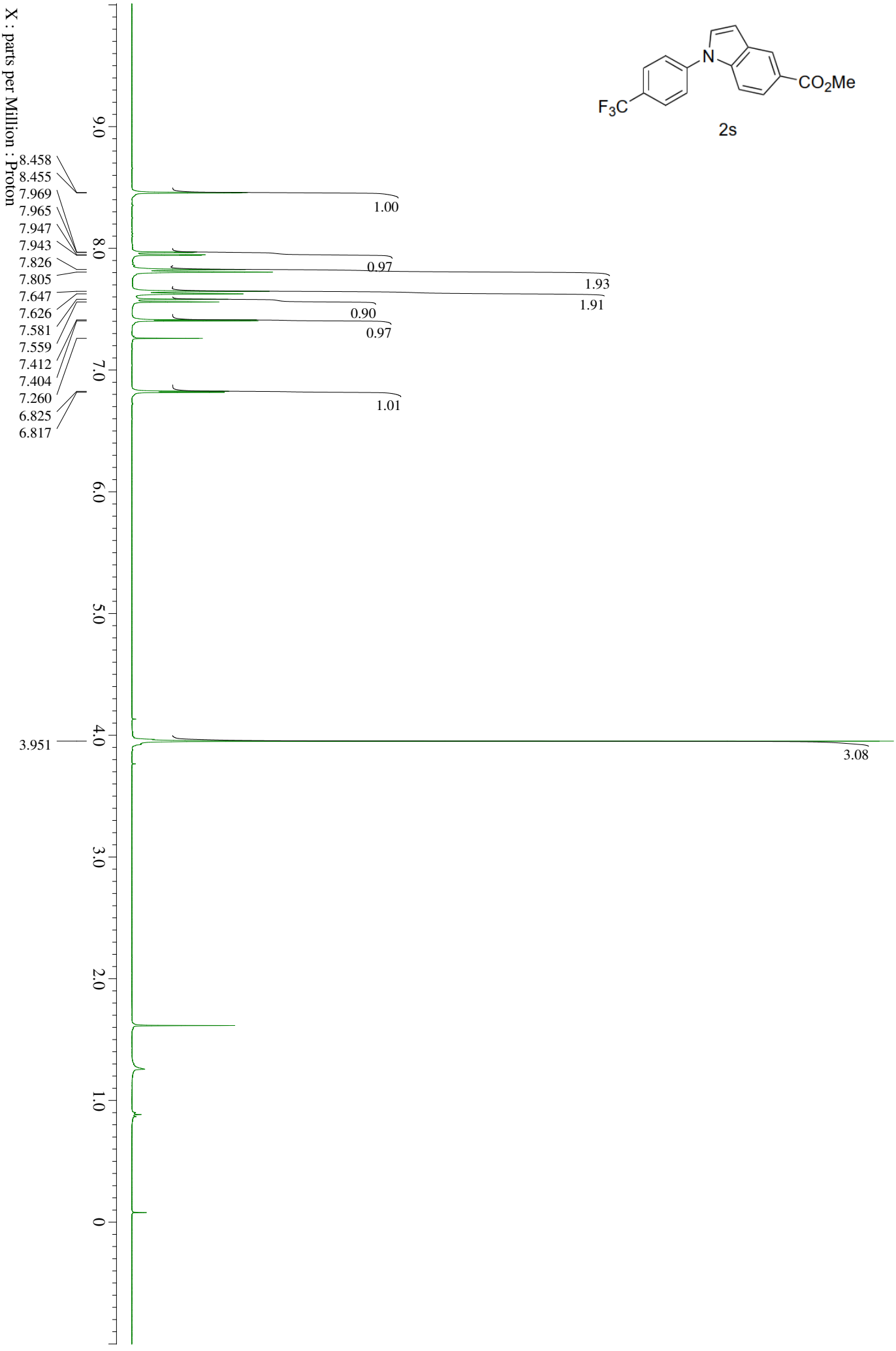
X : parts per Million : aron13

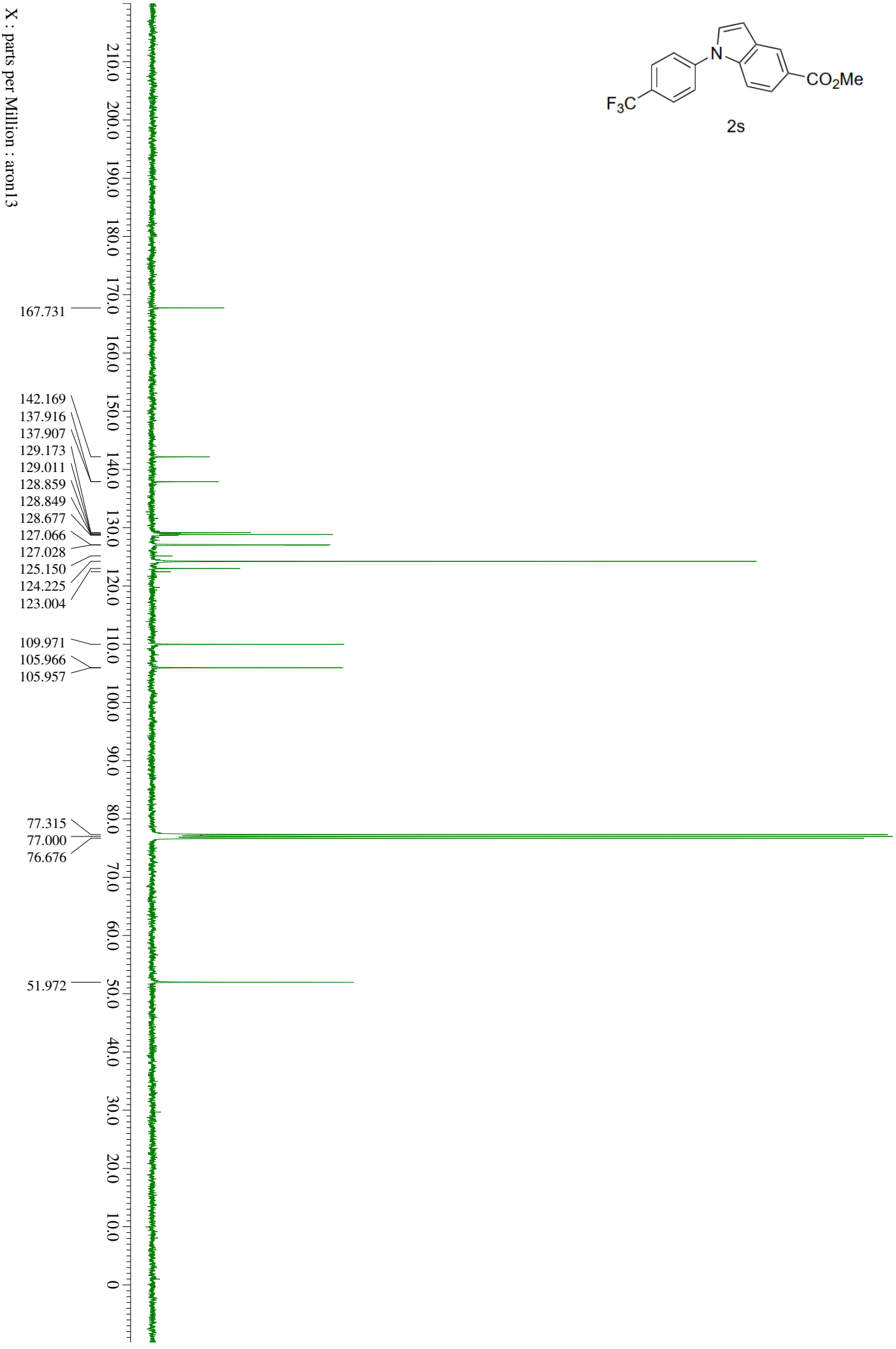
2q

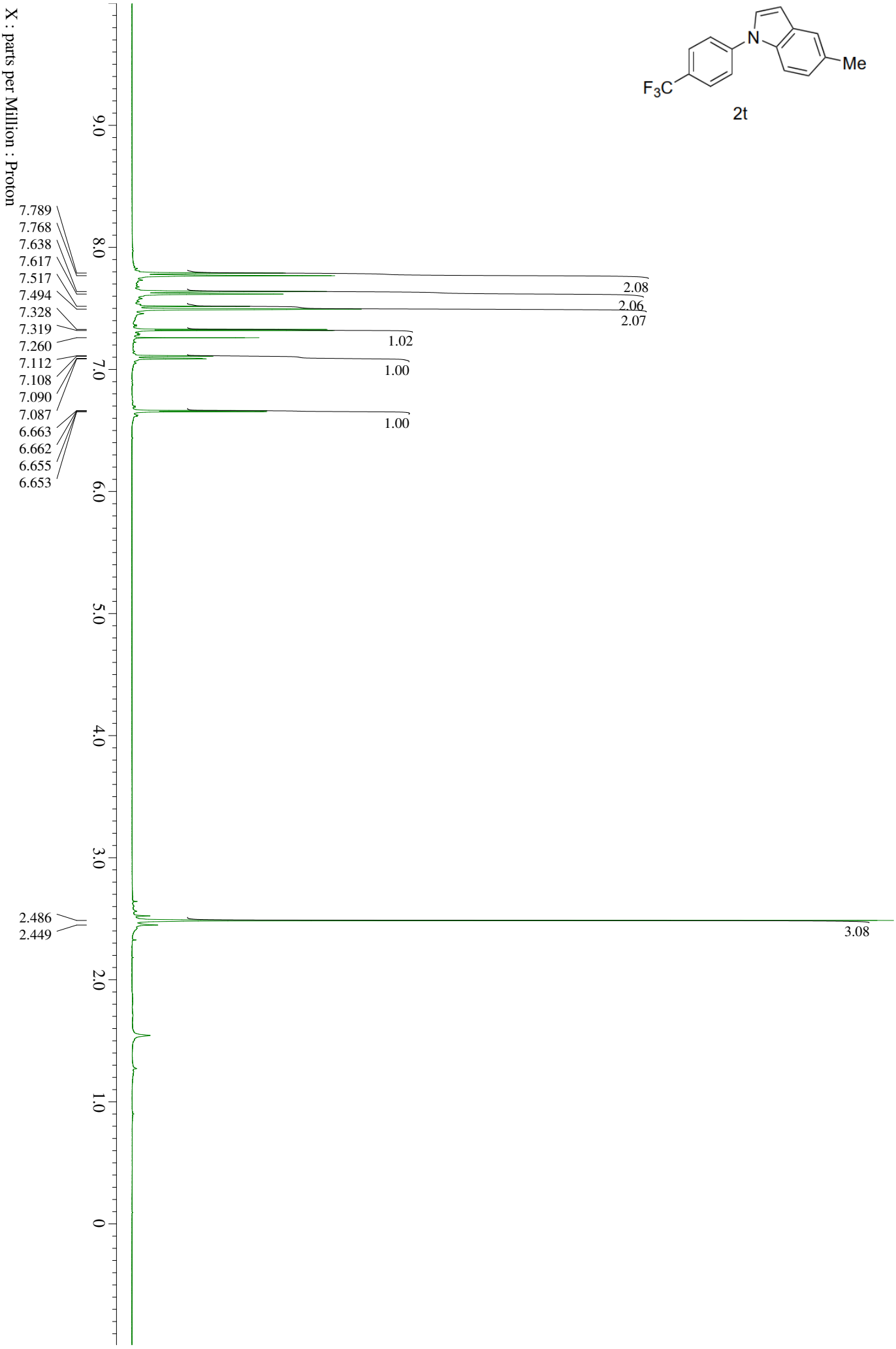

X : parts per Million : Proton
8.970
8.967
8.960
8.956
8.284
8.262
7.930
7.908
7.653
7.495
7.485
7.456
7.448
7.260
7.221
6.768
6.760
1.262
1.00
1.03
1.05
2.09
1.04
1.06
2.11
1.19
1.06
1.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
N
N
2r

X : parts per Million : aron13

2r


X : parts per Million : Proton
8.458
8.455
7.969
7.965
7.947
7.943
7.826
7.805
7.647
7.626
7.581
7.559
7.412
7.404
7.260
6.825
6.817
3.951
1.00
0.97
1.93
1.91
0.90
0.97
1.01
3.08
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
N
CO2Me
F3C
2s

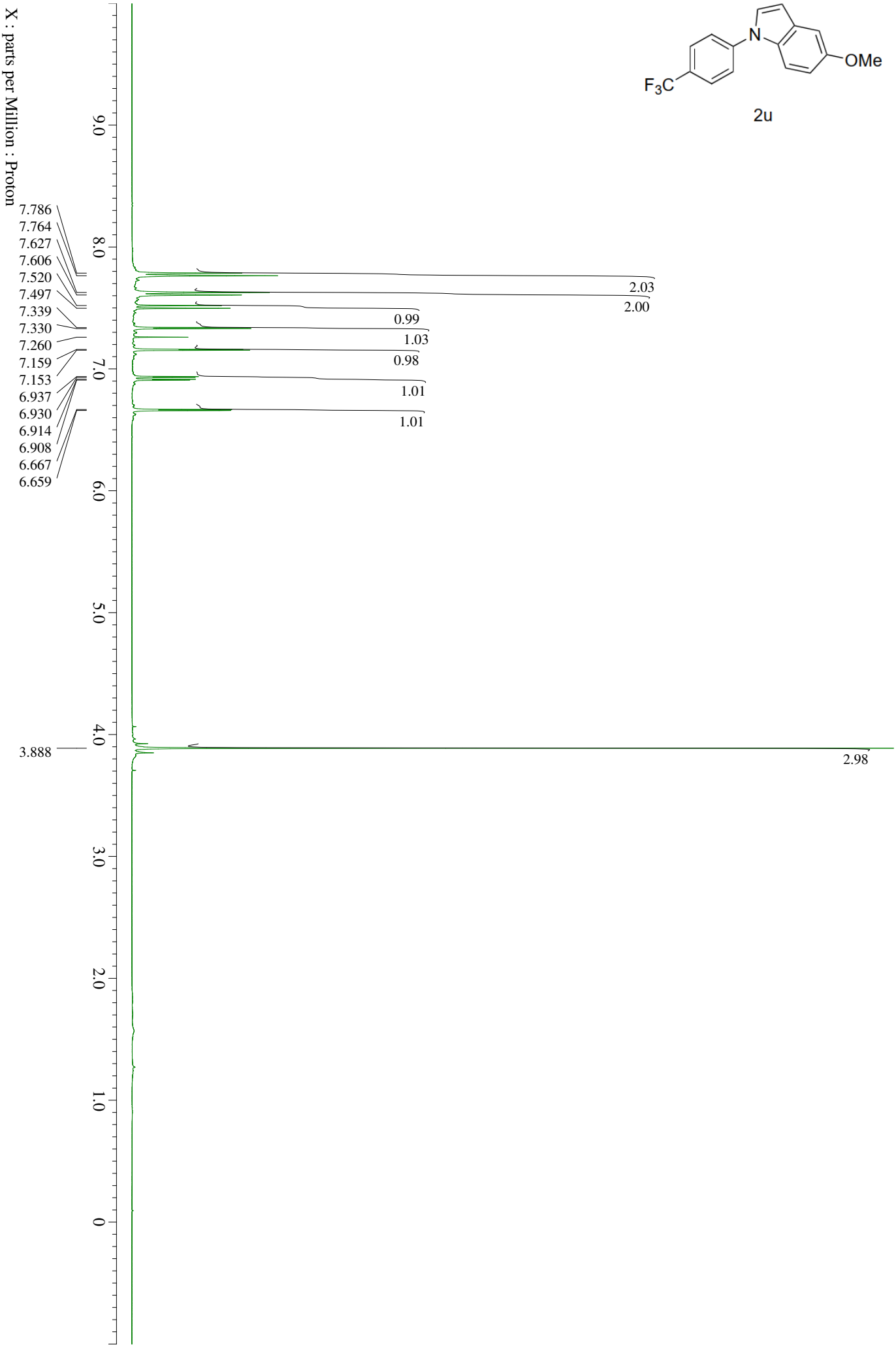

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
167.731
142.169
137.916
137.907
129.173
129.011
128.859
128.849
128.677
127.066
127.028
125.150
124.225
123.004
109.971
105.966
105.957
77.315
77.000
76.676
51.972
N
F3C
CO2Me
2s


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.789
7.768
7.638
7.617
7.517
7.494
7.328
7.319
7.260
7.112
7.108
7.090
7.087
6.663
6.662
6.655
6.653
2.486
2.449
2.08
2.06
2.07
1.02
1.00
1.00
3.08
N
Me
F3C
2t

X : parts per Million : aron13

2t

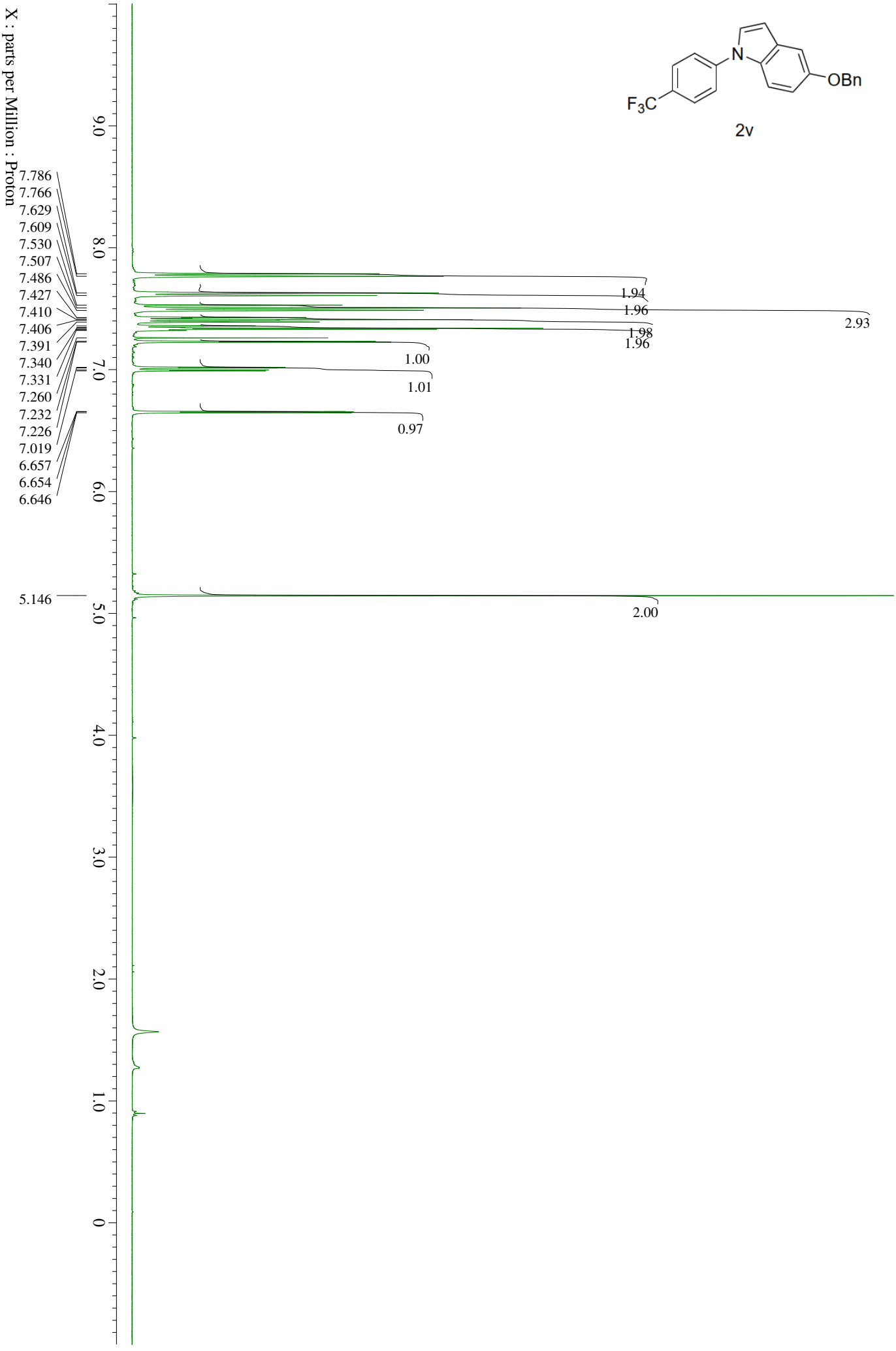
142.941
133.778
130.365
130.012
128.344
128.020
127.686
127.352
126.885
126.847
125.331
124.463
123.586
122.623
121.069
119.944
110.028
104.488
77.315
77.000
76.676
21.309

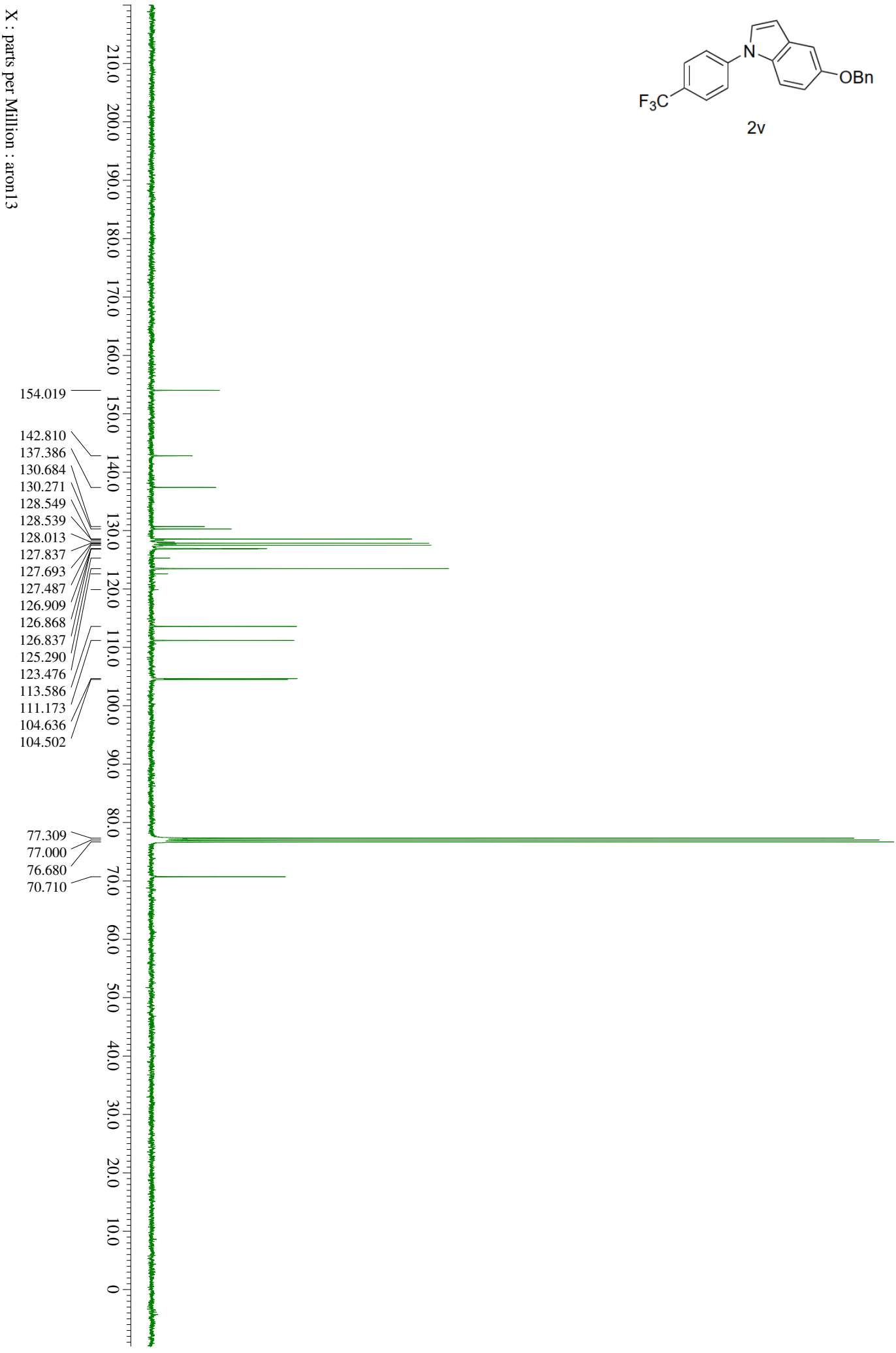

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.786
7.764
7.627
7.606
7.520
7.497
7.339
7.330
7.260
7.159
7.153
6.937
6.930
6.914
6.908
6.667
6.659
3.888
2.03
2.00
0.99
1.03
0.98
1.01
1.01
2.98
N
OMe
F3C
2u

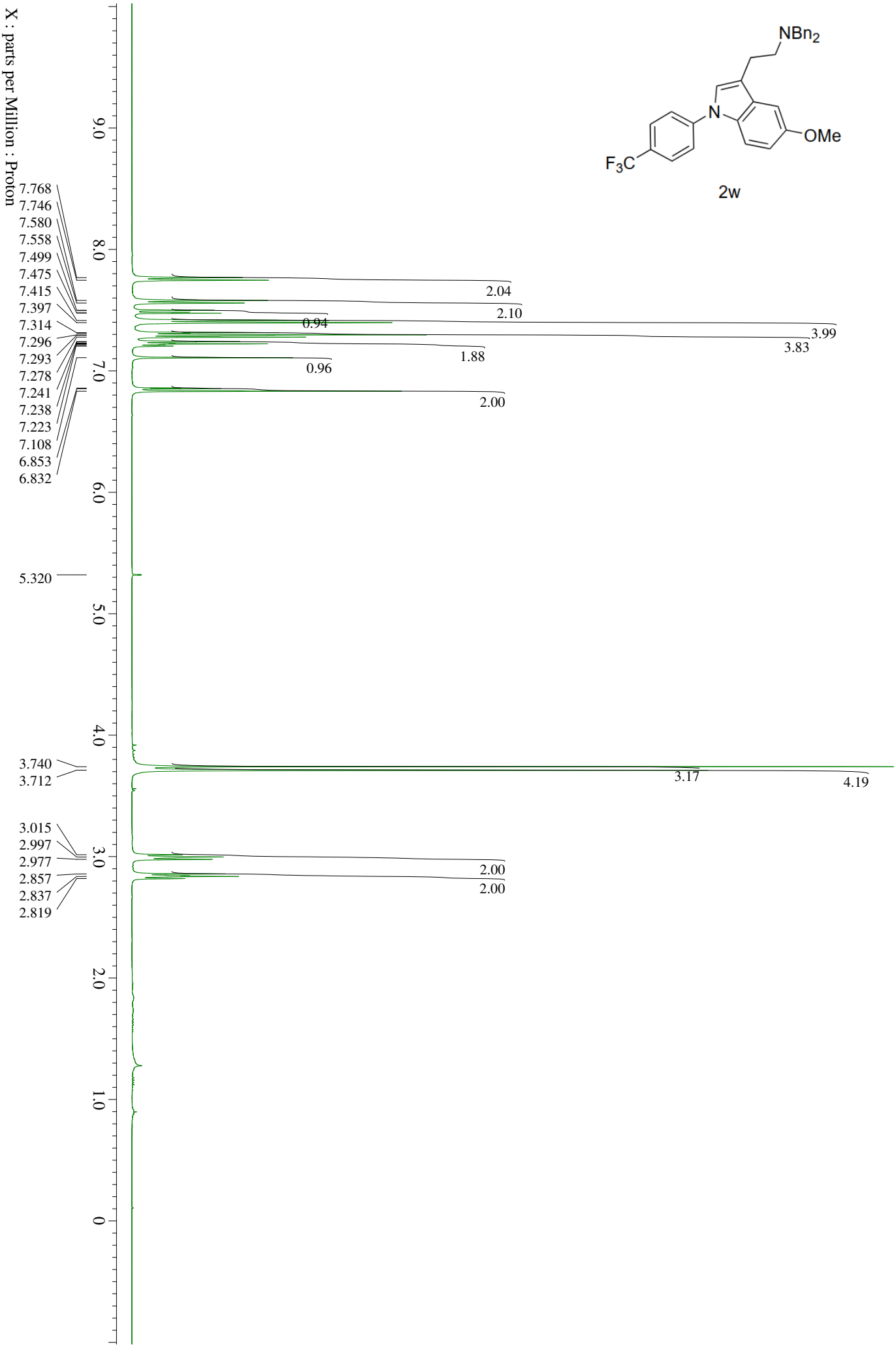
X : parts per Million : aron13

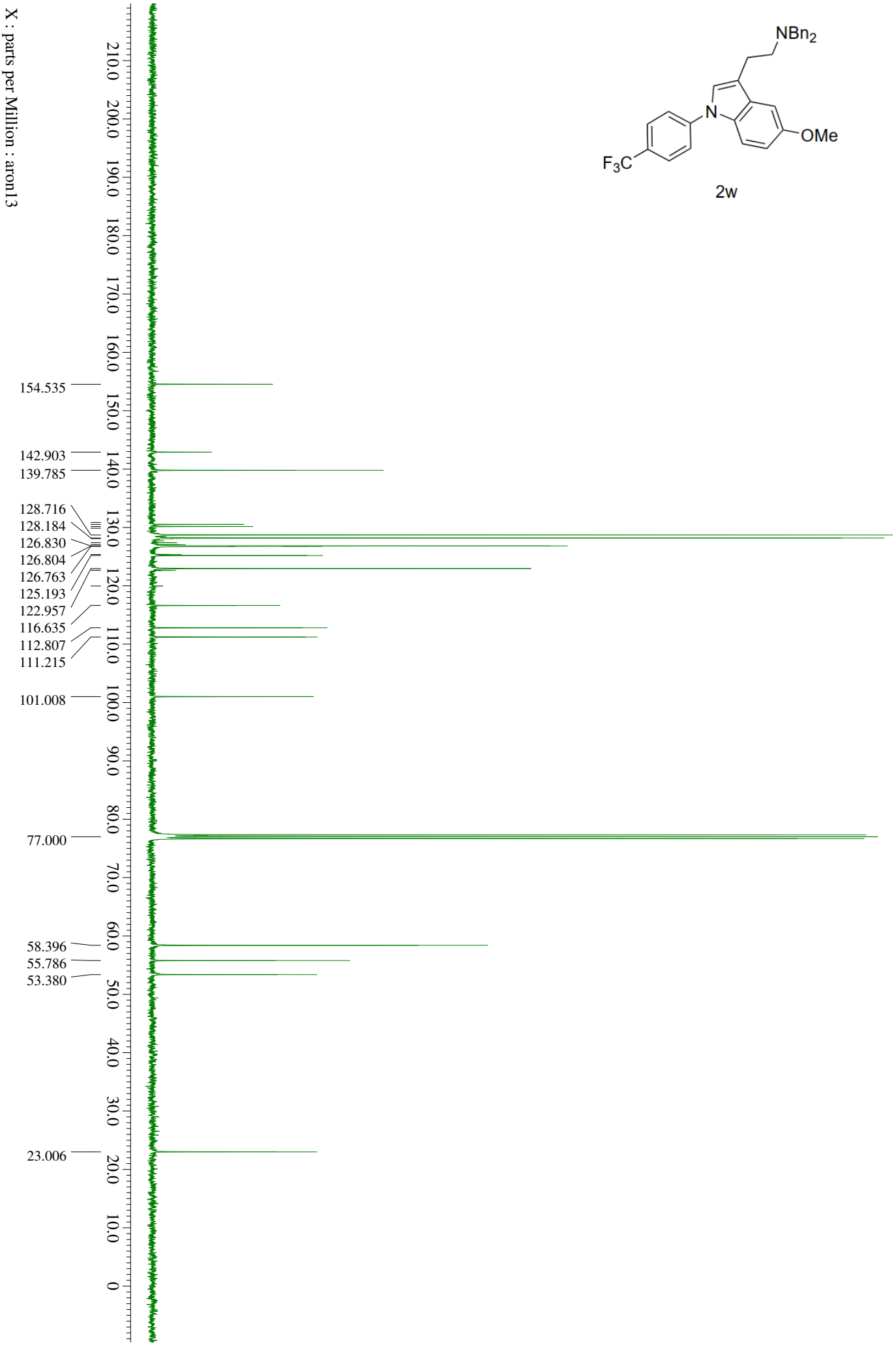
2u

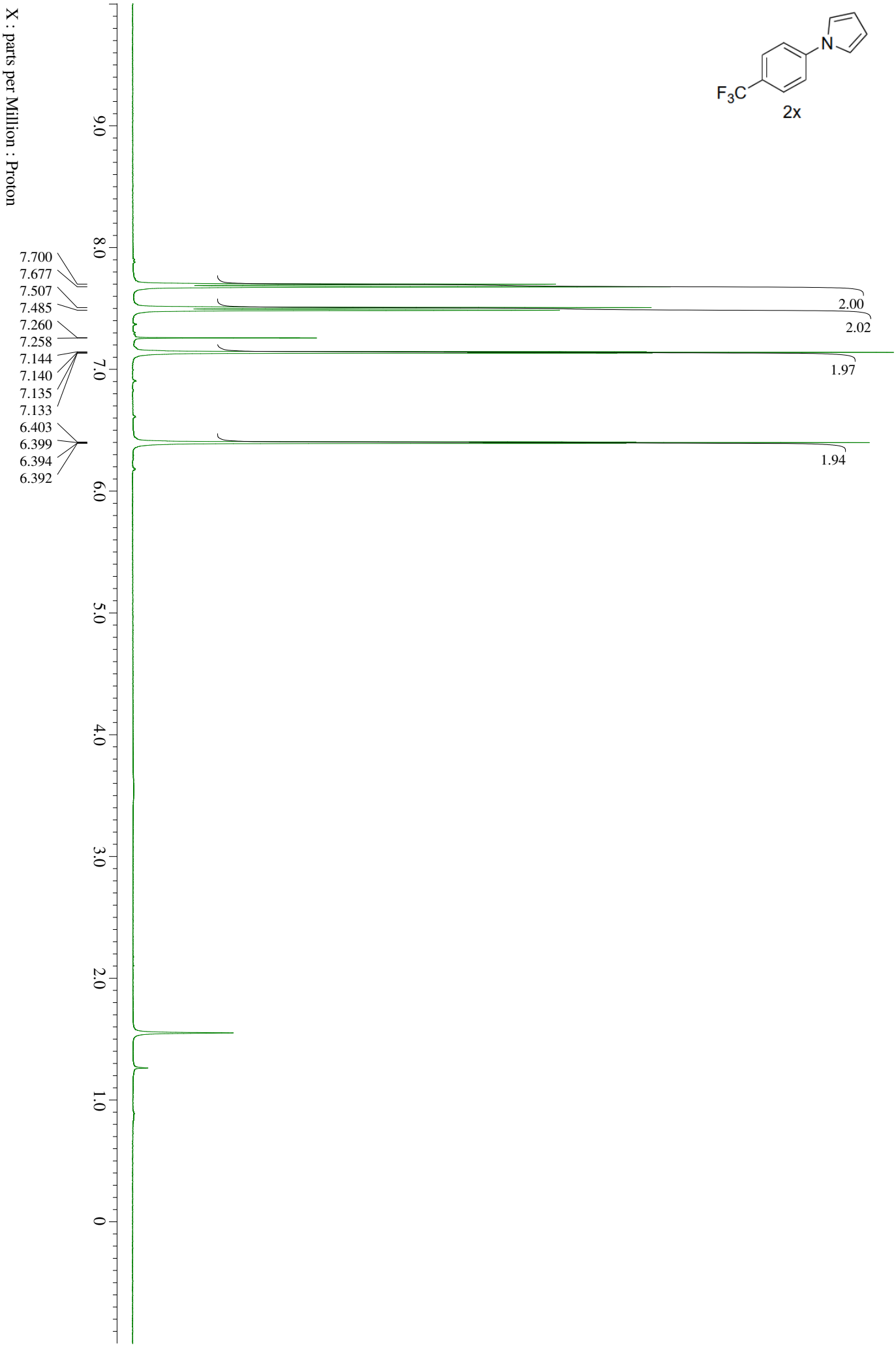
154.884
142.849
130.335
127.796
126.908
126.871
126.836
123.457
112.885
111.176
104.597
102.960
77.318
77.000
76.682
55.782


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.786
7.766
7.629
7.609
7.530
7.507
7.486
7.427
7.410
7.406
7.391
7.340
7.331
7.260
7.232
7.226
7.019
6.657
6.654
6.646
5.146
1.94
1.96
2.93
1.98
1.96
1.00
1.01
0.97
2.00
N
OBn
F3C
2v


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
154.019
142.810
137.386
130.684
130.271
128.549
128.539
128.013
127.837
127.693
127.487
126.909
126.868
126.837
125.290
123.476
113.586
111.173
104.636
104.502
77.309
77.000
76.680
70.710
N
OBn
F3C
2v

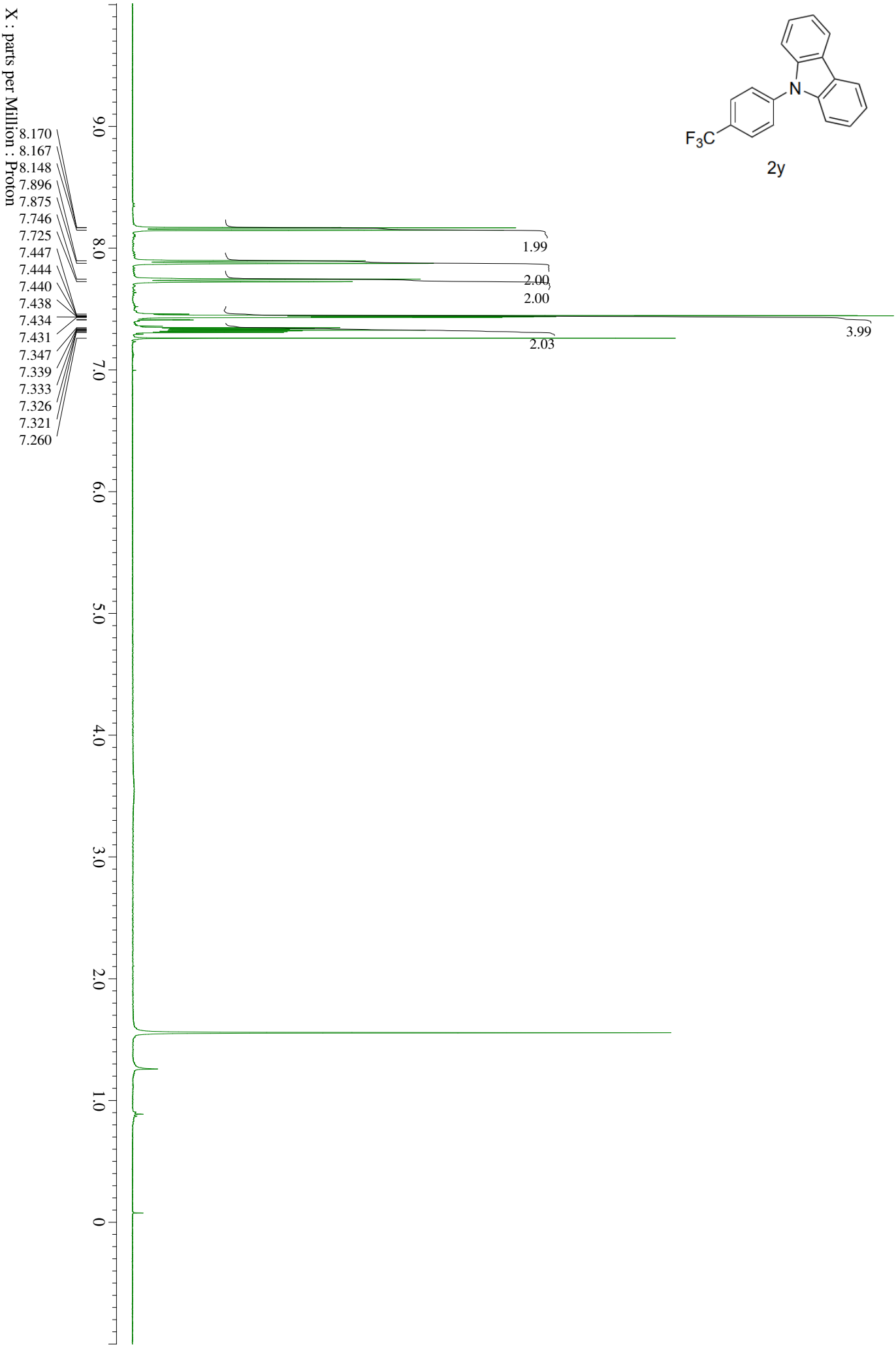

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.768
7.746
7.580
7.558
7.499
7.475
7.415
7.397
7.314
7.296
7.293
7.278
7.241
7.238
7.223
7.108
6.853
6.832
5.320
3.740
3.712
3.015
2.997
2.977
2.857
2.837
2.819
2.04
2.10
0.94
3.99
3.83
1.88
0.96
2.00
3.17
4.19
2.00
2.00
NBn2
N
OMe
F3C
2w


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
154.535
142.903
139.785
128.716
128.184
126.830
126.804
126.763
125.193
122.957
116.635
112.807
111.215
101.008
77.000
58.396
55.786
53.380
23.006
NBn2
N
OMe
F3C
2w


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.700
7.677
7.507
7.485
7.260
7.258
7.144
7.140
7.135
7.133
6.403
6.399
6.394
6.392
2.00
2.02
1.97
1.94
N
F3C
2x

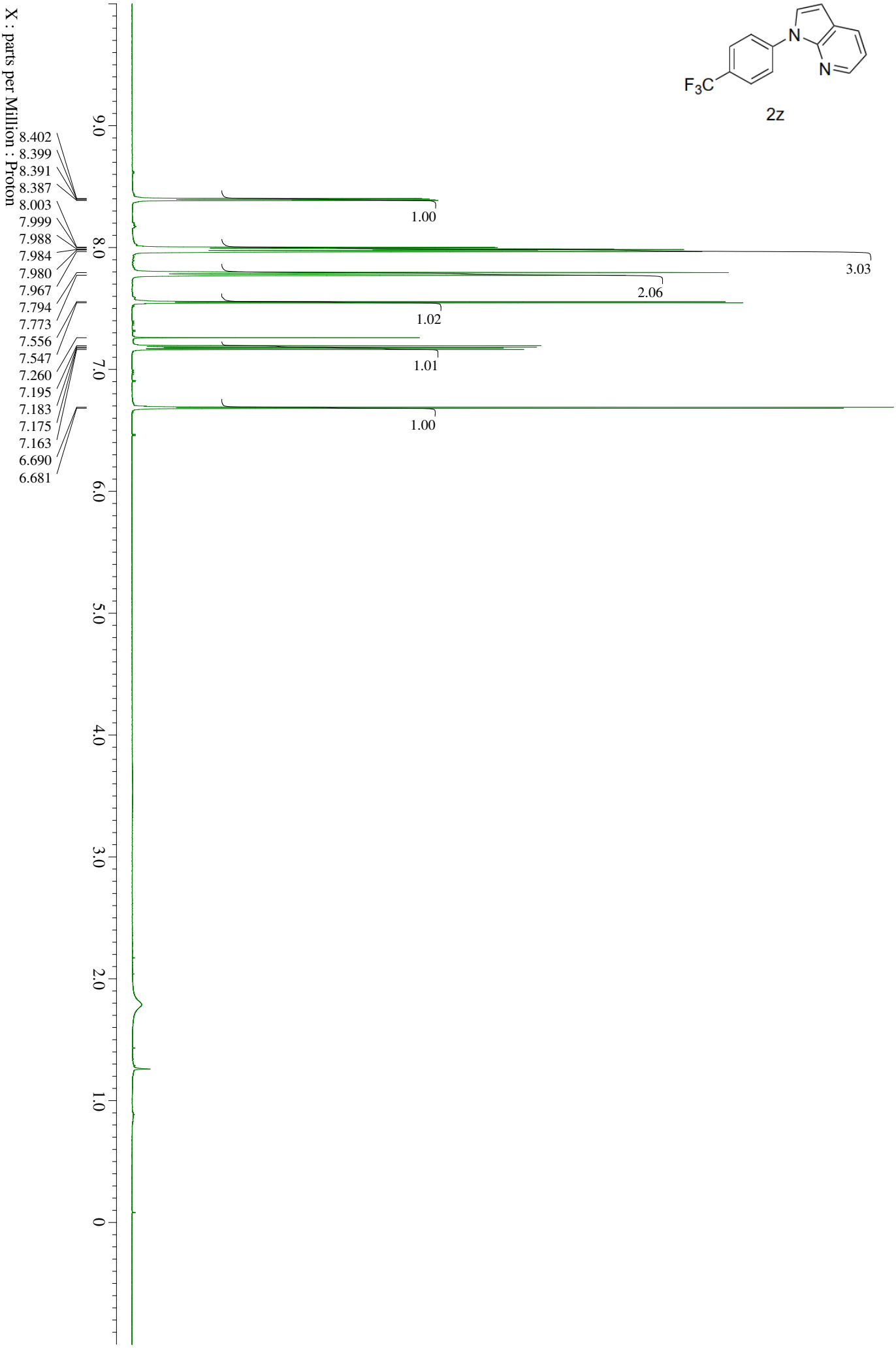
X : parts per Million : aron13

2x


X : parts per Million : Proton
8.170
8.167
8.148
7.896
7.875
7.746
7.725
7.447
7.444
7.440
7.438
7.434
7.431
7.347
7.339
7.333
7.326
7.321
7.260
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.99
2.00
2.00
3.99
2.03
N
F3C
2y

X : parts per Million : aron13

2y

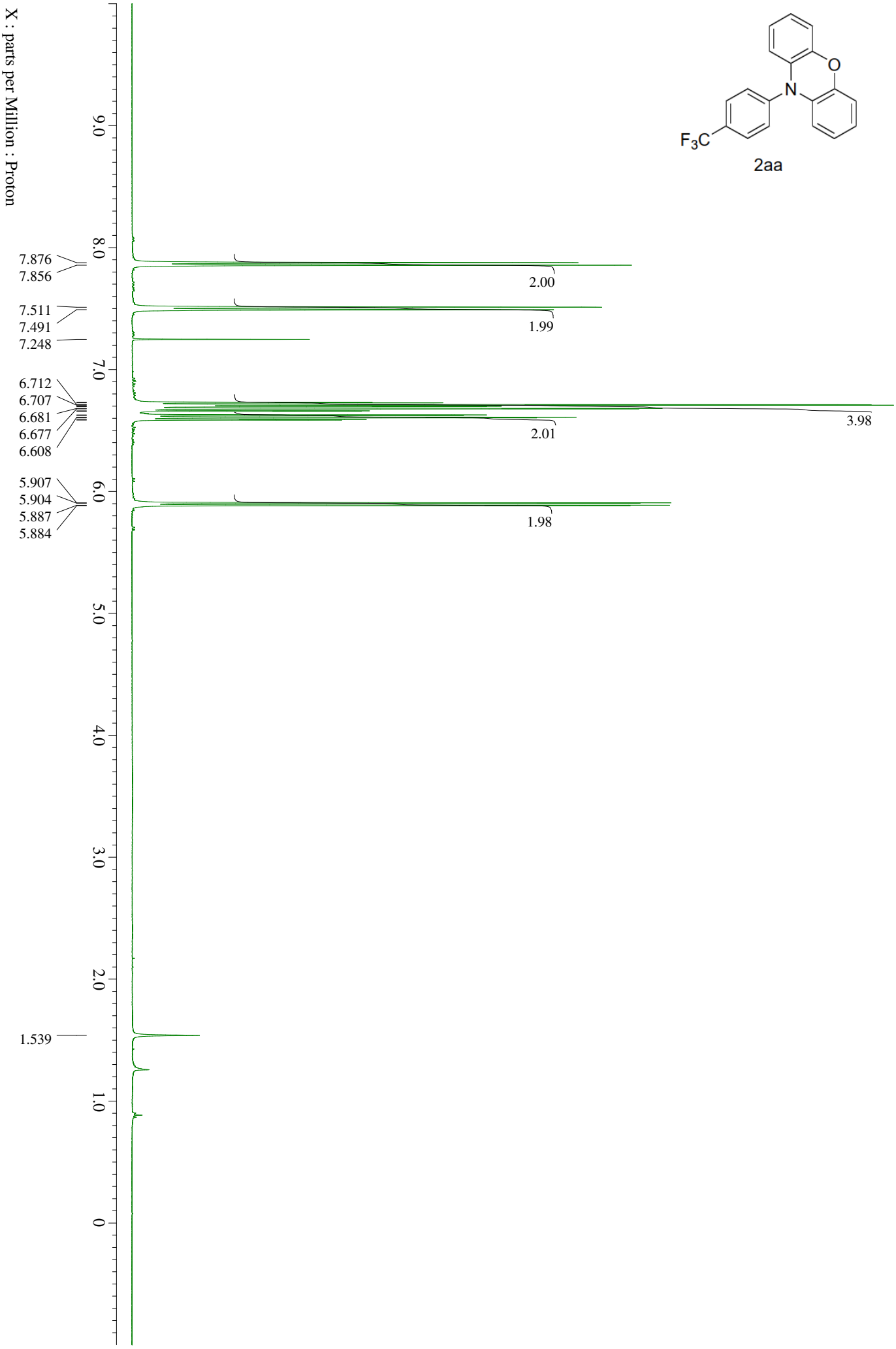

X : parts per Million : Proton
8.402
8.399
8.391
8.387
8.003
7.999
7.988
7.984
7.980
7.967
7.794
7.773
7.556
7.547
7.260
7.195
7.183
7.175
7.163
6.690
6.681
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
3.03
2.06
1.02
1.01
1.00
N
N
F3C
2z

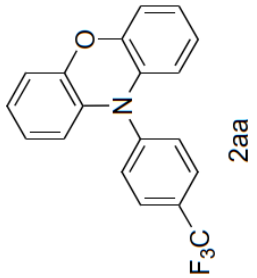
X : parts per Million : aron13

2z

147.430
143.769
141.356
129.384
126.992
126.600
126.569
126.528
123.331
121.908
117.268
102.893
77.320
77.000
76.680

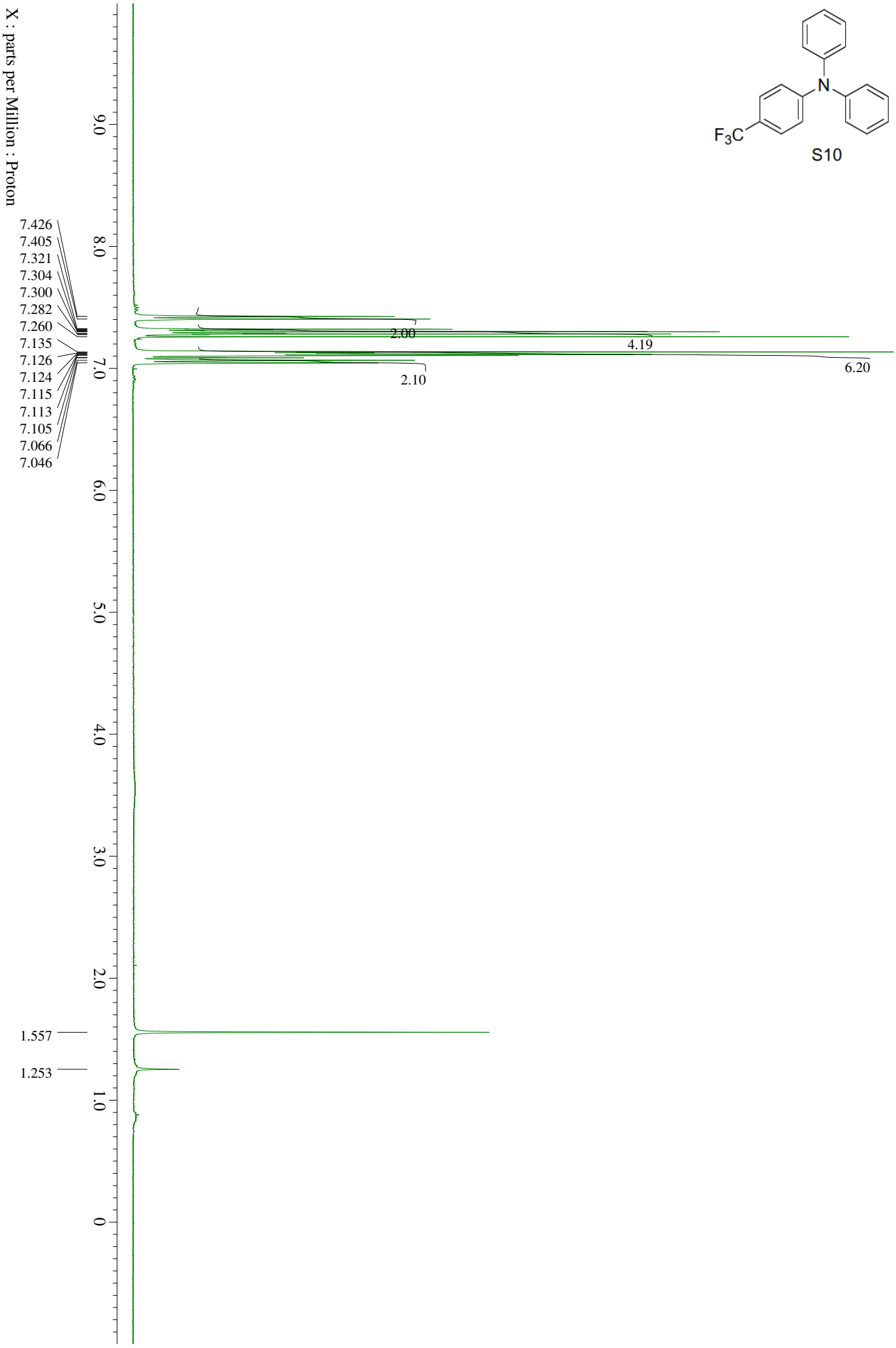
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

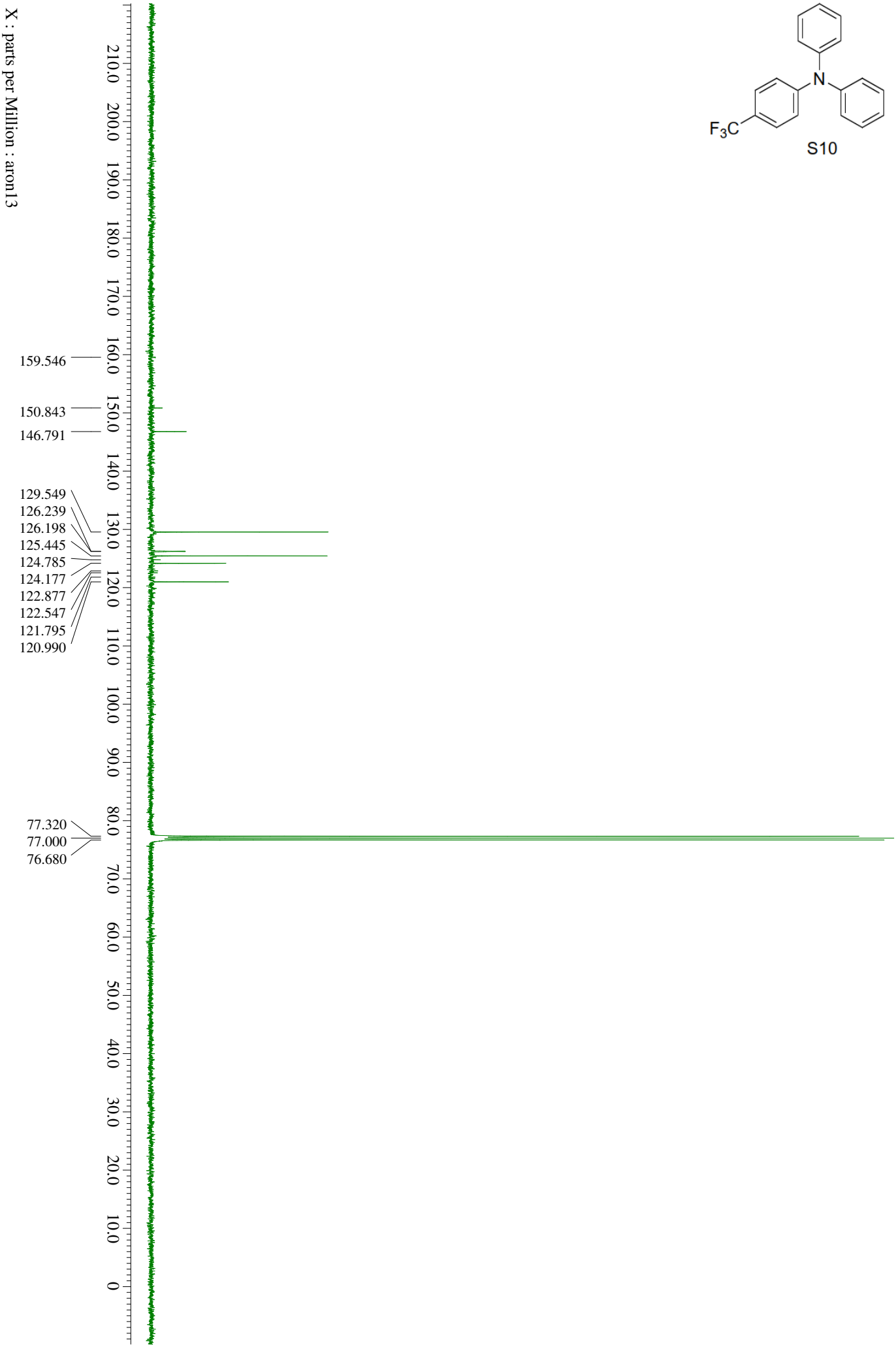

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.876
7.856
7.511
7.491
7.248
6.712
6.707
6.681
6.677
6.608
5.907
5.904
5.887
5.884
1.539
2.00
1.99
3.98
2.01
1.98
O
N
F3C
2aa



2aa

X : parts per Million : aron13


X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.426
7.405
7.321
7.304
7.300
7.282
7.260
7.135
7.126
7.124
7.115
7.113
7.105
7.066
7.046
1.557
1.253
2.00
4.19
2.10
6.20
N
F3C
S10


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.546
150.843
146.791
129.549
126.239
126.198
125.445
124.785
124.177
122.877
122.547
121.795
120.990
77.320
77.000
76.680
N
F3C
S10

X : parts per Million : Proton

2ab

7.562
7.541
7.260
7.195
7.174

5.96

6.00

9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

X : parts per Million : aron13

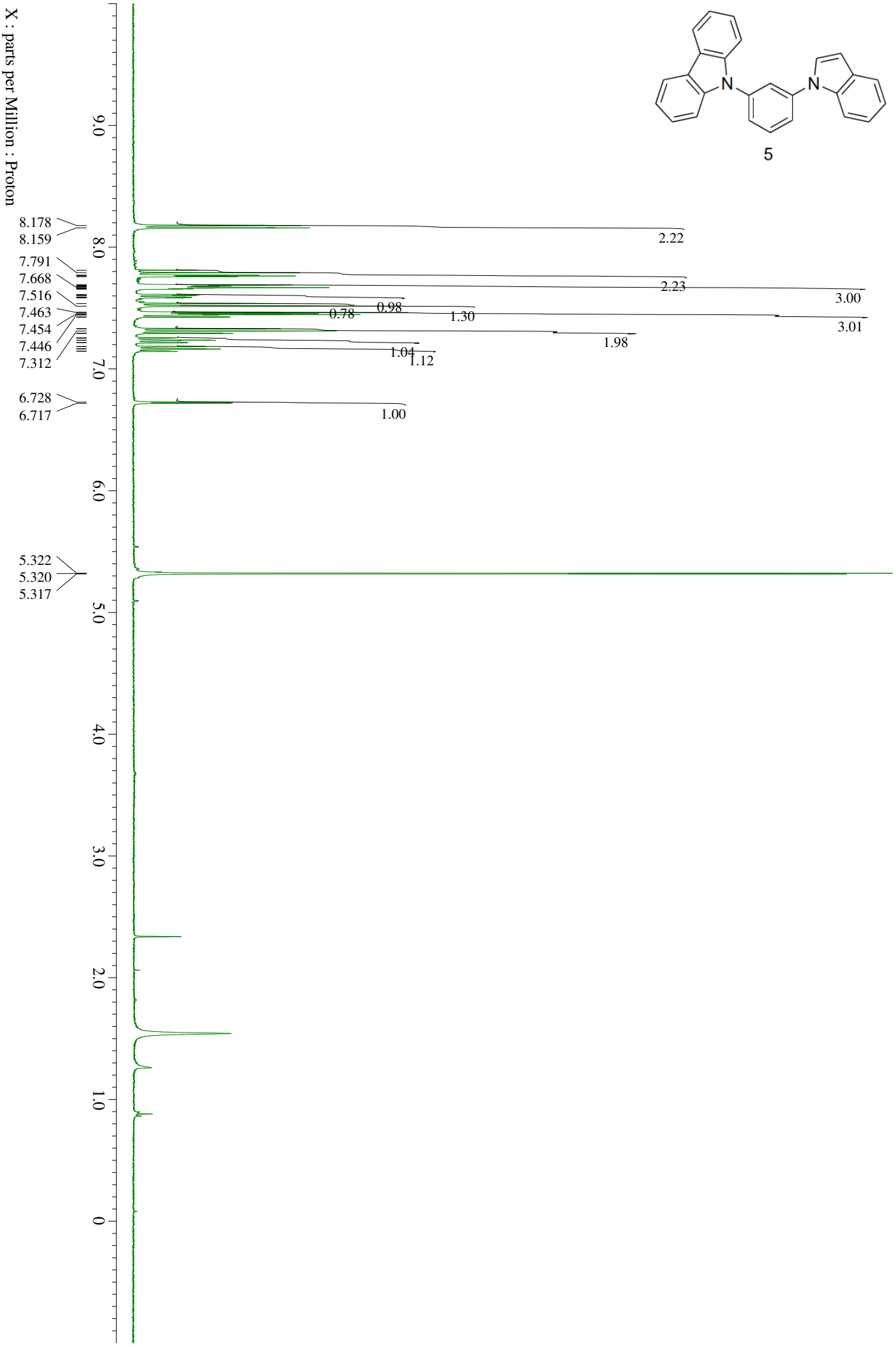
2ab

149.372

128.051
126.964
126.930
126.892
126.856
126.394
126.067
125.741
125.414
125.350
124.129
122.647

77.000

210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0


X : parts per Million : Proton
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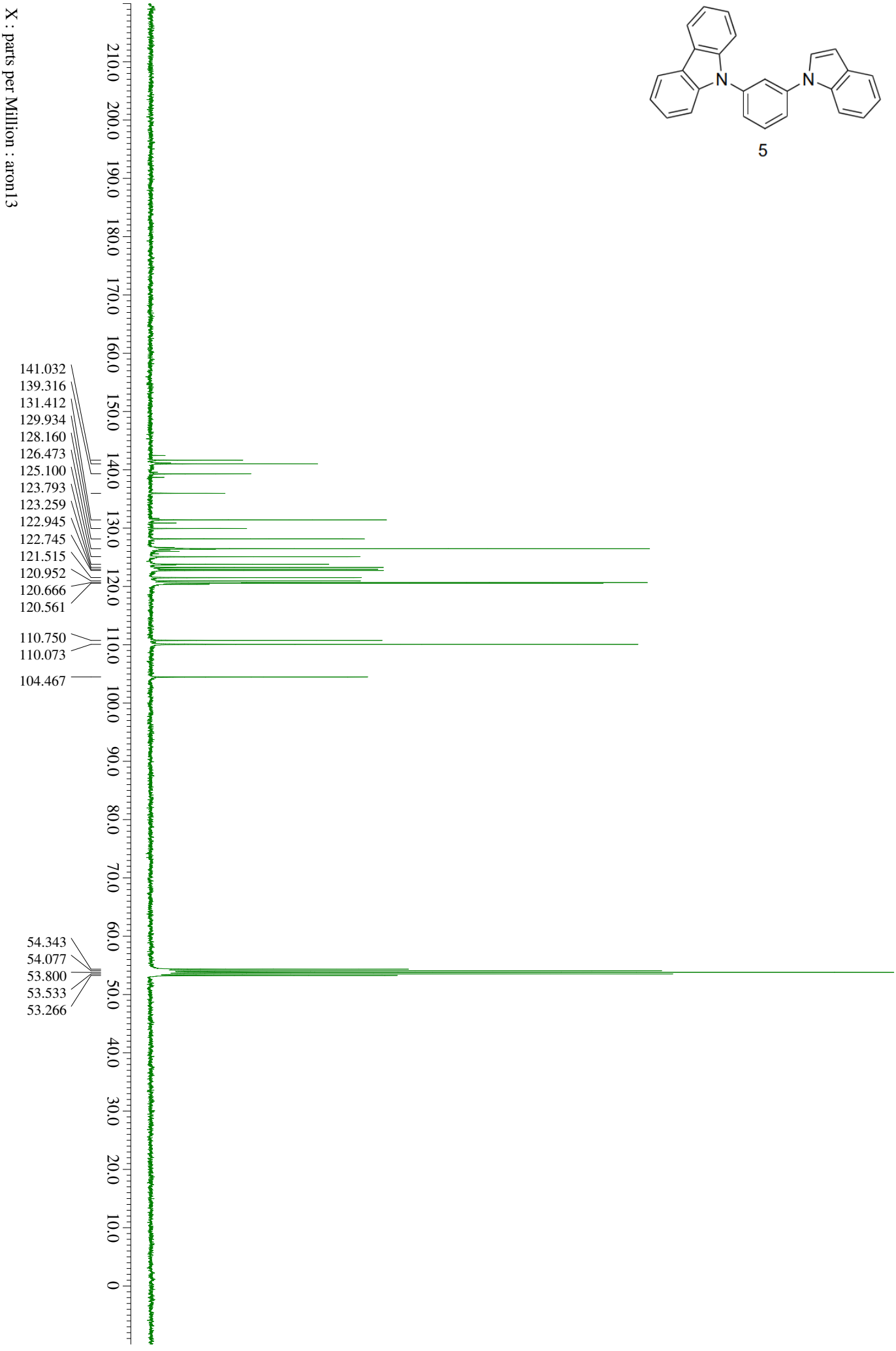
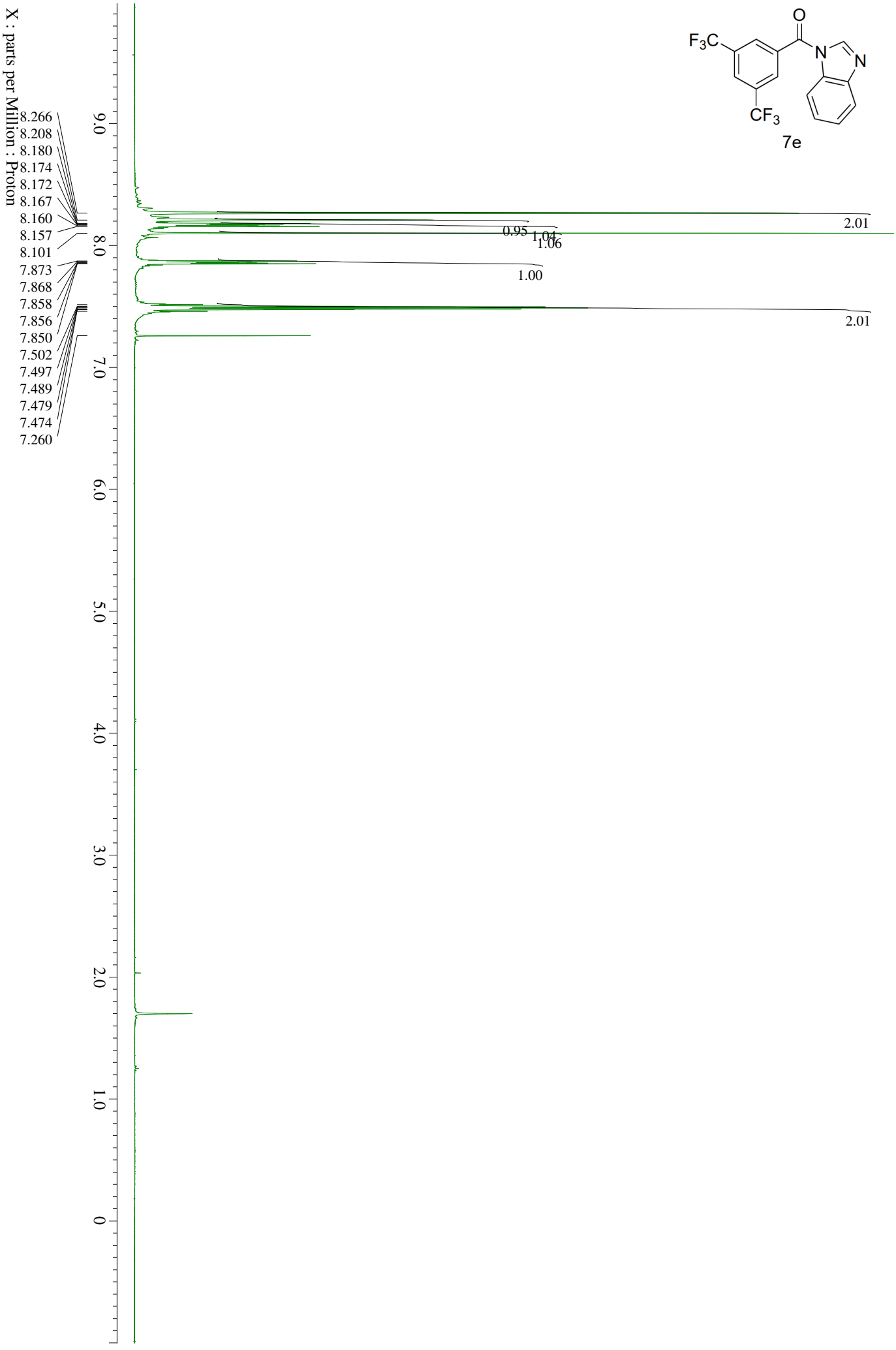
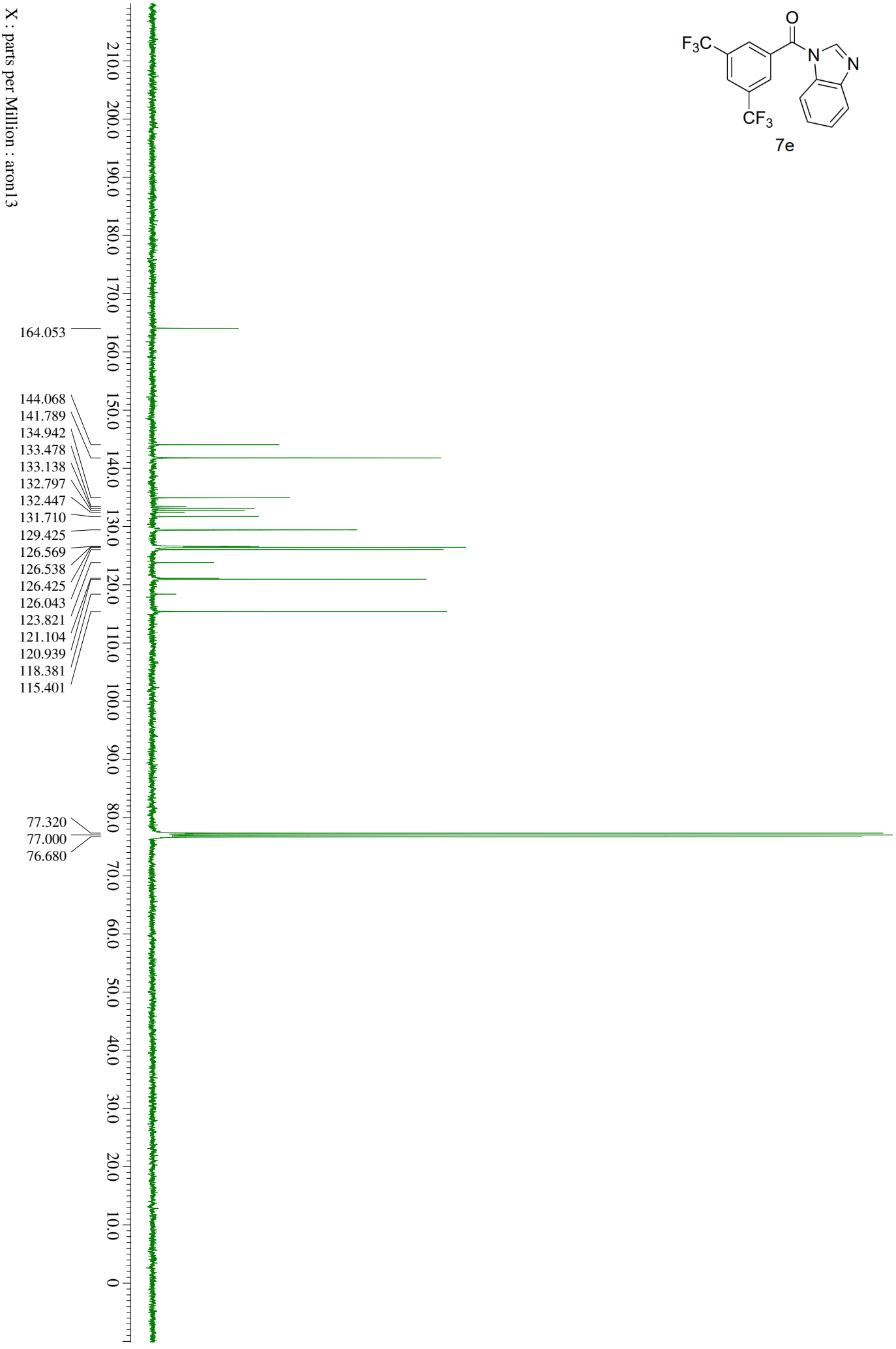
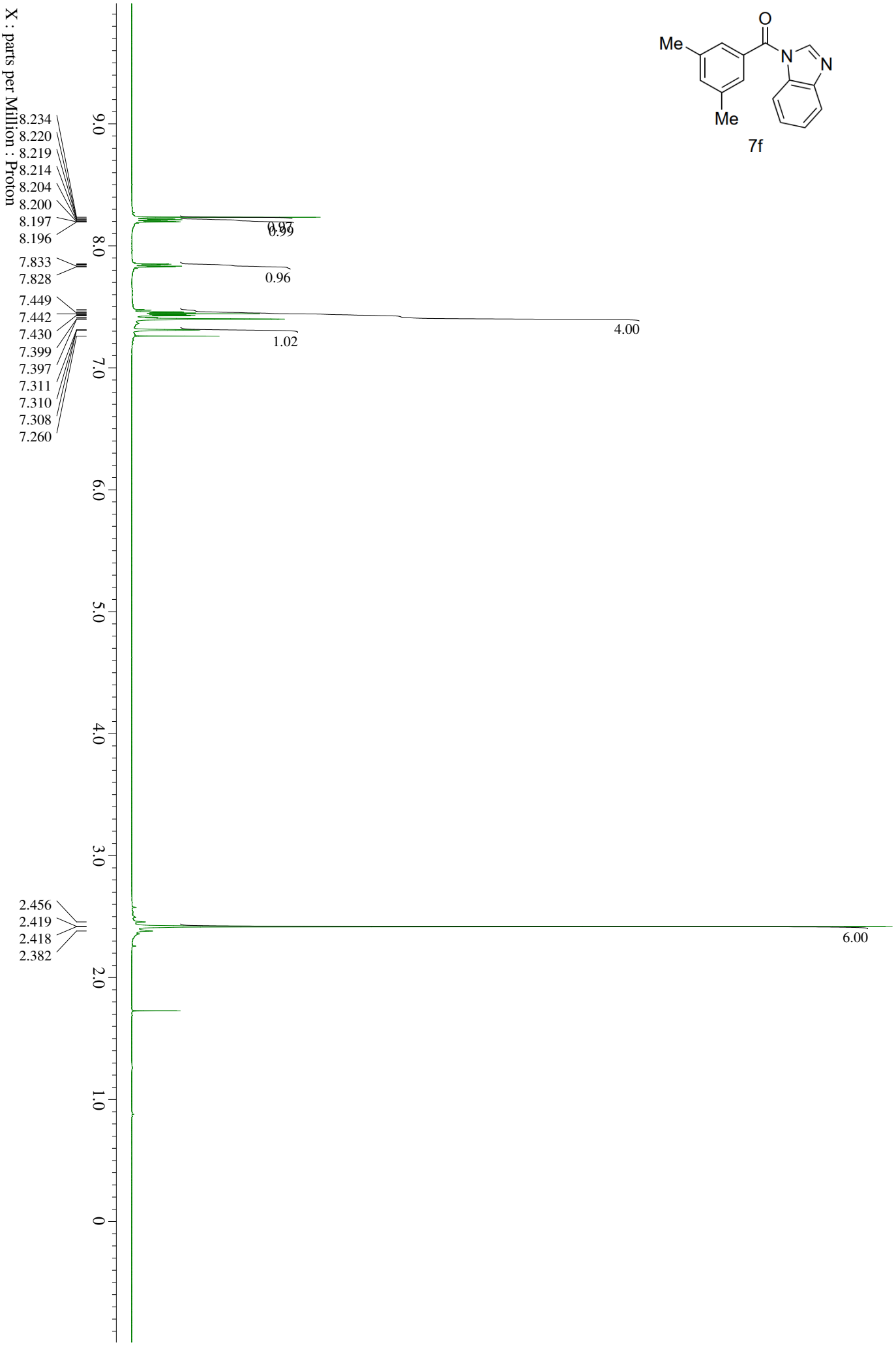
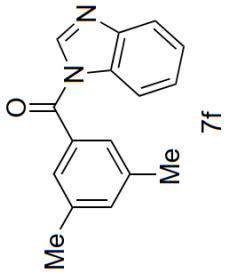
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.178
8.159
7.791
7.668
7.516
7.463
7.454
7.446
7.312
6.728
6.717
5.322
5.320
5.317
2.22
2.23
3.00
3.01
0.78
0.98
1.30
1.98
1.04
1.12
1.00
N
N
5


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
141.032
139.316
131.412
129.934
128.160
126.473
125.100
123.793
123.259
122.945
122.745
121.515
120.952
120.666
120.561
110.750
110.073
104.467
54.343
54.077
53.800
53.533
53.266
N
N
5


X : parts per Million : Proton
8.266
8.208
8.180
8.174
8.172
8.167
8.160
8.157
8.101
7.873
7.868
7.858
7.856
7.850
7.502
7.497
7.489
7.479
7.474
7.260
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.95
1.04
1.06
2.01
1.00
2.01
O
F3C
N
N
CF3
7e

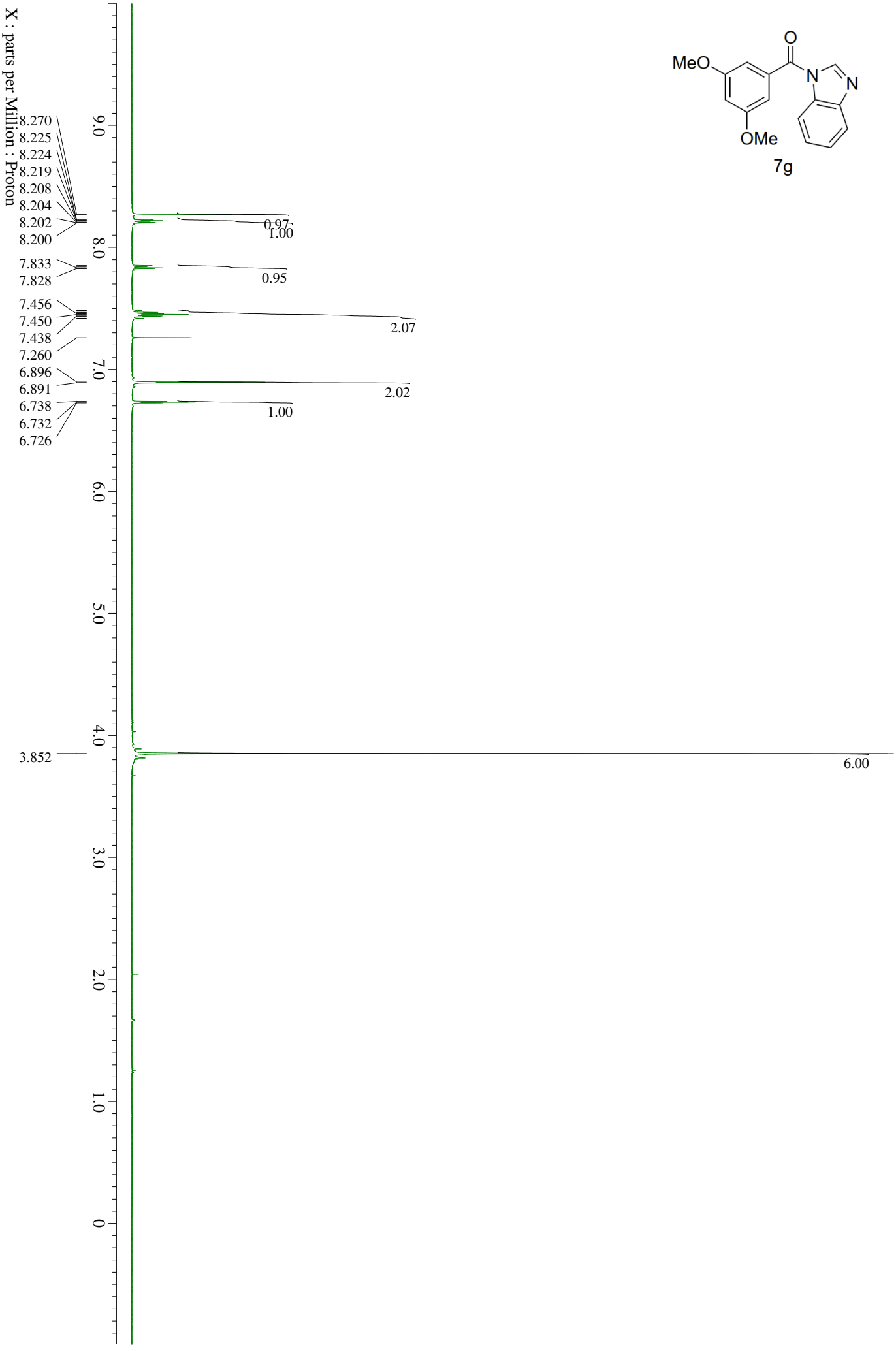

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.053
144.068
141.789
134.942
133.478
133.138
132.797
132.447
131.710
129.425
126.569
126.538
126.425
126.043
123.821
121.104
120.939
118.381
115.401
77.320
77.000
76.680
O
F3C
N
N
CF3
7e

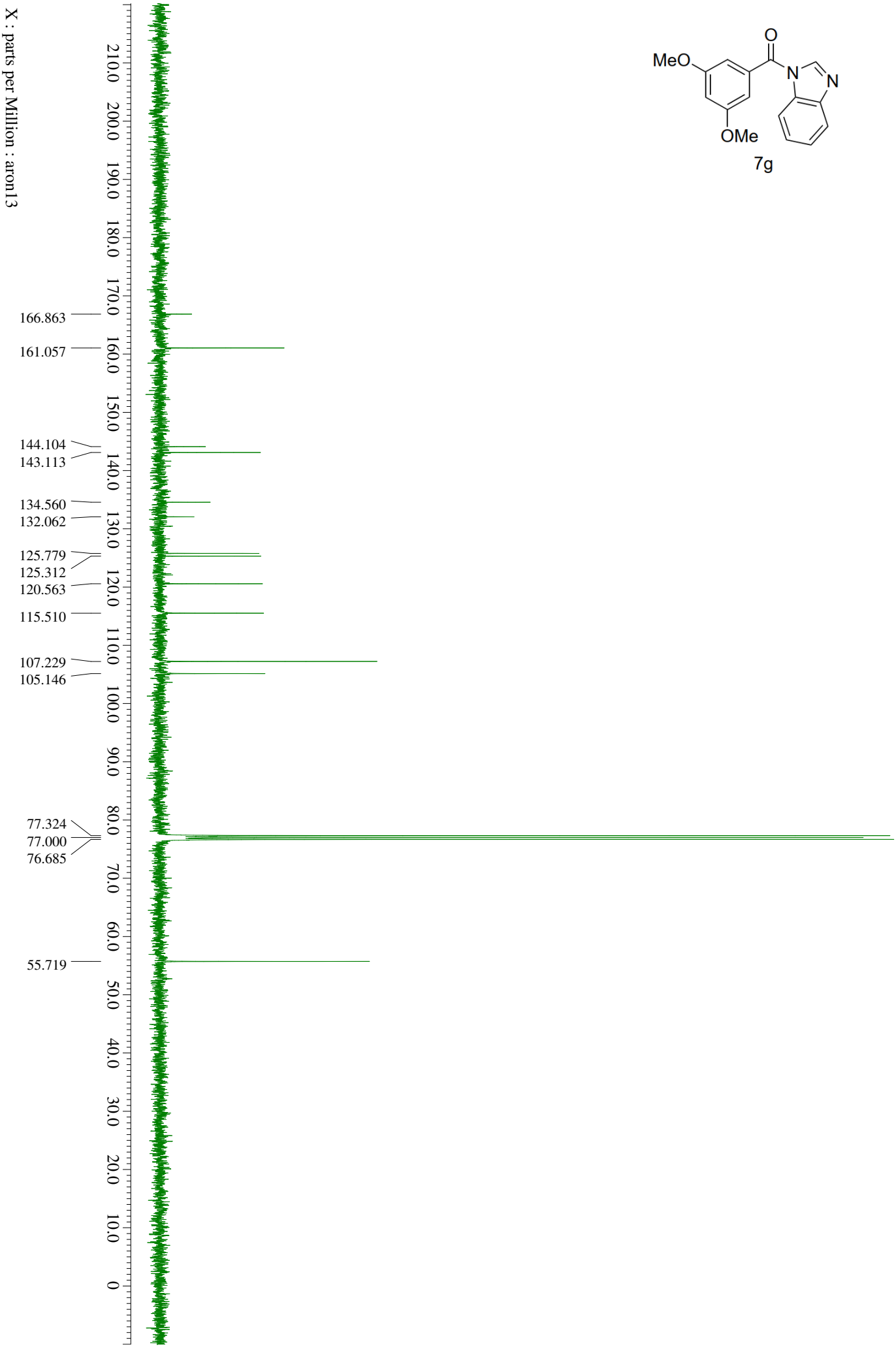

X : parts per Million : Proton
8.234
8.220
8.219
8.214
8.204
8.200
8.197
8.196
7.833
7.828
7.449
7.442
7.430
7.399
7.397
7.311
7.310
7.308
7.260
2.456
2.419
2.418
2.382
0.97
0.99
0.96
4.00
1.02
6.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Me
Me
O
N
N
7f

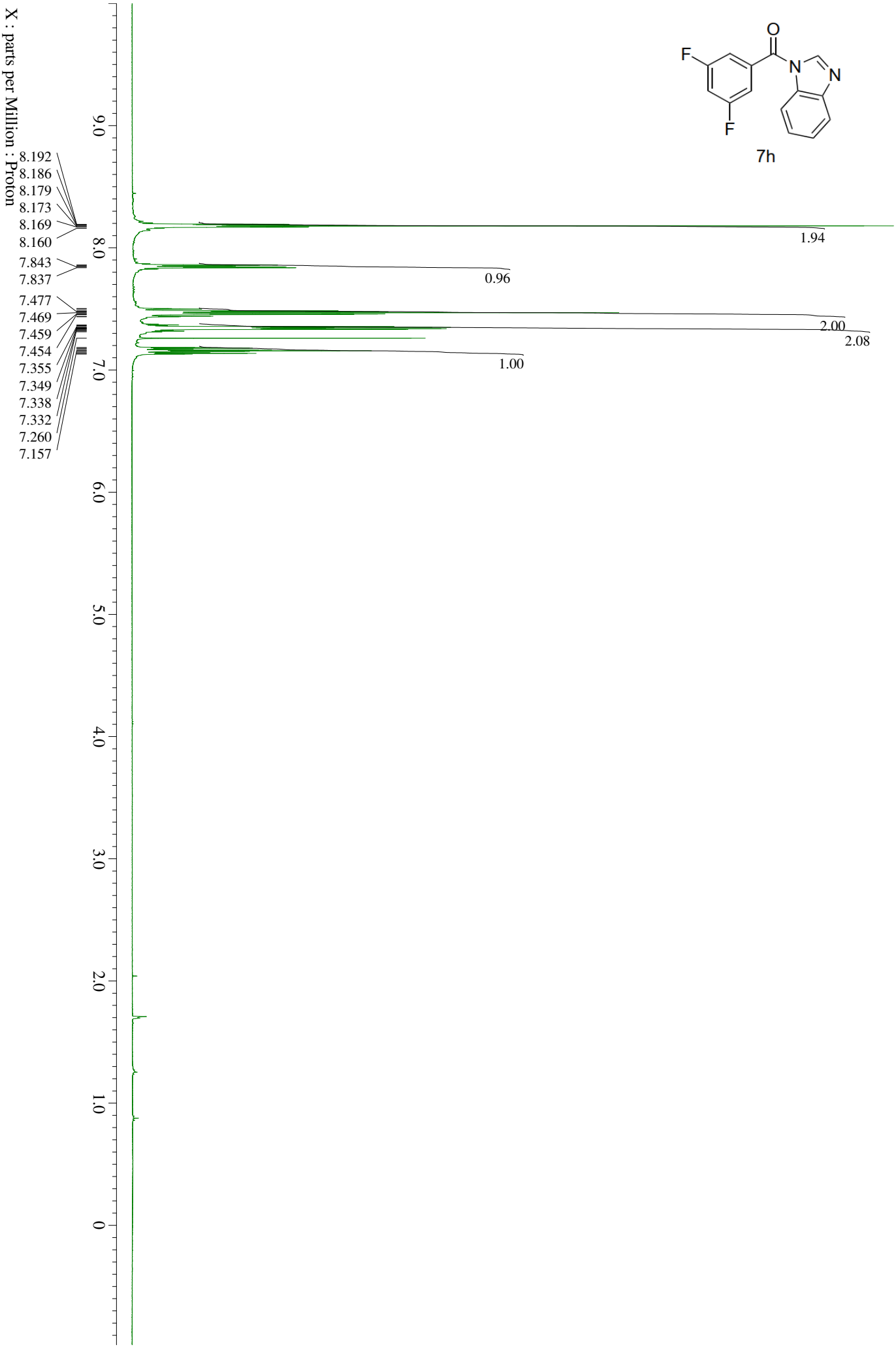


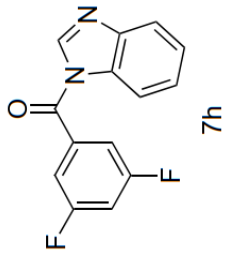
7f

X : parts per Million : aron13


X : parts per Million : Proton
8.270
8.225
8.224
8.219
8.208
8.204
8.202
8.200
7.833
7.828
7.456
7.450
7.438
7.260
6.896
6.891
6.738
6.732
6.726
3.852
0.97
1.00
0.95
2.07
2.02
1.00
6.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
MeO
O
N
N
OMe
7g

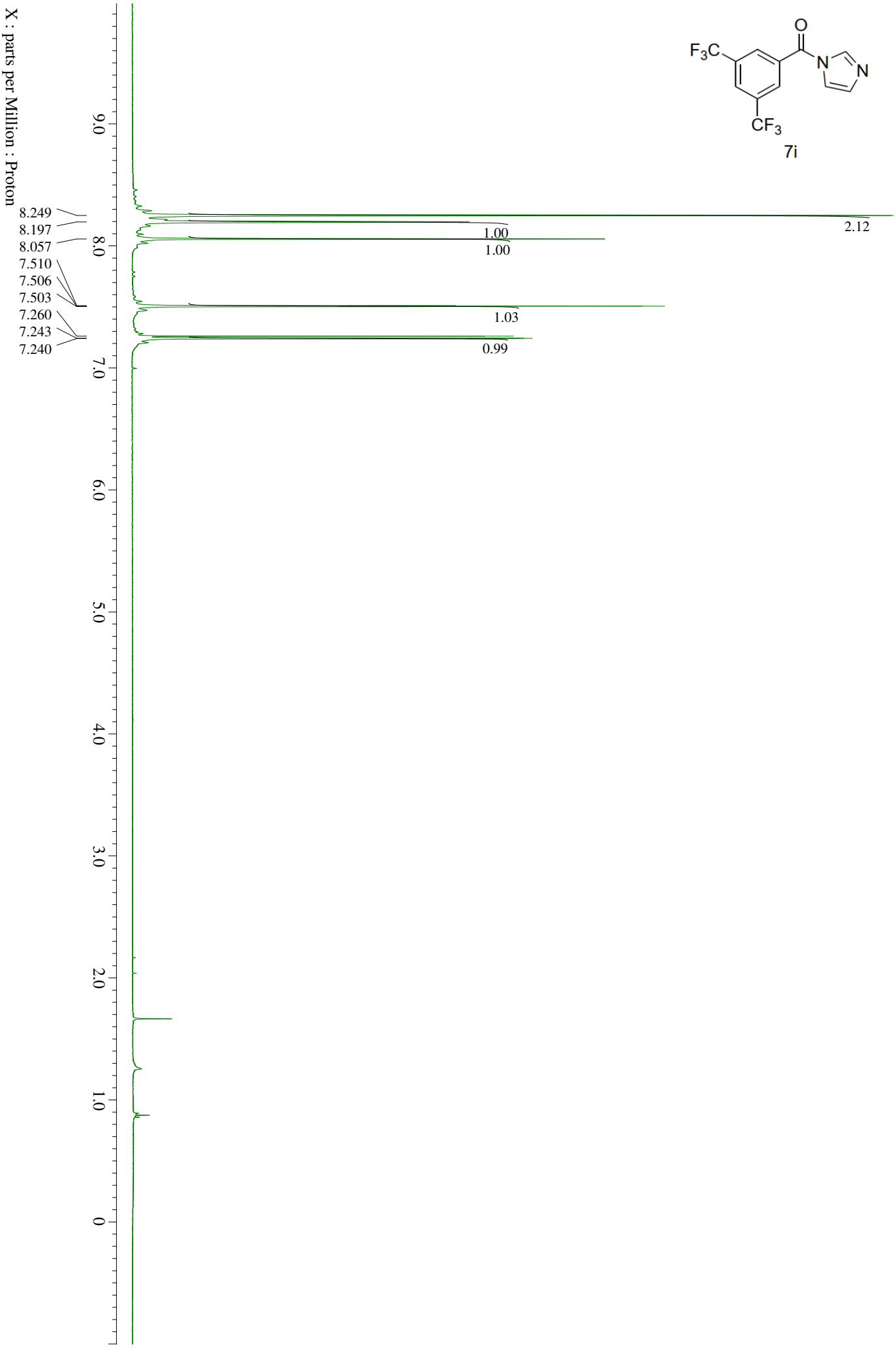

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.863
161.057
144.104
143.113
134.560
132.062
125.779
125.312
120.563
115.510
107.229
105.146
77.324
77.000
76.685
55.719
MeO
OMe
O
N
N
7g


X : parts per Million : Proton
8.192
8.186
8.179
8.173
8.169
8.160
7.843
7.837
7.477
7.469
7.459
7.454
7.355
7.349
7.338
7.332
7.260
7.157
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.94
0.96
2.00
2.08
1.00
F
F
O
N
N
7h



7h

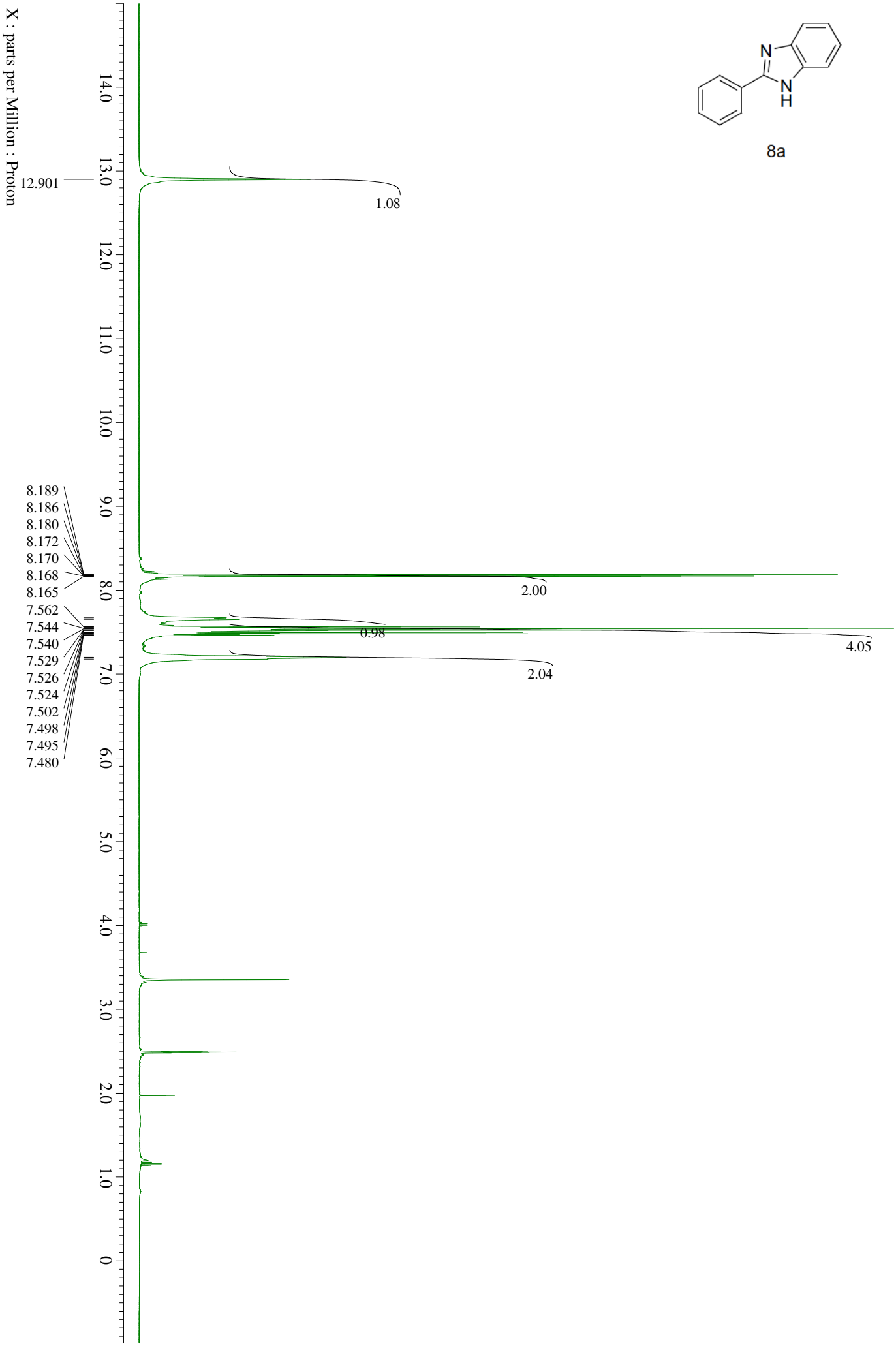
X : parts per Million : aron13

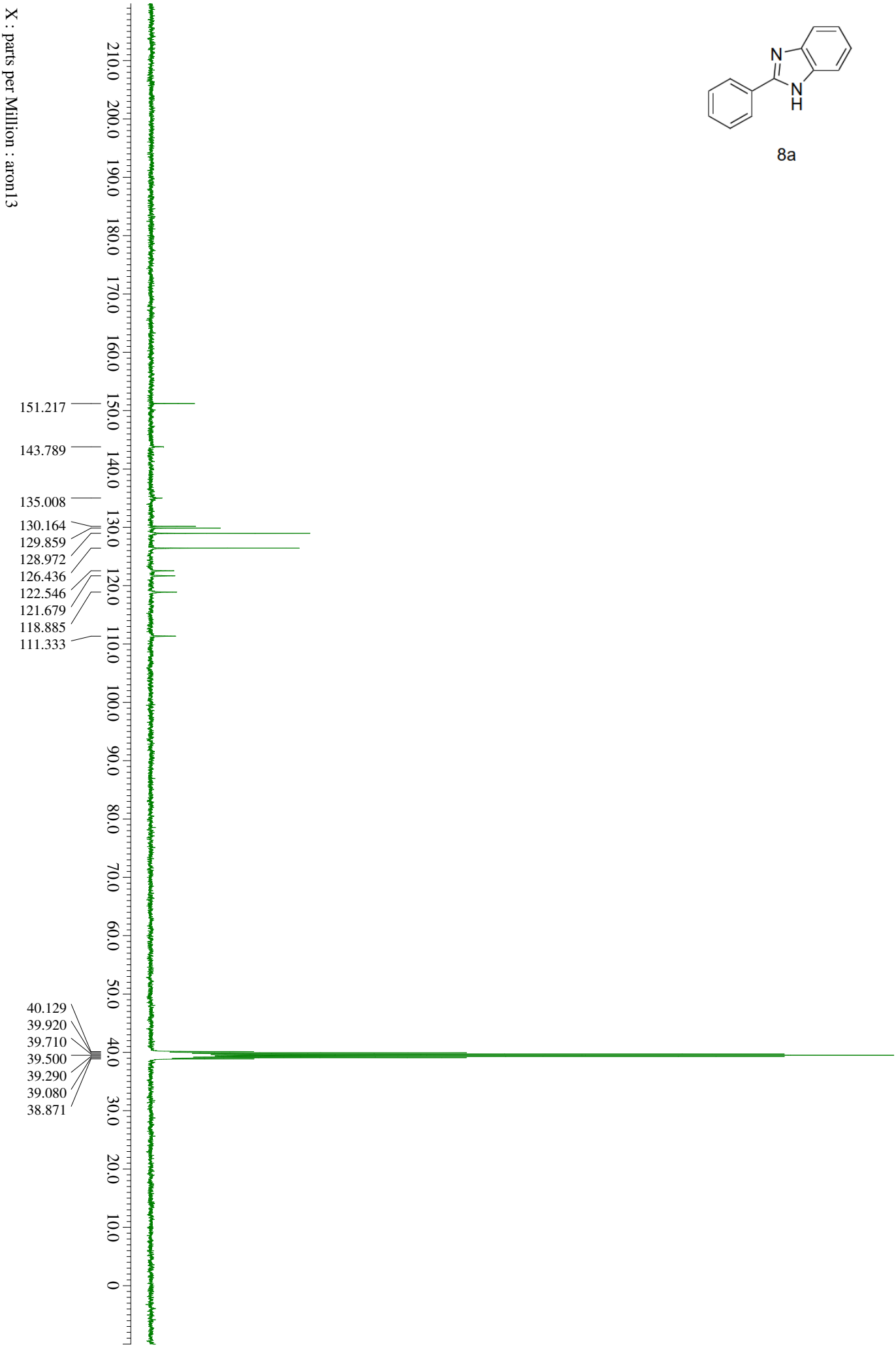

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.249
8.197
8.057
7.510
7.506
7.503
7.260
7.243
7.240
1.00
1.00
1.03
0.99
2.12
O
F3C
N
N
CF3
7i

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
163.352
137.678
133.999
133.451
133.106
132.763
132.019
129.657
129.632
129.596
129.586
129.550
126.976
126.940
126.903
123.777
121.058
117.725
77.317
77.205
77.000
76.682

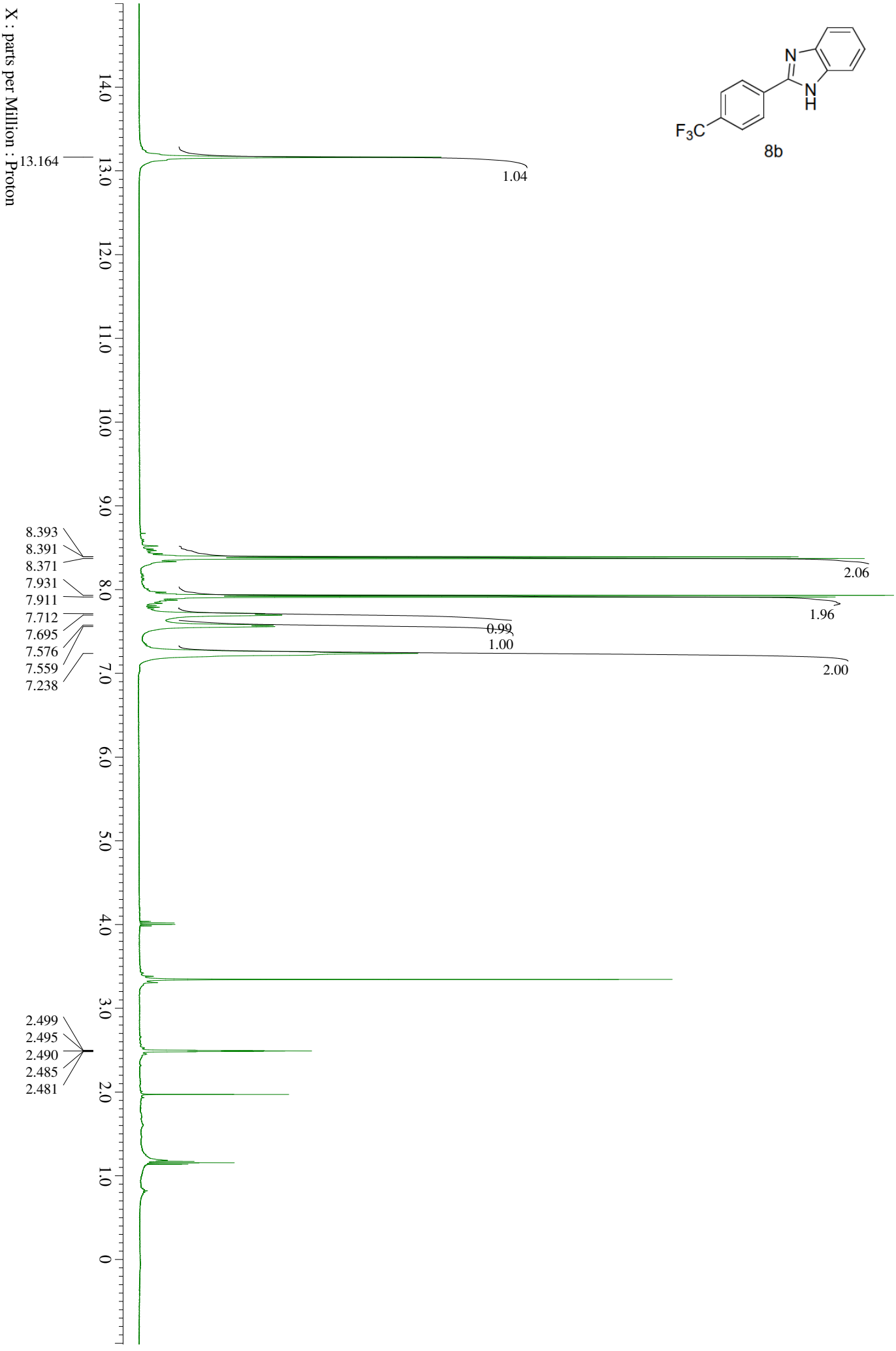
O
F3C
N
N
CF3

7i


X : parts per Million : Proton
12.901
8.189
8.186
8.180
8.172
8.170
8.168
8.165
7.562
7.544
7.540
7.529
7.526
7.524
7.502
7.498
7.495
7.480
1.08
2.00
0.98
4.05
2.04
N
N
H
8a

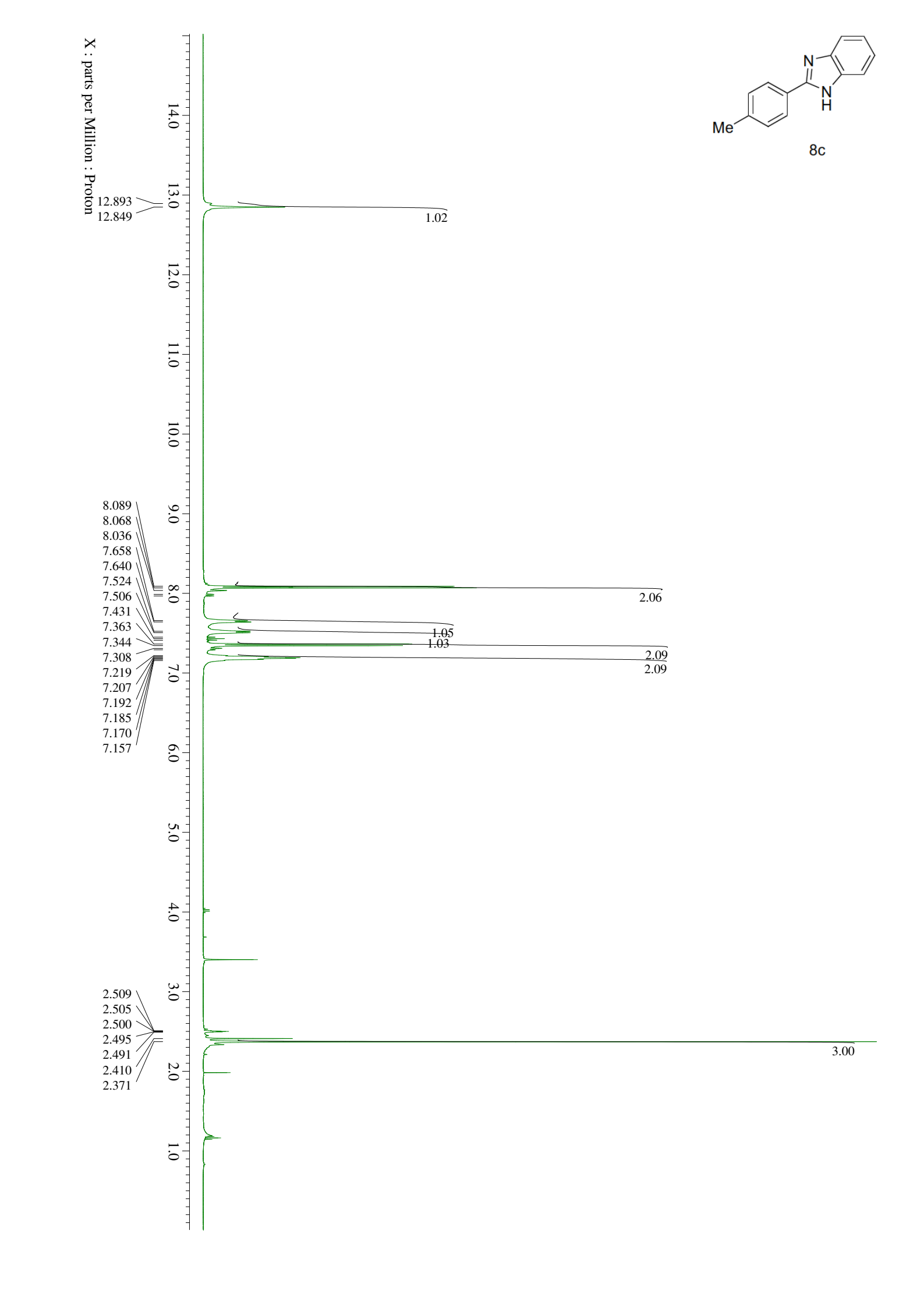

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
151.217
143.789
135.008
130.164
129.859
128.972
126.436
122.546
121.679
118.885
111.333
40.129
39.920
39.710
39.500
39.290
39.080
38.871
N
N
H

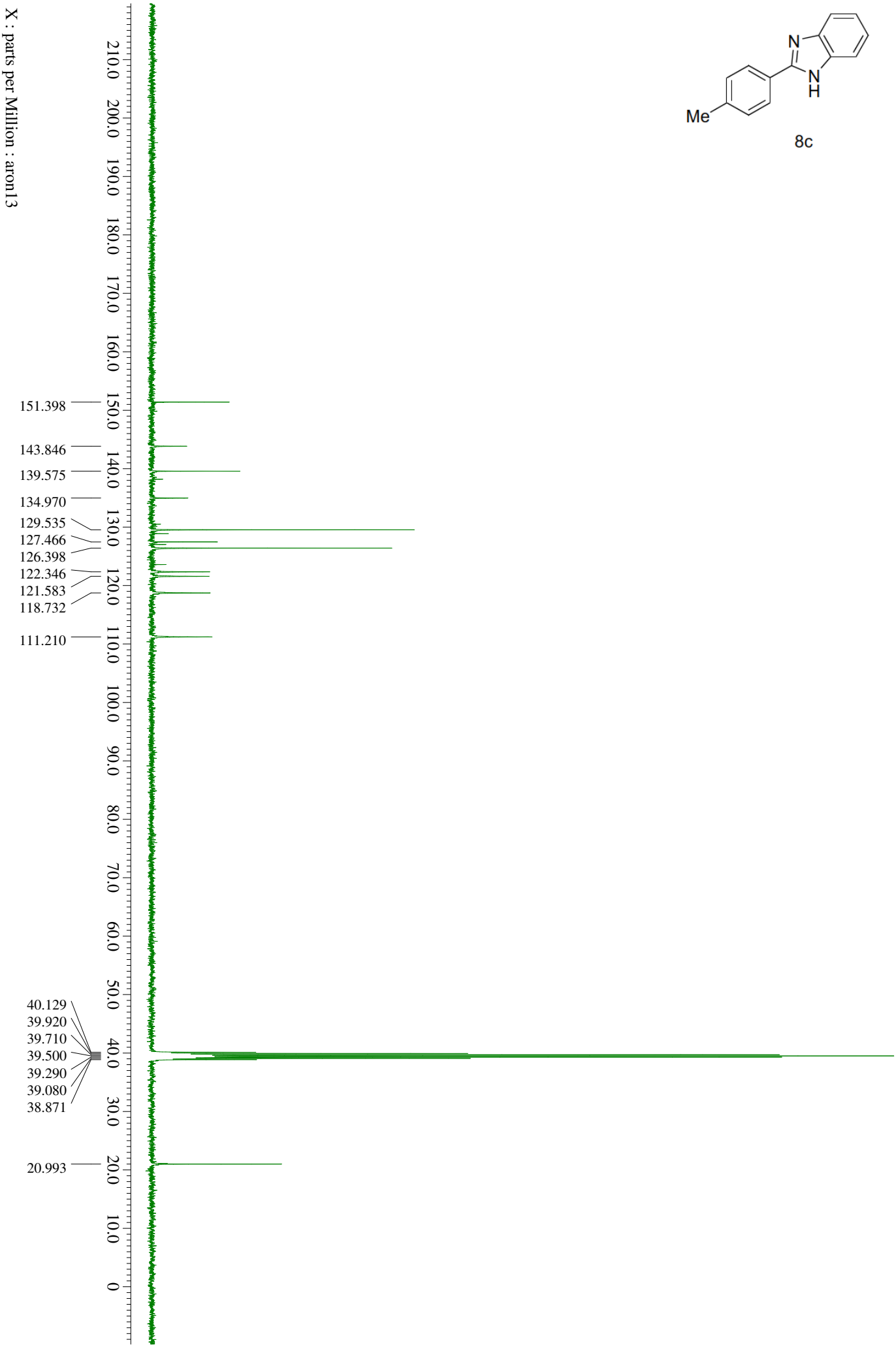
8a

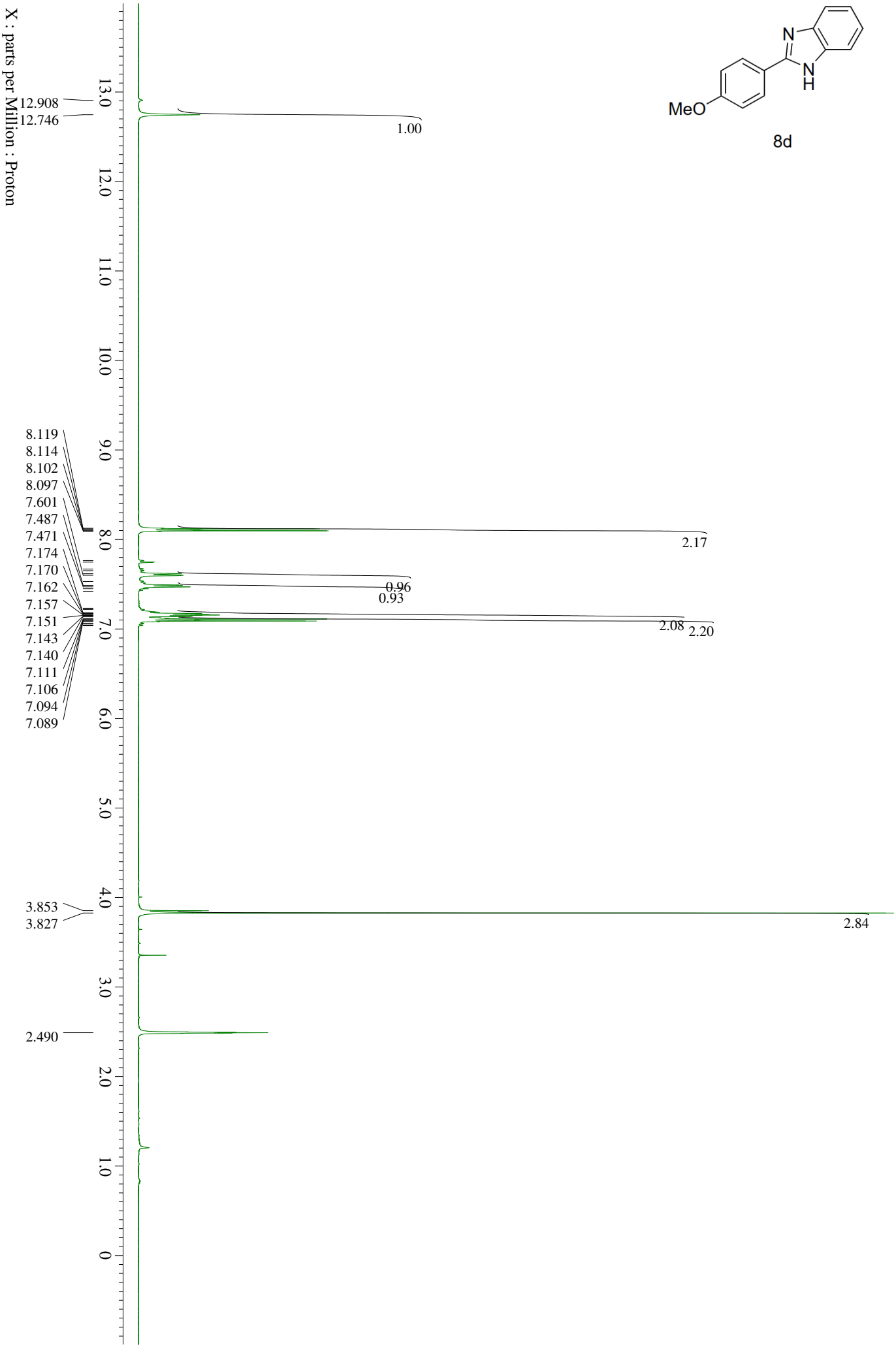

X : parts per Million : Proton
13.164
1.04
8.393
8.391
8.371
7.931
7.911
7.712
7.695
7.576
7.559
7.238
2.06
1.96
0.99
1.00
2.00
2.499
2.495
2.490
2.485
2.481
N
N
H
F3C
8b

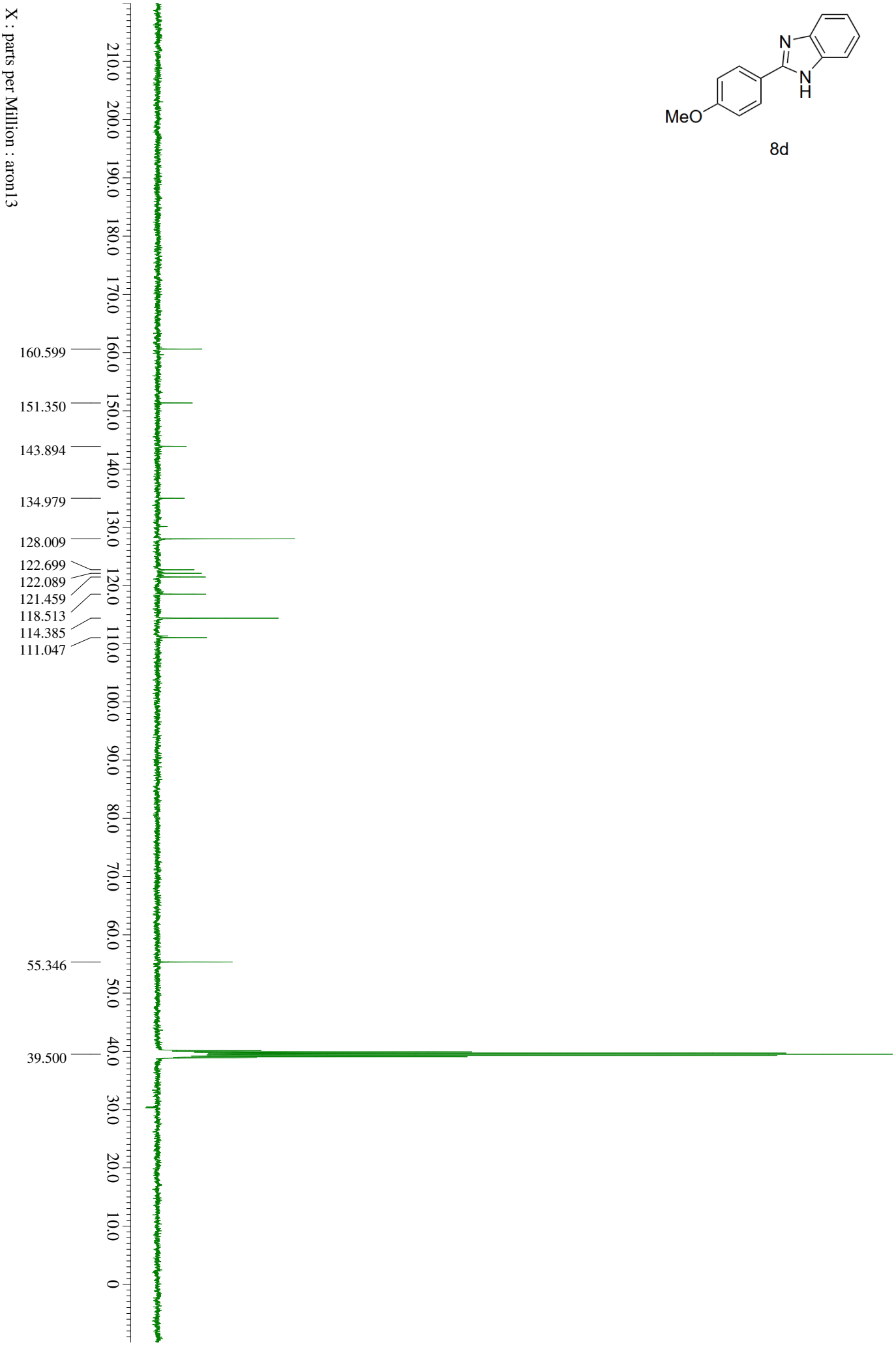
X : parts per Million : aron13

8b

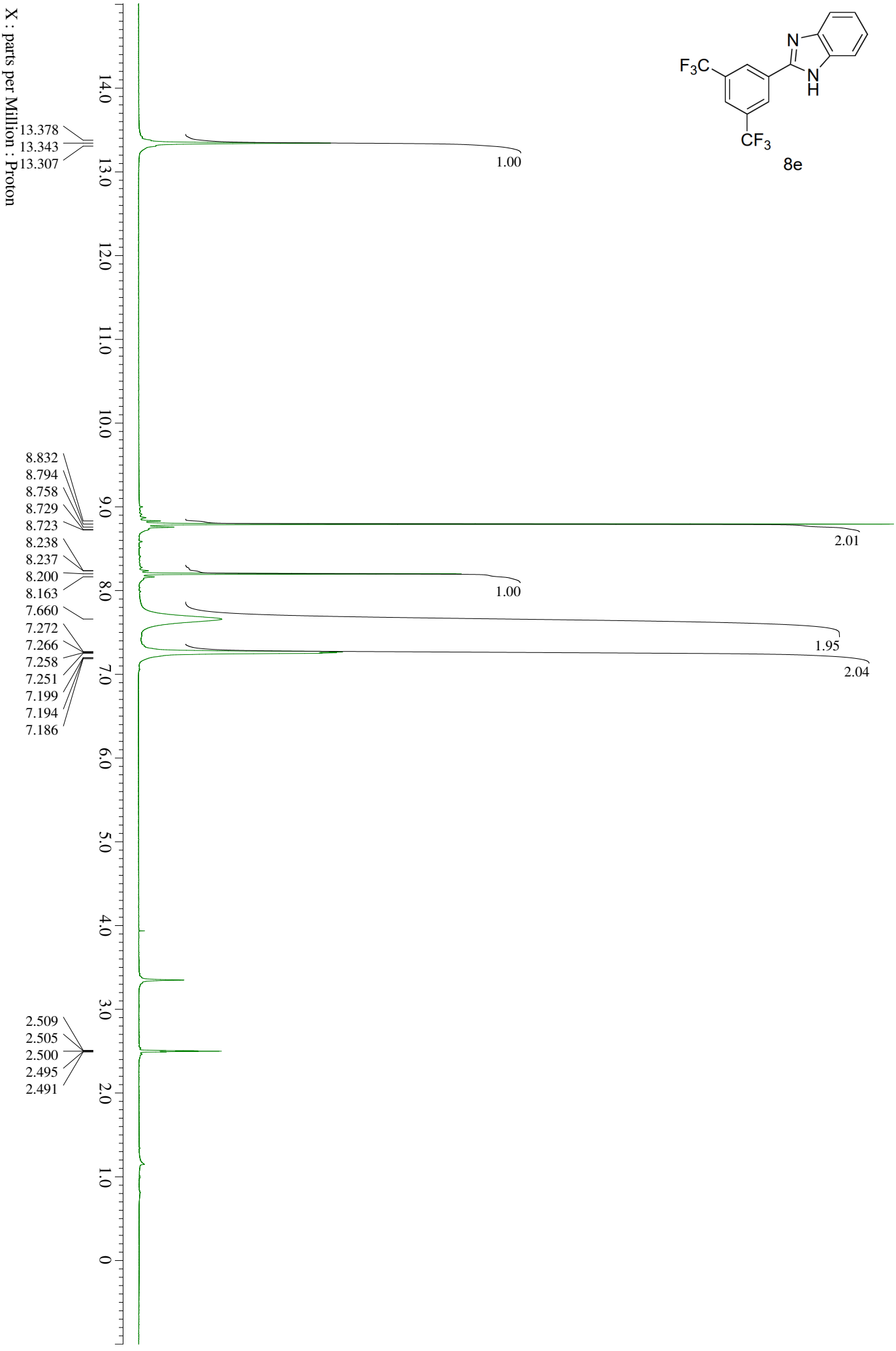

X : parts per Million : Proton
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
12.893
12.849
1.02
8.089
8.068
8.036
7.658
7.640
7.524
7.506
7.431
7.363
7.344
7.308
7.219
7.207
7.192
7.185
7.170
7.157
2.06
1.05
1.03
2.09
2.09
2.509
2.505
2.500
2.495
2.491
2.410
2.371
3.00
N
N
H
Me
8c

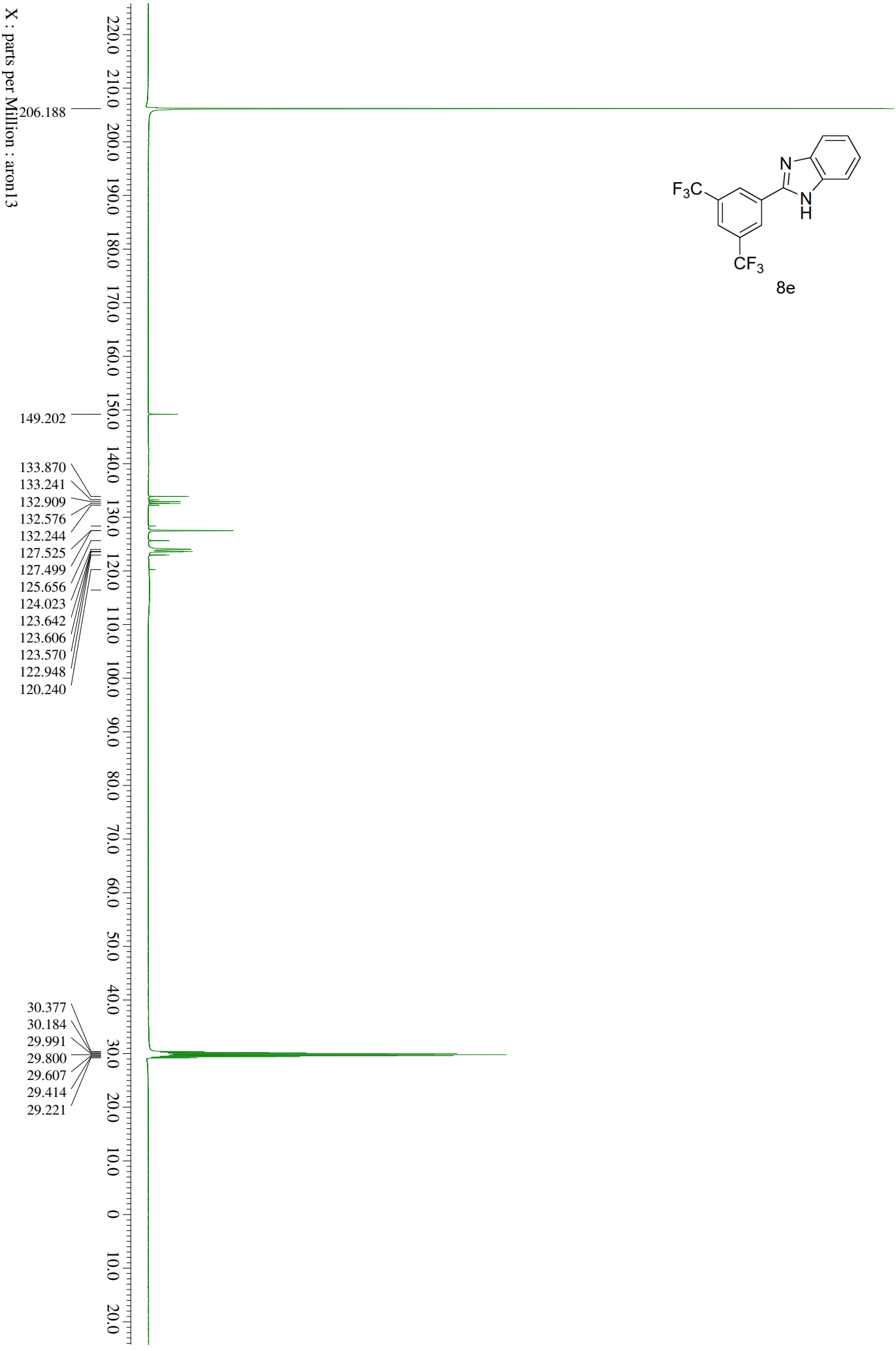

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
151.398
143.846
139.575
134.970
129.535
127.466
126.398
122.346
121.583
118.732
111.210
40.129
39.920
39.710
39.500
39.290
39.080
38.871
20.993
N
N
H
Me
8c

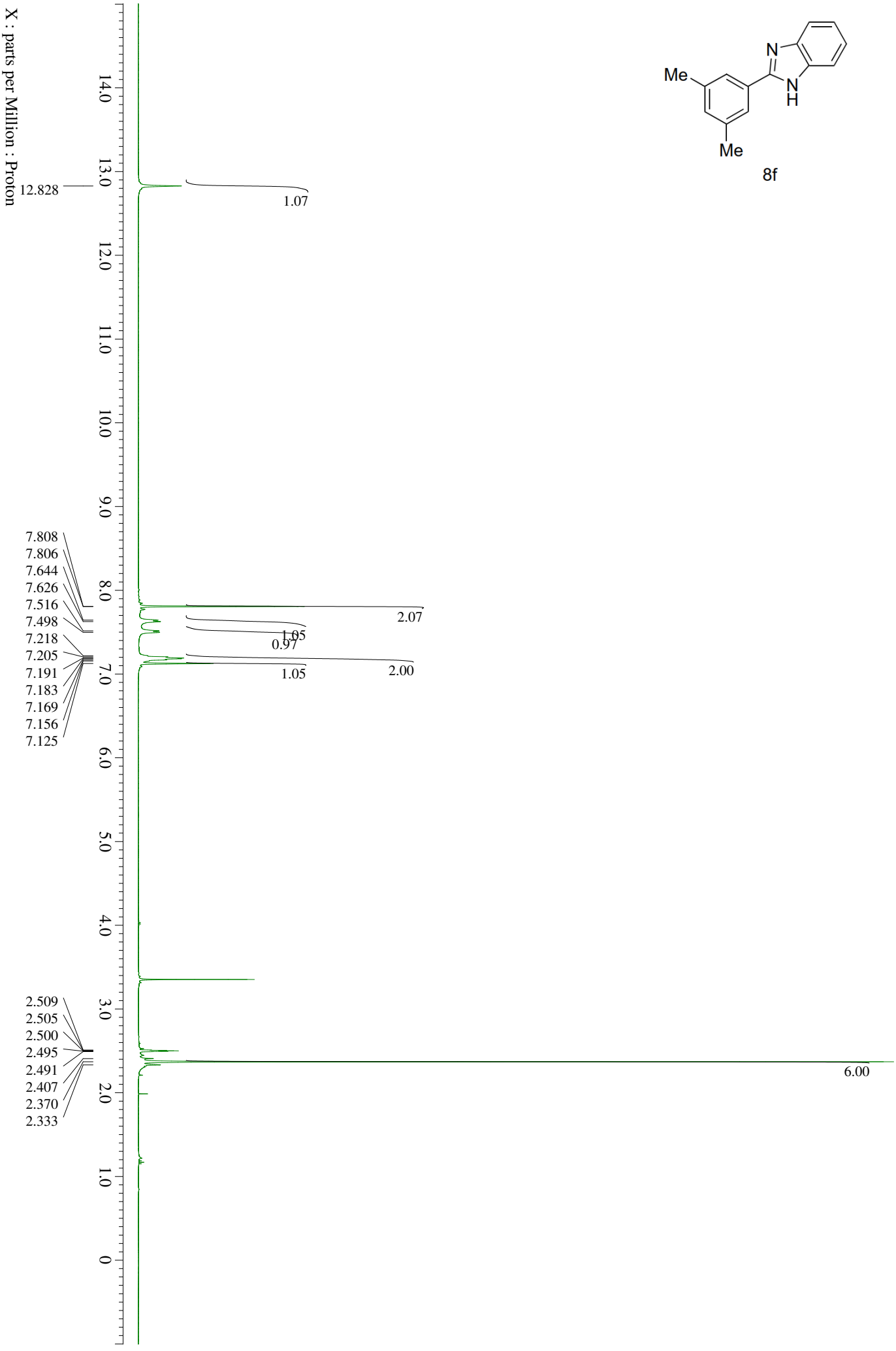

X : parts per Million : Proton
12.908
12.746
1.00
8.119
8.114
8.102
8.097
7.601
7.487
7.471
7.174
7.170
7.162
7.157
7.151
7.143
7.140
7.111
7.106
7.094
7.089
2.17
0.96
0.93
2.08
2.20
3.853
3.827
2.84
2.490
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
N
N
H
MeO
8d

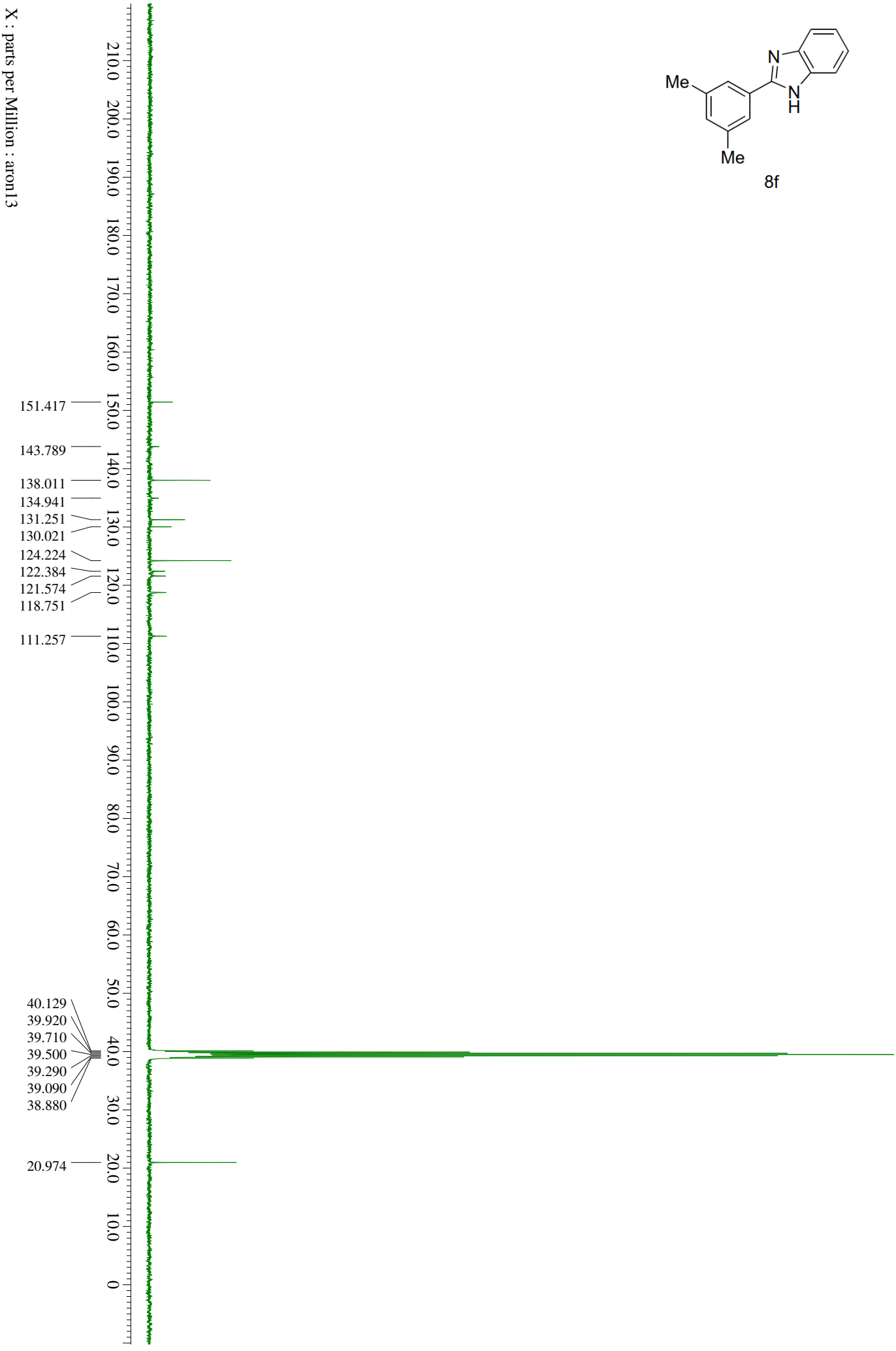

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.599
151.350
143.894
134.979
128.009
122.699
122.089
121.459
118.513
114.385
111.047
55.346
39.500
N
N
H
MeO

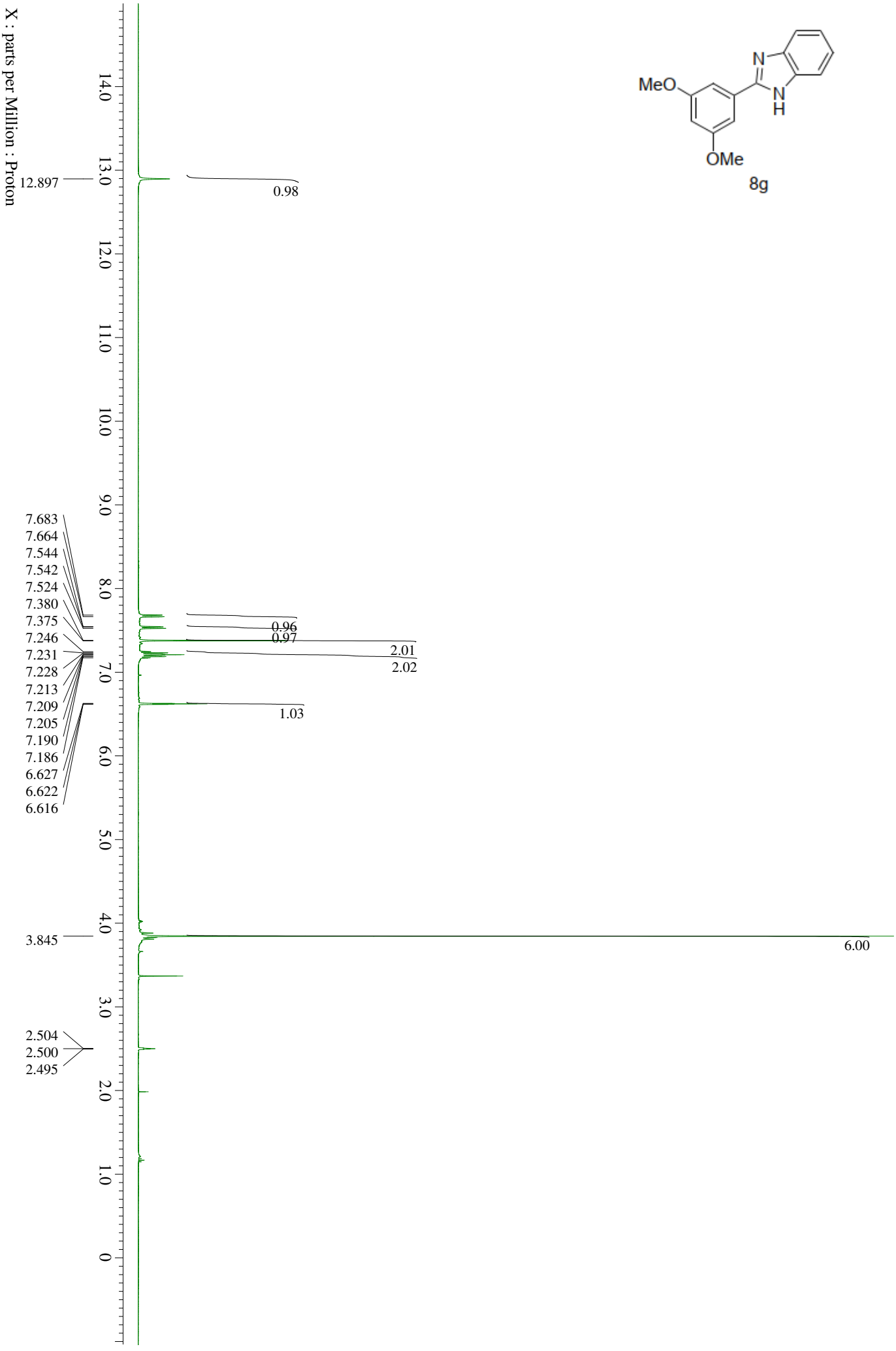
8d

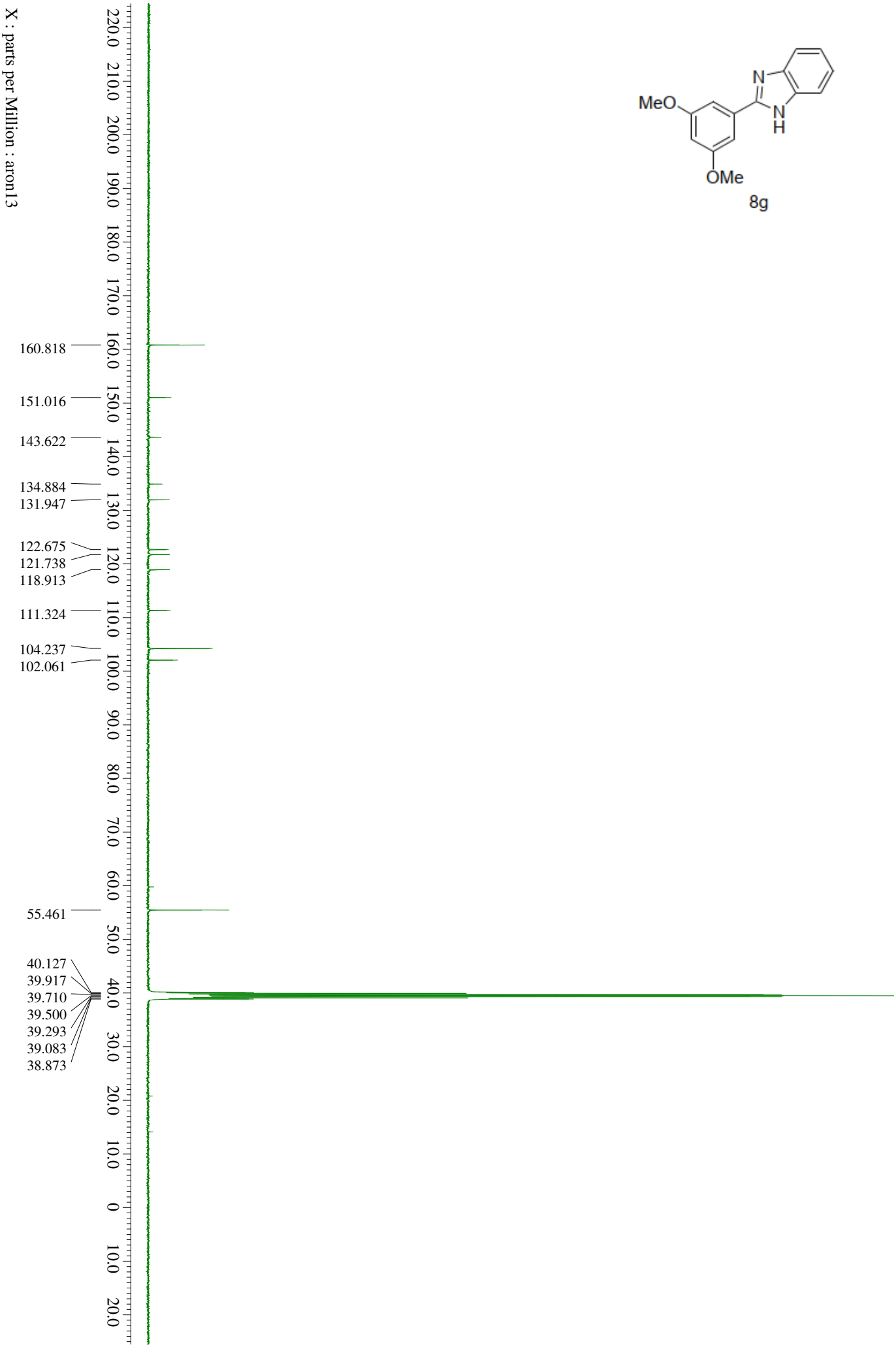

X : parts per Million : Proton
13.378
13.343
13.307
8.832
8.794
8.758
8.729
8.723
8.238
8.237
8.200
8.163
7.660
7.272
7.266
7.258
7.251
7.199
7.194
7.186
2.509
2.505
2.500
2.495
2.491
1.00
2.01
1.00
1.95
2.04
F3C
CF3
N
N
H
8e

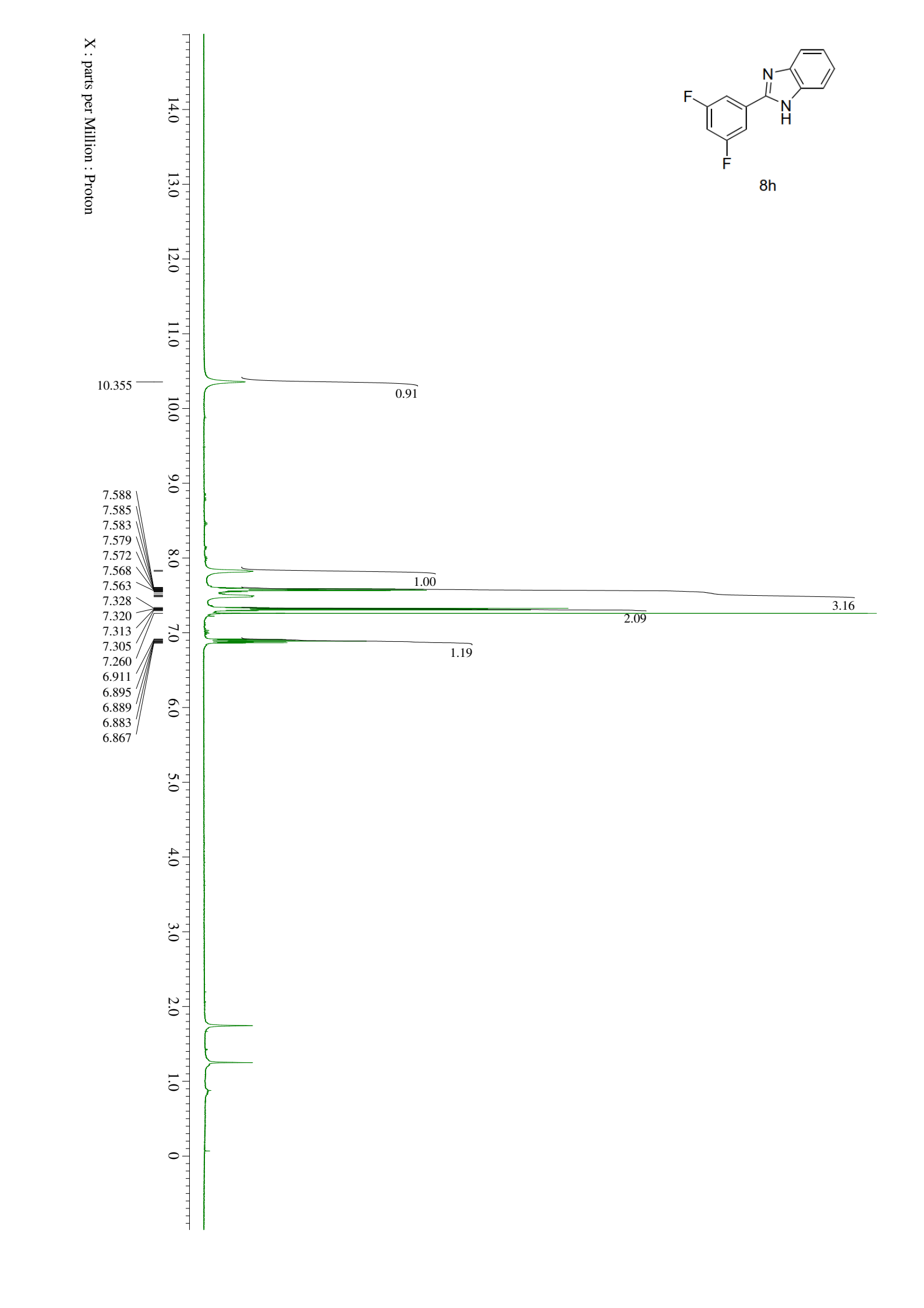

X : parts per Million : aron13
206.188
149.202
133.870
133.241
132.909
132.576
132.244
127.525
127.499
125.656
124.023
123.642
123.606
123.570
122.948
120.240
30.377
30.184
29.991
29.800
29.607
29.414
29.221
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
10.0
20.0
F3C
CF3
N
N
H
8e


X : parts per Million : Proton
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
12.828
1.07
7.808
7.806
7.644
7.626
7.516
7.498
7.218
7.205
7.191
7.183
7.169
7.156
7.125
2.07
1.05
0.97
1.05
2.00
2.509
2.505
2.500
2.495
2.491
2.407
2.370
2.333
6.00
Me
N
N
H
Me
8f


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
151.417
143.789
138.011
134.941
131.251
130.021
124.224
122.384
121.574
118.751
111.257
40.129
39.920
39.710
39.500
39.290
39.090
38.880
20.974
Me
Me
N
N
H
8f

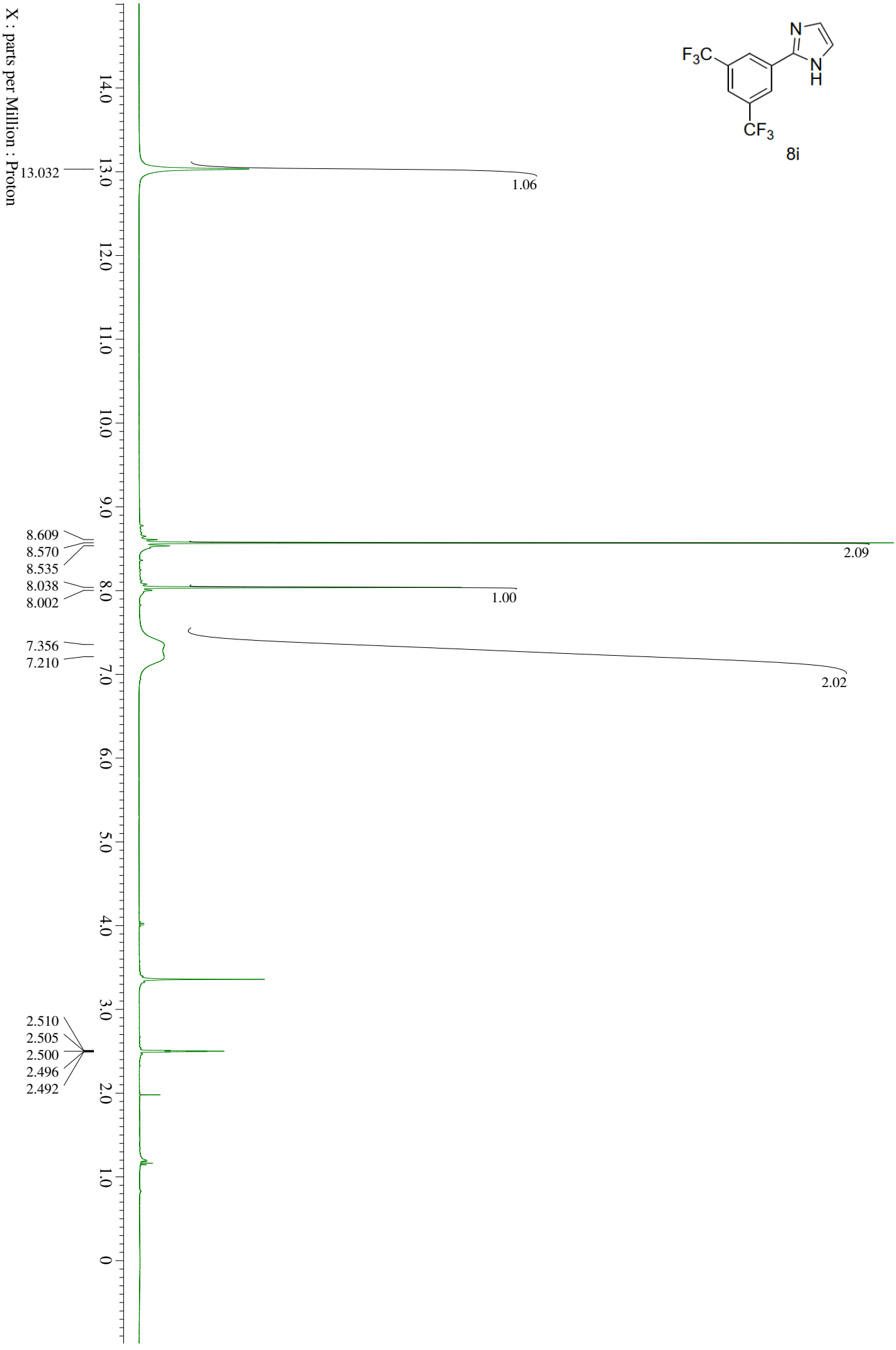

X : parts per Million : Proton
12.897
7.683
7.664
7.544
7.542
7.524
7.380
7.375
7.246
7.231
7.228
7.213
7.209
7.205
7.190
7.186
6.627
6.622
6.616
3.845
2.504
2.500
2.495
0.98
0.96
0.97
2.01
2.02
1.03
6.00
MeO
OMe
N
N
H
8g

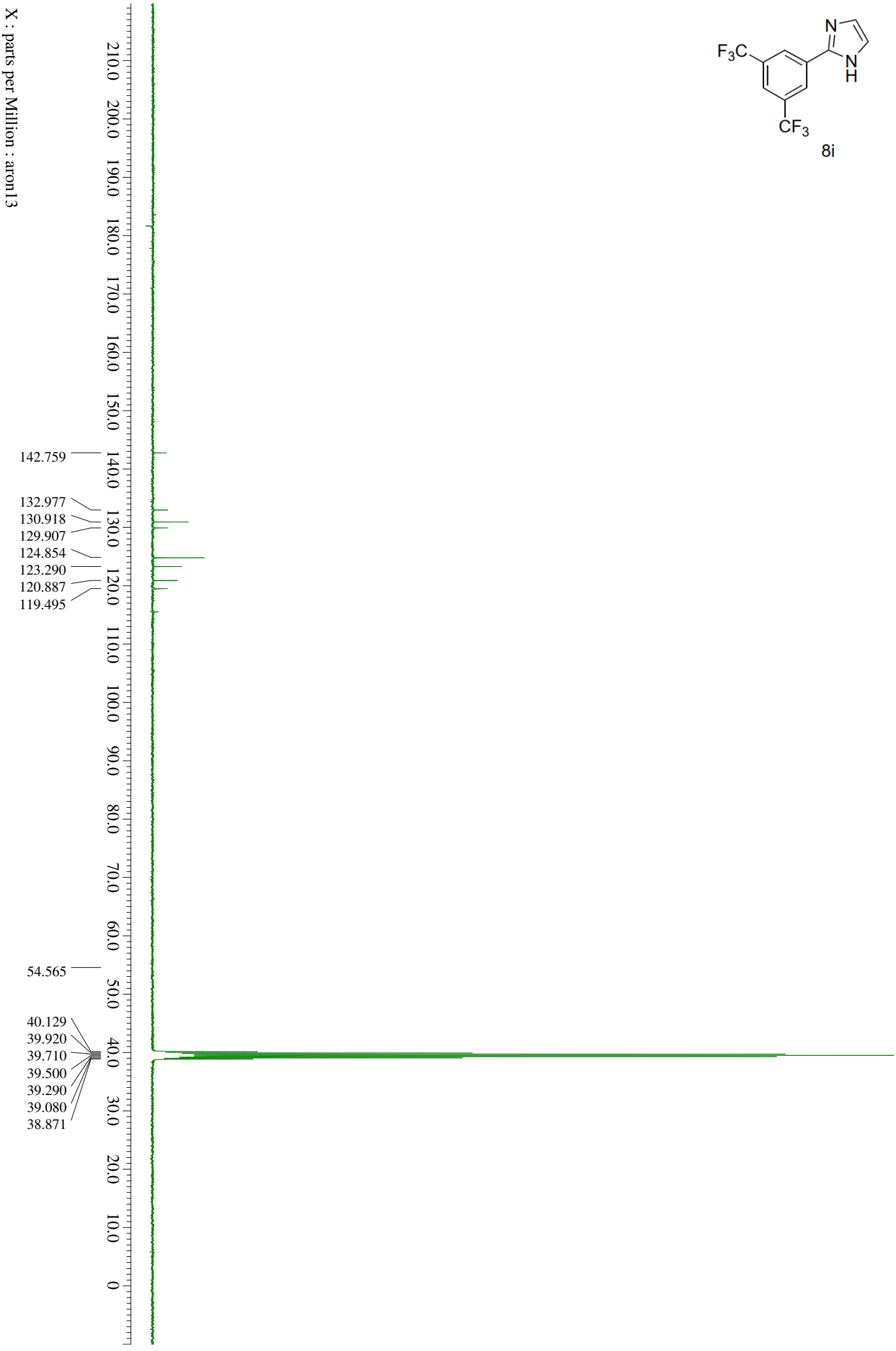

X : parts per Million : aron13
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
10.0
20.0
160.818
151.016
143.622
134.884
131.947
122.675
121.738
118.913
111.324
104.237
102.061
55.461
40.127
39.917
39.710
39.500
39.293
39.083
38.873
MeO
N
N
H
OMe
8g

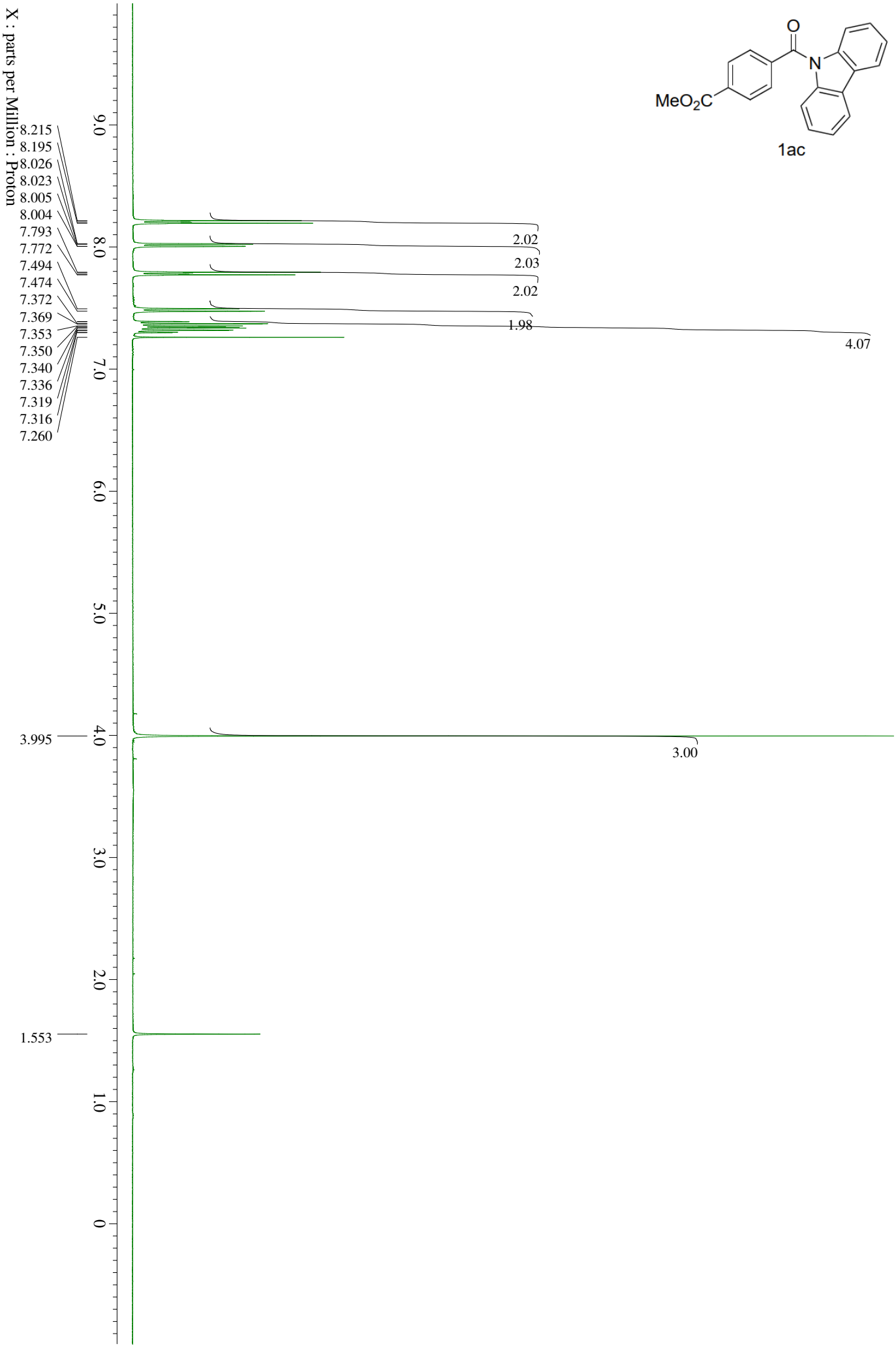

X : parts per Million : Proton
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.355
0.91
7.588
7.585
7.583
7.579
7.572
7.568
7.563
7.328
7.320
7.313
7.305
7.260
6.911
6.895
6.889
6.883
6.867
1.00
3.16
2.09
1.19
F
N
N
H
F
8h

X : parts per Million : aron13

8h


X : parts per Million : Proton
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
13.032
1.06
8.609
8.570
8.535
8.038
8.002
2.09
1.00
7.356
7.210
2.02
2.510
2.505
2.500
2.496
2.492
N
F3C
N
H
CF3
8i


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
142.759
132.977
130.918
129.907
124.854
123.290
120.887
119.495
54.565
40.129
39.920
39.710
39.500
39.290
39.080
38.871
F3C
N
N
H
CF3
8i

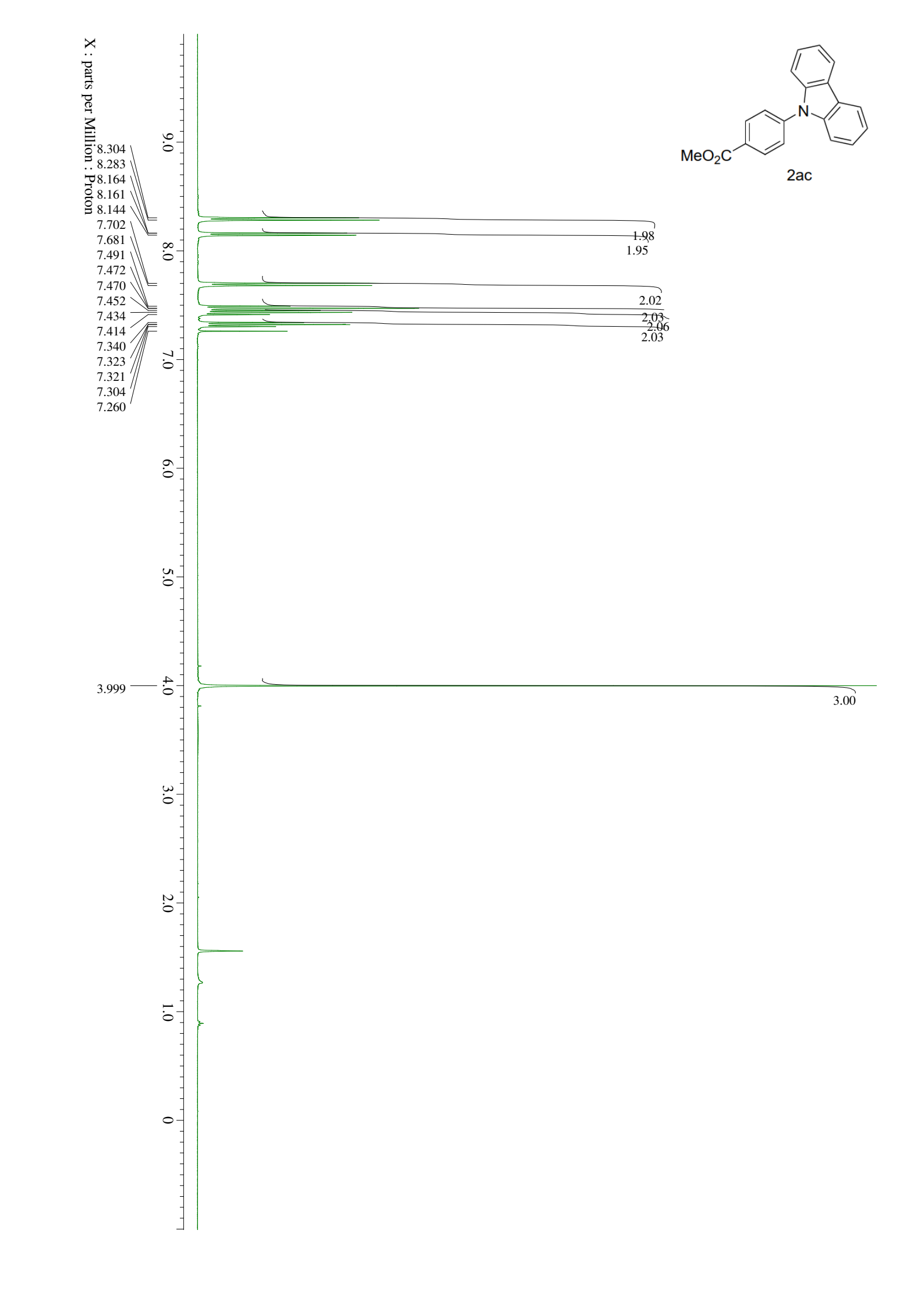

X : parts per Million : Proton
8.215
8.195
8.026
8.023
8.005
8.004
7.793
7.772
7.494
7.474
7.372
7.369
7.353
7.350
7.340
7.336
7.319
7.316
7.260
3.995
1.553
2.02
2.03
2.02
1.98
4.07
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
N
MeO2C
1ac

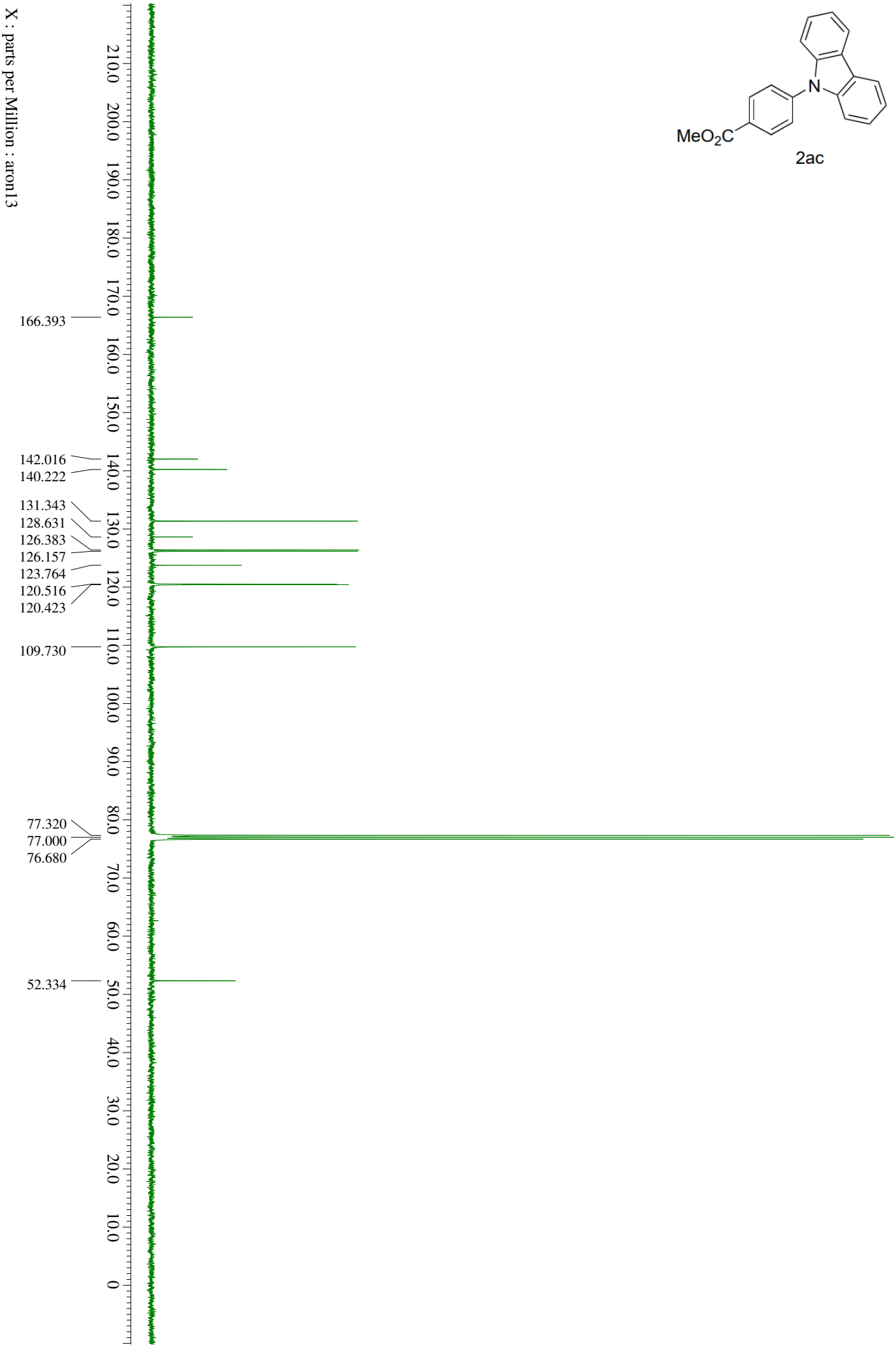
X : parts per Million : aron13

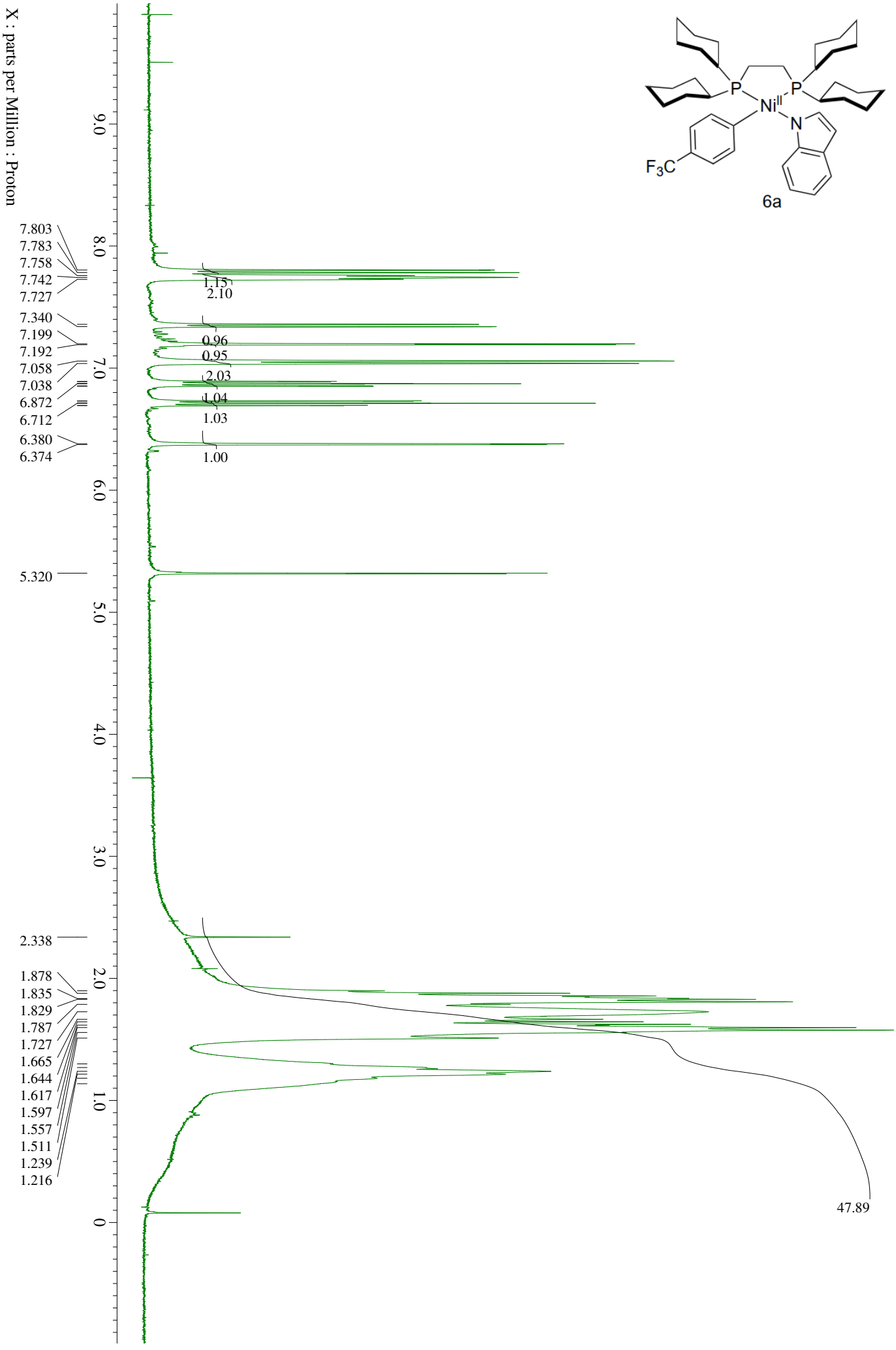
1ac

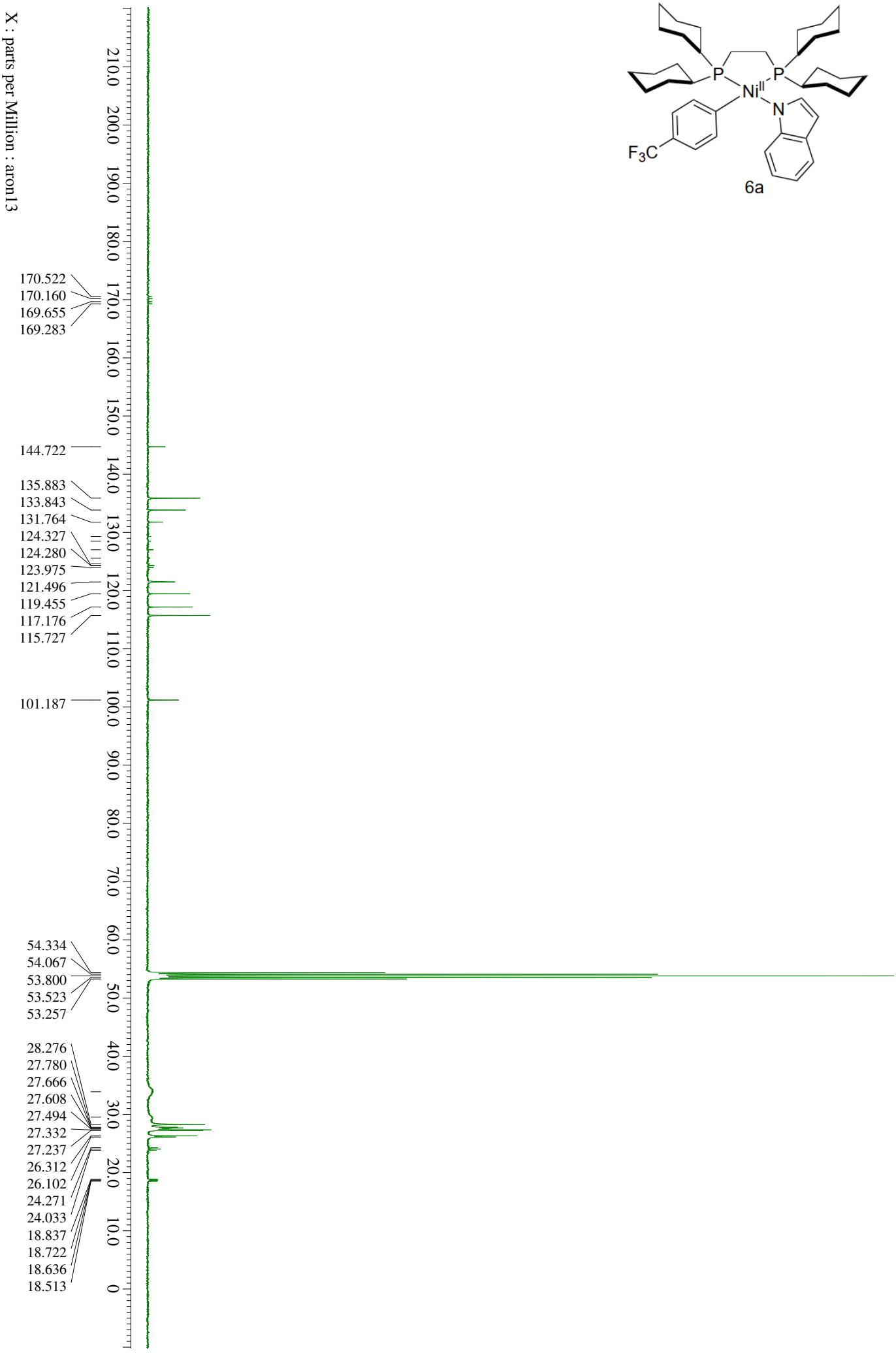
168.641
166.136
139.675
138.820
133.261
130.137
128.848
126.899
126.177
123.775
119.918
115.793
77.320
77.000
76.691
52.571

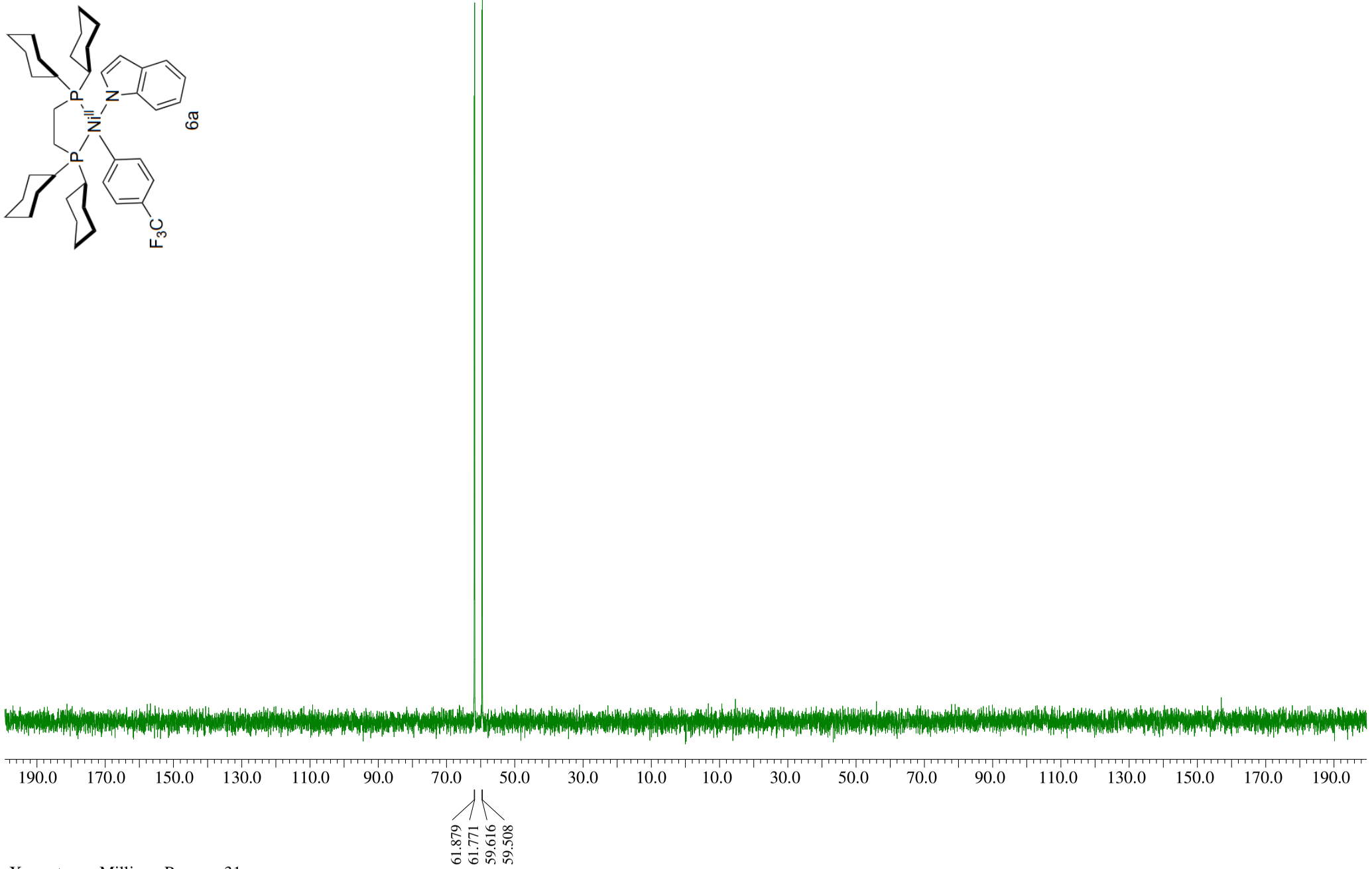
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0

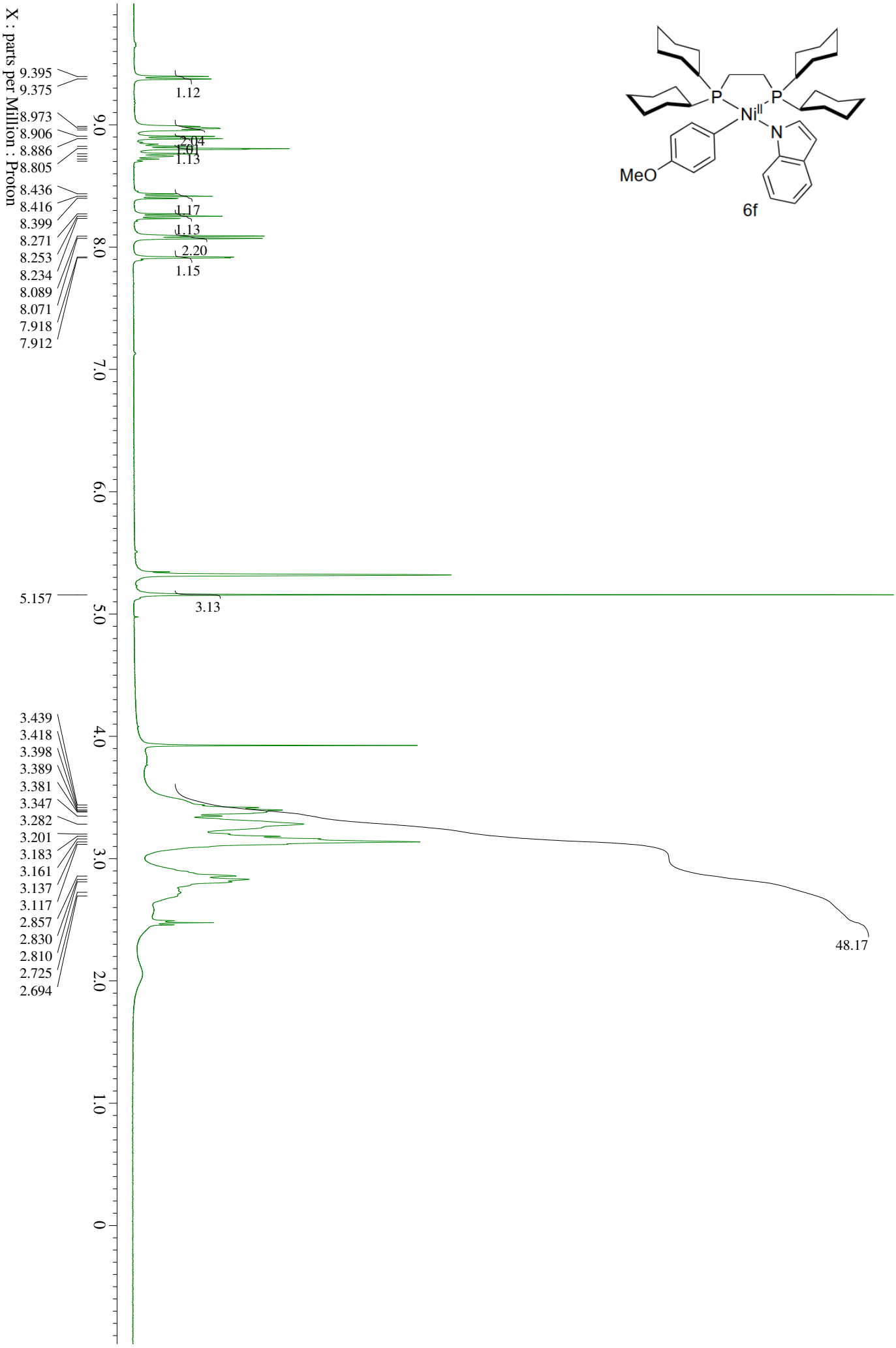

X : parts per Million : Proton
8.304
8.283
8.164
8.161
8.144
7.702
7.681
7.491
7.472
7.470
7.452
7.434
7.414
7.340
7.323
7.321
7.304
7.260
3.999
1.98
1.95
2.02
2.03
2.06
2.03
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
N
MeO2C
2ac

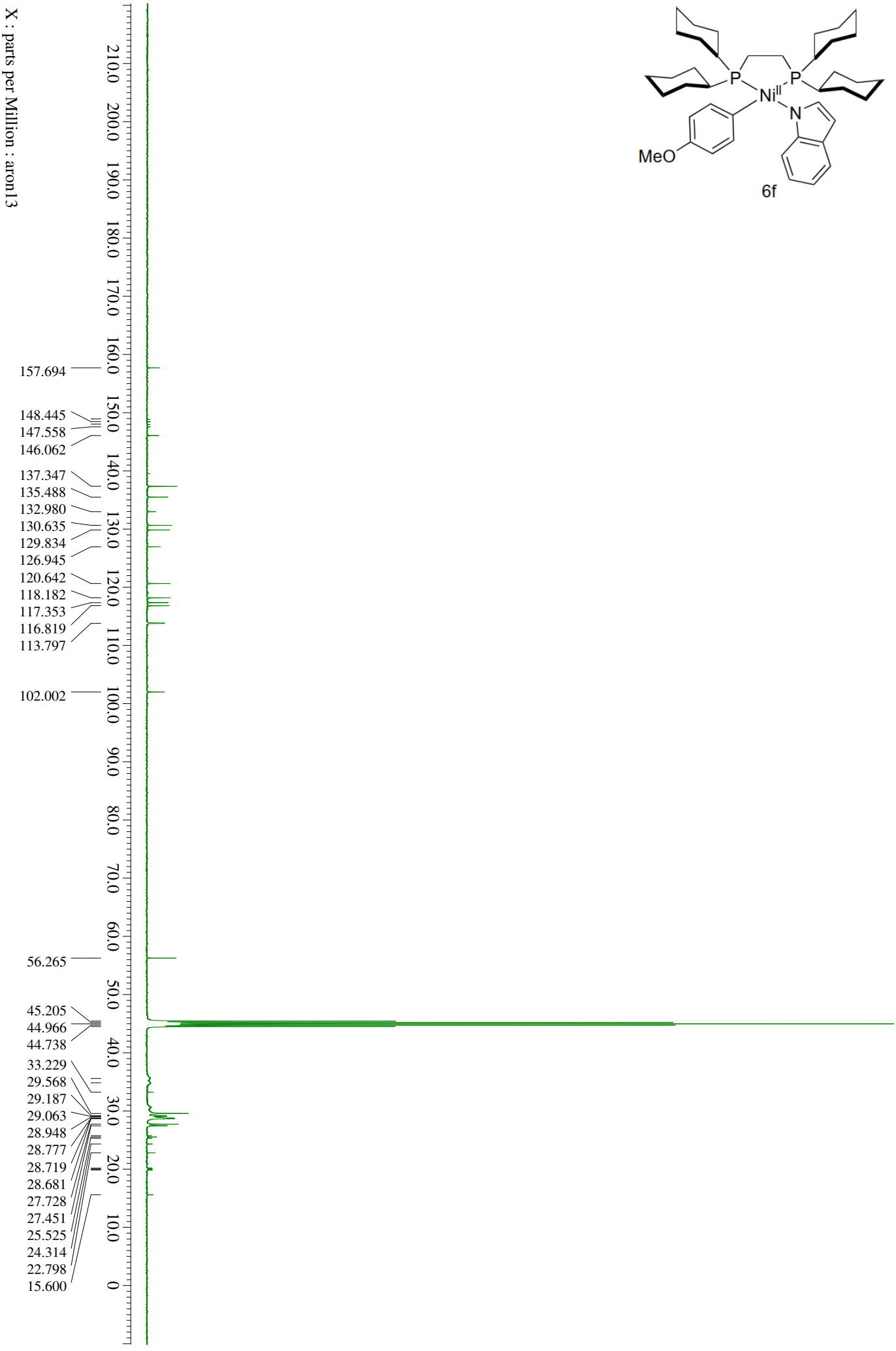

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.393
142.016
140.222
131.343
128.631
126.383
126.157
123.764
120.516
120.423
109.730
77.320
77.000
76.680
52.334
N
MeO2C
2ac

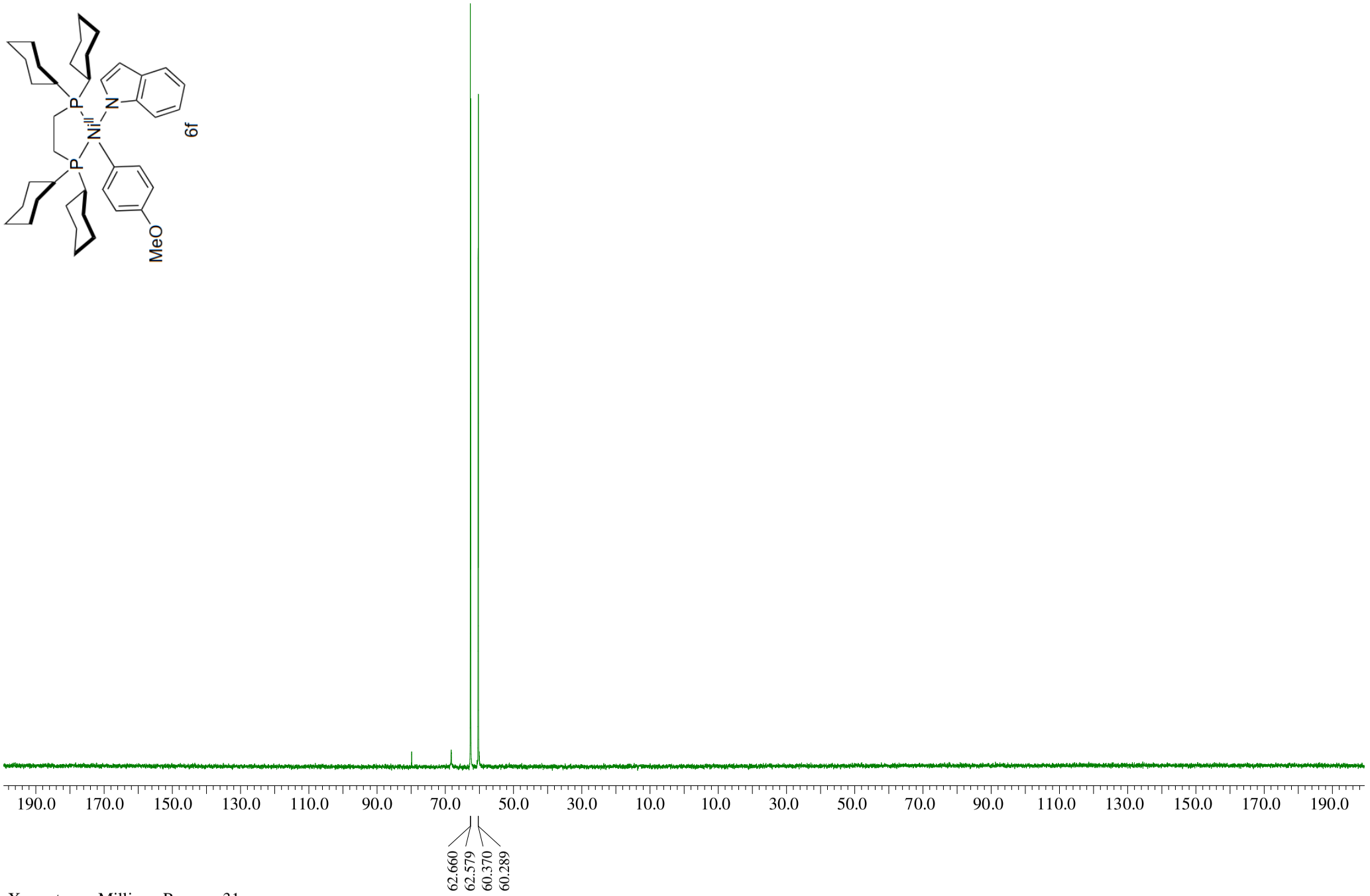

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.803
7.783
7.758
7.742
7.727
7.340
7.199
7.192
7.058
7.038
6.872
6.712
6.380
6.374
5.320
2.338
1.878
1.835
1.829
1.787
1.727
1.665
1.644
1.617
1.597
1.557
1.511
1.239
1.216
1.15
2.10
0.96
0.95
2.03
1.04
1.03
1.00
47.89
P
Ni
II
P
N
F3C
6a

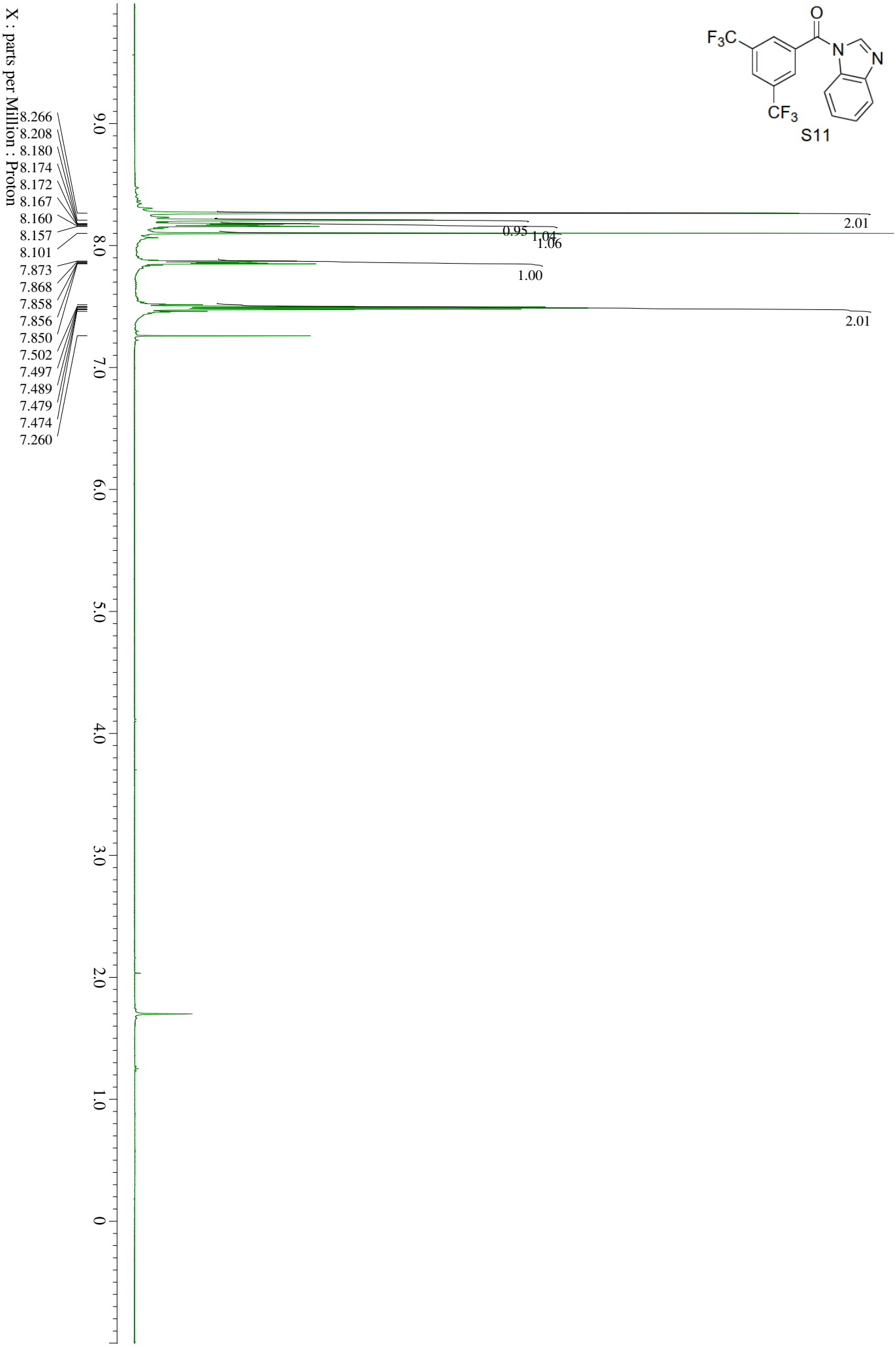

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.522
170.160
169.655
169.283
144.722
135.883
133.843
131.764
124.327
124.280
123.975
121.496
119.455
117.176
115.727
101.187
54.334
54.067
53.800
53.523
53.257
28.276
27.780
27.666
27.608
27.494
27.332
27.237
26.312
26.102
24.271
24.033
18.837
18.722
18.636
18.513
P
Ni
II
P
N
F3C
6a

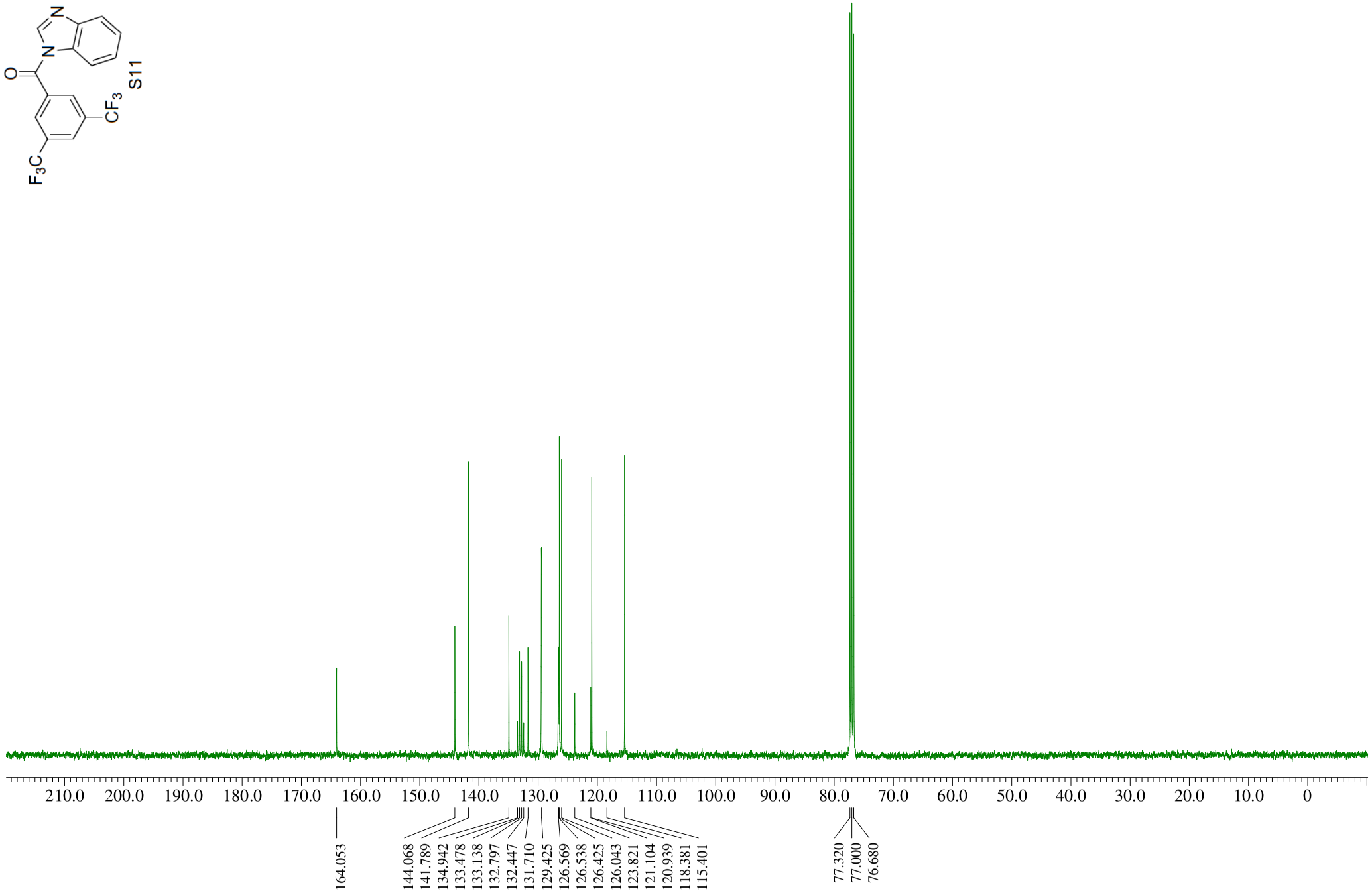

P
Ni
N
P
F3C
6a
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
10.0
30.0
50.0
70.0
90.0
110.0
130.0
150.0
170.0
190.0
61.879
61.771
59.616
59.508
X : parts per Million : Pospor s31

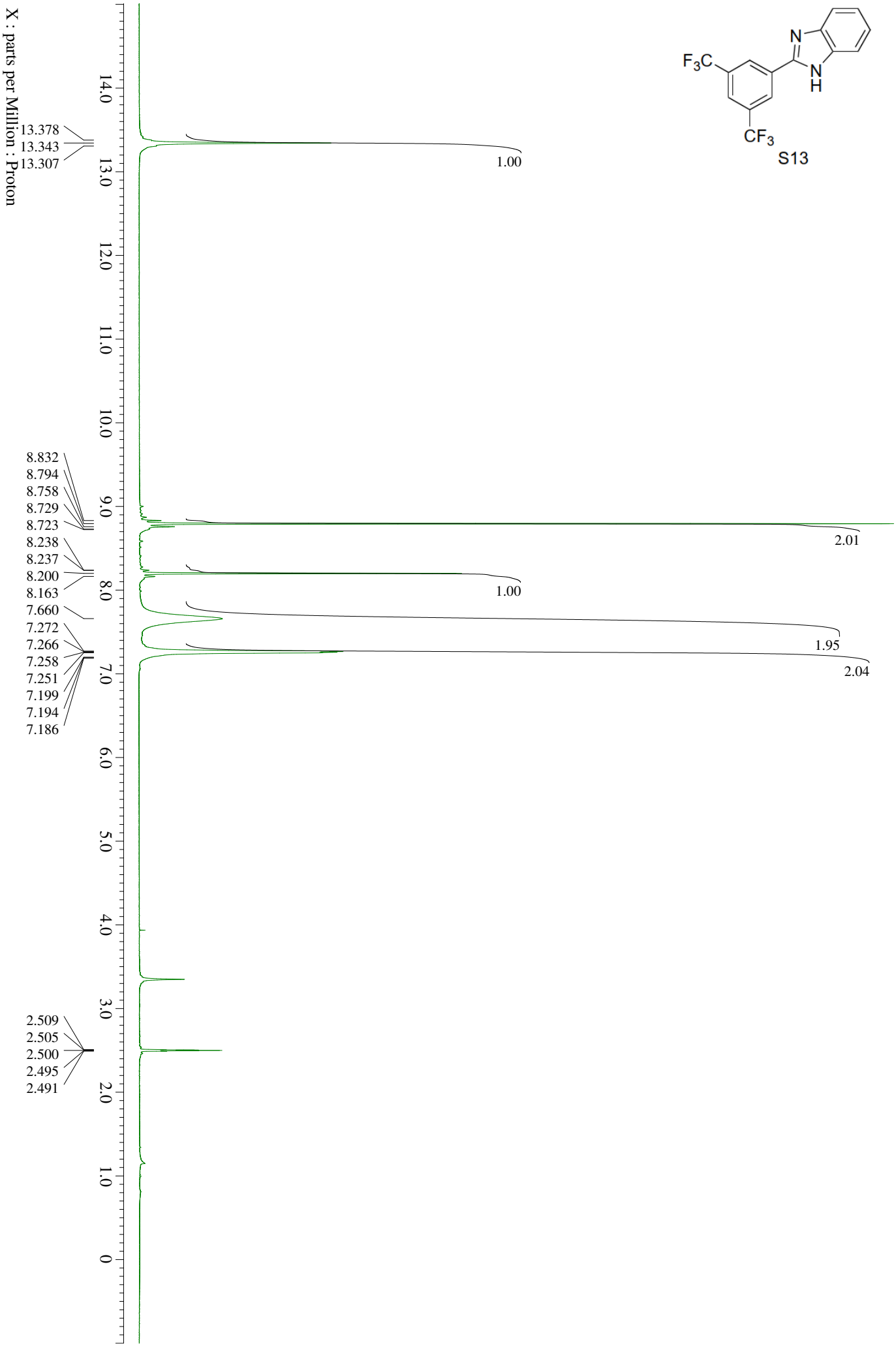

X : parts per Million : Proton
9.395
9.375
8.973
8.906
8.886
8.805
8.436
8.416
8.399
8.271
8.253
8.234
8.089
8.071
7.918
7.912
5.157
3.439
3.418
3.398
3.389
3.381
3.347
3.282
3.201
3.183
3.161
3.137
3.117
2.857
2.830
2.810
2.725
2.694
1.12
2.04
1.01
1.13
1.17
1.13
2.20
1.15
3.13
48.17
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
P
Ni
II
P
N
MeO
6f


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
157.694
148.445
147.558
146.062
137.347
135.488
132.980
130.635
129.834
126.945
120.642
118.182
117.353
116.819
113.797
102.002
56.265
45.205
44.966
44.738
33.229
29.568
29.187
29.063
28.948
28.777
28.719
28.681
27.728
27.451
25.525
24.314
22.798
15.600
P
Ni
II
P
N
MeO
6f


P
Ni
II
N
P
MeO
6f
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
10.0
30.0
50.0
70.0
90.0
110.0
130.0
150.0
170.0
190.0
62.660
62.579
60.370
60.289
X : parts per Million : Pospor s31


X : parts per Million : Proton
8.266
8.208
8.180
8.174
8.172
8.167
8.160
8.157
8.101
7.873
7.868
7.858
7.856
7.850
7.502
7.497
7.489
7.479
7.474
7.260
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.95
1.04
1.06
1.00
2.01
2.01
O
F3C
N
N
CF3
S11


S11
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.053
144.068
141.789
134.942
133.478
133.138
132.797
132.447
131.710
129.425
126.569
126.538
126.425
126.043
123.821
121.104
120.939
118.381
115.401
77.320
77.000
76.680
X : parts per Million : aron13


X : parts per Million : Proton
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
13.378
13.343
13.307
1.00
8.832
8.794
8.758
8.729
8.723
2.01
8.238
8.237
8.200
8.163
1.00
7.660
7.272
7.266
7.258
7.251
7.199
7.194
7.186
1.95
2.04
2.509
2.505
2.500
2.495
2.491
N
F3C
N
H
CF3
S13

X : parts per Million : aron13

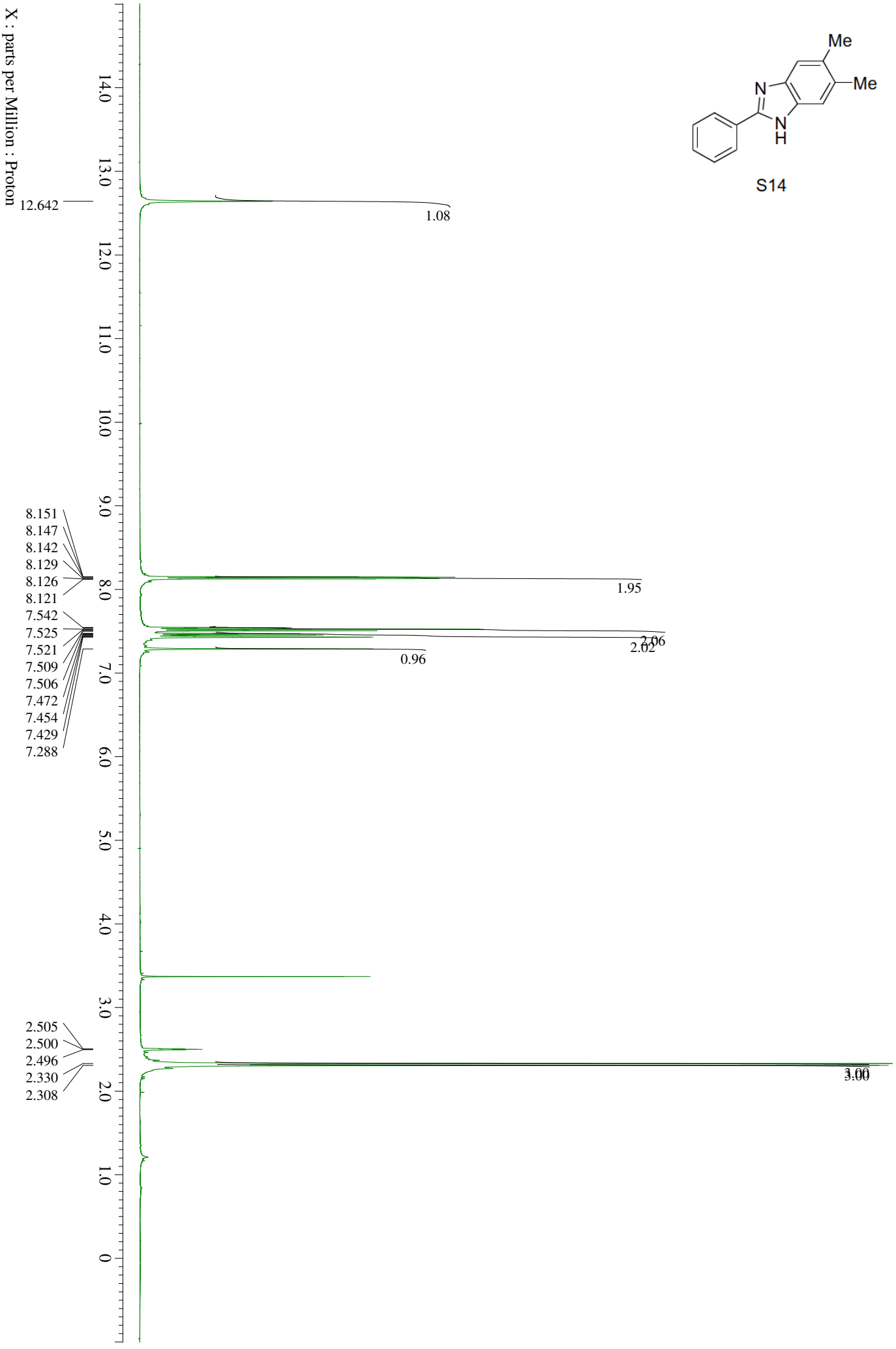
206.188

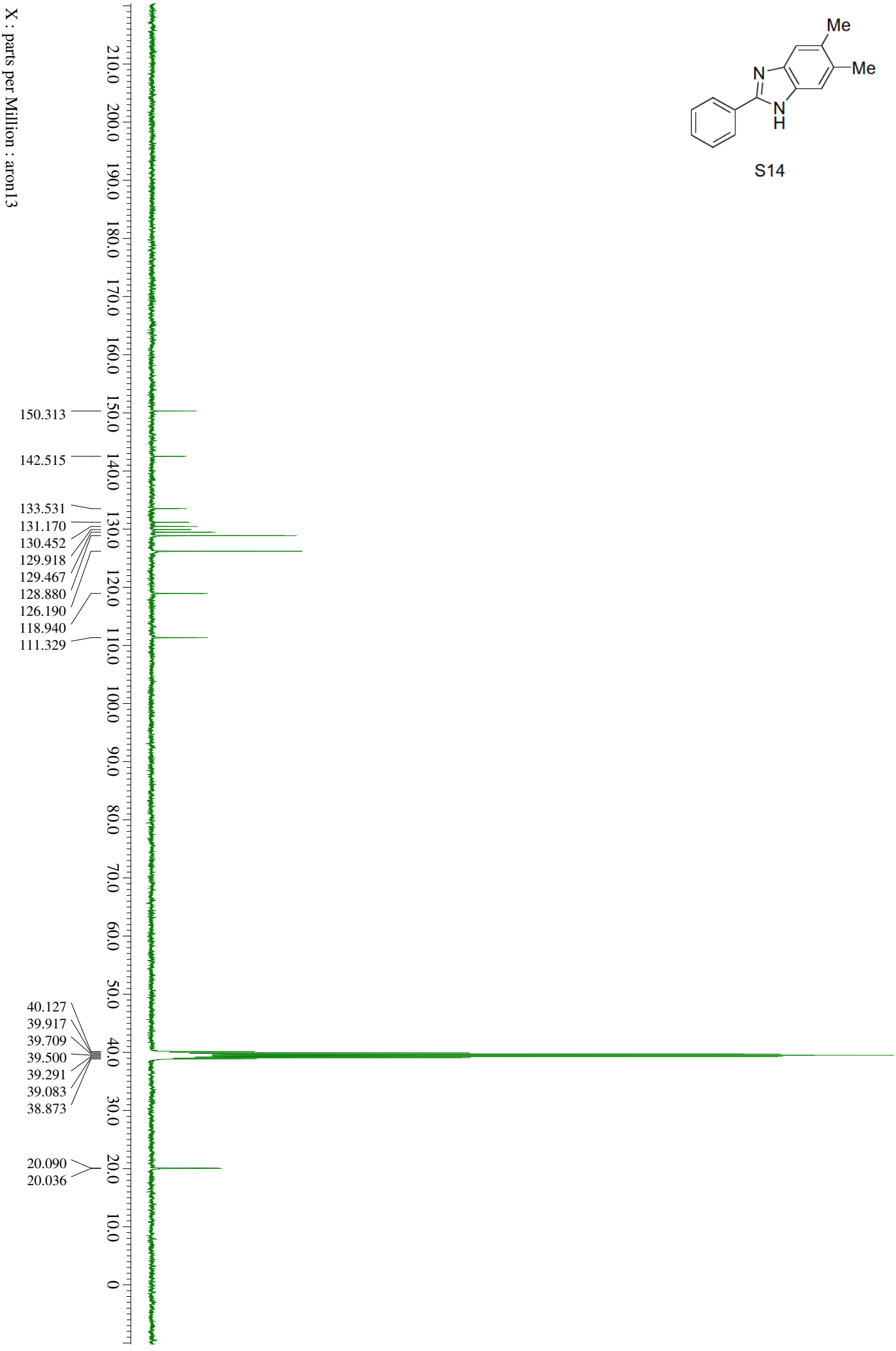
149.202

133.870
133.241
132.909
132.576
132.244
127.525
127.499
125.656
124.023
123.642
123.606
123.570
122.948
120.240

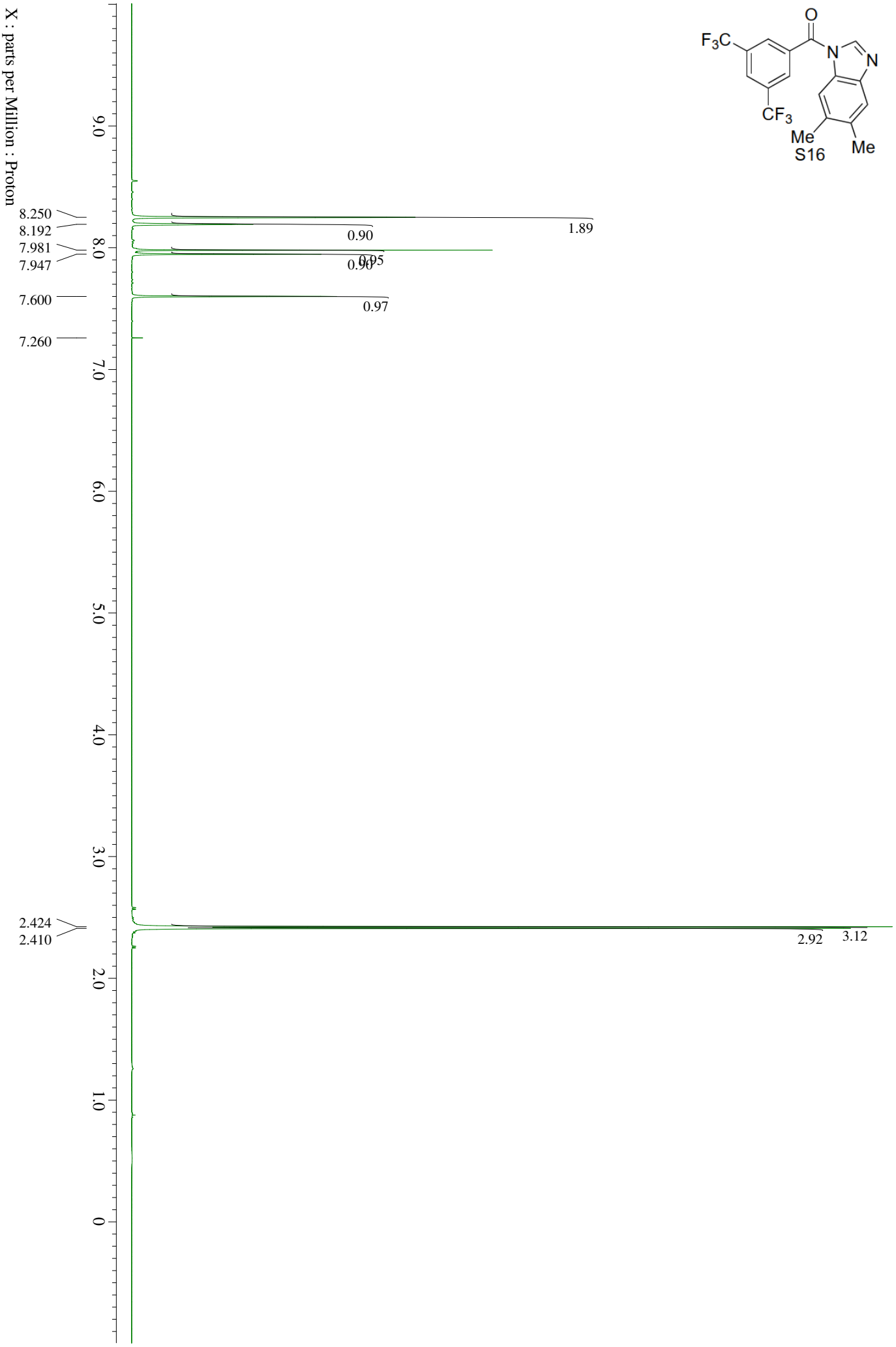
30.377
30.184
29.991
29.800
29.607
29.414
29.221

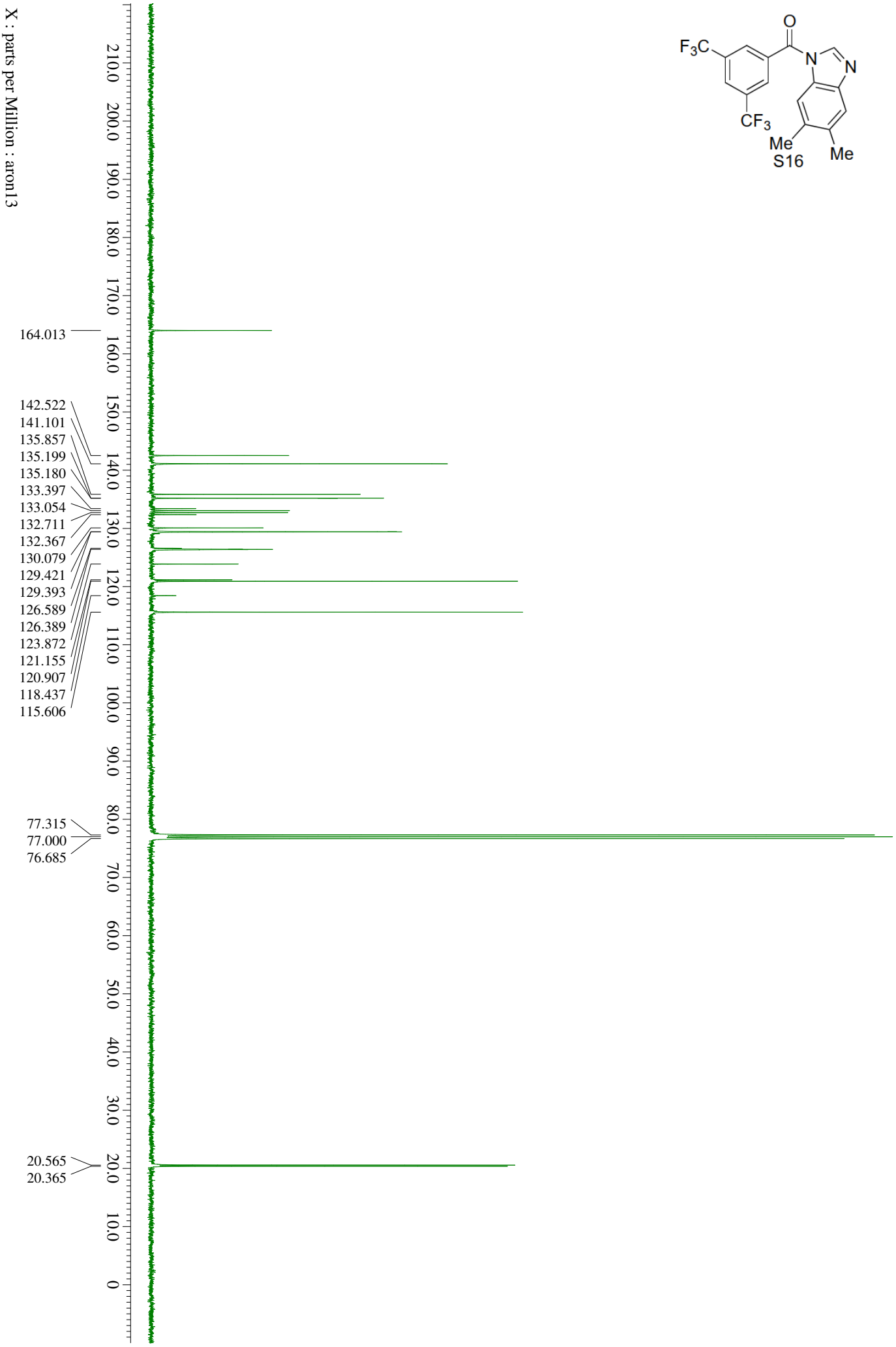
S13

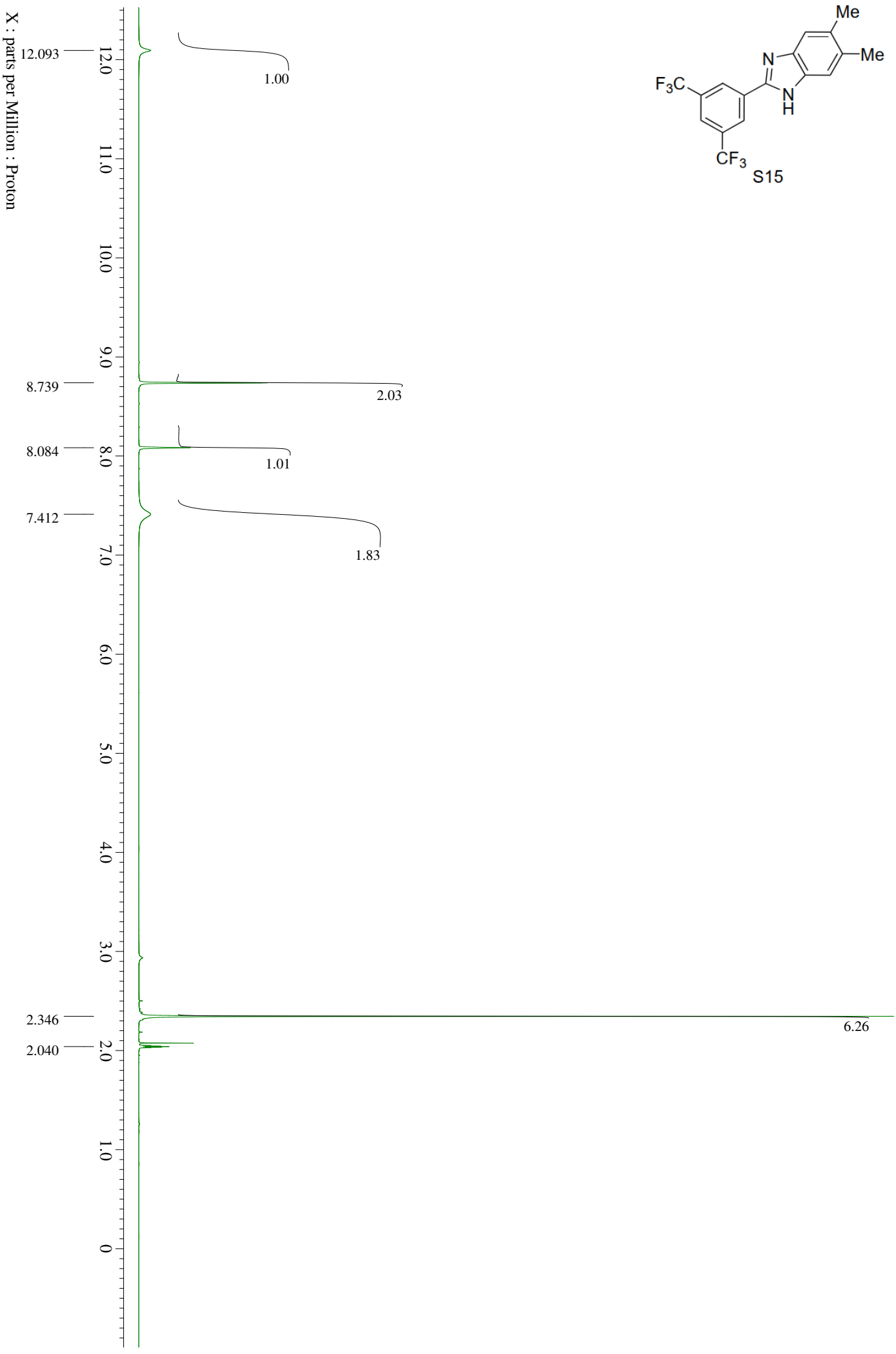

X : parts per Million : Proton
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
12.642
1.08
8.151
8.147
8.142
8.129
8.126
8.121
1.95
7.542
7.525
7.521
7.509
7.506
7.472
7.454
7.429
7.288
2.06
2.02
0.96
2.505
2.500
2.496
2.330
2.308
3.00
Me
Me
N
N
H
S14

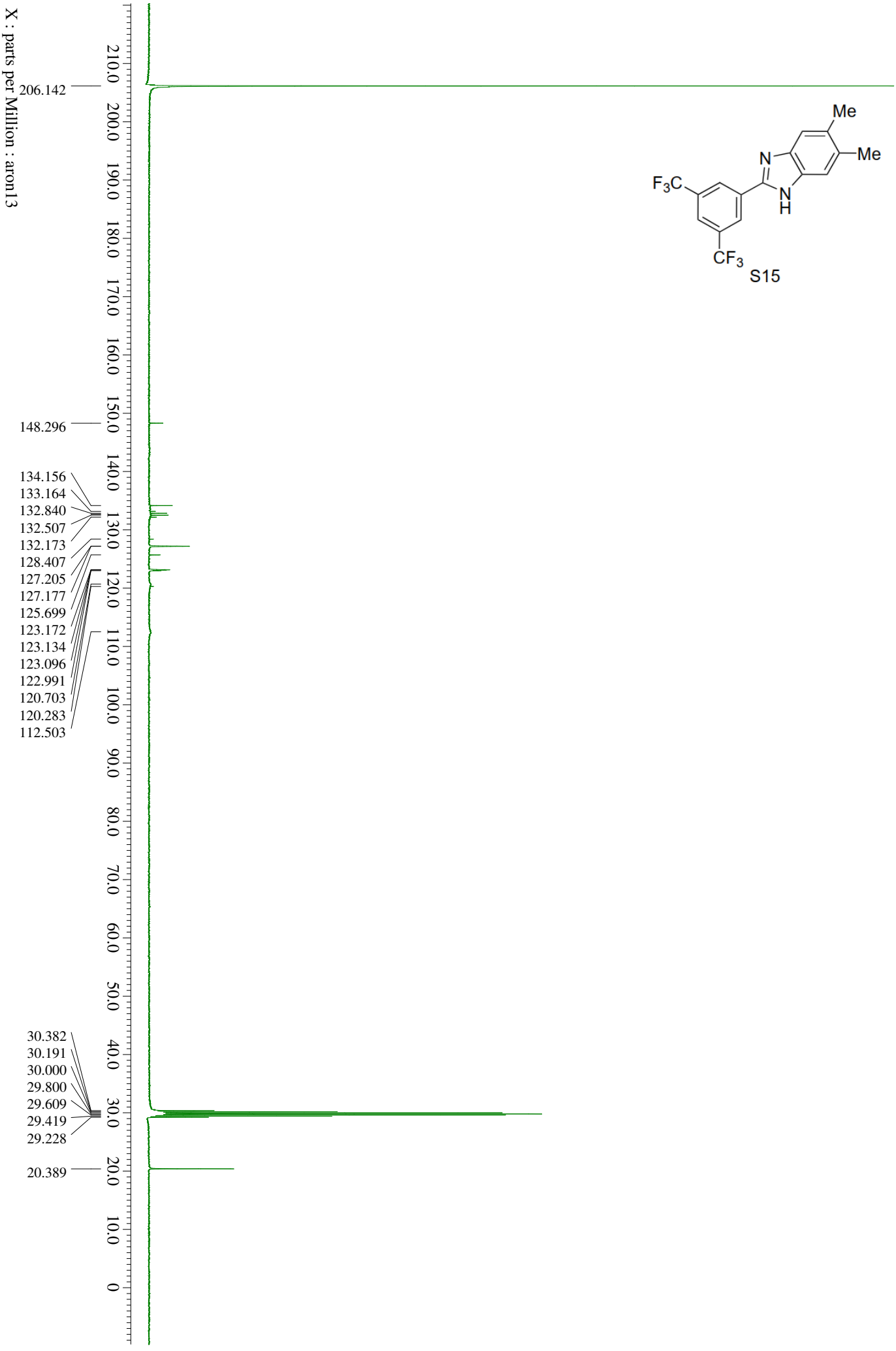

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
150.313
142.515
133.531
131.170
130.452
129.918
129.467
128.880
126.190
118.940
111.329
40.127
39.917
39.709
39.500
39.291
39.083
38.873
20.090
20.036
Me
Me
N
N
H

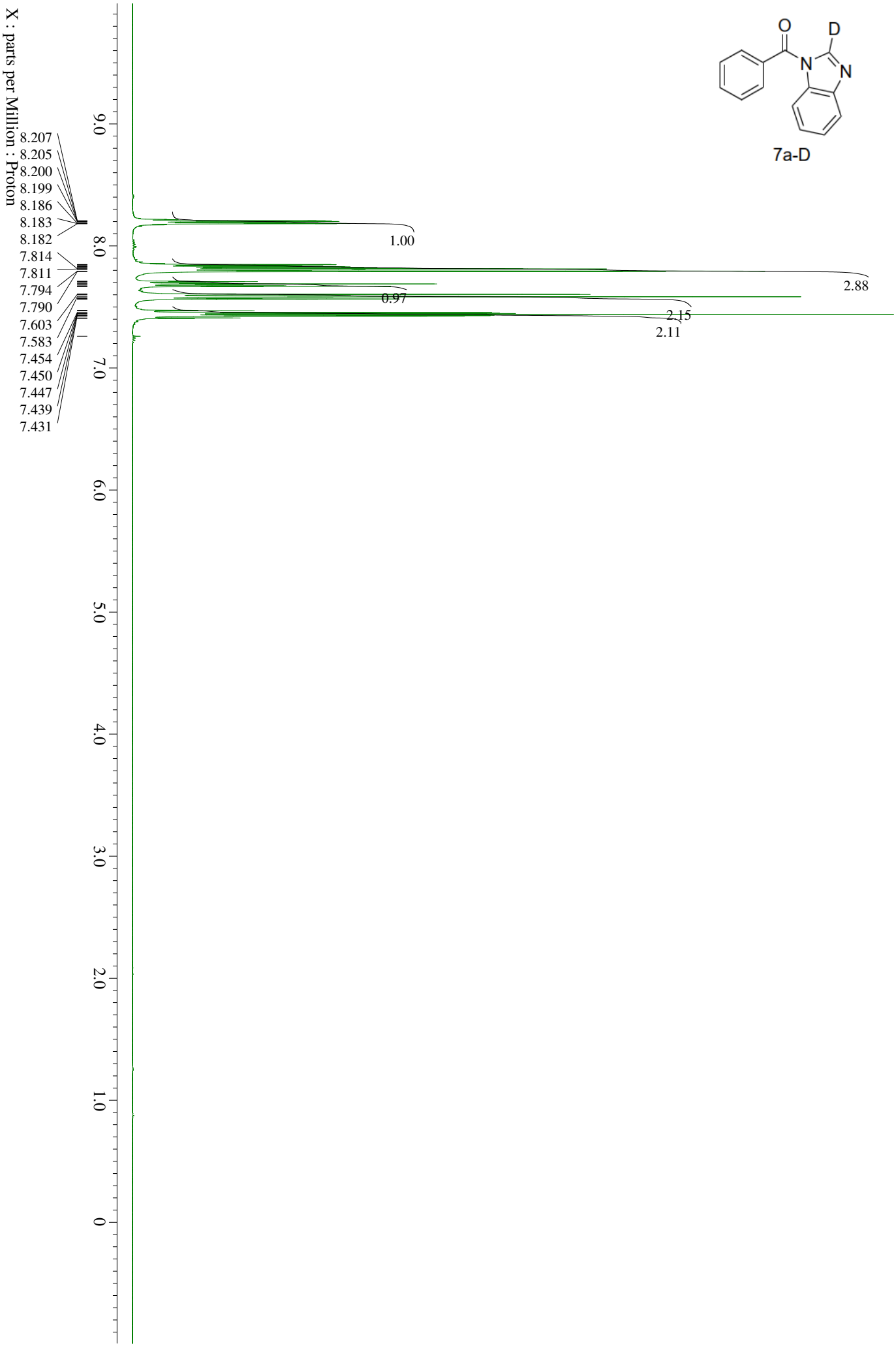
S14

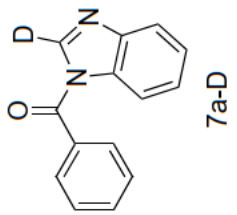

X : parts per Million : Proton
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.250
8.192
7.981
7.947
7.600
7.260
2.424
2.410
1.89
0.90
0.95
0.90
0.97
2.92
3.12
O
F3C
N
N
CF3
Me
Me
S16


X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.013
142.522
141.101
135.857
135.199
135.180
133.397
133.054
132.711
132.367
130.079
129.421
129.393
126.589
126.389
123.872
121.155
120.907
118.437
115.606
77.315
77.000
76.685
20.565
20.365
O
F3C
N
N
CF3
Me
Me
S16


X : parts per Million : Proton
12.093
8.739
8.084
7.412
2.346
2.040
1.00
2.03
1.01
1.83
6.26
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Me
Me
N
N
H
F3C
CF3
S15


X : parts per Million : aron13
206.142
148.296
134.156
133.164
132.840
132.507
132.173
128.407
127.205
127.177
125.699
123.172
123.134
123.096
122.991
120.703
120.283
112.503
30.382
30.191
30.000
29.800
29.609
29.419
29.228
20.389
Me
Me
N
N
H
F3C
CF3
S15


X : parts per Million : Proton
8.207
8.205
8.200
8.199
8.186
8.183
8.182
7.814
7.811
7.794
7.790
7.603
7.583
7.454
7.450
7.447
7.439
7.431
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
0.97
2.88
2.15
2.11
O
D
N
N
7a-D



7a-D

X : parts per Million : e teri

X : parts per Million : aron13
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
167.045
144.038
143.103
142.770
142.455
133.178
132.815
132.062
129.507
129.011
125.712
125.235
120.525
115.424
77.324
77.000
76.685
O
D
N
N
7a-D