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Supporting Information

Cobalt-Catalyzed Chelation Assisted C-H Allylation of Aromatic Amides with Unactivated Olefins

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Contents

I. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer in $CDCl_3$ with tetramethylsilane as the internal standard. Data are reported as follows: chemical shifts in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, and m = multiplet), coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra and high resolution mass spectra (HRMS) were obtained using a JEOL JMS-700 spectrometer. Column chromatography was performed with SiO_2 (Silicycle SiliaFlash F60 (230-400 mesh)). Some compounds were purified by HPLC (Phenomenex Luna 5u Silica (2) 100 × 21.20 mm column with hexane/EtOAc (30/1) as an eluent).

II. Materials

$Co(OAc)_2 \cdot 4H_2O$ (CAS 6147-53-1) was purchased from Wako Pure Chemical Industries, Ltd. Ag_2CO_3 (CAS 534-16-7) was purchased from Nacalai Tesque. 1-Octene (CAS 111-66-0) and 8-aminoquinoline were purchased from Tokyo Chemical Industry Co., Ltd. DCE (CAS 107-06-2) was purchased from Sigma-Aldrich. These reagents were used as received.

III. Synthesis of Starting Amides

All amides bearing an 8-aminoquinoline moiety were prepared by reacting the corresponding acid or acid chloride with 8-aminoquinoline.[1]

General Procedure for the Preparation of Starting Amides.

(1) Synthesis of amides from acid chlorides.

The appropriate acid chloride (15 mmol) was dissolved in CH_2Cl_2 (20 mL). After cooling the reaction mixture to 0 °C, a solution of 8-aminoquinoline (17 mmol) and triethylamine (30 mmol) in 10 mL of CH_2Cl_2 was added dropwise. The resulting mixture was allowed to warm to rt and was then stirred overnight. The crude mixture was then washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x20 mL). The combined organic layers were washed with 1 M HCl aq. (20 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solution evaporated to dryness.The resulting crude amide was purified by flash chromatography on silica gel (eluent: hexane/EtOAc = 5/1).

(2) Synthesis of amides from carboxylic acids.

[1] (a) Ano, Y.; Tobisu, M.; Chatani, N. *Org. Lett.* **2012**, *14*, 354. (b) Aihara, Y.; Chatani, N. *Chem. Sci.* **2012**, *4*, 664. (c) Shibata, K.; Chatani, N. *Org. Lett.* **2014**, *16*, 5148.

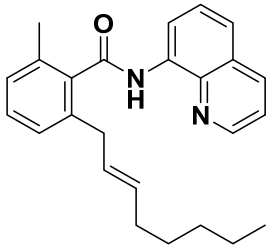
To a stirred solution of a carboxylic acid (15 mmol) and DMF (5 drops) in CH_2Cl_2 (10 mL), $(COCl)_2$ (1.5 mL, 18 mmol) was added dropwise. The solution was magnetically stirred at room temperature for 2 h. The solvent was then removed by evaporation under reduced pressure, and the resulting residue was dissolved in CH_2Cl_2 (15 mL). After cooling the reaction mixture to 0 °C, a solution of 8-Aminoquinoline (17 mmol) and triethylamine (30 mmol) in 10 mL of the same solvent was added dropwise. The resulting mixture was allowed to warm to rt and stirred overnight. The solution containing the crude product was washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x20 mL). The combined organic phase was washed with 1 M HCl aq. (20 mL).The organic phase was dried over anhydrous Na_2SO_4 and the solvent removed by evaporation. The resulting crude amide was purified by flash chromatography on silica gel (eluent: hexane/EtOAc = 5/1).

IV. General Procedure for the Direct Allylation of C-H Bonds in Aromatic Amides with 1-Octene

To a 5 mL screw-capped vial, 2-methyl-*N*-(8-quinolinyl)benzamide **1a** (39 mg, 0.15 mmol), $Co(OAc)_2 \cdot 4H_2O$ (7.5 mg, 0.03 mmol), Ag_2CO_3 (83 mg, 0.3 mmol), 1-octene (34 mg, 0.3 mmol), and DCE (0.5 mL) were added in air. The mixture was stirred for 12 h at 100 °C followed by cooling. The mixture was filtered through a celite pad and the filtrate was concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 30/1) to afford the allylation product **3aa** (44 mg, 79%, E/Z = 21:1) as a colorless oil. The E/Z ratio was determined by the integration of Ar-C<u>H$_2$</u>-C=.

V. Spectroscopic Data

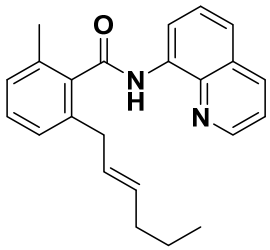
(*E*)-2-Methyl-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3aa) [CAS:1620466-49-0]



79% yield (E/Z = 21:1). Colorless oil. R_f 0.21 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.79 (t, *J* = 6.9 Hz, 3H), 1.06-1.20 (m, 6H), 1.80-1.85 (m, 2H), 2.44 (s, 3H), 3.45 (d, *J* = 6.4 Hz, 2H), 5.37-5.44 (m, 1H), 5.56 (dt, *J* = 15.1, 6.9 Hz, 1H), 7.12-7.15 (m, 2H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55-7.63 (m, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.73 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.99 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.92 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.99, 19.48, 22.40, 28.82, 31.37, 32.33, 36.65, 116.76, 121.60, 121.86, 127.00, 127.41, 127.99, 128.03,

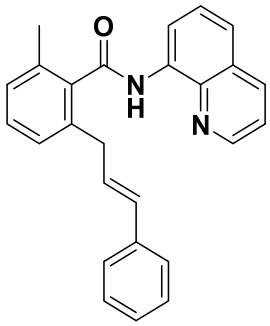
128.07, 129.06, 132.44, 134.40, 134.65, 136.29, 137.68, 137.74, 138.50, 148.18, 168.65. IR (ATR): 3346 w, 2955 w, 2925 w, 2854 w, 1677 m, 1520 s, 1482 m, 1424 m, 1385 m, 1326 m, 1263 w, 1126 w, 970 w, 897 w, 826 w. MS, *m/z* (relative intensity, %): 373 (10), 372 (M^+, 36), 371 (23), 185 (10), 171 (14), 159 (32), 158 (100), 157 (13), 145 (20), 144 (61), 143 (12), 131 (12), 129 (16), 128 (20), 115 (12), 55 (11). HRMS Calcd for $C_{25}H_{28}N_2O$ 372.2202, found 372.2194.

(*E*)-2-(Hex-2-en-1-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3ab) [CAS:1620466-12-7]



76% yield (E/Z = 21:1). Colorless oil. R_f 0.63 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.74 (t, *J* = 7.3 Hz, 3H), 1.16-1.26 (m, 2H), 1.80-1.85 (m, 2H), 2.44 (s, 3H), 3.45 (d, *J* = 6.4 Hz, 2H), 5.37-5.44 (m, 1H), 5.53-5.61 (m, 1H), 7.12-7.16 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55-7.63 (m, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.73 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.99 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.92 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.60, 19.48, 22.29, 34.44, 36.62, 116.76, 121.61, 121.88, 126.98, 127.40, 127.99, 128.03, 128.31, 129.06, 132.20, 134.39, 134.65, 136.28, 137.66, 137.71, 138.51, 148.19, 168.67. IR (ATR): 3346 w, 2956 w, 2925 w, 2870 w, 1675 m, 1518 s, 1482 s, 1424 m, 1385 m, 1326 m, 1263 w, 1126 w, 969 w, 897 w, 826 w. MS, *m/z* (relative intensity, %): 345 (10), 344 (M^+, 37), 343 (22), 201 (10), 185 (10), 171 (13), 159 (26), 158 (100), 157 (15), 145 (26), 144 (63), 143 (10), 131 (25), 129 (14), 128 (17), 115 (12), 55 (10). HRMS Calcd for $C_{23}H_{24}N_2O$ 344.1889, found 344.1886.

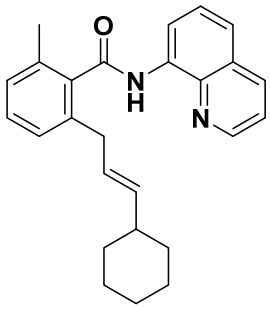
2-Cinnamyl-6-methyl-*N*-(quinolin-8-yl)benzamide (3ac) [CAS:1620466-04-7]



85% yield (E/Z = 29:1). Colorless oil. R_f 0.44 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 2.46 (s, 3H), 3.64 (d, *J* = 6.0 Hz, 2H), 6.27-6.39 (m, 2H), 7.06-7.13 (m, 5H), 7.16-7.21 (m, 2H), 7.29-7.35 (m, 2H), 7.53-7.61 (m, 2H), 8.11 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.48 (dd, *J* = 4.1, 1.4 Hz, 1H),

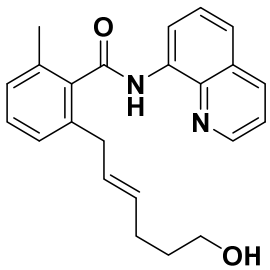
9.00 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.96 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.47, 37.09, 116.72, 121.55, 121.97, 125.97, 126.78, 127.27, 127.30, 127.92, 128.13, 128.38, 128.60, 129.21, 131.24, 134.28, 134.89, 136.12, 136.72, 137.21, 137.88, 138.36, 148.15, 168.56. IR (ATR): 3343 w, 3025 w, 2922 w, 1675 m, 1518 s, 1482 s, 1424 m, 1385 m, 1326 m, 1262 w, 1126 w, 967 w, 897 w, 826 w. MS, *m/z* (relative intensity, %): 378 (M^+, 26), 235 (21), 234 (100), 233 (29), 206 (10), 191 (20), 144 (37), 115 (11), 91 (50). HRMS Calcd for $C_{26}H_{22}N_2O$ 378.1732, found 378.1729.

(*E*)-2-(3-Cyclohexylallyl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3ad)



72% yield. Colorless oil. R_f 0.60 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.80-0.90 (m, 2H), 0.97-1.15 (m, 3H), 1.50-1.58 (m, 5H), 1.73-1.74 (m, 1H), 2.44 (s, 3H), 3.44 (d, *J* = 6.9 Hz, 2H), 5.37 (dd, *J* = 15.1, 6.4 Hz, 1H), 5.47-5.55 (m, 1H), 7.12-7.15 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55 -7.63 (m, 2H), 8.17 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.72 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.99 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.91 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.47, 25.97, 26.09, 32.73, 36.71, 40.33, 116.75, 121.58, 121.85, 125.61, 126.96, 127.40, 127.98, 128.02, 129.05, 134.41, 134.62, 136.27, 137.69, 137.86, 138.24, 138.51, 148.18, 168.65. IR (ATR): 3347 w, 2923 m, 2849 w, 1678 m, 1520 s, 1482 m, 1424 w, 1385 w, 1326 m, 1261 w, 970 w, 897 w, 826 w. MS, *m/z* (relative intensity, %): 384 (M^+, 24), 383 (10), 159 (23), 158 (100), 145 (10), 144 (39), 95 (19). HRMS Calcd for $C_{26}H_{28}N_2O$ 384.2202, found 384.2200.

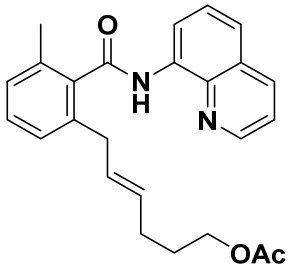
(*E*)-2-(6-Hydroxyhex-2-en-1-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3ae)



65% yield. Colorless oil. R_f 0.29 (hexane/EtOAc = 4/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.42-1.49 (m, 2H), 1.91-1.96 (m, 2H), 2.43 (s, 3H), 3.44-3.49 (m, 4H), 5.37-5.44 (m, 1H), 5.58-5.63 (m, 1H), 7.12-7.14 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55-7.63 (m, 2H), 8.18 (d,

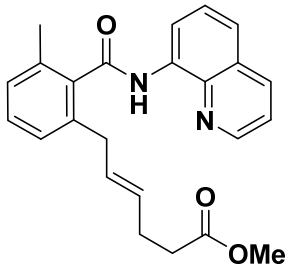
J = 8.2 Hz, 1H), 8.73 (d, *J* = 4.1 Hz, 1H), 8.98 (d, *J* = 7.3 Hz, 1H), 9.92 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.46, 28.61, 31.98, 36.63, 62.30, 116.78, 121.65, 121.94, 127.02, 127.41, 127.98, 128.13, 128.98, 129.13, 131.34, 134.32, 134.71, 136.32, 137.43, 137.63, 138.46, 148.24, 168.63. IR (ATR): 3348 w, 2953 w, 2925 w, 2854 w, 1678 m, 1520 s, 1482 s, 1424 m, 1385 m, 1326 m, 1246 m, 1126 w, 971 w, 897 w, 826 w. MS, *m/z* (relative intensity, %): 360 (M^+, 28), 359 (21), 216 (13), 199 (10), 198 (43), 171 (19), 170 (16), 157 (12), 145 (23), 144 (100), 143 (15), 129 (18), 128 (19), 115 (12), 71 (38). HRMS Calcd for $C_{23}H_{24}N_2O_2$ 360.1838, found 360.1831.

(*E*)-6-(3-Methyl-2-(quinolin-8-ylcarbamoyl)phenyl)hex-4-en-1-yl acetate (3af)



85% yield (E/Z = 25:1). Colorless oil. R_f 0.33 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.48-1.56 (m, 2H), 1.89-1.94 (m, 2H), 1.99 (s, 3H), 2.44 (s, 3H), 3.45 (d, *J* = 6.4 Hz, 2H), 3.91 (t, *J* = 6.6 Hz, 2H), 5.39 (dt, *J* = 15.3, 6.6 Hz, 1H), 5.58-5.65 (m, 1H), 7.12-7.15 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.45 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55-7.63 (m, 2H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.73 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.99 (dd, *J* = 7.6, 1.6 Hz, 1H), 9.91 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.47, 20.93, 28.04, 28.64, 36.62, 63.93, 116.77, 121.64, 121.92, 127.01, 127.42, 127.99, 128.15, 129.13, 129.32, 130.66, 134.34, 134.72, 136.31, 137.36, 137.68, 138.47, 148.21, 168.58, 171.06. IR (ATR): 3347 w, 2926 w, 1736 m, 1676 m, 1520 s, 1482 s, 1424 m, 1385 m, 1326 m, 1243 m, 1127 w, 1042 w, 970 w, 897 w, 827 w. MS, *m/z* (relative intensity, %): 403 (10), 402 (M^+, 33), 401 (18), 199 (30), 198 (100), 171 (11), 170 (14), 157 (12), 145 (16), 144 (49), 143 (17), 129 (15), 128 (14), 71 (14). HRMS Calcd for $C_{25}H_{26}N_2O_3$ 402.1943, found 402.1942.

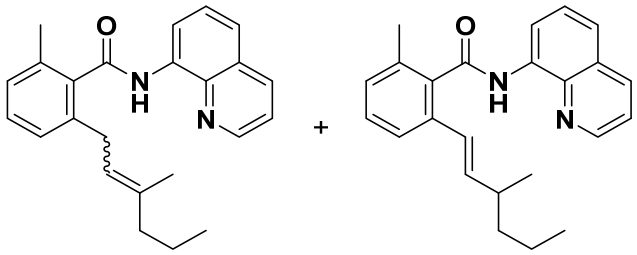
Methyl (*E*)-6-(3-methyl-2-(quinolin-8-ylcarbamoyl)phenyl)hex-4-enoate (3ag)



65% yield. Colorless oil. R_f 0.20 (hexane/EtOAc = 5/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 2.16-2.24 (m, 4H), 2.43 (s, 3H), 3.44 (d, *J* = 6.4 Hz, 2H), 3.58 (s, 3H), 5.37-5.44 (m, 1H), 5.60-5.67 (m, 1H),

7.11-7.15 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.45 (dd, *J* = 8.2, 4.6 Hz, 1H), 7.56-7.63 (m, 2H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.74 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.98 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.91 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.46, 27.58, 33.61, 36.53, 51.39, 116.76, 121.66, 121.96, 126.99, 127.40, 128.00, 128.18, 129.11, 129.66, 129.89, 134.31, 134.73, 136.31, 137.20, 137.67, 138.45, 148.28, 168.57, 173.51. IR (ATR): 3345 w, 2950 w, 2929 w, 2850 w, 1735 m, 1674 m, 1518 s, 1481 s, 1424 m, 1384 m, 1325 m, 1261 m, 1168 m, 970 w, 897 w, 827 m. MS, *m/z* (relative intensity, %): 388 (M^+, 21), 387 (12), 213 (41), 212 (100), 185 (52), 184 (23), 171 (28), 170 (49), 169 (13), 167 (23), 157 (19), 155 (10), 145 (20), 144 (94), 143 (24), 142 (30), 141 (24), 129 (27), 128 (41), 127 (10), 117 (10), 116 (13), 115 (21), 91 (11), 55 (31). HRMS Calcd for $C_{24}H_{24}N_2O_3$ 388.1787, found 388.1784.

2-Methyl-6-(3-methylhex-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ah) and (*E*)-2-methyl-6-(3-methylhex-1-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ah')



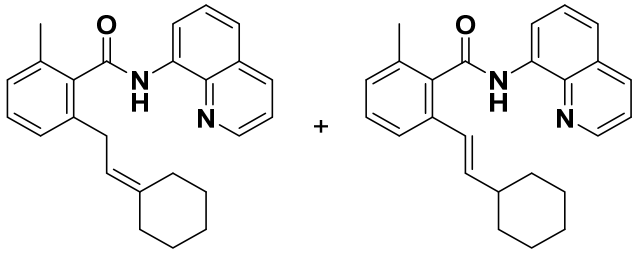
3ah **3ah'**

The spectra were obtained from the mixture (**3ah-E**/**3ah-Z**/**3ah'** = 3.4:1.0:1.6). The E/Z ratio was determined by the integration of -C=C(C<u>H</u>$_3$)-^{n}Pr.

55% yield. Colorless oil. R_f 0.63 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.59 (t, *J* = 6.9 Hz, **3ah'**), 0.71-0.75 (m, **3ah**), 0.89 (d, *J* = 6.9 Hz, **3ah'**), 1.10-1.19 (m), 1.22-1.29 (m, **3ah**), 1.49 (s, **3ah-E**), 1.53 (s, **3ah-Z**), 1.79 (t, *J* = 7.6 Hz, **3ah-E**), 1.89 (t, *J* = 7.8 Hz, **3ah-Z**), 2.11-2.18 (m, **3ah'**), 2.43 (s, **3ah+3ah'**), 3.45-3.49 (m, **3ah**), 5.31 (t, *J* = 6.9 Hz, **3ah**), 6.06 (dd, *J* = 15.6, 8.2 Hz, **3ah'**), 6.50 (d, *J* = 15.6 Hz, **3ah'**), 7.11-7.15 (m), 7.25-7.30 (m), 7.39-7.45 (m), 7.55-7.63 (m), 8.17 (dd, *J* = 8.2, 1.4 Hz, **3ah+3ah'**), 8.70-8.73 (m, **3ah+3ah'**), 8.98-9.02 (m, **3ah+3ah'**), 9.92 (brs, **3ah+3ah'**). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.69, 13.87, 16.00, 19.46, 20.26, 20.52, 20.81, 20.98, 23.27, 31.74, 31.92, 33.73, 37.16, 39.07, 41.64, 116.69, 116.75, 121.58, 121.82, 122.40, 123.22, 123.33, 125.20, 126.71, 127.40, 127.85, 127.95, 128.64, 129.04, 129.08, 134.49, 134.53, 134.57, 135.01, 135.39, 136.18, 136.24, 136.27, 136.60, 136.72, 137.73, 138.51, 140.16, 148.17, 168.63, 168.77. IR (ATR): 3346 w, 2956 w, 2926 w, 2869 w, 1677 m, 1520 s, 1482 m, 1424 m, 1385 m, 1326 m, 1247 w, 898 w. MS, *m/z* (relative intensity, %): 359 (12), 358 (M^+, 43), 315 (12), 288 (14), 287 (61), 215 (14), 214 (57), 199 (24), 186 (12), 185 (10), 173 (10), 172 (44), 171 (30), 159 (11), 157 (12), 146 (11), 145 (61), 144 (100), 143 (15), 142 (11), 141 (11), 129 (16), 128 (20), 115 (14),

69 (25). HRMS Calcd for $C_{24}H_{26}N_2O$ 358.2045, found 358.2040.

2-(2-Cyclohexylideneethyl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3ai) and (*E*)-2-(2-cyclohexylvinyl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3ai')

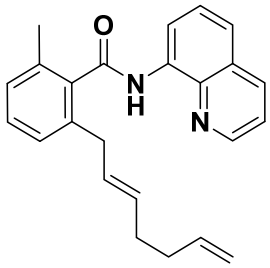


3ai **3ai'**

The spectra were obtained from the mixture (**3ai**/**3ai'** = 3.2:1).

69% yield. Colorless oil. R_f 0.60 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.34-1.39 (m, 6H), 1.96 (t, *J* = 5.3 Hz, 2H), 2.06 (t, *J* = 6.0 Hz, 2H), 2.43 (s, 3H), 3.47 (d, *J* = 7.3 Hz, 2H), 5.27 (t, *J* = 7.1 Hz, 1H), 6.17 (dd, *J* = 15.8, 7.1 Hz, **3ai'**), 6.52 (d, *J* = 16.0 Hz, **3ai'**), 7.11-7.15 (m, 2H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.44 (dd, *J* = 8.5, 4.4 Hz, 1H), 7.55-7.62 (m, 2H), 8.17 (dd, *J* = 8.2, 0.9 Hz, 1H), 8.73 (dd, *J* = 4.1, 0.9 Hz, 1H), 8.99 (d, *J* = 7.3 Hz, 1H), 9.93 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.44, 25.71, 25.97, 26.75, 27.54, 28.34, 28.63, 31.00, 32.62, 37.00, 41.20, 116.74, 119.36, 121.60, 121.85, 123.05, 124.37, 126.71, 127.38, 127.81, 127.96, 128.63, 129.04, 129.09, 134.45, 134.54, 134.93, 135.43, 136.27, 137.69, 138.51, 138.61, 139.84, 140.74, 148.19, 168.61, 168.77. IR (ATR): 3347 w, 2925 w, 2851 w, 1678 m, 1521 s, 1483 m, 1424 w, 1386 w, 1326 w, 1246 m, 826 w. MS, *m/z* (relative intensity, %): 370 (M^+, 4), 287 (15), 226 (22), 146 (10), 145 (45), 144 (100), 115 (11), 81 (49), 55 (15). HRMS Calcd for $C_{25}H_{26}N_2O$ 370.2045, found 370.2046.

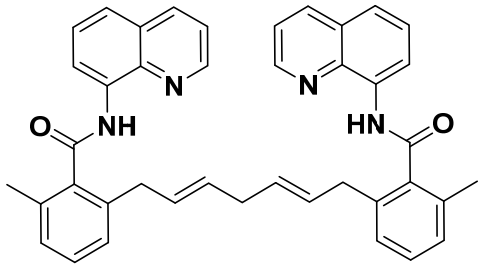
(*E*)-2-(Hepta-2,6-dien-1-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3aj)



62% yield (E/Z = 23:1). Colorless oil. R_f 0.58 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.93-1.95 (m, 4H), 2.44 (s, 3H), 3.45 (d, *J* = 6.4 Hz, 2H), 4.83-4.88 (m, 2H), 5.40-5.43 (m, 1H), 5.56-5.70 (m, 2H), 7.13-7.15 (m, 2H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.63-7.55 (m, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.72 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.99 (dd, *J* = 7.6, 1.1 Hz, 1H), 9.92 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.46, 31.69, 33.32, 36.61, 114.36,

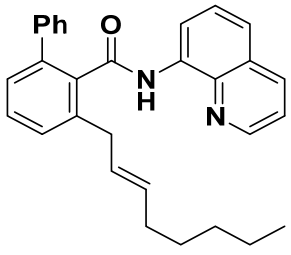
116.75, 121.62, 121.89, 127.01, 127.40, 127.99, 128.08, 128.72, 129.07, 131.40, 134.37, 134.67, 136.29, 137.54, 137.67, 138.30, 138.48, 148.20, 168.63. IR (ATR): 3347 w, 2922 w, 2847 w, 1675 m, 1518 s, 1482 s, 1424 m, 1385 m, 1325 m, 1262 w, 1126 w, 971 w, 901 w, 826 w. MS, *m/z* (relative intensity, %): 356 (M^+, 8), 212 (14), 171 (47), 170 (37), 159 (23), 158 (77), 157 (15), 145 (32), 144 (100), 143 (32), 141 (10), 131 (11), 129 (29), 128 (47), 127 (12), 117 (12), 116 (15), 115 (21), 105 (12), 91 (15), 77 (10), 67 (53), 55 (17). HRMS Calcd for $C_{24}H_{24}N_2O$ 356.1889, found 356.1888.

6,6'-((2*E*,5*E*)-Hepta-2,5-diene-1,7-diyl)bis(2-methyl-*N*-(quinolin-8-yl)benzamide) (3aj')



6% yield. Colorless oil. R_f 0.30 (hexane/EtOAc = 7/3). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 2.39-2.41 (m, 8H), 3.31 (d, *J* = 6.4 Hz, 4H), 5.19-5.26 (m, 2H), 5.40-5.47 (m, 2H), 7.03 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 7.3 Hz, 2H), 7.24 (t, *J* = 8.0 Hz, 2H), 7.40 (dd, *J* = 8.0, 4.4 Hz, 2H), 7.52-7.60 (m, 4H), 8.14 (dd, *J* = 8.2, 1.4 Hz, 2H), 8.68 (dd, *J* = 4.1, 0.9 Hz, 2H), 8.96 (dd, *J* = 7.3, 0.9 Hz, 2H), 9.87 (brs, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 19.46, 35.25, 36.44, 116.74, 121.66, 121.92, 126.96, 127.39, 127.99, 128.07, 129.05 (two overlapping peaks), 130.11, 134.34, 134.64, 136.31, 137.40, 137.62, 138.46, 148.22, 168.58. IR (ATR): 3344 w, 2923 w, 2852 w, 1675 m, 1520 s, 1481 m, 1424 m, 1385 m, 1325 m, 1245 m, 1127 w, 970 w, 898 w, 827 w. MS, *m/z* (relative intensity, %): 183 (M^+-433, 41), 182 (16), 171 (29), 159 (12), 158 (12), 157 (11), 155 (14), 146 (10), 145 (28), 144 (100), 143 (15), 129 (22), 128 (22), 115 (12). HRMS Calcd for $C_{41}H_{36}N_4O_2$ 616.2838, found 616.2834.

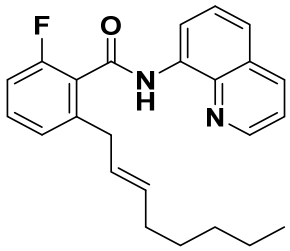
(*E*)-3-(Oct-2-en-1-yl)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (3ba)



68% yield (E/Z = 11:1). Colorless oil. R_f 0.20 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.76 (t, *J* = 6.6 Hz, 3H), 1.03-1.18 (m, 6H), 1.80-1.85 (m, 2H), 3.57 (d, *J* = 6.9 Hz, 2H), 5.44-5.51 (m, 1H), 5.56-5.63 (m, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 2H), 7.30-7.34 (m, 3H),

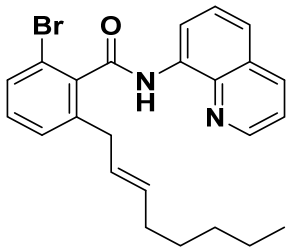
7.42-7.53 (m, 5H), 8.04 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.58 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.76 (dd, *J* = 7.3, 0.9 Hz, 1H), 9.62 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.95, 22.35, 28.81, 31.34, 32.35, 36.70, 116.39, 121.35, 121.54, 127.19 (two overlapping peaks), 127.70, 127.94 (two overlapping peaks), 128.09, 128.65, 128.68, 129.25, 132.58, 134.34, 135.98, 136.54, 138.30, 138.97, 139.73, 140.37, 147.83, 168.01. IR (ATR): 3344 w, 3055 w, 2954 w, 2925 w, 2854 w, 1674 m, 1520 s, 1483 m, 1423 m, 1385 m, 1326 m, 1262 w, 970 w, 896 w, 825 w. MS, *m/z* (relative intensity, %): 434 (M^+, 21), 233 (10), 221 (33), 220 (100), 178 (11), 165 (11), 144 (22). HRMS Calcd for $C_{30}H_{30}N_2O$ 434.2358, found 434.2352.

(*E*)-2-Fluoro-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ca)



43% yield (E/Z = 16:1). Colorless oil. R_f 0.20 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.76 (t, *J* = 6.9 Hz, 3H), 1.04-1.18 (m, 6H), 1.81-1.86 (m, 2H), 3.54 (d, *J* = 6.4 Hz, 2H), 5.43-5.59 (m, 2H), 7.04 (t, *J* = 8.7 Hz, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.36 (td, *J* = 8.0, 5.6 Hz, 1H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55-7.62 (m, 2H), 8.17 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.76 (dd, *J* = 4.0, 1.3 Hz, 1H), 8.96 (dd, *J* = 7.1, 1.6 Hz, 1H), 10.10 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.95, 22.35, 28.80, 31.33, 32.36, 36.30, 113.57 (d, *J* = 21.9 Hz), 116.84, 121.64, 122.06, 125.23 (d, *J* = 17.2 Hz), 125.52 (d, *J* = 2.9 Hz), 127.35 (two overlapping peaks), 127.95, 130.80 (d, *J* = 8.6 Hz), 133.05, 134.33, 136.29, 138.41, 141.76, 148.25, 159.33 (d, *J* = 246.0 Hz), 163.43. IR (ATR): 3345 w, 2955 w, 2925 w, 2854 w, 1679 m, 1523 s, 1484 m, 1460 m, 1424 m, 1386 w, 1327 m, 1247 w, 971 w, 899 w, 825 w. MS, *m/z* (relative intensity, %): 376 (M^+, 32), 375 (12), 175 (18), 163 (26), 162 (100), 149 (10), 147 (12), 146 (11), 145 (10), 144 (60). HRMS Calcd for $C_{24}H_{25}FN_2O$ 376.1951, found 376.1946.

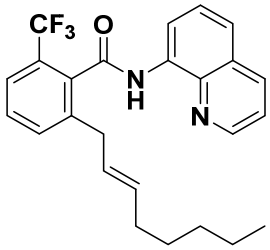
(*E*)-2-Bromo-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3da)



39% yield (E/Z = 19:1). Colorless oil. R_f 0.26 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz)

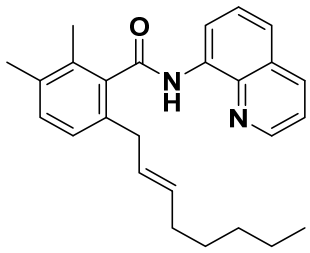
δ: 0.79 (t, *J* = 7.1 Hz, 3H), 1.05-1.20 (m, 6H), 1.80-1.85 (m, 2H), 3.47 (d, *J* = 6.4 Hz, 2H), 5.40-5.57 (m, 2H), 7.22-7.28 (m, 2H), 7.45 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.50 (dd, *J* = 6.9, 2.3 Hz, 1H), 7.56-7.63 (m, 2H), 8.18 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.75 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.98 (dd, *J* = 7.1, 1.6 Hz, 1H), 9.96 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.98, 22.38, 28.75, 31.34, 32.30, 36.84, 116.97, 119.78, 121.66, 122.15, 127.20, 127.39, 127.99, 128.57, 130.44 (two overlapping peaks), 133.23, 134.14, 136.30, 138.48, 138.70, 140.60, 148.26, 166.25. IR (ATR): 3340 w, 2955 w, 2925 w, 2854 w, 1680 m, 1522 s, 1483 m, 1424 m, 1386 w, 1326 m, 1264 w, 970 w, 898 w, 826 w. MS, *m/z* (relative intensity, %): 438 (29), 437 (21), 436 (M^+, 28), 435 (12), 237 (13), 235 (13), 225 (18), 224 (93), 223 (19), 222 (93), 149 (14), 145 (14), 144 (100), 129 (16), 128 (32), 116 (17), 115 (15), 55(19). HRMS Calcd for $C_{24}H_{25}BrN_2O$ 436.1150, found 436.1146.

(*E*)-2-(Oct-2-en-1-yl)-*N*-(quinolin-8-yl)-6-(trifluoromethyl)benzamide (3ea)



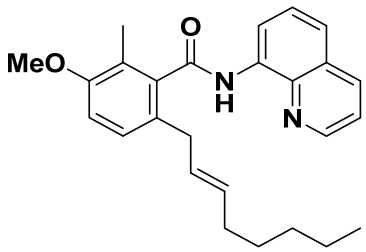
63% yield (E/Z = ~20:1). Colorless oil. R_f 0.24 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.79 (t, *J* = 7.1 Hz, 3H), 1.06-1.21 (m, 6H), 1.81-1.84 (m, 2H), 3.51 (d, *J* = 6.0 Hz, 2H), 5.40-5.58 (m, 2H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.48-7.63 (m, 5H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.73 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.96 (dd, *J* = 7.3, 1.8 Hz, 1H), 9.99 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.98, 22.38, 28.73, 31.34, 32.29, 36.26, 116.94, 121.66, 122.23, 123.83 (q, *J* = 272.7 Hz), 124.00 (q, *J* = 4.8 Hz), 127.09, 127.35 (q, *J* = 31.5 Hz), 127.38, 127.96, 129.33, 133.44 (two overlapping peaks), 134.12, 135.08, 136.29, 138.41, 139.88, 148.26, 165.51. IR (ATR): 3341 w, 2955 w, 2926 w, 2856 w, 1683 m, 1523 s, 1485 m, 1425 w, 1387 w, 1321 s, 1264 w, 1167 m, 1129 m, 970 w, 899 w, 826 w. MS, *m/z* (relative intensity, %): 427 (14), 426 (M^+, 51), 425 (28), 225 (11), 219 (10), 213 (15), 212 (63), 205 (20), 193 (20), 192 (54), 177 (14), 145 (15), 144 (100), 129 (10), 128 (12), 116 (10), 55 (21). HRMS Calcd for $C_{25}H_{25}F_3N_2O$ 426.1919, found 426.1909.

(*E*)-2,3-Dimethyl-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3fa)



73% yield (E/Z = 22:1). Colorless oil. R_f 0.20 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.79 (t, *J* = 6.9 Hz, 3H), 1.08-1.19 (m, 6H), 1.78-1.83 (m, 2H), 2.30 (s, 3H), 2.32 (s, 3H), 3.40 (d, *J* = 6.9 Hz, 2H), 5.35-5.42 (m, 1H), 5.51-5.58 (m, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.54-7.63 (m, 2H), 8.17 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.72 (dd, *J* = 4.1, 1.8 Hz, 1H), 9.01 (dd, *J* = 7.7, 1.5 Hz, 1H), 9.91 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.00, 16.61, 19.91, 22.40, 28.83, 31.38, 32.32, 36.50, 116.74, 121.58, 121.83, 126.82, 127.42, 128.00, 128.30, 130.48, 132.18, 132.88, 134.46, 134.95, 135.14, 136.27, 137.95, 138.51, 148.15, 169.26. IR (ATR): 3348 w, 2954 w, 2925 w, 2854 w, 1678 m, 1520 s, 1481 m, 1424 m, 1384 m, 1326 m, 1269 w, 971 w, 907 w, 825 w. MS, *m/z* (relative intensity, %): 387 (11), 386 (M^+, 39), 385 (18), 242 (11), 185 (10), 173 (34), 172 (100), 171 (20), 159 (16), 157 (11), 145 (21), 144 (58), 143 (10), 142 (11), 129 (11), 128 (11). HRMS Calcd for $C_{26}H_{30}N_2O$ 386.2358, found 386.2352.

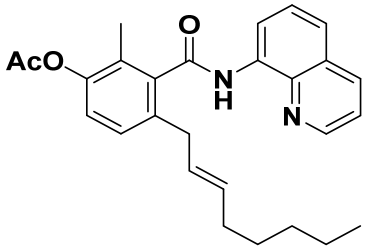
(*E*)-3-Methoxy-2-methyl-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ga)



72% yield (E/Z = 19:1). Colorless oil. R_f 0.20 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.78 (t, *J* = 6.9 Hz, 3H), 1.05-1.18 (m, 6H), 1.78-1.83 (m, 2H), 2.29 (s, 3H), 3.38 (d, *J* = 6.9 Hz, 2H), 3.85 (s, 3H), 5.38 (dt, *J* = 15.0, 6.8 Hz, 1H), 5.50-5.57 (m, 1H), 6.87 (d, *J* = 8.2 Hz, 1H), 7.10 (d, *J* = 8.7 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.6 Hz, 1H), 7.54-7.62 (m, 2H), 8.17 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.71 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.99 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.90 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 12.97, 13.99, 22.40, 28.84, 31.37, 32.31, 36.00, 55.65, 110.89, 116.73, 121.58, 121.83, 123.35, 127.40, 127.66, 127.98, 128.50, 129.36, 132.01, 134.39, 136.25, 138.49, 138.81, 148.15, 156.06, 168.41. IR (ATR): 3347 w, 2955 w, 2925 w, 2853 w, 1678 m, 1522 s, 1479 s, 1425 m, 1384 w, 1326 m, 1268 m, 1096 m, 971 w, 907 w, 825 w. MS, *m/z* (relative intensity, %): 403 (14), 402 (M^+, 41), 401 (13), 259 (16), 258 (68), 215 (14), 202 (10), 201 (24), 189 (39), 188 (100), 187 (96), 176 (10), 175 (22), 174 (10), 173 (14), 161 (16), 159 (11), 158 (10), 149 (14), 145 (22), 144 (98),

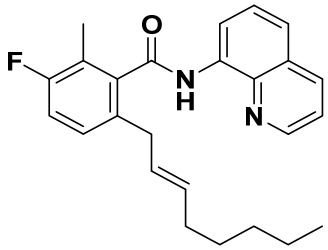
135 (12), 129 (16), 128 (13), 116 (11), 115 (15), 91 (10), 55 (13). HRMS Calcd for $C_{26}H_{30}N_2O_2$ 402.2307, found 402.2309.

(*E*)-2-Methyl-4-(oct-2-en-1-yl)-3-(quinolin-8-ylcarbamoyl)phenyl acetate (3ha)



65% yield (E/Z = 21:1). Colorless oil. R_f 0.20 (hexane/EtOAc = 5/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.79 (t, *J* = 6.6 Hz, 3H), 1.06-1.20 (m, 6H), 1.80-1.85 (m, 2H), 2.25 (s, 3H), 2.34 (s, 3H), 3.42 (d, *J* = 6.9 Hz, 2H), 5.37-5.44 (m, 1H), 5.51-5.58 (m, 1H), 7.06 (d, *J* = 8.2 Hz, 1H), 7.18 (d, *J* = 8.2 Hz, 1H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.55-7.62 (m, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.74 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.97 (dd, *J* = 7.1, 1.6 Hz, 1H), 9.95 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.23, 13.98, 20.81, 22.39, 28.77, 31.35, 32.29, 36.34, 116.80, 121.67, 122.05, 122.74, 126.94, 127.31, 127.68, 127.95, 128.06, 132.72, 134.23, 135.54, 136.23, 138.46, 139.01, 147.58, 148.27, 167.53, 169.38. IR (ATR): 3343 w, 2955 w, 2925 w, 2854 w, 1763 m, 1678 m, 1522 s, 1482 m, 1425 m, 1384 m, 1326 m, 1202 s, 970 w, 898 w, 827 w. MS, *m/z* (relative intensity, %): 431 (11), 430 (M^+, 36), 429 (19), 245 (16), 244 (79), 217 (10), 187 (13), 175 (22), 174 (74), 173 (27), 163 (14), 161 (15), 147 (11), 145 (28), 144 (100), 55 (11). HRMS Calcd for $C_{27}H_{30}N_2O_3$ 430.2256, found 430.2257.

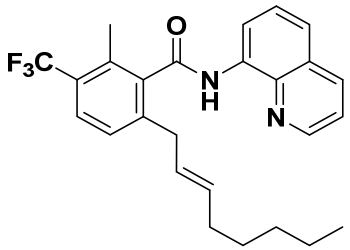
(*E*)-3-Fluoro-2-methyl-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ia)



73% yield (E/Z = 19:1). Colorless oil. R_f 0.26 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.79 (t, *J* = 6.9 Hz, 3H), 1.06-1.26 (m, 6H), 1.80-1.85 (m, 2H), 2.34 (d, *J* = 2.3 Hz, 3H), 3.40 (d, *J* = 6.9 Hz, 2H), 5.36-5.43 (m, 1H), 5.49-5.57 (m, 1H), 7.02-7.12 (m, 2H), 7.45 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.56-7.63 (m, 2H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.74 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.97 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.92 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 11.71 (d, *J* = 3.8 Hz), 13.98, 22.39, 28.79, 31.35, 32.30, 36.11, 115.72 (d, *J* = 21.9 Hz), 116.85, 121.68, 121.87 (d, *J* = 18.1 Hz), 122.12, 127.36, 127.90, 127.99, 128.37 (d, *J* = 8.6 Hz), 132.61, 133.23 (d, *J* = 3.8 Hz), 134.13, 136.32,

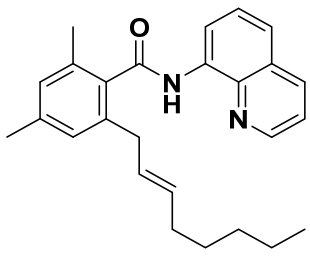
138.44, 139.25 (d, *J* = 2.9 Hz), 148.27, 159.63 (d, *J* = 242.2 Hz), 167.21 (d, *J* = 2.9 Hz). IR (ATR): 3343 w, 2955 w, 2925 w, 2855 w, 1679 m, 1522 s, 1484 s, 1425 w, 1385 w, 1326 m, 1268 w, 969 w, 825 w. MS, *m/z* (relative intensity, %): 391 (11), 390 (M^+, 40), 389 (22), 203 (10), 189 (14), 177 (29), 176 (100), 175 (16), 163 (11), 147 (10), 146 (17), 145 (11), 144 (75), 55 (10). HRMS Calcd for $C_{25}H_{27}FN_2O$ 390.2107, found 390.2101.

(*E*)-2-Methyl-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)-3-(trifluoromethyl)benzamide (3ja)



57% yield (E/Z = 20:1). Colorless oil. R_f 0.31 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.80 (t, *J* = 6.9 Hz, 3H), 1.07-1.21 (m, 6H), 1.81-1.86 (m, 2H), 2.54 (s, 3H), 3.47 (d, *J* = 6.4 Hz, 2H), 5.39-5.57 (m, 2H), 7.25 (d, *J* = 7.3 Hz, 1H), 7.46 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.59-7.66 (m, 3H), 8.19 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.75 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.98 (dd, *J* = 6.9, 1.8 Hz, 1H), 9.94 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.99, 16.09, 22.40, 28.74, 31.35, 32.31, 36.65, 116.96, 121.75, 122.32, 124.41 (q, *J* = 272.7 Hz), 126.55 (q, *J* = 5.7 Hz), 126.94, 127.04, 127.36, 127.49 (q, *J* = 29.6 Hz), 128.02, 133.44, 133.68, 134.02, 136.38, 138.44, 139.76, 141.83, 148.35, 167.46. IR (ATR): 3340 w, 2926 w, 2856 w, 1679 m, 1523 s, 1484 m, 1424 m, 1386 w, 1319 s, 1242 w, 1211 w, 1175 m, 1121 s, 970 w, 904 w, 827 m. MS, *m/z* (relative intensity, %): 441 (11), 440 (M^+, 39), 439 (22), 253 (11), 239 (11), 227 (27), 226 (100), 213 (10), 145 (13), 144 (80), 83 (12), 55 (18). HRMS Calcd for $C_{26}H_{27}F_3N_2O$ 440.2075, found 440.2068.

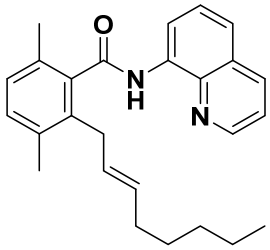
(*E*)-2,4-Dimethyl-6-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ka)



60% yield (E/Z = 20:1). Colorless oil. R_f 0.24 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.79 (t, *J* = 6.9 Hz, 3H), 1.09-1.20 (m, 6H), 1.80-1.85 (m, 2H), 2.35 (s, 3H), 2.40 (s, 3H), 3.41 (d, *J* = 6.4 Hz, 2H), 5.37-5.44 (m, 1H), 5.52-5.59 (m, 1H), 6.95 (s, 2H), 7.43 (dd, *J* = 8.2, 4.6 Hz, 1H), 7.54-7.62 (m, 2H), 8.16 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.71 (dd, *J* = 3.9, 1.6 Hz, 1H), 8.98 (d, *J* = 7.8 Hz,

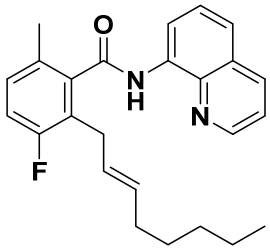
1H), 9.91 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.00, 19.42, 21.22, 22.40, 28.81, 31.38, 32.33, 36.64, 116.66, 121.56, 121.75, 127.41, 127.63, 127.98, 128.20, 128.78, 132.31, 134.49, 134.60, 135.04, 136.25, 137.74, 138.50, 138.83, 148.14, 168.88. IR (ATR): 3349 w, 2954 w, 2924 w, 2854 w, 1677 m, 1520 s, 1482 m, 1423 m, 1384 w, 1325 m, 1262 w, 969 w, 826w. MS, *m/z* (relative intensity, %): 387 (10), 386 (M^+, 35), 385 (21), 243 (14), 185 (10), 173 (37), 172 (100), 171 (11), 159 (16), 157 (10), 145 (20), 144 (54), 83 (12), 55 (12). HRMS Calcd for $C_{26}H_{30}N_2O$ 386.2358, found 386.2352.

(*E*)-3,6-Dimethyl-2-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3la)



67% yield. Colorless oil. R_f 0.25 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.76 (t, *J* = 7.1 Hz, 3H), 1.02-1.15 (m, 6H), 1.77-1.81 (m, 2H), 2.32 (s, 3H), 2.39 (s, 3H), 3.42 (d, *J* = 6.0 Hz, 2H), 5.30 (dt, *J* = 15.1, 6.9 Hz, 1H), 5.51 (dt, *J* = 15.3, 6.2 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 7.8 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.54-7.62 (m, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.71 (dd, *J* = 4.0, 1.5 Hz, 1H), 9.01 (dd, *J* = 7.6, 1.1 Hz, 1H), 9.89 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.99, 19.20, 19.28, 22.39, 28.83, 31.39, 32.37, 34.03, 116.74, 121.56, 121.81, 127.09, 127.42, 128.01, 128.04, 130.90, 131.80, 132.10, 134.46, 134.71, 135.02, 136.25, 138.41, 138.50, 148.11, 169.27. IR (ATR): 3348 w, 2953 w, 2925 w, 2855 w, 1676 m, 1520 s, 1483 m, 1424 w, 1384 w, 1325 m, 972 w, 825 w. MS, *m/z* (relative intensity, %): 387 (10), 386 (M^+, 35), 385 (20), 199 (10), 173 (26), 172 (63), 171 (16), 159 (14), 145 (22), 144 (100), 129 (10), 83 (11), 55 (13). HRMS Calcd for $C_{26}H_{30}N_2O$ 386.2358, found 386.2352.

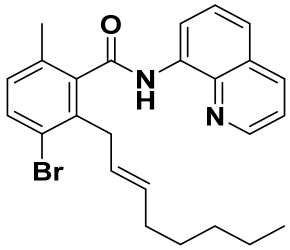
(*E*)-3-Fluoro-6-methyl-2-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3ma)



63% yield (E/Z = 26:1). Colorless oil. R_f 0.23 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.75 (t, *J* = 6.9 Hz, 3H), 0.99-1.14 (m, 6H), 1.73-1.78 (m, 2H), 2.39 (s, 3H), 3.43 (d, *J* = 6.4 Hz,

2H), 5.32-5.39 (m, 1H), 5.50-5.57 (m, 1H), 7.02 (t, *J* = 8.9 Hz, 1H), 7.08-7.11 (m, 1H), 7.45 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.56-7.63 (m, 2H), 8.18 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.73 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.98 (dd, *J* = 7.3, 1.4 Hz, 1H), 9.90 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.96, 18.91, 22.35, 28.65, 30.08 (d, *J* = 2.9 Hz), 31.33, 32.24, 115.84 (d, *J* = 21.9 Hz), 116.85, 121.66, 122.11, 124.88 (d, *J* = 17.2 Hz), 126.58, 127.38, 128.00, 129.42 (d, *J* = 8.6 Hz), 130.24 (d, *J* = 3.8 Hz), 132.30, 134.16, 136.31, 138.44, 139.15 (d, *J* = 3.8 Hz), 148.24, 159.40 (d, *J* = 244.1 Hz), 167.25 (d, *J* = 2.9 Hz). IR (ATR): 3343 w, 2955 w, 2925 w, 2855 w, 1679 m, 1522 s, 1482 m, 1425 w, 1385 w, 1326 m, 1268 w, 970 w, 825 w. MS, *m/z* (relative intensity, %): 391 (12), 390 (M^+, 41), 389 (28), 203 (10), 189 (13), 177 (25), 176 (100), 175 (28), 163 (12), 146 (18), 145 (14), 144 (94), 55 (15). HRMS Calcd for $C_{25}H_{27}FN_2O$ 390.2107, found 390.2111.

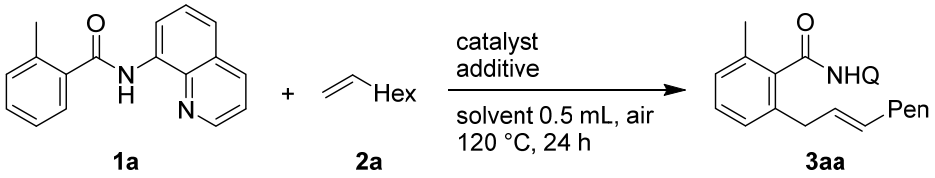
(*E*)-3-Bromo-6-methyl-2-(oct-2-en-1-yl)-*N*-(quinolin-8-yl)benzamide (3na)



46% yield. Colorless oil. R_f 0.23 (hexane/EtOAc = 10/1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.74 (t, *J* = 6.9 Hz, 3H), 1.05-1.11 (m, 6H), 1.72-1.75 (m, 2H), 2.37 (s, 3H), 3.57 (d, *J* = 6.4 Hz, 2H), 5.31-5.38 (m, 1H), 5.54 (dt, *J* = 14.7, 6.7 Hz, 1H), 7.00 (d, *J* = 8.2 Hz, 1H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.63-7.52 (m, 3H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.72 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.98 (d, *J* = 7.3 Hz, 1H), 9.88 (brs, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.98, 19.14, 22.35, 28.63, 31.31, 32.34, 36.89, 116.85, 121.67, 122.15, 122.65, 125.87, 127.38, 128.00, 129.68, 132.82, 133.45, 134.10, 134.23, 136.31, 136.40, 138.42, 139.63, 148.23, 167.51. IR (ATR): 3341 w, 2955 w, 2925 w, 2854 w, 1677 m, 1521 s, 1483 m, 1384 w, 1326 m, 1262 w, 970 w, 825 w. MS, *m/z* (relative intensity, %): 452 (23), 451 (20), 450 (M^+, 22), 449 (14), 238 (29), 237 (12), 236 (28), 145 (15), 144 (100), 142 (10). HRMS Calcd for $C_{25}H_{27}BrN_2O$ 450.1307, found 450.1303.

VI. Optimization Study

Table S1. Optimization of the reaction conditions[a]

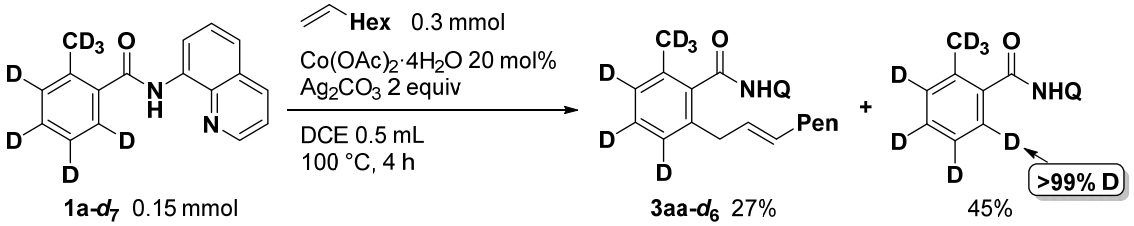


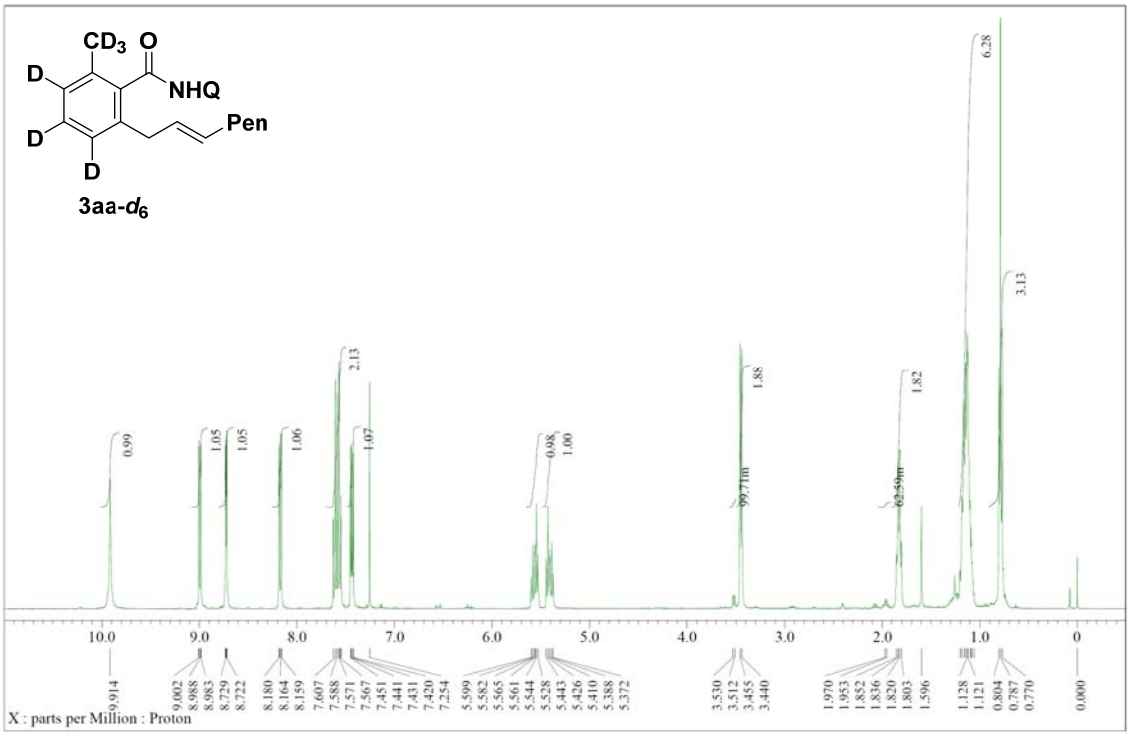
1a **2a** **3aa**

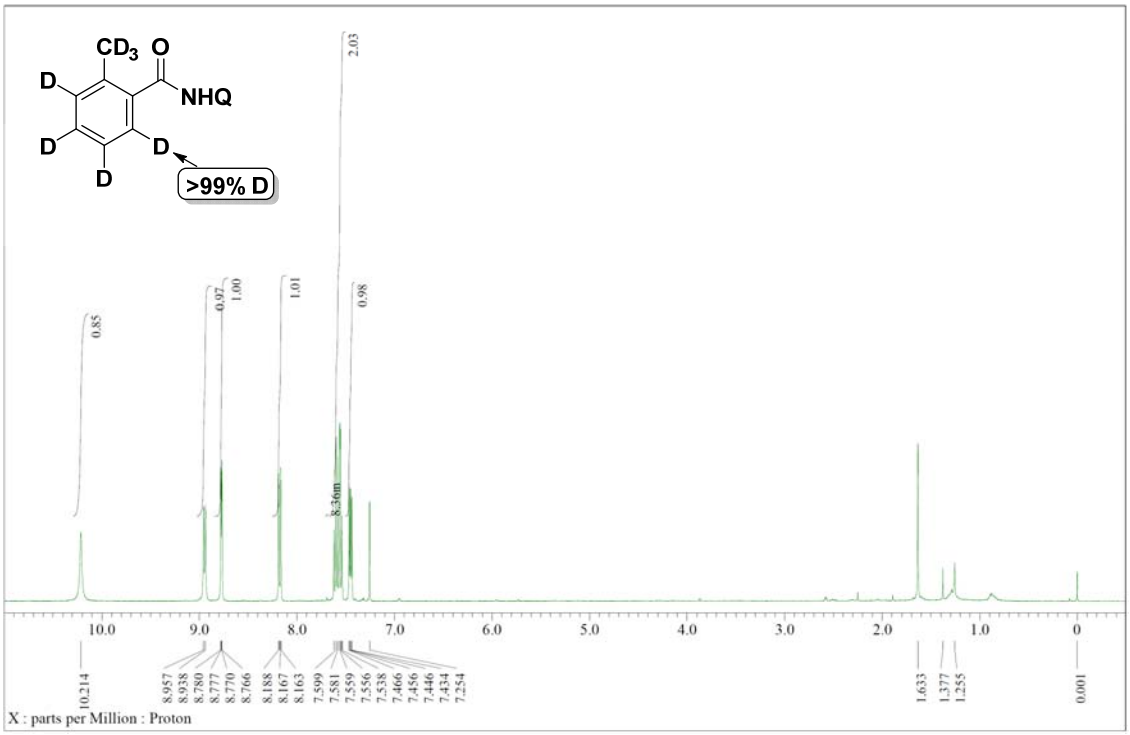
entry	catalyst (mol%)	additive (equiv)	solvent	NMR yield (**3aa/1a**)
1	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DCE	77/14
2	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	toluene	76/trace
3	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DMF	9/22
4[b]	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	$PhCF_3$	55/13
5	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DMF	9/22
6[c]	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DCE	63/17
7	$Co(OAc)_2{\cdot}4H_2O$ (30)	Ag_2CO_3 (1)	DCE	67/12
8	$Co(OAc)_2{\cdot}4H_2O$ (10)	Ag_2CO_3 (1)	DCE	68/13
9	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (2)	DCE	63/0
10	$Co(OAc)_2{\cdot}4H_2O$ (20)	AgOAc (2)	DCE	62/36
11	$Co(OAc)_2{\cdot}4H_2O$ (20)	AgOBz (2)	DCE	messy
12	$Co(OAc)_2{\cdot}4H_2O$ (20)	AgOTf (2)	DCE	0/0
13	$Co(OAc)_2{\cdot}4H_2O$ (20)	AgF (2)	DCE	0/97
14	$Co(OAc)_2{\cdot}4H_2O$ (20)	$AgNO_3$ (2)	DCE	trace/trace
15	$Co(OAc)_2{\cdot}4H_2O$ (20)	$Mn(OAc)_3{\cdot}2H_2O$ (1)	DCE	32/71
16	$CoBr_2$ (20)	Ag_2CO_3 (1)	DCE	0/25
17	$Co(acac)_2$ (20)	Ag_2CO_3 (1)	DCE	10/37
18[d]	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DCE	69/27
19[e]	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DCE	43/56
20[f]	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (1)	DCE	0/100
21[g]	$Co(OAc)_2{\cdot}4H_2O$ (20)	Ag_2CO_3 (2)	DCE	56/0
22[d,g]	**$Co(OAc)_2{\cdot}4H_2O$ (20)**	**Ag_2CO_3 (2)**	**DCE**	**83/6**

[a] Reaction condition: **1a** (0.15 mmol), **2a** (0.3 mmol), catalyst, additive in solvent (0.5 mL) at 120 °C for 24 h. [b] Run at 150 °C. [c] DCE (1 mL) was used. [d] Run at 100 °C. [e] Run at 80 °C. [f] Run at rt. [g] Run for 12 h.

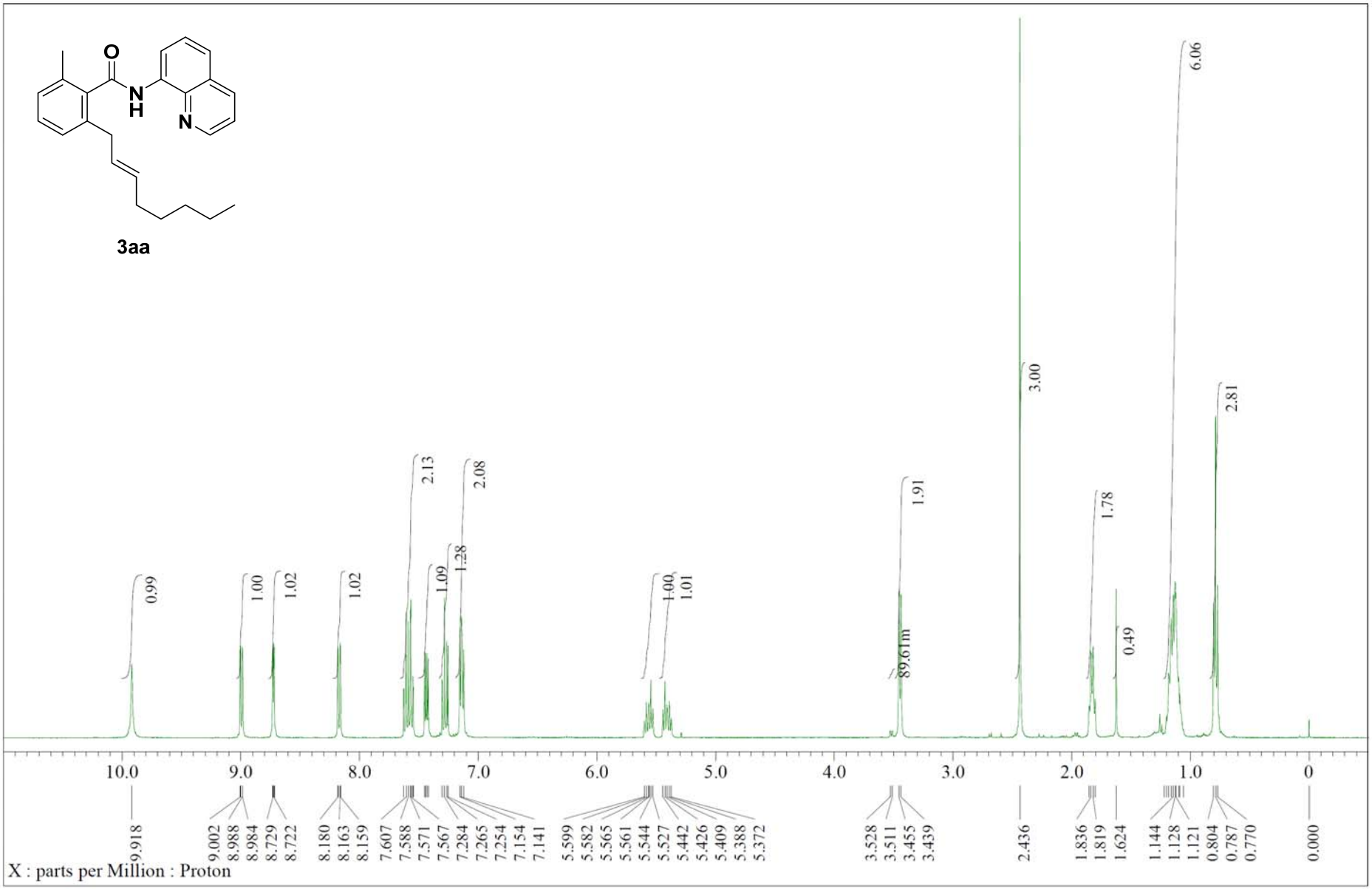
VII. Deuterium Labeling Experiments







VIII. Copies of ^{1}H and ^{13}C NMR Spectra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1.02
2.13
1.09
1.28
2.08
1.00
1.01
89.61m
1.91
3.00
1.78
0.49
6.06
2.81
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.918
9.002
8.988
8.984
8.729
8.722
8.180
8.163
8.159
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7.588
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7.567
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3.528
3.511
3.455
3.439
2.436
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1.819
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1.121
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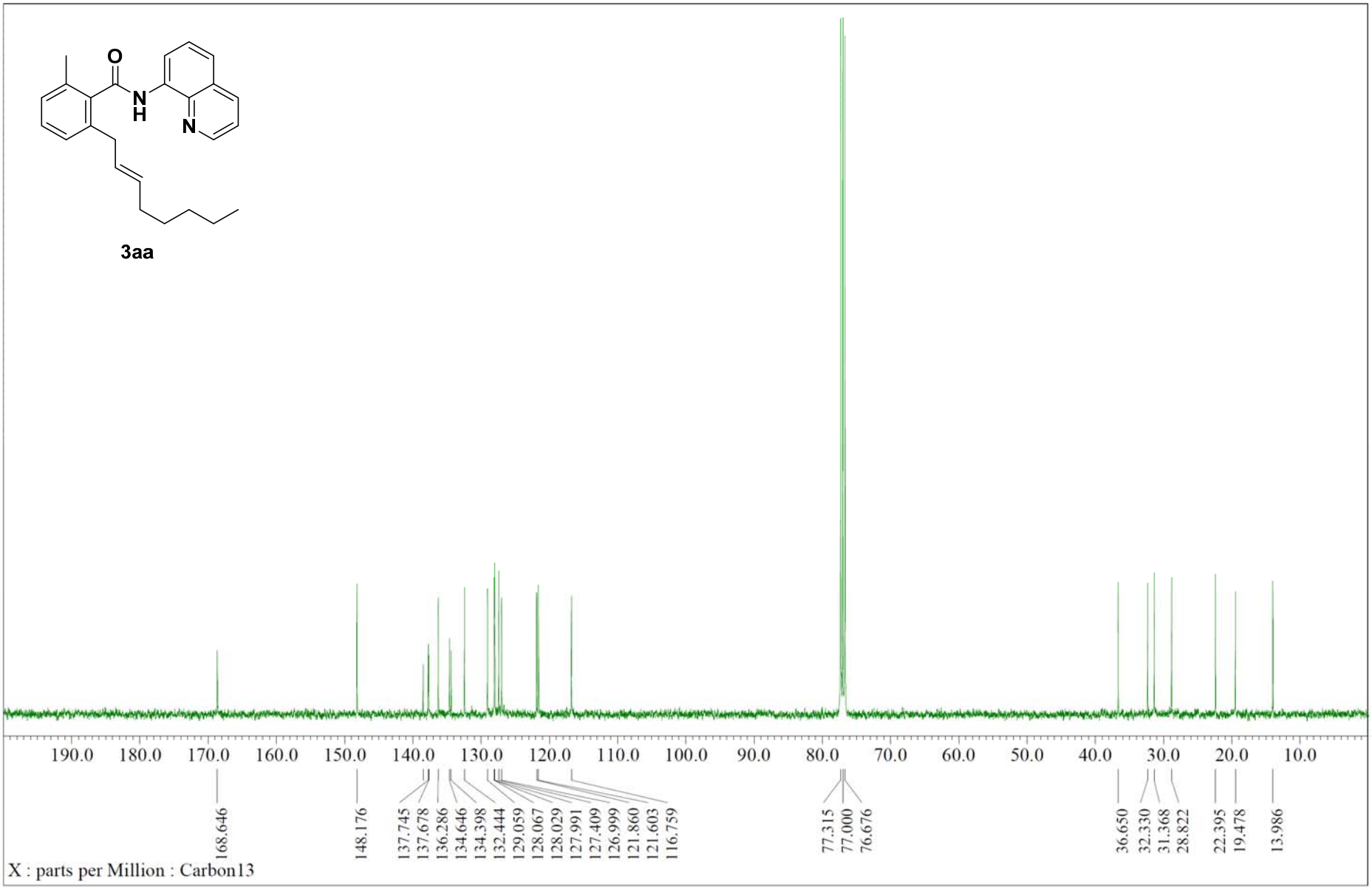
0.787
0.770
0.000
X : parts per Million : Proton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H
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100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
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134.646
134.398
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121.603
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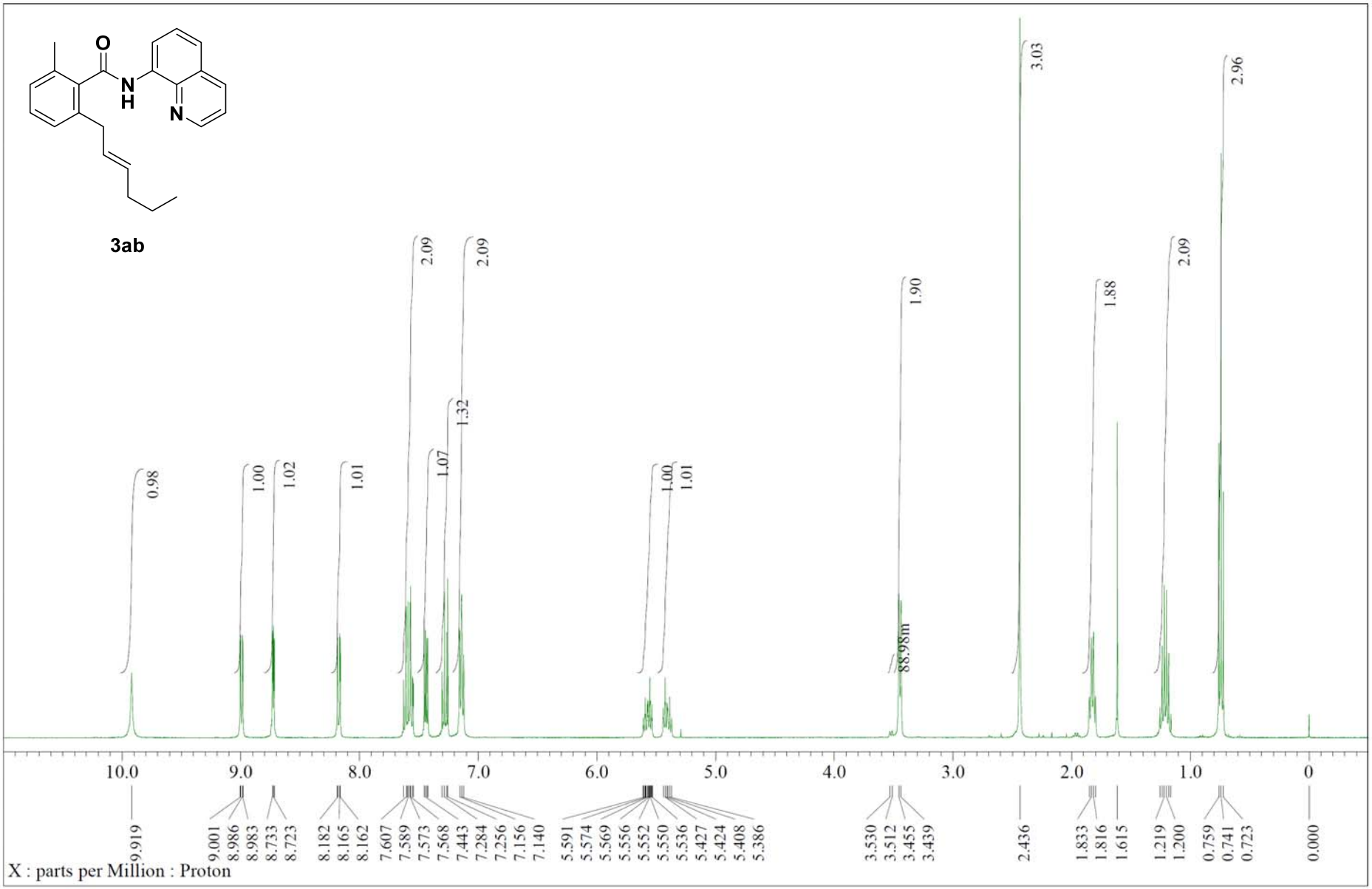
19.478
13.986
X : parts per Million : Carbon13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N
H
N
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1.01
2.09
2.09
1.07
1.32
1.00
1.01
1.90
88.98m
3.03
1.88
2.09
2.96
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.919
9.001
8.986
8.983
8.733
8.723
8.182
8.165
8.162
7.607
7.589
7.573
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7.256
7.156
7.140
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5.574
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5.408
5.386
3.530
3.512
3.455
3.439
2.436
1.833
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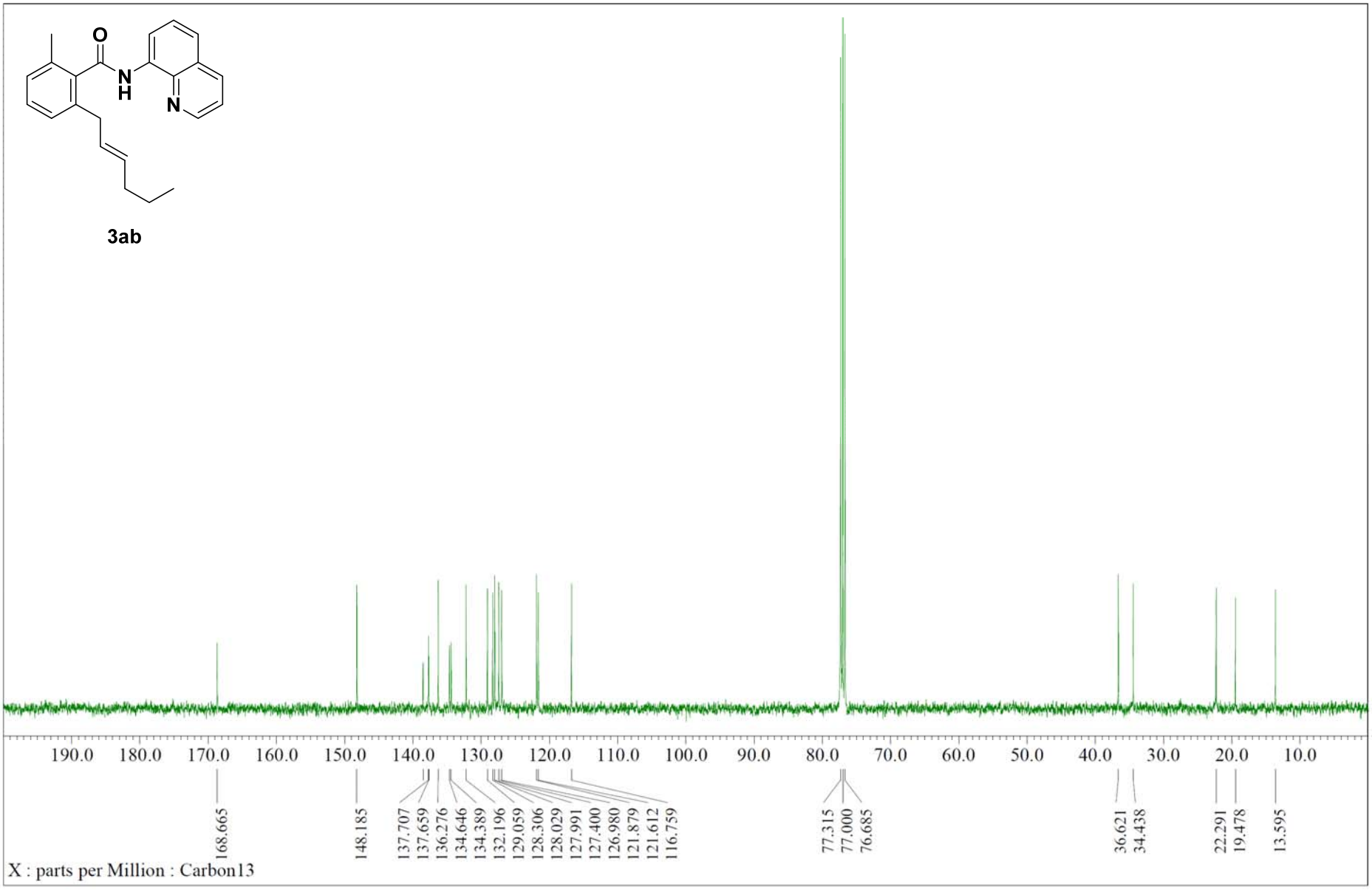
1.615
1.219
1.200
0.759
0.741
0.723
0.000
X : parts per Million : Proton


O
N
H
N
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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
168.665
148.185
137.707
137.659
136.276
134.646
134.389
132.196
129.059
128.306
128.029
127.991
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126.980
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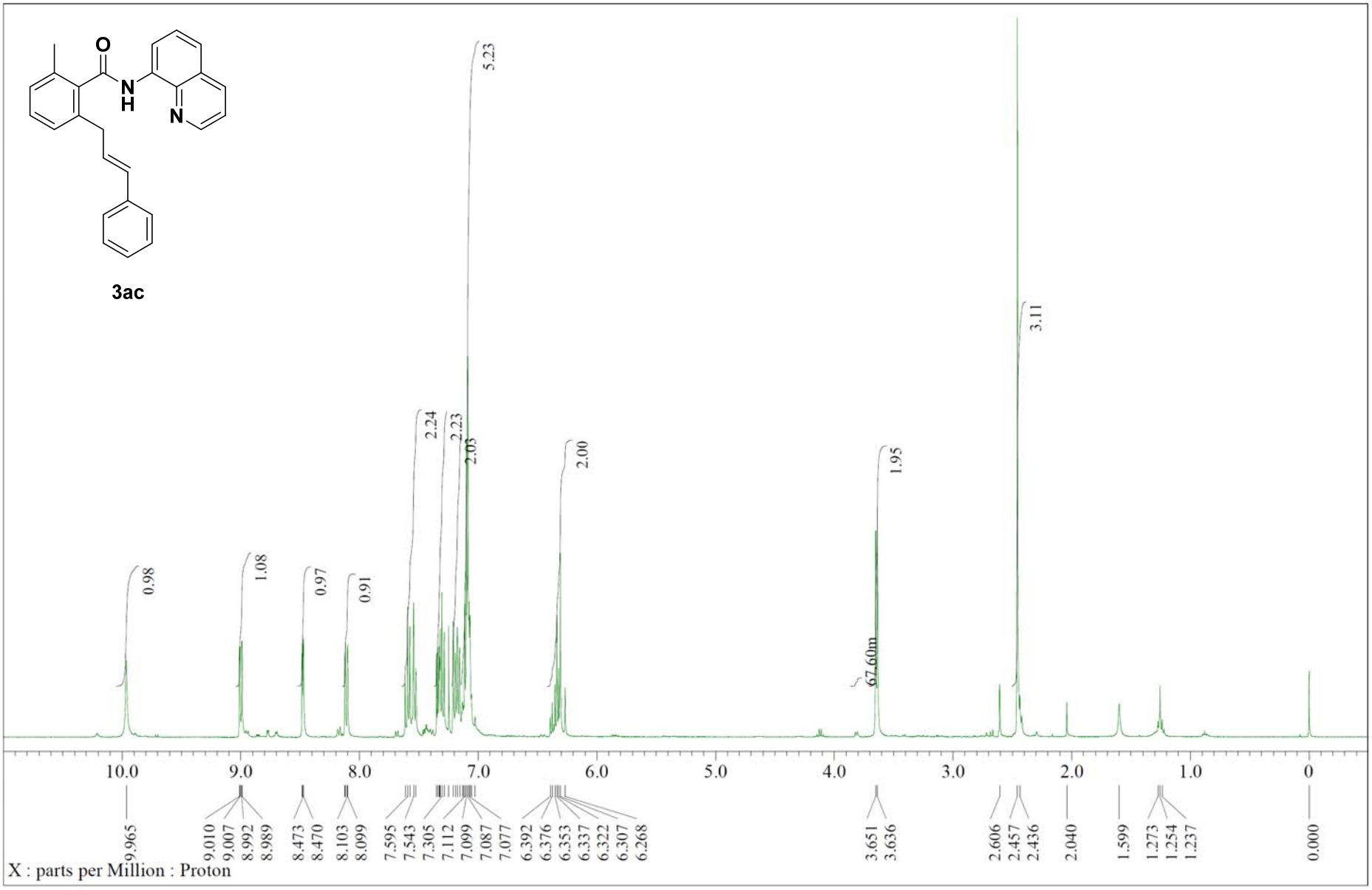
34.438
22.291
19.478
13.595
X : parts per Million : Carbon13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N
H
N
3ac
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3.11
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1.95
1.08
0.98
0.97
0.91
67.60m
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.965
9.010
9.007
8.992
8.989
8.473
8.470
8.103
8.099
7.595
7.543
7.305
7.112
7.099
7.087
7.077
6.392
6.376
6.353
6.337
6.322
6.307
6.268
3.651
3.636
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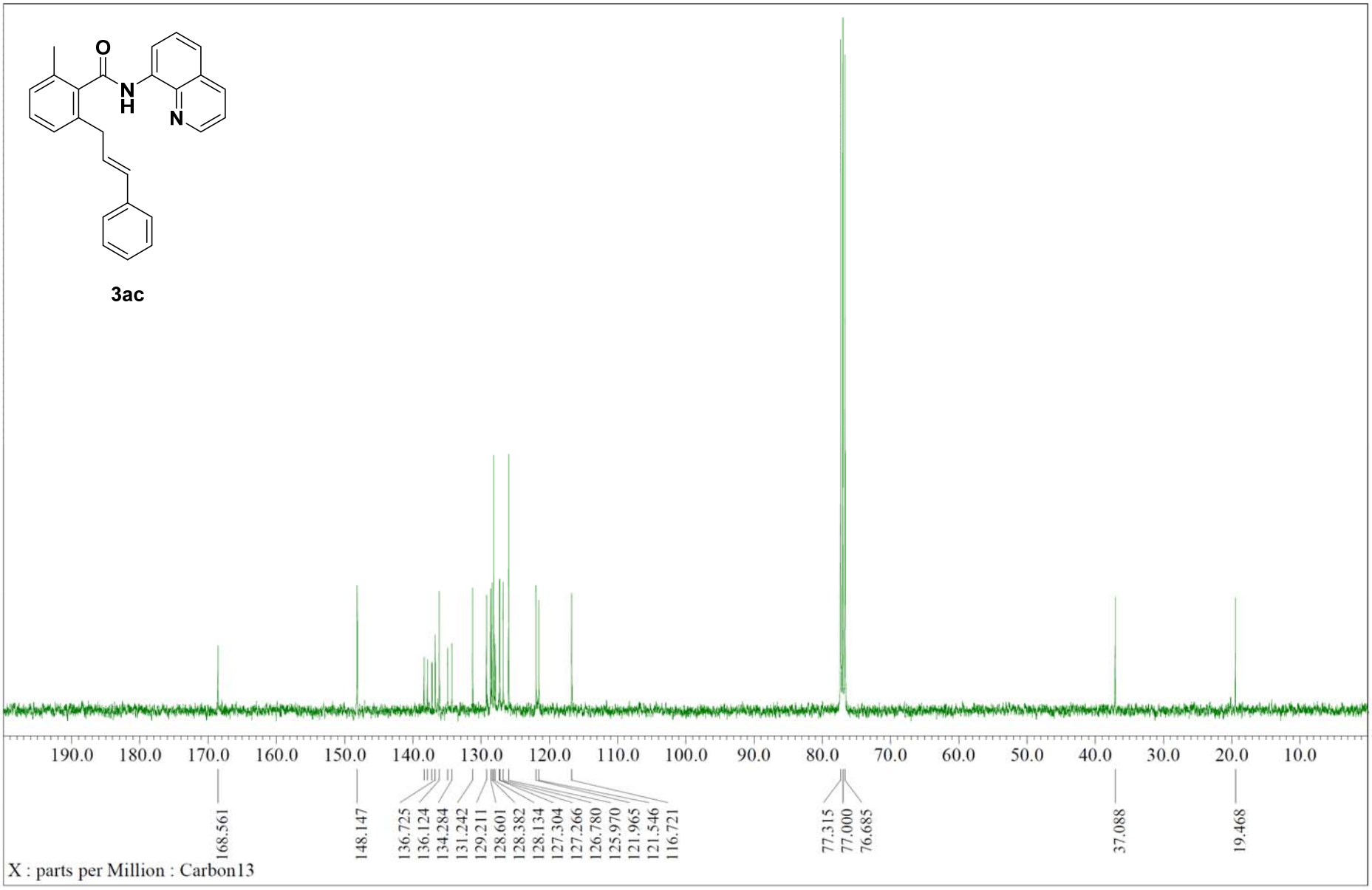
2.457
2.436
2.040
1.599
1.273
1.254
1.237
0.000
X : parts per Million : Proton


O
N
H
N
3ac
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150.0
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120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
168.561
148.147
136.725
136.124
134.284
131.242
129.211
128.601
128.382
128.134
127.304
127.266
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121.546
116.721
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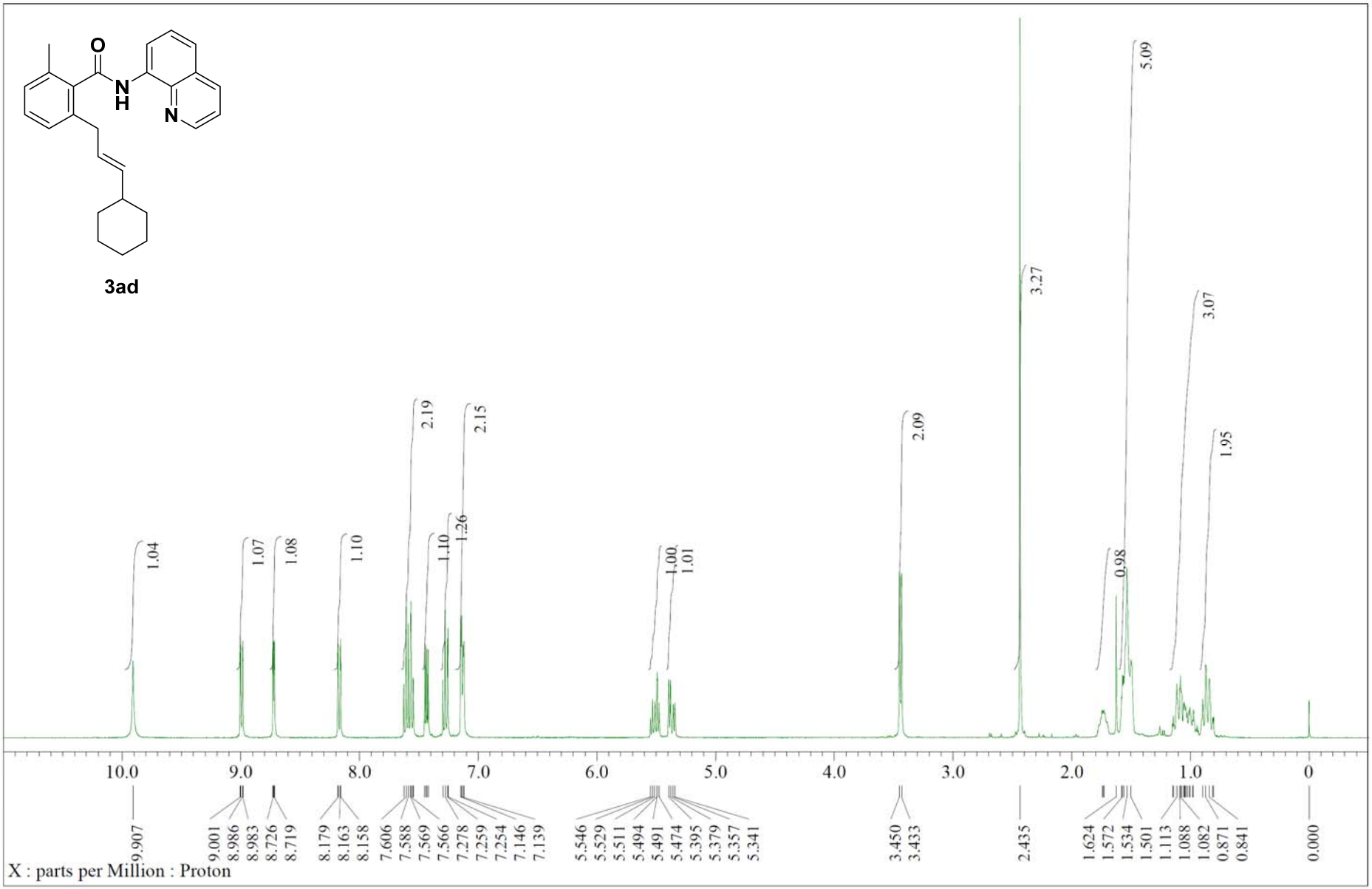
77.000
76.685
37.088
19.468
X : parts per Million : Carbon13


O
N
H
N
3ad
1.04
1.07
1.08
1.10
2.19
1.10
1.26
2.15
1.00
1.01
2.09
3.27
0.98
5.09
3.07
1.95
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.907
9.001
8.986
8.983
8.726
8.719
8.179
8.163
8.158
7.606
7.588
7.569
7.566
7.278
7.259
7.254
7.146
7.139
5.546
5.529
5.511
5.494
5.491
5.474
5.395
5.379
5.357
5.341
3.450
3.433
2.435
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1.572
1.534
1.501
1.113
1.088
1.082
0.871
0.841
0.000
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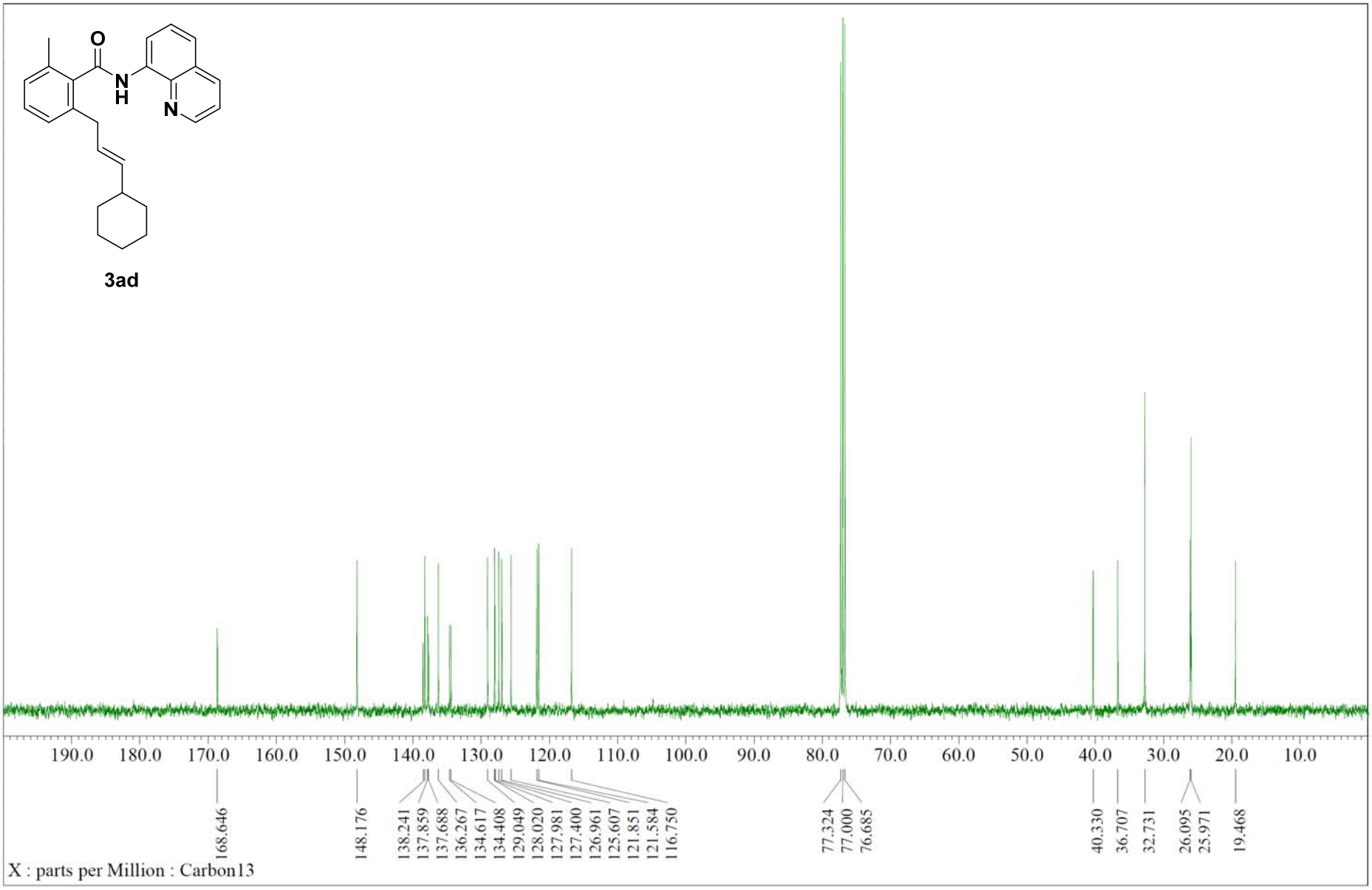
O
N
H
N
3ad
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
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100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
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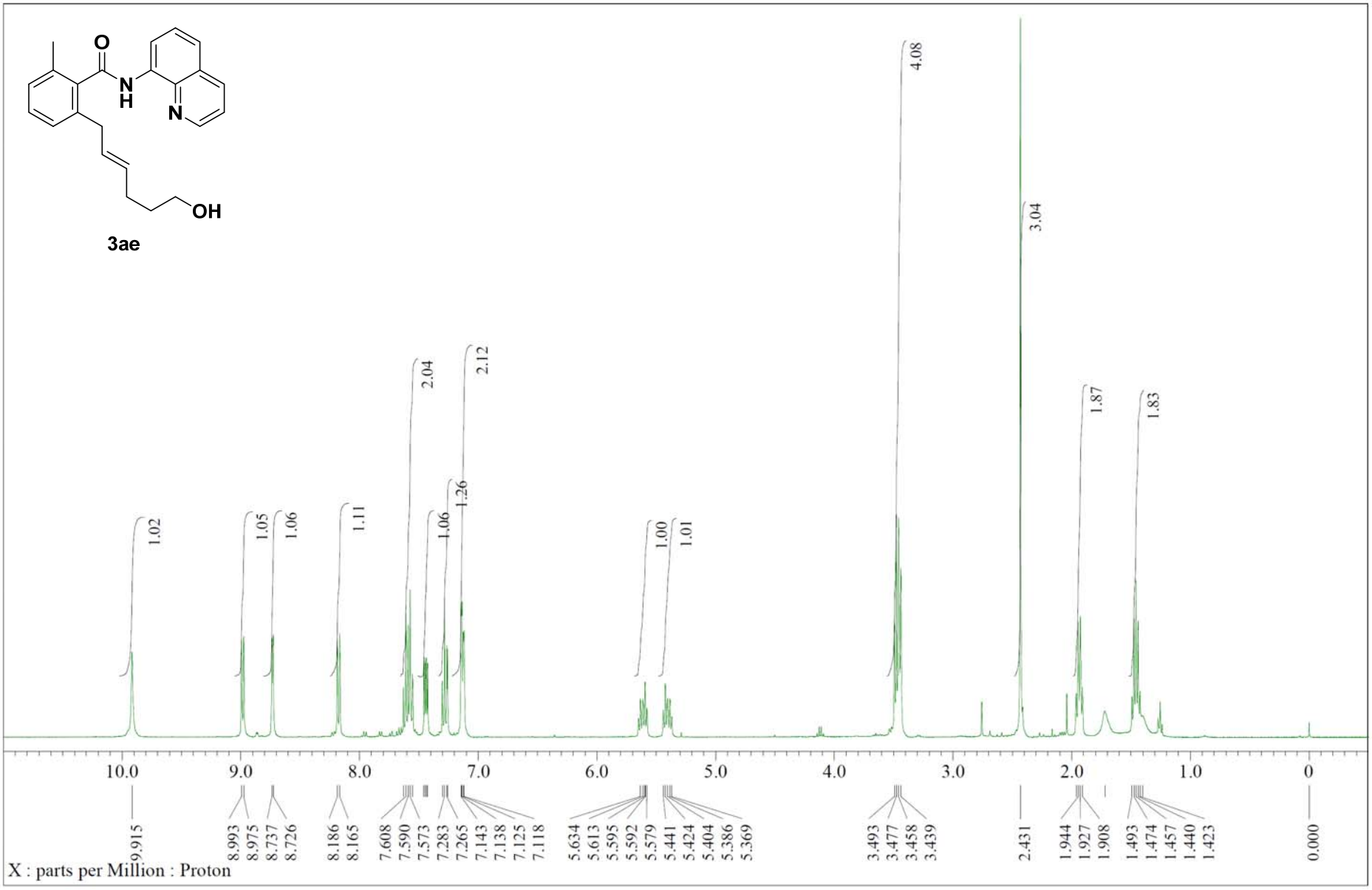
148.176
138.241
137.859
137.688
136.267
134.617
134.408
129.049
128.020
127.981
127.400
126.961
125.607
121.851
121.584
116.750
77.324
77.000
76.685
40.330
36.707
32.731
26.095
25.971
19.468
X : parts per Million : Carbon13


O
N
H
N
OH
3ae
4.08
3.04
2.12
2.04
1.87
1.83
1.26
1.11
1.06
1.06
1.05
1.02
1.01
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.915
8.993
8.975
8.737
8.726
8.186
8.165
7.608
7.590
7.573
7.283
7.265
7.143
7.138
7.125
7.118
5.634
5.613
5.595
5.592
5.579
5.441
5.424
5.404
5.386
5.369
3.493
3.477
3.458
3.439
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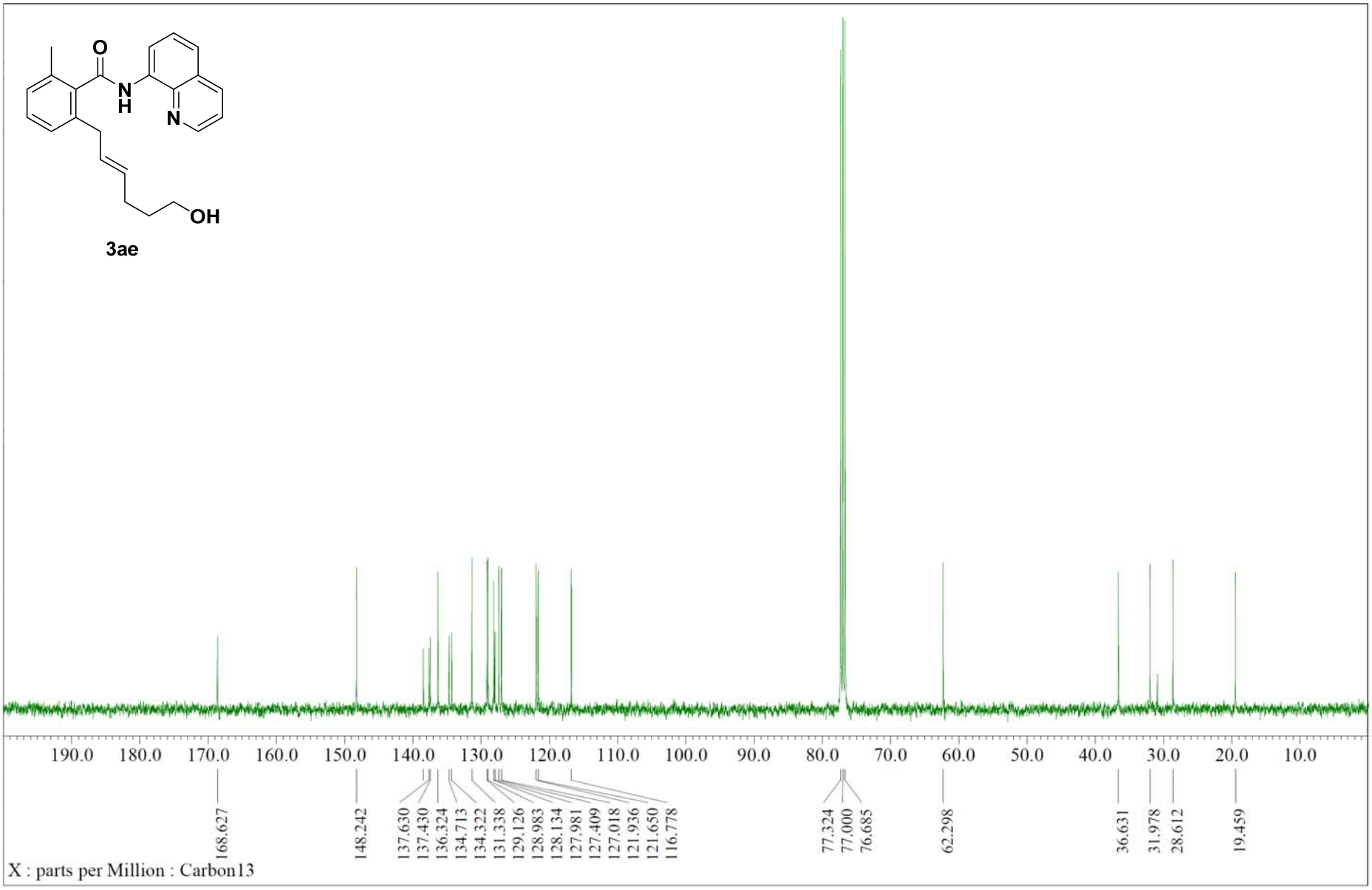
1.440
1.423
0.000
X : parts per Million : Proton


O
N
H
N
OH
3ae
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
168.627
148.242
137.630
137.430
136.324
134.713
134.322
131.338
129.126
128.983
128.134
127.981
127.409
127.018
121.936
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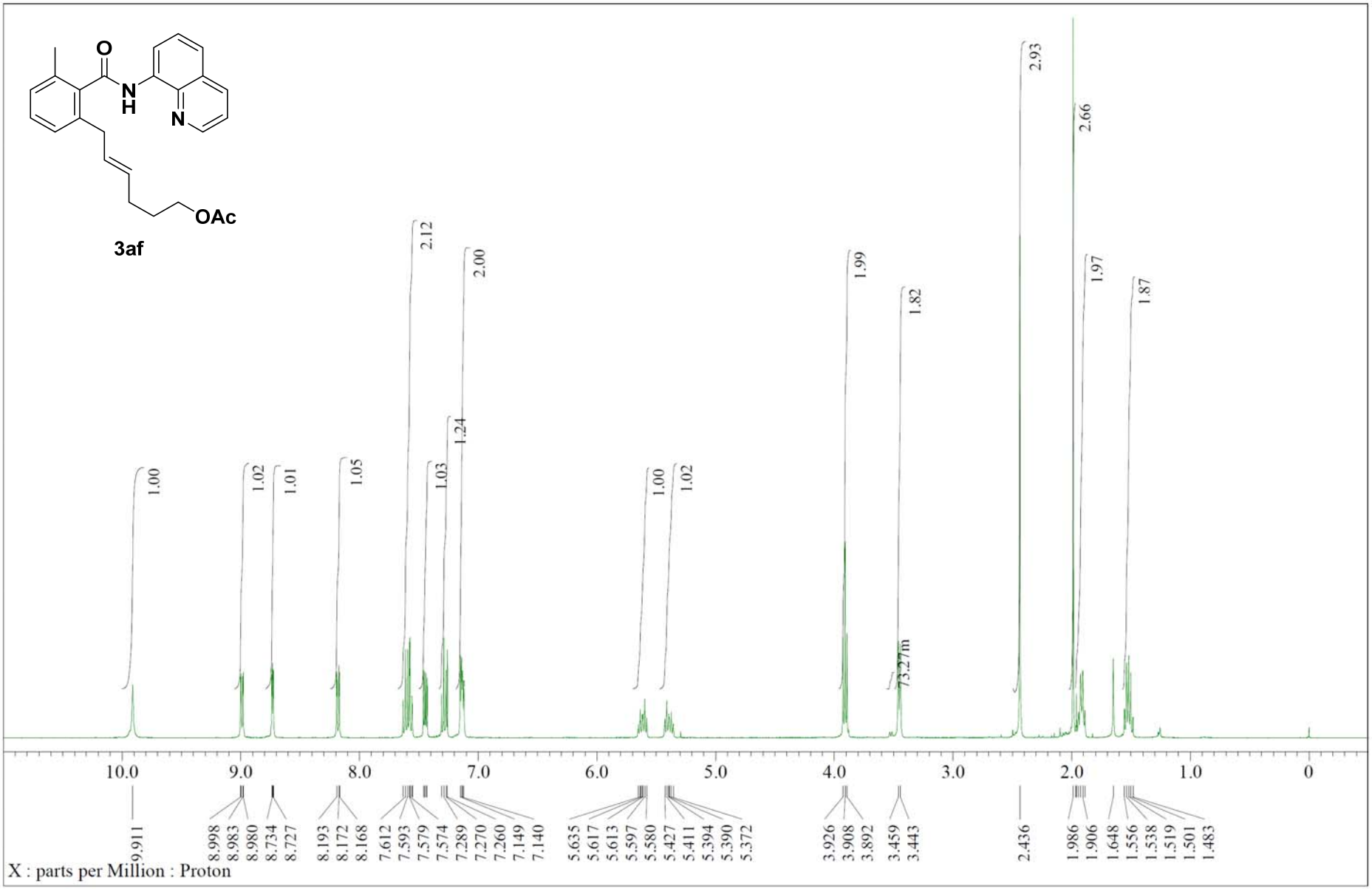
77.000
76.685
62.298
36.631
31.978
28.612
19.459
X : parts per Million : Carbon13


O
N
H
N
OAc
3af
1.00
1.02
1.01
1.05
2.12
1.03
1.24
2.00
1.00
1.02
1.99
1.82
3.27m
2.93
2.66
1.97
1.87
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.911
8.998
8.983
8.980
8.734
8.727
8.193
8.172
8.168
7.612
7.593
7.579
7.574
7.289
7.270
7.260
7.149
7.140
5.635
5.617
5.613
5.597
5.580
5.427
5.411
5.394
5.390
5.372
3.926
3.908
3.892
3.459
3.443
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1.906
1.648
1.556
1.538
1.519
1.501
1.483
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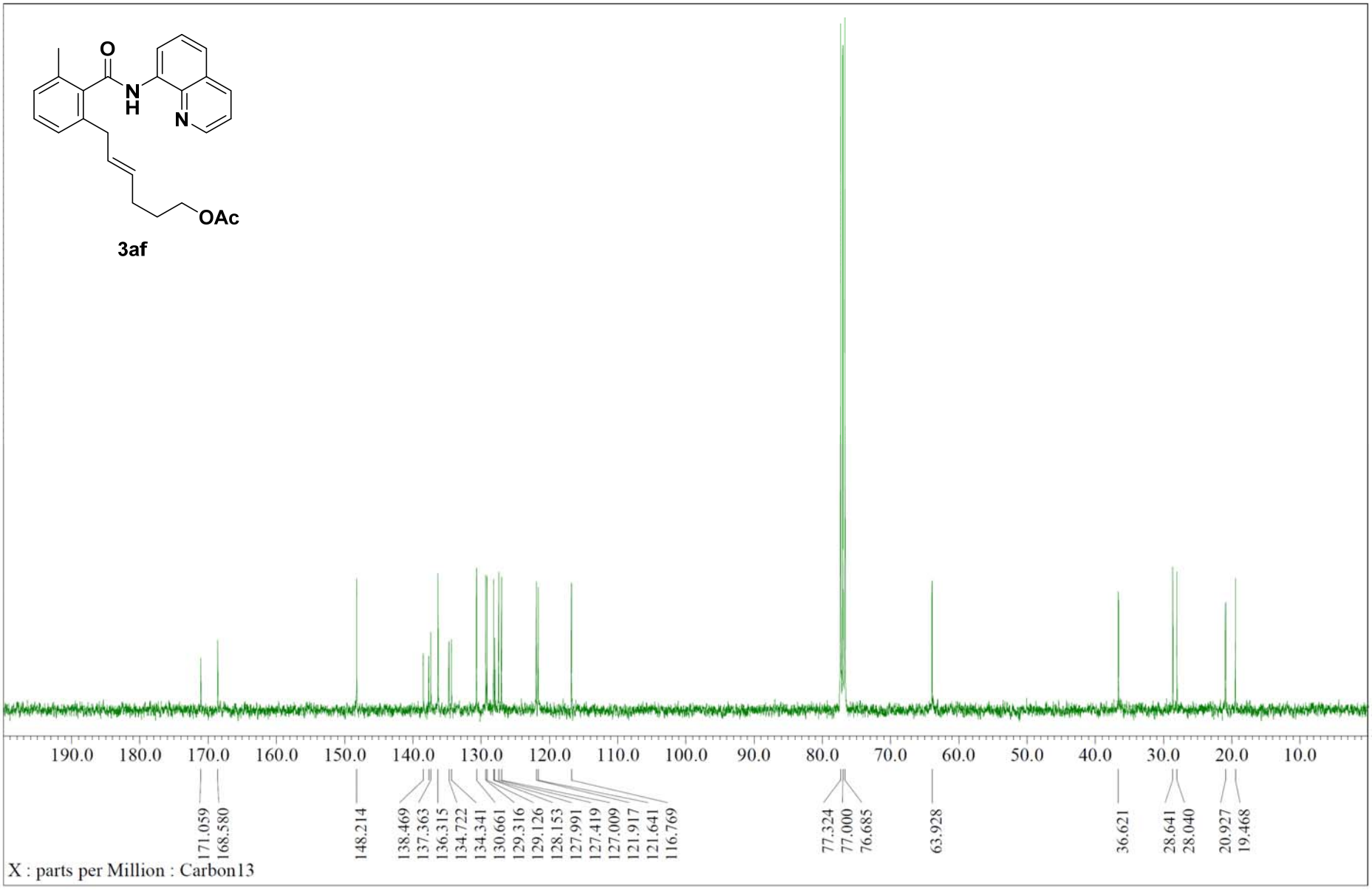
O
N
H
N
OAc
3af
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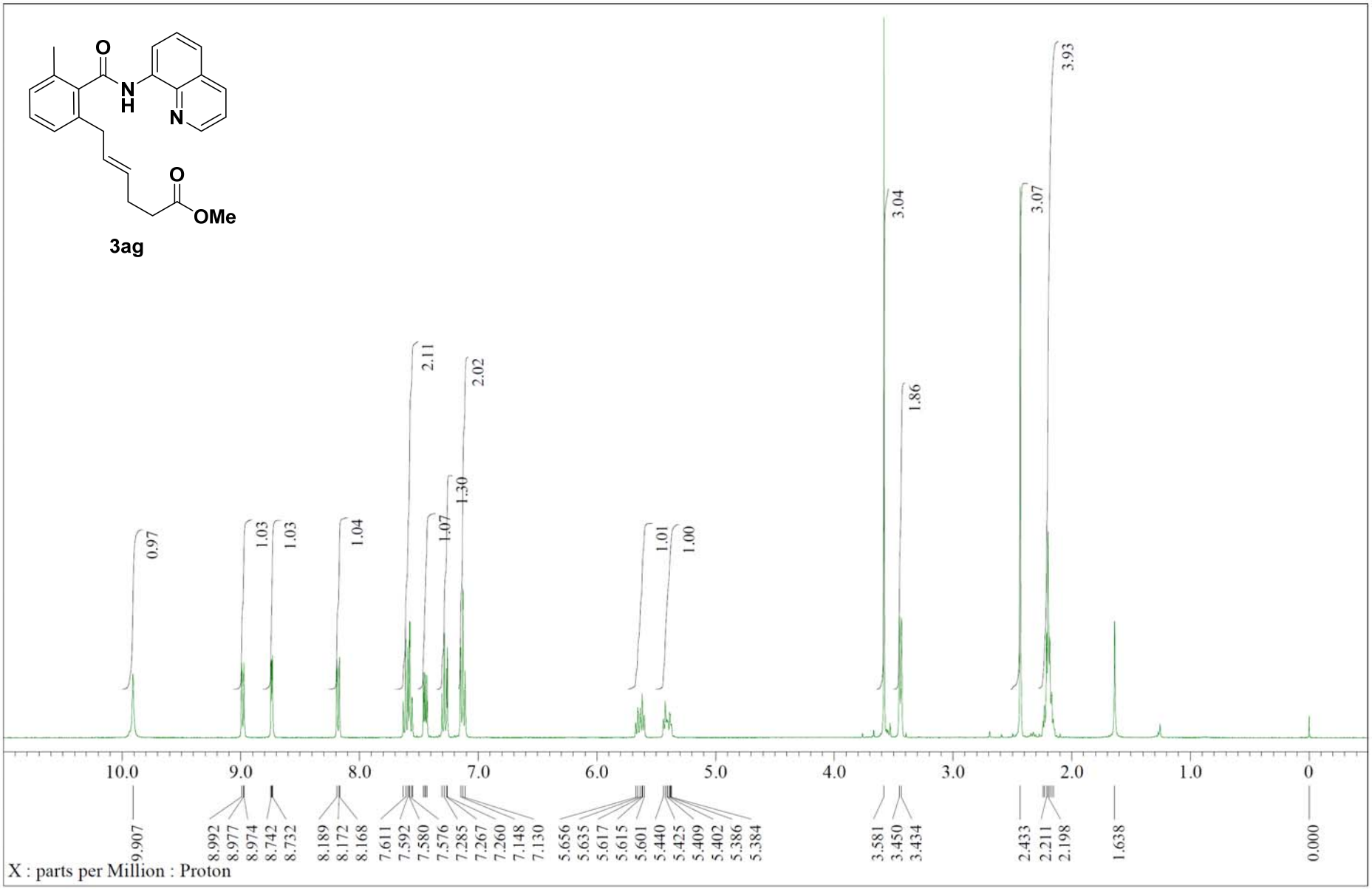
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
171.059
168.580
148.214
138.469
137.363
136.315
134.722
134.341
130.661
129.316
129.126
128.153
127.991
127.419
127.009
121.917
121.641
116.769
77.324
77.000
76.685
63.928
36.621
28.641
28.040
20.927
19.468
X : parts per Million : Carbon13


O
N
H
N
O
OMe
3ag
0.97
1.03
1.03
1.04
2.11
2.02
1.07
1.30
1.01
1.00
3.04
1.86
3.07
3.93
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.907
8.992
8.977
8.974
8.742
8.732
8.189
8.172
8.168
7.611
7.592
7.580
7.576
7.285
7.267
7.260
7.148
7.130
5.656
5.635
5.617
5.615
5.601
5.440
5.425
5.409
5.402
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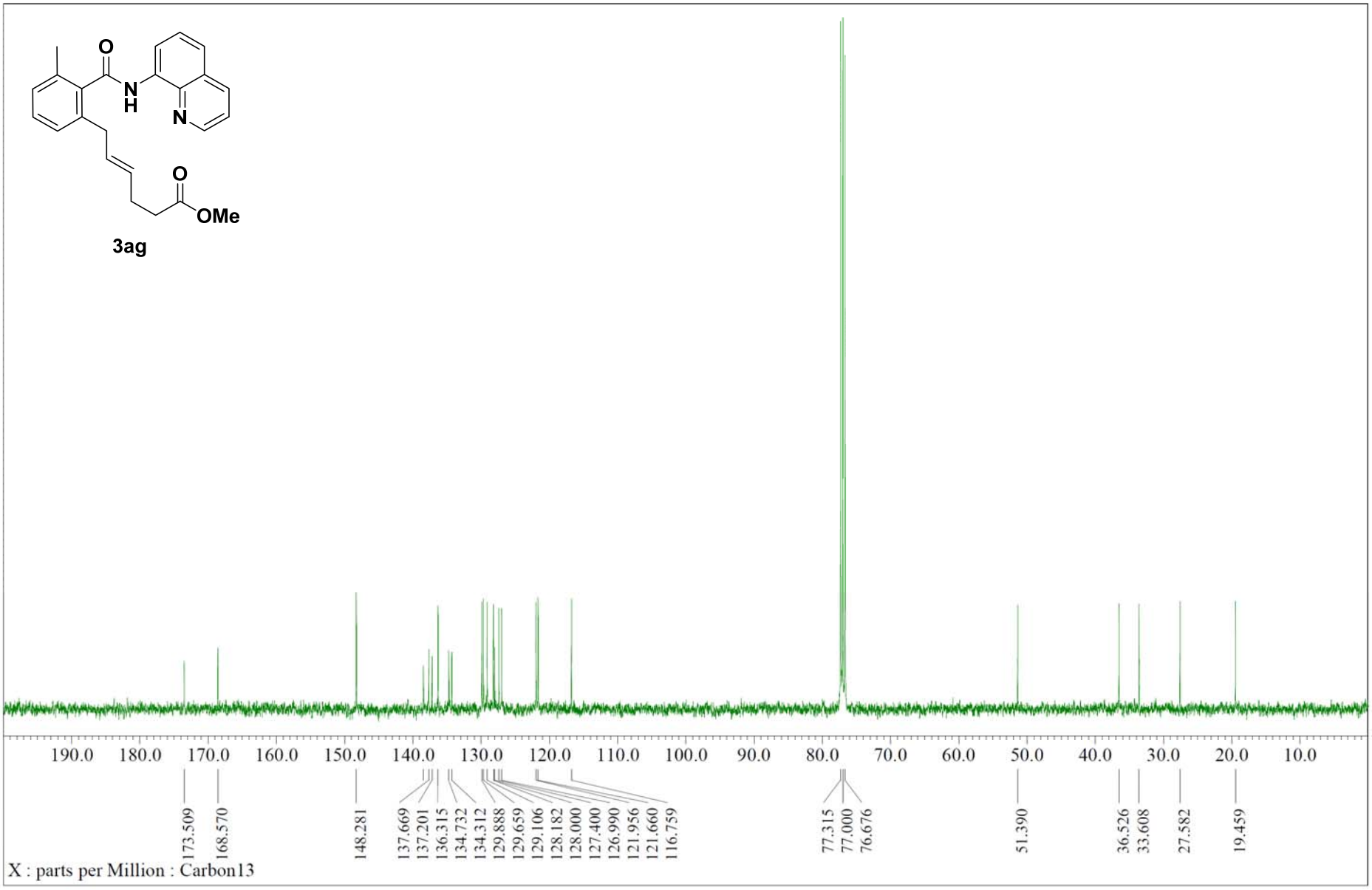
3.450
3.434
2.433
2.211
2.198
1.638
0.000
X : parts per Million : Proton


O
N
H
N
O
OMe
3ag
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
173.509
168.570
148.281
137.669
137.201
136.315
134.732
134.312
129.888
129.659
129.106
128.182
128.000
127.400
126.990
121.956
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77.000
76.676
51.390
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33.608
27.582
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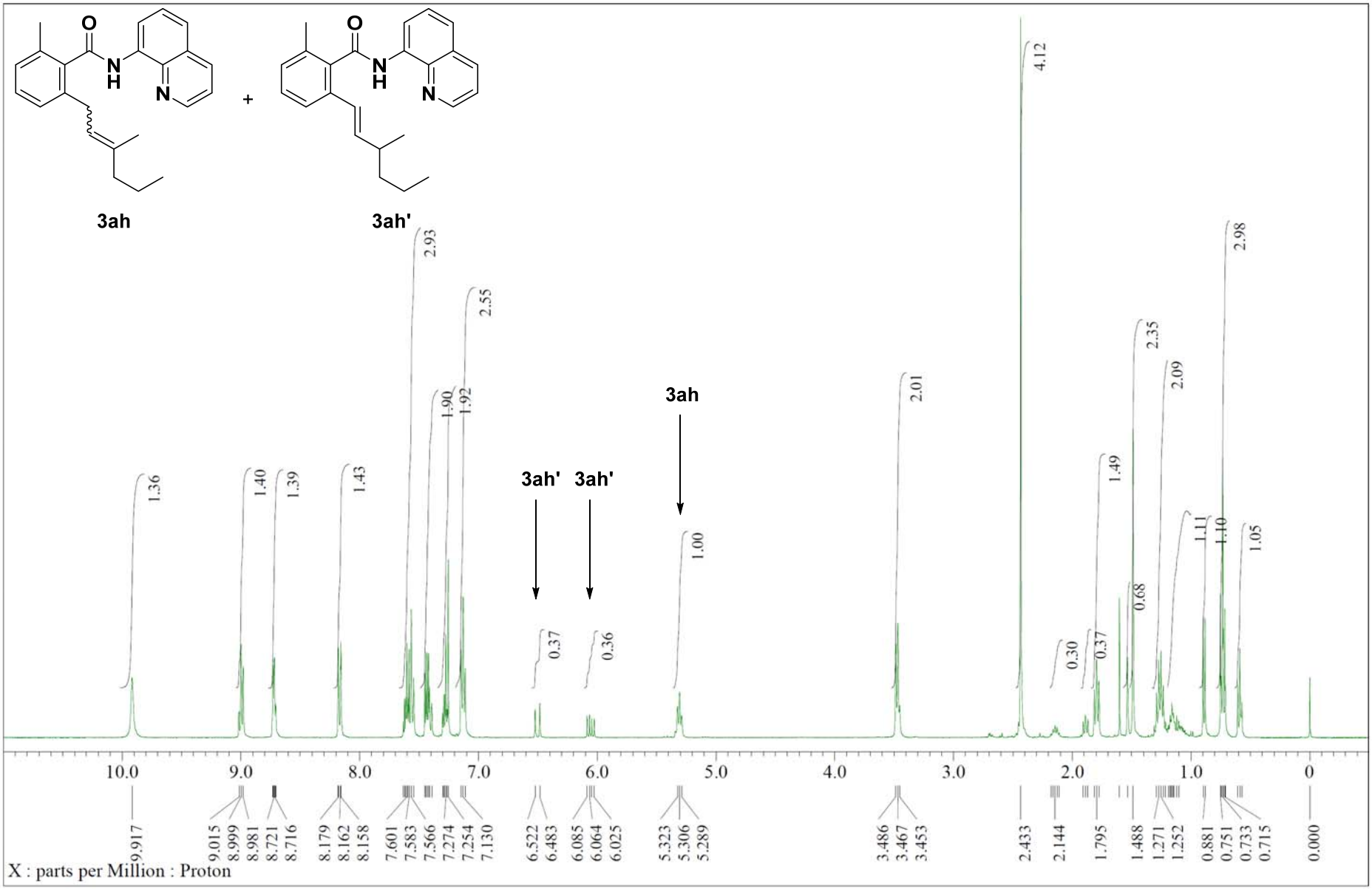
X : parts per Million : Carbon13


3ah
3ah'
3ah
3ah'
3ah'
4.12
2.98
2.93
2.55
2.35
2.09
2.01
1.90
1.92
1.49
1.43
1.40
1.39
1.36
1.11
1.10
1.05
1.00
0.68
0.37
0.36
0.30
0.37
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.917
9.015
8.999
8.981
8.721
8.716
8.179
8.162
8.158
7.601
7.583
7.566
7.274
7.254
7.130
6.522
6.483
6.085
6.064
6.025
5.323
5.306
5.289
3.486
3.467
3.453
2.433
2.144
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1.271
1.252
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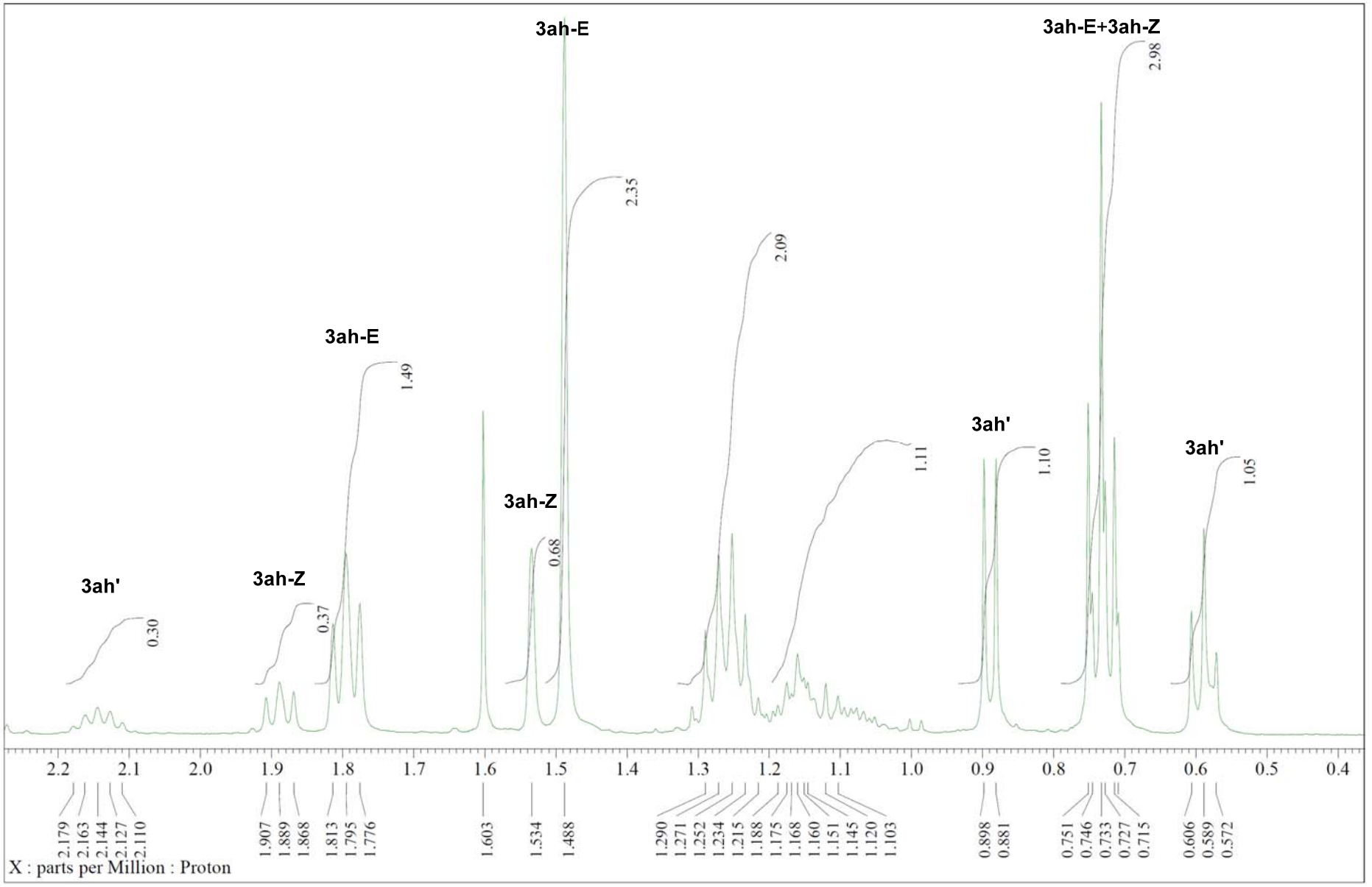
0.751
0.733
0.715
0.000
X : parts per Million : Proton


3ah-E
3ah-E+3ah-Z
3ah-E
3ah-Z
3ah'
3ah-Z
3ah'
3ah'
0.30
0.37
1.49
0.68
2.35
2.09
1.11
1.10
2.98
1.05
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
2.179
2.163
2.144
2.127
2.110
1.907
1.889
1.868
1.813
1.795
1.776
1.603
1.534
1.488
1.290
1.271
1.252
1.234
1.215
1.188
1.175
1.168
1.160
1.151
1.145
1.120
1.103
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0.881
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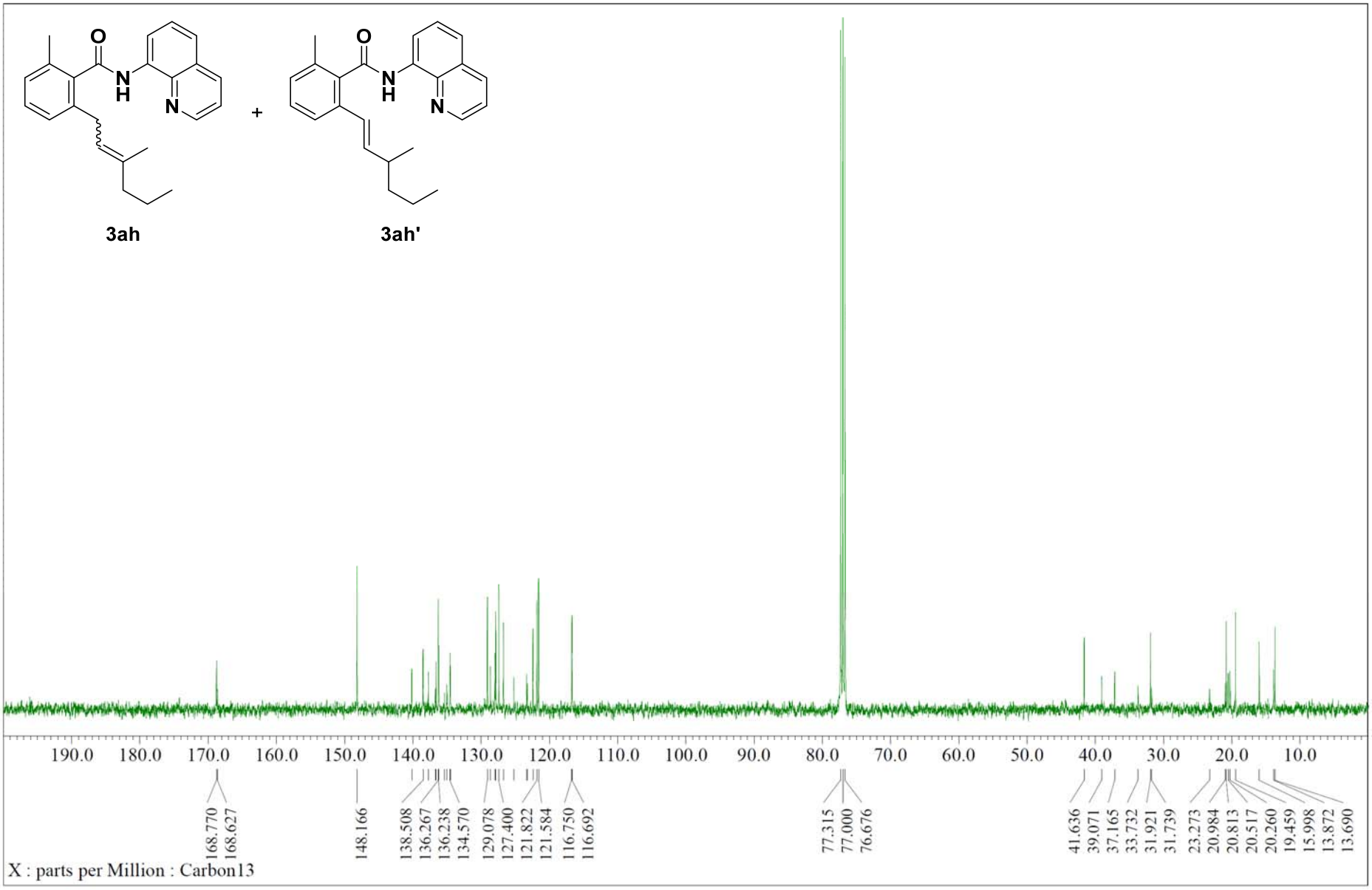
0.746
0.733
0.727
0.715
0.606
0.589
0.572
X : parts per Million : Proton


O
N
H
N
+
O
N
H
N
3ah
3ah'
190.0
180.0
170.0
160.0
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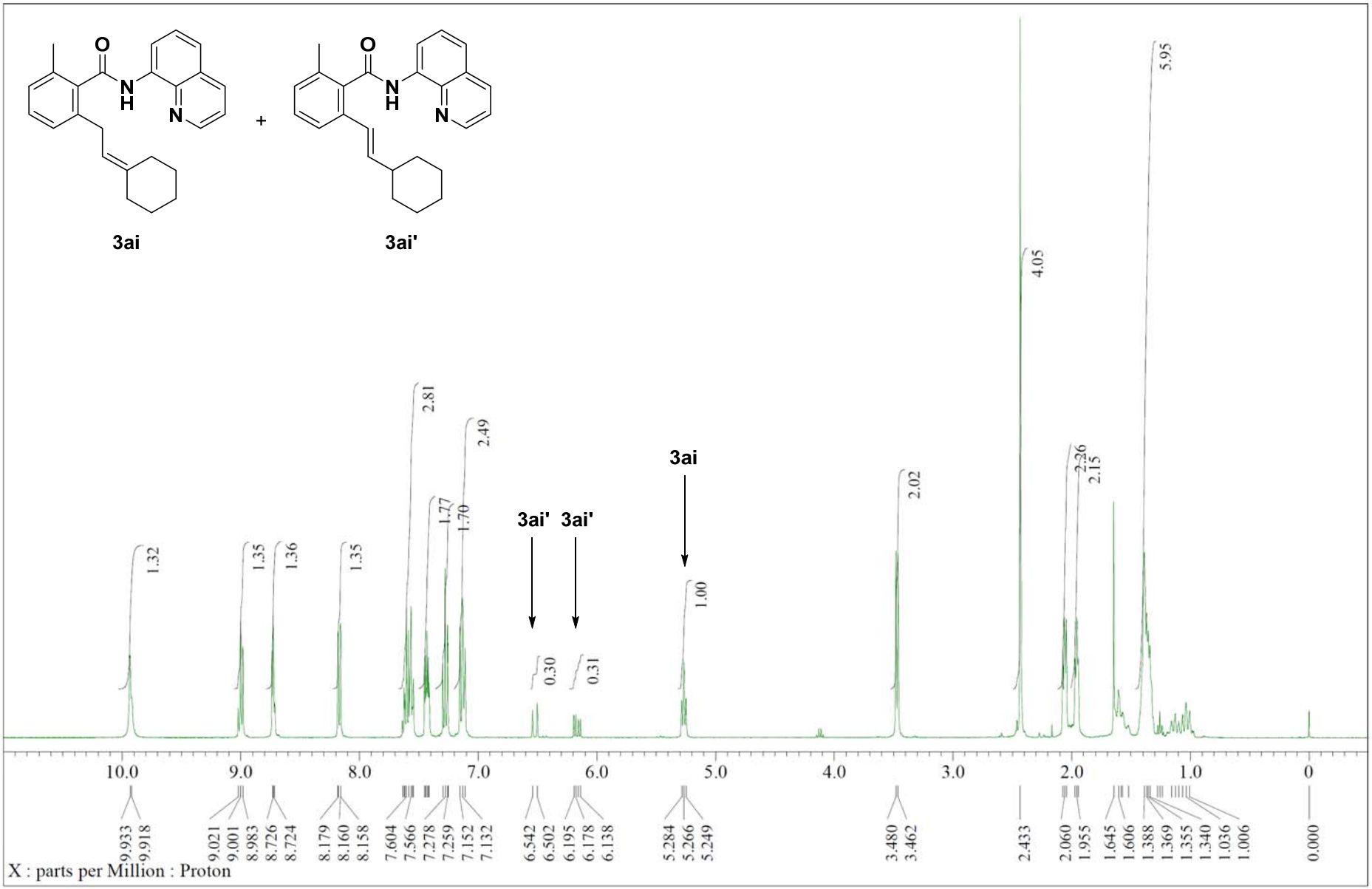
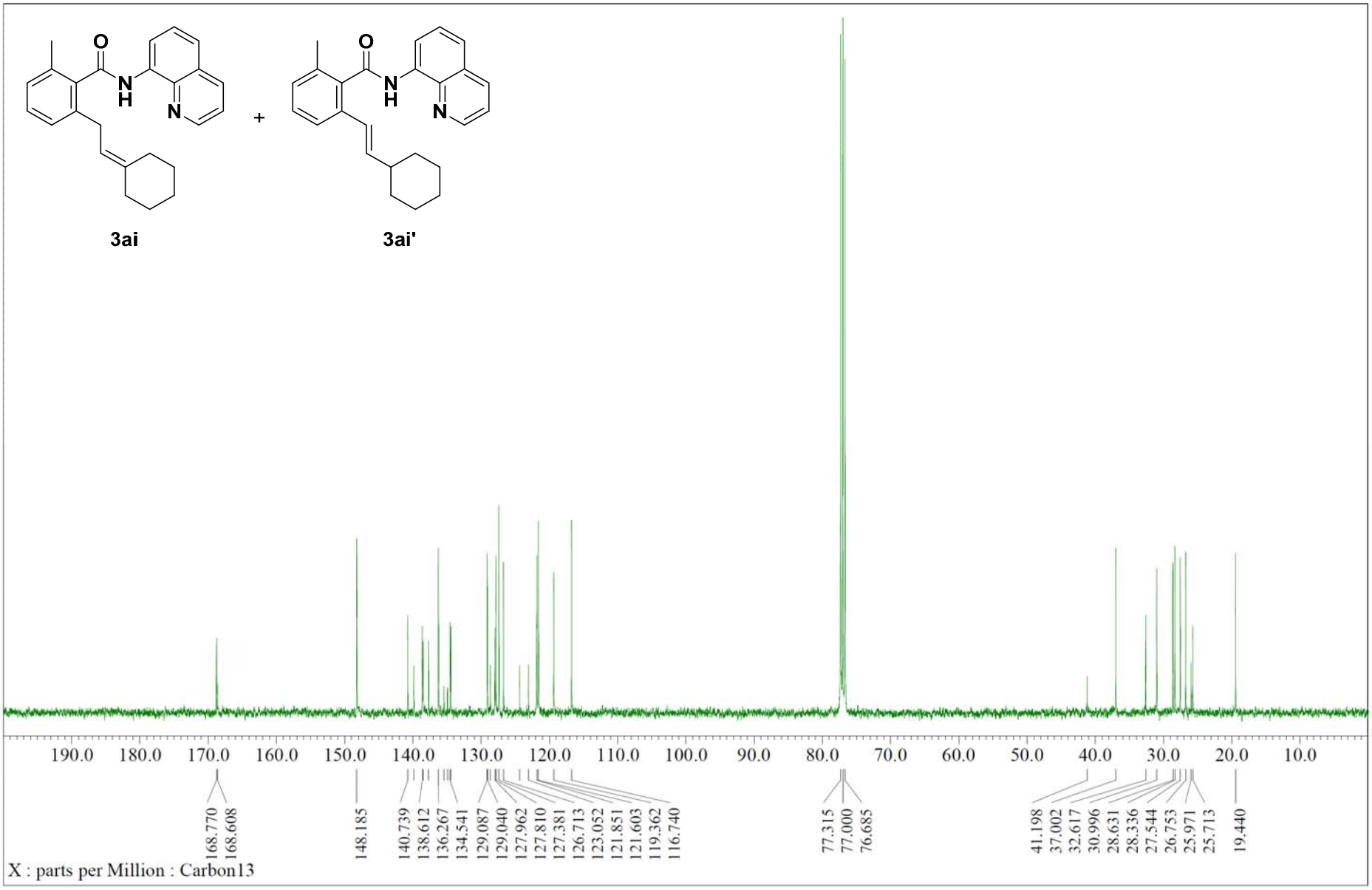
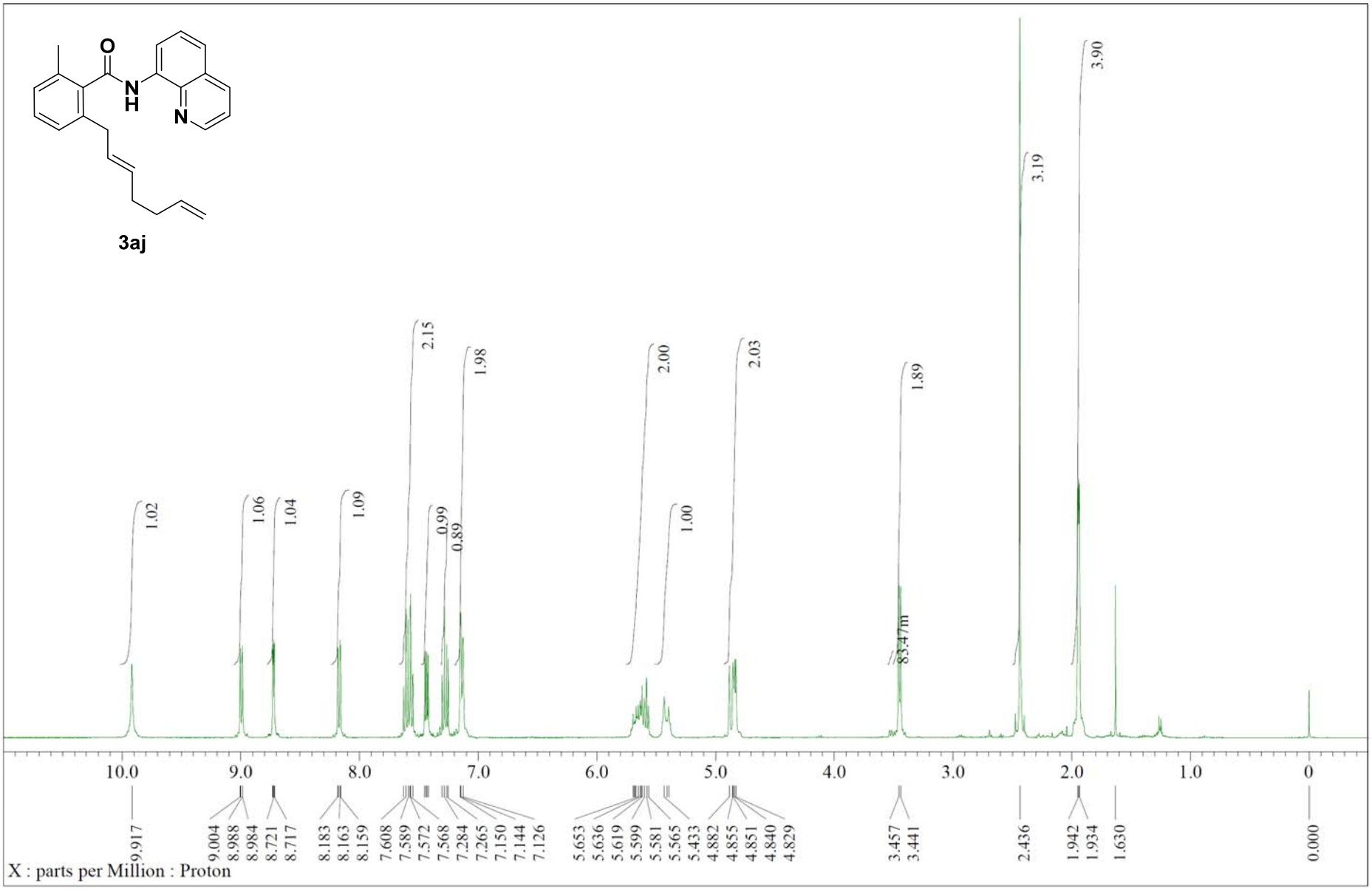
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
168.770
168.627
148.166
138.508
136.267
136.238
134.570
129.078
127.400
121.822
121.584
116.750
116.692
77.315
77.000
76.676
41.636
39.071
37.165
33.732
31.921
31.739
23.273
20.984
20.813
20.517
20.260
19.459
15.998
13.872
13.690
X : parts per Million : Carbon13


3ai
3ai'
3ai' 3ai'
3ai
X : parts per Million : Proton


3ai
3ai'
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
168.770
168.608
148.185
140.739
138.612
136.267
134.541
129.087
129.040
127.962
127.810
127.381
126.713
123.052
121.851
121.603
119.362
116.740
77.315
77.000
76.685
41.198
37.002
32.617
30.996
28.631
28.336
27.544
26.753
25.971
25.713
19.440
X : parts per Million : Carbon13


O
N
H
N
3aj
1.02
1.06
1.04
1.09
2.15
0.99
0.89
1.98
2.00
1.00
2.03
1.89
3.47m
3.19
3.90
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.917
9.004
8.988
8.984
8.721
8.717
8.183
8.163
8.159
7.608
7.589
7.572
7.568
7.284
7.265
7.150
7.144
7.126
5.653
5.636
5.619
5.599
5.581
5.565
5.433
4.882
4.855
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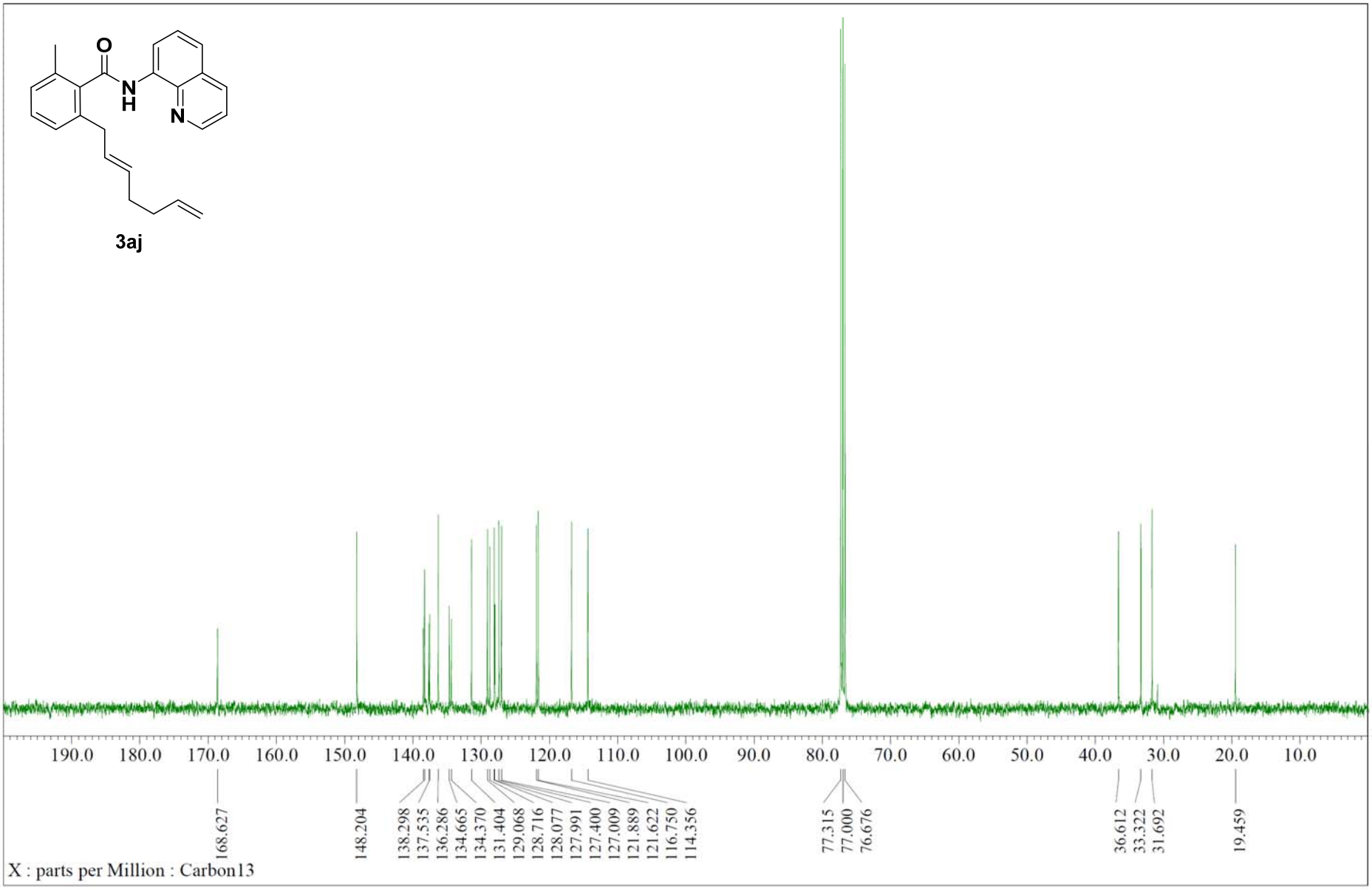
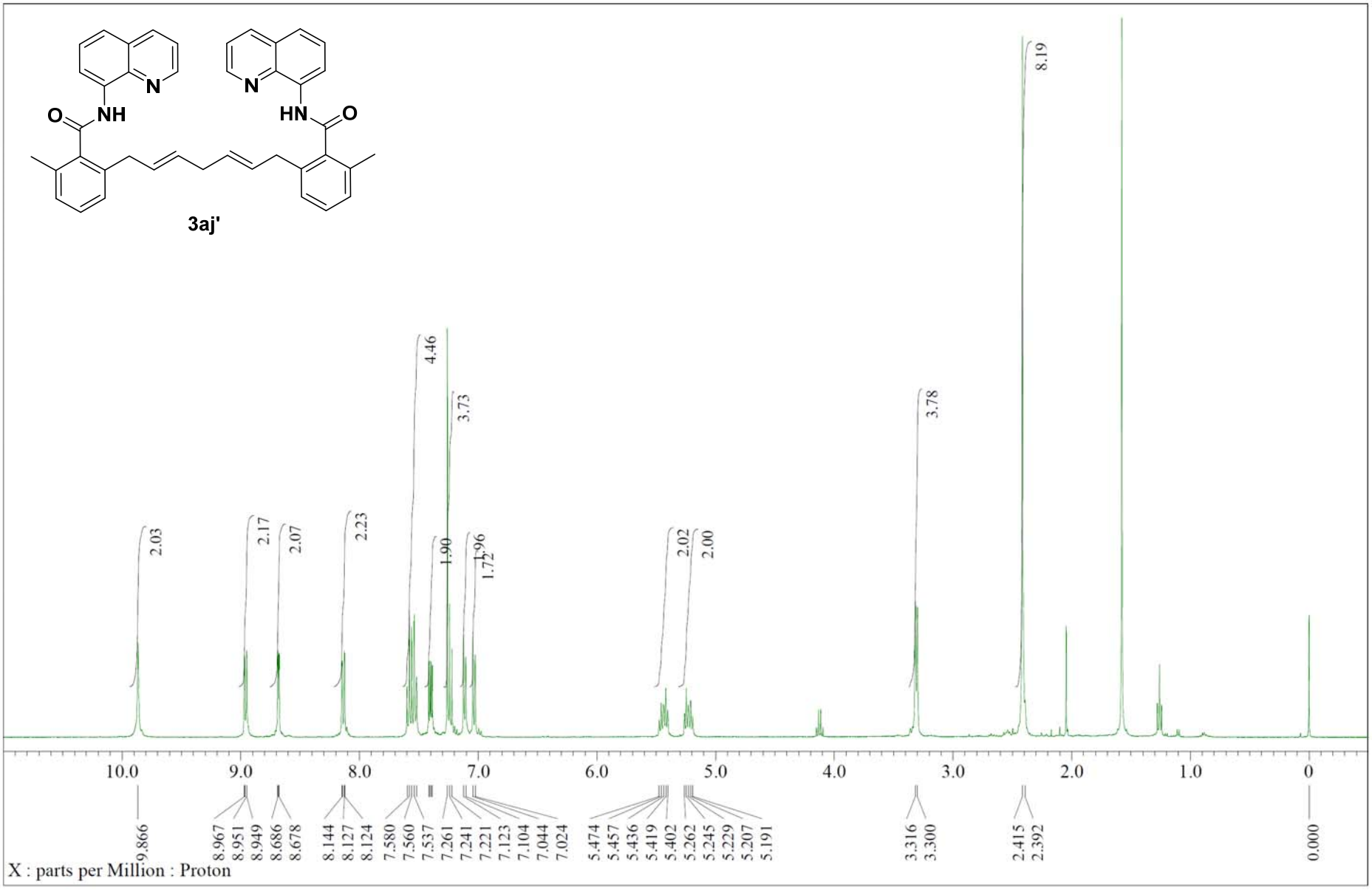
3.457
3.441
2.436
1.942
1.934
1.630
0.000
X : parts per Million : Proton


O
N
H
N
3aj
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
168.627
148.204
138.298
137.535
136.286
134.665
134.370
131.404
129.068
128.716
128.077
127.991
127.400
127.009
121.889
121.622
116.750
114.356
77.315
77.000
76.676
36.612
33.322
31.692
19.459
X : parts per Million : Carbon13


3aj'
2.03
2.17
2.07
2.23
4.46
3.73
1.90
1.96
1.72
2.02
2.00
3.78
8.19
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.866
8.967
8.951
8.949
8.686
8.678
8.144
8.127
8.124
7.580
7.560
7.537
7.261
7.241
7.221
7.123
7.104
7.044
7.024
5.474
5.457
5.436
5.419
5.402
5.262
5.245
5.229
5.207
5.191
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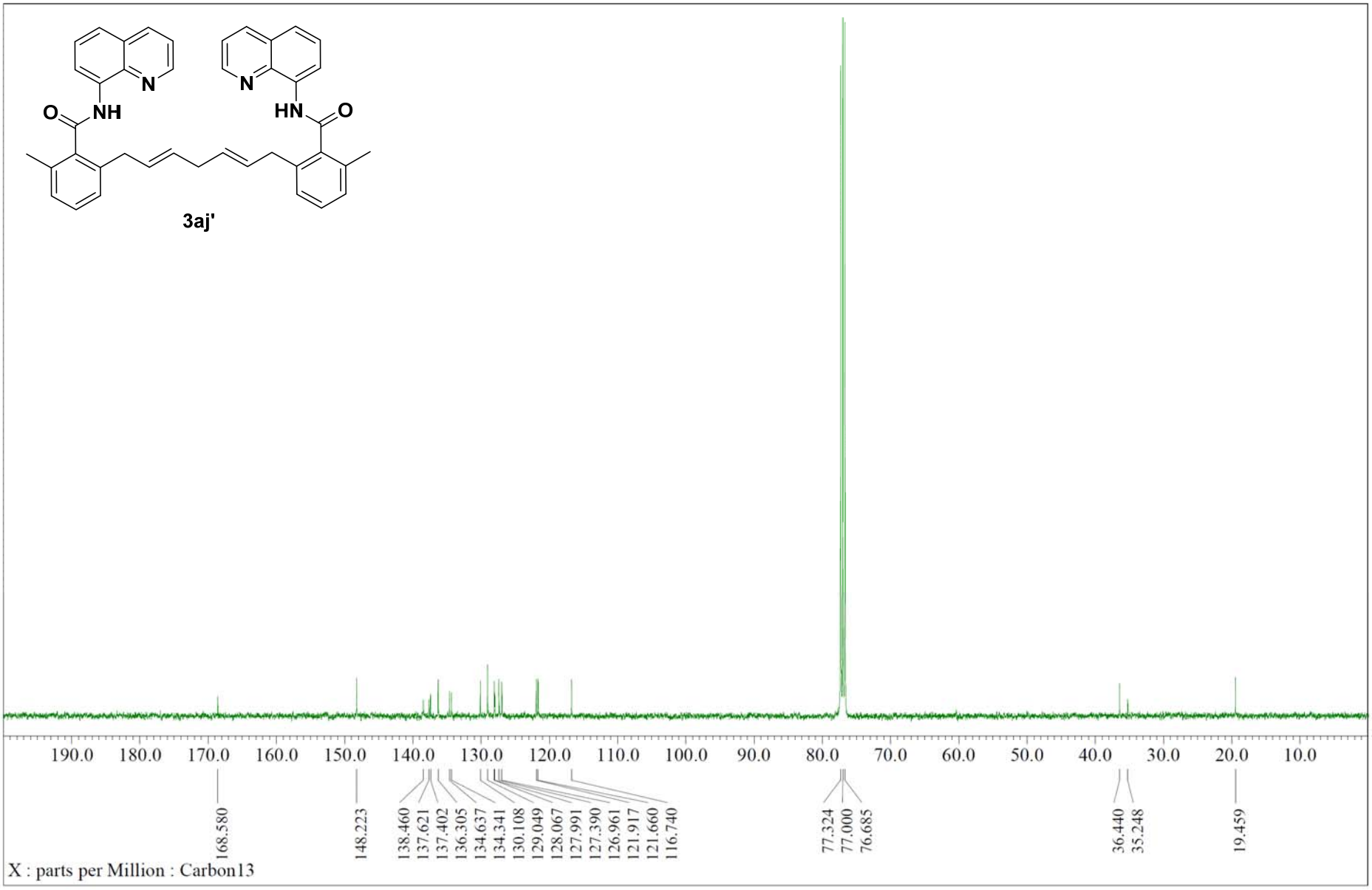
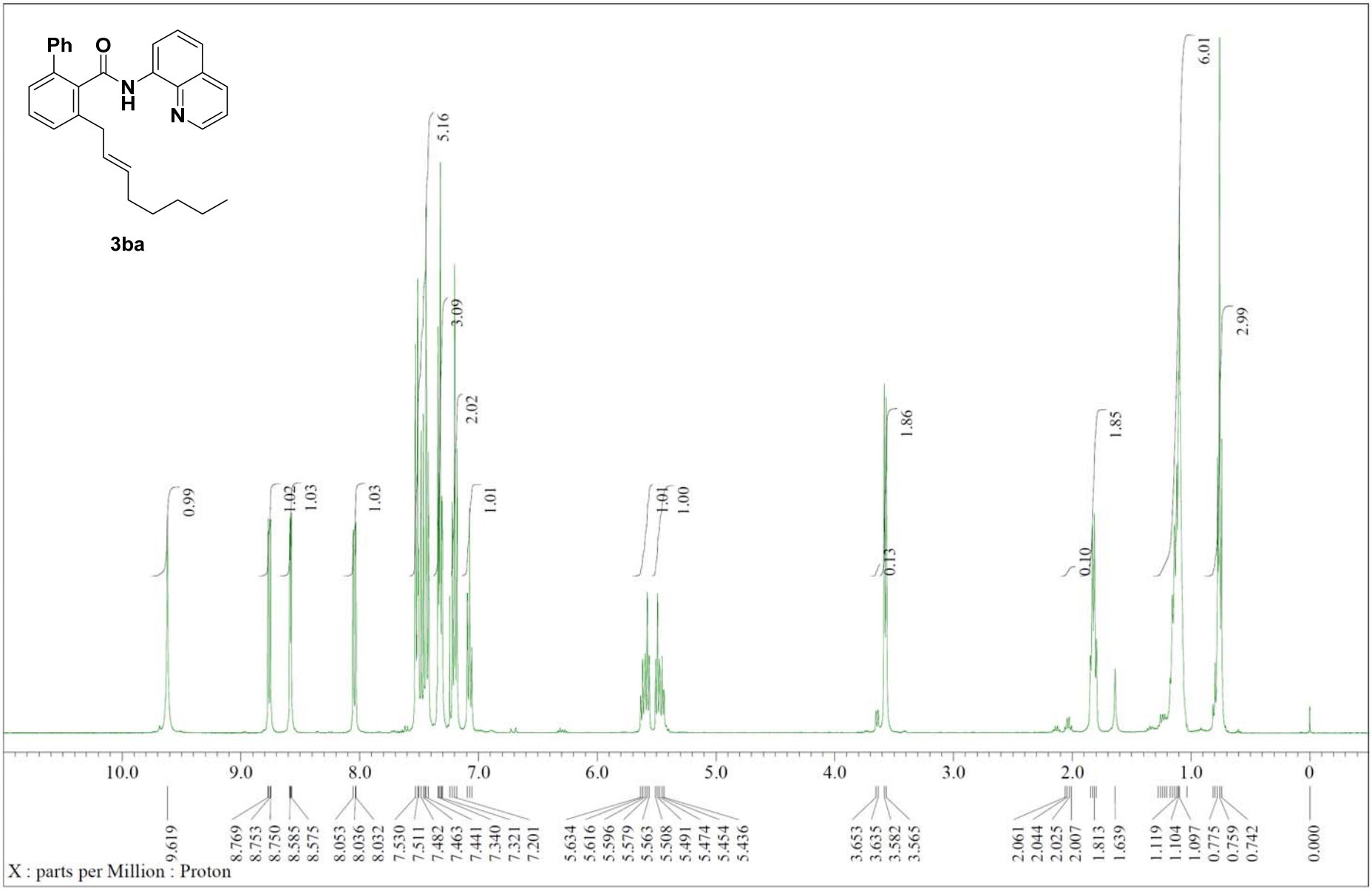
3.300
2.415
2.392
0.000
X : parts per Million : Proton


O
NH
N
HN
O
N
3aj'
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
168.580
148.223
138.460
137.621
137.402
136.305
134.637
134.341
130.108
129.049
128.067
127.991
127.390
126.961
121.917
121.660
116.740
77.324
77.000
76.685
36.440
35.248
19.459
X : parts per Million : Carbon13


Ph
O
N
H
N
3ba
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1.03
1.03
5.16
3.09
2.02
1.01
1.01
1.00
0.13
1.86
0.10
1.85
6.01
2.99
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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8.769
8.753
8.750
8.585
8.575
8.053
8.036
8.032
7.530
7.511
7.482
7.463
7.441
7.340
7.321
7.201
5.634
5.616
5.596
5.579
5.563
5.508
5.491
5.474
5.454
5.436
3.653
3.635
3.582
3.565
2.061
2.044
2.025
2.007
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1.639
1.119
1.104
1.097
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0.759
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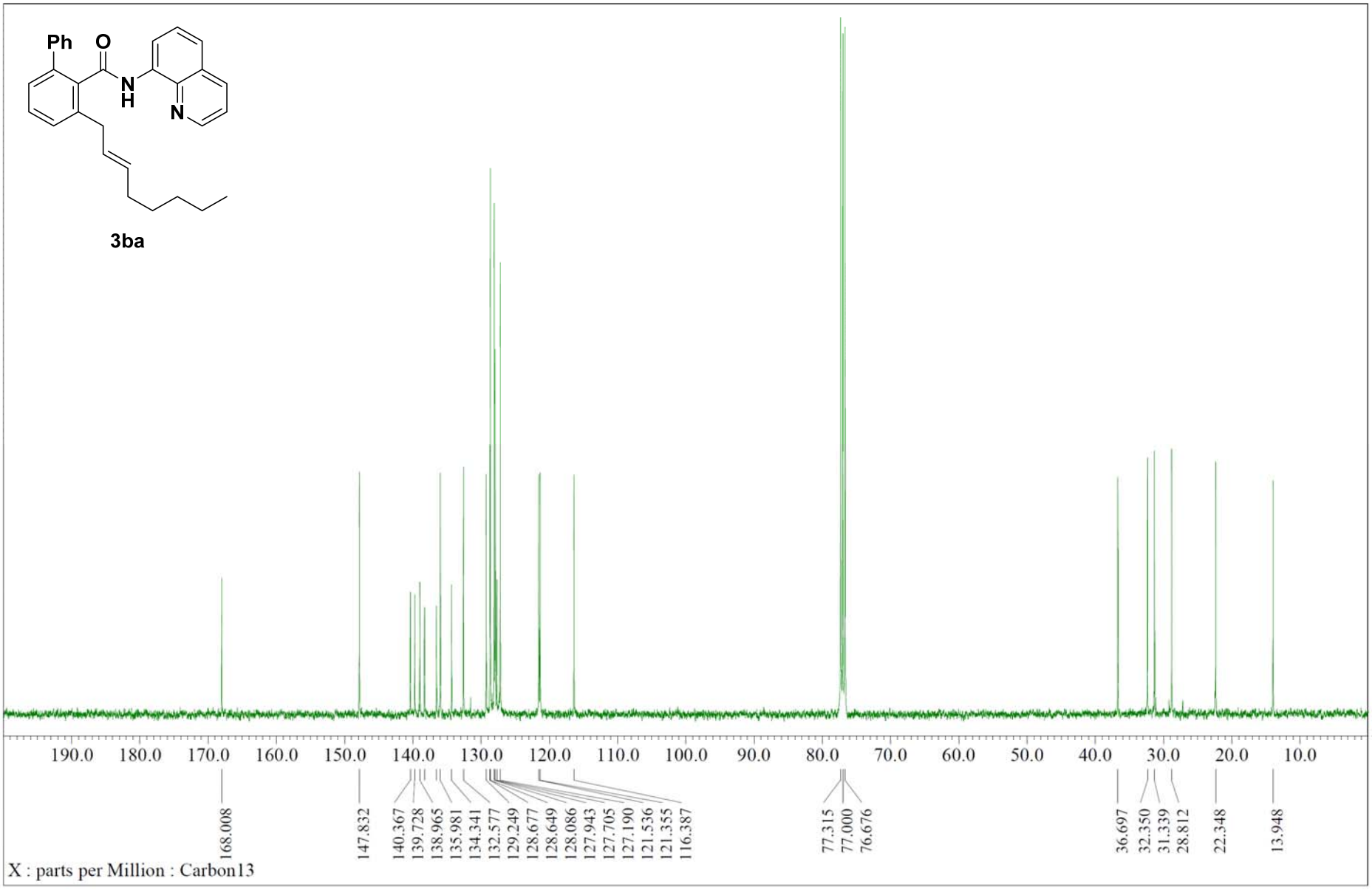
0.000
X : parts per Million : Proton


Ph
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N
H
N
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90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
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140.367
139.728
138.965
135.981
134.341
132.577
129.249
128.677
128.649
128.086
127.943
127.705
127.190
121.536
121.355
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76.676
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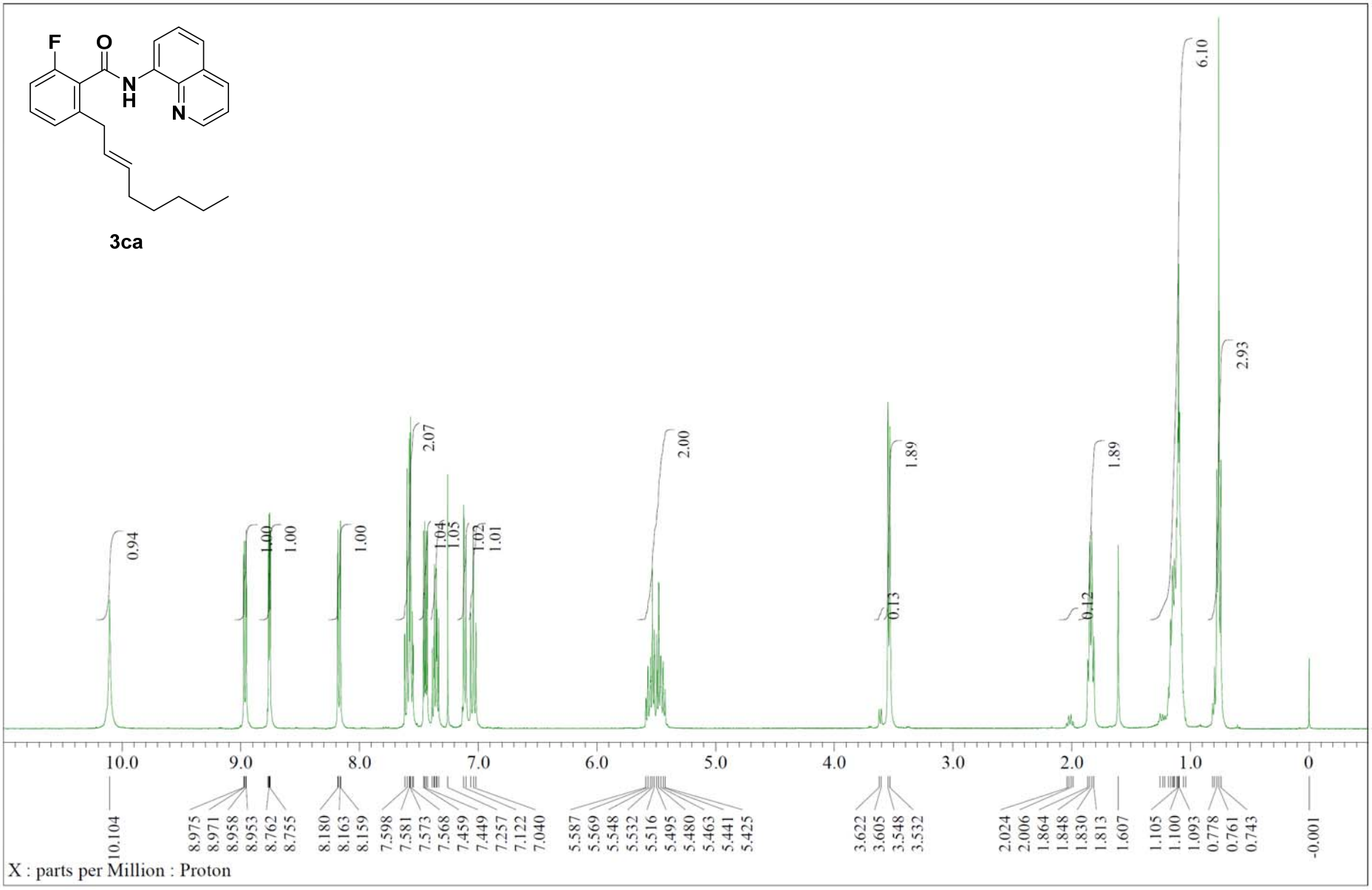
32.350
31.339
28.812
22.348
13.948
X : parts per Million : Carbon13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H
N
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1.00
1.00
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1.04
1.05
1.02
1.01
2.00
1.89
0.13
0.12
1.89
6.10
2.93
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.104
8.975
8.971
8.958
8.953
8.762
8.755
8.180
8.163
8.159
7.598
7.581
7.573
7.568
7.459
7.449
7.257
7.122
7.040
5.587
5.569
5.548
5.532
5.516
5.495
5.480
5.463
5.441
5.425
3.622
3.605
3.548
3.532
2.024
2.006
1.864
1.848
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1.813
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1.105
1.100
1.093
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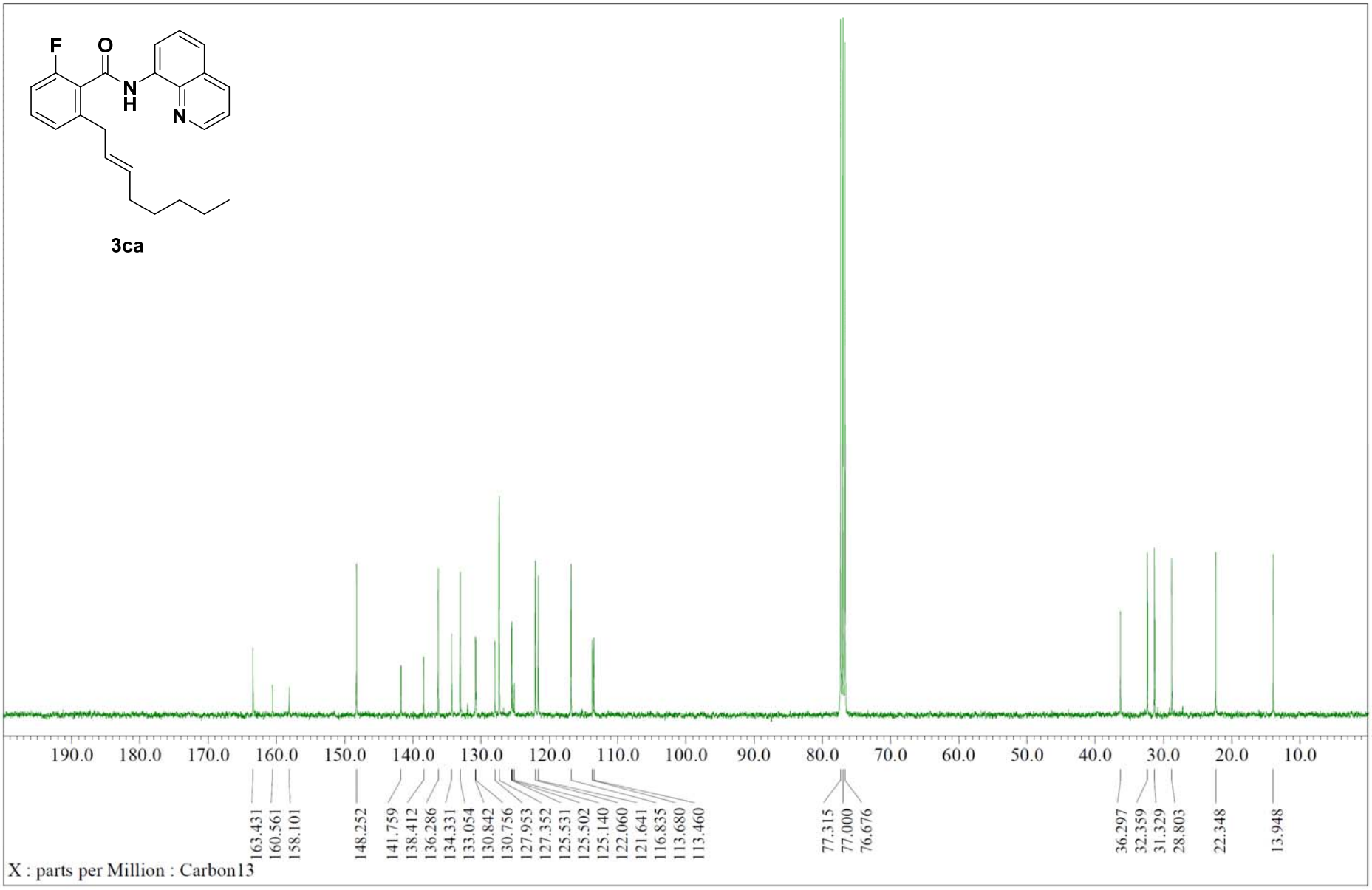
0.743
-0.001
X : parts per Million : Proton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H
N
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160.0
150.0
140.0
130.0
120.0
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80.0
70.0
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50.0
40.0
30.0
20.0
10.0
163.431
160.561
158.101
148.252
141.759
138.412
136.286
134.331
133.054
130.842
130.756
127.953
127.352
125.531
125.502
125.140
122.060
121.641
116.835
113.680
113.460
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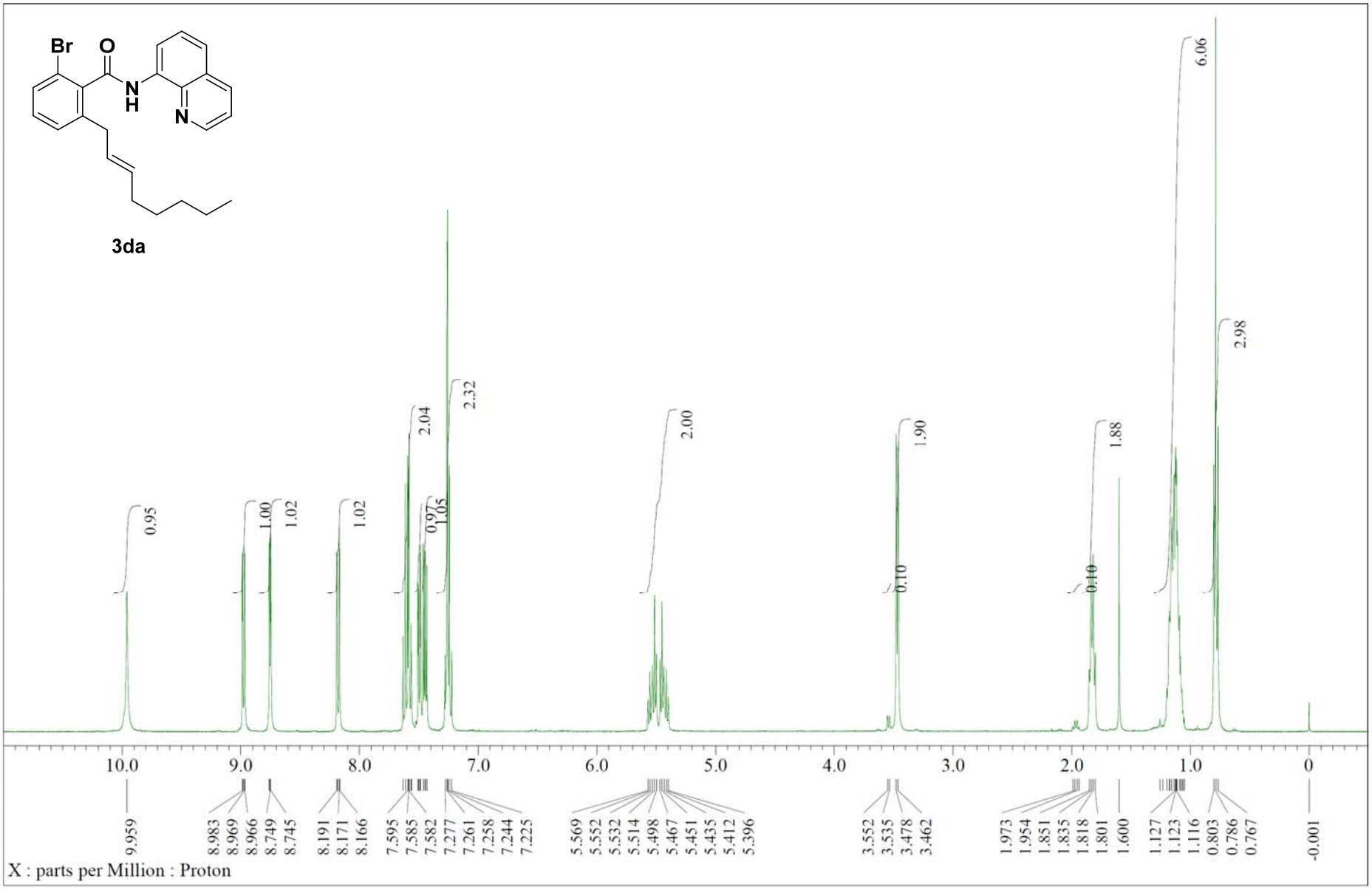
77.000
76.676
36.297
32.359
31.329
28.803
22.348
13.948
X : parts per Million : Carbon13


Br
O
N
H
N
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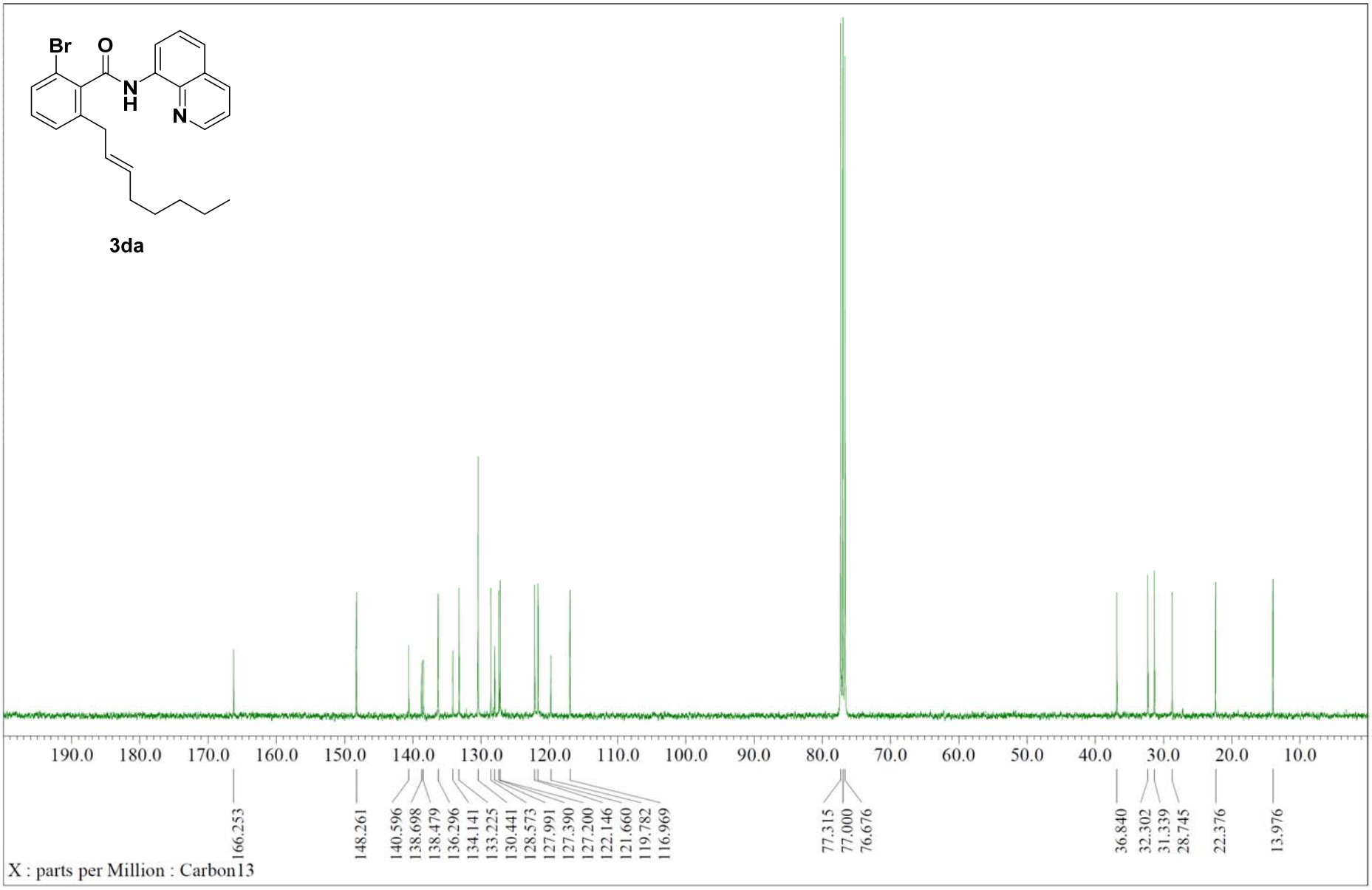
1.00
1.02
1.02
2.04
0.97
1.05
2.32
2.00
1.90
0.10
0.10
1.88
6.06
2.98
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.959
8.983
8.969
8.966
8.749
8.745
8.191
8.171
8.166
7.595
7.585
7.582
7.277
7.261
7.258
7.244
7.225
5.569
5.552
5.532
5.514
5.498
5.467
5.451
5.435
5.412
5.396
3.552
3.535
3.478
3.462
1.973
1.954
1.851
1.835
1.818
1.801
1.600
1.127
1.123
1.116
0.803
0.786
0.767
-0.001
X : parts per Million : Proton


Br
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H
N
3da
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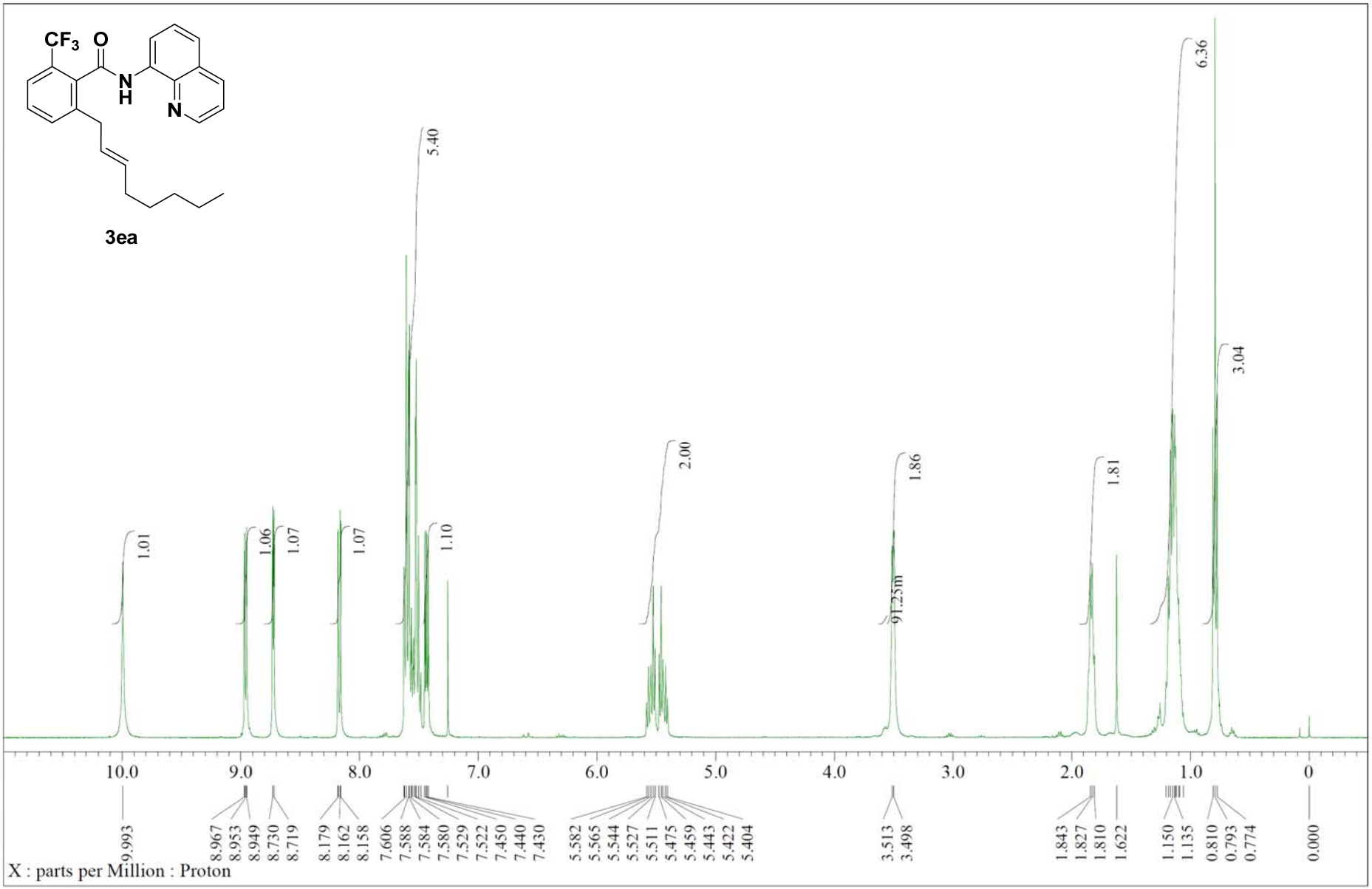
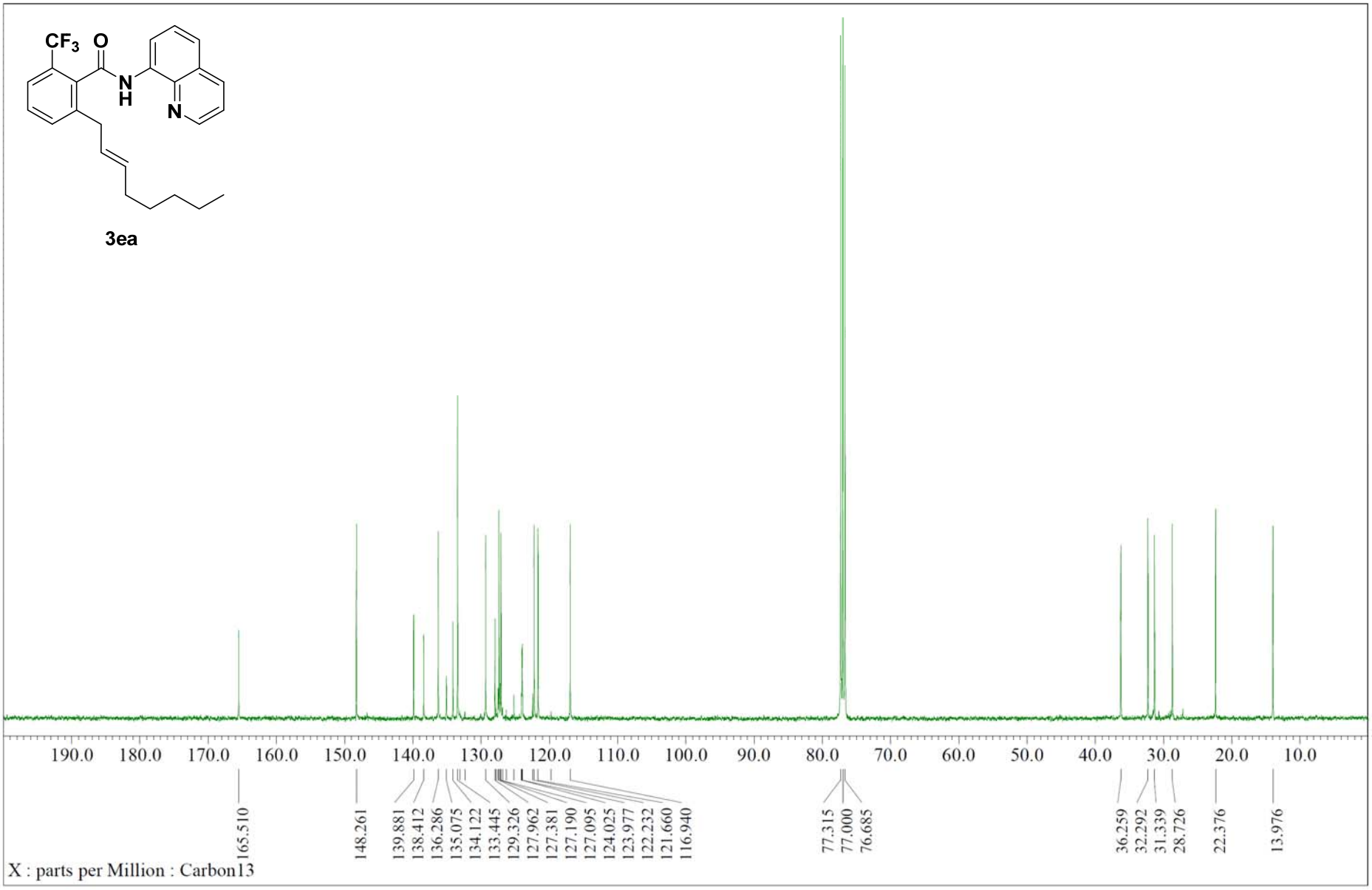
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
166.253
148.261
140.596
138.698
138.479
136.296
134.141
133.225
130.441
128.573
127.991
127.390
127.200
122.146
121.660
119.782
116.969
77.315
77.000
76.676
36.840
32.302
31.339
28.745
22.376
13.976
X : parts per Million : Carbon13


CF3
O
N
H
N
3ea
6.36
5.40
3.04
2.00
1.86
1.81
1.01
1.06
1.07
1.07
1.10
9T.25m
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.993
8.967
8.953
8.949
8.730
8.719
8.179
8.162
8.158
7.606
7.588
7.584
7.580
7.529
7.522
7.450
7.440
7.430
5.582
5.565
5.544
5.527
5.511
5.475
5.459
5.443
5.422
5.404
3.513
3.498
1.843
1.827
1.810
1.622
1.150
1.135
0.810
0.793
0.774
0.000
X : parts per Million : Proton


CF3
O
N
H
N
3ea
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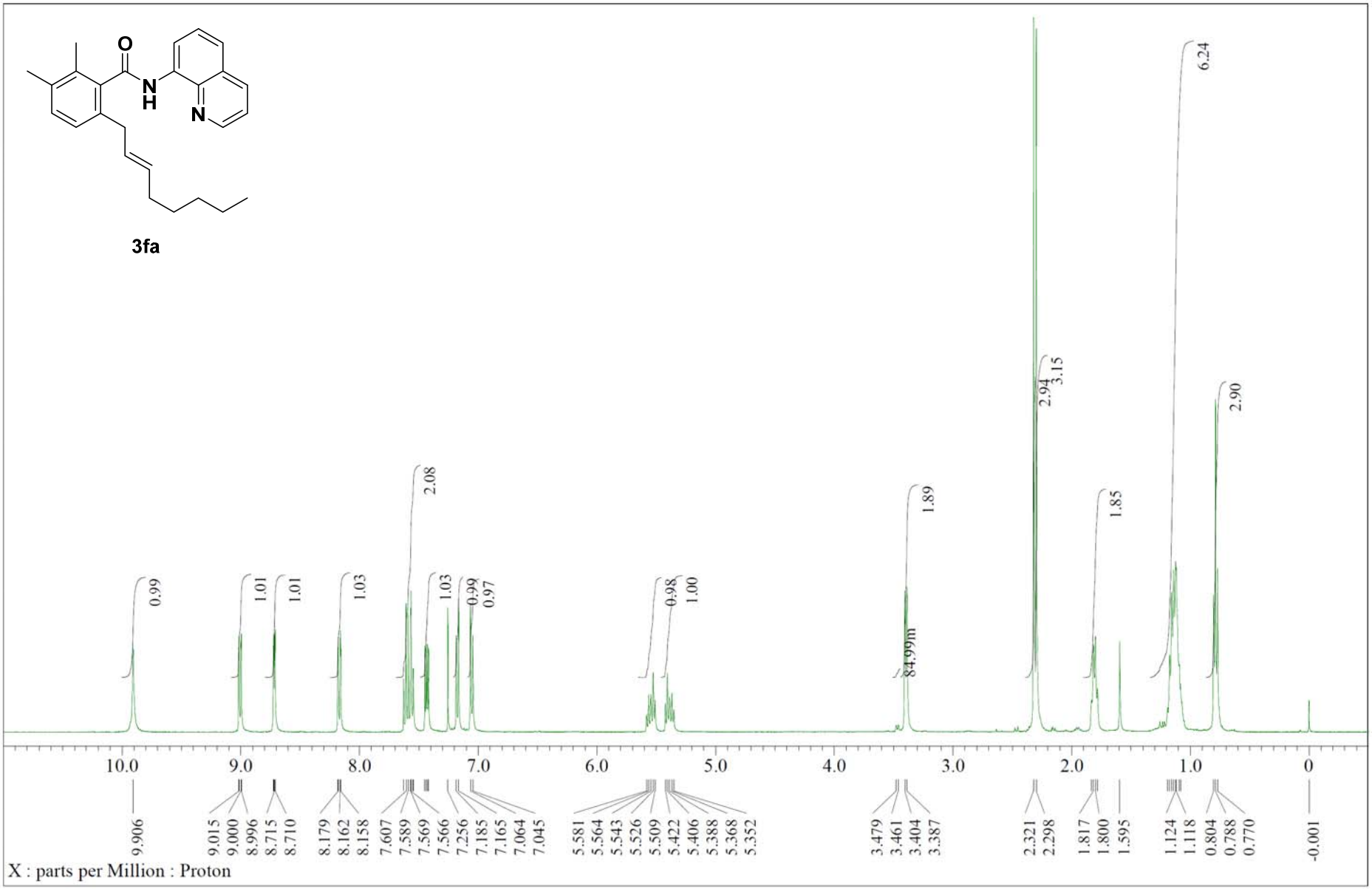
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
165.510
148.261
139.881
138.412
136.286
135.075
134.122
133.445
129.326
127.962
127.381
127.190
127.095
124.025
123.977
122.232
121.660
116.940
77.315
77.000
76.685
36.259
32.292
31.339
28.726
22.376
13.976
X : parts per Million : Carbon13


O
N
H
N
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2.94
3.15
2.90
2.08
1.89
1.85
84.99m
0.99
1.01
1.01
1.03
1.03
0.99
0.97
0.98
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.906
9.015
9.000
8.996
8.715
8.710
8.179
8.162
8.158
7.607
7.589
7.569
7.566
7.256
7.185
7.165
7.064
7.045
5.581
5.564
5.543
5.526
5.509
5.422
5.406
5.388
5.368
5.352
3.479
3.461
3.404
3.387
2.321
2.298
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1.595
1.124
1.118
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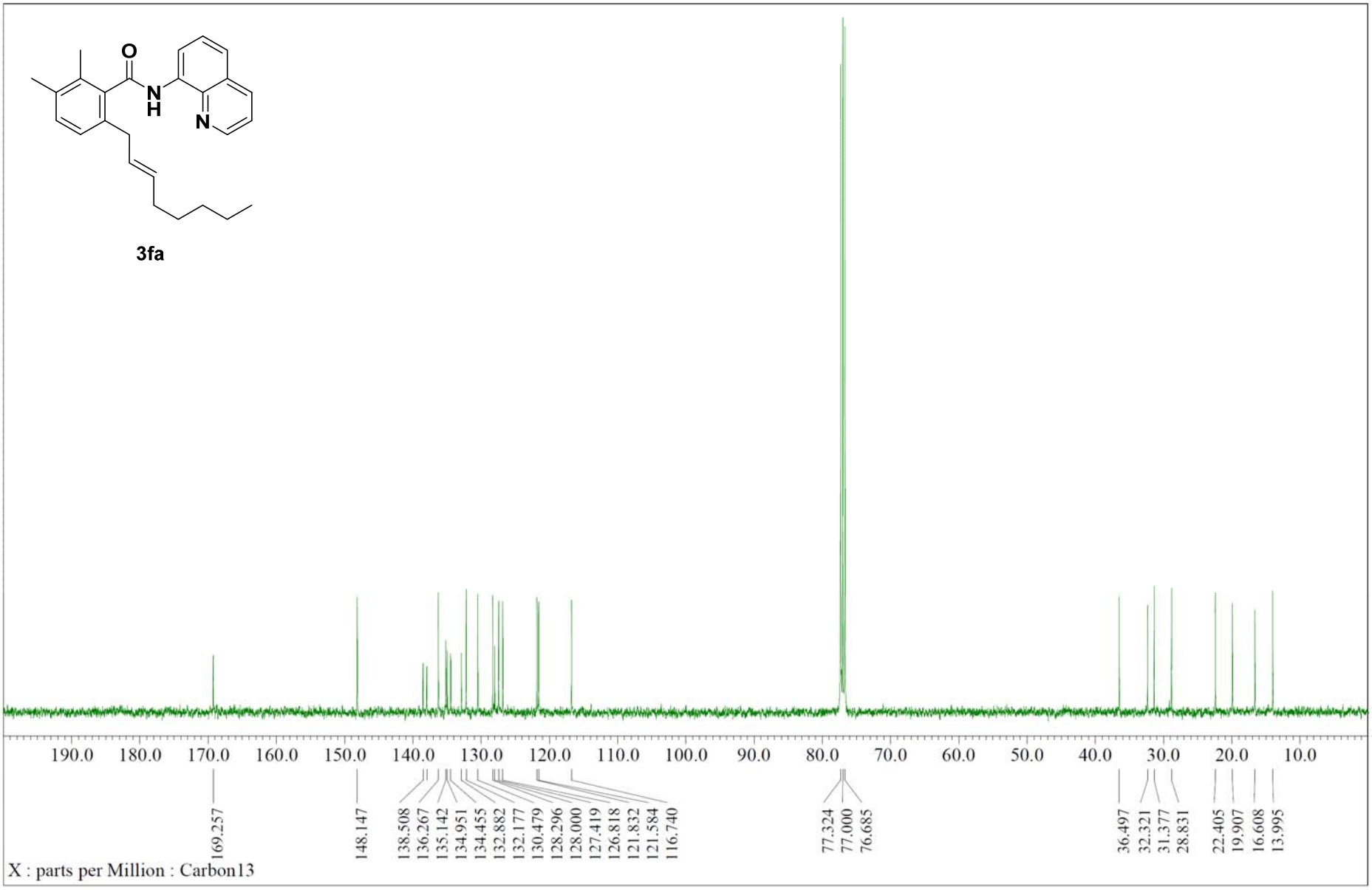
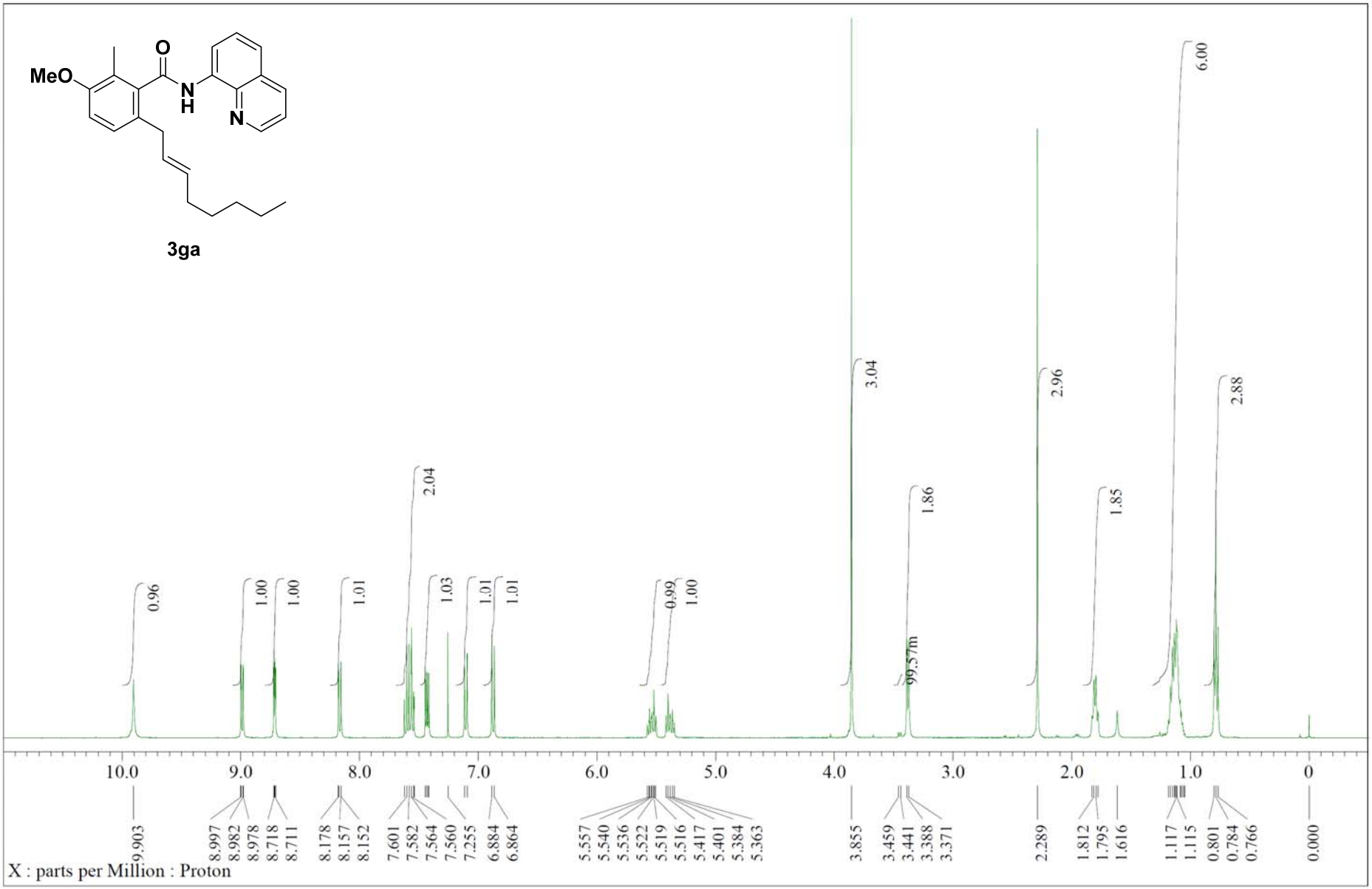
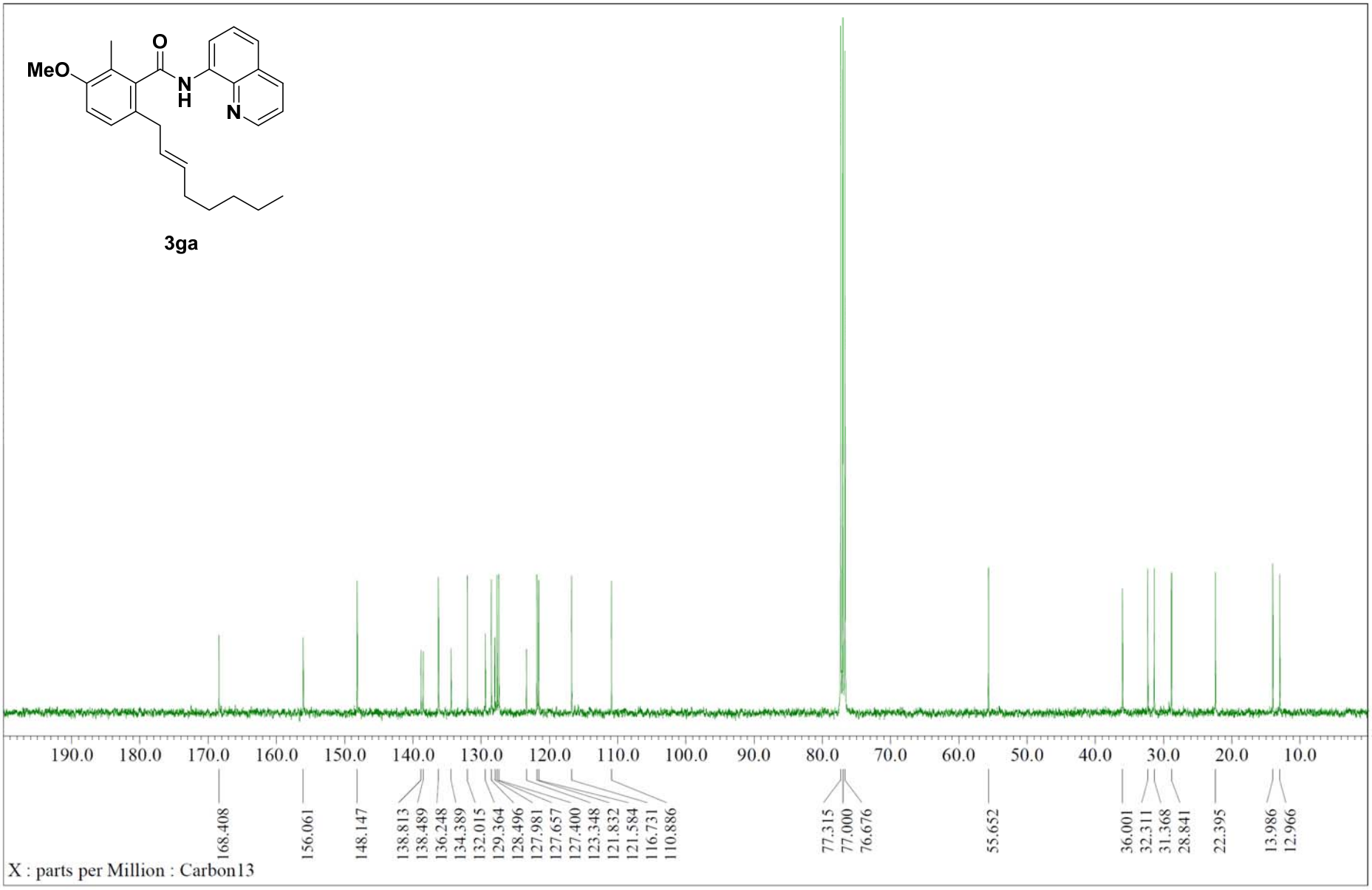
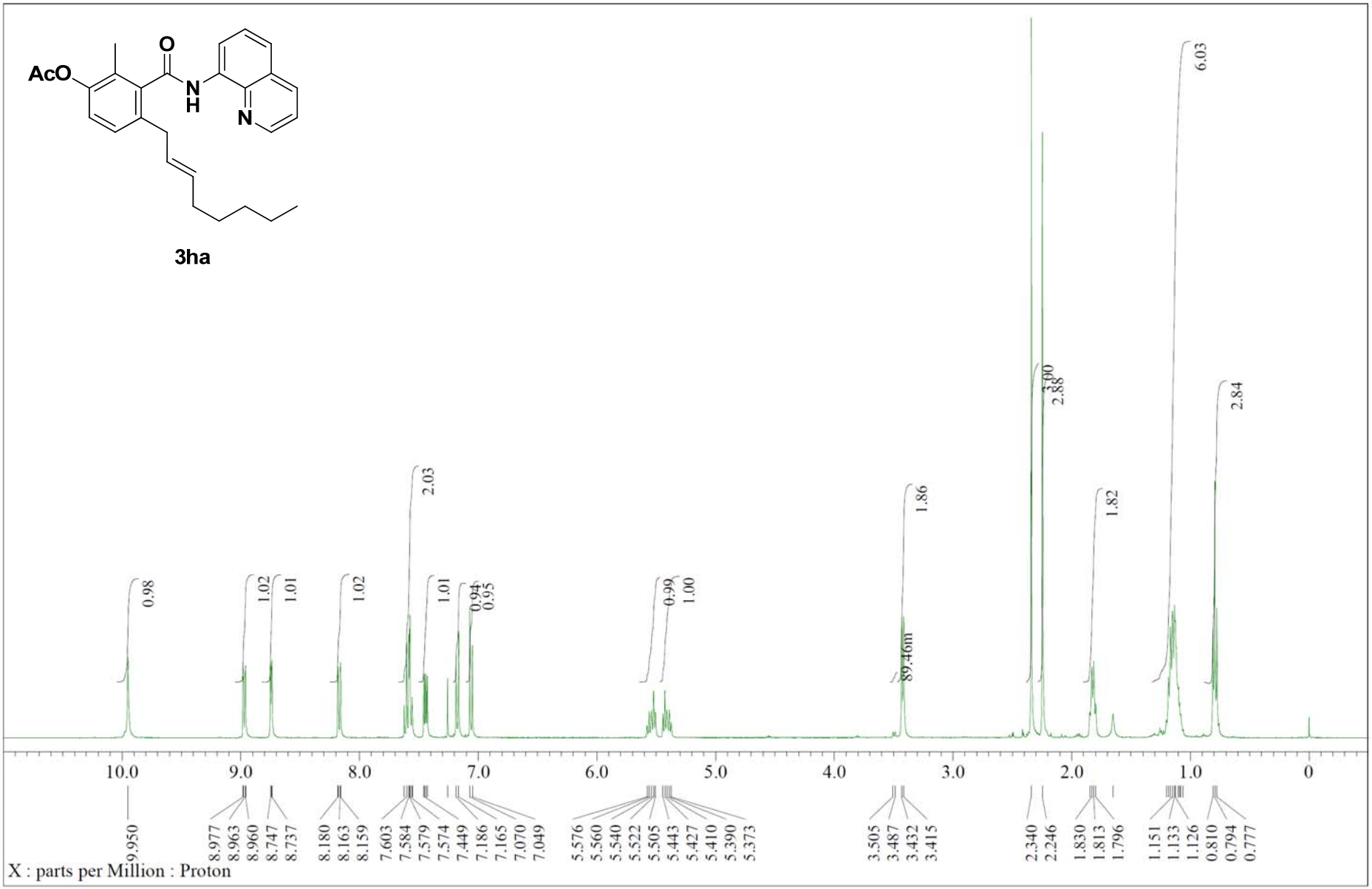
0.788
0.770
-0.001
X : parts per Million : Proton


O
N
H
N
3fa
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
169.257
148.147
138.508
136.267
135.142
134.951
134.455
132.882
132.177
130.479
128.296
128.000
127.419
126.818
121.832
121.584
116.740
77.324
77.000
76.685
36.497
32.321
31.377
28.831
22.405
19.907
16.608
13.995
X : parts per Million : Carbon13


MeO
O
N
H
N
3ga
0.96
1.00
1.00
1.01
2.04
1.03
1.01
1.01
0.99
1.00
3.04
99.57m
1.86
2.96
1.85
6.00
2.88
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.903
8.997
8.982
8.978
8.718
8.711
8.178
8.157
8.152
7.601
7.582
7.564
7.560
7.255
6.884
6.864
5.557
5.540
5.536
5.522
5.519
5.516
5.417
5.401
5.384
5.363
3.855
3.459
3.441
3.388
3.371
2.289
1.812
1.795
1.616
1.117
1.115
0.801
0.784
0.766
0.000
X : parts per Million : Proton


MeO
O
N
H
N
3ga
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
168.408
156.061
148.147
138.813
138.489
136.248
134.389
132.015
129.364
128.496
127.981
127.657
127.400
123.348
121.832
121.584
116.731
110.886
77.315
77.000
76.676
55.652
36.001
32.311
31.368
28.841
22.395
13.986
12.966
X : parts per Million : Carbon13


AcO
O
N
H
N
3ha
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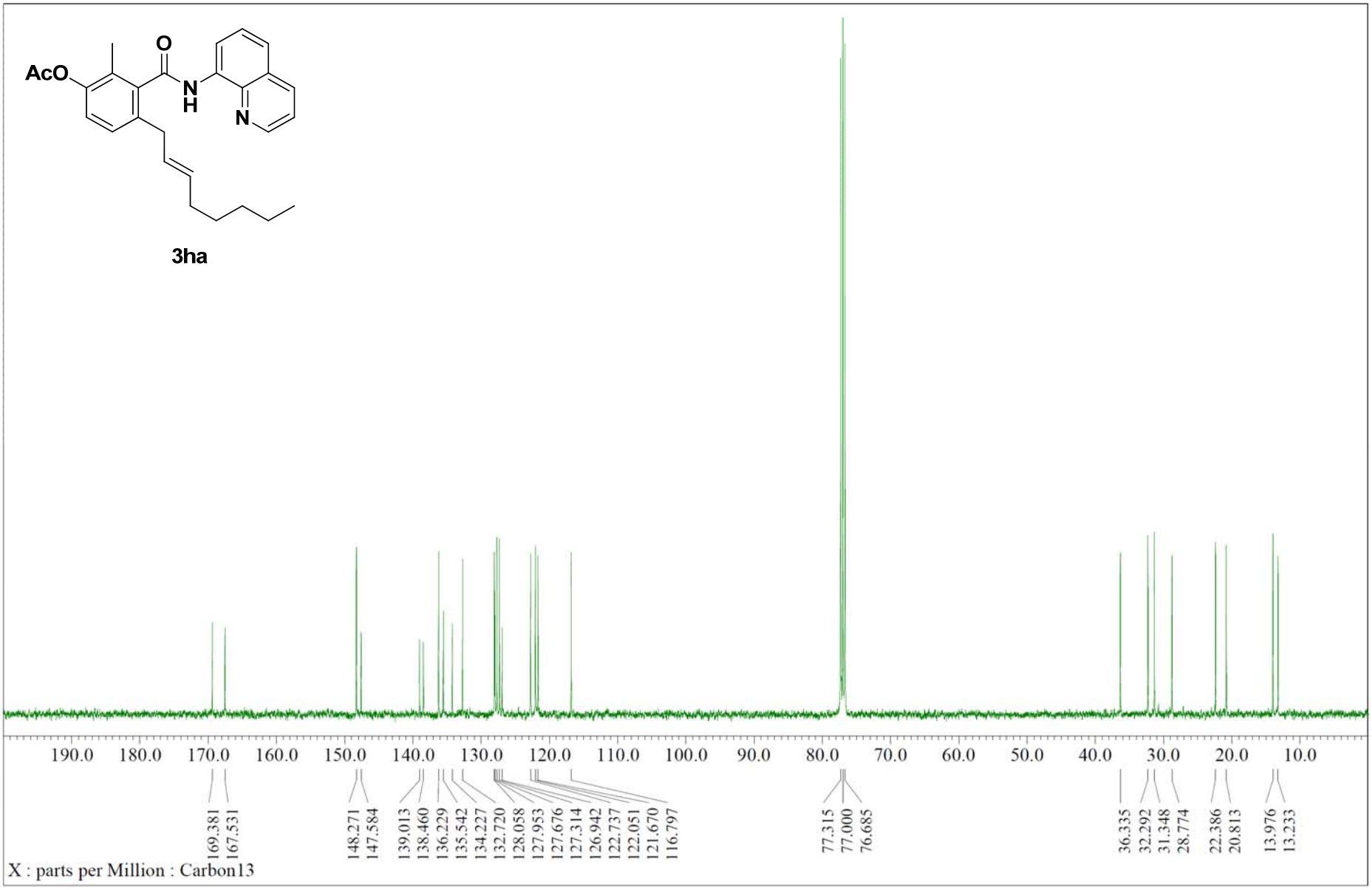
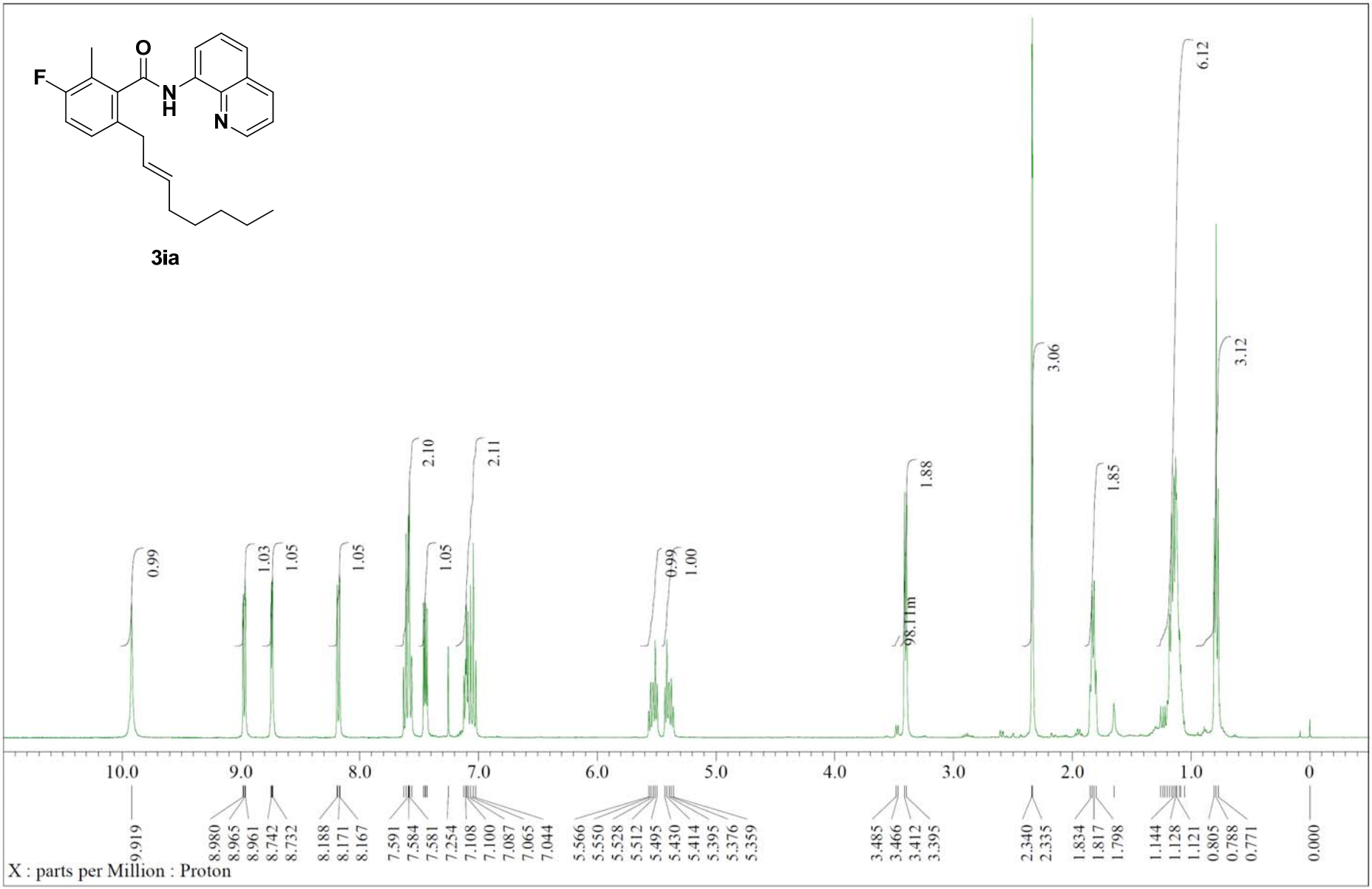
3.00
2.88
2.84
2.03
1.86
1.82
1.02
1.02
1.01
1.01
0.98
0.99
1.00
0.94
0.95
89.46m
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.950
8.977
8.963
8.960
8.747
8.737
8.180
8.163
8.159
7.603
7.584
7.579
7.574
7.449
7.186
7.165
7.070
7.049
5.576
5.560
5.540
5.522
5.505
5.443
5.427
5.410
5.390
5.373
3.505
3.487
3.432
3.415
2.340
2.246
1.830
1.813
1.796
1.151
1.133
1.126
0.810
0.794
0.777
X : parts per Million : Proton


AcO
O
N
H
N
3ha
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
169.381
167.531
148.271
147.584
139.013
138.460
136.229
135.542
134.227
132.720
128.058
127.953
127.676
127.314
126.942
122.737
122.051
121.670
116.797
77.315
77.000
76.685
36.335
32.292
31.348
28.774
22.386
20.813
13.976
13.233
X : parts per Million : Carbon13


F
O
N
H
N
3ia
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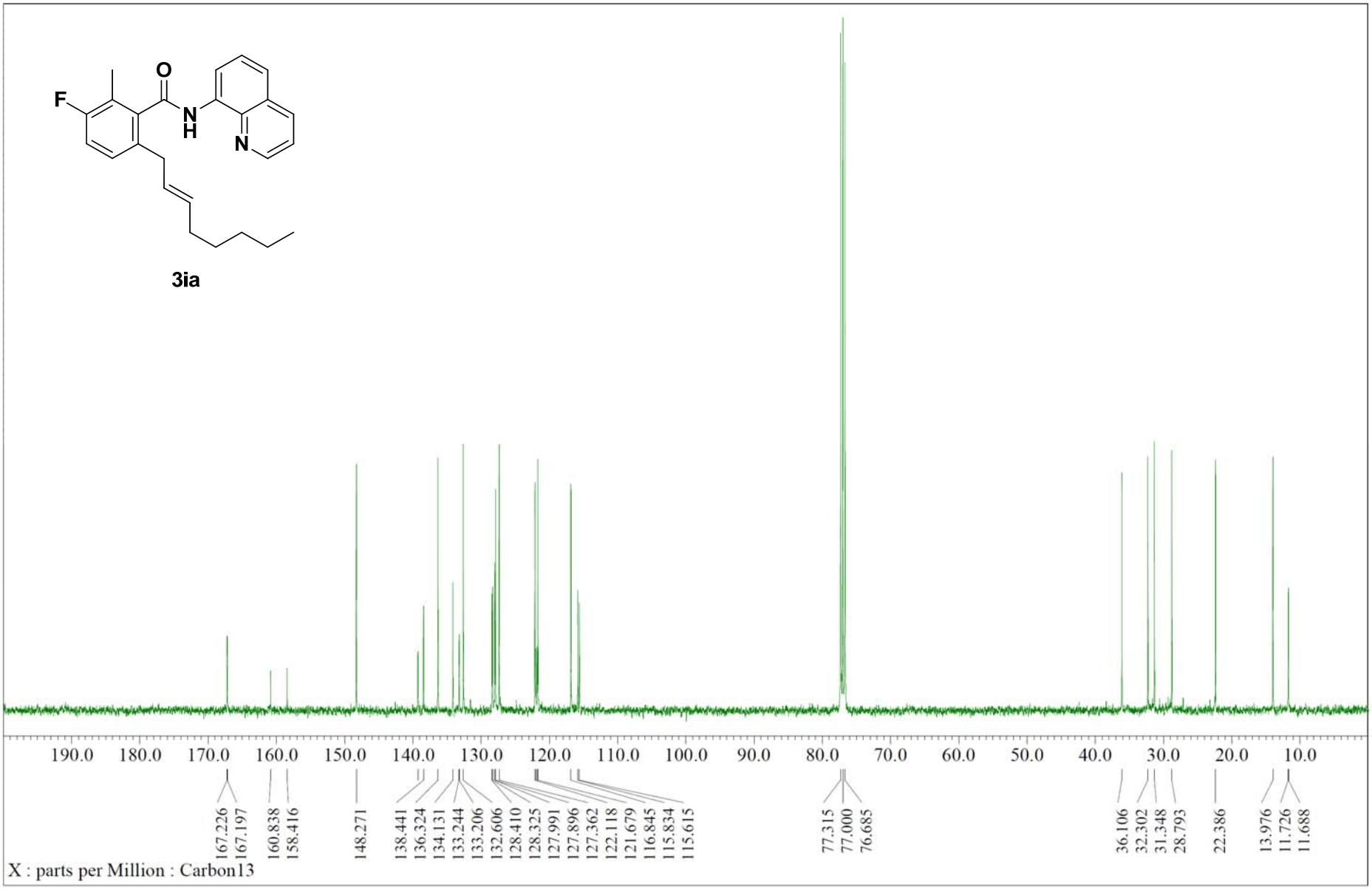
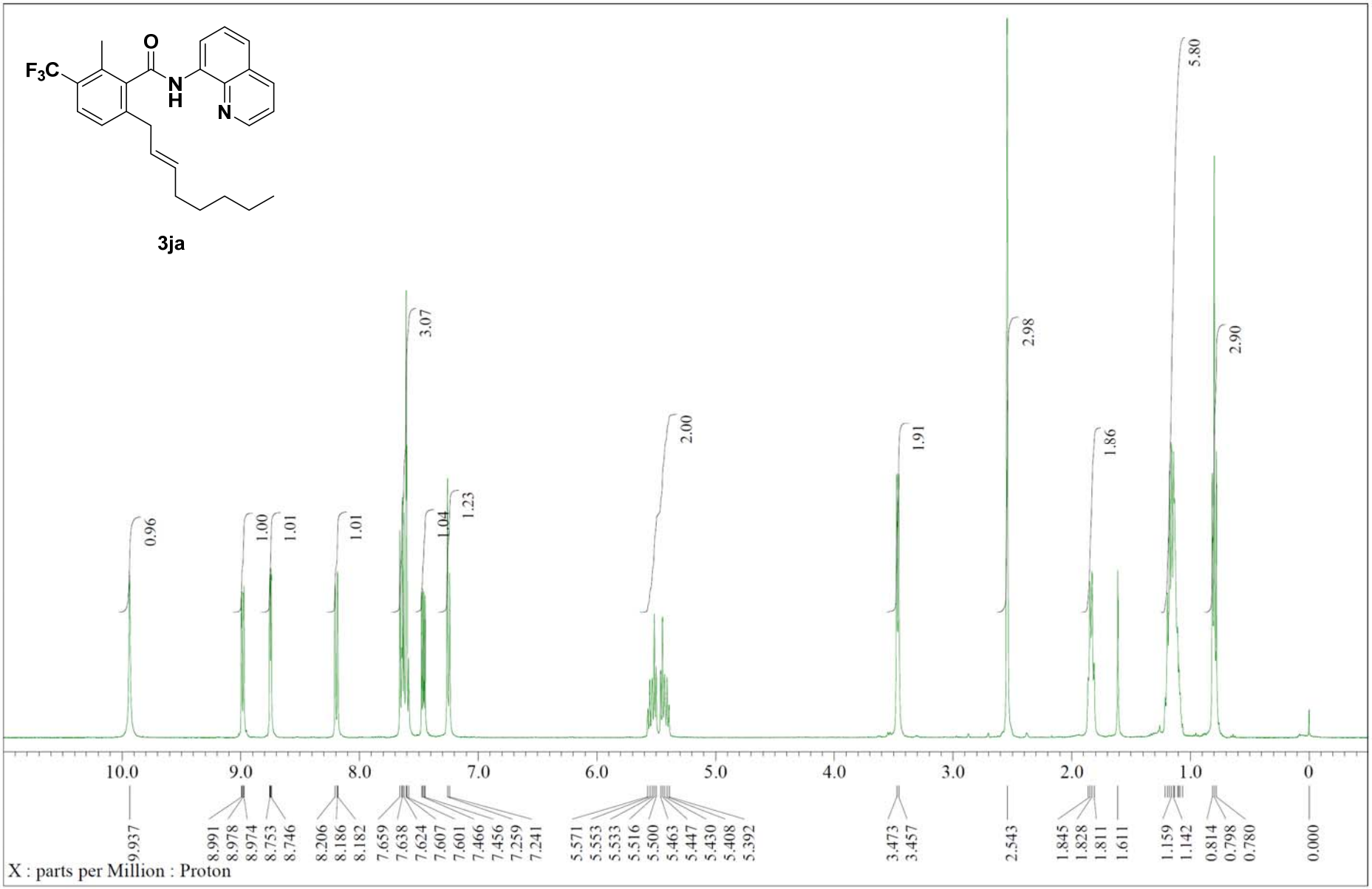
1.03
1.05
1.05
2.10
1.05
2.11
0.99
1.00
98.11m
1.88
3.06
1.85
6.12
3.12
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.919
8.980
8.965
8.961
8.742
8.732
8.188
8.171
8.167
7.591
7.584
7.581
7.254
7.108
7.100
7.087
7.065
7.044
5.566
5.550
5.528
5.512
5.495
5.430
5.414
5.395
5.376
5.359
3.485
3.466
3.412
3.395
2.340
2.335
1.834
1.817
1.798
1.144
1.128
1.121
0.805
0.788
0.771
0.000
X : parts per Million : Proton


F
O
N
H
N
3ia
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
167.226
167.197
160.838
158.416
148.271
138.441
136.324
134.131
133.244
133.206
132.606
128.410
128.325
127.991
127.896
127.362
122.118
121.679
116.845
115.834
115.615
77.315
77.000
76.685
36.106
32.302
31.348
28.793
22.386
13.976
11.726
11.688
X : parts per Million : Carbon13


F3C
O
N
H
N
3ja
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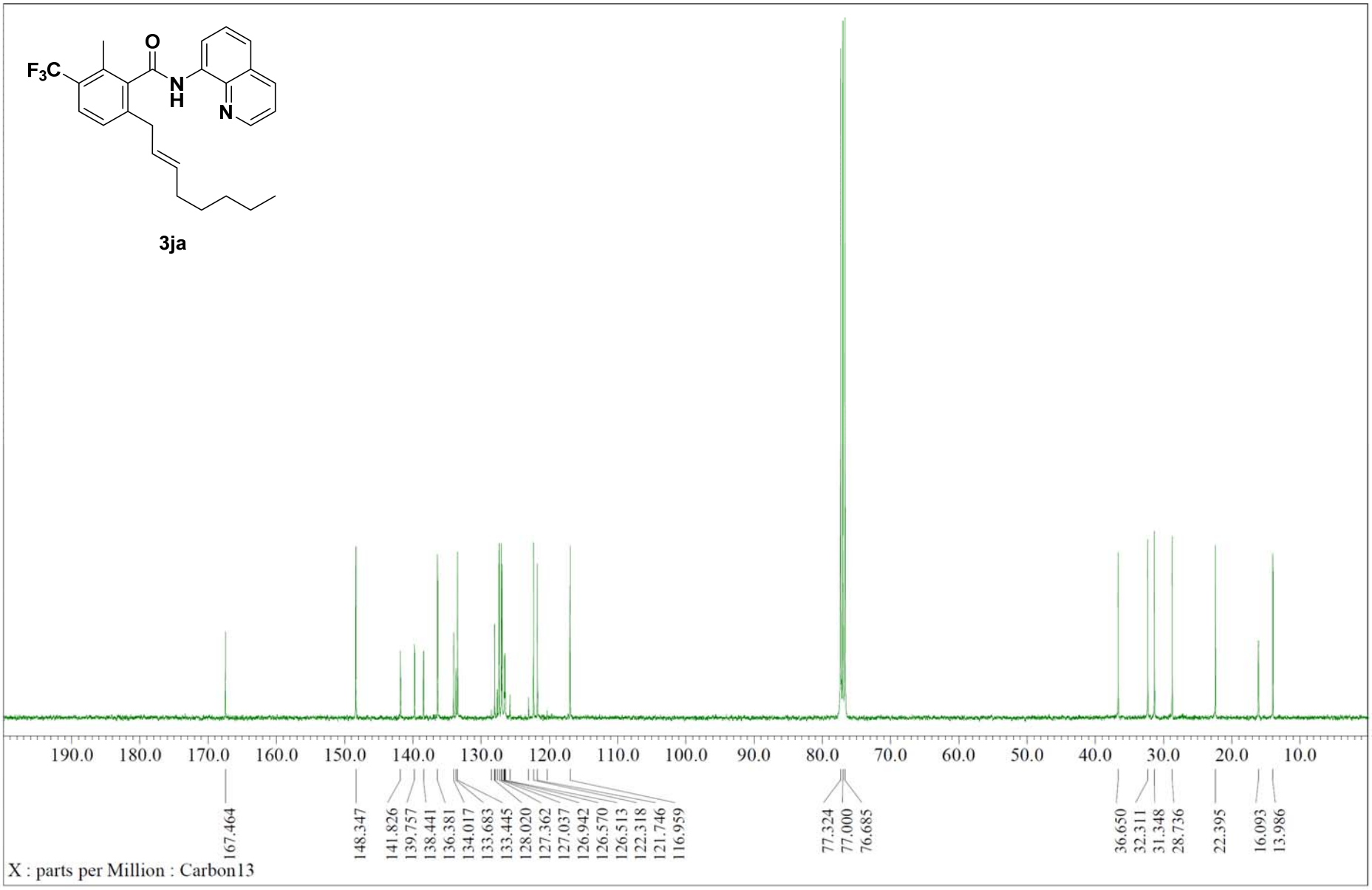
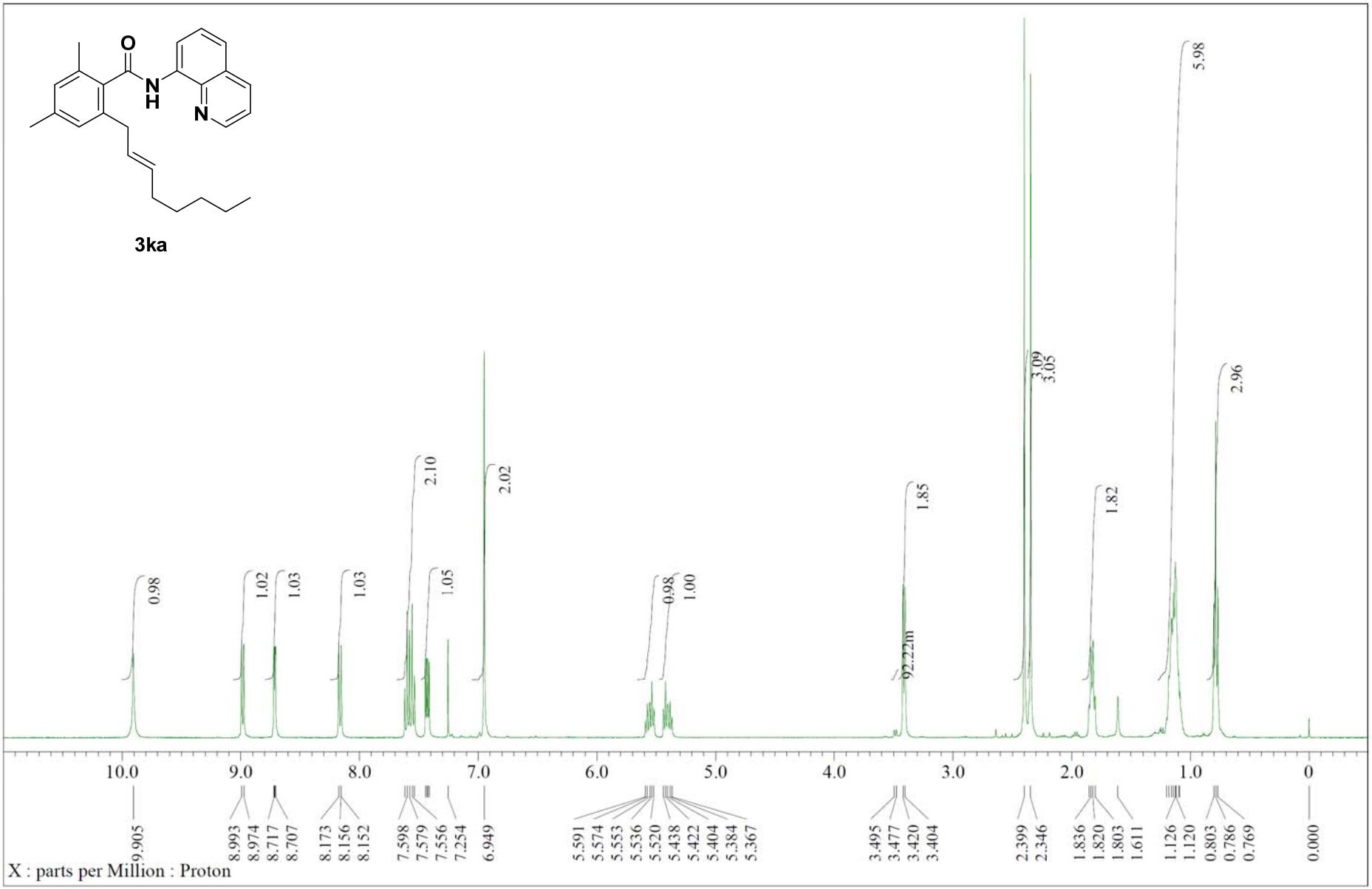
1.00
1.01
1.01
3.07
1.04
1.23
2.00
1.91
2.98
1.86
5.80
2.90
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.937
8.991
8.978
8.974
8.753
8.746
8.206
8.186
8.182
7.659
7.638
7.624
7.607
7.601
7.466
7.456
7.259
7.241
5.571
5.553
5.533
5.516
5.500
5.463
5.447
5.430
5.408
5.392
3.473
3.457
2.543
1.845
1.828
1.811
1.611
1.159
1.142
0.814
0.798
0.780
0.000
X : parts per Million : Proton


O
F3C
N
H
N
3ja
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
167.464
148.347
141.826
139.757
138.441
136.381
134.017
133.683
133.445
128.020
127.362
127.037
126.942
126.570
126.513
122.318
121.746
116.959
77.324
77.000
76.685
36.650
32.311
31.348
28.736
22.395
16.093
13.986
X : parts per Million : Carbon13


O
N
H
N
3ka
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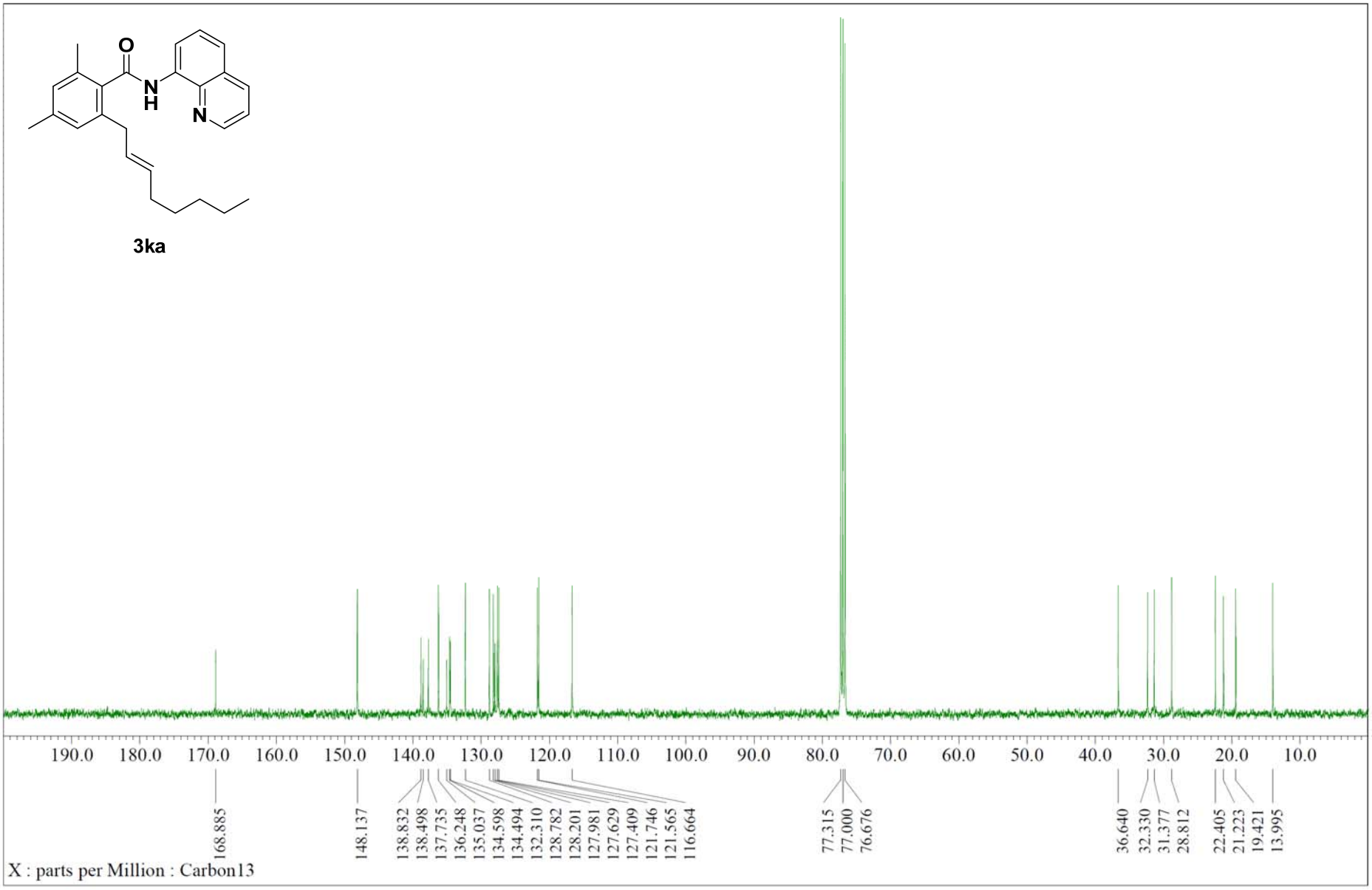
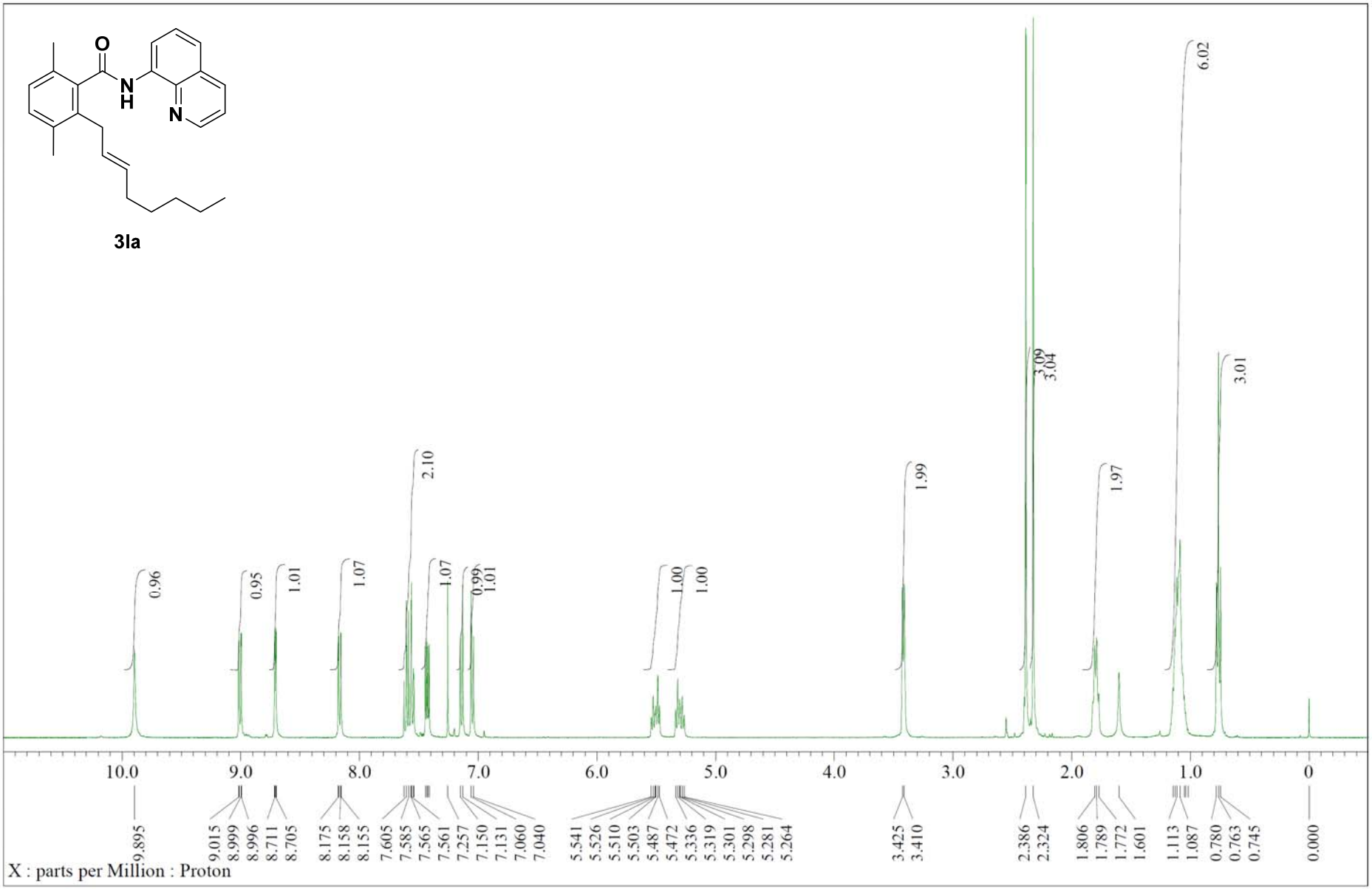
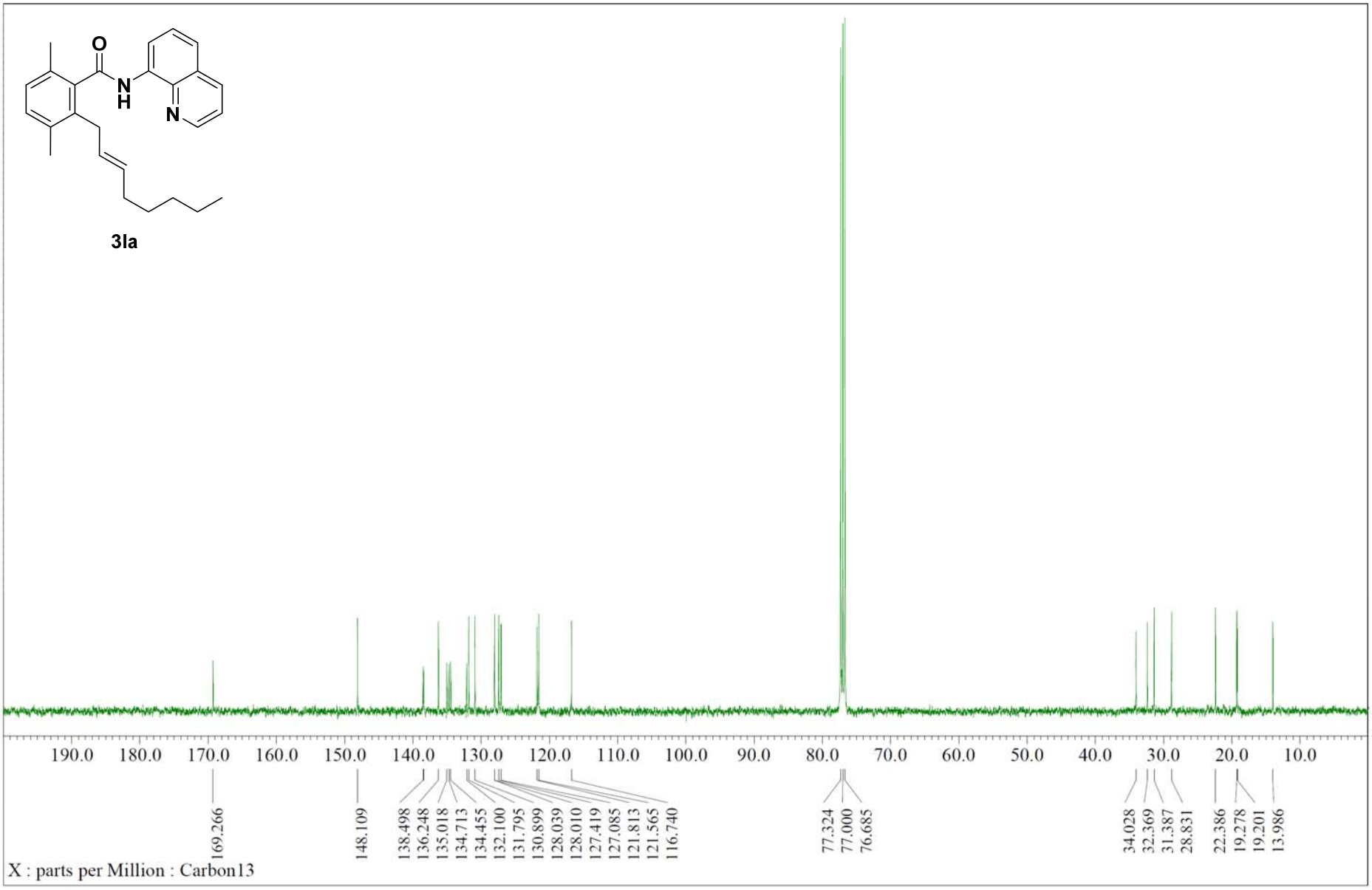
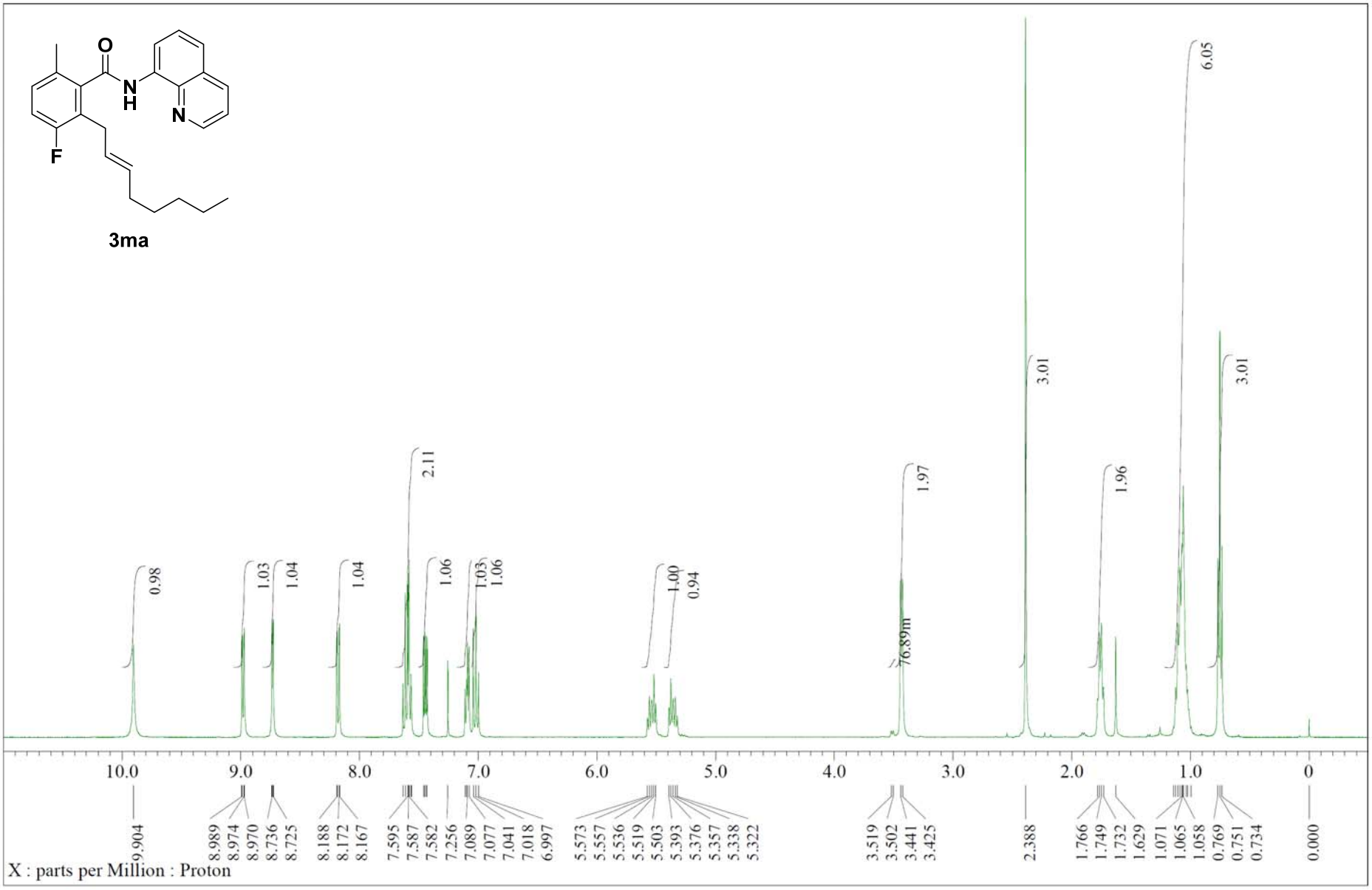
1.03
1.03
2.10
1.05
2.02
0.98
1.00
92.22m
1.85
3.09
3.05
1.82
5.98
2.96
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.905
8.993
8.974
8.717
8.707
8.173
8.156
8.152
7.598
7.579
7.556
7.254
6.949
5.591
5.574
5.553
5.536
5.520
5.438
5.422
5.404
5.384
5.367
3.495
3.477
3.420
3.404
2.399
2.346
1.836
1.820
1.803
1.611
1.126
1.120
0.803
0.786
0.769
0.000
X : parts per Million : Proton


O
N
H
N
3ka
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
168.885
148.137
138.832
138.498
137.735
136.248
135.037
134.598
134.494
132.310
128.782
128.201
127.981
127.629
127.409
121.746
121.565
116.664
77.315
77.000
76.676
36.640
32.330
31.377
28.812
22.405
21.223
19.421
13.995
X : parts per Million : Carbon13


O
N
H
N
3la
0.96
0.95
1.01
1.07
2.10
1.07
0.99
1.01
1.00
1.00
1.99
3.09
3.04
1.97
6.02
3.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.895
9.015
8.999
8.996
8.711
8.705
8.175
8.158
8.155
7.605
7.585
7.565
7.561
7.257
7.150
7.131
7.060
7.040
5.541
5.526
5.510
5.503
5.487
5.472
5.336
5.319
5.301
5.298
5.281
5.264
3.425
3.410
2.386
2.324
1.806
1.789
1.772
1.601
1.113
1.087
0.780
0.763
0.745
0.000
X : parts per Million : Proton


O
N
H
N
3la
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
169.266
148.109
138.498
136.248
135.018
134.713
134.455
132.100
131.795
130.899
128.039
128.010
127.419
127.085
121.813
121.565
116.740
77.324
77.000
76.685
34.028
32.369
31.387
28.831
22.386
19.278
19.201
13.986
X : parts per Million : Carbon13


O
N
H
N
F
3ma
0.98
1.03
1.04
1.04
2.11
1.06
1.03
1.06
1.00
0.94
1.97
76.89m
3.01
1.96
6.05
3.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.904
8.989
8.974
8.970
8.736
8.725
8.188
8.172
8.167
7.595
7.587
7.582
7.256
7.089
7.077
7.041
7.018
6.997
5.573
5.557
5.536
5.519
5.503
5.393
5.376
5.357
5.338
5.322
3.519
3.502
3.441
3.425
2.388
1.766
1.749
1.732
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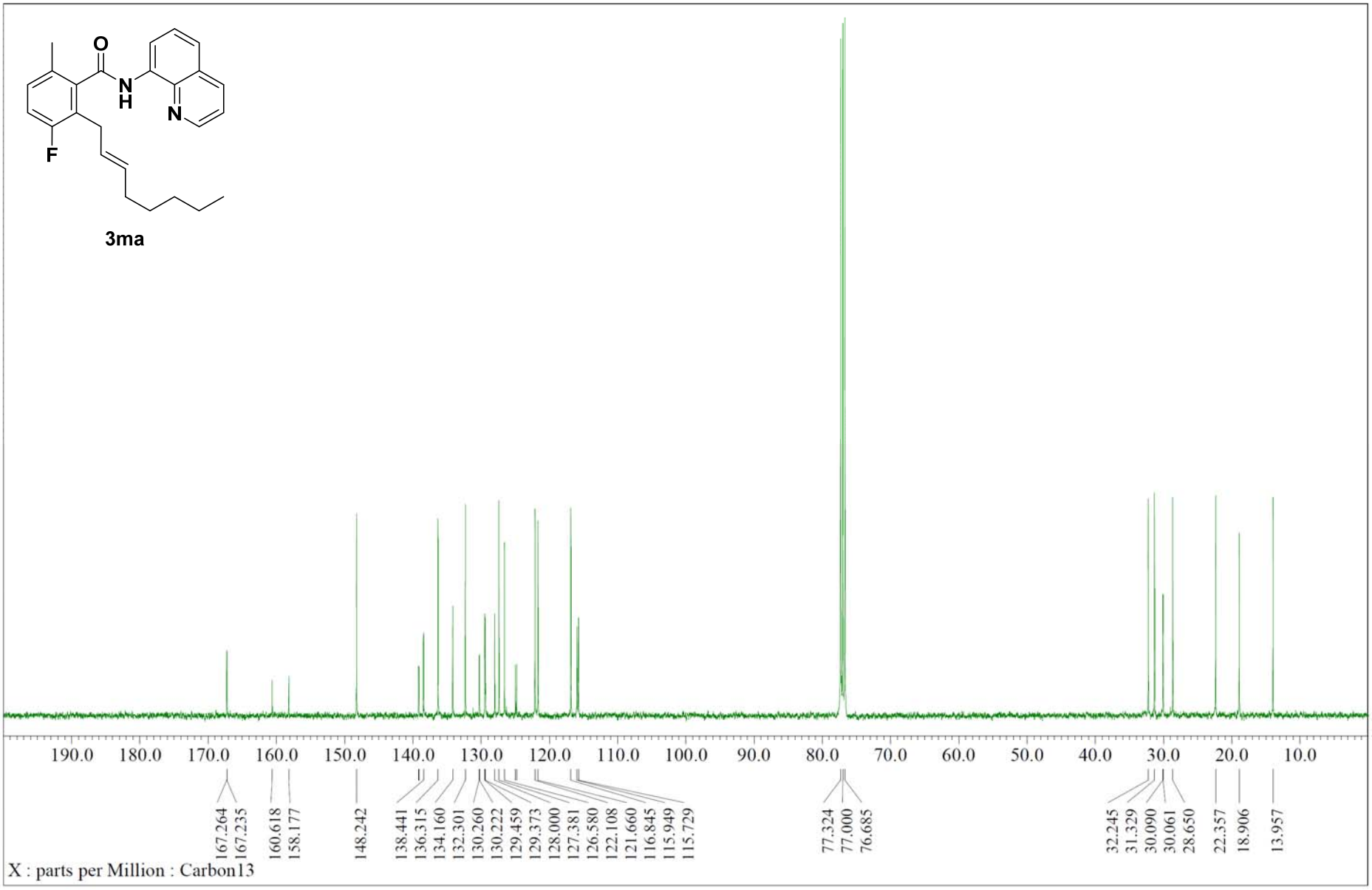
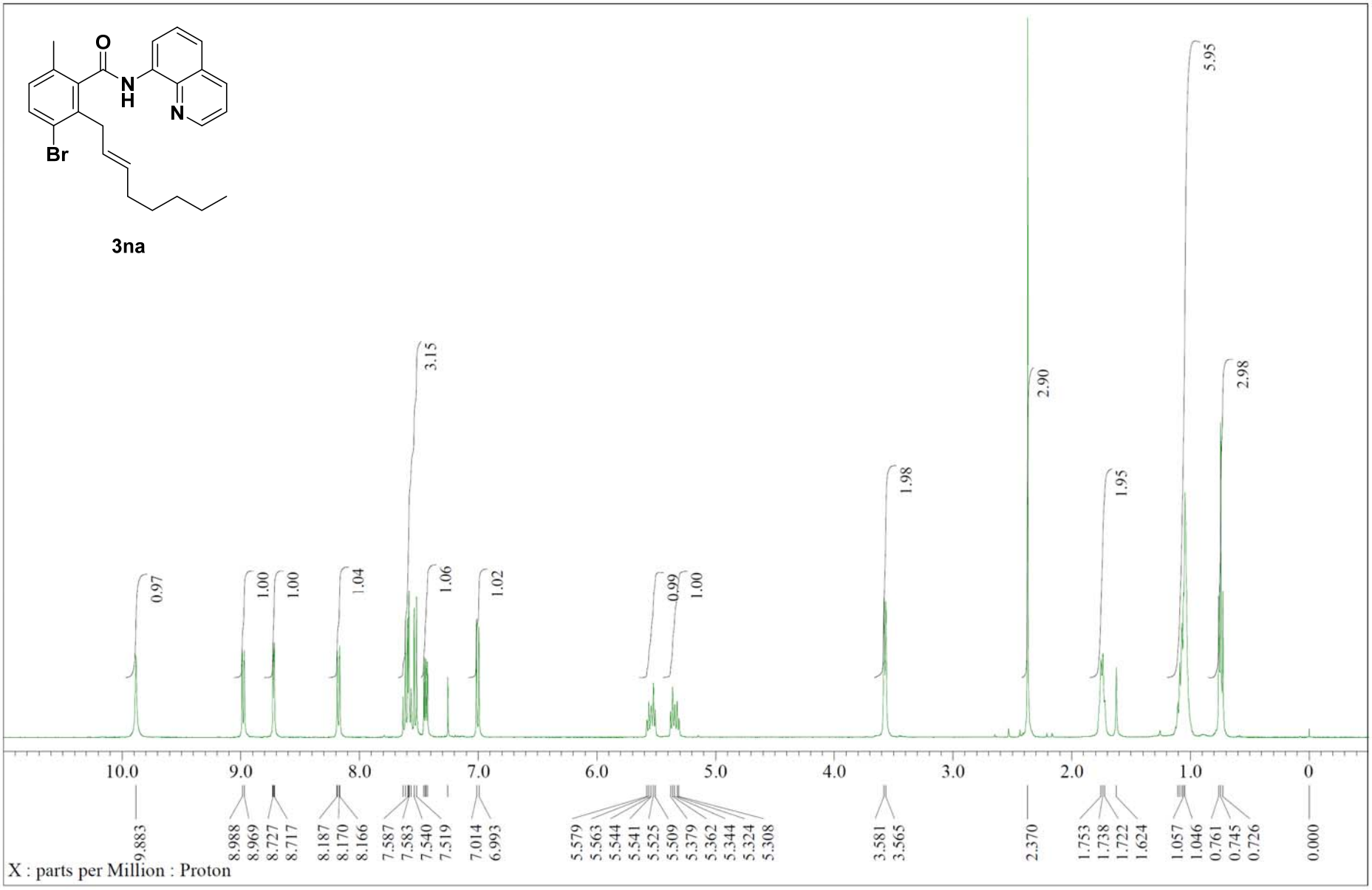
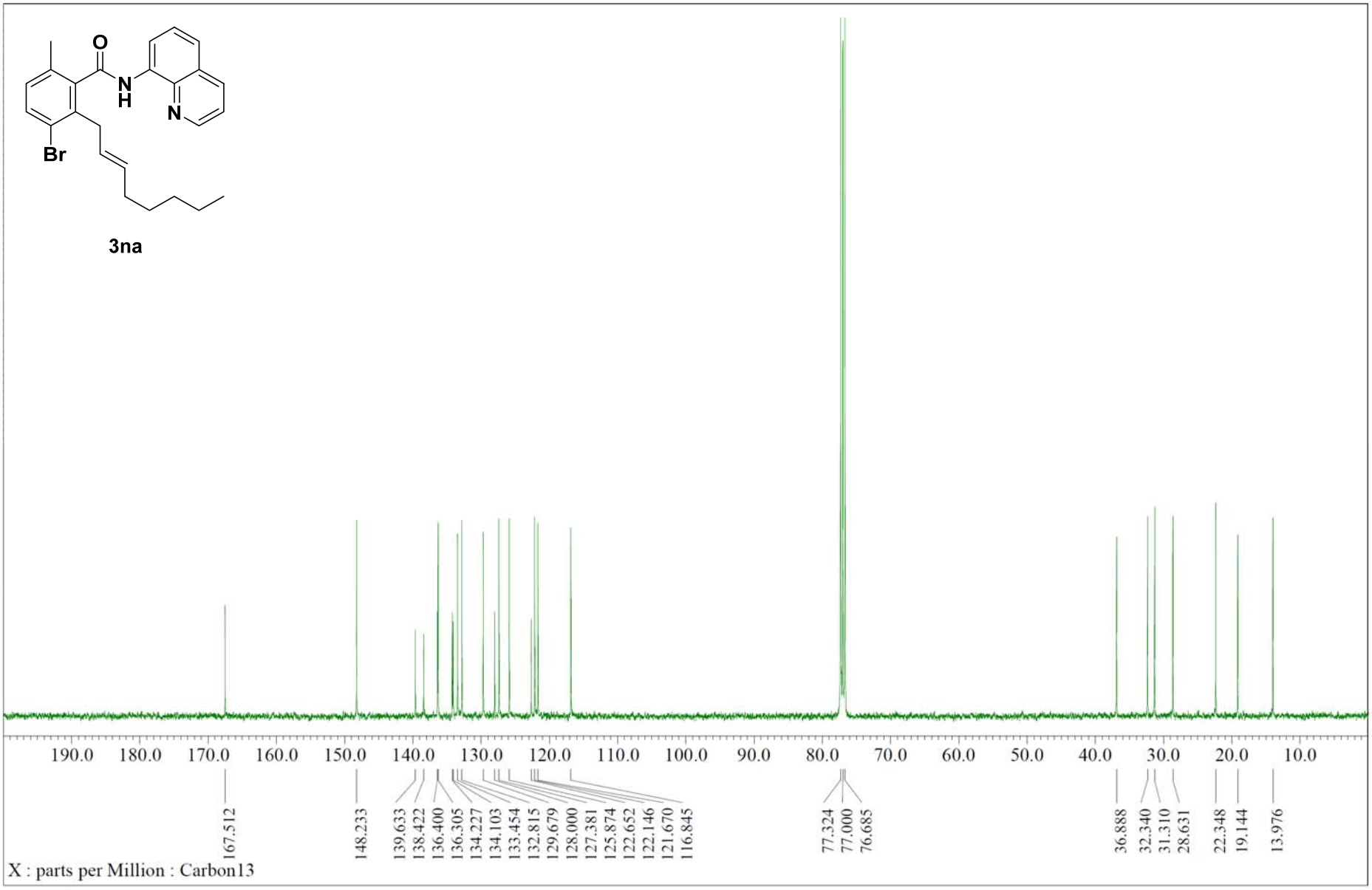
1.071
1.065
1.058
0.769
0.751
0.734
0.000
X : parts per Million : Proton


O
N
H
N
F
3ma
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
167.264
167.235
160.618
158.177
148.242
138.441
136.315
134.160
132.301
130.260
130.222
129.459
129.373
128.000
127.381
126.580
122.108
121.660
116.845
115.949
115.729
77.324
77.000
76.685
32.245
31.329
30.090
30.061
28.650
22.357
18.906
13.957
X : parts per Million : Carbon13


O
N
H
N
Br
3na
0.97
1.00
1.00
1.04
3.15
1.06
1.02
0.99
1.00
1.98
2.90
1.95
5.95
2.98
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.883
8.988
8.969
8.727
8.717
8.187
8.170
8.166
7.587
7.583
7.540
7.519
7.014
6.993
5.579
5.563
5.544
5.541
5.525
5.509
5.379
5.362
5.344
5.324
5.308
3.581
3.565
2.370
1.753
1.738
1.722
1.624
1.057
1.046
0.761
0.745
0.726
0.000
X : parts per Million : Proton


O
N
H
N
Br
3na
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
167.512
148.233
139.633
138.422
136.400
136.305
134.227
134.103
133.454
132.815
129.679
128.000
127.381
125.874
122.652
122.146
121.670
116.845
77.324
77.000
76.685
36.888
32.340
31.310
28.631
22.348
19.144
13.976
X : parts per Million : Carbon13