Electronic Supplementary Information

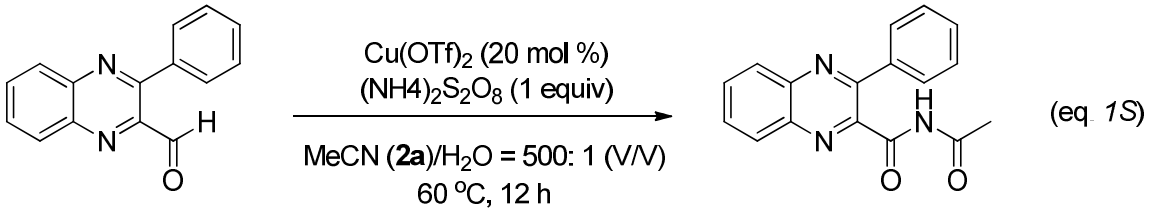
Copper-catalyzed Three-Component Reaction of *N*-Heteroaryl Aldehydes, Nitriles, and Water

Hanyang Bao, Bingwei Zhou, Hongwei Jin,* and Yunkui Liu*

State Key Laboratory Breeding Base of Green Chemistry-Synthesis Technology, College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, P. R. China
Email: jhwei828@zjut.edu.cn; ykuiliu@zjut.edu.cn;

Contents

1. 3 mmol-scale synthesis of 3aa



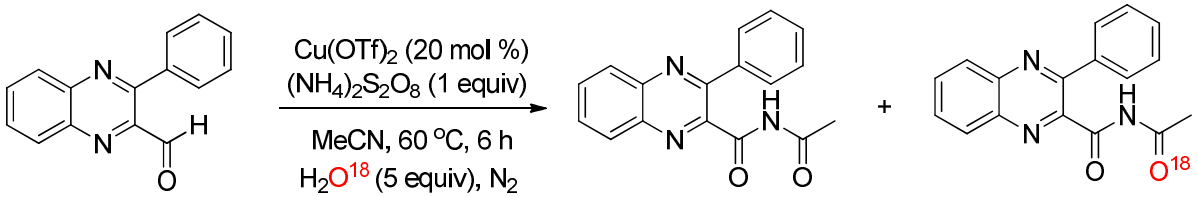
(eq. *1S*)

1a: 3 mmol

3aa: 610 mg, 70%

Procedure: **1a** (702.0 mg, 3 mmol), $Cu(OTf)_2$ (217.0 mg, 0.6 mmol), $(NH4)_2S_2O_8$ (685.0 mg, 3 mmol), and CH_3CN/H_2O = 500/1 (V/V, 30 mL) were added to a 100-mL reaction tube. Then the reaction mixture was stirred at 60 ºC for 12 h. Upon completion, the resulting mixture was diluted with CH_2Cl_2 (50 mL) and filtered through Celite. After evaporation of the solvent under vacuum, the residue was purified by column chromatography on silica gel (100-200 mesh) using petroleum ether-EtOAc (6:1-3:1) as eluent to give pure product **3aa** (610.0 mg, 70%).

2. Reaction of 1a in CH_3CN-H_2O^{18} (5 equiv of H_2O^{18})



1a

2a
(m/z = 291)

2a-O^{18}
(m/z = 293)

MS-analytical Results:

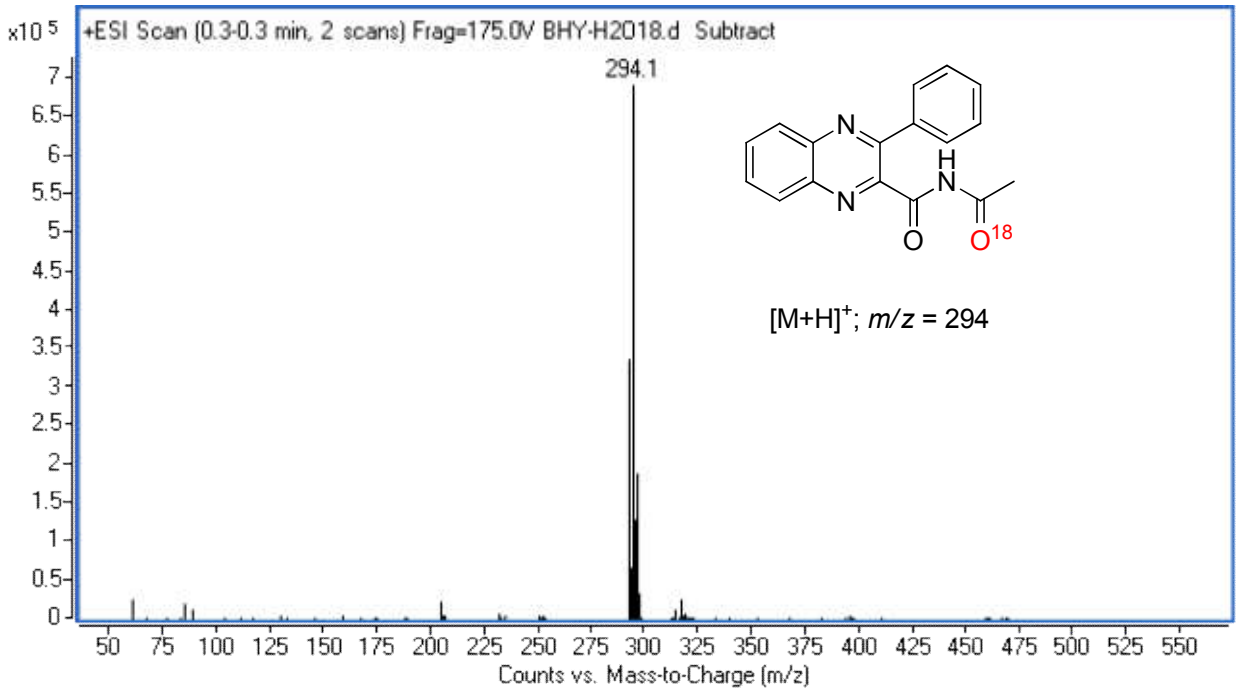
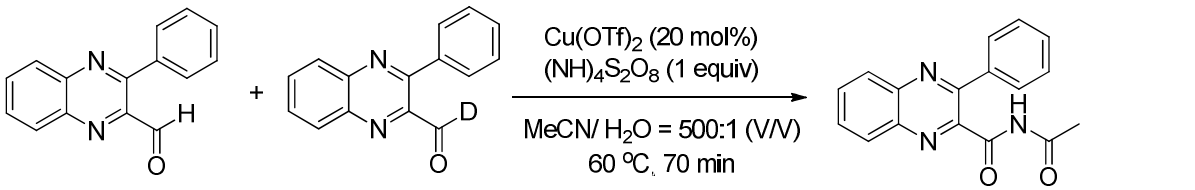


Figure *S1*. The MS-spectrum of **2a**/**2a-O^{18}**

3. Intermolecular Competition Experiment on 1a and 1a-*d*.



1a

0.144 mmol

1a *d* (96% D enrichment)

0.156 mmol

totally 33% of **1a** and **1a** *d* were recovered

k_H/k_D = 1.0

(calculated by ^{1}H NMR analysis)

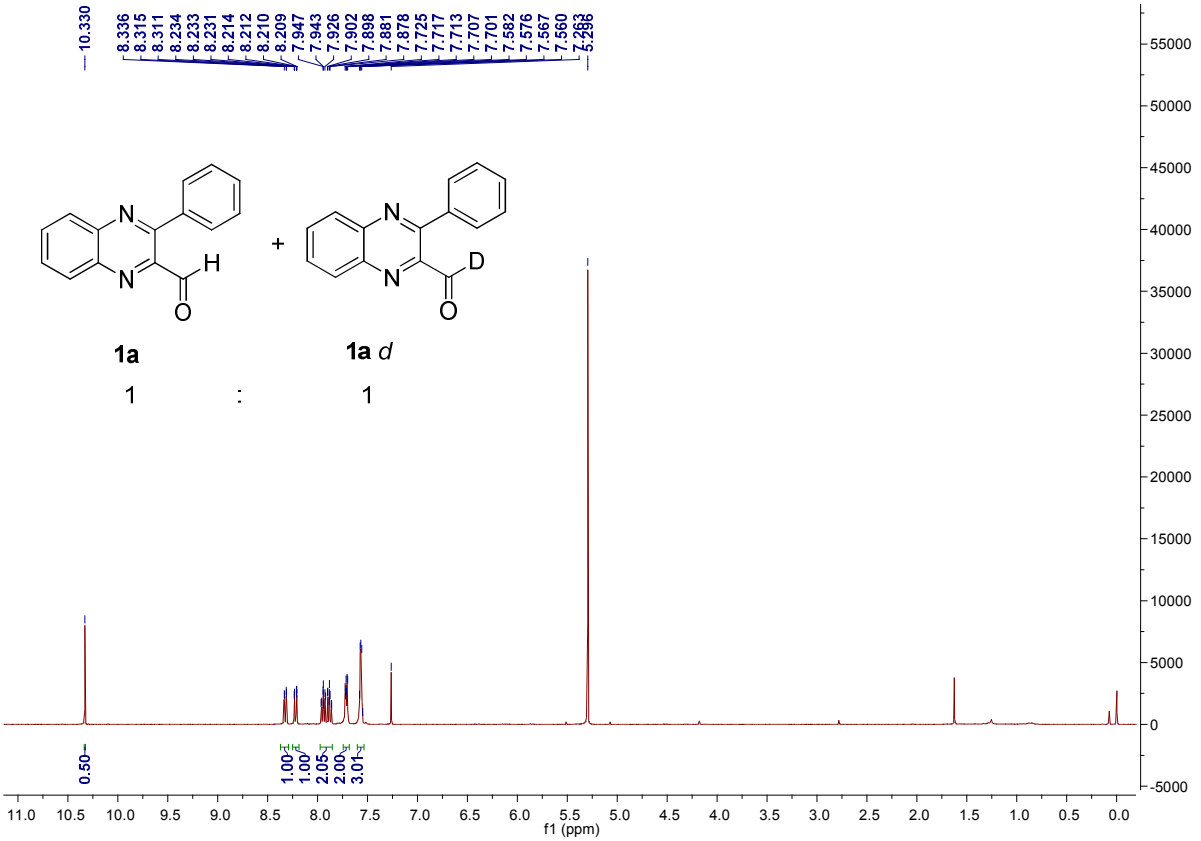


Figure *S2*. The ^{1}H NMR of the Recovered Mixture of 1a and 1a-*d*

4.1 Characterization of unknown starting materials

3-(4-ethylphenyl)quinoxaline-2-carbaldehyde (1f): **1f** was synthesized according to the reported procedure[1] as yellow solid (2.0 mmol scale, 0.29 g, total 55% yield through a two-step process). m.p. 77.9-79.4 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.34 (s, 1H), 8.31 (dd, J_1 = 8.4 Hz, J_2 = 1.1 Hz, 1H), 8.20 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 7.94-7.90 (m, 1H), 7.87-7.84 (m, 1H), 7.66-7.64 (m, 2H), 7.40 (d, J = 8.2 Hz, 2H), 2.77 (q, J = 7.6 Hz, 2H), 1.31 (t, J = 7.6 Hz, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 191.4, 154.6, 146.4, 145.0, 142.9, 140.9, 133.8, 133.0, 130.8, 130.3, 129.9, 129.3, 128.3, 28.8, 15.4. IR (potassium bromide) (ν, cm^{-1}): 1706 (C=O). HRMS (ESI) for $C_{17}H_{15}N_2O$ $[M + H]^+$: calcd: 263.1179, found: 263.1175.

3-(4-(benzyloxy)phenyl)quinoxaline-2-carbaldehyde (1h): 1h was synthesized according to the reported procedure[1] as yellow solid (2.0 mmol scale, 0.41 g, total 60% yield through a two-step process). m.p. 130.5-132.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.34 (s, 1H), 8.30 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 8.19 (dd, J_1 = 8.4 Hz,

J_2 = 0.9 Hz, 1H), 7.93-7.90 (m, 1H), 7.86-7.83 (m, 1H), 7.72-7.69 (m, 2H), 7.49-7.35 (m, 5H), 7.18-7.15 (m, 2H), 5.18 (s, 2H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 191.5, 160.4, 154.0, 145.0, 142.9, 140.8, 136.5, 133.0, 131.6, 130.6, 130.3, 129.3, 129.0, 128.7, 128.2, 127.5, 115.2, 70.14. IR (potassium bromide) (ν, cm^{-1}): 1708 (C=O). HRMS (ESI) for $C_{22}H_{17}N_2O_2$ $[M + H]^+$: calcd: 341.1285, found: 341.1289.

3-(3-bromophenyl)quinoxaline-2-carbaldehyde (1i): **1i** was synthesized according to the reported procedure[1] as white solid (2.0 mmol scale, 0.45 g, total 72% yield through a two-step process). m.p. 176.3-177.1 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 8.32 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 8.22 (dd, J_1 = 8.4 Hz, J_2 = 0.9 Hz, 1H), 7.99-7.89 (m, 1H), 7.93-7.89 (m, 2H), 7.70-7.68 (m, 1H), 7.60-7.58 (m, 1H), 7.42 (t, J = 7.9 Hz, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 191.3, 152.6, 144.8, 142.7, 141.1, 138.7, 133.4, 132.8, 132.5, 131.3, 130.3, 129.9, 129.4, 128.5, 122.7. IR (potassium bromide) (ν, cm^{-1}): 1710 (C=O). HRMS (ESI) for $C_{15}H_{10}BrN_2O$ $[M + H]^+$: calcd: 312.9971, found: 312.9978.

3-(3-chlorophenyl)quinoxaline-2-carbaldehyde (1j): **1j** was synthesized according to the reported procedure[1] as yellow solid (2.0 mmol scale, 0.36 g, total 68% yield through a two-step process). m.p. 172.9-174.5 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 8.32 (dd, J_1 = 8.3 Hz, J_2 = 1.1 Hz, 1H), 8.22 (dd, J_1 = 8.2 Hz, J_2 = 1.2 Hz, 1H), 7.99-7.96 (m, 1H), 7.93-7.90 (m, 1H), 7.74 (t, J = 1.7 Hz, 1H), 7.55-7.47 (m, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 191.3, 152.7, 144.8, 142.7, 141.1, 138.5, 134.7, 133.4, 131.3, 130.3, 129.9, 129.70, 129.66, 129.4, 128.0. IR (potassium bromide) (ν, cm^{-1}): 1705 (C=O). HRMS (ESI) for $C_{15}H_{10}ClN_2O$ $[M + H]^+$: calcd: 269.0476, found: 269.0471.

3-(2-fluorophenyl)quinoxaline-2-carbaldehyde (1l): **1l** was synthesized according to the reported procedure[1] as yellow solid (2 mmol scale, 0.40 g, total 79% yield through a two-step process). m.p. 124.3-126.1 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.29 (d, J =1.1 Hz, 1H), 8.31 (dd, J_1 = 8.3 Hz, J_2 = 1.1 Hz, 1H), 8.23 (dd, J_1 = 8.3 Hz, J_2 = 1.0 Hz, 1H), 7.96-7.88 (m, 2H), 7.75-7.71 (m, 1H), 7.56-7.51 (m, 1H), 7.38 (td, J_1 = 7.5 Hz, J_2 =1.0 Hz, 1H), 7.21-7.18 (m, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 191.2, 160.0 (d, J = 247.9 Hz), 148.4, 145.6, 143.2, 141.0, 133.1, 131.8 (d,

J = 8.4 Hz), 131.2, 131.1 (d, *J* = 2.8 Hz), 130.2, 129.5, 125.5 (d, *J* = 14.7 Hz), 124.9 (d, *J* = 3.4 Hz), 115.5 (d, *J* = 21.6 Hz). IR (potassium bromide) (ν, cm^{-1}): 1708 (C=O). HRMS (ESI) for $C_{15}H_{10}FN_2O$ $[M + H]^+$: calcd: 253.0772, found: 253.0777.

3-(2-bromophenyl)quinoxaline-2-carbaldehyde (1n): **1n** was synthesized according to the reported procedure[1] as yellow solid (2 mmol scale, 0.38 g, total 61% yield through a two-step process). m.p. 81.2-82.4 ºC. ^1H NMR (500 MHz, $CDCl_3$): 10.24 (s, 1H), 8.36-8.34 (m, 1H), 8.25-8.23 (m, 1H), 7.99-7.92 (m, 2H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.55-7.54 (m, 2H), 7.44-7.40 (m, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 190.9, 153.1, 145.3, 142.8, 141.3, 138.3, 133.2, 132.7, 131.3, 130.9, 130.6, 130.3, 129.5, 128.0, 122.3. IR (potassium bromide) (ν, cm^{-1}): 1713 (C=O). HRMS (ESI) for $C_{15}H_{10}BrN_2O$ $[M + H]^+$: calcd: 312.9971, found: 312.9978.

3-chloroquinoxaline-2-carbaldehyde (1q): **1q** was synthesized according to the reported procedure[1] as white solid (2.0 mmol scale, 0.17 g, total 45% yield through a two-step process). m.p. 141.6-143.0 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.45 (s, 1H), 8.30 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 8.12 (dd, J_1 = 8.4 Hz, J_2 = 0.9 Hz, 1H), 8.01-7.97 (m, 1H), 7.94-7.90 (m, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 189.0, 145.5, 143.1, 142.9, 140.7, 134.2, 131.4, 130.4, 128.4. IR (potassium bromide) (ν, cm^{-1}): 1706 (C=O). HRMS (ESI) for $C_9H_6ClN_2O$ $[M + H]^+$: calcd: 193.0163, found: 193.0167.

6,7-dibromo-3-phenylquinoxaline-2-carbaldehyde (1s): **1s** was synthesized according to the reported procedure[1] as yellow solid (2.0 mmol scale, 0.59 g, total 75% yield through a two-step process). m.p. 178.7-179.9 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.28 (s, 1H), 8.61 (s, 1H), 8.54 (s, 1H), 7.71-7.69 (m, 2H), 7.60-7.56 (m, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 190.6, 155.3, 145.8, 141.8, 140.0, 135.9, 134.0, 133.4, 130.5, 130.4, 129.8, 128.8, 127.9. IR (potassium bromide) (ν, cm^{-1}): 1710 (C=O). HRMS (ESI) for $C_{15}H_9Br_2N_2O$ $[M + H]^+$: calcd: 390.9076, found: 390.9081.

3-(4-methoxyphenyl)-6,7-dimethylquinoxaline-2-carbaldehyde (1v): **1v** was synthesized according to the reported procedure[1] as yellow solid (2.0 mmol scale, 0.40 g, total 69% yield through a two-step process). m.p. 144.4-146.5 ºC. ^1H NMR

(500 MHz, $CDCl_3$): δ 10.28 (s, 1H), 8.00 (s, 1H), 7.91 (s, 1H), 7.65 (d, *J* = 8.7 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H), 2.53 (s, 6H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 191.6, 160.9, 153.5, 144.4, 144.0, 141.9, 141.5, 139.9, 131.4, 129.1, 129.0, 128.1, 114.1, 55.4, 20.7, 20.4. IR (potassium bromide) (ν, cm^{-1}): 1711 (C=O). HRMS (ESI) for $C_{18}H_{17}N_2O_2$ $[M + H]^+$: calcd: 293.1285, found: 293.1279.

8-methyl-7-(trifluoromethyl)quinoline-2-carbaldehyde (6g): **6g** was synthesized from the oxidation of 2,8-dimethyl-7-(trifluoromethyl)quinolone with SeO_2 as white solid (2.0 mmol scale, 0.35 g, 73% yield). m.p. 94.3-97.2 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.26 (d, *J* = 0.8 Hz, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.83 (d, *J* = 8.7 Hz, 1H), 3.09 (d, *J* = 1.9 Hz, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 193.7, 152.4, 146.7, 139.6, 137.7, 131.1, 130.0 (q, *J* = 29.9 Hz), 125.8, 125.0 (q, *J* = 5.4 Hz), 124.3 (q, *J* = 273.75 Hz), 118.6, 13.4 (d, *J* = 2.0 Hz). IR (potassium bromide) (ν, cm^{-1}): 1708 (C=O). HRMS (ESI) for $C_{12}H_9F_3NO$ $[M + H]^+$: calcd: 240.0631, found: 240.0637.

5,7-dimethylquinoline-2-carbaldehyde (6i): **6i** was synthesized from the oxidation of 2,5,7-trimethylquinoline with SeO_2 as white solid (2.0 mmol scale, 0.30 g, 81% yield). m.p. 88.6-89.9 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.20 (s, 1H), 8.37 (d, *J* = 8.6 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.85 (s, 1H), 7.33 (s, 1H), 2.67 (s, 3H), 2.55 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 194.0, 152.1, 148.6, 140.5, 134.4, 133.5, 132.0, 127.6, 127.4, 116.2, 21.8, 18.6. IR (potassium bromide) (ν, cm^{-1}): 1701 (C=O). HRMS (ESI) for $C_{12}H_{12}NO$ $[M + H]^+$: calcd: 186.0913, found: 186.0917.

3-chlorophenanthridine-6-carbaldehyde (6k): **6k** was synthesized from the oxidation of 3-chloro-6-methylphenanthridine with SeO_2 as white solid (2.0 mmol scale, 0.31 g, 64% yield). m.p. 134.8-135.8 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.27 (s, 1H), 9.28 (d, *J* = 8.3 Hz, 1H), 8.44 (d, *J* = 8.3 Hz, 1H), 8.35 (d, *J* = 8.8 Hz, 1H), 8.16 (d, *J* = 2.0 Hz, 1H), 7.84 (t, *J* = 7.7 Hz, 1H), 7.73 (t, *J* = 7.7 Hz, 1H), 7.66-7.64 (m, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 195.4, 151.2, 144.0, 135.0, 133.2, 131.6, 130.4, 130.3, 129.1, 127.2, 124.1, 123.7, 123.5, 121.9. IR (potassium bromide) (ν, cm^{-1}): 1708 (C=O). HRMS (ESI) for $C_{14}H_{19}ClNO$ $[M + H]^+$: calcd: 242.0367, found: 242.0361.

2-methylphenanthridine-6-carbaldehyde (6l): **6l** was synthesized from the oxidation of 2,6-dimethylphenanthridine with SeO_2 as white solid (2.0 mmol scale, 0.37 g, 84% yield). m.p. 134.8-135.8 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.35 (s, 1H), 9.36 (d, *J* = 8.4 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 8.28 (s, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 7.85-7.82 (m, 1H), 7.75-7.72 (m, 1H), 7.61 (dd, J_1 = 8.3 Hz, J_2 = 1.6 Hz, 1H), 2.65 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 195.7, 149.3, 141.6, 140.4, 132.9, 130.92, 130.91, 130.8, 128.5, 126.7, 125.3, 123.6, 121.78, 121.76, 22.29. IR (potassium bromide) (ν, cm^{-1}): 1690 (C=O). HRMS (ESI) for $C_{15}H_{12}NO$ $[M + H]^+$: calcd: 222.0913, found: 222.0918.

8-methylphenanthridine-6-carbaldehyde (6m): **6m** was synthesized from the oxidation of 6,8-dimethylphenanthridine with SeO_2 as white solid (2.0 mmol scale, 0.3 g, 69% yield). m.p. 111.3-112.2 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.43 (s, 1H), 9.23 (s, 1H), 8.61-8.57 (m, 2H), 8.34-8.32 (m, 1H), 7.83-7.81 (m, 2H), 7.75(dd, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 2.65 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 195.9, 150.0, 143.1, 139.1, 133.0, 131.5, 131.2, 129.8, 128.8, 126.2, 125.8, 123.8, 122.1, 121.8, 22.0. IR (potassium bromide) (ν, cm^{-1}): 1701 (C=O). HRMS (ESI) for $C_{15}H_{12}NO$ $[M + H]^+$: calcd: 222.0913, found: 222.0915.

4.2 Characterization of 3ba-3va

***N*-acetyl-3-(4-bromophenyl)quinoxaline-2-carboxamide (3ba):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (105.5 mg, 95%). m.p. 212.9−213.8 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.22 (s, 1H), 8.23–8.19 (m, 2H), 7.99–7.90 (m, 2H), 7.68–7.66 (m, 2H), 7.56–7.54 (m, 2H), 2.57 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.2, 162.6, 153.4, 143.1, 141.3, 139.0, 137.3, 133.2, 131.48, 131.46, 130.6, 129.42, 129.41, 124.1, 25.4; IR (potassium bromide) (ν, cm^{-1}): 3345 (N-H), 1748 (C=O). HRMS (ESI) for $C_{17}H_{13}BrN_3O_2$ $[M + H]^+$: calcd: 370.0186, found: 370.0180.

***N*-acetyl-3-(4-chlorophenyl)quinoxaline-2-carboxamide (3ca):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (94.2 mg, 97%). m.p. 187.2−188.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.31 (s, 1H), 8.22–8.19

(m, 2H), 7.98–7.95 (m, 1H), 7.93–7.89 (m, 1H), 7.61 (d, J = 8.5 Hz, 2H), 7.51 (d, J = 8.0 Hz, 2H), 2.57 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.1, 162.7, 153.3, 143.1, 141.4, 139.0, 136.8, 135.7, 133.2, 131.4, 130.4, 129.40, 129.38, 128.5, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3349 (N-H), 1748 (C=O). HRMS (ESI) for $C_{17}H_{13}ClN_3O_2$ $[M + H]^+$: calcd: 326.0691, found: 326.0684.

***N*-acetyl-3-(4-fluorophenyl)quinoxaline-2-carboxamide (3da):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (90.9 mg, 98%). m.p. 180.7–182.8 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 8.20 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.17 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.96–7.87 (m, 2H), 7.68–7.65 (m, 2H), 7.24–7.19 (m, 2H), 2.55 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.1, 163.5 (d, $J_{C\text{-}F}$ = 247.5 Hz), 153.3, 143.0, 141.6, 138.9, 134.3 (d, $J_{C\text{-}F}$ = 3.75 Hz), 133.0, 131.2, 131.0, 130.9, 129.315, 129.307, 115.4 (d, $J_{C\text{-}F}$ = 21.25 Hz), 25.3; IR (potassium bromide) (ν, cm^{-1}): 3357 (N-H), 1748 (C=O. HRMS (ESI) for $C_{17}H_{13}FN_3O_2$ $[M + H]^+$: calcd: 310.0986, found: 310.0994.

***N*-acetyl-3-(*p*-tolyl)quinoxaline-2-carboxamide (3ea):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (61.4 mg, 67%). m.p. 162.3–164.0 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.25 (s, 1H), 8.21 (dd, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 8.17 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.95–7.85 (m, 2H), 7.58 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 2.57 (s, 3H), 2.47 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 163.0, 154.3, 143.1, 142.0, 139.5, 138.8, 135.4, 132.8, 130.9, 129.4, 129.3, 129.1, 128.8, 25.4, 21.5. IR (potassium bromide) (ν, cm^{-1}): 3335 (N-H), 1750 (C=O). HRMS (ESI) for $C_{18}H_{16}N_3O_2$ $[M + H]^+$: calcd: 306.1237, found: 306.1245.

***N*-acetyl-3-(4-ethylphenyl)quinoxaline-2-carboxamide (3fa):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (60.0 mg, 63%). m.p. 165.4–166.1 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.28 (s, 1H), 8.20 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.16 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 7.93–7.90 (m, 1H), 7.87–7.84 (m, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 2.77 (q, J = 7.5 Hz, 2H), 2.56 (s, 3H), 1.31 (t, J = 7.5 Hz, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.2, 163.1, 154.2, 145.7, 143.0, 142.0, 138.7, 135.5, 132.7, 130.9, 129.3, 129.2,

128.9, 127.9, 28.7, 25.4, 15.2. IR (potassium bromide) (ν, cm^{-1}): 3239 (N-H), 1738 (C=O). HRMS (ESI) for $C_{19}H_{18}N_3O_2$ $[M + H]^+$: calcd: 320.1394, found: 320.1387.

***N*-acetyl-3-(4-methoxyphenyl)quinoxaline-2-carboxamide (3ga):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (64.0 mg, 66%). m.p. 136.7–138.3 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.23 (s, 1H), 8.19 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.15 (dd, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 1H), 7.94–7.90 (m, 1H), 7.87–7.84 (m, 1H), 7.66 (d, J = 8.5 Hz, 2H), 7.05 (d, J = 8.5 Hz, 2H), 3.90 (s, 3H), 2.58 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 163.2, 160.8, 153.8, 143.1, 141.9, 138.6, 132.8, 130.8, 130.6, 130.4, 129.29, 129.27, 113.9, 55.4, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3330 (N-H), 1712 (C=O). HRMS (ESI) for $C_{18}H_{16}N_3O_3$ $[M + H]^+$: calcd: 322.1186, found: 322.1181.

***N*-acetyl-3-(4-(benzyloxy)phenyl)quinoxaline-2-carboxamide (3ha):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (103.0 mg, 86%). m.p. 149.2–150.2 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.25 (s, 1H), 8.20–8.14 (m, 2H), 7.94–7.84 (m, 2H), 7.68–7.65 (m, 2H), 7.49–7.35 (m, 5H), 7.15–7.12 (m, 2H), 5.16 (s, 2H), 2.58 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 163.2, 160.0, 153.7, 143.1, 141.9, 138.6, 136.7, 132.8, 130.8, 130.63, 130.58, 129.3, 129.2, 128.6, 128.1, 127.5, 114.7, 70.0, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3325 (N-H), 1708 (C=O). HRMS (ESI) for $C_{24}H_{20}N_3O_3$ $[M + H]^+$: calcd: 398.1499, found: 398.1504.

***N*-acetyl-3-(3-bromophenyl)quinoxaline-2-carboxamide (3ia):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (98.2 mg, 88%). m.p. 179.8–181.6 ºC. ^1H NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 8.22 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.20(dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.99–7.95 (m, 1H), 7.94–7.90 (m, 1H), 7.83 (t, J = 2.0 Hz, 1H), 7.86–7.64 (m, 1H), 7.57–7.54 (m, 1H), 7.39 (t, J = 8.0 Hz, 1H), 2.57 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.2, 162.6, 152.9, 143.0, 141.5, 140.3, 139.1, 133.2, 132.3, 131.8, 131.6, 129.6, 129.5, 129.4, 127.7, 122.4, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3301 (N-H), 1744 (C=O). HRMS (ESI) for $C_{17}H_{13}BrN_3O_2$ $[M + H]^+$: calcd: 370.0186, found: 370.0180.

***N*-acetyl-3-(3-chlorophenyl)quinoxaline-2-carboxamide (3ja):** Purified by

column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (93.0 mg, 95%). m.p. 169.4–171.1 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.33 (s, 1H), 8.23–8.18 (m, 2H), 7.98–7.90 (m, 2H), 7.67 (t, J = 1.5 Hz, 1H), 7.52–7.43 (m, 3H), 2.56 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.1, 162.6, 152.9, 142.9, 141.5, 140.0, 139.0, 134.2, 133.1, 131.5, 129.38, 129.35, 128.9, 127.1, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3312 (N-H), 1745 (C=O). HRMS (ESI) for $C_{17}H_{13}ClN_3O_2$ $[M + H]^+$: calcd: 326.0691, found: 326.0683.

***N*-acetyl-3-(3-methoxyphenyl)quinoxaline-2-carboxamide (3ka):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (75.0 mg, 78%); m.p. 142.4–143.1 ºC; ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.22 (s, 1H), 8.23 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.19 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 7.97–7.88 (m, 2H), 7.44 (t, J = 8.0 Hz, 1H), 7.23–7.19 (m, 2H), 7.09–7.06 (m, 1H), 3.90 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.2, 162.8, 159.5, 154.1, 143.0, 142.1, 139.6, 139.0, 132.9, 131.2, 129.4, 129.34, 129.33, 121.3, 115.1, 114.4, 55.4, 25.4; IR (potassium bromide) (ν, cm^{-1}): 3286 (N-H), 1712 (C=O). HRMS (ESI) for $C_{18}H_{16}N_3O_3$ $[M + H]^+$: calcd: 322.1186, found: 322.1190.

***N*-acetyl-3-(2-fluorophenyl)quinoxaline-2-carboxamide (3la):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (80.0 mg, 86%). m.p. 123.3–125.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.29 (s, 1H), 8.24–8.18 (m, 2H), 7.97–7.89 (m, 2H), 7.78–7.75 (m, 1H), 7.55–7.50 (m, 1H), 7.40–7.37 (m, 1H), 7.17 (t, J= 4.0 Hz, 1H), 2.58 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.2, 162.4, 160.0 (d, J = 245.0 Hz), 149.0, 143.4, 142.4, 138.9, 132.9, 131.43, 131.35, 130.4 (d, J = 2.5 Hz), 129.41, 129.39, 126.8 (d, J = 15.0 Hz), 124.7 (d, J = 2.5 Hz), 115.2 (d, J = 22.5 Hz), 25.3. IR (potassium bromide) (ν, cm^{-1}): 3248 (N-H), 1733 (C=O). HRMS (ESI) for $C_{17}H_{13}FN_3O_2$ $[M + H]^+$: calcd: 310.0986, found: 310.0980.

***N*-acetyl-3-(2-methoxyphenyl)quinoxaline-2-carboxamide (3ma):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (81.9 mg, 85%). m.p. 143.8–144.9 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.05 (s, 1H), 8.22 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.17 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.92–7.85 (m, 2H), 7.74 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.53–7.49 (m, 1H), 7.24–7.21 (m, 1H), 6.98 (d,

J = 8.5 Hz, 1H), 3.76 (s, 3H), 2.57 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.4, 163.1, 156.4, 151.3, 144.2, 143.5, 138.7, 132.2, 131.2, 130.7, 130.0, 129.34, 129.31, 127.8, 121.6, 110.5, 55.0, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3309 (N-H), 1709 (C=O). HRMS (ESI) for $C_{18}H_{16}N_3O_3$ $[M + H]^+$: calcd: 322.1186, found: 322.1180.

***N*-acetyl-3-(2-bromophenyl)quinoxaline-2-carboxamide (3na):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (98.8 mg, 89%). m.p. 165.9–167.0 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.41 (s, 1H), 8.26–8.22 (m, 2H), 7.99–7.93 (m, 2H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.57–7.53 (m, 2H), 7.42–7.38 (m, 1H) 2.56 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.2, 162.0, 153.5, 143.1, 141.8, 139.8, 139.1, 133.0, 132.3, 131.6, 130.4, 129.8, 129.5, 129.4, 127.8, 122.1, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3275 (N-H), 1740 (C=O). HRMS (ESI) for $C_{17}H_{13}BrN_3O_2$ $[M + H]^+$: calcd: 370.0186, found: 370.0192.

***N*-acetylquinoxaline-2-carboxamide (3oa):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (55.0 mg, 85%). m.p. 101.3–103.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.31 (s, 1H), 9.66 (s, 1H), 8.20 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.14 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 7.94–7.87 (m, 2H), 2.69 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 171.8, 162.0, 144.4, 143.5, 141.5, 139.9, 132.7, 131.4, 129.8, 129.5, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3247 (N-H), 1711 (C=O). HRMS (ESI) for $C_{11}H_{10}N_3O_2$ $[M + H]^+$: calcd: 216.0768, found: 216.0775.

***N*-acetyl-3-methylquinoxaline-2-carboxamide (3pa):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (30.7 mg, 45%). m.p. 144.8–147.9 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.80 (s, 1H), 8.11–8.08 (m, 2H), 7.92–7.80 (m, 2H), 3.14 (s, 3H), 2.66 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.1, 163.0, 154.6, 143.5, 140.7, 138.8, 132.8, 130.4, 129.4, 128.5, 25.4, 24.9. IR (potassium bromide) (ν, cm^{-1}): 3255 (N-H), 1711 (C=O). HRMS (ESI) for $C_{12}H_{12}N_3O_2$ $[M + H]^+$: calcd: 230.0924, found: 230.0931.

***N*-acetyl-3-chloroquinoxaline-2-carboxamide (3qa):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a red solid (47.0 mg, 63%). m.p. 162.5–163.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.21 (s, 1H), 8.16 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.11 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 7.99–7.89 (m, 2H), 2.66 (s,

3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.0, 162.8, 145.2, 143.1, 140.1, 138.5, 134.0, 131.7, 129.4, 128.4, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3301 (N-H), 1742 (C=O). HRMS (ESI) for $C_{11}H_9ClN_3O_2$ $[M + H]^+$: calcd: 250.0378, found: 250.0385.

***N*-acetyl-6,7-dichloro-3-phenylquinoxaline-2-carboxamide (3ra):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (98.5 mg, 91%). m.p. 174.0–175.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.01 (s, 1H), 8.34 (s, 1H), 8.30 (s, 1H), 7.67–7.65 (m, 2H), 7.56–7.52 (m, 3H), 2.52 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 171.9, 162.8, 156.1, 143.5, 141.6, 137.8, 137.5, 137.4, 136.0, 129.94, 129.87, 129.7, 128.9, 128.4, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3250 (N-H), 1712 (C=O). HRMS (ESI) for $C_{17}H_{12}Cl_2N_3O_2$ $[M + H]^+$: calcd: 360.0301, found: 360.0309.

***N*-acetyl-6,7-dibromo-3-phenylquinoxaline-2-carboxamide (3sa):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (84.8 mg, 73%). m.p. 198.9–201.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.99 (s, 1H), 8.53 (s, 1H), 8.49 (s, 1H), 7.67–7.65 (m, 2H), 7.56–7.51 (m, 3H), 2.52 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 171.8, 162.8, 156.1, 143.6, 141.9, 138.0, 137.4, 133.4, 133.1, 130.1, 129.9, 128.9, 128.4, 128.1, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3256 (N-H), 1711 (C=O). HRMS (ESI) for $C_{17}H_{12}Br_2N_3O_2$ $[M + H]^+$: calcd: 447.9291, found: 447.9283.

***N*-acetyl-6,7-dimethyl-3-phenylquinoxaline-2-carboxamide (3ta):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (60.3 mg, 63%). m.p. 138.0–139.4 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.37 (s, 1H), 7.96 (s, 1H), 7.90 (s, 1H), 7.64–7.62 (m, 2H), 7.52–7.51 (m, 3H), 2.56–2.55 (m, 9H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 163.0, 153.6, 144.3, 142.13, 142.08, 140.6, 138.6, 137.9, 129.1, 128.8, 128.3, 128.14, 128.05, 25.4, 20.7, 20.4. IR (potassium bromide) (ν, cm^{-1}): 3307 (N-H), 1708 (C=O). HRMS (ESI) for $C_{19}H_{18}N_3O_2$ $[M + H]^+$: calcd: 320.1394, found: 320.1399.

***N*-acetyl-6,7-dimethyl-3-(p-tolyl)quinoxaline-2-carboxamide (3ua):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (58.4 mg, 58%). m.p. 177.2–177.9 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 7.94 (s, 1H), 7.88 (s, 1H), 7.54 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 8.0 Hz, 2H), 2.56 (s, 3H),

2.550 (s, 3H), 2.548 (s, 3H), 2.45 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.4, 163.2, 153.6, 144.2, 142.1, 141.9, 140.7, 139.1, 137.8, 135.7, 128.9, 128.8, 128.2, 128.0, 25.4, 21.4, 20.7, 20.4. IR (potassium bromide) (ν, cm^{-1}): 3329 (N-H), 1738 (C=O). HRMS (ESI) for $C_{20}H_{20}N_3O_2$ $[M + H]^+$: calcd: 334.1550, found: 334.1557.

***N*-acetyl-3-(4-methoxyphenyl)-6,7-dimethylquinoxaline-2-carboxamide (3va):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (61.2 mg, 58%). m.p. 150.0–151.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.32 (s, 1H), 7.93 (s, 1H), 7.88 (s, 1H), 7.63–7.61 (m, 2H), 7.05–7.02 (m, 2H), 3.90 (s, 3H), 2.57 (s, 3H), 2.56 (s, 6H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.4, 163.4, 160.5, 153.1, 144.2, 142.2, 141.8, 140.7, 137.7, 130.9, 130.5, 128.2, 128.1, 113.8, 55.3, 25.4, 20.7, 20.4. IR (potassium bromide) (ν, cm^{-1}): 3378 (N-H), 1655 (C=O). HRMS (ESI) for $C_{20}H_{20}N_3O_3$ $[M + H]^+$: calcd: 350.1499, found: 350.1491.

4.3 Characterization of 3ad-3ag

***N*-(3-methoxypropanoyl)-3-phenylquinoxaline-2-carboxamide (3ad):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (29.8 mg, 30%). m.p. 128.5–130.0 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.38 (s, 1H), 8.22 (d, J = 8.0 Hz, 1H), 8.19–8.17 (m, 1H), 7.95–7.86 (m, 2H), 7.69–7.67 (m, 2H), 7.53–7.52 (m, 3H), 3.72 (t, J = 6.0 Hz, 2H), 3.42 (s, 3H), 3.046 (t, J = 5.5 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.2, 163.3, 154.0, 142.9, 139.0, 138.1, 132.6, 131.0, 129.4, 129.35, 129.30, 128.9, 128.3, 67.2, 58.9, 37.9. IR (potassium bromide) (ν, cm^{-1}): 3276 (N-H), 1693 (C=O). HRMS (ESI) for $C_{19}H_{18}N_3O_3$ $[M + H]^+$: calcd: 336.1343, found: 336.1350.

***N*-acryloyl-3-phenylquinoxaline-2-carboxamide (3ae):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (25.1 mg, 27%). m.p. 193.0 – 194.2 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.27 (s, 1H), 8.25–8.21 (m, 2H), 7.97–7.89 (m, 2H), 7.69–7.67 (m, 2H), 7.54–7.53 (m, 3H), 7.25–7.22 (m, 1H), 6.61 (dd, J_1 = 17.0 Hz, J_2 = 1.5 Hz, 1H), 5.93 (dd, J_1 = 10.0 Hz, J_2 = 1.5 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 166.1, 154.4, 143.1, 138.9, 138.3, 132.9, 132.1, 131.1, 129.6, 129.5, 129.4, 128.9, 128.3, 113.6. IR (potassium bromide) (ν, cm^{-1}):

3235 (N-H), 1727 (C=O). HRMS (ESI) for $C_{18}H_{14}N_3O_2$ $[M + H]^+$: calcd: 304.1081, found: 304.1089.

***N*-benzoyl-3-phenylquinoxaline-2-carboxamide (3af):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (88.0 mg, 83%). m.p. 145.7−148.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.53 (s, 1H), 8.23(dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 8.18–8.16 (m, 1H), 7.91–7.82 (m, 4H), 7.78–7.76 (m, 2H), 7.61–7.58 (m, 1H), 7.49–7.45 (m, 5H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 165.3, 165.8, 153.1, 145.2, 142.6, 139.2, 137.6, 133.4, 132.3, 132.0, 130.6, 129.43, 129.40, 129.2, 129.0, 128.9, 128.4, 127.9. IR (potassium bromide) (ν, cm^{-1}): 3251 (N-H), 1681 (C=O). HRMS (ESI) for $C_{22}H_{16}N_3O_2$ $[M + H]^+$: calcd: 354.1237, found: 354.1242.

***N*-(4-methoxybenzoyl)-3-phenylquinoxaline-2-carboxamide (3ag):** Purified by column chromatography (petroleum ether/EtOAc, 6/1-3/1) as a white solid (67.8 mg, 59%). m.p. 140.3-142.1 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.38 (s, 1H), 8.22 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 8.16 (dd, J_1 = 8.3 Hz, J_2 = 1.1 Hz, 1H), 7.89-7.77 (m, 6H), 7.47-7.43 (m, 3H), 6.92 (d, J = 8.9 Hz, 2H), 3.86 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 166.8, 164.7, 163.9, 152.9, 146.0, 142.5, 139.4, 137.7, 131.8, 130.6, 130.3, 129.5, 129.5, 129.3, 129.1, 128.5, 124.3, 114.2, 55.60. IR (potassium bromide) (ν, cm^{-1}): 3277 (N-H), 1694 (C=O). HRMS (ESI) for $C_{23}H_{18}N_3O_3$ $[M + H]^+$: calcd: 384.1343, found: 384.1351.

4.4 Characterization of 7ba-7na

***N*-acetyl-6-methylquinoline-2-carboxamide (7ba):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (58.9 mg, 72%). m.p. 135.3−136.7 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.70 (s, 1H), 8.24 (s, 2H), 8.00 (d, J = 8.5 Hz, 1H), 7.64–7.62 (m, 2H), 2.66 (s, 3H), 2.57 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.1, 163.1, 146.7, 144.8, 139.4, 137.2, 133.1, 129.9, 129.5, 126.5, 118.7, 25.3, 21.8. IR (potassium bromide) (ν, cm^{-1}): 3323 (N-H), 1706 (C=O). HRMS (ESI) for $C_{13}H_{13}N_2O_2$ $[M + H]^+$: calcd: 229.0972, found: 229.0964.

***N*-acetyl-6-methoxyquinoline-2-carboxamide (7ca):** Purified by column

chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (52.0 mg, 71%). m.p. 138.4 – 139.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.60 (s, 1H), 8.19–8.15 (m, 2H), 7.94 (d, J = 9.0 Hz, 1H), 7.40 (dd, J_1 = 9.5 Hz, J_2 = 2.5 Hz, 1H), 7.07 (d, J = 2.5 Hz, 1H), 3.94 (s, 3H), 2.64 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.1, 163.1, 159.6, 145.1, 142.2, 136.3, 131.23, 131.20, 123.9, 119.1, 104.7, 55.6, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3329 (N-H), 1709 (C=O). HRMS (ESI) for $C_{13}H_{13}N_2O_3$ [M + H]$^+$: calcd: 245.0921, found: 245.0930.

***N*-acetyl-6-fluoroquinoline-2-carboxamide (7da):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (64.0 mg, 92%). m.p. 143.3 – 145.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.61 (s, 1H), 8.31 (s, 2H), 8.16–8.13 (m, 1H), 7.61–7.57 (m, 1H), 7.52 (dd,J_1 = 8.5 Hz, J_2 = 3.0 Hz, 1H), 2.87 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.1, 162.8, 161.8 (d, $J_{C\text{-}F}$ = 252.5 Hz), 147.2(d, $J_{C\text{-}F}$ = 3.75 Hz), 143.3, 137.4(d, $J_{C\text{-}F}$ = 5.0 Hz), 132.6(d, $J_{C\text{-}F}$ = 10.0 Hz), 130.7(d, $J_{C\text{-}F}$ = 10.0 Hz), 121.3(d, $J_{C\text{-}F}$ = 26.25 Hz), 119.5, 110.9(d, $J_{C\text{-}F}$ = 21.25 Hz), 25.3. IR (potassium bromide) (ν, cm^{-1}): 3318 (N-H), 1713 (C=O). HRMS (ESI) for $C_{12}H_{10}FN_2O_2$ [M + H]$^+$: calcd: 233.0721, found: 233.0730.

***N*-acetyl-6-bromoquinoline-2-carboxamide (7ea):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (61.4 mg, 70%). m.p. 141.3 – 143.4 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.59 (s, 1H), 8.30 (d, J = 8.5 Hz, 1H), 8.26 (d, J = 8.5 Hz, 1H), 8.05 (d, J = 2.0 Hz, 1H), 7.97 (d, J = 9.0 Hz, 1H), 7.85 (dd, J_1 = 9.0 Hz, J_2 = 2.0 Hz, 1H), 2.66 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.1, 162.7, 148.0, 144.7, 137.1, 134.3, 131.4, 130.7, 129.8, 123.4, 119.6, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3311 (N-H), 1711 (C=O). HRMS (ESI) for $C_{12}H_{10}BrN_2O_2$ [M + H]$^+$: calcd: 292.9920, found: 292.9929.

***N*-acetyl-6-iodoquinoline-2-carboxamide (7fa):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (72.0 mg, 71%). m.p. 179.0 – 180.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.62 (s, 1H), 8.24–8.32 (m, 2H), 8.27 (d, J = 8.5 Hz, 1H), 8.06 (dd, J_1 = 9.0 Hz, J_2 =2.0 Hz, 1H), 7.87 (d, J = 9.0 Hz, 1H), 2.68 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 172.1, 162.8, 148.2, 145.2, 139.6, 136.9, 136.6, 131.3, 131.2, 119.6, 95.4, 25.4. IR (potassium bromide) (ν, cm^{-1}):

3325 (N-H), 1691 (C=O). HRMS (ESI) for $C_{12}H_{10}IN_2O_2$ $[M + H]^+$: calcd: 340.9781, found: 340.9786.

***N*-acetyl-7-methyl-8-(trifluoromethyl)quinoline-2-carboxamide (7ga):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (28.2 mg, 35%). m.p. 148.2–149.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.47 (s, 1H), 8.41 (s, 2H), 7.88–7.83 (m, 2H), 3.00 (d, J = 2.0 Hz, 3H), 2.69 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 171.9, 162.7, 147.8, 145.0, 138.7, 138.5 (d, J_{C-F} = 1.25 Hz), 130.9, 130.4 (q, J_{C-F} = 28.75 Hz), 125.9, 124.9 (q, J_{C-F} = 5.0 Hz), 124.1 (q, J_{C-F} = 273.75 Hz), 120.3, 25.4, 13.6 (d, J_{C-F} = 1.25 Hz). IR (potassium bromide) (ν, cm^{-1}): 3344 (N-H), 1716 (C=O). HRMS (ESI) for $C_{14}H_{12}F_3N_2O_2$ $[M + H]^+$: calcd: 297.0845, found: 297.0850.

***N*-acetyl-8-bromoquinoline-2-carboxamide (7ha):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (27.7 mg, 31%). m.p. 145.9–147.4 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.72 (s, 1H), 8.42 (d, J = 8.5 Hz, 1H), 8.38 (d, J = 8.5 Hz, 1H), 8.16 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.91 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.58–7.55 (m, 1H), 2.68 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 171.8, 162.7, 148.3, 143.4, 138.9, 134.3, 131.1, 129.4, 127.5, 125.6, 119.7, 25.4. IR (potassium bromide) (ν, cm^{-1}): 3341 (N-H), 1707 (C=O). HRMS (ESI) for $C_{12}H_{10}BrN_2O_2$ $[M + H]^+$: calcd: 292.9920, found: 292.9928.

***N*-acetyl-5,7-dimethylquinoline-2-carboxamide (7ia):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (45.0 mg, 62%). m.p. 128.1–130.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.74 (s, 1H), 8.45 (d, J = 8.5 Hz, 1H), 8.23 (d, J = 8.5 Hz, 1H), 7.75 (s, 1H), 7.34 (s, 1H), 2.69 (s, 3H), 2.67 (s, 3H), 2.55 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.1, 163.3, 147.0, 146.9, 140.9, 134.32, 134.28, 131.8, 127.4, 126.9, 117.6, 25.4, 21.8, 18.5. IR (potassium bromide) (ν, cm^{-1}): 3312 (N-H), 1703 (C=O). HRMS (ESI) for $C_{14}H_{15}N_2O_2$ $[M + H]^+$: calcd: 243.1128, found: 243.1136.

***N*-acetylphenanthridine-6-carboxamide (7ja):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (55.4 mg, 70%). m.p. 148.9–150.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.93 (s, 1H), 9.58 (d, J = 8.5

Hz, 1H), 8.69 (d, J = 8.5 Hz, 1H), 8.63–8.61 (m, 1H), 8.23–8.21 (m, 1H), 7.95–7.92 (m, 1H), 7.83–7.78 (m, 3H), 2.72 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 164.2, 146.1, 141.3, 134.0, 131.4, 130.8, 129.6, 129.3, 128.5, 128.2, 126.1, 124.2, 122.2, 122.1, 25.5. IR (potassium bromide) (ν, cm^{-1}): 3258 (N-H), 1709 (C=O). HRMS (ESI) for $C_{16}H_{13}N_2O_2$ $[M + H]^+$: calcd: 265.0972, found: 265.0968.

***N*-acetyl-3-chlorophenanthridine-6-carboxamide (7ka):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (49.0 mg, 55%). m.p. 223.9−225.0 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.78 (s, 1H), 9.55 (d, J = 8.5 Hz, 1H), 8.62 (d, J = 8.0 Hz, 1H), 8.52 (d, J = 9.0 Hz, 1H), 8.19 (d, J = 2.5 Hz, 1H), 7.96–7.93 (m, 1H), 7.83–7.80 (m, 1H), 7.75 (dd, J_1 = 8.5 Hz, J_2 = 2.5 Hz, 1H), 2.71 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.1, 163.8, 147.3, 141.8, 136.2, 133.7, 131.9, 130.2, 129.7, 128.8, 128.5, 124.5, 124.0, 123.6, 122.1, 25.5. IR (potassium bromide) (ν, cm^{-1}): 3239 (N-H), 1705 (C=O). HRMS (ESI) for $C_{16}H_{12}ClN_2O_2$ $[M + H]^+$: calcd: 299.0582, found: 299.0576.

***N*-acetyl-2-methylphenanthridine-6-carboxamide (7la):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (50.4 mg, 61%). m.p. 131.9−133.7 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.93 (s, 1H), 9.57 (dd, J_1 = 8.5 Hz, J_2 = 0.5 Hz, 1H), 8.65 (d, J = 8.5 Hz, 1H), 8.37 (s, 1H), 8.07 (d, J = 8.5 Hz, 1H), 7.91–7.88 (m, 1H), 7.79–7.75 (m, 1H), 7.63 (dd, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 1H), 2.71 (s, 3H), 2.68 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 164.3, 145.0, 140.2, 139.6, 133.7, 131.2, 131.0, 130.5, 128.3, 128.1, 126.0, 124.4, 122.1, 121.7, 25.5, 22.3. IR (potassium bromide) (ν, cm^{-1}): 3305 (N-H), 1708 (C=O). HRMS (ESI) for $C_{17}H_{15}N_2O_2$ $[M + H]^+$: calcd: 279.1128, found: 279.1135.

***N*-acetyl-8-methylphenanthridine-6-carboxamide (7ma):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (52.3 mg, 63%). m.p. 135.7 − 137.6 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.95 (s, 1H), 9.37 (s, 1H), 8.59–8.58 (m, 2H), 8.21–8.18 (m, 1H), 7.81–7.78 (m, 2H), 7.76 (dd, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 2.72 (s, 3H), 2.65 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 172.3, 164.3, 145.7, 140.9, 138.8, 133.2, 132.0, 130.7, 129.6, 128.9, 127.5, 126.2, 124.4, 122.0, 25.5, 22.0. IR (potassium bromide) (ν, cm^{-1}): 3308 (N-H), 1714 (C=O). HRMS

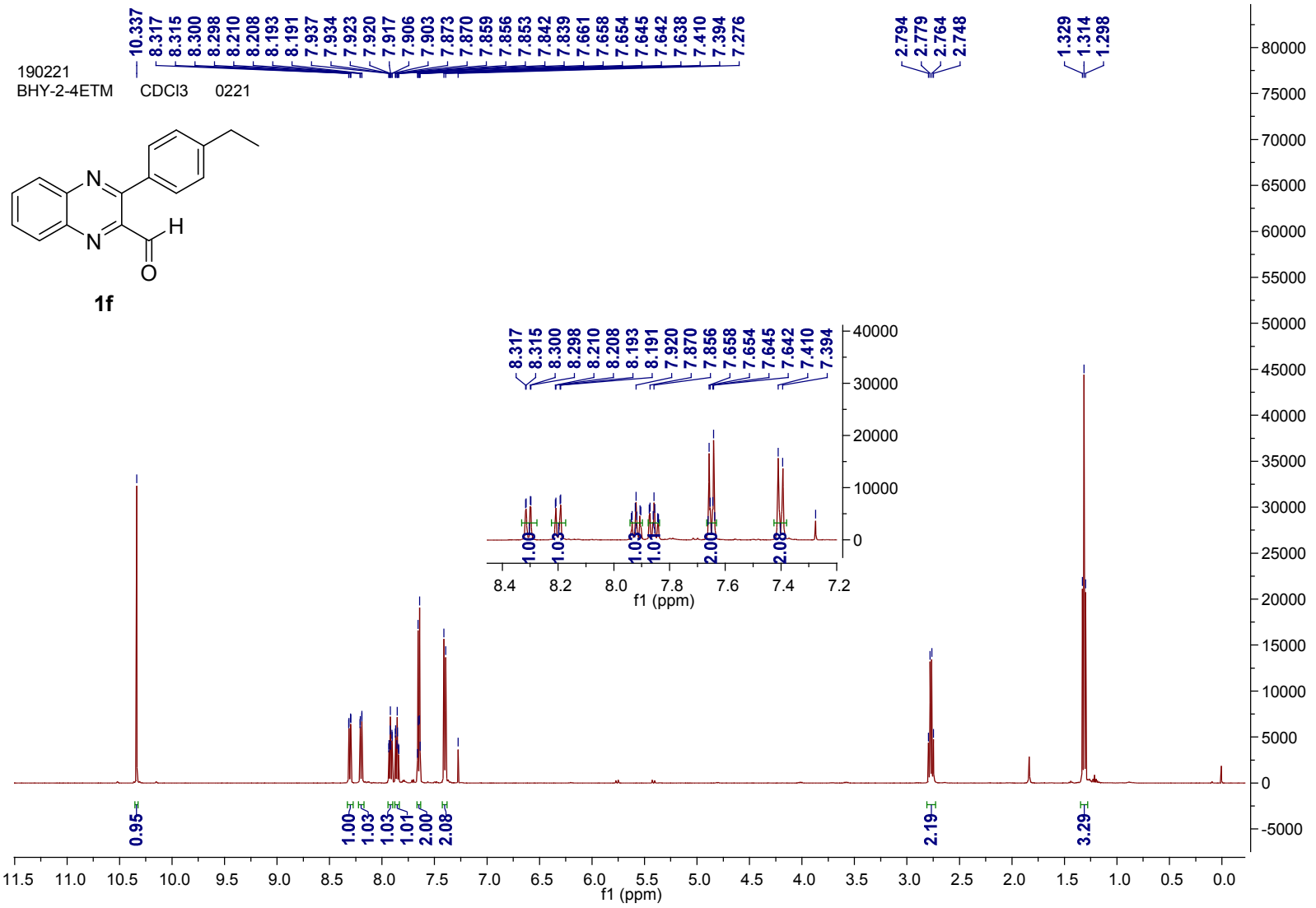
(ESI) for $C_{17}H_{15}N_2O_2$ $[M + H]^+$: calcd: 279.1128, found: 279.1133.

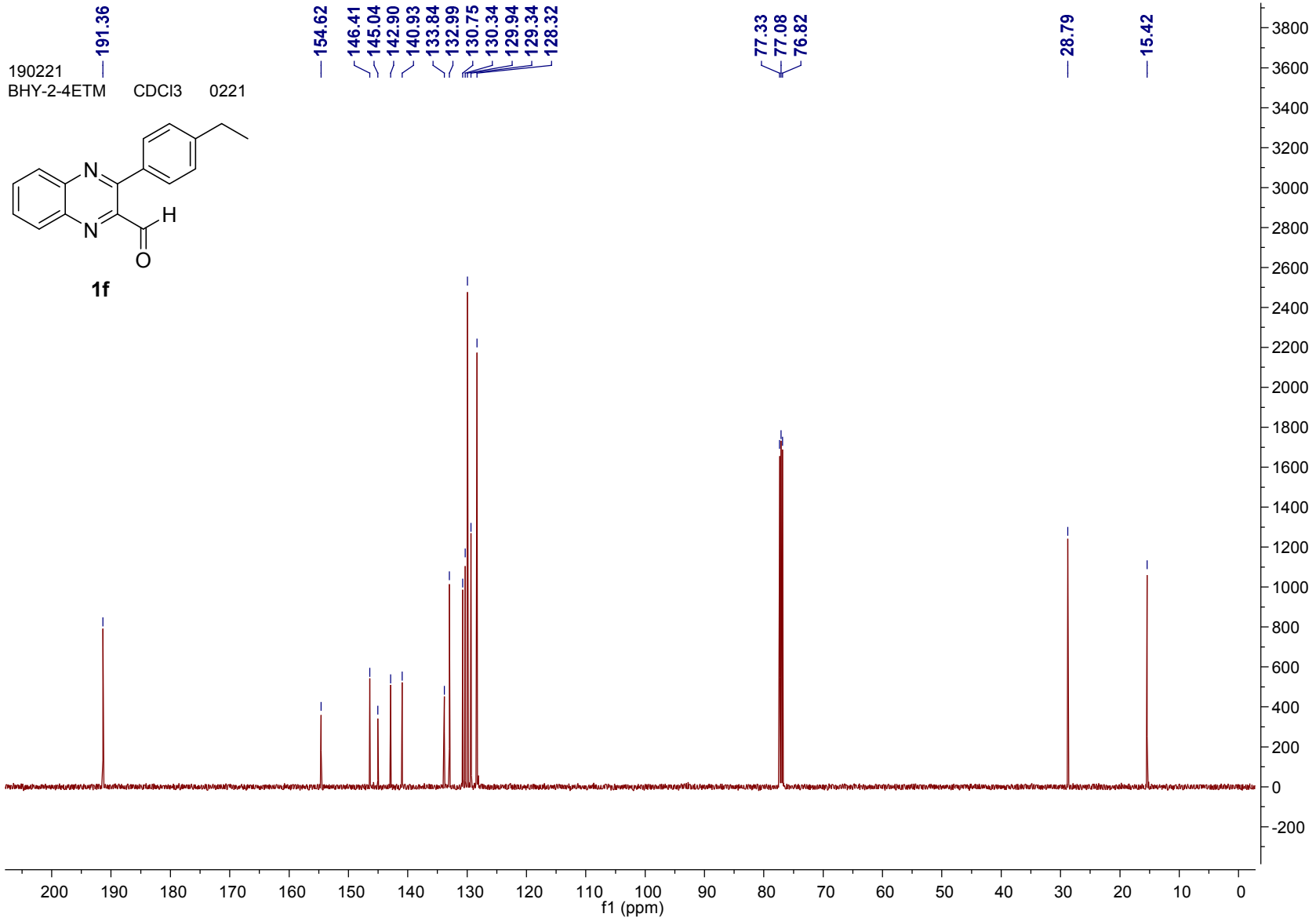
***N*-acetylpicolinamide (7na):** Purified by column chromatography (petroleum ether/EtOAc, 10/1-6/1) as a white solid (27.0 mg, 55%). m.p. 74.1-76.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.47 (s, 1H), 8.62 (ddd, J_1 = 4.8 Hz, J_2 = 1.6 Hz, J_3 =0.9 Hz, 1H), 8.26 (dt, J_1 = 7.8 Hz, J_2 = 1.0 Hz, 1H), 7.93 (td, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.55 (ddd, J_1 = 7.6 Hz, J_2 = 4.8 Hz, J_3 = 1.2 Hz, 1H), 2.52 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.0, 162.9, 148.4, 148.2, 137.8, 127.6, 123.1, 25.3. IR (potassium bromide) (ν, cm^{-1}): 3348 (N-H), 1711 (C=O). HRMS (ESI) for $C_8H_9N_2O_2$ $[M + H]^+$: calcd: 165.0659, found: 165.0654.

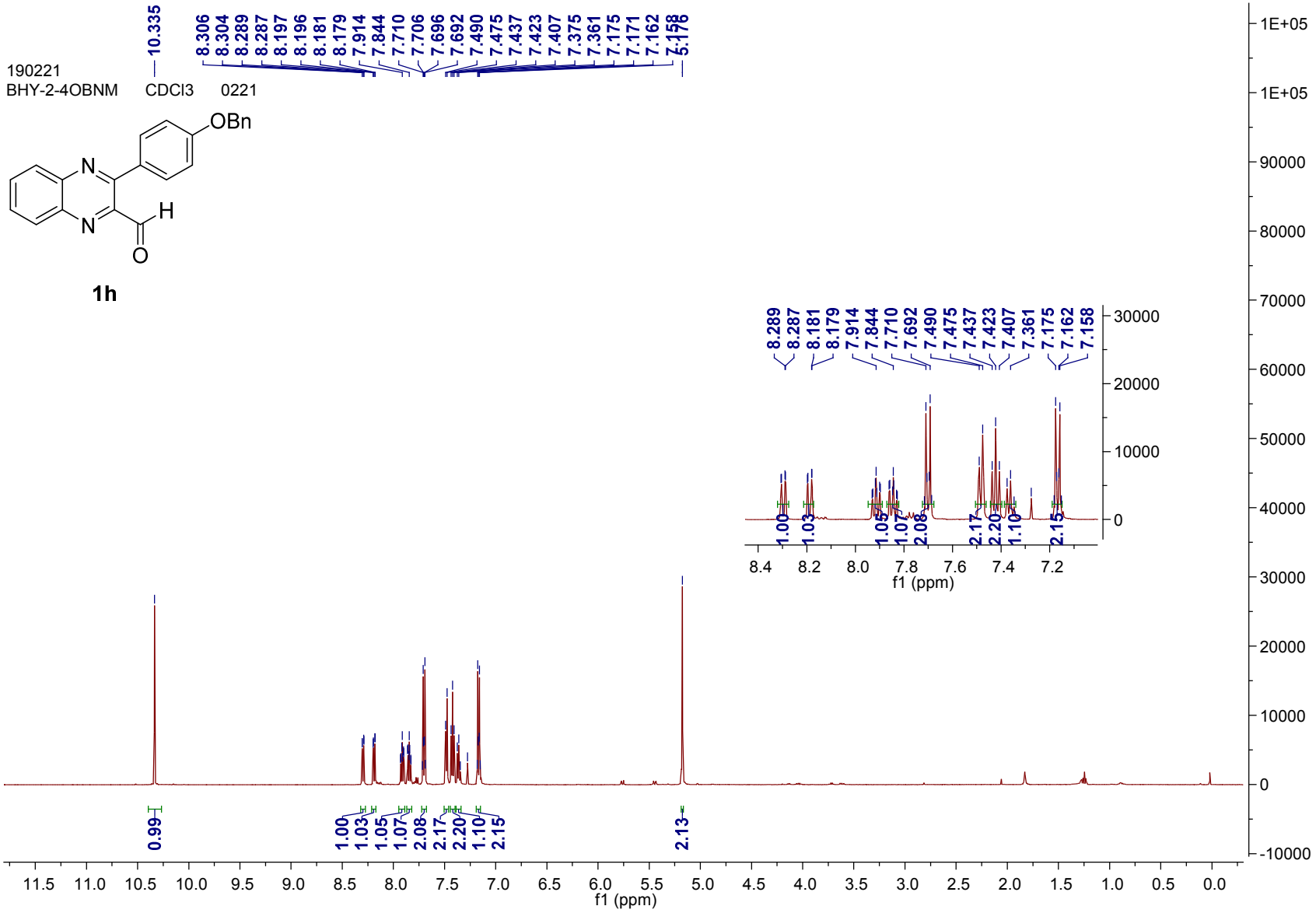
5. References

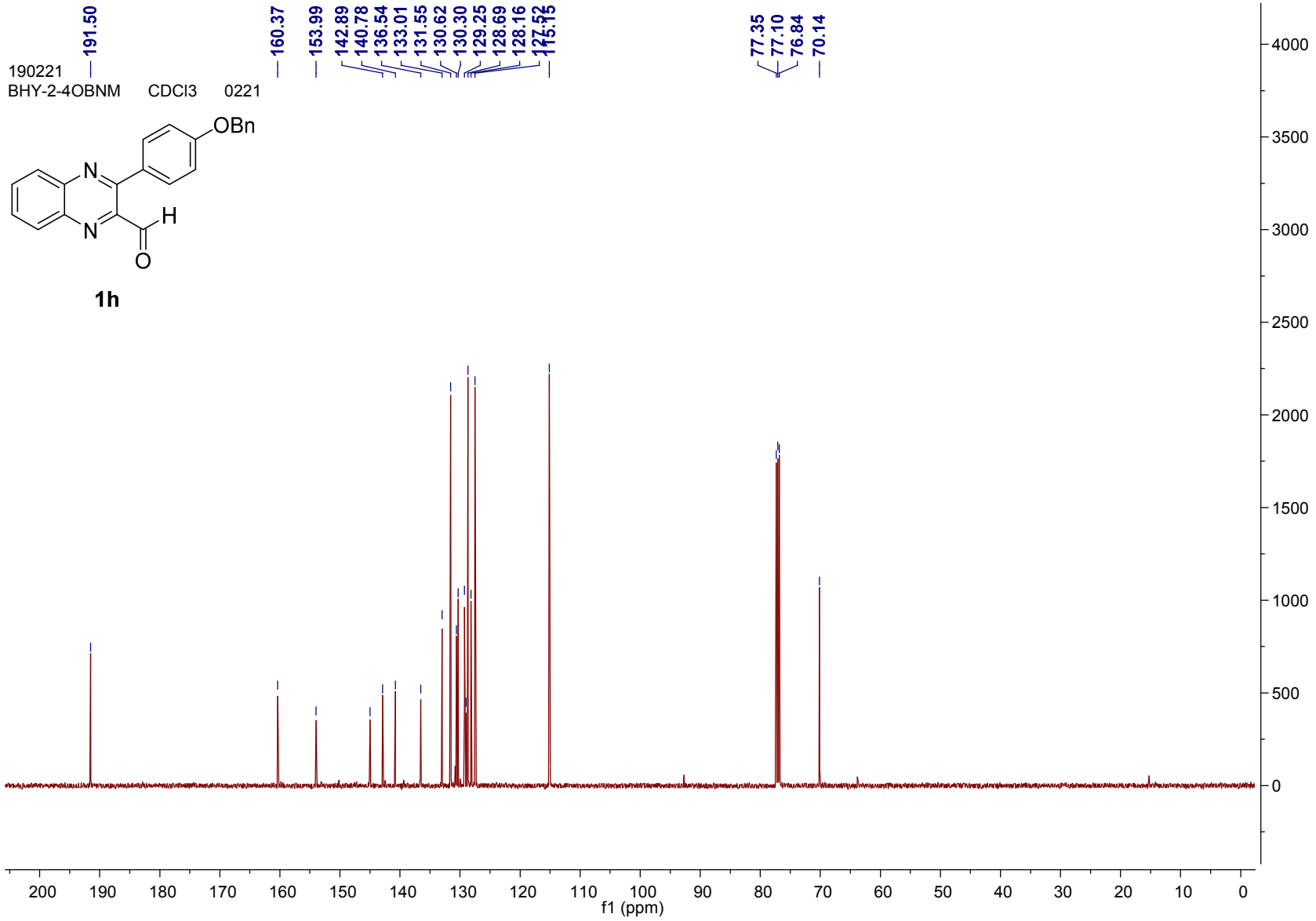
[1] Y. Liu, B. Jiang, W. Zhang and Z. Xu, *J. Org. Chem.,* 2013, **78**, 966.

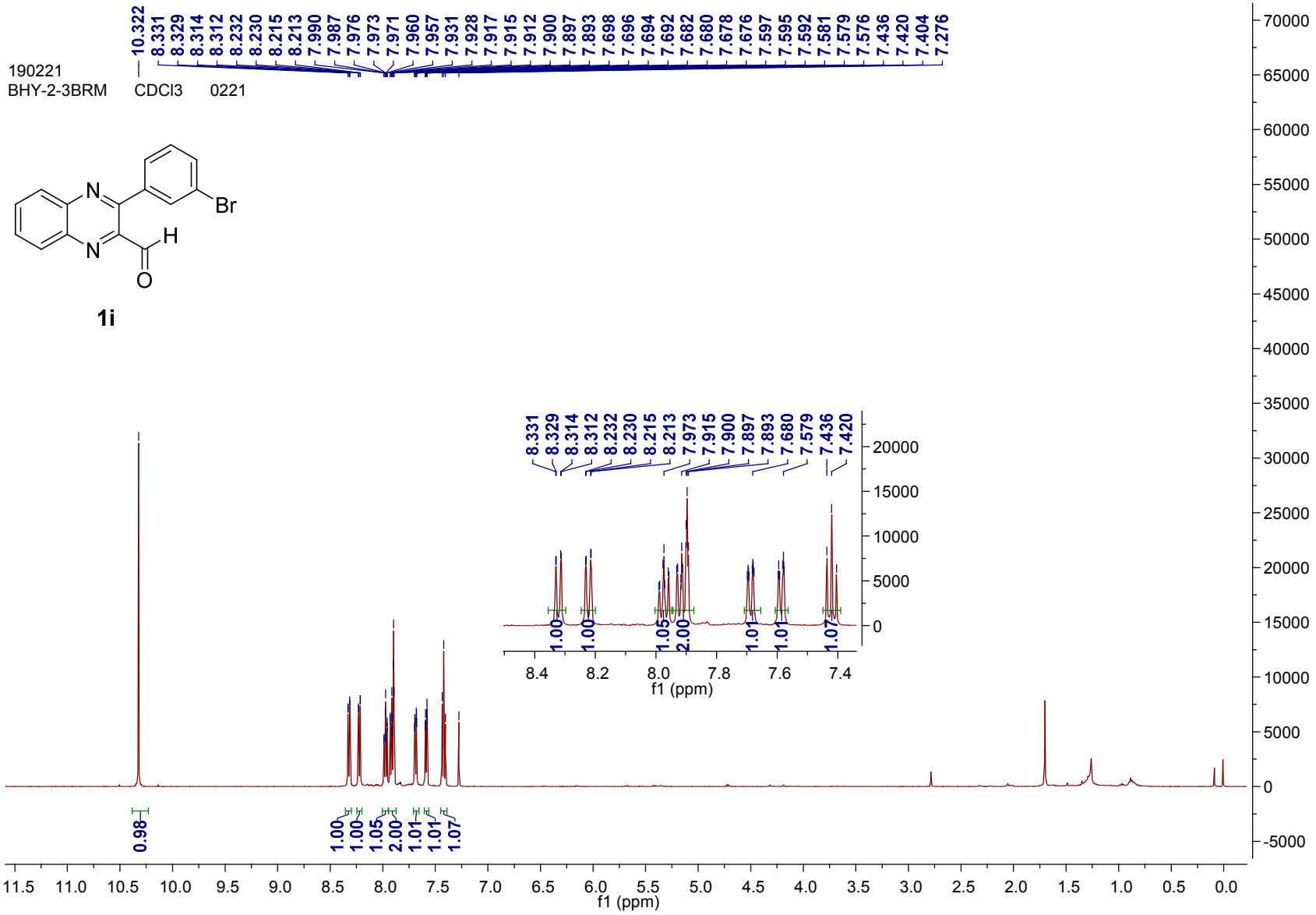
6. ^{1}H and ^{13}C NMR spectra of unknown starting materials.

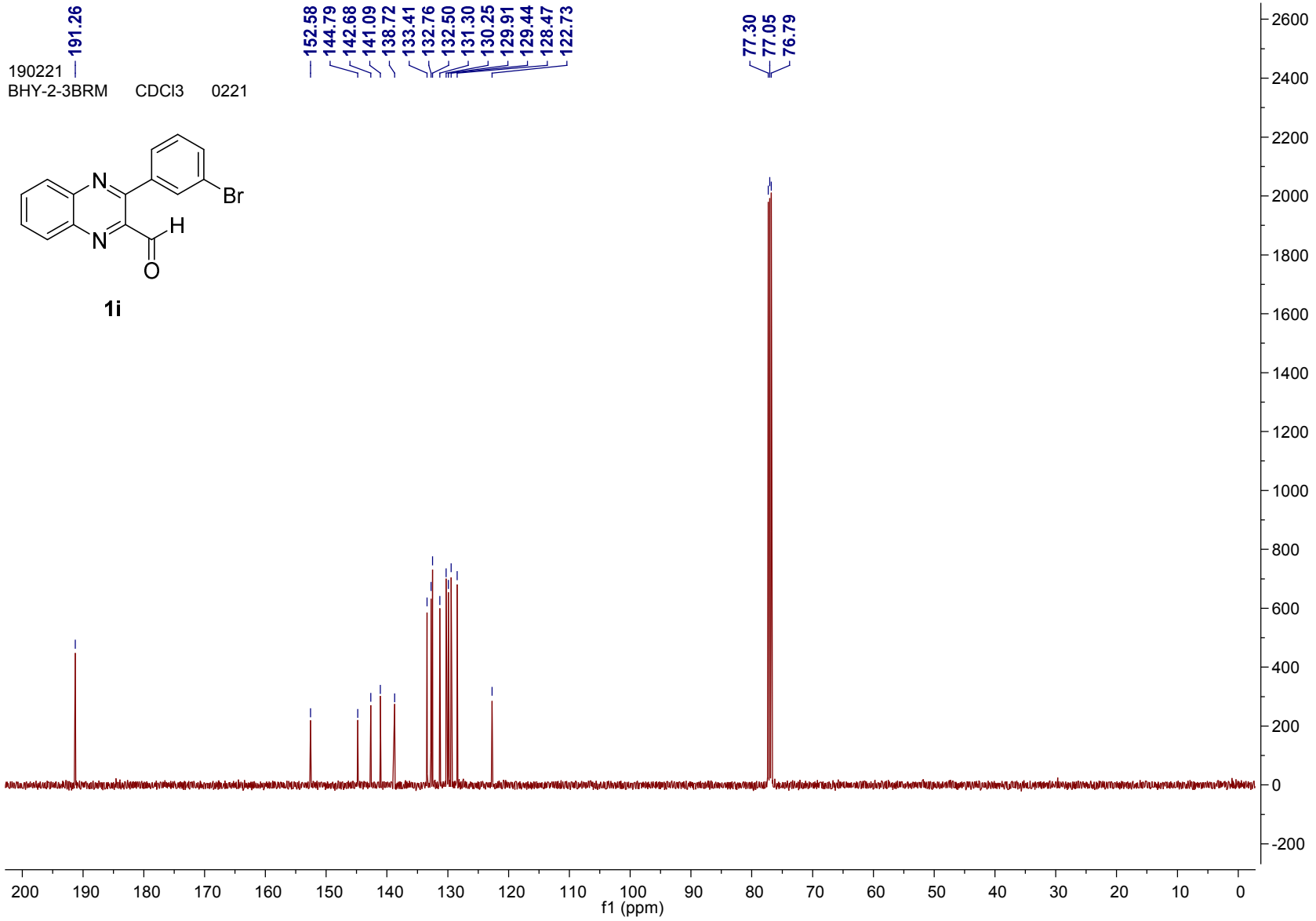


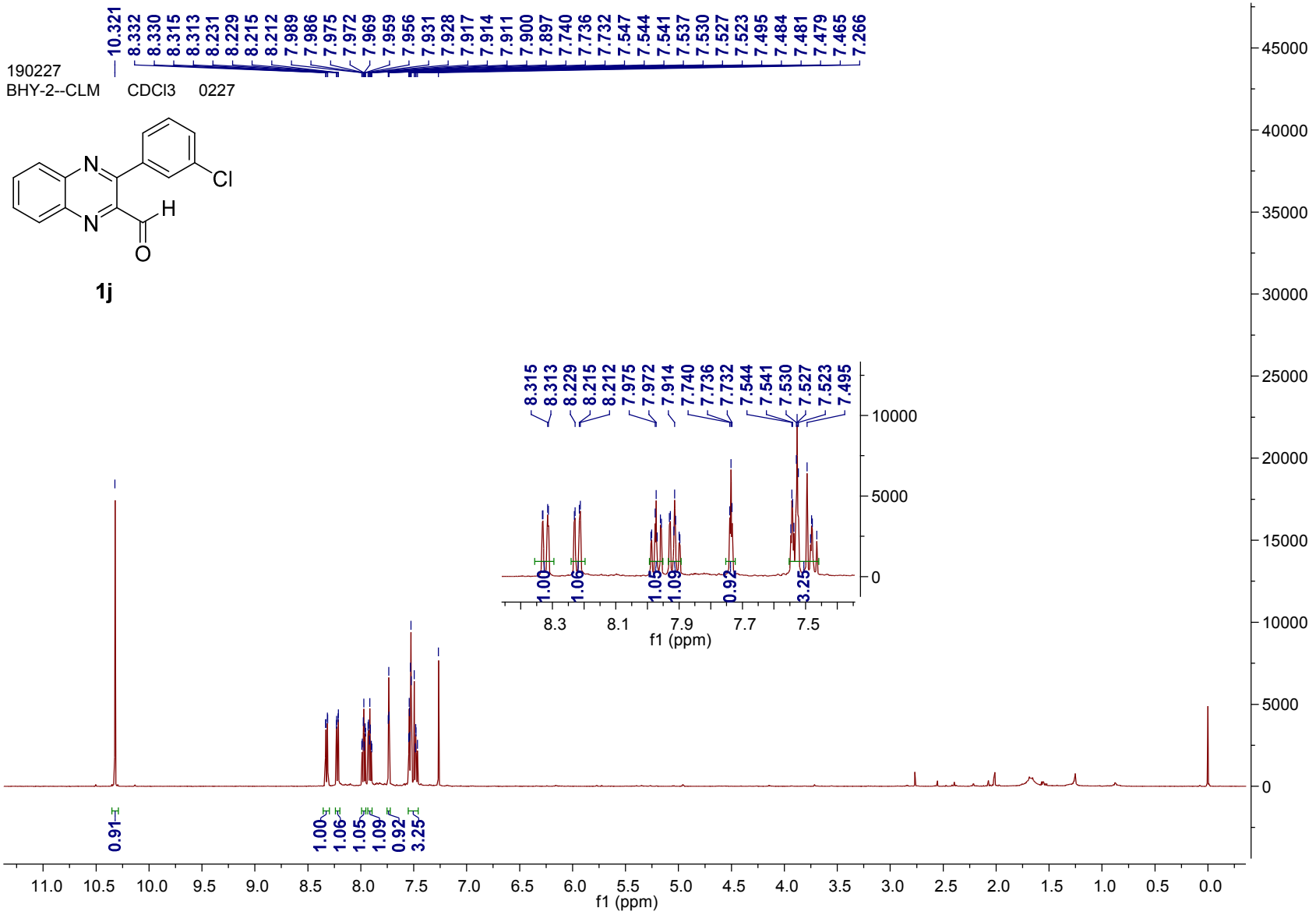

191.36
154.62
146.41
145.04
142.90
140.93
133.84
132.99
130.75
130.34
129.94
129.34
128.32
77.33
77.08
76.82
28.79
15.42
190221
BHY-2-4ETM CDCl3 0221
N
N
H
O
1f
f1 (ppm)

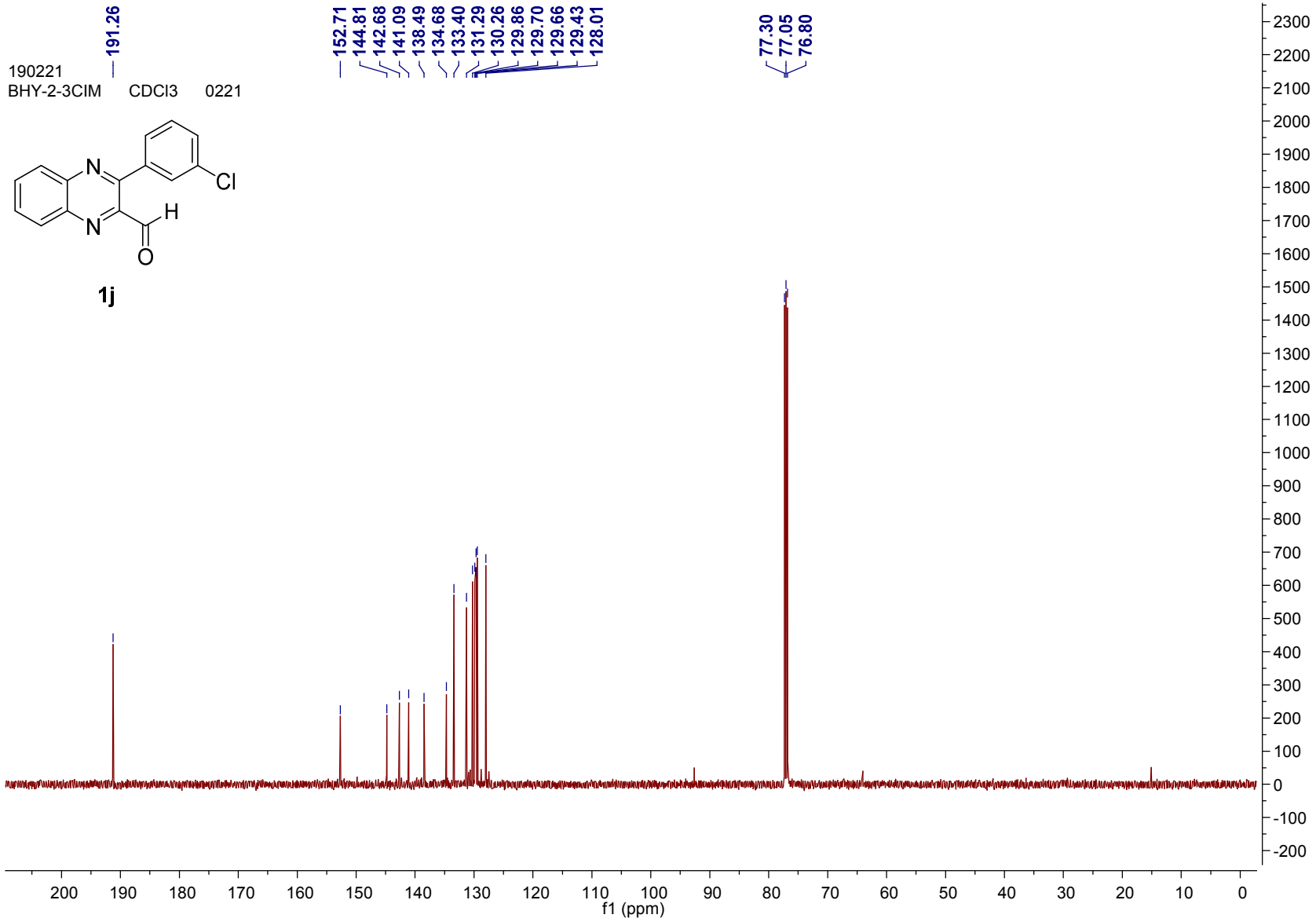

190221
BHY-2-4OBNM CDCl3 0221
10.335
8.306 8.304 8.289 8.287 8.197 8.196 8.181 8.179 7.914 7.844 7.710 7.706 7.696 7.692 7.490 7.475 7.437 7.423 7.407 7.375 7.361 7.175 7.171 7.162 7.158
OBn
N
N
H
O
1h
0.99 1.00 1.03 1.05 1.07 2.08 2.17 2.20 1.10 2.15 2.13
f1 (ppm)

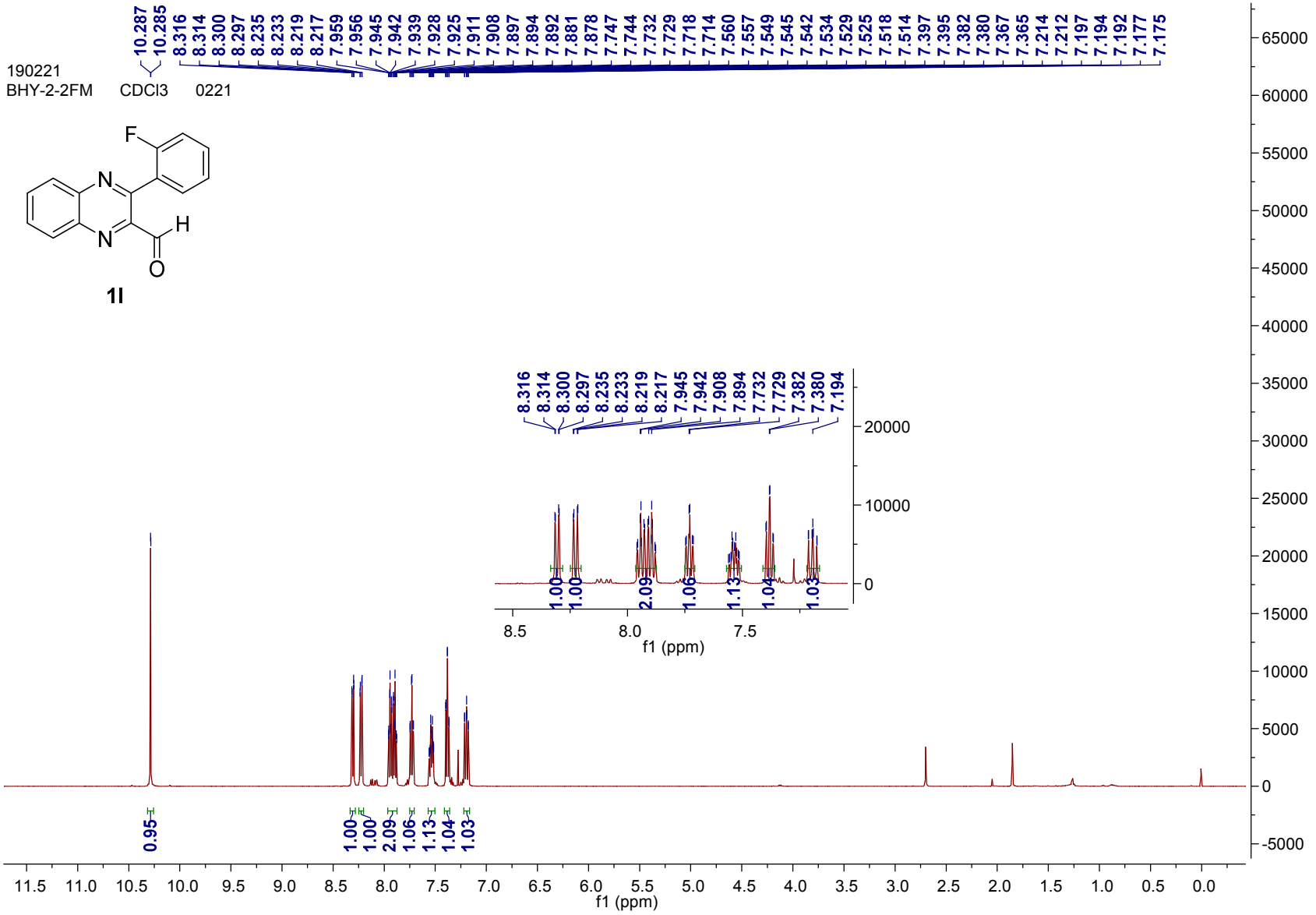

191.50
160.37
153.99
142.89
140.78
136.54
133.01
131.55
130.62
130.30
129.25
128.69
128.16
77.35
77.10
76.84
70.14
190221
BHY-2-4OBNM CDCl3 0221
OBn
N
N
H
O
1h
4000
3500
3000
2500
2000
1500
1000
500
0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

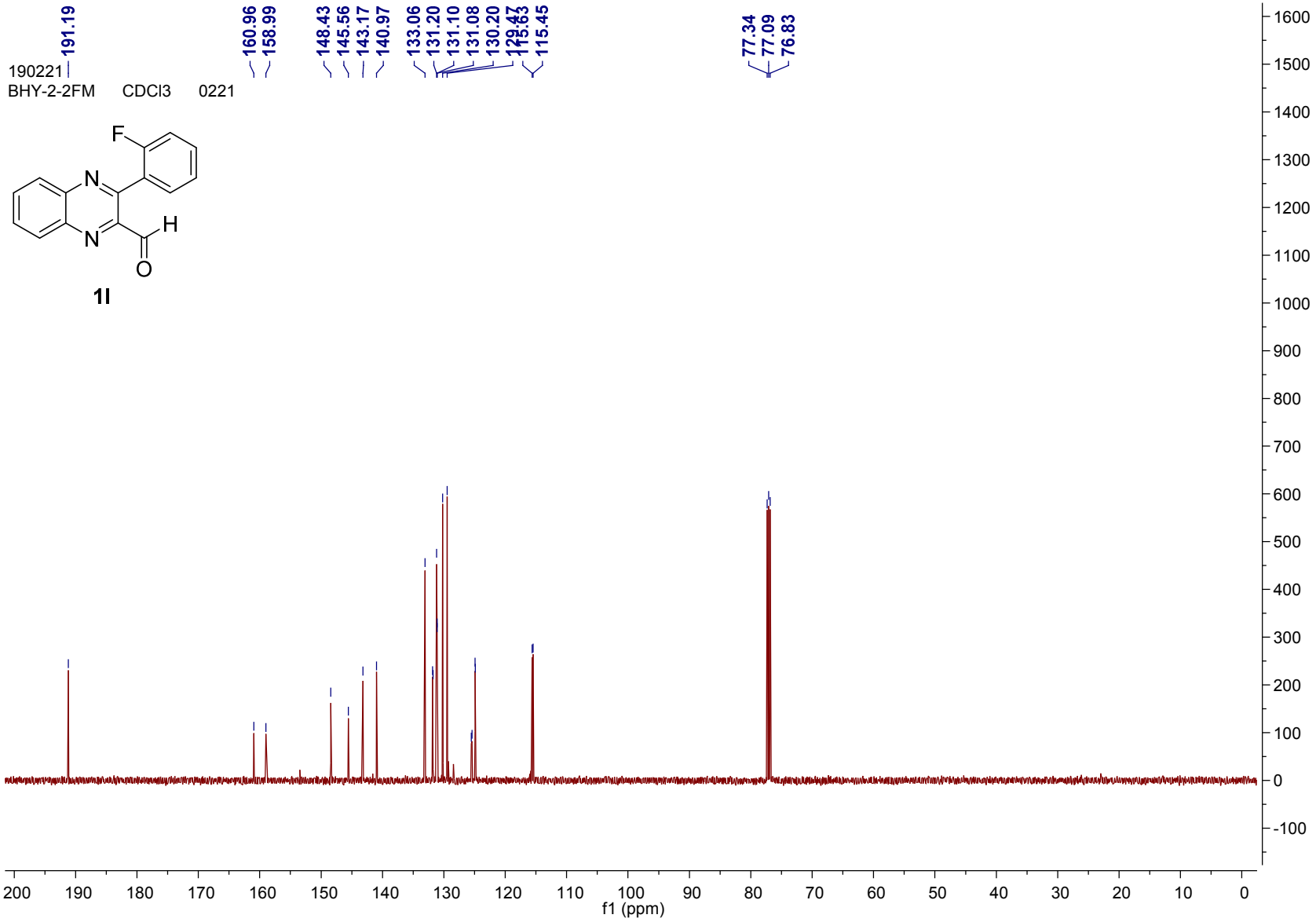

190221
BHY-2-3BRM CDCl3 0221
10.322
8.331
8.329
8.314
8.312
8.232
8.230
8.215
8.213
7.990
7.987
7.976
7.973
7.971
7.960
7.957
7.931
7.928
7.917
7.915
7.912
7.900
7.897
7.893
7.698
7.696
7.694
7.692
7.682
7.680
7.678
7.676
7.597
7.595
7.592
7.581
7.579
7.576
7.436
7.420
7.404
7.276
N
N
Br
H
O
1i
0.98
1.00
1.00
1.05
2.00
1.01
1.01
1.07
f1 (ppm)

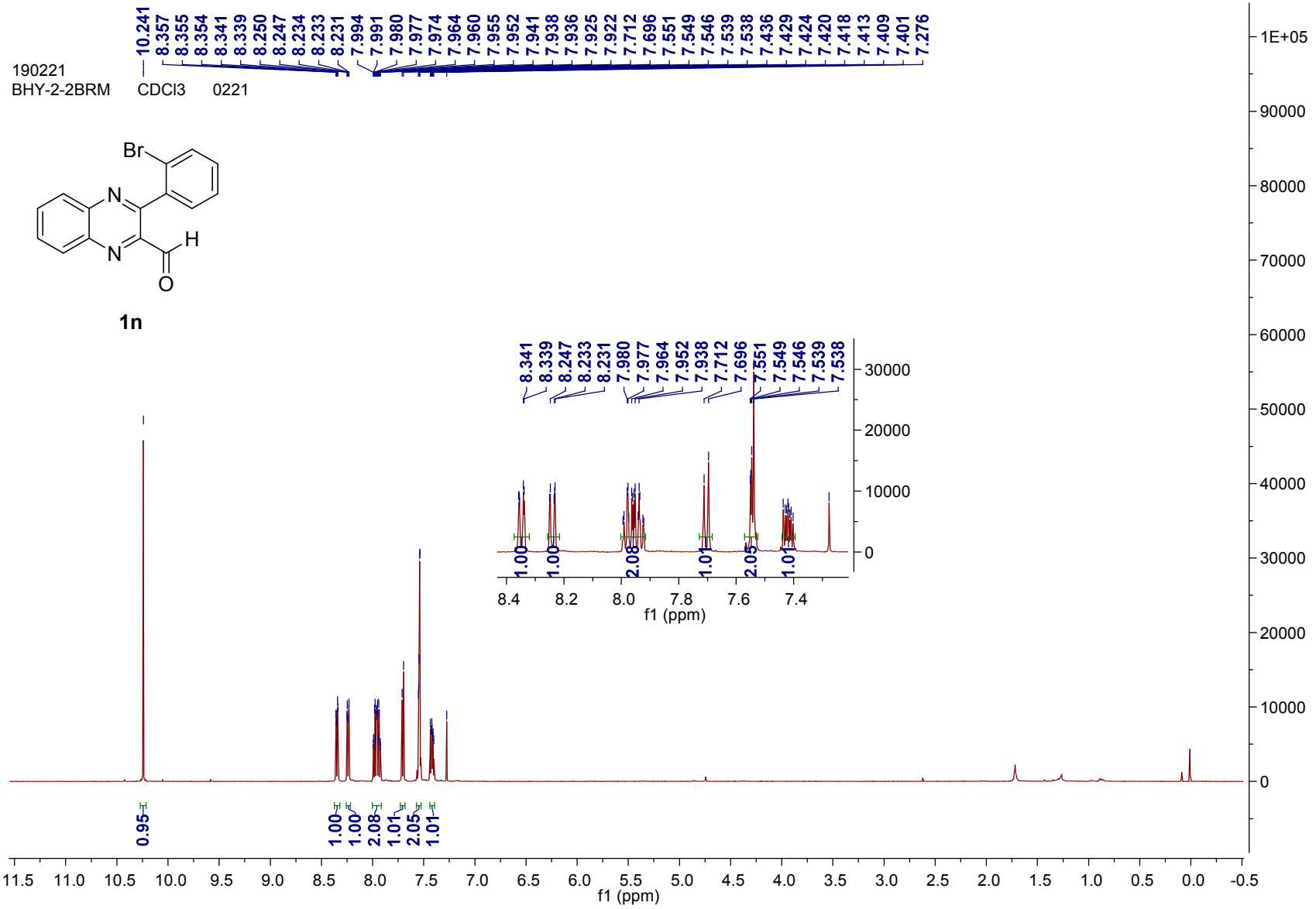

191.26
152.58
144.79
142.68
141.09
138.72
133.41
132.76
132.50
131.30
130.25
129.91
129.44
128.47
122.73
77.30
77.05
76.79
190221
BHY-2-3BRM CDCl3 0221
N
N
Br
H
O
1i
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

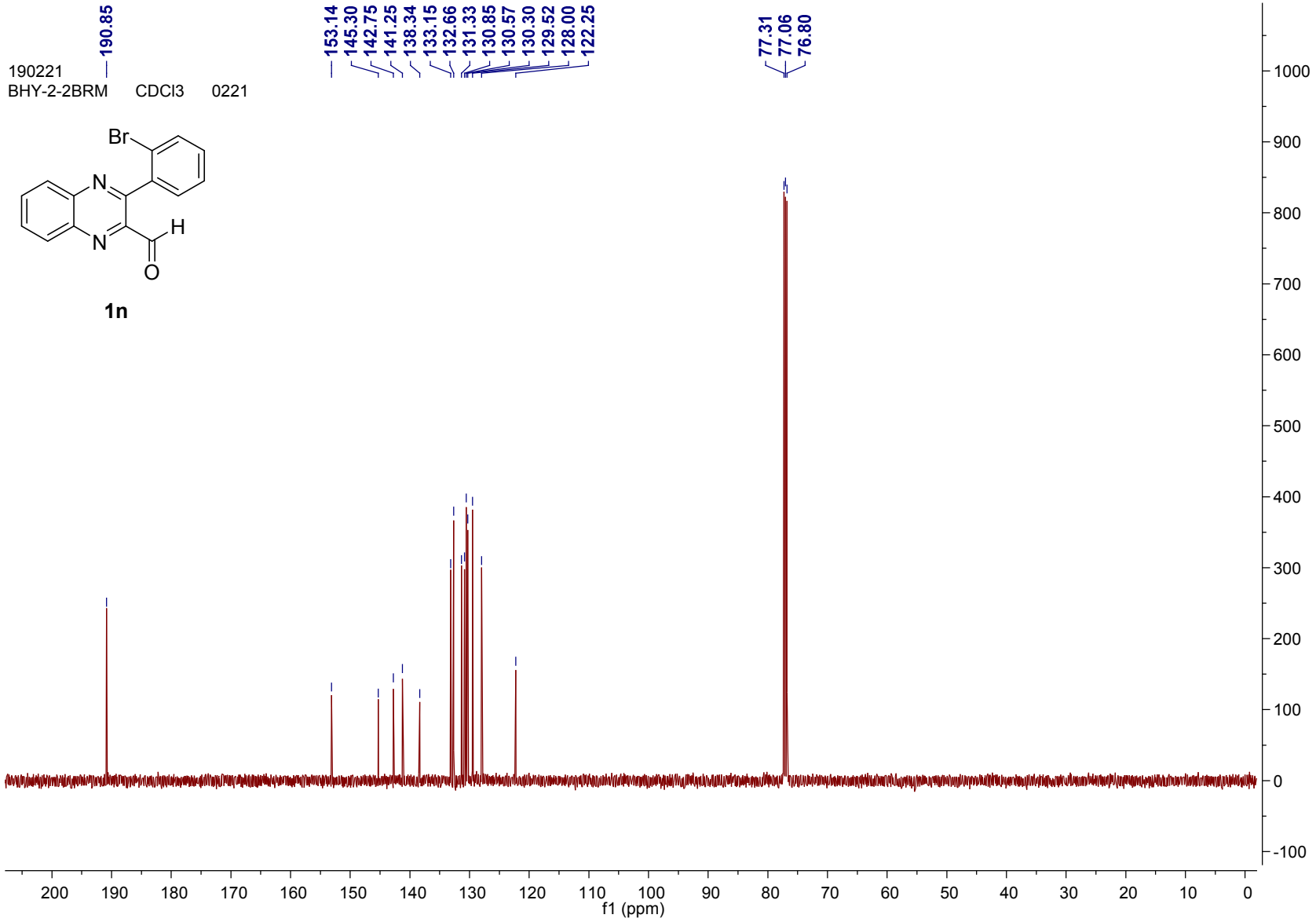

10.321
8.332
8.330
8.315
8.313
8.231
8.229
8.215
8.212
7.989
7.986
7.975
7.972
7.969
7.959
7.956
7.931
7.928
7.917
7.914
7.911
7.900
7.897
7.740
7.736
7.732
7.547
7.544
7.541
7.537
7.530
7.527
7.523
7.495
7.484
7.481
7.479
7.465
7.266
190227
BHY-2--CLM CDCl3 0227
N
N
Cl
H
O
1j
0.91
1.00
1.06
1.05
1.09
0.92
3.25
f1 (ppm)

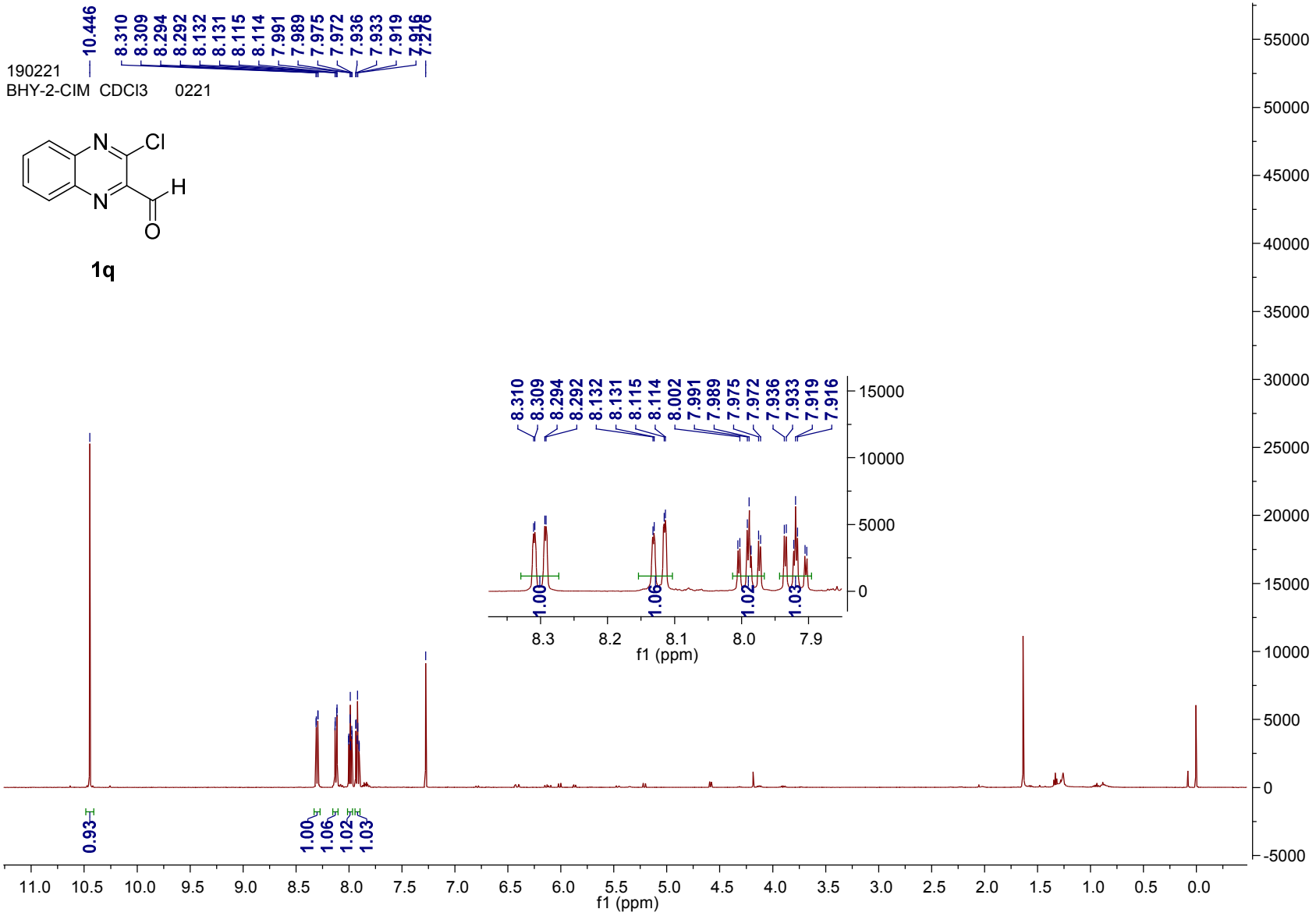

191.26
152.71
144.81
142.68
141.09
138.49
134.68
133.40
131.29
130.26
129.86
129.70
129.66
129.43
128.01
77.30
77.05
76.80
190221
BHY-2-3CIM CDCl3 0221
N
N
Cl
H
O
1j
f1 (ppm)

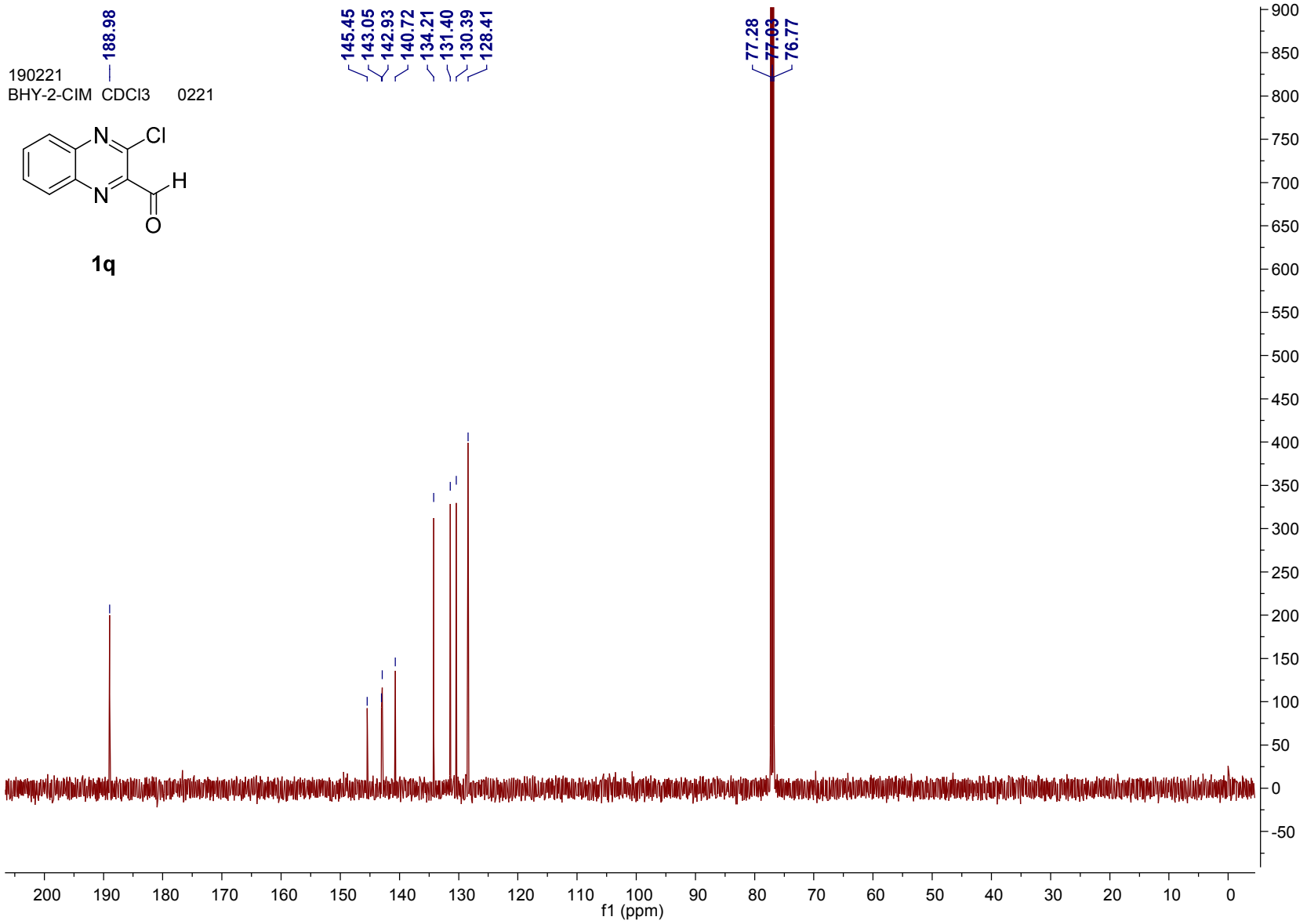

190221
BHY-2-2FM CDCl3 0221
10.287 10.285 8.316 8.314 8.300 8.297 8.235 8.233 8.219 8.217 7.959 7.956 7.945 7.942 7.939 7.928 7.925 7.911 7.908 7.897 7.894 7.892 7.881 7.878 7.747 7.744 7.732 7.729 7.718 7.714 7.560 7.557 7.549 7.545 7.542 7.534 7.529 7.525 7.518 7.514 7.397 7.395 7.382 7.380 7.367 7.365 7.214 7.212 7.197 7.194 7.192 7.177 7.175
F
N
N
H
O
1l
8.316 8.314 8.300 8.297 8.235 8.233 8.219 8.217 7.945 7.942 7.908 7.894 7.732 7.729 7.382 7.380 7.194
1.00 1.00 2.09 1.06 1.13 1.04 1.03
8.5 8.0 7.5
f1 (ppm)
0.95 1.00 1.00 2.09 1.06 1.13 1.04 1.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

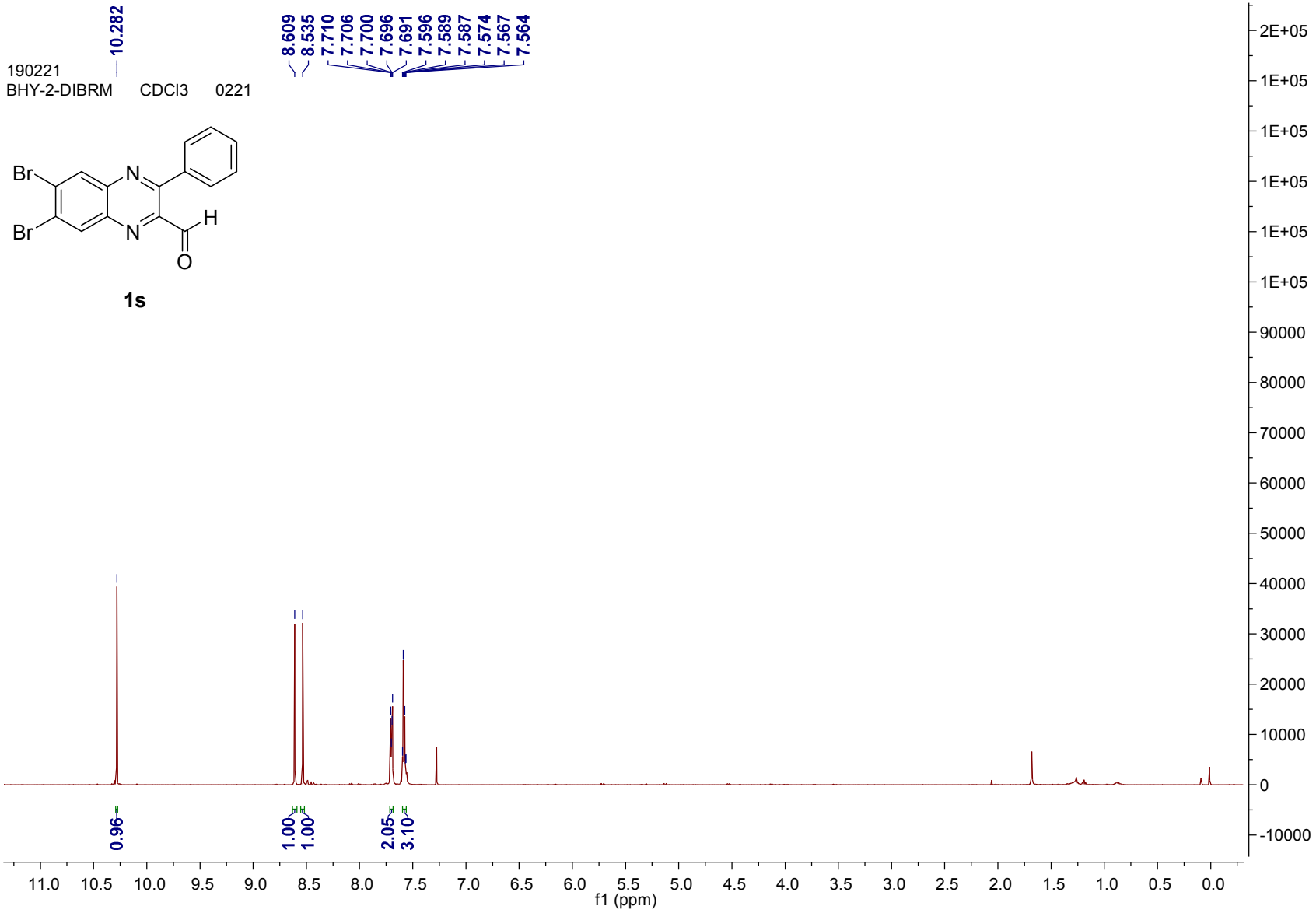

191.19
160.96
158.99
148.43
145.56
143.17
140.97
133.06
131.20
131.10
131.08
130.20
129.47
115.83
115.45
77.34
77.09
76.83
190221
BHY-2-2FM CDCl3 0221
F
N
N
H
O
1l
f1 (ppm)

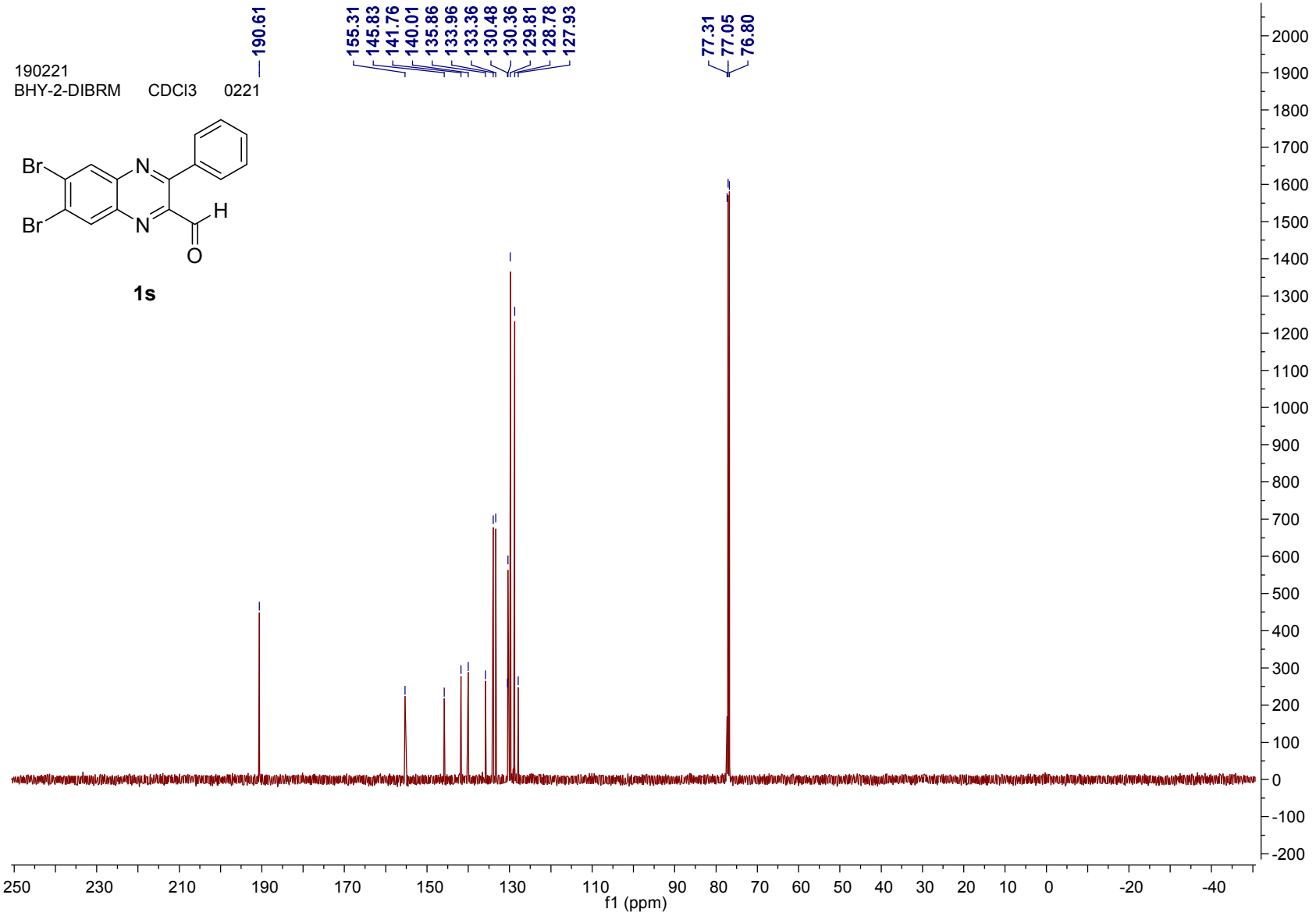

190221
BHY-2-2BRM CDCl3 0221
10.241 8.357 8.355 8.354 8.341 8.339 8.250 8.247 8.234 8.233 8.231 7.994 7.991 7.980 7.977 7.974 7.964 7.960 7.955 7.952 7.941 7.938 7.936 7.925 7.922 7.712 7.696 7.551 7.549 7.546 7.539 7.538 7.436 7.429 7.424 7.420 7.418 7.413 7.409 7.401 7.276
Br
N
N
H
O
1n
0.95 1.00 1.00 2.08 1.01 2.05 1.01
f1 (ppm)

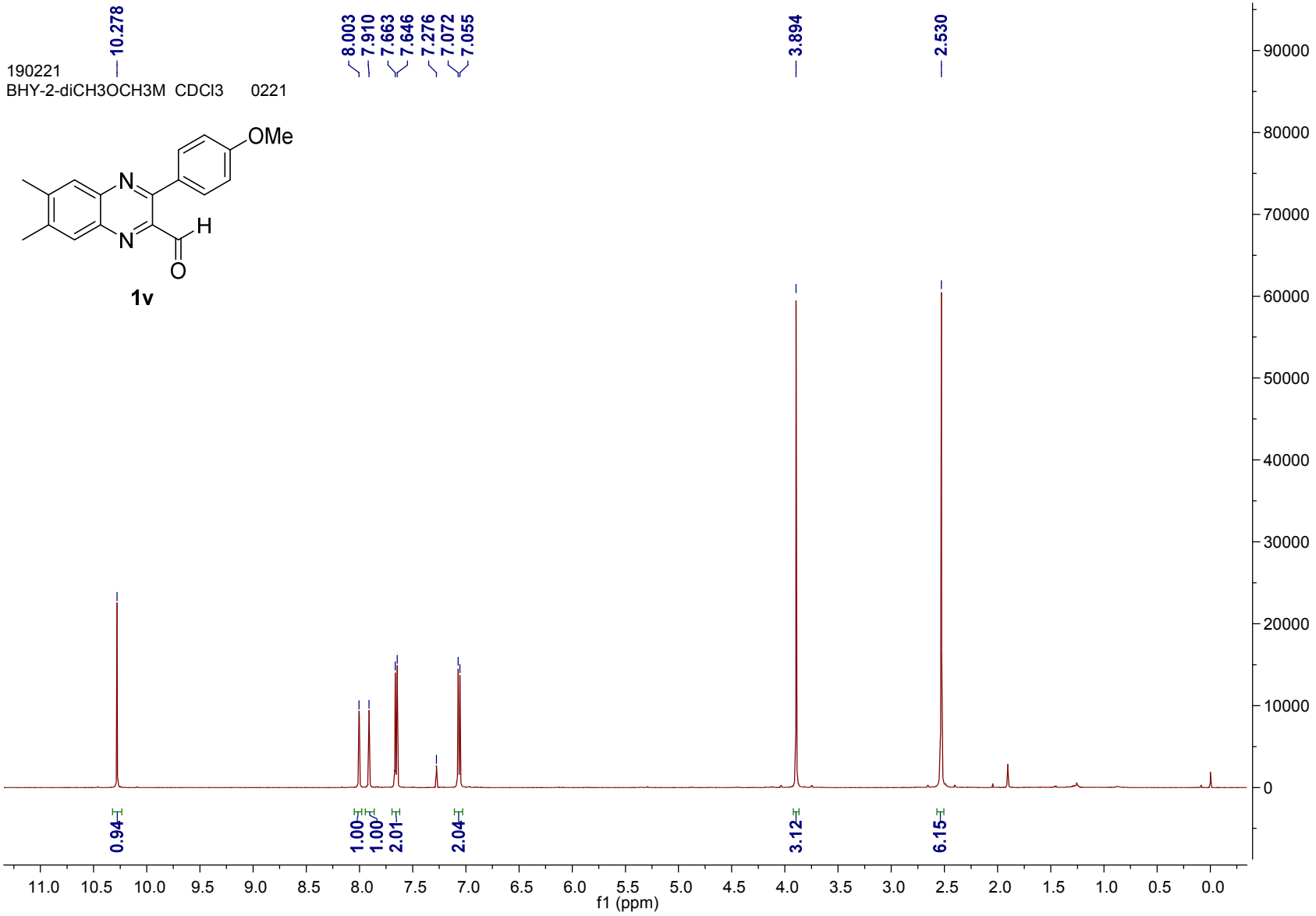

190.85
153.14
145.30
142.75
141.25
138.34
133.15
132.66
131.33
130.85
130.57
130.30
129.52
128.00
122.25
77.31
77.06
76.80
190221
BHY-2-2BRM CDCl3 0221
Br
N
N
H
O
1n
1000
900
800
700
600
500
400
300
200
100
0
-100
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

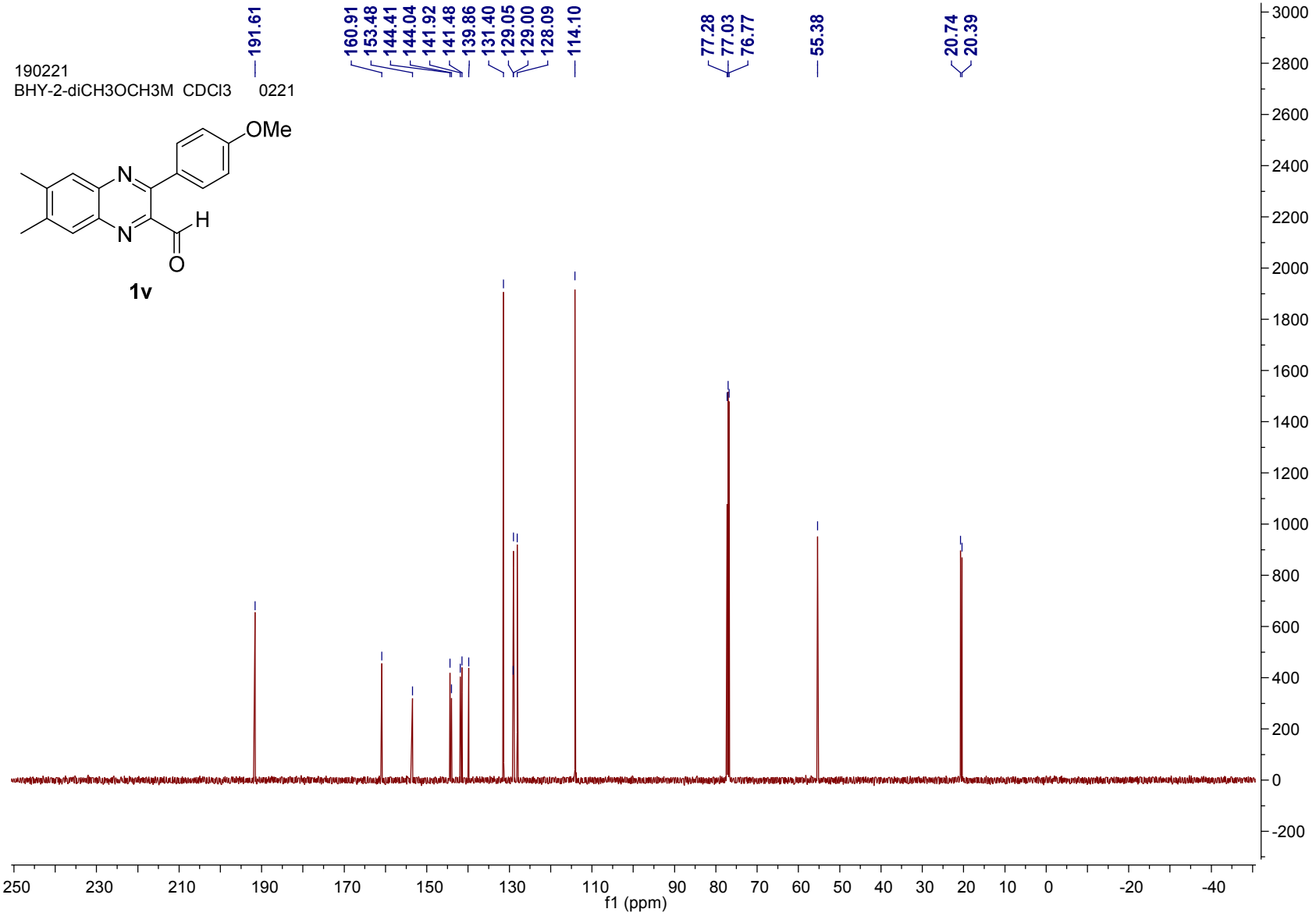

190221
BHY-2-CIM CDCl3 0221
10.446
8.310
8.309
8.294
8.292
8.132
8.131
8.115
8.114
7.991
7.989
7.975
7.972
7.936
7.933
7.919
7.916
7.276
N
Cl
N
H
O
1q
0.93
1.00
1.06
1.02
1.03
f1 (ppm)
8.002
1.00
1.06
1.02
1.03
f1 (ppm)

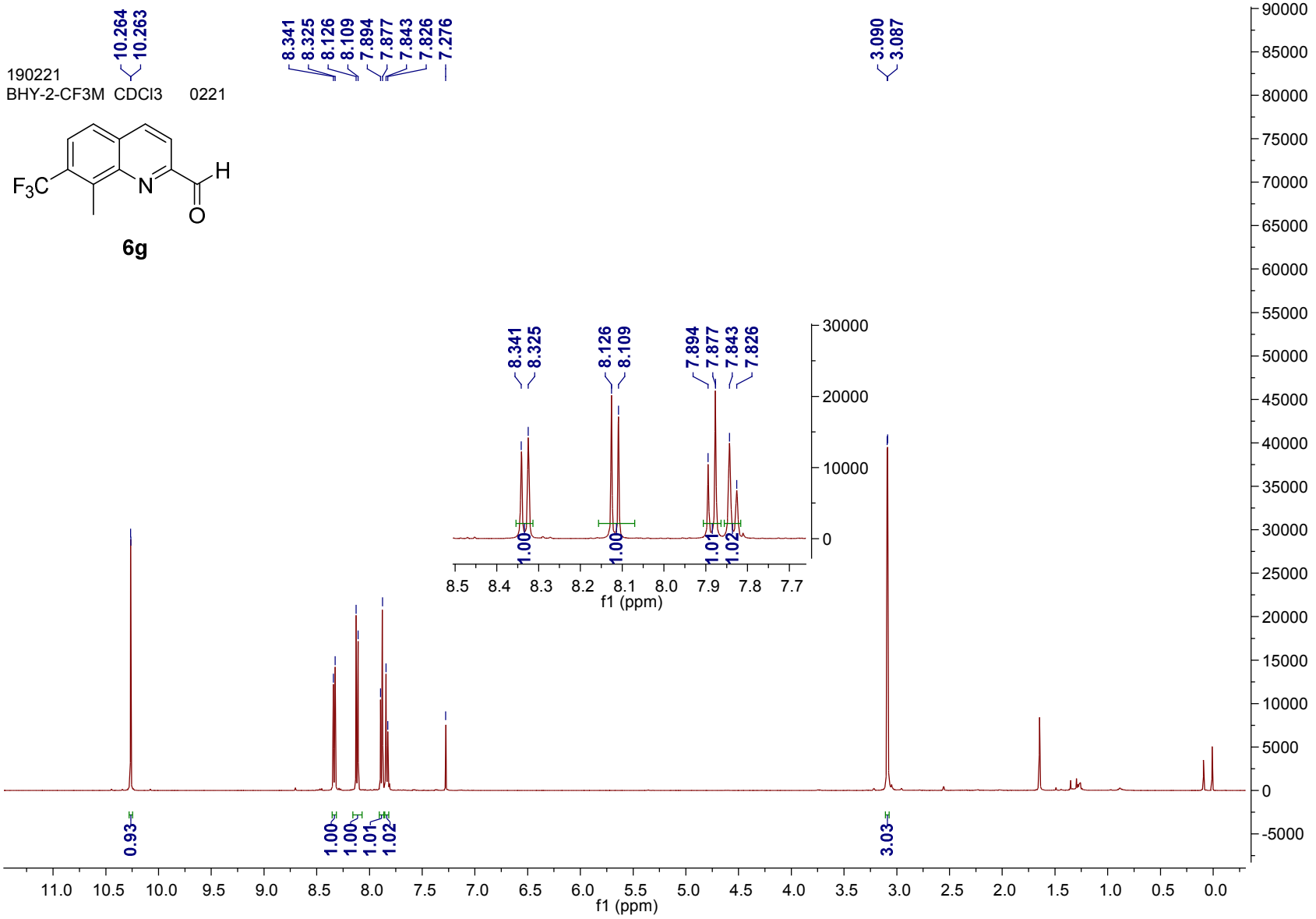

190221
BHY-2-CIM CDCl3 0221
188.98
145.45
143.05
142.93
140.72
134.21
131.40
130.39
128.41
77.28
77.03
76.77
N
Cl
H
N
O
1q
f1 (ppm)

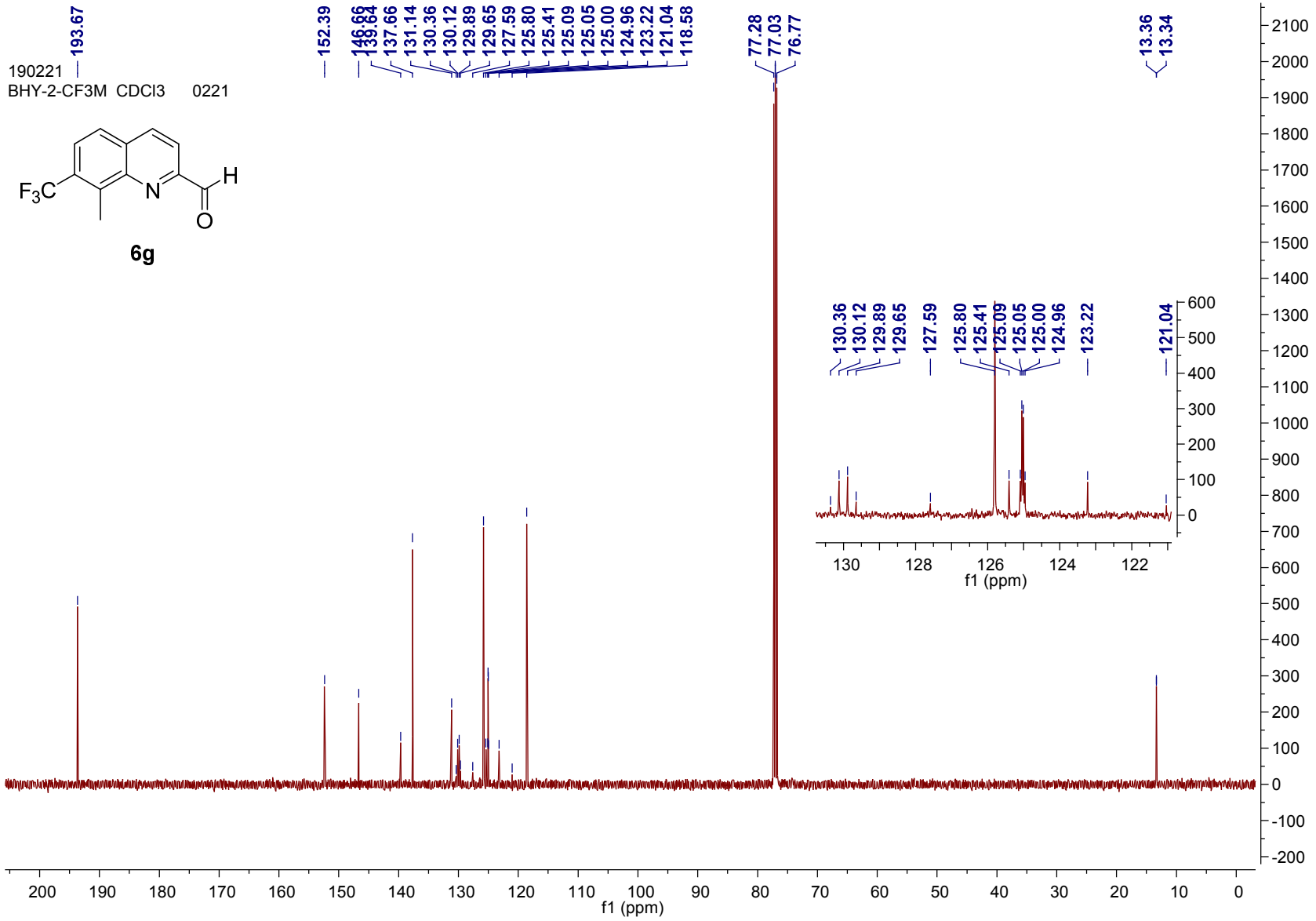

190221
BHY-2-DIBRM CDCl3 0221
10.282
8.609
8.535
7.710
7.706
7.700
7.696
7.691
7.596
7.589
7.587
7.574
7.567
7.564
Br
Br
N
N
H
O
1s
0.96
1.00
1.00
2.05
3.10
f1 (ppm)

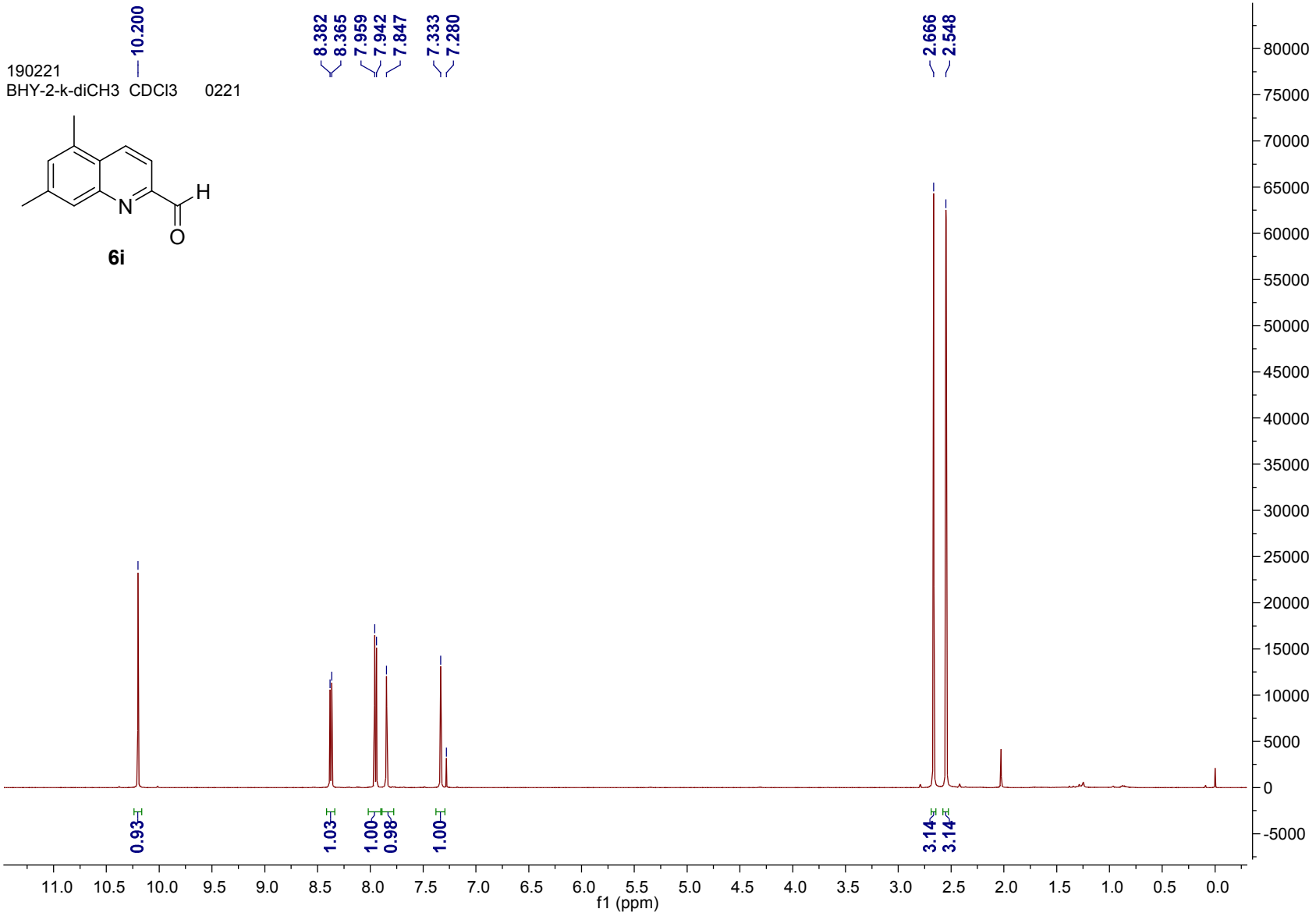

190221
BHY-2-DIBRM CDCl3 0221
190.61
155.31
145.83
141.76
140.01
135.86
133.96
133.36
130.48
130.36
129.81
128.78
127.93
77.31
77.05
76.80
Br
Br
N
N
H
O
1s
f1 (ppm)

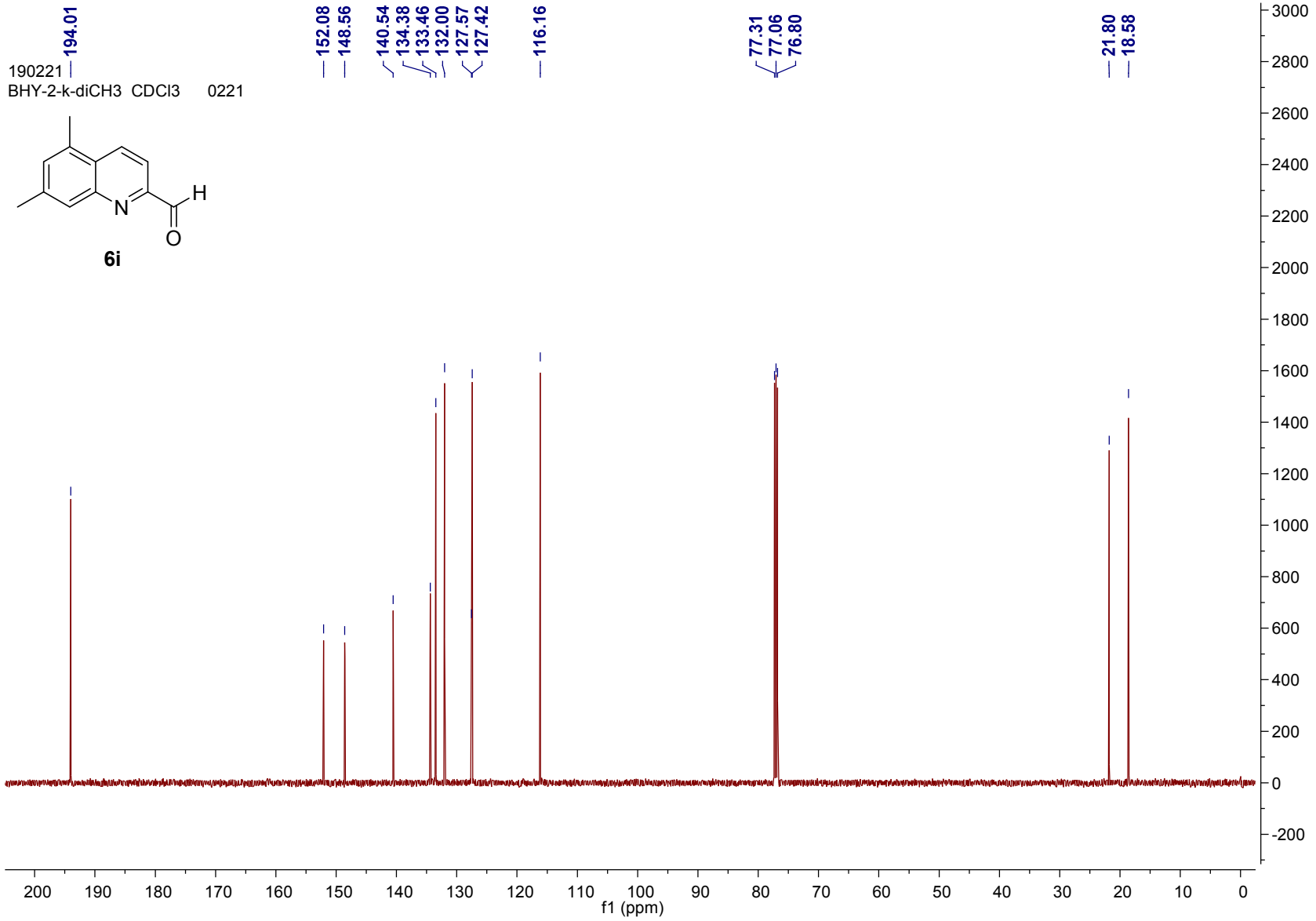

190221
BHY-2-diCH3OCH3M CDCl3 0221
10.278
8.003
7.910
7.663
7.646
7.276
7.072
7.055
3.894
2.530
OMe
N
N
H
O
1v
0.94
1.00
1.00
2.01
2.04
3.12
6.15
f1 (ppm)

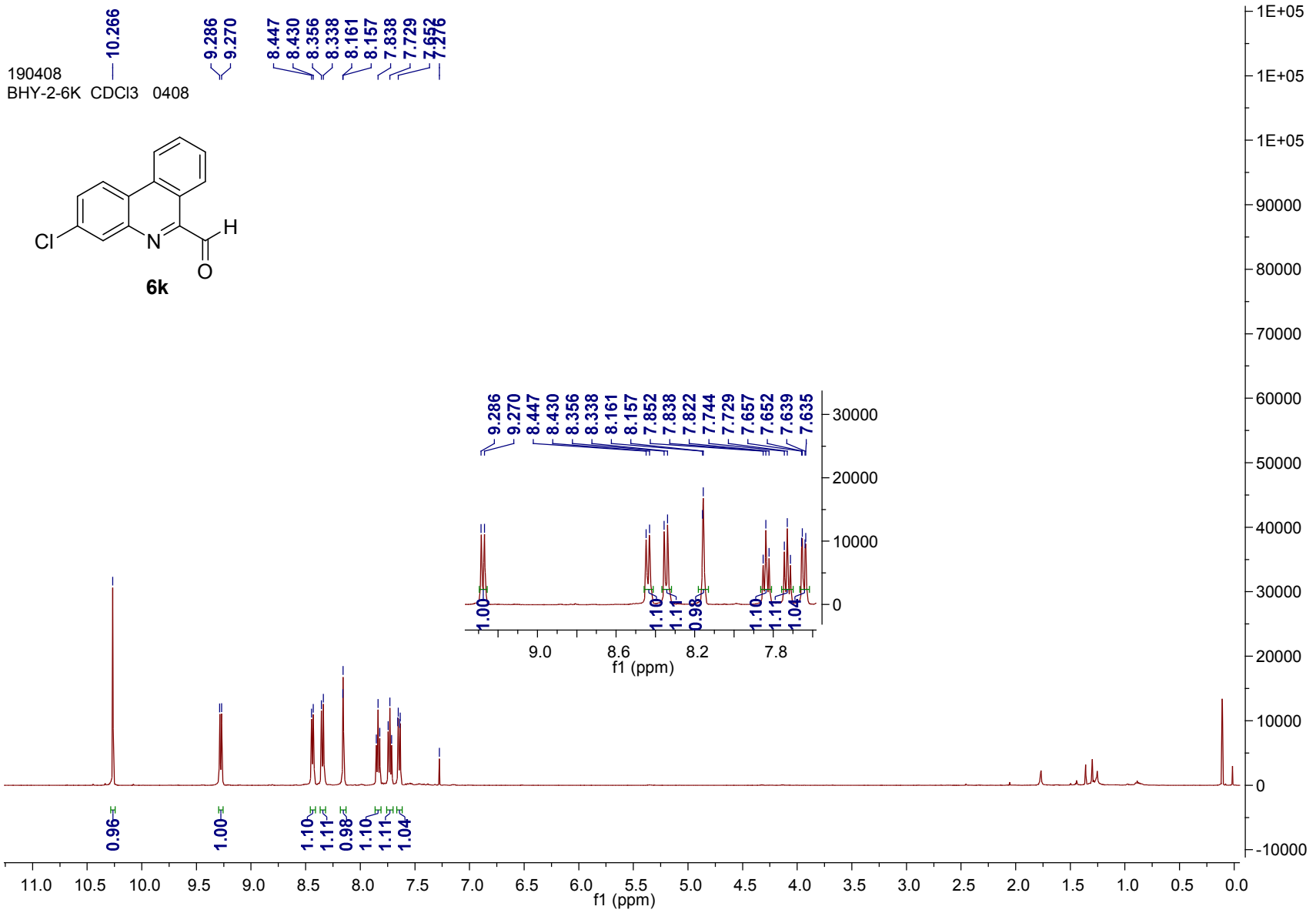

191.61
160.91
153.48
144.41
144.04
141.92
141.48
139.86
131.40
129.05
129.00
128.09
114.10
77.28
77.03
76.77
55.38
20.74
20.39
190221
BHY-2-diCH3OCH3M CDCl3 0221
OMe
N
N
H
O
1v
f1 (ppm)

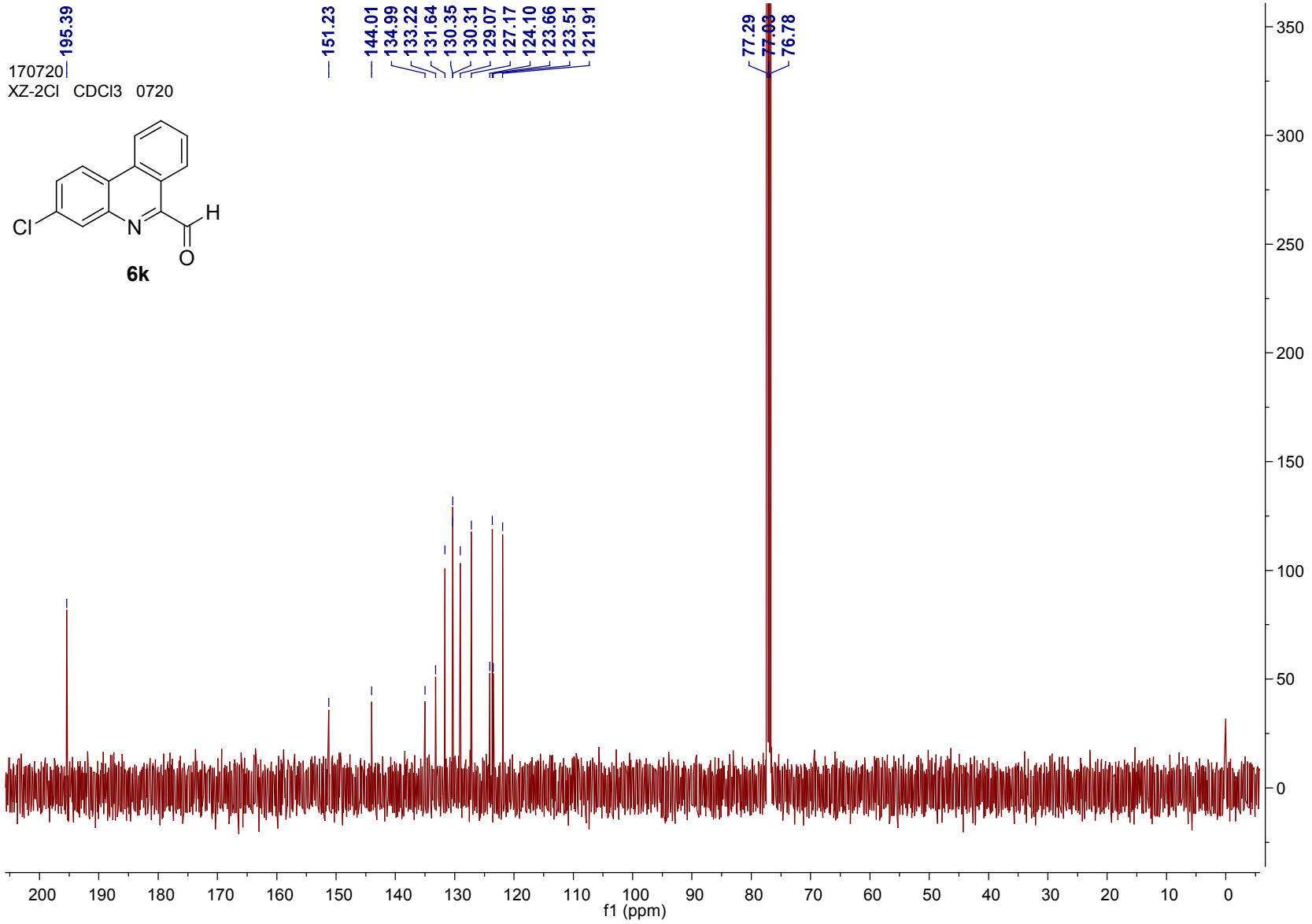

190221
BHY-2-CF3M CDCl3 0221
10.264
10.263
8.341
8.325
8.126
8.109
7.894
7.877
7.843
7.826
7.276
3.090
3.087
F3C
N
H
O
6g
0.93
1.00
1.00
1.01
1.02
3.03
f1 (ppm)

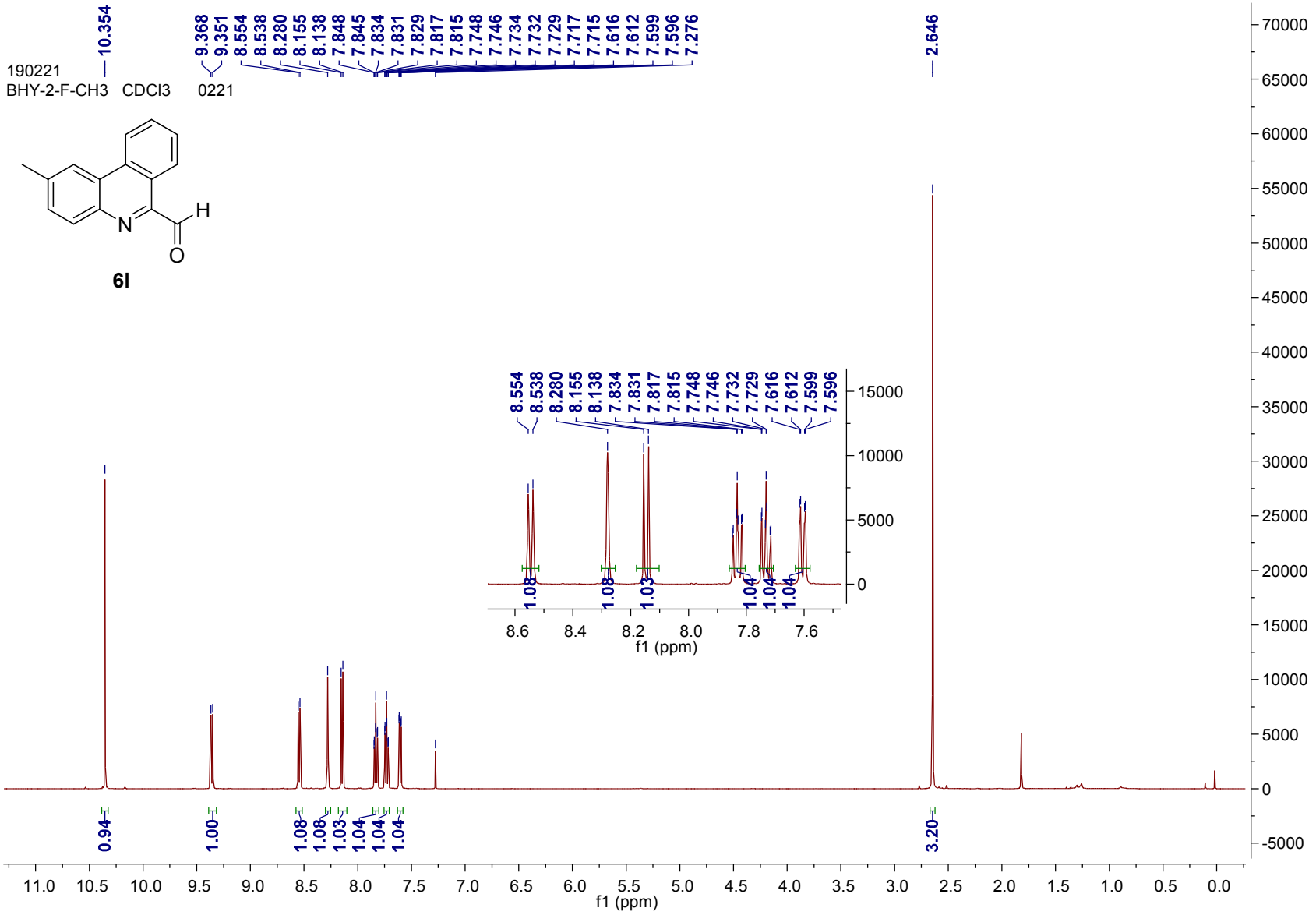

190221
BHY-2-CF3M CDCl3 0221
193.67
152.39
146.66
139.64
137.66
131.14
130.36
130.12
129.89
129.65
127.59
125.80
125.41
125.09
125.05
125.00
124.96
123.22
121.04
118.58
77.28
77.03
76.77
13.36
13.34
F3C
N
O
H
6g
f1 (ppm)

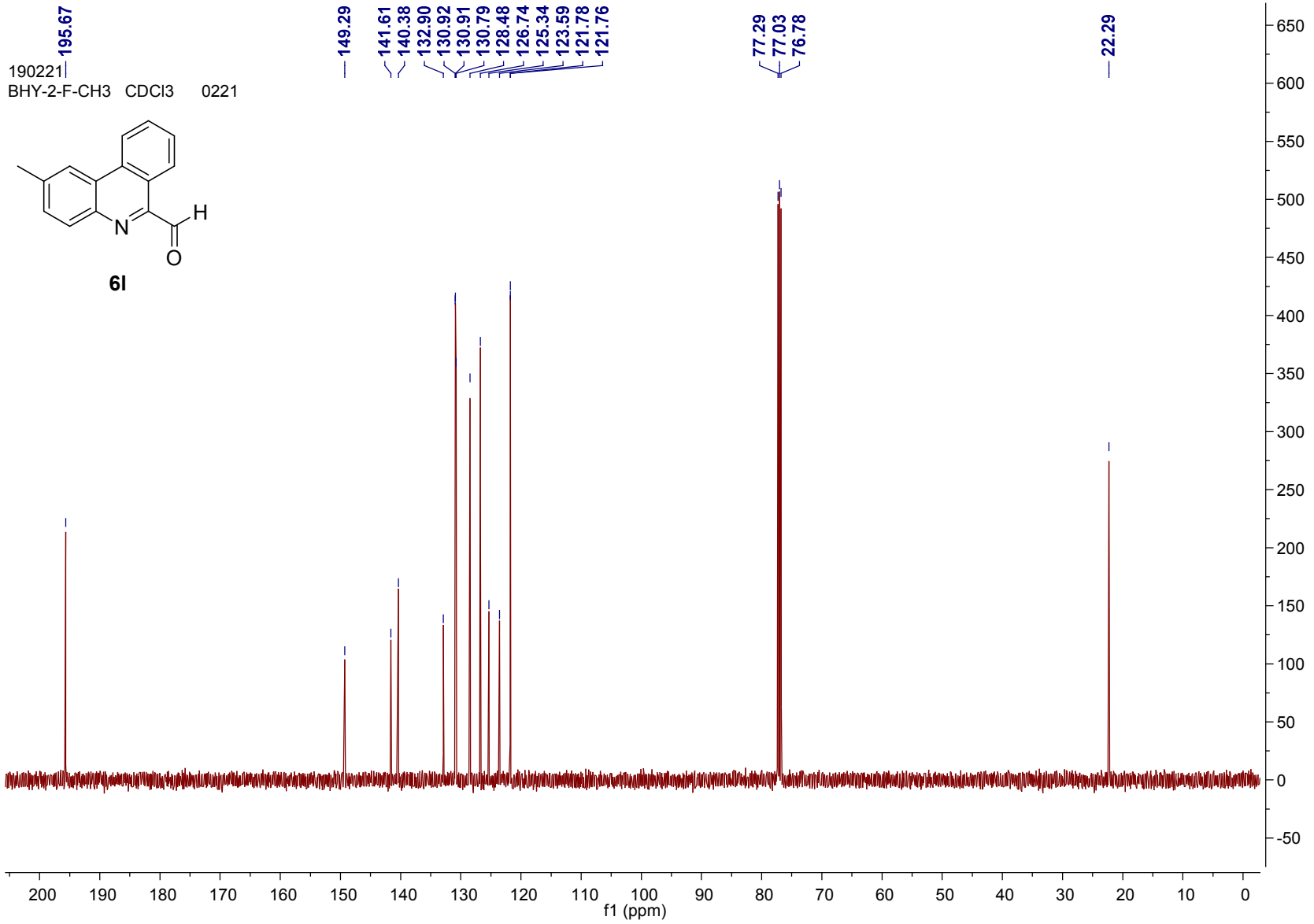

190221
BHY-2-k-diCH3 CDCl3 0221
10.200
8.382
8.365
7.959
7.942
7.847
7.333
7.280
2.666
2.548
N
H
O
6i
0.93
1.03
1.00
0.98
1.00
3.14
3.14
f1 (ppm)

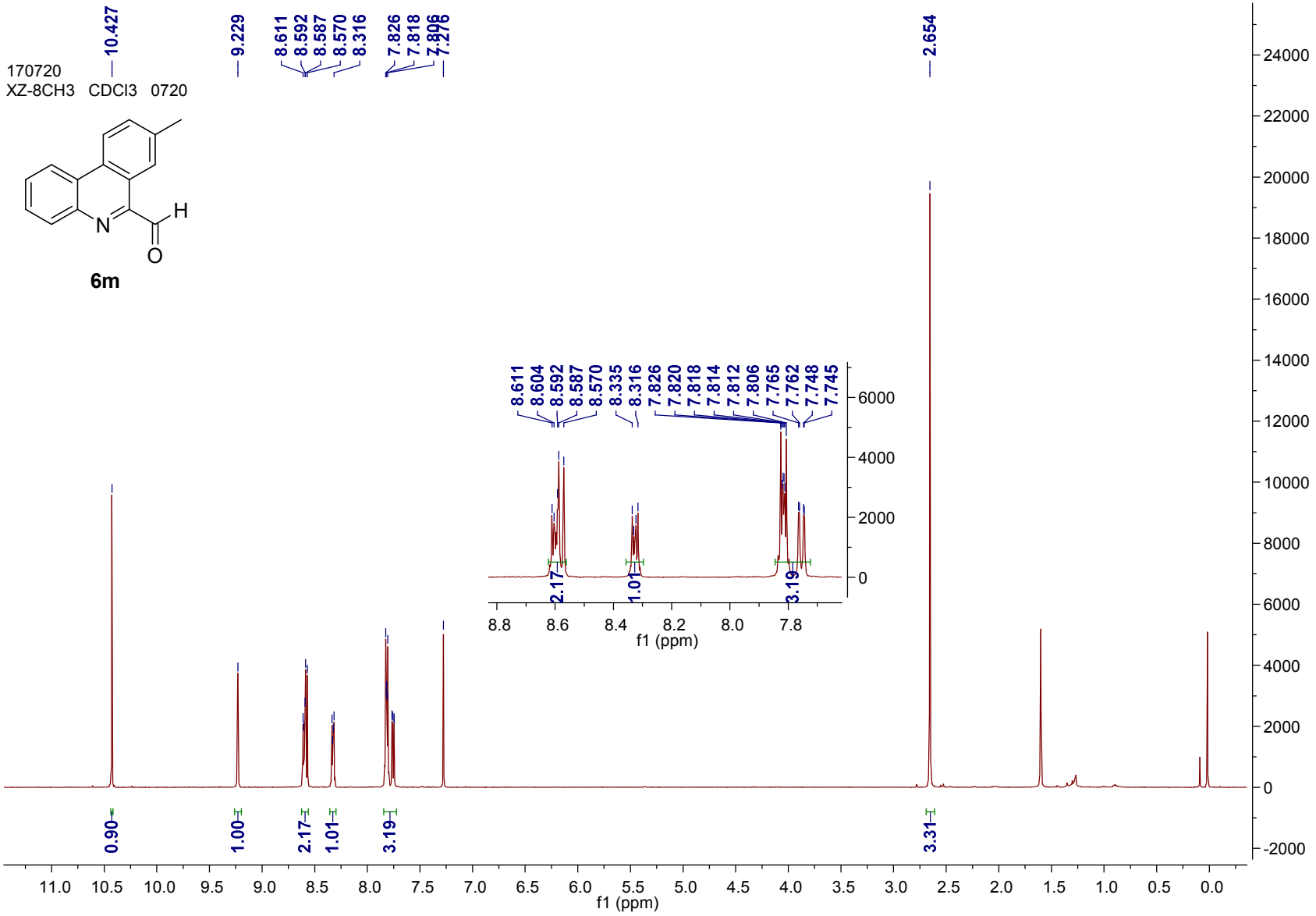

194.01
152.08
148.56
140.54
134.38
133.46
132.00
127.57
127.42
116.16
77.31
77.06
76.80
21.80
18.58
190221
BHY-2-k-diCH3 CDCl3 0221
N
H
O
6i
f1 (ppm)

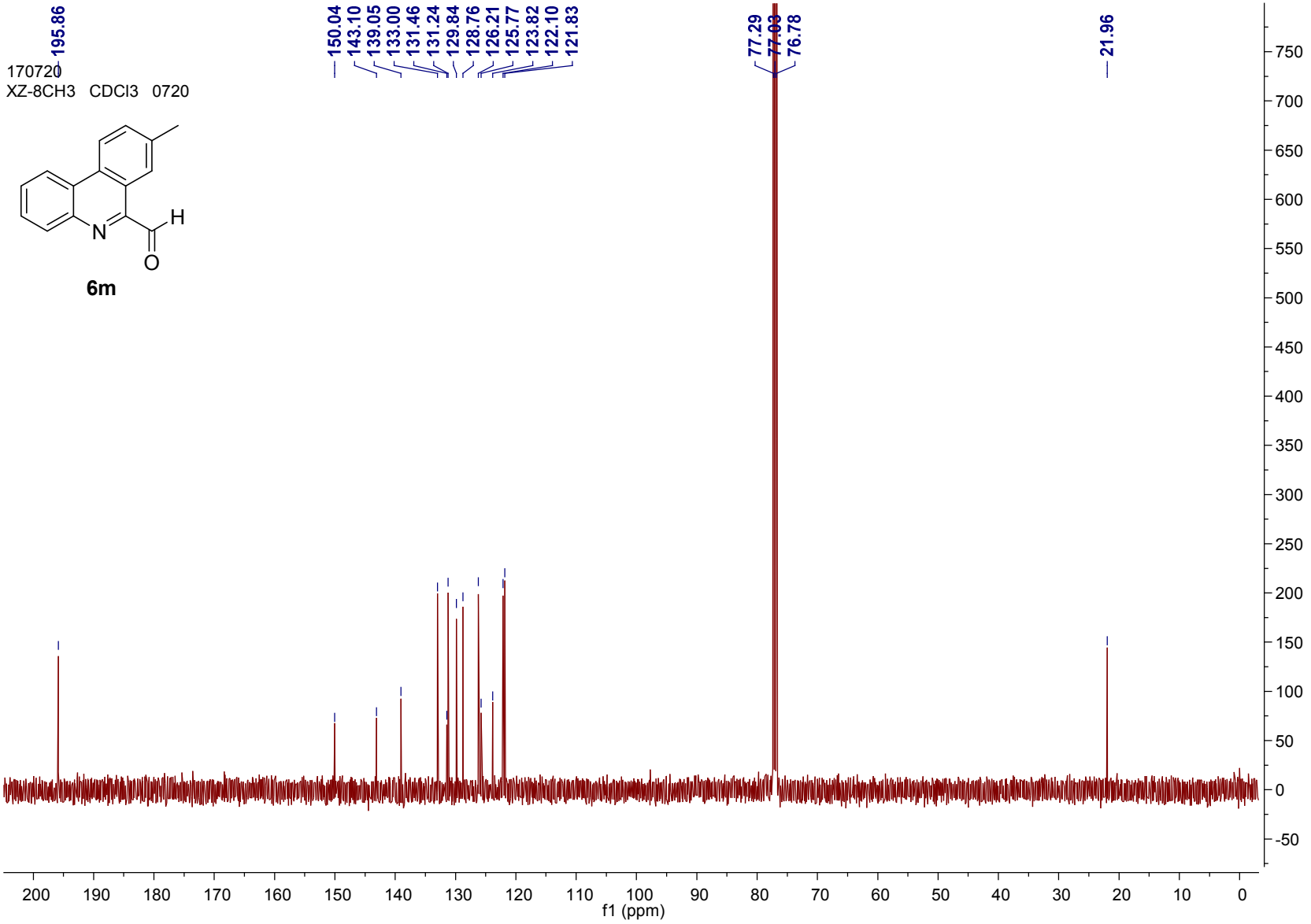

190408
BHY-2-6K CDCl3 0408
10.266
9.286
9.270
8.447
8.430
8.356
8.338
8.161
8.157
7.838
7.729
7.657
7.652
7.276
Cl
N
H
O
6k
9.286
9.270
8.447
8.430
8.356
8.338
8.161
8.157
7.852
7.838
7.822
7.744
7.729
7.657
7.652
7.639
7.635
1.00
1.10
1.11
0.98
1.10
1.11
1.04
f1 (ppm)
0.96
1.00
1.10
1.11
0.98
1.10
1.11
1.04
f1 (ppm)


195.39
151.23
144.01
134.99
133.22
131.64
130.35
130.31
129.07
127.17
124.10
123.66
123.51
121.91
77.29
77.00
76.78
170720
XZ-2Cl CDCl3 0720
Cl
N
H
O
6k
350
300
250
200
150
100
50
0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

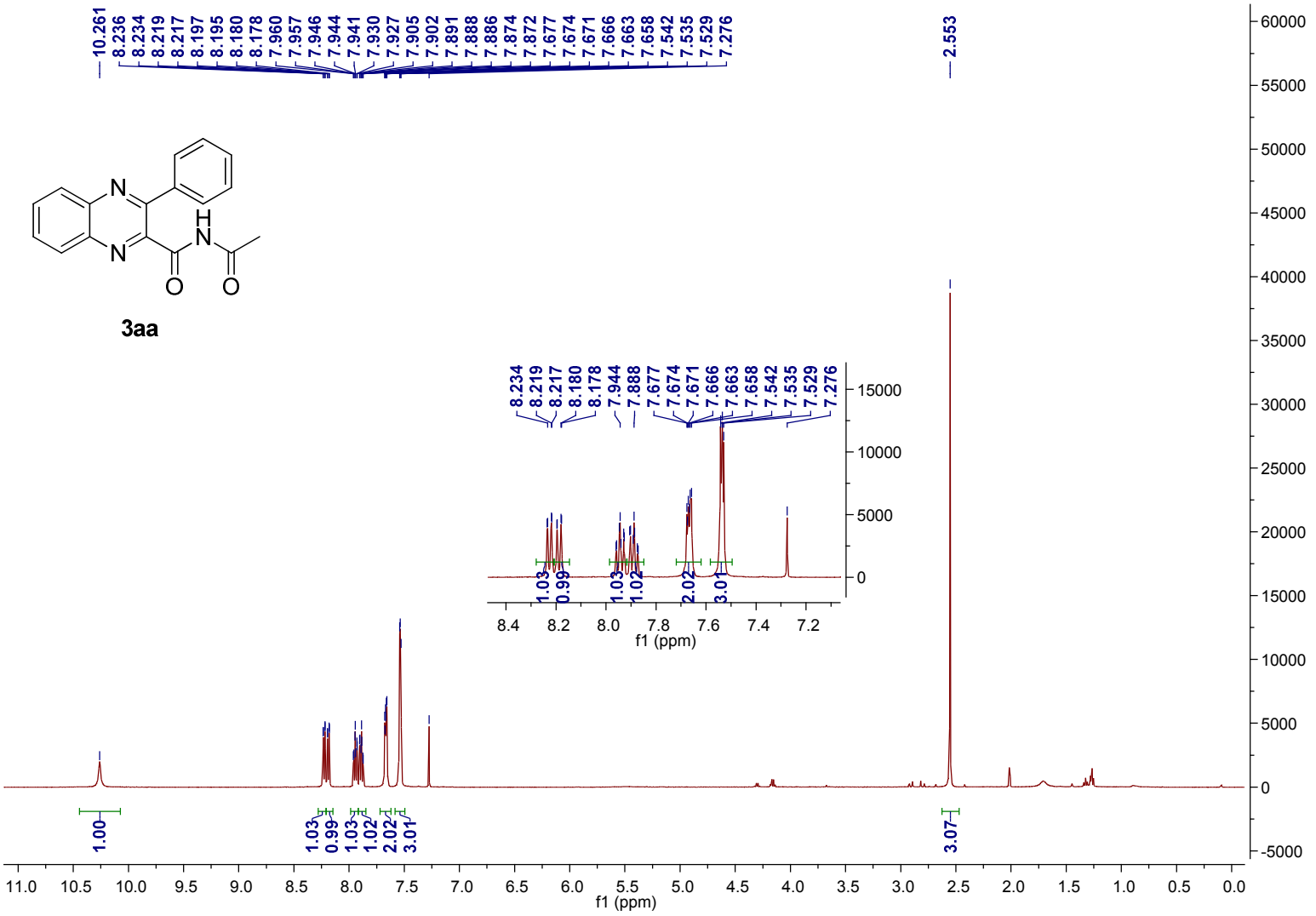

190221
BHY-2-F-CH3 CDCl3 0221
10.354
9.368
9.351
8.554
8.538
8.280
8.155
8.138
7.848
7.845
7.834
7.831
7.829
7.817
7.815
7.748
7.746
7.734
7.732
7.729
7.717
7.715
7.616
7.612
7.599
7.596
7.276
2.646
N
H
O
6l
0.94
1.00
1.08
1.08
1.03
1.04
1.04
1.04
3.20
f1 (ppm)

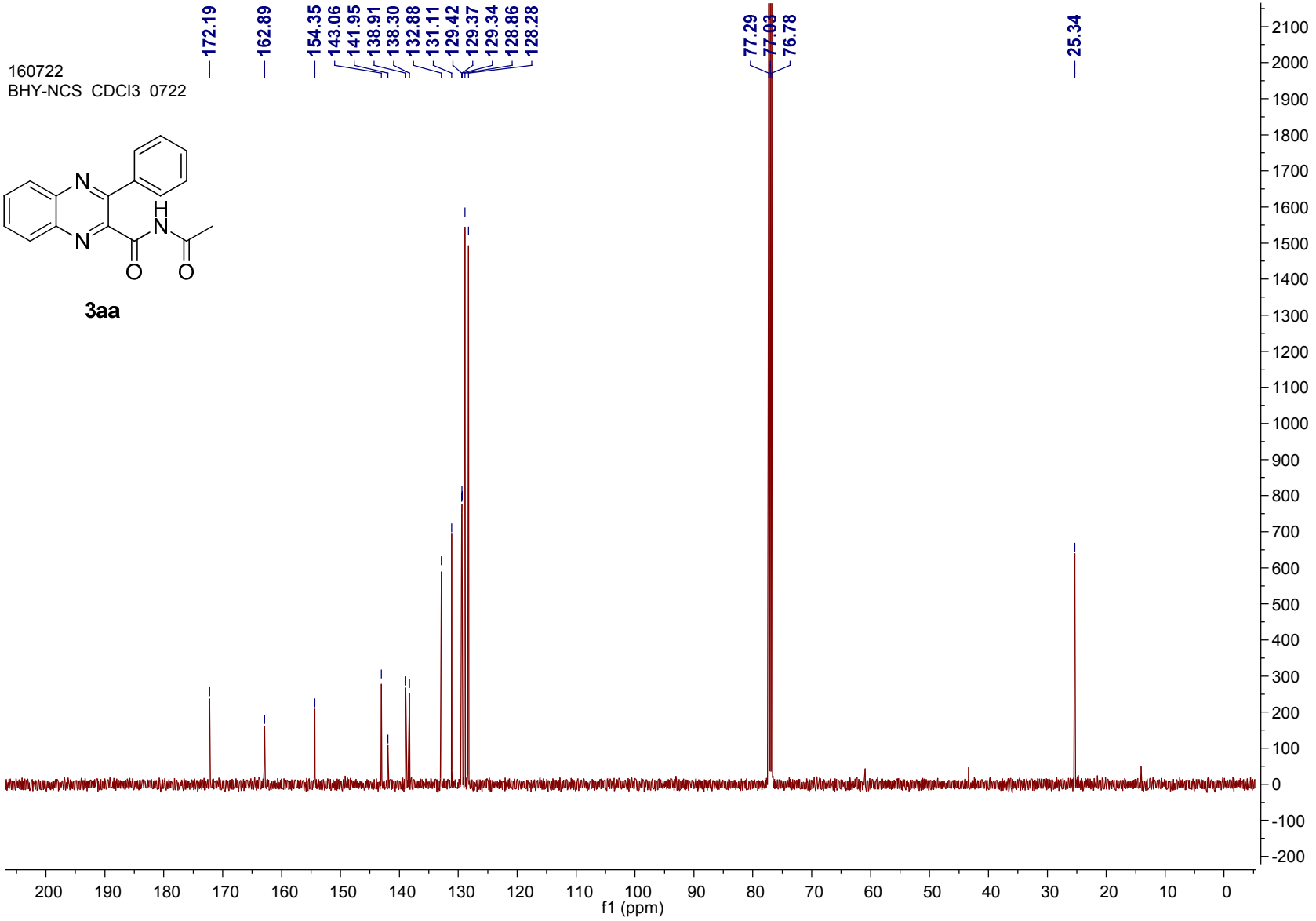

195.67
149.29
141.61
140.38
132.90
130.92
130.91
130.79
128.48
126.74
125.34
123.59
121.78
121.76
77.29
77.03
76.78
22.29
190221
BHY-2-F-CH3 CDCl3 0221
N
H
O
6l
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

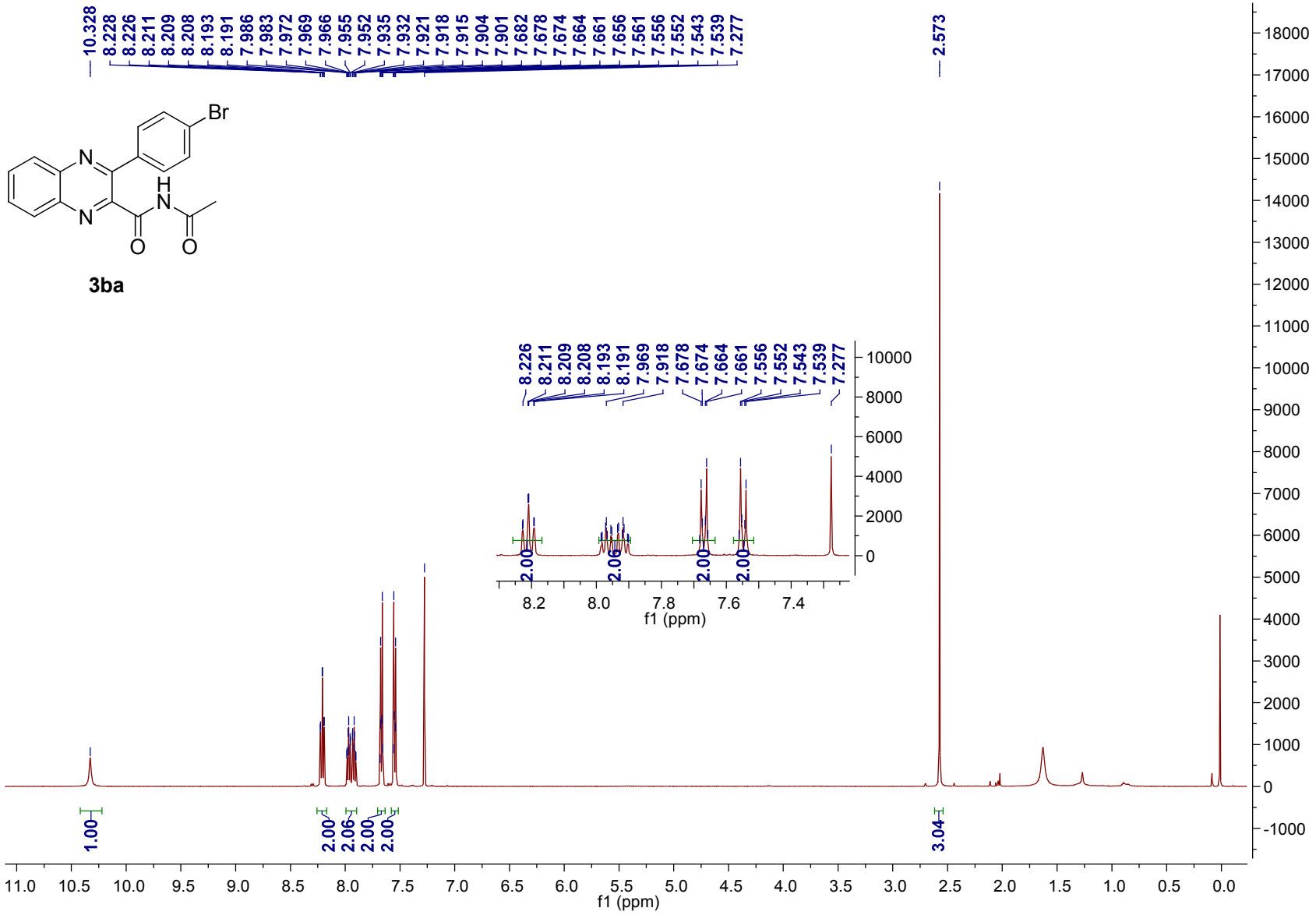

170720
XZ-8CH3 CDCl3 0720
10.427
9.229
8.611
8.592
8.587
8.570
8.316
7.826
7.818
7.806
7.276
2.654
6m
8.611
8.604
8.592
8.587
8.570
8.335
8.316
7.826
7.820
7.818
7.814
7.812
7.806
7.765
7.762
7.748
7.745
2.17
1.01
3.19
f1 (ppm)
0.90
1.00
2.17
1.01
3.19
3.31
f1 (ppm)

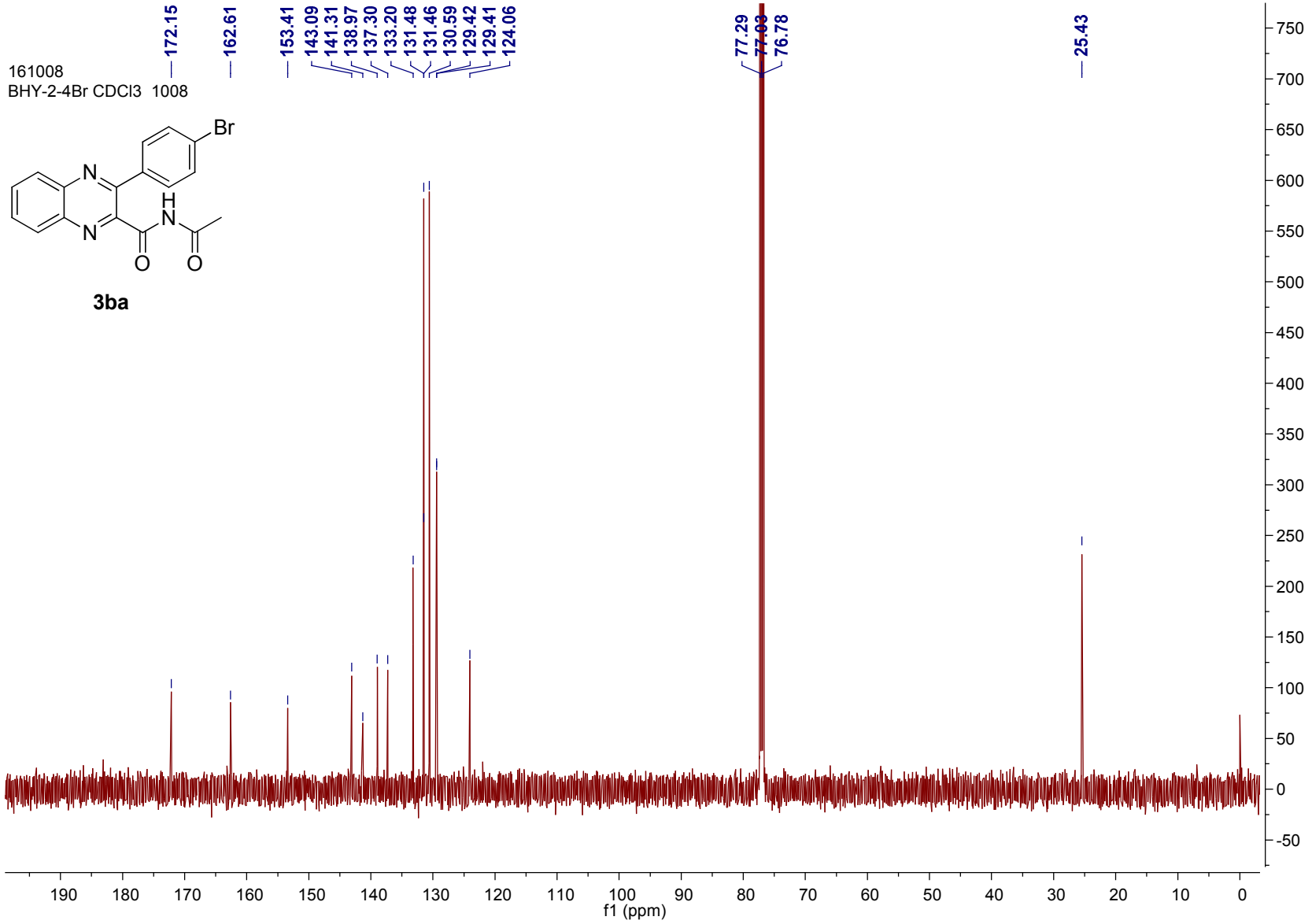

195.86
150.04
143.10
139.05
133.00
131.46
131.24
129.84
128.76
126.21
125.77
123.82
122.10
121.83
77.29
77.03
76.78
21.96
170720
XZ-8CH3 CDCl3 0720
N
H
O
6m
f1 (ppm)

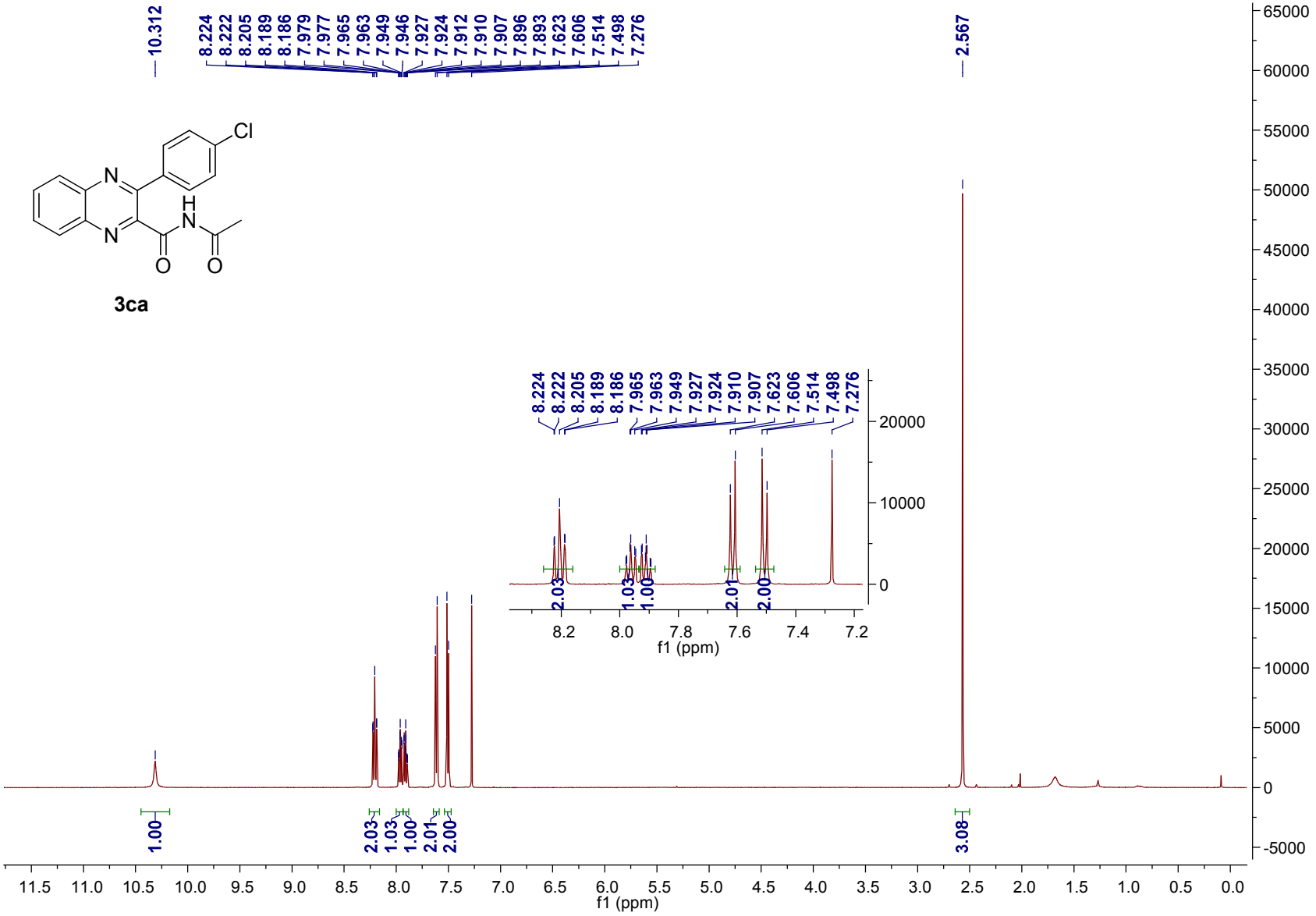
7. ^{1}H and ^{13}C NMR spectra of 3aa-va, 3ab-ag, 7aa-na, 8a, 1a-*d*

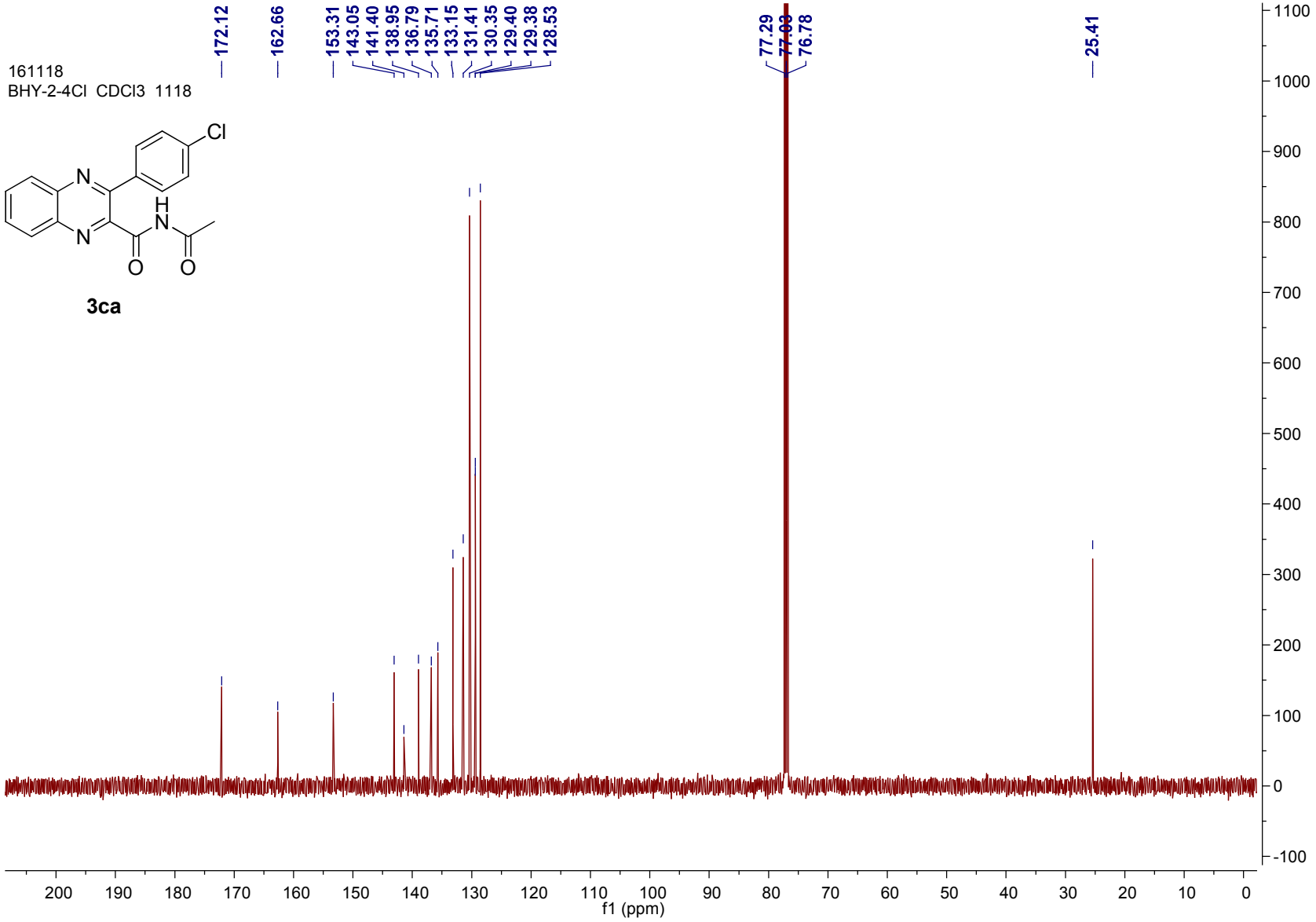


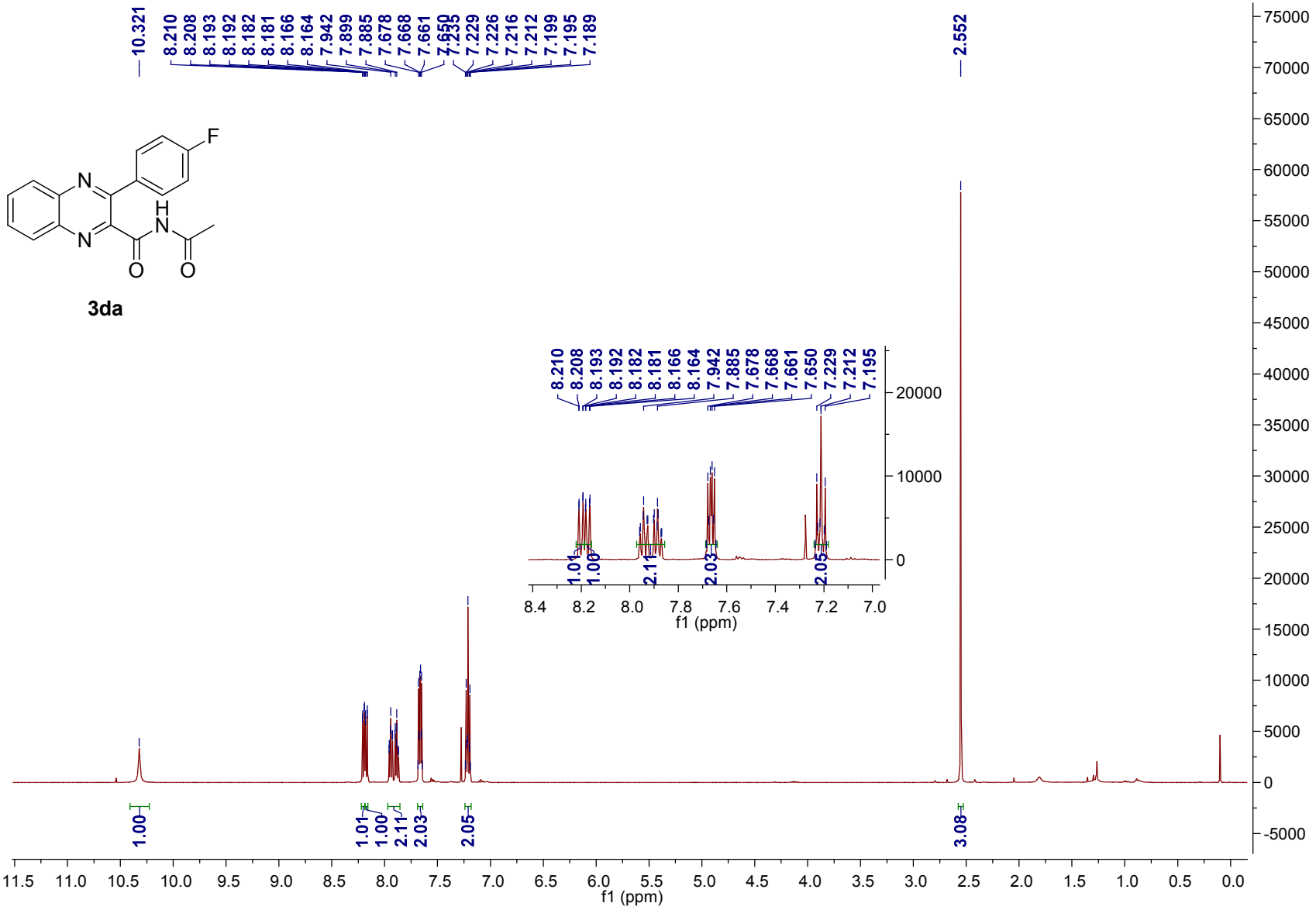

160722
BHY-NCS CDCl3 0722
172.19
162.89
154.35
143.06
141.95
138.91
138.30
132.88
131.11
129.42
129.37
129.34
128.86
128.28
77.29
77.03
76.78
25.34
3aa
f1 (ppm)

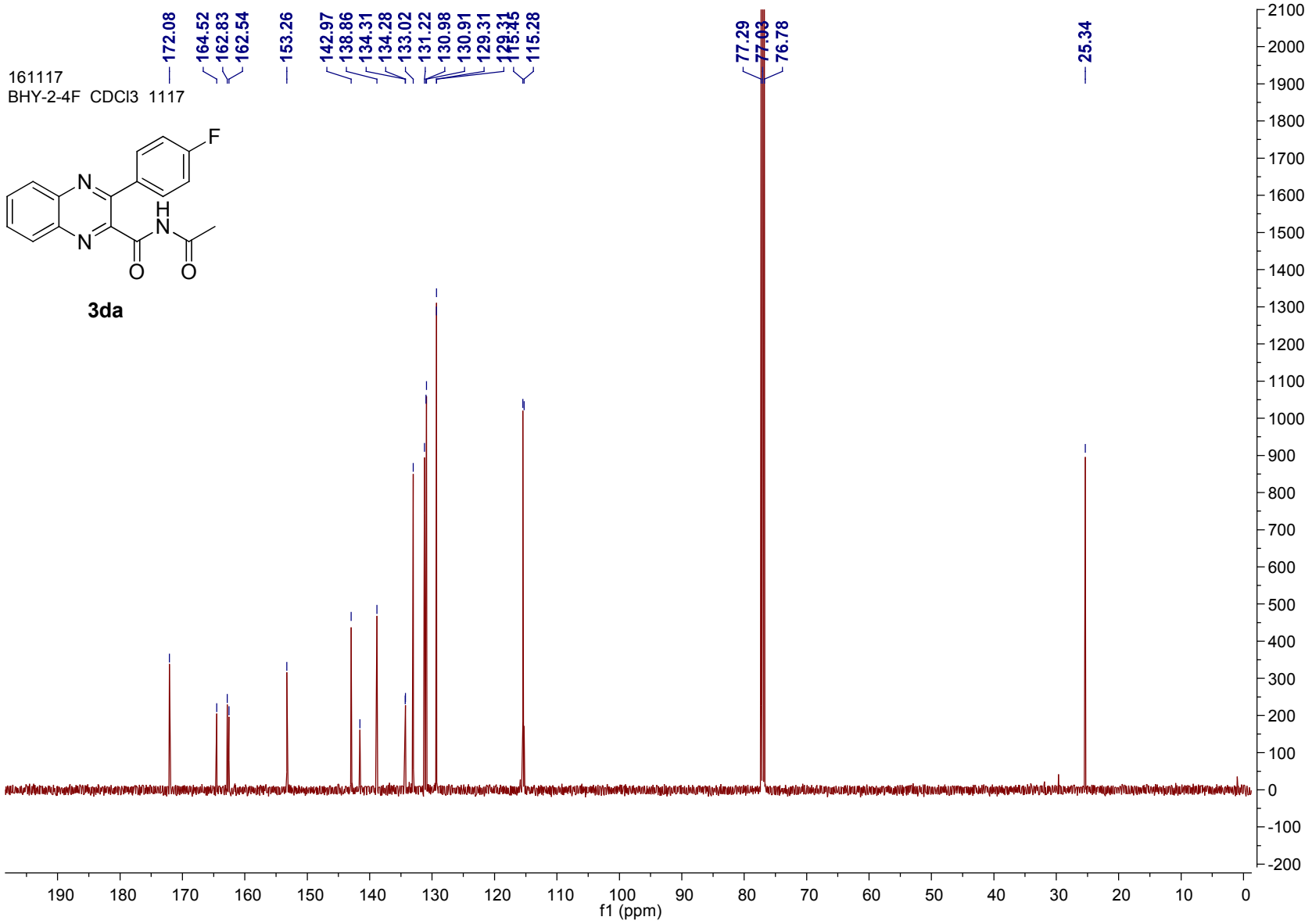

10.328
8.228
8.226
8.211
8.209
8.208
8.193
8.191
7.986
7.983
7.972
7.969
7.966
7.955
7.952
7.935
7.932
7.921
7.918
7.915
7.904
7.901
7.682
7.678
7.674
7.664
7.661
7.656
7.561
7.556
7.552
7.543
7.539
7.277
2.573
Br
N
H
N
N
O
O
3ba
f1 (ppm)
1.00
2.00
2.06
2.00
2.00
3.04

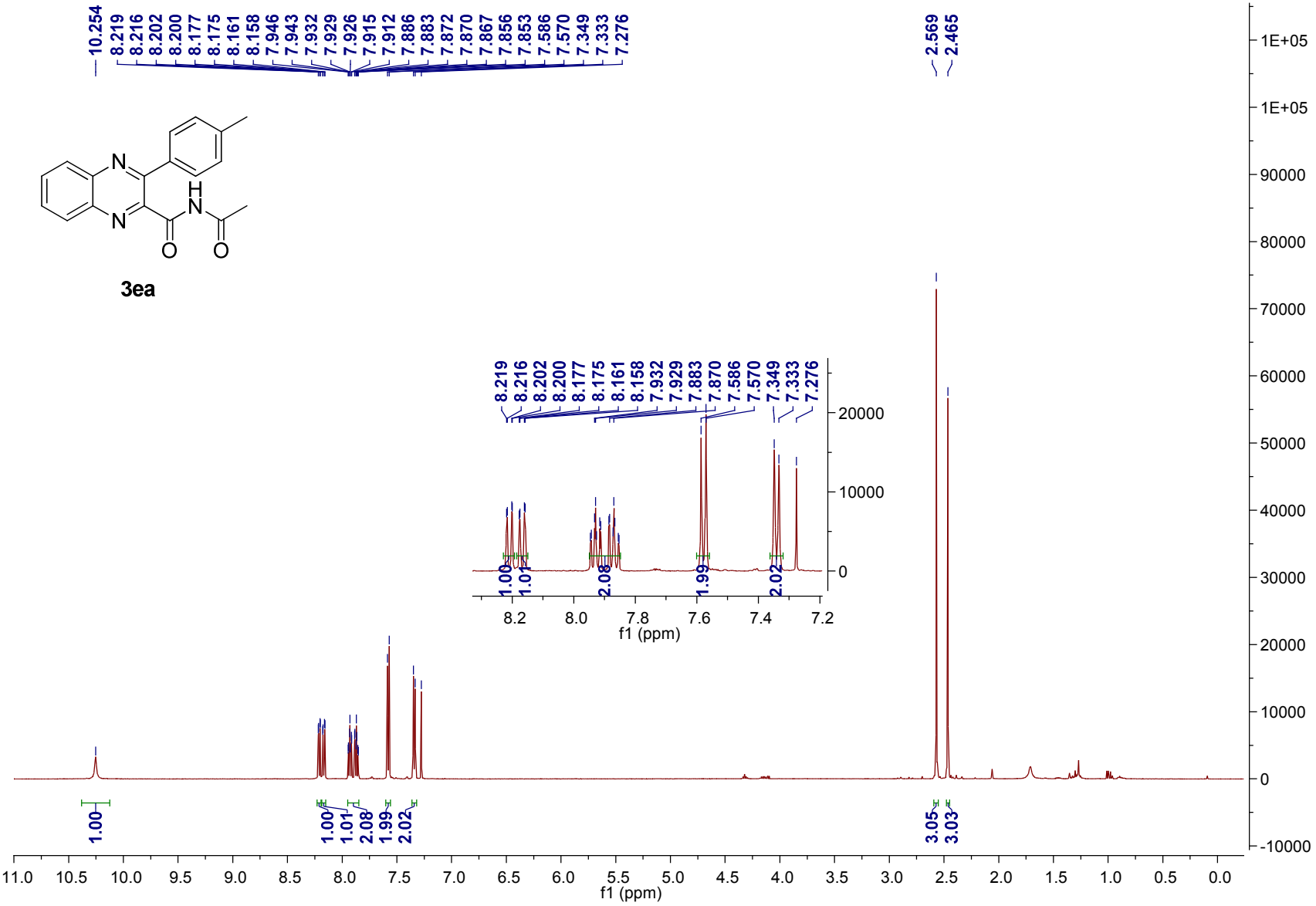

161008
BHY-2-4Br CDCl3 1008
172.15
162.61
153.41
143.09
141.31
138.97
137.30
133.20
131.48
131.46
130.59
129.42
129.41
124.06
77.29
77.03
76.78
25.43
Br
N
N
H
N
O
O
3ba
f1 (ppm)

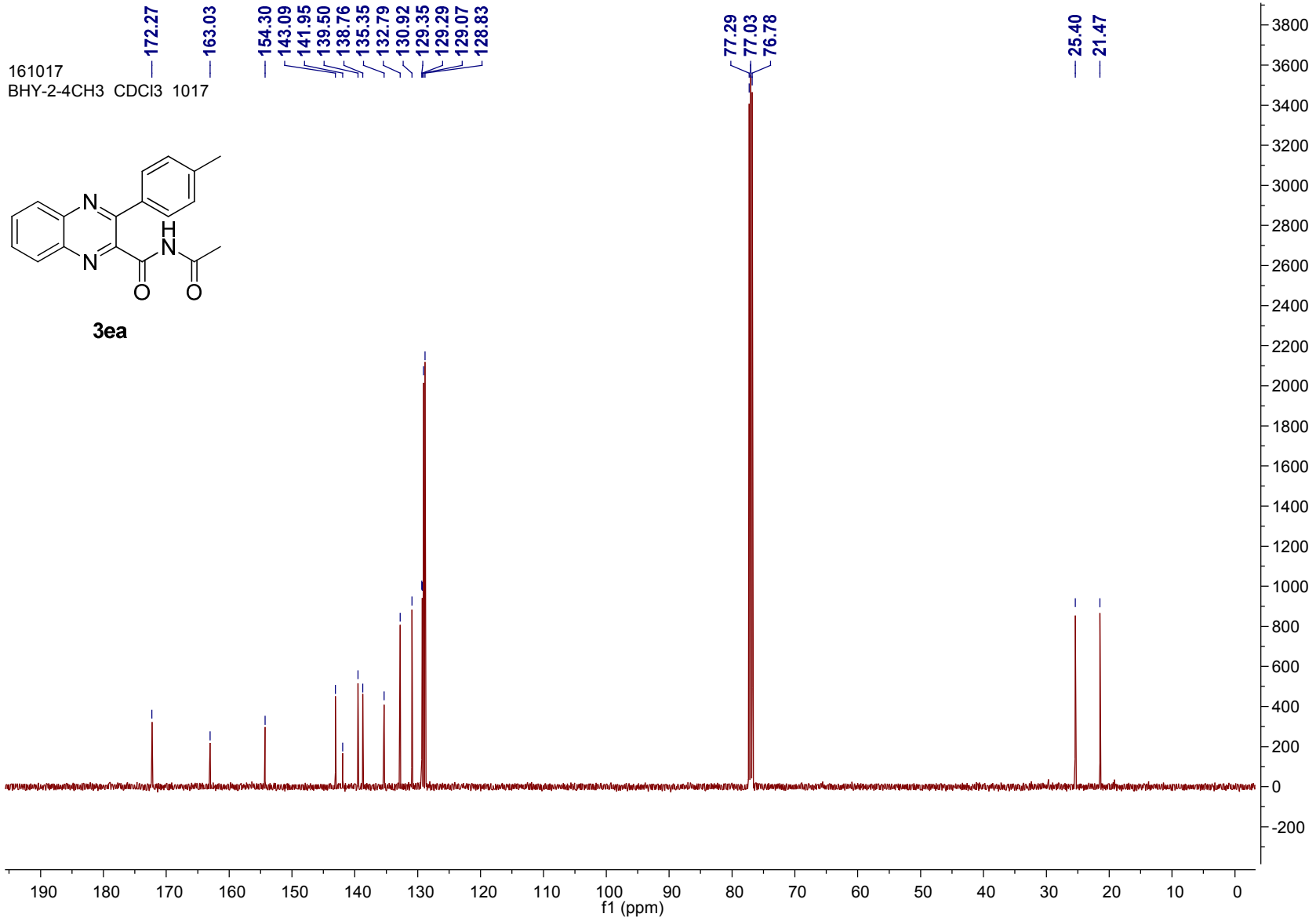

10.312
8.224
8.222
8.205
8.189
8.186
7.979
7.977
7.965
7.963
7.949
7.946
7.927
7.924
7.912
7.910
7.907
7.896
7.893
7.623
7.606
7.514
7.498
7.276
2.567
Cl
N
H
N
N
O
O
3ca
f1 (ppm)
1.00
2.03
1.03
1.00
2.01
2.00
3.08

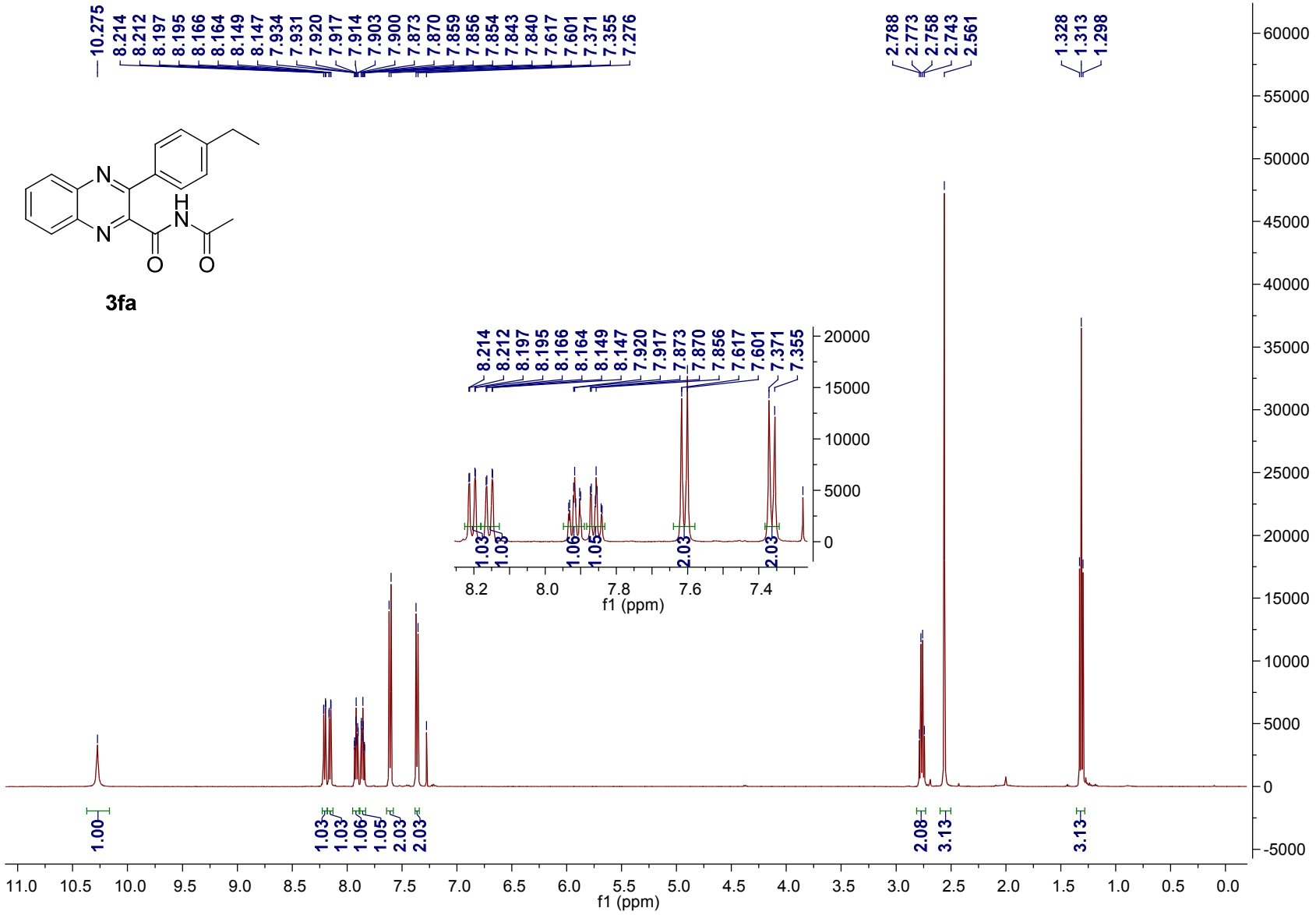

161118
BHY-2-4Cl CDCl3 1118
172.12
162.66
153.31
143.05
141.40
138.95
136.79
135.71
133.15
131.41
130.35
129.40
129.38
128.53
77.29
77.03
76.78
25.41
Cl
N
N
H
N
O
O
3ca
f1 (ppm)

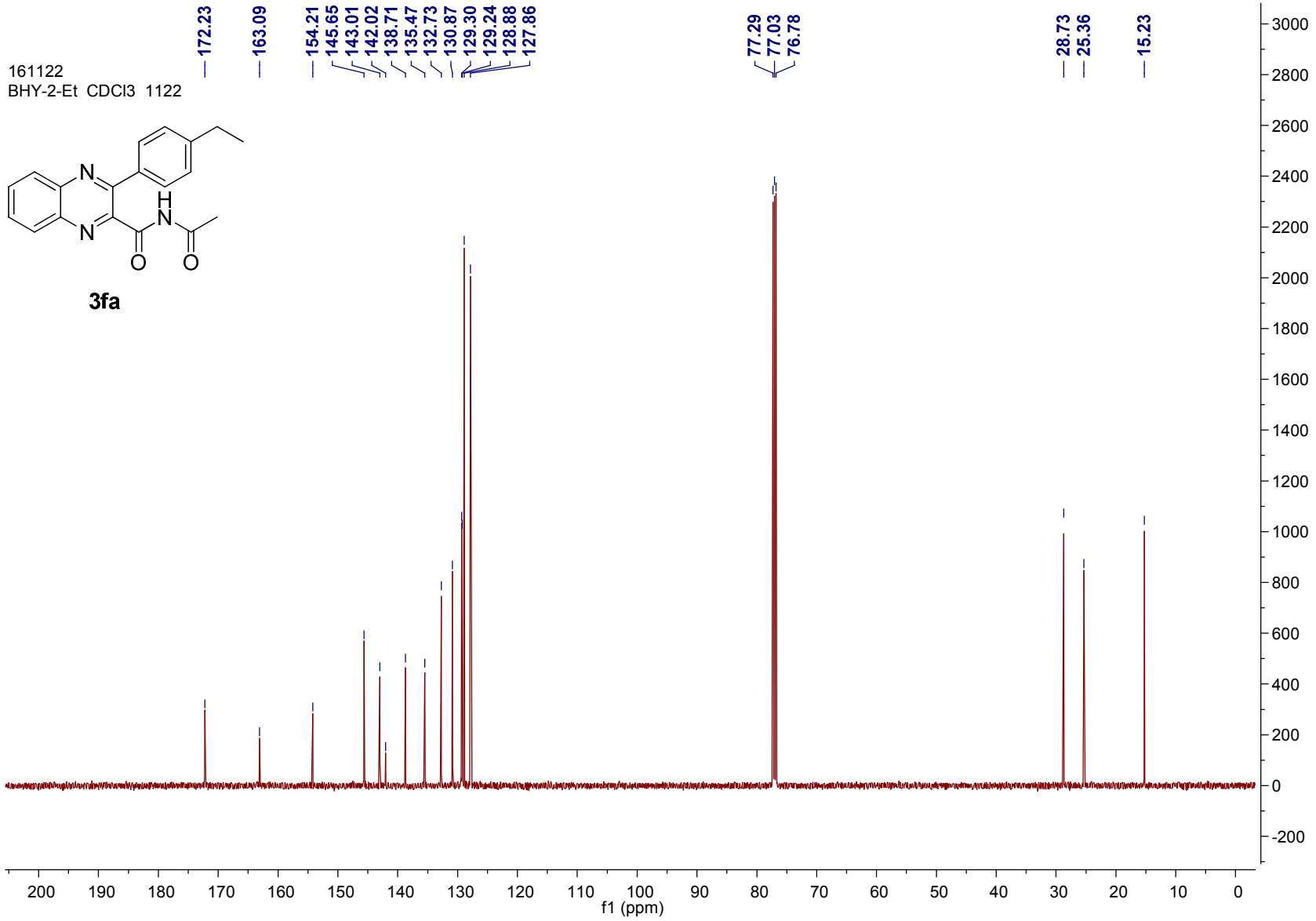

10.321
8.210
8.208
8.193
8.192
8.182
8.181
8.166
8.164
7.942
7.899
7.885
7.678
7.668
7.661
7.650
7.235
7.229
7.226
7.216
7.212
7.199
7.195
7.189
2.552
F
N
H
N
O
O
3da
1.00
1.01
1.00
2.11
2.03
2.05
3.08
f1 (ppm)

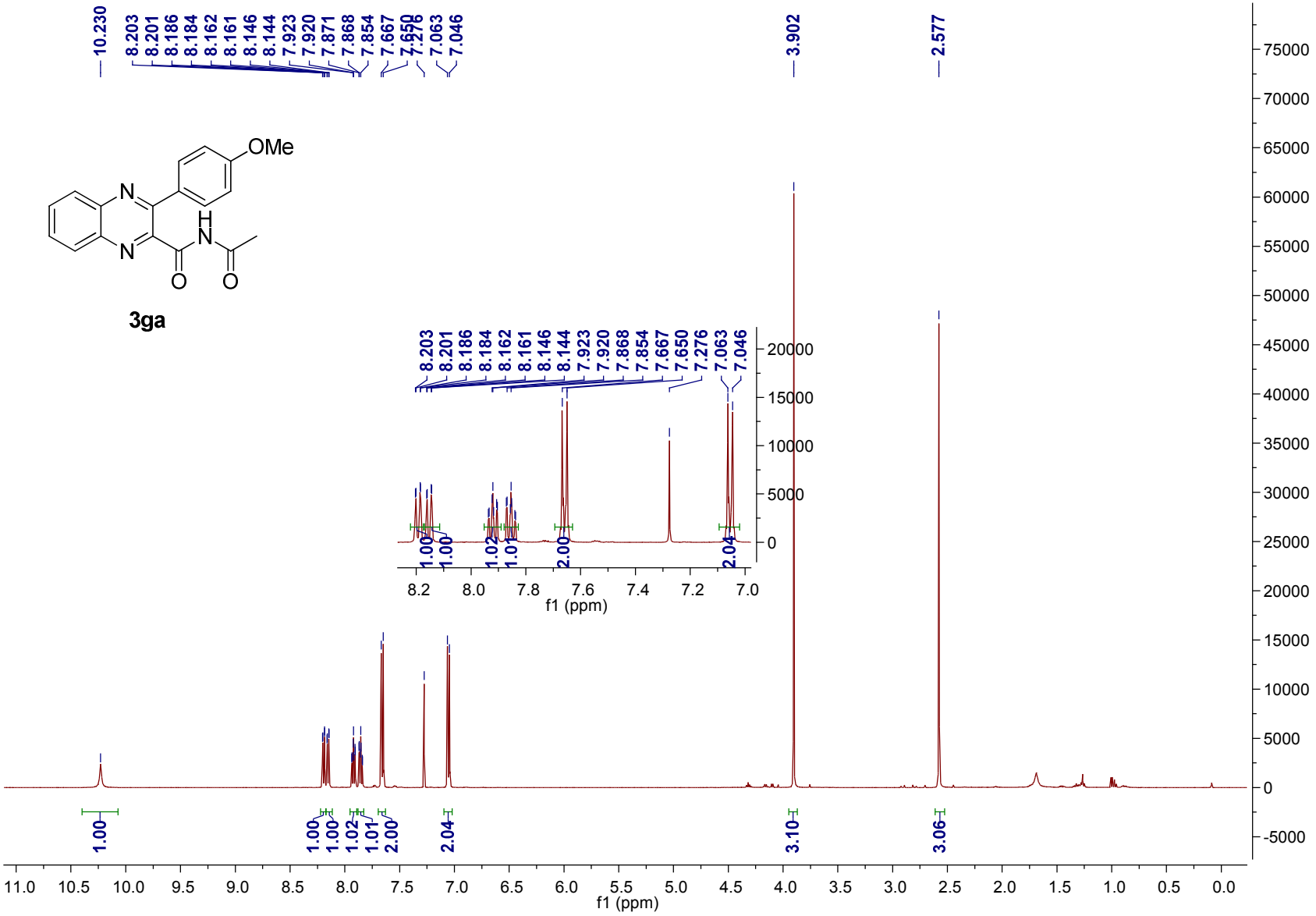

161117
BHY-2-4F CDCl3 1117
172.08
164.52
162.83
162.54
153.26
142.97
138.86
134.31
134.28
133.02
131.22
130.98
130.91
129.31
115.28
77.29
77.03
76.78
25.34
F
N
N
H
N
O
O
3da
f1 (ppm)

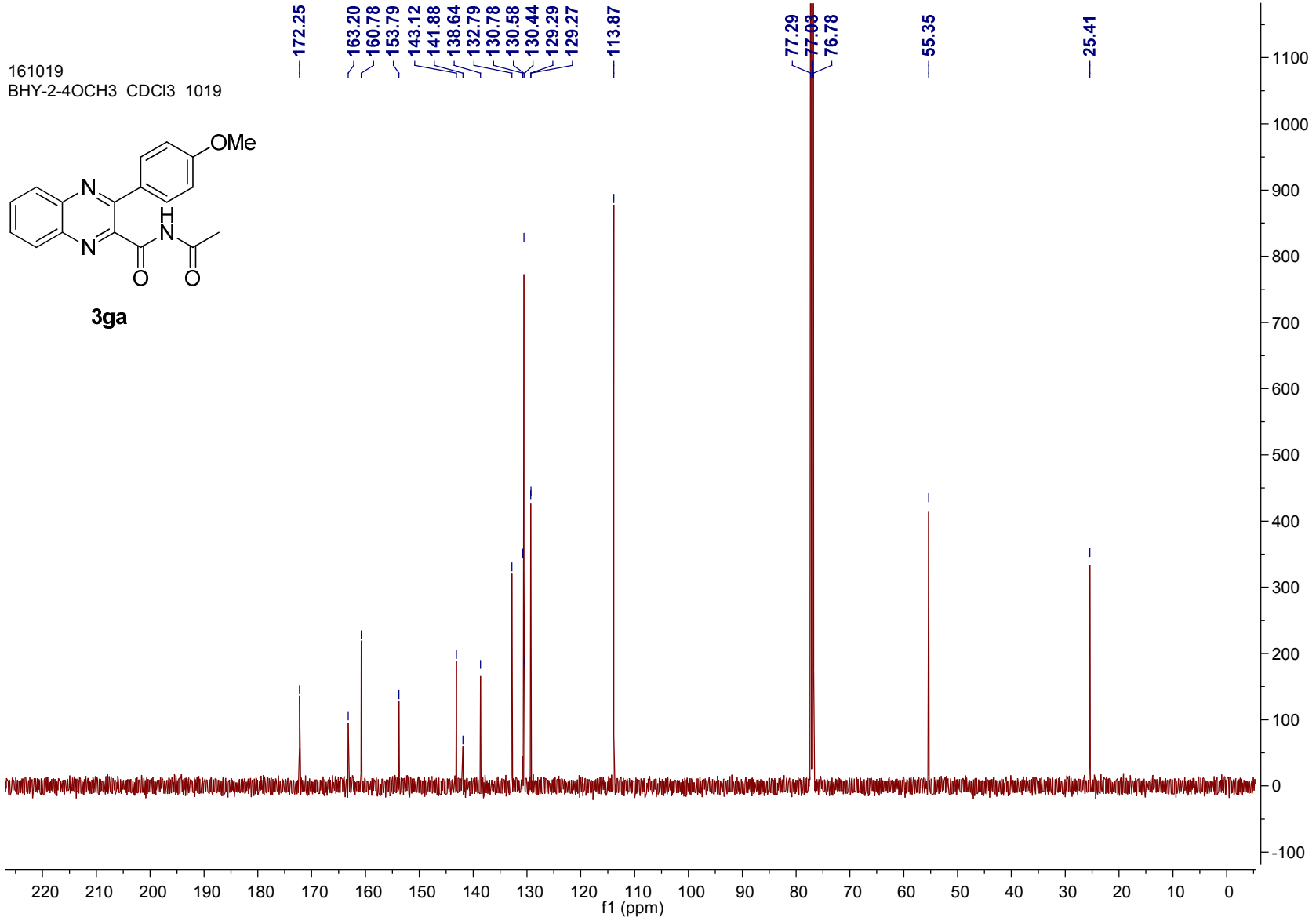

10.254
8.219
8.216
8.202
8.200
8.177
8.175
8.161
8.158
7.946
7.943
7.932
7.929
7.926
7.915
7.912
7.886
7.883
7.872
7.870
7.867
7.856
7.853
7.586
7.570
7.349
7.333
7.276
2.569
2.465
3ea
f1 (ppm)

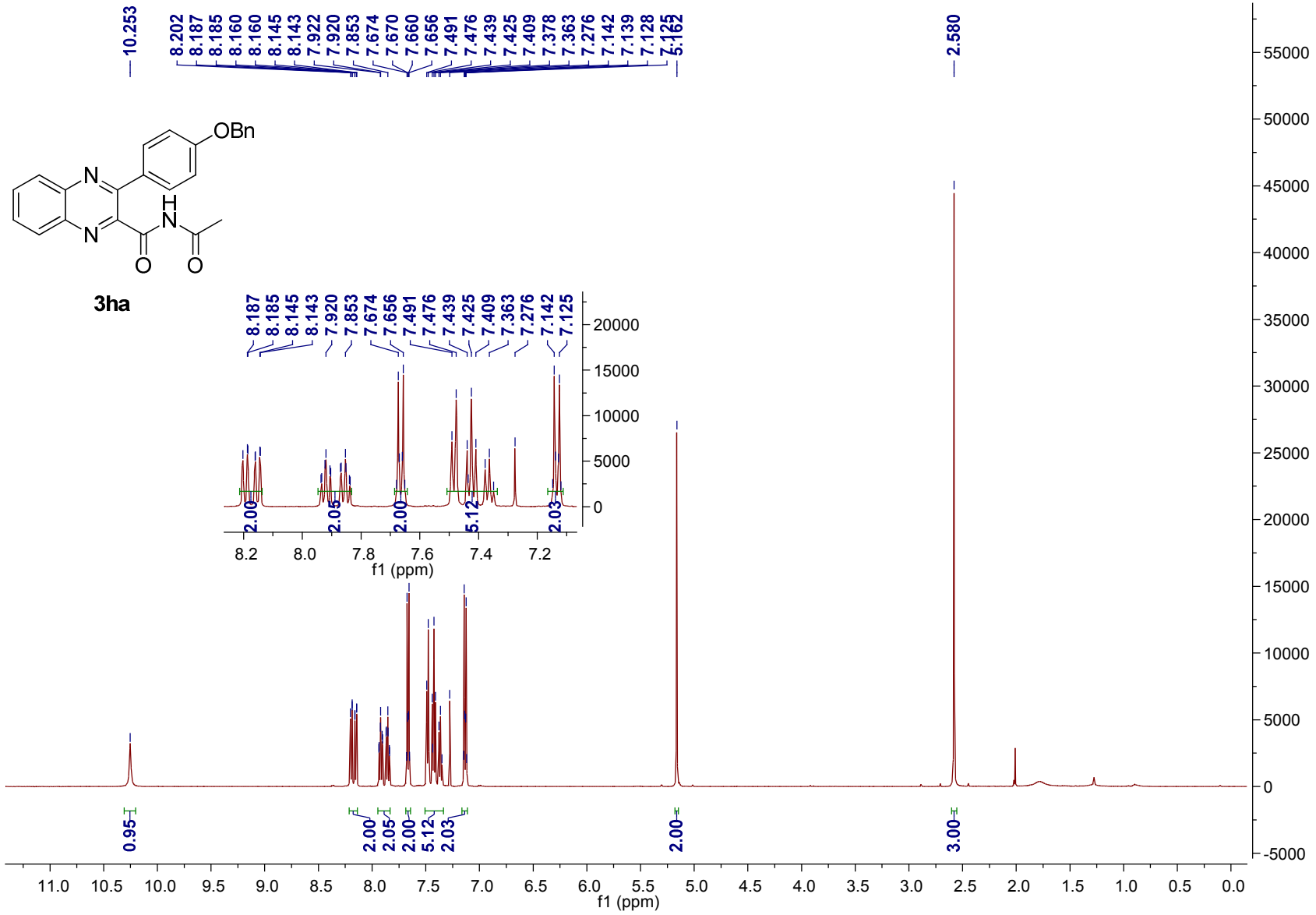

161017
BHY-2-4CH3 CDCl3 1017
172.27
163.03
154.30
143.09
141.95
139.50
138.76
135.35
132.79
130.92
129.35
129.29
129.07
128.83
77.29
77.03
76.78
25.40
21.47
3ea
f1 (ppm)

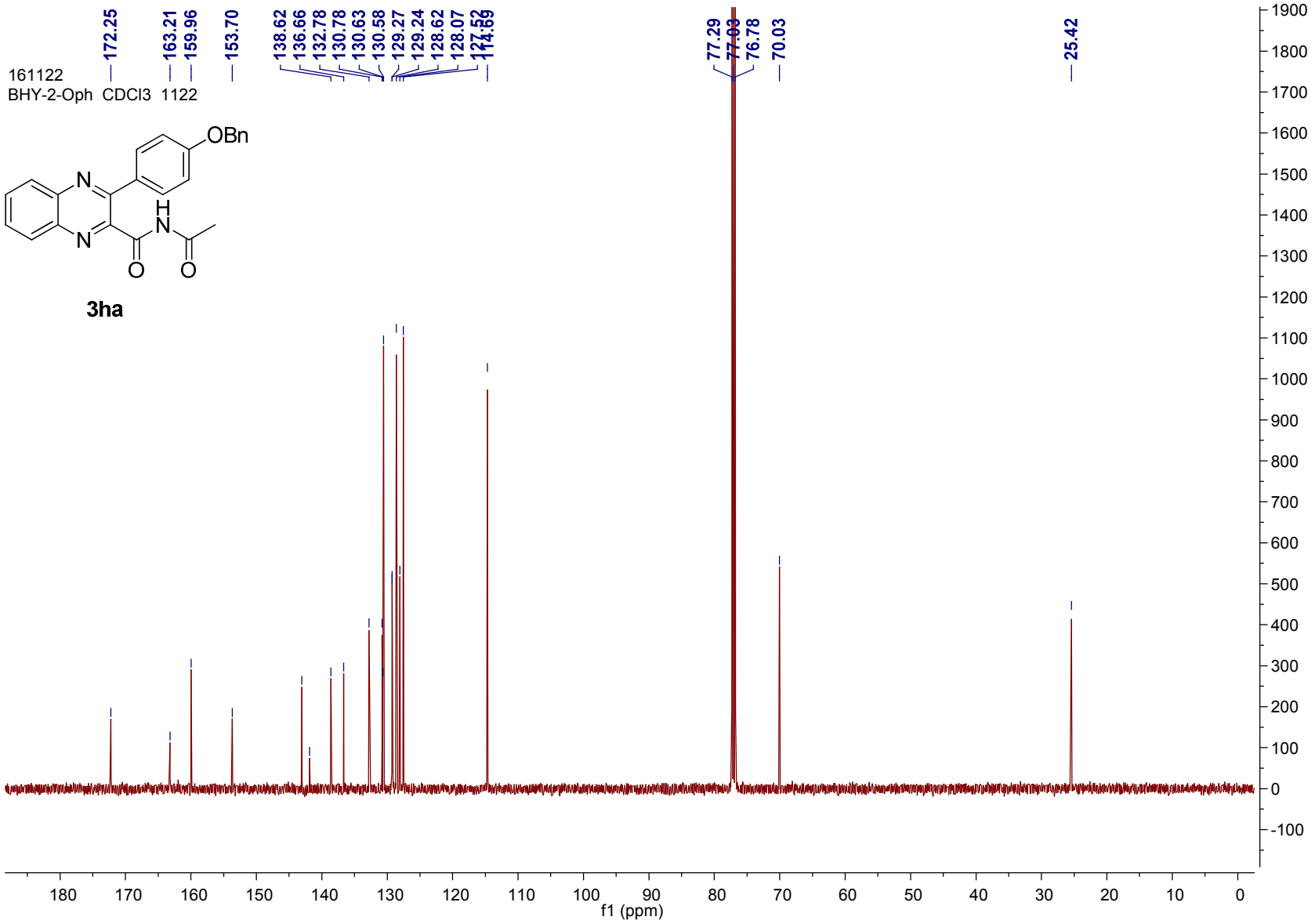

10.275
8.214
8.212
8.197
8.195
8.166
8.164
8.149
8.147
7.934
7.931
7.920
7.917
7.914
7.903
7.900
7.873
7.870
7.859
7.856
7.854
7.843
7.840
7.617
7.601
7.371
7.355
7.276
2.788
2.773
2.758
2.743
2.561
1.328
1.313
1.298
N
H
N
N
O
O
3fa
1.00
1.03
1.03
1.06
1.05
2.03
2.03
2.08
3.13
3.13
f1 (ppm)

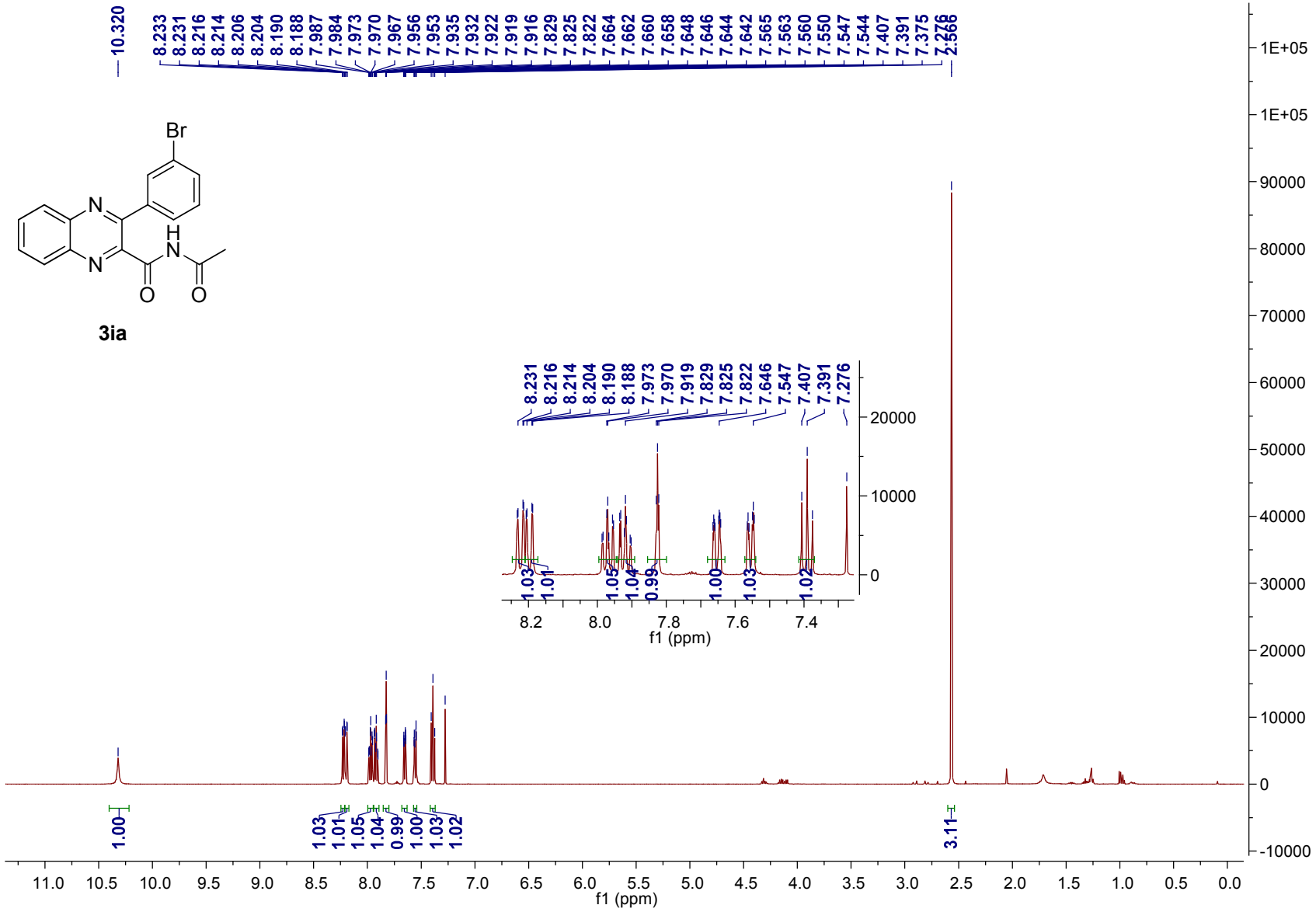

161122
BHY-2-Et CDCl3 1122
172.23
163.09
154.21
145.65
143.01
142.02
138.71
135.47
132.73
130.87
129.30
129.24
128.88
127.86
77.29
77.03
76.78
28.73
25.36
15.23
3fa
f1 (ppm)

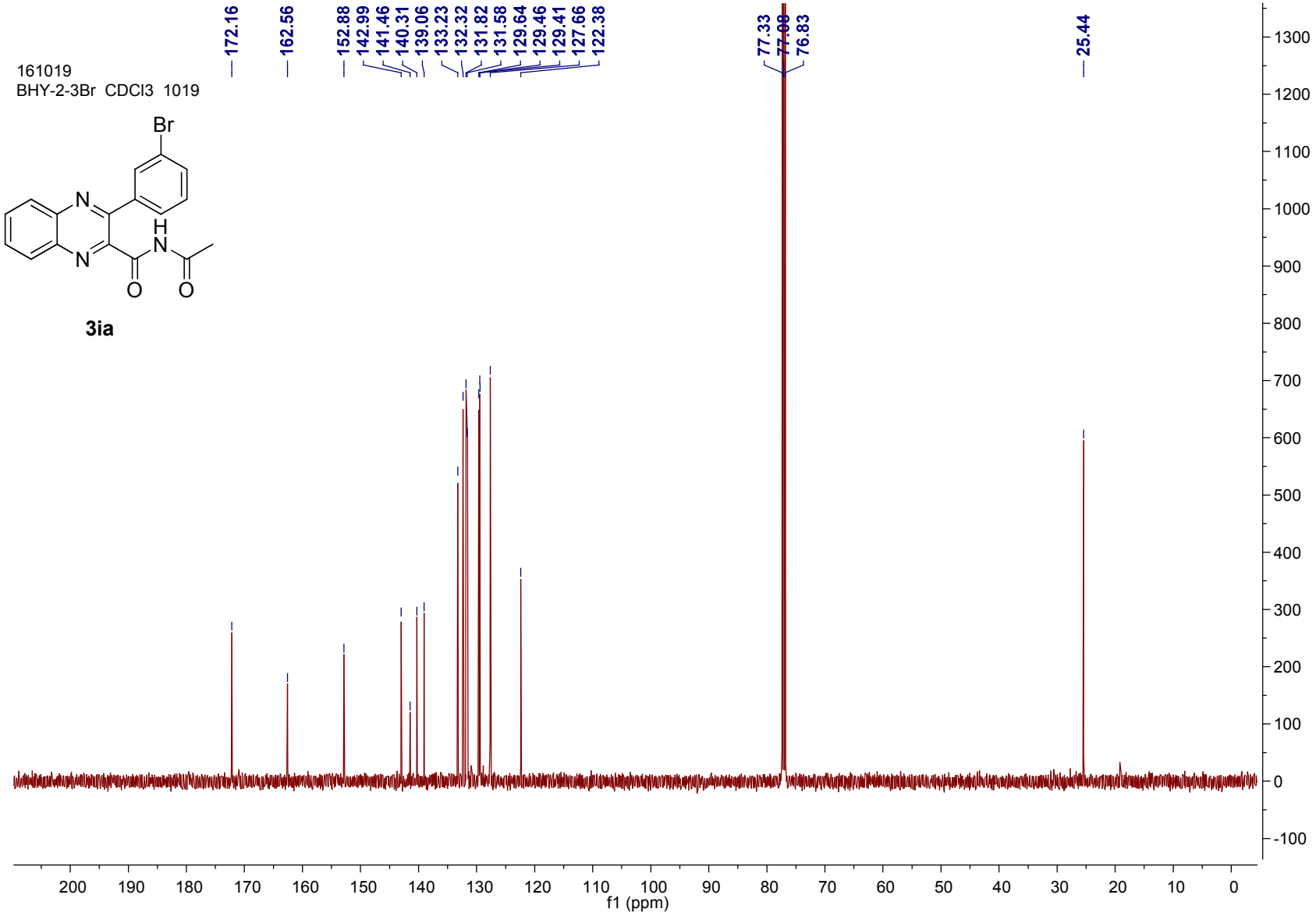

10.230
8.203
8.201
8.186
8.184
8.162
8.161
8.146
8.144
7.923
7.920
7.871
7.868
7.854
7.667
7.650
7.276
7.063
7.046
3.902
2.577
OMe
N
H
N
N
O
O
3ga
f1 (ppm)
1.00
1.00
1.00
1.02
1.01
2.00
2.04
3.10
3.06

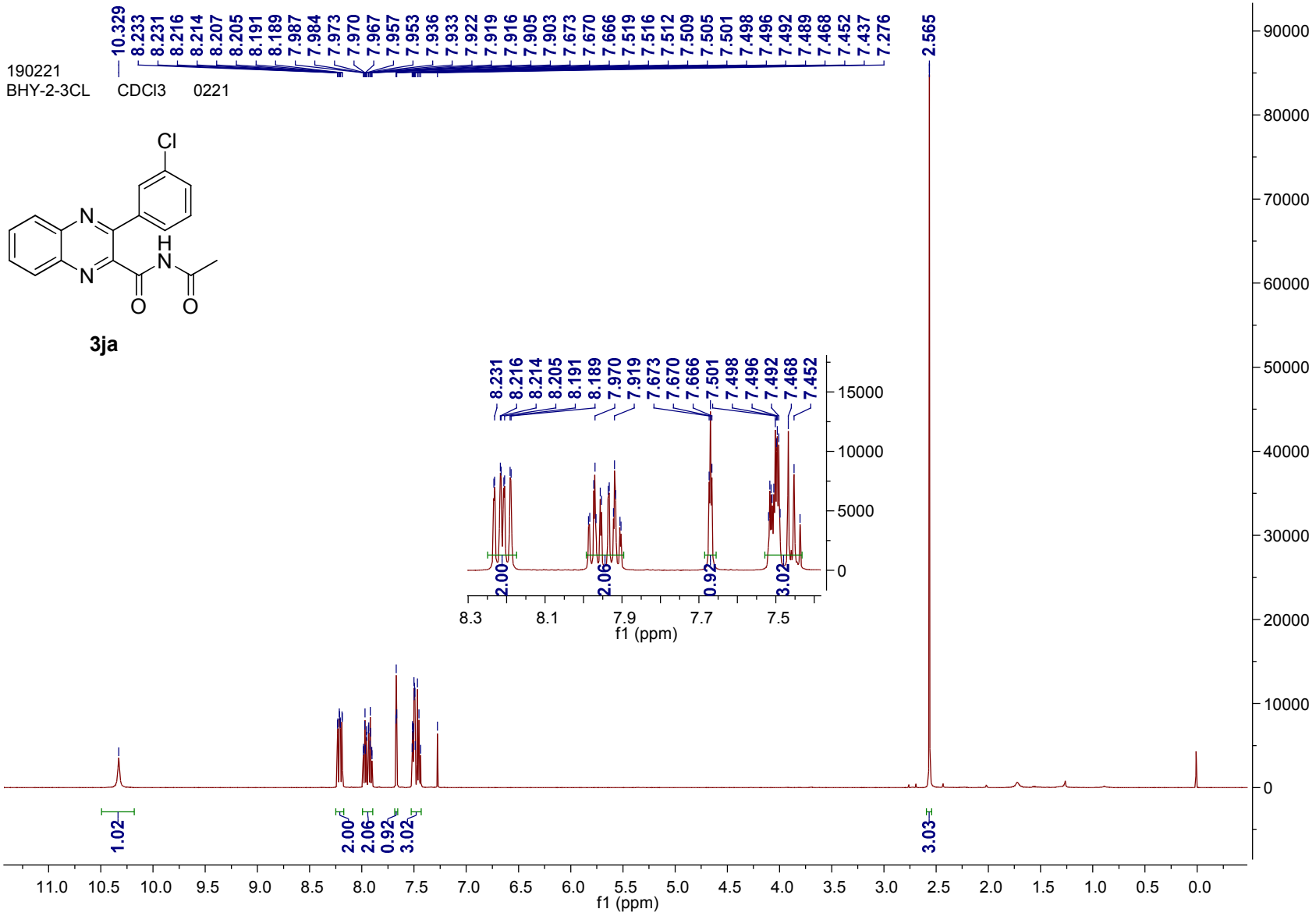

161019
BHY-2-4OCH3 CDCl3 1019
OMe
N
N
H
N
O
O
3ga
172.25
163.20
160.78
153.79
143.12
141.88
138.64
132.79
130.78
130.58
130.44
129.29
129.27
113.87
77.29
77.03
76.78
55.35
25.41
f1 (ppm)

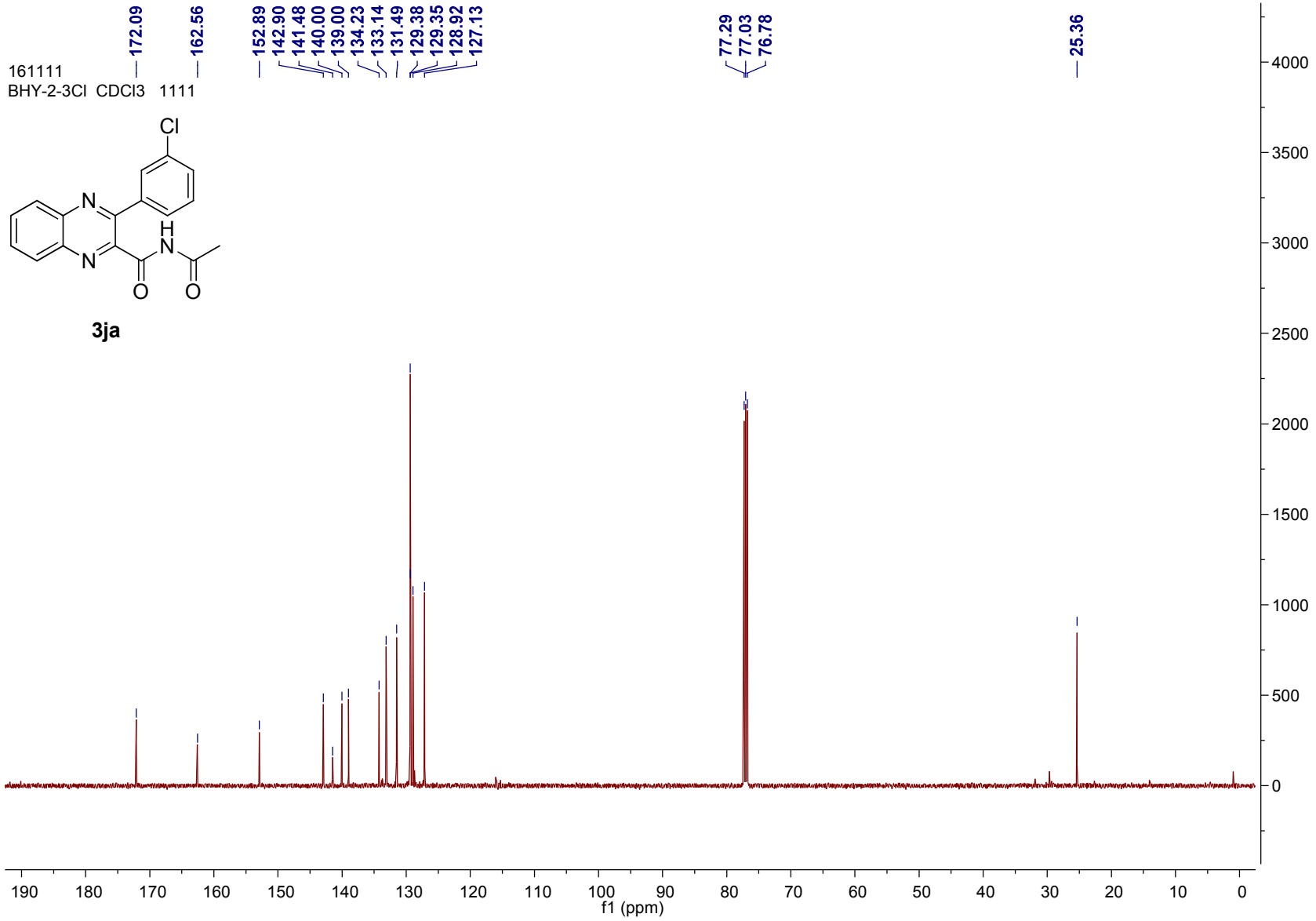

10.253
8.202
8.187
8.185
8.160
8.160
8.145
8.143
7.922
7.920
7.853
7.674
7.670
7.660
7.656
7.491
7.476
7.439
7.425
7.409
7.378
7.363
7.276
7.142
7.139
7.128
7.125
5.162
2.580
OBn
N
H
N
N
O
O
3ha
f1 (ppm)
0.95
2.00
2.05
2.00
5.12
2.03
2.00
3.00

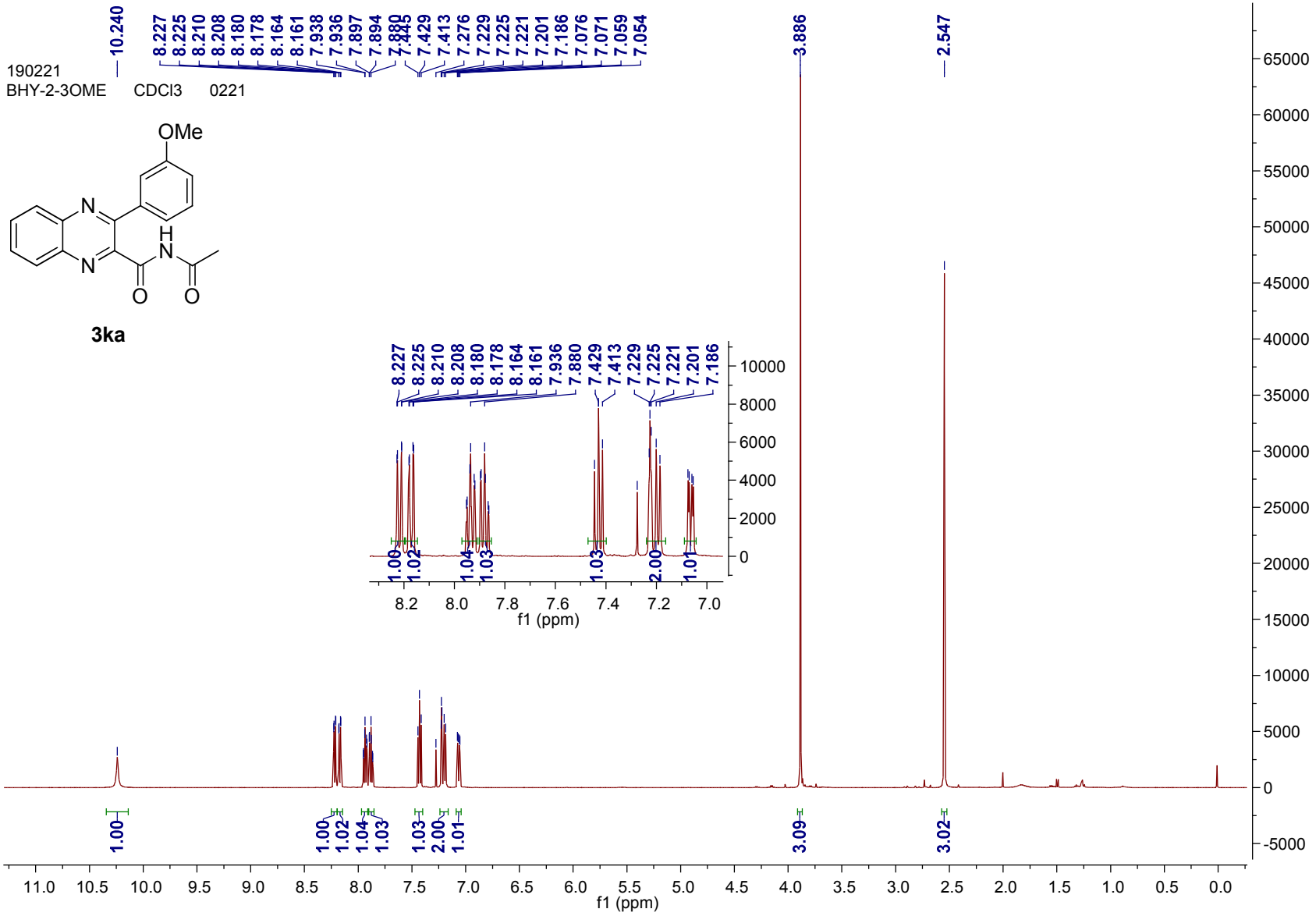

172.25
163.21
159.96
153.70
138.62
136.66
132.78
130.78
130.63
130.58
129.27
129.24
128.62
128.07
77.29
77.03
76.78
70.03
25.42
161122
BHY-2-Oph CDCl3 1122
OBn
N
H
N
N
O
O
3ha
f1 (ppm)

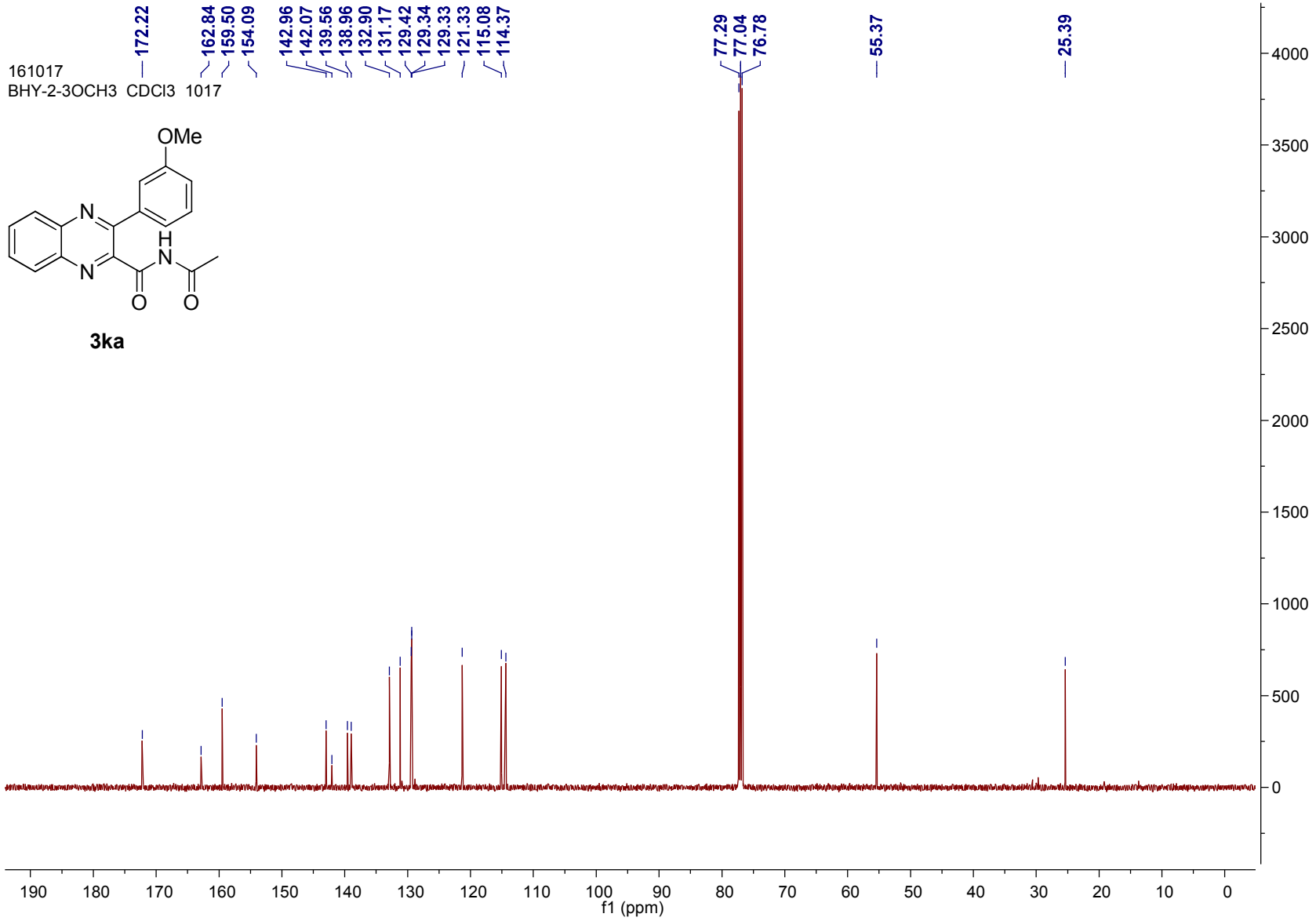

10.320
8.233
8.231
8.216
8.214
8.206
8.204
8.190
8.188
7.987
7.984
7.973
7.970
7.967
7.956
7.953
7.935
7.932
7.922
7.919
7.916
7.829
7.825
7.822
7.664
7.662
7.660
7.658
7.648
7.646
7.644
7.642
7.565
7.563
7.560
7.550
7.547
7.544
7.407
7.391
7.375
7.276
2.568
Br
N
H
N
N
O
O
3ia
1.00
1.03
1.01
1.05
1.04
0.99
1.00
1.03
1.02
3.11
f1 (ppm)

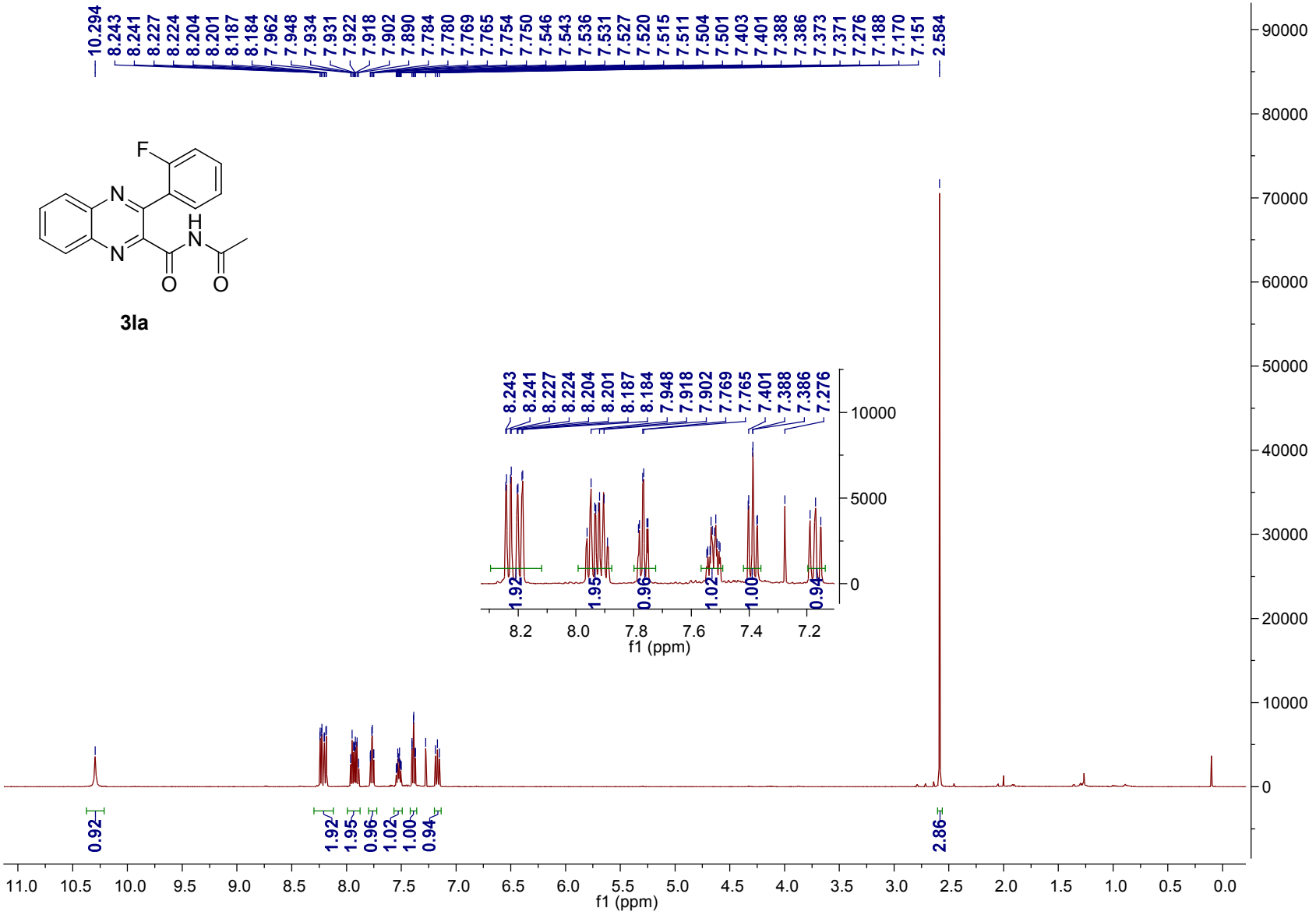

161019
BHY-2-3Br CDCl3 1019
Br
N
N
H
N
O
O
3ia
172.16
162.56
152.88
142.99
141.46
140.31
139.06
133.23
132.32
131.82
131.58
129.64
129.46
129.41
127.66
122.38
77.33
77.08
76.83
25.44
f1 (ppm)

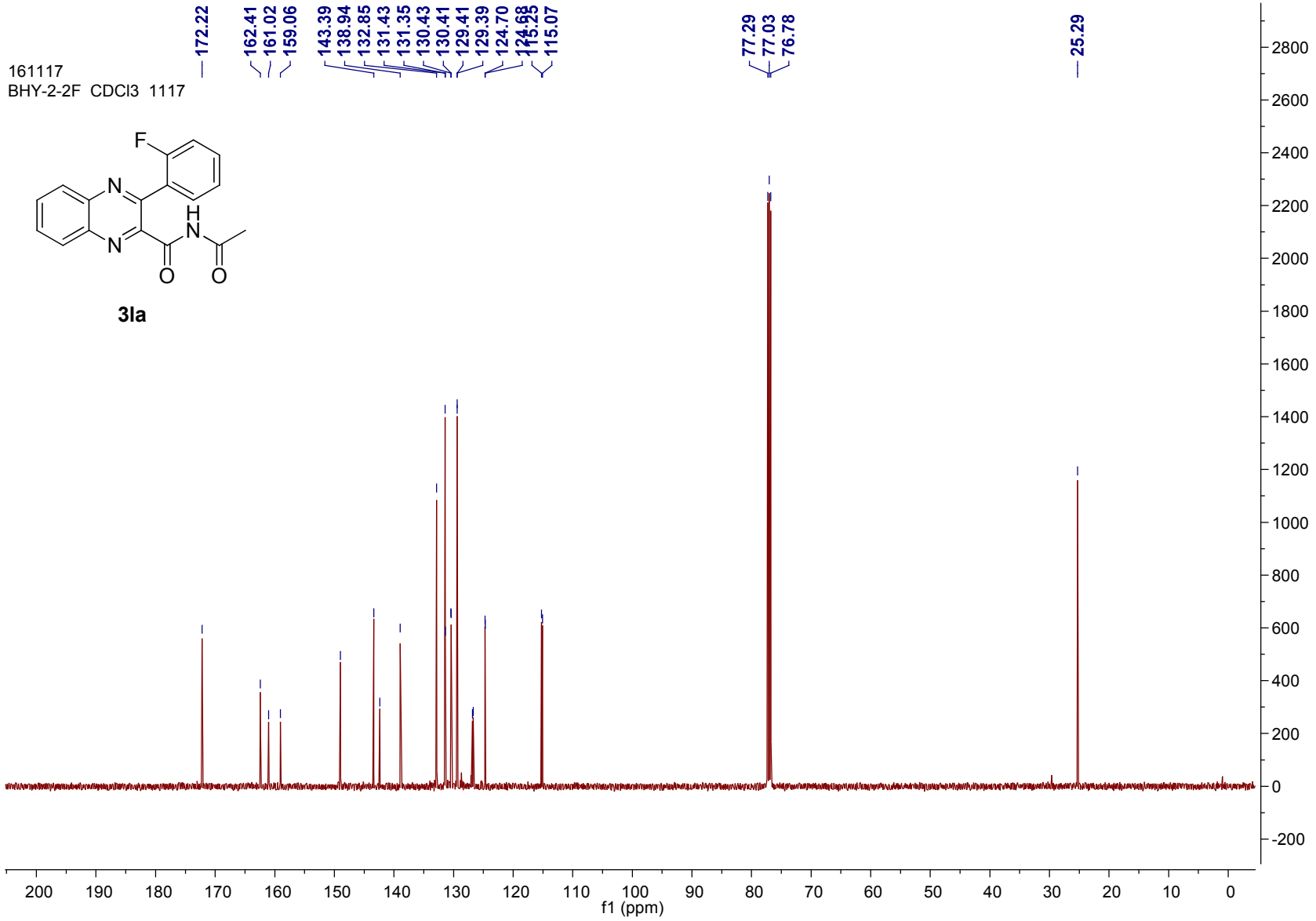

190221
BHY-2-3CL CDCl3 0221
10.329
8.233
8.231
8.216
8.214
8.207
8.205
8.191
8.189
7.987
7.984
7.973
7.970
7.967
7.957
7.953
7.936
7.933
7.922
7.919
7.916
7.905
7.903
7.673
7.670
7.666
7.519
7.516
7.512
7.509
7.505
7.501
7.498
7.496
7.492
7.489
7.468
7.452
7.437
7.276
2.565
Cl
N
H
N
N
O
O
3ja
1.02
2.00
2.06
0.92
3.02
3.03
f1 (ppm)

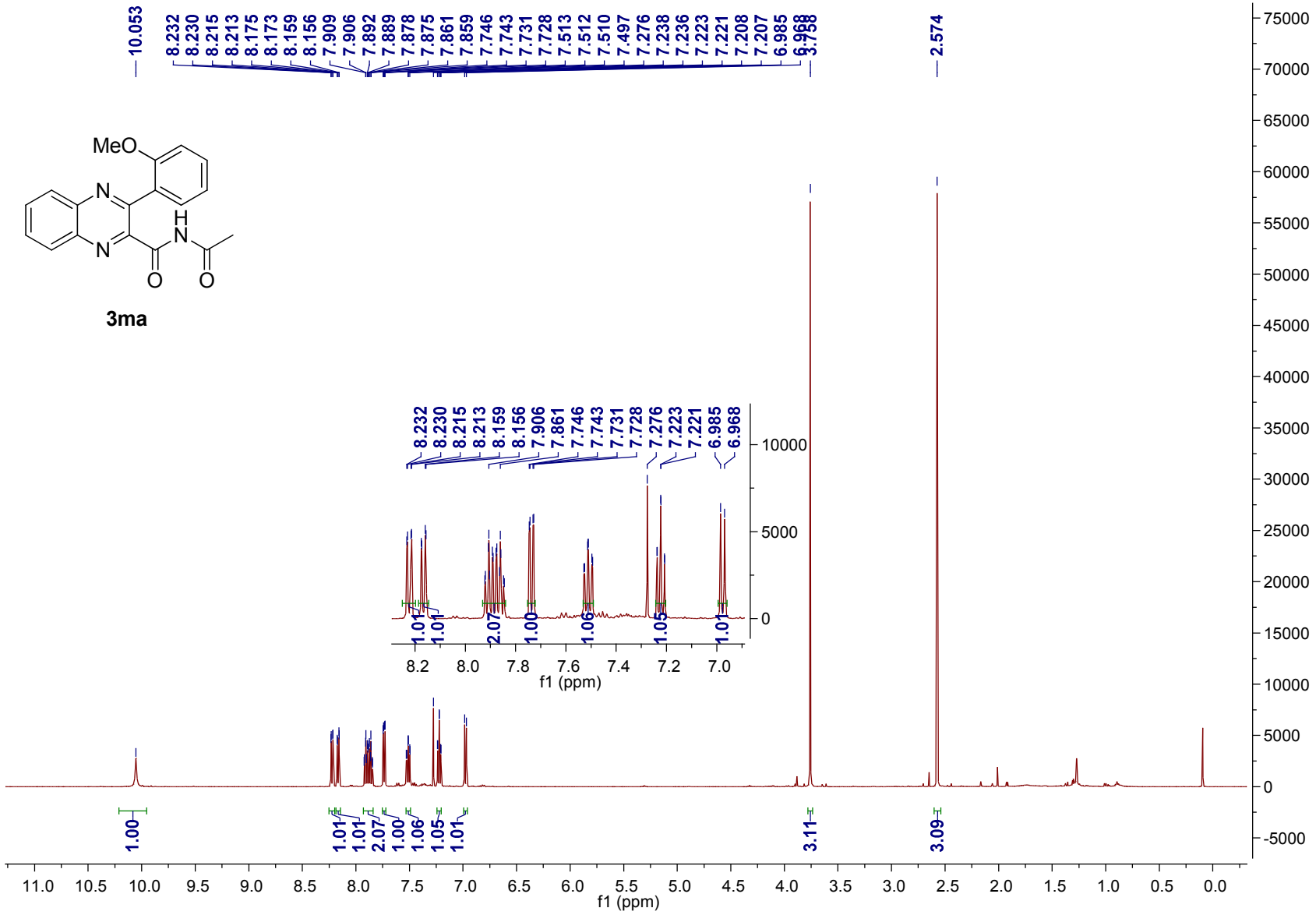

161111
BHY-2-3Cl CDCl3 1111
172.09
162.56
152.89
142.90
141.48
140.00
139.00
134.23
133.14
131.49
129.38
129.35
128.92
127.13
77.29
77.03
76.78
25.36
Cl
N
N
H
N
O
O
3ja
4000
3500
3000
2500
2000
1500
1000
500
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

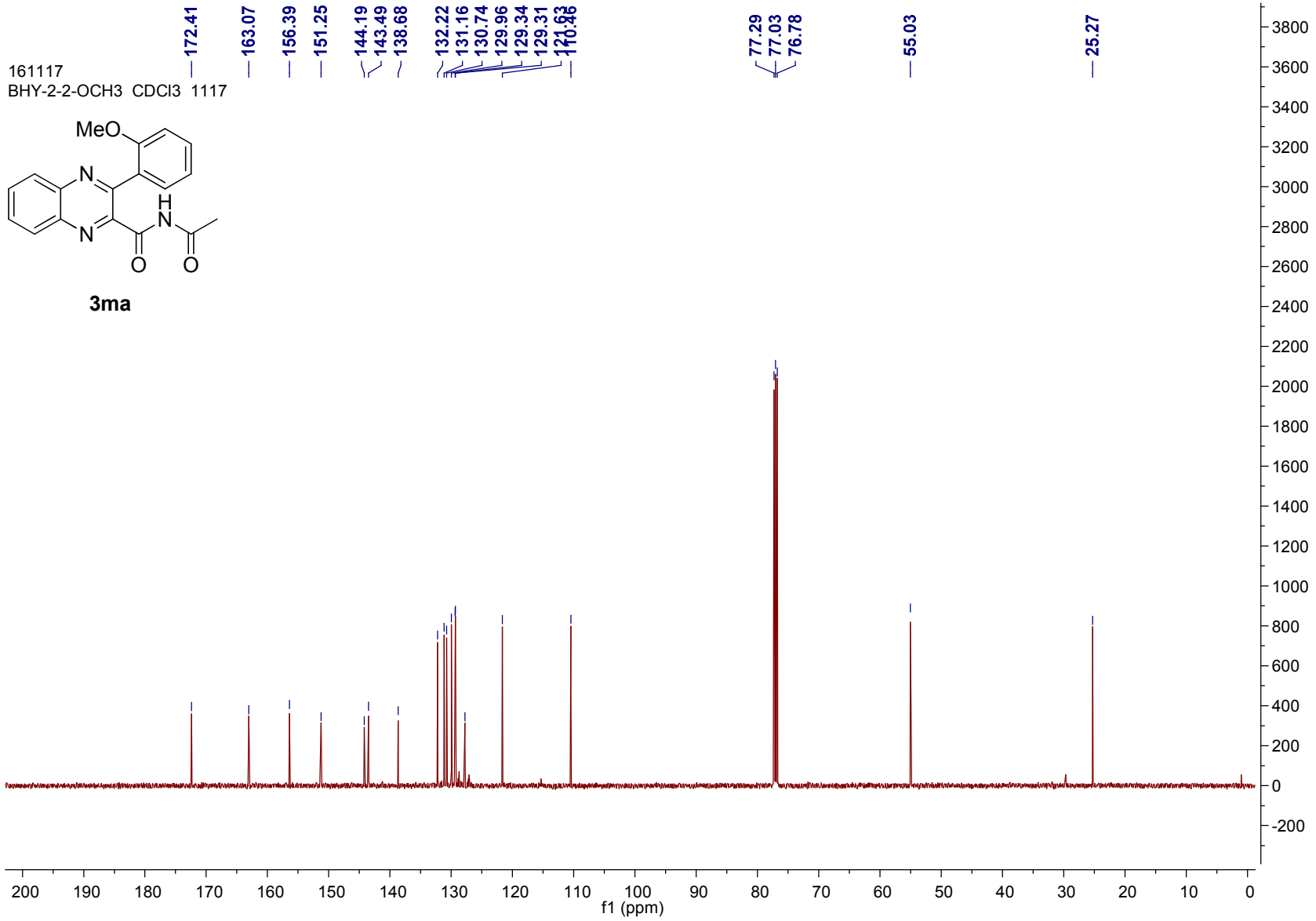

190221
BHY-2-3OME CDCl3 0221
OMe
N
H
N
N
O
O
3ka
10.240
8.227
8.225
8.210
8.208
8.180
8.178
8.164
8.161
7.938
7.936
7.897
7.894
7.429
7.413
7.276
7.229
7.225
7.221
7.201
7.186
7.076
7.071
7.059
7.054
3.886
2.547
1.00
1.00
1.02
1.04
1.03
1.03
2.00
1.01
3.09
3.02
f1 (ppm)

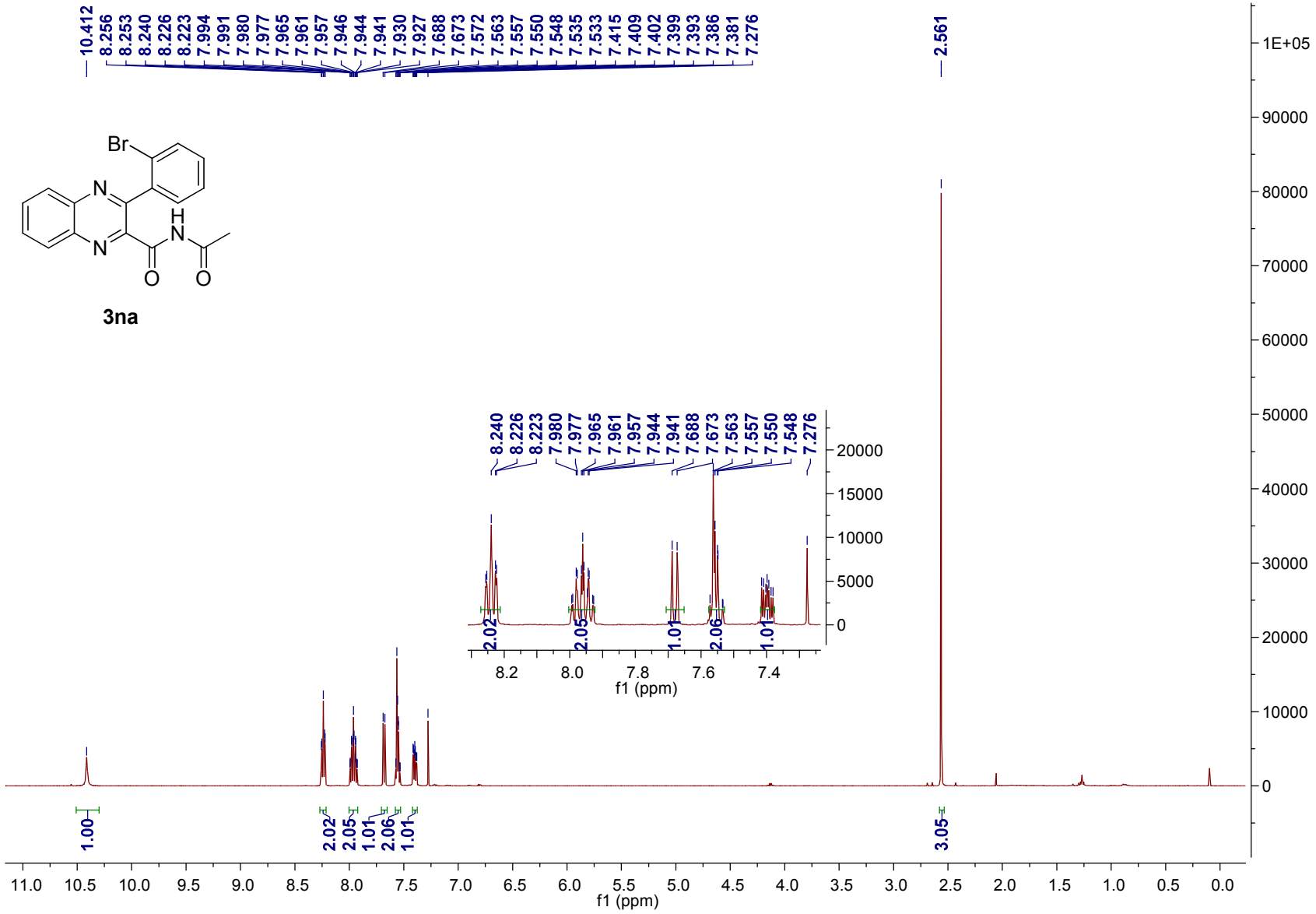

161017
BHY-2-3OCH3 CDCl3 1017
172.22
162.84
159.50
154.09
142.96
142.07
139.56
138.96
132.90
131.17
129.42
129.34
129.33
121.33
115.08
114.37
77.29
77.04
76.78
55.37
25.39
OMe
N
H
N
N
O
O
3ka
4000
3500
3000
2500
2000
1500
1000
500
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

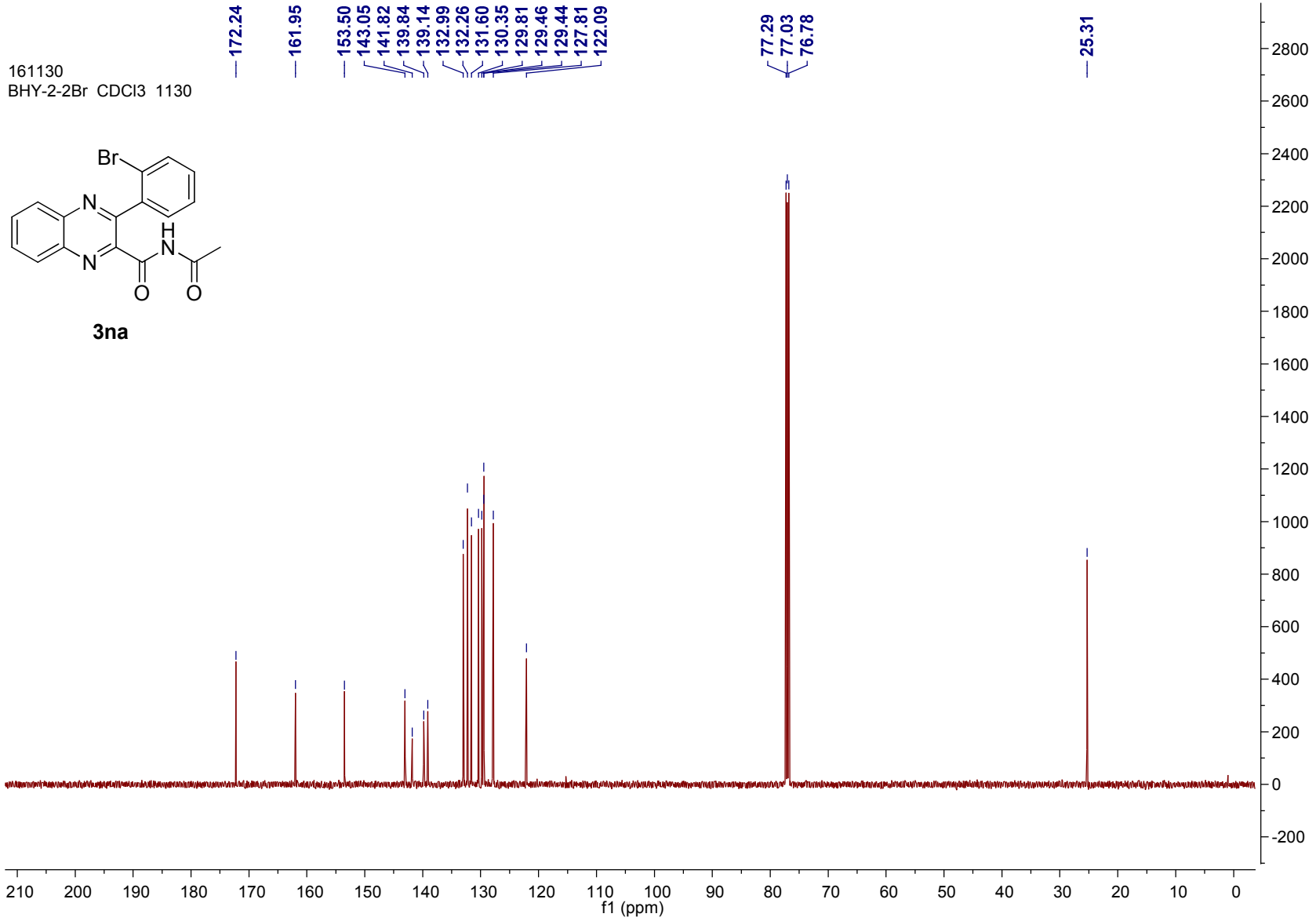

10.294
8.243
8.241
8.227
8.224
8.204
8.201
8.187
8.184
7.962
7.948
7.934
7.931
7.922
7.918
7.902
7.890
7.784
7.780
7.769
7.765
7.754
7.750
7.546
7.543
7.536
7.531
7.527
7.520
7.515
7.511
7.504
7.501
7.403
7.401
7.388
7.386
7.373
7.371
7.276
7.188
7.170
7.151
2.584
F
N
N
H
N
O
O
3la
0.92
1.92
1.95
0.96
1.02
1.00
0.94
2.86
f1 (ppm)

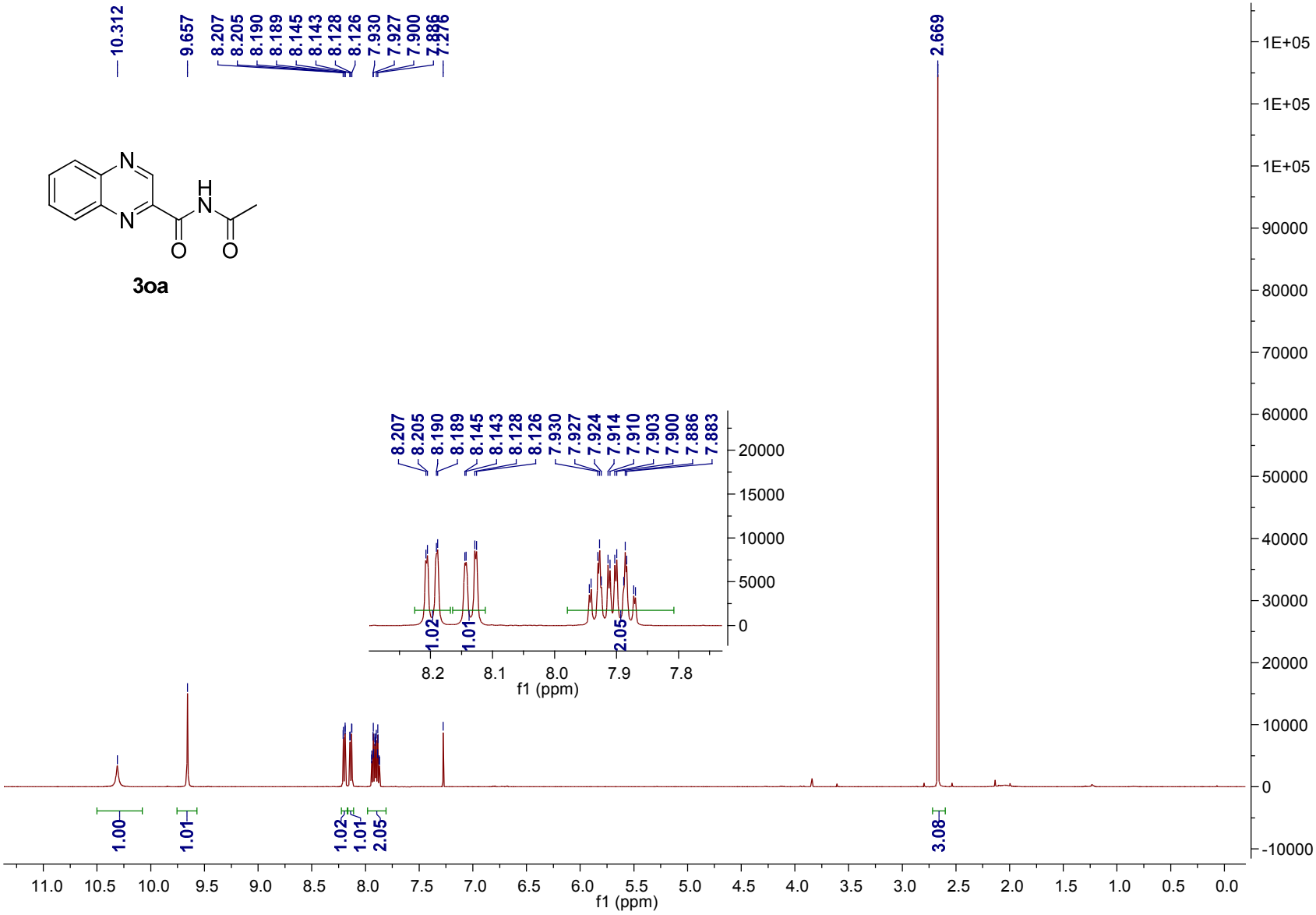

161117
BHY-2-2F CDCl3 1117
172.22
162.41
161.02
159.06
143.39
138.94
132.85
131.43
131.35
130.43
130.41
129.41
129.39
124.70
115.25
115.07
77.29
77.03
76.78
25.29
F
N
N
H
N
O
O
3la
f1 (ppm)

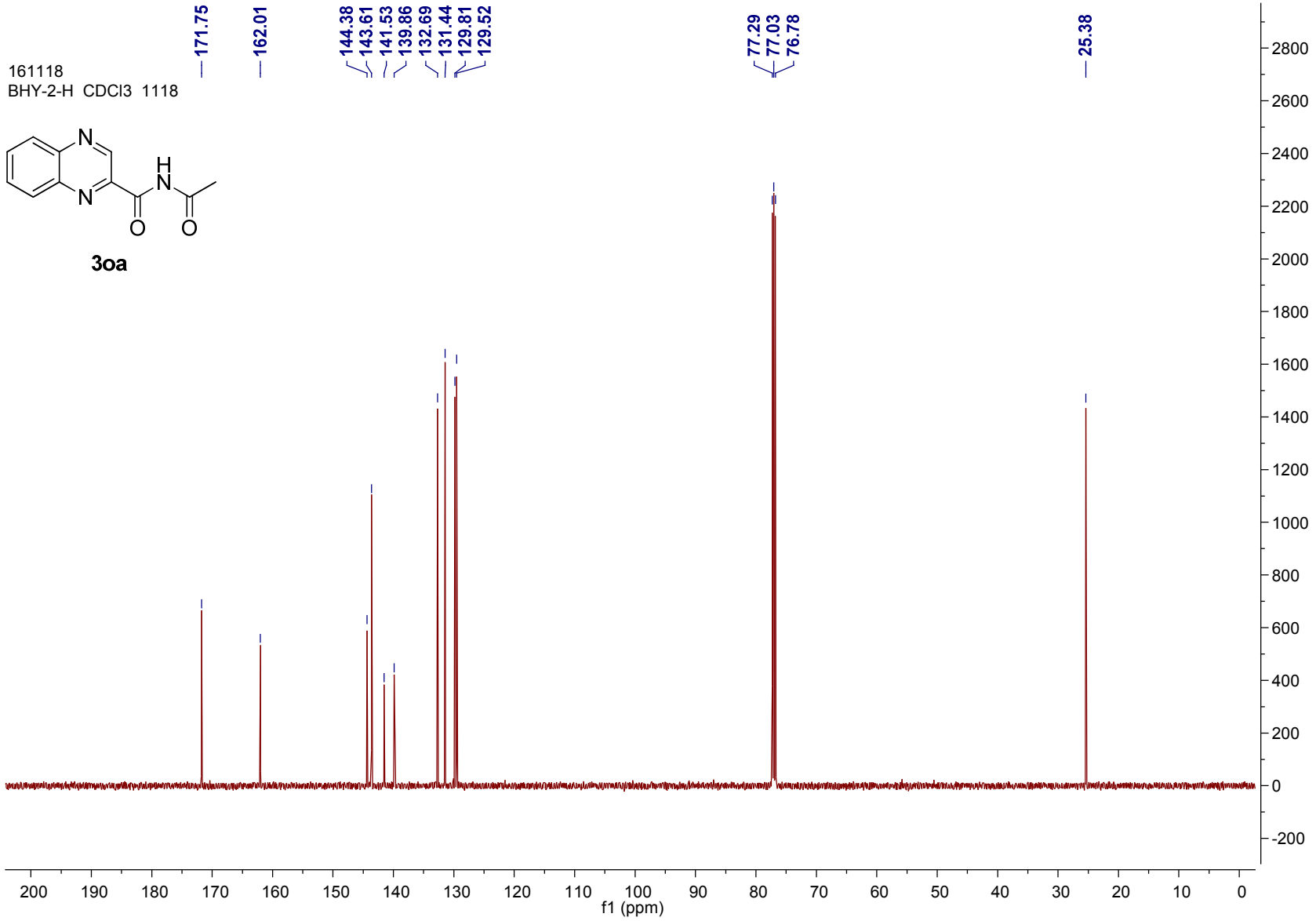

10.053
8.232
8.230
8.215
8.213
8.175
8.173
8.159
8.156
7.909
7.906
7.892
7.889
7.878
7.875
7.861
7.859
7.746
7.743
7.731
7.728
7.513
7.512
7.510
7.497
7.276
7.238
7.236
7.223
7.221
7.208
7.207
6.985
6.968
3.758
2.574
MeO
N
H
N
N
O
O
3ma
f1 (ppm)
1.00
1.01
1.01
2.07
1.00
1.06
1.05
1.01
3.11
3.09

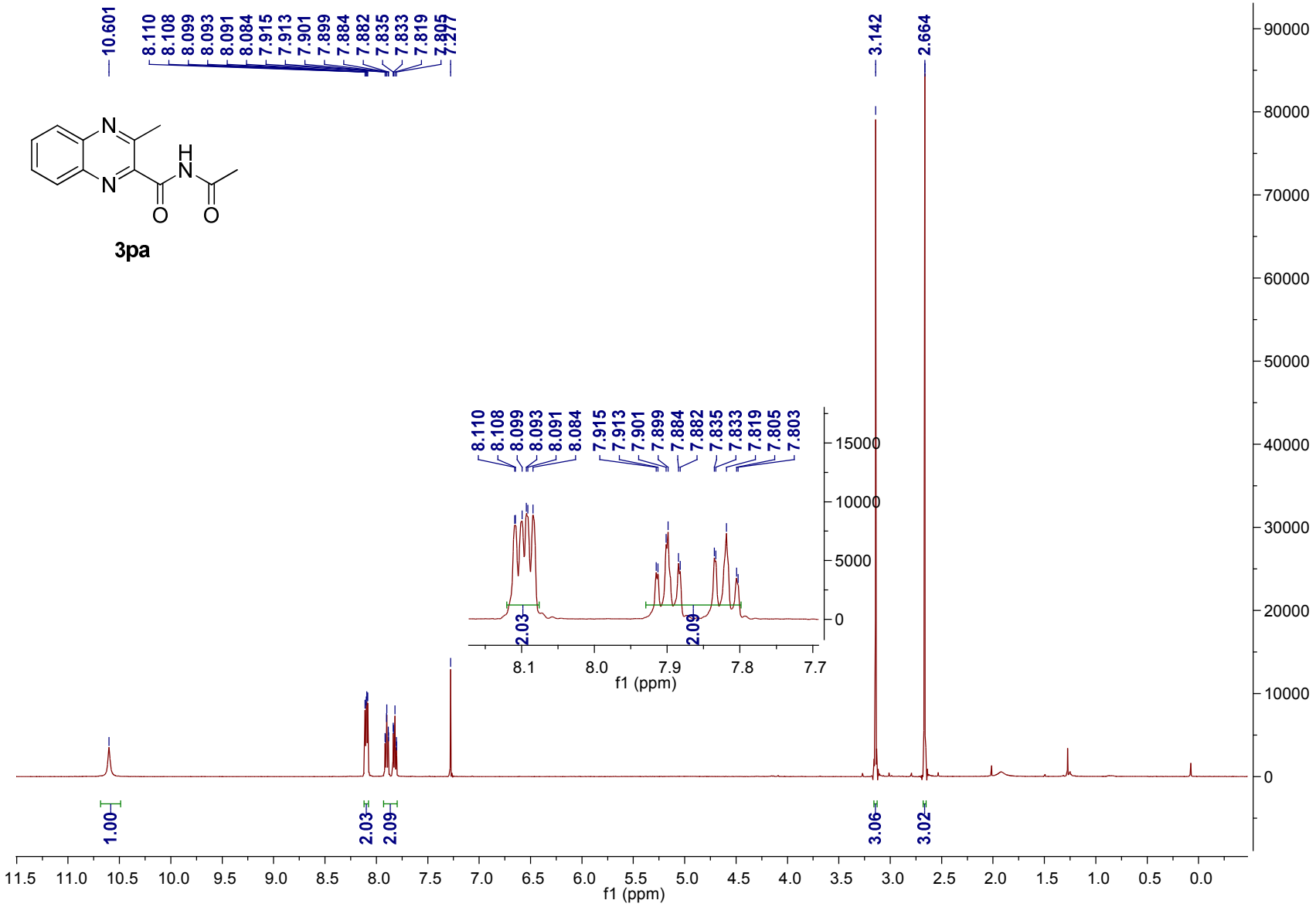

172.41
163.07
156.39
151.25
144.19
143.49
138.68
132.22
131.16
130.74
129.96
129.34
129.31
121.63
110.48
77.29
77.03
76.78
55.03
25.27
161117
BHY-2-2-OCH3 CDCl3 1117
MeO
N
N
H
N
O
O
3ma
f1 (ppm)

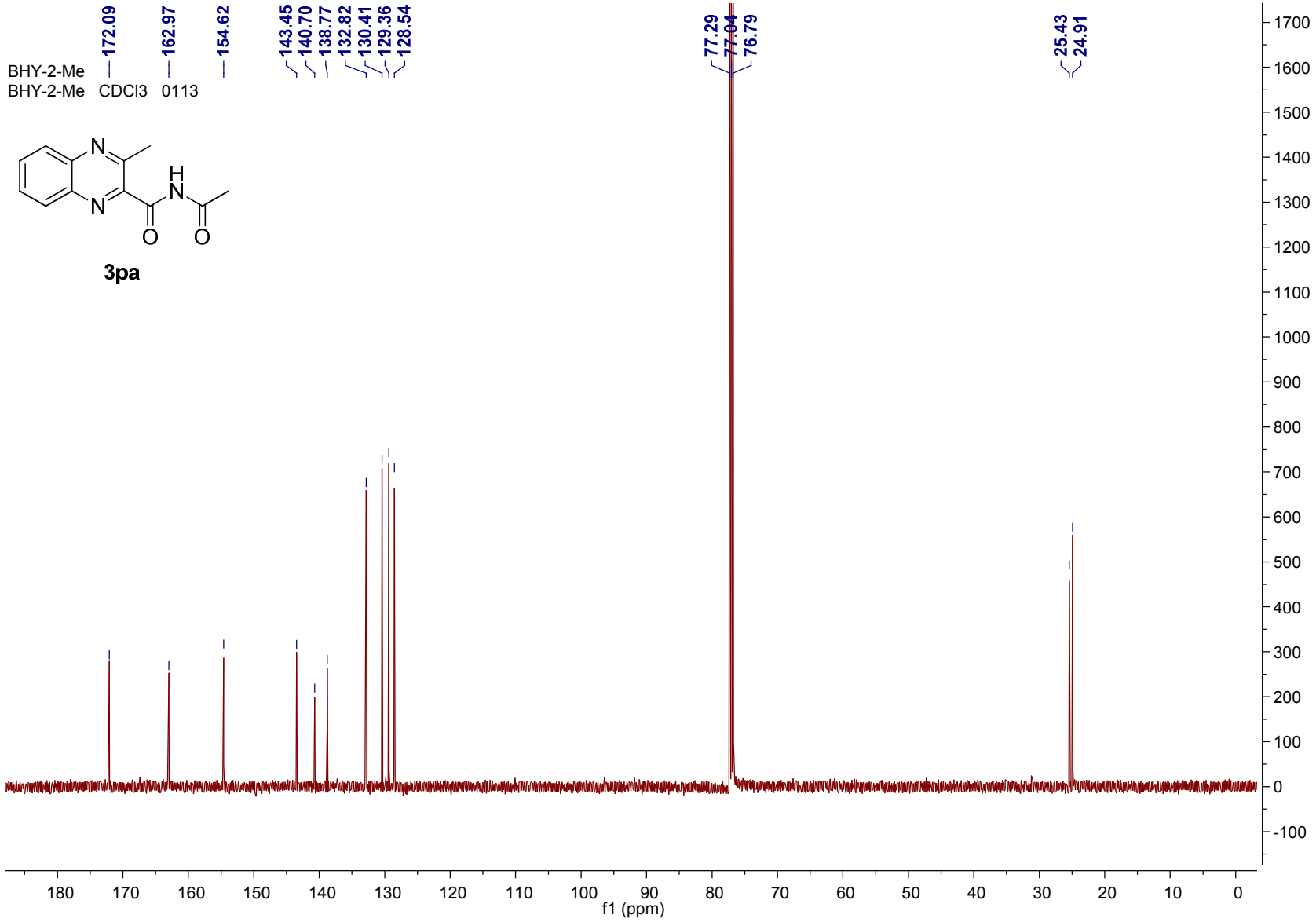

10.412
8.256
8.253
8.240
8.226
8.223
7.994
7.991
7.980
7.977
7.965
7.961
7.957
7.946
7.944
7.941
7.930
7.927
7.688
7.673
7.572
7.563
7.557
7.550
7.548
7.535
7.533
7.415
7.409
7.402
7.399
7.393
7.386
7.381
7.276
2.561
Br
N
N
H
N
O
O
3na
1.00
2.02
2.05
1.01
2.06
1.01
3.05
f1 (ppm)

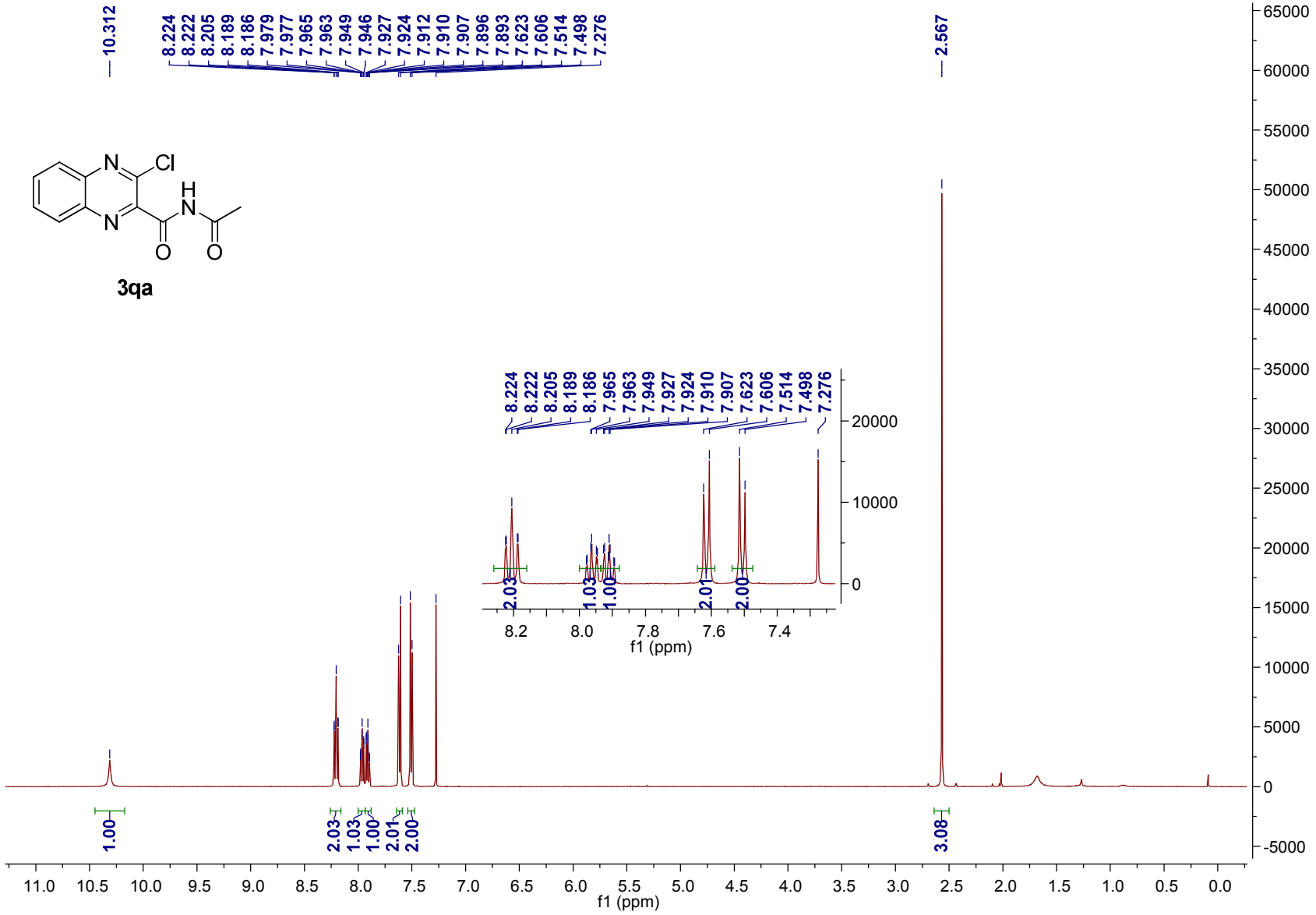

161130
BHY-2-2Br CDCl3 1130
172.24
161.95
153.50
143.05
141.82
139.84
139.14
132.99
132.26
131.60
130.35
129.81
129.46
129.44
127.81
122.09
77.29
77.03
76.78
25.31
Br
N
N
H
N
O
O
3na
f1 (ppm)

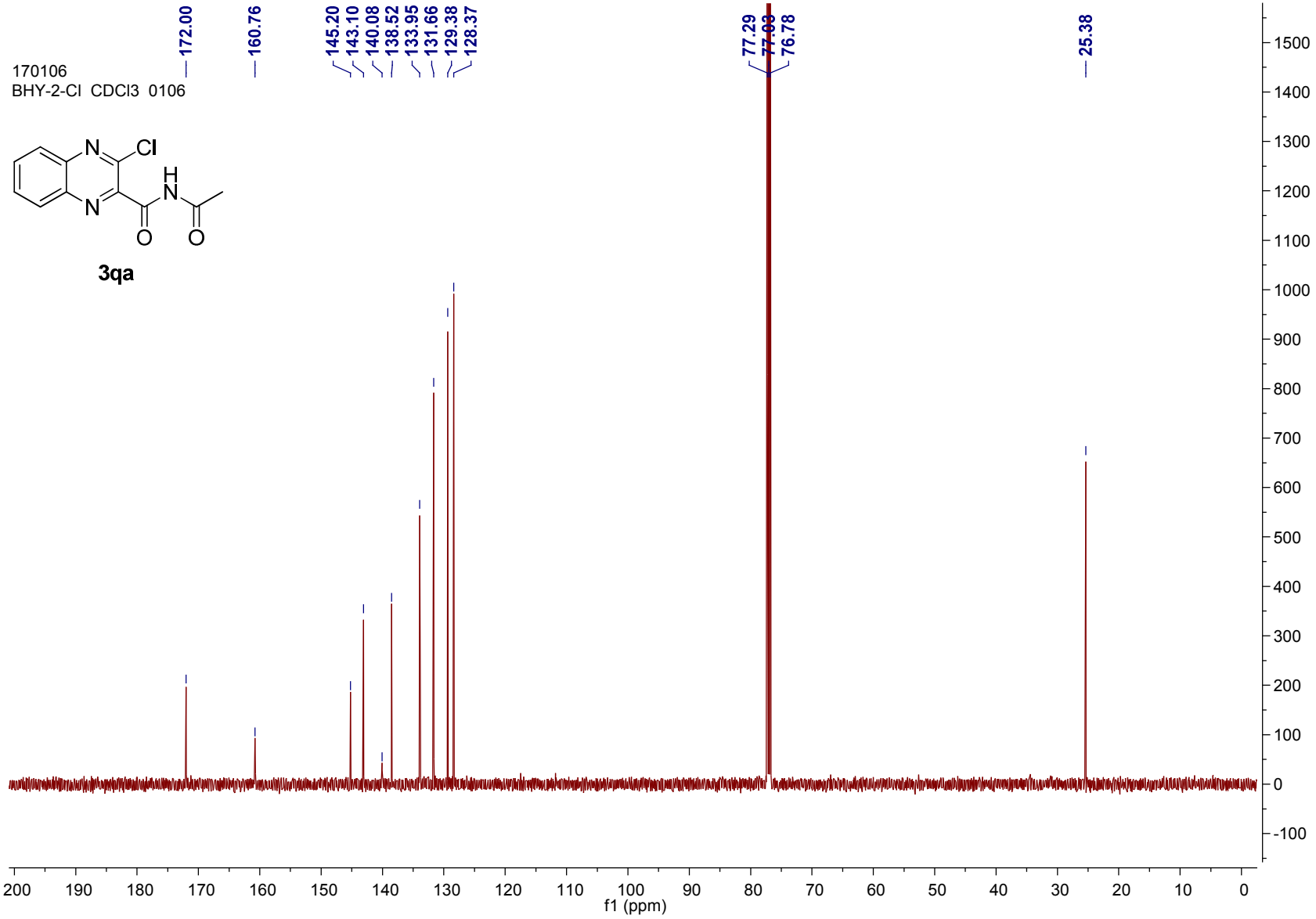

10.312
9.657
8.207
8.205
8.190
8.189
8.145
8.143
8.128
8.126
7.930
7.927
7.900
2.669
3oa
1.00
1.01
1.02
1.01
2.05
3.08
f1 (ppm)

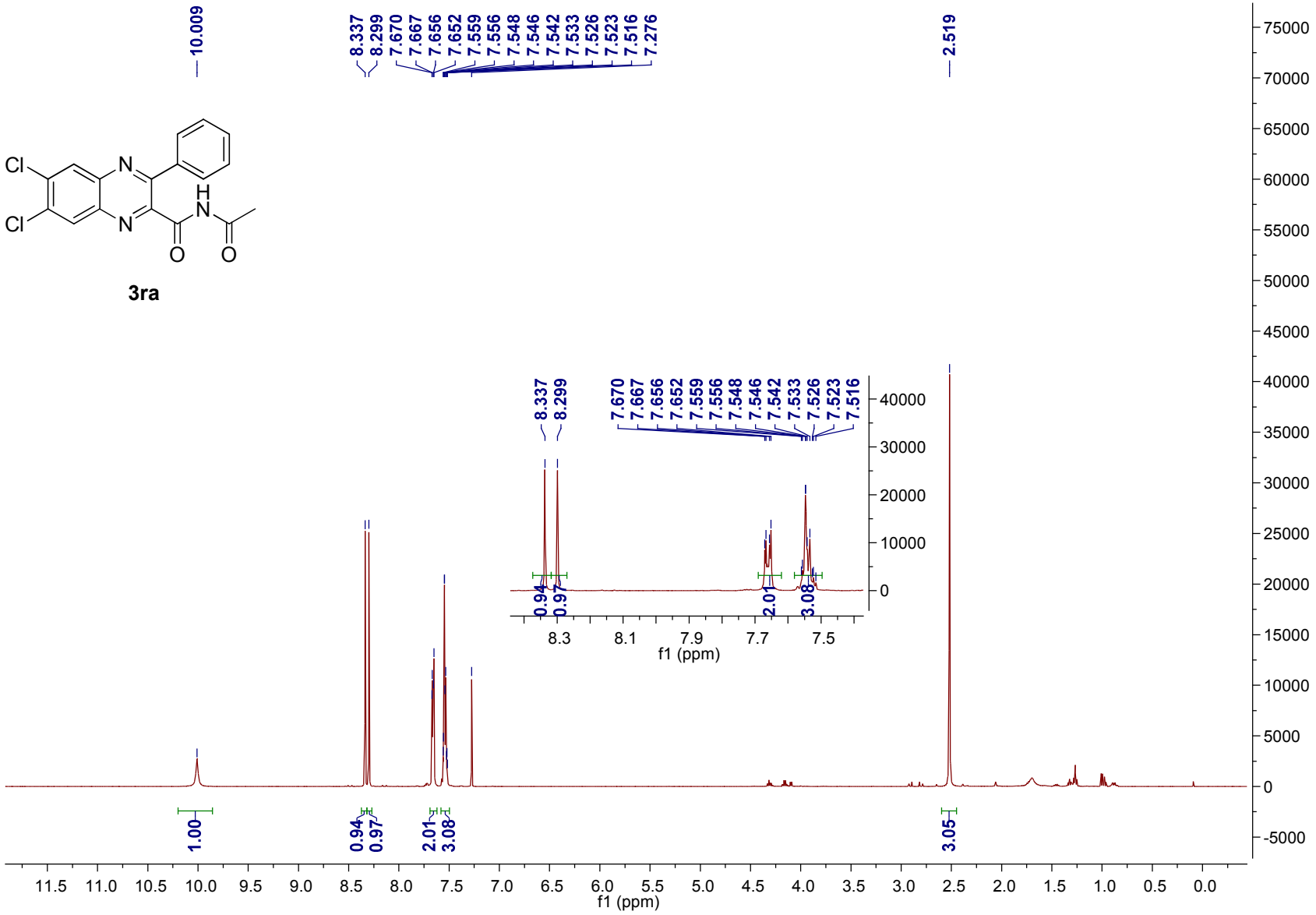

171.75
162.01
144.38
143.61
141.53
139.86
132.69
131.44
129.81
129.52
77.29
77.03
76.78
25.38
161118
BHY-2-H CDCl3 1118
3oa
f1 (ppm)

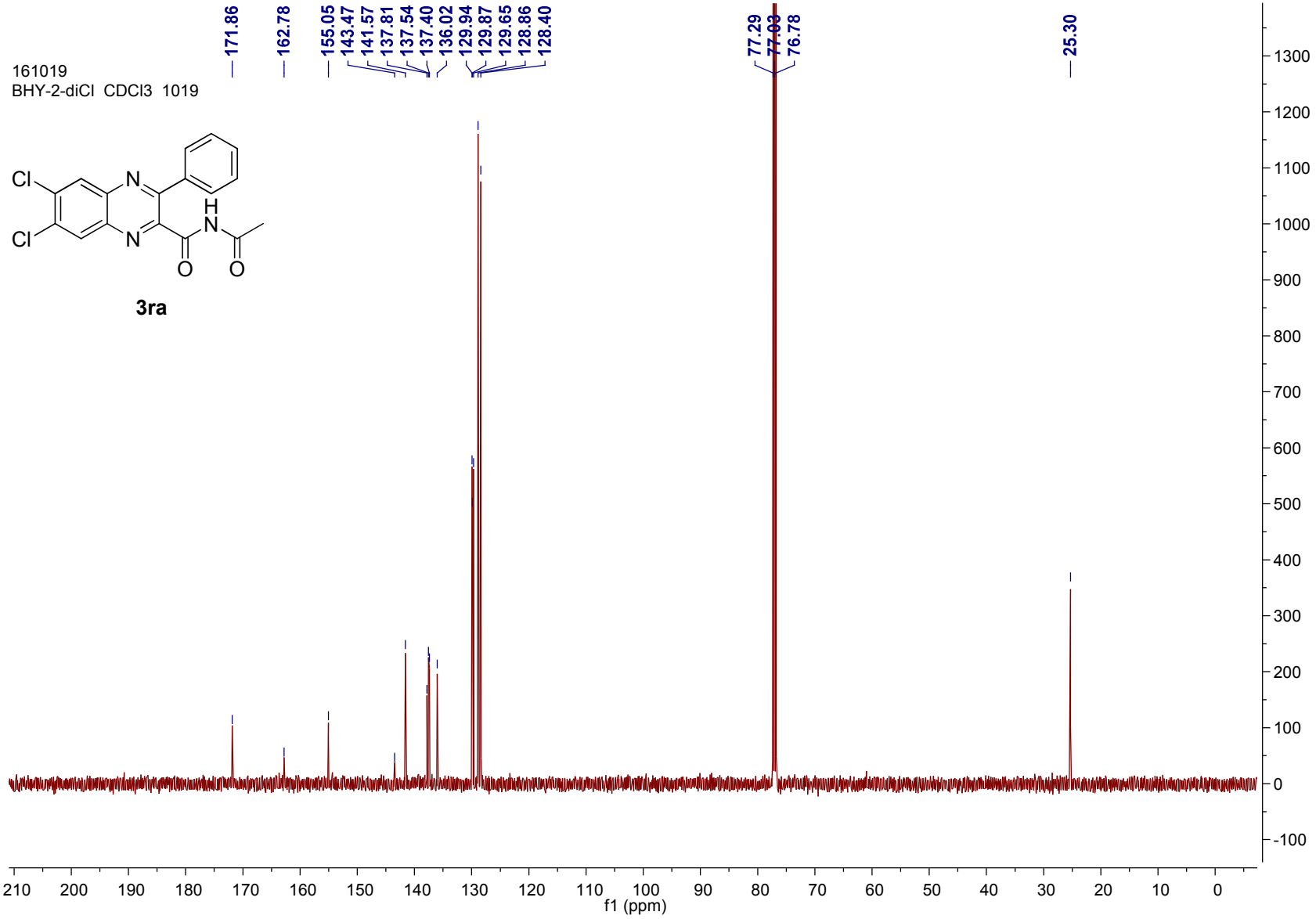

10.601
8.110
8.108
8.099
8.093
8.091
8.084
7.915
7.913
7.901
7.899
7.884
7.882
7.835
7.833
7.819
7.805
7.277
3.142
2.664
N
N
H
N
O
O
3pa
8.110
8.108
8.099
8.093
8.091
8.084
7.915
7.913
7.901
7.899
7.884
7.882
7.835
7.833
7.819
7.805
7.803
2.03
2.09
f1 (ppm)
1.00
2.03
2.09
3.06
3.02
f1 (ppm)

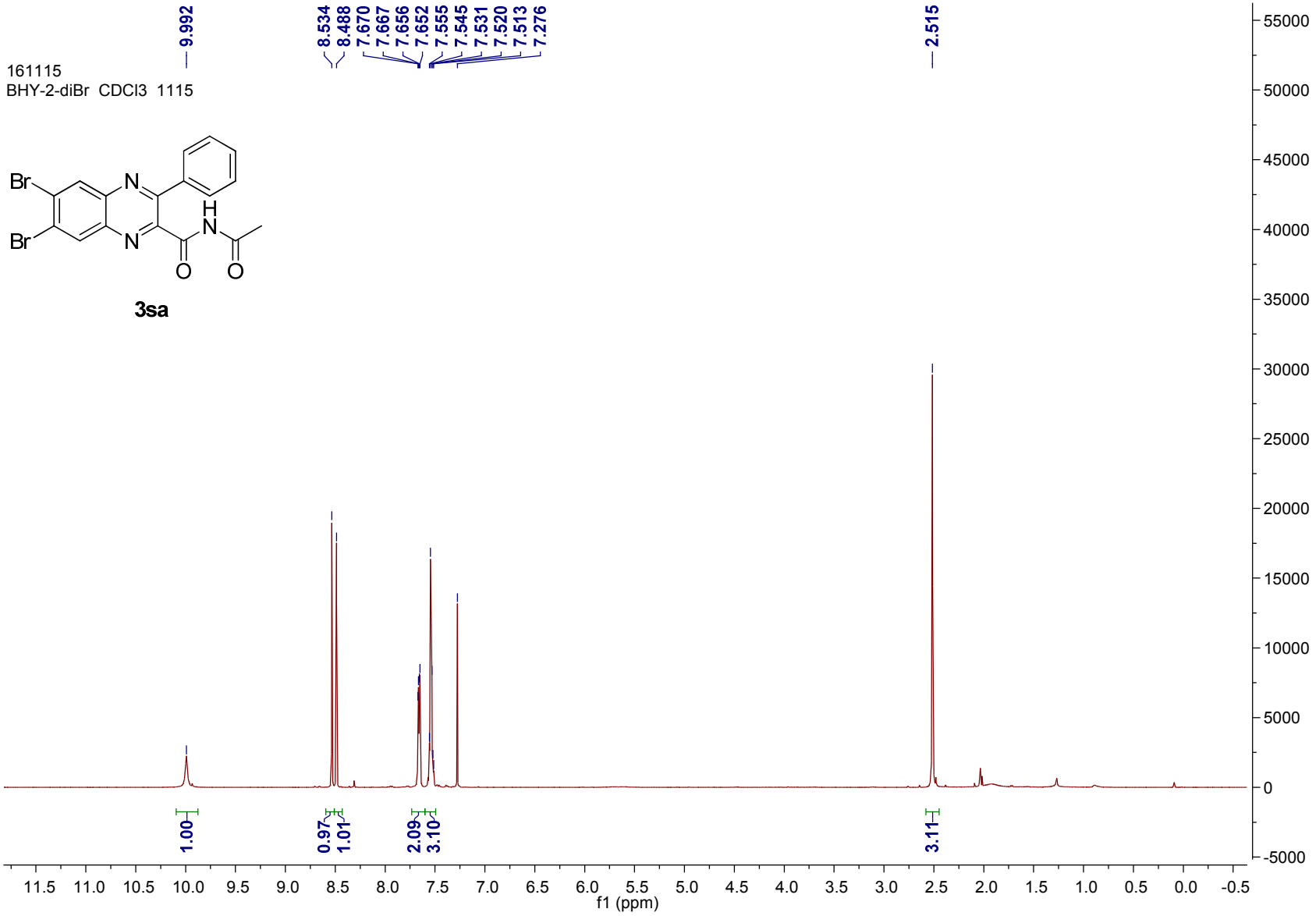

172.09
162.97
154.62
143.45
140.70
138.77
132.82
130.41
129.36
128.54
77.29
77.04
76.79
25.43
24.91
BHY-2-Me
BHY-2-Me CDCl3 0113
N
N
H
N
O
O
3pa
f1 (ppm)

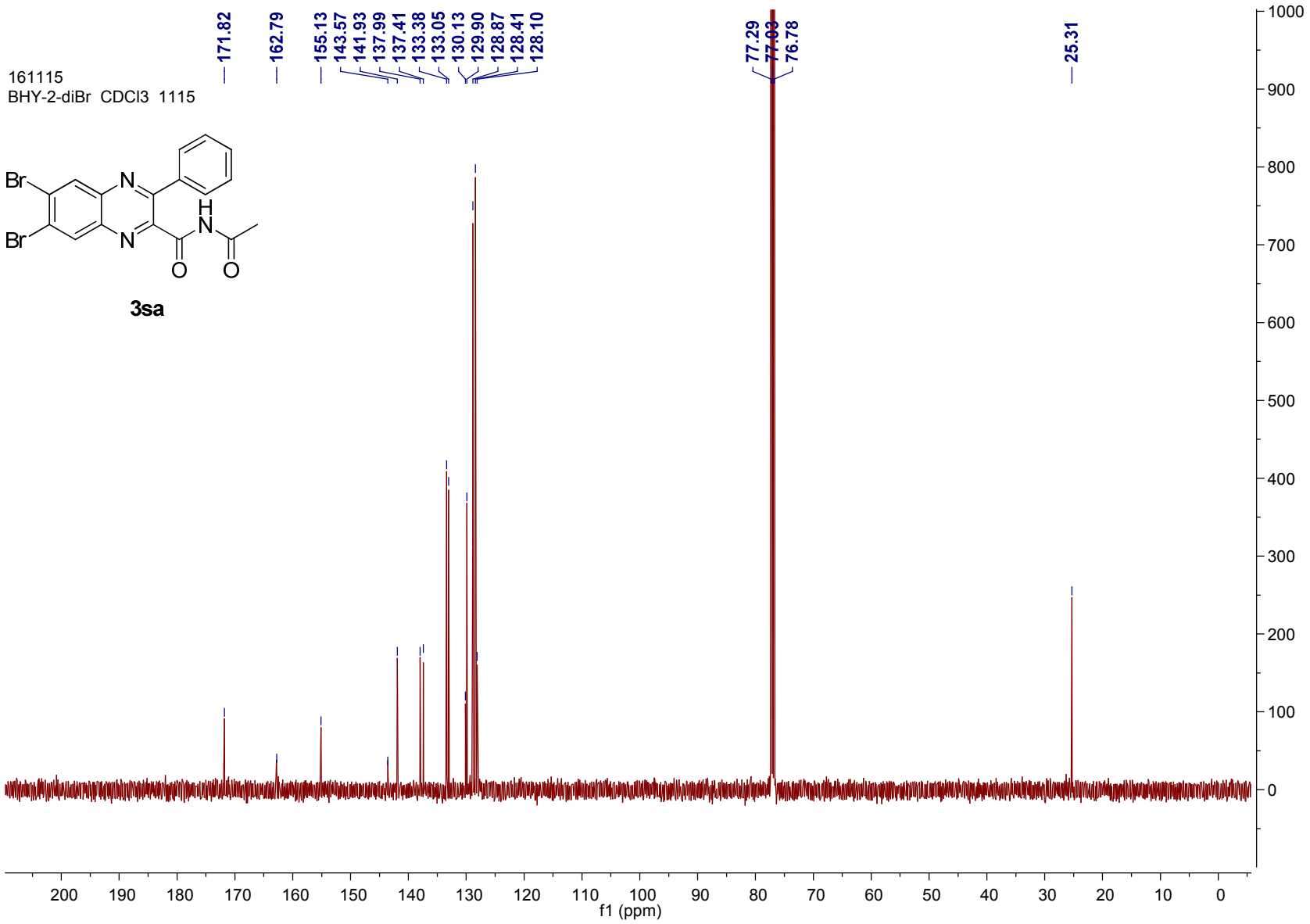

10.312
8.224
8.222
8.205
8.189
8.186
7.979
7.977
7.965
7.963
7.949
7.946
7.927
7.924
7.912
7.910
7.907
7.896
7.893
7.623
7.606
7.514
7.498
7.276
2.567
Cl
N
H
N
O
O
3qa
f1 (ppm)
1.00
2.03
1.03
1.00
2.01
2.00
3.08

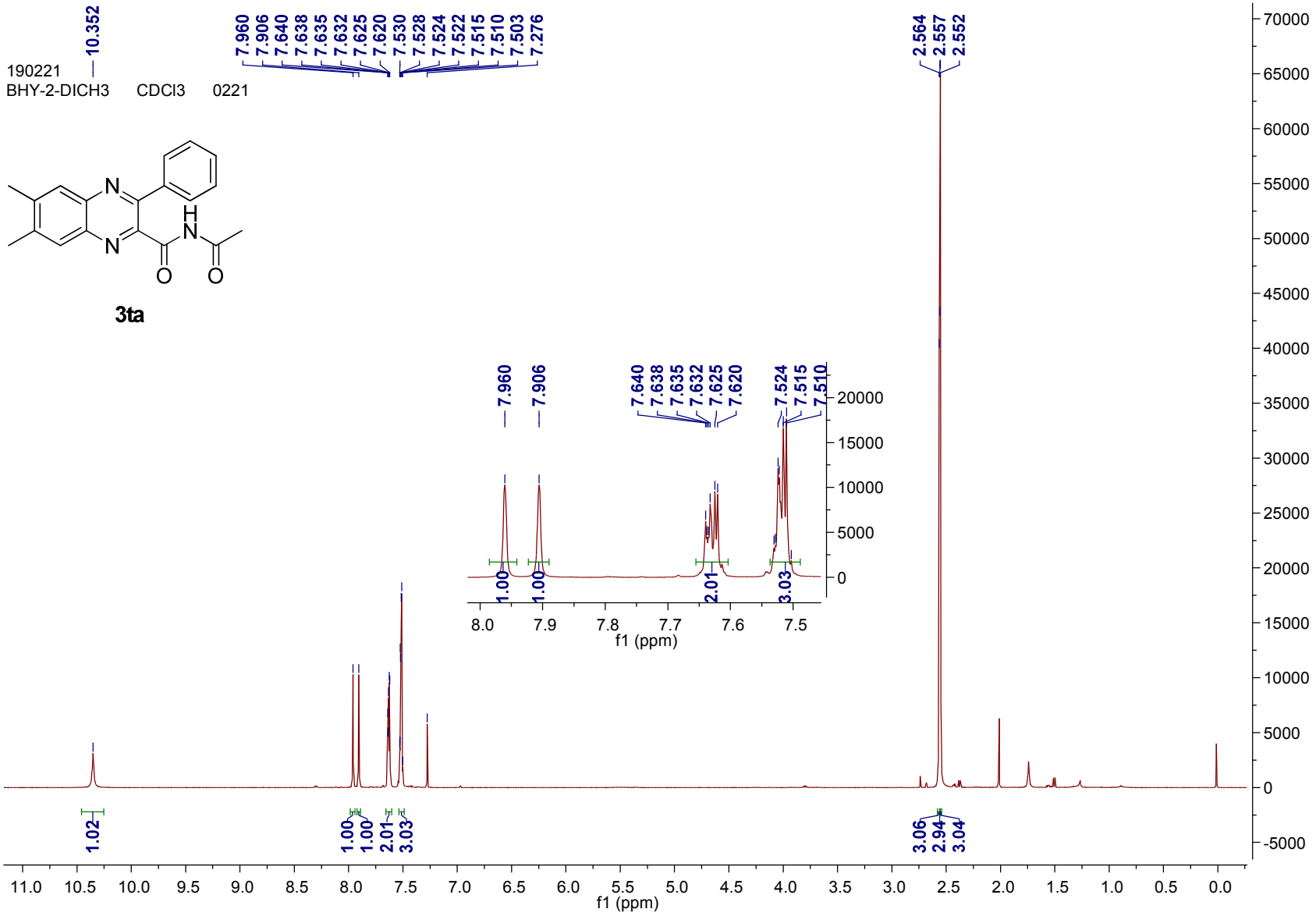

172.00
160.76
145.20
143.10
140.08
138.52
133.95
131.66
129.38
128.37
77.29
77.03
76.78
25.38
170106
BHY-2-Cl CDCl3 0106
N
Cl
H
N
N
O
O
3qa
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

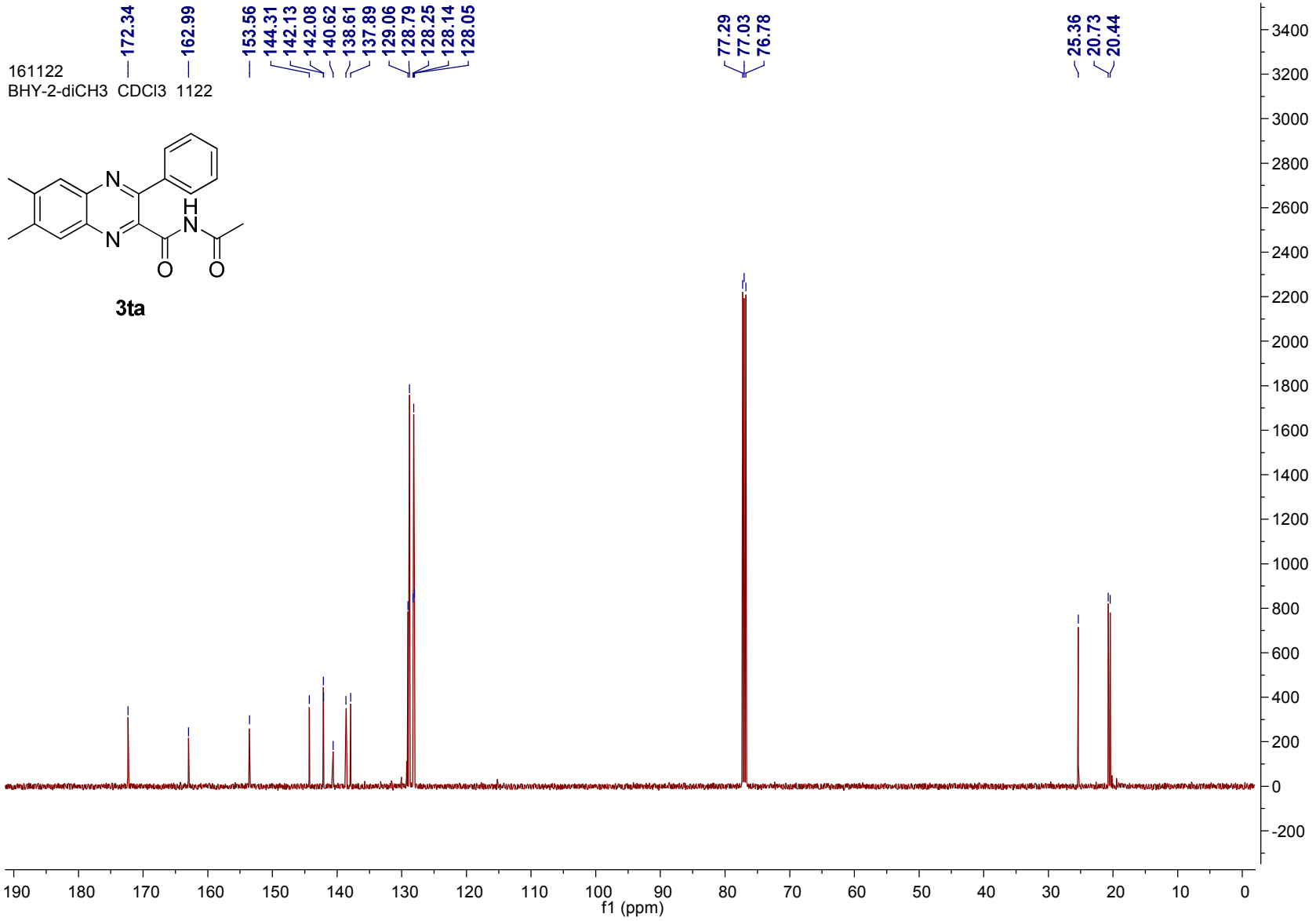

10.009
8.337
8.299
7.670
7.667
7.656
7.652
7.559
7.556
7.548
7.546
7.542
7.533
7.526
7.523
7.516
7.276
2.519
Cl
Cl
N
N
H
N
O
O
3ra
1.00
0.94
0.97
2.01
3.08
3.05
f1 (ppm)

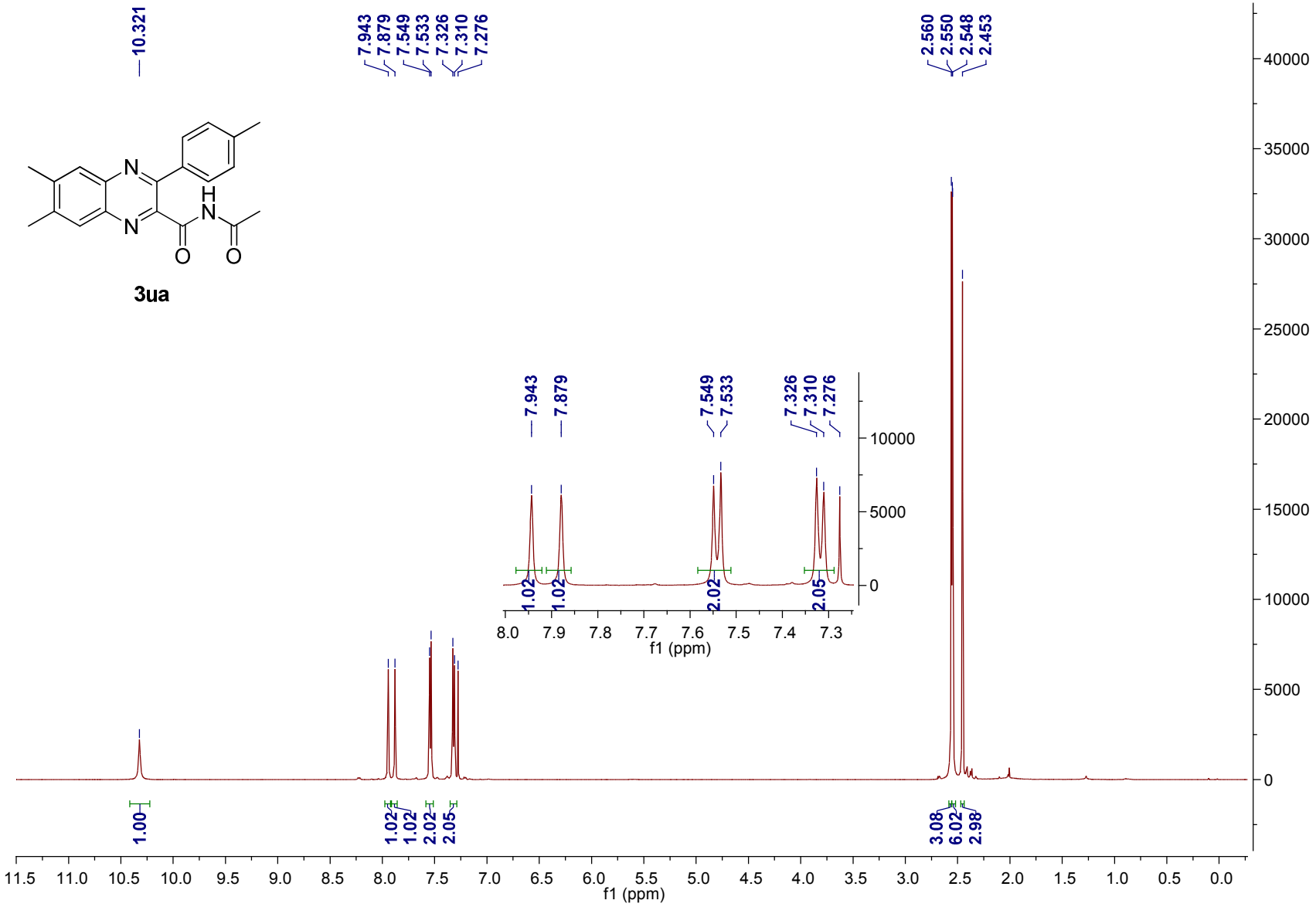

171.86
162.78
155.05
143.47
141.57
137.81
137.54
137.40
136.02
129.94
129.87
129.65
128.86
128.40
77.29
77.03
76.78
25.30
161019
BHY-2-diCl CDCl3 1019
Cl
Cl
N
N
H
N
O
O
3ra
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

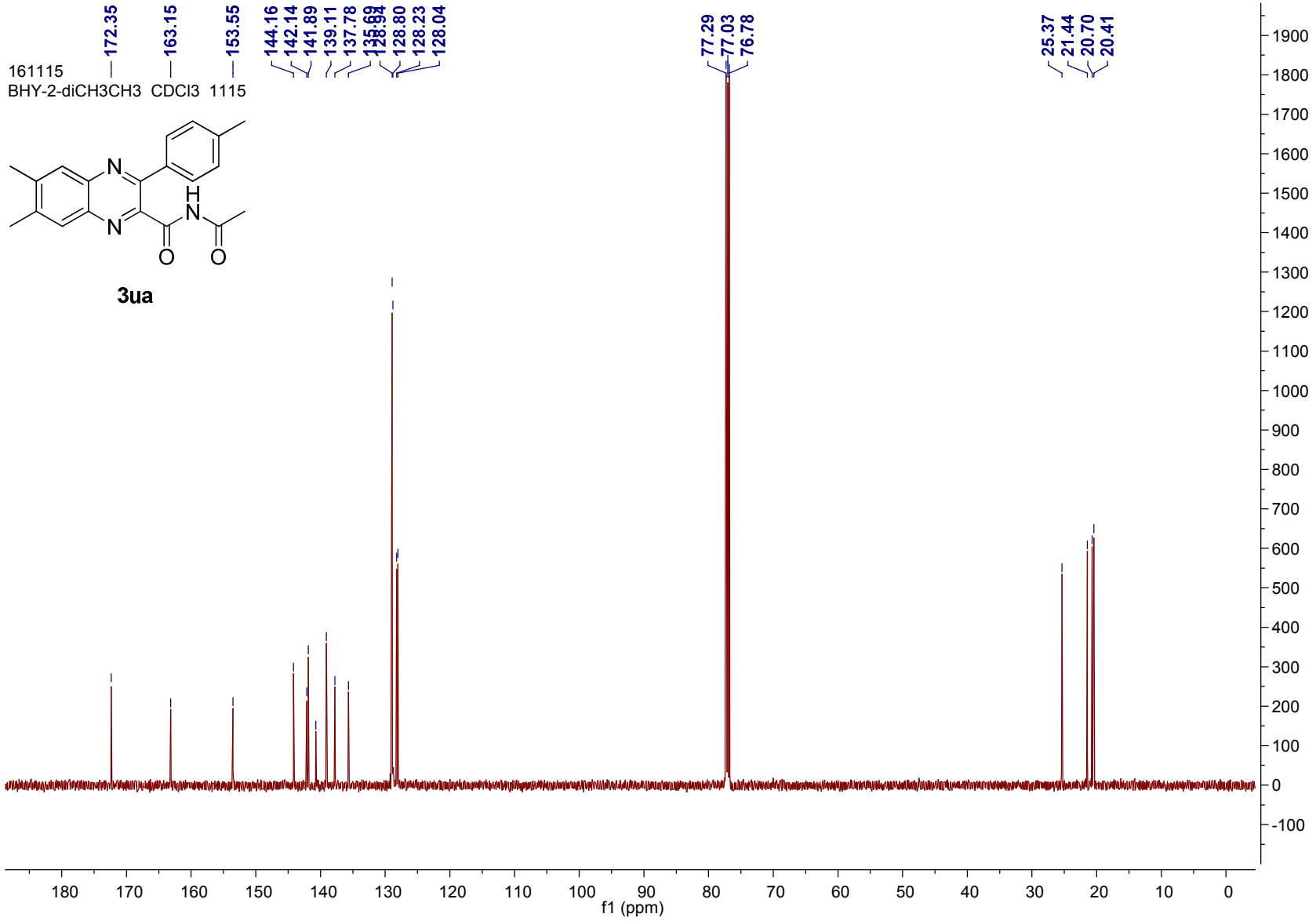

161115
BHY-2-diBr CDCl3 1115
9.992
8.534
8.488
7.670
7.667
7.656
7.652
7.555
7.545
7.531
7.520
7.513
7.276
2.515
Br
Br
N
N
H
N
O
O
3sa
1.00
0.97
1.01
2.09
3.10
3.11
f1 (ppm)

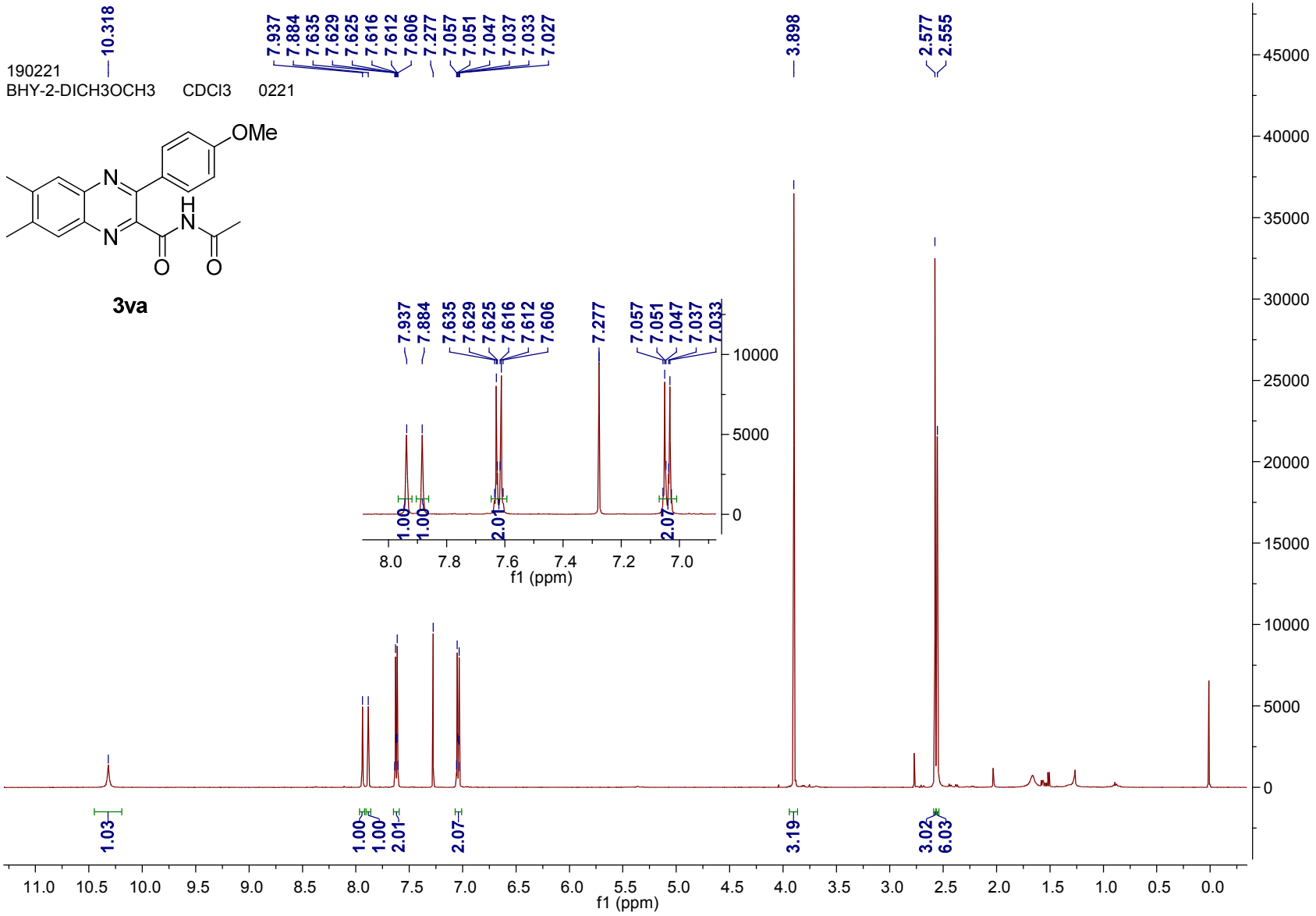

161115
BHY-2-diBr CDCl3 1115
171.82
162.79
155.13
143.57
141.93
137.99
137.41
133.38
133.05
130.13
129.90
128.87
128.41
128.10
77.29
77.03
76.78
25.31
Br
Br
N
N
H
N
O
O
3sa
f1 (ppm)

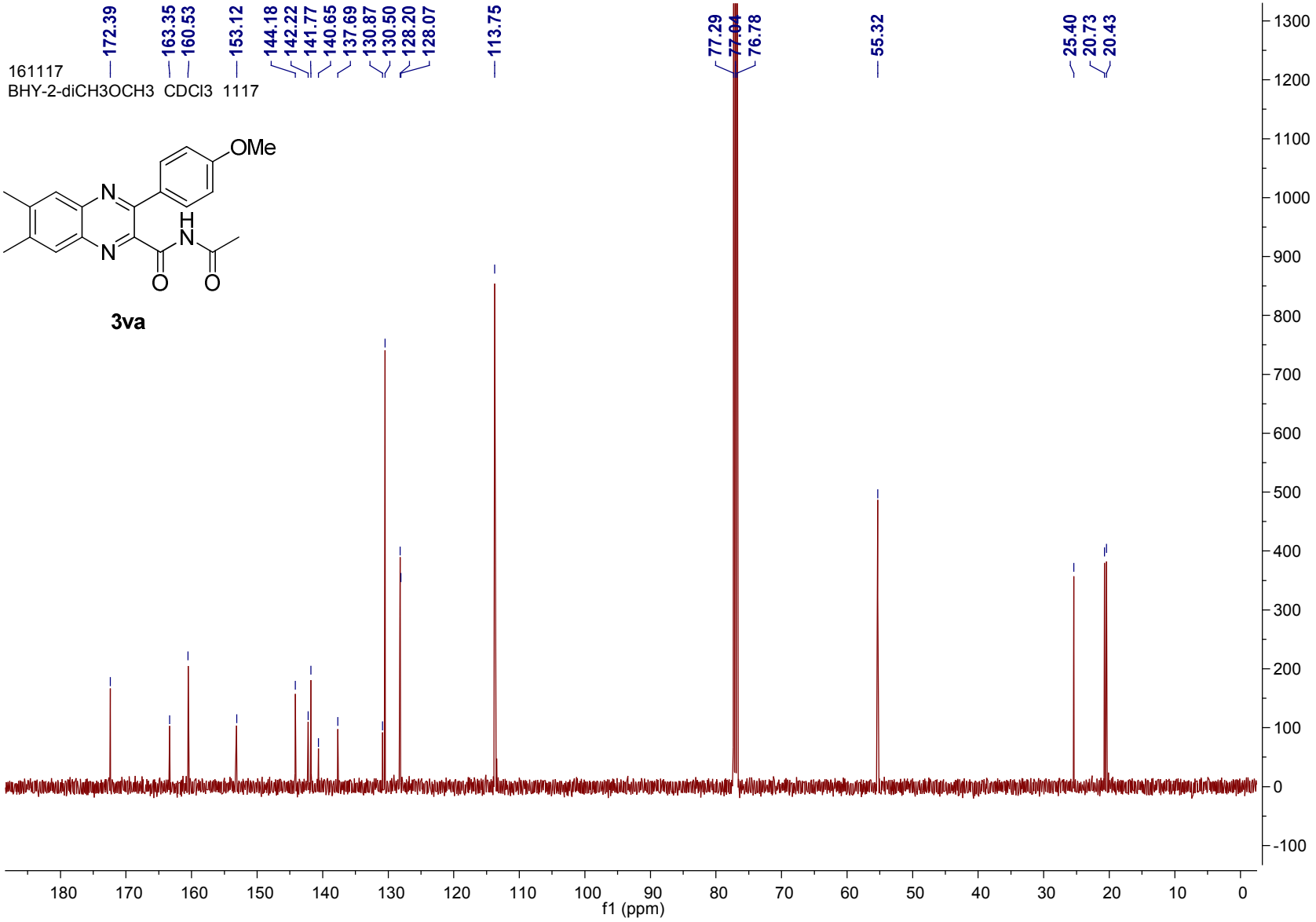

190221
BHY-2-DICH3 CDCl3 0221
10.352
7.960
7.906
7.640
7.638
7.635
7.632
7.625
7.620
7.530
7.528
7.524
7.522
7.515
7.510
7.503
7.276
2.564
2.557
2.552
3ta
1.02
1.00
1.00
2.01
3.03
3.06
2.94
3.04
f1 (ppm)

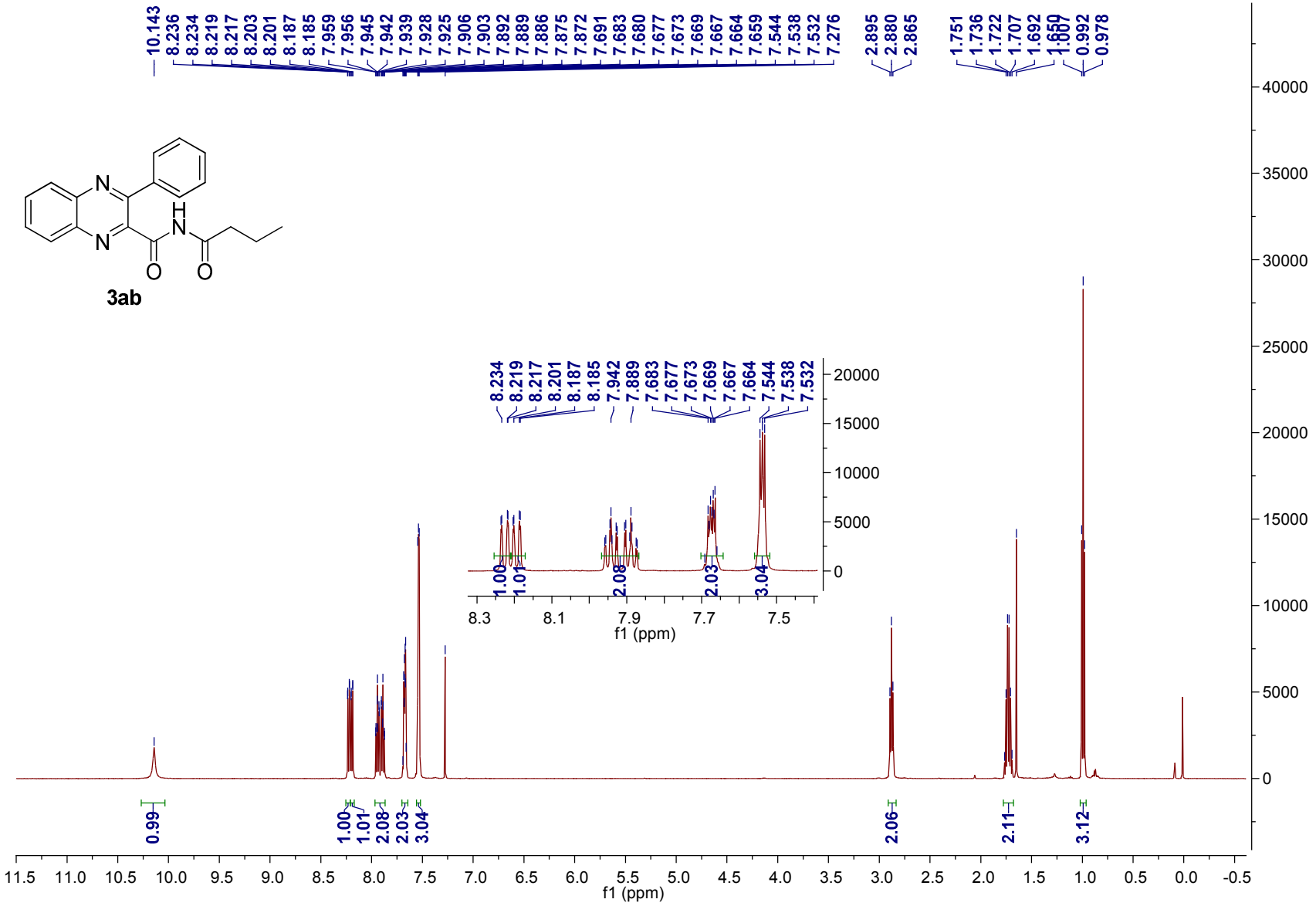

172.34
162.99
153.56
144.31
142.13
142.08
140.62
138.61
137.89
129.06
128.79
128.25
128.14
128.05
77.29
77.03
76.78
25.36
20.73
20.44
161122
BHY-2-diCH3 CDCl3 1122
N
H
N
N
O
O
3ta
f1 (ppm)

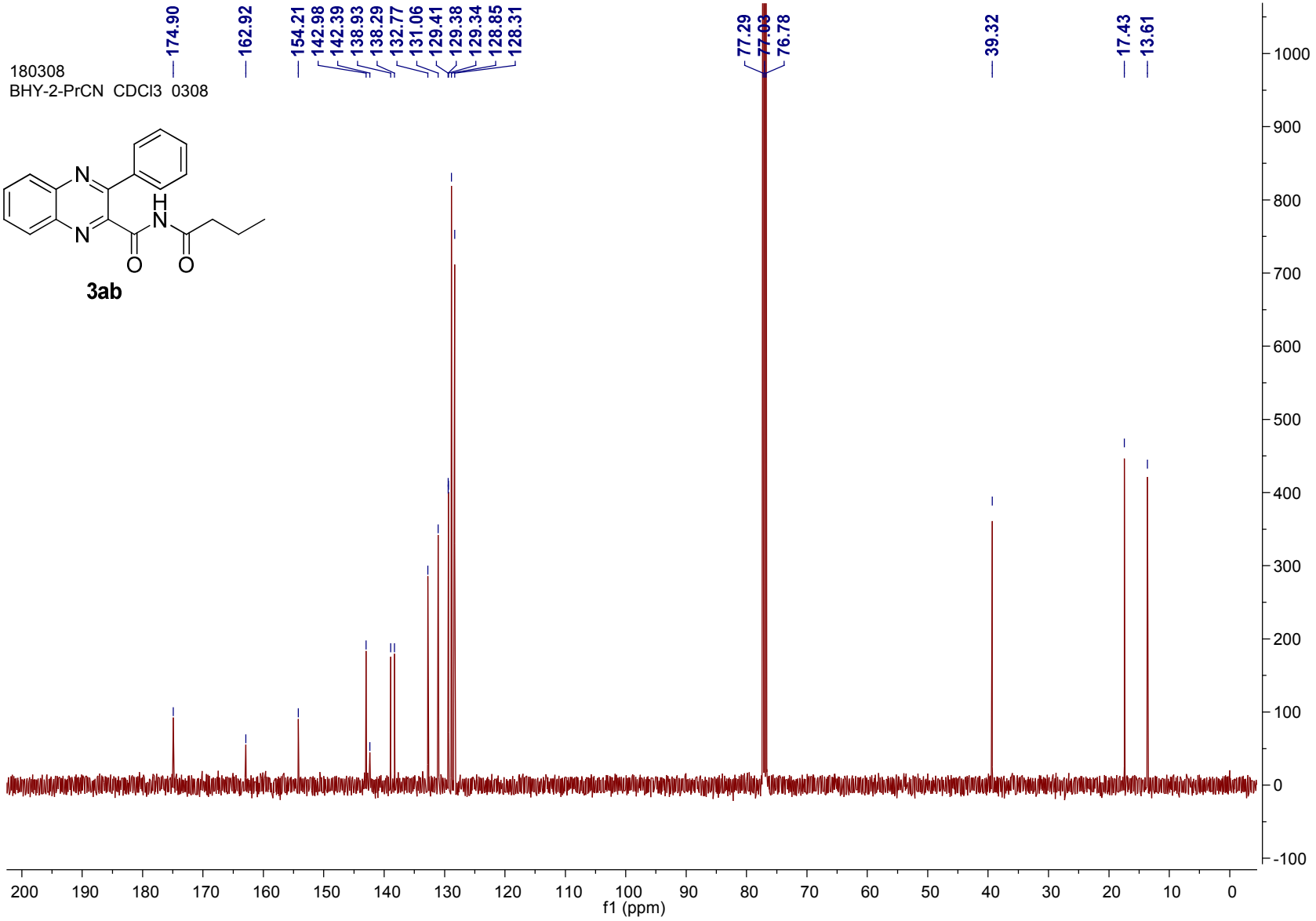

10.321
7.943
7.879
7.549
7.533
7.326
7.310
7.276
2.560
2.550
2.548
2.453
3ua
1.00
1.02
1.02
2.02
2.05
3.08
6.02
2.98
f1 (ppm)

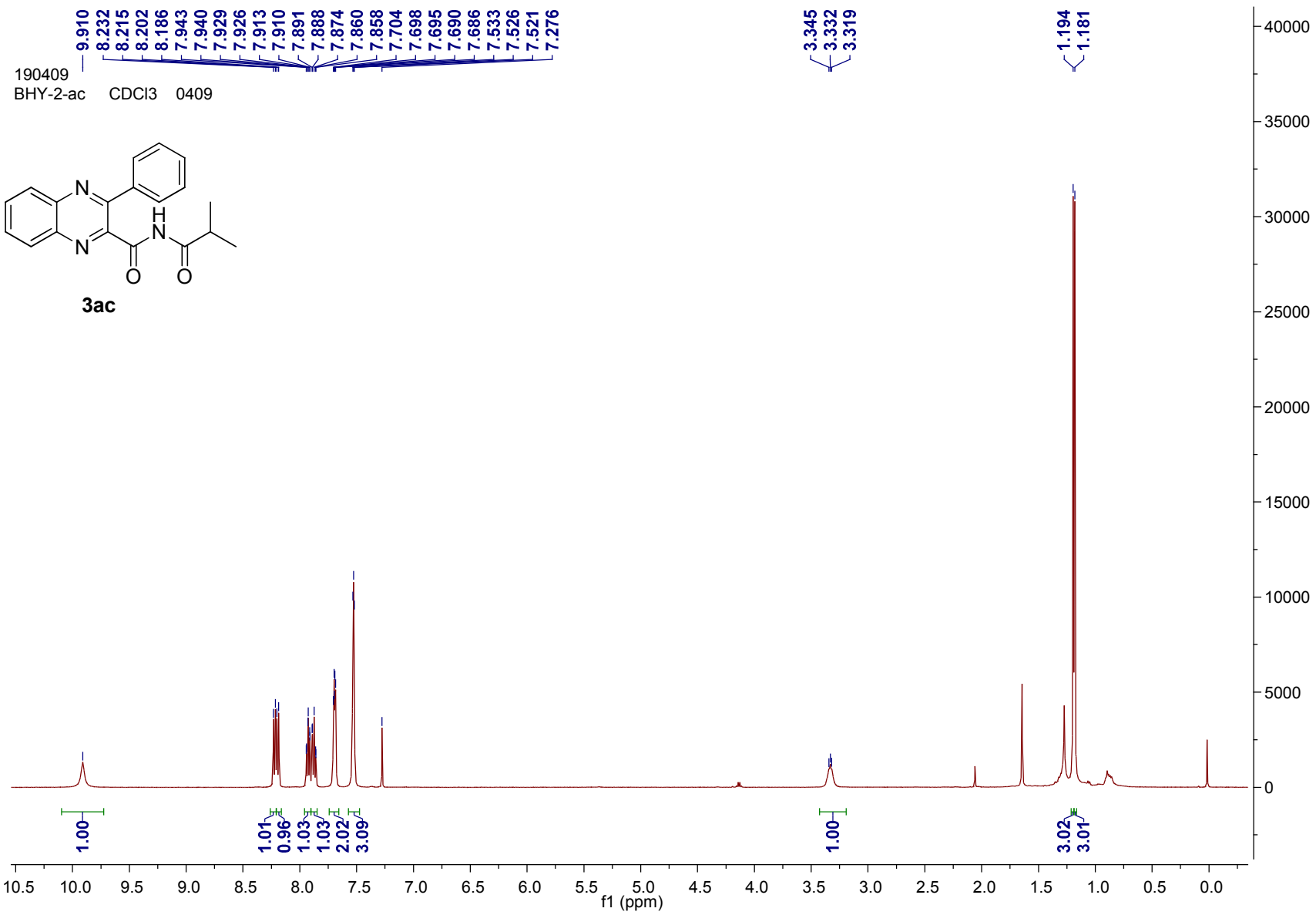

172.35
163.15
153.55
144.16
142.14
141.89
139.11
137.78
135.69
128.94
128.80
128.23
128.04
77.29
77.03
76.78
25.37
21.44
20.70
20.41
161115
BHY-2-diCH3CH3 CDCl3 1115
N
N
H
N
O
O
3ua
f1 (ppm)

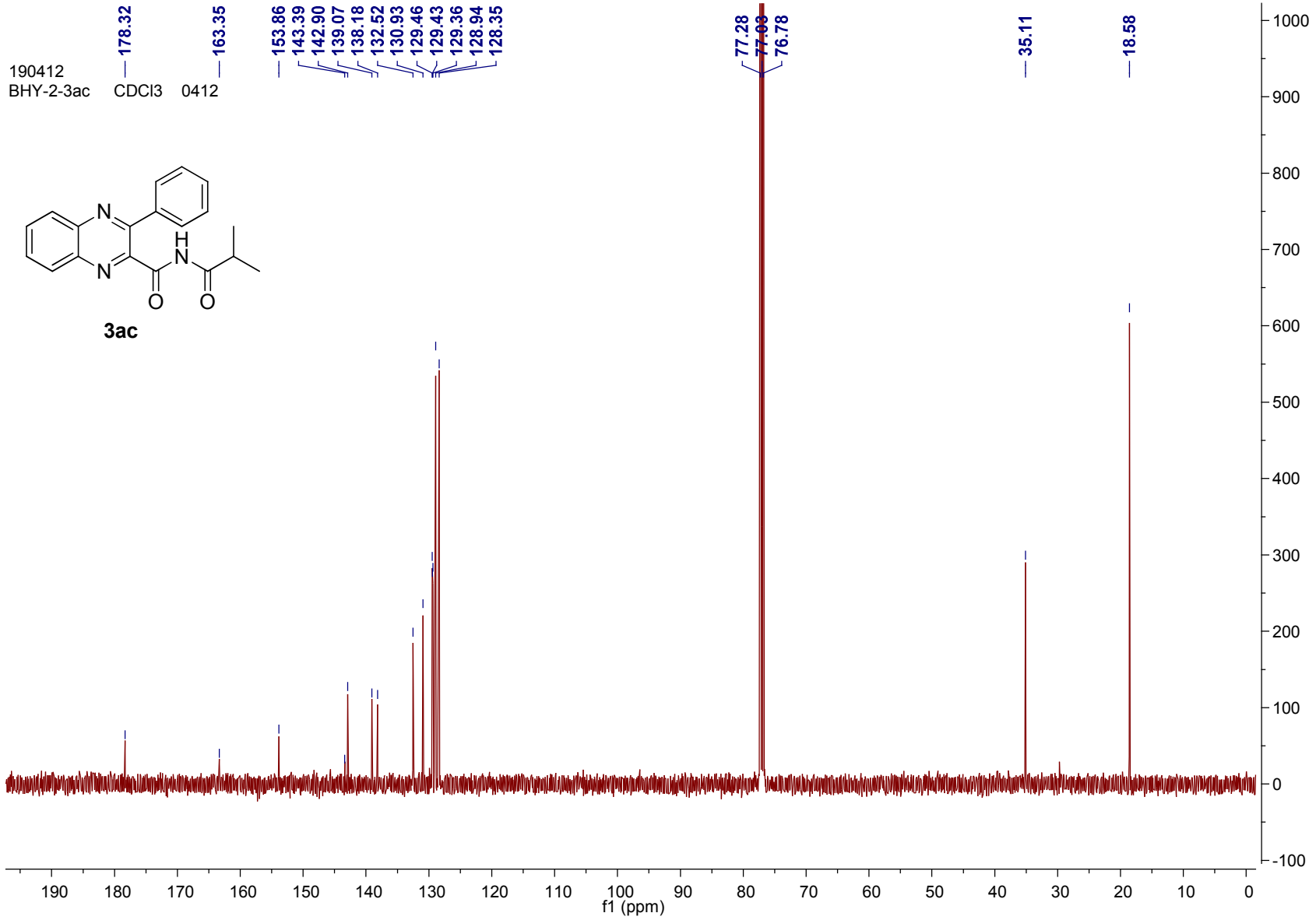

190221
BHY-2-DICH3OCH3 CDCl3 0221
10.318
7.937
7.884
7.635
7.629
7.625
7.616
7.612
7.606
7.277
7.057
7.051
7.047
7.037
7.033
7.027
3.898
2.577
2.555
OMe
N
H
N
N
O
O
3va
f1 (ppm)
1.03
1.00
1.00
2.01
2.07
3.19
3.02
6.03

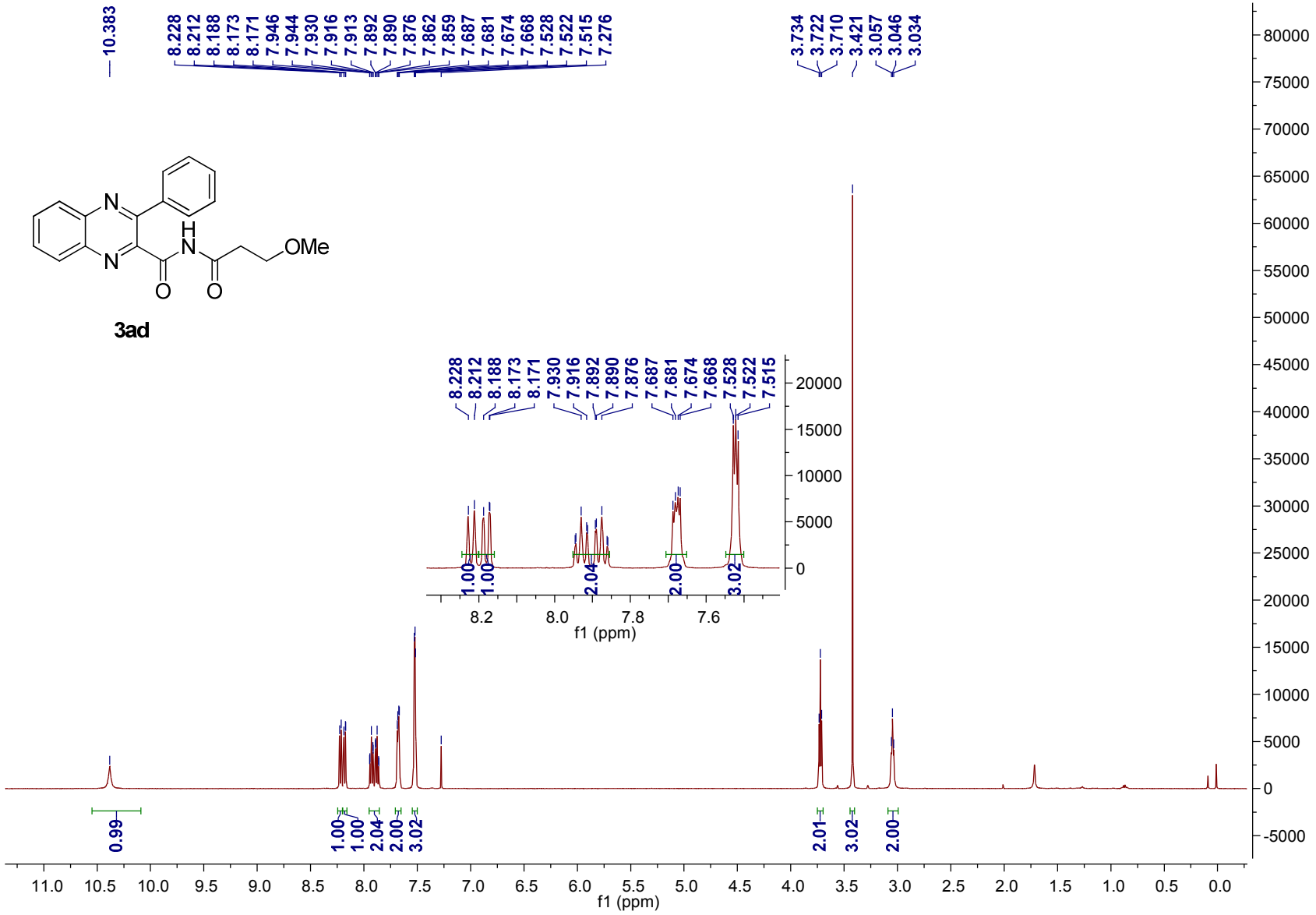

172.39
163.35
160.53
153.12
144.18
142.22
141.77
140.65
137.69
130.87
130.50
128.20
128.07
113.75
77.29
77.04
76.78
55.32
25.40
20.73
20.43
161117
BHY-2-diCH3OCH3 CDCl3 1117
OMe
N
H
N
N
O
O
3va
f1 (ppm)

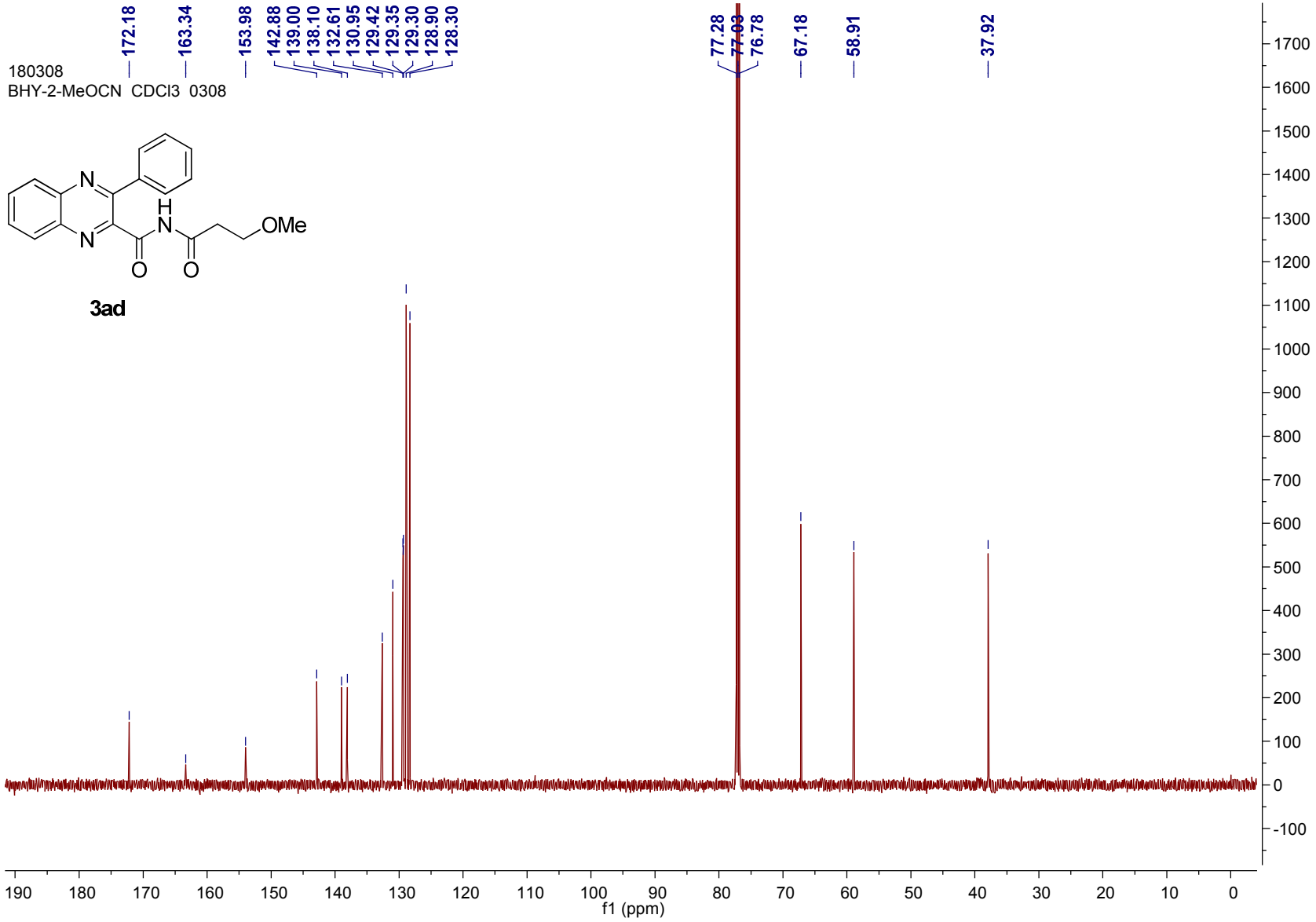

10.143
8.236
8.234
8.219
8.217
8.203
8.201
8.187
8.185
7.959
7.956
7.945
7.942
7.939
7.928
7.925
7.906
7.903
7.892
7.889
7.886
7.875
7.872
7.691
7.683
7.680
7.677
7.673
7.669
7.667
7.664
7.659
7.544
7.538
7.532
7.276
2.895
2.880
2.865
1.751
1.736
1.722
1.707
1.692
1.659
1.007
0.992
0.978
3ab
f1 (ppm)
0.99
1.00
1.01
2.08
2.03
3.04
2.06
2.11
3.12

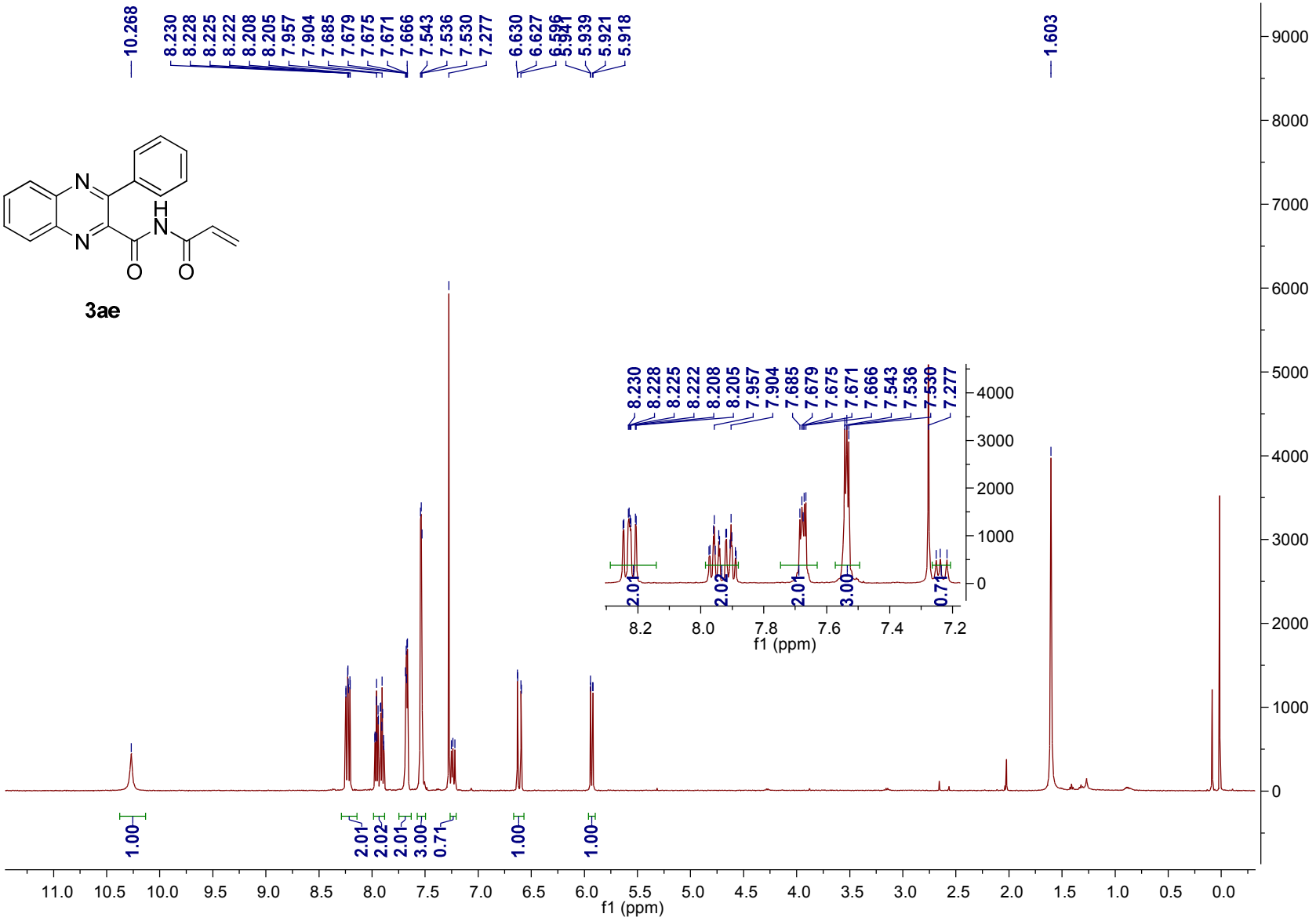

180308
BHY-2-PrCN CDCl3 0308
174.90
162.92
154.21
142.98
142.39
138.93
138.29
132.77
131.06
129.41
129.38
129.34
128.85
128.31
77.29
77.03
76.78
39.32
17.43
13.61
3ab
f1 (ppm)

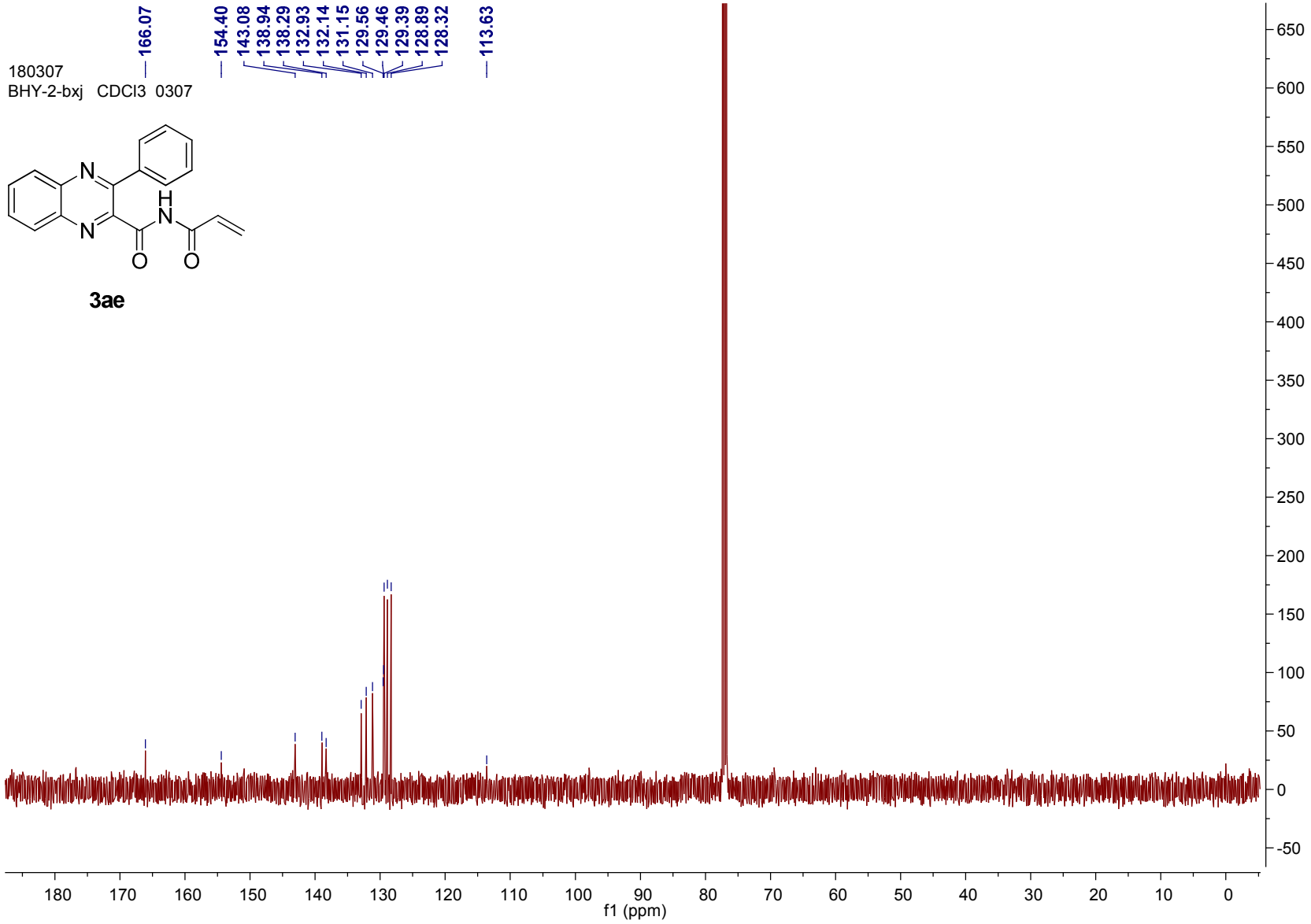

9.910
8.232
8.215
8.202
8.186
7.943
7.940
7.929
7.926
7.913
7.910
7.891
7.888
7.874
7.860
7.858
7.704
7.698
7.695
7.690
7.686
7.533
7.526
7.521
7.276
3.345
3.332
3.319
1.194
1.181
190409
BHY-2-ac CDCl3 0409
3ac
1.00
1.01
0.96
1.03
1.03
2.02
3.09
1.00
3.02
3.01
f1 (ppm)

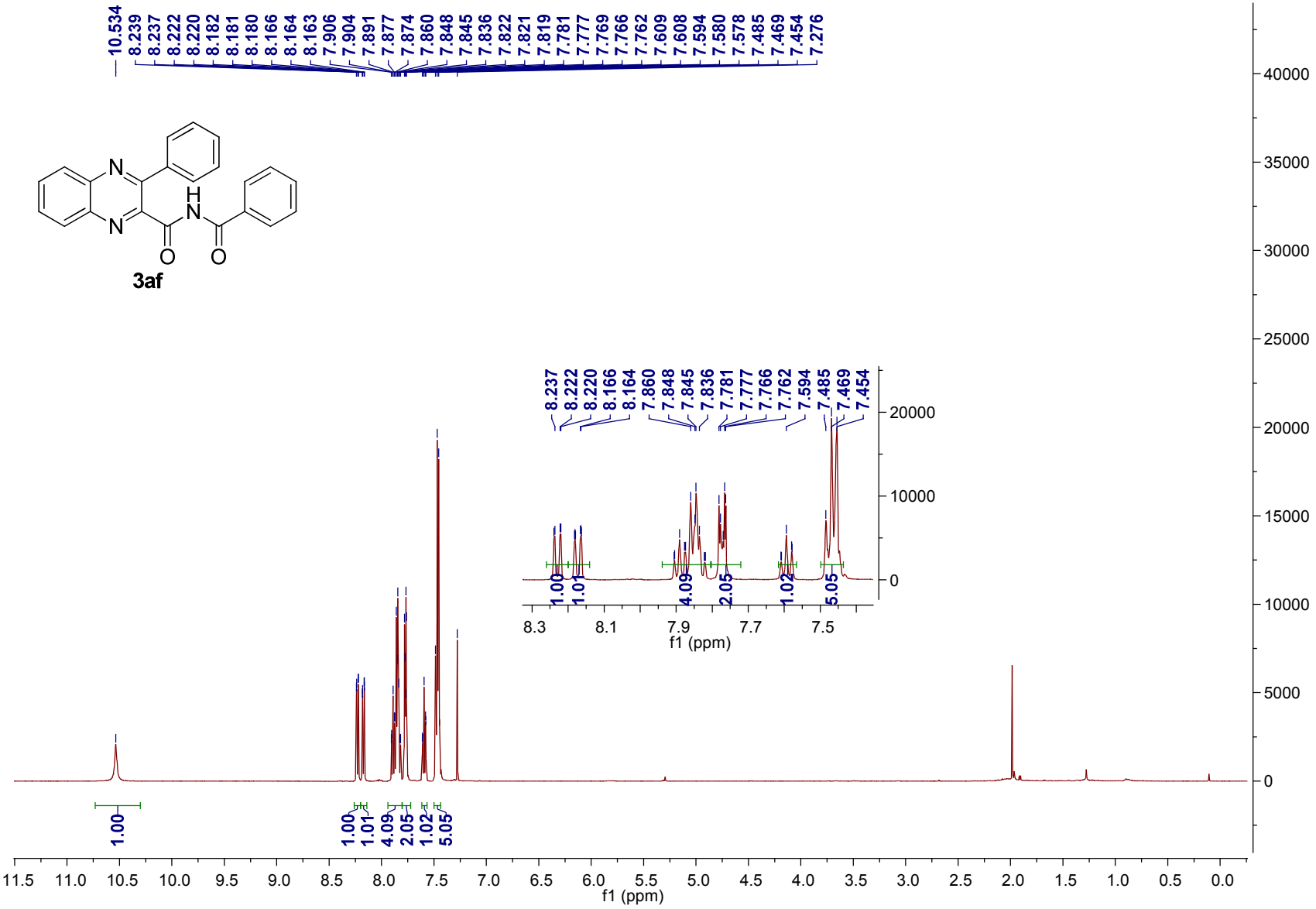

190412
BHY-2-3ac CDCl3 0412
178.32
163.35
153.86
143.39
142.90
139.07
138.18
132.52
130.93
129.46
129.43
129.36
128.94
128.35
77.28
77.03
76.78
35.11
18.58
3ac
f1 (ppm)

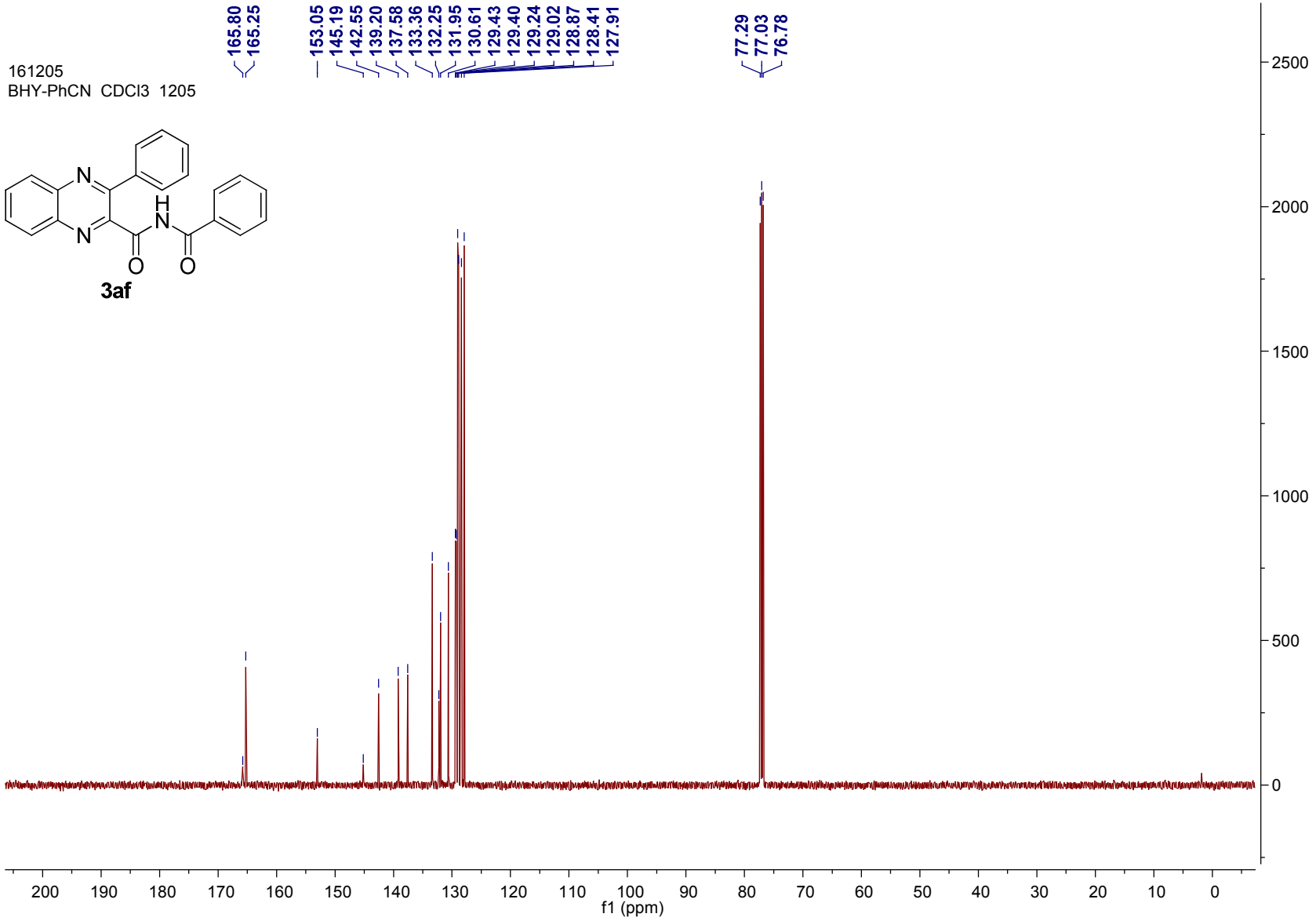

10.383
8.228
8.212
8.188
8.173
8.171
7.946
7.944
7.930
7.916
7.913
7.892
7.890
7.876
7.862
7.859
7.687
7.681
7.674
7.668
7.528
7.522
7.515
7.276
3.734
3.722
3.710
3.421
3.057
3.046
3.034
N
H
N
N
OMe
O
O
3ad
f1 (ppm)
0.99
1.00
1.00
2.04
2.00
3.02
2.01
3.02
2.00

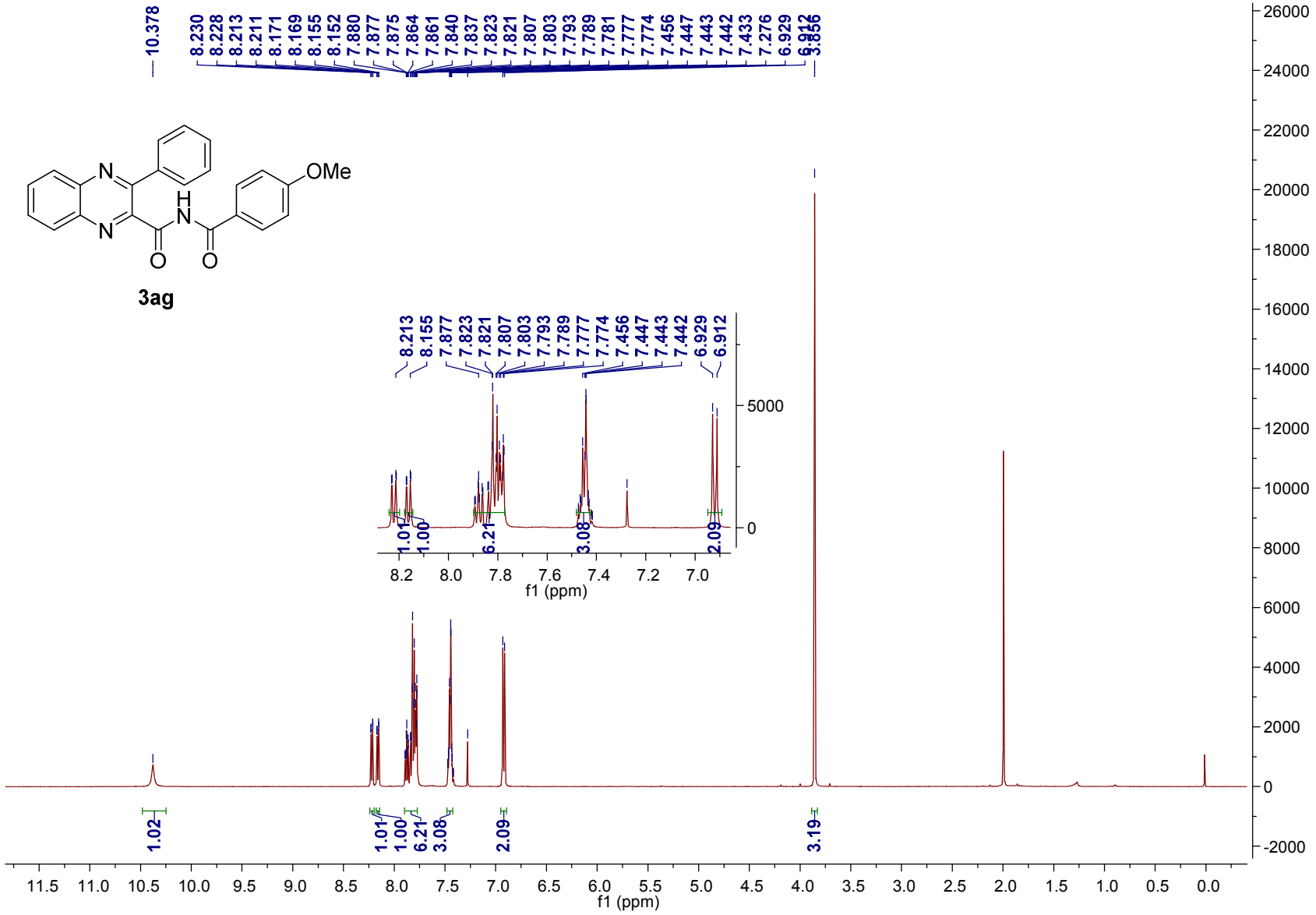

172.18
163.34
153.98
142.88
139.00
138.10
132.61
130.95
129.42
129.35
129.30
128.90
128.30
77.28
77.03
76.78
67.18
58.91
37.92
180308
BHY-2-MeOCN CDCl3 0308
N
N
H
N
OMe
O
O
3ad
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

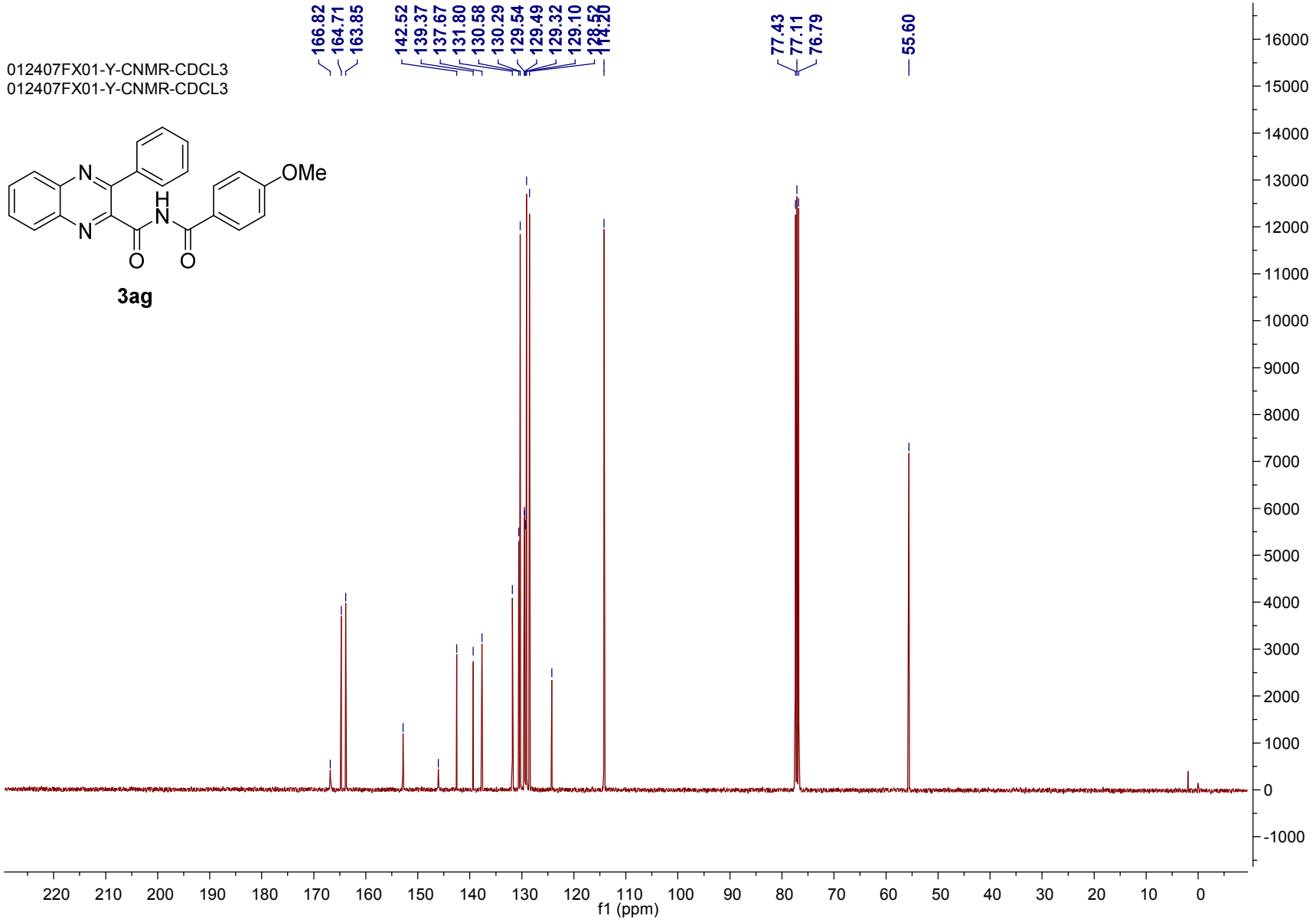

10.268
8.230
8.228
8.225
8.222
8.208
8.205
7.957
7.904
7.685
7.679
7.675
7.671
7.666
7.543
7.536
7.530
7.277
6.630
6.627
6.596
5.941
5.939
5.921
5.918
1.603
3ae
1.00
2.01
2.02
2.01
3.00
0.71
1.00
1.00
f1 (ppm)

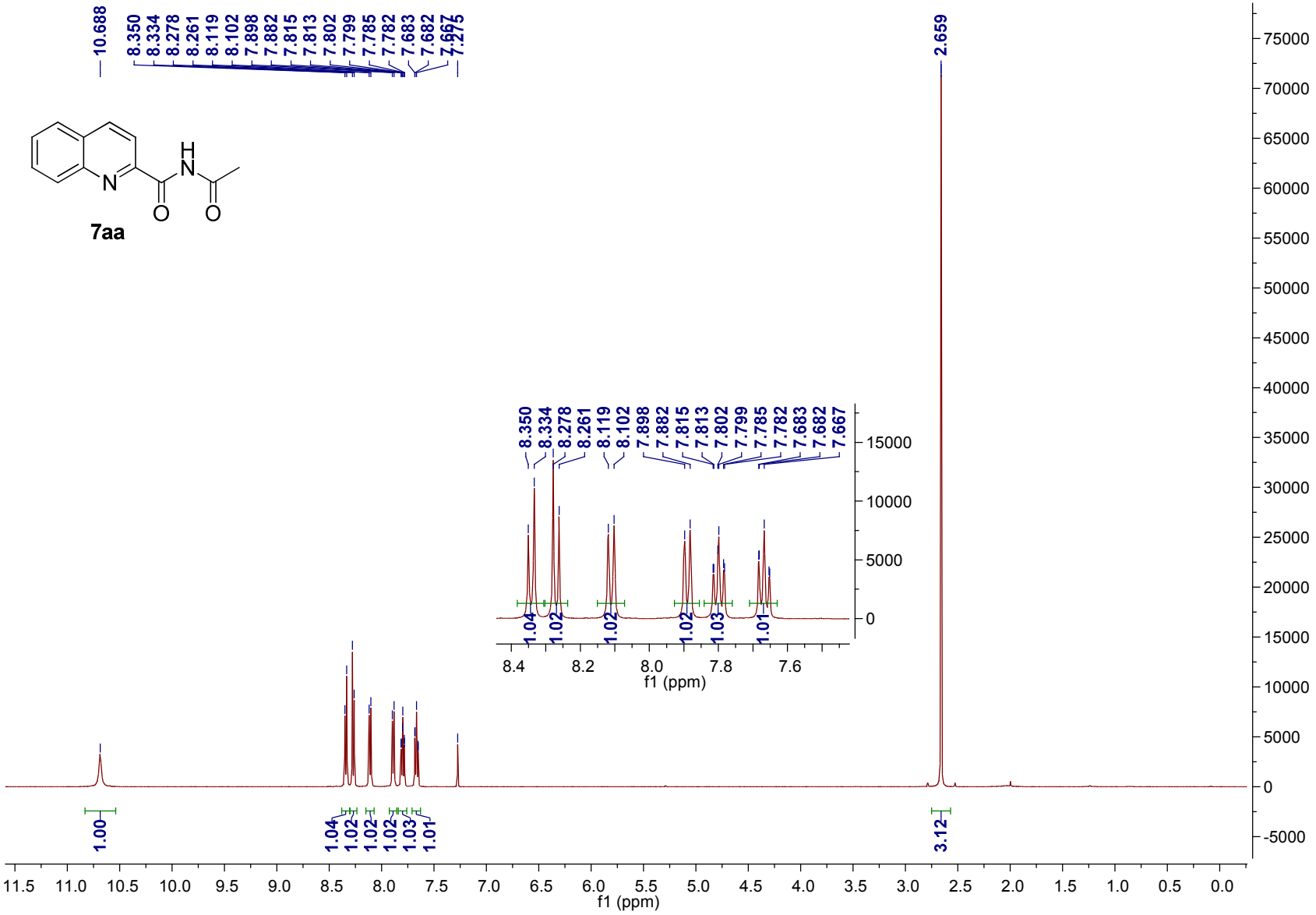

166.07
154.40
143.08
138.94
138.29
132.93
132.14
131.15
129.56
129.46
129.39
128.89
128.32
113.63
180307
BHY-2-bxj CDCl3 0307
N
N
H
N
O
O
3ae
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

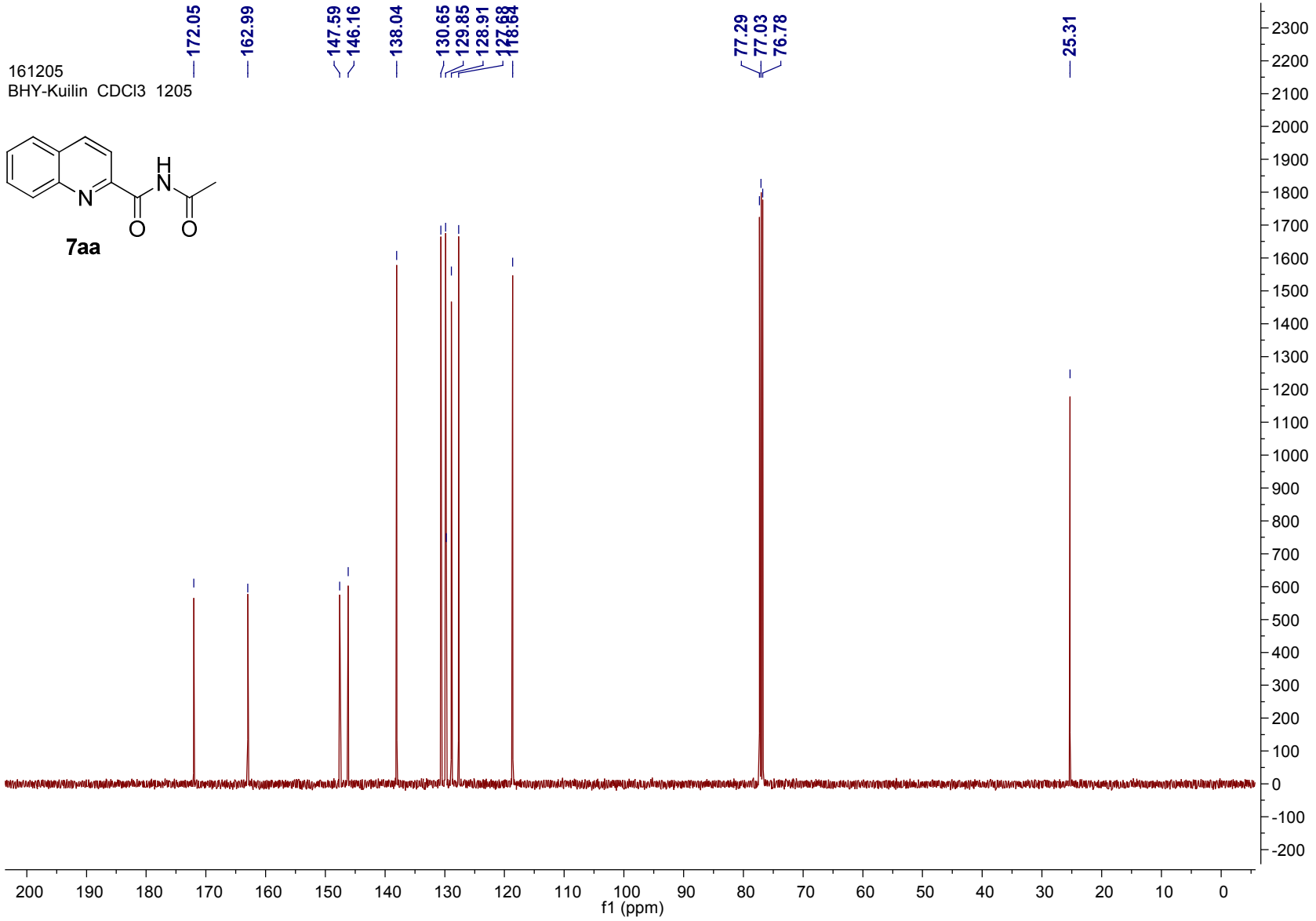

10.534
8.239
8.237
8.222
8.220
8.182
8.181
8.180
8.166
8.164
8.163
7.906
7.904
7.891
7.877
7.874
7.860
7.848
7.845
7.836
7.822
7.821
7.819
7.781
7.777
7.769
7.766
7.762
7.609
7.608
7.594
7.580
7.578
7.485
7.469
7.454
7.276
N
H
N
N
O
O
3af
1.00
1.00
1.01
4.09
2.05
1.02
5.05
f1 (ppm)

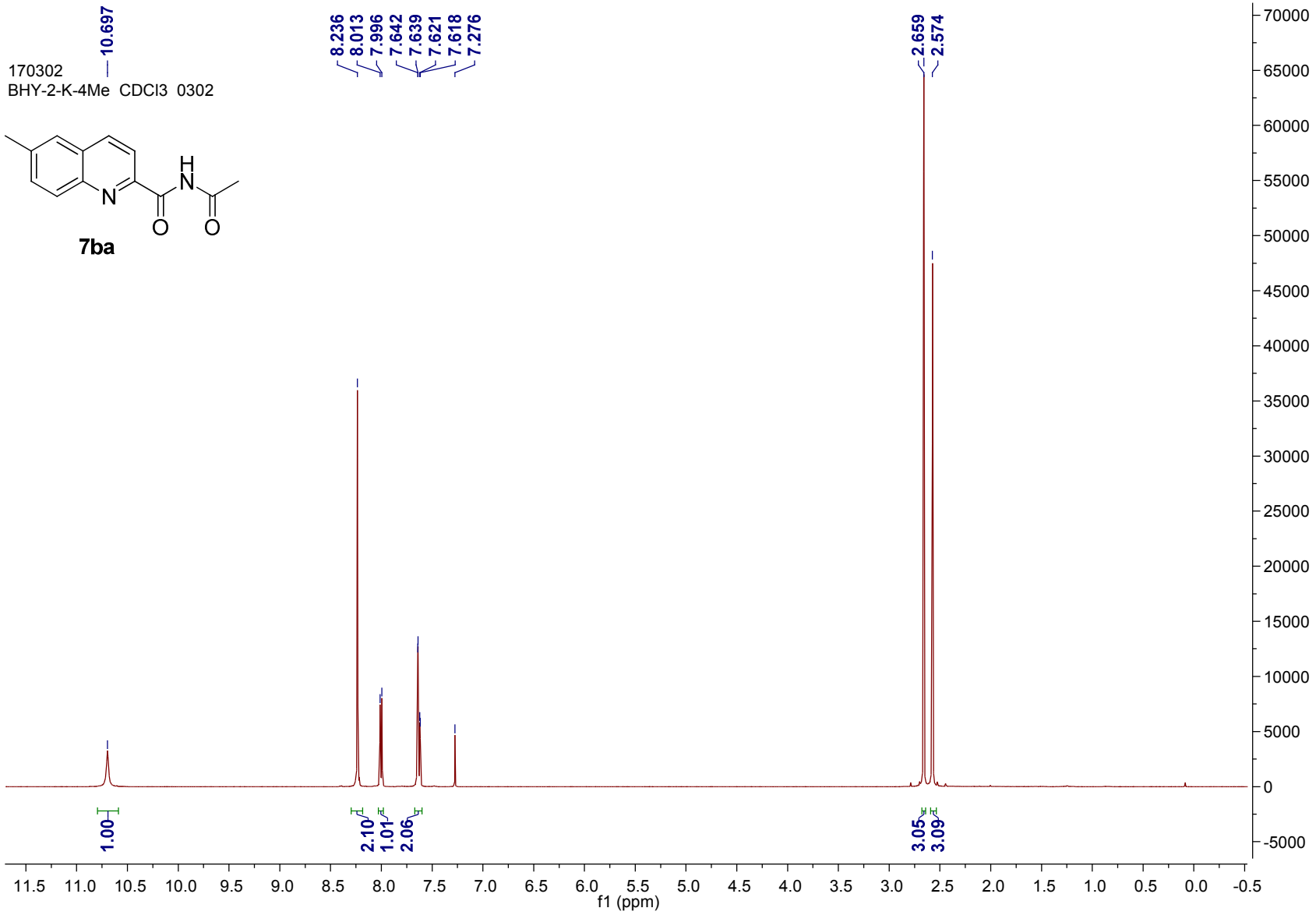

165.80
165.25
153.05
145.19
142.55
139.20
137.58
133.36
132.25
131.95
130.61
129.43
129.40
129.24
129.02
128.87
128.41
127.91
77.29
77.03
76.78
161205
BHY-PhCN CDCl3 1205
N
N
H
N
O
O
3af
2500
2000
1500
1000
500
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

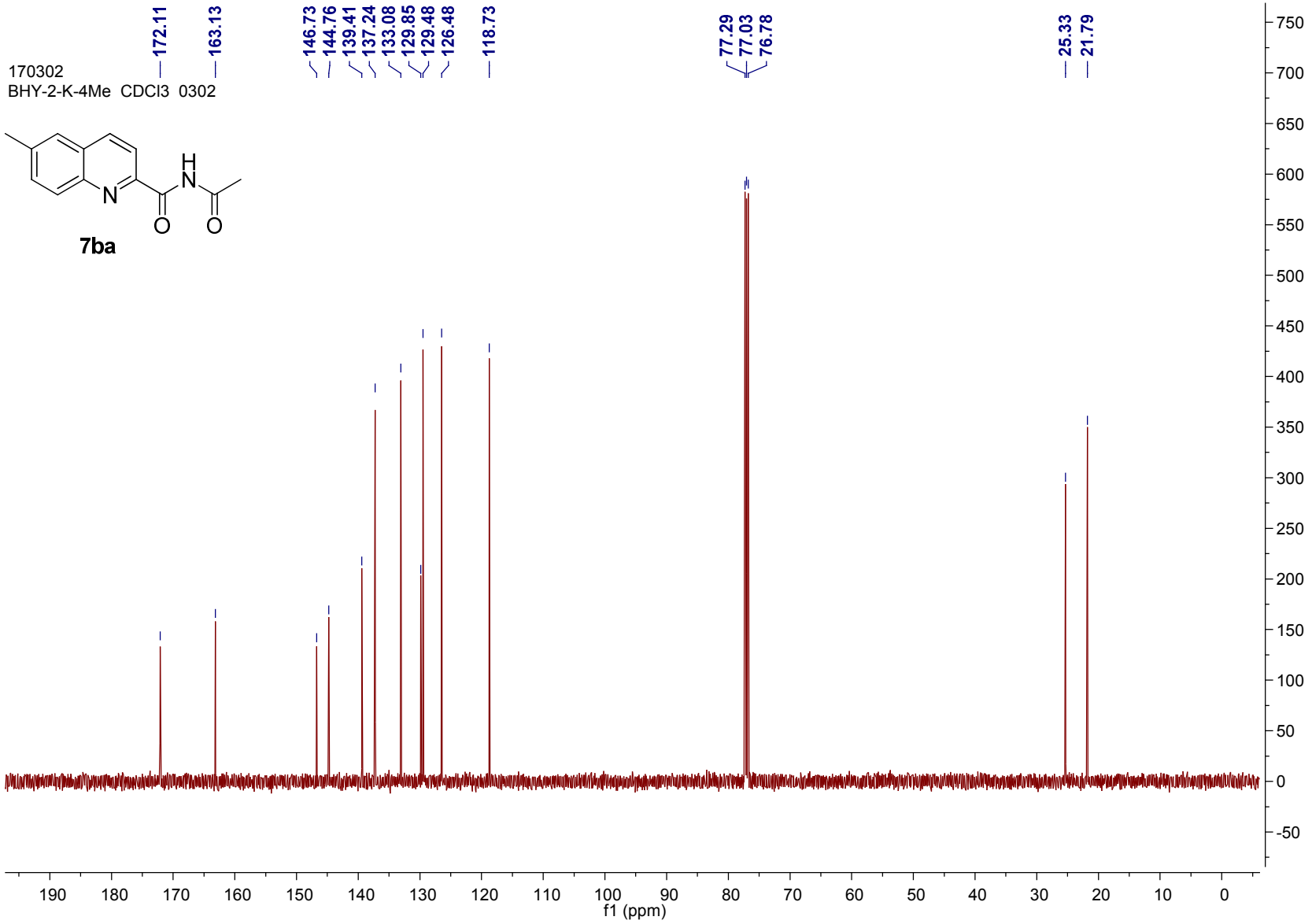

10.378
8.230
8.228
8.213
8.211
8.171
8.169
8.155
8.152
7.880
7.877
7.875
7.864
7.861
7.840
7.837
7.823
7.821
7.807
7.803
7.793
7.789
7.781
7.777
7.774
7.456
7.447
7.443
7.442
7.433
7.276
6.929
6.912
3.856
OMe
N
H
N
O
O
3ag
8.213
8.155
7.877
7.823
7.821
7.807
7.803
7.793
7.789
7.777
7.774
7.456
7.447
7.443
7.442
6.929
6.912
5000
0
1.01
1.00
6.21
3.08
2.09
8.2
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
1.02
1.01
1.00
6.21
3.08
2.09
3.19
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

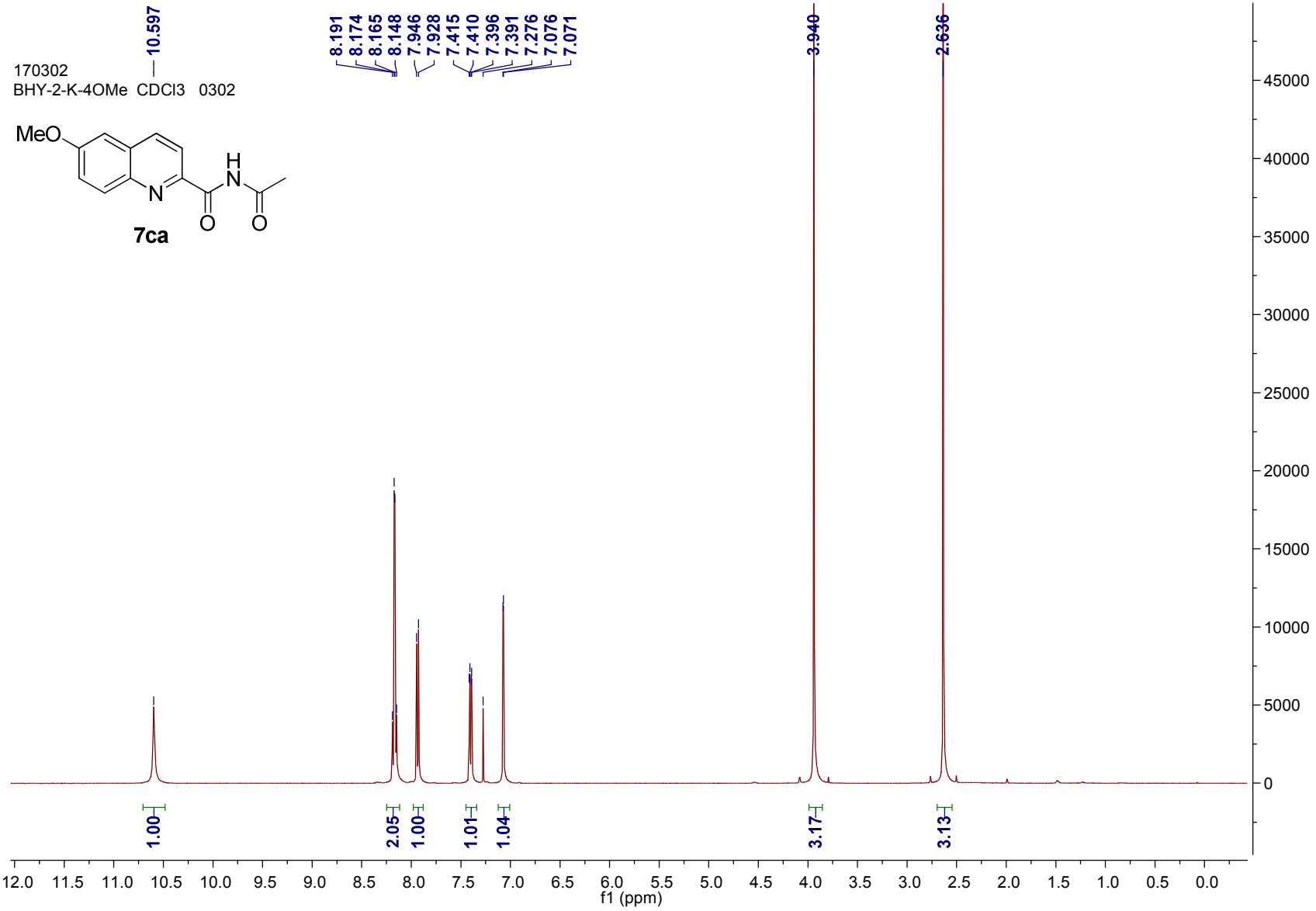

012407FX01-Y-CNMR-CDCL3
012407FX01-Y-CNMR-CDCL3
166.82
164.71
163.85
142.52
139.37
137.67
131.80
130.58
130.29
129.54
129.49
129.32
129.10
77.43
77.11
76.79
55.60
OMe
N
H
N
O
O
3ag
f1 (ppm)

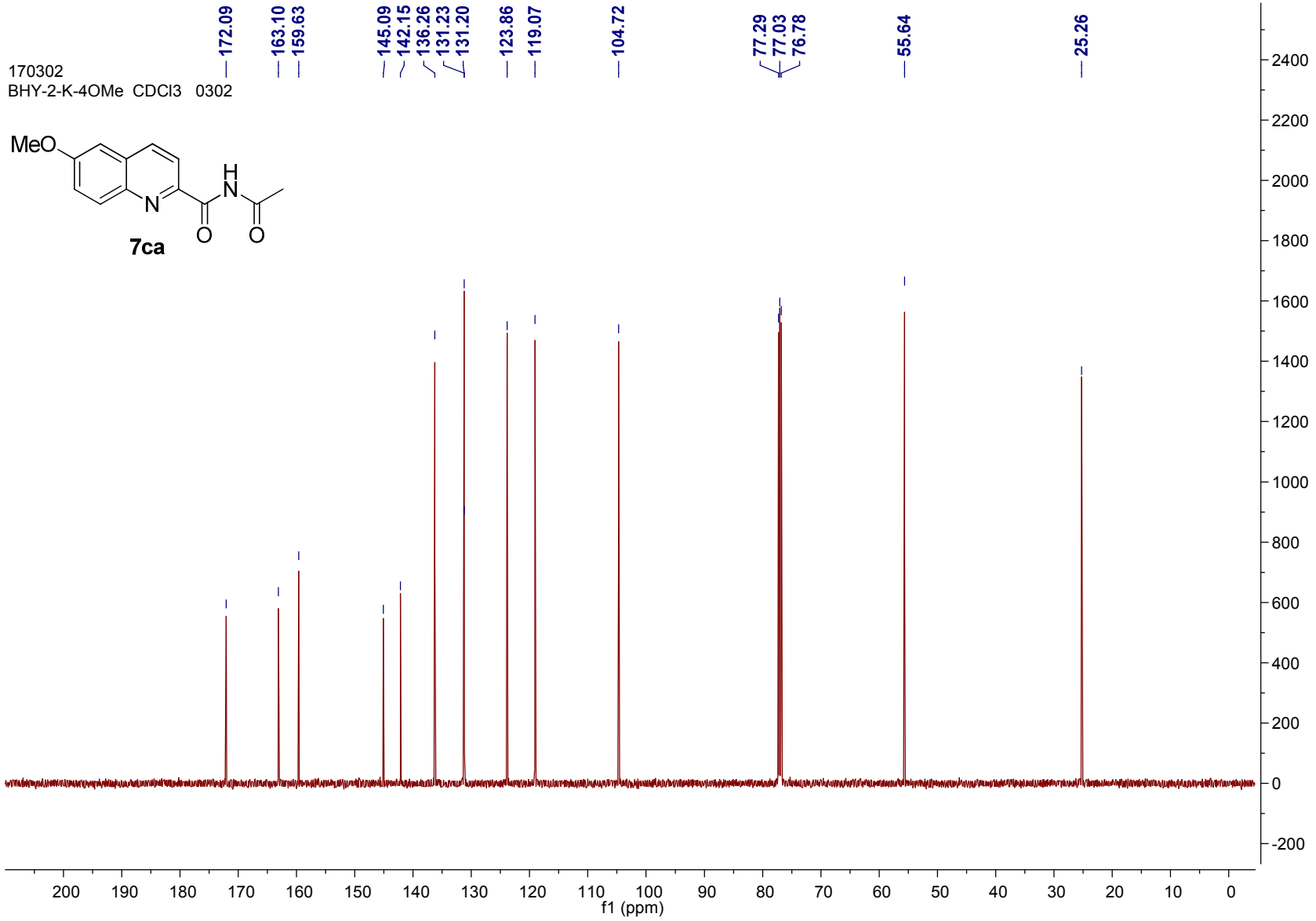

10.688
8.350
8.334
8.278
8.261
8.119
8.102
7.898
7.882
7.815
7.813
7.802
7.799
7.785
7.782
7.683
7.682
7.667
2.659
7aa
1.00
1.04
1.02
1.02
1.02
1.03
1.01
3.12
f1 (ppm)

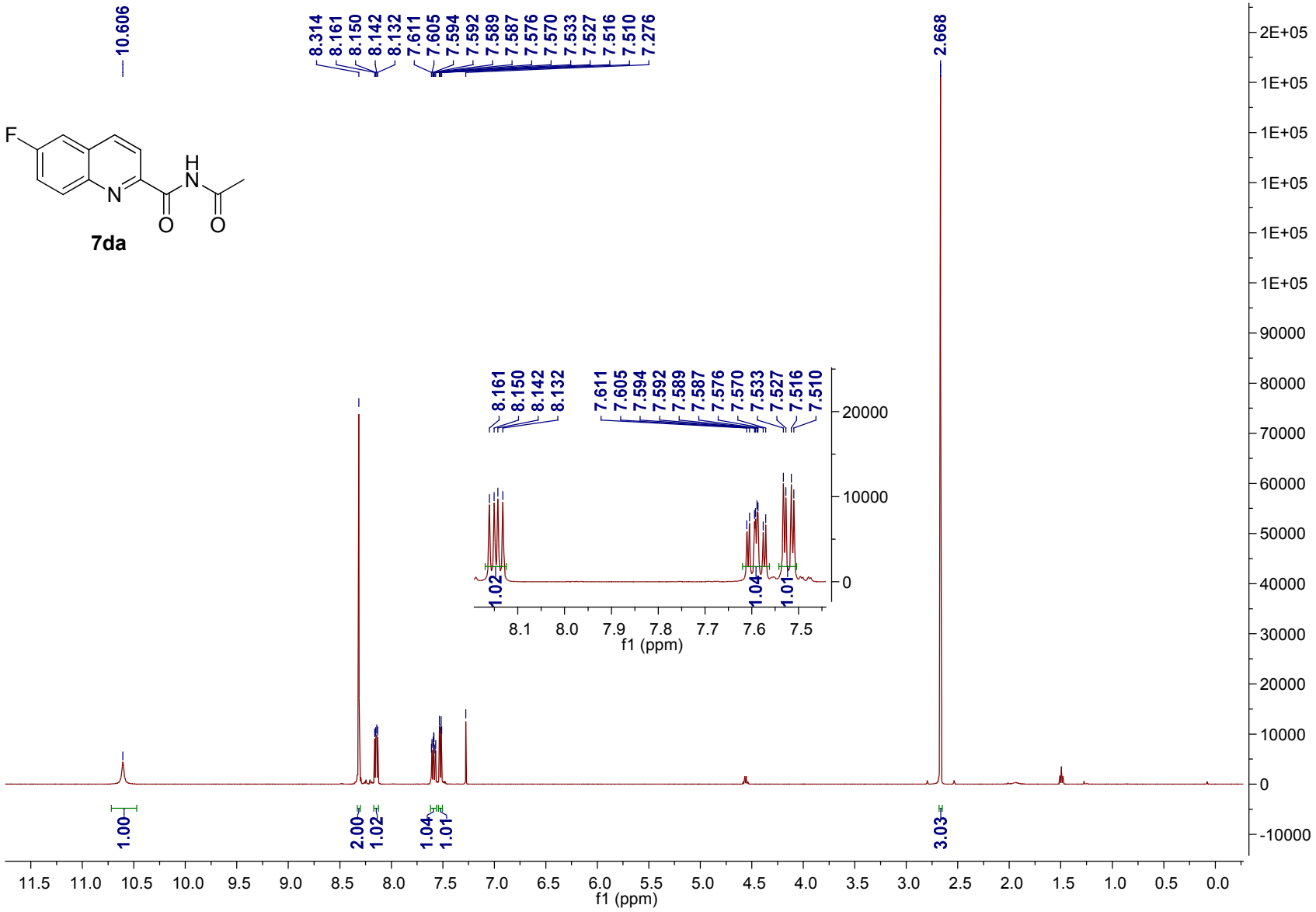

161205
BHY-Kuilin CDCl3 1205
172.05
162.99
147.59
146.16
138.04
130.65
129.85
128.91
77.29
77.03
76.78
25.31
7aa
f1 (ppm)

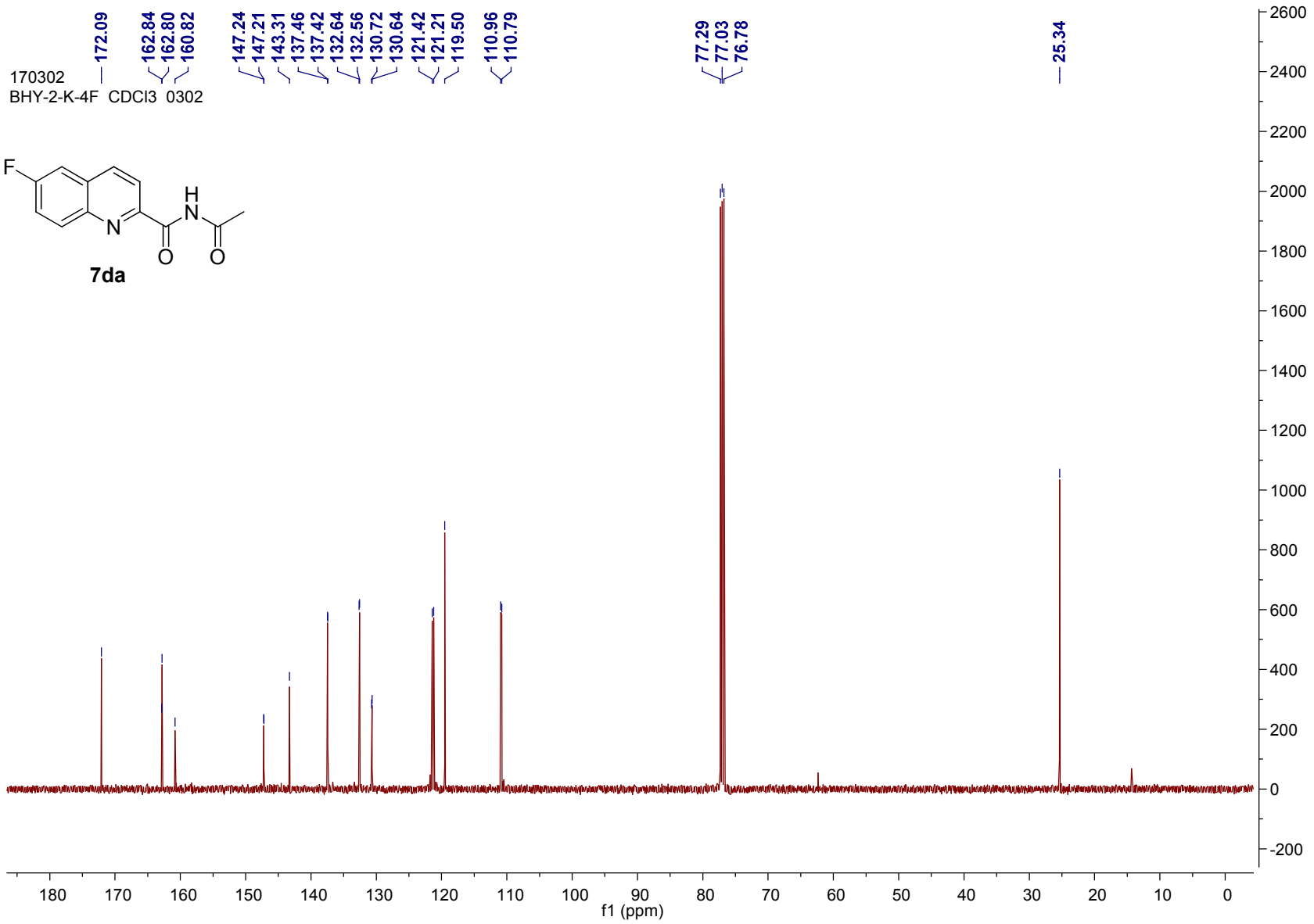

170302
BHY-2-K-4Me CDCl3 0302
10.697
8.236
8.013
7.996
7.642
7.639
7.621
7.618
7.276
2.659
2.574
7ba
1.00
2.10
1.01
2.06
3.05
3.09
f1 (ppm)

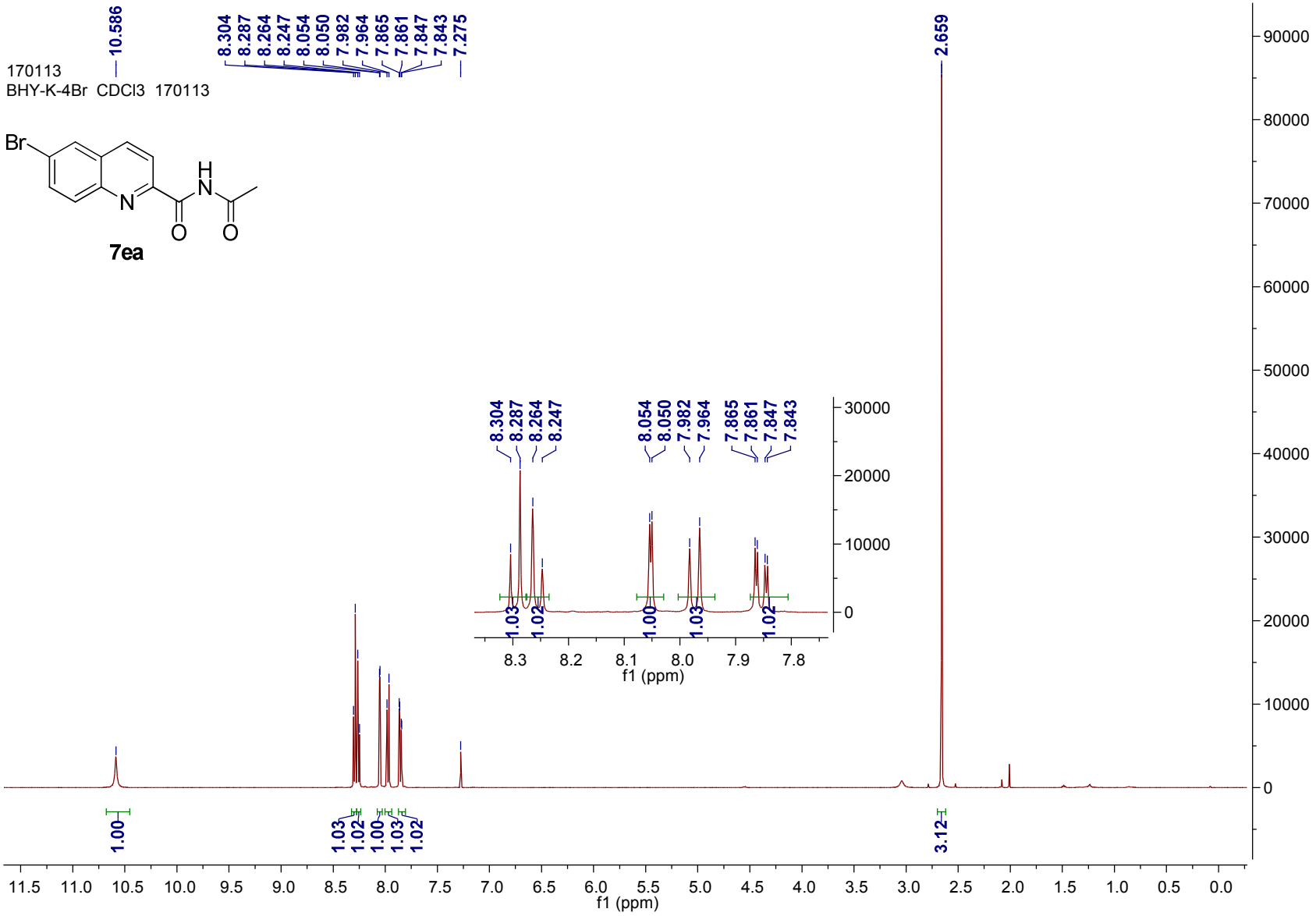

170302
BHY-2-K-4Me CDCl3 0302
172.11
163.13
146.73
144.76
139.41
137.24
133.08
129.85
129.48
126.48
118.73
77.29
77.03
76.78
25.33
21.79
7ba
f1 (ppm)

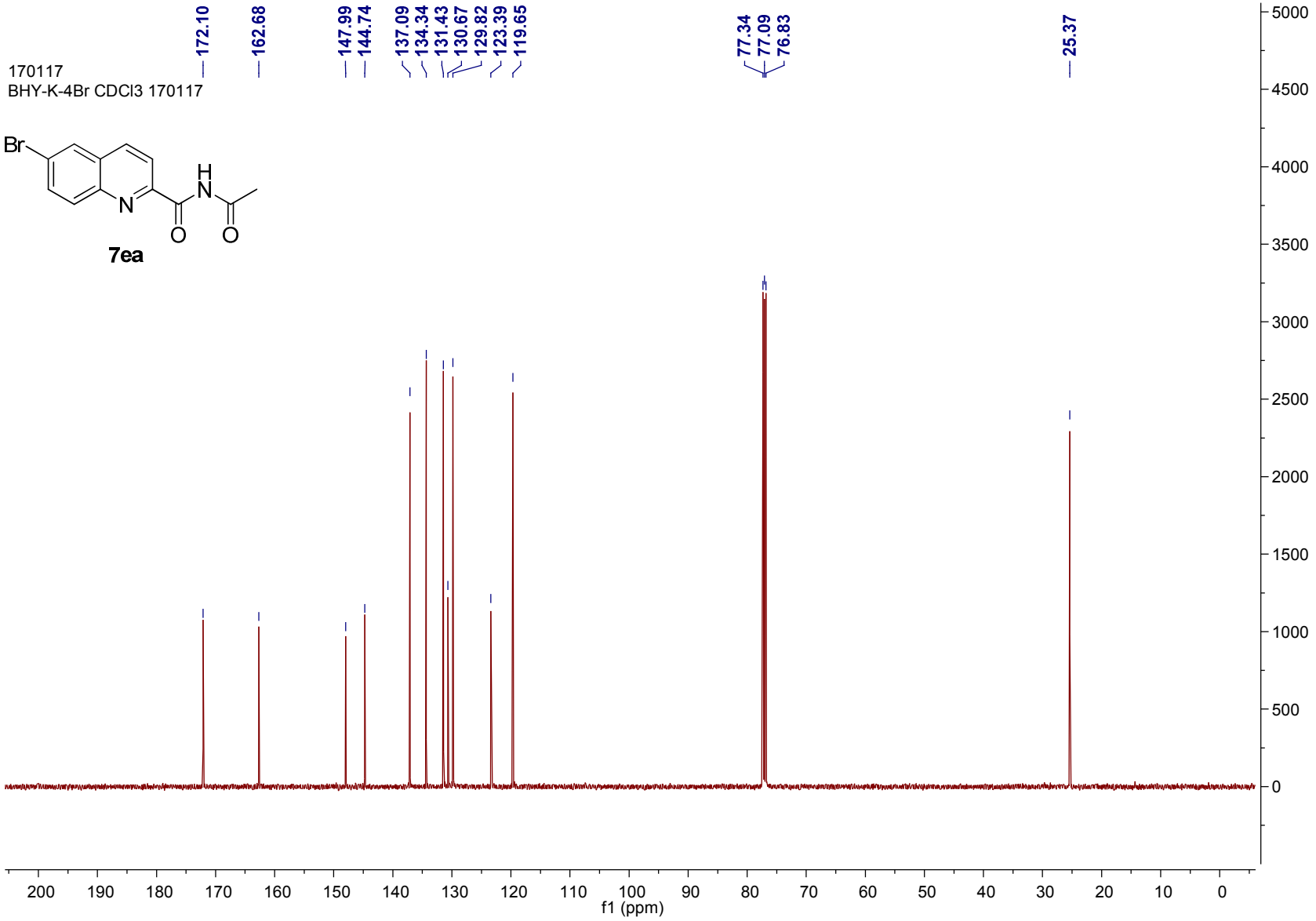

170302
BHY-2-K-4OMe CDCl3 0302
10.597
8.191
8.174
8.165
8.148
7.946
7.928
7.415
7.410
7.396
7.391
7.276
7.076
7.071
3.940
2.636
MeO
N
H
N
O
O
7ca
1.00
2.05
1.00
1.01
1.04
3.17
3.13
f1 (ppm)

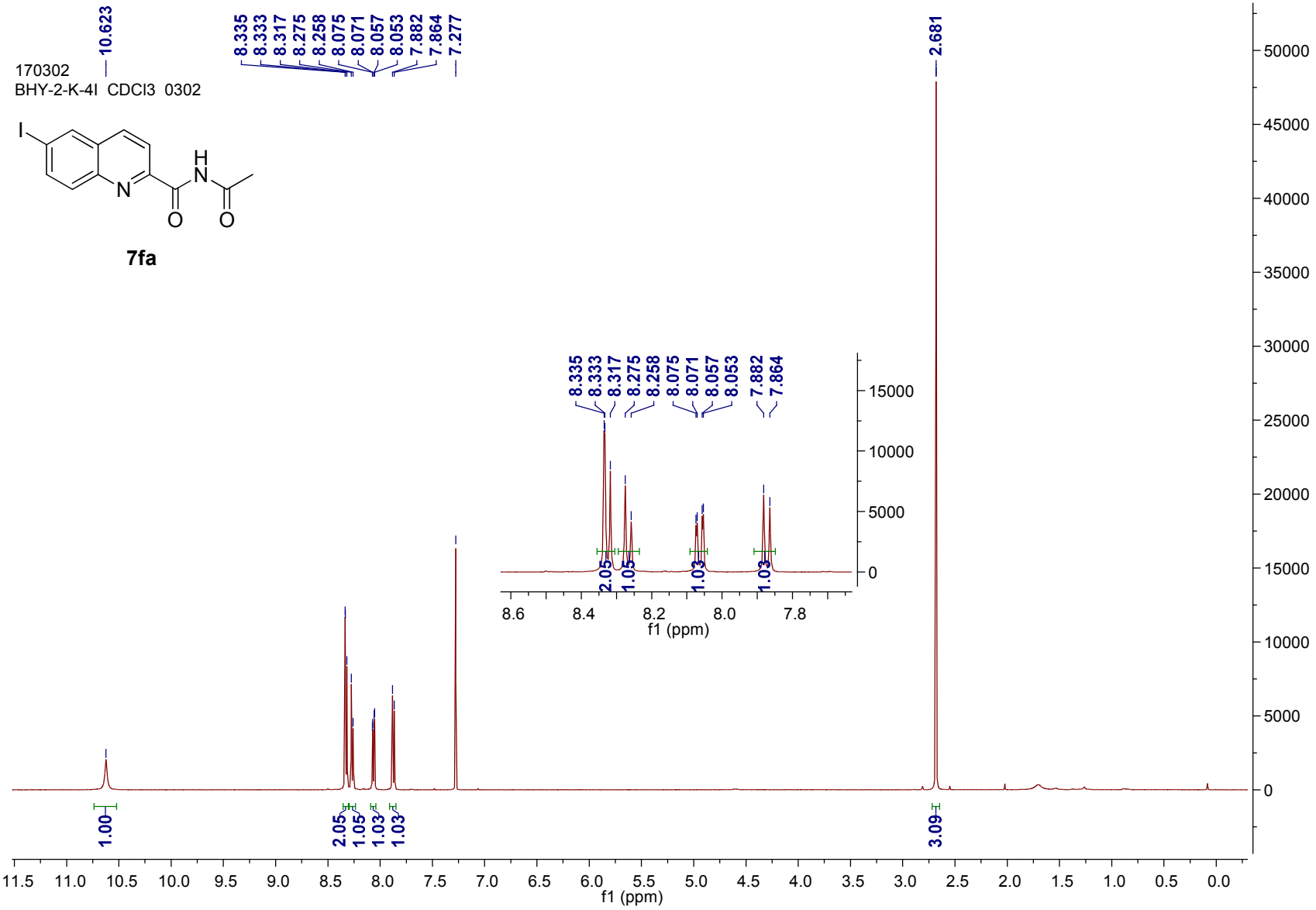

172.09
163.10
159.63
145.09
142.15
136.26
131.23
131.20
123.86
119.07
104.72
77.29
77.03
76.78
55.64
25.26
170302
BHY-2-K-4OMe CDCl3 0302
MeO
N
H
N
O
O
7ca
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

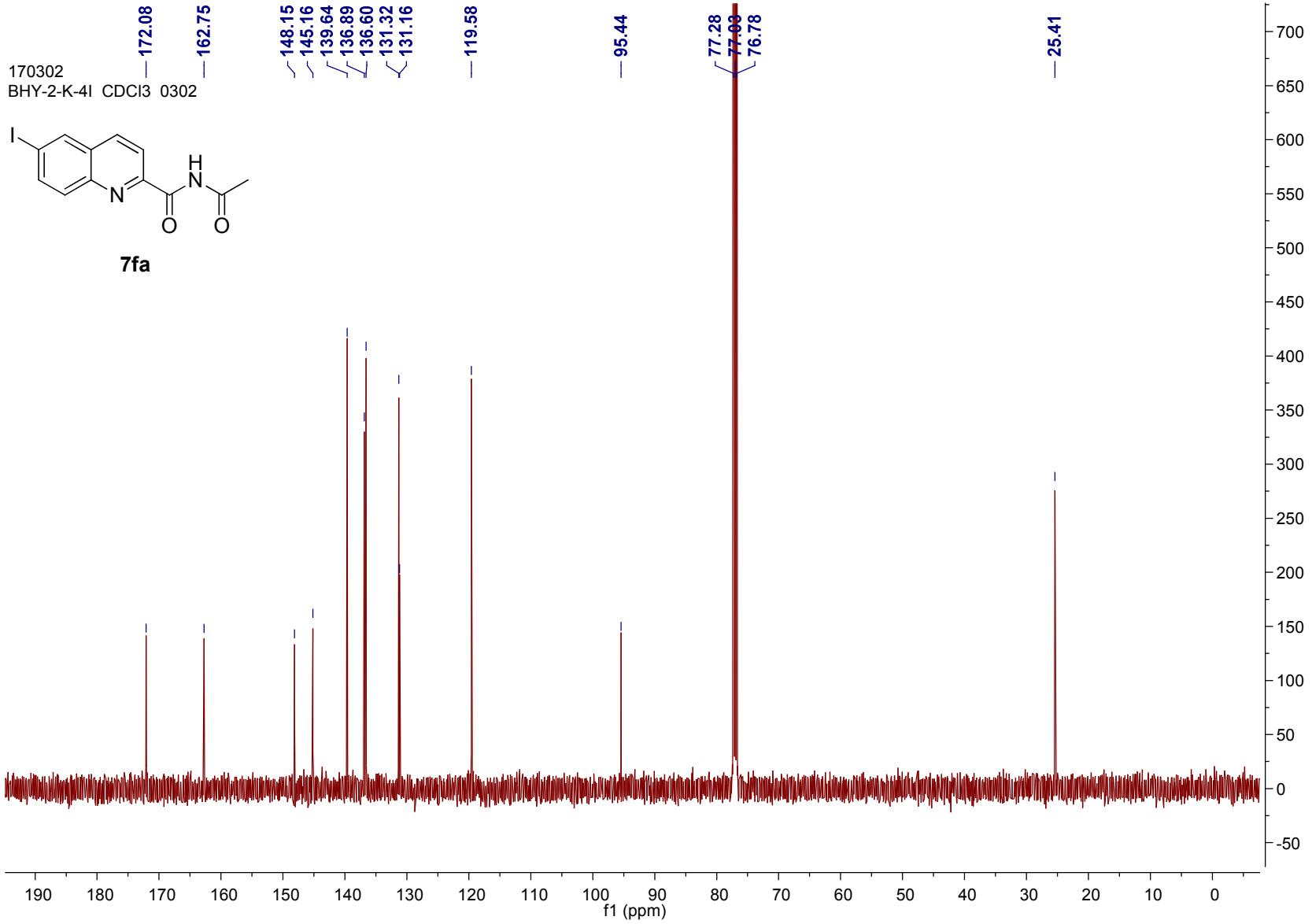

10.606
8.314
8.161
8.150
8.142
8.132
7.611
7.605
7.594
7.592
7.589
7.587
7.576
7.570
7.533
7.527
7.516
7.510
7.276
2.668
F
N
H
N
O
O
7da
1.00
2.00
1.02
1.04
1.01
3.03
f1 (ppm)

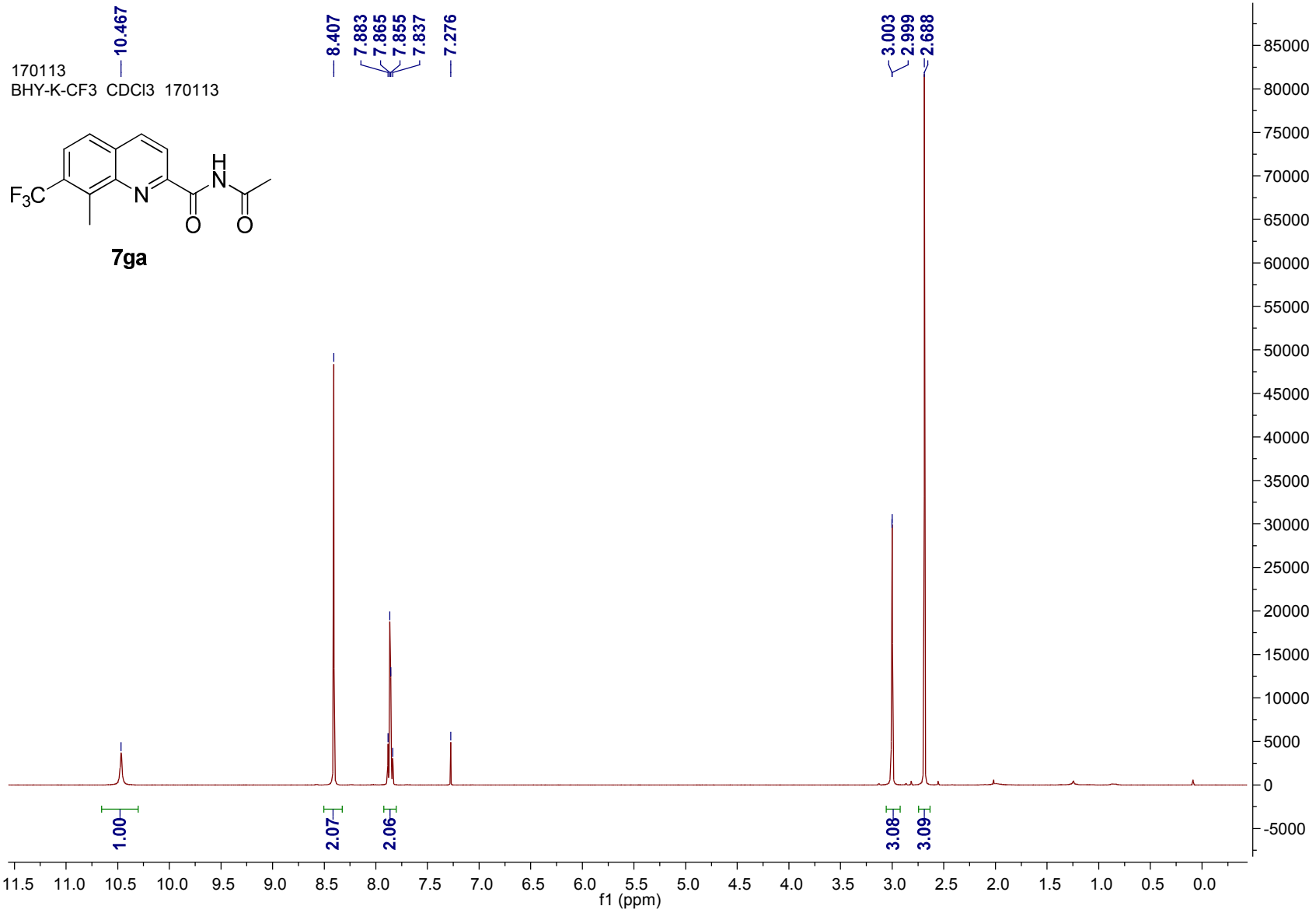

172.09
162.84
162.80
160.82
147.24
147.21
143.31
137.46
137.42
132.64
132.56
130.72
130.64
121.42
121.21
119.50
110.96
110.79
77.29
77.03
76.78
25.34
170302
BHY-2-K-4F CDCl3 0302
F
N
H
N
O
O
7da
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

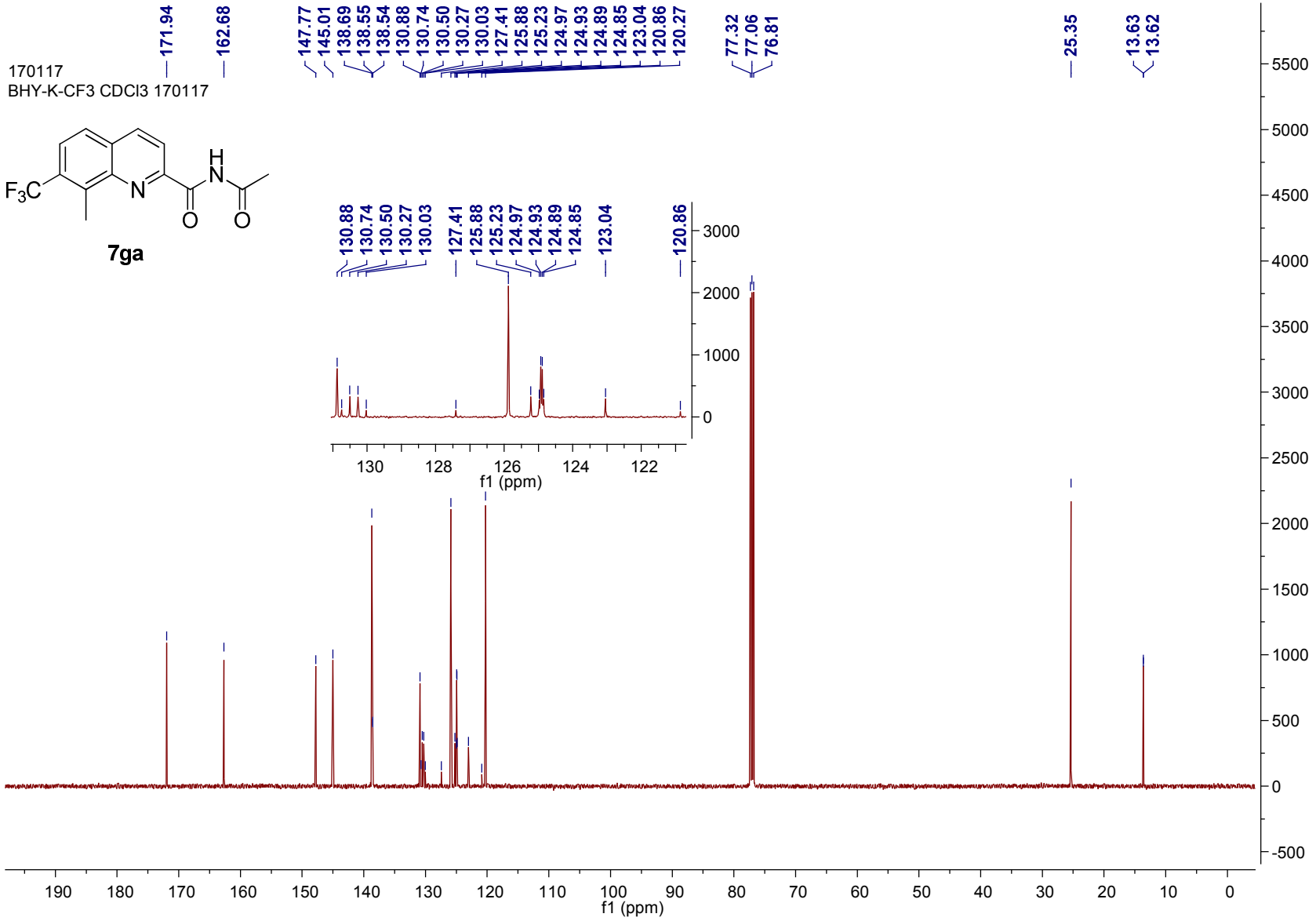

170113
BHY-K-4Br CDCl3 170113
10.586
8.304
8.287
8.264
8.247
8.054
8.050
7.982
7.964
7.865
7.861
7.847
7.843
7.275
2.659
Br
N
H
N
O
O
7ea
f1 (ppm)
1.00
1.03
1.02
1.00
1.03
1.02
3.12

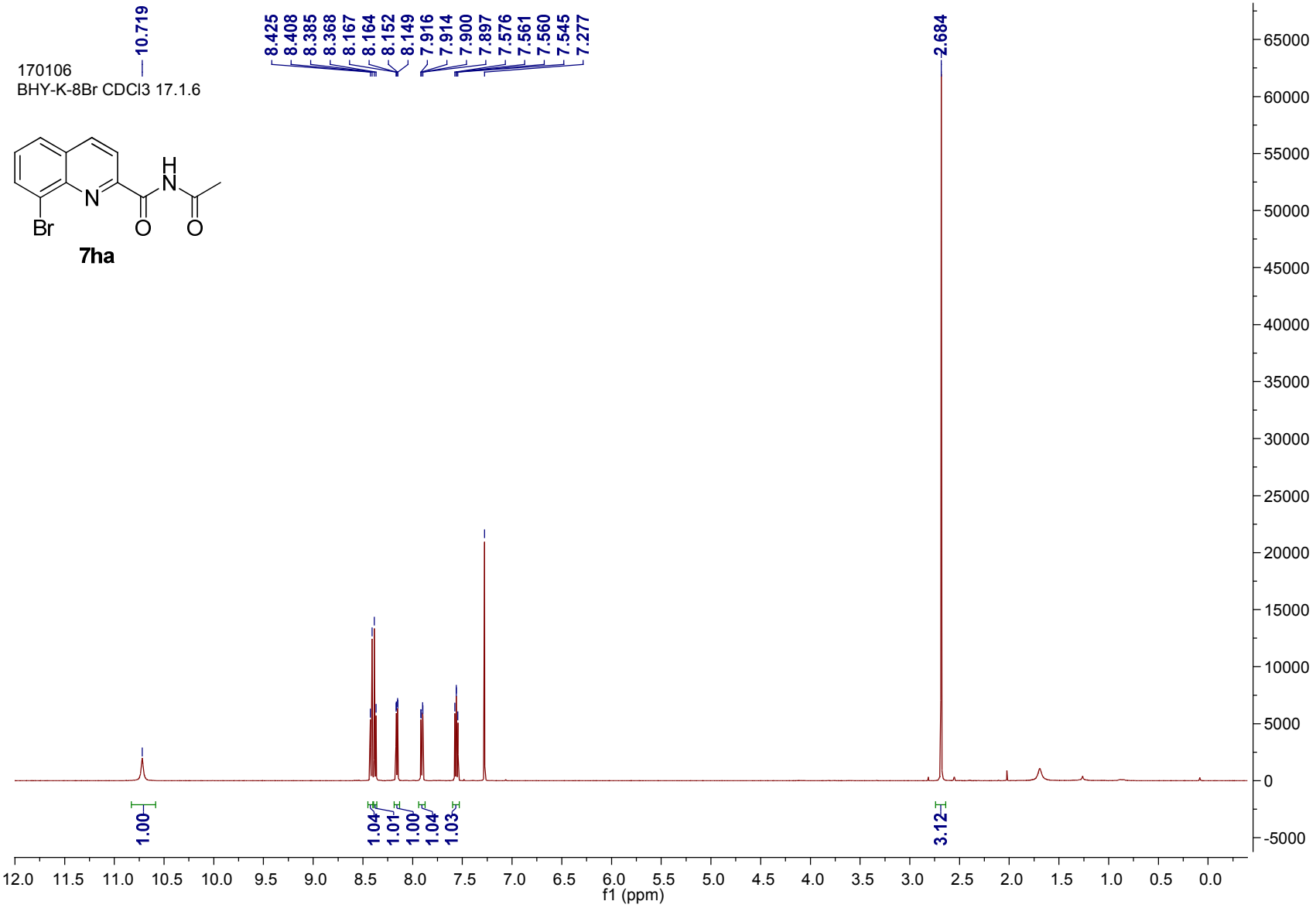

172.10
162.68
147.99
144.74
137.09
134.34
131.43
130.67
129.82
123.39
119.65
77.34
77.09
76.83
25.37
170117
BHY-K-4Br CDCl3 170117
Br
N
H
N
O
O
7ea
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

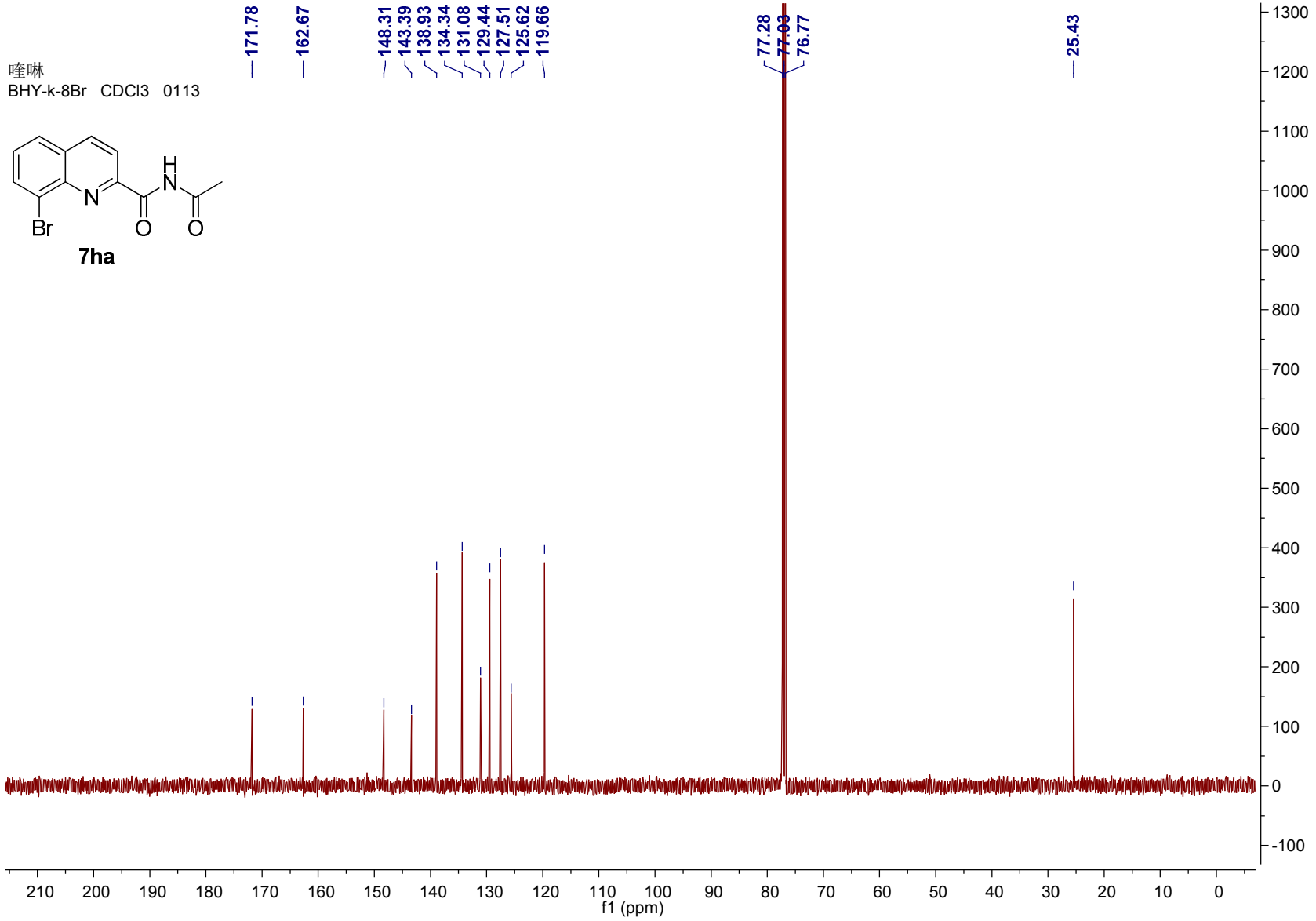

170302
BHY-2-K-4I CDCl3 0302
10.623
8.335
8.333
8.317
8.275
8.258
8.075
8.071
8.057
8.053
7.882
7.864
7.277
2.681
I
H
N
N
O
O
7fa
1.00
2.05
1.05
1.03
1.03
3.09
f1 (ppm)

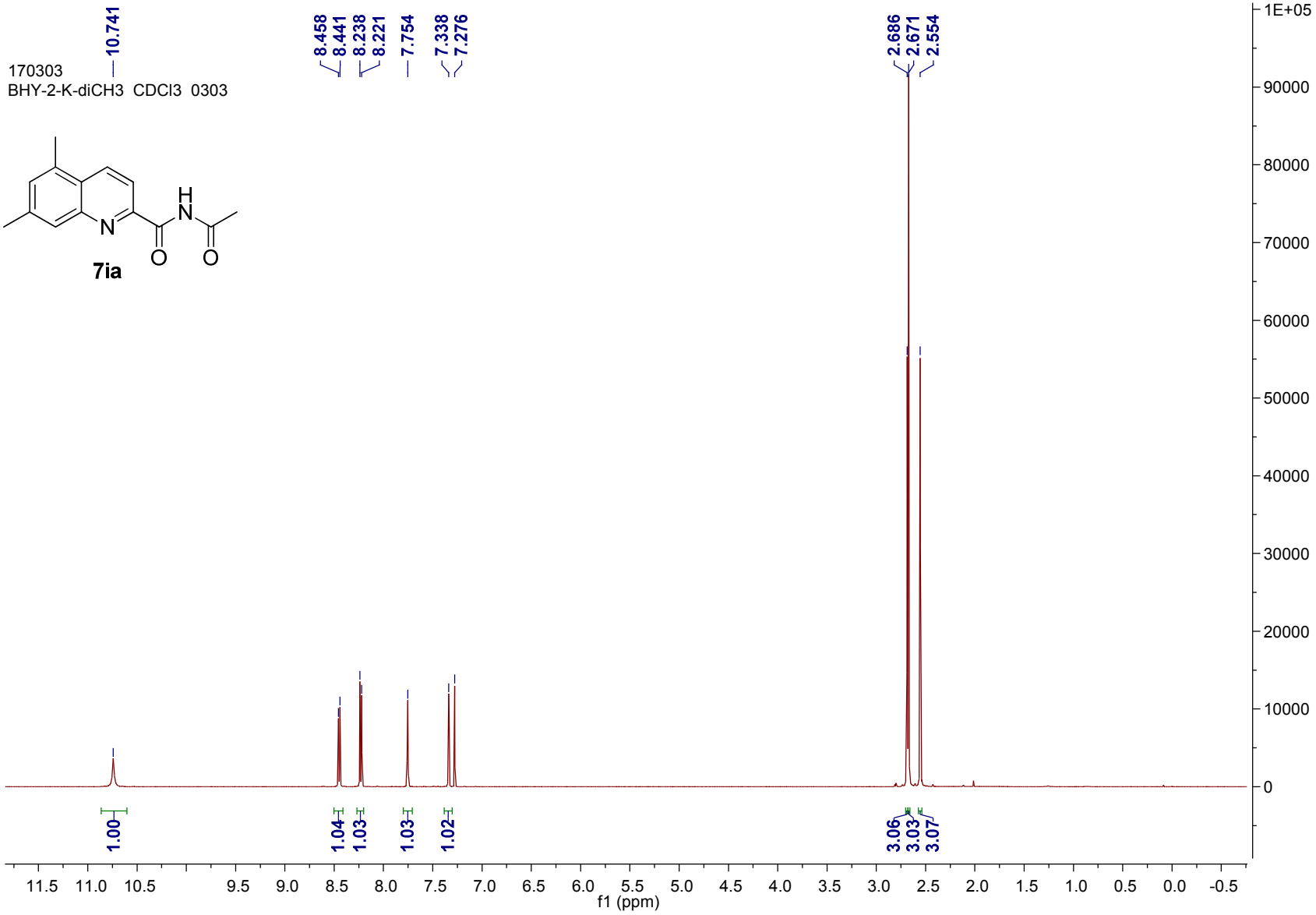

172.08
162.75
148.15
145.16
139.64
136.89
136.60
131.32
131.16
119.58
95.44
77.28
77.03
76.78
25.41
170302
BHY-2-K-4I CDCl3 0302
I
H
N
N
O
O
7fa
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

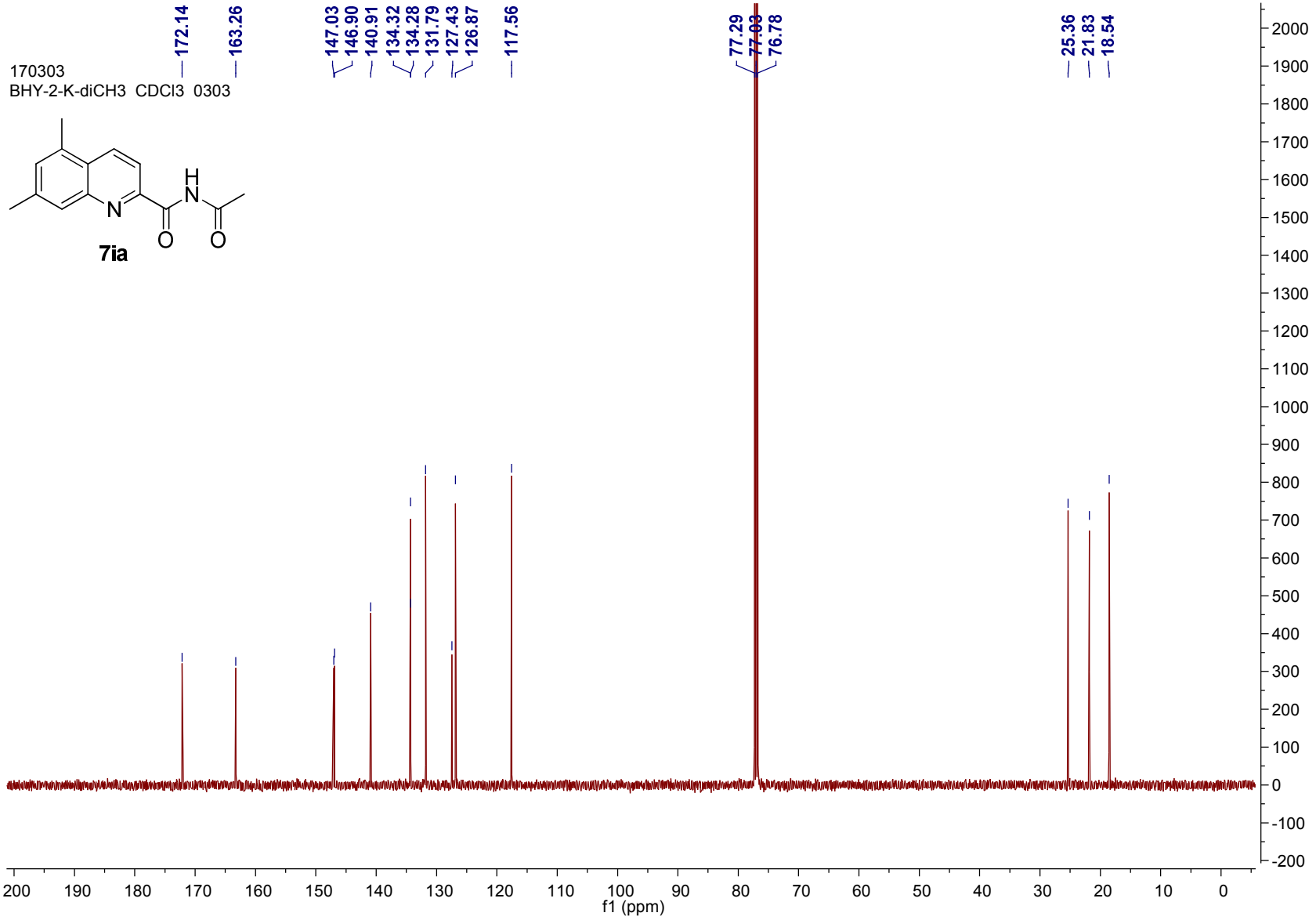

170113
BHY-K-CF3 CDCl3 170113
10.467
8.407
7.883
7.865
7.855
7.837
7.276
3.003
2.999
2.688
F3C
N
H
N
O
O
7ga
1.00
2.07
2.06
3.08
3.09
f1 (ppm)

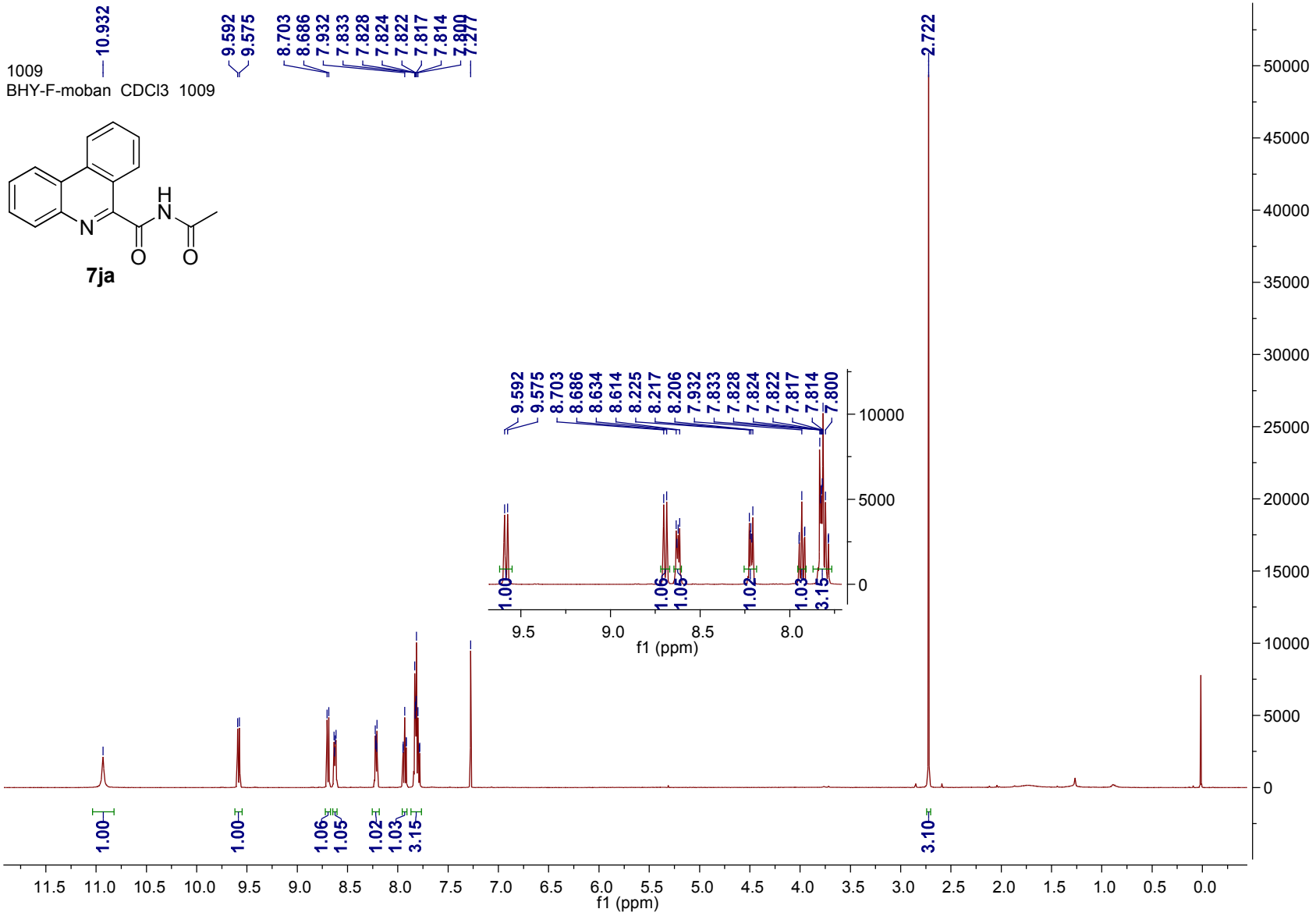

171.94
162.68
147.77
145.01
138.69
138.55
138.54
130.88
130.74
130.50
130.27
130.03
127.41
125.88
125.23
124.97
124.93
124.89
124.85
123.04
120.86
120.27
77.32
77.06
76.81
25.35
13.63
13.62
170117
BHY-K-CF3 CDCl3 170117
F3C
N
H
N
O
O
7ga
f1 (ppm)
f1 (ppm)

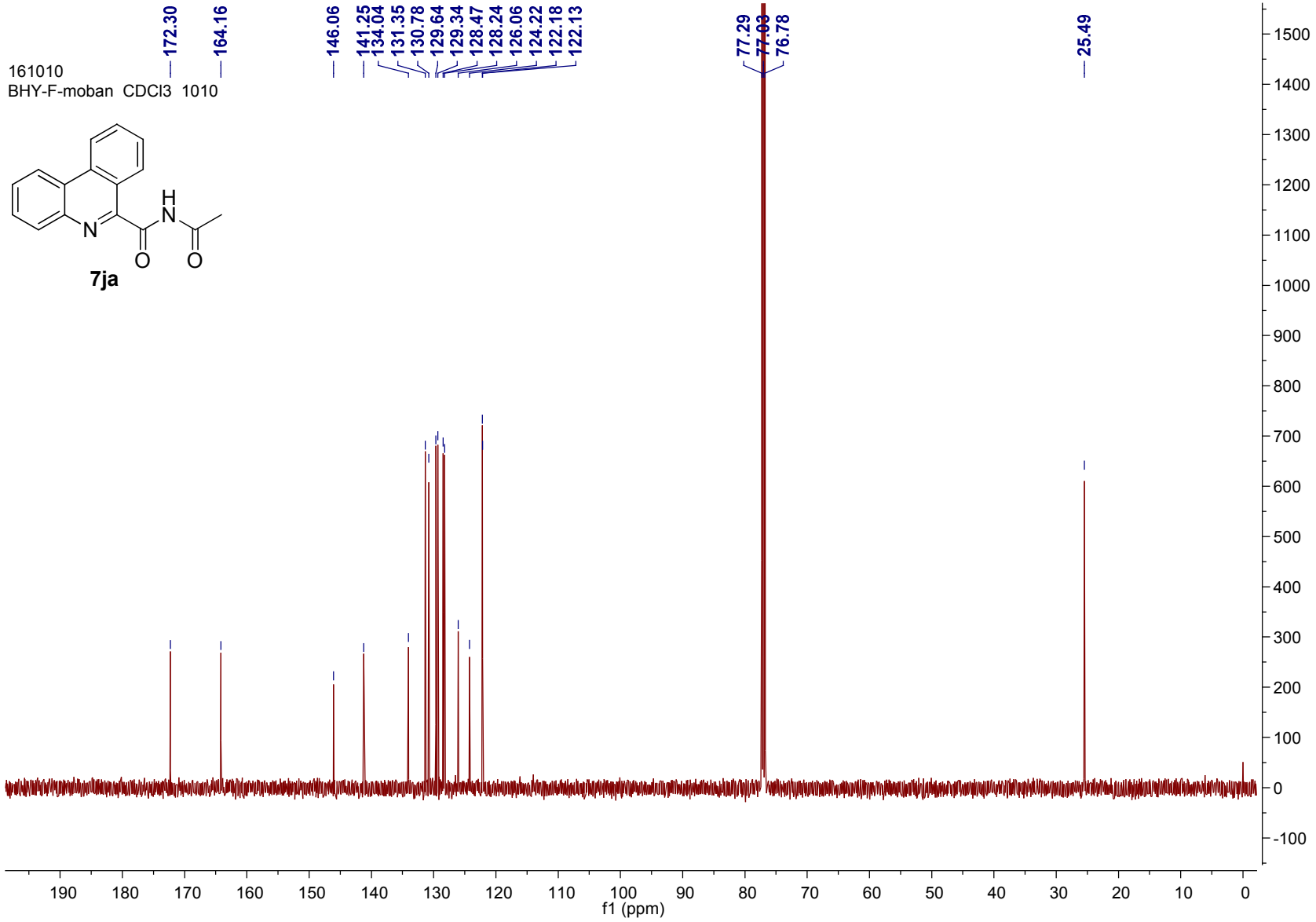

170106
BHY-K-8Br CDCl3 17.1.6
10.719
8.425
8.408
8.385
8.368
8.167
8.164
8.152
8.149
7.916
7.914
7.900
7.897
7.576
7.561
7.560
7.545
7.277
2.684
Br
N
H
N
O
O
7ha
1.00
1.04
1.01
1.00
1.04
1.03
3.12
f1 (ppm)

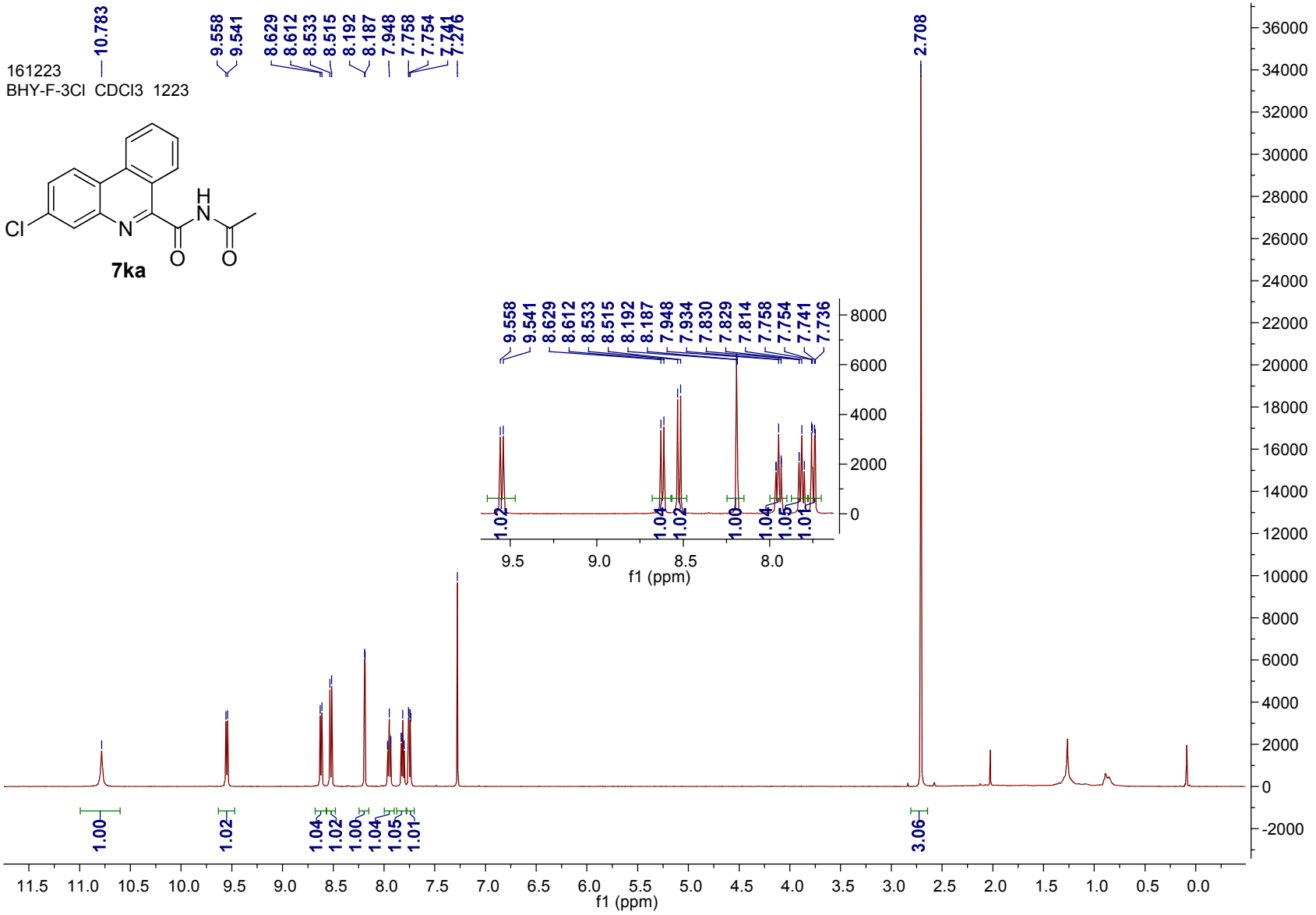

喹啉
BHY-k-8Br CDCl3 0113
171.78
162.67
148.31
143.39
138.93
134.34
131.08
129.44
127.51
125.62
119.66
77.28
77.03
76.77
25.43
Br
N
H
N
O
O
7ha
f1 (ppm)

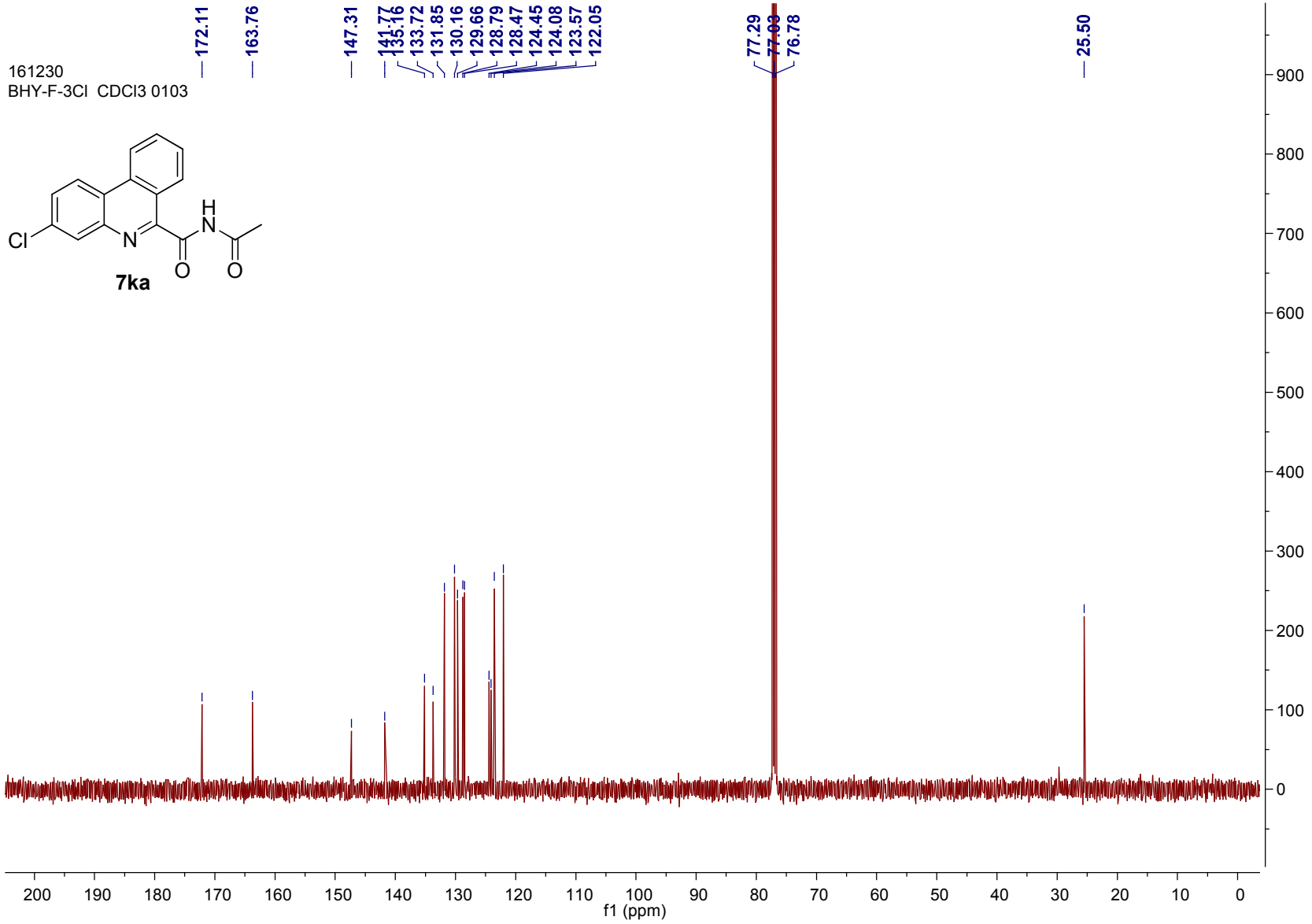

170303
BHY-2-K-diCH3 CDCl3 0303
10.741
8.458
8.441
8.238
8.221
7.754
7.338
7.276
2.686
2.671
2.554
7ia
1.00
1.04
1.03
1.03
1.02
3.06
3.03
3.07
f1 (ppm)

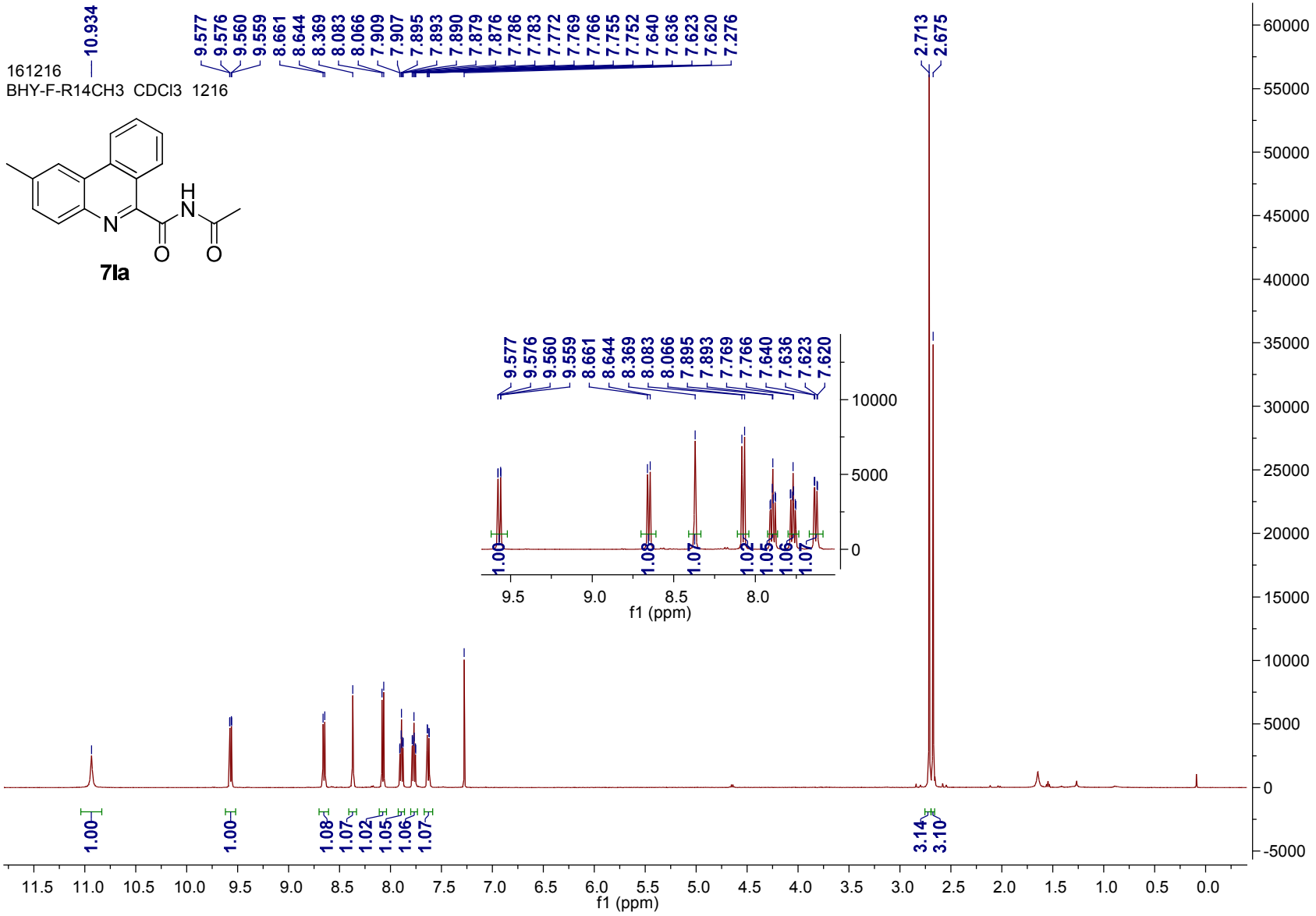

172.14
163.26
147.03
146.90
140.91
134.32
134.28
131.79
127.43
126.87
117.56
77.29
77.03
76.78
25.36
21.83
18.54
170303
BHY-2-K-diCH3 CDCl3 0303
7ia
f1 (ppm)

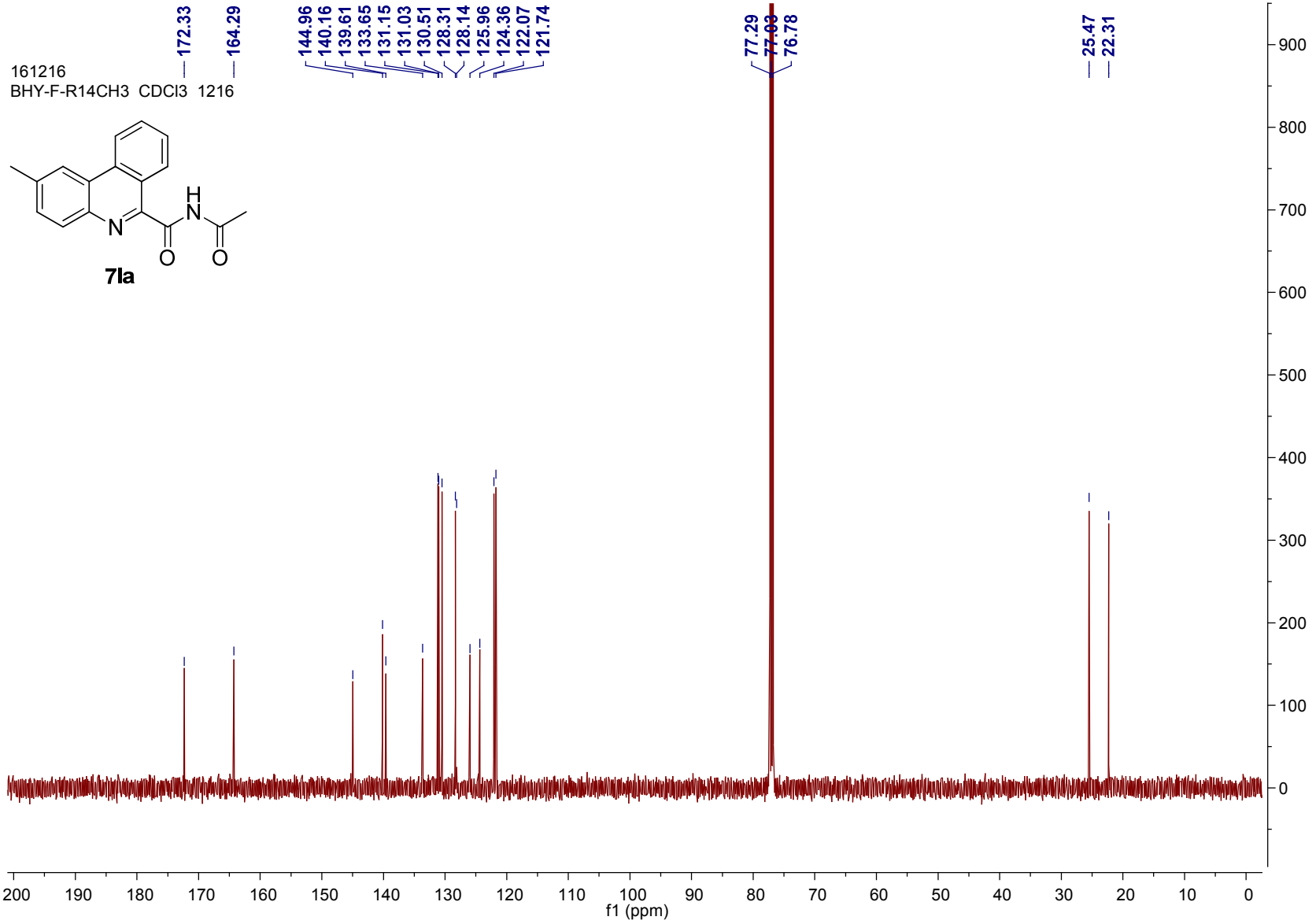

1009
BHY-F-moban CDCl3 1009
10.932
9.592
9.575
8.703
8.686
8.634
8.614
8.225
8.217
8.206
7.932
7.833
7.828
7.824
7.822
7.817
7.814
7.800
7.277
2.722
7ja
f1 (ppm)

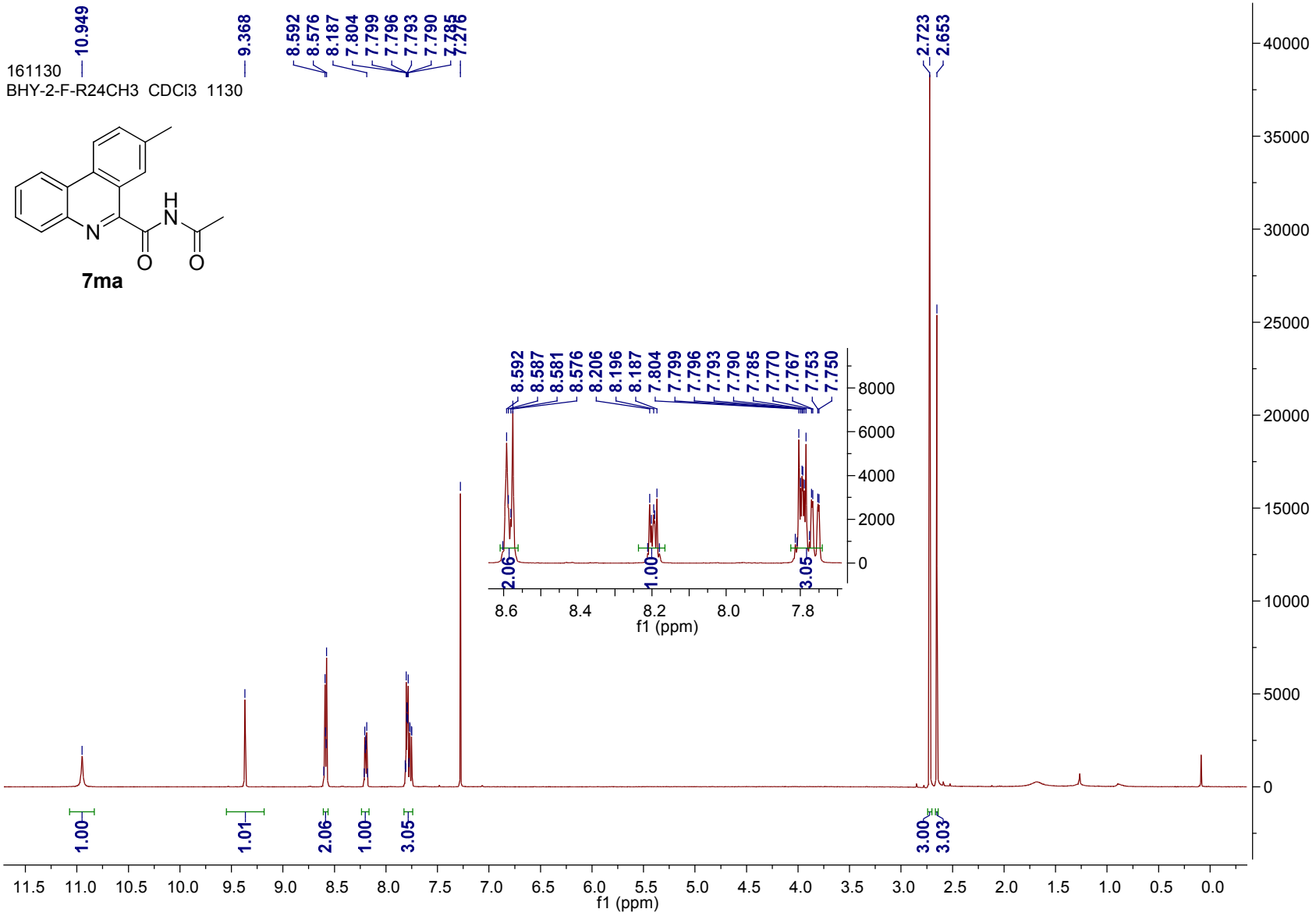

161010
BHY-F-moban CDCl3 1010
172.30
164.16
146.06
141.25
134.04
131.35
130.78
129.64
129.34
128.47
128.24
126.06
124.22
122.18
122.13
77.29
77.03
76.78
25.49
7ja
f1 (ppm)

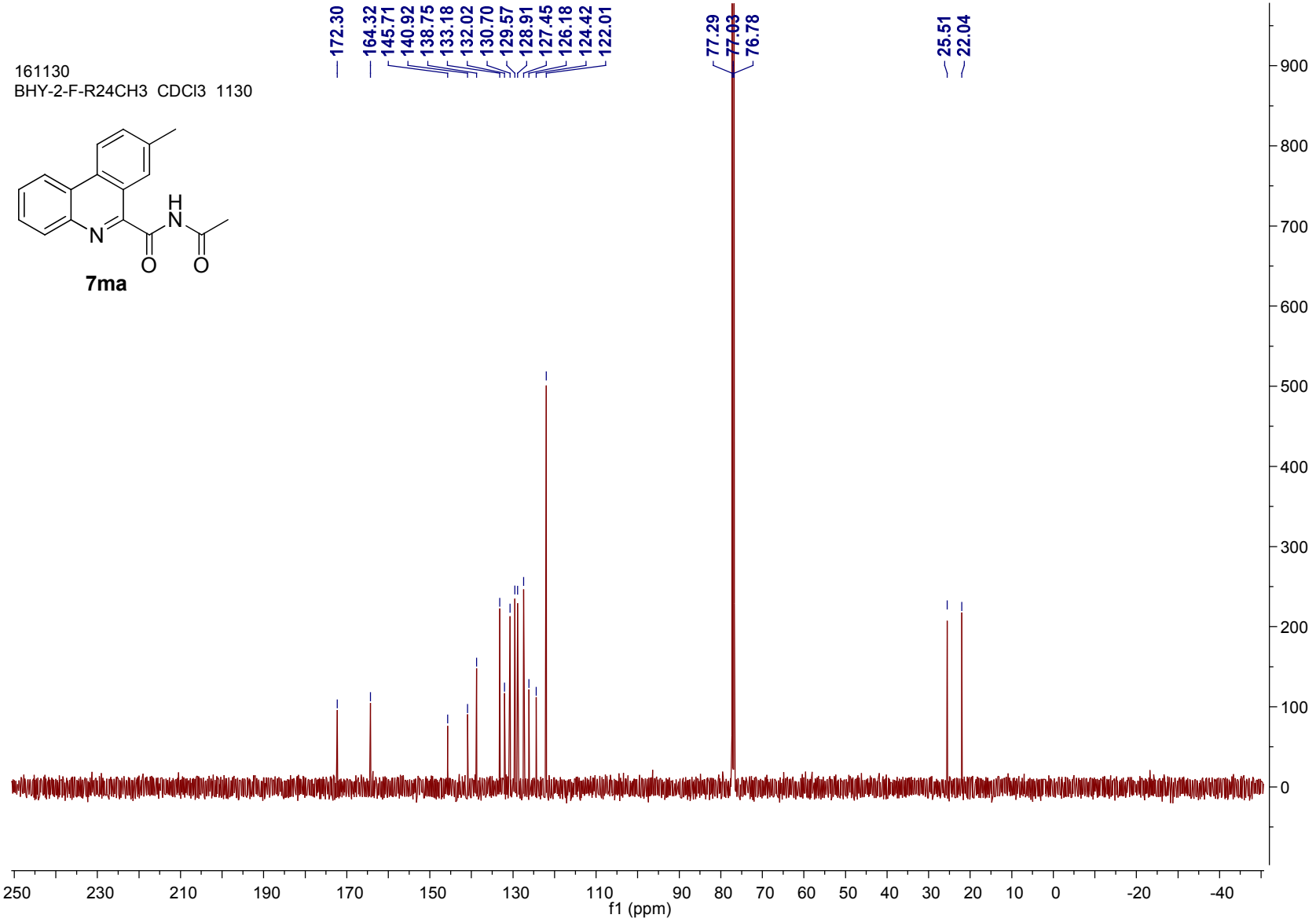

161223
BHY-F-3Cl CDCl3 1223
7ka
10.783
9.558
9.541
8.629
8.612
8.533
8.515
8.192
8.187
7.948
7.758
7.754
7.741
7.276
2.708
1.00
1.02
1.04
1.02
1.00
1.04
1.05
1.01
3.06
f1 (ppm)

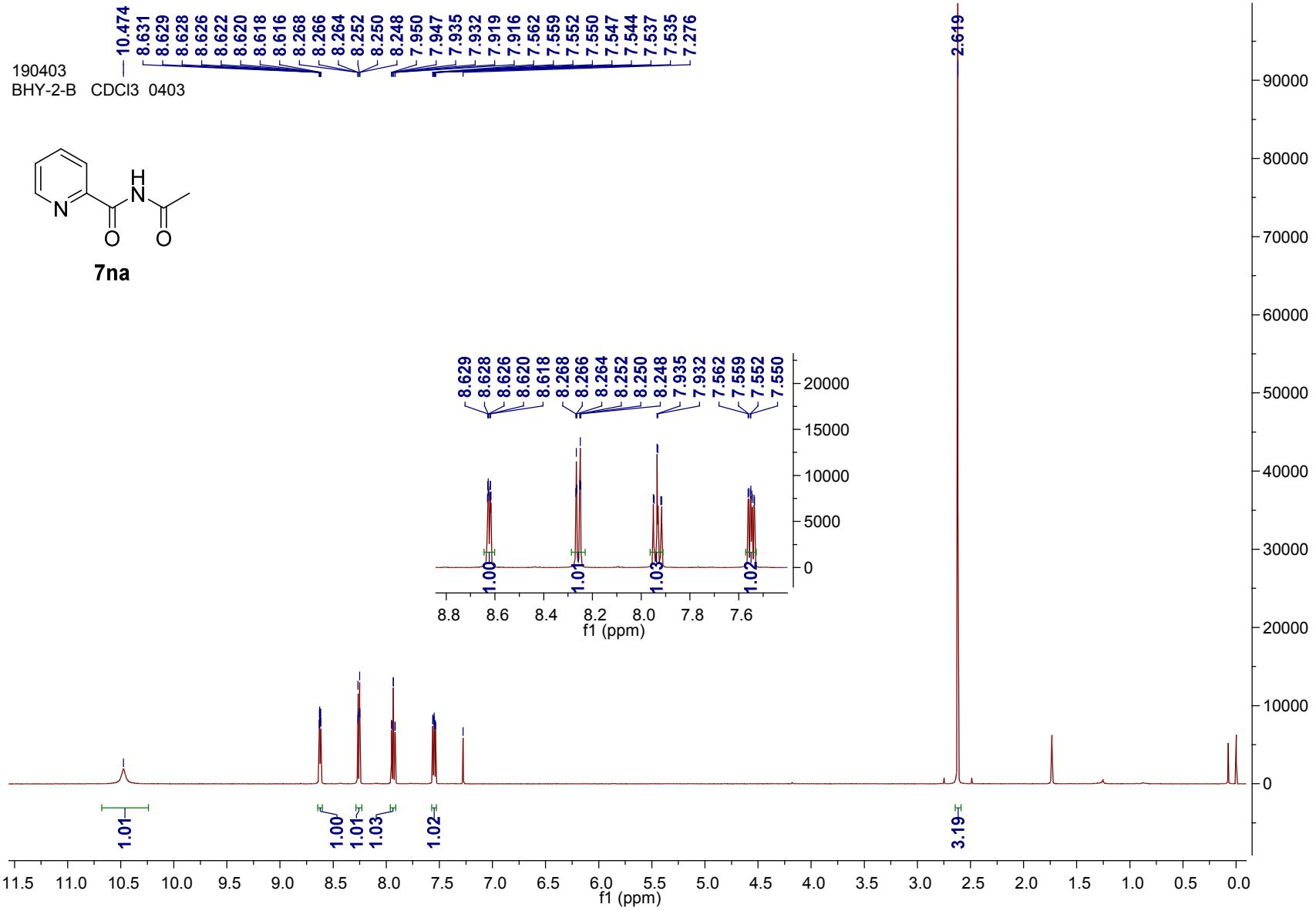

161230
BHY-F-3Cl CDCl3 0103
172.11
163.76
147.31
141.77
135.16
133.72
131.85
130.16
129.66
128.79
128.47
124.45
124.08
123.57
122.05
77.29
77.03
76.78
25.50
Cl
N
H
N
O
O
7ka
f1 (ppm)

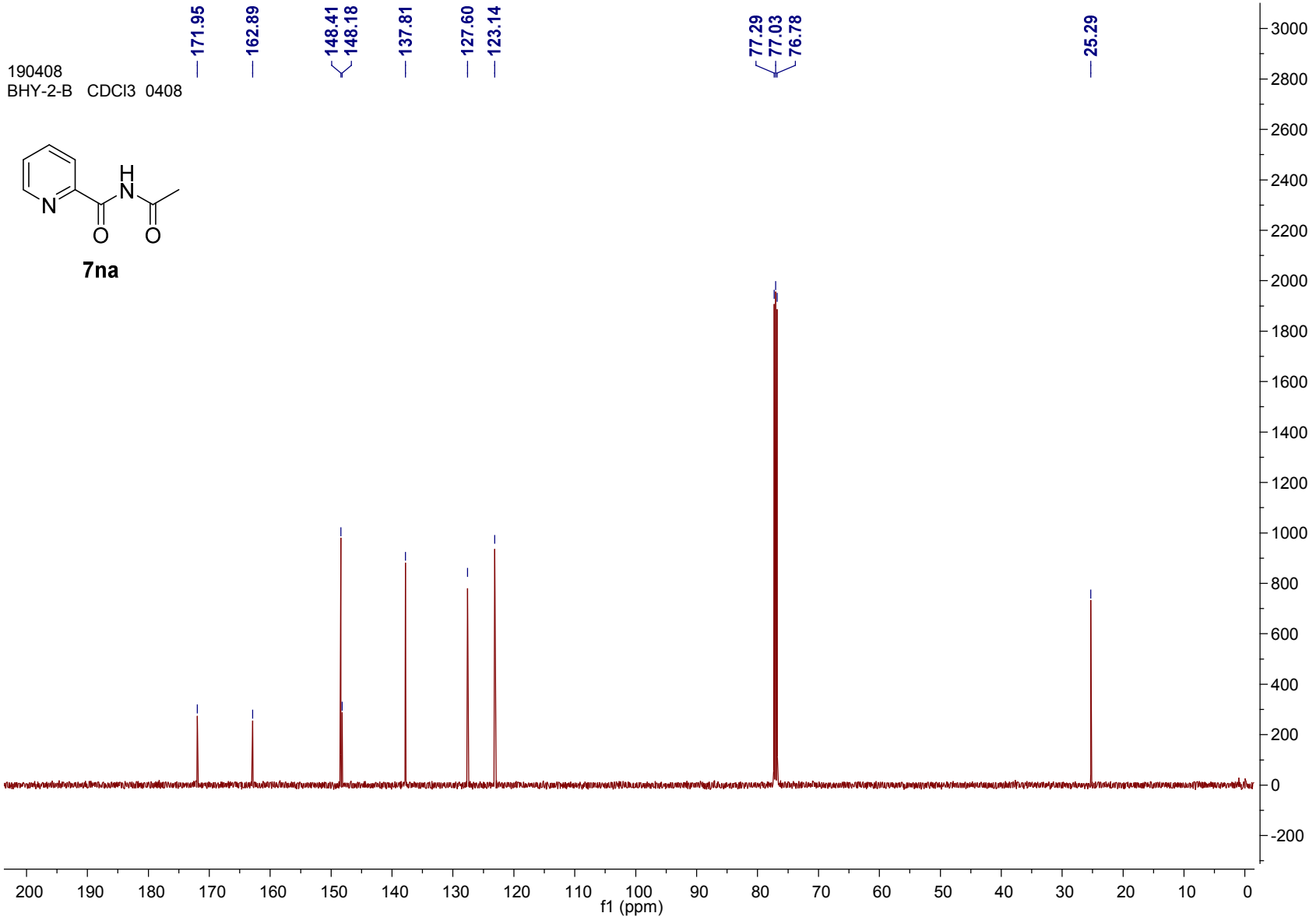

161216
BHY-F-R14CH3 CDCl3 1216
10.934
9.577
9.576
9.560
9.559
8.661
8.644
8.369
8.083
8.066
7.909
7.907
7.895
7.893
7.890
7.879
7.876
7.786
7.783
7.772
7.769
7.766
7.755
7.752
7.640
7.636
7.623
7.620
7.276
2.713
2.675
7la
1.00
1.00
1.08
1.07
1.02
1.05
1.06
1.07
3.14
3.10
f1 (ppm)

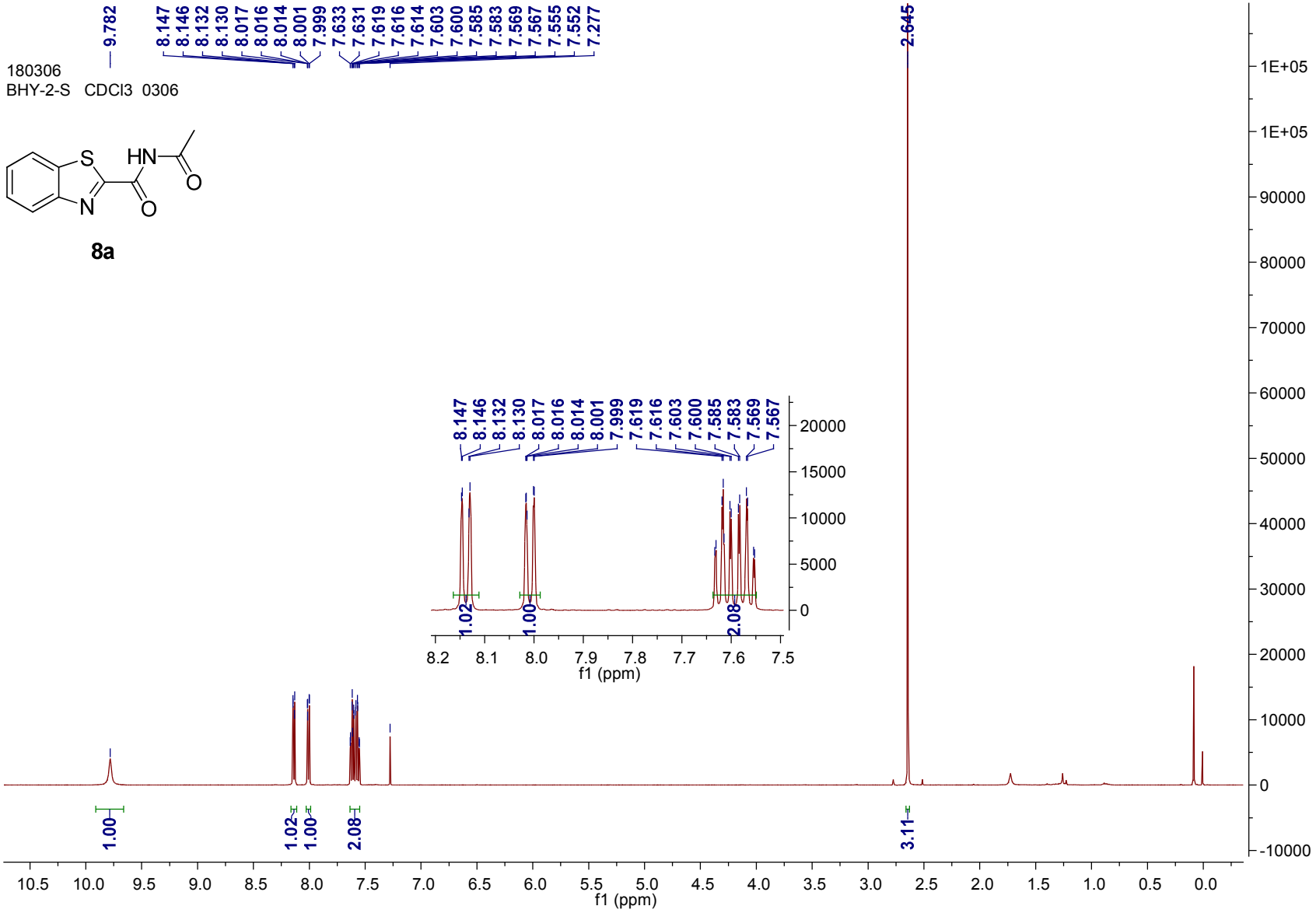

161216
BHY-F-R14CH3 CDCl3 1216
172.33
164.29
144.96
140.16
139.61
133.65
131.15
131.03
130.51
128.31
128.14
125.96
124.36
122.07
121.74
77.29
77.03
76.78
25.47
22.31
H
N
N
O
O
7la
f1 (ppm)

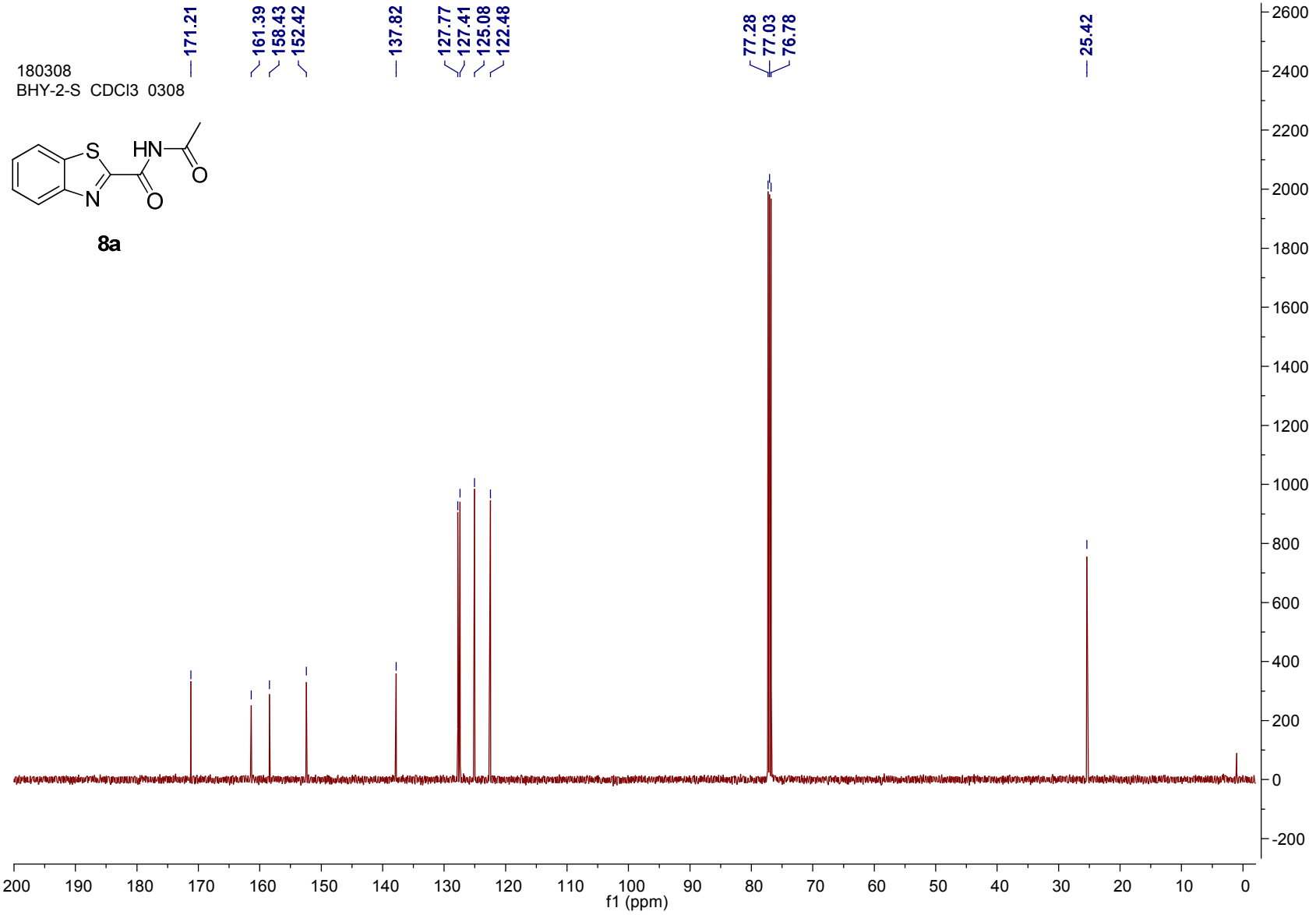

161130
BHY-2-F-R24CH3 CDCl3 1130
10.949
9.368
8.592
8.576
8.187
7.804
7.799
7.796
7.793
7.790
7.276
2.723
2.653
7ma
f1 (ppm)

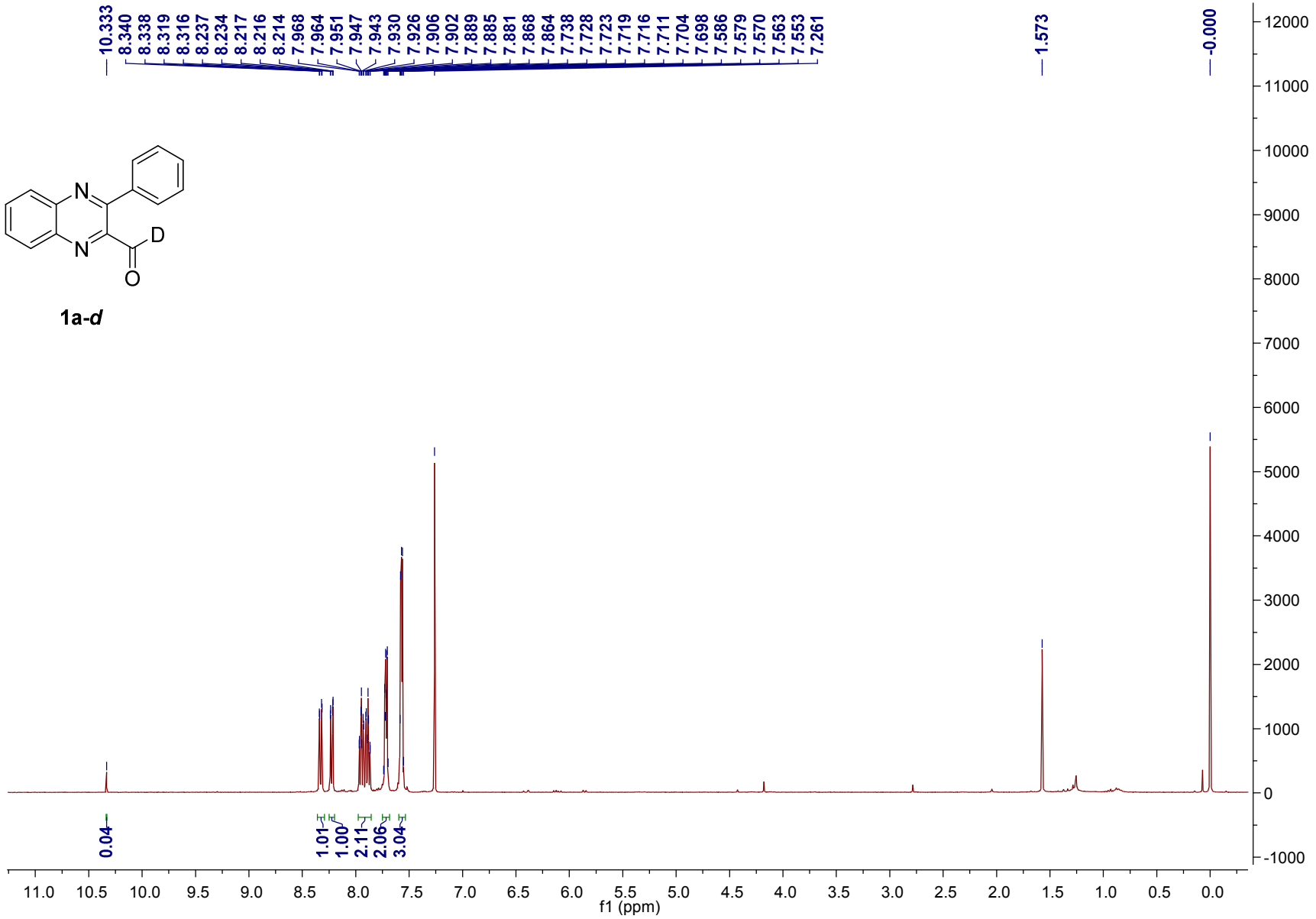

161130
BHY-2-F-R24CH3 CDCl3 1130
7ma
172.30
164.32
145.71
140.92
138.75
133.18
132.02
130.70
129.57
128.91
127.45
126.18
124.42
122.01
77.29
77.03
76.78
25.51
22.04
f1 (ppm)


10.474
8.631
8.629
8.628
8.626
8.622
8.620
8.618
8.616
8.268
8.266
8.264
8.252
8.250
8.248
7.950
7.947
7.935
7.932
7.919
7.916
7.562
7.559
7.552
7.550
7.547
7.544
7.537
7.535
7.276
2.619
190403
BHY-2-B CDCl3 0403
7na
f1 (ppm)
1.01
1.00
1.01
1.03
1.02
3.19


171.95
162.89
148.41
148.18
137.81
127.60
123.14
77.29
77.03
76.78
25.29
190408
BHY-2-B CDCl3 0408
7na
f1 (ppm)


180306
BHY-2-S CDCl3 0306
8a
9.782
8.147
8.146
8.132
8.130
8.017
8.016
8.014
8.001
7.999
7.633
7.631
7.619
7.616
7.614
7.603
7.600
7.585
7.583
7.569
7.567
7.555
7.552
7.277
2.645
1.00
1.02
1.00
2.08
3.11
f1 (ppm)


171.21
161.39
158.43
152.42
137.82
127.77
127.41
125.08
122.48
77.28
77.03
76.78
25.42
180308
BHY-2-S CDCl3 0308
S
HN
O
N
O
8a
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.333
8.340
8.338
8.319
8.316
8.237
8.234
8.217
8.216
8.214
7.968
7.964
7.951
7.947
7.943
7.930
7.926
7.906
7.902
7.889
7.885
7.881
7.868
7.864
7.738
7.728
7.723
7.719
7.716
7.711
7.704
7.698
7.586
7.579
7.570
7.563
7.553
7.261
1.573
-0.000
N
N
D
O
1a-d
0.04
1.01
1.00
2.11
2.06
3.04
f1 (ppm)