Supporting Information

Metal-free photo-induced heteroarylations of C-H and C-C bonds of alcohols by flow chemistry

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Contents

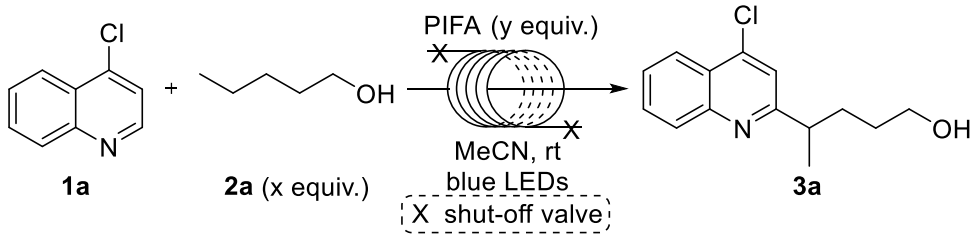
1. General experimental details

Commercially available reagents were used without further purification. THF was distilled from sodium. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26, CD_3OD: 3.31). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, q = quadruplet, br = broad, m = multiplet), coupling constants (Hz) and integration. ^{13}C-NMR spectra were recorded on a BRUKER AVANCE III HD (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.00, CD_3OD: 49.00). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. Mass spectra were measured with an Agilent Technologies 6120 Quadrupole LC/MS. High resolution mass spectrometry (HRMS) were measured with a GCT Premier^{TM} and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR and values are uncorrected.

Peristaltic pump of continuous-flow system was manufactured by Nanjing Runze Fluid Control Equipment Co. Ltd (LM60B-RZ1030-4 type), and was set at 65 rpm. Microreactor was used commercially available PFA (perfluoroalkoxyalkane) tube with an inner diameter of 760 μm (3.5 mL). Blue LED lamp parameters: rated power 50 W, rated voltage 220 V, rated current 300 mA, rated frequency 50 Hz, λ_{max} = 450 nm. The distance between light source and the reaction is 10 cm.

2. Reaction conditions survey

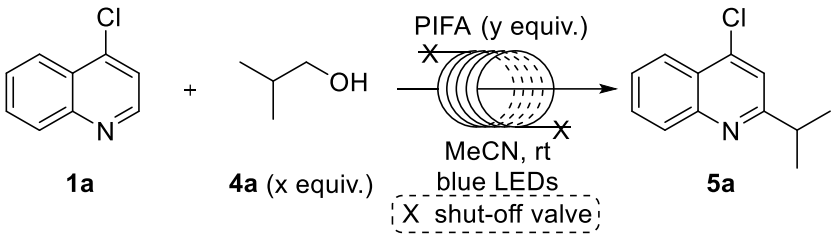
Table S1 Reaction conditions survey about 1,5-HAT pathway[a]



Entry	x (equiv.)	y (equiv.)	Yield[b] (%)
1	5.0	2.3	68
2[c]	5.0	2.3	62
3	5.0	2.5	68
4	5.0	2.1	75
5	5.0	1.9	72
6	4.0	2.1	69
7	6.0	2.1	72
8[d]	5.0	2.1	58
9[e]	5.0	2.1	0
10[f]	5.0	2.1	0

[a]Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), **2a** (5.0 equiv.), PIFA (2.1 equiv.) in MeCN (1.0 mL), irradiated by 2 × 50 W blue LEDs at rt for 12 h. [b]Isolated yield. [c]MeCN (2.0 mL). [d]2 × 30 W blue LEDs. [e]30 W green LEDs. [f]In dark. PIFA = Bis(trifluoroacetoxy)iodobenzene.

Table S2 Reaction conditions survey about β-C-C scission pathway[a]



Entry	x (equiv.)	y (equiv.)	Yield[b] (%)
1	5.0	2.1	75
2[c]	5.0	2.1	70
3	5.0	1.9	70
4	5.0	2.3	68
5	4.0	2.1	69
6	6.0	2.1	71
7[d]	5.0	2.1	56
8[e]	5.0	2.1	0
9[f]	5.0	2.1	0

[a]Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), **4a** (5.0 equiv.), PIFA (2.1 equiv.) in MeCN (1.0 mL), irradiated by 2 × 50 W blue LEDs at rt for 12 h. [b]Isolated yield. [c]MeCN (2.0 mL). [d]2 × 30 W blue LEDs. [e]30 W green LEDs. [f]In dark. PIFA = Bis(trifluoroacetoxy)iodobenzene.

3. General procedure for synthesizing 3 and 5

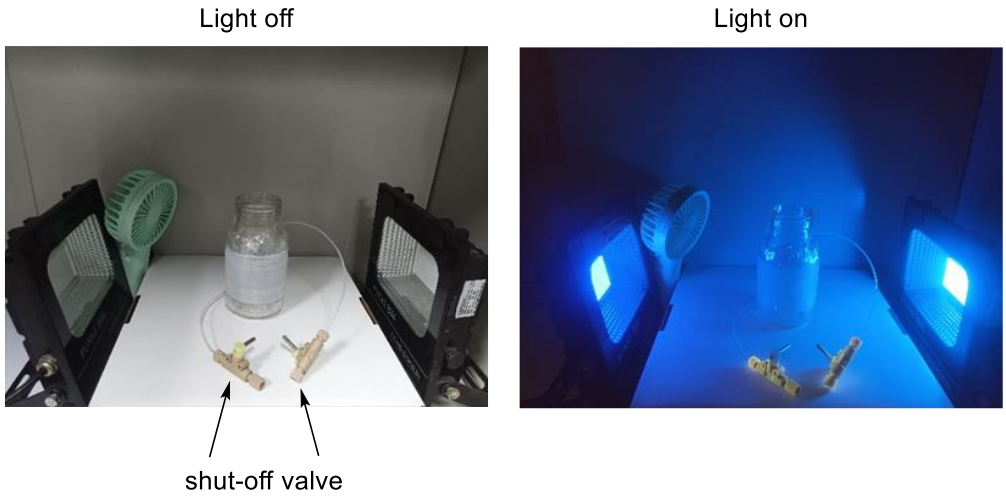


Figure S1 Reaction equipment

Heteroarene **1** (0.2 mmol, 1.0 equiv.), alcohol **2** or **4** (1.0 mmol, 5.0 equiv.) and PIFA (Bis(trifluoroacetoxy)iodobenzene, 0.42 mmol, 2.1 equiv.) were dissolved in MeCN (1.0 mL). Then the solution was transferred into the microreactor (PFA tube, ID = 760 μm) *via* syringe. The reaction was irradiated with 2 x 50 W blue LEDs at room temperature. After 12 hours, the reaction solution was collected in a flask and the microreactor was washed with EtOAc and water *via* syringe. The mixture was quenched by addition of aq. KOH until pH > 8 and then extracted with EtOAc. The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered,

concentrated, and purified by flash column chromatography on silica gel to give the desired product **3** or **5**.

4. Gram-scale preparations

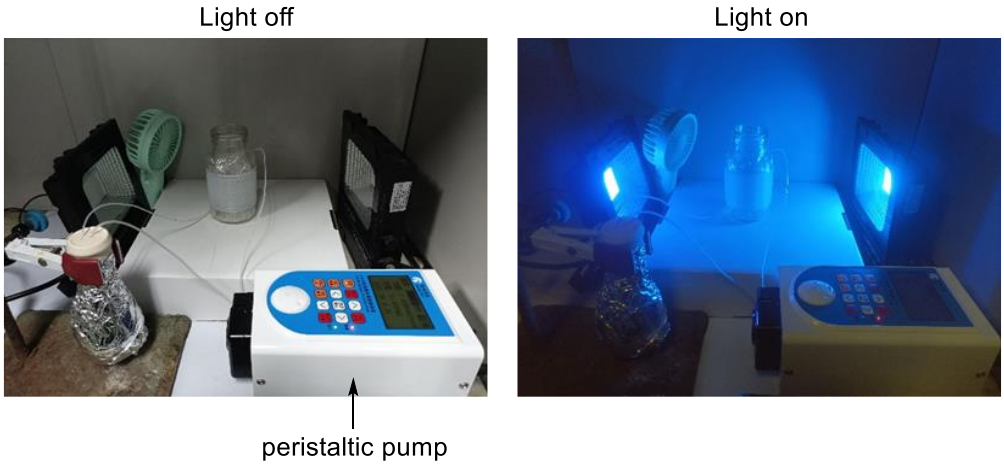
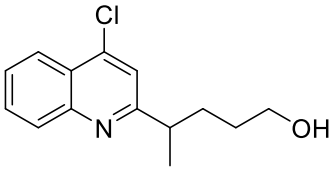


Figure S2 Reaction equipment of gram-scale reactions

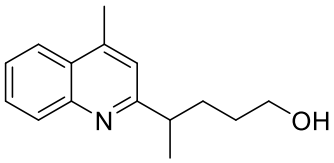
Heteroarene **1c** (8.0 mmol, 1.0 equiv.) and alcohol **2a** (40.0 mmol, 5.0 equiv.) were loaded in a tin foil wrapped flask. Then MeCN (40 mL) followed by PIFA (4.2 mmol, 0.525 equiv.) was added to the mixture (PIFA was added in four batches, one batch every 12 hours, 4.2 mmol per batch). Then the solution was injected to the microreactor (PFA tube, ID = 760 μm) by a peristaltic pump, flow rate (3.0 mL/min). The reaction was irradiated with 2 x 50 W blue LEDs at room temperature. After 48 hours, the reaction solution was collected in a flask and the microreactor was washed with EtOAc and water *via* syringe. The mixture was quenched by addition of aq. KOH until pH > 8 and then extracted with EtOAc. The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel to give the desired product product **3c** (1.16 g, 63% yield).

Heteroarene **1a** (7.0 mmol, 1.0 equiv.) and alcohol **4t** (35.0 mmol, 5.0 equiv.) were loaded in a tin foil wrapped flask. Then MeCN (35 mL) followed by PIFA (14.7 mmol, 2.1 equiv.) was added to the mixture. Then the solution was injected to the microreactor (PFA tube, ID = 760 μm) by a peristaltic pump, flow rate (3.0 mL/min). The reaction was irradiated with 2 x 50 W blue LEDs at room temperature. After 12 hours, the reaction solution was collected in a flask and the microreactor was washed with EtOAc and water *via* syringe. The mixture was quenched by addition of aq. KOH until pH > 8 and then extracted with EtOAc. The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel to give the desired product product **5t** (1.27 g, 82% yield).

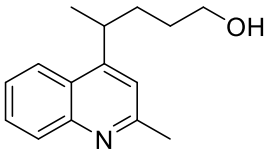
5. Characterization of products[1]



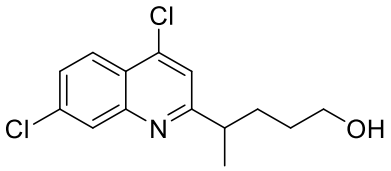
3a: 37.3 mg, 75% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.06-8.02 (m, 1H), 7.75-7.69 (m 1H), 7.60-7.54 (m, 1H), 7.40 (s, 1H), 3.68-3.56 (m, 2H), 3.16-3.05 (m, 1H), 2.37 (br, 1H), 1.98-1.87 (m, 1H), 1.82-1.71 (m, 1H), 1.68-1.56 (m, 1H), 1.54-1.42 (m, 1H), 1.37 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 148.4, 142.9, 130.3, 129.1, 126.8, 125.1, 123.9, 119.8, 62.6, 42.3, 32.8, 30.6, 20.8.



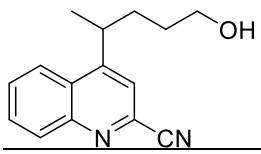
3b: 31.9 mg, 70% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.94 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.69-7.62 (m, 1H), 7.53-7.46 (m, 1H), 7.15 (s, 1H), 3.67-3.55 (m, 2H), 3.15-3.04 (m, 1H), 2.68 (d, *J* = 0.8 Hz, 3H), 2.58 (br, 1H), 2.00-1.89 (m, 1H), 1.82-1.71 (m, 1H), 1.69-1.57 (m, 1H), 1.54-1.42 (m, 1H), 1.37 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 147.3, 144.6, 129.3, 129.1, 127.0, 125.5, 123.6, 120.3, 62.6, 42.2, 32.9, 30.7, 21.1, 18.8.



3c: 36.7 mg, 80% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether/MeOH = 1/1/0-4/4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-7.99 (m, 2H), 7.65-7.60 (m, 1H), 7.48-7.43 (m, 1H), 7.14 (s, 1H), 3.62 (t, *J* = 6.4 Hz, 2H), 3.59-3.51 (m, 1H), 2.89 (br, 1H), 2.68 (s, 3H), 1.89-1.71 (m, 2H), 1.65-1.49 (m, 2H), 1.35 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 153.6, 147.8, 129.2, 128.9, 125.4, 125.4, 122.7, 118.4, 62.4, 33.4, 33.1, 30.6, 25.2, 21.2.



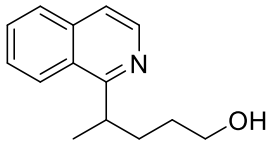
3d: 38.5 mg, 68% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.8 Hz, 1H), 8.04 (d, *J* = 2.0 Hz, 1H), 7.51 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.38 (s, 1H), 3.67-3.57 (m, 2H), 3.13-3.02 (m, 1H), 2.16 (br, 1H), 1.96-1.86 (m, 1H), 1.81-1.71 (m, 1H), 1.66-1.55 (m, 1H), 1.52-1.42 (m, 1H), 1.36 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 148.8, 142.8, 136.3, 128.2, 127.7, 125.3, 123.6, 120.1, 62.6, 42.3, 32.8, 30.6, 20.7. FT-IR: ν (cm^{-1}) δ 2931, 2869, 1608, 1588, 1490, 1405, 1301, 1159, 1072. HRMS [ESI] calcd for $C_{14}H_{15}Cl_2NNaO$ $[M+Na]^+$ 306.0423, found 306.0428.



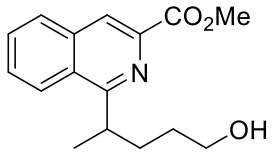
3e: 20.7 mg, 43% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/1). ^{1}H NMR

[1] Characterization of product **3a**-**3c** and **3e**-**3m** refers to: X. Wu, H. Zhang, N. Tang, Z. Wu, D. Wang, M. Ji, Y. Xu, M. Wang and C. Zhu, *Nat. Commun*., 2018, **9**, 3343. Characterization of product **5ae** refers to: Y. Wang, L. Yang, S. Liu, L. Huang and Z.-Q. Liu, *Adv. Synth. Catal*., 2019, **361**, 4568.

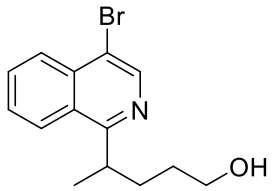
(400 MHz, $CDCl_3$) δ 8.20-8.14 (m, 2H), 7.84-7.79 (m, 1H), 7.73-7.68 (m, 1H), 7.59 (s, 1H), 3.71-3.63 (m, 3H), 1.94-1.78 (m, 2H), 1.67-1.50 (m, 3H), 1.42 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 148.4, 133.7, 131.0, 130.6, 129.1, 127.7, 123.0, 120.1, 117.8, 62.5, 33.5, 33.4, 30.4, 21.1.



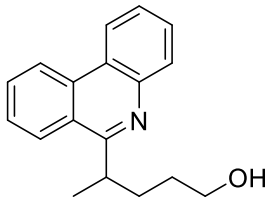
3f: 26.7 mg, 62% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/1-2/1). ^1H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 6.0 Hz, 1H), 8.22 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.68-7.63 (m, 1H), 7.61-7.55 (m, 1H), 7.49 (d, *J* = 5.6 Hz, 1H), 3.87-3.77 (m, 1H), 3.63-3.50 (m, 2H), 2.21-2.11 (m, 2H), 1.87-1.76 (m, 1H), 1.70-1.58 (m, 1H), 1.54-1.43 (m, 1H), 1.40 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 141.7, 136.4, 129.7, 127.5, 127.0, 126.7, 124.6, 119.1, 62.7, 36.0, 31.9, 30.9, 21.2.



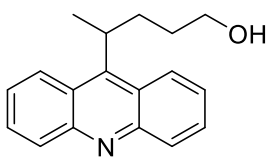
3g: 33.9 mg, 62% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/1-3/2). ^1H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 8.29-8.25 (m, 1H), 7.97-7.93 (m, 1H), 7.76-7.69 (m, 2H), 4.02 (s, 3H), 3.84-3.76 (m, 1H), 3.59-3.53 (m, 1H), 3.46-3.39 (m, 1H), 2.54 (br, 1H), 2.49-2.39 (m, 1H), 1.87-1.70 (m, 2H), 1.51-1.43 (m, 1H), 1.41 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 165.7, 140.2, 136.1, 130.3, 129.3, 129.1, 128.1, 124.9, 122.6, 62.1, 52.6, 36.9, 31.2, 30.4, 21.8.



3h: 30.4 mg, 52% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/6-1/2). ^1H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.24-8.16 (m, 2H), 7.80-7.74 (m, 1H), 7.68-7.62 (m, 1H), 3.84-3.73 (m, 1H), 3.64-3.52 (m, 2H), 2.17-2.06 (m, 1H), 1.92 (br, 1H), 1.85-1.74 (m, 1H), 1.67-1.55 (m, 1H), 1.53-1.42 (m, 1H), 1.39 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 143.5, 134.9, 130.9, 128.1, 127.9, 126.9, 125.0, 117.6, 62.7, 35.9, 32.0, 30.8, 21.1.

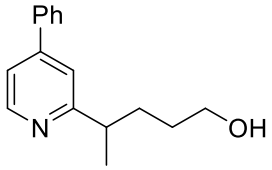


3i: 36.1 mg, 68% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/2-2/3). ^1H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 8.4 Hz, 1H), 8.54 (d, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.86-7.80 (m, 1H), 7.74-7.67 (m, 2H), 7.64-7.59 (m, 1H), 3.92-3.82 (m, 1H), 3.66-3.49 (m, 2H), 2.45-2.34 (m, 2H), 1.92-1.82 (m, 1H), 1.81-1.69 (m, 1H), 1.63-1.52 (m, 1H), 1.47 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 143.5, 133.1, 130.1, 129.6, 128.6, 127.2, 126.3, 125.6, 125.0, 123.4, 122.6, 121.8, 62.6, 36.6, 31.0, 30.9, 21.3.

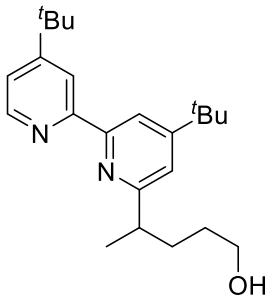


3j: 22.8 mg, 43% yield, yellow solid, m.p. 156-157 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 2/3-3/2). ^1H NMR (400 MHz, $CDCl_3$) δ 8.52-8.32 (m, 2H), 8.22 (d, *J* = 8.8 Hz, 2H), 7.77-7.67 (m, 2H), 7.56-7.43 (m, 2H), 4.40-4.27 (m, 1H),

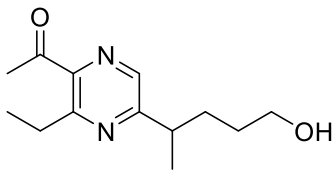
3.57 (t, *J* = 6.4 Hz, 2H), 2.36-2.20 (m, 2H), 1.90 (br, 1H), 1.73 (d, *J* = 7.2 Hz, 3H), 1.71-1.59 (m, 1H), 1.39-1.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.8, 148.9, 148.7, 130.8, 130.5, 129.5, 126.0, 125.8, 125.5, 125.4, 124.5, 124.3, 123.6, 62.5, 34.0, 33.6, 31.9, 21.3.



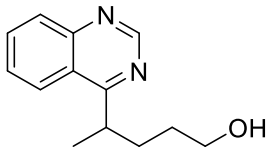
3k: 21.2 mg, 44% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether/MeOH = 1/1/0-6/6/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 5.2 Hz, 1H), 7.65-7.60 (m, 2H), 7.51-7.40 (m, 3H), 7.37-7.35 (m, 1H), 7.34-7.31 (m, 1H), 3.68-3.58 (m, 2H), 3.05-2.95 (m, 1H), 2.09 (br, 1H), 1.94-1.83 (m, 1H), 1.78-1.68 (m, 1H), 1.67-1.55 (m, 1H), 1.54-1.44 (m, 1H), 1.36 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 149.4, 149.0, 138.5, 129.0, 128.9, 127.0, 119.6, 119.4, 62.7, 41.6, 33.2, 30.7, 21.0.



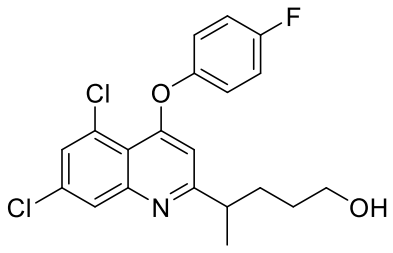
3l: 21.0 mg, 30% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/3-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 5.2 Hz, 1H), 8.46 (d, *J* = 1.2 Hz, 1H), 8.20 (d, *J* = 1.6 Hz, 1H), 7.29-7.26 (m, 1H), 7.13 (d, *J* = 2.0 Hz, 1H), 3.69-3.58 (m, 2H), 3.07-2.98 (m, 1H), 1.96-1.87 (m, 2H), 1.78-1.69 (m, 2H), 1.65-1.56 (m, 1H), 1.39-1.36 (m, 21H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 161.3, 160.7, 156.9, 155.5, 148.9, 120.5, 118.4, 118.4, 115.7, 63.1, 41.5, 35.0, 34.9, 33.5, 30.7, 30.6, 21.2.



3m: 15.1 mg, 32% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/2-2/3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 3.65-3.59 (m, 2H), 3.14 (q, *J* = 7.2 Hz, 2H), 3.06-2.95 (m, 1H), 2.68 (s, 3H), 1.91-1.83 (m, 1H), 1.78-1.68 (m, 1H), 1.61-1.52 (m, 2H), 1.48-1.39 (m, 1H), 1.33 (d, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.3, 163.0, 158.0, 144.4, 139.1, 62.7, 39.4, 32.5, 30.5, 28.9, 28.1, 20.4, 13.2.

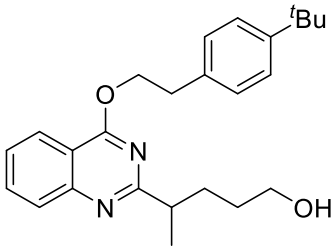


3n: 17.3 mg, 40% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 2/1-4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (s, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.90-7.84 (m, 1H), 7.66-7.60 (m, 1H), 3.86-3.77 (m, 1H), 3.66-3.56 (m, 2H), 2.17-2.07 (m, 1H), 1.96 (br, 1H), 1.87-1.77 (m, 1H), 1.68-1.56 (m, 1H), 1.54-1.44 (m, 1H), 1.41 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.2, 154.6, 150.0, 133.5, 129.3, 127.5, 124.1, 123.7, 62.6, 35.9, 31.9, 30.7, 20.6. FT-IR: ν (cm^{-1}) δ 2932, 2870, 1569, 1496, 1346, 1268, 1057, 1029. HRMS [ESI] calcd for $C_{13}H_{16}N_2NaO$ $[M+Na]^+$ 239.1155, found 239.1150.

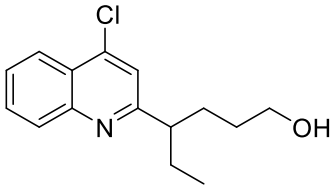


3o: 33.2 mg, 42% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 2.0 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.19-7.07 (m, 4H), 6.51 (s, 1H), 3.63-3.52 (m, 2H), 2.95-2.86 (m, 1H), 2.04 (br, 1H),

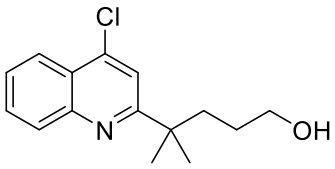
1.84-1.74 (m, 1H), 1.68-1.51 (m, 2H), 1.45-1.37 (m, 1H), 1.23 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 162.5, 159.9 (d, $J_{C\text{-}F}$ = 242.9 Hz), 151.2, 150.2 (d, $J_{C\text{-}F}$ = 2.7 Hz), 134.9, 129.9, 128.8, 127.4, 121.9 (d, $J_{C\text{-}F}$ = 8.4 Hz), 117.0 (d, $J_{C\text{-}F}$ = 23.4 Hz), 117.0, 105.7, 62.6, 42.2, 32.4, 30.5, 20.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.2 (s). FT-IR: ν (cm^{-1}) δ 2930, 2870, 1599, 1501, 1427, 1361, 1193, 1100, 1057. HRMS [ESI] calcd for $C_{20}H_{19}Cl_2FNO_2$ $[M+H]^+$ 394.0771, found 394.0778.



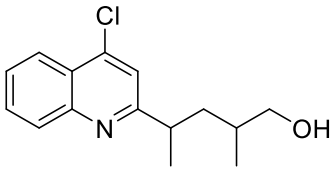
3p: 47.1 mg, 60% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/2-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.09 (m, 1H), 7.87-7.84 (m, 1H), 7.79-7.74 (m, 1H), 7.51-7.46 (m, 1H), 7.39-7.35 (m, 2H), 7.31-7.27 (m, 2H), 4.81-4.74 (m, 2H), 3.68-3.58 (m, 2H), 3.18 (t, J = 7.2 Hz, 2H), 3.14-3.04 (m, 1H), 2.41 (br, 1H), 2.07-1.97 (m, 1H), 1.80-1.69 (m, 1H), 1.68-1.60 (m, 1H), 1.56-1.46 (m, 1H), 1.38 (d, J = 6.8 Hz, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 166.7, 151.1, 149.4, 134.9, 133.3, 128.7, 127.0, 126.0, 125.4, 123.4, 115.0, 67.4, 62.8, 42.9, 34.7, 34.4, 32.0, 31.4, 30.7, 20.2. FT-IR: ν (cm^{-1}) δ 3032, 2920, 1620, 1469, 1368, 1298, 1174, 1150, 1087. HRMS [ESI] calcd for $C_{25}H_{32}N_2NaO_2$ $[M+Na]^+$ 415.2356, found 415.2346.



3q: 34.4 mg, 65% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.4, 1.2 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.75-7.69 (m, 1H), 7.60-7.54 (m, 1H), 7.37 (s, 1H), 3.63-3.53 (m, 2H), 2.92-2.84 (m, 1H), 2.36 (br, 1H), 1.88-1.74 (m, 4H), 1.59-1.50 (m, 1H), 1.44-1.33 (m, 1H), 0.83 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 148.5, 142.8, 130.2, 129.2, 126.7, 125.1, 123.9, 120.2, 62.6, 49.8, 31.2, 30.6, 28.6, 12.0. FT-IR: ν (cm^{-1}) δ 2931, 2872, 1616, 1554, 1457, 1374, 1218, 1151, 1059. HRMS [ESI] calcd for $C_{15}H_{18}ClNNaO$ $[M+Na]^+$ 286.0969, found 286.0974.

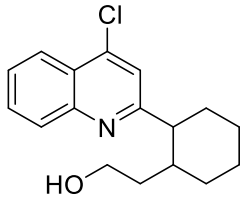


3r: 34.7 mg, 66% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/6-1/3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.4, 1.2 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.75-7.69 (m, 1H), 7.60-7.54 (m, 2H), 3.55 (t, J = 6.0 Hz, 2H), 2.33 (br, 1H), 1.96-1.90 (m, 2H), 1.50-1.44 (m, 2H), 1.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 148.0, 142.6, 130.1, 129.4, 126.8, 124.6, 123.7, 118.9, 63.0, 41.0, 38.1, 28.1. FT-IR: ν (cm^{-1}) δ 2945, 2869, 1684, 1588, 1492, 1365, 1289, 1209, 1102. HRMS [ESI] calcd for $C_{15}H_{19}ClNO$ $[M+H]^+$ 264.1150, found 264.1158.

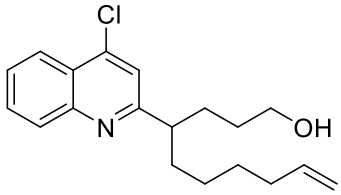


3s: (*d.r.* = 1:1): 31.7 mg, 60% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/4-1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H, two isomers), 8.06-8.02 (m, 2H, two isomers), 7.76-7.70 (m, 2H, two isomers), 7.61-7.55 (m, 2H, two isomers), 7.43 (s, 1H, one isomer), 7.41 (s, 1H, one isomer), 3.54-3.44 (m, 2H, two isomers), 3.44-3.36 (m, 2H, two isomers),

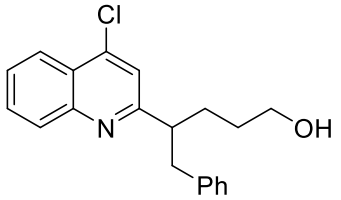
3.34-3.24 (m, 1H, one isomer), 3.24-3.15 (m, 1H, one isomer), 2.89 (br, 1H, one isomer), 2.62 (br, 1H, one isomer), 2.21-2.13 (m, 1H, one isomer), 1.78-1.64 (m, 3H, two isomers), 1.56-1.47 (m, 1H, one isomer), 1.46-1.38 (m, 1H, one isomer), 1.36 (d, J = 6.8 Hz, 3H, one isomer), 1.36 (d, J = 7.2 Hz, 3H, one isomer), 0.97 (d, J = 6.4 Hz, 3H, one isomer), 0.89 (d, J = 6.8 Hz, 3H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9 & 166.5 (two isomers), 148.4 & 148.2 (two isomers), 143.1 & 142.9 (two isomers), 130.4 & 130.4 (two isomers), 129.1 (overlap, two isomers), 126.8 & 126.8 (two isomers), 125.1 & 125.1 (two isomers), 123.9 (overlap, two isomers), 120.3 & 119.6 (two isomers), 68.2 & 67.8 (two isomers), 40.8 & 40.3 (two isomers), 39.6 & 39.5 (two isomers), 34.3 & 33.5 (two isomers), 22.4 & 20.8 (two isomers), 17.3 & 17.2 (two isomers). FT-IR: ν (cm^{-1}) δ 2926, 2871, 1588, 1495, 1377, 1223, 1150, 1031. HRMS [ESI] calcd for $C_{15}H_{19}ClNO$ $[M+H]^+$ 264.1150, found 264.1155.



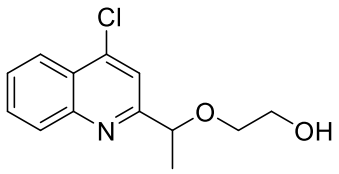
3t: 40.4 mg, 70% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/9-1/3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.4, 0.8 Hz, 1H), 8.03 (d, J = 8.4 Hz, 1H), 7.75-7.69 (m, 1H), 7.60-7.55 (m, 1H), 7.40 (s, 1H), 3.56-3.49 (m, 2H), 2.75-2.63 (m, 2H), 2.12-2.01 (m, 1H), 2.01-1.91 (m, 2H), 1.88-1.78 (m, 2H), 1.58-1.14 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 148.3, 143.0, 130.4, 129.0, 126.8, 125.1, 123.9, 120.8, 60.4, 52.7, 37.6, 37.5, 34.6, 32.5, 26.4, 26.2. FT-IR: ν (cm^{-1}) δ 2925, 2853, 1733, 1699, 1588, 1494, 1373, 1223, 1083. HRMS [ESI] calcd for $C_{17}H_{20}ClNNaO$ $[M+Na]^+$ 312.1126, found 312.1118.



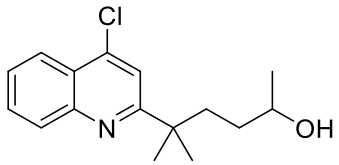
3u: 33.7 mg, 53% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/6-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, J = 8.4, 1.2 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.75-7.69 (m, 1H), 7.61-7.54 (m, 1H), 7.36 (s, 1H), 5.79-5.67 (m, 1H), 4.97-4.85 (m, 2H), 3.65-3.53 (m 2H), 3.00-2.91 (m, 1H), 2.23 (br, 1H), 2.01-1.93 (m, 2H), 1.88-1.69 (m, 4H), 1.60-1.49 (m, 1H), 1.45-1.25 (m, 4H), 1.21-1.11 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 148.5, 142.8, 138.8, 130.2, 129.2, 126.7, 125.1, 123.9, 120.2, 114.3, 62.6, 48.2, 35.5, 33.5, 31.6, 30.6, 28.9, 27.0. FT-IR: ν (cm^{-1}) δ 2928, 2856, 1638, 1588, 1494, 1375, 1220, 1150, 1057. HRMS [ESI] calcd for $C_{19}H_{25}ClNO$ $[M+H]^+$ 318.1619, found 318.1627.



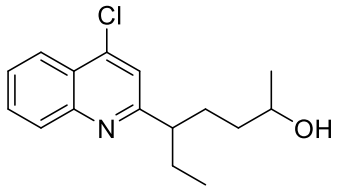
3v: 35.0 mg, 51% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/5-2/3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 8.4, 1.2 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.76-7.71 (m, 1H), 7.61-7.56 (m, 1H), 7.27 (s, 1H), 7.23-7.17 (m, 2H), 7.17-7.08 (m, 3H), 3.60-3.49 (m, 2H), 3.31-3.23 (m, 1H), 3.20-3.12 (m, 1H), 3.03-2.96 (m, 1H), 2.02-1.91 (m, 2H), 1.90-1.80 (m, 1H), 1.58-1.46 (m, 1H), 1.46-1.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 148.6, 142.5, 139.8, 130.3, 129.3, 129.1, 128.2, 126.8, 126.1, 125.1, 123.9, 121.0, 62.6, 49.9, 42.0, 30.5, 30.5. FT-IR: ν (cm^{-1}) δ 2931, 2858, 1616, 1587, 1474, 1374, 1221, 1151, 1057. HRMS [ESI] calcd for $C_{20}H_{21}ClNO$ $[M+H]^+$ 326.1306, found 326.1311.



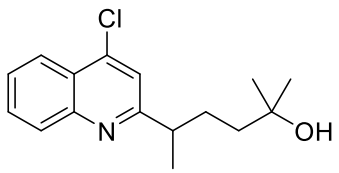
3w: 23.2 mg, 46% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/3-1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.79-7.73 (m, 1H), 7.65-7.59 (m, 2H), 4.74 (q, *J* = 6.8 Hz, 1H), 3.84-3.77 (m, 1H), 3.77-3.65 (m, 2H), 3.55-3.49 (m, 1H), 2.92 (br, 1H), 1.57 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 148.2, 143.7, 130.6, 129.3, 127.4, 125.7, 124.0, 118.2, 79.3, 70.8, 61.9, 22.3. FT-IR: ν (cm^{-1}) δ 2927, 2867, 1616, 1589, 1457, 1342, 1258, 1175, 1110, 1059. HRMS [ESI] calcd for $C_{13}H_{14}ClNNaO_2$ $[M+Na]^+$ 274.0605, found 274.0601.



3x: 39.5 mg, 71% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/10-1/6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0, 0.8 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.75-7.69 (m, 1H), 7.60-7.55 (m, 2H), 3.77-3.68 (m, 1H), 2.68 (br, 1H), 2.07-1.99 (m, 1H), 1.96-1.87 (m, 1H), 1.42 (s, 3H), 1.42 (s, 3H), 1.40-1.27 (m, 2H), 1.13 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 148.0, 142.7, 130.2, 129.4, 126.8, 124.6, 123.7, 119.1, 68.1, 41.1, 37.6, 34.5, 28.4, 28.2, 23.4. FT-IR: ν (cm^{-1}) δ 2964, 2929, 1616, 1588, 1473, 1366, 1209, 1103. HRMS [ESI] calcd for $C_{16}H_{21}ClNO$ $[M+H]^+$ 278.1306, found 278.1297.

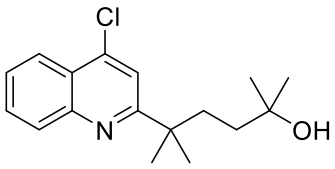


3y: (*d.r.* = 1:1): 37.4 mg, 67% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/8-1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.4 Hz, 2H, two isomers), 8.06 (d, *J* = 8.4 Hz, 2H, two isomers), 7.77-7.70 (m, 2H, two isomers), 7.62-7.55 (m, 2H, two isomers), 7.37 (s, 1H, one isomer), 7.37 (s, 1H, one isomer), 3.83-3.75 (m, 1H, one isomer), 3.73-3.65 (m, 1H, one isomer), 2.91-2.82 (m, 2H, two isomers), 2.19 (br, 1H, one isomer), 1.95-1.74 (m, 9H, two isomers), 1.51-1.40 (m, 2H, two isomers), 1.33-1.20 (m, 2H, two isomers), 1.13 (d, *J* = 5.6 Hz, 3H, one isomer), 1.11 (d, *J* = 6.0 Hz, 3H, one isomer), 0.84 (t, *J* = 7.2 Hz, 6H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7 & 165.6 (two isomers), 148.5 & 148.4 (two isomers), 142.7 & 142.7 (two isomers), 130.2 & 130.2 (two isomers), 129.3 & 129.2 (two isomers), 126.7 & 126.7 (two isomers), 125.1 (overlap, two isomers), 123.9 (overlap, two isomers), 120.3 (overlap, two isomers), 67.9 & 67.8 (two isomers), 50.0 & 50.0 (two isomers), 37.1 & 37.0 (two isomers), 30.9 & 30.8 (two isomers), 28.7 (overlap, two isomers), 23.5 & 23.4 (two isomers), 12.0 & 12.0 (two isomers). FT-IR: ν (cm^{-1}) δ 2962, 2929, 1616, 1588, 1457, 1373, 1219, 1122, 1028. HRMS [ESI] calcd for $C_{16}H_{21}ClNO$ $[M+H]^+$ 278.1306, found 278.1310.

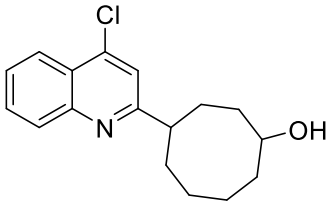


3z: 36.5 mg, 66% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/9-1/3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.07-8.03 (m, 1H), 7.75-7.69 (m, 1H), 7.60-7.55 (m, 1H), 7.40 (s, 1H), 3.11-3.01 (m, 1H), 1.99-1.88 (m, 2H), 1.83-1.73 (m, 1H), 1.61-1.52 (m, 1H), 1.37 (d, *J* = 7.2 Hz, 3H), 1.36-1.28 (m, 1H), 1.18 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 148.5, 142.8, 130.2, 129.2, 126.7, 125.1, 123.9, 119.9, 70.7,

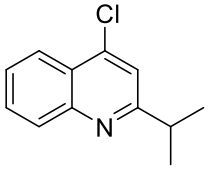
42.7, 41.4, 31.0, 29.3, 29.2, 21.0. FT-IR: ν (cm^{-1}) δ 2966, 2931, 1589, 1494, 1375, 1281, 1220, 1053. HRMS [ESI] calcd for $C_{16}H_{21}ClNO$ $[M+H]^+$ 278.1306, found 278.1310.



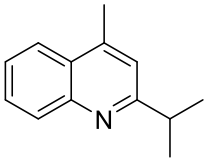
3aa: 32.8 mg, 56% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/20-1/10). ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.75-7.70 (m, 1H), 7.61-7.55 (m, 2H), 2.80 (br, 1H), 2.02-1.96 (m, 2H), 1.42 (s, 6H), 1.41-1.35 (m, 2H), 1.19 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 148.0, 142.7, 130.2, 129.3, 126.8, 124.6, 123.7, 119.2, 70.7, 41.1, 38.6, 35.9, 29.3, 28.4. FT-IR: ν (cm^{-1}) δ 2966, 2930, 1617, 1589, 1458, 1365, 1268, 1192, 1091. HRMS [ESI] calcd for $C_{17}H_{22}ClNNaO$ $[M+Na]^+$ 314.1282, found 314.1284.



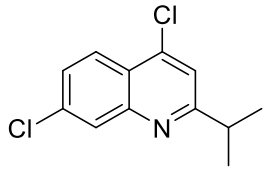
3ab: (*d.r.* = 1:1): 41.8 mg, 72% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/2-1/1). ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0, 0.8 Hz, 2H, two isomers), 8.04 (d, *J* = 8.4 Hz, 2H, two isomers), 7.76-7.70 (m, 2H, two isomers), 7.60-7.54 (m, 2H, two isomers), 7.40 (s, 1H, one isomer), 7.37 (s, 1H, one isomer), 4.06-3.95 (m, 2H, two isomers), 3.16-3.03 (m, 2H, two isomers), 2.17-1.55 (m, 26H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0 & 167.8 (two isomers), 148.4 & 148.4 (two isomers), 142.7 & 142.6 (two isomers), 130.2 & 130.2 (two isomers), 129.3 & 129.3 (two isomers), 126.7 (overlap, two isomers), 125.0 & 125.0 (two isomers), 123.9 & 123.9 (two isomers), 120.2 & 120.0 (two isomers), 72.2 & 71.3 (two isomers), 48.1 & 47.8 (two isomers), 34.7 & 34.2 (two isomers), 33.9 & 33.2 (two isomers), 31.6 & 31.4 (two isomers), 29.2 & 28.3 (two isomers), 26.5 & 26.4 (two isomers), 22.9 & 22.3 (two isomers). FT-IR: ν (cm^{-1}) δ 2924, 2855, 1616, 1588, 1494, 1375, 1218, 1150, 1044. HRMS [ESI] calcd for $C_{17}H_{21}ClNO$ $[M+H]^+$ 290.1306, found 290.1301.



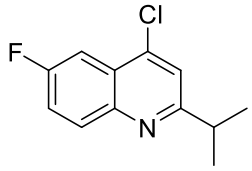
5a: 30.9 mg, 75% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.08-8.04 (m, 1H), 7.75-7.69 (m, 1H), 7.59-7.54 (m, 1H), 7.43 (s, 1H), 3.29-3.17 (m, 1H), 1.39 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 148.6, 142.6, 130.1, 129.3, 126.6, 125.1, 123.9, 119.4, 37.2, 22.3. FT-IR: ν (cm^{-1}) δ 2963, 1615, 1553, 1409, 1328, 1253, 1217, 1148, 1024. HRMS [ESI] calcd for $C_{12}H_{13}ClN$ $[M+H]^+$ 206.0731, found 206.0739.



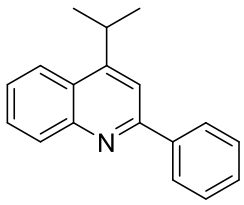
5b: 28.5 mg, 77% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/60). ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.4, 0.4 Hz, 1H), 7.94 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.69-7.64 (m, 1H), 7.52-7.46 (m, 1H), 7.19-7.16 (m, 1H), 3.28-3.16 (m, 1H), 2.68 (d, *J* = 0.8 Hz, 3H), 1.39 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 147.6, 144.3, 129.5, 128.9, 127.0, 125.4, 123.5, 119.7, 37.2, 22.5, 18.8. FT-IR: ν (cm^{-1}) δ 2962, 1603, 1561, 1471, 1412, 1341, 1261, 1188, 1152, 1089, 1033. HRMS [ESI] calcd for $C_{13}H_{16}N$ $[M+H]^+$ 186.1277, found 186.1270.



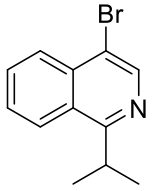
5c: 35.1 mg, 73% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 9.2 Hz, 1H), 8.05 (d, *J* = 2.0 Hz, 1H), 7.50 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.40 (s, 1H), 3.25-3.14 (m, 1H), 1.37 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 149.0, 142.5, 136.2, 128.3, 127.5, 125.2, 123.5, 119.7, 37.1, 22.2. FT-IR: ν (cm^{-1}) δ 2964, 1607, 1547, 1458, 1386, 1302, 1265, 1146, 1091, 1048. HRMS [ESI] calcd for $C_{12}H_{12}Cl_2N$ $[M+H]^+$ 240.0341, found 240.0344.



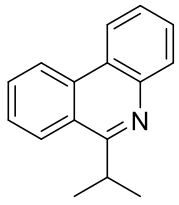
5d: 26.9 mg, 60% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 9.2, 5.2 Hz, 1H), 7.78 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.51-7.45 (m, 1H), 7.44 (s, 1H), 3.27-3.15 (m, 1H), 1.38 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9 (d, $J_{C\text{-}F}$ = 2.5 Hz), 160.7 (d, $J_{C\text{-}F}$ = 246.5 Hz), 145.6, 141.8 (d, $J_{C\text{-}F}$ = 5.6 Hz), 131.9 (d, $J_{C\text{-}F}$ = 9.1 Hz), 125.9 (d, $J_{C\text{-}F}$ = 10.0 Hz), 120.3 (d, $J_{C\text{-}F}$ = 25.5 Hz), 120.1, 107.7 (d, $J_{C\text{-}F}$ = 24.3 Hz), 37.0, 22.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.5 (s). FT-IR: ν (cm^{-1}) δ 2965, 1626, 1560, 1459, 1386, 1313, 1224, 1146, 1088, 1046. HRMS [ESI] calcd for $C_{12}H_{12}ClFN$ $[M+H]^+$ 224.0637, found 224.0632.



5e: 33.6 mg, 68% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/80). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25-8.20 (m, 1H), 8.20-8.15 (m, 2H), 8.13-8.09 (m, 1H), 7.80 (s, 1H), 7.75-7.69 (m, 1H), 7.58-7.52 (m, 3H), 7.51-7.45 (m, 1H), 3.86-3.75 (m, 1H), 1.48 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 154.9, 148.5, 140.2, 130.7, 129.1, 129.0, 128.7, 127.6, 125.9, 125.8, 122.9, 114.9, 28.5, 23.0. FT-IR: ν (cm^{-1}) δ 2902, 1615, 1550, 1508, 1458, 1364, 1292, 1181, 1058. HRMS [ESI] calcd for $C_{18}H_{18}N$ $[M+H]^+$ 248.1434, found 248.1432.

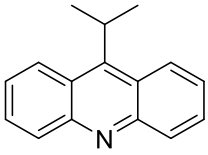


5f: 29.8 mg, 60% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.23-8.17 (m, 2H), 7.79-7.73 (m, 1H), 7.67-7.61 (m, 1H), 3.97-3.85 (m, 1H), 1.43 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 143.6, 134.9, 130.8, 127.7, 127.5, 126.8, 125.1, 117.6, 31.0, 22.1. FT-IR: ν (cm^{-1}) δ 2964, 1616, 1563, 1467, 1387, 1285, 1189, 1124, 1065, 1008. HRMS [ESI] calcd for $C_{12}H_{13}BrN$ $[M+H]^+$ 250.0226, found 250.0217.

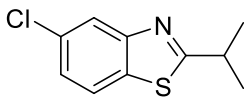


5g: 35.2 mg, 80% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68-8.63 (m, 1H), 8.54 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.35-8.30 (m, 1H), 8.17 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.85-7.78 (m, 1H), 7.75-7.66 (m, 2H), 7.65-7.58 (m, 1H), 4.07-3.95 (m, 1H), 1.54 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 143.8, 133.0, 129.9, 129.9, 128.3, 127.0, 126.1, 125.6, 124.7,

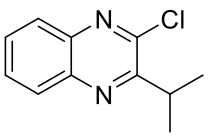
123.4, 122.5, 121.8, 31.4, 21.9. FT-IR: ν (cm^{-1}) δ 2964, 1611, 1526, 1486, 1382, 1289, 1211, 1162, 1110, 1006. HRMS [ESI] calcd for $C_{16}H_{16}N$ $[M+H]^+$ 222.1277, found 222.1286.



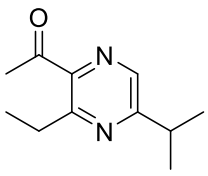
5h: 19.0 mg, 43% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/50-1/10). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 9.2 Hz, 2H), 8.24 (dd, *J* = 8.8, 0.4 Hz, 2H), 7.77-7.71 (m, 2H), 7.55-7.49 (m, 2H), 4.60-4.47 (m, 1H), 1.76 (d, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 149.0, 130.8, 129.4, 125.0, 124.5, 28.4, 22.8. FT-IR: ν (cm^{-1}) δ 2929, 1626, 1590, 1458, 1384, 1274, 1158, 1026. HRMS [ESI] calcd for $C_{16}H_{16}N$ $[M+H]^+$ 222.1277, found 222.1285.



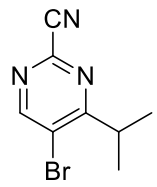
5i: 12.7 mg, 30% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 2.0 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.31 (dd, *J* = 8.8, 2.0 Hz, 1H), 3.47-3.35 (m, 1H), 1.47 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.6, 154.0, 133.0, 131.8, 125.0, 122.5, 122.2, 34.2, 22.8. FT-IR: ν (cm^{-1}) δ 2967, 1589, 1510, 1462, 1384, 1247, 1144, 1095, 1004. HRMS [ESI] calcd for $C_{10}H_{10}ClNNaS$ $[M+Na]^+$ 234.0115, found 234.0106.



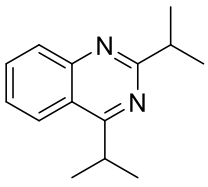
5j: 25.2 mg, 61% yield, white solid, m.p. 61-62 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-8.03 (m, 1H), 7.98-7.94 (m, 1H), 7.75-7.66 (m, 2H), 3.76-3.64 (m, 1H), 1.41 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 147.3, 141.1, 140.7, 129.9, 129.8, 128.8, 128.0, 32.6, 21.0. FT-IR: ν (cm^{-1}) δ 2967, 1610, 1562, 1467, 1443, 1359, 1311, 1266, 1159, 1020. HRMS [ESI] calcd for $C_{11}H_{12}ClN_2$ $[M+H]^+$ 207.0684, found 207.0691.



5k: 15.3 mg, 40% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/80). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 3.19-3.07 (m, 3H), 2.68 (s, 3H), 1.34 (d, *J* = 6.8 Hz, 6H), 1.27 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.3, 163.9, 157.9, 144.3, 138.4, 34.3, 28.9, 28.1, 21.9, 13.2. FT-IR: ν (cm^{-1}) δ 2968, 1698, 1552, 1459, 1386, 1281, 1147, 1100, 1017. HRMS [ESI] calcd for $C_{11}H_{17}N_2O$ $[M+H]^+$ 193.1335, found 193.1337.

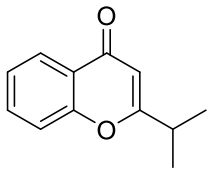


5l: 16.3 mg, 36% yield, white solid, m.p. 57-58 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/60). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 3.56-3.45 (m, 1H), 1.30 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.3, 159.4, 143.1, 123.8, 115.4, 34.2, 20.4. FT-IR: ν (cm^{-1}) δ 2929, 1590, 1470, 1430, 1382, 1330, 1219, 1095, 1007. HRMS [EI] calcd for $C_8H_8BrN_3$ $[M]^+$ 224.9896, found 224.9899.

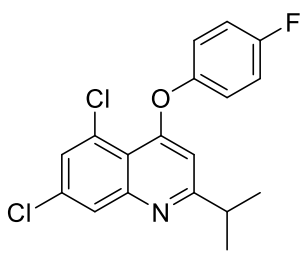


5m: 15.4 mg, 36% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/80). ^{1}H NMR

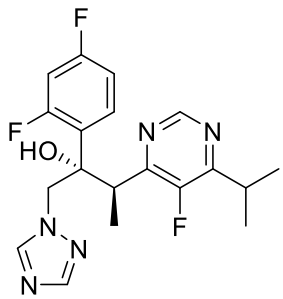
(400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.81-7.76 (m, 1H), 7.55-7.50 (m, 1H), 3.94-3.82 (m, 1H), 3.37-3.26 (m, 1H), 1.42 (d, *J* = 6.8 Hz, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.3, 170.9, 150.4, 132.7, 128.9, 126.1, 123.9, 121.3, 38.0, 30.9, 21.8, 21.7. FT-IR: ν (cm^{-1}) δ 2965, 1616, 1558, 1456, 1391, 1240, 1163, 1131, 1094, 1009. HRMS [ESI] calcd for $C_{14}H_{19}N_2$ $[M+H]^+$ 215.1543, found 215.1534.



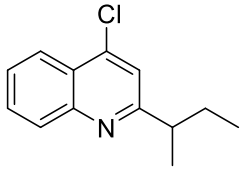
5n: 11.3 mg, 30% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/30-1/15). ^1H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.67-7.61 (m, 1H), 7.45-7.42 (m, 1H), 7.40-7.34 (m, 1H), 6.19 (s, 1H), 2.92-2.81 (m, 1H), 1.32 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.7, 174.2, 156.5, 133.4, 125.6, 124.8, 123.7, 117.8, 107.6, 33.2, 20.1. FT-IR: ν (cm^{-1}) δ 2970, 1633, 1569, 1464, 1395, 1247, 1210, 1123, 1037. HRMS [ESI] calcd for $C_{12}H_{13}O_2$ $[M+H]^+$ 189.0910, found 189.0916.



5o: 37.5 mg, 54% yield, yellow solid, m.p. 49-50 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/80). ^1H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 2.0 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.18-7.08 (m, 4H), 6.54 (s, 1H), 3.09-2.97 (m, 1H), 1.25 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 162.4, 159.8 (d, J_{C-F} = 242.6 Hz), 151.4, 150.3 (d, J_{C-F} = 2.8 Hz), 134.8, 129.9, 128.6, 127.5, 121.9 (d, J_{C-F} = 8.3 Hz), 117.0 (d, J_{C-F} = 23.5 Hz), 117.0, 105.3, 37.0, 22.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.4 (s). FT-IR: ν (cm^{-1}) δ 2966, 1599, 1502, 1426, 1342, 1318, 1235, 1142, 1091, 1012. HRMS [ESI] calcd for $C_{18}H_{15}Cl_2FNO$ $[M+H]^+$ 350.0509, found 350.0508.

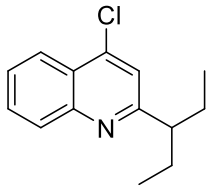


5p: 24.5 mg, 31% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/2-1/1). ^1H NMR (400 MHz, CD_3OD) δ 8.87 (d, *J* = 1.6 Hz, 1H), 8.29 (s, 1H), 7.57-7.49 (m, 2H), 7.01-6.93 (m, 1H), 6.90-6.83 (m, 1H), 4.81 (d, *J* = 14.4 Hz, 1H), 4.38 (d, *J* = 14.0 Hz, 1H), 4.19-4.12 (m, 1H), 3.51-3.39 (m, 1H), 1.34 (d, *J* = 6.8 Hz, 3H), 1.32 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 164.7 (d, *J* = 14.1 Hz), 164.2 (dd, *J* = 246.8, 12.6 Hz), 160.4 (dd, *J* = 245.1, 11.8 Hz), 158.8 (d, *J* = 14.5 Hz), 155.0 (d, *J* = 260.5 Hz), 154.2 (d, *J* = 9.7 Hz), 150.9, 145.8, 131.7 (dd, *J* = 9.4, 5.7 Hz), 125.4 (dd, *J* = 12.0, 3.7 Hz), 112.1 (dd, *J* = 20.7, 3.3 Hz), 105.0 (dd, *J* = 27.9, 26.0 Hz), 78.5 (d, *J* = 5.0 Hz), 58.1 (d, *J* = 5.0 Hz), 38.4 (d, *J* = 5.4 Hz), 30.4, 20.9 (d, *J* = 6.3 Hz), 15.9; ^{19}F NMR (376 MHz, CD_3OD) δ -109.5 (d, *J* = 8.6 Hz, 1F), -112.8 (d, *J* = 8.6 Hz, 1F), -140.7 (s, 1F). FT-IR: ν (cm^{-1}) δ 2974, 1618, 1591, 1500, 1408, 1337, 1205, 1137, 1054. HRMS [EI] calcd for $C_{19}H_{20}F_3N_5O$ $[M]^+$ 391.1620, found 391.1618.

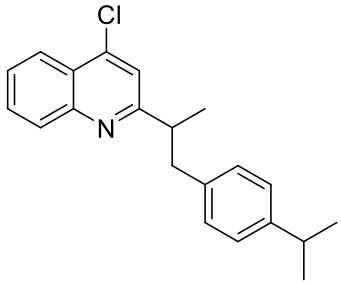


5q: 24.3 mg, 55% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0, 0.8 Hz, 1H), 8.09-8.04 (m, 1H), 7.75-7.69 (m, 1H), 7.59-7.54 (m, 1H), 7.39 (s, 1H), 3.03-2.93 (m, 1H),

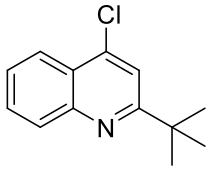
1.91-1.79 (m, 1H), 1.77-1.65 (m, 1H), 1.36 (d, *J* = 6.8 Hz, 3H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 148.6, 142.6, 130.1, 129.3, 126.6, 125.1, 123.9, 119.7, 44.5, 29.8, 20.2, 12.1. FT-IR: ν (cm^{-1}) δ 2962, 1615, 1589, 1456, 1376, 1283, 1148, 1084, 1025. HRMS [ESI] calcd for $C_{13}H_{15}ClN$ $[M+H]^+$ 220.0888, found 220.0889.



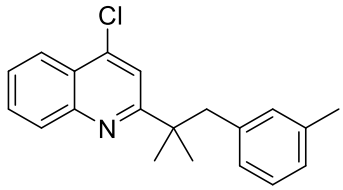
5r: 26.3 mg, 56% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.10-8.06 (m, 1H), 7.74-7.68 (m, 1H), 7.58-7.52 (m, 1H), 7.35 (s, 1H), 2.80-2.70 (m, 1H), 1.83-1.73 (m, 4H), 0.83 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 148.7, 142.4, 130.0, 129.4, 126.5, 125.1, 123.8, 120.2, 52.1, 28.1, 12.1. FT-IR: ν (cm^{-1}) δ 2961, 1615, 1553, 1458, 1410, 1372, 1286, 1169, 1104, 1057. HRMS [EI] calcd for $C_{14}H_{16}ClN$ $[M]^+$ 233.0966, found 233.0965.



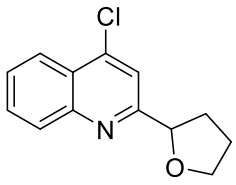
5s: 43.6 mg, 67% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.13-8.09 (m, 1H), 7.78-7.72 (m, 1H), 7.62-7.56 (m, 1H), 7.35 (s, 1H), 7.14-7.08 (m, 4H), 3.42-3.32 (m, 1H), 3.22 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.93-2.83 (m, 2H), 1.37 (d, *J* = 7.2 Hz, 3H), 1.24 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 148.7, 146.5, 142.4, 137.4, 130.1, 129.4, 129.0, 126.6, 126.3, 125.1, 123.9, 120.4, 44.4, 42.4, 33.6, 24.0, 24.0, 19.9. FT-IR: ν (cm^{-1}) δ 2960, 1615, 1553, 1493, 1363, 1220, 1162, 1094. HRMS [ESI] calcd for $C_{21}H_{23}ClN$ $[M+H]^+$ 324.1514, found 324.1510.



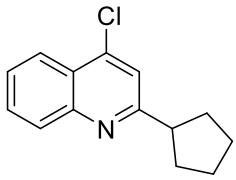
5t: 39.7 mg, 90% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.75-7.69 (m, 1H), 7.60 (s, 1H), 7.60-7.54 (m, 1H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 148.3, 142.3, 129.9, 129.7, 126.6, 124.7, 123.7, 118.5, 38.3, 30.0. FT-IR: ν (cm^{-1}) δ 2957, 1617, 1551, 1461, 1364, 1302, 1245, 1148, 1024. HRMS [ESI] calcd for $C_{13}H_{15}ClN$ $[M+H]^+$ 220.0888, found 220.0884.



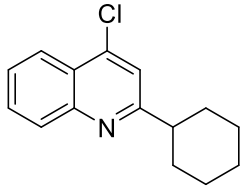
5u: 49.7 mg, 80% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.16-8.10 (m, 1H), 7.79-7.73 (m, 1H), 7.64-7.57 (m, 1H), 7.46 (s, 1H), 7.08-7.01 (m, 1H), 7.00-6.95 (m, 1H), 6.76 (s, 1H), 6.73-6.68 (m, 1H), 3.10 (s, 2H), 2.23 (s, 3H), 1.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 148.3, 142.0, 138.6, 137.0, 131.4, 129.9, 129.8, 127.5, 127.4, 126.7, 126.7, 124.6, 123.7, 119.2, 48.9, 42.4, 27.3, 21.3. FT-IR: ν (cm^{-1}) δ 2921, 1607, 1586, 1492, 1406, 1386, 1290, 1221, 1141, 1101, 1050. HRMS [EI] calcd for $C_{20}H_{20}ClN$ $[M]^+$ 309.1279, found 309.1277.



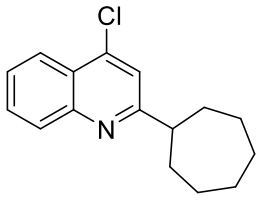
5v: 18.6 mg, 40% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/30-1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.18 (m, 1H), 8.07-8.03 (m, 1H), 7.76-7.71 (m, 1H), 7.71 (s, 1H), 7.61-7.56 (m, 1H), 5.17-5.12 (m, 1H), 4.20-4.13 (m, 1H), 4.07-4.00 (m, 1H), 2.56-2.46 (m, 1H), 2.13-1.97 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 148.4, 143.2, 130.3, 129.3, 127.0, 125.5, 124.0, 118.2, 81.5, 69.3, 33.3, 25.9. FT-IR: ν (cm^{-1}) δ 2872, 1615, 1553, 1461, 1363, 1262, 1201, 1107. HRMS [ESI] calcd for $C_{13}H_{13}ClNO$ $[M+H]^+$ 234.0680, found 234.0674.



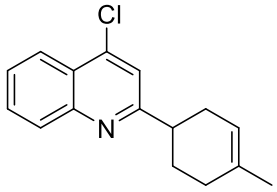
5w: 30.0 mg, 65% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0, 0.8 Hz, 1H), 8.07-8.02 (m, 1H), 7.75-7.69 (m, 1H), 7.59-7.54 (m, 1H), 7.43 (s, 1H), 3.40-3.30 (m, 1H), 2.24-2.12 (m, 2H), 1.94-1.83 (m, 4H), 1.80-1.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 148.5, 142.4, 130.1, 129.3, 126.5, 125.0, 123.8, 120.2, 48.6, 33.5, 25.9. FT-IR: ν (cm^{-1}) δ 2950, 1696, 1588, 1493, 1364, 1277, 1149, 1043. HRMS [ESI] calcd for $C_{14}H_{15}ClN$ $[M+H]^+$ 232.0888, found 232.0880.



5x: 31.5 mg, 64% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.08-8.03 (m, 1H), 7.74-7.69 (m, 1H), 7.58-7.53 (m, 1H), 7.42 (s, 1H), 2.93-2.84 (m, 1H), 2.06-1.98 (m, 2H), 1.94-1.85 (m, 2H), 1.83-1.74 (m, 1H), 1.67-1.55 (m, 2H), 1.52-1.40 (m, 2H), 1.38-1.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 148.7, 142.6, 130.1, 129.3, 126.5, 125.1, 123.8, 119.8, 47.4, 32.7, 26.4, 26.0. FT-IR: ν (cm^{-1}) δ 2925, 1598, 1493, 1410, 1372, 1214, 1149, 1119, 1039. HRMS [ESI] calcd for $C_{15}H_{17}ClN$ $[M+H]^+$ 246.1044, found 246.1037.

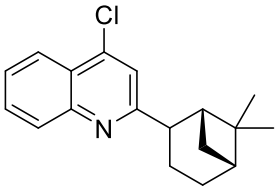


5y: 21.4 mg, 41% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.07-8.02 (m, 1H), 7.75-7.69 (m, 1H), 7.59-7.53 (m, 1H), 7.39 (s, 1H), 3.09-3.01 (m, 1H), 2.08-2.00 (m, 2H), 1.92-1.60 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 148.4, 142.6, 130.1, 129.2, 126.5, 125.0, 123.9, 119.8, 49.4, 34.9, 27.9, 27.3. FT-IR: ν (cm^{-1}) δ 2920, 1588, 1492, 1409, 1375, 1303, 1282, 1216, 1116, 1025. HRMS [ESI] calcd for $C_{16}H_{19}ClN$ $[M+H]^+$ 260.1201, found 260.1206.

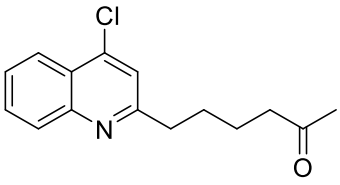


5z: 21.3 mg, 41% yield, white solid, m.p. 66-67 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.16 (m, 1H), 8.08-8.03 (m, 1H), 7.76-7.70 (m, 1H), 7.60-7.55 (m, 1H), 7.43 (s, 1H), 5.54-5.49 (m, 1H), 3.14-3.04 (m, 1H), 2.42-2.35 (m, 2H), 2.28-2.15 (m, 1H), 2.14-2.02 (m, 2H), 1.98-1.86 (m, 1H), 1.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 148.6, 142.6, 134.0, 130.2, 129.3, 126.6, 125.1, 123.9, 120.1, 119.9, 42.9, 31.4, 30.3, 28.8, 23.6. FT-IR: ν (cm^{-1}) δ

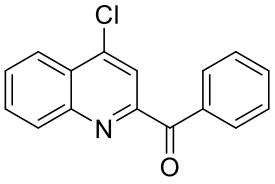
2927, 1590, 1493, 1436, 1375, 1312, 1273, 1215, 1163, 1120, 1017. HRMS [ESI] calcd for $C_{16}H_{17}ClN$ $[M+H]^+$ 258.1044, found 258.1050.



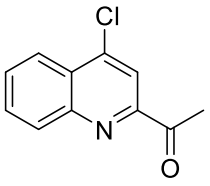
5aa: 35.5 mg, 62% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.75-7.68 (m, 1H), 7.59-7.53 (m, 1H), 7.42 (s, 1H), 3.58-3.51 (m, 1H), 2.29-2.16 (m, 3H), 2.05-1.91 (m, 4H), 1.86-1.82 (m, 1H), 1.29 (s, 3H), 1.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 148.5, 142.5, 130.0, 129.4, 126.5, 125.1, 123.8, 120.2, 45.9, 43.9, 40.0, 39.8, 26.7, 24.5, 24.0, 20.8, 20.3. FT-IR: ν (cm^{-1}) δ 2909, 1726, 1615, 1553, 1460, 1302, 1260, 1165, 1117, 1025. HRMS [ESI] calcd for $C_{18}H_{21}ClN$ $[M+H]^+$ 286.1357, found 286.1352.



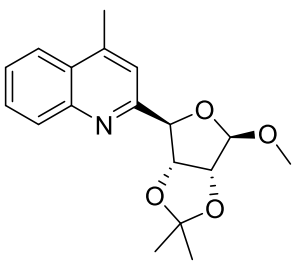
5ab: 27.5 mg, 53% yield, yellow oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/80-1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.76-7.70 (m, 1H), 7.60-7.55 (m, 1H), 7.39 (s, 1H), 2.95 (t, *J* = 7.6 Hz, 2H), 2.49 (t, *J* = 7.2 Hz, 2H), 2.13 (s, 3H), 1.87-1.78 (m, 2H), 1.73-1.64 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.8, 162.2, 148.7, 142.6, 130.3, 129.1, 126.7, 124.9, 123.9, 121.3, 43.4, 38.7, 29.9, 29.0, 23.4. FT-IR: ν (cm^{-1}) δ 2929, 1713, 1615, 1589, 1459, 1358, 1292, 1164, 1073, 1024. HRMS [ESI] calcd for $C_{15}H_{16}ClNNaO$ $[M+Na]^+$ 284.0813, found 284.0806.



5ac: 18.8 mg, 35% yield, white solid, m.p. 133-134 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/50). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34-8.30 (m, 1H), 8.27-8.20 (m, 4H), 7.87-7.82 (m, 1H), 7.79-7.74 (m, 1H), 7.67-7.61 (m, 1H), 7.55-7.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 154.4, 147.6, 143.8, 135.7, 133.3, 131.4, 130.9, 129.4, 128.2, 127.1, 124.1, 121.0. FT-IR: ν (cm^{-1}) δ 2923, 1661, 1514, 1447, 1323, 1263, 1207, 1158, 1077. HRMS [ESI] calcd for $C_{16}H_{10}ClNNaO$ $[M+Na]^+$ 290.0343, found 290.0340.



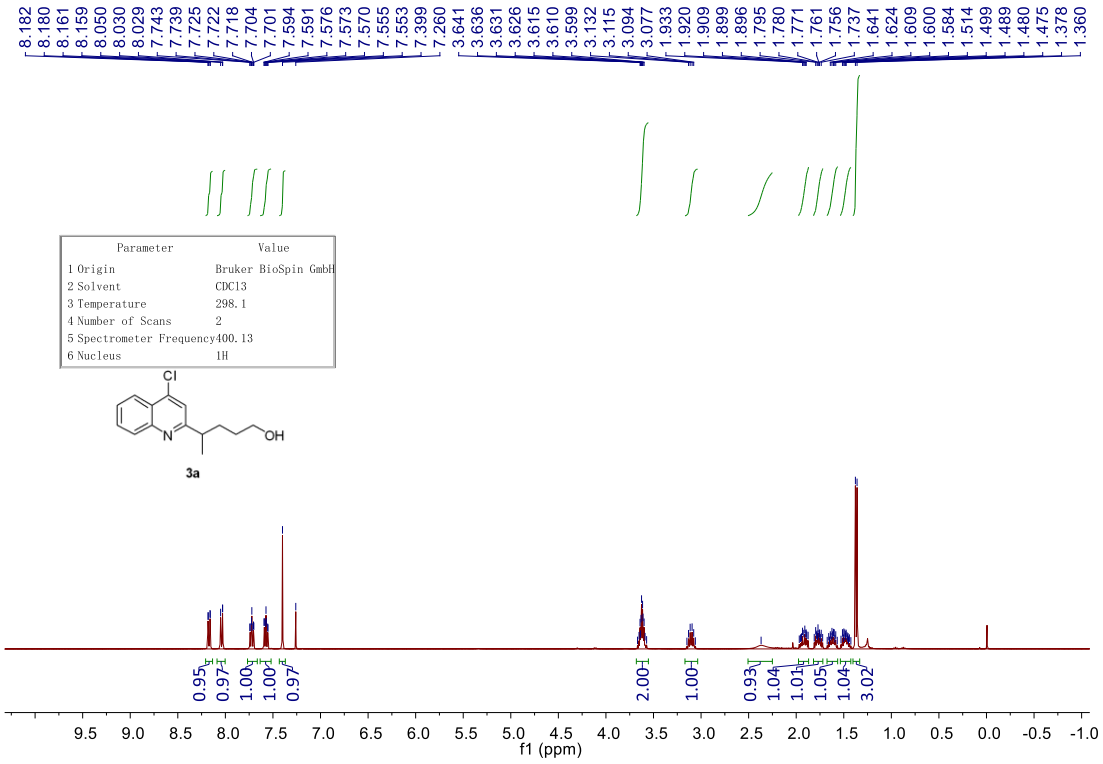
5ad: 12.2 mg, 30% yield, white solid, m.p. 89-90 °C. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/100-1/50). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30-8.26 (m, 1H), 8.24-8.21 (m, 1H), 8.20 (s, 1H), 7.87-7.82 (m, 1H), 7.78-7.73 (m, 1H), 2.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 152.9, 148.0, 143.7, 130.9, 130.8, 129.6, 127.6, 124.2, 118.2, 25.4. FT-IR: ν (cm^{-1}) δ 2921, 1654, 1577, 1496, 1406, 1306, 1242, 1155, 1086. HRMS [ESI] calcd for $C_{11}H_9ClNO$ $[M+H]^+$ 206.0367, found 206.0366.

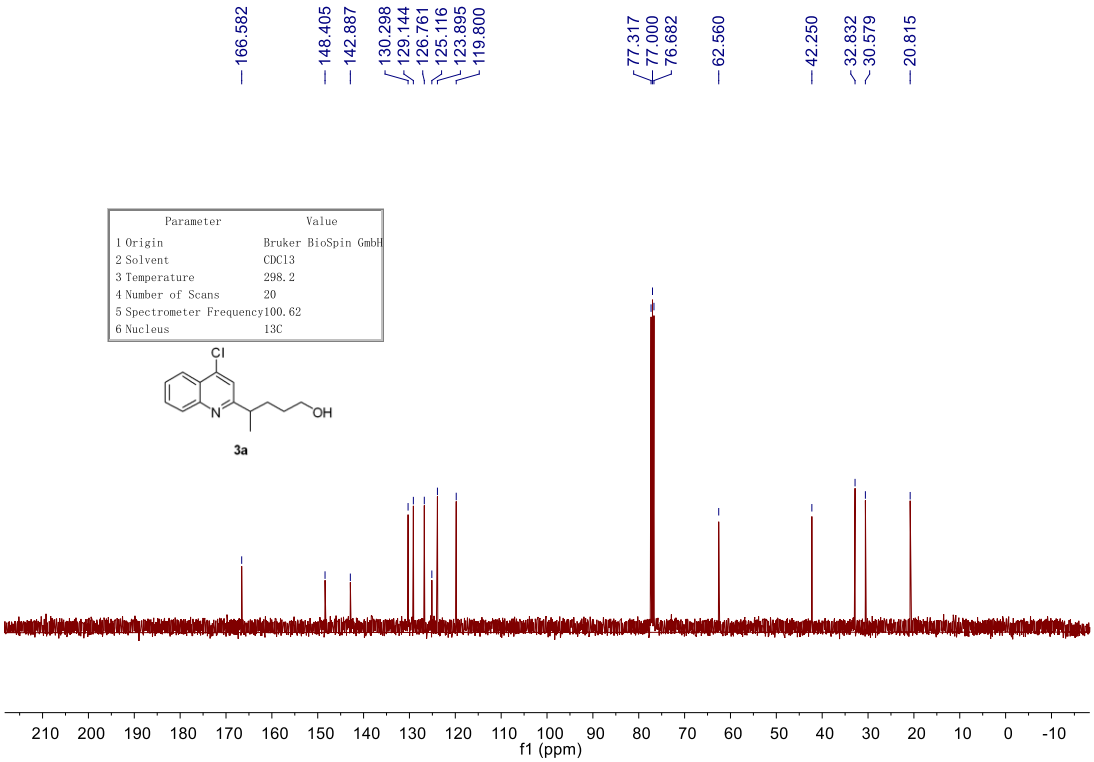


5ae: (*d.r.* > 20:1): 19.7 mg, 31% yield, colorless oil. Purification by flash column chromatography (eluent: EtOAc/Petroleum ether = 1/80-1/40). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.96 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.71-7.65 (m, 1H), 7.56-7.49 (m, 2H),

5.76 (dd, *J* = 6.0, 1.2 Hz, 1H), 5.42 (brs, 1H), 5.16 (brs, 1H), 4.64 (d, *J* = 6.0 Hz, 1H), 3.29 (s, 3H), 2.71 (d, *J* = 0.8 Hz, 3H), 1.60 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 147.1, 144.2, 130.1, 129.0, 127.3, 126.1, 123.5, 119.6, 112.5, 110.5, 88.8, 85.3, 83.6, 55.4, 26.7, 25.3, 18.8.

6. ^{1}H, ^{13}C and ^{19}F NMR spectra

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142.887
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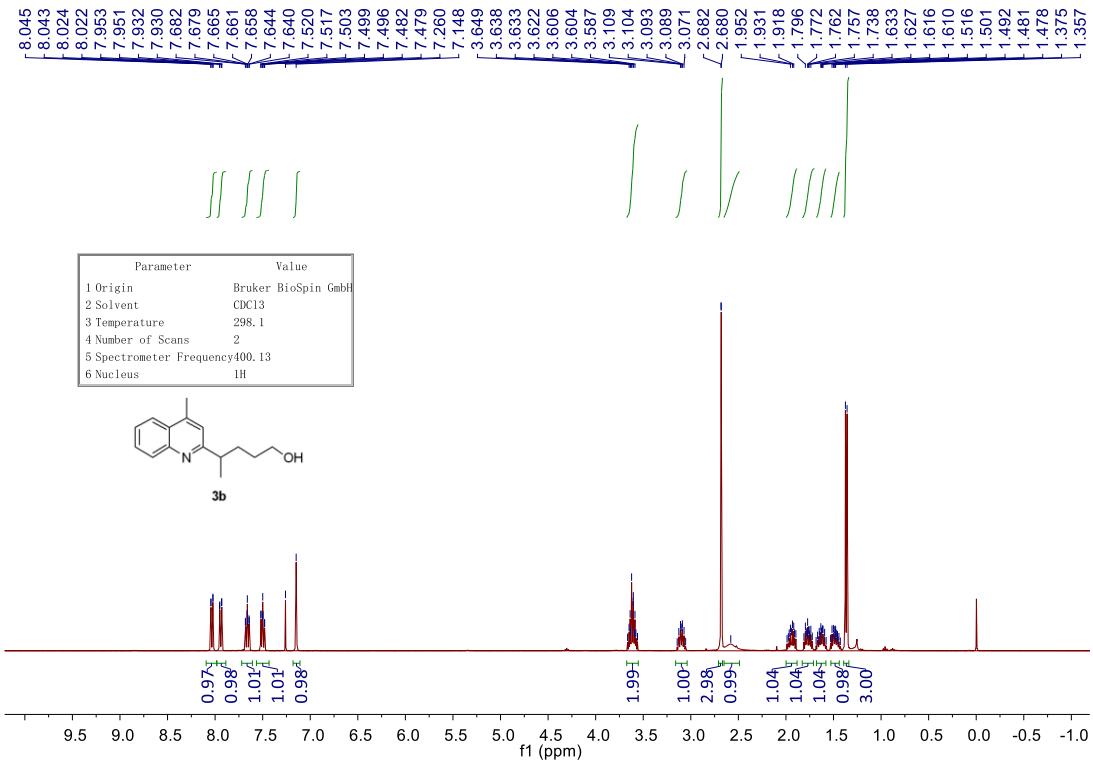
125.116
123.895
119.800
77.317
77.000
76.682
62.560
42.250
32.832
30.579
20.815
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3a
f1 (ppm)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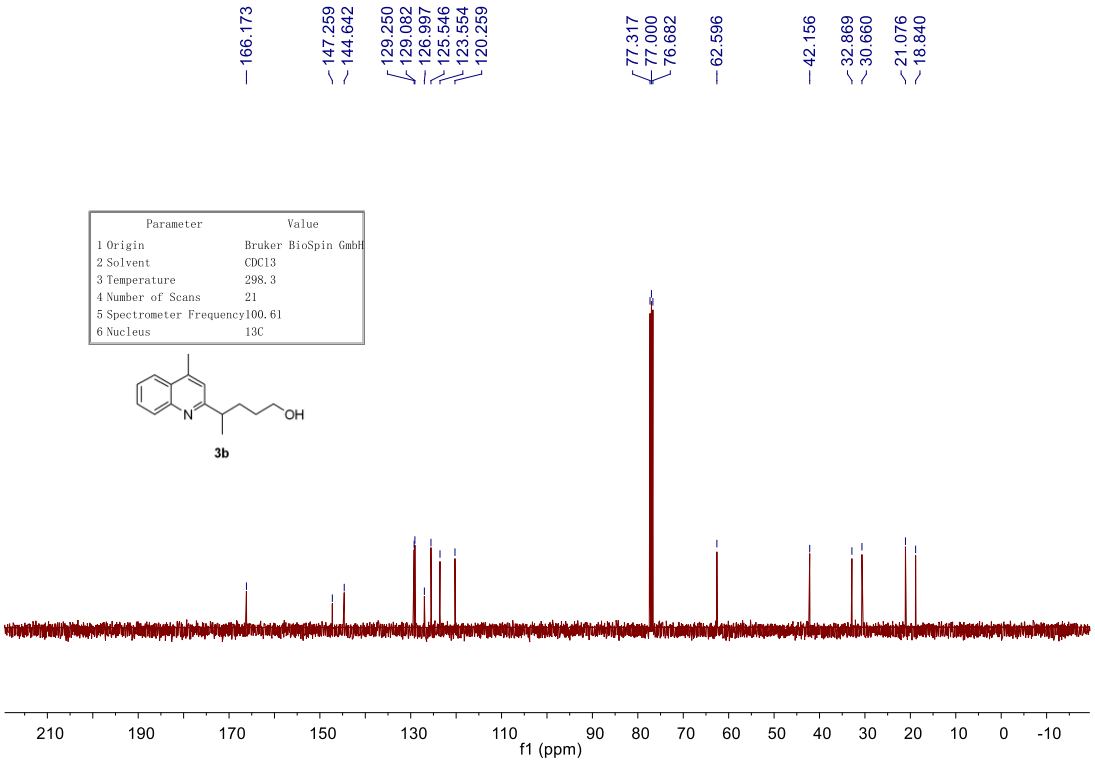
7.930
7.682
7.679
7.665
7.661
7.658
7.644
7.640
7.520
7.517
7.503
7.499
7.496
7.482
7.479
7.260
7.148
3.649
3.638
3.633
3.622
3.606
3.604
3.587
3.109
3.104
3.093
3.089
3.071
2.682
2.680
1.952
1.931
1.918
1.796
1.772
1.762
1.757
1.738
1.633
1.627
1.616
1.610
1.516
1.501
1.492
1.481
1.478
1.375
1.357
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
N
OH
3b
0.97
0.98
1.01
1.01
0.98
1.99
1.00
2.98
0.99
1.04
1.04
1.04
0.98
3.00
f1 (ppm)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129.082
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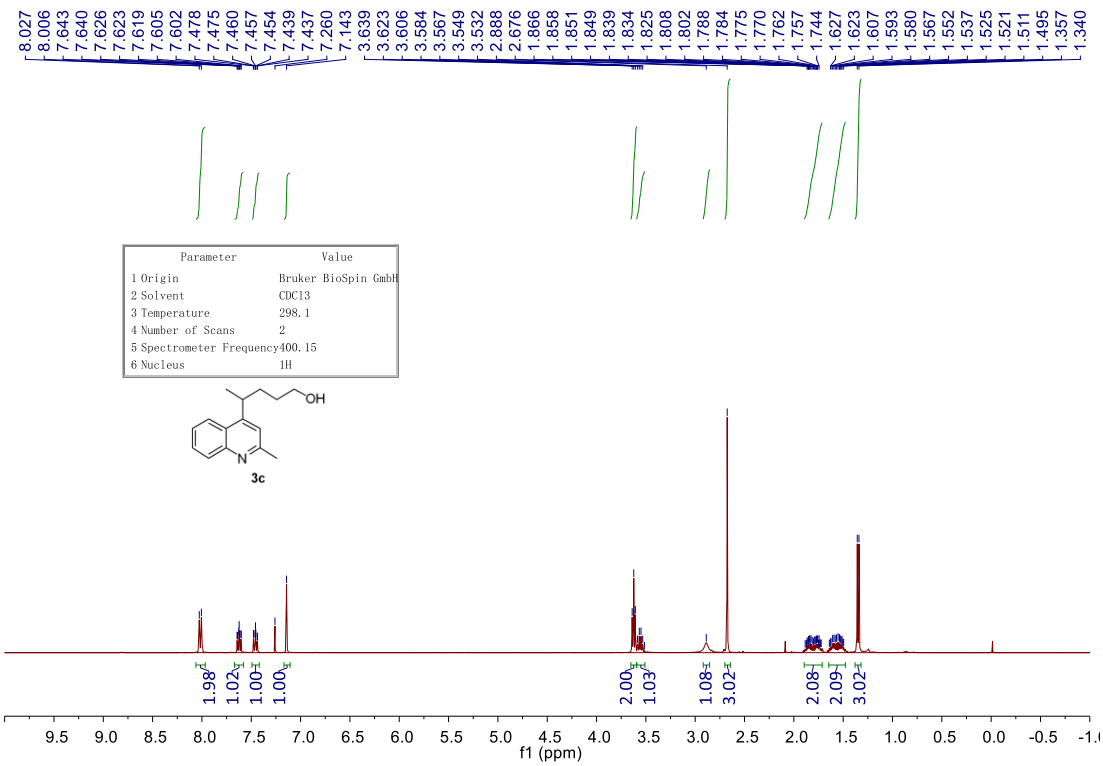
125.546
123.554
120.259
77.317
77.000
76.682
62.596
42.156
32.869
30.660
21.076
18.840
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 21
5 Spectrometer Frequency 100.61
6 Nucleus 13C
OH
N
3b
f1 (ppm)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8.006
7.643
7.640
7.626
7.623
7.619
7.605
7.602
7.478
7.475
7.460
7.457
7.454
7.439
7.437
7.260
7.143
3.639
3.623
3.606
3.584
3.567
3.549
3.532
2.888
2.676
1.866
1.858
1.851
1.849
1.839
1.834
1.825
1.808
1.802
1.788
1.784
1.775
1.770
1.762
1.757
1.744
1.627
1.623
1.607
1.593
1.580
1.567
1.552
1.537
1.525
1.521
1.511
1.495
1.357
1.340
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
OH
N
3c
1.98
1.02
1.00
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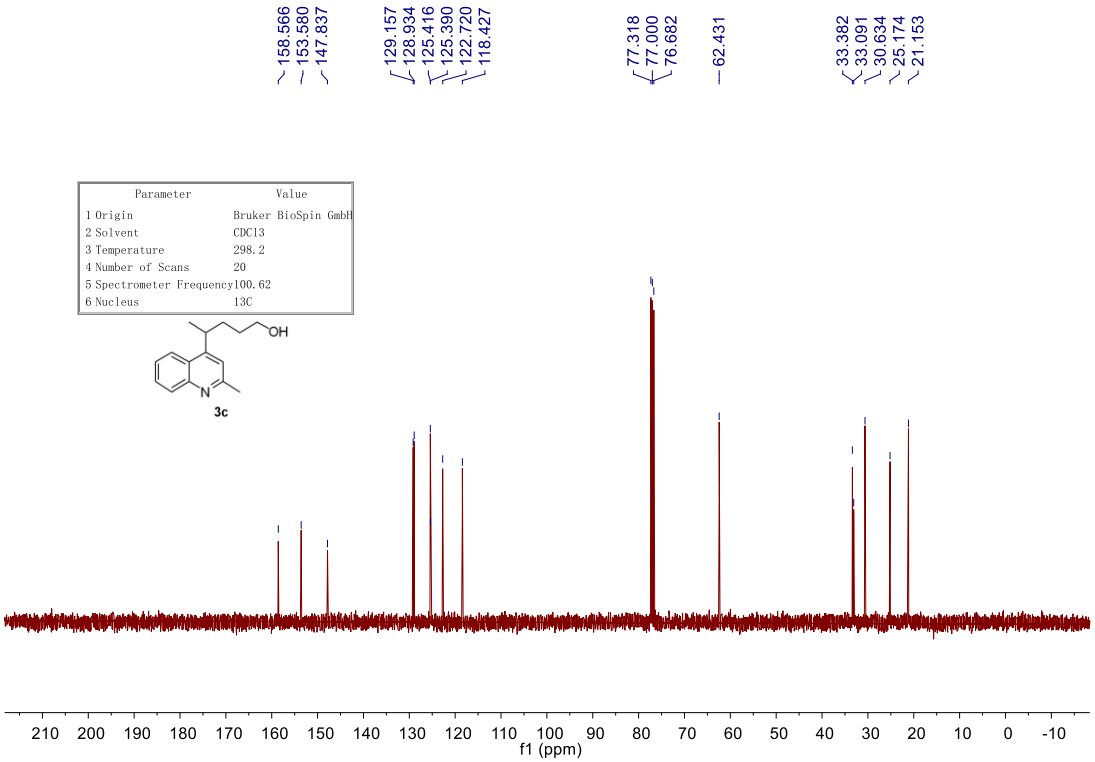
3.02
2.08
2.09
3.02
f1 (ppm)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147.837
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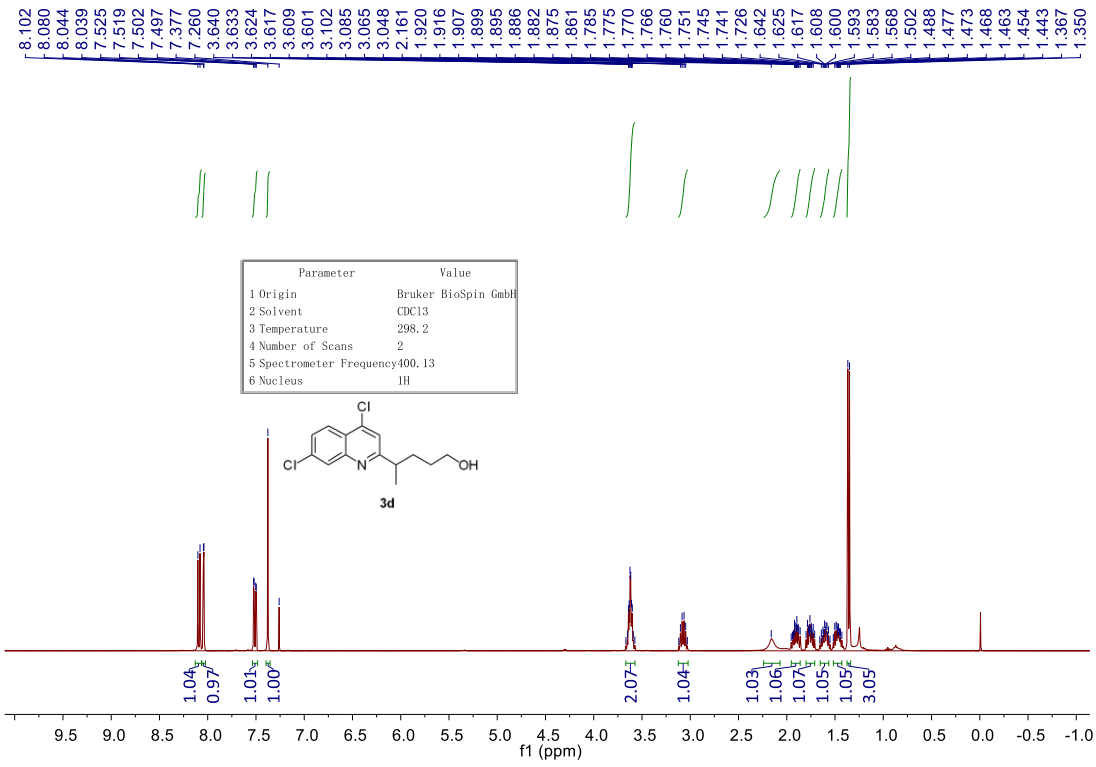
128.934
125.416
125.390
122.720
118.427
77.318
77.000
76.682
62.431
33.382
33.091
30.634
25.174
21.153
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
N
3c
f1 (ppm)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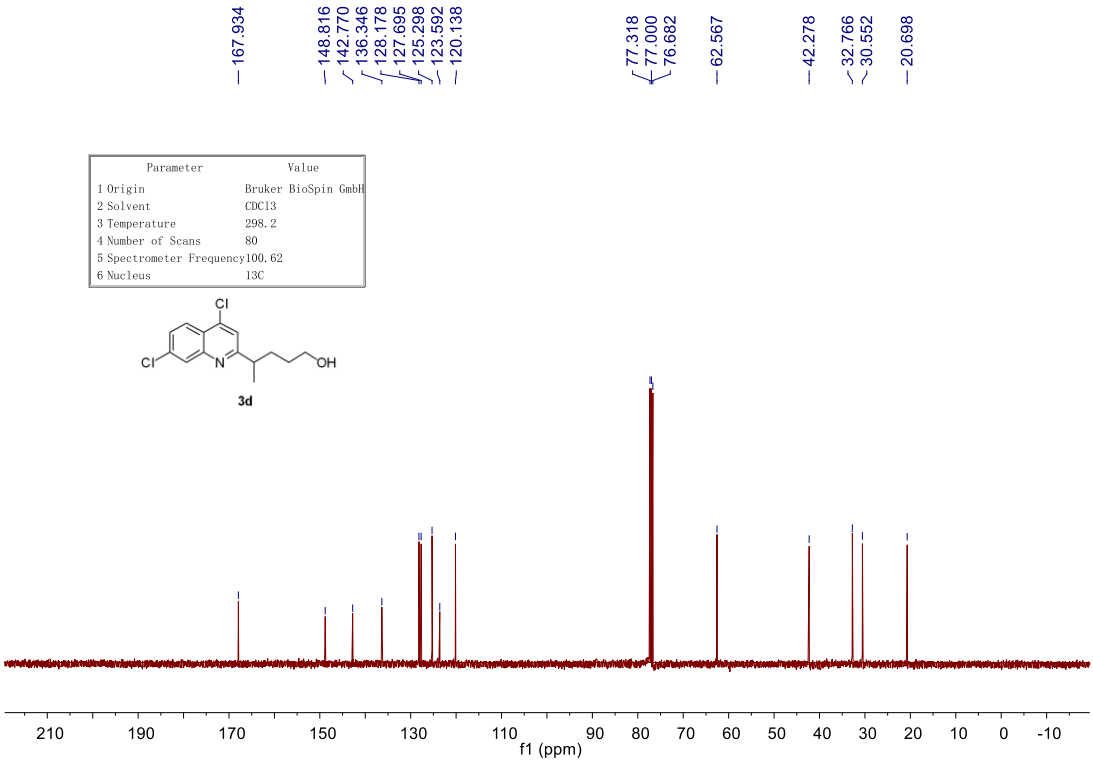
8.044
8.039
7.525
7.519
7.502
7.497
7.377
7.260
3.640
3.633
3.624
3.617
3.609
3.601
3.102
3.085
3.065
3.048
2.161
1.920
1.916
1.907
1.899
1.895
1.886
1.882
1.875
1.861
1.785
1.775
1.770
1.766
1.760
1.751
1.745
1.741
1.726
1.642
1.625
1.617
1.608
1.600
1.593
1.583
1.568
1.502
1.488
1.477
1.473
1.468
1.463
1.454
1.443
1.367
1.350
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
Cl
N
OH
3d
1.04
0.97
1.01
1.00
2.07
1.04
1.03
1.06
1.07
1.05
1.05
3.05
f1 (ppm)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142.770
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127.895
125.298
123.592
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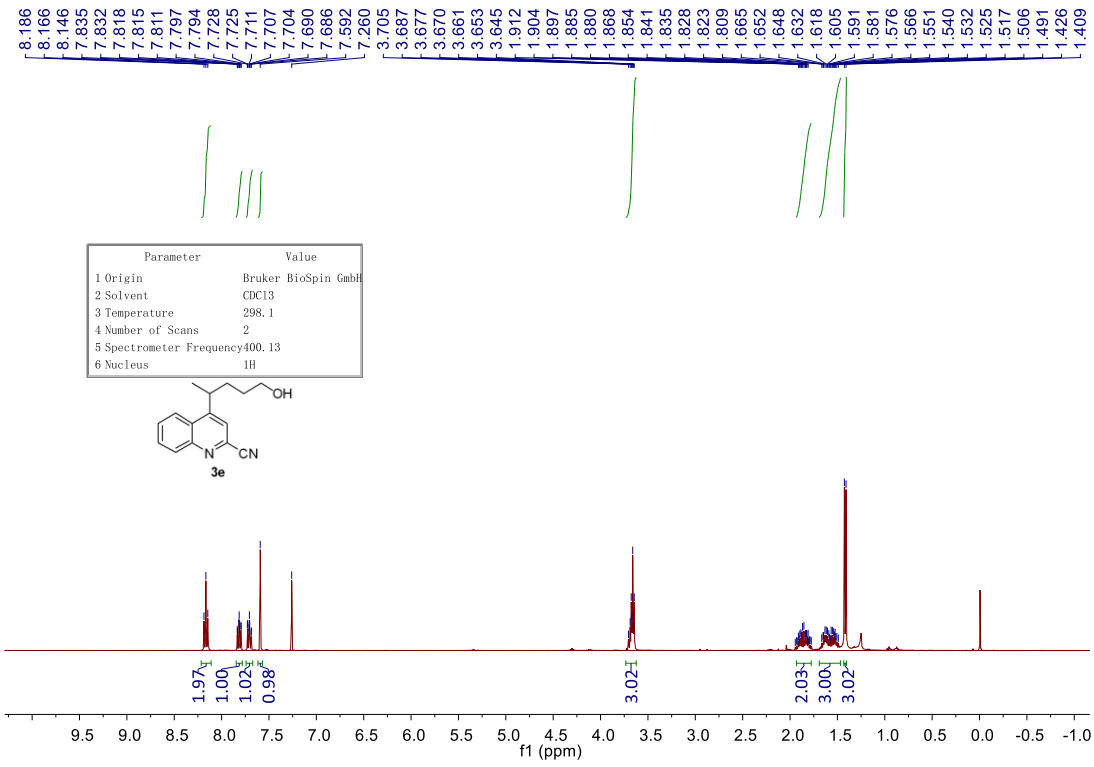
77.318
77.000
76.682
62.567
42.278
32.766
30.552
20.698
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
Cl
N
OH
3d
f1 (ppm)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8.166
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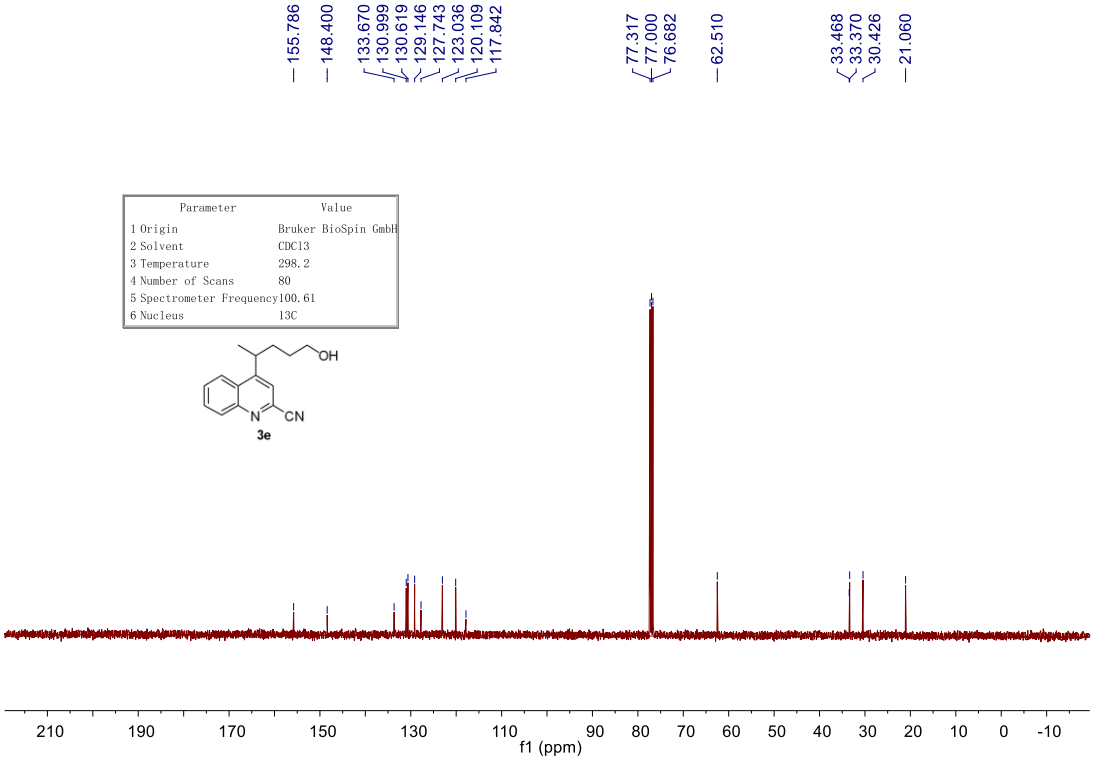
7.818
7.815
7.811
7.797
7.794
7.728
7.725
7.711
7.707
7.704
7.690
7.686
7.592
7.260
3.705
3.687
3.677
3.670
3.661
3.653
3.645
1.912
1.904
1.897
1.885
1.880
1.868
1.854
1.841
1.835
1.828
1.823
1.809
1.665
1.652
1.648
1.632
1.618
1.605
1.591
1.581
1.576
1.566
1.551
1.540
1.532
1.525
1.517
1.506
1.491
1.426
1.409
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
N
CN
3e
1.97
1.00
1.02
0.98
3.02
2.03
3.00
3.02
f1 (ppm)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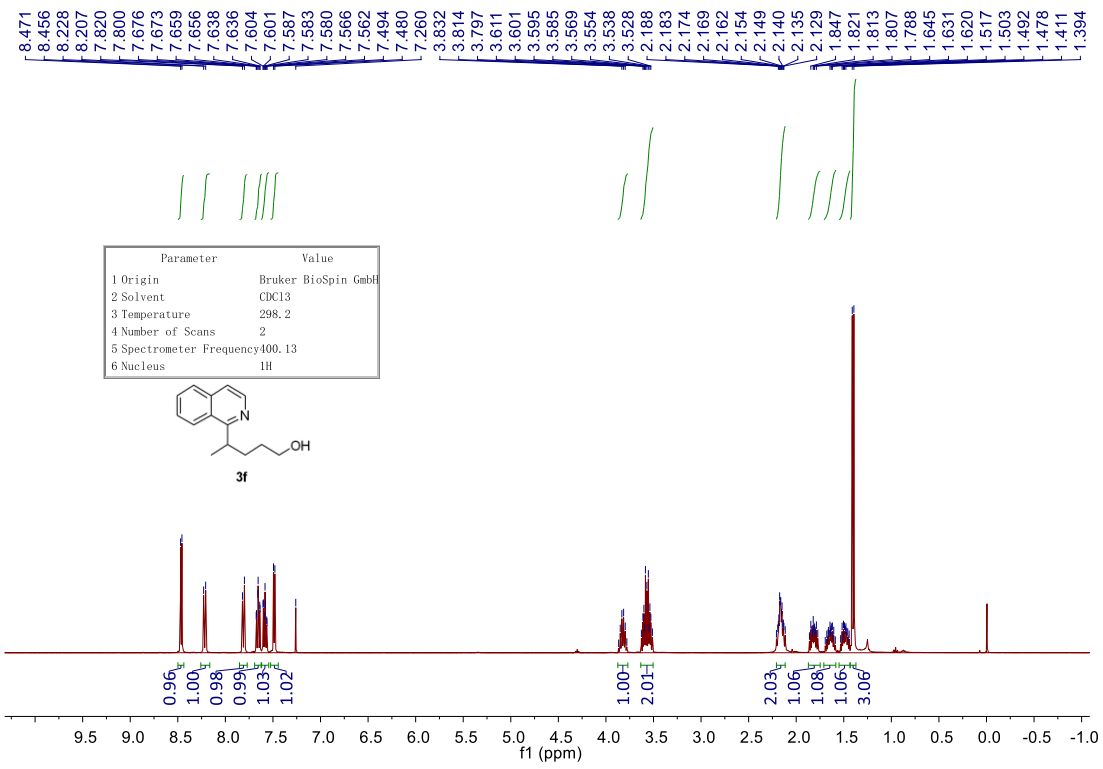
129.146
127.743
123.036
120.109
117.842
77.317
77.000
76.682
62.510
33.468
33.370
30.426
21.060
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.61
6 Nucleus 13C
OH
N
CN
3e
f1 (ppm)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7.604
7.601
7.587
7.583
7.580
7.566
7.562
7.494
7.480
7.260
3.832
3.814
3.797
3.611
3.601
3.595
3.585
3.569
3.554
3.538
3.528
2.188
2.183
2.174
2.169
2.162
2.154
2.149
2.140
2.135
2.129
1.847
1.821
1.813
1.807
1.788
1.645
1.631
1.620
1.517
1.503
1.492
1.478
1.411
1.394
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
N
OH
3f
0.96
1.00
0.98
0.99
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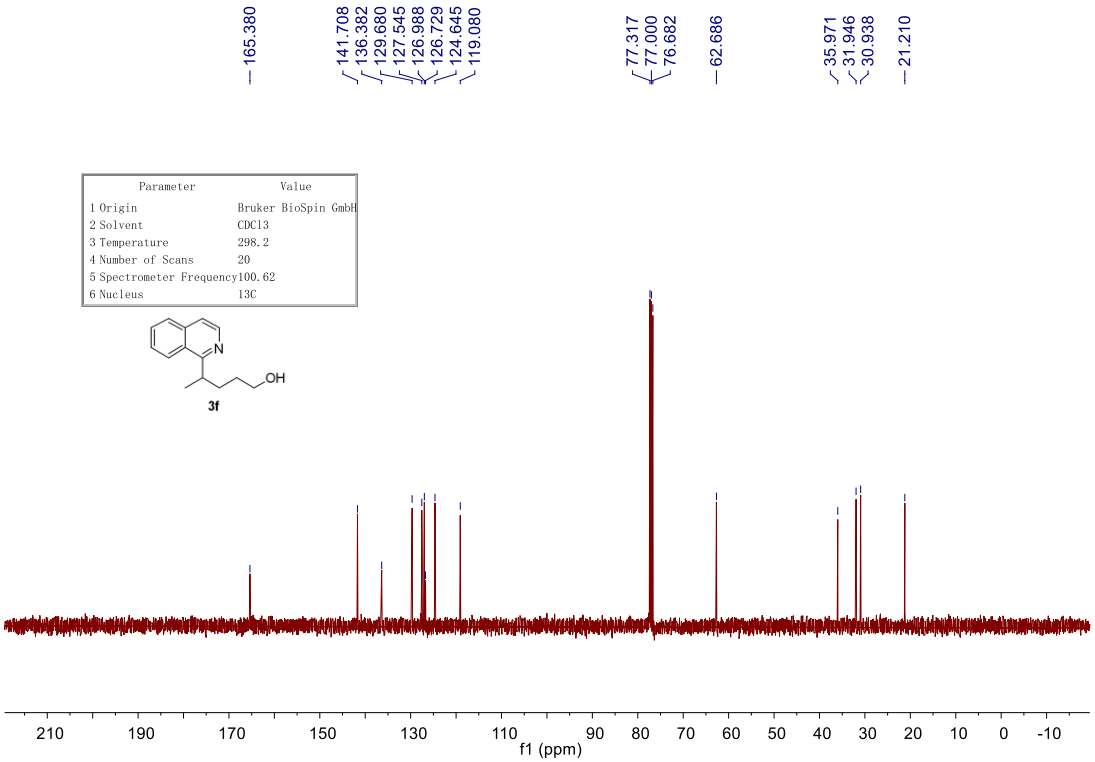
1.02
1.00
2.01
2.03
1.06
1.08
1.06
3.06
f1 (ppm)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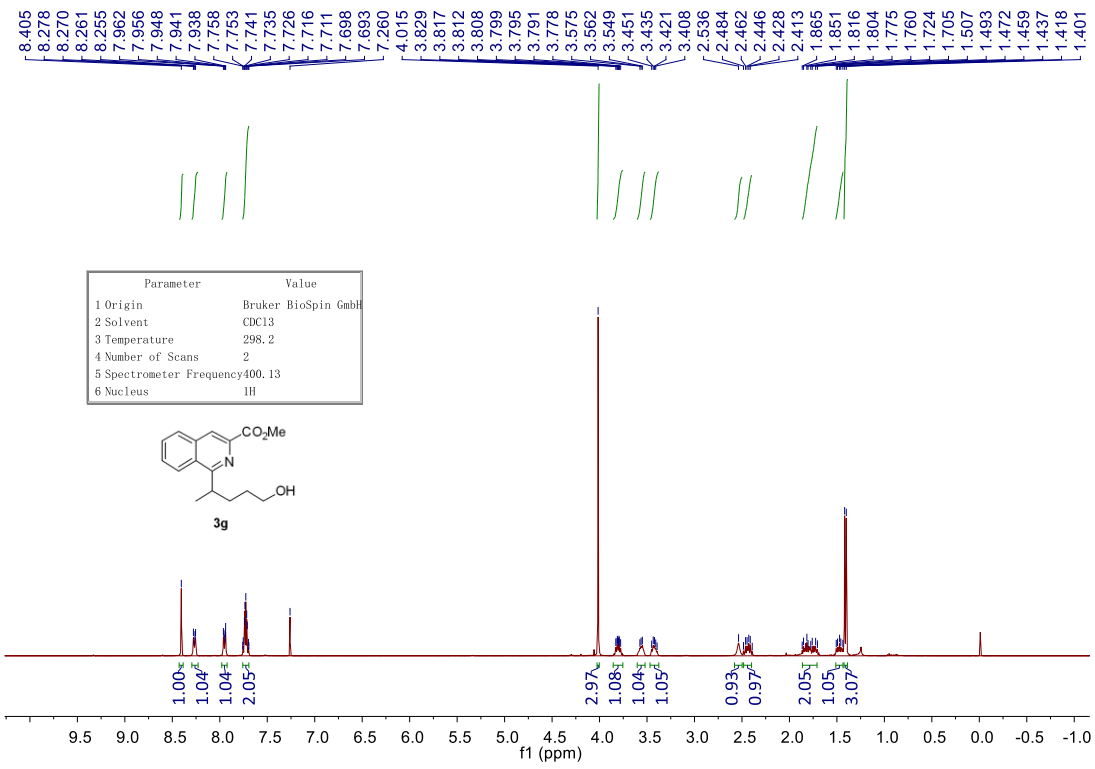
77.317
77.000
76.682
62.686
35.971
31.946
30.938
21.210
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N
OH
3f
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.938
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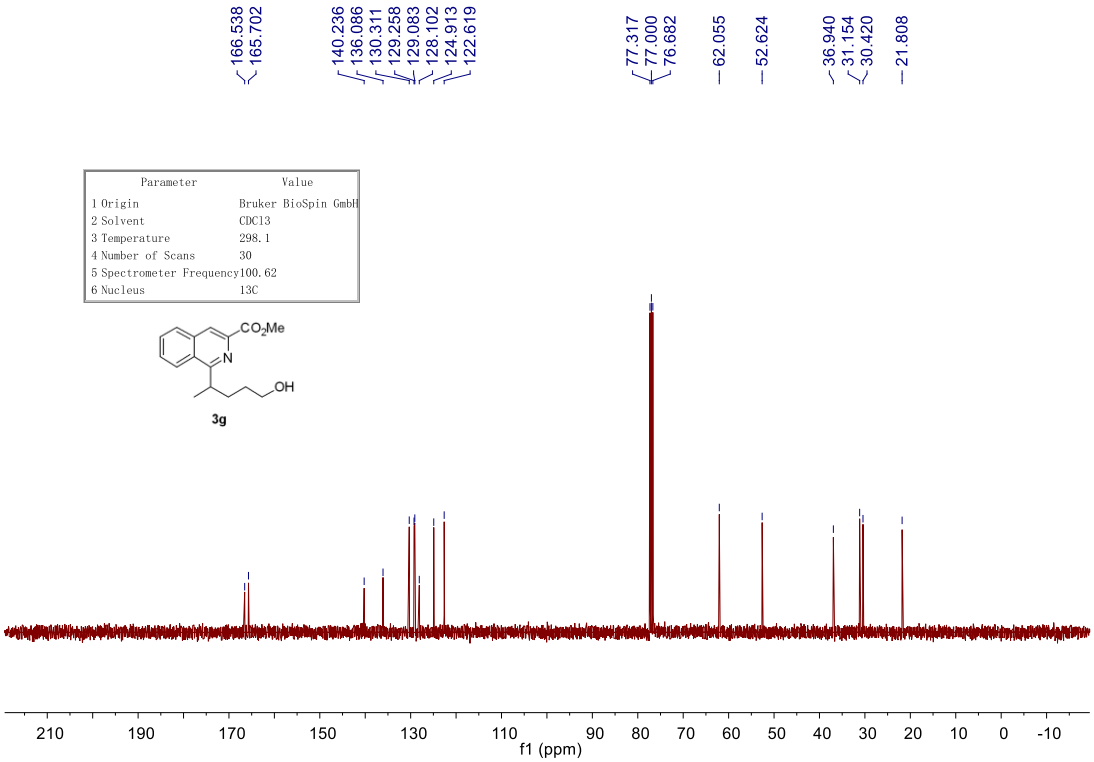
7.753
7.741
7.735
7.726
7.716
7.711
7.698
7.693
7.260
4.015
3.829
3.817
3.812
3.808
3.799
3.795
3.791
3.778
3.575
3.562
3.549
3.451
3.435
3.421
3.408
2.536
2.484
2.462
2.446
2.428
2.413
1.865
1.851
1.816
1.804
1.775
1.760
1.724
1.705
1.507
1.493
1.472
1.459
1.437
1.418
1.401
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CO2Me
N
OH
3g
1.00 1.04 1.04 2.05 2.97 1.08 1.04 1.05 0.93 0.97 2.05 1.05 3.07
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 -0.5 -1.0
f1 (ppm)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129.083
128.102
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122.619
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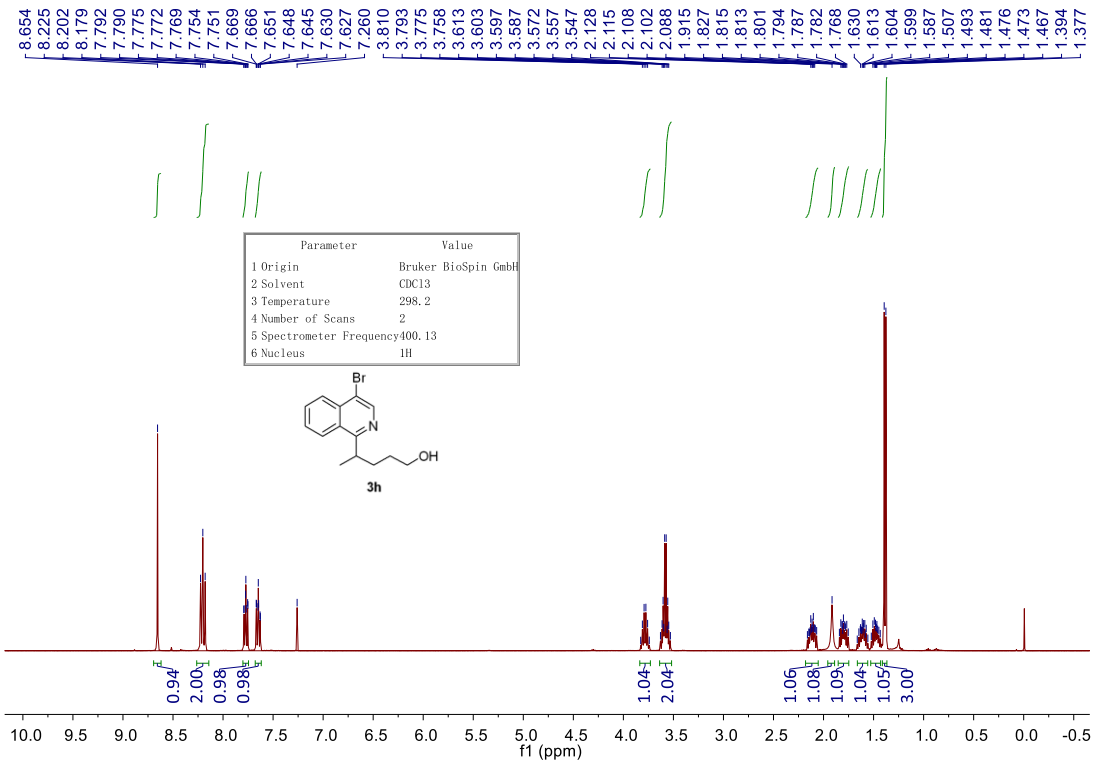
77.000
76.682
62.055
52.624
36.940
31.154
30.420
21.808
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CO2Me
N
OH
3g
f1 (ppm)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7.790
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7.772
7.769
7.754
7.751
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7.666
7.651
7.648
7.645
7.630
7.627
7.260
3.810
3.793
3.775
3.758
3.613
3.603
3.597
3.587
3.572
3.557
3.547
2.128
2.115
2.108
2.102
2.088
1.915
1.827
1.815
1.813
1.801
1.794
1.787
1.782
1.768
1.630
1.613
1.604
1.599
1.587
1.507
1.493
1.481
1.476
1.473
1.467
1.394
1.377
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Br
N
OH
3h
0.94
2.00
0.98
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1.04
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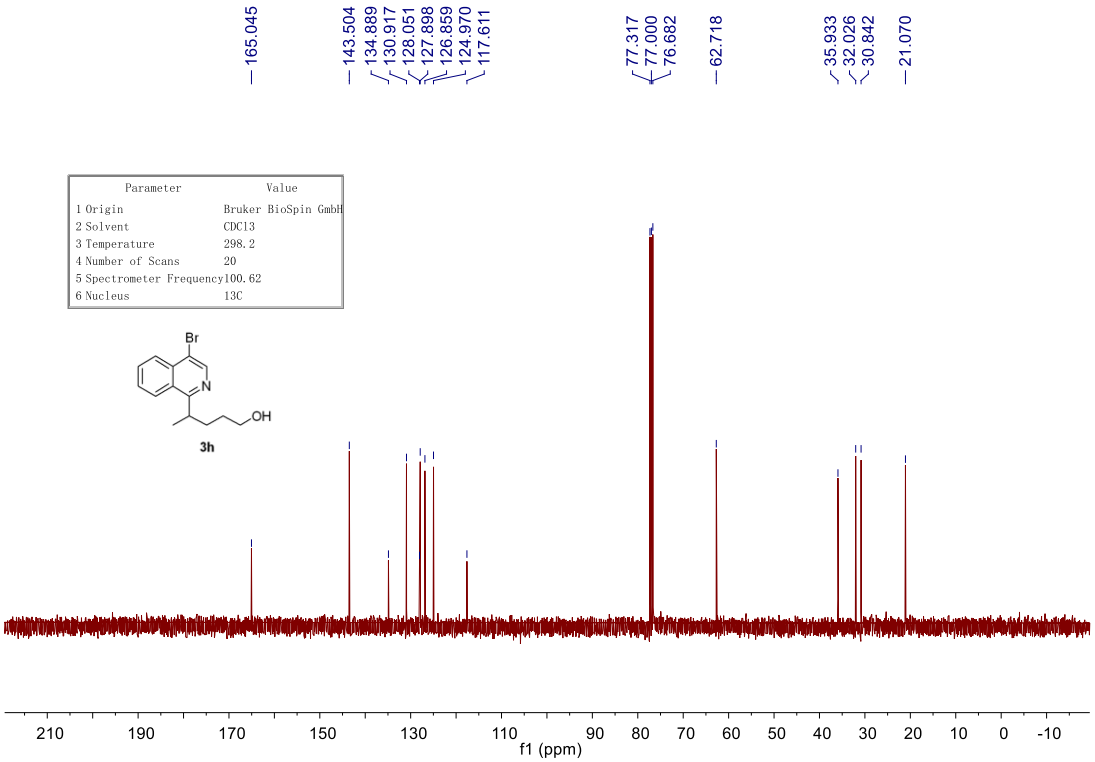
1.06
1.08
1.05
1.04
1.05
3.00
f1 (ppm)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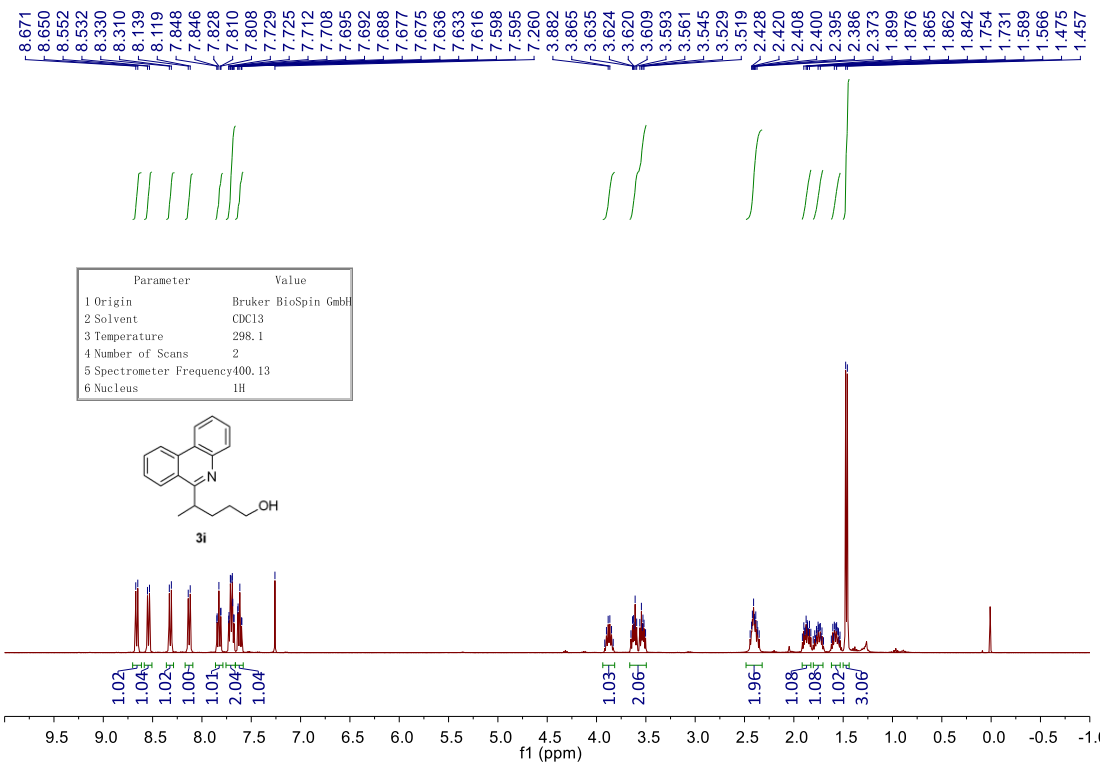
130.917
128.051
127.898
126.859
124.970
117.611
77.317
77.000
76.682
62.718
35.933
32.026
30.842
21.070
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Br
N
OH
3h
f1 (ppm)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7.828
7.810
7.808
7.729
7.725
7.712
7.708
7.695
7.692
7.688
7.677
7.675
7.636
7.633
7.616
7.598
7.595
7.260
3.882
3.865
3.635
3.624
3.620
3.609
3.593
3.561
3.545
3.529
3.519
2.428
2.420
2.408
2.400
2.395
2.386
2.373
1.899
1.876
1.865
1.862
1.842
1.754
1.731
1.589
1.566
1.475
1.457
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
N
OH
3i
1.02
1.04
1.02
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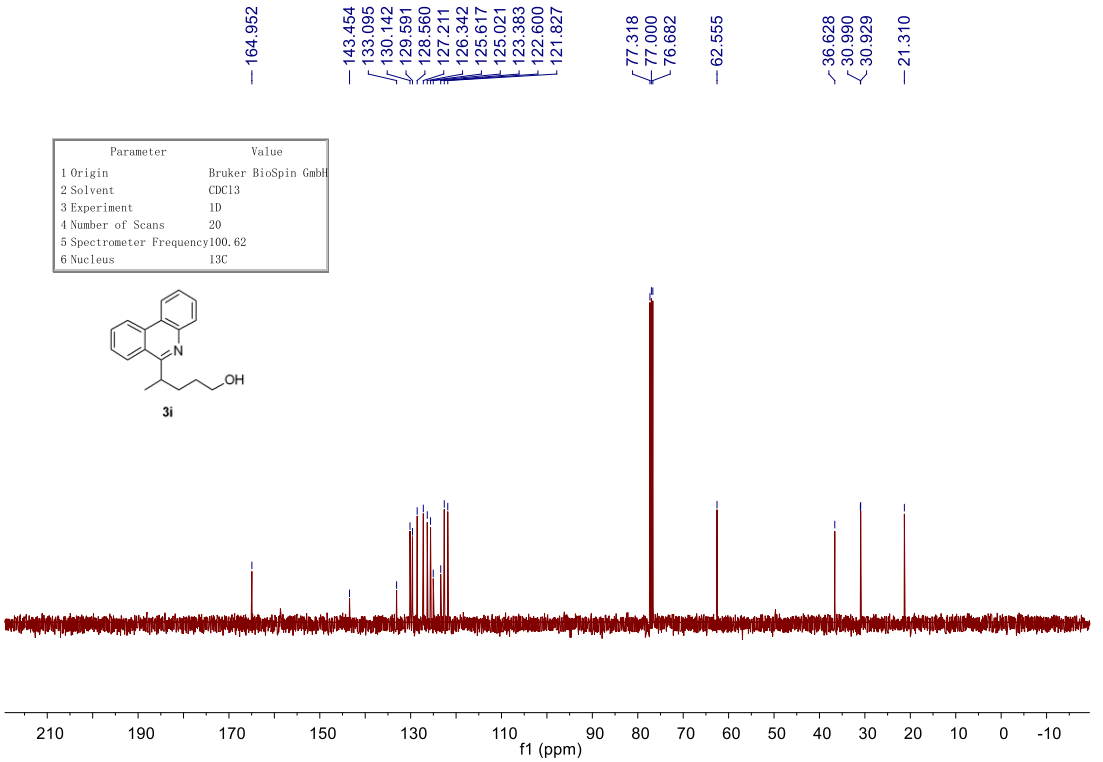
1.08
1.08
1.02
3.06
f1 (ppm)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126.342
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125.021
123.383
122.600
121.827
77.318
77.000
76.682
62.555
36.628
30.990
30.929
21.310
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Experiment 1D
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N
OH
3i
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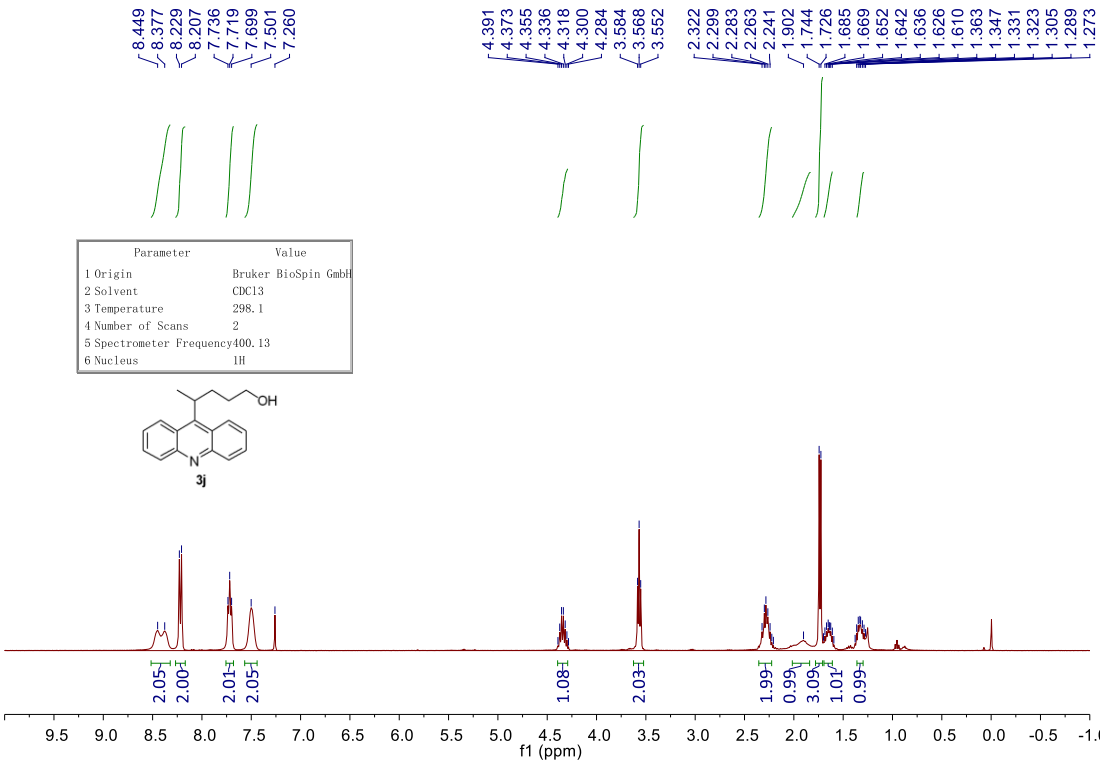
f1 (ppm)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8.207
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7.719
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7.501
7.260
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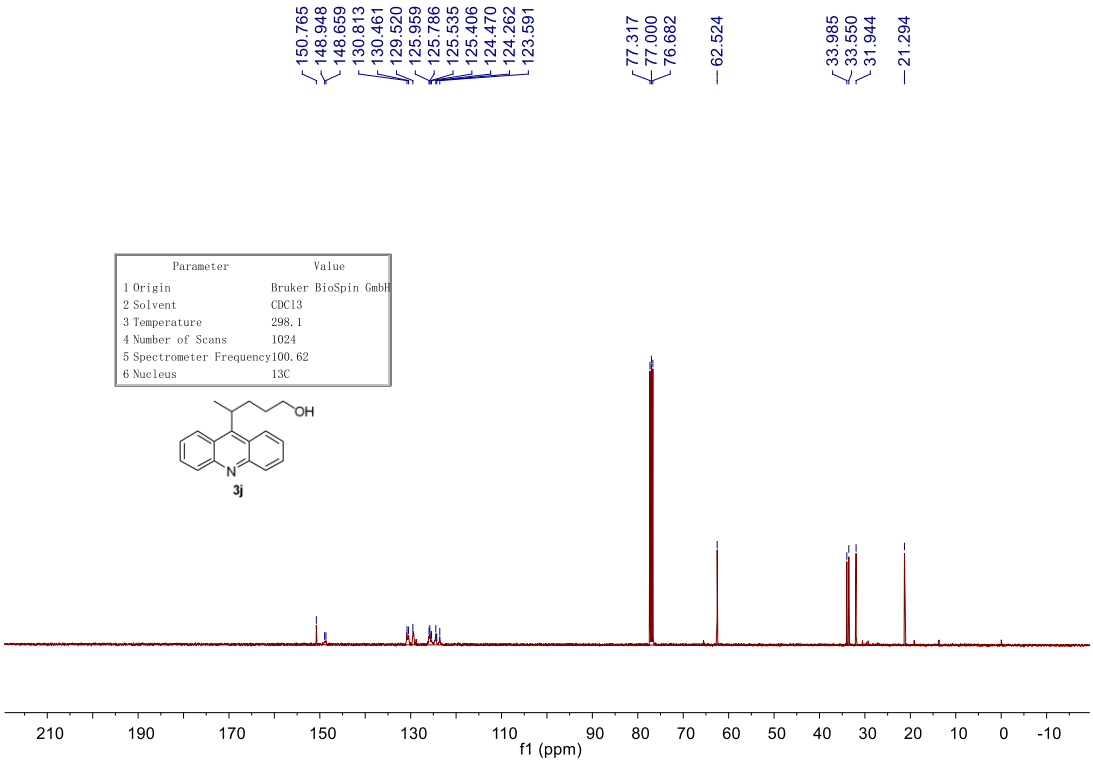
4.373
4.355
4.336
4.318
4.300
4.284
3.584
3.568
3.552
2.322
2.299
2.283
2.263
2.241
1.902
1.744
1.726
1.685
1.669
1.652
1.642
1.636
1.626
1.610
1.363
1.347
1.331
1.323
1.305
1.289
1.273
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
N
OH
3j
2.05 2.00 2.01 2.05 1.08 2.03 1.99 0.99 3.09 1.01 0.99
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 -0.5
f1 (ppm)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125.786
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125.406
124.470
124.262
123.591
77.317
77.000
76.682
62.524
33.985
33.550
31.944
21.294
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
N
3j
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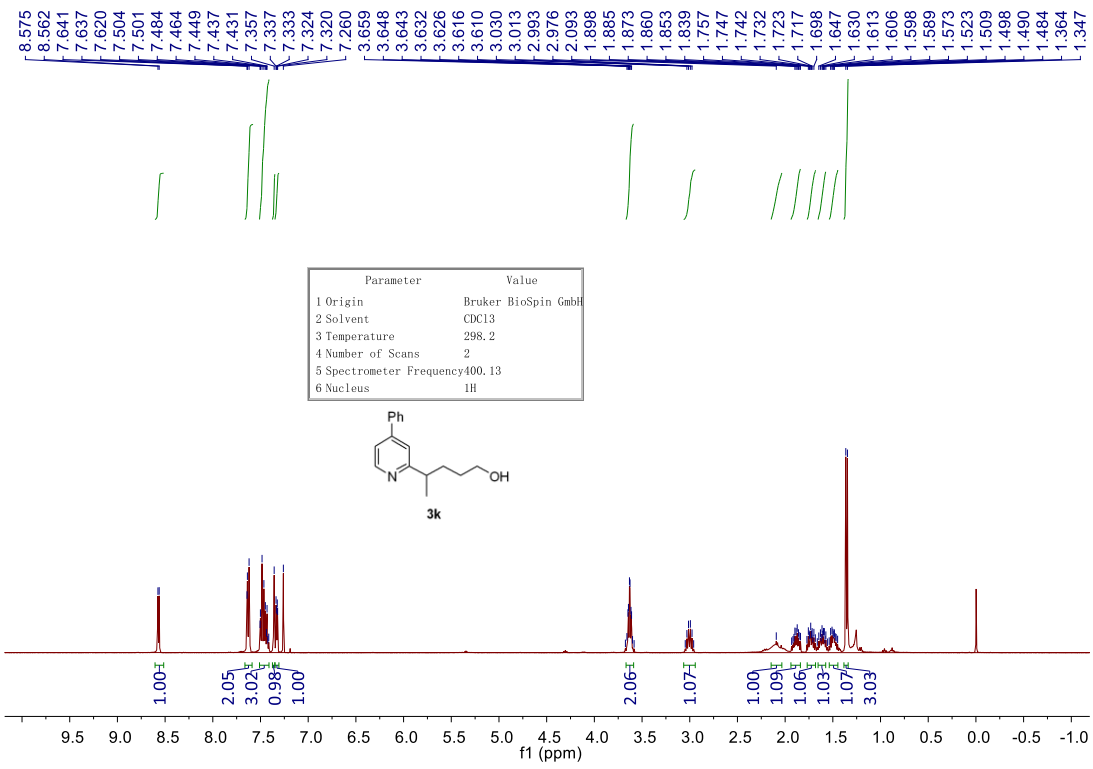
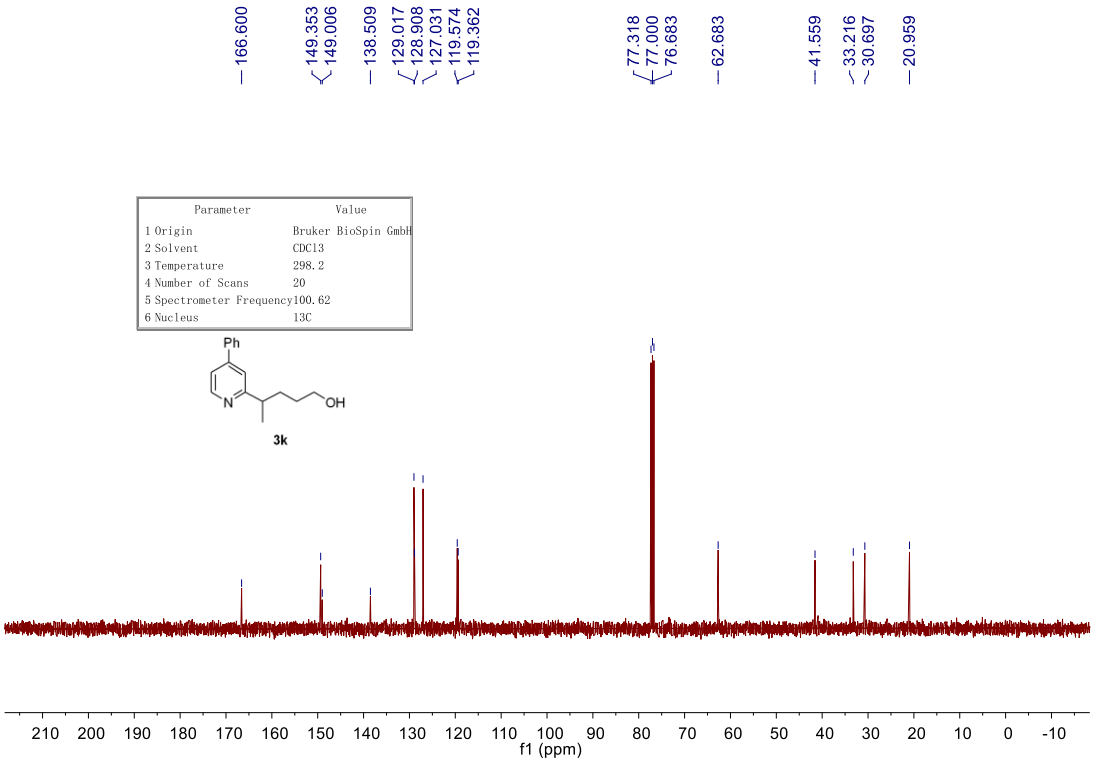
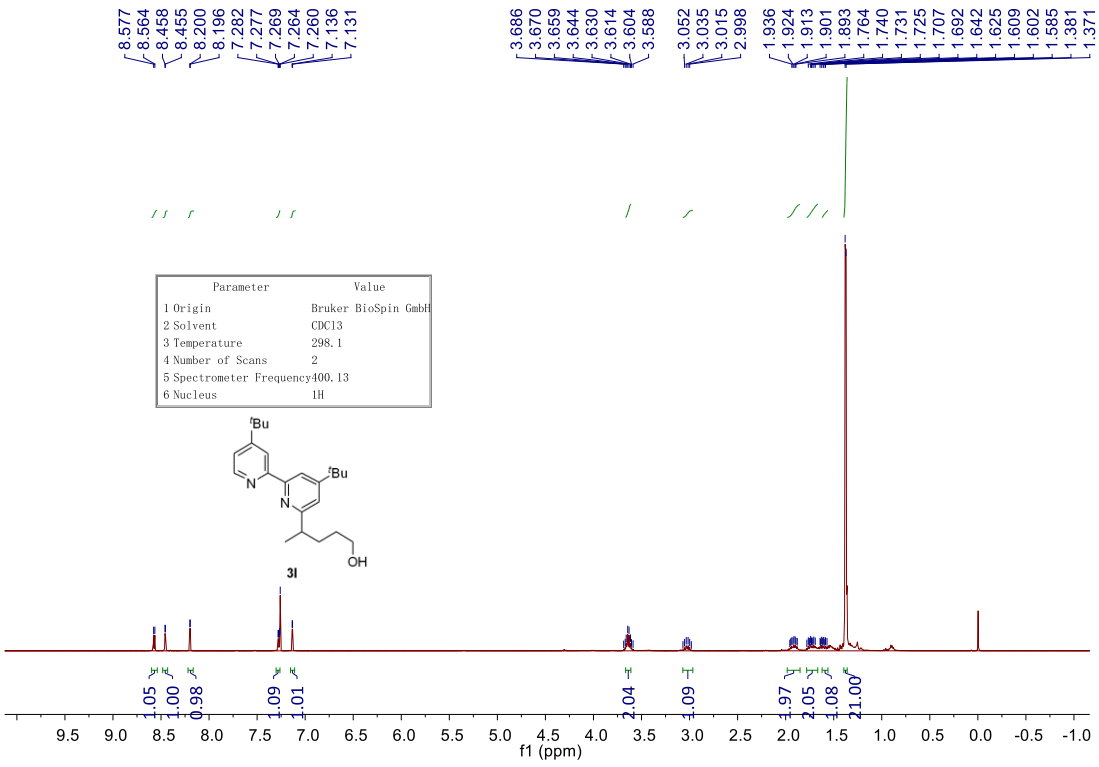
f1 (ppm)


8.575
8.562
7.641
7.637
7.620
7.504
7.501
7.484
7.464
7.449
7.437
7.431
7.357
7.337
7.333
7.324
7.320
7.260
3.659
3.648
3.643
3.632
3.626
3.616
3.610
3.030
3.013
2.993
2.976
2.093
1.898
1.885
1.873
1.860
1.853
1.839
1.757
1.747
1.742
1.732
1.723
1.717
1.698
1.647
1.630
1.613
1.606
1.598
1.589
1.573
1.523
1.509
1.498
1.490
1.484
1.364
1.347
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Ph
N
OH
3k
1.00
2.05
3.02
0.98
1.00
2.06
1.07
1.00
1.09
1.06
1.03
1.07
3.03
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 -0.5 -1.0
f1 (ppm)


166.600
149.353
149.006
138.509
129.017
128.908
127.031
119.574
119.362
77.318
77.000
76.683
62.683
41.559
33.216
30.697
20.959
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Ph
N
OH
3k
f1 (ppm)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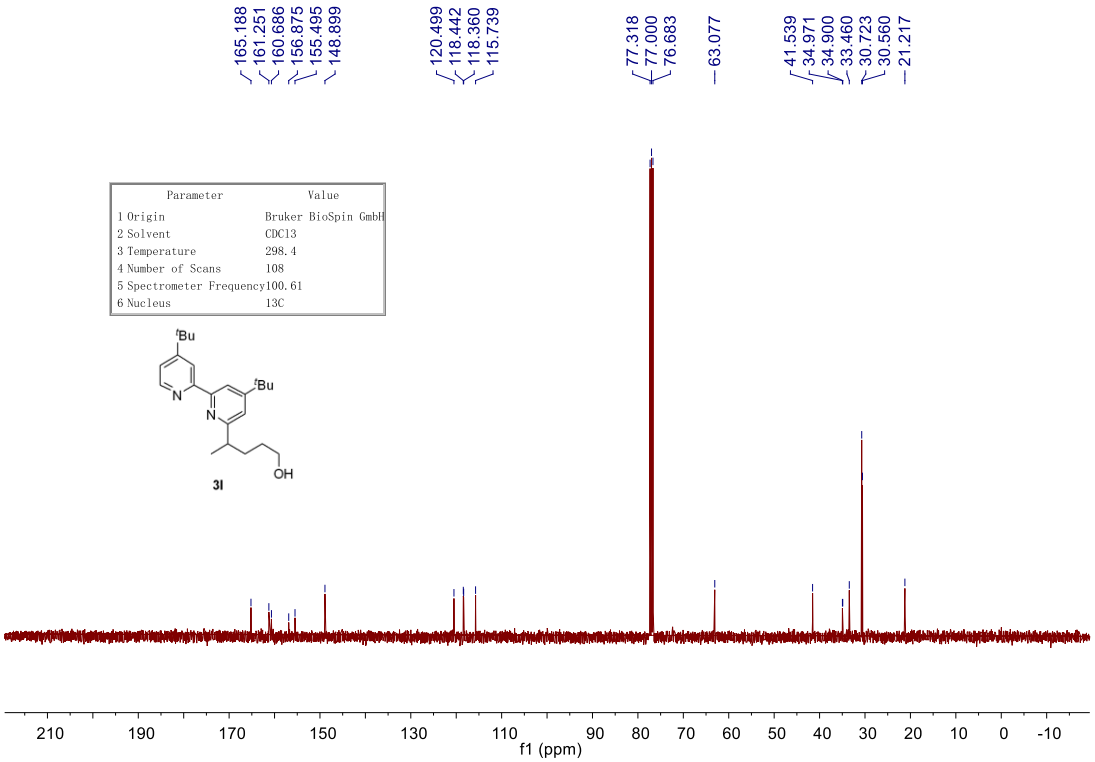
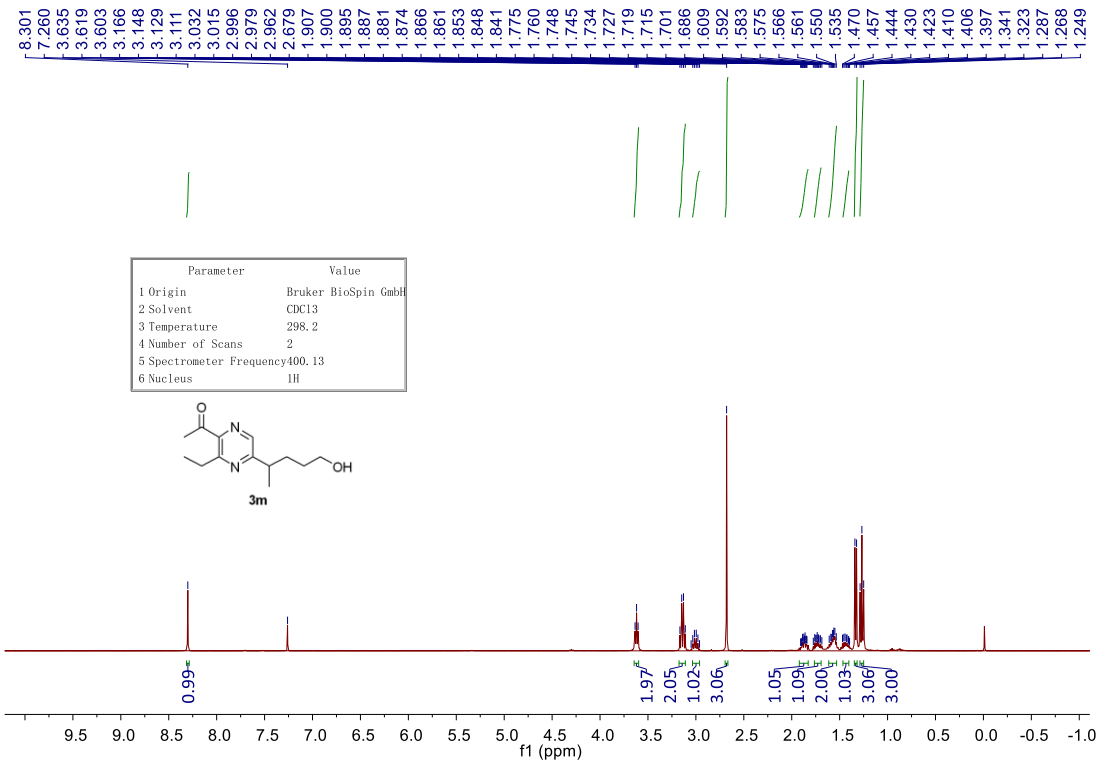
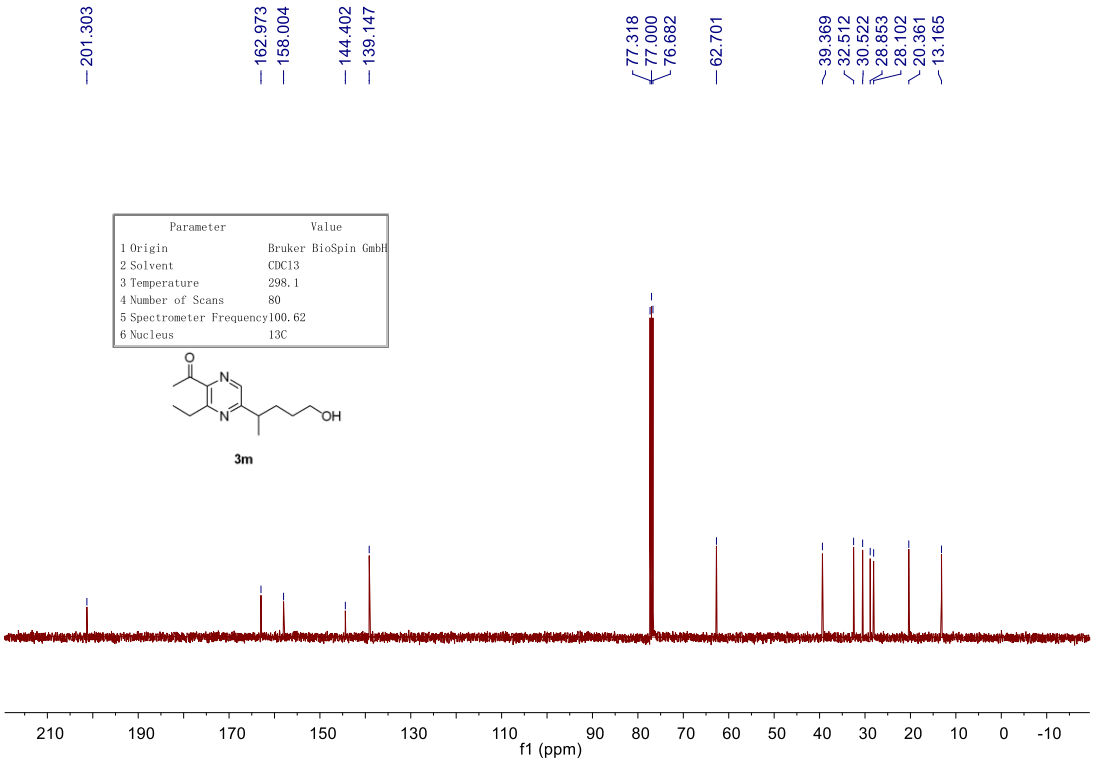
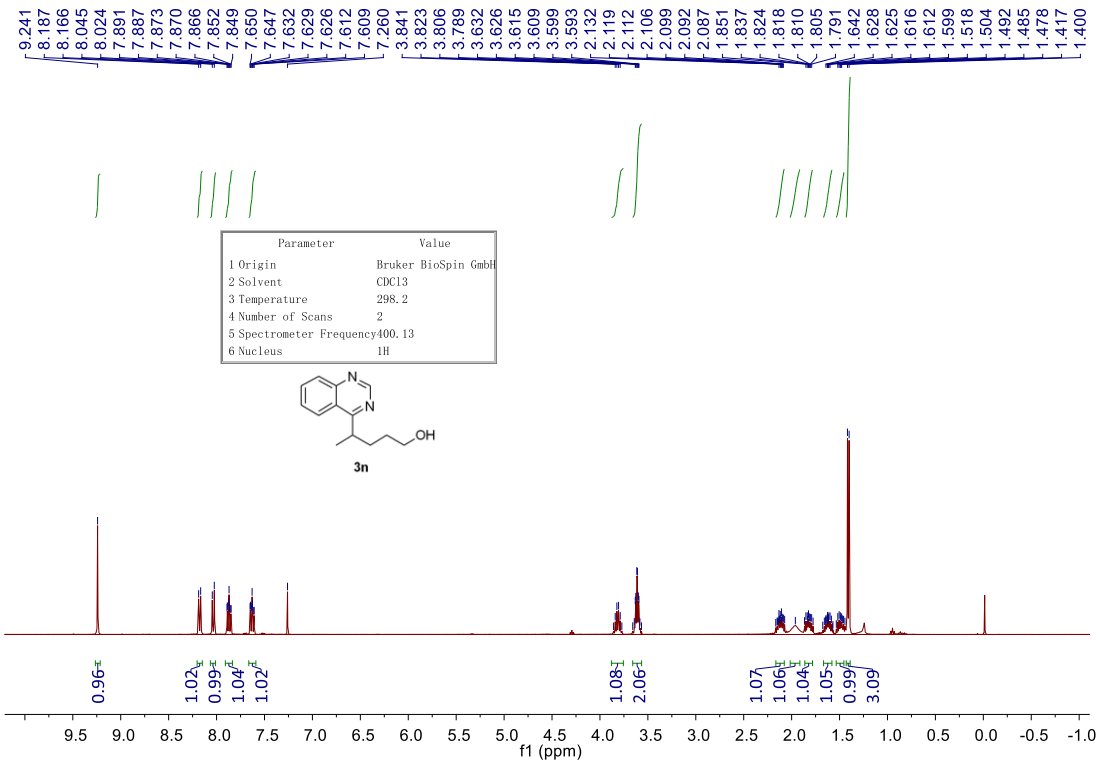
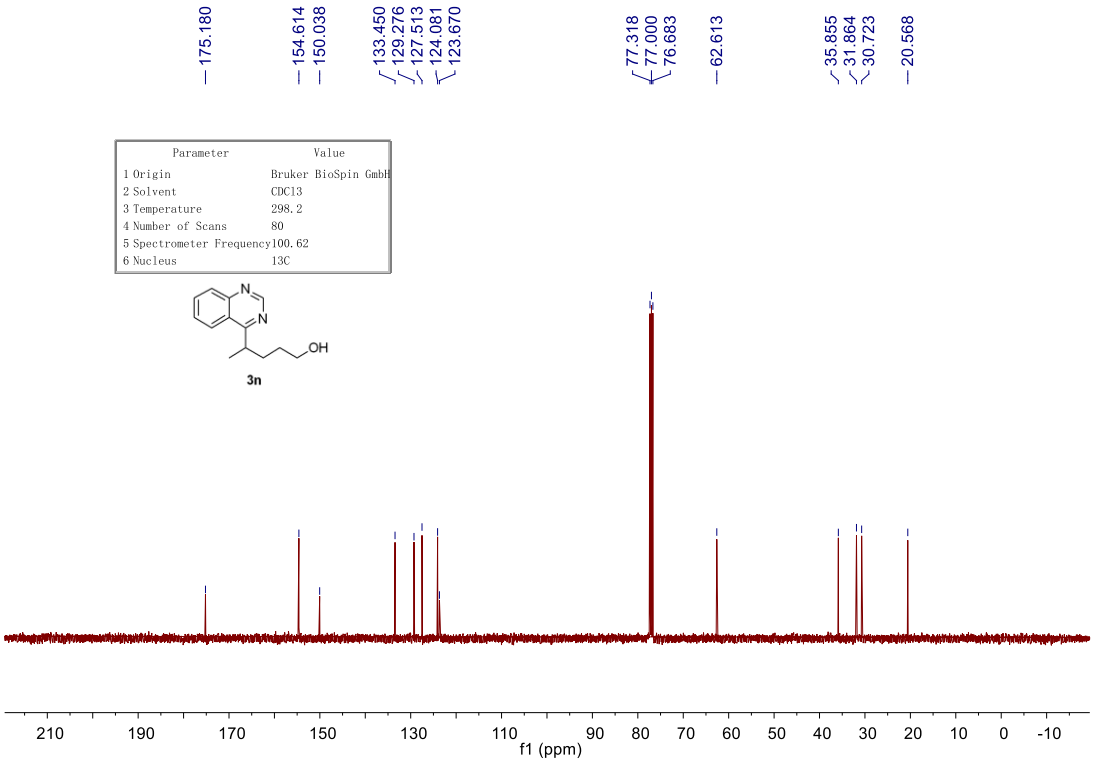
8.564
8.458
8.455
8.200
8.196
7.282
7.277
7.269
7.264
7.260
7.136
7.131
3.686
3.670
3.659
3.644
3.630
3.614
3.604
3.588
3.052
3.035
3.015
2.998
1.936
1.924
1.913
1.901
1.893
1.764
1.740
1.731
1.725
1.707
1.692
1.642
1.625
1.609
1.602
1.585
1.381
1.371
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
tBu
tBu
N
N
OH
3l
1.05
1.00
0.98
1.09
1.01
2.04
1.09
1.97
2.05
1.08
21.00
f1 (ppm)

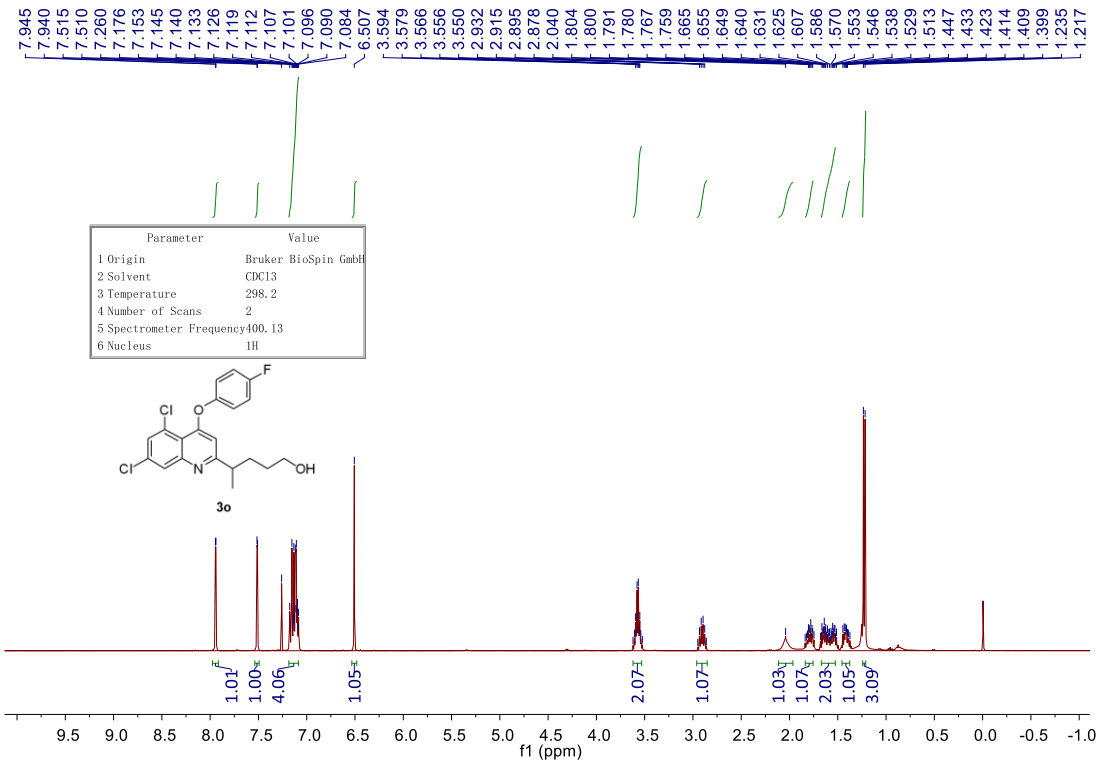

165.188
161.251
160.686
156.875
155.495
148.899
120.499
118.442
118.360
115.739
77.318
77.000
76.683
63.077
41.539
34.971
34.900
33.460
30.723
30.560
21.217
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 108
5 Spectrometer Frequency 100.61
6 Nucleus 13C
tBu
tBu
N
N
OH
3l
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

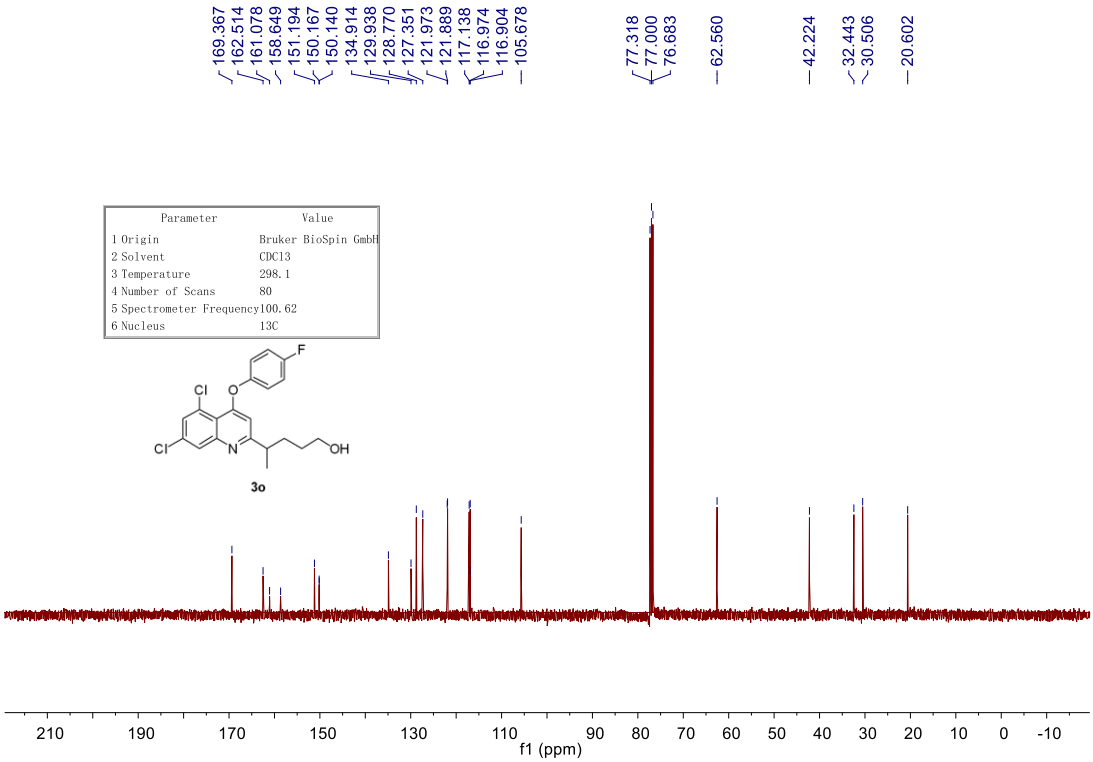

8.301
7.260
3.635
3.619
3.603
3.166
3.148
3.129
3.111
3.032
3.015
2.996
2.979
2.962
2.679
1.907
1.900
1.895
1.887
1.881
1.874
1.866
1.861
1.853
1.848
1.841
1.775
1.760
1.748
1.745
1.734
1.727
1.719
1.715
1.701
1.686
1.609
1.592
1.583
1.575
1.566
1.561
1.550
1.535
1.470
1.457
1.444
1.430
1.423
1.410
1.406
1.397
1.341
1.323
1.287
1.268
1.249
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N
N
OH
3m
0.99
1.97
2.05
1.02
3.06
1.05
1.09
2.00
1.03
3.06
3.00
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 -0.5 -1.0
f1 (ppm)

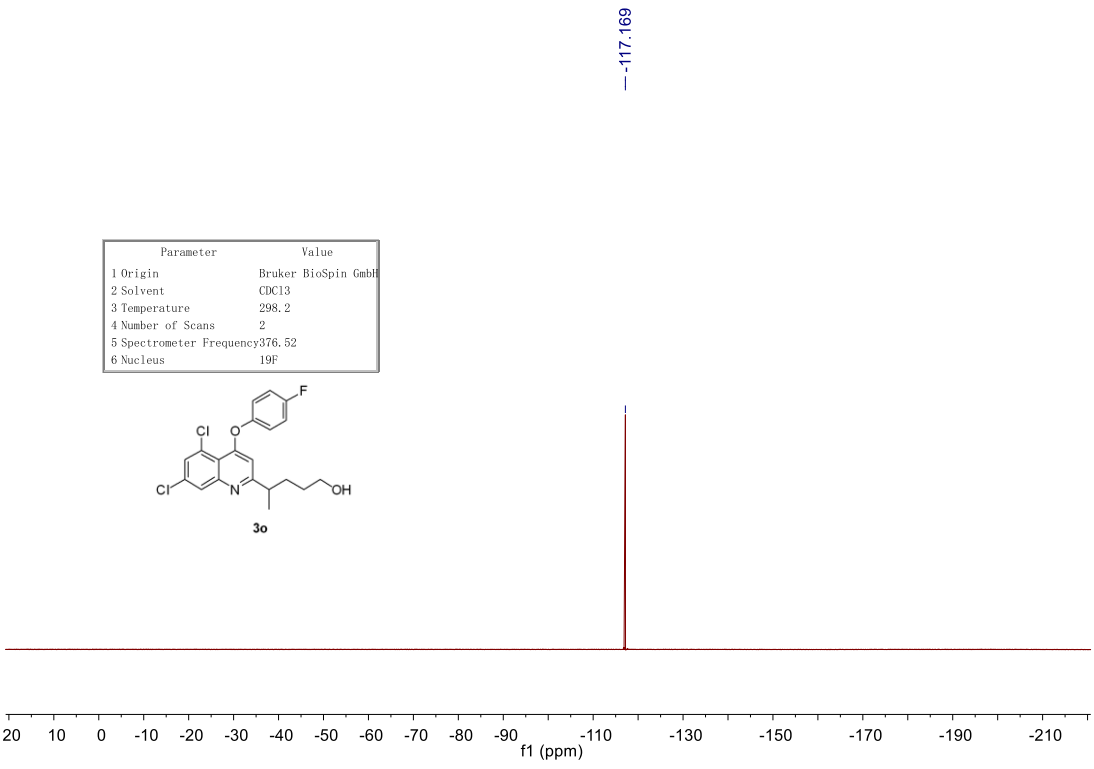

201.303
162.973
158.004
144.402
139.147
77.318
77.000
76.682
62.701
39.369
32.512
30.522
28.853
28.102
20.361
13.165
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
N
N
OH
3m
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

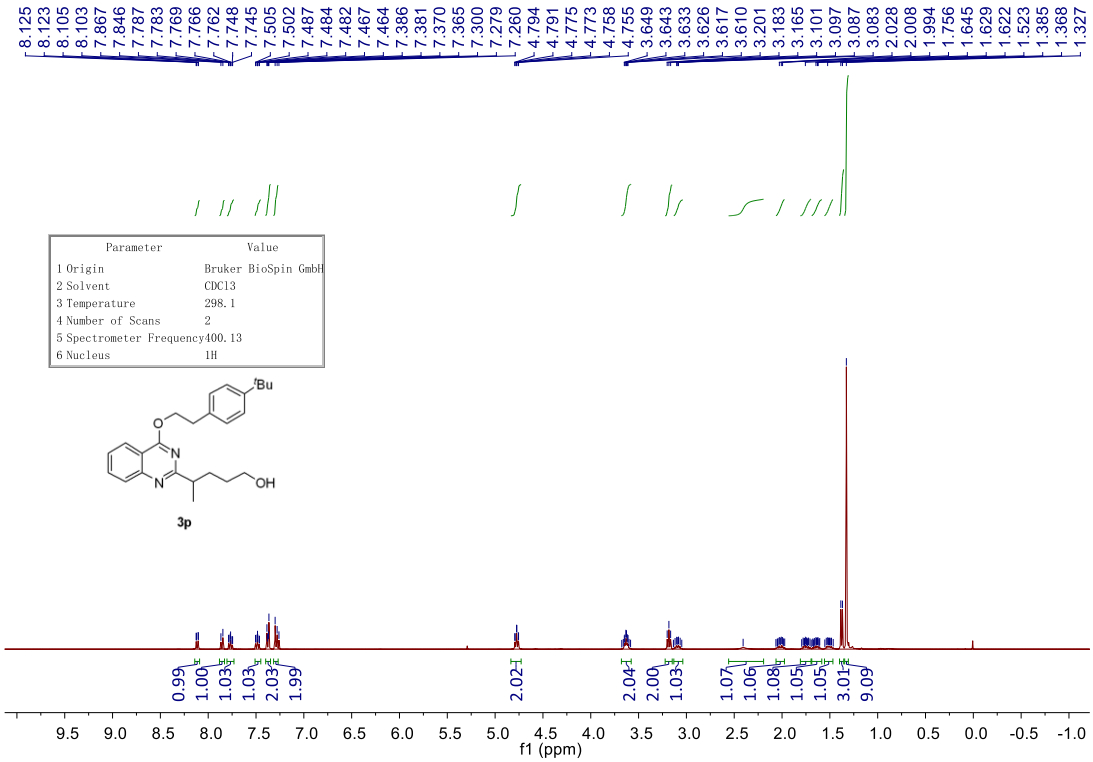

9.241
8.187
8.166
8.045
8.024
7.891
7.887
7.873
7.870
7.866
7.852
7.849
7.650
7.647
7.632
7.629
7.626
7.612
7.609
7.260
3.841
3.823
3.806
3.789
3.632
3.626
3.615
3.609
3.599
3.593
2.132
2.119
2.112
2.106
2.099
2.092
2.087
1.851
1.837
1.824
1.818
1.810
1.805
1.791
1.642
1.628
1.625
1.616
1.612
1.599
1.518
1.504
1.492
1.485
1.478
1.417
1.400
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
N
N
OH
3n
0.96
1.02
0.99
1.04
1.02
1.08
2.06
1.07
1.06
1.04
1.05
0.99
3.09
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 -0.5 -1.0
f1 (ppm)

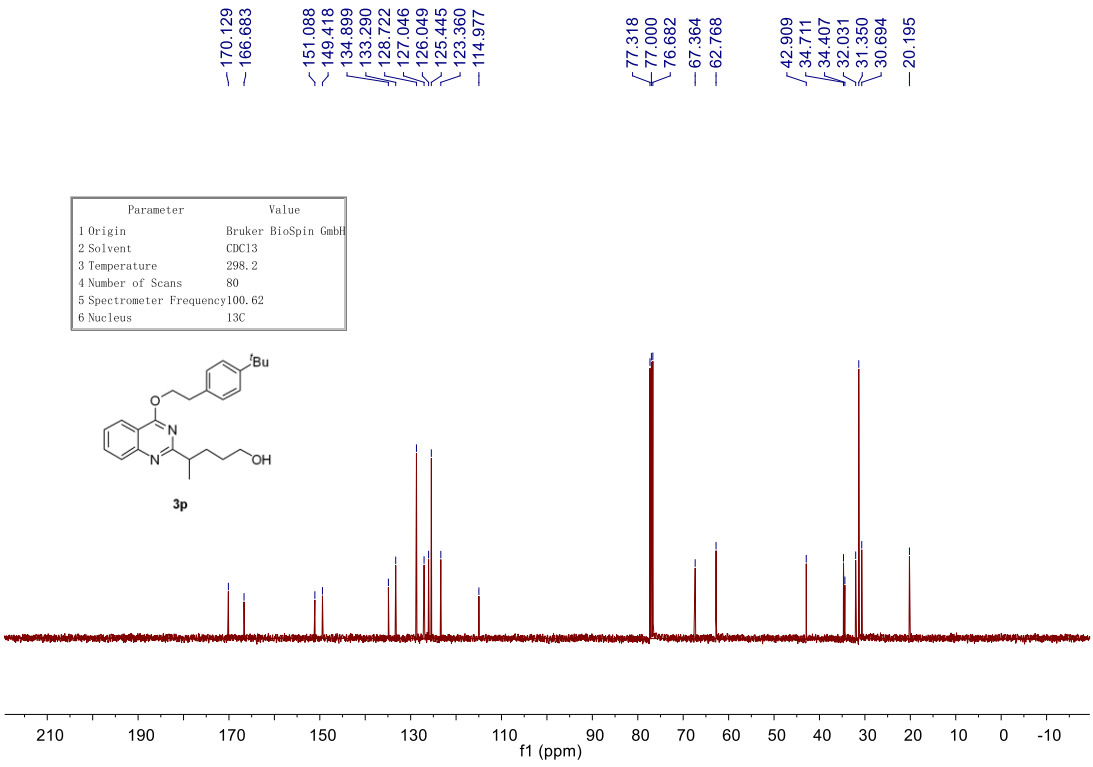

175.180
154.614
150.038
133.450
129.276
127.513
124.081
123.670
77.318
77.000
76.683
62.613
35.855
31.864
30.723
20.568
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N
N
OH
3n
f1 (ppm)

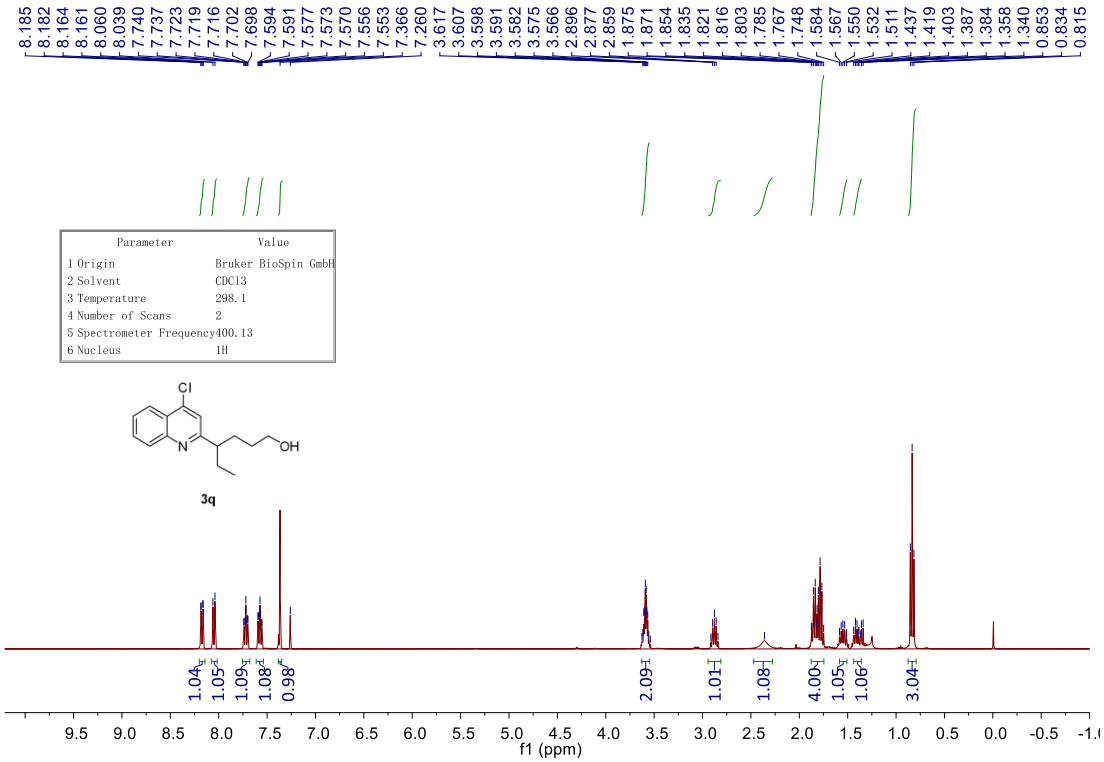

7.945
7.940
7.515
7.510
7.260
7.176
7.153
7.145
7.140
7.133
7.126
7.119
7.112
7.107
7.101
7.096
7.090
7.084
6.507
3.594
3.579
3.566
3.556
3.550
2.932
2.915
2.895
2.878
2.040
1.804
1.800
1.791
1.780
1.767
1.759
1.665
1.655
1.649
1.640
1.631
1.625
1.607
1.586
1.570
1.553
1.546
1.538
1.529
1.513
1.447
1.433
1.423
1.414
1.409
1.399
1.235
1.217
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
F
Cl
O
Cl
N
OH
3o
1.01
1.00
4.06
1.05
2.07
1.07
1.03
1.07
2.03
1.05
3.09
f1 (ppm)


169.367
162.514
161.078
158.649
151.194
150.167
150.140
134.914
129.938
128.770
127.351
121.973
121.889
117.138
116.974
116.904
105.678
77.318
77.000
76.683
62.560
42.224
32.443
30.506
20.602
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
F
Cl
O
Cl
N
OH
3o
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-117.169
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
F
Cl
O
Cl
N
OH
3o
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


8.125 8.123 8.105 8.103 7.867 7.846 7.787 7.783 7.769 7.766 7.762 7.748 7.745 7.505 7.502 7.487 7.484 7.482 7.467 7.464 7.386 7.381 7.370 7.365 7.300 7.279 7.260 4.794 4.791 4.775 4.773 4.758 4.755 3.649 3.643 3.633 3.626 3.617 3.610 3.201 3.183 3.165 3.101 3.097 3.087 3.083 2.028 2.008 1.994 1.756 1.645 1.629 1.622 1.523 1.385 1.368 1.327
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
tBu
O
N
N
OH
3p
0.99 1.00 1.03 1.03 2.03 1.99 2.02 2.04 2.00 1.03 1.07 1.06 1.08 1.05 1.05 3.01 9.09
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 -0.5 -1.0
f1 (ppm)


170.129 166.683 151.088 149.418 134.899 133.290 128.722 127.046 126.049 125.445 123.360 114.977 77.318 77.000 76.682 67.364 62.768 42.909 34.711 34.407 32.031 31.350 30.694 20.195
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
tBu
O
N
N
OH
3p
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.161
8.060
8.039
7.740
7.737
7.723
7.719
7.716
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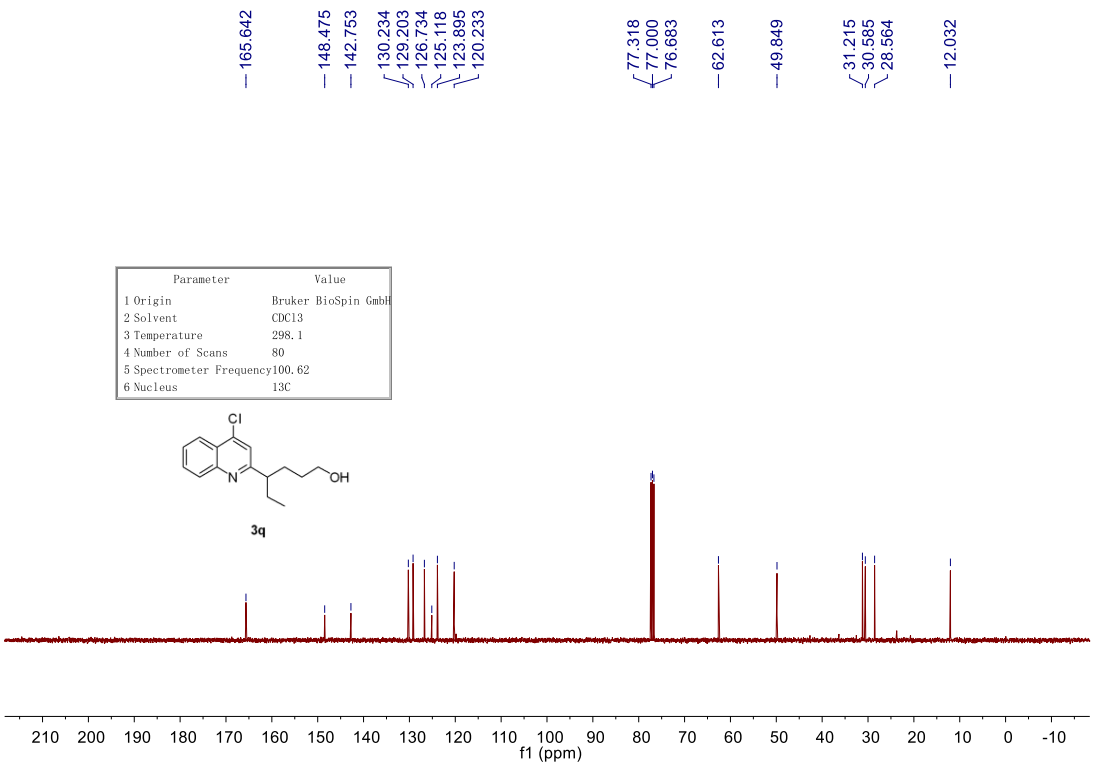
7.594
7.591
7.577
7.573
7.570
7.556
7.553
7.366
7.260
3.617
3.607
3.598
3.591
3.582
3.575
3.566
2.896
2.877
2.859
1.875
1.871
1.854
1.835
1.821
1.816
1.803
1.785
1.767
1.748
1.584
1.567
1.550
1.532
1.511
1.437
1.419
1.403
1.387
1.384
1.358
1.340
0.853
0.834
0.815
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3q
1.04
1.05
1.09
1.08
0.98
2.09
1.01
1.08
4.00
1.05
1.06
3.04
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 -0.5
f1 (ppm)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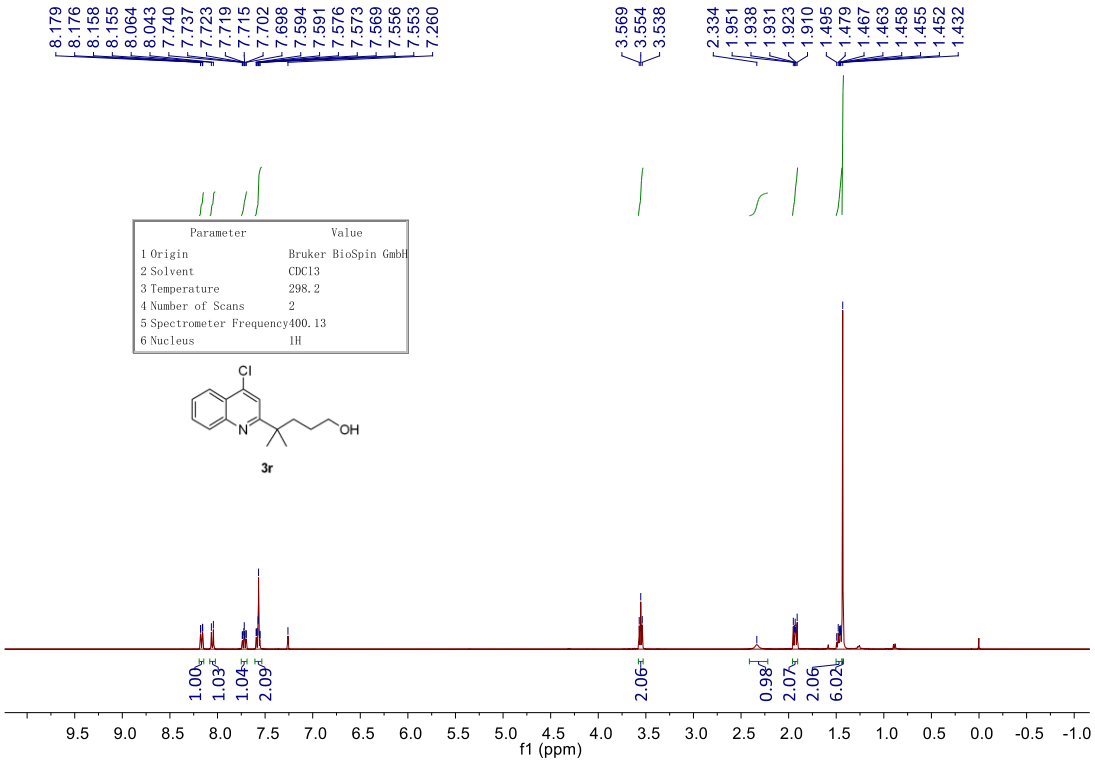
142.753
130.234
129.203
126.734
125.118
123.895
120.233
77.318
77.000
76.683
62.613
49.849
31.215
30.585
28.564
12.032
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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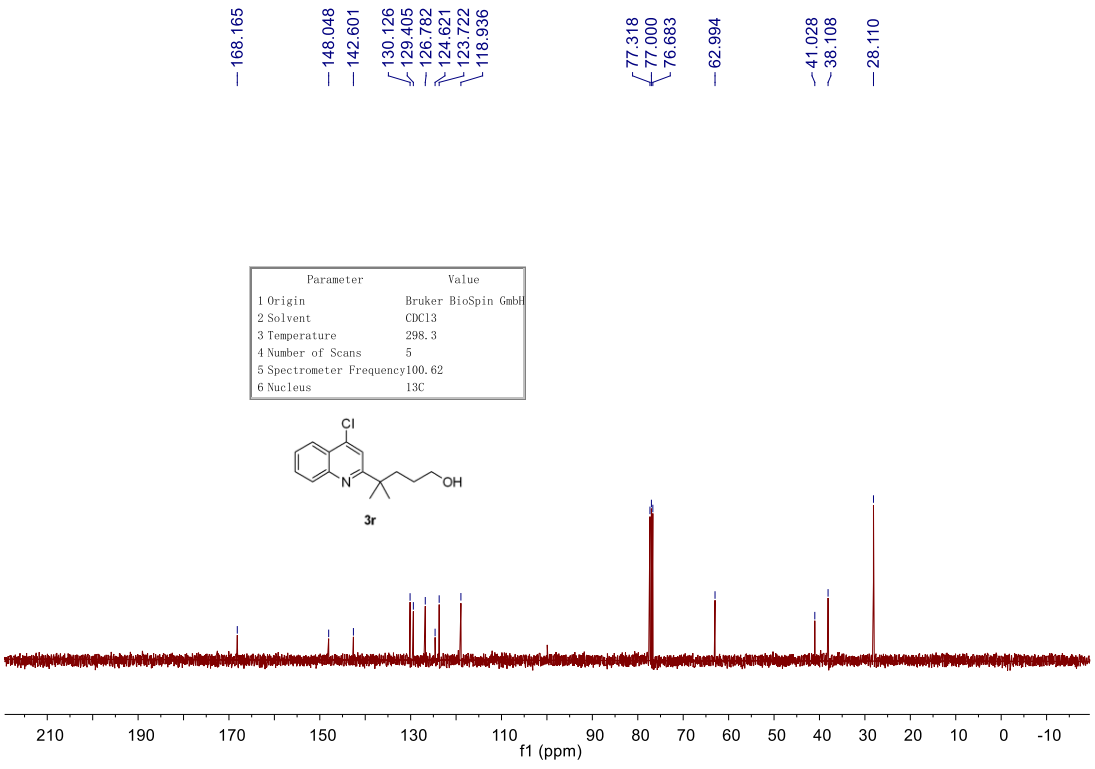
8.176
8.158
8.155
8.064
8.043
7.740
7.737
7.723
7.719
7.715
7.702
7.698
7.594
7.591
7.576
7.573
7.569
7.556
7.553
7.260
3.569
3.554
3.538
2.334
1.951
1.938
1.931
1.923
1.910
1.495
1.479
1.467
1.463
1.458
1.455
1.452
1.432
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3r
1.00
1.03
1.04
2.09
2.06
0.98
2.07
2.06
6.02
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 -0.5 -1.0
f1 (ppm)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148.048
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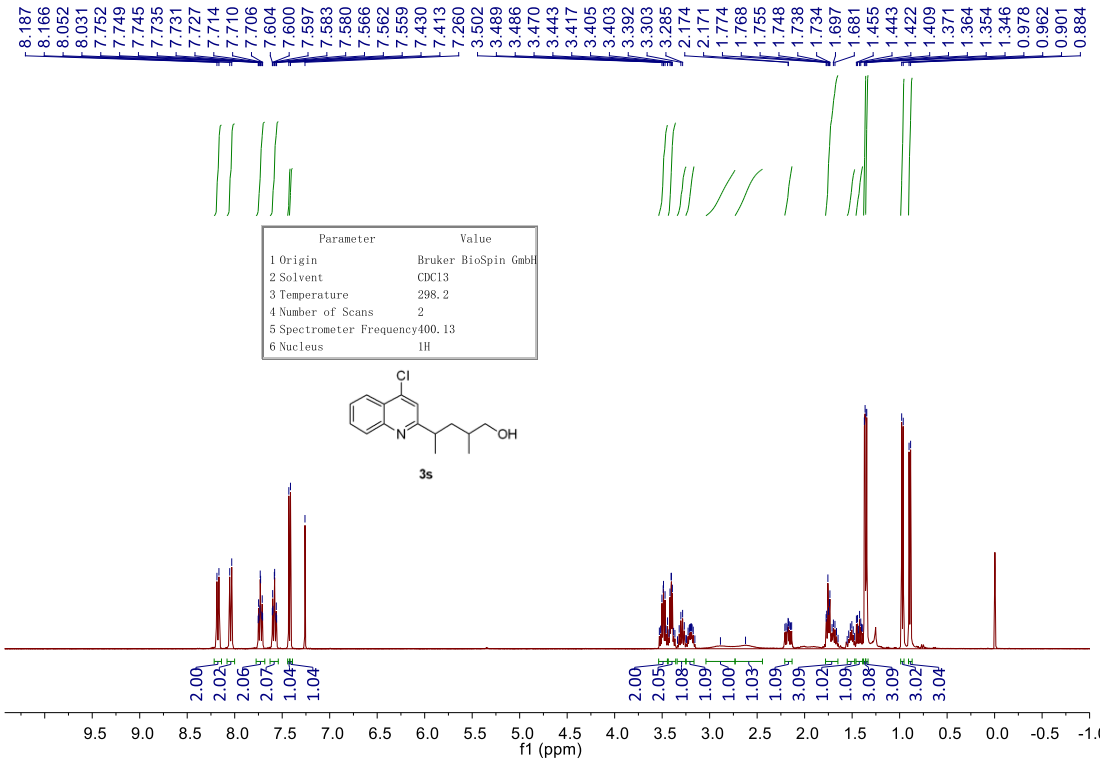
130.126
129.405
126.782
124.621
123.722
118.936
77.318
77.000
76.683
62.994
41.028
38.108
28.110
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 5
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3r
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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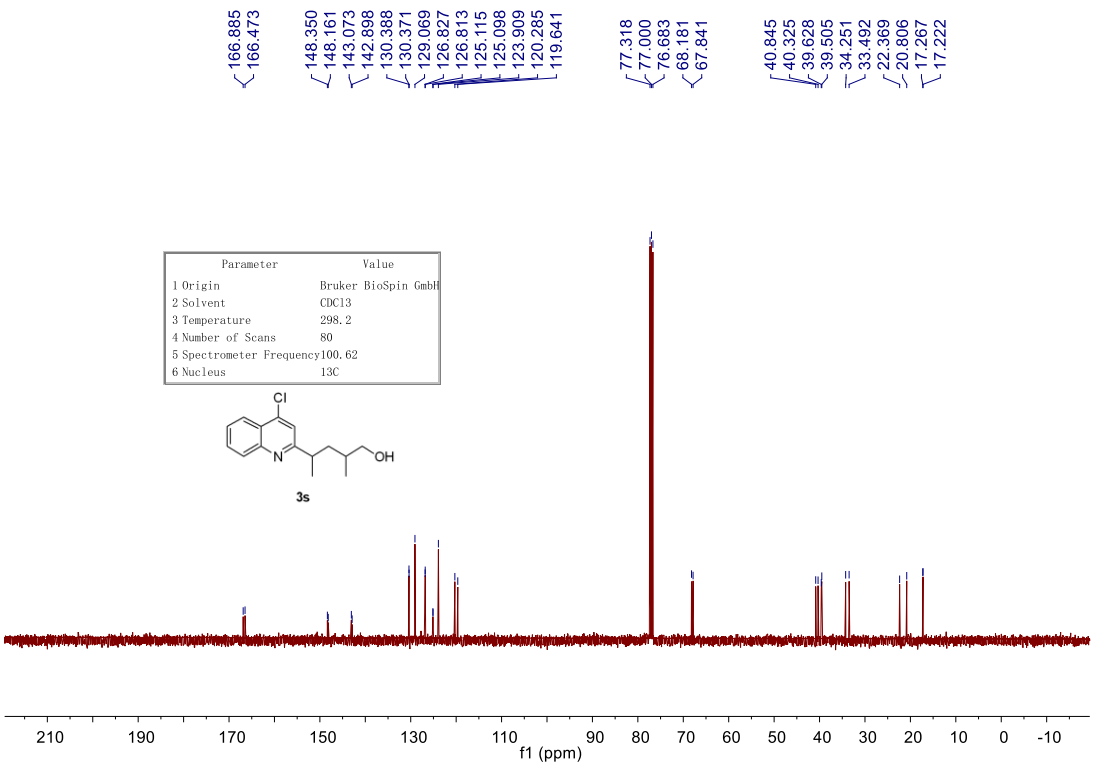
8.166
8.052
8.031
7.752
7.749
7.745
7.735
7.731
7.727
7.714
7.710
7.706
7.604
7.600
7.597
7.583
7.580
7.566
7.562
7.559
7.430
7.413
7.260
3.502
3.489
3.486
3.470
3.443
3.417
3.405
3.403
3.392
3.303
3.285
2.174
2.171
1.774
1.768
1.755
1.748
1.738
1.734
1.697
1.681
1.455
1.443
1.422
1.409
1.371
1.364
1.354
1.346
0.978
0.962
0.901
0.884
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3s
2.00
2.02
2.06
2.07
1.04
1.04
2.00
2.05
1.08
1.09
1.00
1.03
1.09
3.09
1.02
1.09
3.08
3.09
3.02
3.04
f1 (ppm)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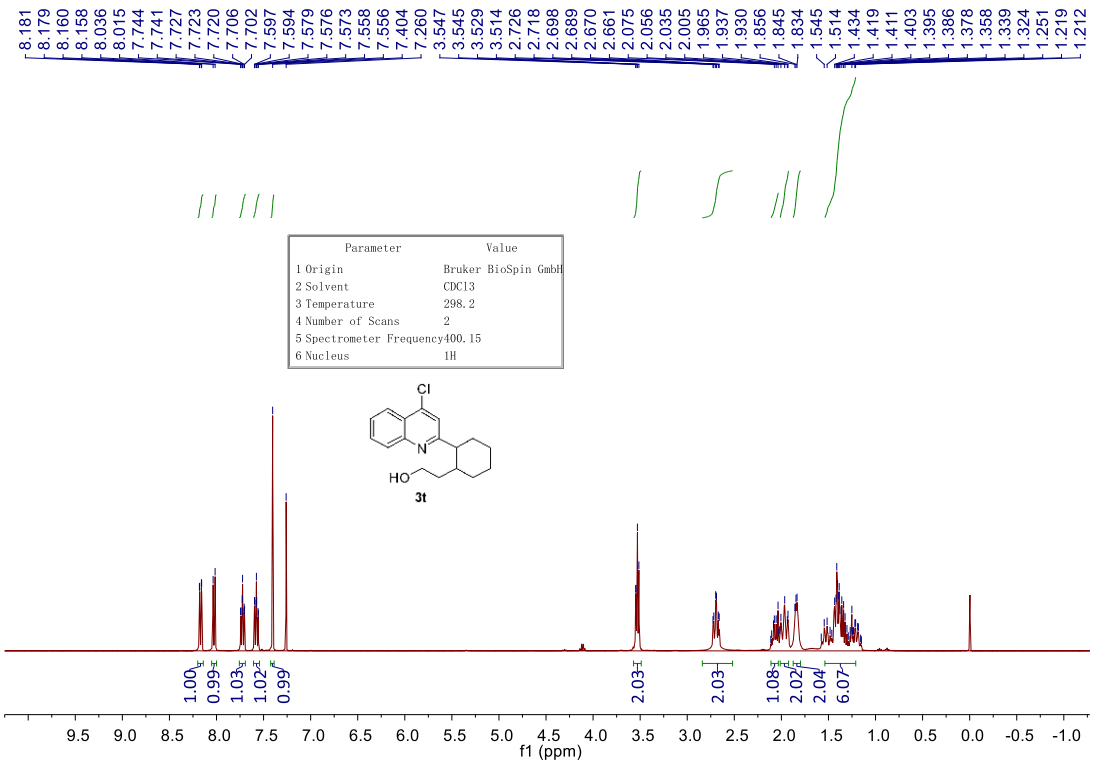
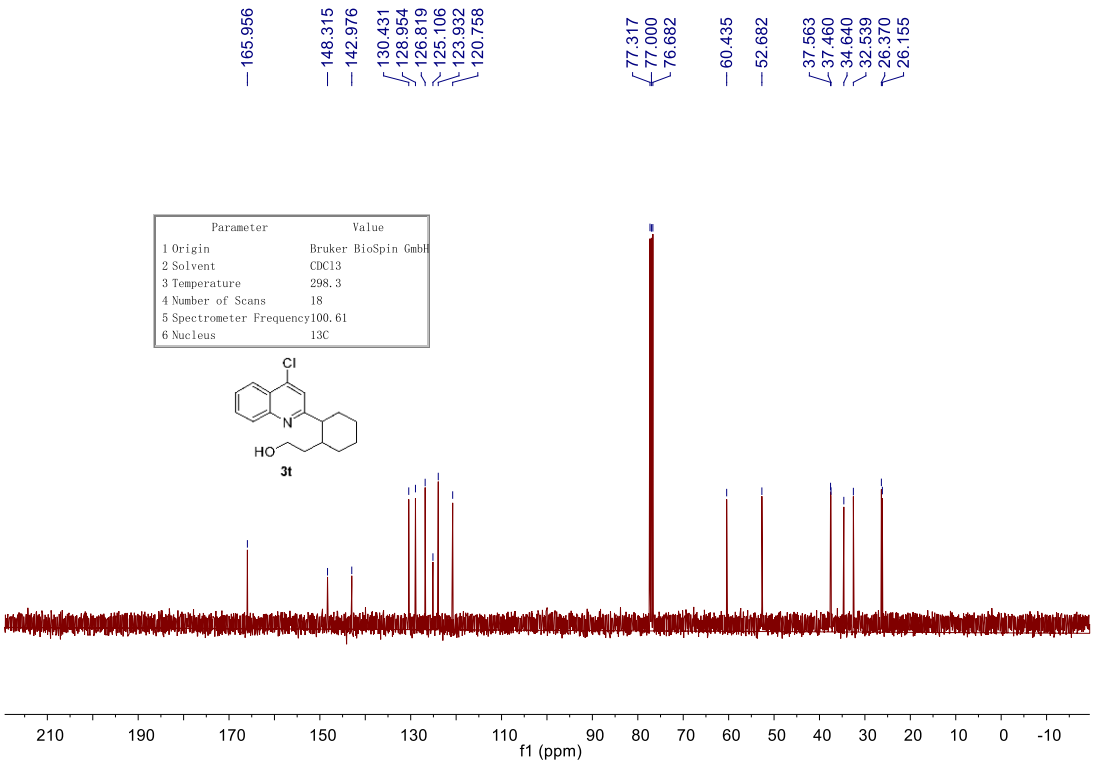
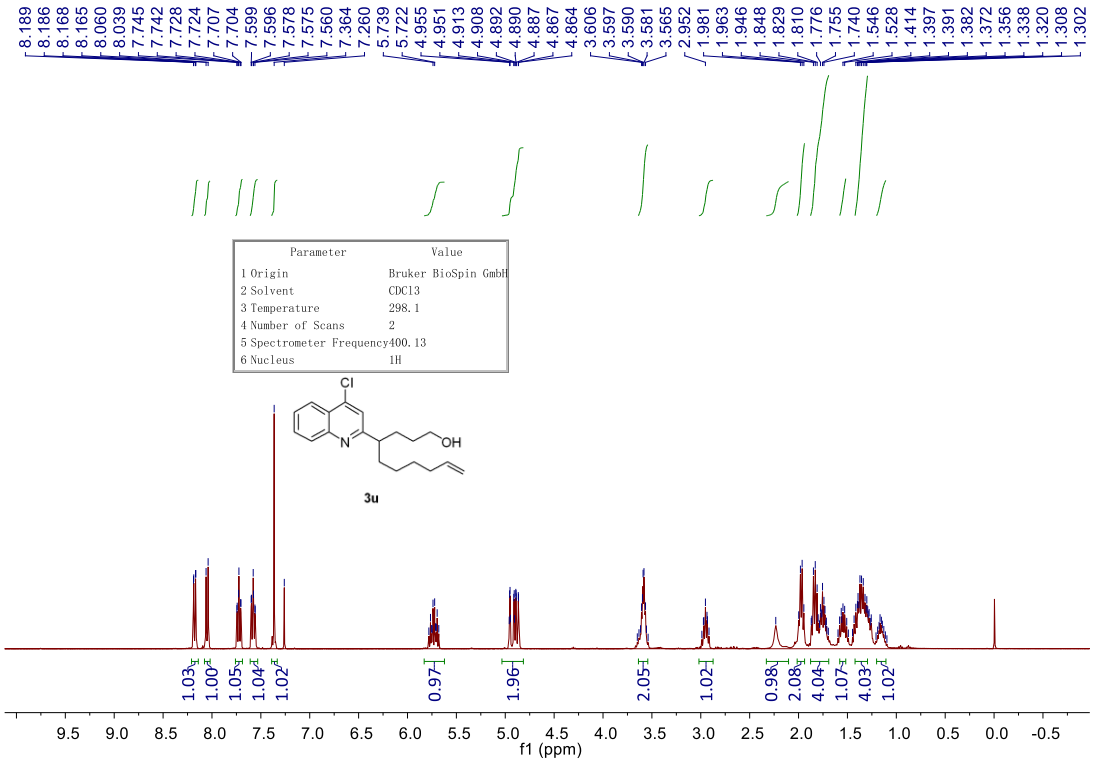
148.161
143.073
142.898
130.388
130.371
129.069
126.827
126.813
125.115
125.098
123.909
120.285
119.641
77.318
77.000
76.683
68.181
67.841
40.845
40.325
39.628
39.505
34.251
33.492
22.369
20.806
17.267
17.222
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3s
f1 (ppm)


8.181
8.179
8.160
8.158
8.036
8.015
7.744
7.741
7.727
7.723
7.720
7.706
7.702
7.597
7.594
7.579
7.576
7.573
7.558
7.556
7.404
7.260
3.547
3.545
3.529
3.514
2.726
2.718
2.698
2.689
2.670
2.661
2.075
2.056
2.035
2.005
1.965
1.937
1.930
1.856
1.845
1.834
1.545
1.514
1.434
1.419
1.411
1.403
1.395
1.386
1.378
1.358
1.339
1.324
1.251
1.219
1.212
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
HO
3t
1.00
0.99
1.03
1.02
0.99
2.03
2.03
1.08
2.02
2.04
6.07
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 -0.5 -1.0
f1 (ppm)


165.956
148.315
142.976
130.431
128.954
126.819
125.106
123.932
120.758
77.317
77.000
76.682
60.435
52.682
37.563
37.460
34.640
32.539
26.370
26.155
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 18
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
N
HO
3t
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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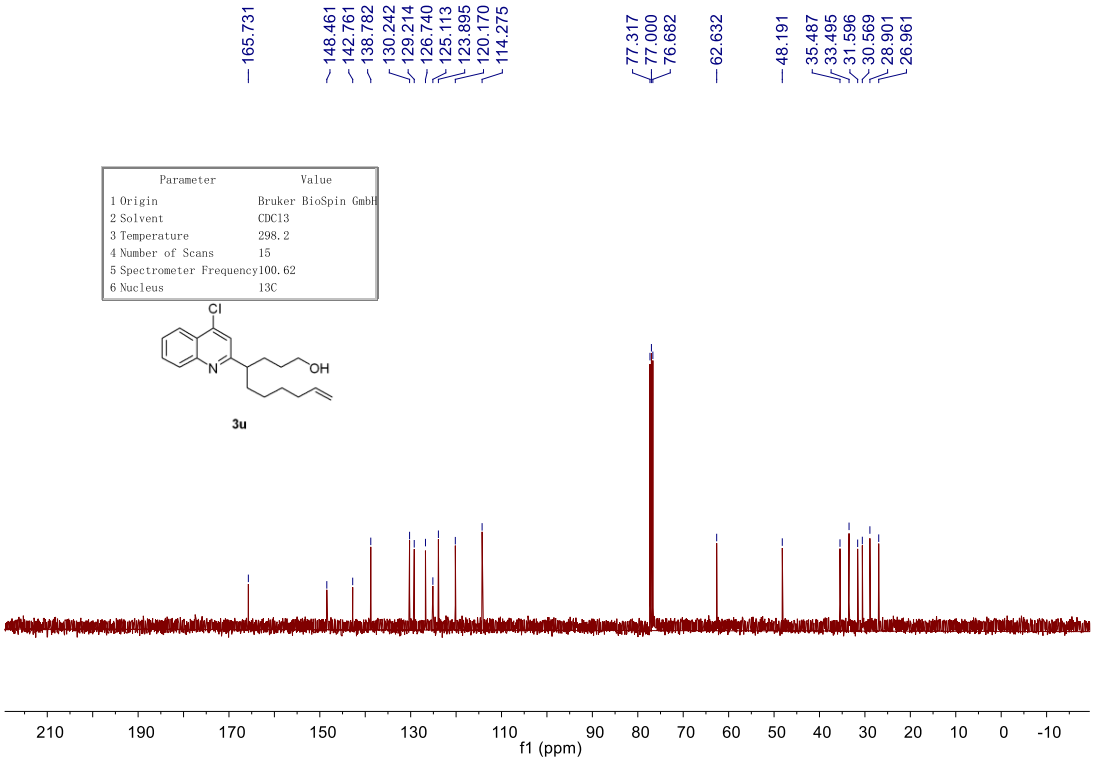
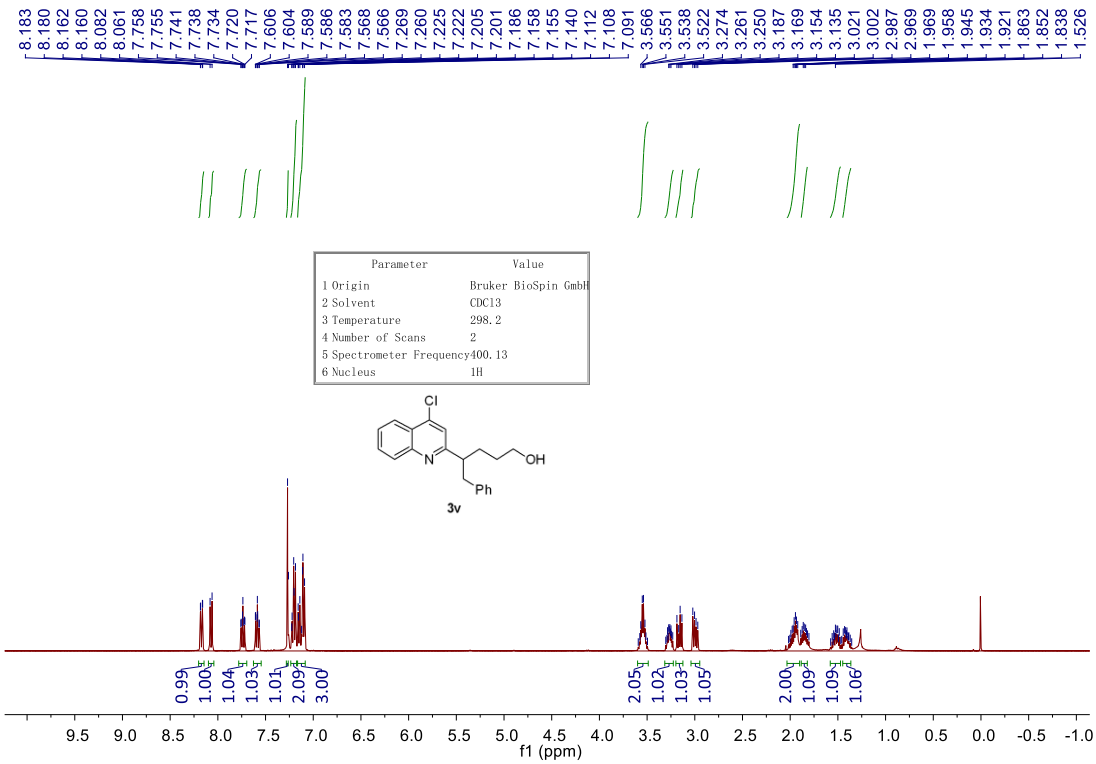
8.186
8.168
8.165
8.060
8.039
7.745
7.742
7.728
7.724
7.707
7.704
7.599
7.596
7.578
7.575
7.560
7.364
7.260
5.739
5.722
4.955
4.951
4.913
4.908
4.892
4.890
4.887
4.867
4.864
3.606
3.597
3.590
3.581
3.565
2.952
1.981
1.963
1.946
1.848
1.829
1.810
1.776
1.755
1.740
1.546
1.528
1.414
1.397
1.391
1.382
1.372
1.356
1.338
1.320
1.308
1.302
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3u
1.03
1.00
1.05
1.04
1.02
0.97
1.96
2.05
1.02
0.98
2.08
4.04
1.07
4.03
1.02
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 -0.5
f1 (ppm)


165.731
148.461
142.761
138.782
130.242
129.214
126.740
125.113
123.895
120.170
114.275
77.317
77.000
76.682
62.632
48.191
35.487
33.495
31.596
30.569
28.901
26.961
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 15
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3u
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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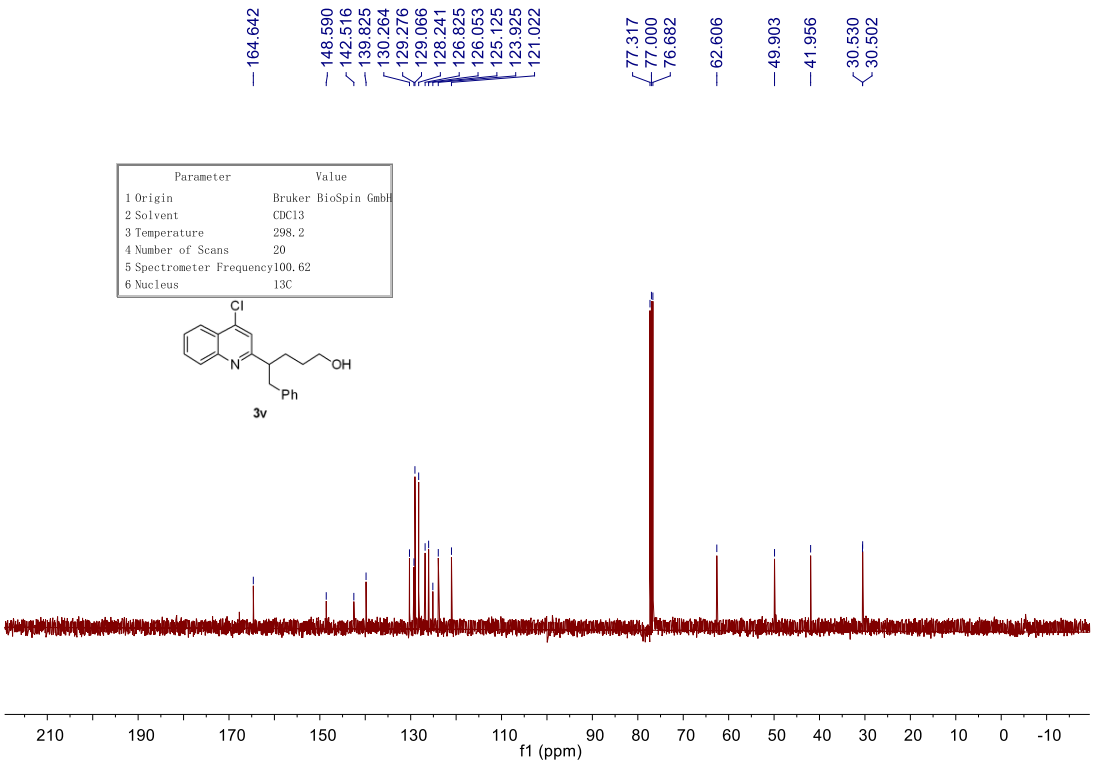
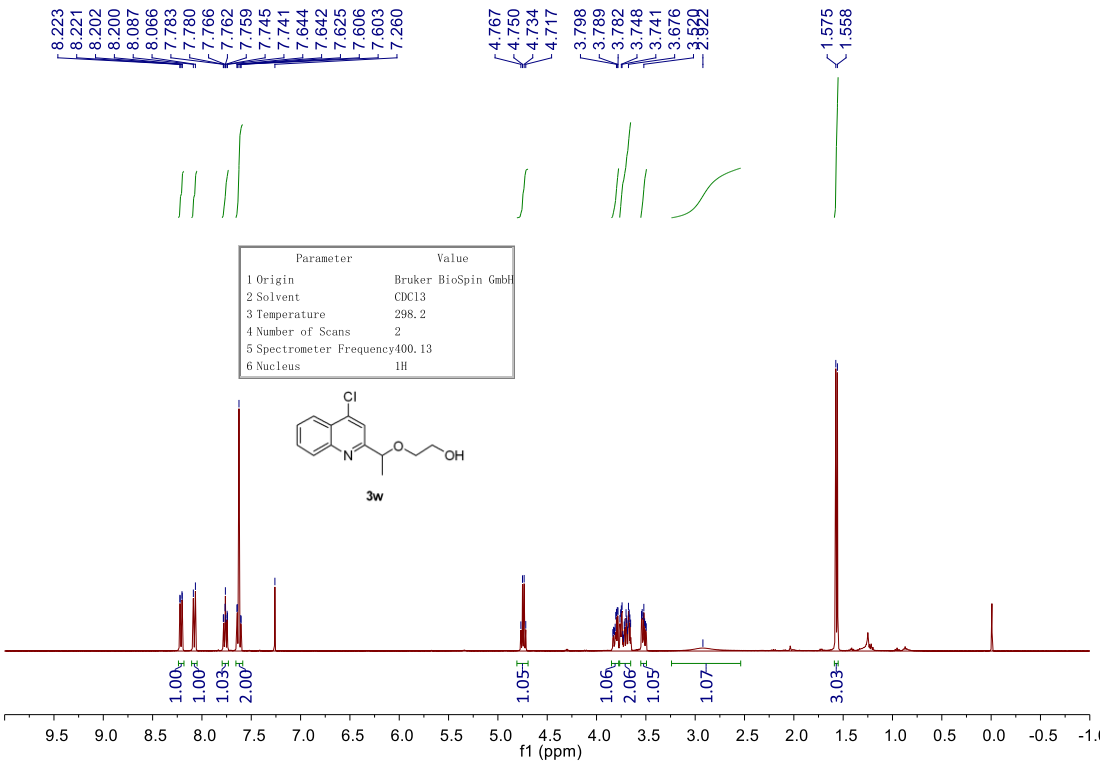
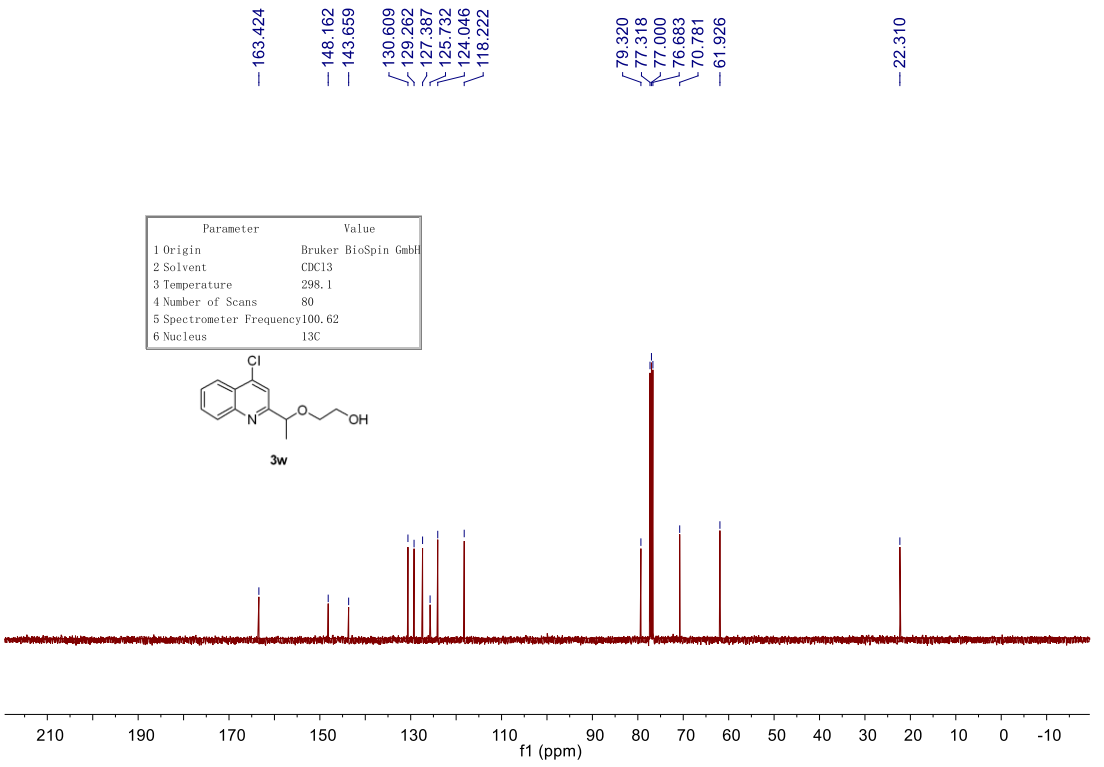
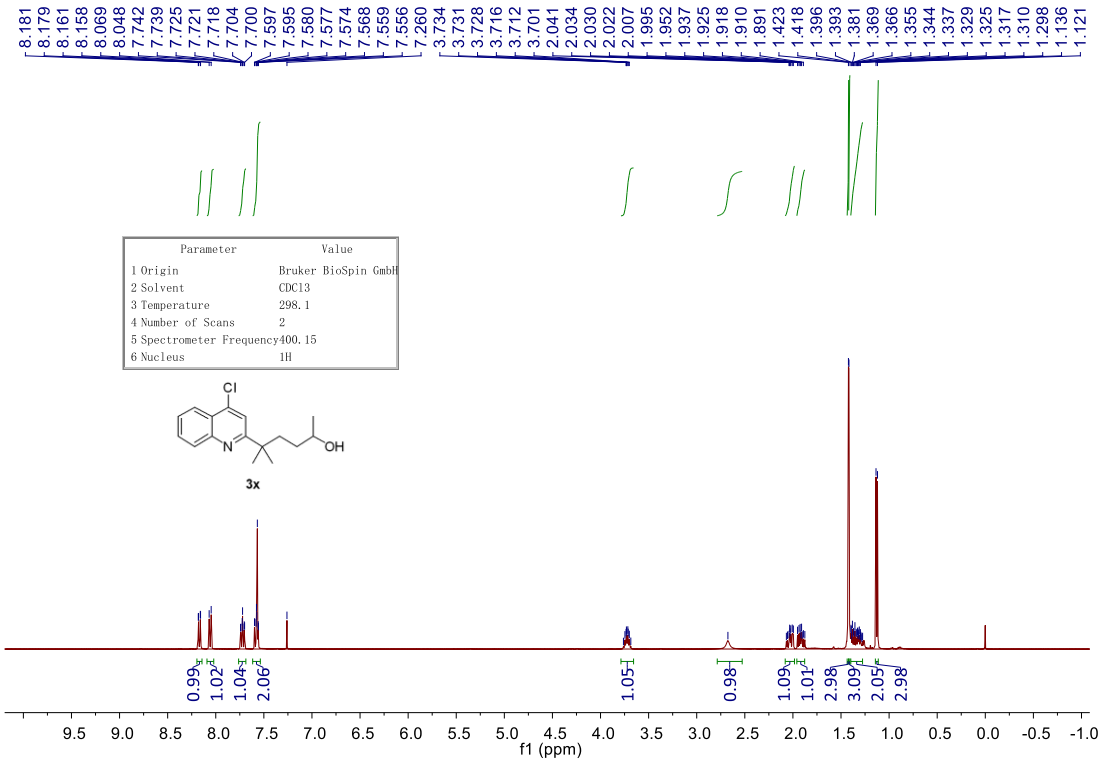
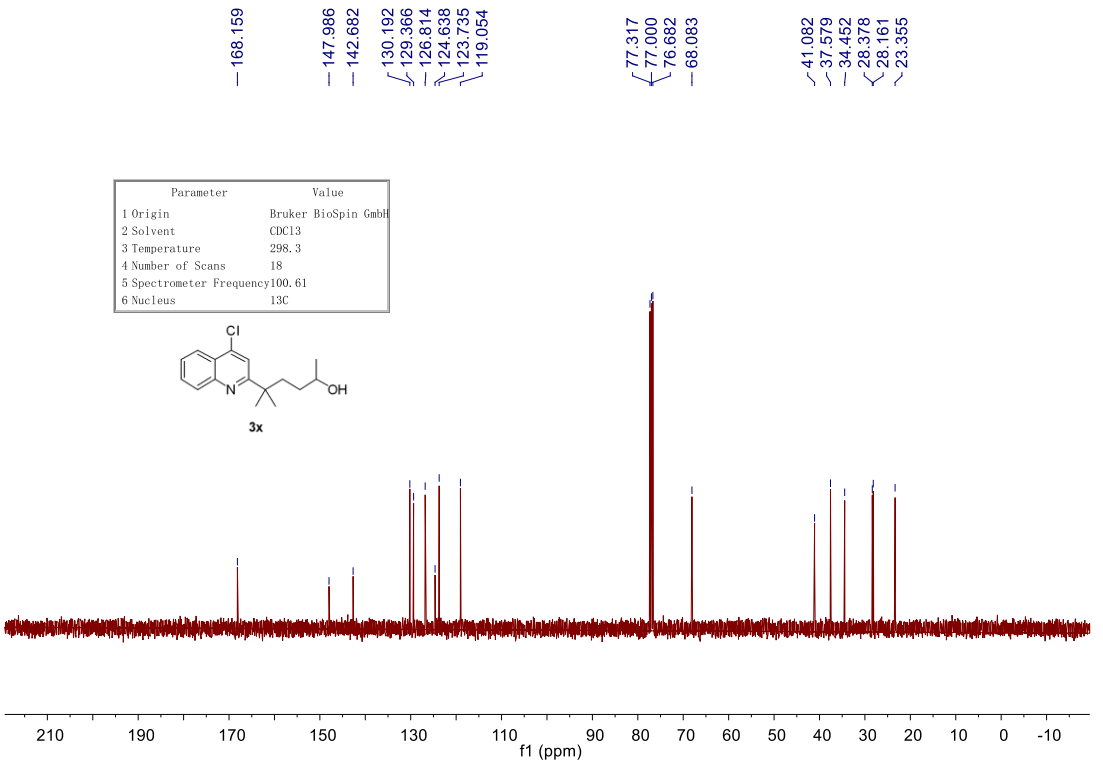
8.180
8.162
8.160
8.082
8.061
7.758
7.755
7.741
7.738
7.734
7.720
7.717
7.606
7.604
7.589
7.586
7.583
7.568
7.566
7.269
7.260
7.225
7.222
7.205
7.201
7.186
7.158
7.155
7.140
7.112
7.108
7.091
3.566
3.551
3.538
3.522
3.274
3.261
3.250
3.187
3.169
3.154
3.135
3.021
3.002
2.987
2.969
1.969
1.958
1.945
1.934
1.921
1.863
1.852
1.838
1.526
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
Ph
3v
0.99
1.00
1.04
1.03
1.01
2.09
3.00
2.05
1.02
1.03
1.05
2.00
1.09
1.09
1.06
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 -0.5 -1.0
f1 (ppm)

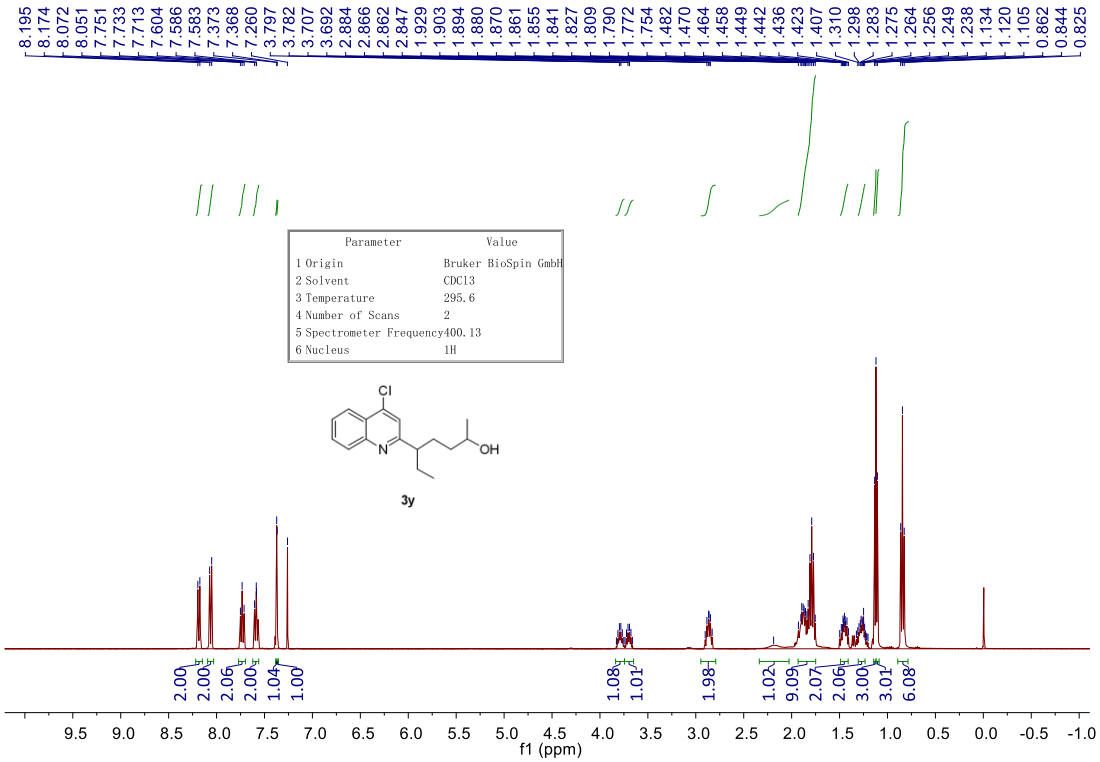

164.642
148.590
142.516
139.825
130.264
129.276
129.066
128.241
126.825
126.053
125.125
123.925
121.022
77.317
77.000
76.682
62.606
49.903
41.956
30.530
30.502
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
Ph
3v
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

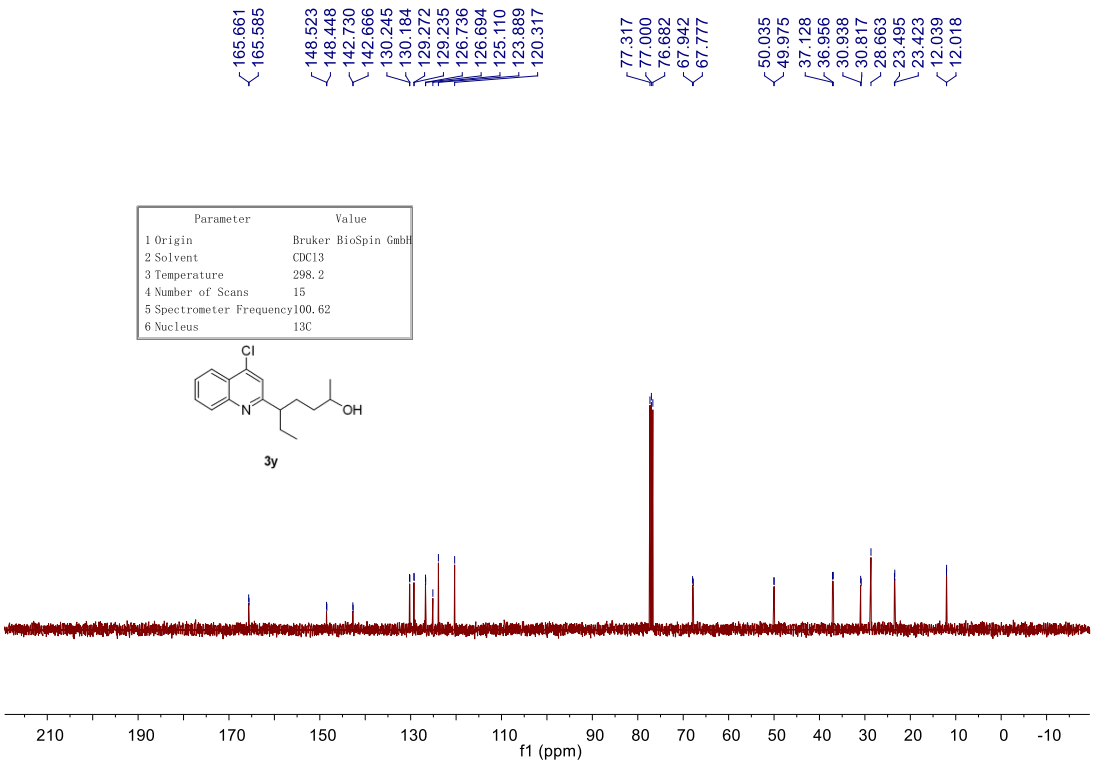

8.223
8.221
8.202
8.200
8.087
8.066
7.783
7.780
7.766
7.762
7.759
7.745
7.741
7.644
7.642
7.625
7.606
7.603
7.260
4.767
4.750
4.734
4.717
3.798
3.789
3.782
3.748
3.741
3.676
3.622
3.622
2.922
1.575
1.558
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
O
OH
3w
1.00
1.00
1.03
2.00
1.05
1.06
2.06
1.05
1.07
3.03
f1 (ppm)

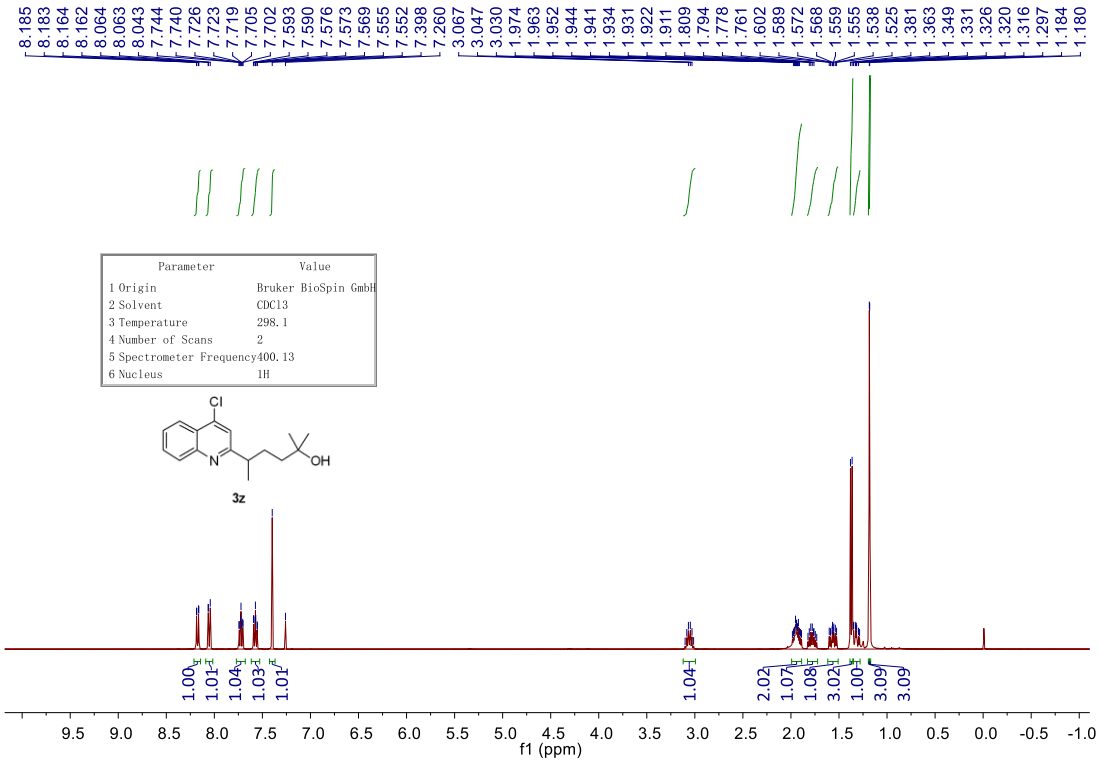

163.424
148.162
143.659
130.609
129.262
127.387
125.732
124.046
118.222
79.320
77.318
77.000
76.683
70.781
61.926
22.310
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
O
OH
3w
f1 (ppm)

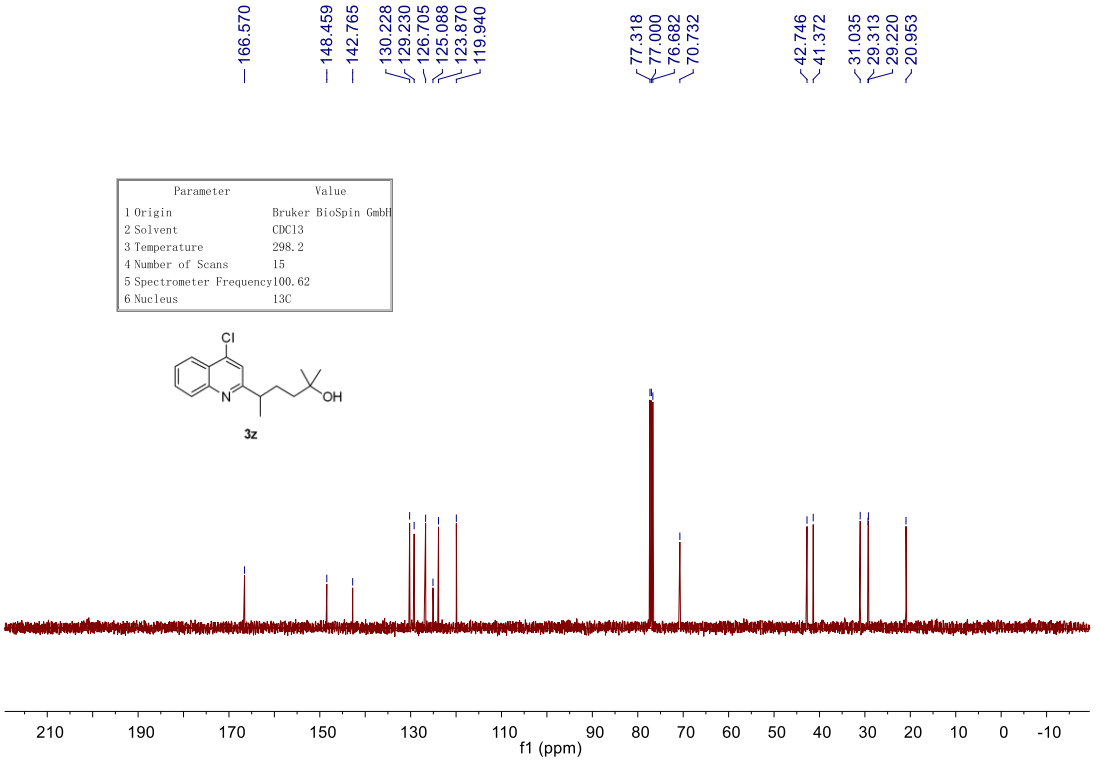

8.181
8.179
8.161
8.158
8.069
8.048
7.742
7.739
7.725
7.721
7.718
7.704
7.700
7.597
7.595
7.580
7.577
7.574
7.568
7.559
7.556
7.260
3.734
3.731
3.728
3.716
3.712
3.701
2.041
2.034
2.030
2.022
2.007
1.995
1.952
1.937
1.925
1.918
1.910
1.891
1.423
1.418
1.396
1.393
1.381
1.369
1.366
1.355
1.344
1.337
1.329
1.325
1.317
1.310
1.298
1.136
1.121
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
OH
3x
0.99
1.02
1.04
2.06
1.05
0.98
1.09
1.01
2.98
3.09
2.05
2.98
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 -0.5 -1.0
f1 (ppm)

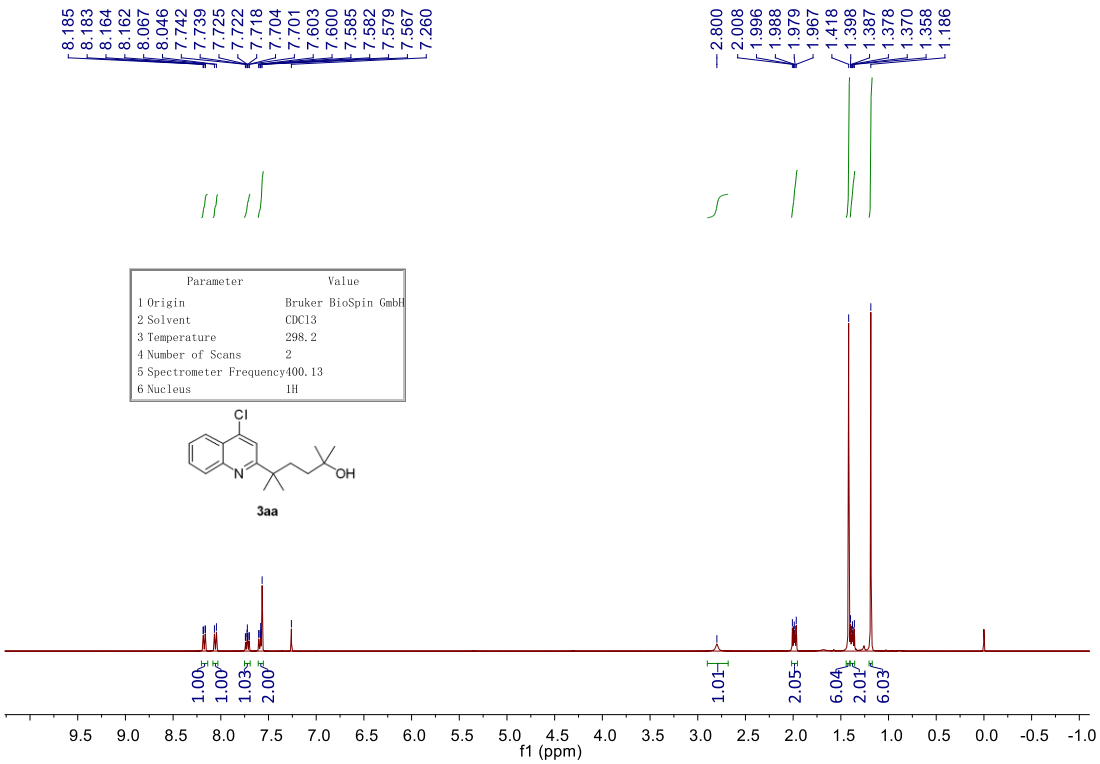

168.159
147.986
142.682
130.192
129.366
126.814
124.638
123.735
119.054
77.317
77.000
76.682
68.083
41.082
37.579
34.452
28.378
28.161
23.355
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 18
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
N
OH
3x
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

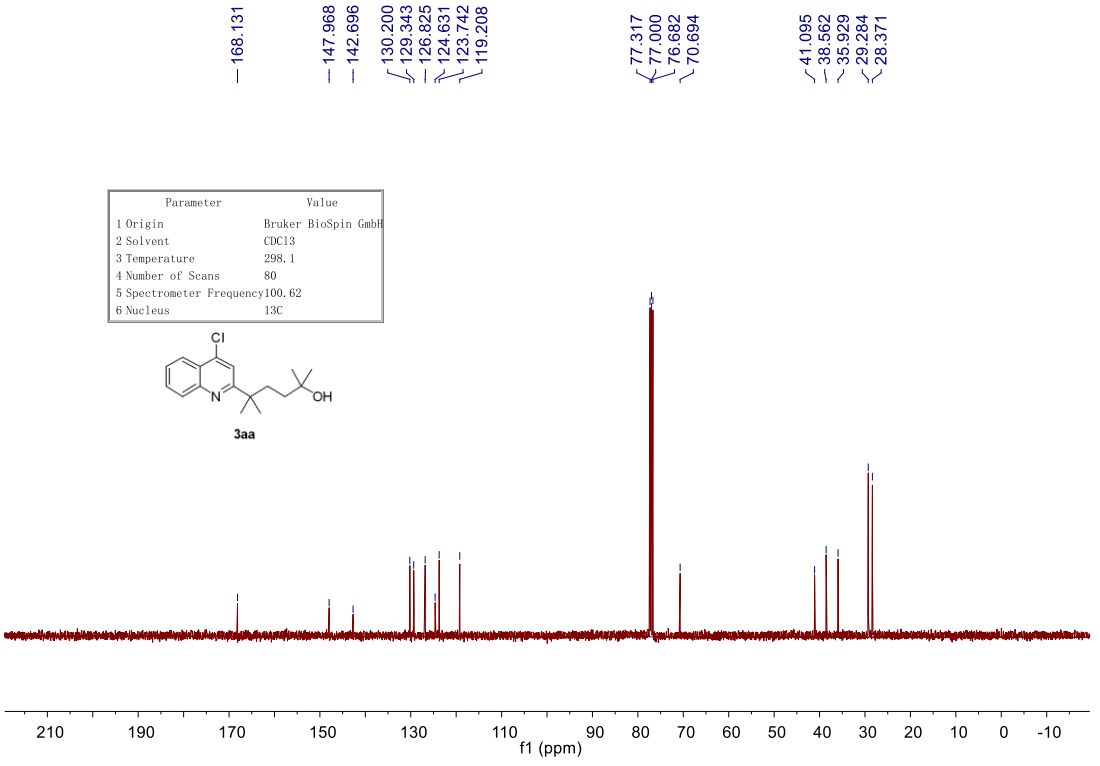

8.195
8.174
8.072
8.051
7.751
7.733
7.713
7.604
7.586
7.583
7.373
7.368
7.260
3.797
3.782
3.707
3.692
2.884
2.866
2.862
2.847
1.929
1.903
1.894
1.880
1.870
1.861
1.855
1.841
1.827
1.809
1.790
1.772
1.754
1.482
1.470
1.464
1.458
1.449
1.442
1.436
1.423
1.407
1.310
1.298
1.283
1.275
1.264
1.256
1.249
1.238
1.134
1.120
1.105
0.862
0.844
0.825
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.6
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3y
2.00
2.00
2.06
2.00
1.04
1.00
1.08
1.01
1.98
1.02
9.09
2.07
2.06
3.00
3.01
6.08
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 -0.5 -1.0
f1 (ppm)

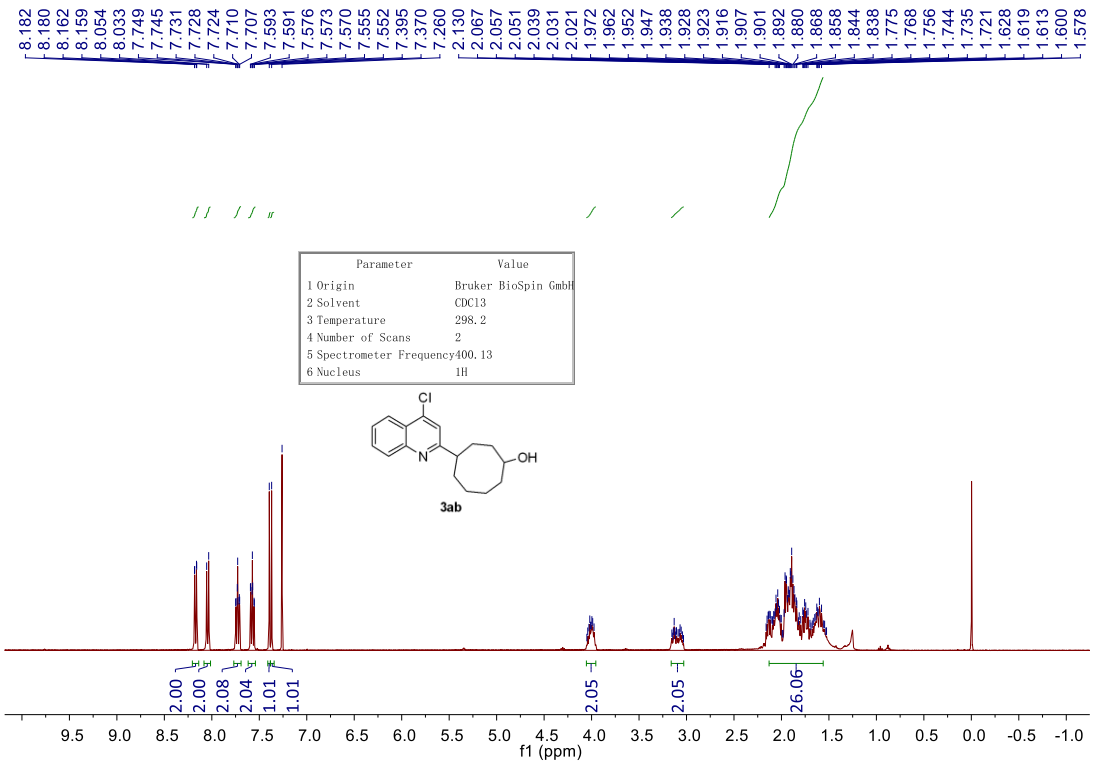

165.661
165.585
148.523
148.448
142.730
142.666
130.245
130.184
129.272
129.235
126.736
126.694
125.110
123.889
120.317
77.317
77.000
76.682
67.942
67.777
50.035
49.975
37.128
36.956
30.938
30.817
28.663
23.495
23.423
12.039
12.018
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 15
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3y
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

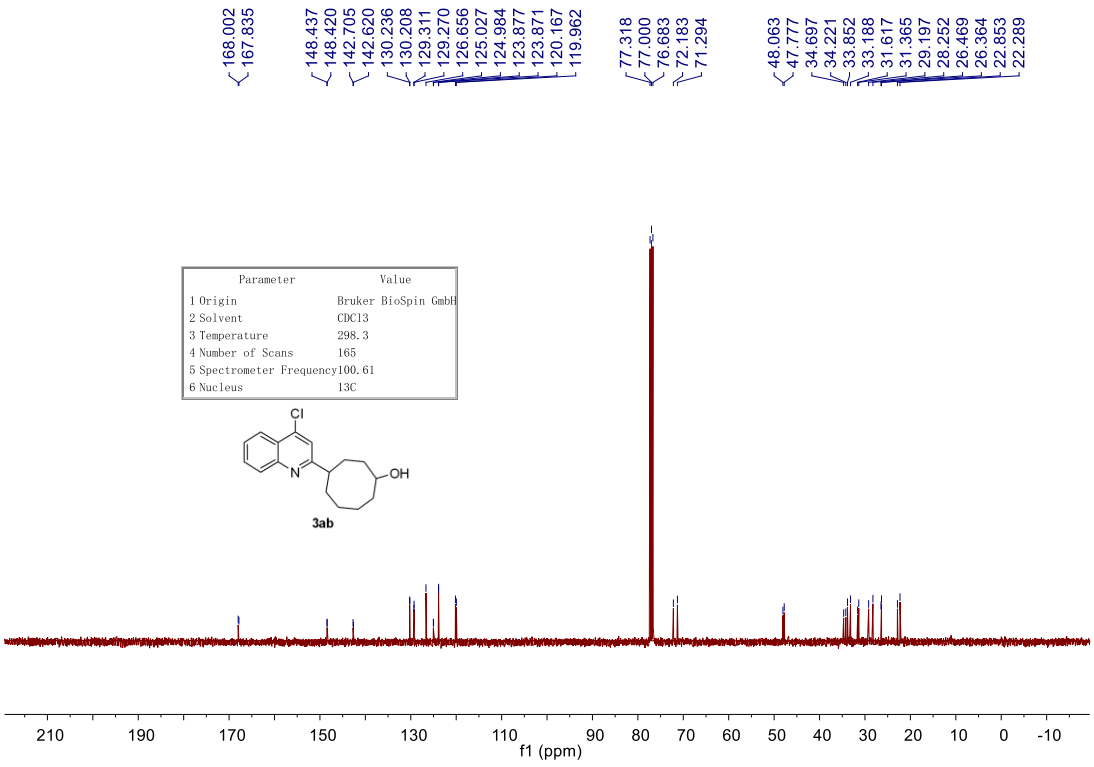

8.185 8.183 8.164 8.162 8.064 8.063 8.043 7.744 7.740 7.726 7.723 7.719 7.705 7.702 7.593 7.590 7.576 7.573 7.569 7.555 7.552 7.398 7.260
3.067 3.047 3.030 1.974 1.963 1.952 1.944 1.941 1.934 1.931 1.922 1.911 1.809 1.794 1.778 1.761 1.602 1.589 1.572 1.568 1.559 1.555 1.538 1.525 1.381 1.363 1.349 1.331 1.326 1.320 1.316 1.297 1.184 1.180
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3z
1.00 1.01 1.04 1.03 1.01 1.04 2.02 1.07 1.08 3.02 1.00 3.09 3.09
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 -0.5 -1.0
f1 (ppm)

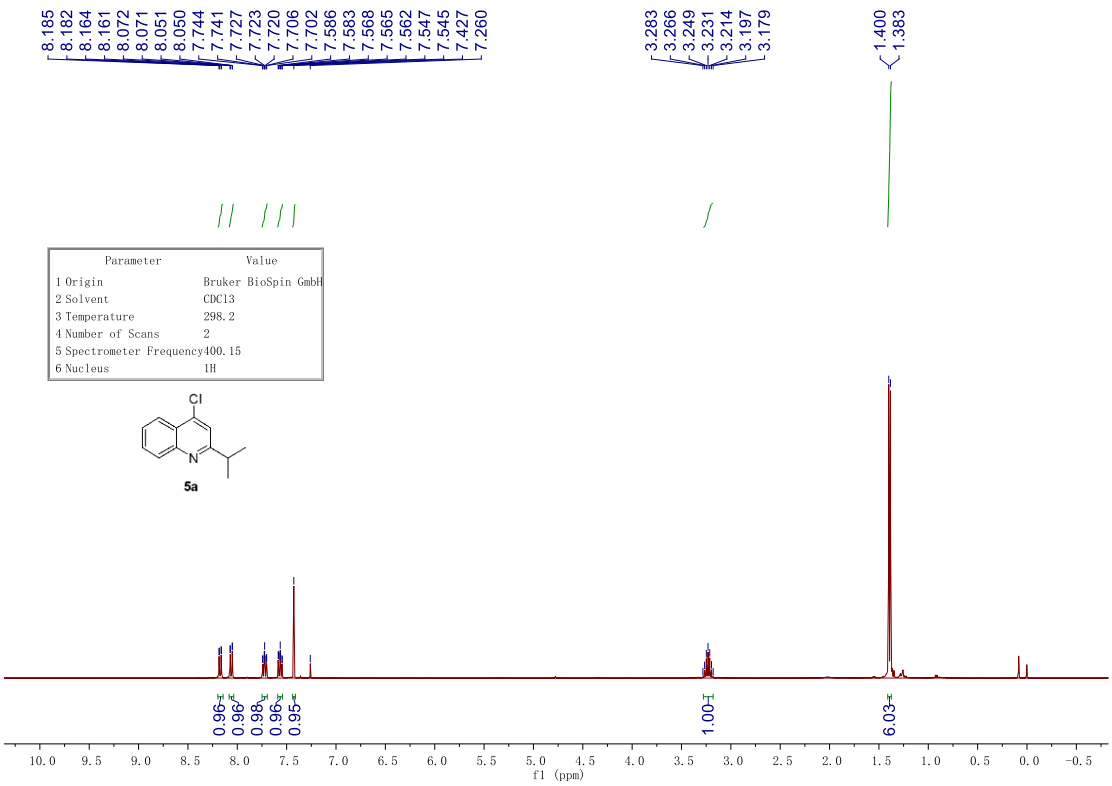

166.570 148.459 142.765 130.228 129.230 126.705 125.088 123.870 119.940
77.318 77.000 76.682 70.732
42.746 41.372 31.035 29.313 29.220 20.953
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 15
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3z
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

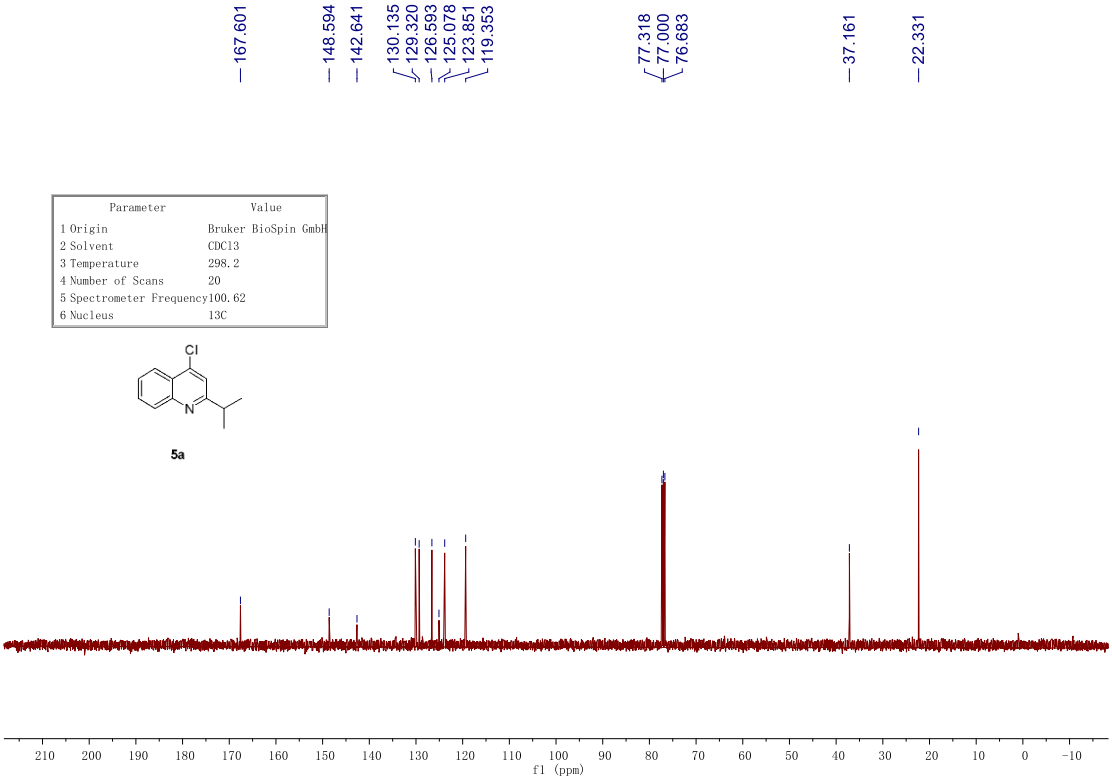

8.185
8.183
8.164
8.162
8.067
8.046
7.742
7.739
7.725
7.722
7.718
7.704
7.701
7.603
7.600
7.585
7.582
7.579
7.567
7.260
2.800
2.008
1.996
1.988
1.979
1.967
1.418
1.398
1.387
1.378
1.370
1.358
1.186
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3aa
1.00
1.00
1.03
2.00
1.01
2.05
6.04
2.01
6.03
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 -0.5 -1.0
f1 (ppm)

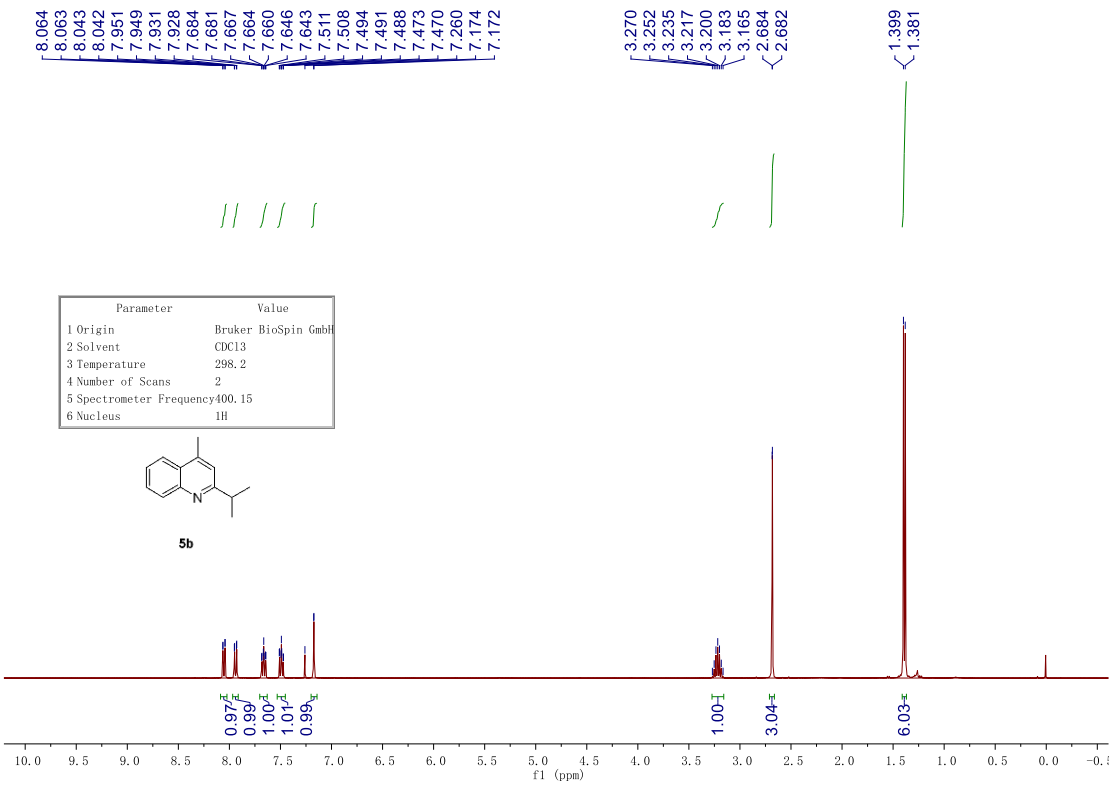

168.131
147.968
142.696
130.200
129.343
126.825
124.631
123.742
119.208
77.317
77.000
76.682
70.694
41.095
38.562
35.929
29.284
28.371
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
OH
3aa
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

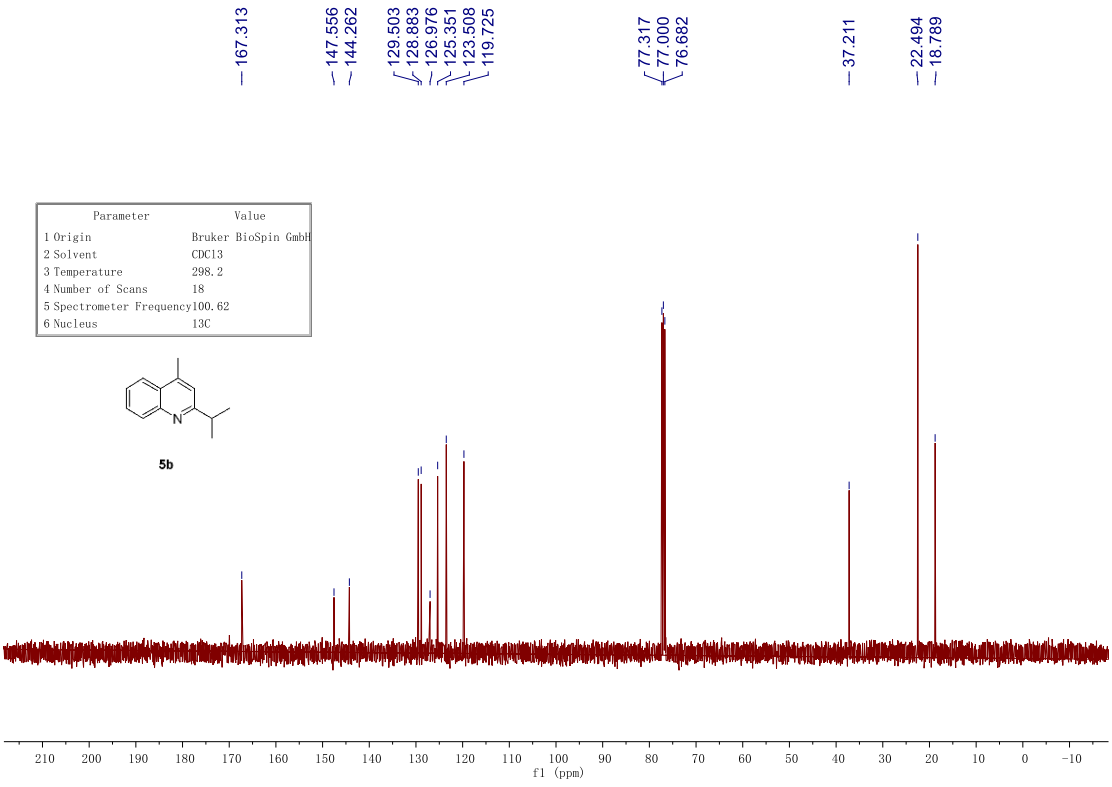

8.182 8.180 8.162 8.159 8.054 8.033 7.749 7.745 7.731 7.728 7.724 7.710 7.707 7.593 7.591 7.576 7.573 7.570 7.555 7.552 7.395 7.370 7.260
2.130 2.067 2.057 2.051 2.039 2.031 2.021 1.972 1.962 1.952 1.947 1.938 1.928 1.923 1.916 1.907 1.901 1.892 1.880 1.868 1.858 1.844 1.838 1.775 1.768 1.756 1.744 1.735 1.721 1.628 1.619 1.613 1.600 1.578
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
OH
3ab
2.00 2.00 2.08 2.04 1.01 1.01 2.05 2.05 26.06
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 -0.5 -1.0
f1 (ppm)

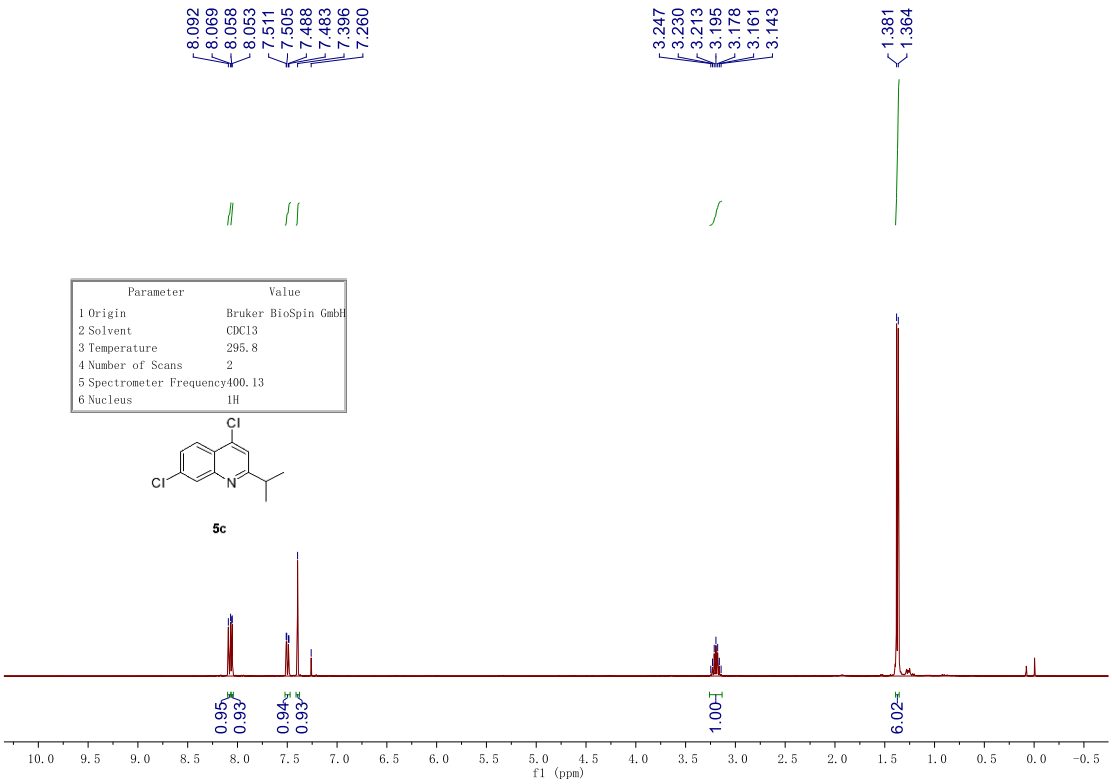

168.002 167.835 148.437 148.420 142.705 142.620 130.236 130.208 129.311 129.270 126.656 125.027 124.984 123.877 123.871 120.167 119.962
77.318 77.000 76.683 72.183 71.294
48.063 47.777 34.697 34.221 33.852 33.188 31.617 31.365 29.197 28.252 26.469 26.364 22.853 22.289
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 165
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
N
OH
3ab
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

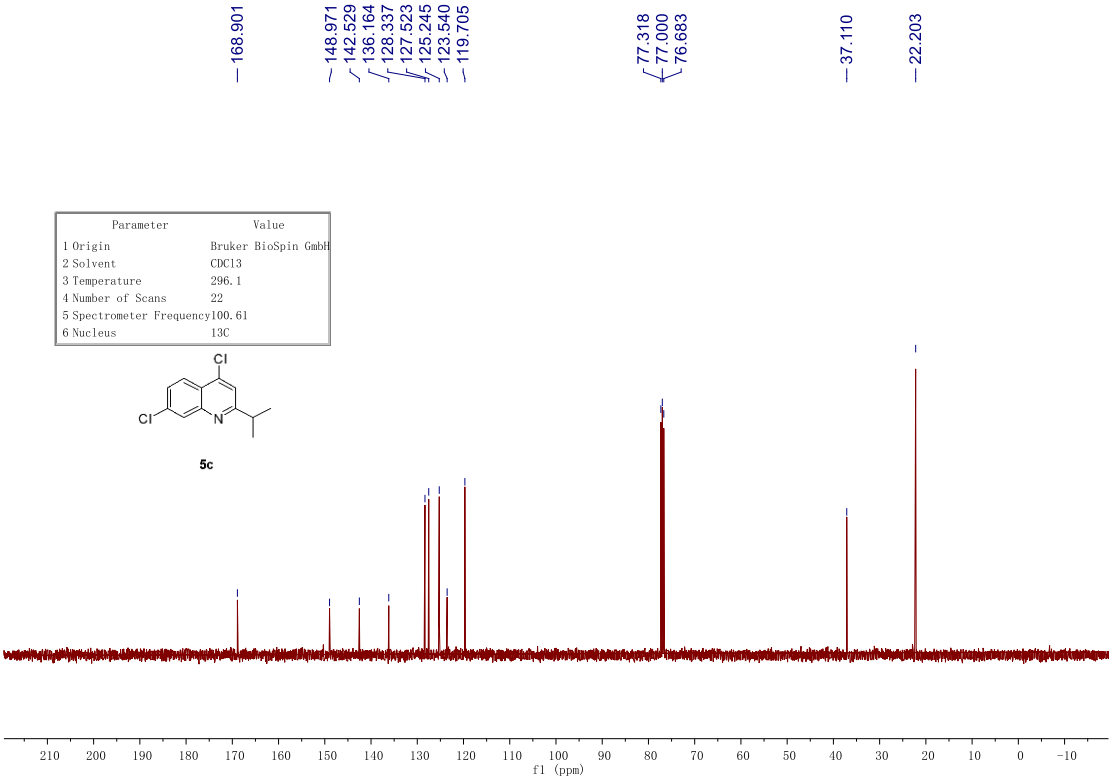

8.185
8.182
8.164
8.161
8.072
8.071
8.051
8.050
7.744
7.741
7.727
7.723
7.720
7.706
7.702
7.586
7.583
7.568
7.565
7.562
7.547
7.545
7.427
7.260
3.283
3.266
3.249
3.231
3.214
3.197
3.179
1.400
1.383
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
5a
0.96
0.96
0.98
0.96
0.95
1.00
6.03
f1 (ppm)

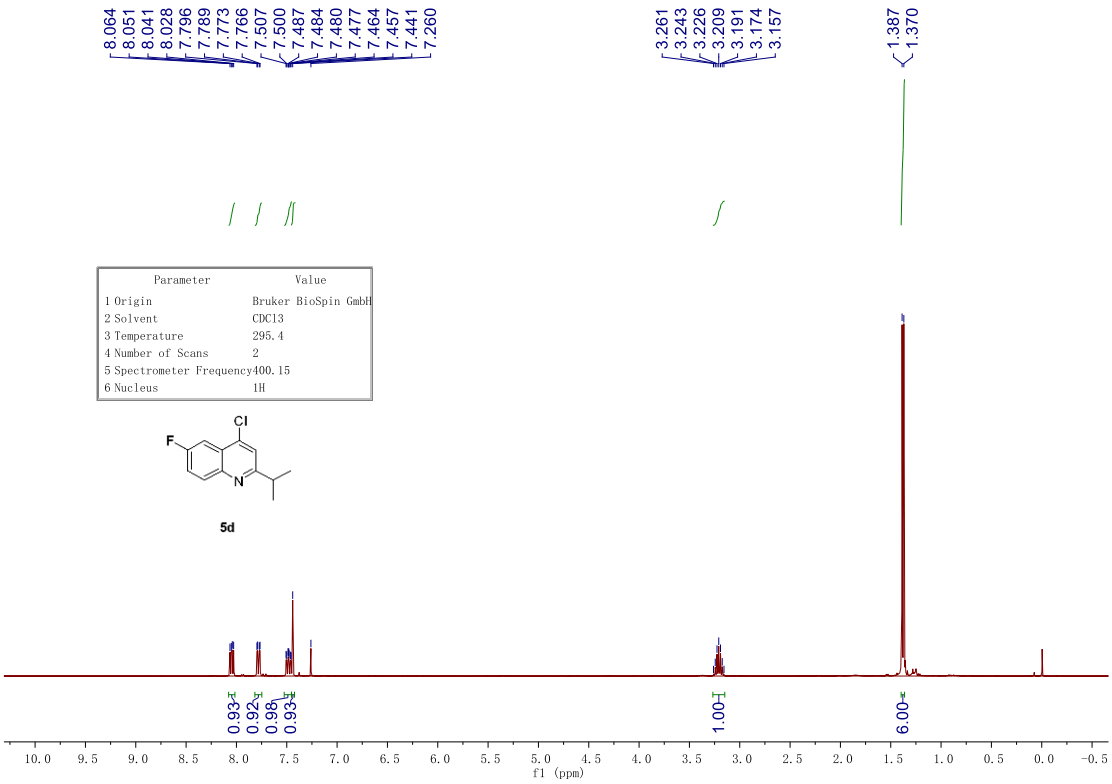

167.601
148.594
142.641
130.135
129.320
126.593
125.078
123.851
119.353
77.318
77.000
76.683
37.161
22.331
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5a
f1 (ppm)

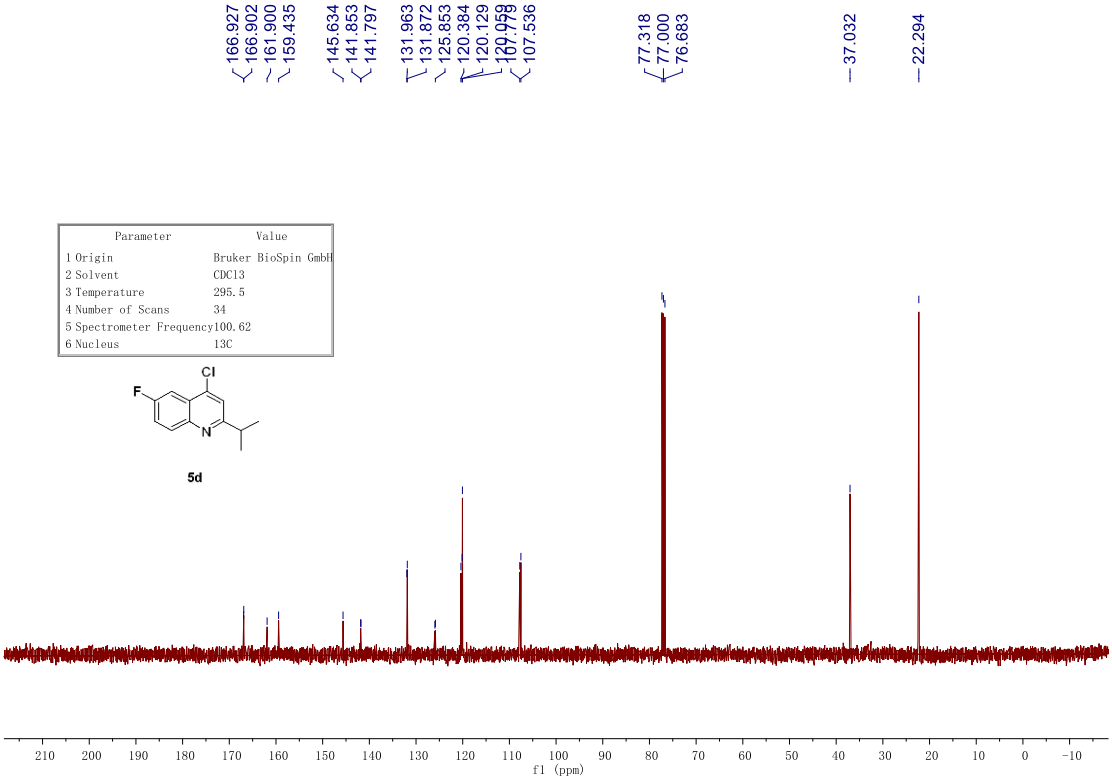

8.064
8.063
8.043
8.042
7.951
7.949
7.931
7.928
7.684
7.681
7.667
7.664
7.660
7.646
7.643
7.511
7.508
7.494
7.491
7.488
7.473
7.470
7.260
7.174
7.172
3.270
3.252
3.235
3.217
3.200
3.183
3.165
2.684
2.682
1.399
1.381
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
5b
0.97
0.99
1.00
1.01
0.99
1.00
3.04
6.03
f1 (ppm)

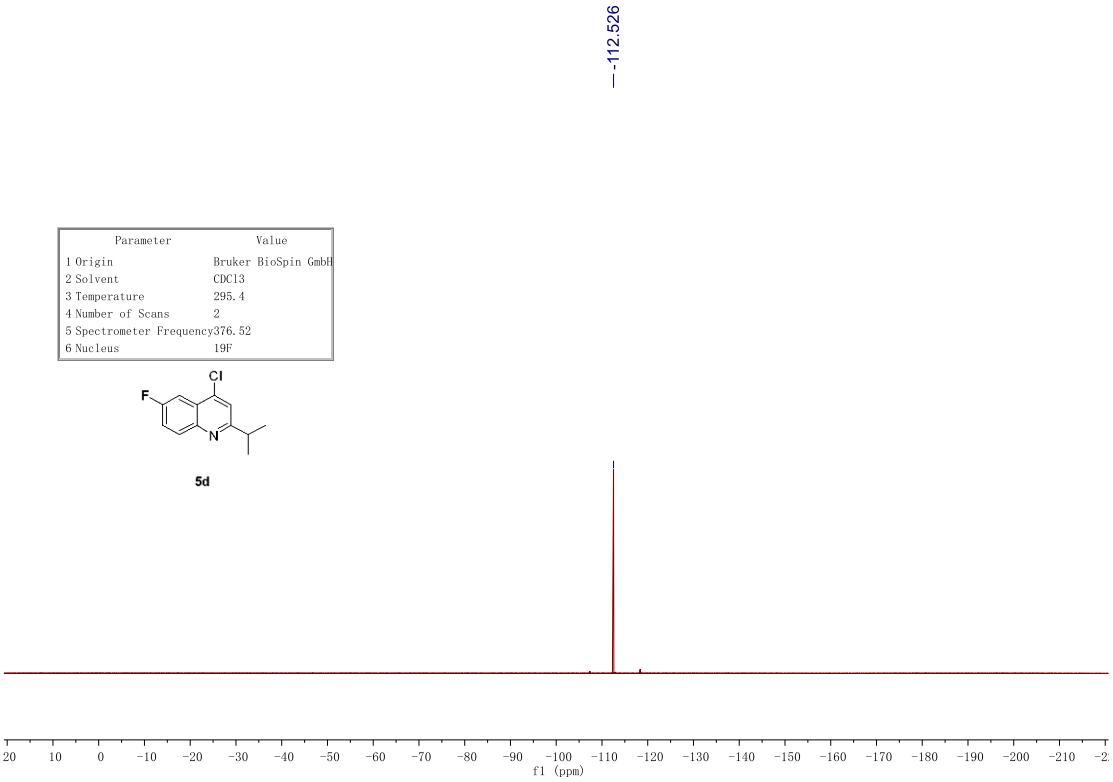

167.313
147.556
144.262
129.503
128.883
126.976
125.351
123.508
119.725
77.317
77.000
76.682
37.211
22.494
18.789
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 18
5 Spectrometer Frequency 100.62
6 Nucleus 13C
5b
f1 (ppm)

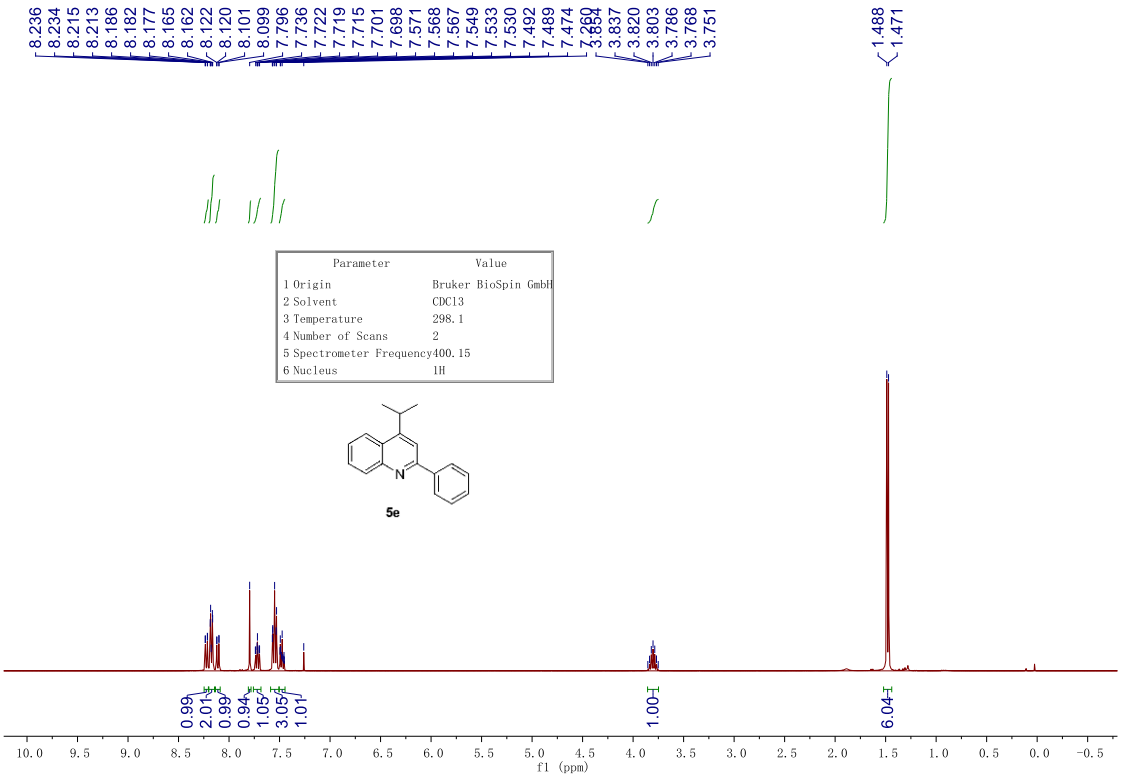

8.092
8.069
8.058
8.053
7.511
7.505
7.488
7.483
7.396
7.260
3.247
3.230
3.213
3.195
3.178
3.161
3.143
1.381
1.364
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.8
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
Cl
N
5c
0.95
0.93
0.94
0.93
1.00
6.02
f1 (ppm)

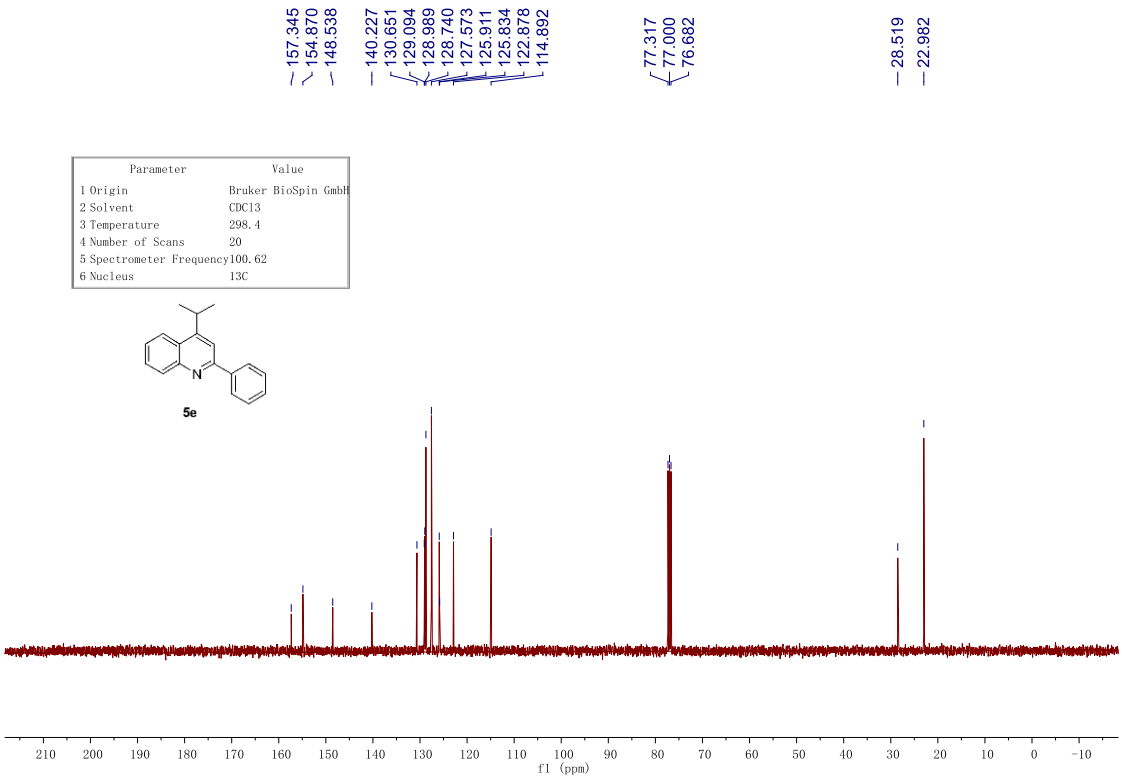

168.901
148.971
142.529
136.164
128.337
127.523
125.245
123.540
119.705
77.318
77.000
76.683
37.110
22.203
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.1
4 Number of Scans 22
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
Cl
N
5c
f1 (ppm)

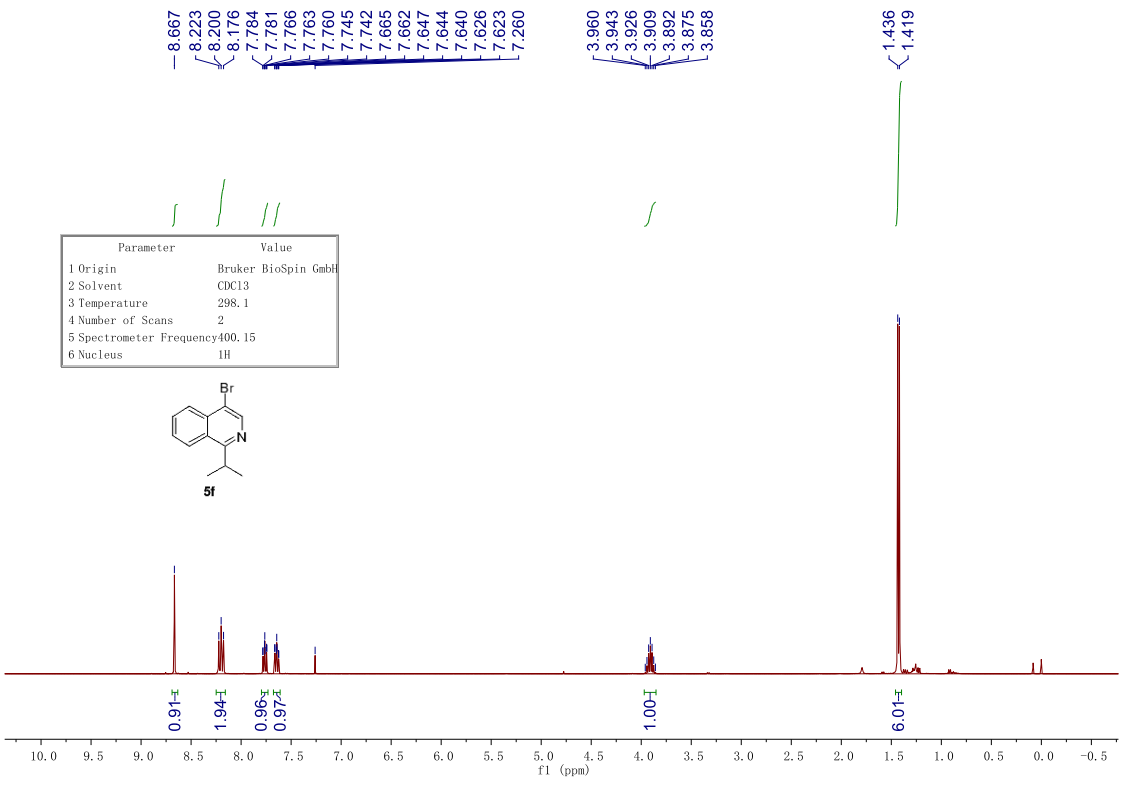

8.064
8.051
8.041
8.028
7.796
7.789
7.773
7.766
7.507
7.500
7.487
7.484
7.480
7.477
7.464
7.457
7.441
7.260
3.261
3.243
3.226
3.209
3.191
3.174
3.157
1.387
1.370
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.4
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
F
N
5d
0.93
0.92
0.98
0.93
1.00
6.00
f1 (ppm)

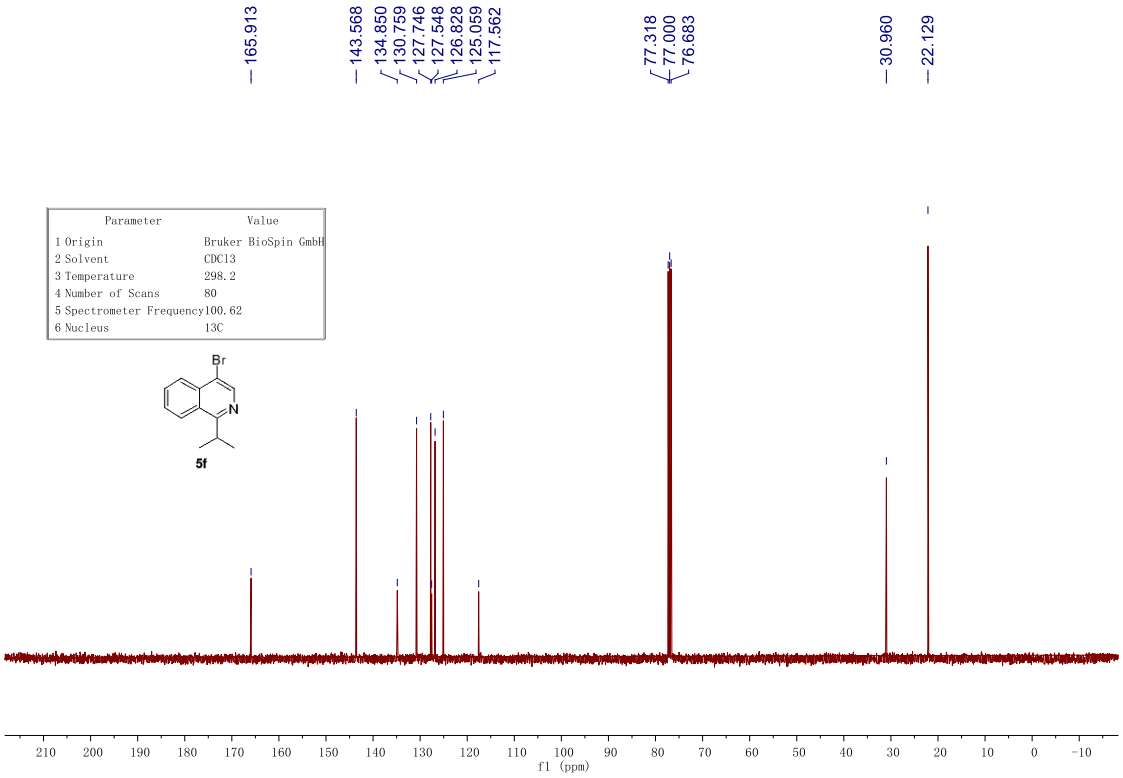

166.927
166.902
161.900
159.435
145.634
141.853
141.797
131.963
131.872
125.853
120.384
120.129
120.059
107.779
107.536
77.318
77.000
76.683
37.032
22.294
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.5
4 Number of Scans 34
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
F
N
5d
f1 (ppm)

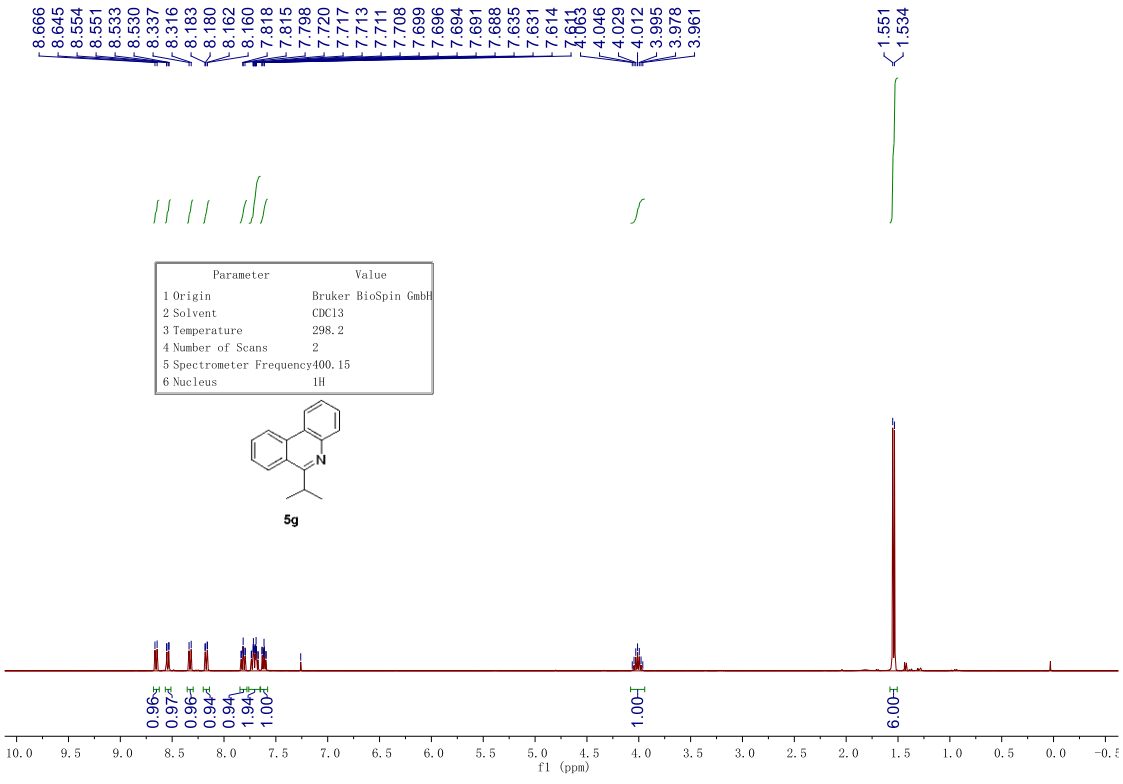

-112.526
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.4
4 Number of Scans 2
5 Spectrometer Frequency376.52
6 Nucleus 19F
Cl
F
N
5d
f1 (ppm)


8.236
8.234
8.215
8.213
8.186
8.182
8.177
8.165
8.162
8.122
8.120
8.101
8.099
7.796
7.736
7.722
7.719
7.715
7.701
7.698
7.571
7.568
7.567
7.549
7.533
7.530
7.492
7.489
7.474
7.260
3.854
3.837
3.820
3.803
3.786
3.768
3.751
1.488
1.471
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency400.15
6 Nucleus 1H
N
5e
0.99
2.01
0.99
0.94
1.05
3.05
1.01
1.00
6.04
f1 (ppm)


157.345
154.870
148.538
140.227
130.651
129.094
128.989
128.740
127.573
125.911
125.834
122.878
114.892
77.317
77.000
76.682
28.519
22.982
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N
5e
f1 (ppm)


8.667
8.223
8.200
8.176
7.784
7.781
7.766
7.763
7.760
7.745
7.742
7.665
7.662
7.647
7.644
7.640
7.626
7.623
7.260
3.960
3.943
3.926
3.909
3.892
3.875
3.858
1.436
1.419
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Br
N
5f
0.91
1.94
0.96
0.97
1.00
6.01
f1 (ppm)


165.913
143.568
134.850
130.759
127.746
127.548
126.828
125.059
117.562
77.318
77.000
76.683
30.960
22.129
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency100.62
6 Nucleus 13C
Br
N
5f
f1 (ppm)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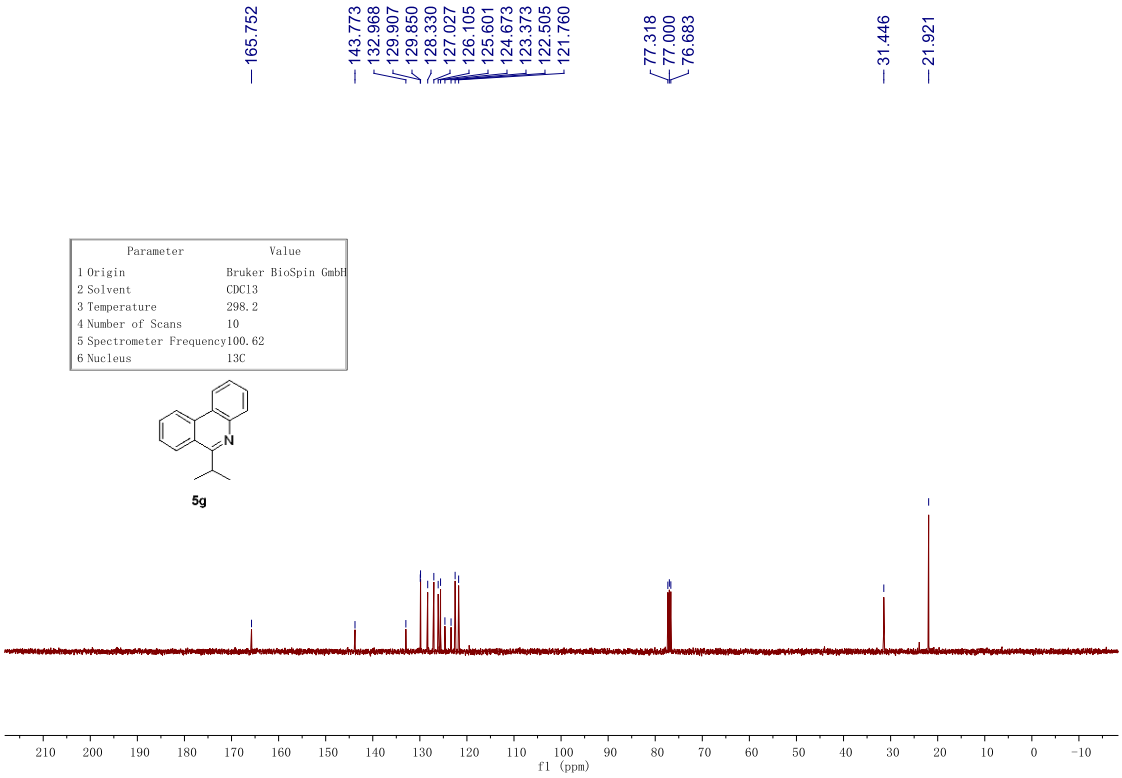
8.645
8.554
8.551
8.533
8.530
8.337
8.316
8.183
8.180
8.162
8.160
7.818
7.815
7.798
7.720
7.717
7.713
7.711
7.708
7.699
7.696
7.694
7.691
7.688
7.635
7.631
7.614
7.611
4.063
4.046
4.029
4.012
3.995
3.978
3.961
1.551
1.534
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency400.15
6 Nucleus 1H
N
5g
0.96
0.97
0.96
0.94
0.94
1.94
1.00
1.00
6.00
f1 (ppm)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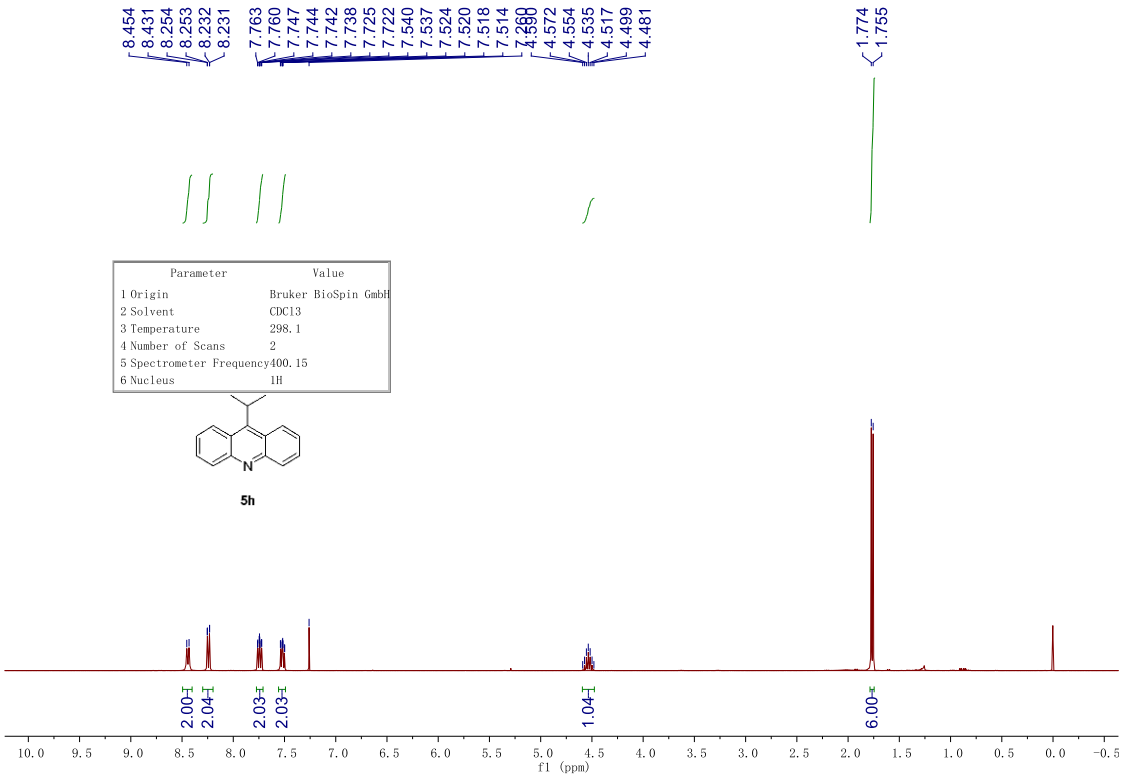
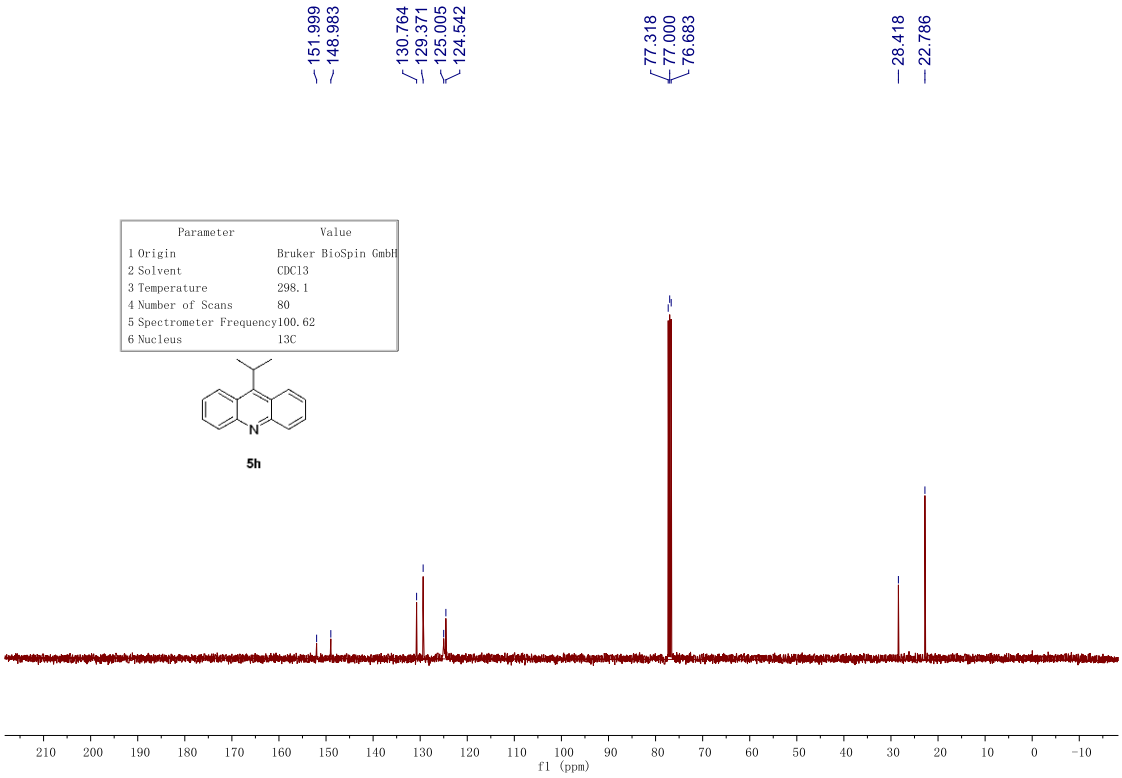
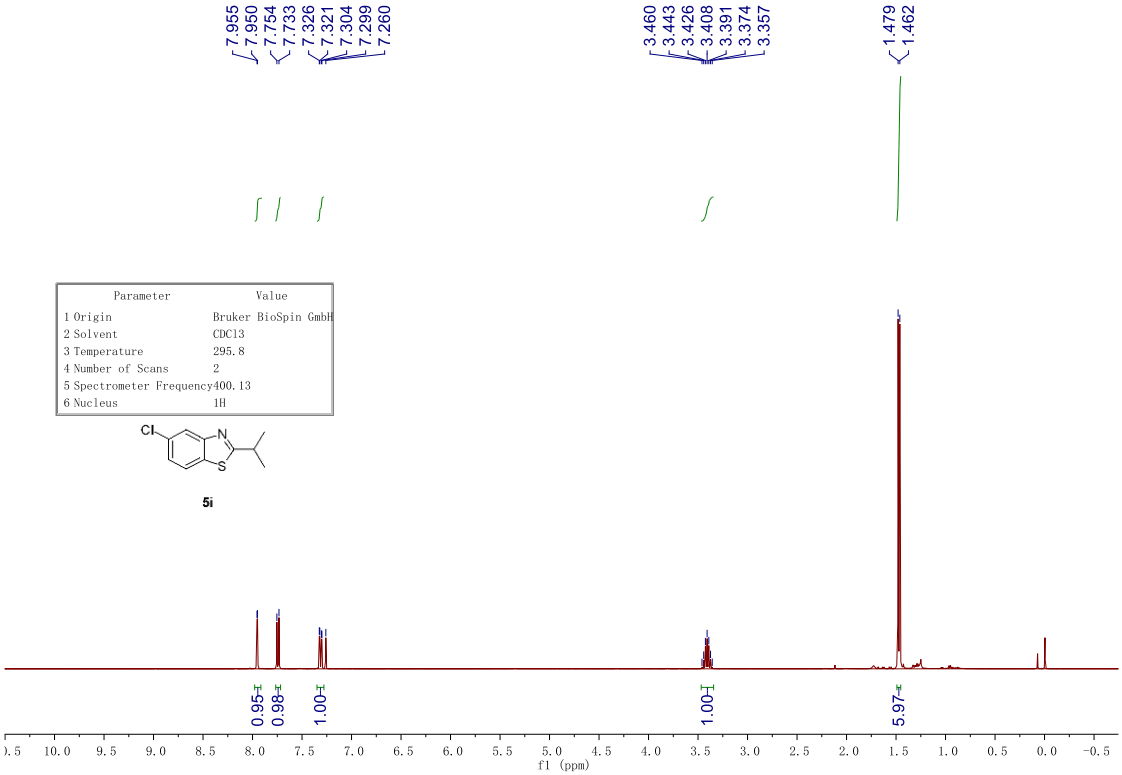
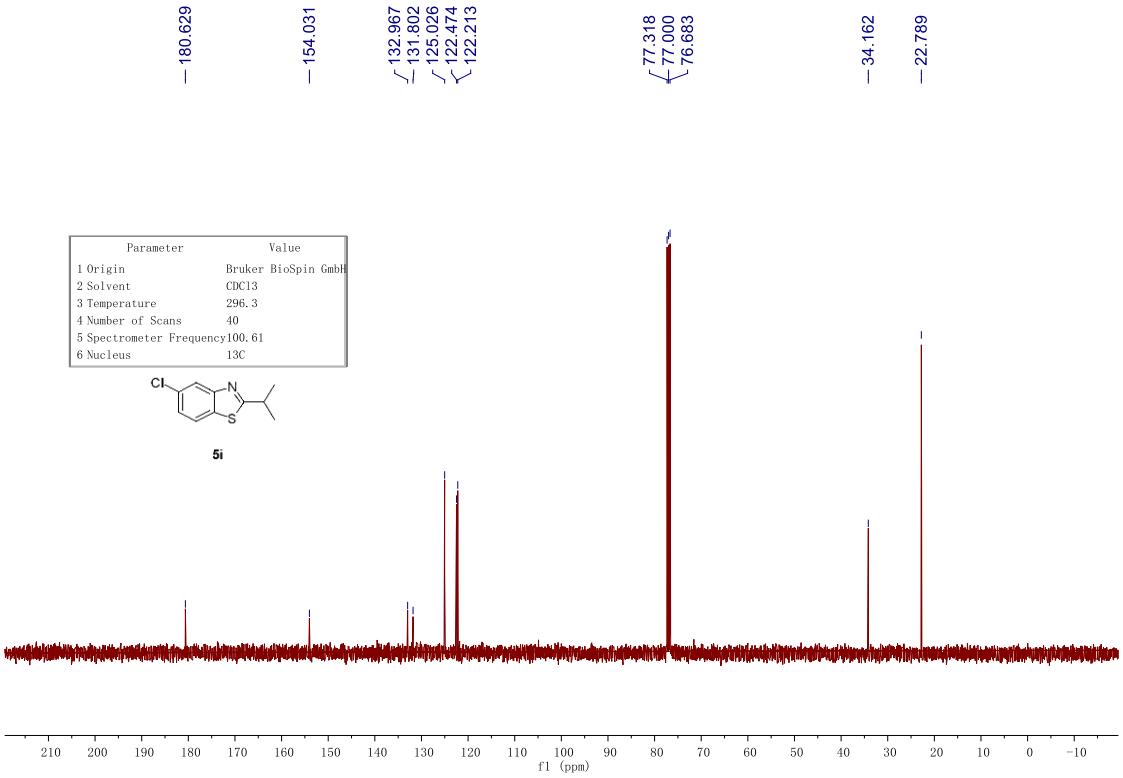
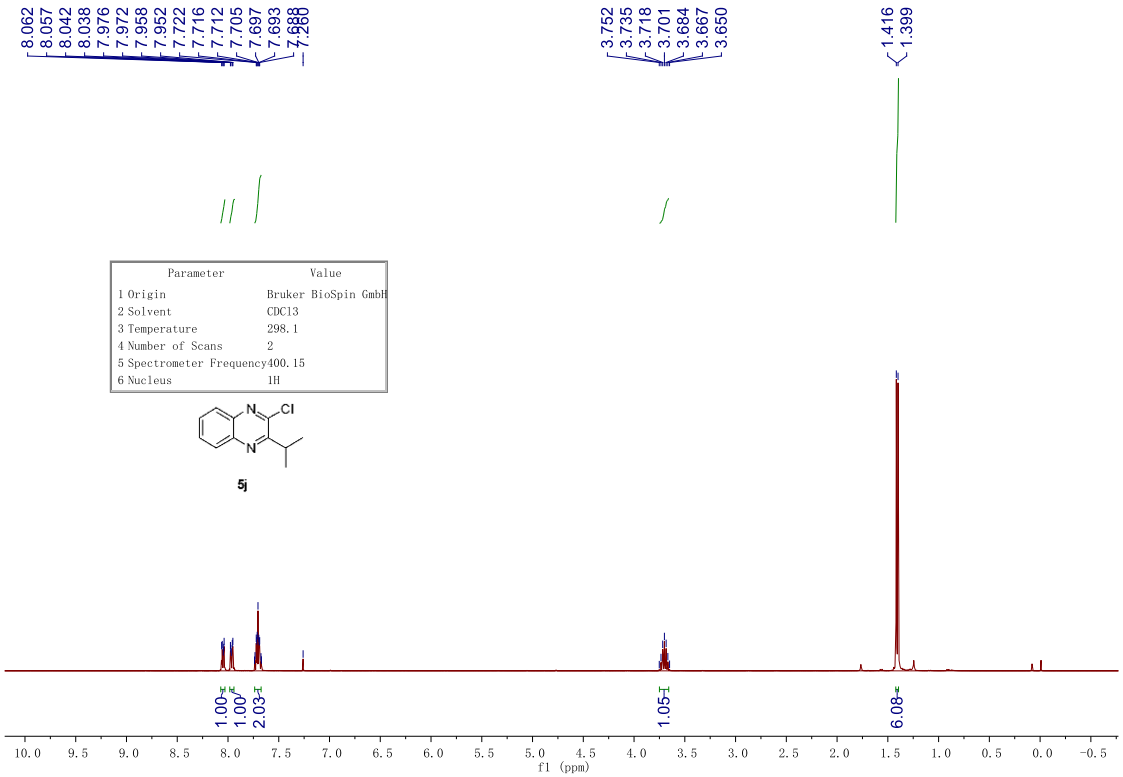
143.773
132.968
129.907
129.850
128.330
127.027
126.105
125.601
124.673
123.373
122.505
121.760
77.318
77.000
76.683
31.446
21.921
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N
5g
f1 (ppm)

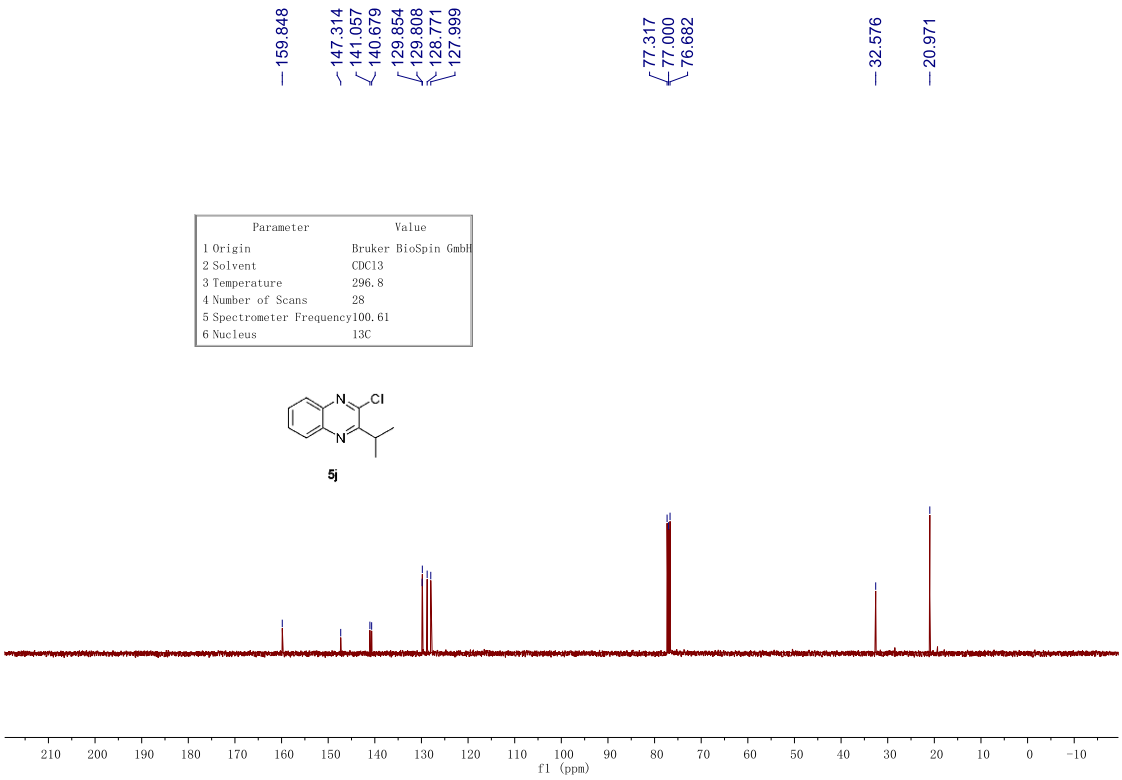

8.454
8.431
8.254
8.253
8.232
8.231
7.763
7.760
7.747
7.744
7.742
7.738
7.725
7.722
7.540
7.537
7.524
7.520
7.518
7.514
4.572
4.554
4.535
4.517
4.499
4.481
1.774
1.755
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
N
5h
2.00
2.04
2.03
2.03
1.04
6.00
f1 (ppm)

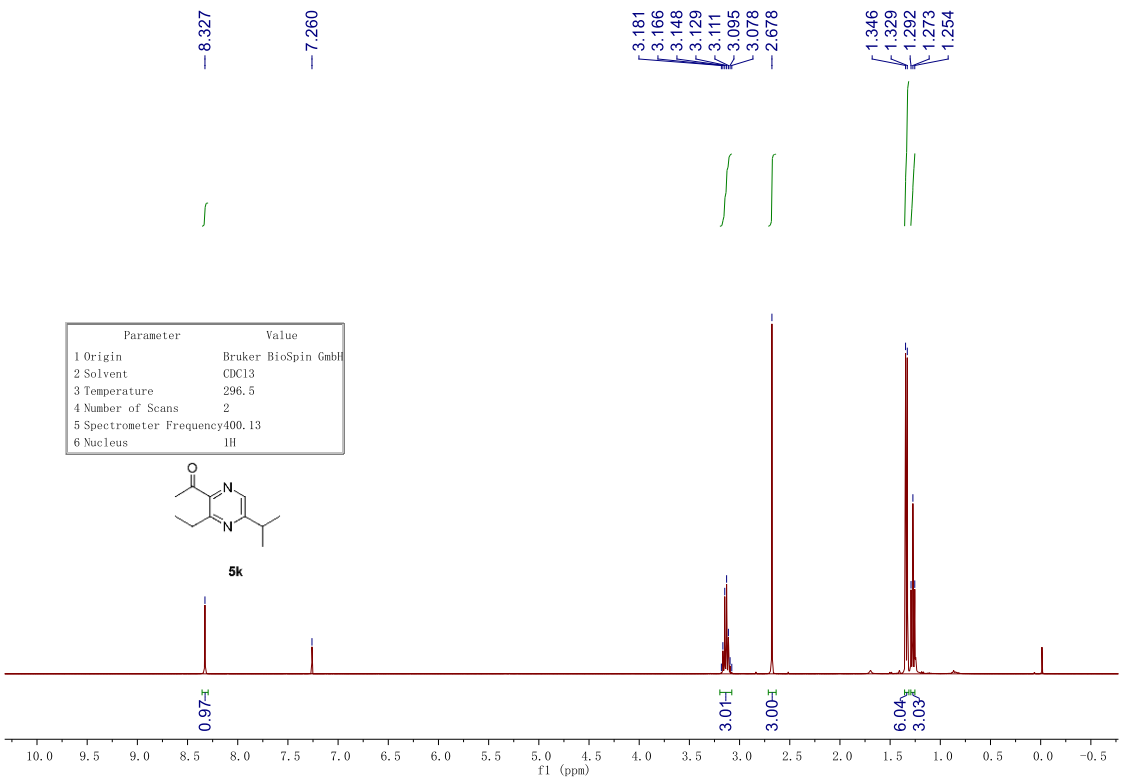

151.999
148.983
130.764
129.371
125.005
124.542
77.318
77.000
76.683
28.418
22.786
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N
5h
f1 (ppm)

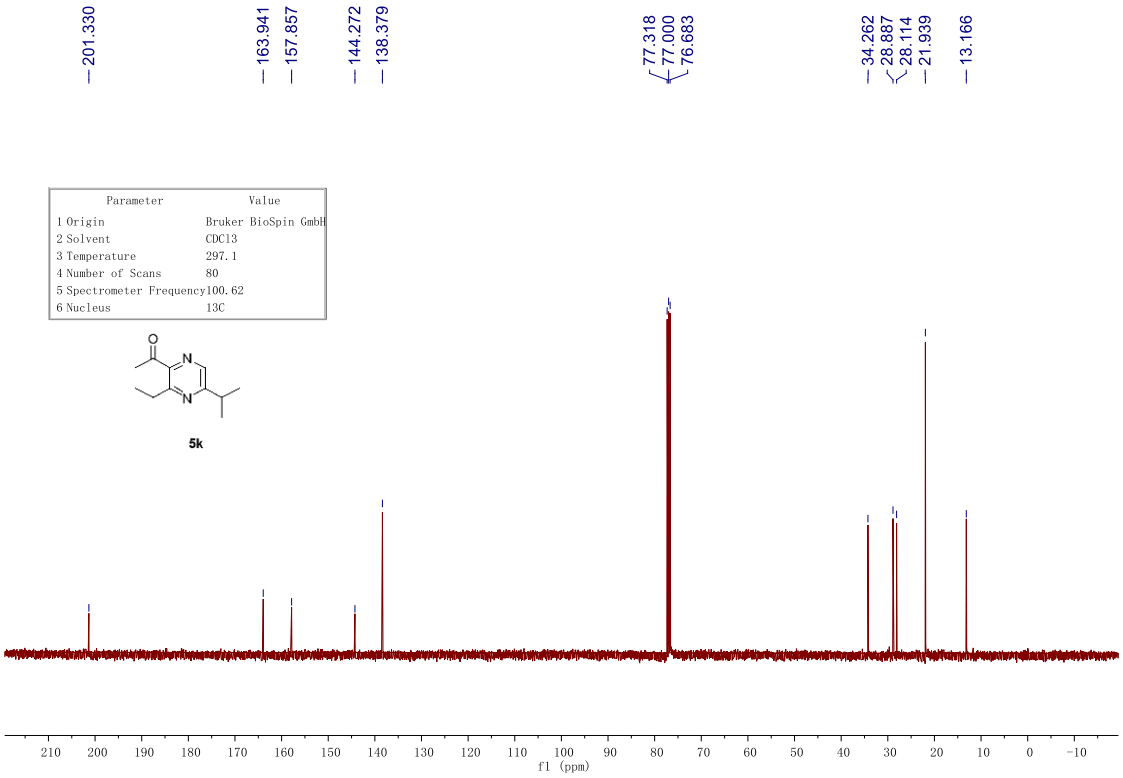

7.955
7.950
7.754
7.733
7.326
7.321
7.304
7.299
7.260
3.460
3.443
3.426
3.408
3.391
3.374
3.357
1.479
1.462
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.8
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
S
5i
0.95
0.98
1.00
1.00
5.97
f1 (ppm)


180.629
154.031
132.967
131.802
125.026
122.474
122.213
77.318
77.000
76.683
34.162
22.789
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.3
4 Number of Scans 40
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
N
S
5i
f1 (ppm)


8.062
8.057
8.042
8.038
7.976
7.972
7.958
7.952
7.722
7.716
7.712
7.705
7.697
7.693
7.688
7.680
3.752
3.735
3.718
3.701
3.684
3.667
3.650
1.416
1.399
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
N
Cl
N
5j
1.00
1.00
2.03
1.05
6.08
f1 (ppm)


159.848
147.314
141.057
140.679
129.854
129.808
128.771
127.999
77.317
77.000
76.682
32.576
20.971
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.8
4 Number of Scans 28
5 Spectrometer Frequency 100.61
6 Nucleus 13C
N
N
Cl
5j
f1 (ppm)


8.327
7.260
3.181
3.166
3.148
3.129
3.111
3.095
3.078
2.678
1.346
1.329
1.292
1.273
1.254
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.5
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N
N
5k
0.97
3.01
3.00
6.04
3.03
f1 (ppm)


201.330
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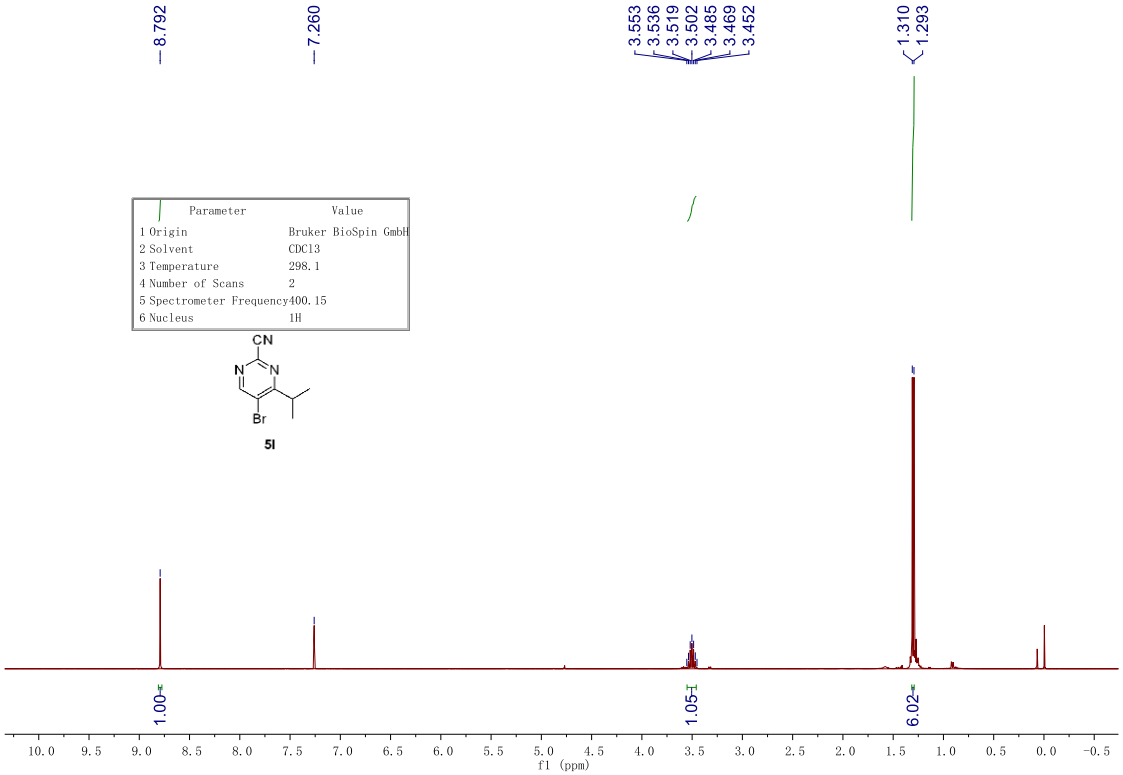
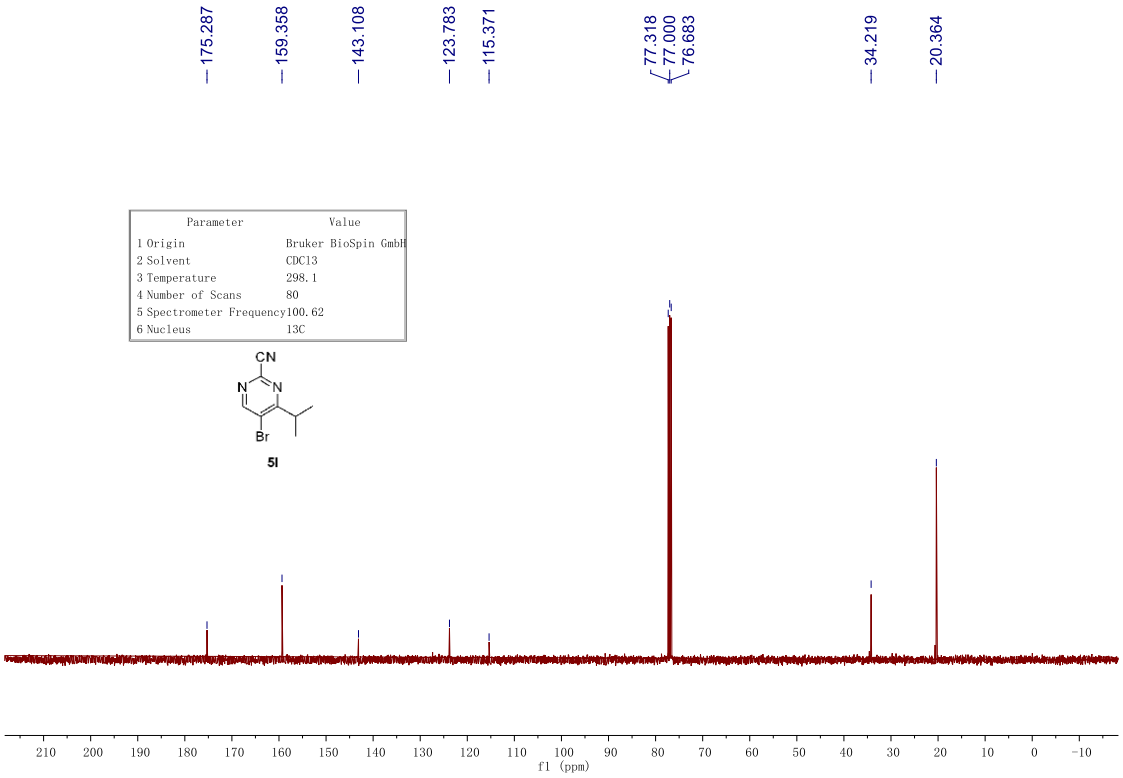
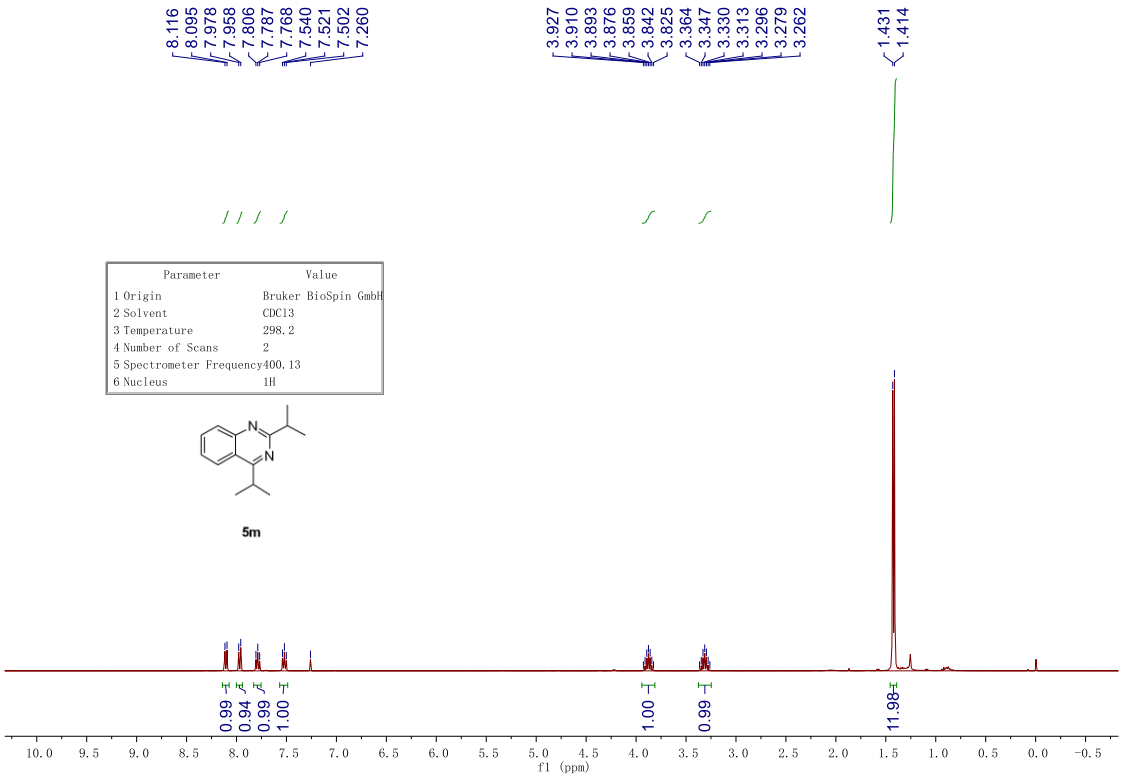
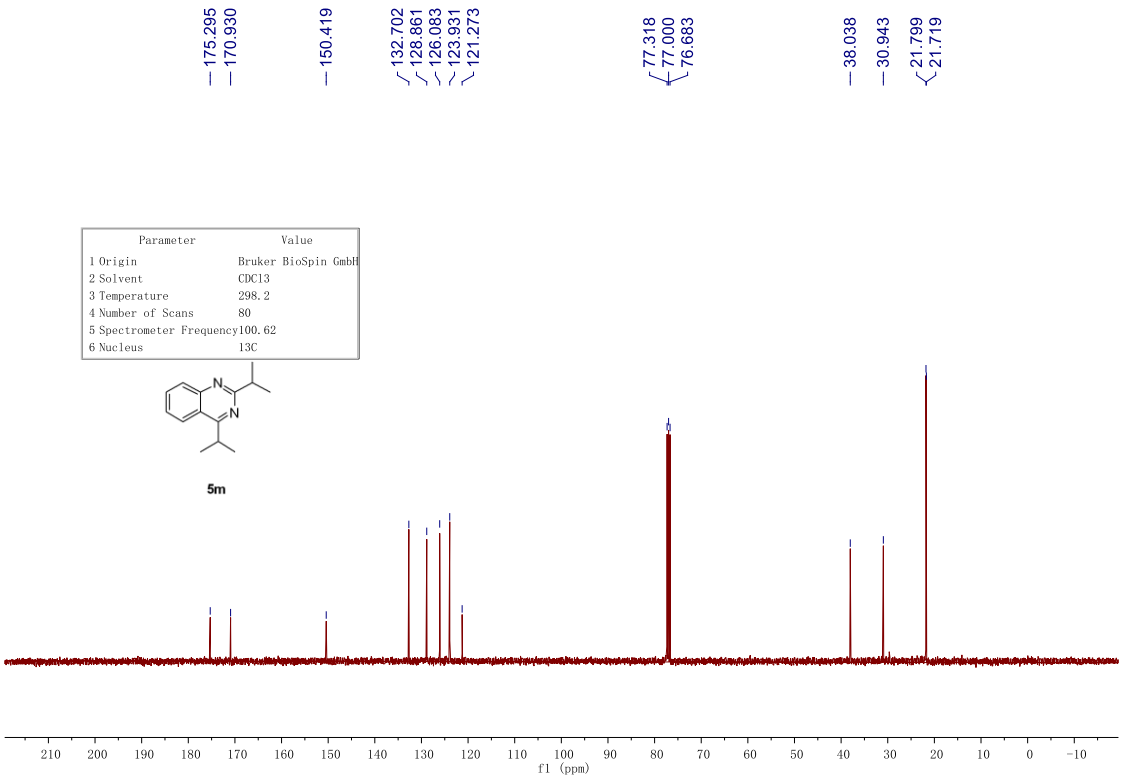
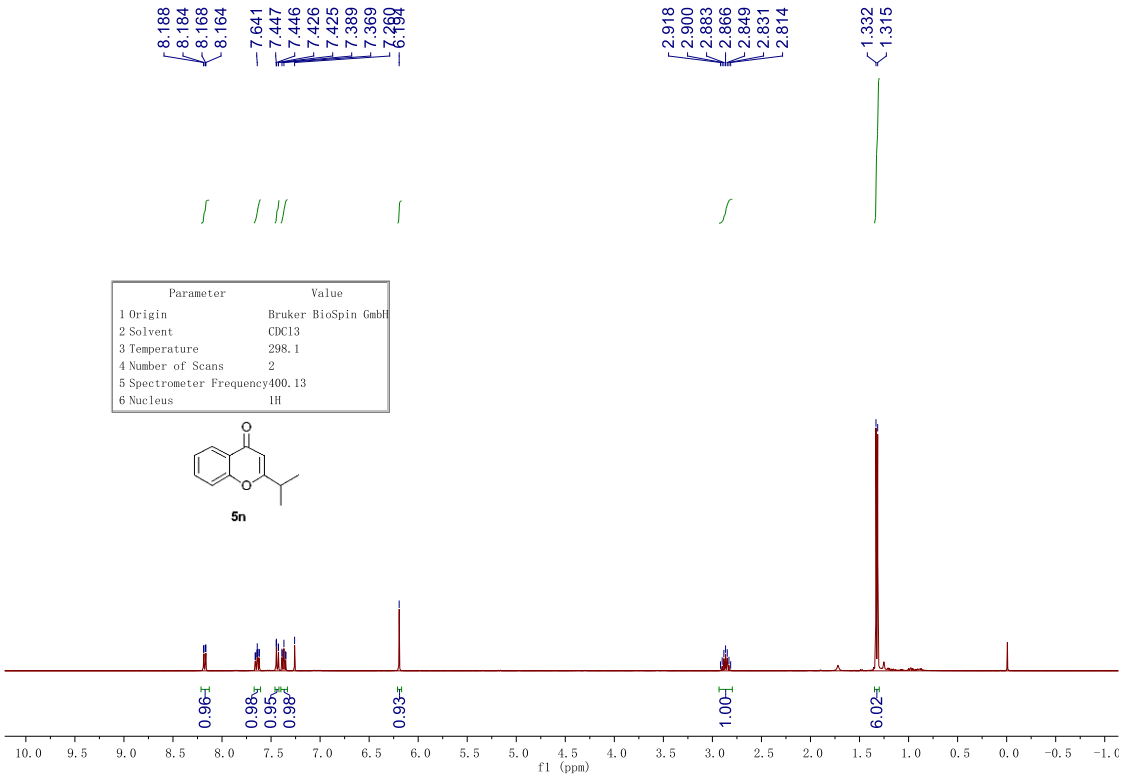
157.857
144.272
138.379
77.318
77.000
76.683
34.262
28.887
28.114
21.939
13.166
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
N
N
5k
f1 (ppm)

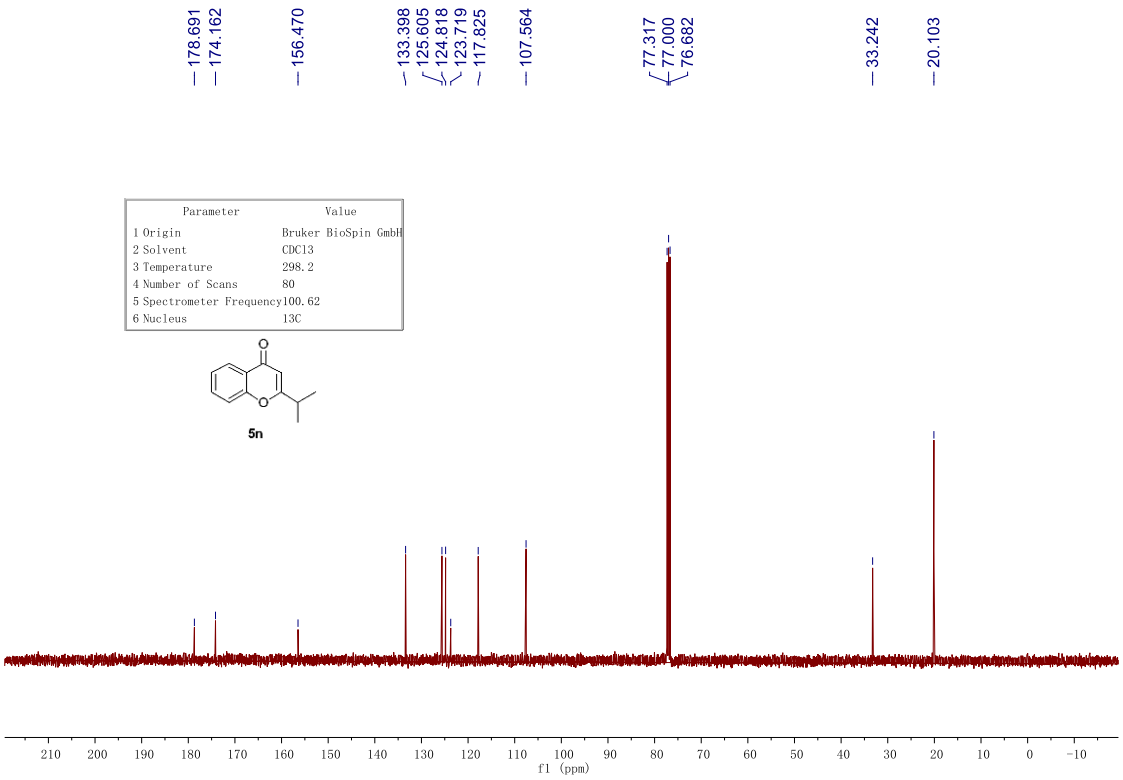

8.792
7.260
3.553
3.536
3.519
3.502
3.485
3.469
3.452
1.310
1.293
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N
N
Br
5l
1.00
1.05
6.02
f1 (ppm)

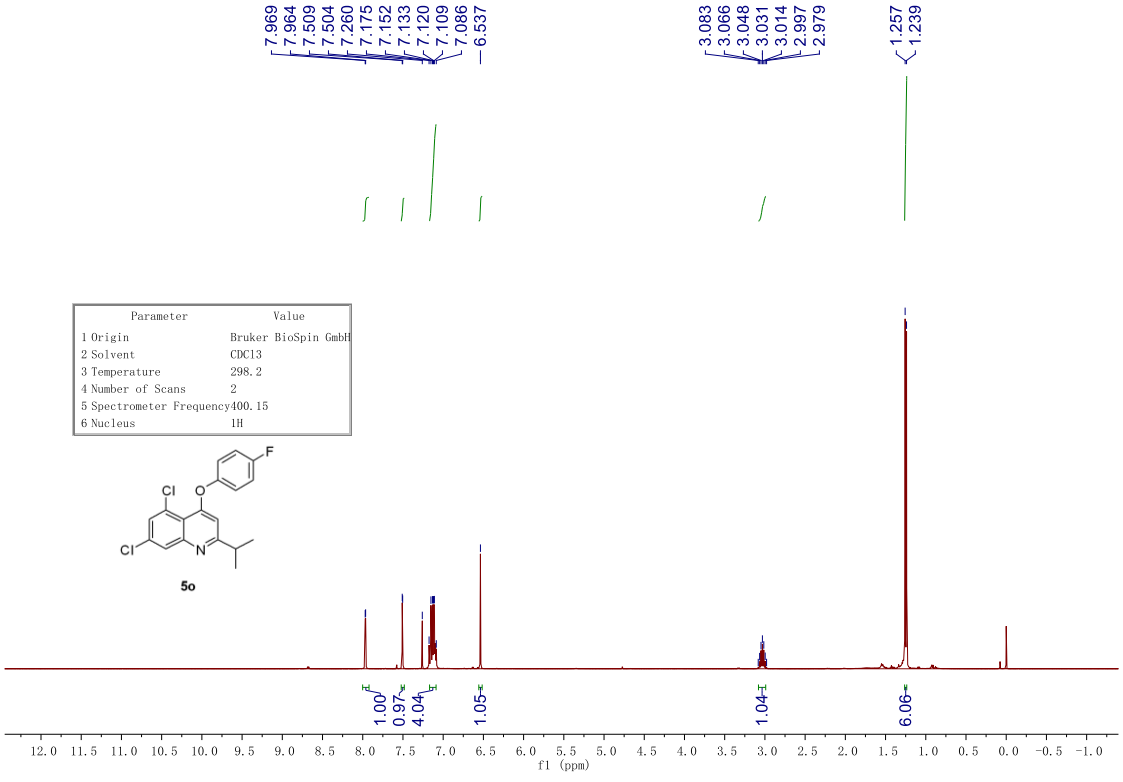

175.287
159.358
143.108
123.783
115.371
77.318
77.000
76.683
34.219
20.364
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N
N
Br
5l
f1 (ppm)

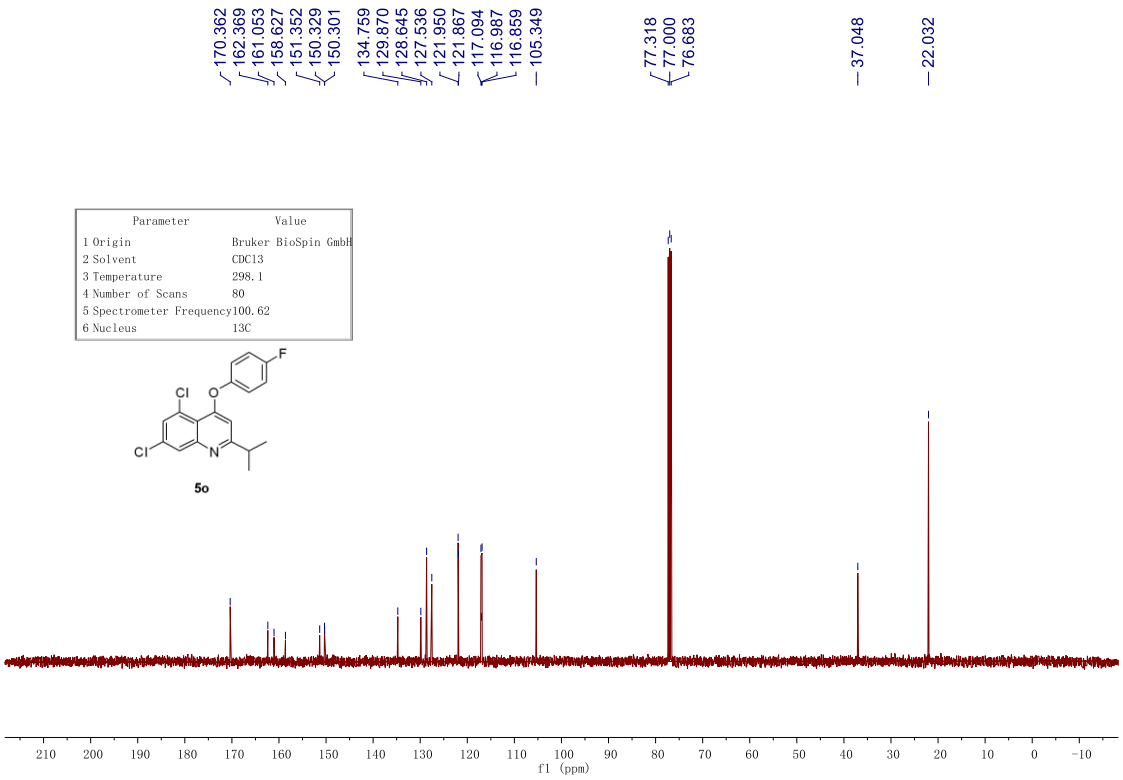

8.116
8.095
7.978
7.958
7.806
7.787
7.768
7.540
7.521
7.502
7.260
3.927
3.910
3.893
3.876
3.859
3.842
3.825
3.364
3.347
3.330
3.313
3.296
3.279
3.262
1.431
1.414
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
N
N
5m
0.99
0.94
0.99
1.00
1.00
0.99
11.98
f1 (ppm)

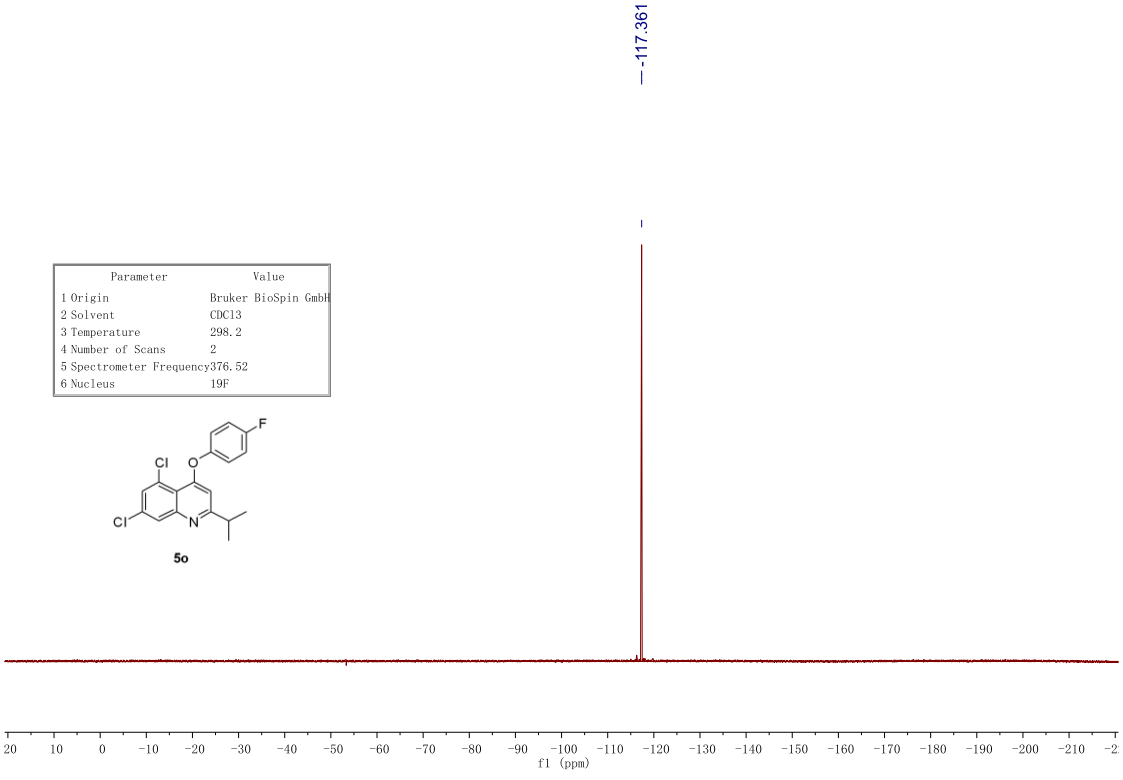

175.295
170.930
150.419
132.702
128.861
126.083
123.931
121.273
77.318
77.000
76.683
38.038
30.943
21.799
21.719
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
5m
f1 (ppm)

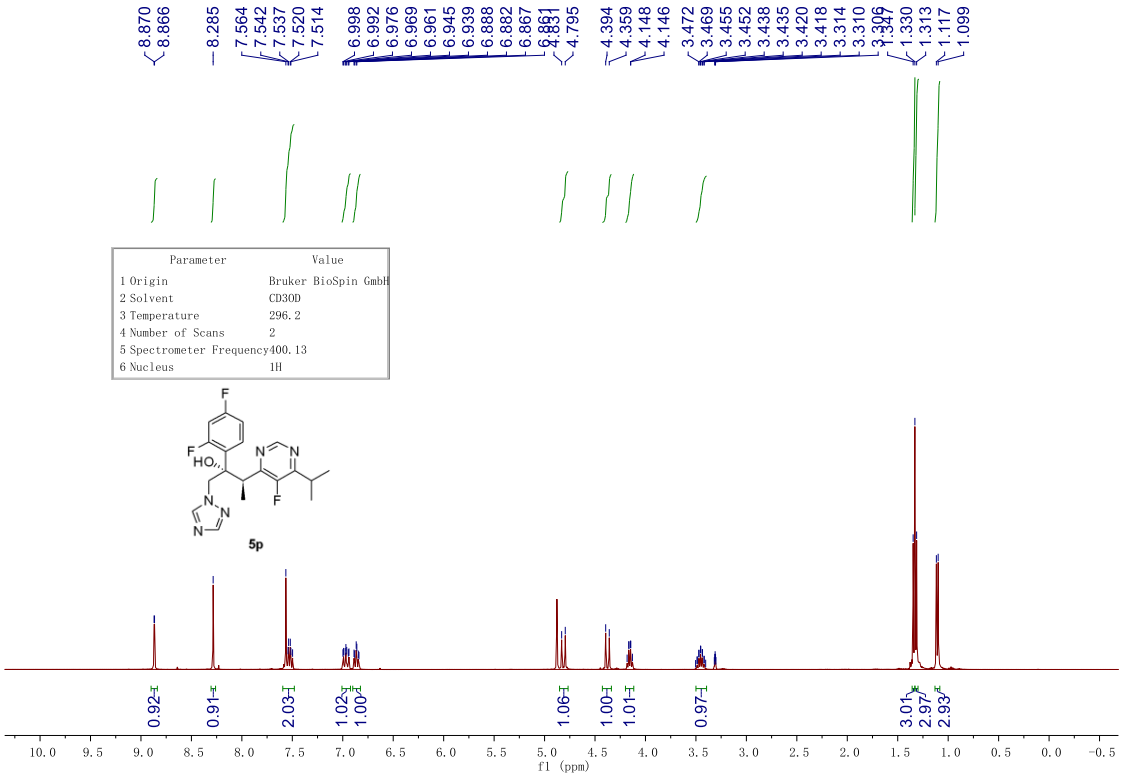

8.188
8.184
8.168
8.164
7.641
7.447
7.446
7.426
7.425
7.389
7.369
7.260
6.194
2.918
2.900
2.883
2.866
2.849
2.831
2.814
1.332
1.315
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5n
0.96
0.98
0.95
0.98
0.93
1.00
6.02
f1 (ppm)

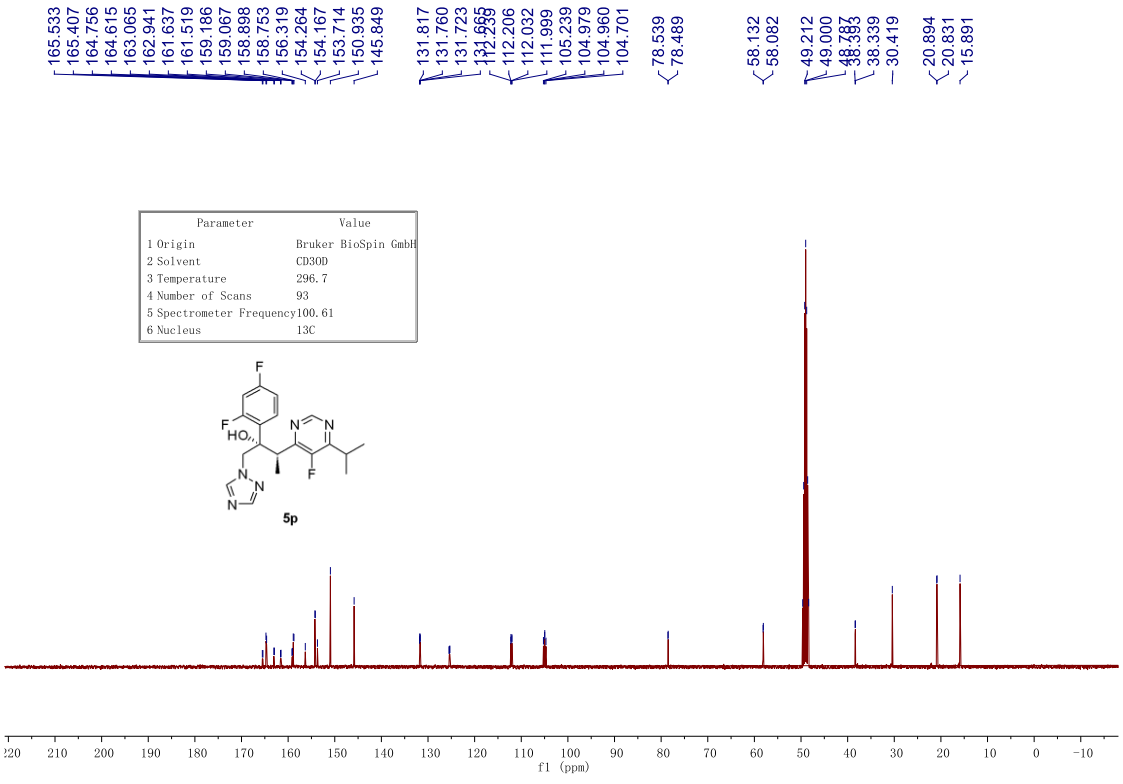

178.691
174.162
156.470
133.398
125.605
124.818
123.719
117.825
107.564
77.317
77.000
76.682
33.242
20.103
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
O
5n
f1 (ppm)

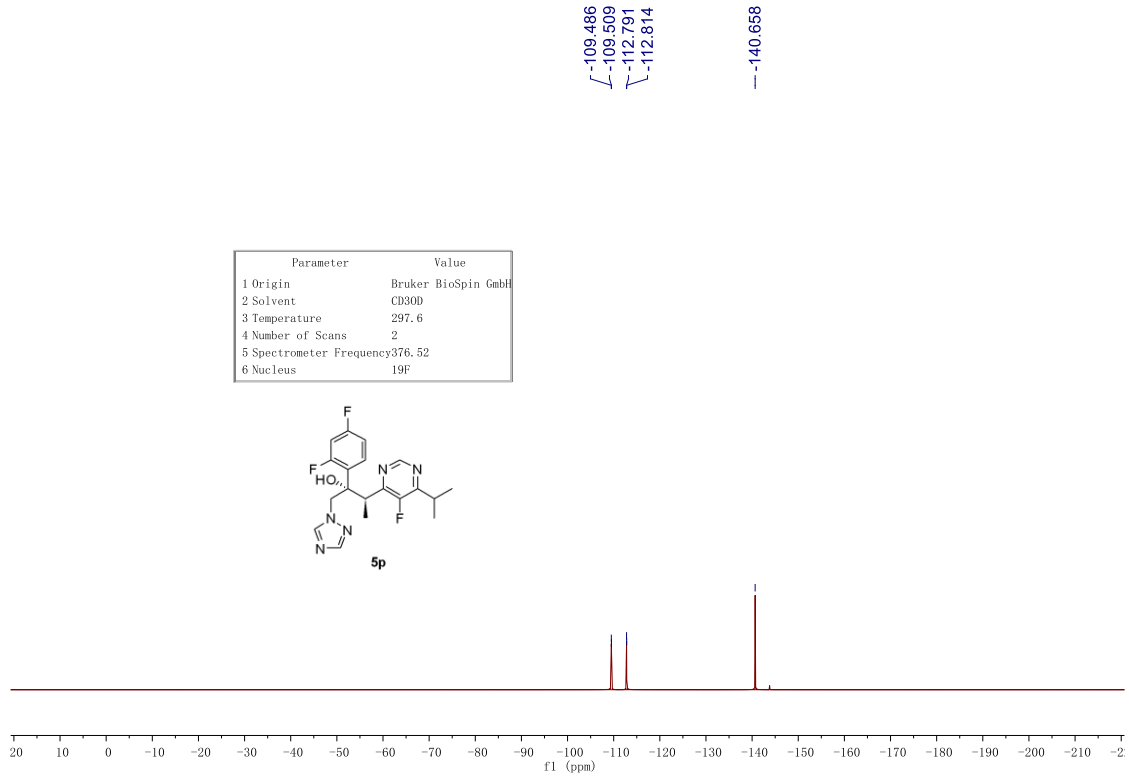

7.969
7.964
7.509
7.504
7.260
7.175
7.152
7.133
7.120
7.109
7.086
6.537
3.083
3.066
3.048
3.031
3.014
2.997
2.979
1.257
1.239
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
F
O
Cl
Cl
N
5o
1.00
0.97
4.04
1.05
1.04
6.06
f1 (ppm)

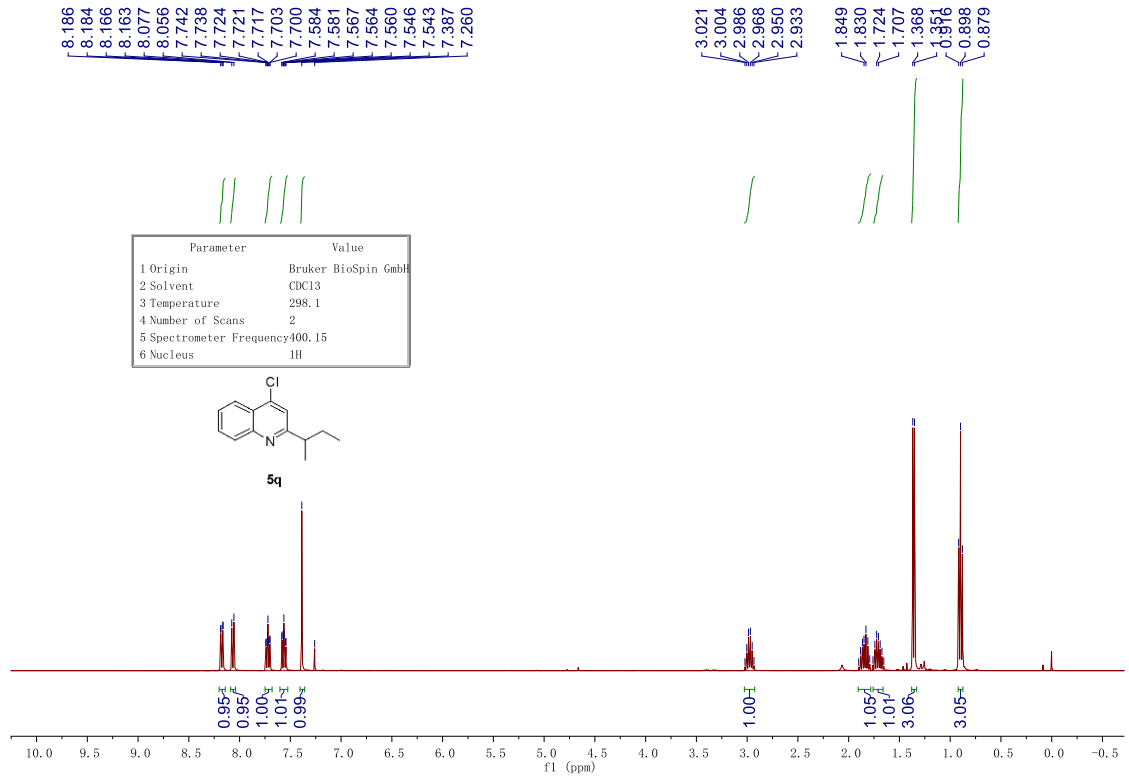

170.362
162.369
161.053
158.627
151.352
150.329
150.301
134.759
129.870
128.645
127.536
121.950
121.867
117.094
116.987
116.859
105.349
77.318
77.000
76.683
37.048
22.032
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
F
Cl
O
Cl
N
5o
f1 (ppm)

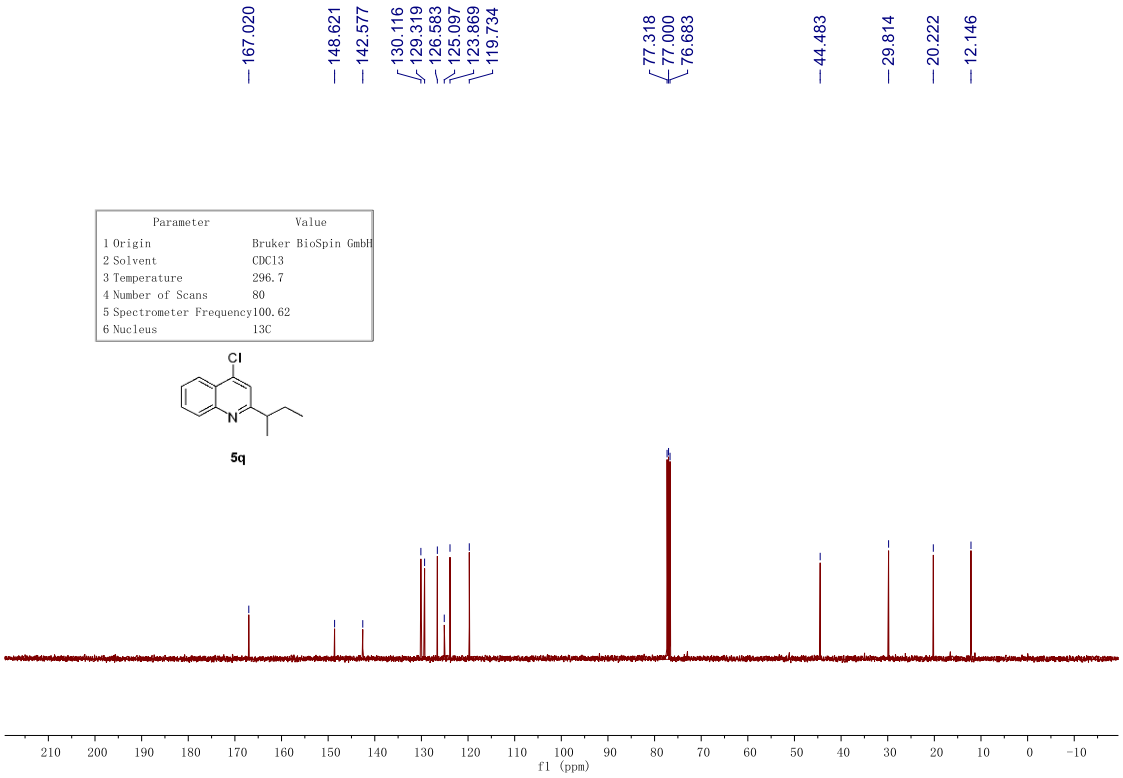

-117.361
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
F
Cl
O
Cl
N
5o
f1 (ppm)

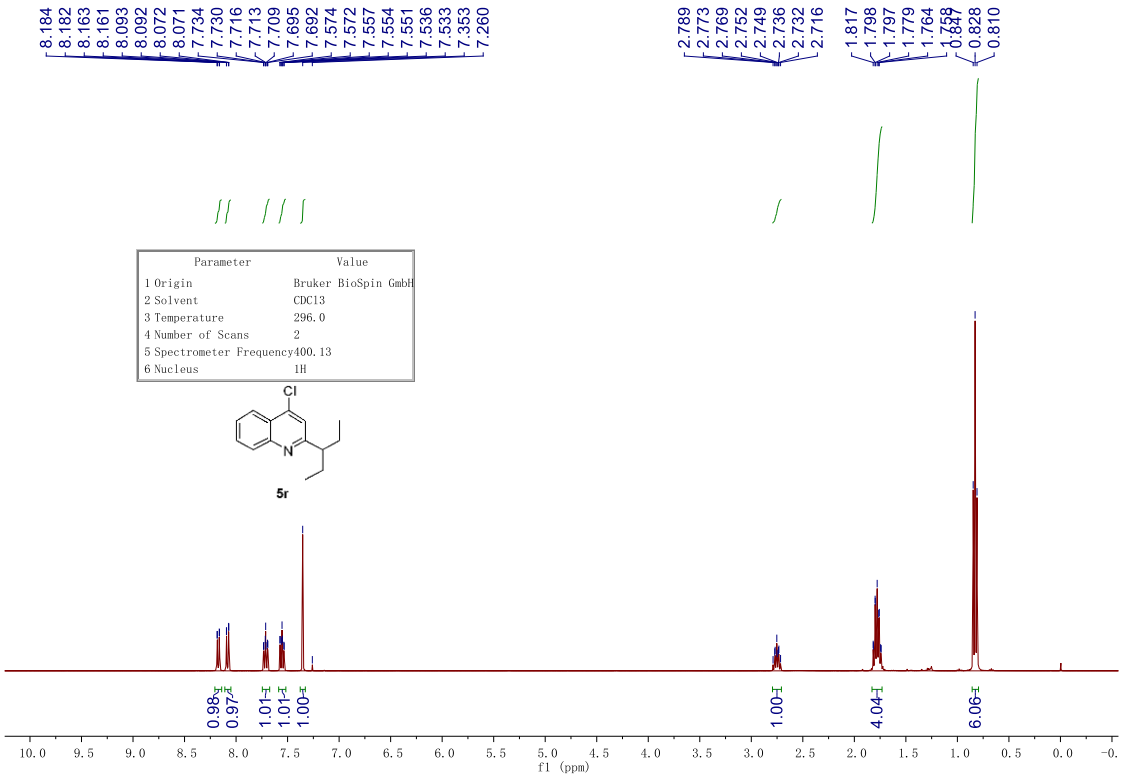

8.870
8.866
8.285
7.564
7.542
7.537
7.520
7.514
6.998
6.992
6.976
6.969
6.961
6.945
6.939
6.888
6.882
6.867
4.795
4.394
4.359
4.148
4.146
3.472
3.469
3.455
3.452
3.438
3.435
3.420
3.418
3.314
3.310
1.330
1.313
1.117
1.099
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CD3OD
3 Temperature 296.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5p
0.92
0.91
2.03
1.02
1.00
1.06
1.00
1.01
0.97
3.01
2.97
2.93
f1 (ppm)

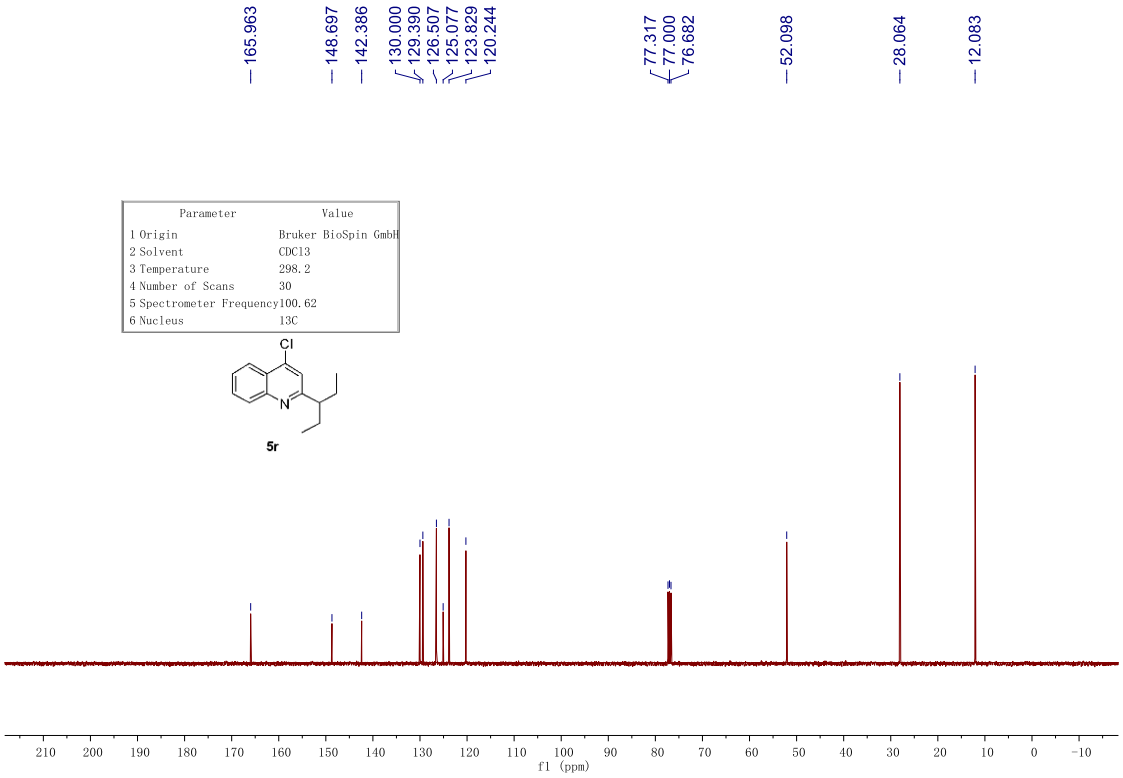

165.533
165.407
164.756
164.615
163.065
162.941
161.637
161.519
159.186
159.067
158.898
158.753
156.319
154.264
154.167
153.714
150.935
145.849
131.817
131.760
131.723
112.206
112.032
111.999
105.239
104.979
104.960
104.701
78.539
78.489
58.132
58.082
49.212
49.000
38.339
30.419
20.894
20.831
15.891
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CD3OD
3 Temperature 296.7
4 Number of Scans 93
5 Spectrometer Frequency 100.61
6 Nucleus 13C
5p
f1 (ppm)

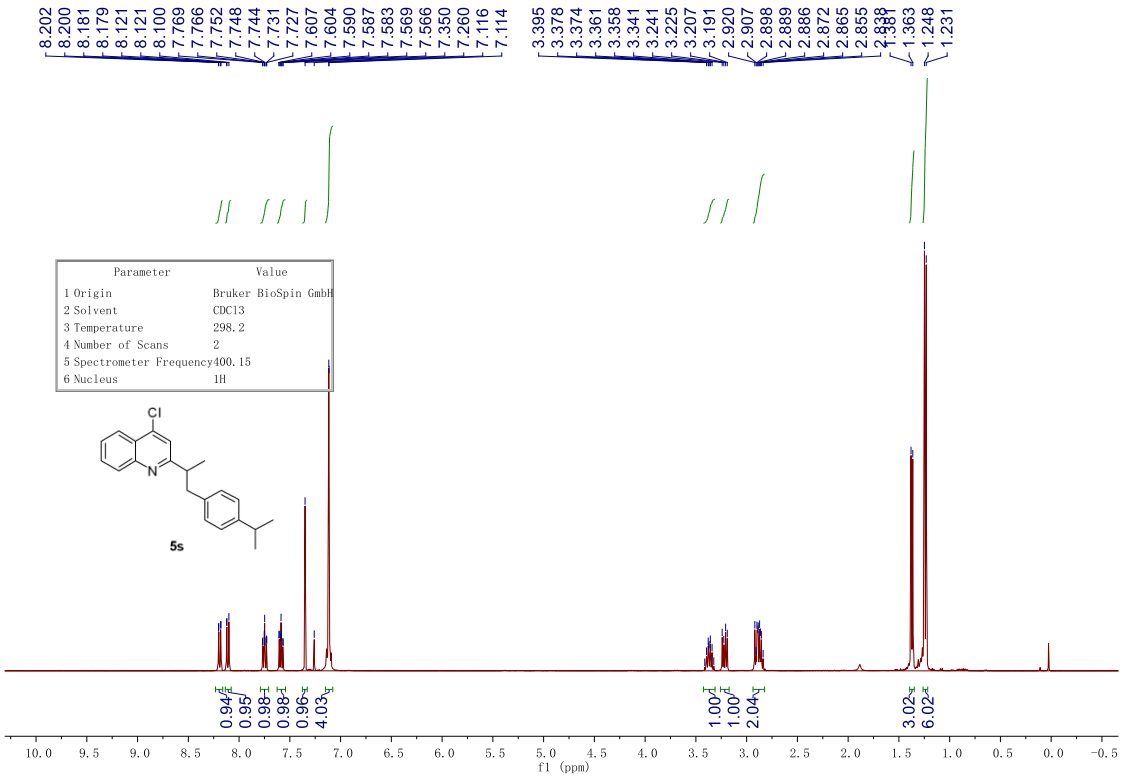

-109.486
-109.509
-112.791
-112.814
-140.658
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CD3OD
3 Temperature 297.6
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
5p
f1 (ppm)

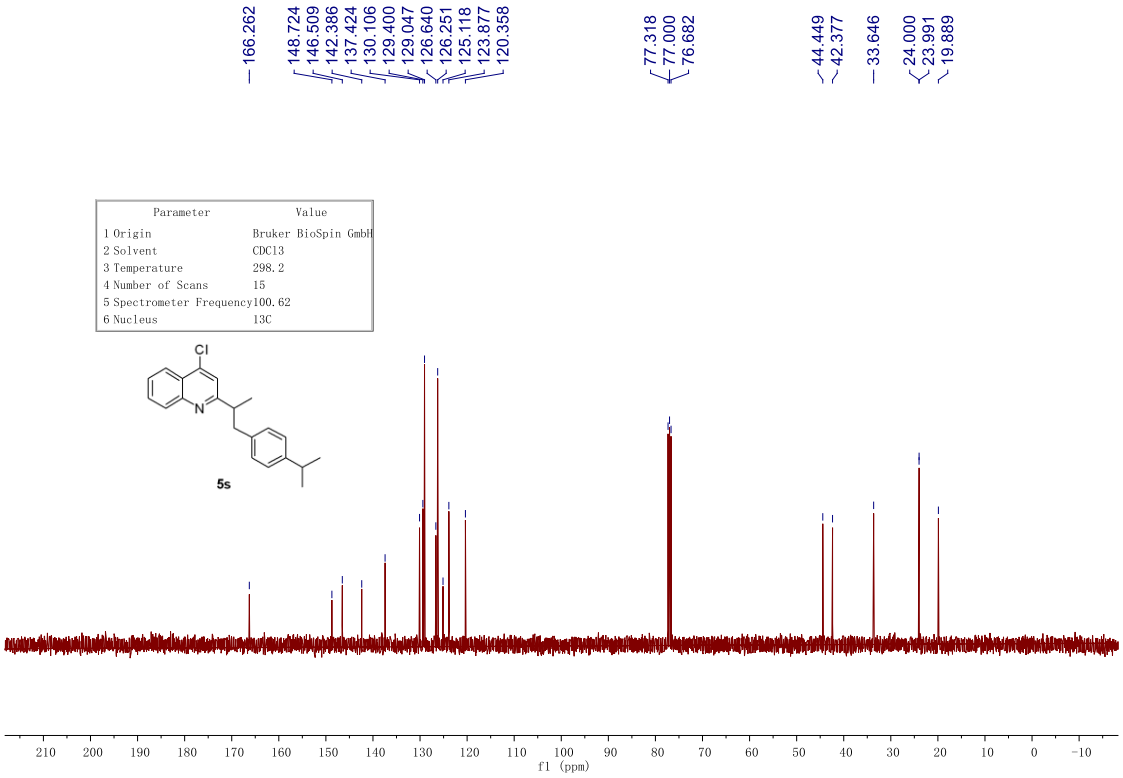

8.186
8.184
8.166
8.163
8.077
8.056
7.742
7.738
7.724
7.721
7.717
7.703
7.700
7.584
7.581
7.567
7.564
7.560
7.546
7.543
7.387
7.260
3.021
3.004
2.986
2.968
2.950
2.933
1.849
1.830
1.724
1.707
1.368
0.916
0.898
0.879
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
5q
0.95
0.95
1.00
1.01
0.99
1.00
1.05
1.01
3.06
3.05
f1 (ppm)

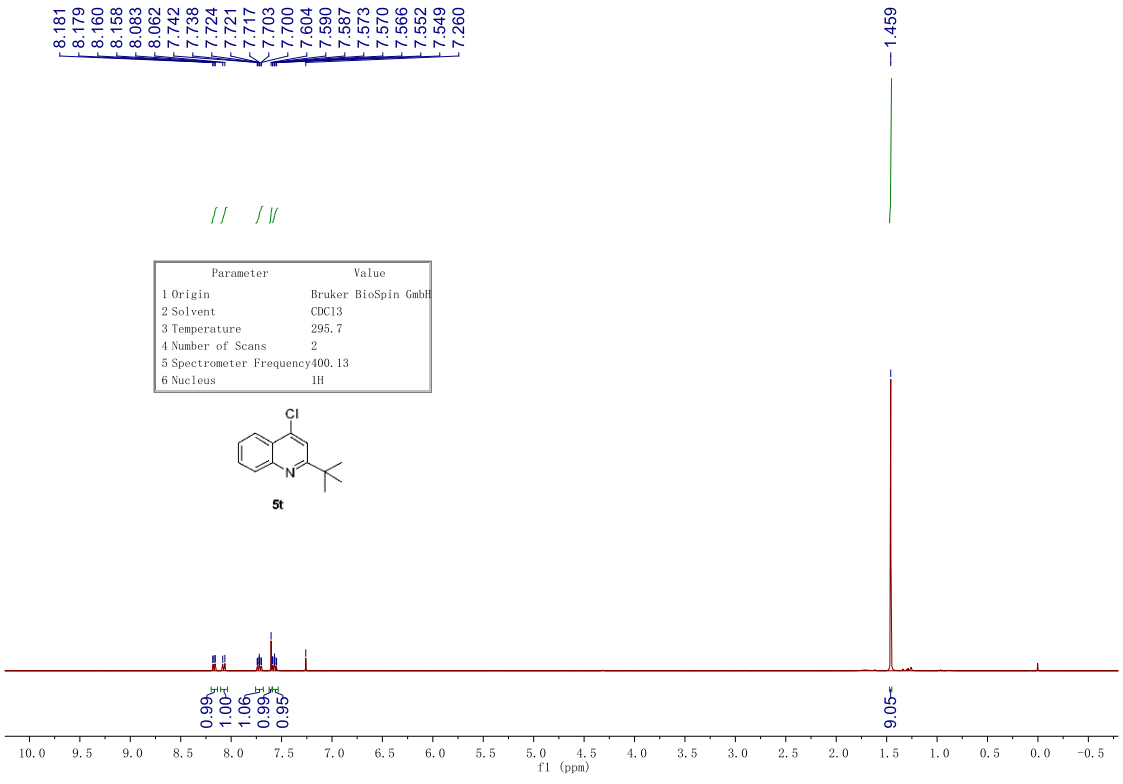

167.020
148.621
142.577
130.116
129.319
126.583
125.097
123.869
119.734
77.318
77.000
76.683
44.483
29.814
20.222
12.146
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5q
f1 (ppm)

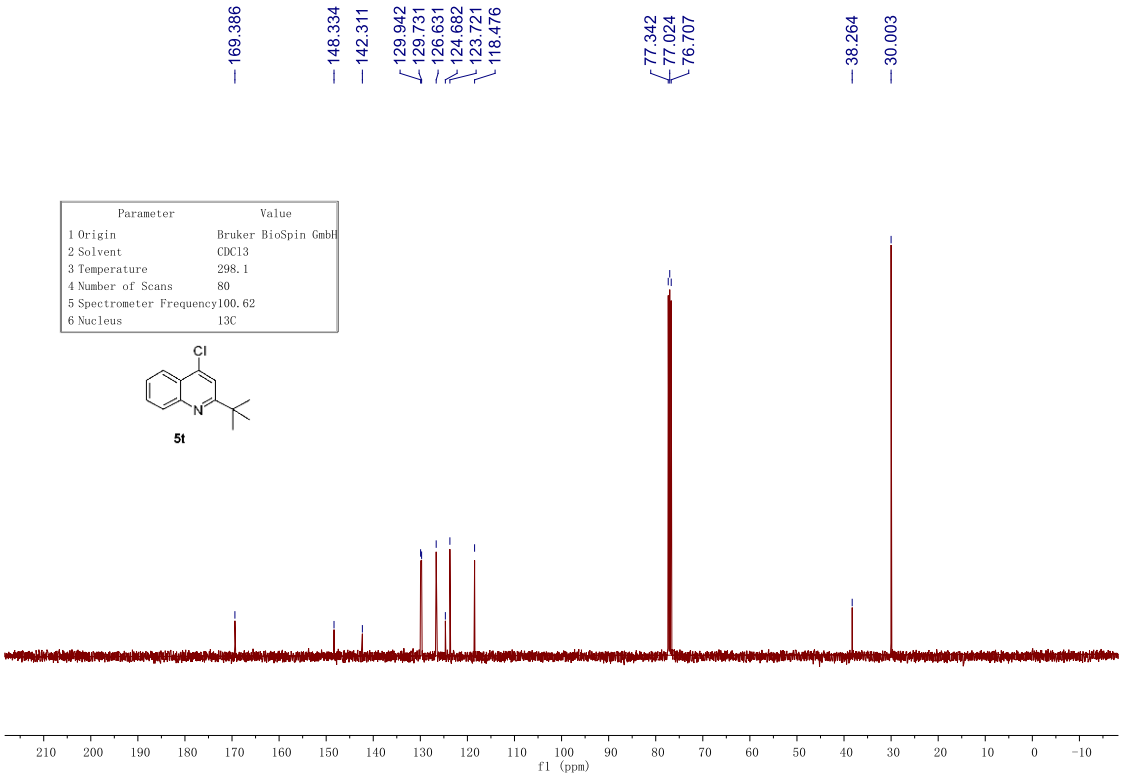

8.184
8.182
8.163
8.161
8.093
8.092
8.072
8.071
7.734
7.730
7.716
7.713
7.709
7.695
7.692
7.574
7.572
7.557
7.554
7.551
7.536
7.533
7.353
7.260
2.789
2.773
2.769
2.752
2.749
2.736
2.732
2.716
1.817
1.798
1.797
1.779
1.764
0.847
0.828
0.810
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
5r
0.98
0.97
1.01
1.01
1.00
1.00
4.04
6.06
f1 (ppm)

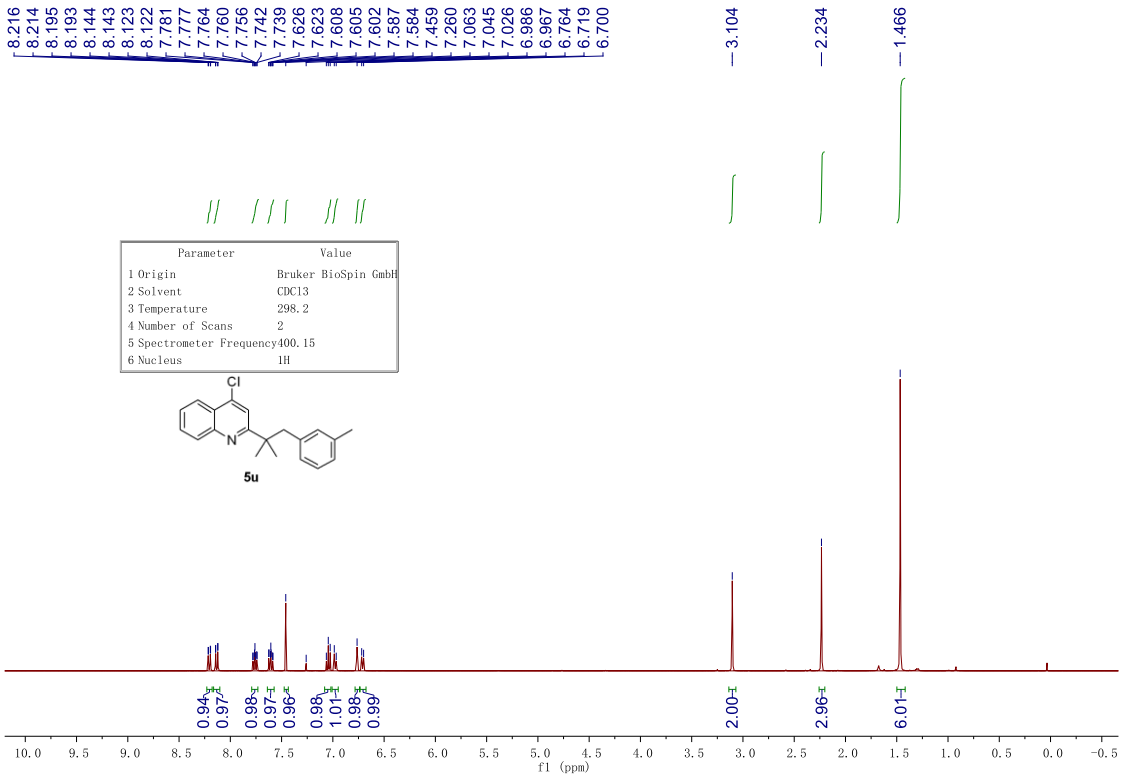

165.963
148.697
142.386
130.000
129.390
126.507
125.077
123.829
120.244
77.317
77.000
76.682
52.098
28.064
12.083
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5r
f1 (ppm)

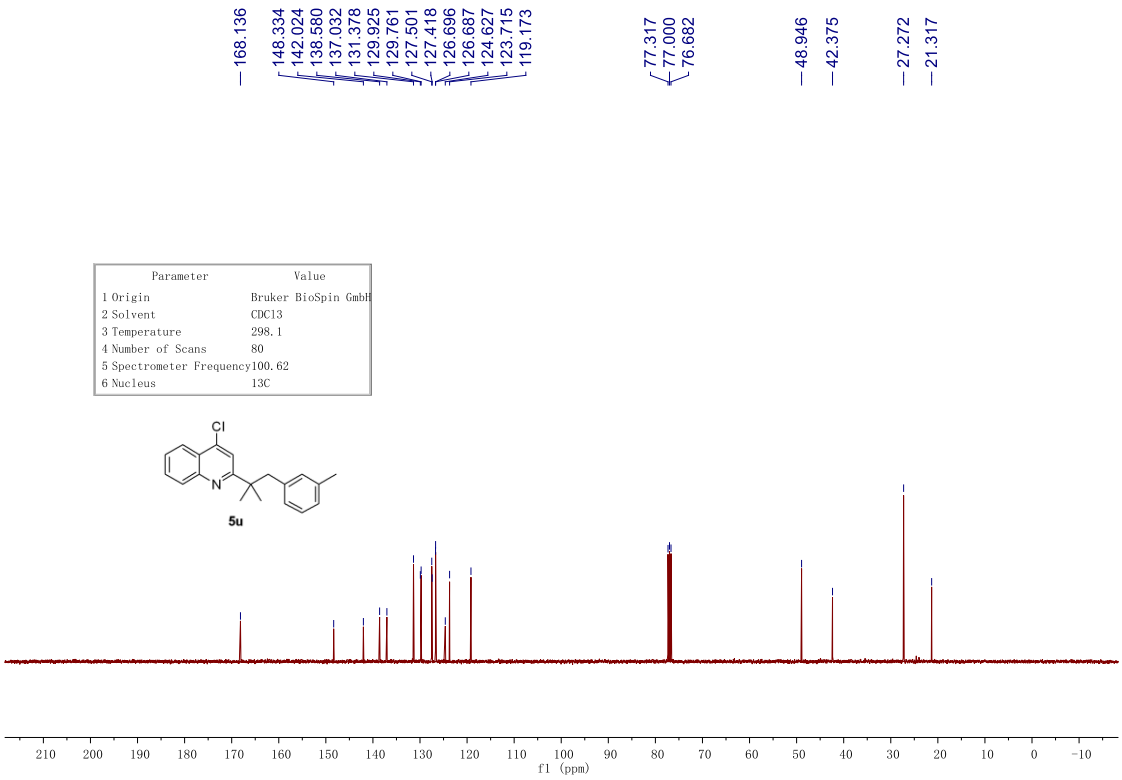

8.202
8.200
8.181
8.179
8.121
8.121
8.100
7.769
7.766
7.752
7.748
7.744
7.731
7.727
7.607
7.604
7.590
7.587
7.583
7.569
7.566
7.350
7.260
7.116
7.114
3.395
3.378
3.374
3.361
3.358
3.341
3.241
3.225
3.207
3.191
2.920
2.907
2.898
2.889
2.886
2.872
2.865
2.855
1.363
1.248
1.231
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
5s
0.94
0.95
0.98
0.98
0.96
4.03
1.00
1.00
2.04
3.02
6.02
f1 (ppm)

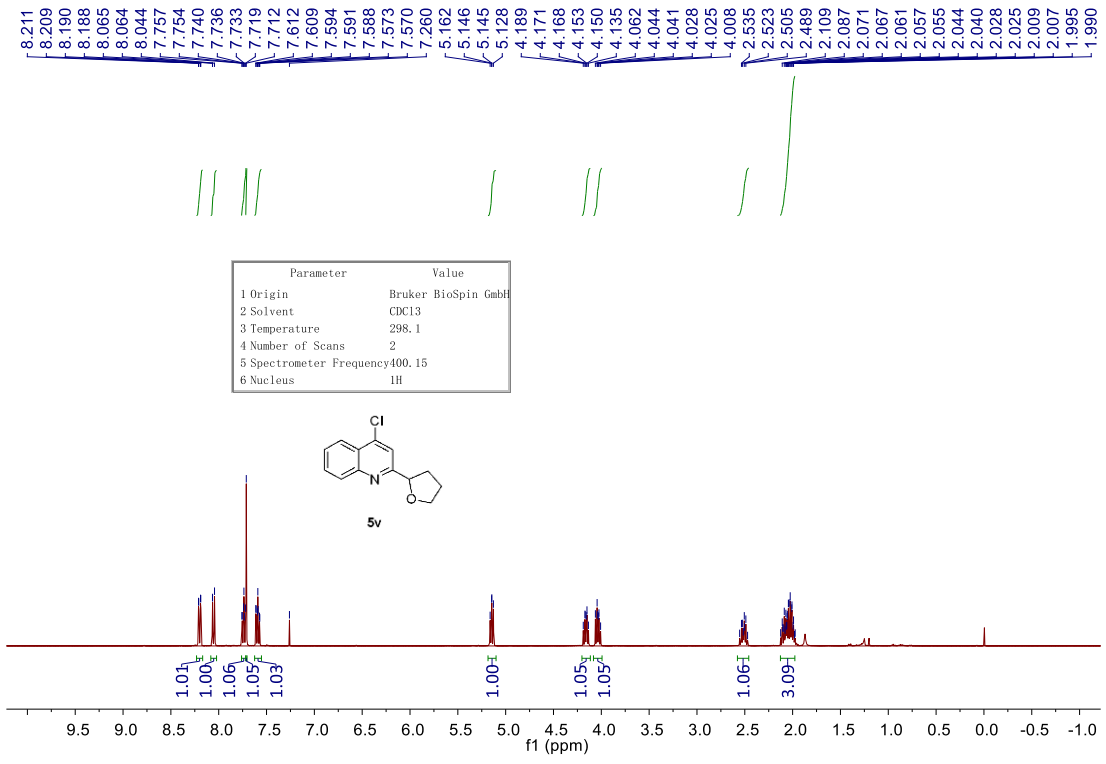

166.262
148.724
146.509
142.386
137.424
130.106
129.400
129.047
126.640
126.251
125.118
123.877
120.358
77.318
77.000
76.682
44.449
42.377
33.646
24.000
23.991
19.889
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 15
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5s
f1 (ppm)


8.181
8.179
8.160
8.158
8.083
8.062
7.742
7.738
7.724
7.721
7.717
7.703
7.700
7.604
7.590
7.587
7.573
7.570
7.566
7.552
7.549
7.260
1.459
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.7
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
5t
0.99
1.00
1.06
0.99
0.95
9.05
f1 (ppm)


169.386
148.334
142.311
129.942
129.731
126.631
124.682
123.721
118.476
77.342
77.024
76.707
38.264
30.003
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5t
f1 (ppm)


8.216
8.214
8.195
8.193
8.144
8.143
8.123
8.122
7.781
7.777
7.764
7.760
7.756
7.742
7.739
7.626
7.623
7.608
7.605
7.602
7.587
7.584
7.459
7.260
7.063
7.045
7.026
6.986
6.967
6.764
6.719
6.700
3.104
2.234
1.466
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
5u
0.94
0.97
0.98
0.97
0.96
0.98
1.01
0.98
0.99
2.00
2.96
6.01
f1 (ppm)


168.136
148.334
142.024
138.580
137.032
131.378
129.925
129.761
127.501
127.418
126.696
126.687
124.627
123.715
119.173
77.317
77.000
76.682
48.946
42.375
27.272
21.317
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5u
f1 (ppm)


8.211
8.209
8.190
8.188
8.065
8.064
8.044
7.757
7.754
7.740
7.736
7.733
7.719
7.712
7.612
7.609
7.594
7.591
7.588
7.573
7.570
7.260
5.162
5.146
5.145
5.128
4.189
4.171
4.168
4.153
4.150
4.135
4.062
4.044
4.041
4.028
4.025
4.008
2.535
2.523
2.505
2.489
2.109
2.087
2.071
2.067
2.061
2.057
2.055
2.044
2.040
2.028
2.025
2.009
2.007
1.995
1.990
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
O
5v
1.01
1.00
1.06
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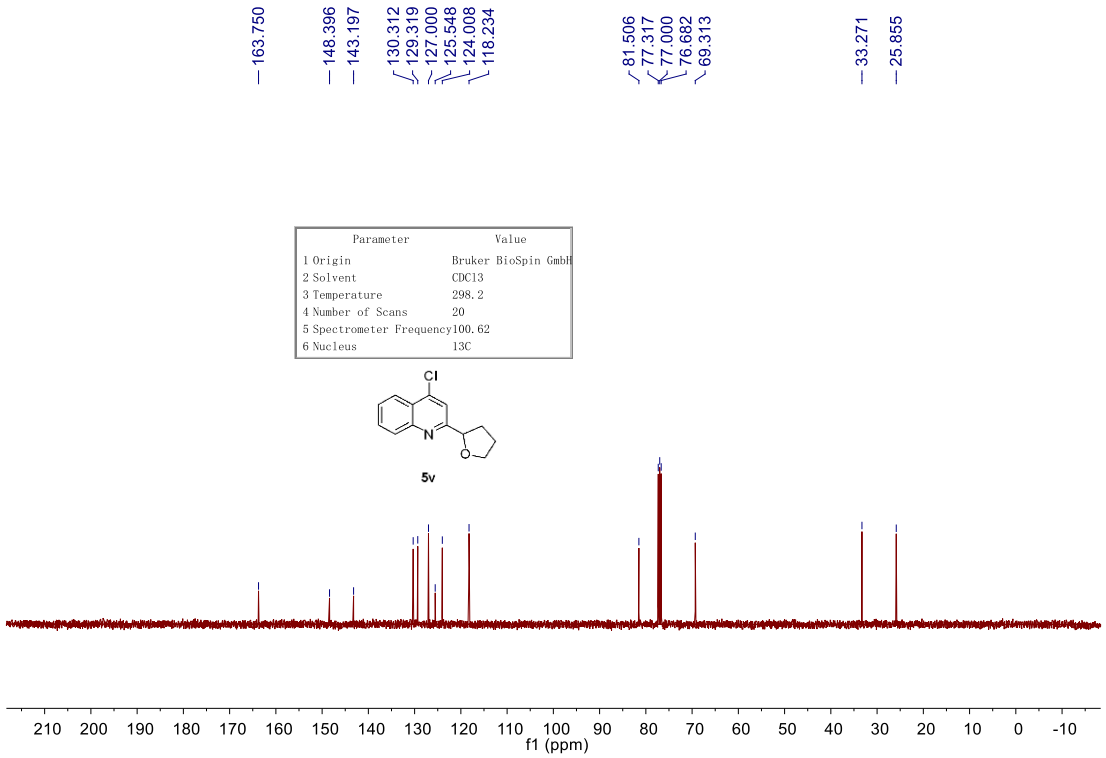
1.05
1.05
1.06
3.09
f1 (ppm)


163.750
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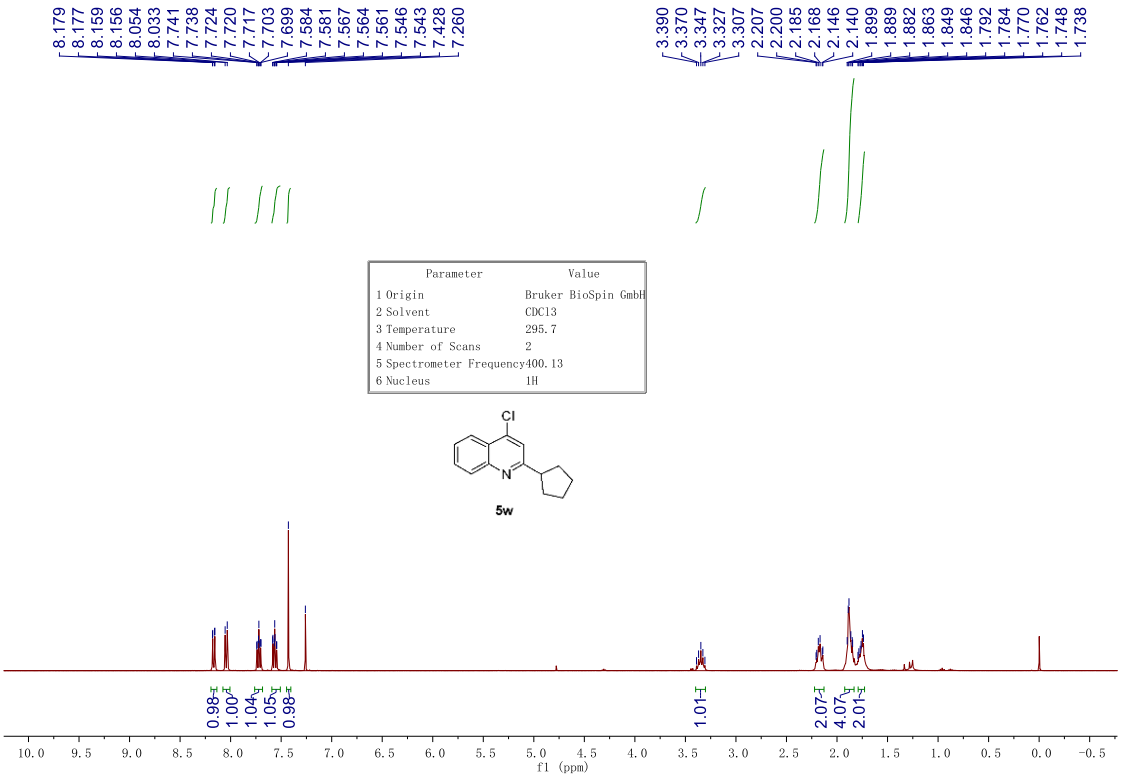
143.197
130.312
129.319
127.000
125.548
124.008
118.234
81.506
77.317
77.000
76.682
69.313
33.271
25.855
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
O
5v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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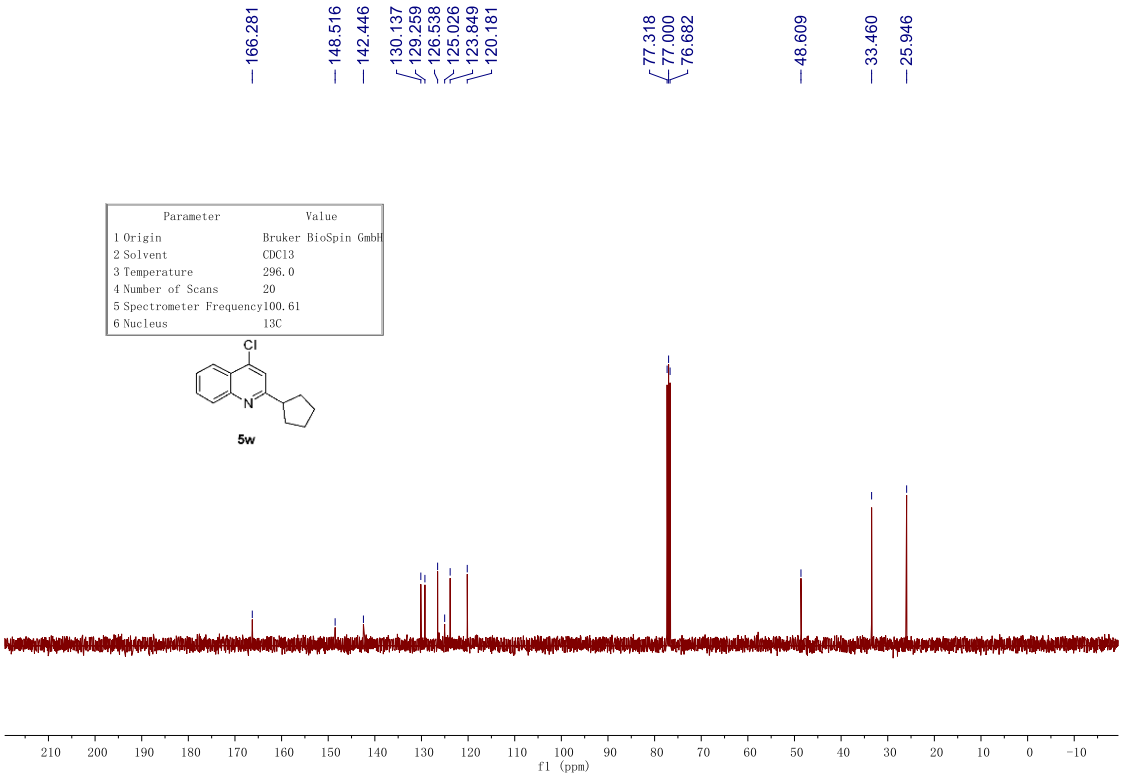
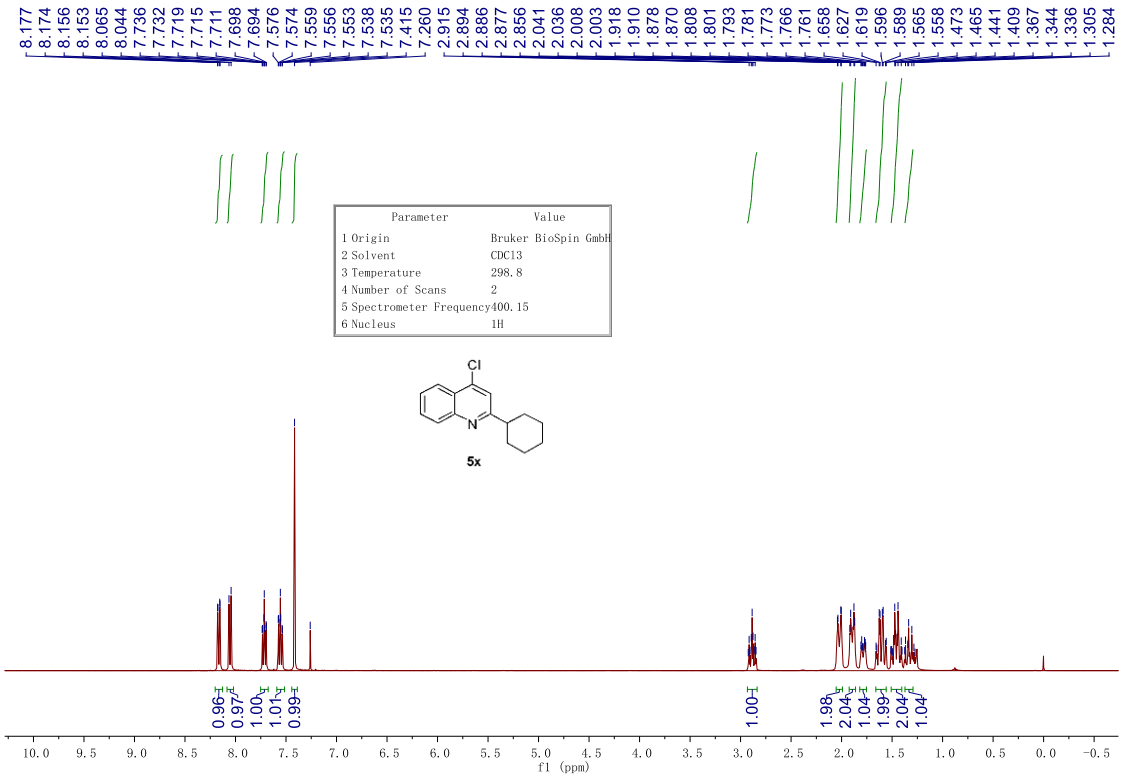
8.177
8.159
8.156
8.054
8.033
7.741
7.738
7.724
7.720
7.717
7.703
7.699
7.584
7.581
7.567
7.564
7.561
7.546
7.543
7.428
7.260
3.390
3.370
3.347
3.327
3.307
2.207
2.200
2.185
2.168
2.146
2.140
1.899
1.889
1.882
1.863
1.849
1.846
1.792
1.784
1.770
1.762
1.748
1.738
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.7
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
5w
0.98
1.00
1.04
1.05
0.98
1.01
2.07
4.07
2.01
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 -0.5
f1 (ppm)


166.281
148.516
142.446
130.137
129.259
126.538
125.026
123.849
120.181
77.318
77.000
76.682
48.609
33.460
25.946
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.0
4 Number of Scans 20
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
N
5w
f1 (ppm)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8.174
8.156
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8.065
8.044
7.736
7.732
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7.715
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7.694
7.576
7.574
7.559
7.556
7.553
7.538
7.535
7.415
7.260
2.915
2.894
2.886
2.877
2.856
2.041
2.036
2.008
2.003
1.918
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1.870
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1.801
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1.781
1.773
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1.658
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1.619
1.596
1.589
1.565
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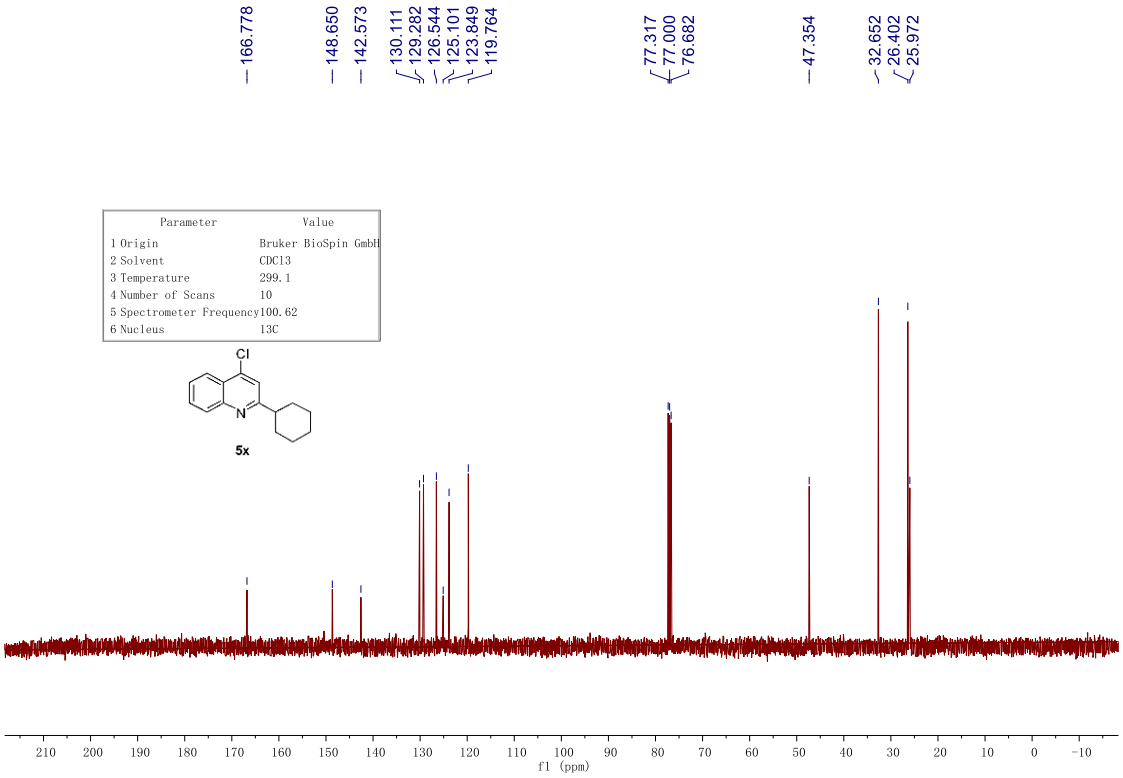
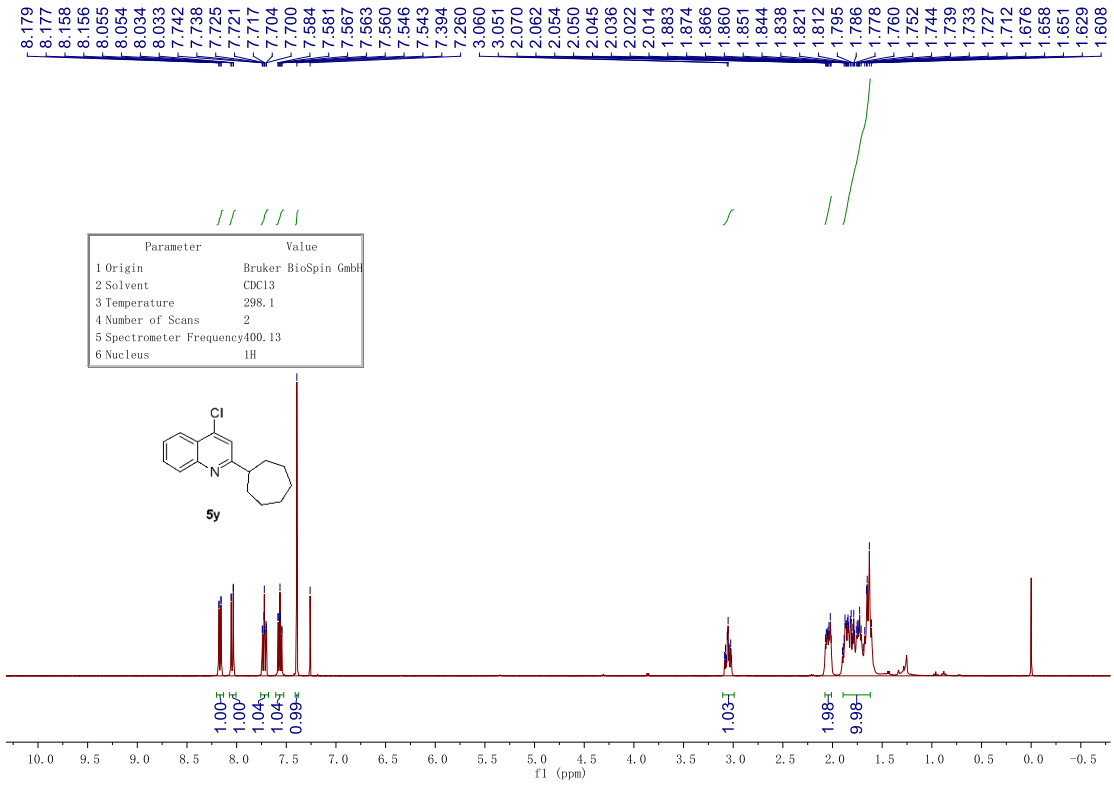
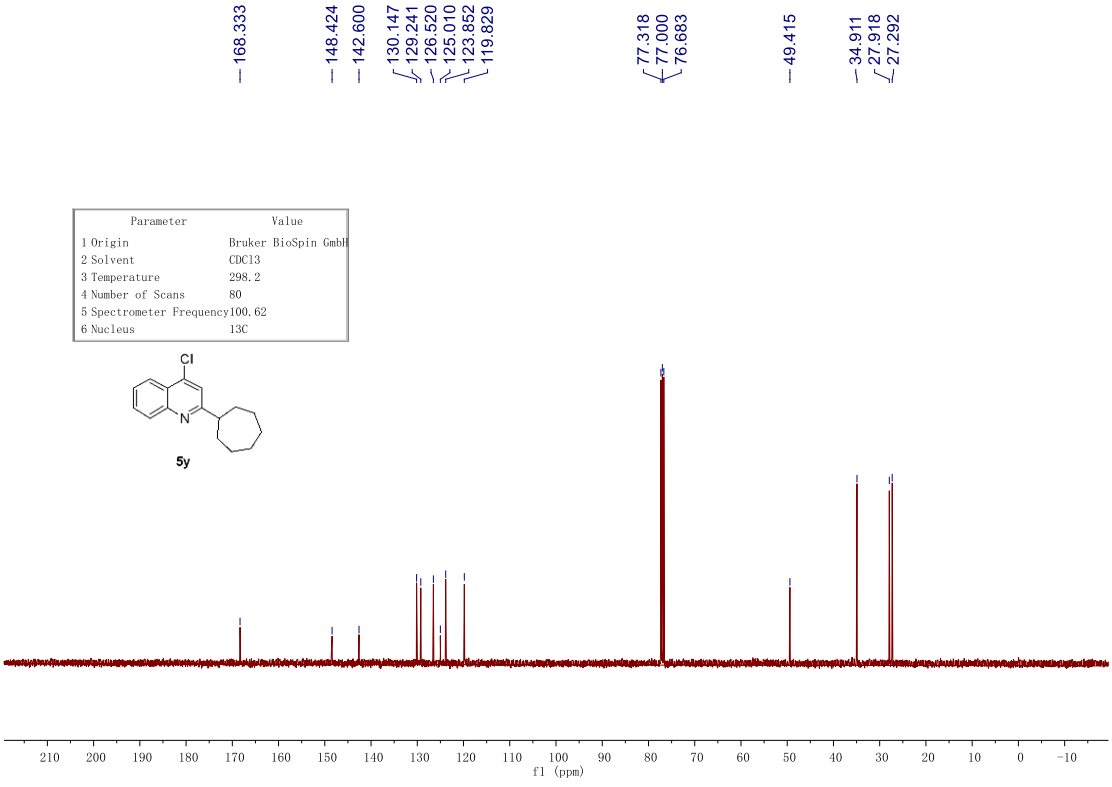
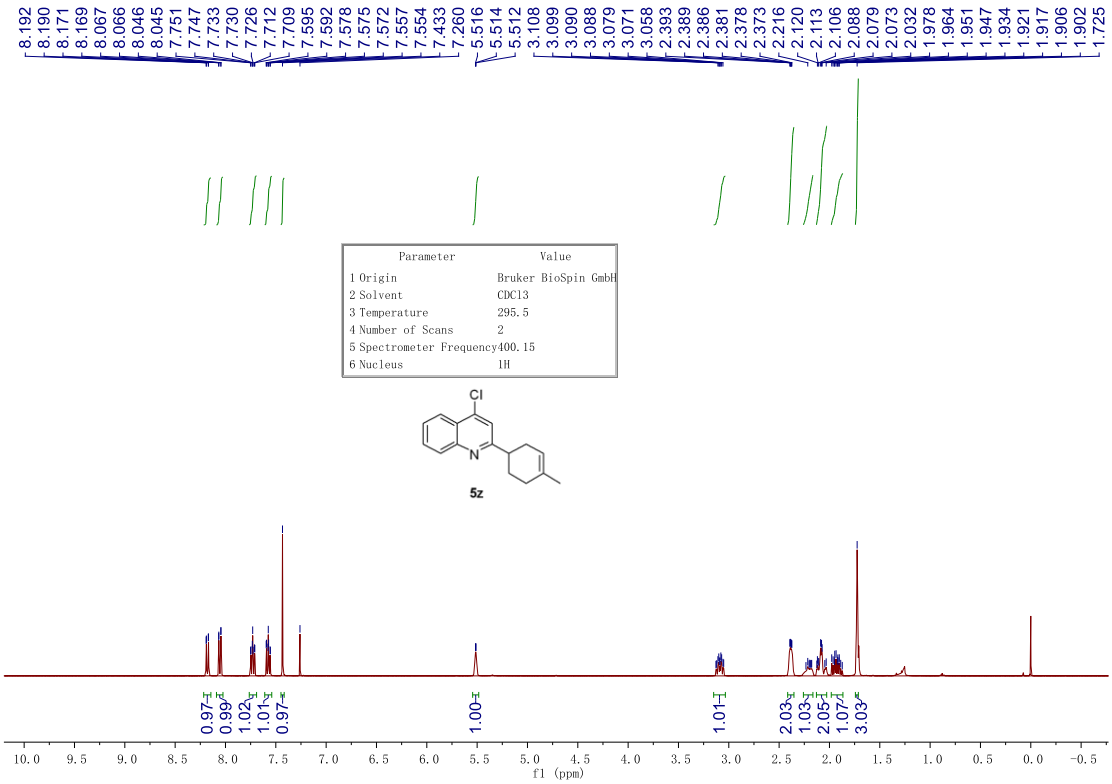
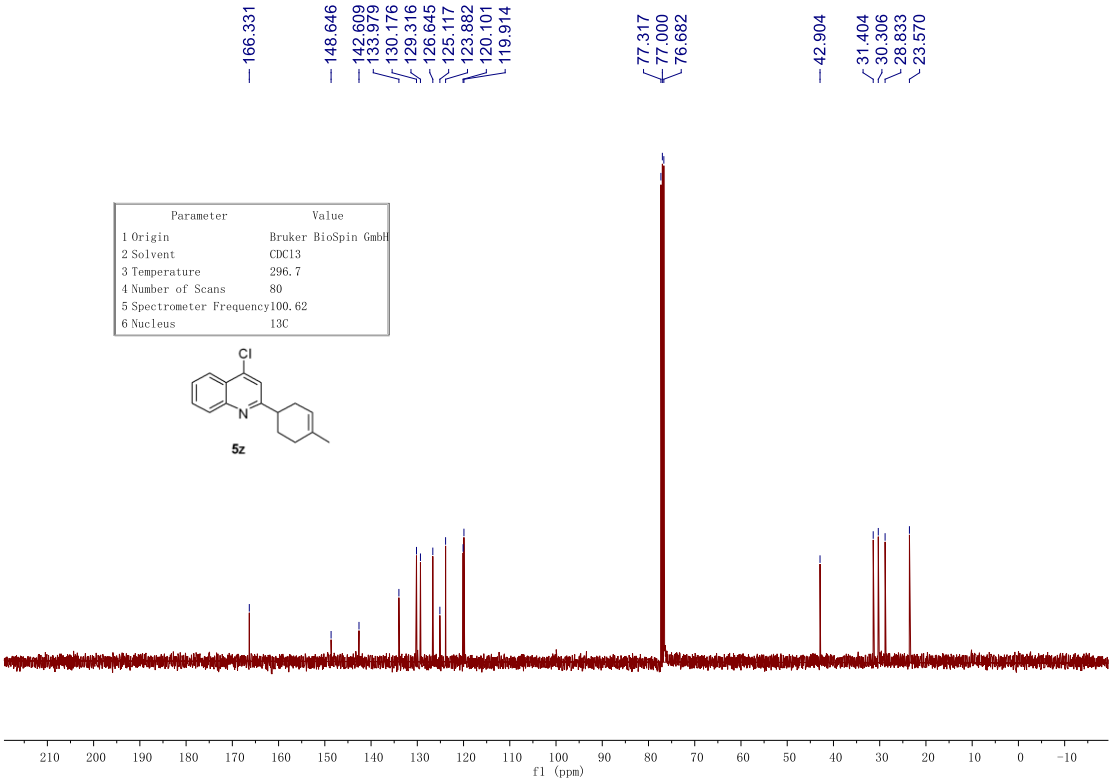
1.473
1.465
1.441
1.409
1.367
1.344
1.336
1.305
1.284
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.8
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
5x
0.96
0.97
1.00
1.01
0.99
1.00
1.98
2.04
1.04
1.99
2.04
1.04
f1 (ppm)

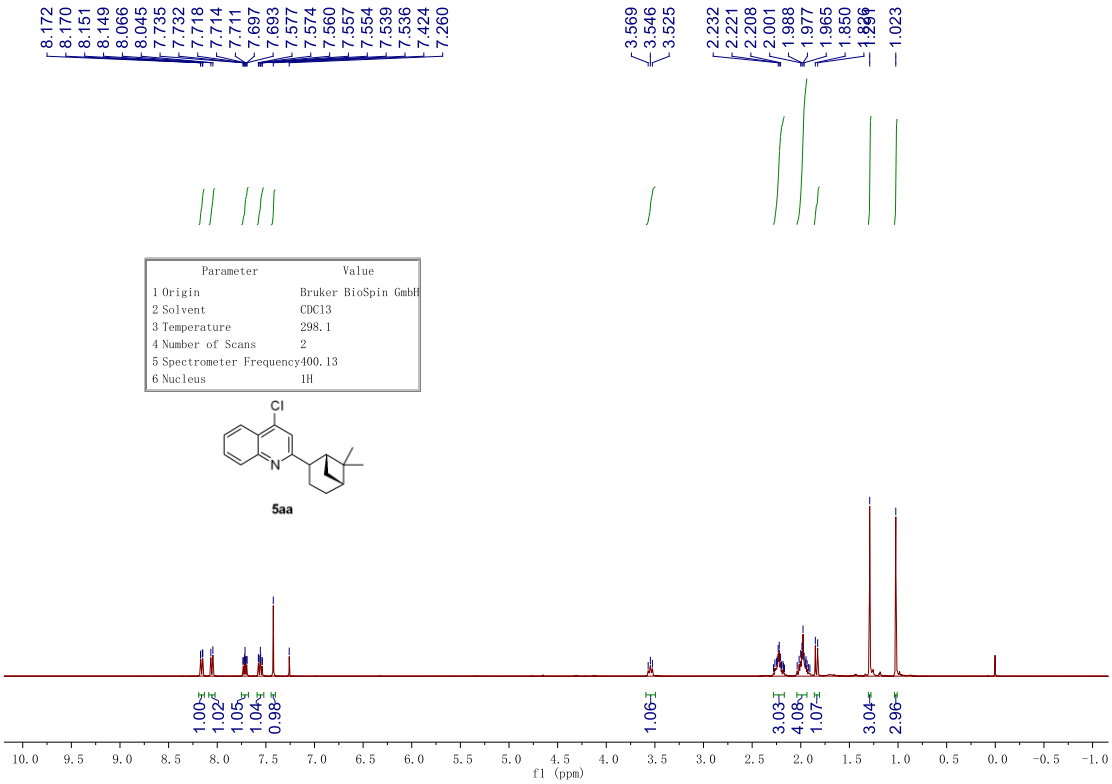

166.778
148.650
142.573
130.111
129.282
126.544
125.101
123.849
119.764
77.317
77.000
76.682
47.354
32.652
26.402
25.972
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5x
f1 (ppm)

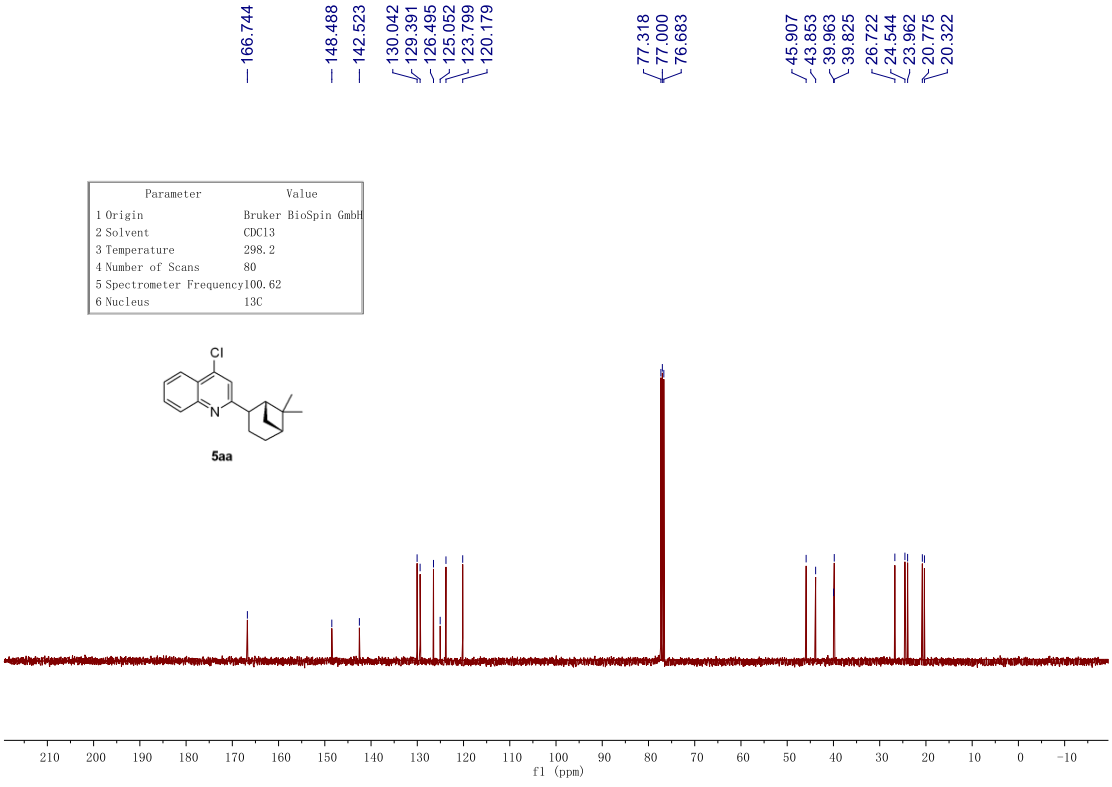

8.179
8.177
8.158
8.156
8.055
8.054
8.034
8.033
7.742
7.738
7.725
7.721
7.717
7.704
7.700
7.584
7.581
7.567
7.563
7.560
7.546
7.543
7.394
7.260
3.060
3.051
2.070
2.062
2.054
2.050
2.045
2.036
2.022
2.014
1.883
1.874
1.866
1.860
1.851
1.844
1.838
1.821
1.812
1.795
1.786
1.778
1.760
1.752
1.744
1.739
1.733
1.727
1.712
1.676
1.658
1.651
1.629
1.608
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
5y
1.00
1.00
1.04
1.04
0.99
1.03
1.98
9.98
f1 (ppm)

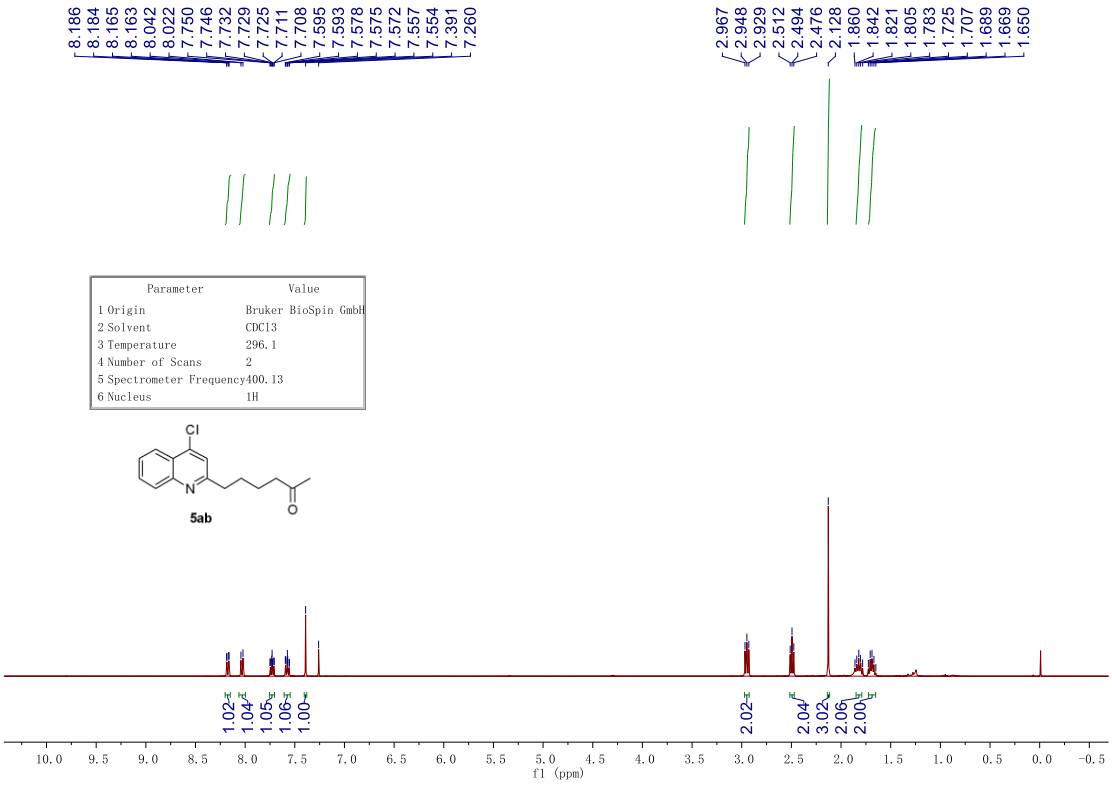

168.333
148.424
142.600
130.147
129.241
126.520
125.010
123.852
119.829
77.318
77.000
76.683
49.415
34.911
27.918
27.292
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5y
f1 (ppm)

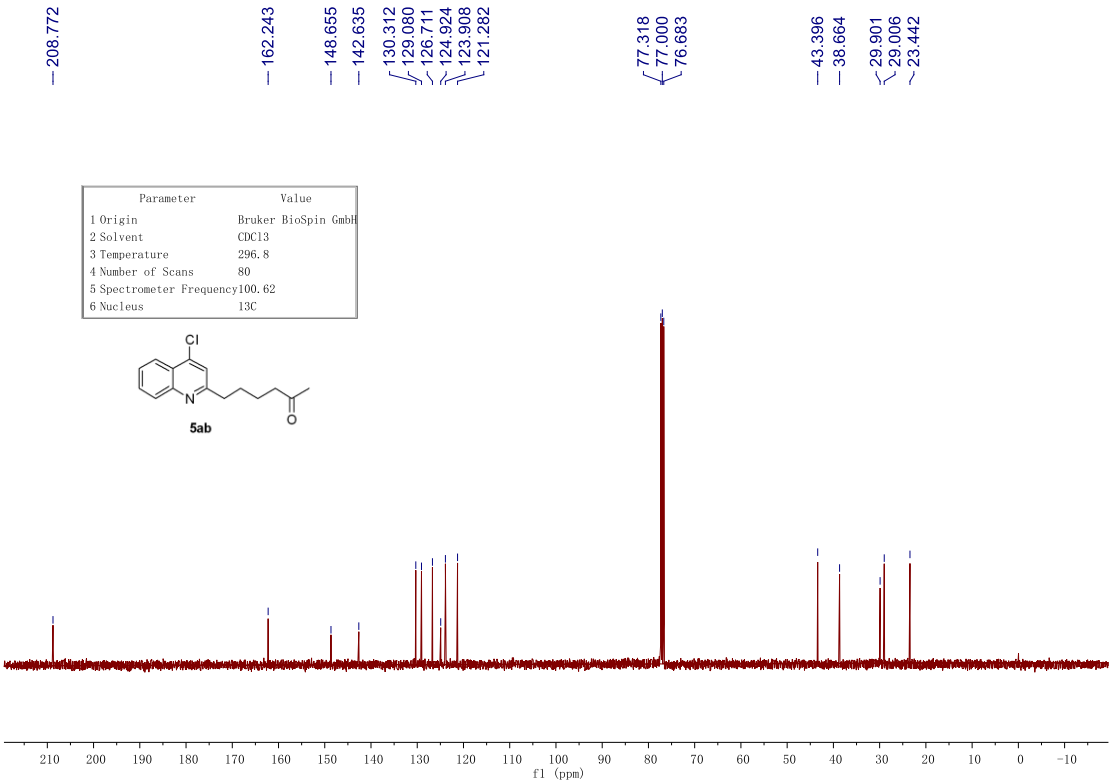

8.192
8.190
8.171
8.169
8.067
8.066
8.046
8.045
7.751
7.747
7.733
7.730
7.726
7.712
7.709
7.595
7.592
7.578
7.575
7.572
7.557
7.554
7.433
7.260
5.516
5.514
5.512
3.108
3.099
3.090
3.088
3.079
3.071
3.058
2.393
2.389
2.386
2.381
2.378
2.373
2.216
2.120
2.113
2.106
2.088
2.079
2.073
2.032
1.978
1.964
1.951
1.947
1.934
1.921
1.917
1.906
1.902
1.725
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
5z
0.97
0.99
1.02
1.01
0.97
1.00
1.01
2.03
1.03
2.05
1.07
3.03
f1 (ppm)

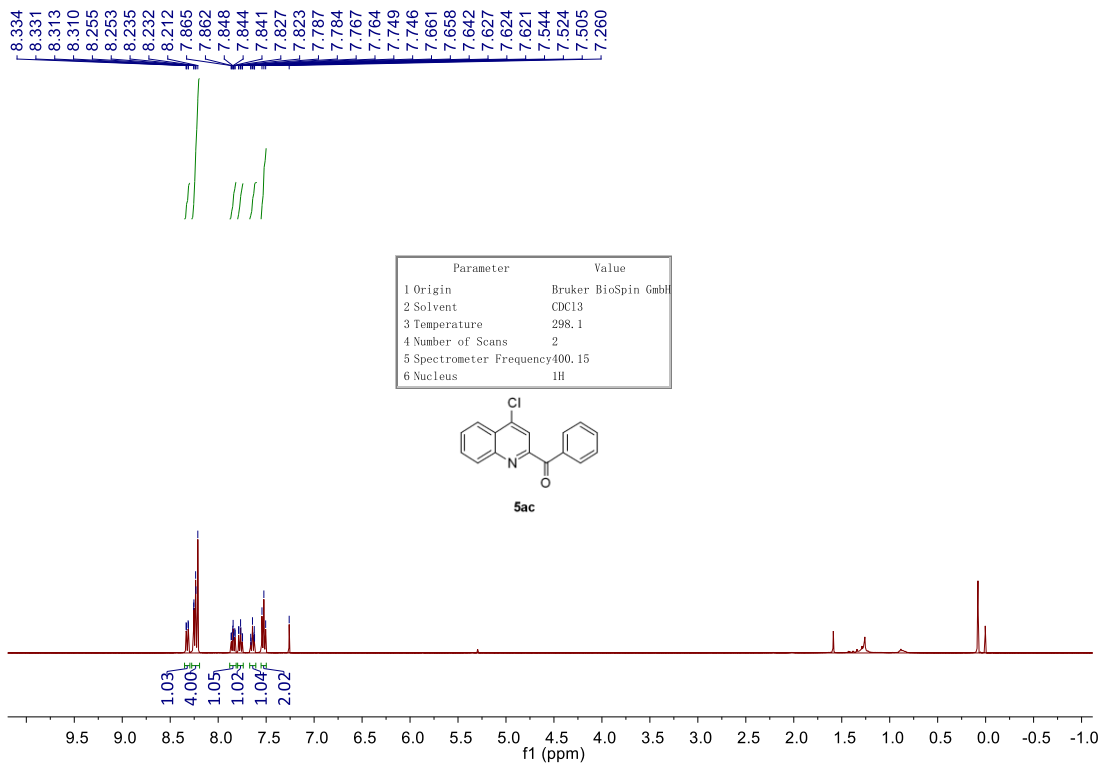

166.331
148.646
142.609
133.979
130.176
129.316
126.645
125.117
123.882
120.101
119.914
77.317
77.000
76.682
42.904
31.404
30.306
28.833
23.570
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5z
f1 (ppm)

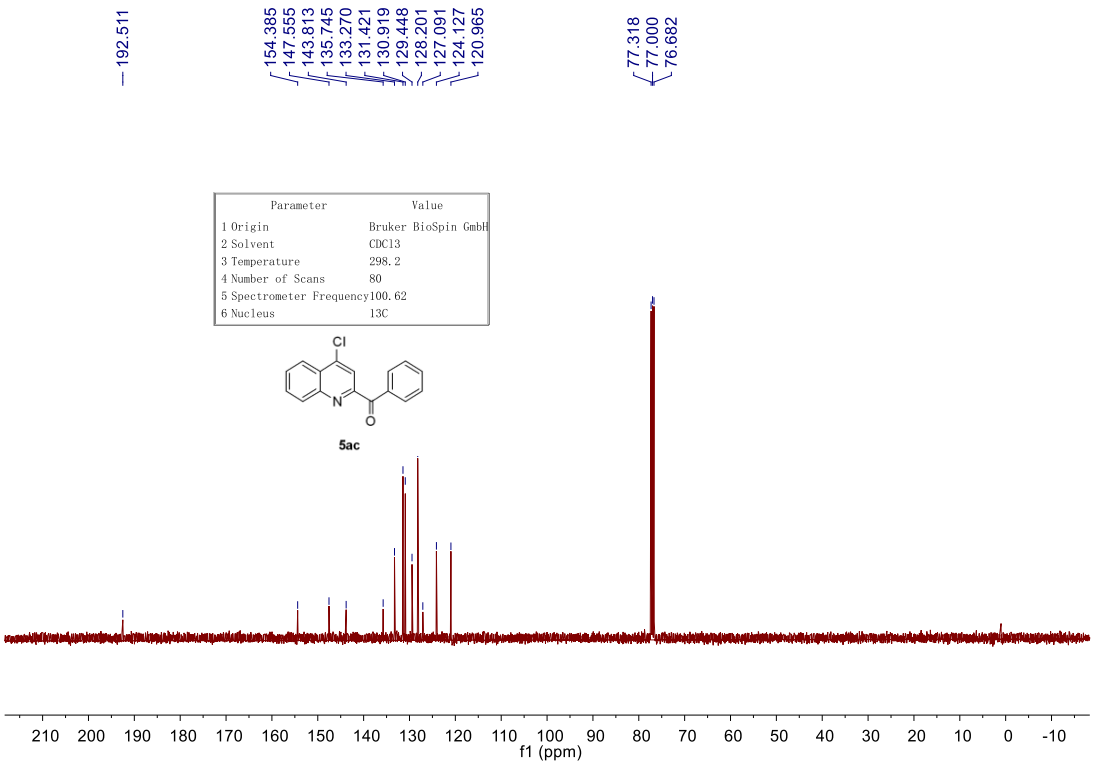

8.172
8.170
8.151
8.149
8.066
8.045
7.735
7.732
7.718
7.714
7.711
7.697
7.693
7.577
7.574
7.560
7.557
7.554
7.539
7.536
7.424
7.260
3.569
3.546
3.525
2.232
2.221
2.208
2.001
1.988
1.977
1.965
1.850
1.023
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
5aa
1.00
1.02
1.05
1.04
0.98
1.06
3.03
4.08
1.07
3.04
2.96
f1 (ppm)

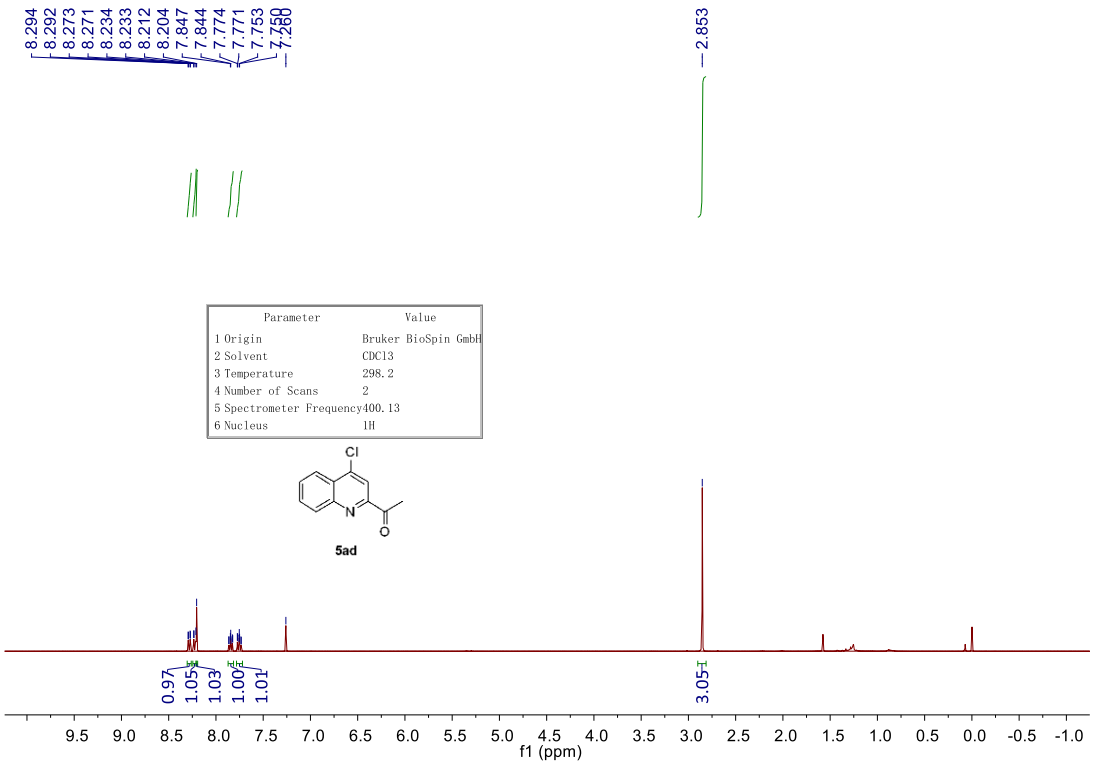

166.744
148.488
142.523
130.042
129.391
126.495
125.052
123.799
120.179
77.318
77.000
76.683
45.907
43.853
39.963
39.825
26.722
24.544
23.962
20.775
20.322
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
5aa
f1 (ppm)

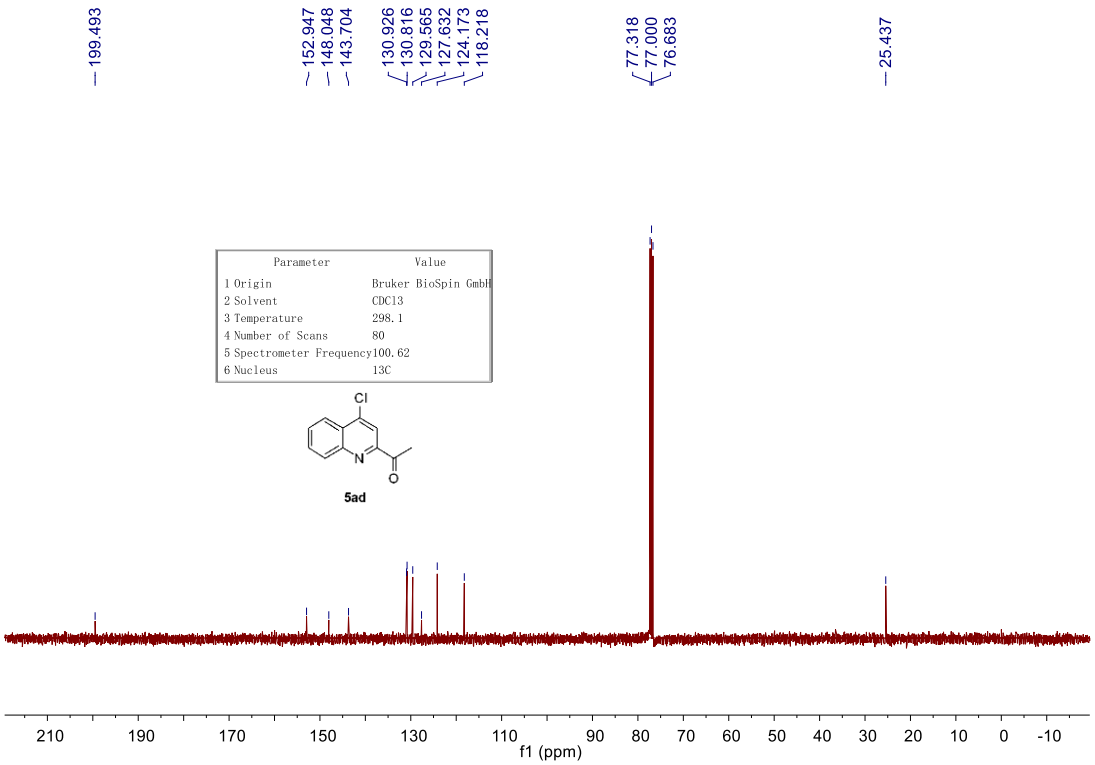

8.186
8.184
8.165
8.163
8.042
8.022
7.750
7.746
7.732
7.729
7.725
7.711
7.708
7.595
7.593
7.578
7.575
7.572
7.557
7.554
7.391
7.260
2.967
2.948
2.929
2.512
2.494
2.476
2.128
1.860
1.842
1.821
1.805
1.783
1.725
1.707
1.689
1.669
1.650
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
O
5ab
1.02
1.04
1.05
1.06
1.00
2.02
2.04
3.02
2.06
2.00
f1 (ppm)

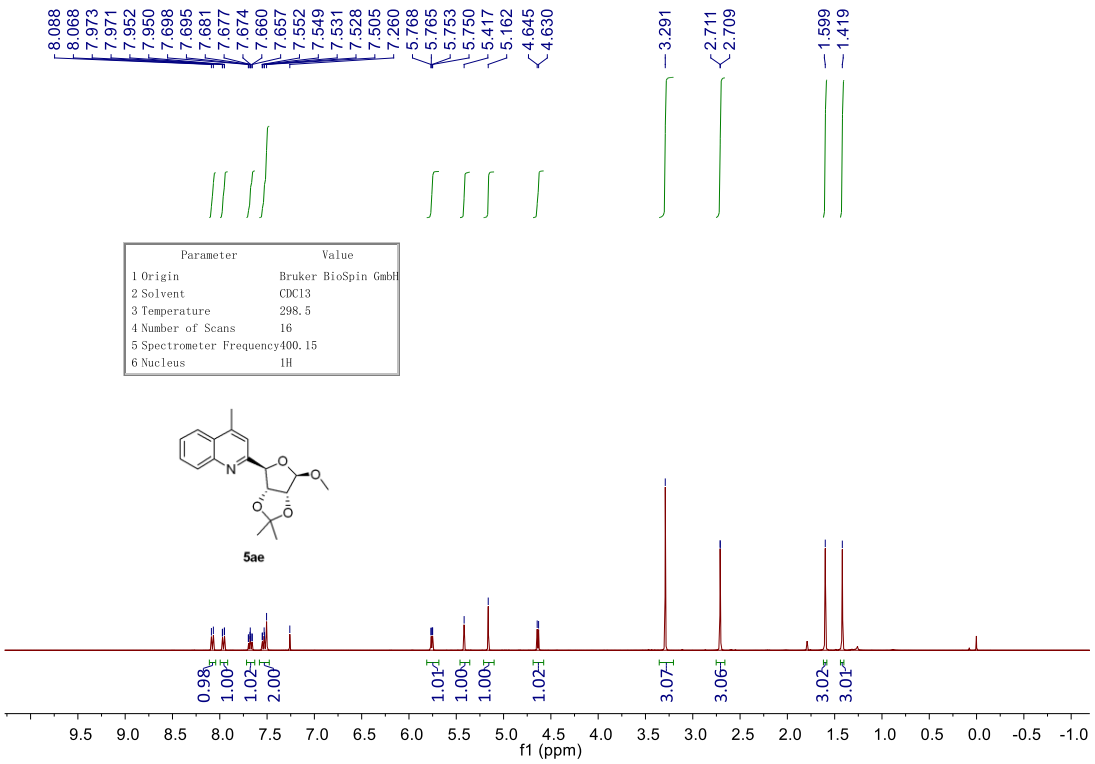

208.772
162.243
148.655
142.635
130.312
129.080
126.711
124.924
123.908
121.282
77.318
77.000
76.683
43.396
38.664
29.901
29.006
23.442
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.8
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
O
5ab
f1 (ppm)

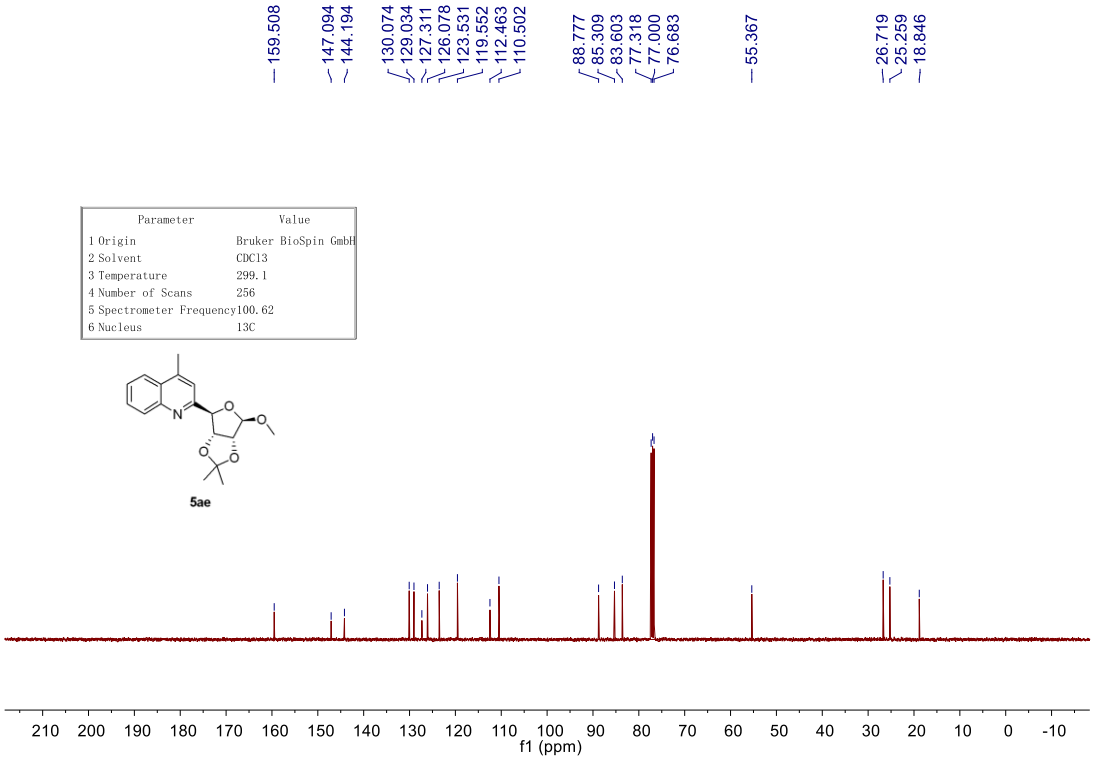

8.334
8.331
8.313
8.310
8.255
8.253
8.235
8.232
8.212
7.865
7.862
7.848
7.844
7.841
7.827
7.823
7.787
7.784
7.767
7.764
7.749
7.746
7.661
7.658
7.642
7.627
7.624
7.621
7.544
7.524
7.505
7.260
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
N
O
5ac
1.03
4.00
1.05
1.02
1.04
2.02
f1 (ppm)


192.511
154.385
147.555
143.813
135.745
133.270
131.421
130.919
129.448
128.201
127.091
124.127
120.965
77.318
77.000
76.682
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
O
5ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.294
8.292
8.273
8.271
8.234
8.233
8.212
8.204
7.847
7.844
7.774
7.771
7.753
7.750
7.280
2.853
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
N
O
5ad
0.97
1.05
1.03
1.00
1.01
3.05
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 -0.5 -1.0
f1 (ppm)


199.493
152.947
148.048
143.704
130.926
130.816
129.565
127.632
124.173
118.218
77.318
77.000
76.683
25.437
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
N
O
5ad
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.088
8.068
7.973
7.971
7.952
7.950
7.698
7.695
7.681
7.677
7.674
7.660
7.657
7.552
7.549
7.531
7.528
7.505
7.260
5.768
5.765
5.753
5.750
5.417
5.162
4.645
4.630
3.291
2.711
2.709
1.599
1.419
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.5
4 Number of Scans 16
5 Spectrometer Frequency 400.15
6 Nucleus 1H
N
O
O
O
O
5ae
0.98
1.00
1.02
2.00
1.01
1.00
1.00
1.02
3.07
3.06
3.02
3.01
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 -0.5 -1.0
f1 (ppm)


159.508
147.094
144.194
130.074
129.034
127.311
126.078
123.531
119.552
112.463
110.502
88.777
85.309
83.603
77.318
77.000
76.683
55.367
26.719
25.259
18.846
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.1
4 Number of Scans 256
5 Spectrometer Frequency 100.62
6 Nucleus 13C
5ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)