Supplementary Material

Pyridinic-N-Co single-atom catalysts unlock sustainable and efficient quinoline synthesis via hydrogen-transfer-coupled annulation

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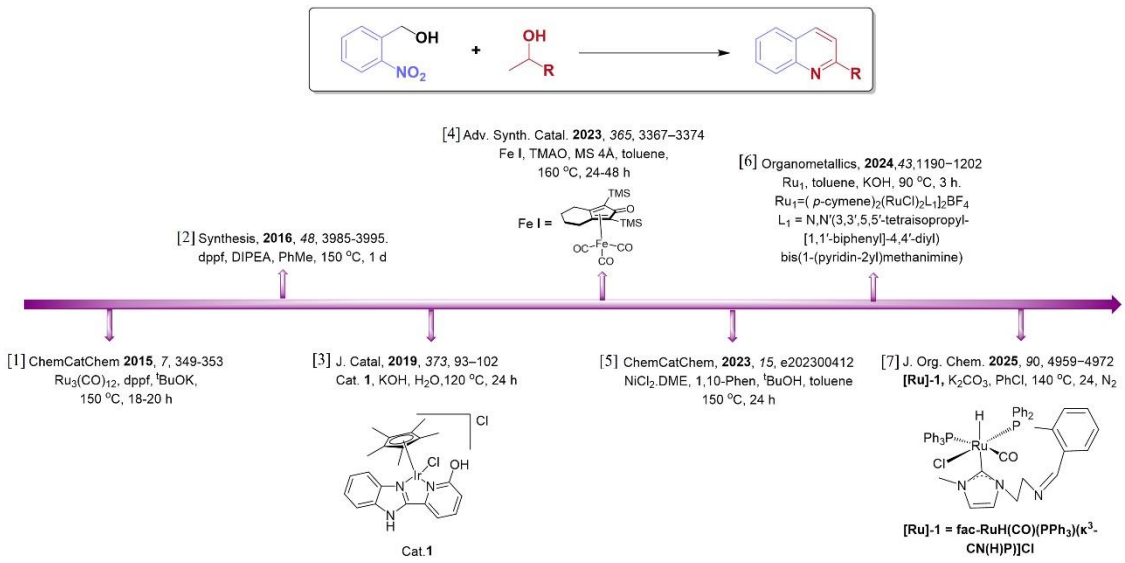
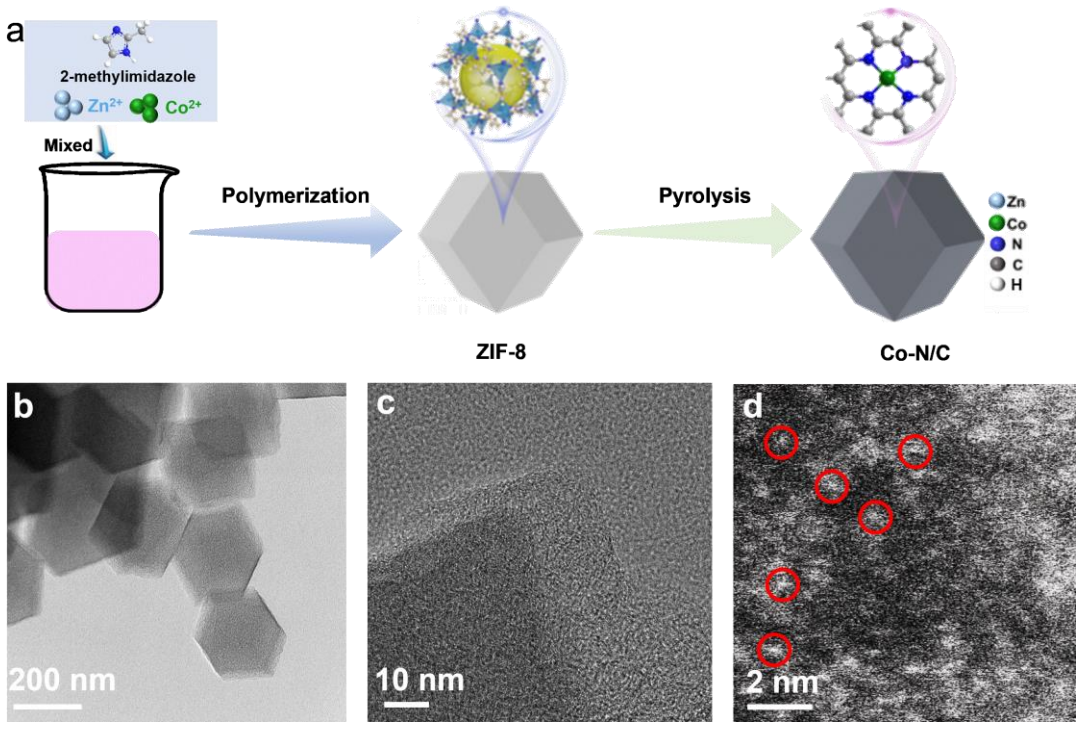
MAIN TEXT

Preparation of Cavosonstat: To a solution of Cavosonstat building block (118 mg, 0.36 mmol) in MeOH (5 mL) at 0 °C was slowly added aqueous LiOH (1 M, 4.8 mL, 4.8 mmol) over 15 min. The reaction mixture was allowed to warm to room temperature and stirred overnight. The organic solvent was removed in vacuo, and the residual aqueous solution was partitioned with Et_2O. The organic phase was extracted with H_2O (two times). The combined aqueous extract was acidified to pH 2 with 1 N HCl. The aqueous phase was then extracted with $CHCl_3$ (three times). The combined organic extract was

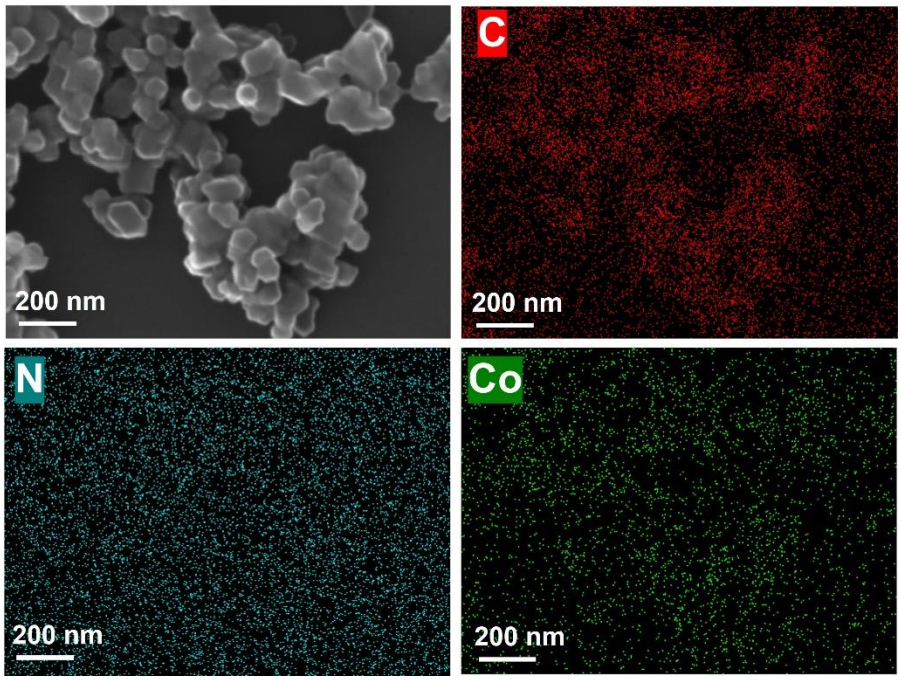
dried over $MgSO_4$ and concentrated to afford the desired product (85.84 mg, 76%).



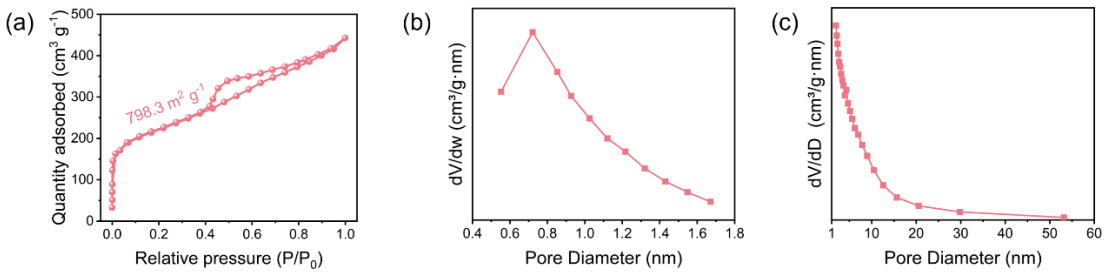
Supplementary Figure 1. The reported methods for synthesizing quinoline via a hydrogen transfer reaction. [1-7]



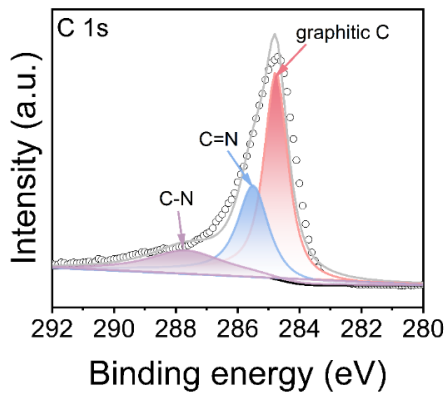
Supplementary Figure 2. (a) Schematic illustration of the synthesis procedure of Co-N/C. (b) TEM and (c) HR-TEM images of Co-N/C. (d) AC HAADF-STEM image of Co-N/C.



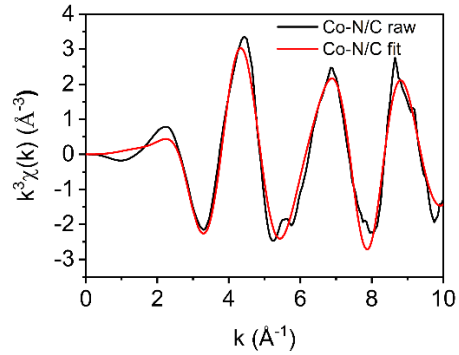
Supplementary Figure 3. EDS element mapping images of Co-N/C



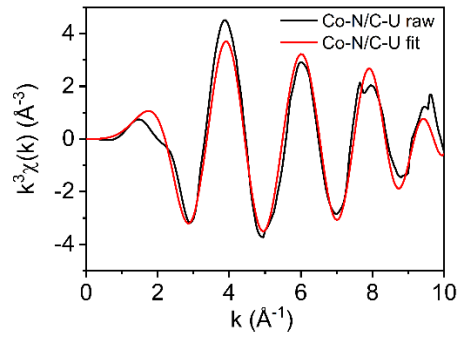
Supplementary Figure 4. Texture structure of the *as*-prepared Co-N/C catalyst. (a) N_2 adsorption-desorption isotherm curves, (b) mesoporous and (c) microporous pore-size distribution.



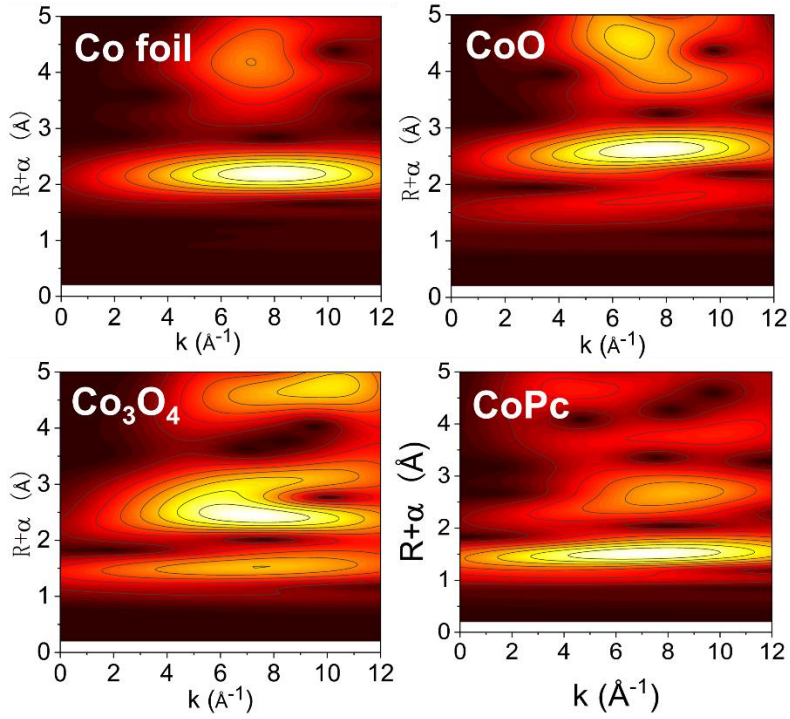
Supplementary Figure 5. XPS spectrum of C 1s for Co-N/C-U.



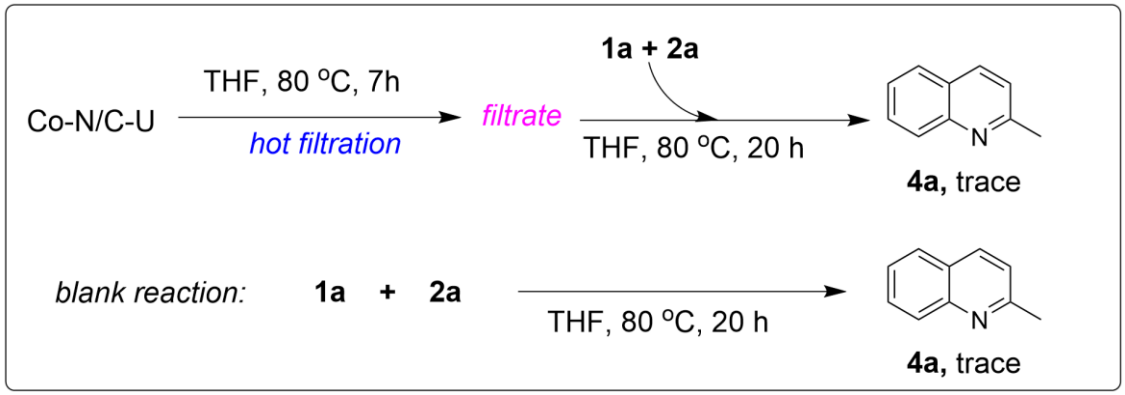
Supplementary Figure 6. EXAFS curve fitting of Co-N/C at the k space



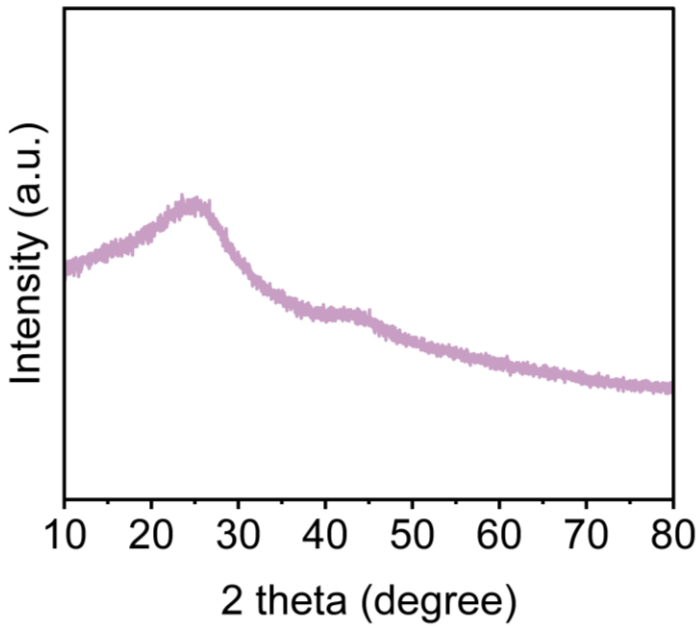
Supplementary Figure 7. EXAFS curve fitting of Co-N/C-U at the k space



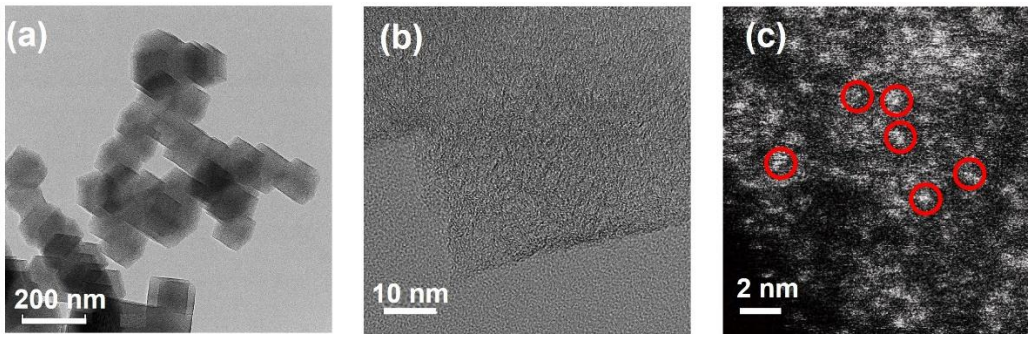
Supplementary Figure 8. Wavelet transform of Co foil, CoO, Co_3O_4 and CoPc.



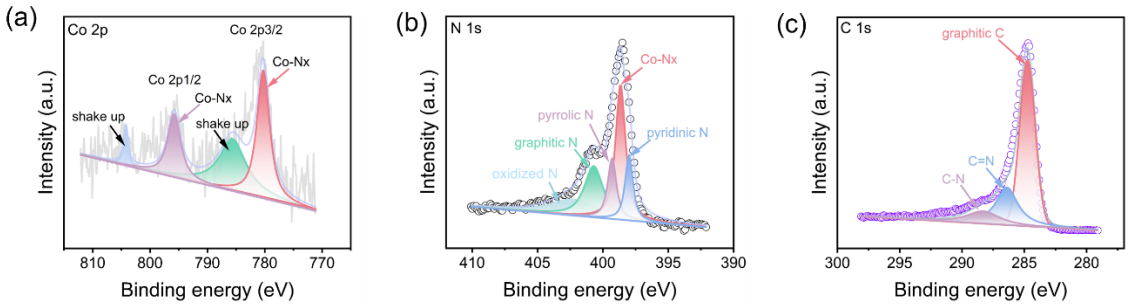
Supplementary Figure 9. Hot filtration experiments



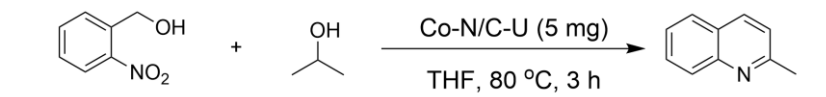
Supplementary Figure 10. XRD pattern of the spent Co-N/C-U catalyst.



Supplementary Figure 11. Structural characterization of the spent Co-N/C-U catalyst. (a & b) TEM images, (c) AC-HAADF-STEM images.

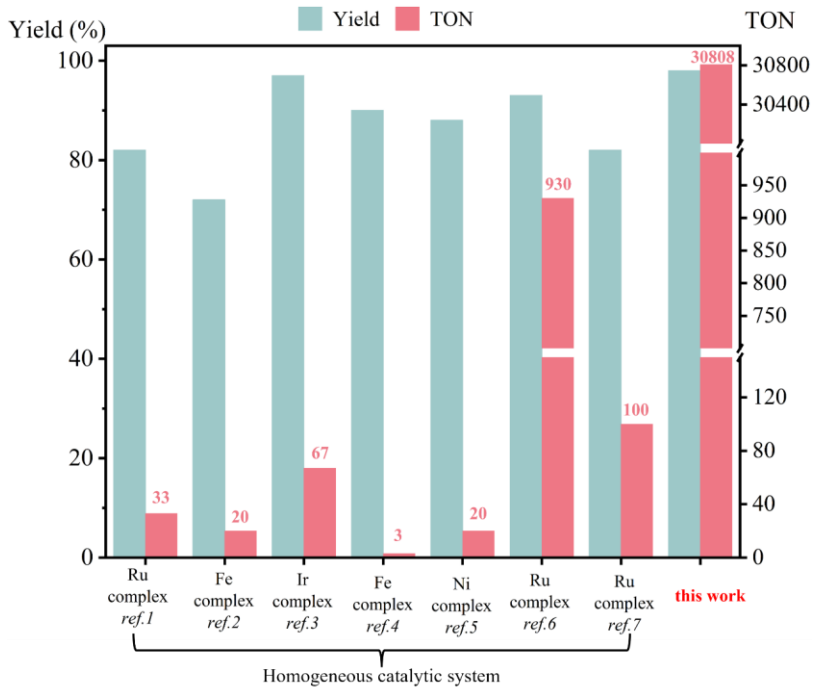


Supplementary Figure 12. XPS spectra of the spent Co-N/C-U catalyst. (a) Co 2*p*, (b) N 1*s*, and (c) C 1*s*.

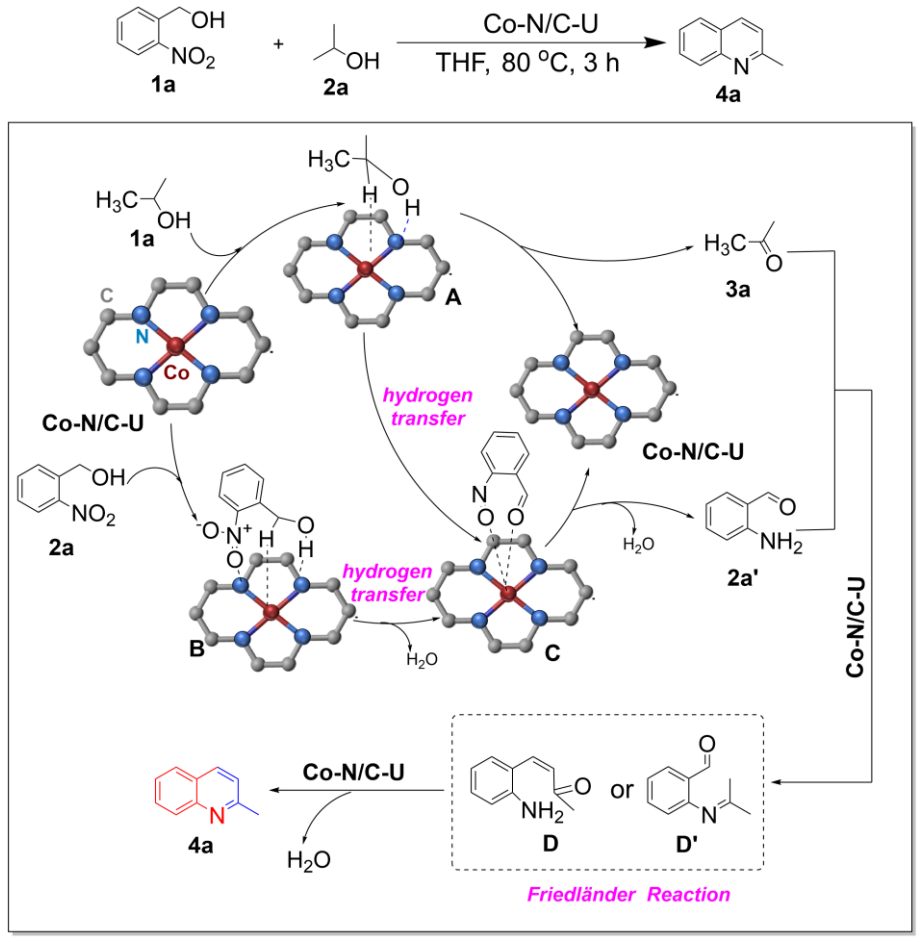


1a	**2a**	**4a**
10 mmol	22 mmol	Yield = 94%
1.53 g	1.32 g	1.35 g
100 mmol	220 mmol	Yield = 61%
15.31 g	13.22 g	8.73 g

Supplementary Figure 13. Scale-up reaction



Supplementary Figure 14. Yield and TON value compared with the reported catalytic systems.



Supplementary Figure 15. Proposed mechanism

Initially, the dissociation of the Co-N4 moiety and the coordination of the oxygen atom from 2-nitroaryl alcohol **1a** to the nitrogen atoms in the Co-N/C-U catalyst, as well as to the metal center, resulted in the formation of structure **B**. Under Co-catalysis conditions, the relatively active alcohol unit of **1a** firstly undergoes a hydrogen transfer to form a nitrosobenzene complex **C**. And the presence of excess alcohol **2a** would proceed through two successive hydrogen transfers to give ketone **3a**, and 2-aminoketone **2a′**, respectively. Then, the a-Aldol condensation or carbonyl imination of **2a′** with **3a** gives intermediate **D** or **D′**; Finally, the intramolecular condensation of **D** or **D′** affords the desired quinoline product **4a**.

Supplementary Table 1. EXAFS fitting parameters at the Co K-edge for the Co single atom catalysts with Co-N_4 sites.

Sample	Scattering path	S_0^2	CN	R (A)	$\sigma^2(10^{-3}$ Å$^2)$	ΔE_0 (eV)	R fator
Co-N/C-U	Co-N	0.74	3.9+0.1	1.92+0.02	3.9+4.2	9.2+0.5	0.0052
Co-N/C	Co-N	0.76	3.9+0.3	1.91+.0.1	3.9+4.0	9.1+0.5	0.0050

CN is the coordination number; R is the interatomic distance between absorber and backscattering atoms;

σ^2 is the Debye-Waller factor, which accounts for both thermal and structural disorders; ΔE_0 is the inner potential correction; R factor measures the goodness of fit. An E_0 value of 7709.0 eV was used to calibrate all data with respect to the first inflection point of the Co K-edge absorption of Co foil.

Supplementary Table 2. DFT-calculated single point energies, expressed in kcal/mol, for the pristine catalysts and their adsorption complexes with **1a** and **2a** across various spin states.

	Spin multiplicity	Total energy (a.u.)	Total energy (kcal/mol)	Relative energy (kcal/mol)
		Catalyst		
Co-N/C-U	2	-3900.658171	-2447702.01	0
	4	-3900.651485	-2447697.81	4.20
	6	-3900.653555	-2447699.11	2.90
Co-N/C	2	-3134.319319	-1966816.72	2.47
	4	-3134.323252	-1966819.18	0
	6	-3134.282323	-1966793.5	25.68
Co-N/C-U-1a	2	-4451.476712	-2793346.15	0
	4	-4451.471711	-2793343.01	3.13
	6	-4451.474866	-2793344.99	1.15
Co-N/C-U-2a	2	-4094.816316	-2569538.19	0
	4	-4094.809538	-2569533.93	4.25
	6	-4094.815383	-2569537.6	0.58
Co-N/C-1a	2	-3685.152313	-2312469.93	0.00
	4	-3685.150945	-2312469.07	0.86
	6	-3685.085585	-2312428.06	41.87
Co-N/C-2a	2	-3328.480819	-2088655	0.84
	4	-3328.482151	-2088655.83	0.00
	6	-3328.47194	-2088649.43	6.41

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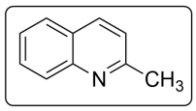
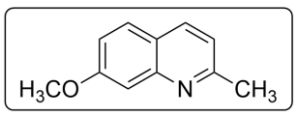
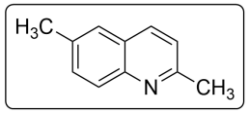
3. Spectra Data of Products



2-methylquinoline (4a): colorless oil, Rf = 0.63 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.31 (d, J = 8.4 Hz, 1H), 8.10 (dd, J = 8.1, 1.1 Hz, 1H), 7.81 – 7.78 (m, 1H), 7.63 - 7.50 (m, 2H), 7.20 (dd, J = 8.4, 0.9 Hz, 1H), 2.75 (d, J = 0.7 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 160.22, 145.10, 132.86, 129.11, 128.53, 126.65, 126.39, 124.37, 120.98, 25.63. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_9N + H^+$: 144.0813 $[M+H]^+$; found:144.0819.

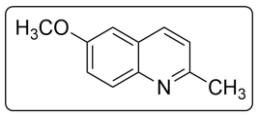


7-methoxy-2-methylquinoline (4b): colorless oil, Rf = 0.61 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13 – 8.09 (m, 1H), 7.78 (d, *J* = 8.9 Hz, 1H), 7.32 (d, *J* = 2.5 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 1H), 7.15 (dd, *J* = 8.9, 2.6 Hz, 1H), 3.88 (s, 3H), 2.60 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.60, 159.25, 149.52, 136.16, 129.25, 121.67, 120.17, 118.52, 107.31, 55.77, 25.22. **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}NO + H^+$: 174.0919 $[M+H]^+$; found:174.0901.

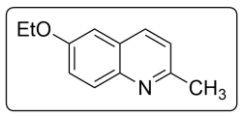


2,6-dimethylquinoline (4c): white solid, Rf = 0.60 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.63 (s, 1H), 7.51 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 2.61 (s, 3H), 2.44 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 158.12, 146.37, 135.84, 135.32, 131.87, 128.43, 126.91, 126.60, 122.51, 25.19,

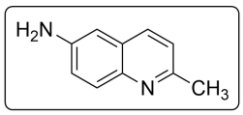
21.46. **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}N + H^+$: 158.0970 $[M+H]^+$; found:158.0921.



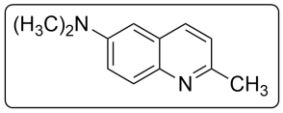
6-methoxy-2-methylquinoline (4d): white solid, Rf = 0.54 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.10 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 9.1 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.28 (d, J = 2.8 Hz, 1H), 3.86 (s, 3H), 2.59 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 157.04, 156.33, 143.75, 135.43, 130.07, 127.57, 122.70, 122.03, 106.06, 55.82, 24.97. **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}NO + H^+$: 174.0919 $[M+H]^+$; found:174.0963.



2-methyl-6-ethoxyquinoline (4e): white solid, Rf = 0.50 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.10 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 9.1 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.28 (d, J = 2.8 Hz, 1H), 4.12 (q, J = 7.0 Hz, 2H), 2.59 (s, 3H), 1.38 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 156.59, 156.28, 143.65, 135.44, 130.04, 127.60, 122.69, 122.24, 106.67, 63.81, 24.99, 15.08. **HRMS** (ESI-TOF): Calcd. for $C_{12}H_{13}NO + H^+$: 188.1075 $[M+H]^+$; found:188.1083.

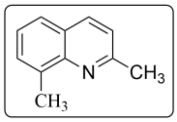


2-methylquinolin-6-amine (4f): yellow solid, Rf = 0.55 (Petroleum ether/EtOAc, v/v = 5/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.82 (d, J = 8.4 Hz, 1H), 7.64 (d, J = 8.9 Hz, 1H), 7.21 – 7.08 (m, 2H), 6.78 (d, J = 2.4 Hz, 1H), 5.49 (s, 2H), 2.52 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 153.36, 146.83, 141.96, 133.90, 129.34, 128.39, 122.34, 121.87, 105.69, 24.84. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_{10}N_2 + H^+$: 159.0922 $[M+H]^+$; found:159. 1007.

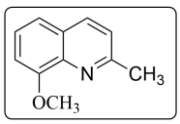


N,N,2-trimethylquinolin-6-amine (4g): brown solid, Rf = 0.51 (Petroleum ether/EtOAc, v/v = 5/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.97 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 9.2 Hz, 1H), 7.38 (dd, J = 9.2, 2.9 Hz, 1H), 7.23 (d, J = 8.4 Hz, 1H), 6.89 (d, J = 2.9 Hz, 1H), 2.99 (s, 6H),

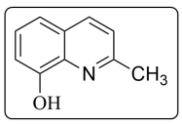
2.55 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 154.31, 148.41, 141.79, 134.70, 129.18, 128.01, 122.57, 119.73, 105.68, 40.88, 24.95. **HRMS** (ESI-TOF): Calcd. for $C_{12}H_{14}N_2$ + H^+: 187.1235 $[M+H]^+$; found:123. 1209.



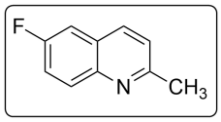
2,8-dimethylquinoline (4h): white solid, Rf = 0.59 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.12 (d, J = 8.4 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 7.0 Hz, 1H), 7.39 – 7.34 (m, 1H), 7.32 (d, J = 8.4 Hz, 1H), 2.69 (s, 3H), 2.64 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 157.95, 146.68, 136.71, 136.07, 129.76, 126.48, 126.12, 125.65, 122.20, 25.64, 18.17. **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}N$ + H^+: 158.0970 $[M+H]^+$; found:158. 0993.



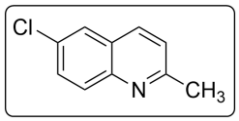
8-Methoxy-2-methylquinoline (4i): white solid, Rf = 0.58 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.17 (d, J = 8.3 Hz, 1H), 7.44 – 7.38 (m, 3H), 7.13 (dd, J = 5.7, 3.3 Hz, 1H), 3.94 (s, 3H), 2.63 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 157.62, 155.16, 139.50, 136.38, 127.64, 126.25, 122.92, 119.70, 108.77, 55.91, 25.36**.** (126 MHz, DMSO-d_6) δ . **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}NO$+ H^+: 174.0919 $[M+H]^+$; found:174. 0957.



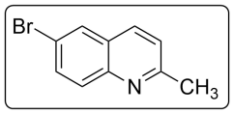
8-Hydroxyquinaldine (4j): white solid, Rf = 0.39 (Petroleum ether/EtOAc, v/v = 5/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.46 (s, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.37 – 7.30 (m, 2H), 7.06 (dd, J = 7.1, 1.8 Hz, 1H), 2.67 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 157.13, 152.99, 138.26, 136.59, 127.41, 126.84, 123.06, 118.01, 111.56, 25.18. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_9NO$+ H^+: 160.0762 $[M+H]^+$; found:160. 0793.



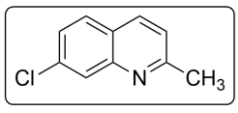
6-Fluoroquinaldine (4k): white solid, Rf = 0.59 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.20 (d, J = 8.5 Hz, 1H), 7.96 (dd, J = 9.2, 5.5 Hz, 1H), 7.69 (dd, J = 9.4, 2.9 Hz, 1H), 7.59 (td, J = 8.9, 2.9 Hz, 1H), 7.41 (d, J = 8.5 Hz, 1H), 2.62 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.81, 158.65, 144.90, 136.08, 131.28, 127.23, 123.35, 119.76, 111.13, 25.14. **^{19}F NMR** (470 MHz, DMSO-d_6) δ -110.14. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_8NF$ + H^+: 162.0719 $[M+H]^+$; found:162. 0733.



6-Chloro-2-methylquinoline (4l): white solid, Rf = 0.56 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.22 (d, J = 8.5 Hz, 1H), 8.04 (d, J = 2.4 Hz, 1H), 7.92 (d, J = 9.0 Hz, 1H), 7.70 (dd, J = 9.0, 2.4 Hz, 1H), 7.46 (d, J = 8.4 Hz, 1H), 2.64 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 159.98, 146.21, 135.93, 130.81, 130.39, 130.34, 127.48, 126.97, 123.66, 25.36. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_8NCl$+ H^+: 178.0424 $[M+H]^+$; found:178. 0439.

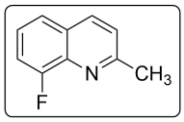


6-Bromo-2-methylquinoline (4m): white solid, Rf = 0.51 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.21 – 8.15 (m, 2H), 7.83 (dt, J = 9.0, 0.6 Hz, 1H), 7.78 (dd, J = 8.9, 2.2 Hz, 1H), 7.43 (d, J = 8.5 Hz, 1H), 2.62 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.11, 146.40, 135.85, 132.89, 130.94, 130.25, 128.07, 123.63, 118.90, 25.41. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_8NBr$+ H^+: 221.9918 $[M+H]^+$; found:221. 1103.

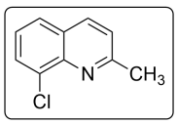


7-chloro-2-methylquinoline (4n): white solid, Rf = 0.53 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.28 (dd, J = 8.4, 0.7 Hz, 1H), 8.01 – 7.90 (m, 2H), 7.55 (dd, J = 8.6, 2.2 Hz, 1H), 7.44 (d, J = 8.4 Hz, 1H), 2.65 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.80, 148.16, 136.64, 134.38, 130.28, 127.40, 126.77, 125.32, 123.14, 25.40. **HRMS** (ESI-TOF):

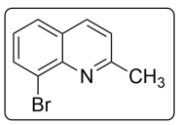
Calcd. for $C_{10}H_8NCl + H^+$: 178.0424 $[M+H]^+$; found:178. 0419.



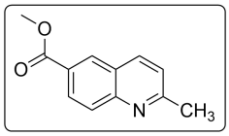
8-fluoro-2-methyl-Quinoline (4o): white solid, Rf = 0.52 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.30 (d, J = 8.5 Hz, 1H), 7.74 (d, J = 7.5 Hz, 1H), 7.56 – 7.46 (m, 3H), 2.68 (s, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 159.80, 137.57, 136.50, 128.43, 126.04, 125.96, 124.18, 123.72, 113.98, 25.45. **^{19}F NMR** (470 MHz, DMSO-d_6) δ -134.96. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_8NF + H^+$: 162.0719 $[M+H]^+$; found:162.0733.



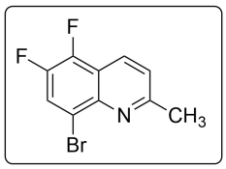
8-chloro-2-methylquinoline (4p): white solid, Rf = 0.55 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.28 (d, J = 8.4 Hz, 1H), 7.89 - 7.86 (m, 1.0 Hz), 7.49 - 7.46 (m, 2H), 2.68 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.40, 143.57, 137.22, 132.16, 129.99, 128.15, 127.77, 126.31, 123.63, 25.65.. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_8NCl + H^+$: 178.0424 $[M+H]^+$; found:178.0410.



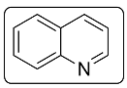
8-bromo-2-methylquinoline (4q): white solid, Rf = 0.52 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.27 (d, J = 8.4 Hz, 1H), 8.07 (dd, J = 7.5, 1.3 Hz, 1H), 7.93 (dd, J = 8.1, 1.2 Hz, 1H), 7.48 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 7.8 Hz, 1H), 2.69 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.66, 144.37, 137.36, 133.49, 128.53, 128.15, 126.92, 123.89, 123.65, 25.68.. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_8NBr + H^+$: 221.9918 $[M+H]^+$; found:221.1107.



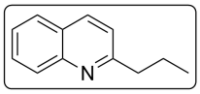
Methyl 2-methyl-6-quinolinecarboxylate (4r): white solid, Rf = 0.48 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.59 (d, J = 1.8 Hz, 1H), 8.41 (d, J = 8.5 Hz, 1H), 8.13 (dd, J = 8.7, 2.0 Hz, 1H), 7.96 (d, J = 8.7 Hz, 1H), 7.49 (d, J = 8.5 Hz, 1H), 3.90 (s, 1H), 2.67 (s, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.46, 162.17, 149.61, 137.97, 131.17, 129.24, 128.84, 126.93, 125.94, 123.60, 52.85, 25.60. **HRMS** (ESI-TOF): Calcd. for $C_{12}H_{11}NO_2$+ H^+: 202.0868 $[M+H]^+$; found:202.0851.



8-bromo-5,6-difluoro-2-methylquinoline (4s): brown solid, Rf = 0.48 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.38 (d, J = 8.3 Hz, 1H), 8.30 (t, J = 9.3 Hz, 1H), 7.60 (d, J = 8.5 Hz, 1H), 2.70 (s, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.07, 146.29, 143.83, 141.11, 129.73, 124.45, 123.49, 123.26, 118.89, 25.53. **^{19}F NMR** (470 MHz, DMSO-d_6) δ -107.62, -109.21. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_6NBrF_2$+ H^+: 257.9730 $[M+H]^+$; found:257.9716.

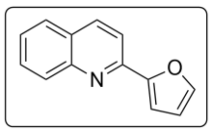


Quinoline (4t): white oli, Rf = 0.63 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.91 (dd, J = 4.2, 1.7 Hz, 1H), 8.33 (d, J = 8.3 Hz, 1H), 8.04 (d, J = 8.5 Hz, 1H), 7.95 (d, J = 9.0 Hz, 1H), 7.74 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.58 (ddd, J = 8.0, 7.1, 1.1 Hz, 1H), 7.50 (dd, J = 8.3, 4.2 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 151.06, 148.27, 136.49, 130.00, 129.47, 128.59, 128.44, 127.04, 121.95. **HRMS** (ESI-TOF): Calcd. for C_9H_7N + H^+: 130.0657 $[M+H]^+$; found: 130.0664.

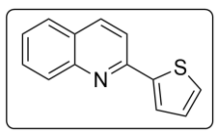


2-propylquinoline (4u): white oli, Rf = 0.63 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** NMR (500 MHz, Chloroform-d) δ 8.04 (d, J = 8.4 Hz, 1H, 1H), 7.88 (s, 1H), 7.74 (d, J = 1.2 Hz, 1H), 7.73 (d, J = 1.2 Hz, 1H), 7.62 (t, J = 7.7 Hz, 1H), 7.47 -7.44 (m, 1H), 2.84 (q, J = 7.8 Hz, 2H), 1.87 -1.79 (m,

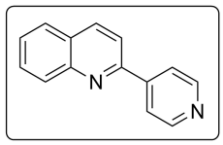
2H), 1.07 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 162.11, 146.17, 135.51, 134.29, 128.62, 128.27, 127.43, 127.02, 125.79, 37.77, 23.12, 14.51**. HRMS** (ESI-TOF): Calcd. for $C_{12}H_{13}N + H^+$: 172.1126 $[M+H]^+$; found:172.1119.



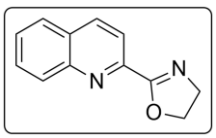
2-(furan-2-yl)quinoline (4v): yellow solid, Rf = 0.65 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-*d*$_6$) δ 8.36 (dd, J = 8.6, 0.8 Hz, 1H), 7.96 (dd, J = 8.4, 1.0 Hz, 1H), 7.94 – 7.87 (m, 3H), 7.71 (d, J = 8.4 Hz, 1H), 7.52 (m, 1H), 7.32 (dd, J = 3.4, 0.8 Hz, 1H), 6.68 (dd, J = 3.4, 1.8 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-*d*$_6$) δ 153.62, 148.94, 147.96, 145.49, 137.60, 130.69, 129.12, 128.49, 127.35, 126.85, 117.88, 113.12, 111.17. **HRMS** (ESI-TOF): Calcd. for $C_{13}H_9NO + H^+$: 196.0757 $[M+H]^+$; found: 196.0726.



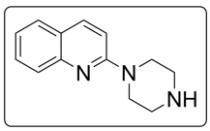
2-(thiophen-2-yl)quinoline (4w): white solid, Rf = 0.60 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.27 (d, J = 8.4 Hz, 1H), 8.05 – 7.99 (m, 1H), 7.89 – 7.83 (m, 1H), 7.85 – 7.77 (m, 2H), 7.53 (td, J = 7.3, 1.2 Hz, 1H), 7.25 (dd, J = 4.7, 1.9 Hz, 1H), 7.21 – 7.14 (m, 2H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 151.35, 148.94, 141.75, 129.76, 129.16, 128.31, 127.96, 127.78, 127.53, 126.25, 124.48, 123.60, 117.65. **HRMS** (ESI-TOF): Calcd. for $C_{13}H_9NS + H^+$: 212.0534 $[M+H]^+$; found:212.0525



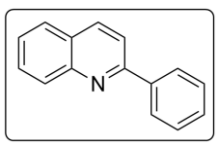
2-(pyridin-4-yl)quinoline (4x): white solid, Rf = 0.53 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.67 – 8.61 (m, 2H), 8.32 (d, *J* = 8.4 Hz, 1H), 8.17 – 8.07 (m, 3H), 7.91 – 7.83 (m, 2H), 7.84 – 7.77 (m, 1H), 7.54 (td, *J* = 7.6, 1.3 Hz, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 153.22, 149.46, 149.02, 134.30, 129.42, 129.03, 127.39, 126.95, 126.25, 124.58, 121.20, 120.35. **HRMS** (ESI-TOF): Calcd. for $C_{14}H_{10}N_2 + H^+$: 207.0922 $[M+H]^+$; found:207.0931.



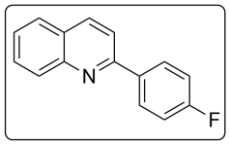
2-(quinolin-2-yl)-4,5-dihydrooxazole (4y): white solid, Rf = 0.56 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.46 (d, J = 8.6 Hz, 1H), 8.10 (t, J = 8.5 Hz, 2H), 8.03 (d, J = 8.1 Hz, 1H), 7.89 – 7.73 (m, 1H), 7.68 (t, J = 7.5 Hz, 1H), 4.49 (t, J = 9.7 Hz, 2H), 4.06 (t, J = 9.6 Hz, 2H). **^{13}C NMR NMR** (126 MHz, DMSO-d_6) δ 163.83, 147.38, 147.13, 137.46, 130.87, 129.93, 128.76, 128.53, 128.50, 121.18, 68.32, 55.22. **HRMS** (ESI-TOF): Calcd. for $C_{12}H_{10}N_2O$ + H^+: 119.0871 $[M+H]^+$; found:119.0827.



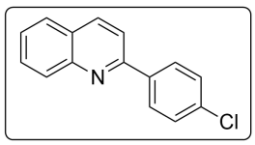
2-(piperazin-1-yl)quinoline (4z): white solid, Rf = 0.57 (Petroleum ether/EtOAc, v/v = 10/1) **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.1 (d, J = 8.4 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.72 (dt, J = 7.6, 0.8 Hz, 1H), 7.54 – 7.47 (m, 1H), 7.34 – 7.28 (m, 1H), 7.24 (d, J = 8.4 Hz, 1H), 3.62 (t, J = 5.1 Hz, 4H), 2.69 (dtd, J = 7.9, 5.0, 4.0 Hz, 4H). **^{13}C NMR NMR** (126 MHz, DMSO-d_6) δ 157.80, 147.79, 137.78, 129.88, 127.90, 126.50, 123.21, 122.42, 110.61, 46.20, 46.05. **HRMS** (ESI-TOF): Calcd. for $C_{13}H_{15}N_3$ + H^+: 214.1344 $[M+H]^+$; found:214.1369.



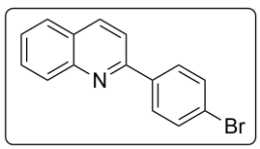
2-phenylquinoline (4aa): white solid, Rf = 0.61 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-d) δ 8.26 (d, J = 8.6 Hz, 1H), 8.21 – 8.16 (m, 1H), 7.87 (dd, J = 22.6, 8.9 Hz, 1H), 7.78 – 7.72 (m, 1H), 7.58 – 7.52 (m, 2H), 7.51 – 7.44 (m, 1H), 7.40 – 7.31 (m, 2H), 7.21 – 7.13 (m, 1H), 6.77 – 6.60 (m, 1H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 154.68, 152.02, 148.90, 147.93, 137.32, 130.53, 128.92, 128.38, 127.08, 126.50, 117.65, 112.45, 109.41, 14.09. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{12}N$ + H^+: 206..0970 $[M+H]^+$; found: 206.0943.



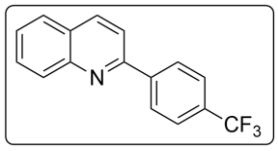
2-(4-fluorophenyl)quinoline (4ab): white solid, Rf = 0.57 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.28 (d, J = 8.5 Hz, 1H), 8.18 (dd, J = 8.9, 5.4 Hz, 1H), 7.86 (d, J = 8.6 Hz, 1H), 7.77 (t, J = 8.4 Hz, 1H), 7.57 (t, J = 8.0 Hz, 1H), 7.37 – 7.30 (m, 1H), 7.25 – 7.15 (m, 2H), 7.02 (t, J = 8.7 Hz, 1H), 6.77 – 6.60 (m, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 156.12, 129.91, 129.40, 129.22, 127.63, 126.85, 118.99, 118.10, 116.14, 115.97, 115.63, 115.46, 113.20. **^{19}F NMR** (470 MHz, Chloroform-*d*) δ -105.17. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{10}NF + H^+$: 224.0876 $[M+H]^+$; found: 224.0877.



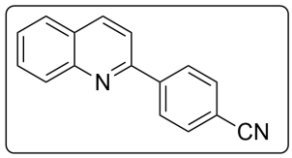
2-(4-chlorophenyl)quinoline (4ac): white solid, Rf = 0.55 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.26 (d, J = 8.6 Hz, 1H), 8.13 (d, J = 8.6 Hz, 2H), 7.85 (dd, J = 8.3, 4.3 Hz, 2H), 7.76 (t, J = 7.0 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.51 (d, J = 8.6 Hz, 2H), 7.30(s, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 156.02, 137.55, 135.88, 130.25, 129.40, 129.19, 129.06, 128.84, 127.62, 127.31, 126.80, 118.82, 113.01. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{10}NCl + H^+$: 240.0580 $[M+H]^+$; found: 240.0581.



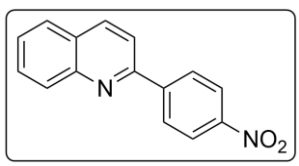
2-(4-bromophenyl)quinoline (4ad): white solid, Rf = 0.54 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.32 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.85 – 7.75 (m, 4H), 7.59 – 7.52 (m, 3H).. **^{13}C NMR** (126 MHz, DMSO-d_6) δ154.55, 149.46, 134.84, 131.48, 129.41, 129.00, 128.69, 127.61, 126.95, 126.32, 124.66, 121.33, 119.54.. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{10}BrN + H^+$: 284.0075 $[M+H]^+$; found: 284.0070.



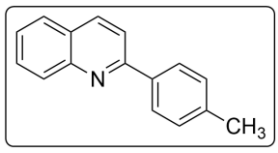
2-(4-(trifluoromethyl)phenyl)quinoline (4ae): white solid, Rf = 0.56 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.30 (t, J = 7.6 Hz, 3H), 8.25 (d, J = 7.9 Hz, 1H), 7.91 (d, J = 8.6 Hz, 1H), 7.88 (d, J = 8.2 Hz, 1H), 7.79 (t, J = 8.3 Hz, 3H), 7.59 (t, J = 7.0 Hz, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 155.74, 137.62, 130.34, 129.67, 129.59, 128.07, 127.66, 127.54, 127.11, 125.95, 125.93, 125.90, 125.87, 119.04. **^{19}F NMR** (470 MHz, Chloroform-*d*) δ -62.86. **HRMS** (ESI-TOF): Calcd. for $C_{16}H_{10}NF_3$ + H^+: 274.0844 $[M+H]^+$; found: 274.0840.



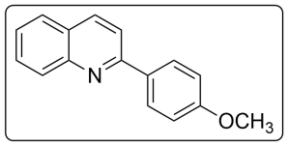
4-(quinolin-2-yl)benzonitrile (4af): white solid, Rf = 0.55 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.42 – 8.34 (m, 4H), 8.32 (d, J = 8.6 Hz, 1H), 8.20 (d, J = 8.6 Hz, 1H), 7.94 (d, J = 8.6 Hz, 1H), 7.88 (d, J = 8.1 Hz, 1H), 7.79 (t, J = 7.0 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 155.33, 149.46, 137.28, 132.51, 129.37, 129.36, 127.72, 127.58, 126.83, 126.27, 124.44, 119.53, 118.51, 112.67. **HRMS** (ESI-TOF): Calcd. for $C_{16}H_{10}N_2$ + H^+: 231.0922 $[M+H]^+$; found: 231.0911.



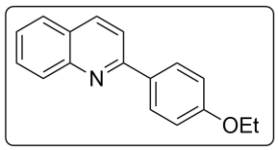
2-(4-nitrophenyl)quinoline (4ag): white solid, Rf = 0.53 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.31 (dd, *J* = 8.7, 3.0 Hz, 3H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.89 (t, *J* = 9.0 Hz, 2H), 7.85 – 7.75 (m, 3H), 7.60 (t, *J* = 7.5 Hz, 1H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 154.93, 147.96, 143.65, 137.67, 132.70, 130.42, 129.66, 128.23, 127.62, 127.57, 127.32, 118.79, 112.88. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{10}N_2O_2$ + H^+: 251.0821 $[M+H]^+$; found: 251.0815.



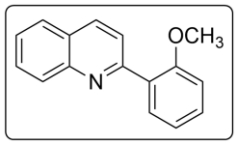
2-(*p*-tolyl)quinoline (4ah): white solid, Rf = 0.64 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 8.5 Hz, 2H), 8.07 (d, *J* = 8.2 Hz, 2H), 7.76 – 7.70 (m, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 2H), 6.74 – 6.57 (m, 2H), 2.43 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 157.32, 148.25, 139.89, 136.37, 130.03, 129.75, 129.35, 127.70, 127.18, 126.42, 119.12, 117.59, 112.92, 21.50. **HRMS** (ESI-TOF): Calcd. for $C_{16}H_{13}N + H^+$: 220.1126 $[M+H]^+$; found: 220.1143.



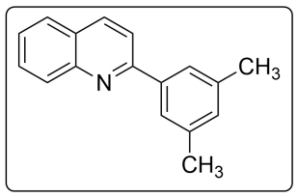
2-(4-methoxyphenyl)quinoline (4ai): white solid, Rf = 0.60 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.16 (dd, *J* = 19.7, 8.8 Hz, 4H), 7.82 (dd, *J* = 15.3, 9.0 Hz, 2H), 7.75 – 7.68 (m, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 8.9 Hz, 2H), 3.89 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 160.88, 157.02, 148.35, 136.77, 132.33, 129.70, 128.99, 127.55, 126.99, 126.03, 118.70, 114.31, 112.90, 55.40. **HRMS** (ESI-TOF): Calcd. for $C_{16}H_{13}NO + H^+$: 236.1075 $[M+H]^+$; found: 236.1043.



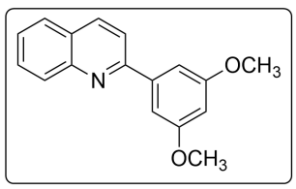
2-(4-ethoxyphenyl)quinoline (4aj): white solid, Rf = 0.58 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*)) δ 8.26 (d, J = 8.5 Hz, 2H), 7.88 (d, J = 8.6 Hz, 2H), 7.75 – 7.68 (m, 2H), 7.56 (d, J = 8.0 Hz, 1H), 7.45 (t, J = 7.9 Hz, 1H), 7.18 (dd, J = 8.5, 7.4 Hz, 2H), 4.31 (s, 2H), 1.25 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 157.15, 148.14, 141.19, 137.38, 129.98, 129.36, 127.59, 126.65, 120.23, 119.36, 117.71, 115.80, 112.79, 55.59, 14.26. **HRMS** (ESI-TOF): Calcd. for $C_{17}H_{15}NO + H^+$: 250.1232 $[M+H]^+$; found: 250.1233.



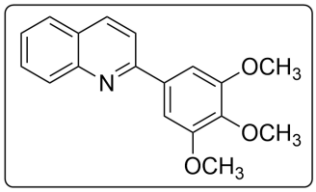
2-(2-methoxyphenyl)quinoline (4ak): white solid, Rf = 0.58 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 22.1, 8.5 Hz, 2H), 7.89 (d, J = 8.6 Hz, 1H), 7.85 (dd, J = 7.6, 1.8 Hz, 2H), 7.72 (t, J = 7.0 Hz, 1H), 7.54 (t, J = 6.9 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.18 – 7.11 (m, 1H), 7.04 (d, J = 9.2 Hz, 1H), 3.87 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 157.26, 157.15, 148.15, 135.43, 131.61, 130.55, 129.52, 129.46, 127.51, 127.14, 126.38, 123.58, 121.38, 111.49, 55.75. **HRMS** (ESI-TOF): Calcd. for $C_{16}H_{13}NO + H^+$: 236.1075 $[M+H]^+$; found: 236.1061.



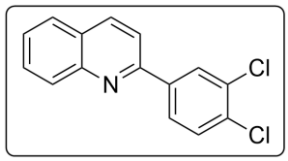
2-(3,5-dimethylphenyl)quinoline (4al): white solid, Rf = 0.52 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.32 (t, J = 9.3 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 8.03 – 7.95 (m, 1H), 7.89 (d, J = 5.5 Hz, 1H), 7.83 (s, 2H) , 7.71 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 6.99 (s, 1H), 2.29 (s, 6H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 156.78, 148.08, 139.09, 138.22, 137.36, 131.40, 130.23, 129.56, 128.20, 127.42, 126.69, 125.48, 119.23, 21.47. **HRMS** (ESI-TOF): Calcd. for $C_{17}H_{15}N + H^+$: 234.1283 $[M+H]^+$; found: 234.1196.



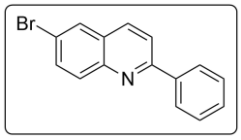
2-(3,5-dimethoxyphenyl)quinoline (4am): white solid, Rf = 0.53 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.25 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.6 Hz, 1H), 7.78 – 7.53 (m, 1H), 7.34 (s, 1H), 7.20 – 7.13 (m, 1H), 6.72 (t, J = 7.3 Hz, 1H), 6.64 (d, J = 8.7 Hz, 1H), 6.54 (d, J = 2.3 Hz, 1H), 6.37 (t, J = 2.3 Hz, 1H), 3.92 (m, 3H), 3.78 (m, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 161.27, 157.06, 142.08, 130.14, 129.35, 127.59, 126.72, 119.40, 117.76, 113.00, 105.86, 105.36, 99.16, 55.43. **HRMS** (ESI-TOF): Calcd. for $C_{17}H_{15}NO_2 + H^+$: 266.1181 $[M+H]^+$; found: 266.1161.



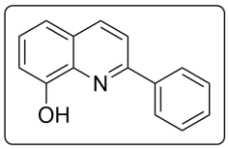
2-(3,4,5-trimethoxyphenyl)quinoline (4an): white solid, Rf = 0.50 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.10 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 8.6 Hz, 1H), 7.65 – 7.33 (m, 1H), 7.26 (s, 1H), 7.07 – 6.98 (m, 2H), 6.51 (d, J = 9.6 Hz, 1H), 6.46 (s, 1H), 3.87 (s, 3H), 3.69 (s, 6H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 156.97, 153.48, 148.18, 135.26, 129.38, 127.60, 126.61, 119.13, 117.89, 115.22, 113.05, 105.02, 104.31, 60.99, 56.18. **HRMS** (ESI-TOF): Calcd. for $C_{18}H_{17}NO_3$ + H^+: 296.1287 $[M+H]^+$; found: 296.1271.



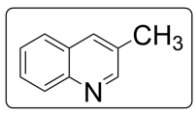
2-(3,4-dichlorophenyl)quinoline (4ao): white solid, Rf = 0.50 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.31 (dd, J = 8.2, 6.1 Hz, 3H), 7.93 – 7.86 (m, 2H), 7.82 (d, J = 8.5 Hz, 2H), 7.78 (t, J = 7.7 Hz, 1H), 7.60 (t, J = 7.5 Hz, 1H).. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 154.97,149.47, 147.93, 143.38, 137.81, 132.76, 130.53, 129.66, 128.31, 127.69, 127.63, 127.41, 118.92, 118.86, 112.97. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_9NCl_2$ + H^+: 274.0190 $[M+H]^+$; found: 274.0193.



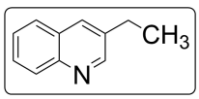
6-bromo-2-phenylquinoline (4ap): white solid, Rf = 0.53(Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.42 (d, J = 8.7 Hz, 1H), 8.28 (d, J = 2.2 Hz, 1H), 8.27 – 8.24 (m, 2H), 8.19 (d, J = 8.7 Hz, 1H), 7.99 (d, J = 9.0 Hz, 1H), 7.87 (dd, J = 8.9, 2.3 Hz, 1H), 7.55 (t, J = 7.2 Hz, 2H), 7.53 – 7.48 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6)**δ** 157.09, 146.60, 138.71, 136.92, 133.40, 131.72, 130.33, 130.27, 129.37, 128.72, 127.74, 120.14, 119.72. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{10}NBr$ + H^+: 284.0075 $[M+H]^+$; found: 284.0044.



2-phenylquinolin-8-ol (4aq): white solid, Rf = 0.55 (Petroleum ether/EtOAc, v/v = 10/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 9.68 (s, 1H), 8.49 (dt, J = 8.4, 1.9 Hz, 2H), 8.38 (d, J = 8.7 Hz, 1H), 8.17 (d, J = 8.7 Hz, 1H), 7.54 (d, J = 7.3 Hz. 2H), 7.49 (d, J = 7.2 Hz. 1H), 7.46 – 7.35 (m, 2H), 7.14 (dd, J = 7.0, 1.9 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 154.36, 153.70, 138.71, 138.54, 137.64, 130.04, 129.18, 128.21, 127.95, 127.84, 119.28, 118.05, 112.00. **HRMS** (ESI-TOF): Calcd. for $C_{15}H_{11}NO$ + H^+: 222.0919 $[M+H]^+$; found: 222.0957.

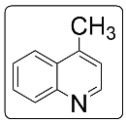


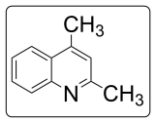
3-methylquinoline (**4ar**): yellow oil, Rf = 0.57 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.74 (d, J = 1.5 Hz, 1H), 8.06 (dt, J = 8.2, 1.0 Hz, 1H), 7.90 – 7.80 (m, 1H), 7.76 – 7.65 (m, 2H), 7.55 – 7.42 (m, 1H), 2.41 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 147.09, 130.24, 128.54, 128.13, 127.49, 18.52. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_9N$ + H^+: 144.0813 $[M+H]^+$; found: 144.0817.



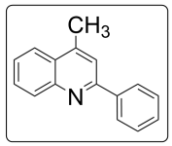
3-ethylquinoline (**4as**): colourless oil, Rf = 0.55 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.75 (d, J = 1.4 Hz, 1H), 8.14 – 8.05 (m, 1H), 8.01 (dd, J = 2.3, 1.4 Hz, 1H), 7.77 – 7.66 (m, 2H), 7.49 (td, J = 7.8, 1.4 Hz, 1H), 2.76 (q, J = 7.2 Hz, 2H), 1.26 (t, J = 7.2 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 148.97, 147.15, 136.99, 132.65, 129.55, 129.33, 128.25, 127.82, 127.49, 26.60, 14.67. **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}N$ + H^+: 158.0970 $[M+H]^+$; found: 158.0953.

4-methylquinoline (**4au**): colourless oil, Rf = 0.56 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.74 (d, J = 5.7 Hz, 1H), 8.05 (dd, J = 8.0, 1.5 Hz, 1H), 8.00 – 7.97 (m, 1H), 7.70 – 7.67 (m, 1H), 7.53 (td, J = 7.6, 1.2 Hz, 1H), 7.28 – 7.19 (m, 1H), 2.69 (d, J = 0.7 Hz, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 149.13, 147.99, 142.91, 128.58, 128.06, 127.76, 127.00, 124.85, 121.52, 18.40. **HRMS** (ESI-TOF): Calcd. for $C_{10}H_9N$ + H^+: 144.0813 $[M+H]^+$; found: 144.0819.

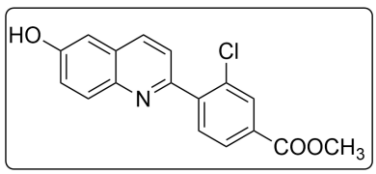




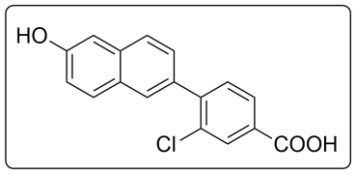
2,4-dimethylquinoline (**4av**): yellow oil,, Rf = 0.51 (Petroleum ether/EtOAc, v/v = 30/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.94 (ddd, J = 8.5, 7.7, 1.4 Hz, 2H), 7.73 (td, J = 7.6, 1.2 Hz, 1H), 7.51 (td, J = 7.6, 1.2 Hz, 1H), 7.03 (d, J = 0.8 Hz, 1H), 2.68 (s, 3H), 2.62 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 156.31, 146.60, 144.17, 129.82, 128.26, 127.13, 124.57, 124.37, 122.27, 24.99, 18.86. **HRMS** (ESI-TOF): Calcd. for $C_{11}H_{11}N + H^+$: 158.0970 $[M+H]^+$; found: 185.0953.



4-methyl-2-phenylquinoline (**4aw**): white solid, Rf = 0.57 (Petroleum ether/EtOAc, v/v = 20/1). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.19 – 8.10 (m, 1H), 7.99 (ddd, J = 15.1, 7.6, 1.7 Hz, 3H), 7.62 (d, J = 0.8 Hz, 1H), 7.54 (dtd, J = 26.2, 7.5, 1.3 Hz, 2H), 7.43 – 7.35 (m, 3H), 2.73 (s, 3H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 154.29, 148.06, 144.78, 137.74, 130.43, 129.59, 129.18, 128.73, 127.67, 126.98, 124.70, 124.26, 120.75, 19.31. **HRMS** (ESI-TOF): Calcd. for $C_{16}H_{13}N + H^+$: 220.1126 $[M+H]^+$; found: 220.1107.

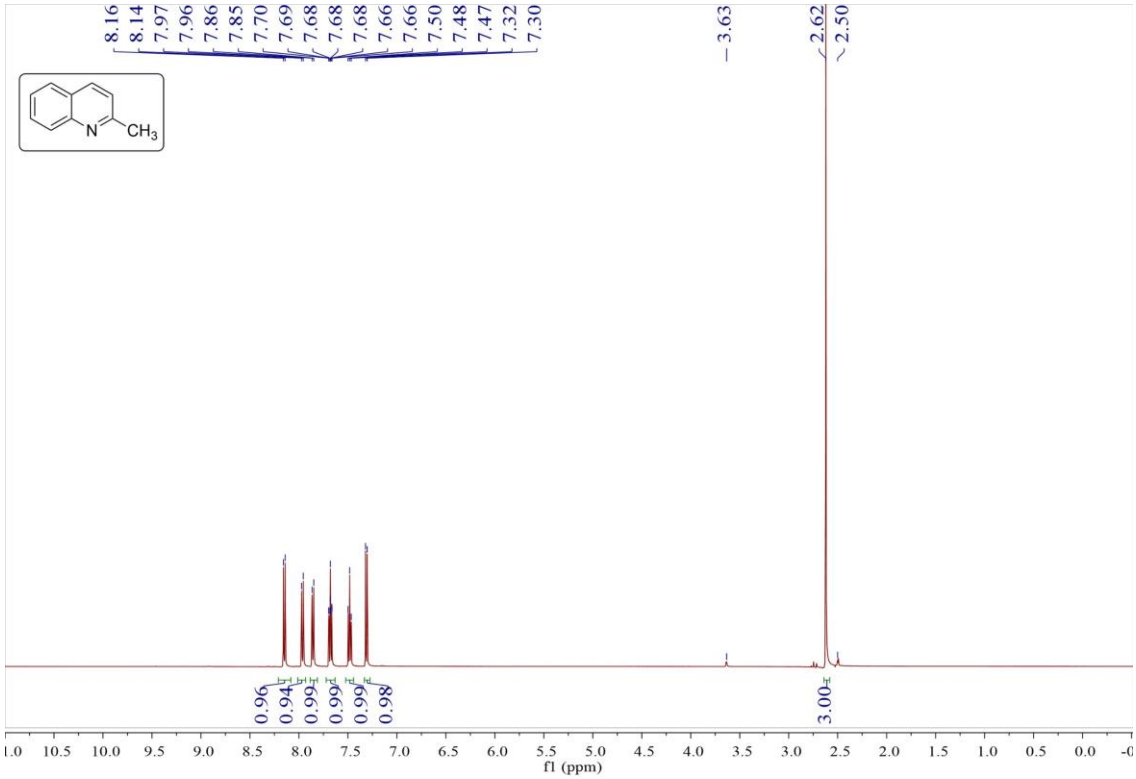


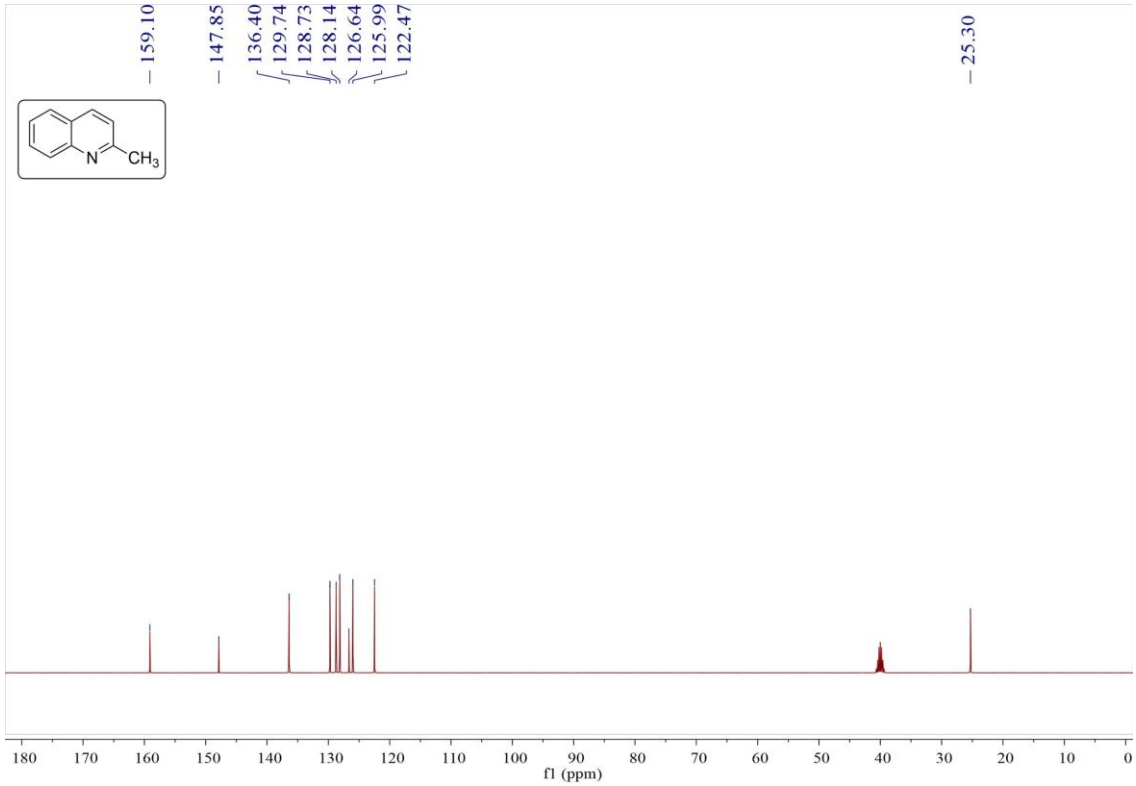
Methyl 3-chloro-4-(6-hydroxyquinolin-2-yl)benzoate (4ar): white solid, Rf = 0.41 (Petroleum ether/EtOAc, v/v = 15/1). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.33 (s, 1H), 8.34 (d, J = 8.6 Hz, 1H), 8.07 (d, J = 1.6 Hz, 1H), 8.05 – 7.92 (m, 2H), 7.78 (dd, J = 25.7, 8.2 Hz, 2H), 7.42 (dd, J = 9.1, 2.7 Hz, 1H), 7.26 (d, J = 2.6 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO- d_6) δ 166.38, 156.89, 152.47, 142.84, 142.20, 135.75, 132.97, 132.71, 132.11, 130.89, 130.42, 129.06, 128.56, 123.56, 122.87, 108.76. **HRMS** (ESI-TOF): Calcd. for $C_{17}H_{12}ClNO_3 + H^+$: 314.0584 $[M+H]^+$; found: 314.0588.



Cavosonstat: ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12 (d, J = 1.9 Hz, 1H), 7.89 (dd, J = 8.4, 1.8 Hz, 1H), 7.82 – 7.78 (m, 3H), 7.54 (dd, J = 9.0, 1.6 Hz, 1H), 7.34 (t, J = 2.3 Hz, 1H), 7.16 – 7.09 (m, 1H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 167.75, 157.30, 141.31, 133.91, 133.06, 132.09, 131.41, 129.50, 129.19, 129.12, 128.73, 128.34, 128.17, 127.43, 127.32, 116.43, 107.24.

4. Spectroscopy

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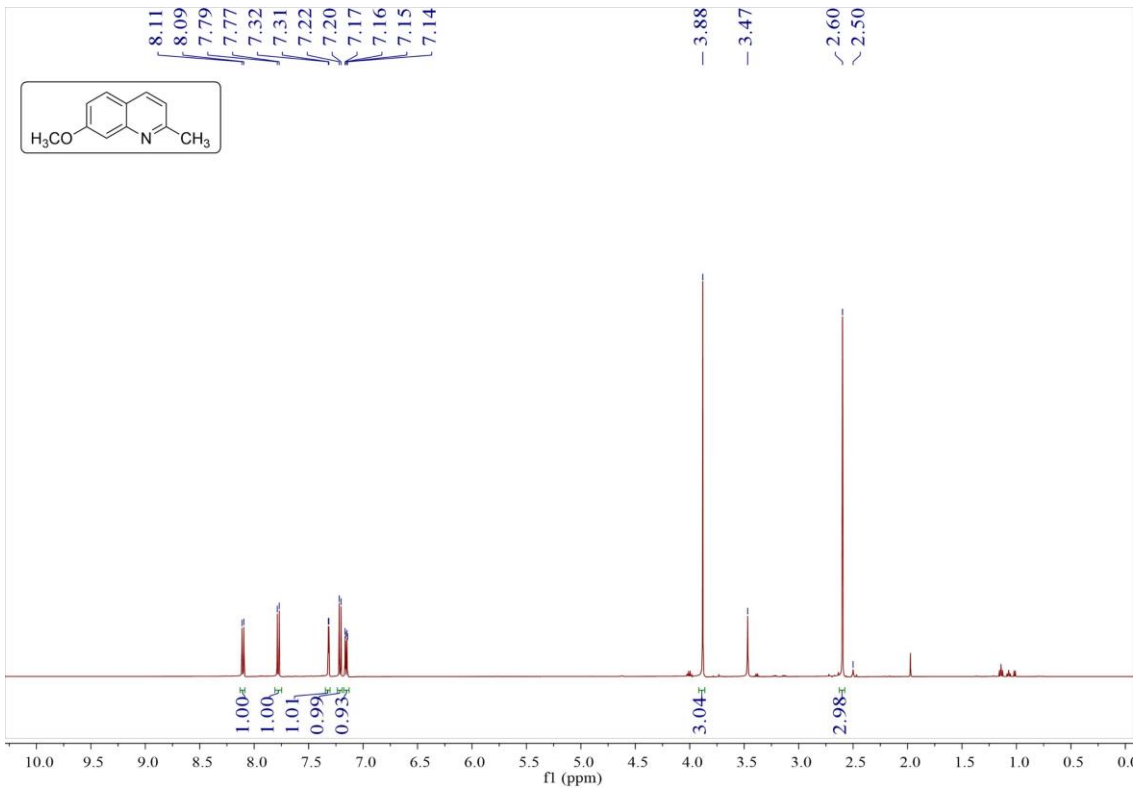
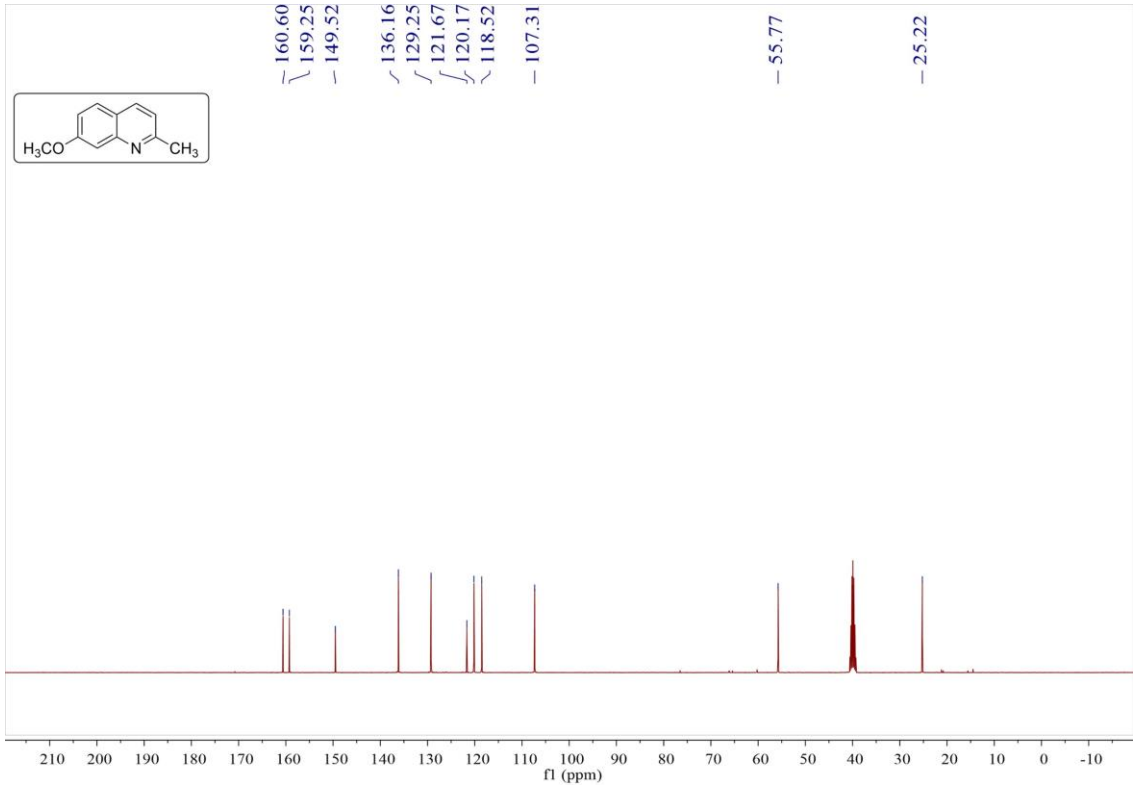
147.85
136.40
129.74
128.73
128.14
126.64
125.99
122.47
25.30
N
CH3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.11
8.09
7.79
7.77
7.32
7.31
7.22
7.20
7.17
7.16
7.15
7.14
3.88
3.47
2.60
2.50
H3CO
N
CH3
1.00
1.00
1.01
0.99
0.93
3.04
2.98
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
f1 (ppm)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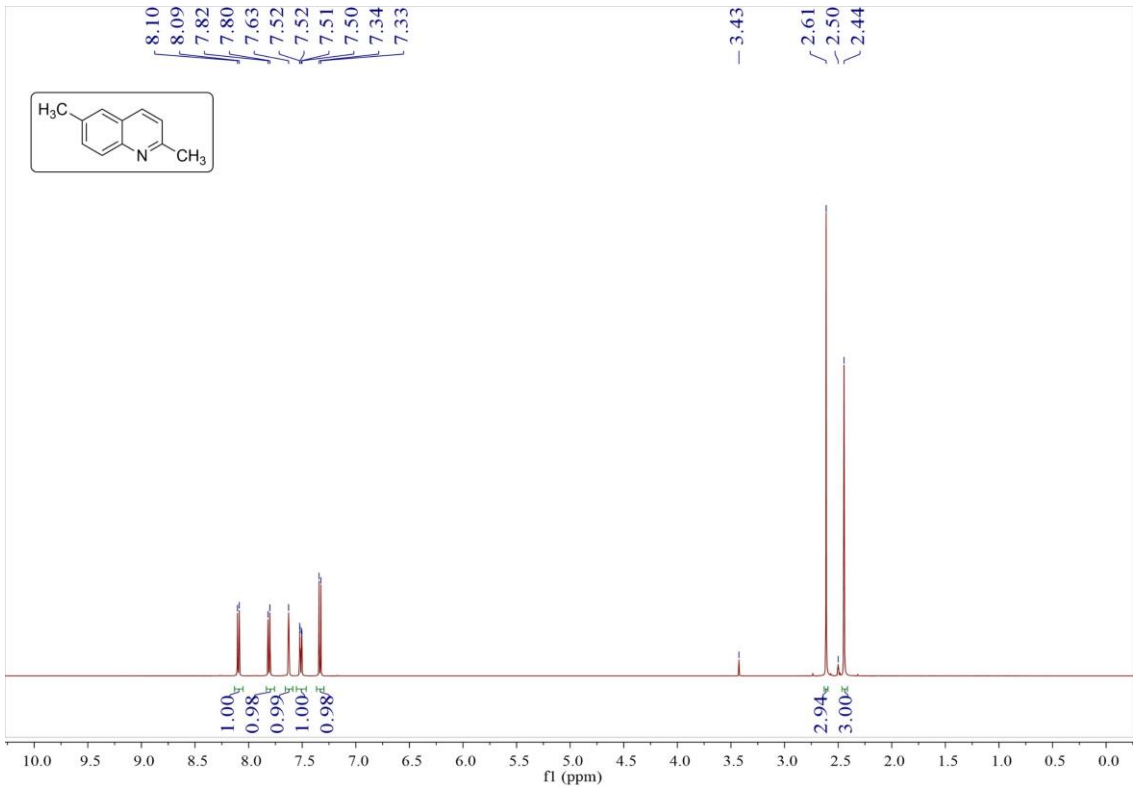
159.25
149.52
136.16
129.25
121.67
120.17
118.52
107.31
55.77
25.22
H3CO
N
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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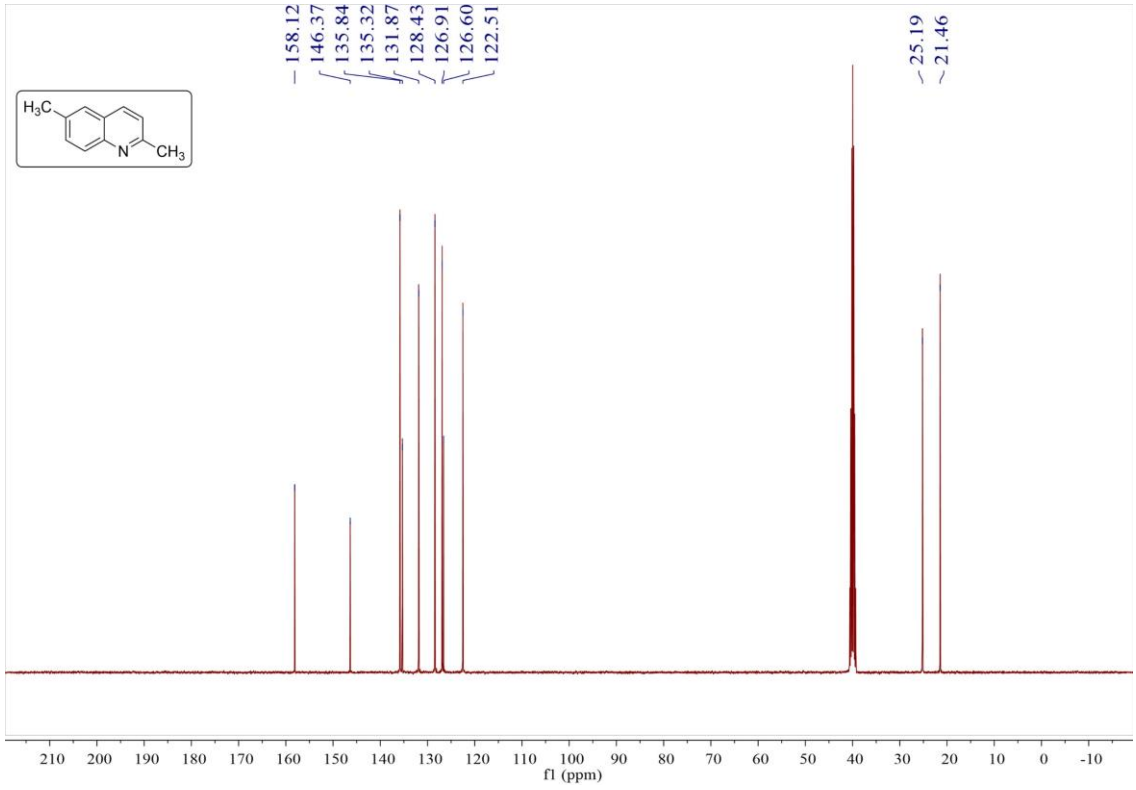
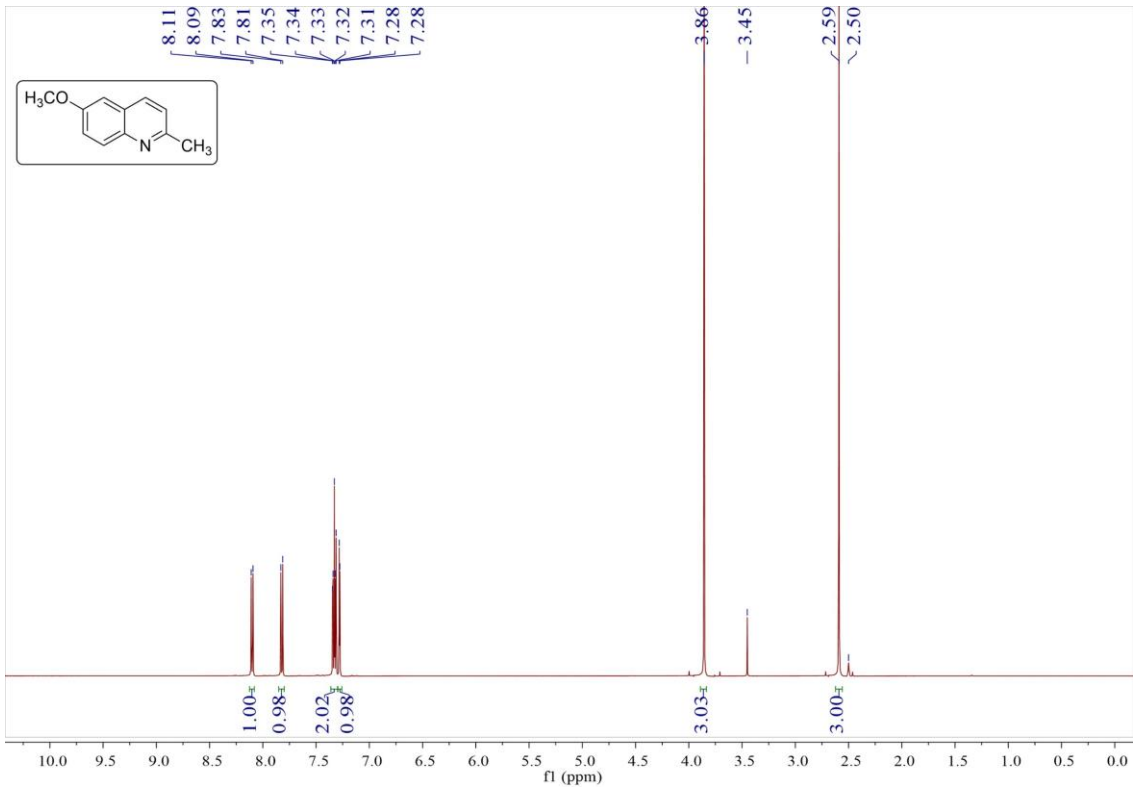
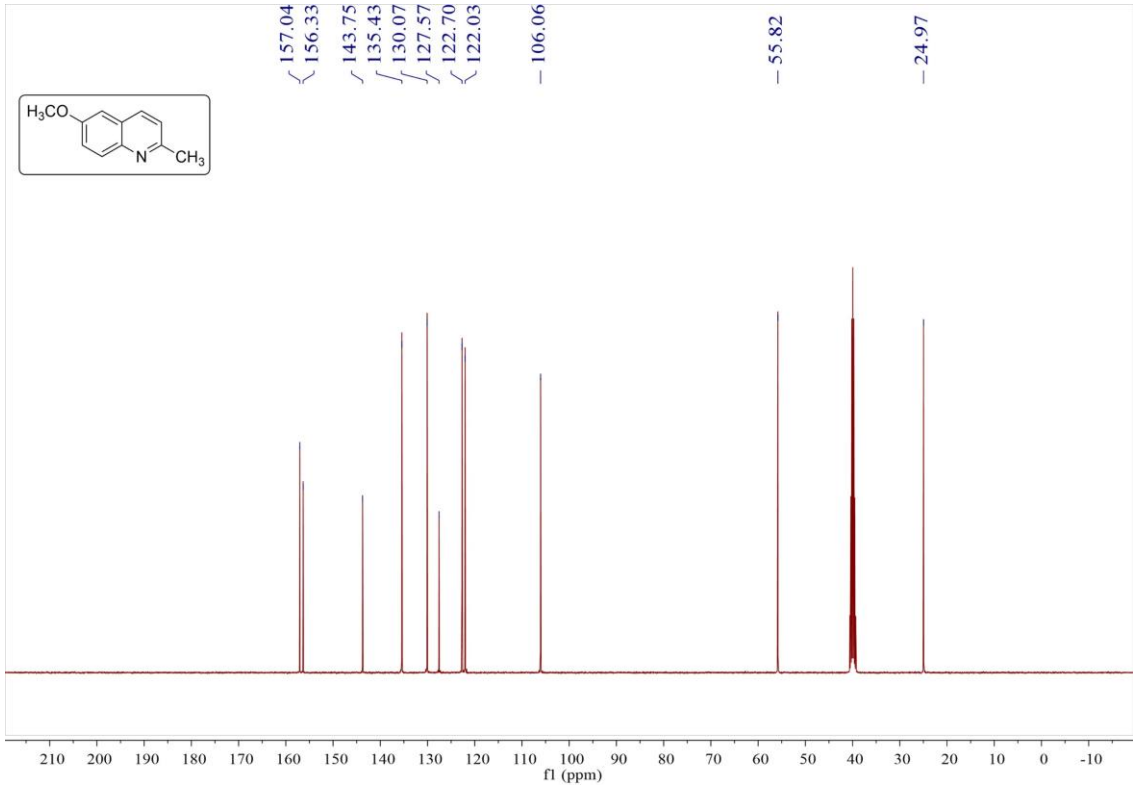
8.09
7.82
7.80
7.63
7.52
7.52
7.51
7.50
7.34
7.33
3.43
2.61
2.50
2.44
H3C
N
CH3
1.00
0.98
0.99
1.00
0.98
2.94
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


158.12
146.37
135.84
135.32
131.87
128.43
126.91
126.60
122.51
25.19
21.46
H3C
N
CH3
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)


8.11
8.09
7.83
7.81
7.35
7.34
7.33
7.32
7.31
7.28
7.28
3.86
3.45
2.59
2.50
H3CO
N
CH3
1.00
0.98
2.02
0.98
3.03
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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156.33
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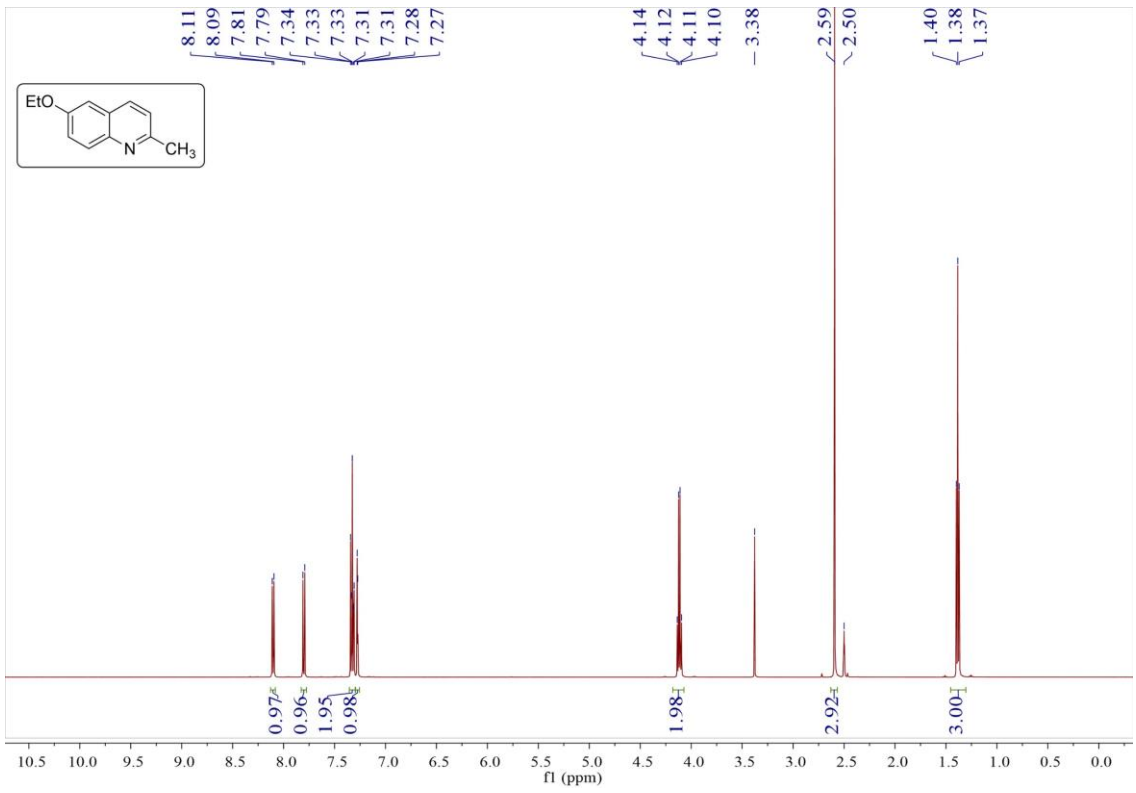
135.43
130.07
127.57
122.70
122.03
106.06
55.82
24.97
H3CO
N
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.09
7.81
7.79
7.34
7.33
7.33
7.31
7.31
7.28
7.27
4.14
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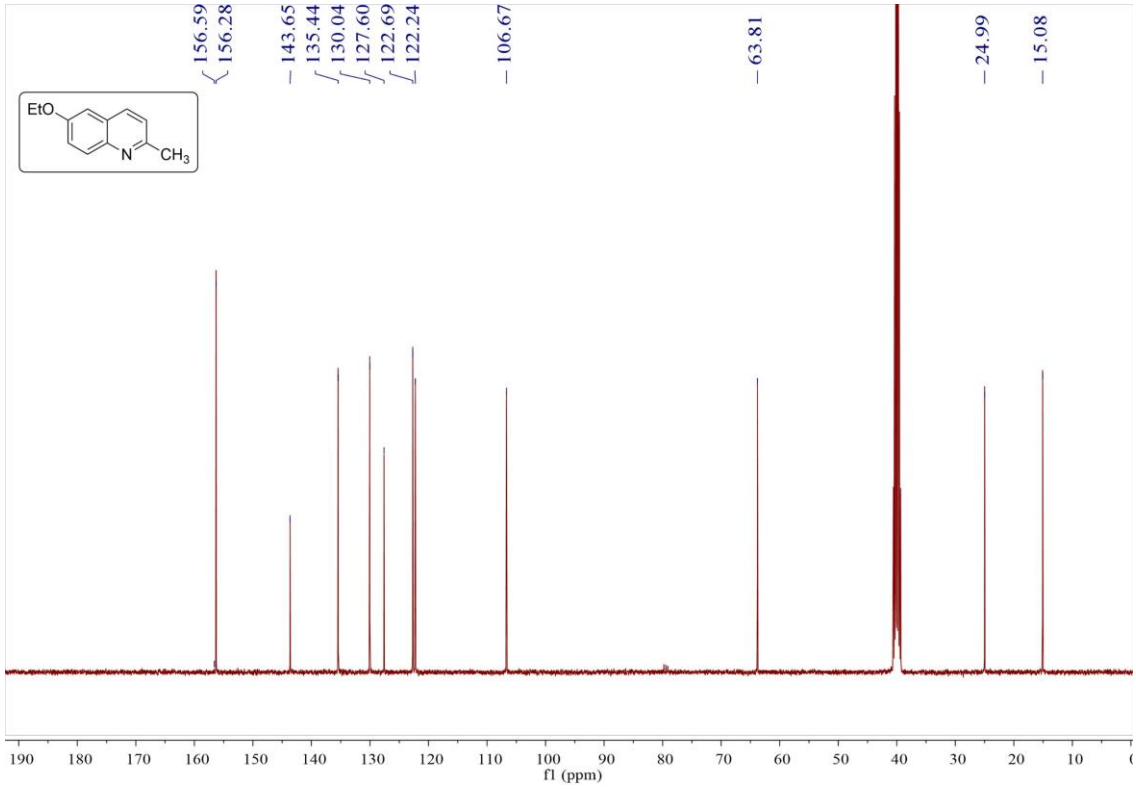
4.11
4.10
3.38
2.59
2.50
1.40
1.38
1.37
EtO
N
CH3
0.97
0.96
1.95
0.98
1.98
2.92
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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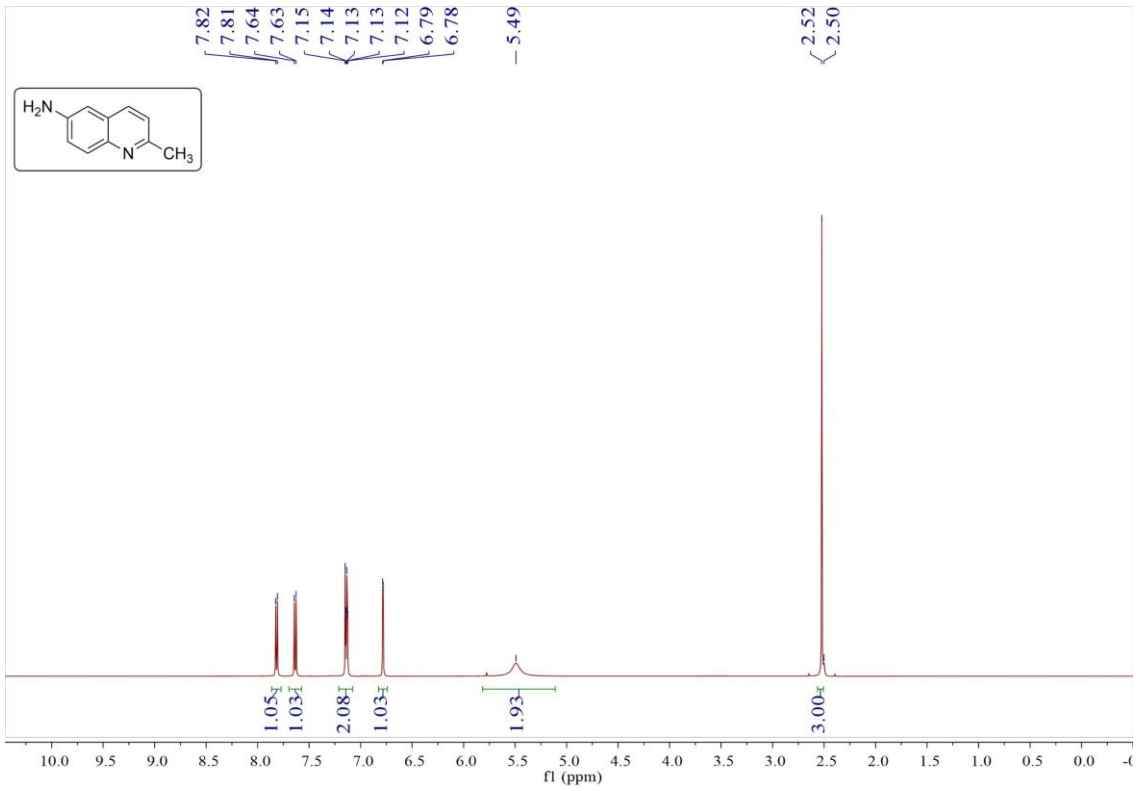
135.44
130.04
127.60
122.69
122.24
106.67
63.81
24.99
15.08
EtO
N
CH3
f1 (ppm)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7.14
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7.13
7.12
6.79
6.78
5.49
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N
CH3
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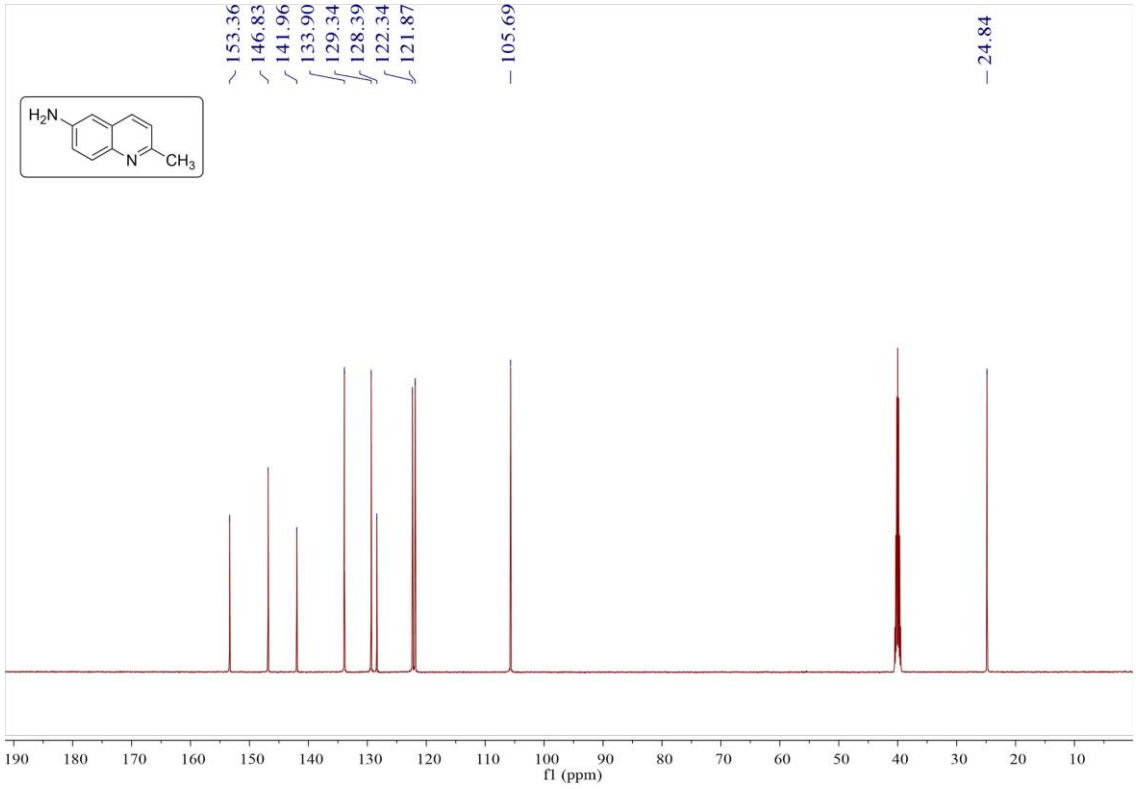
1.03
2.08
1.03
1.93
3.00
f1 (ppm)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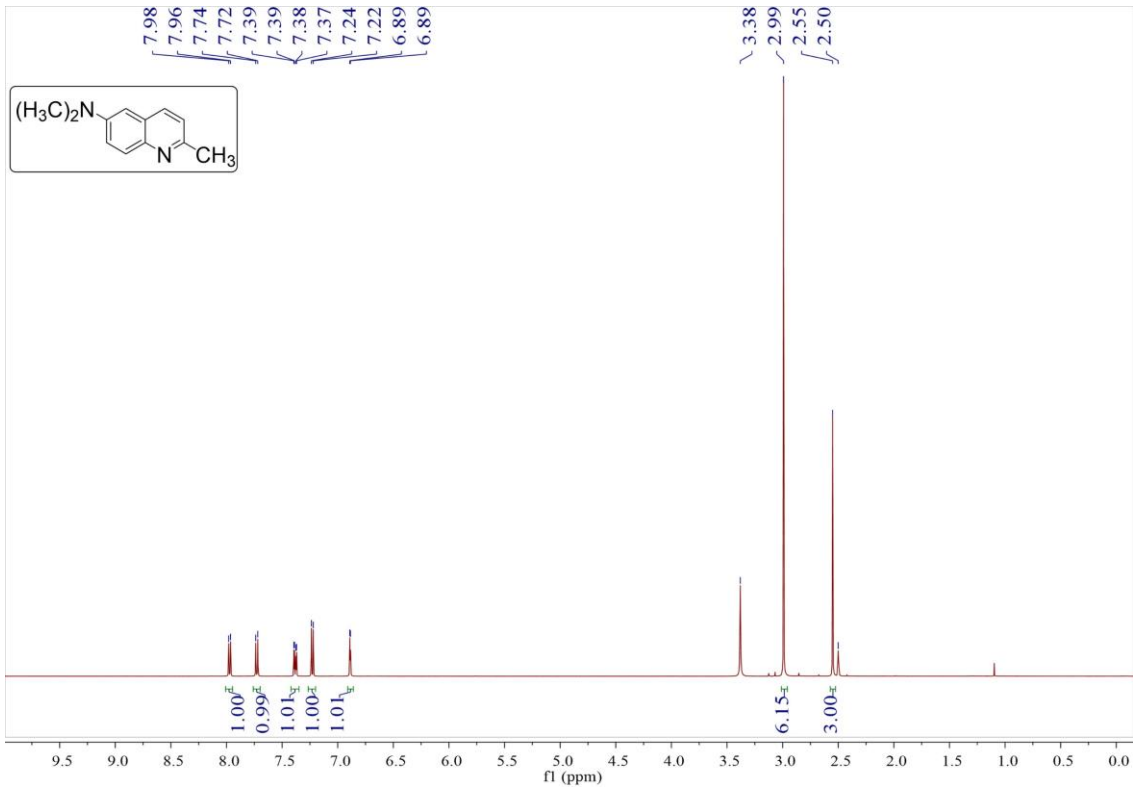
146.83
141.96
133.90
129.34
128.39
122.34
121.87
105.69
24.84
H2N
N
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.37
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6.89
6.89
3.38
2.99
2.55
2.50
(H3C)2N
N
CH3
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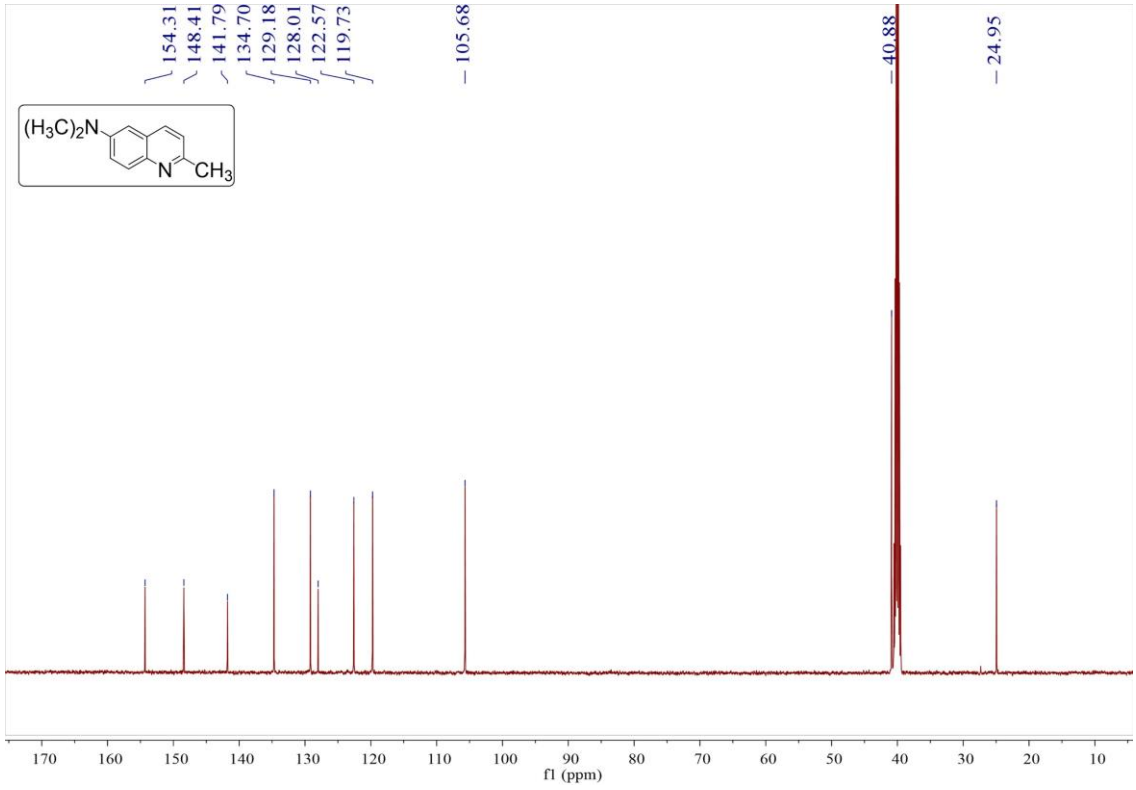
0.99
1.01
1.00
1.01
6.15
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.01
122.57
119.73
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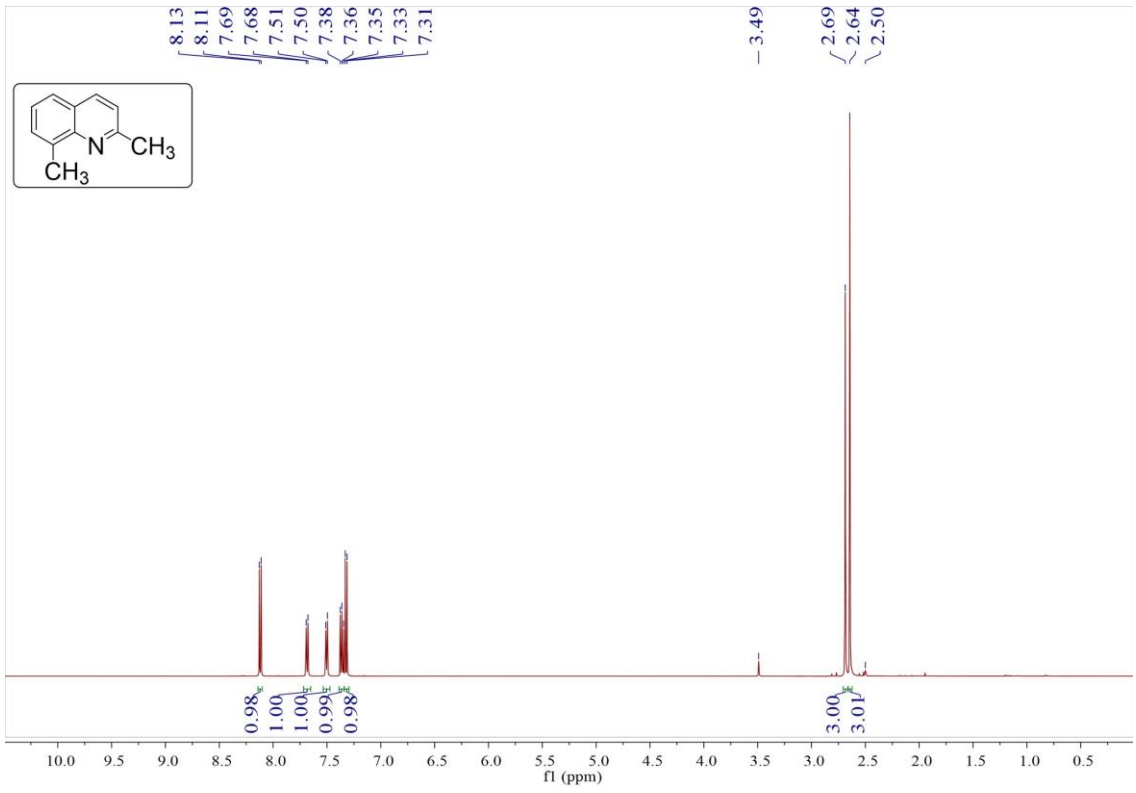
24.95
(H3C)2N
N
CH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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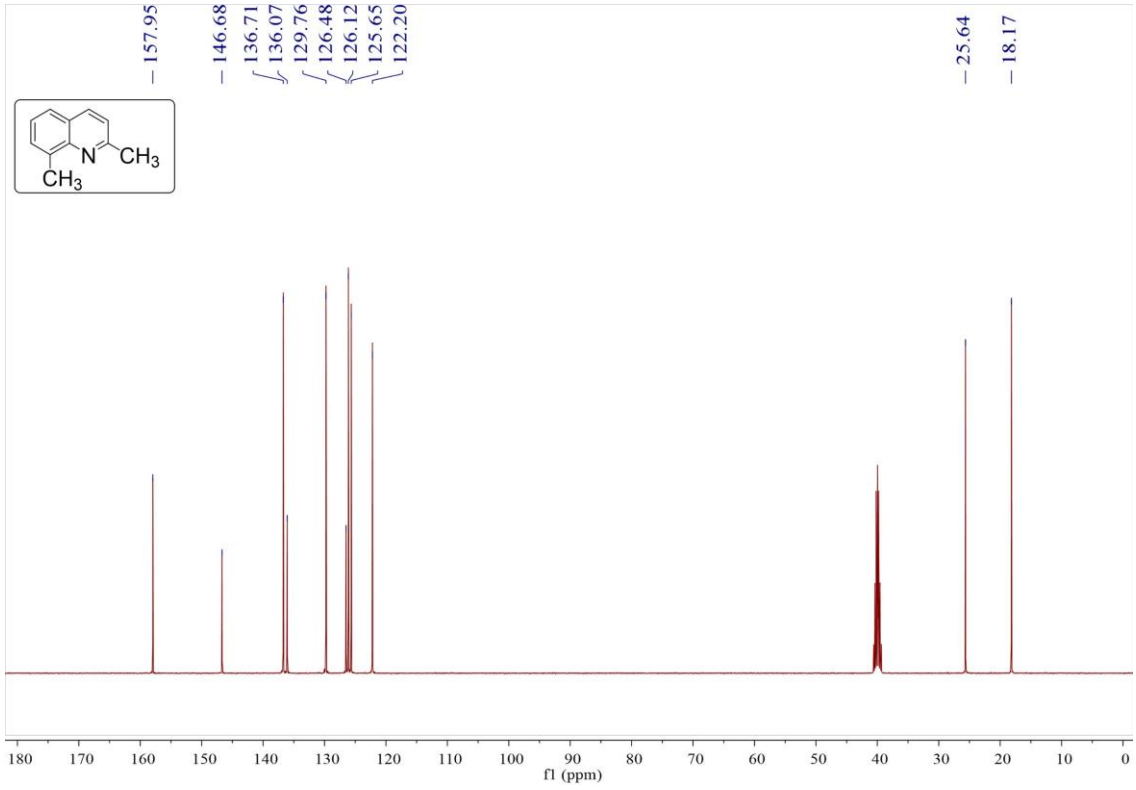
7.36
7.35
7.33
7.31
3.49
2.69
2.64
2.50
N
CH3
CH3
0.98
1.00
1.00
0.99
0.98
3.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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126.12
125.65
122.20
25.64
18.17
N
CH3
CH3
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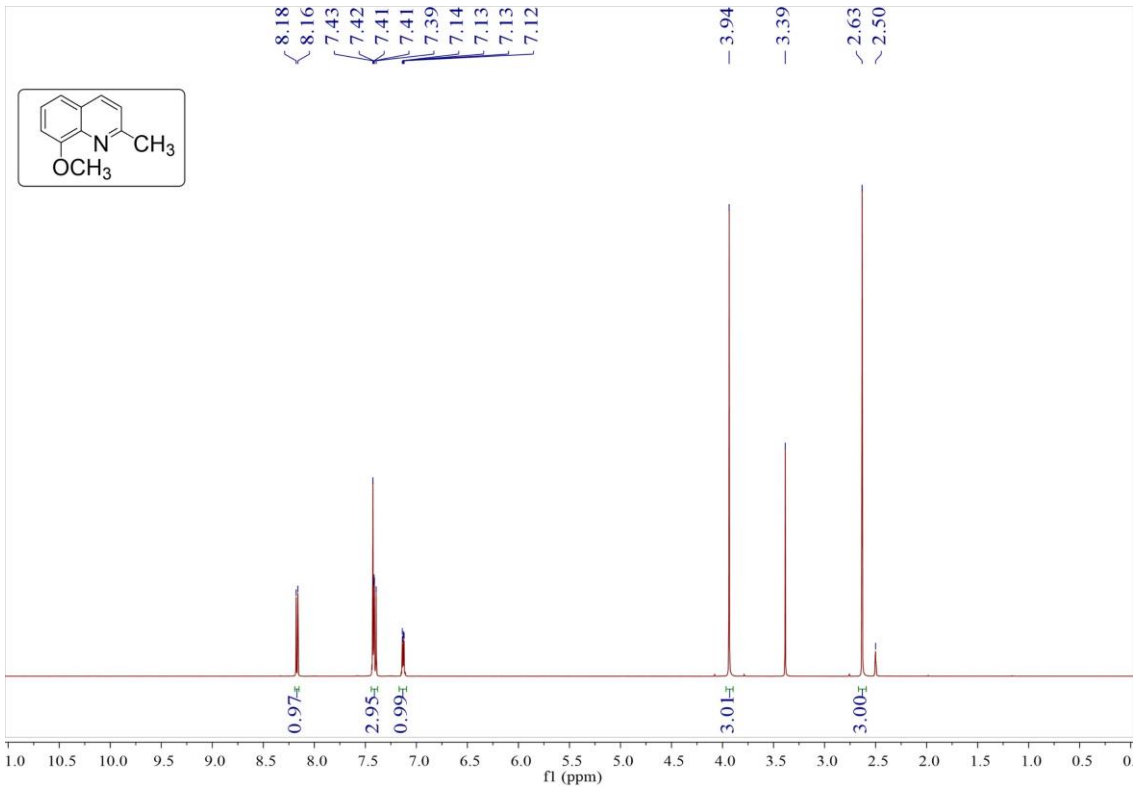
f1 (ppm)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7.41
7.39
7.14
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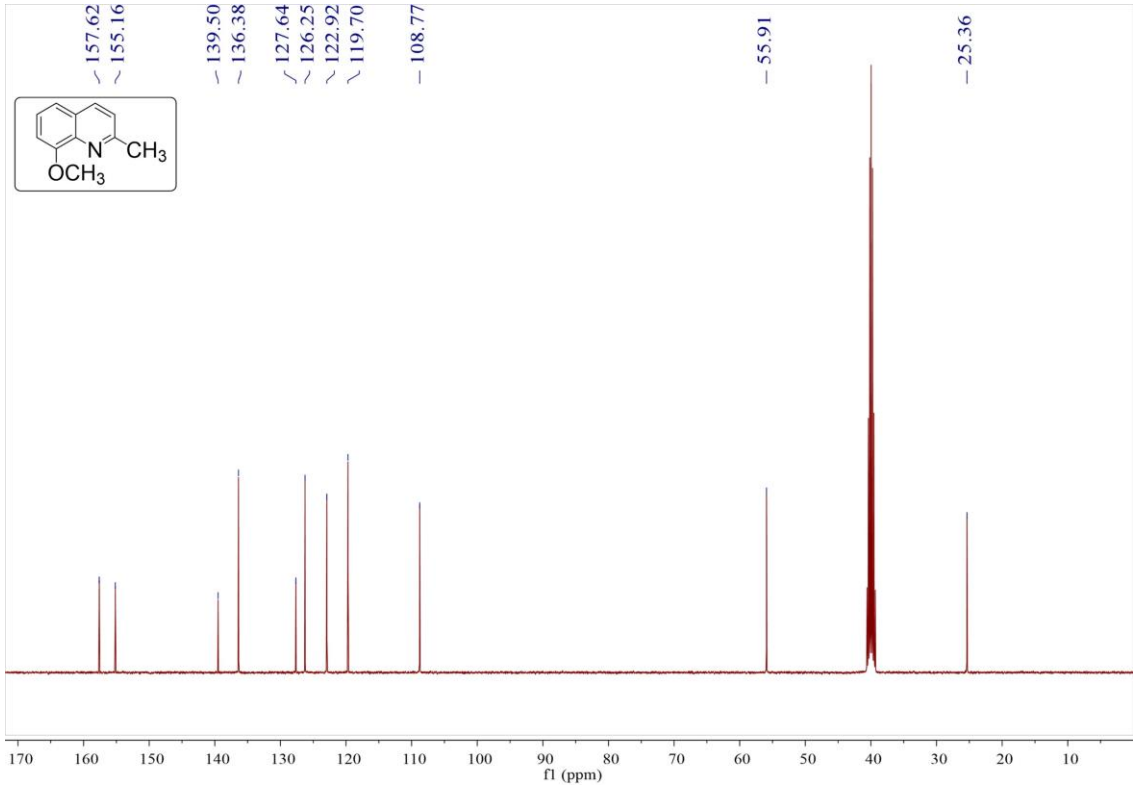
7.13
7.12
3.94
3.39
2.63
2.50
N
CH3
OCH3
0.97
2.95
0.99
3.01
3.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)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127.64
126.25
122.92
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55.91
25.36
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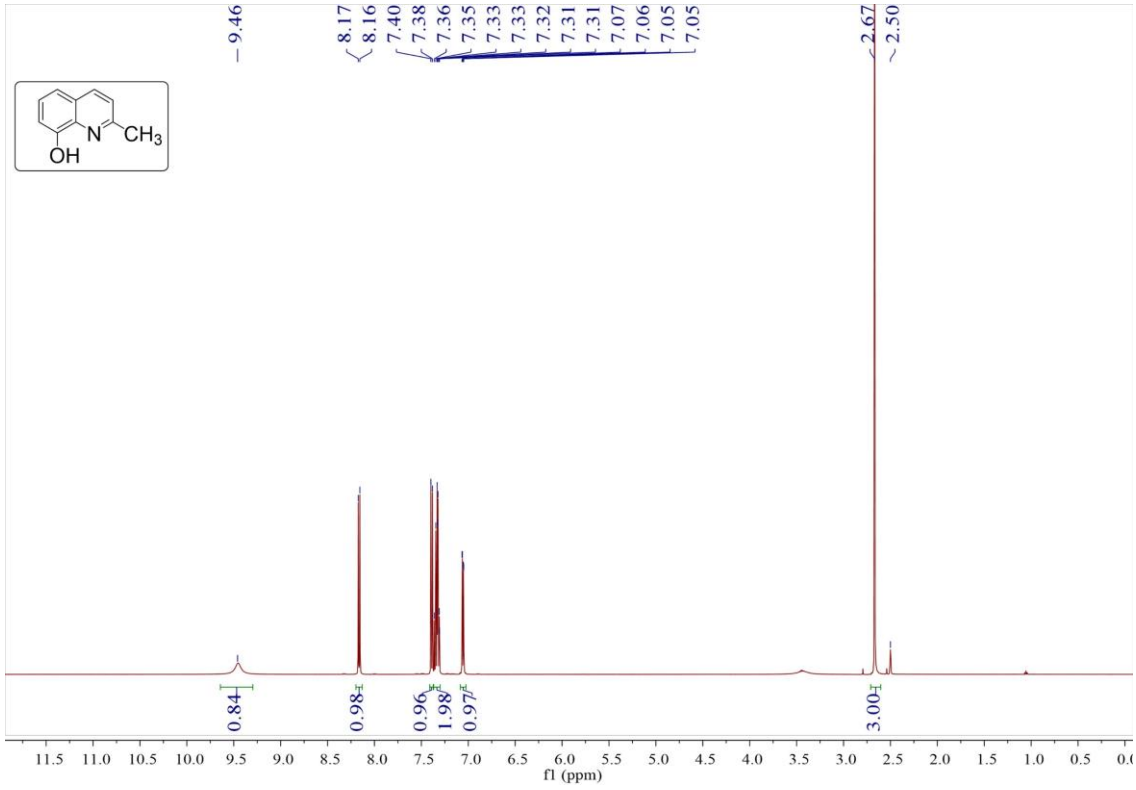
CH3
OCH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.33
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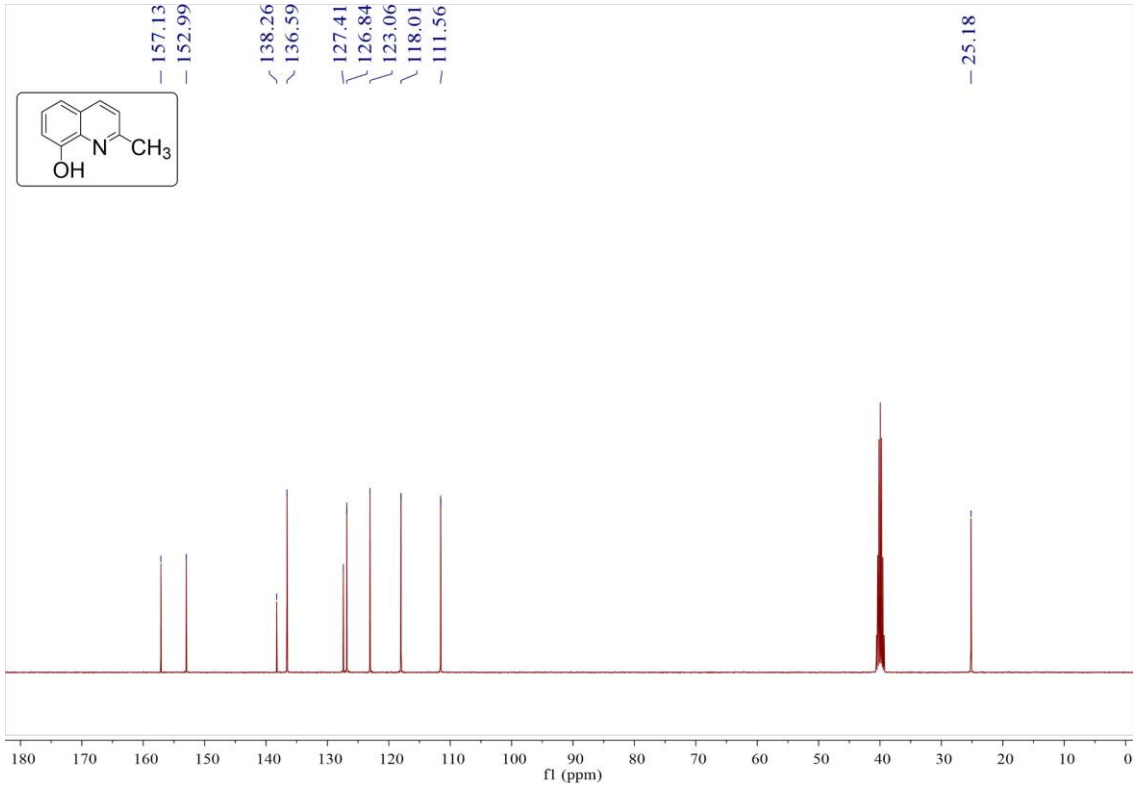
7.32
7.31
7.31
7.07
7.06
7.05
7.05
2.67
2.50
N
CH3
OH
0.84
0.98
0.96
1.98
0.97
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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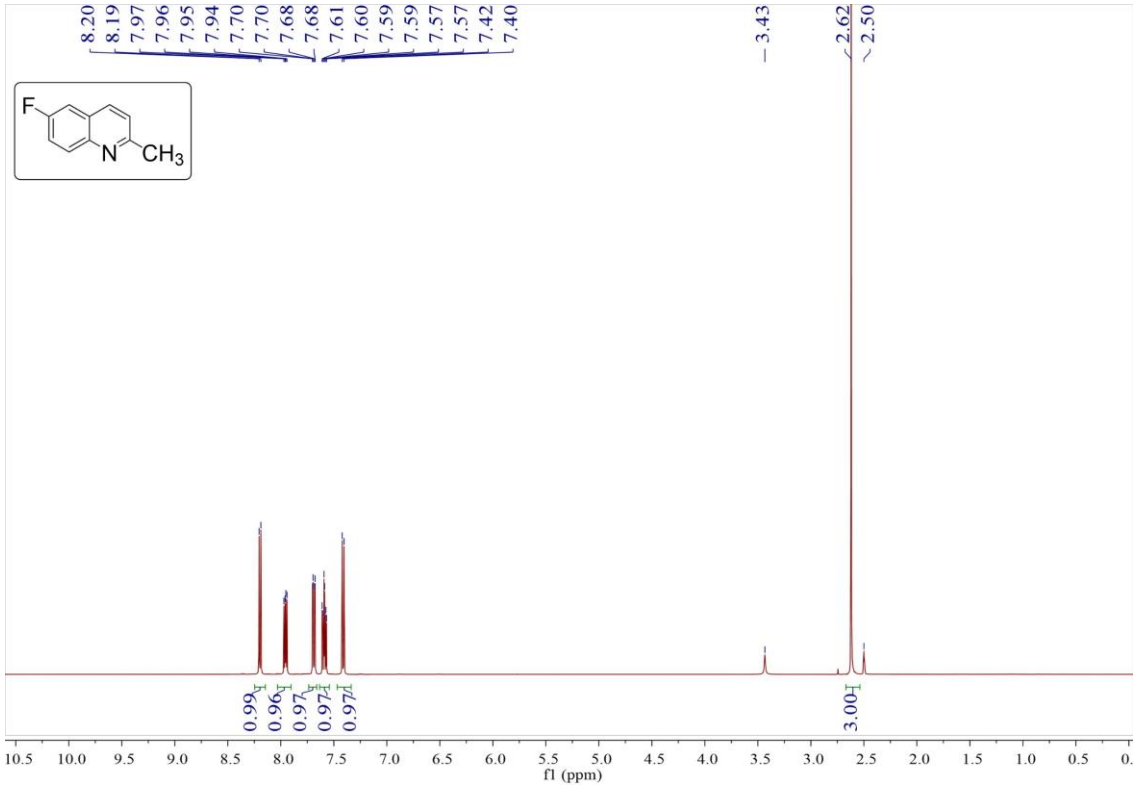
127.41
126.84
123.06
118.01
111.56
25.18
N
CH3
OH
f1 (ppm)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8.19
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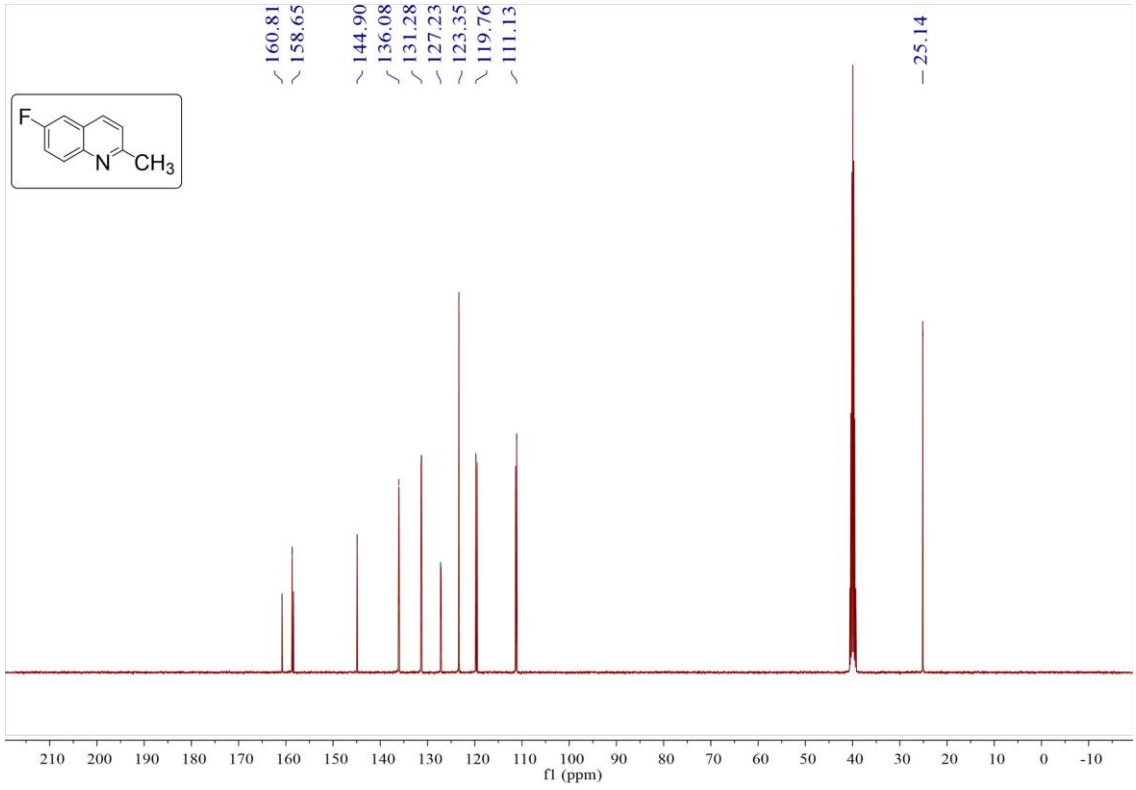
7.95
7.94
7.70
7.70
7.68
7.68
7.61
7.60
7.59
7.59
7.57
7.57
7.42
7.40
3.43
2.62
2.50
F
N
CH3
0.99
0.96
0.97
0.97
0.97
3.00
f1 (ppm)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123.35
119.76
111.13
25.14
F
N
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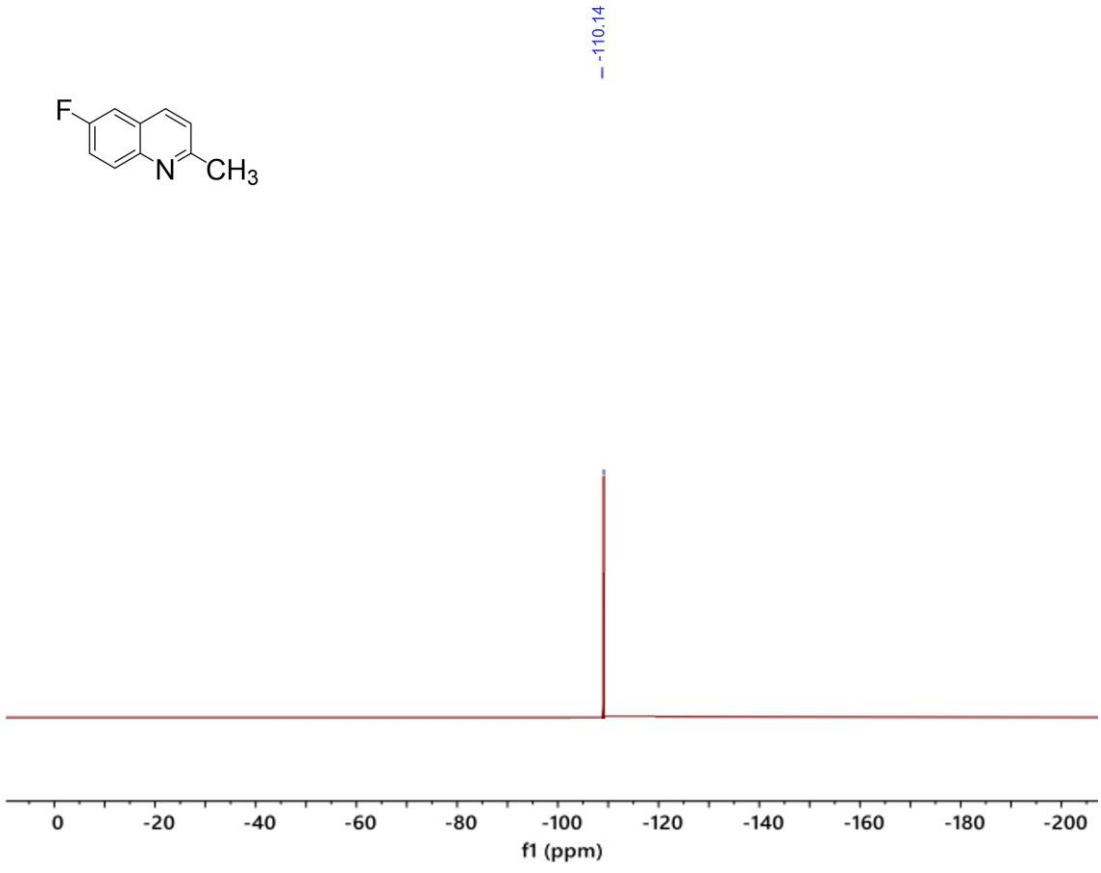
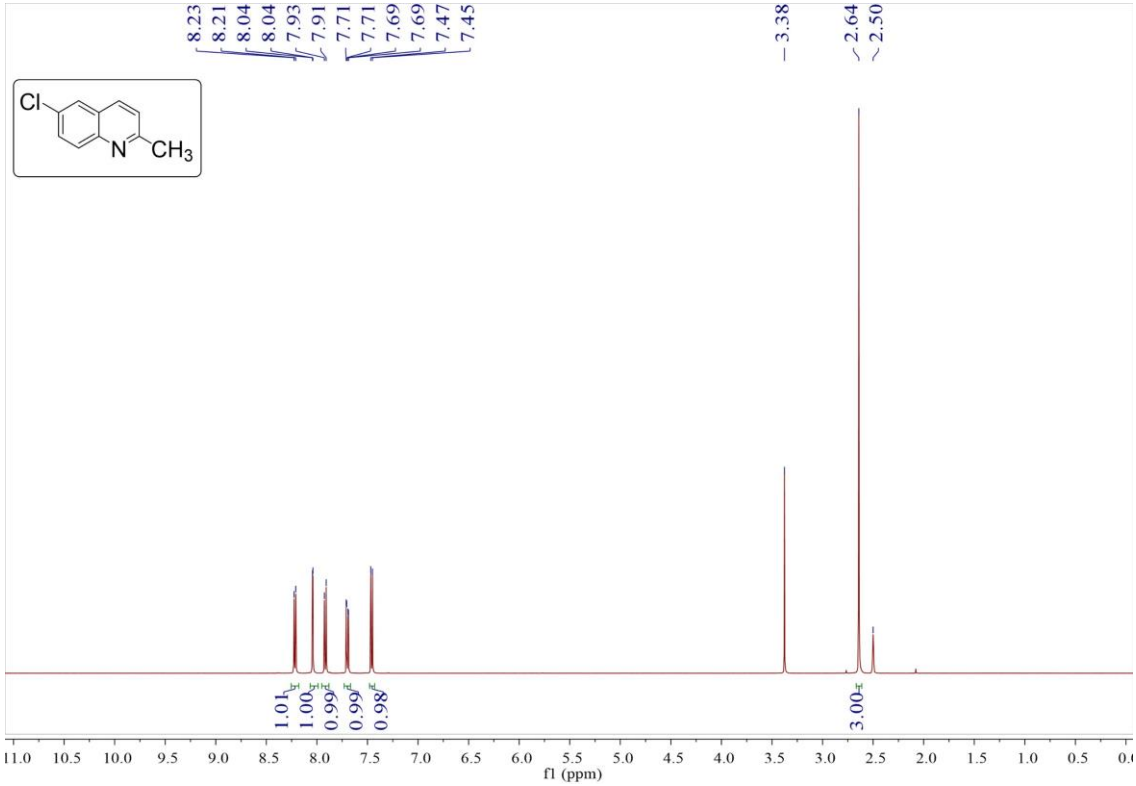
f1 (ppm)


-110.14
F
N
CH3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)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8.04
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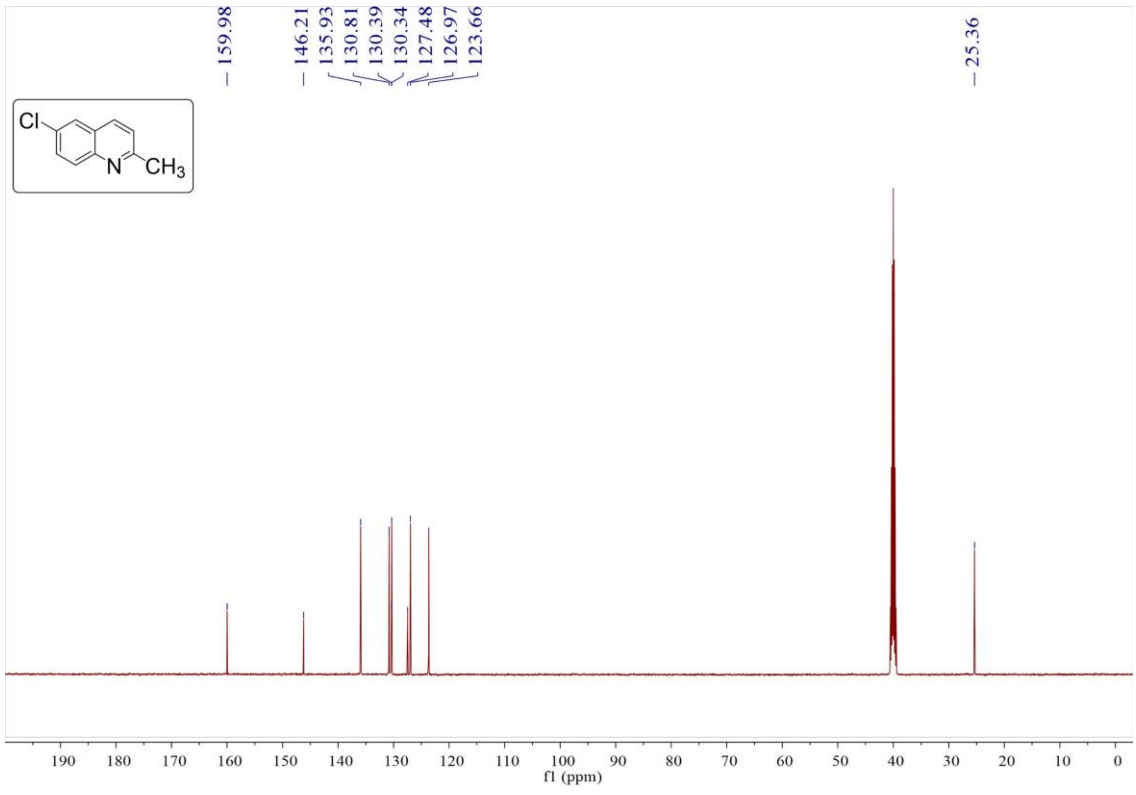
7.91
7.71
7.71
7.69
7.69
7.47
7.45
3.38
2.64
2.50
Cl
N
CH3
1.01
1.00
0.99
0.99
0.98
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


159.98
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135.93
130.81
130.39
130.34
127.48
126.97
123.66
25.36
Cl
N
CH3
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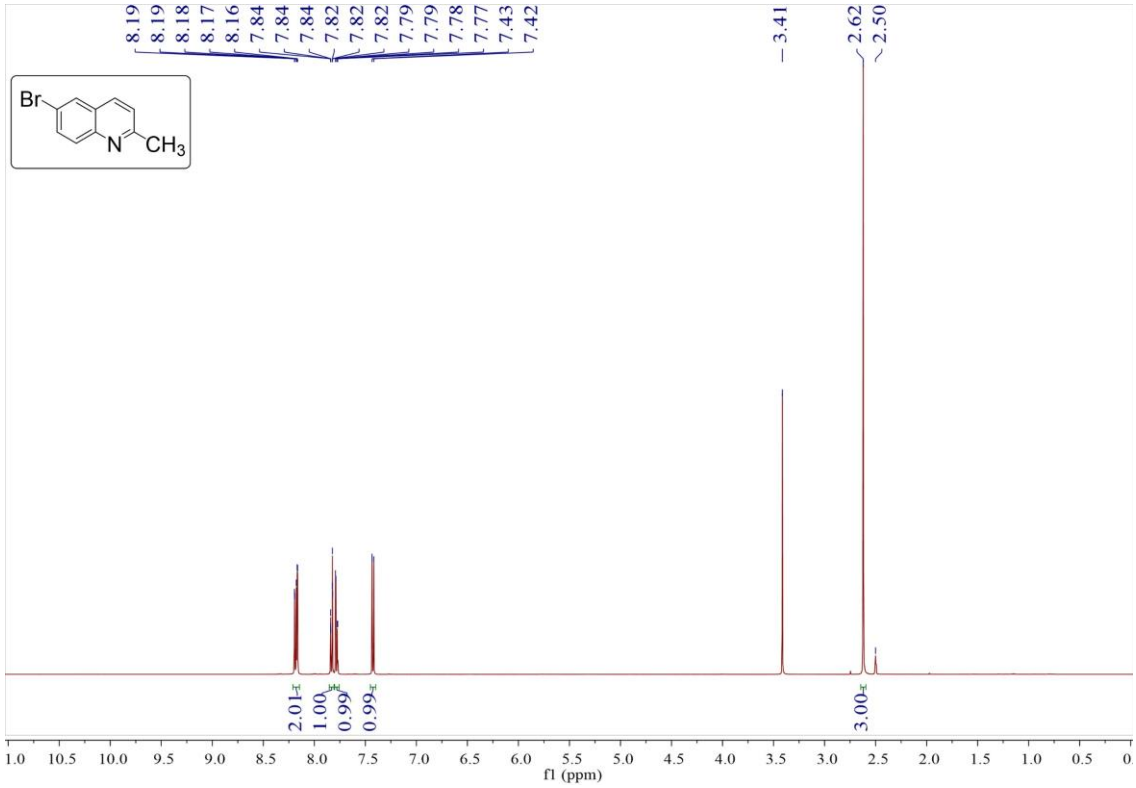
f1 (ppm)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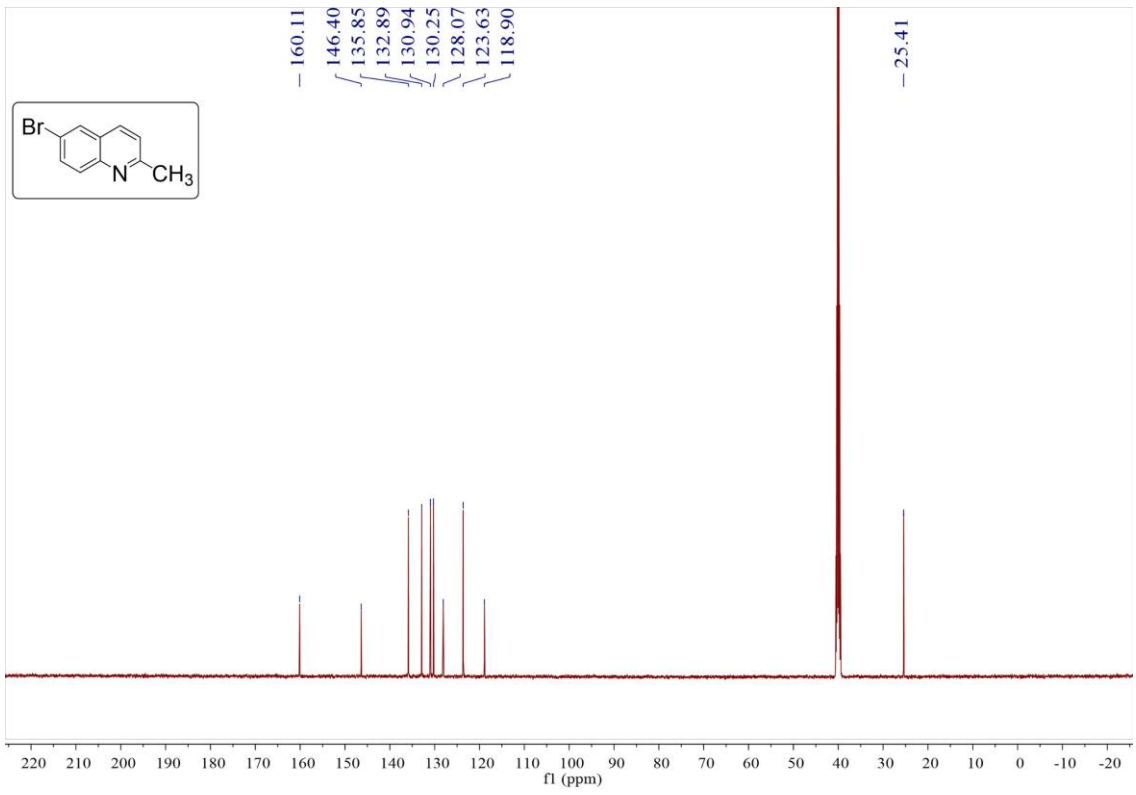
7.84
7.84
7.84
7.82
7.82
7.82
7.79
7.79
7.78
7.77
7.43
7.42
3.41
2.62
2.50
Br
N
CH3
2.01
1.00
0.99
0.99
3.00
f1 (ppm)


160.11
146.40
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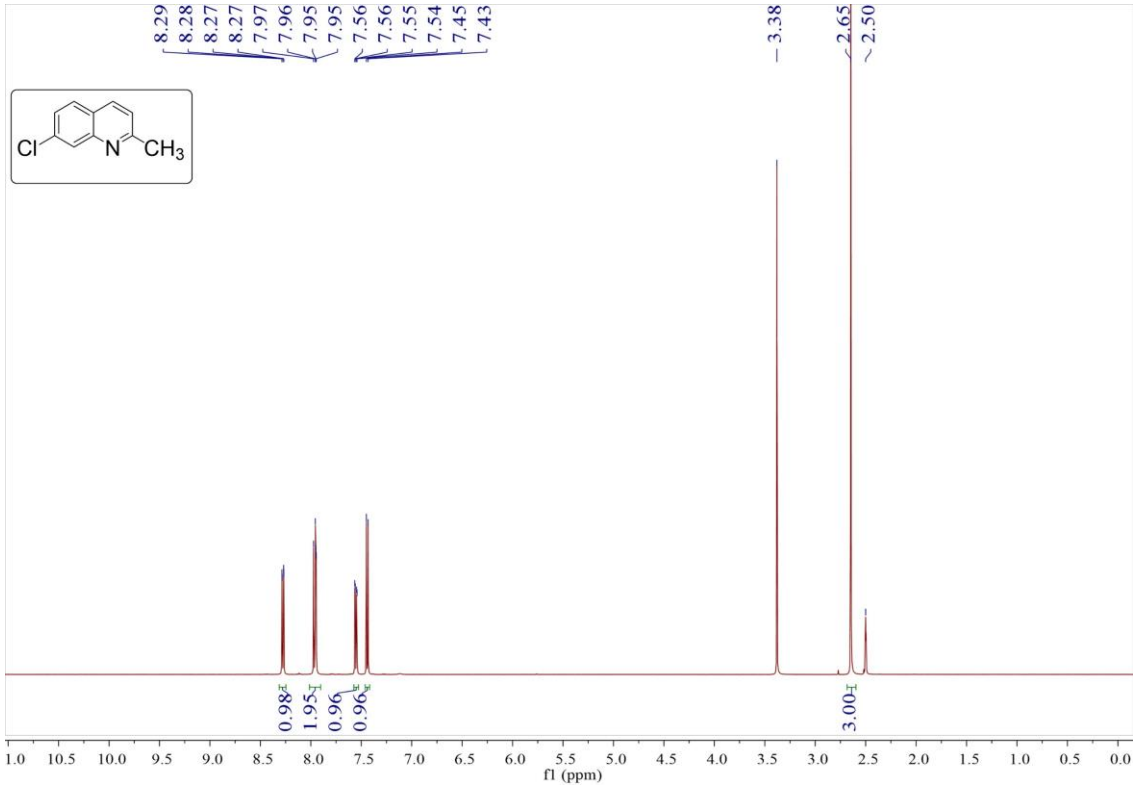
130.25
128.07
123.63
118.90
25.41
Br
N
CH3
f1 (ppm)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7.95
7.95
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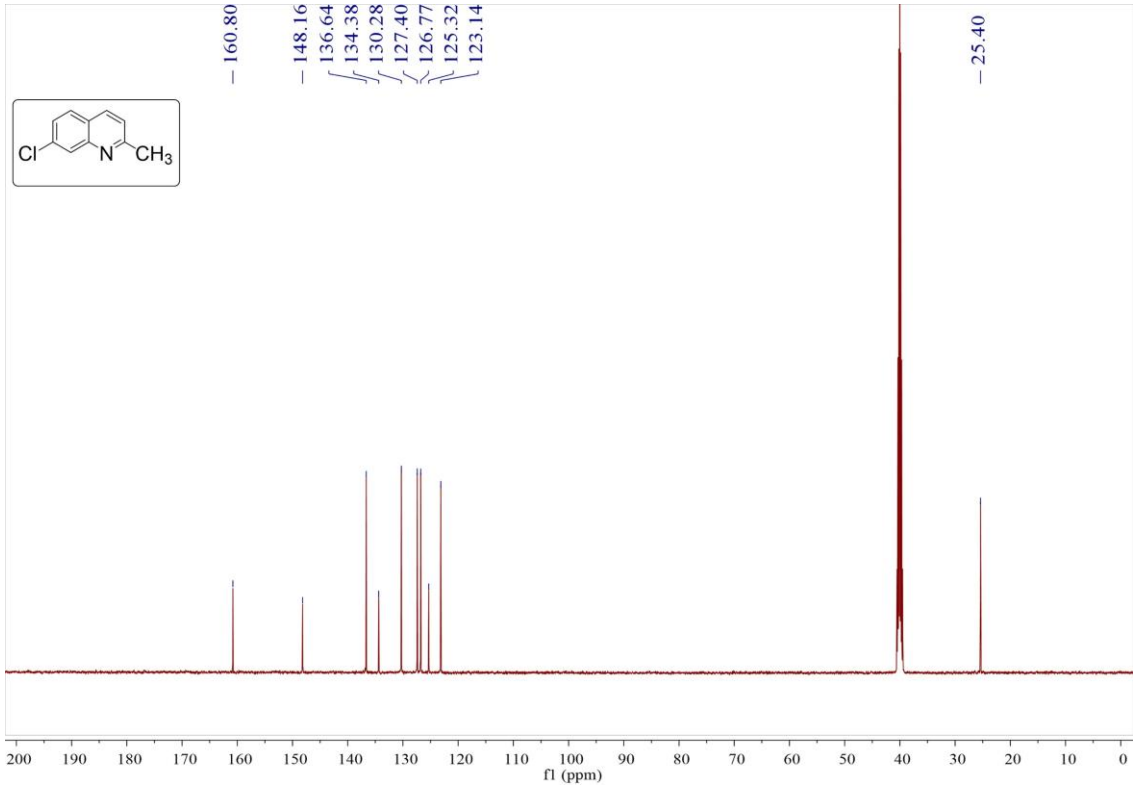
7.56
7.55
7.54
7.45
7.43
3.38
2.65
2.50
Cl
N
CH3
0.98
1.95
0.96
0.96
3.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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148.16
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130.28
127.40
126.77
125.32
123.14
25.40
Cl
N
CH3
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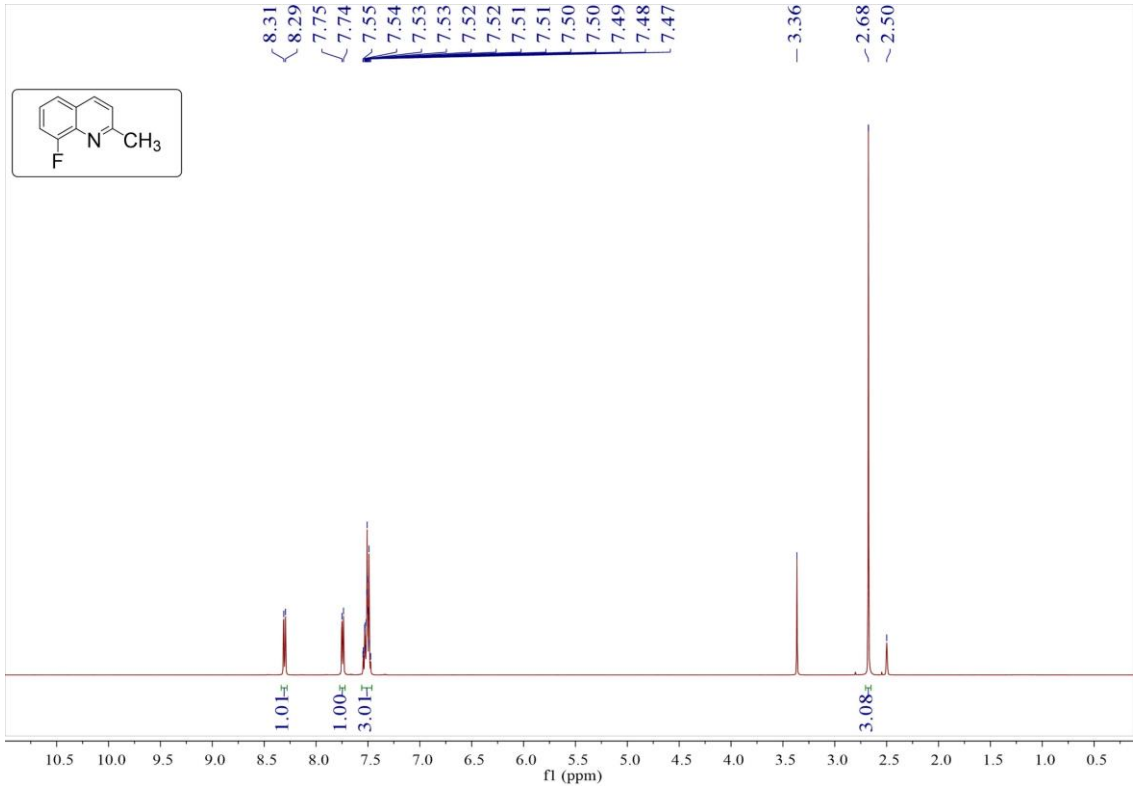
f1 (ppm)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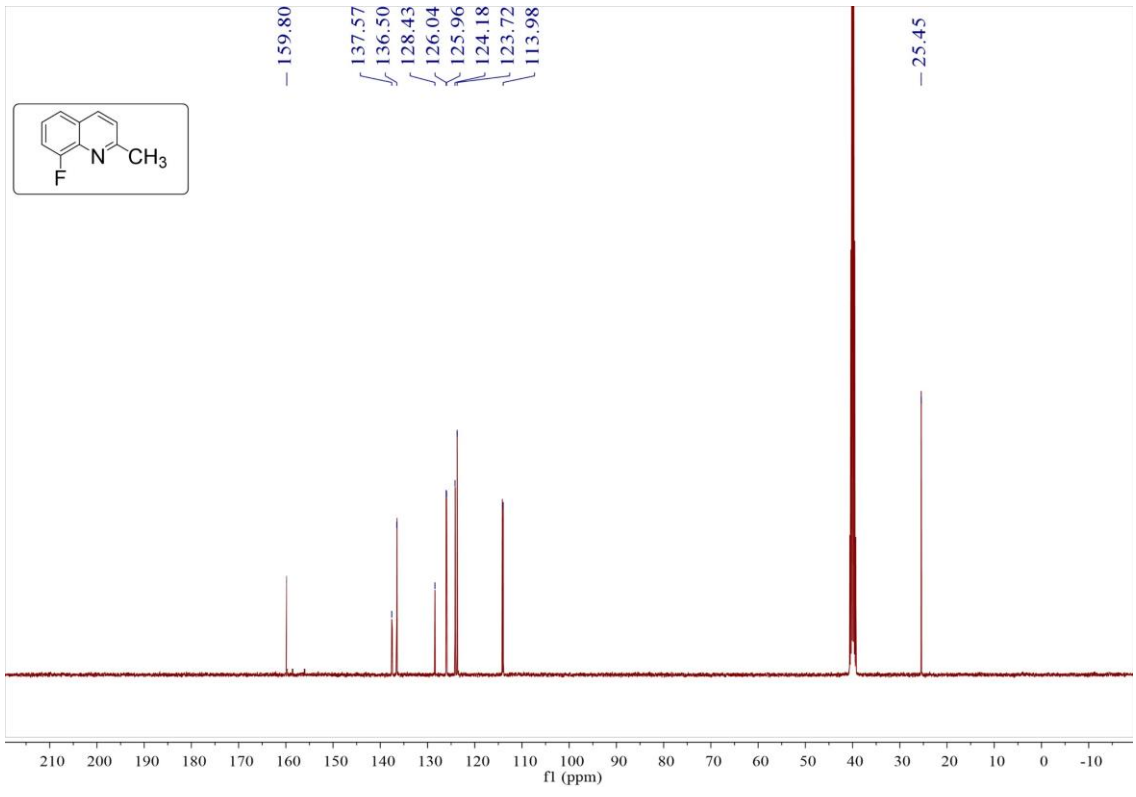
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.48
7.47
3.36
2.68
2.50
N
CH3
F
1.01
1.00
3.01
3.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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137.57
136.50
128.43
126.04
125.96
124.18
123.72
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25.45
N
CH3
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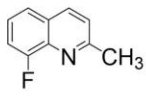
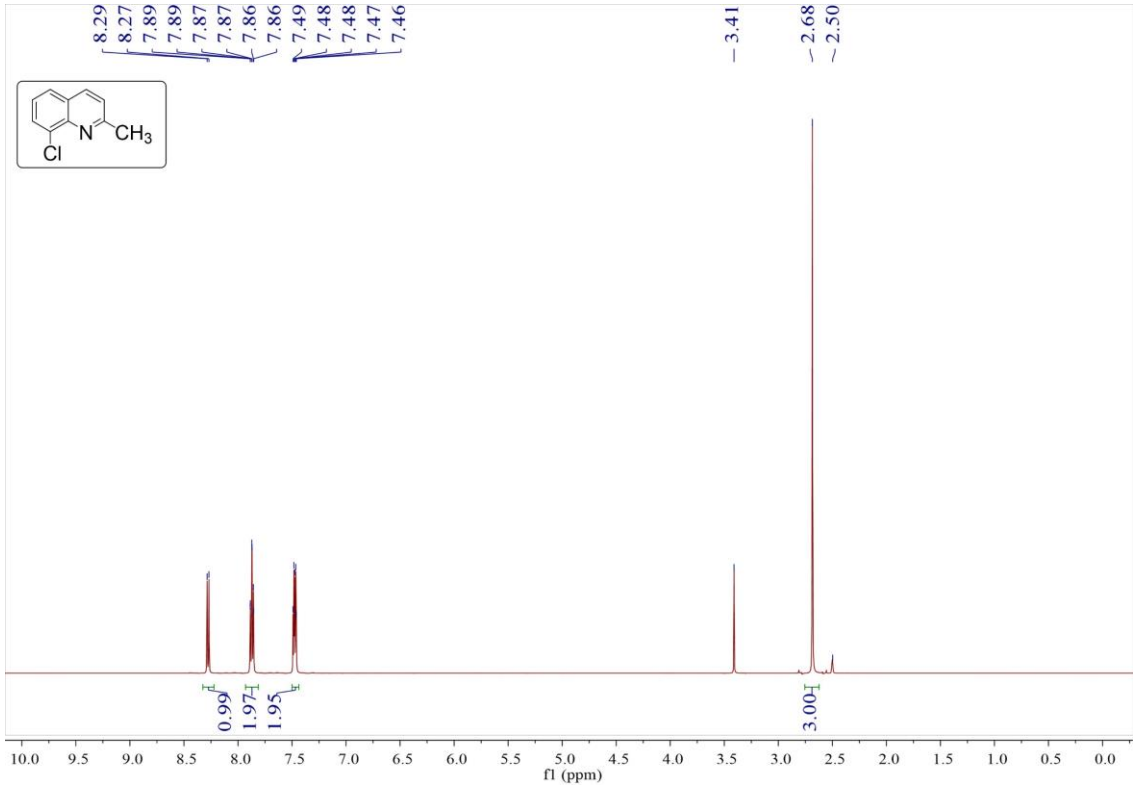
f1 (ppm)


N
CH3
F

-134.96
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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7.86
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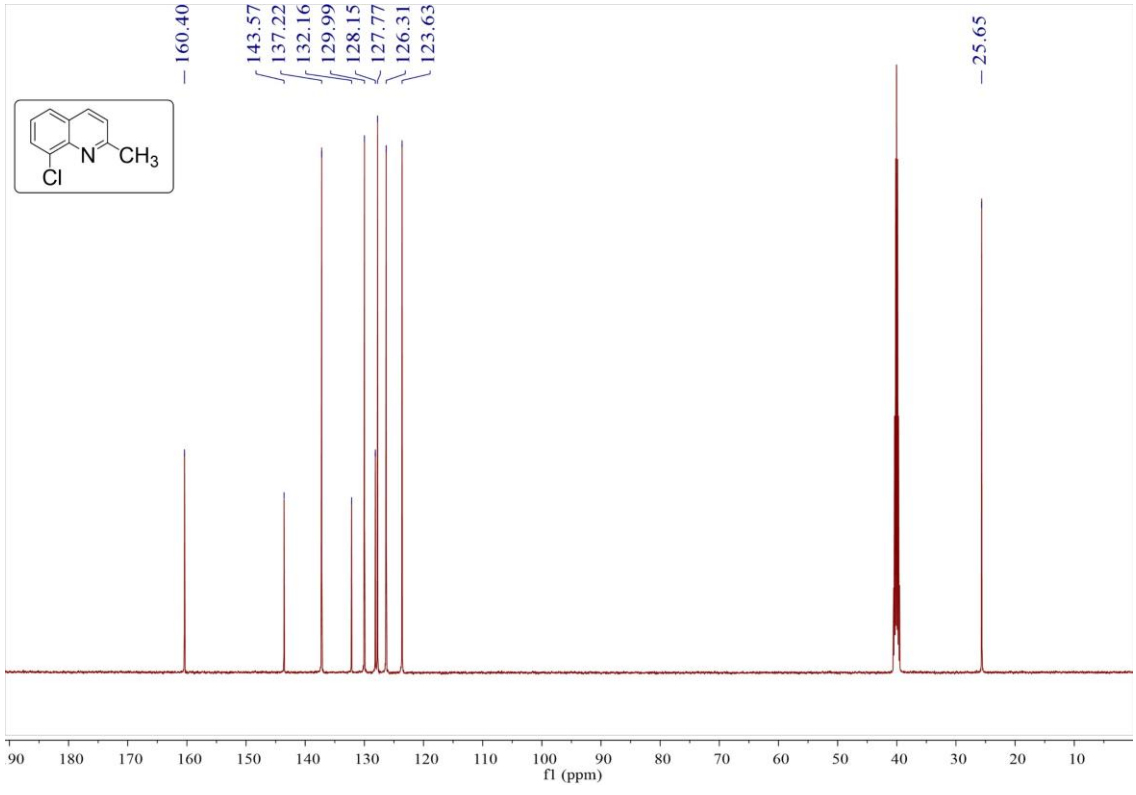
7.48
7.48
7.47
7.46
3.41
2.68
2.50
N
CH3
Cl
0.99
1.97
1.95
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.99
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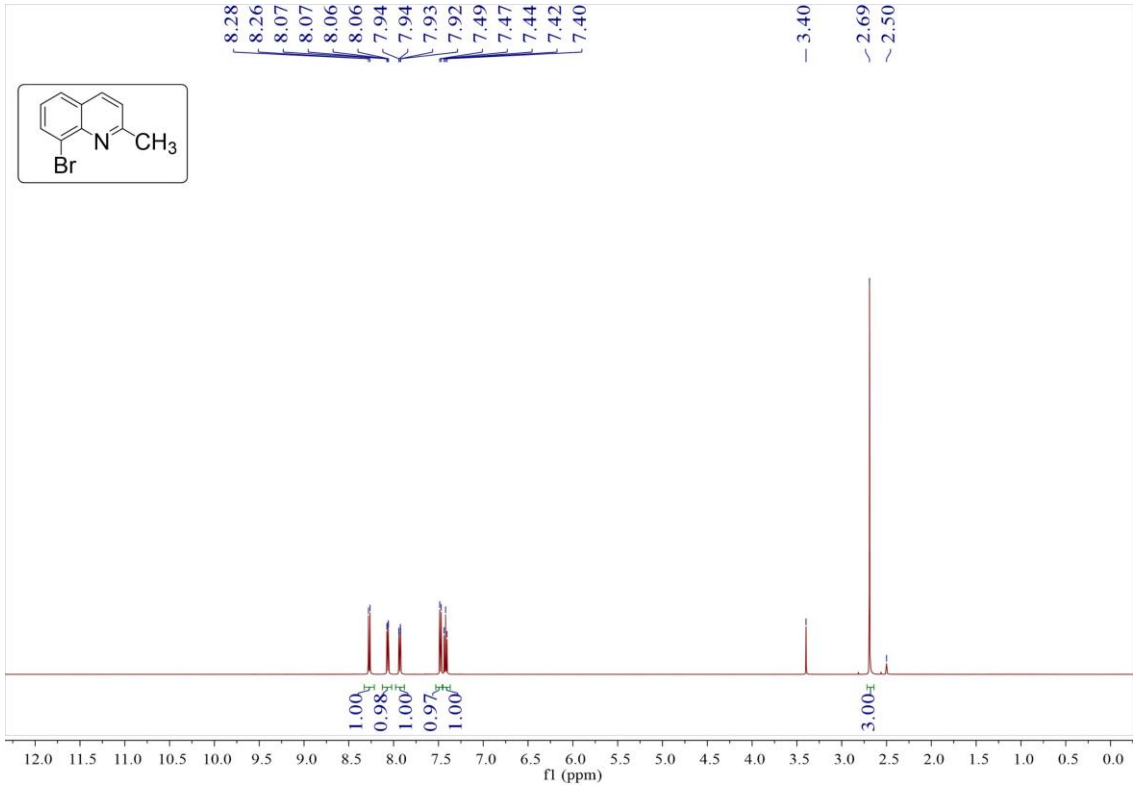
127.77
126.31
123.63
25.65
N
CH3
Cl
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.26
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8.07
8.06
8.06
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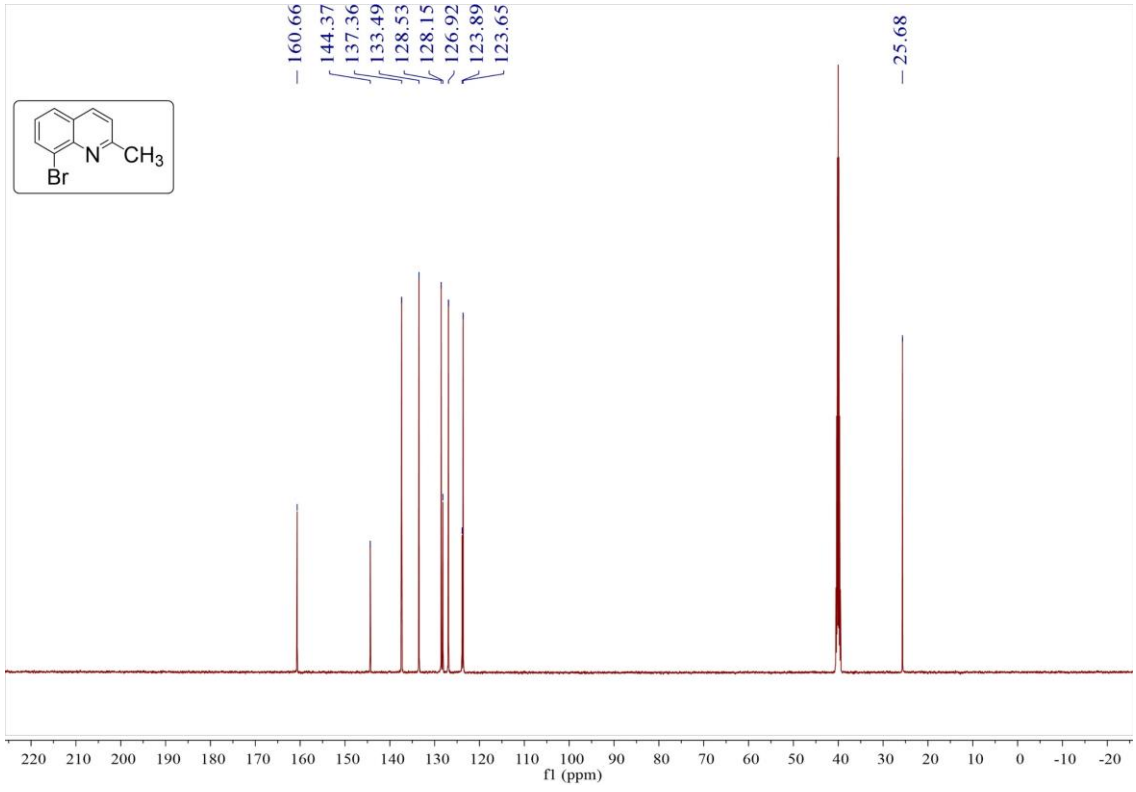
7.94
7.93
7.92
7.49
7.47
7.44
7.42
7.40
3.40
2.69
2.50
N
CH3
Br
1.00
0.98
1.00
0.97
1.00
3.00
f1 (ppm)


160.66
144.37
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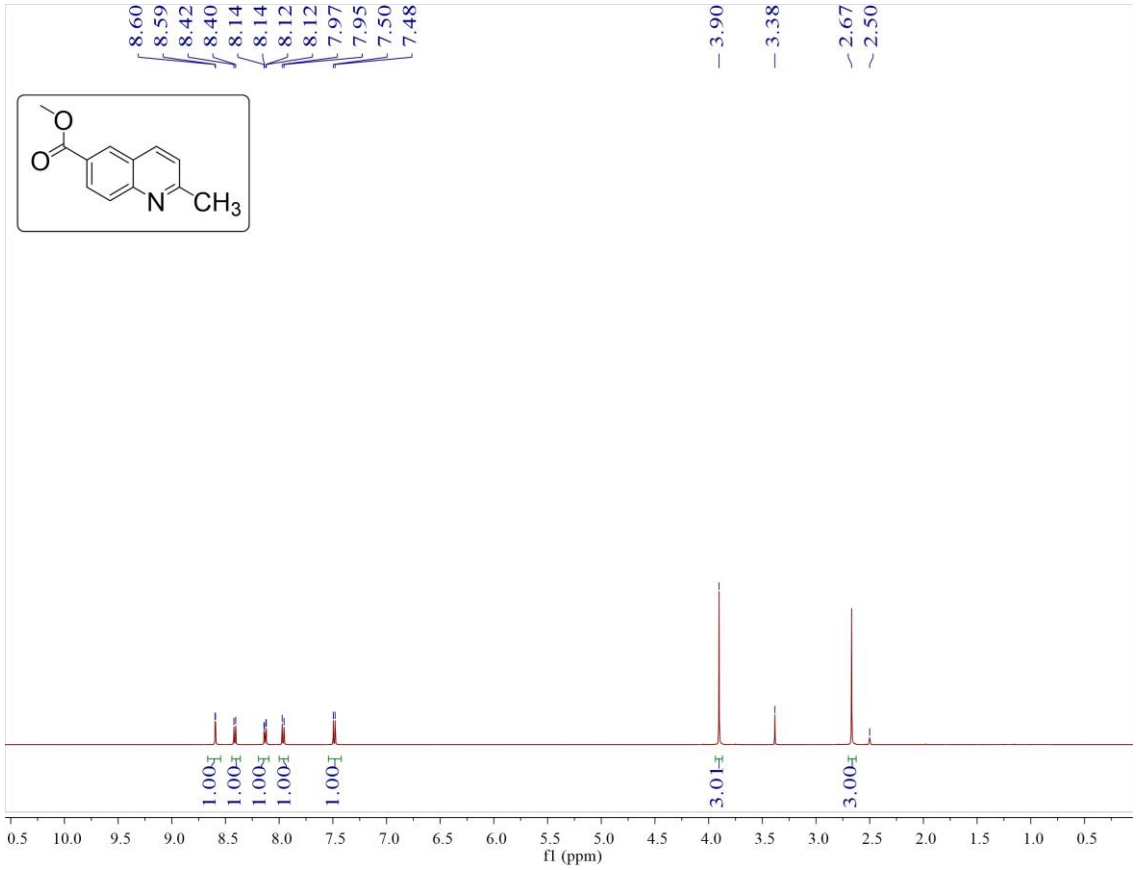
133.49
128.53
128.15
126.92
123.89
123.65
25.68
N
CH3
Br
f1 (ppm)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8.59
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8.14
8.12
8.12
7.97
7.95
7.50
7.48
3.90
3.38
2.67
2.50
O
O
N
CH3
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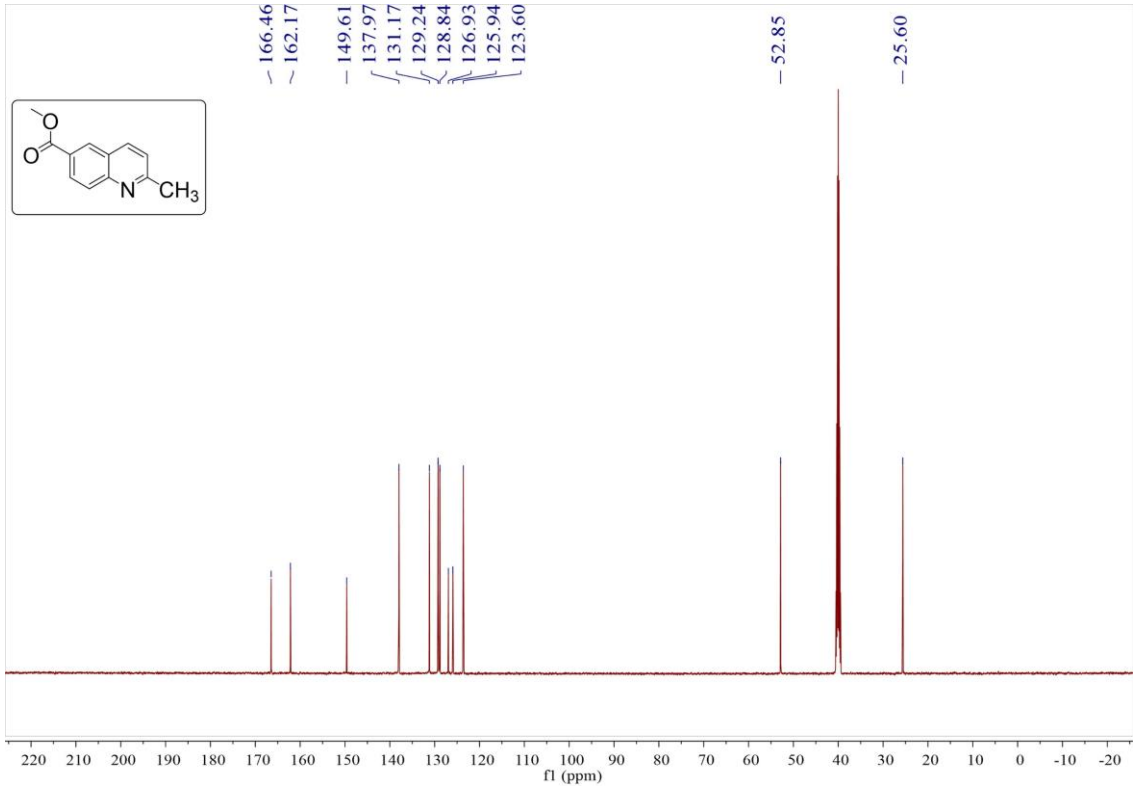
1.00
1.00
1.00
1.00
3.01
3.00
f1 (ppm)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162.17
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137.97
131.17
129.24
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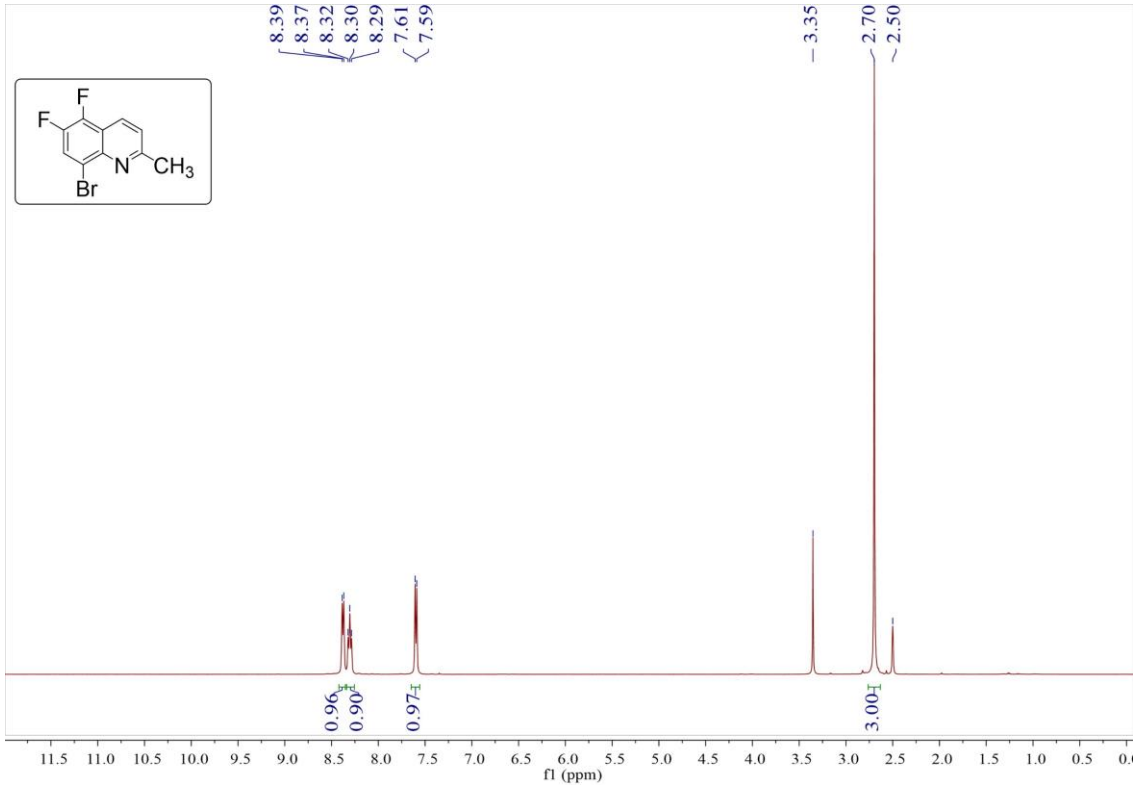
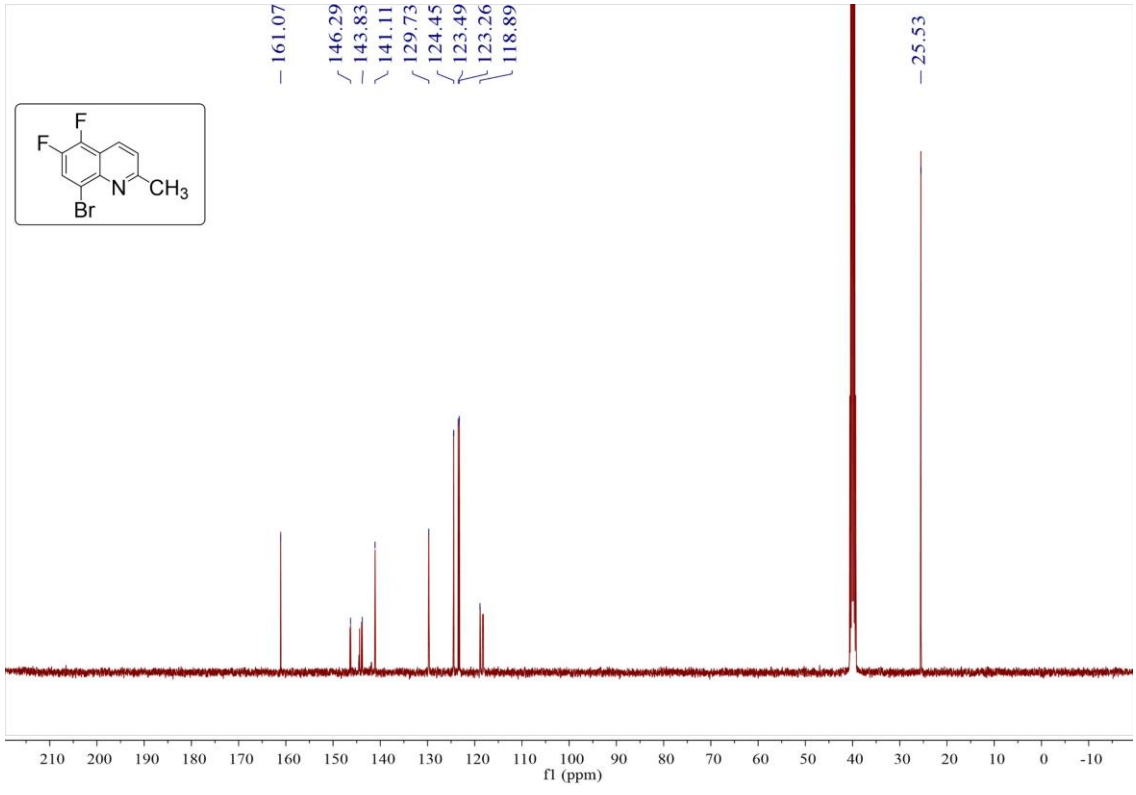
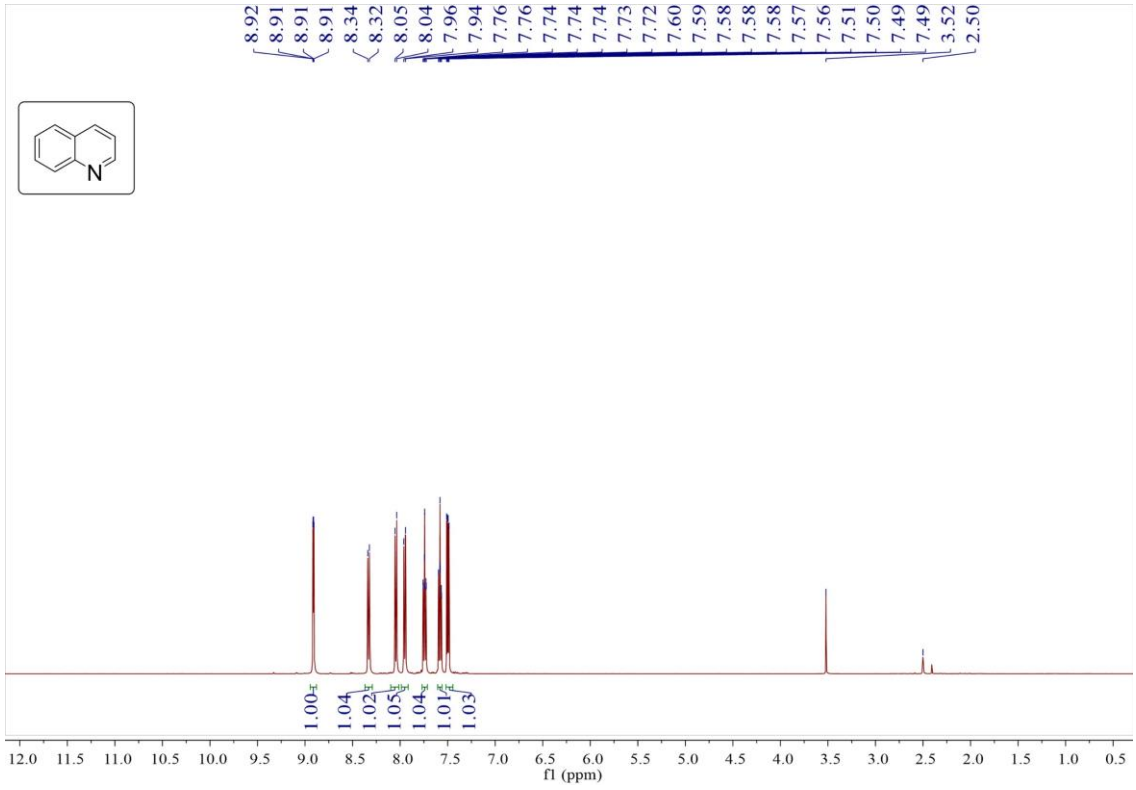
126.93
125.94
123.60
52.85
25.60
O
O
N
CH3
f1 (ppm)


8.39
8.37
8.32
8.30
8.29
7.61
7.59
3.35
2.70
2.50
F
F
N
CH3
Br
0.96
0.90
0.97
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


161.07
146.29
143.83
141.11
129.73
124.45
123.49
123.26
118.89
25.53
F
F
N
CH3
Br
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)


F
F
N
CH3
Br

-107.62
-109.21
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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8.91
8.91
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8.32
8.05
8.04
7.96
7.94
7.76
7.76
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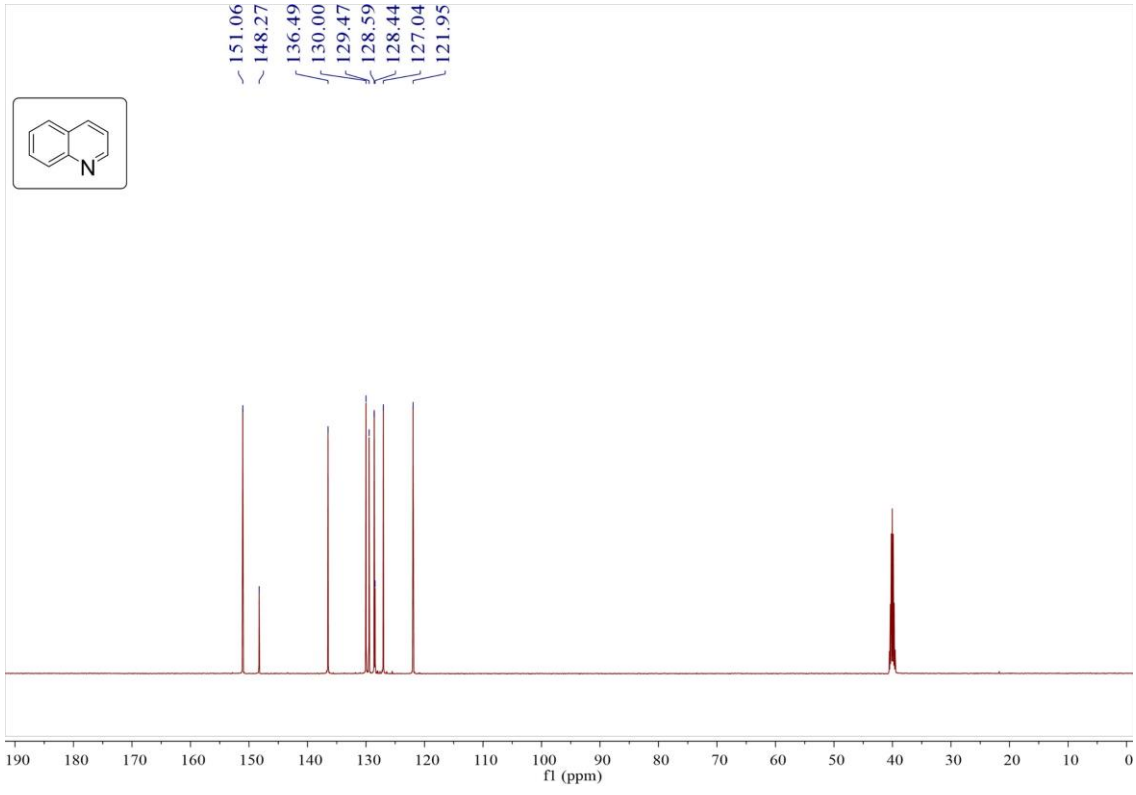
7.74
7.74
7.73
7.72
7.60
7.59
7.58
7.58
7.58
7.57
7.56
7.51
7.50
7.49
7.49
3.52
2.50
1.00
1.04
1.02
1.05
1.04
1.01
1.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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148.27
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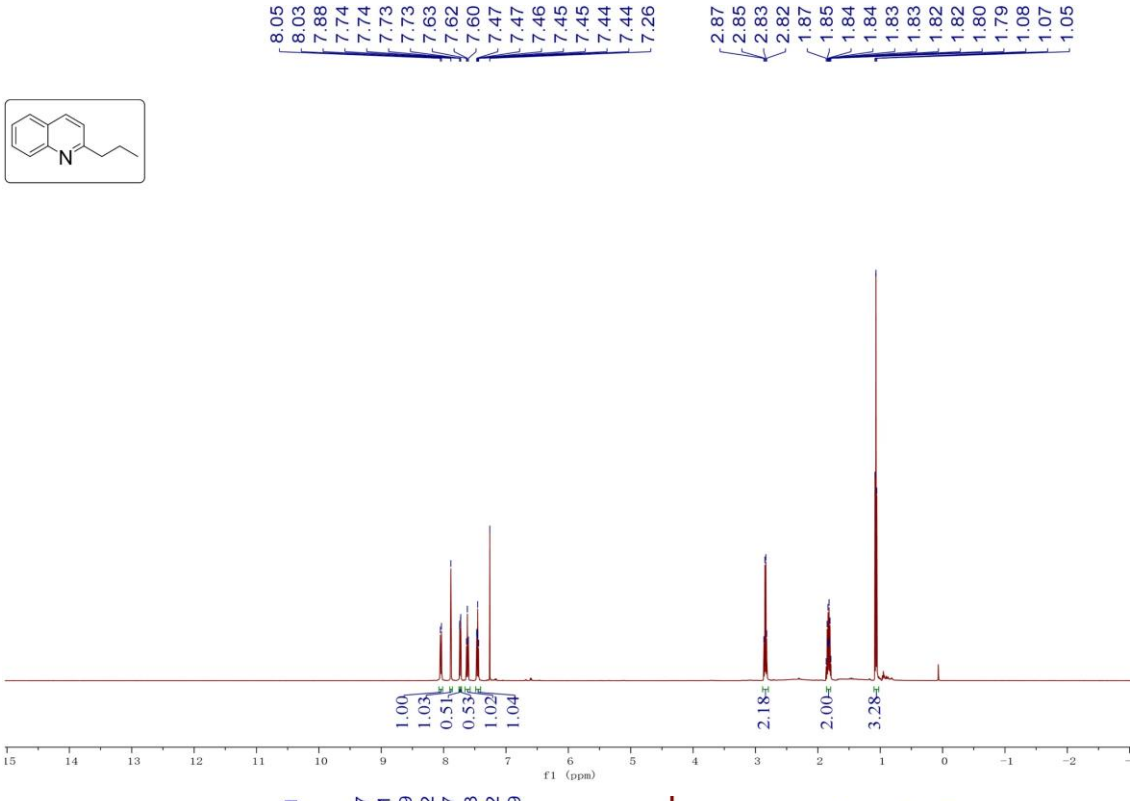
130.00
129.47
128.59
128.44
127.04
121.95
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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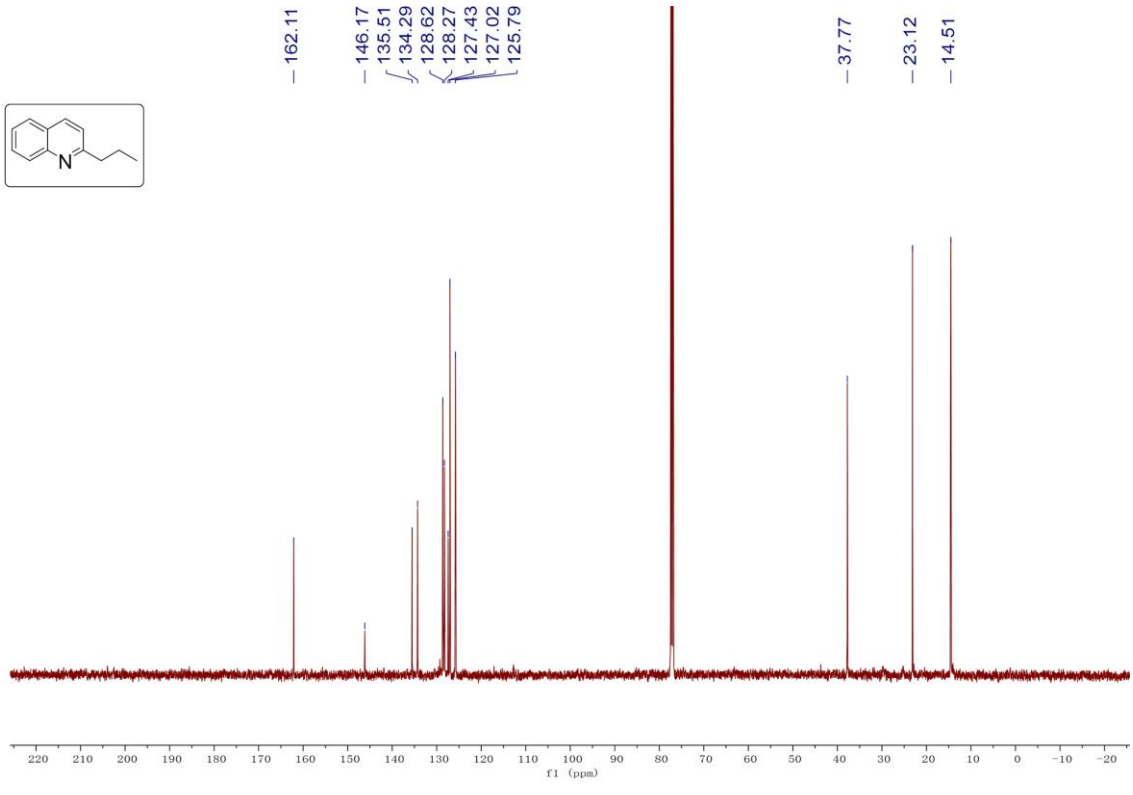
7.73
7.63
7.62
7.60
7.47
7.47
7.46
7.45
7.45
7.44
7.44
7.26
2.87
2.85
2.83
2.82
1.87
1.85
1.84
1.84
1.83
1.83
1.82
1.82
1.80
1.79
1.08
1.07
1.05
1.00
1.03
0.51
0.53
1.02
1.04
2.18
2.00
3.28
f1 (ppm)


162.11
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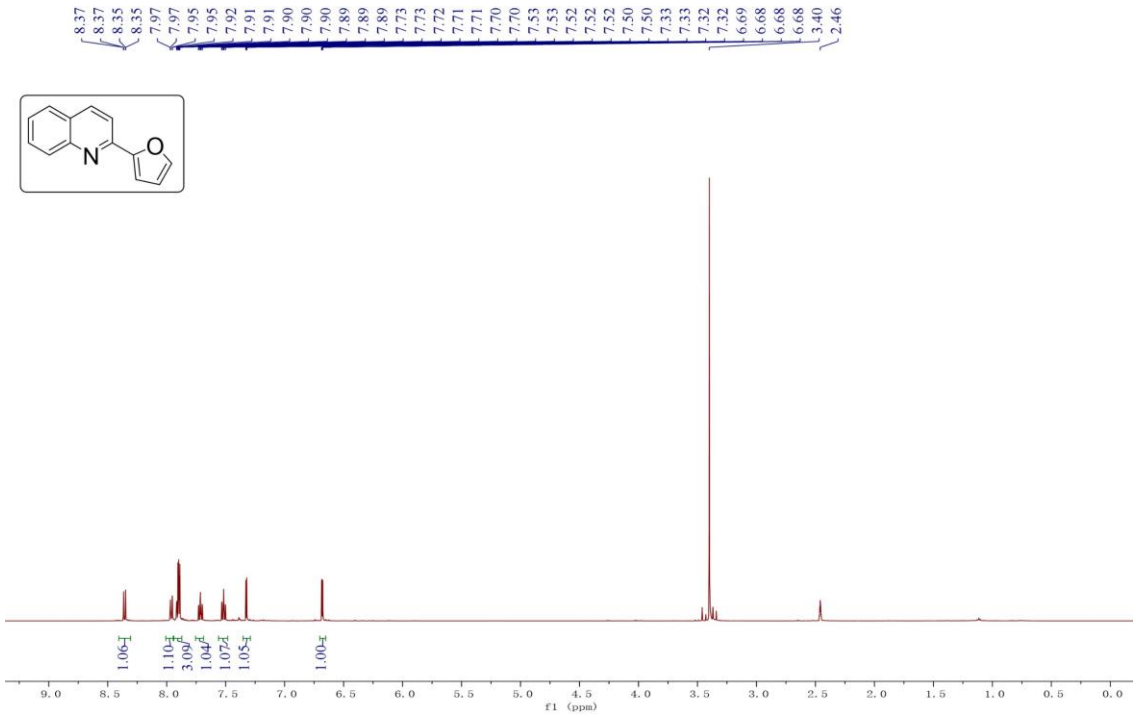
128.62
128.27
127.43
127.02
125.79
37.77
23.12
14.51
f1 (ppm)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7.32
7.32
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6.68
6.68
3.40
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N
O
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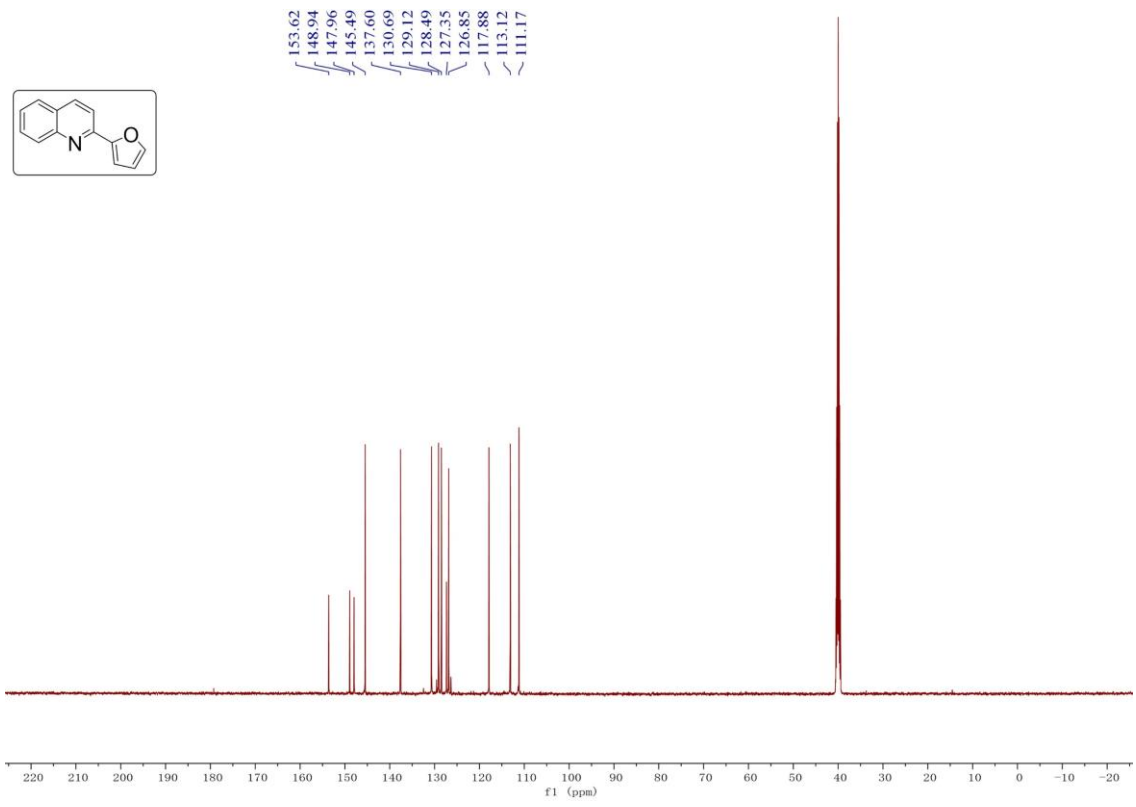
1.10
3.09
1.04
1.07
1.05
1.00
f1 (ppm)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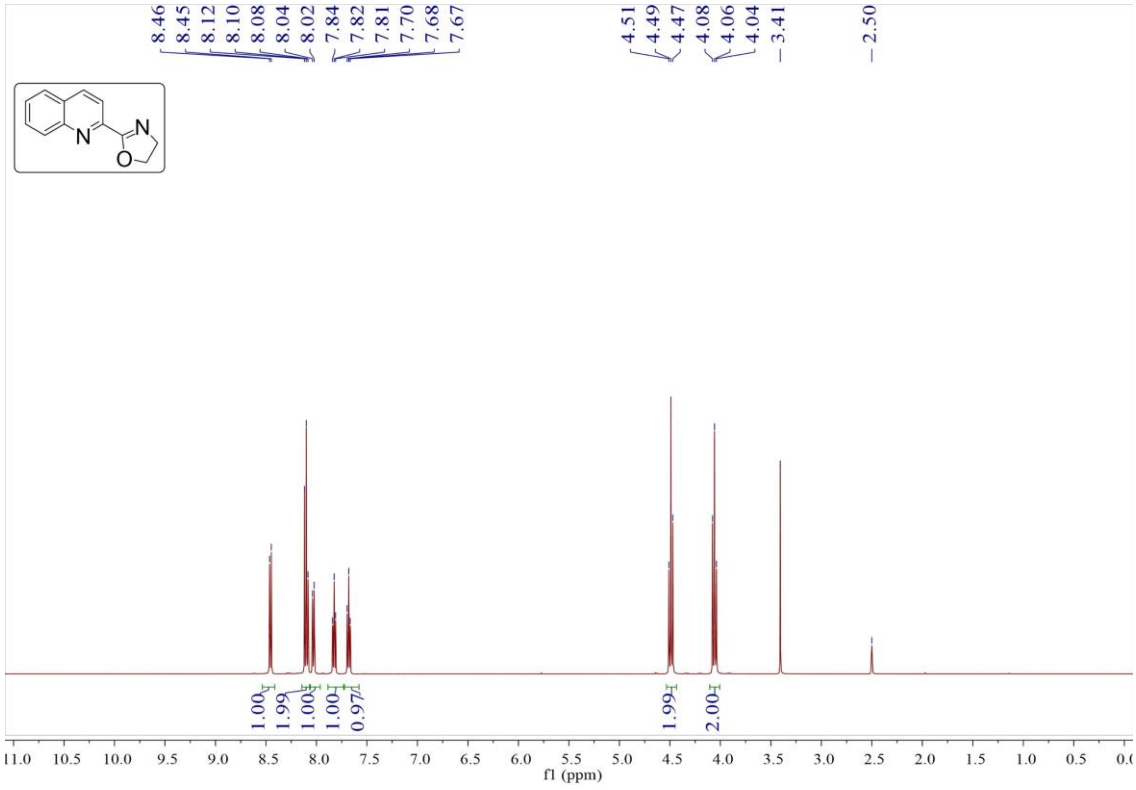
128.49
127.35
126.85
117.88
113.12
111.17
N
O
f1 (ppm)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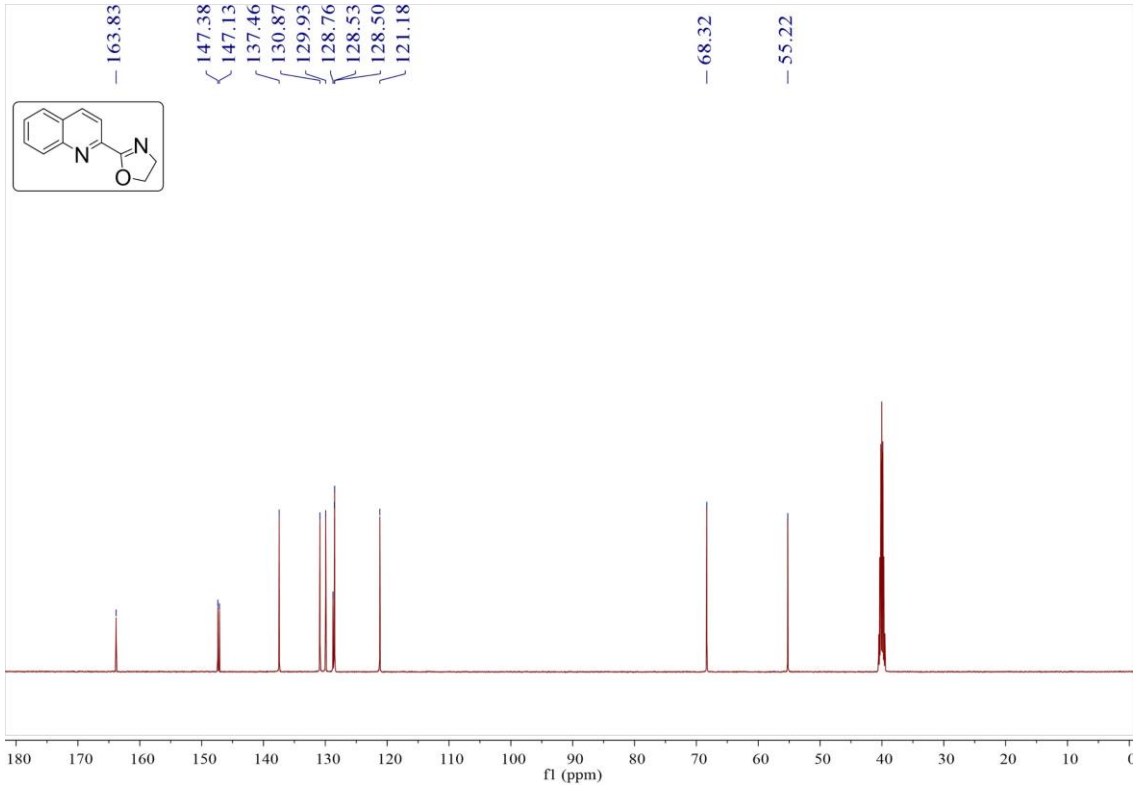
8.12
8.10
8.08
8.04
8.02
7.84
7.82
7.81
7.70
7.68
7.67
4.51
4.49
4.47
4.08
4.06
4.04
3.41
2.50
1.00
1.99
1.00
1.00
0.97
1.99
2.00
fl (ppm)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128.76
128.53
128.50
121.18
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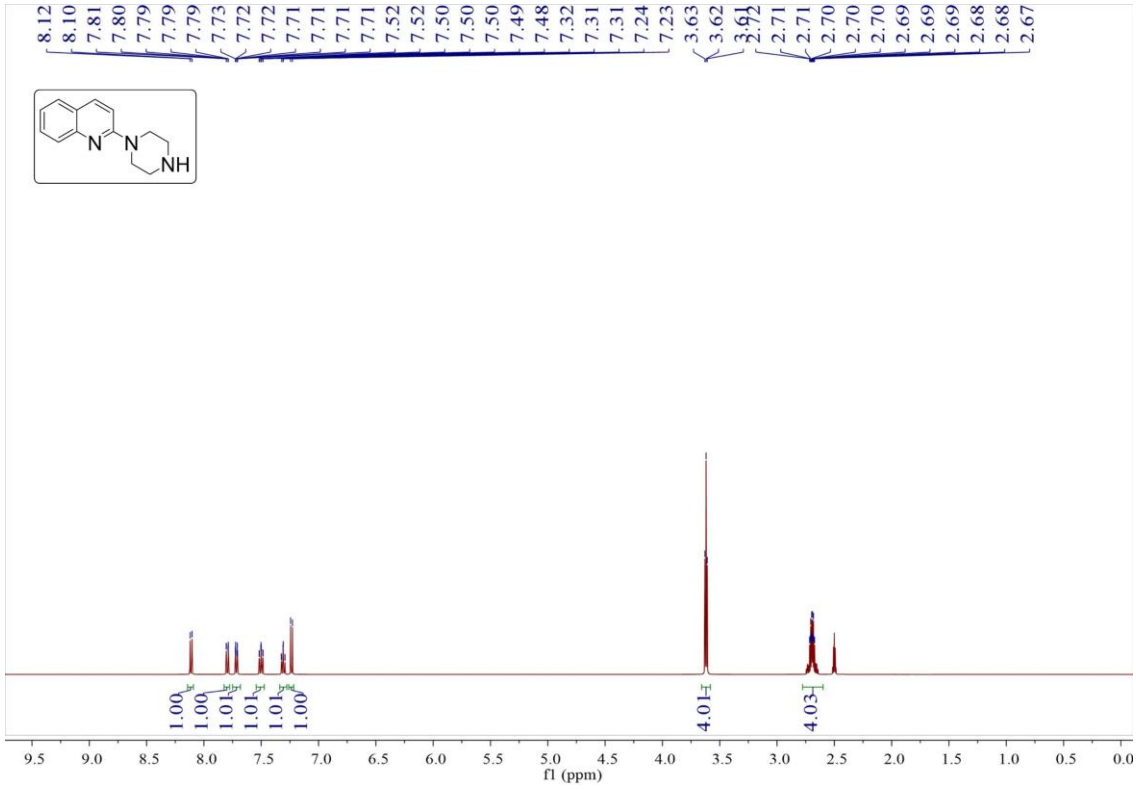
55.22
fl (ppm)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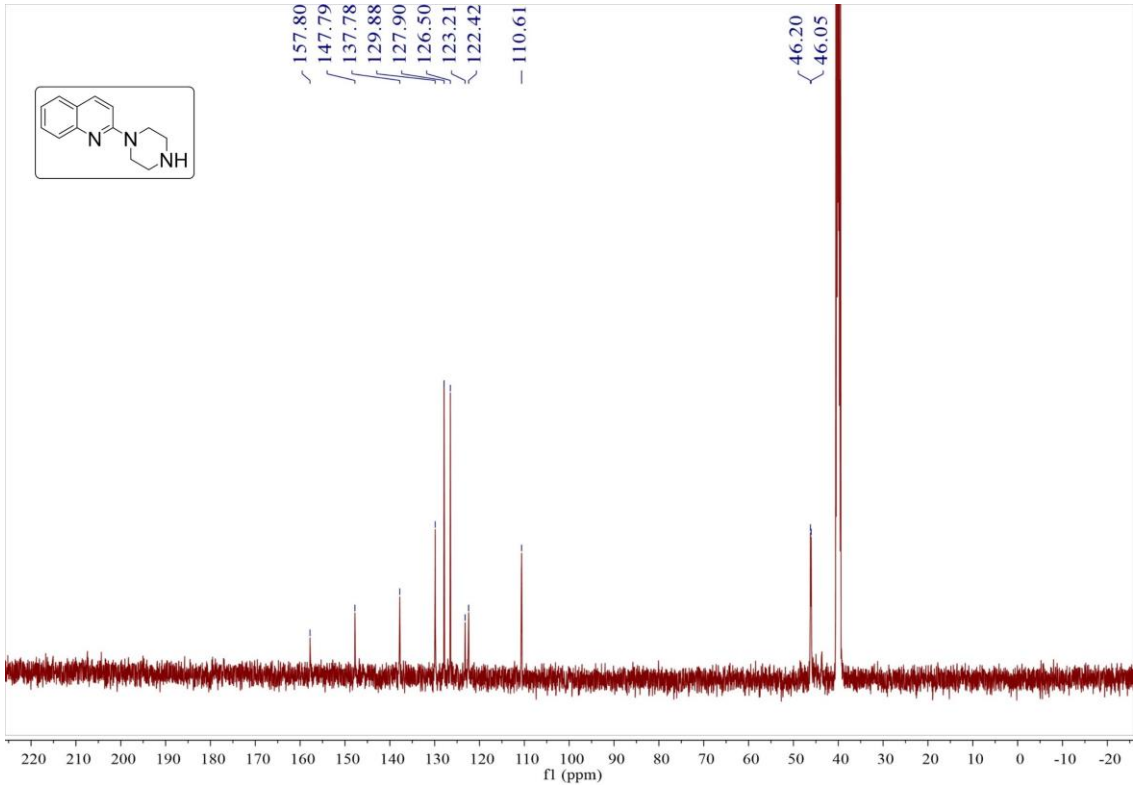
1.01
1.00
4.01
4.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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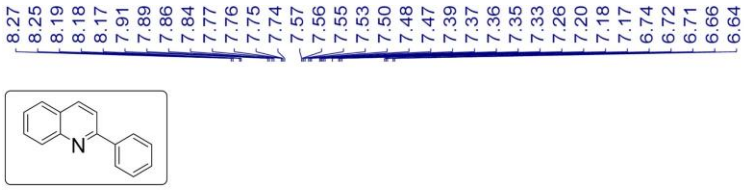
127.90
126.50
123.21
122.42
110.61
46.20
46.05
N
N
NH
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.76
7.75
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7.57
7.56
7.55
7.53
7.50
7.48
7.47
7.39
7.37
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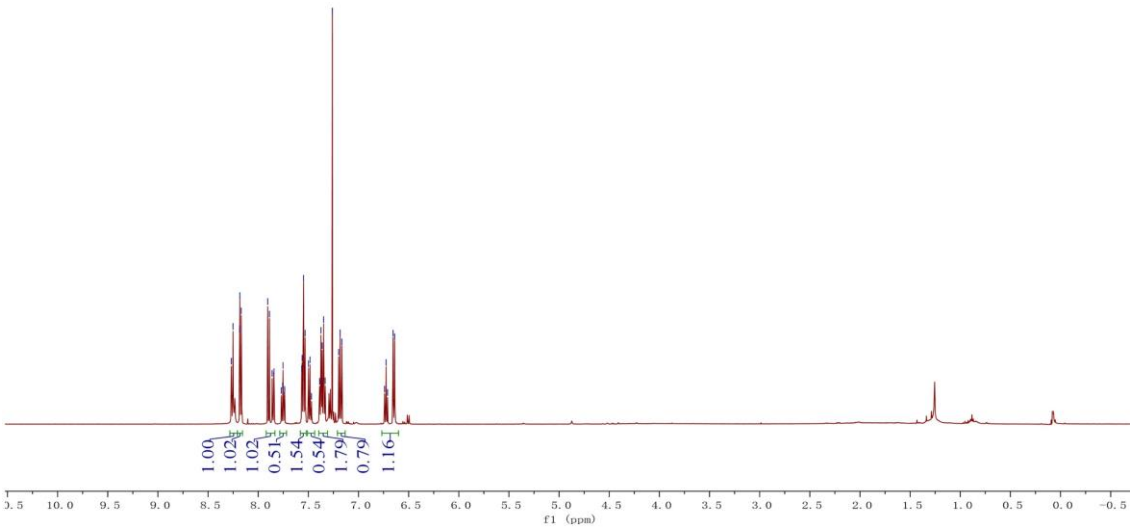
7.26
7.20
7.18
7.17
6.74
6.72
6.71
6.66
6.64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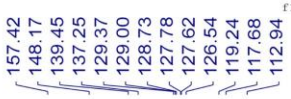
1.02
1.02
0.51
1.54
0.54
1.79
0.79
1.16
f1 (ppm)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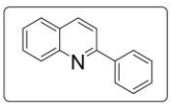
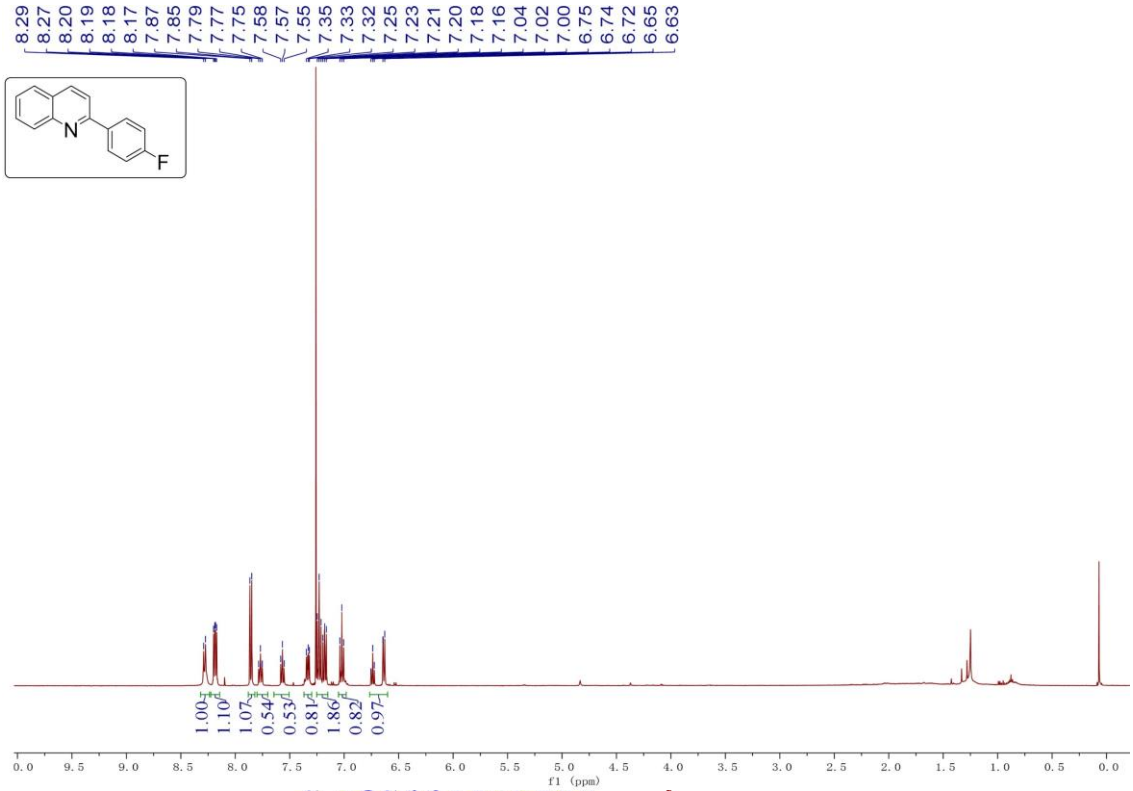
127.78
127.62
126.54
119.24
117.68
112.94



f1 (ppm)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7.57
7.55
7.35
7.33
7.32
7.25
7.23
7.21
7.20
7.18
7.16
7.04
7.02
7.00
6.75
6.74
6.72
6.65
6.63
N
F
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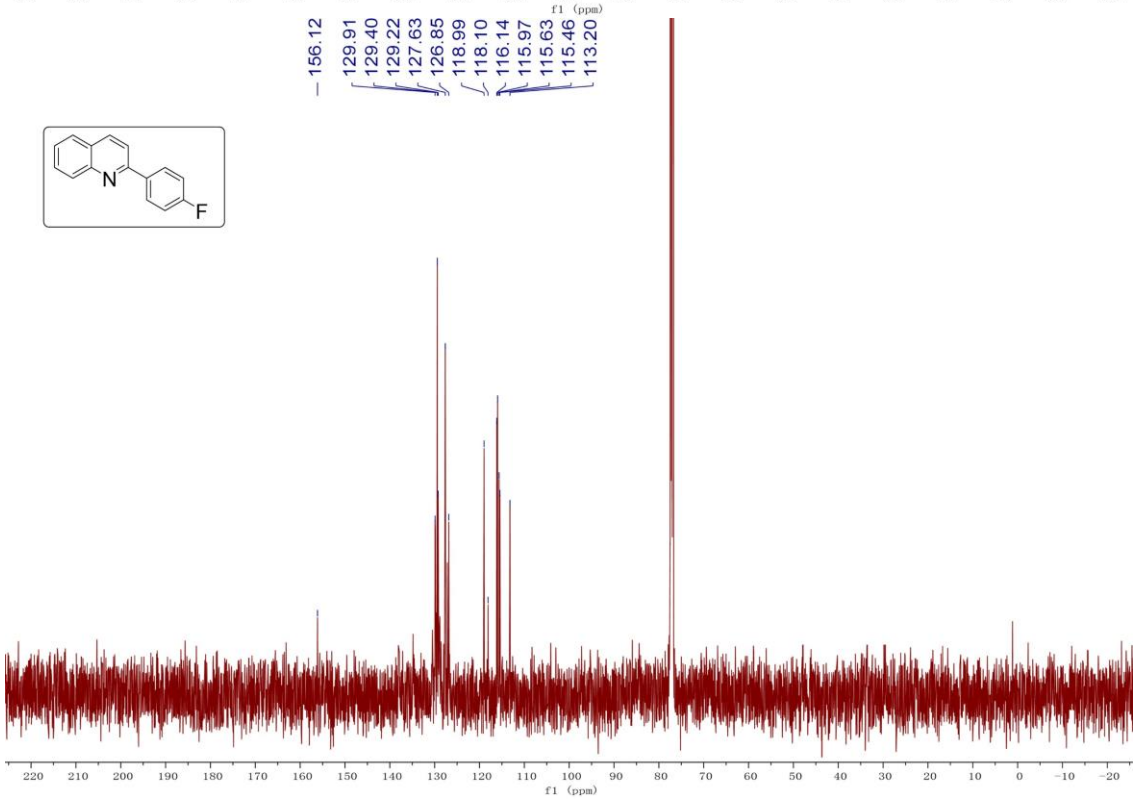
1.10
1.07
0.54
0.53
0.81
1.86
0.82
0.97
f1 (ppm)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126.85
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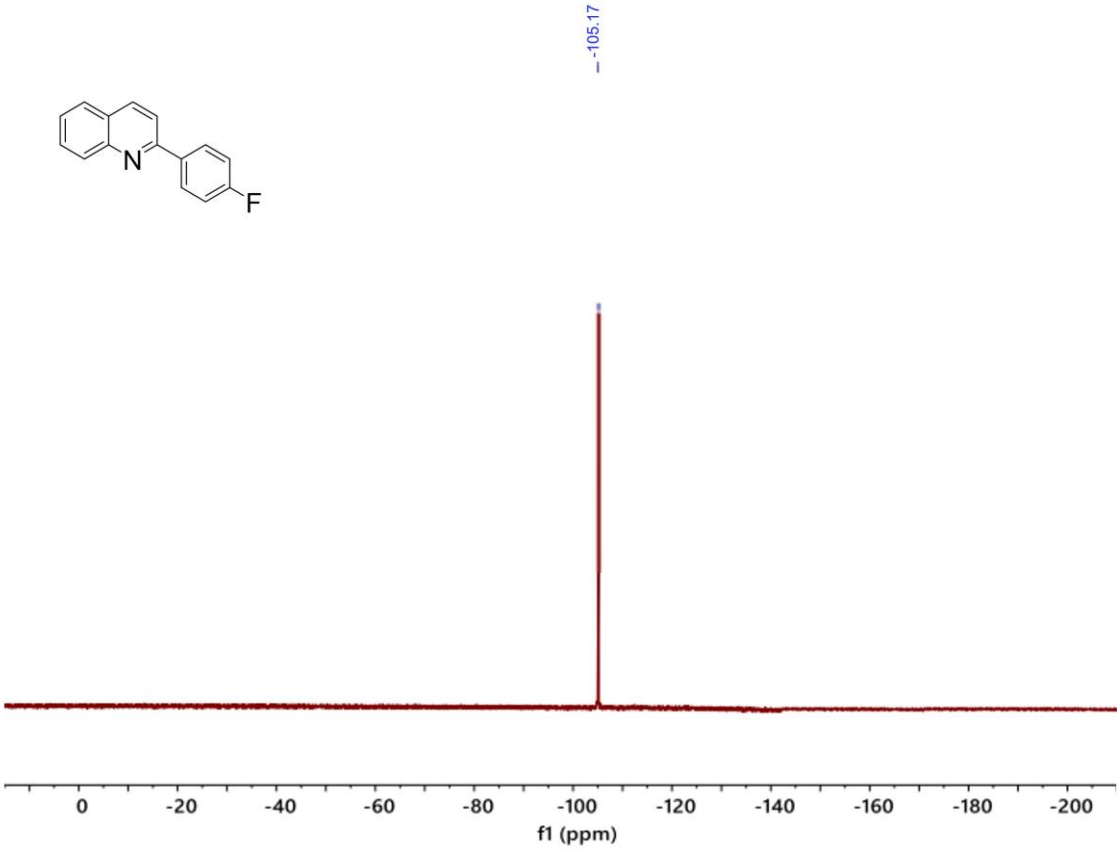
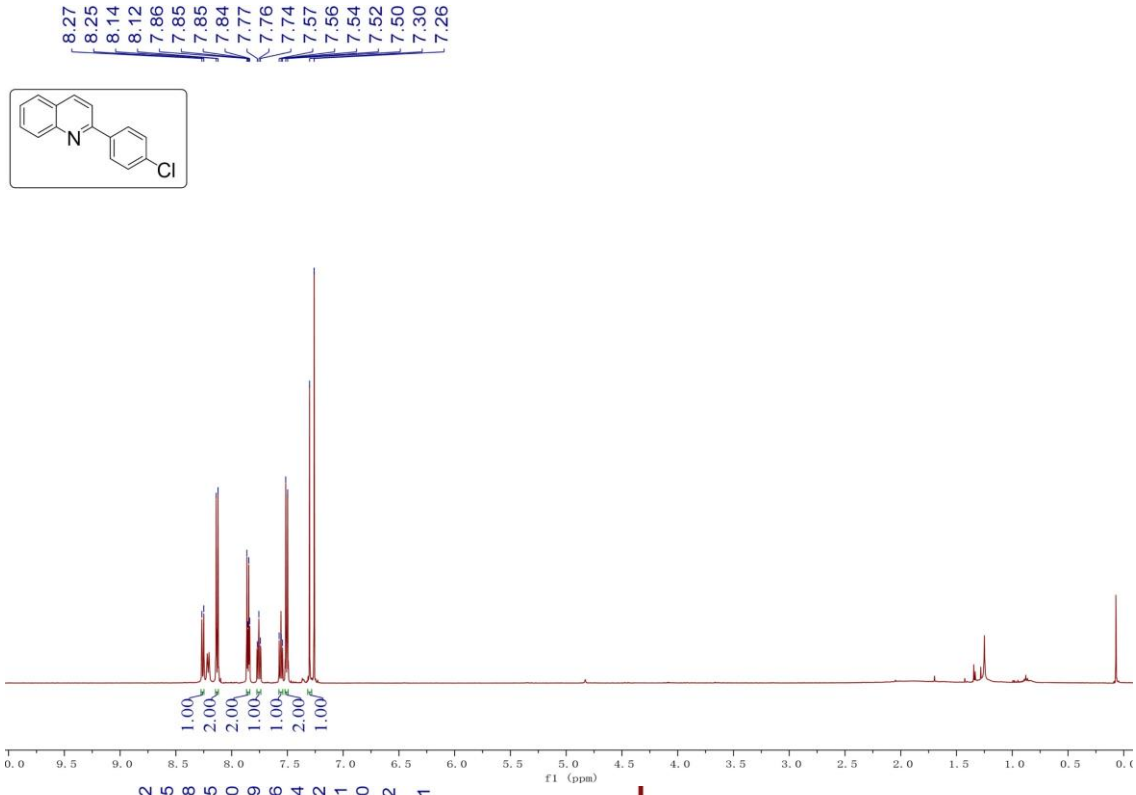
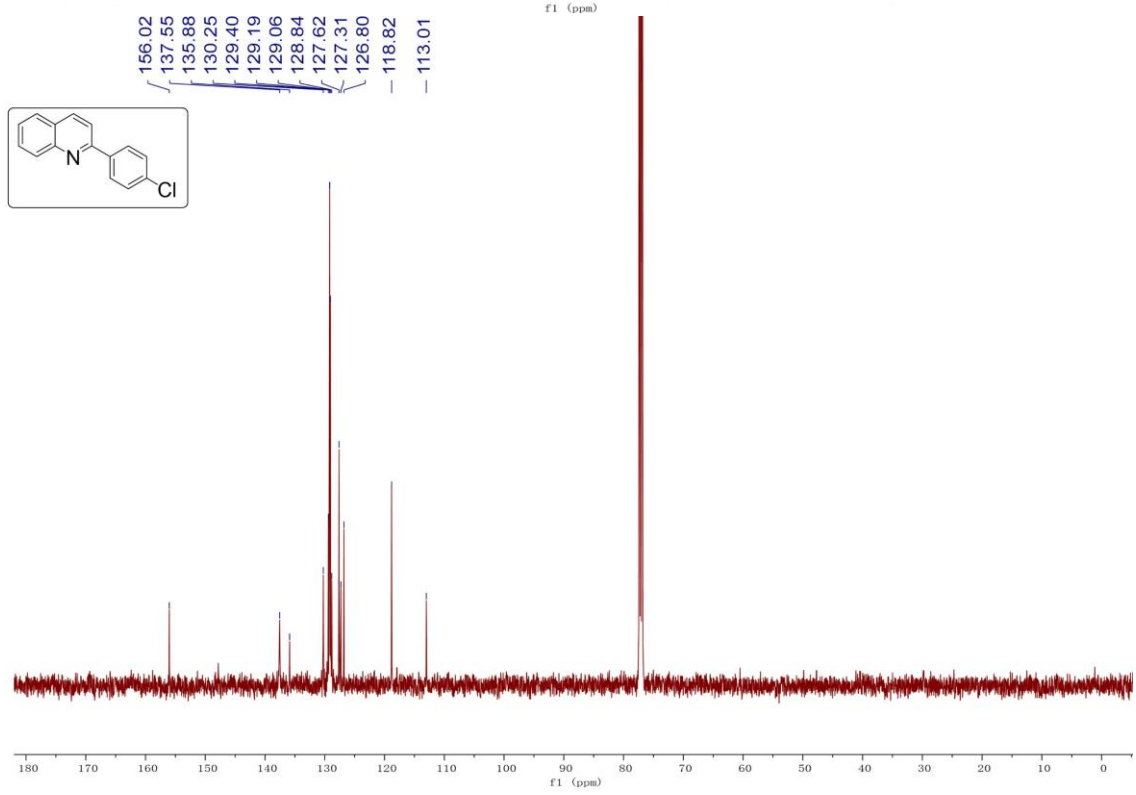
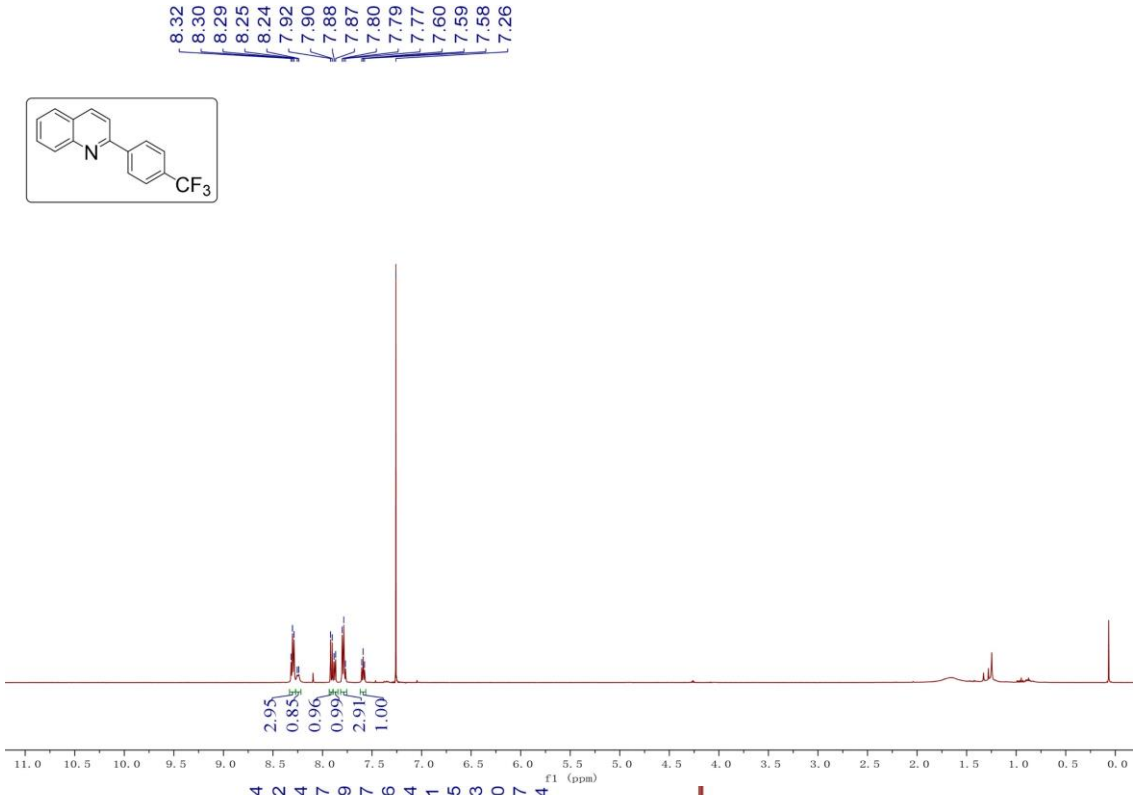
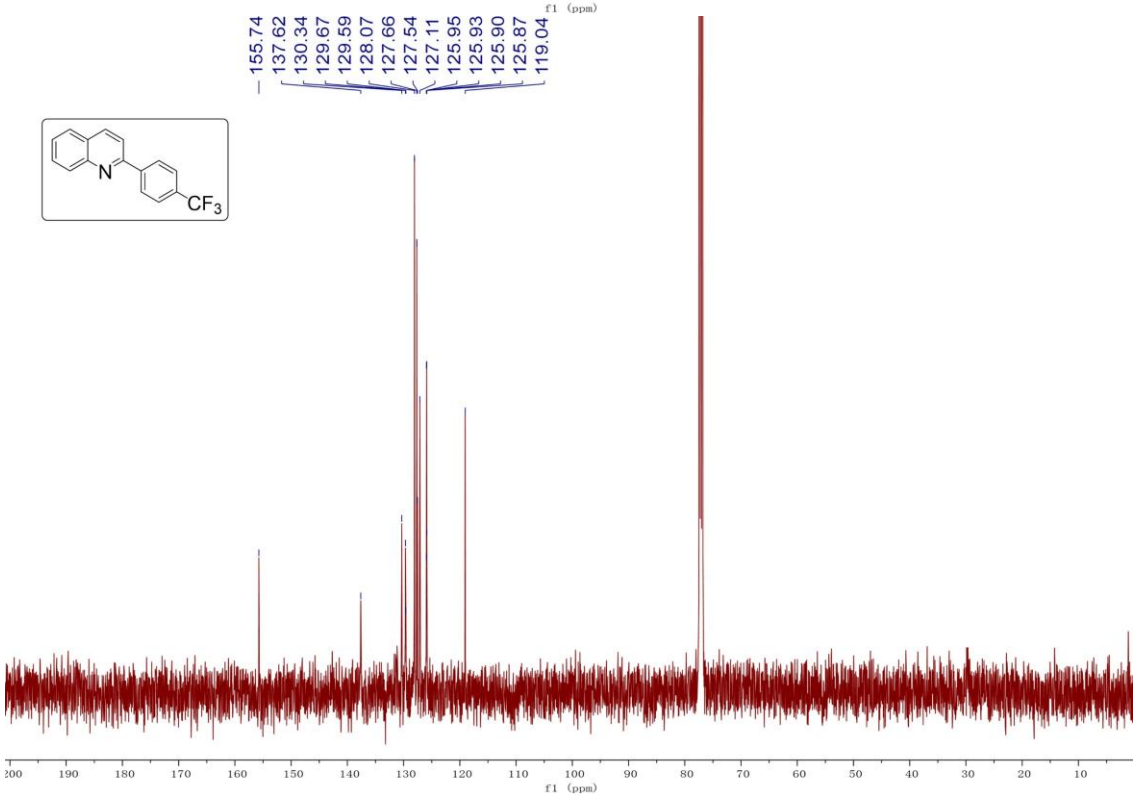
118.10
116.14
115.97
115.63
115.46
113.20
N
F
f1 (ppm)

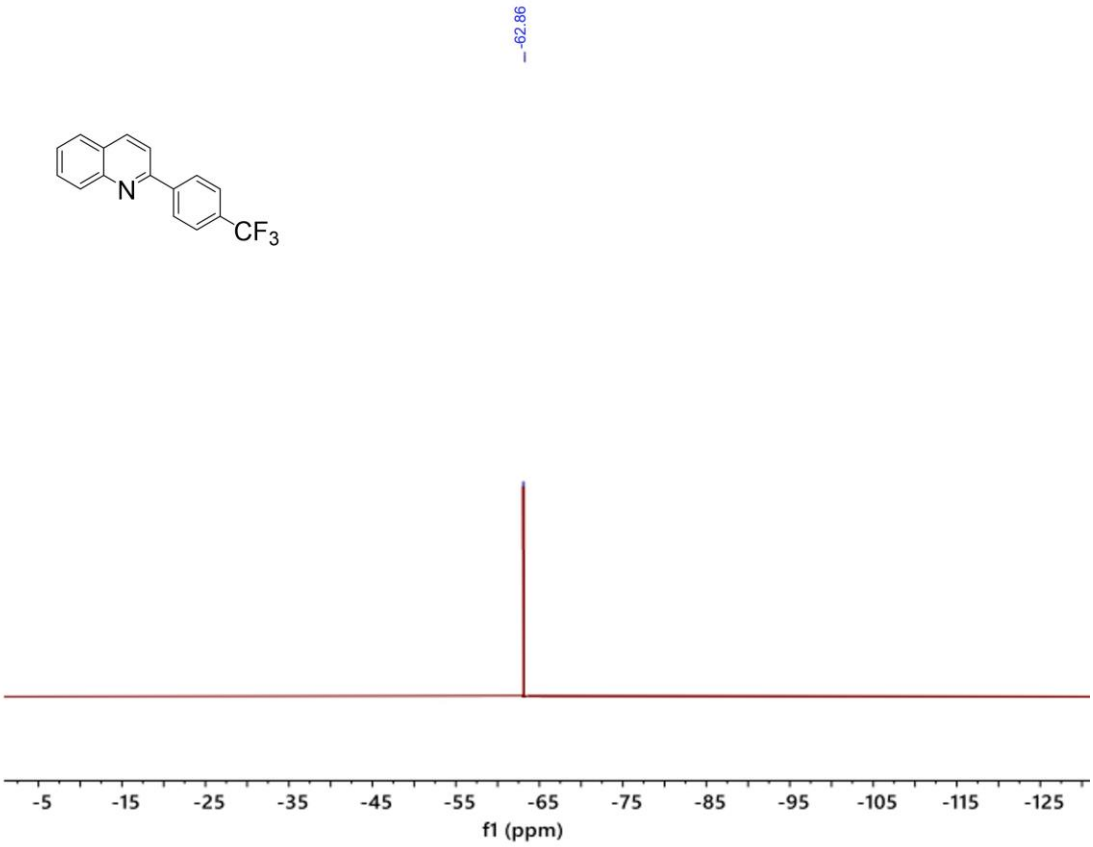

-105.17
N
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

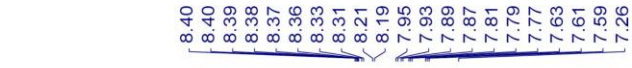

8.27
8.25
8.14
8.12
7.86
7.85
7.85
7.84
7.77
7.76
7.74
7.57
7.56
7.54
7.52
7.50
7.30
7.26
N
Cl
1.00
2.00
2.00
1.00
1.00
2.00
1.00
f1 (ppm)


156.02
137.55
135.88
130.25
129.40
129.19
129.06
128.84
127.62
127.31
126.80
118.82
113.01
N
Cl
f1 (ppm)


8.32
8.30
8.29
8.25
8.24
7.92
7.90
7.88
7.87
7.80
7.79
7.77
7.60
7.59
7.58
7.26
N
CF3
2.95
0.85
0.96
0.99
2.91
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


155.74
137.62
130.34
129.67
129.59
128.07
127.66
127.54
127.11
125.95
125.93
125.90
125.87
119.04
N
CF3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


-62.86
N
CF3
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-115
-125
f1 (ppm)


8.40
8.40
8.39
8.38
8.37
8.36
8.33
8.31
8.21
8.19
7.95
7.93
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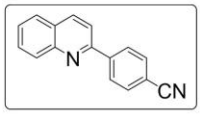
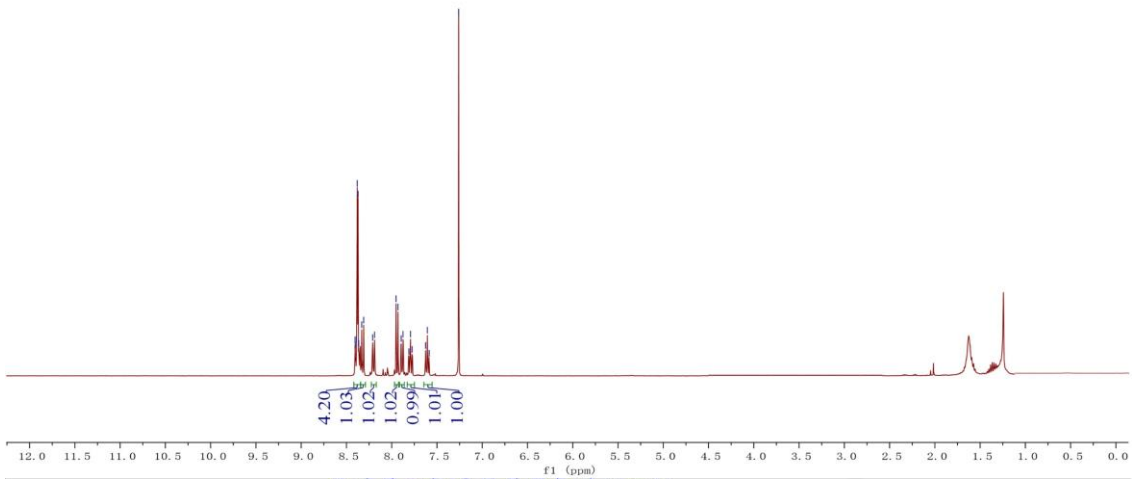
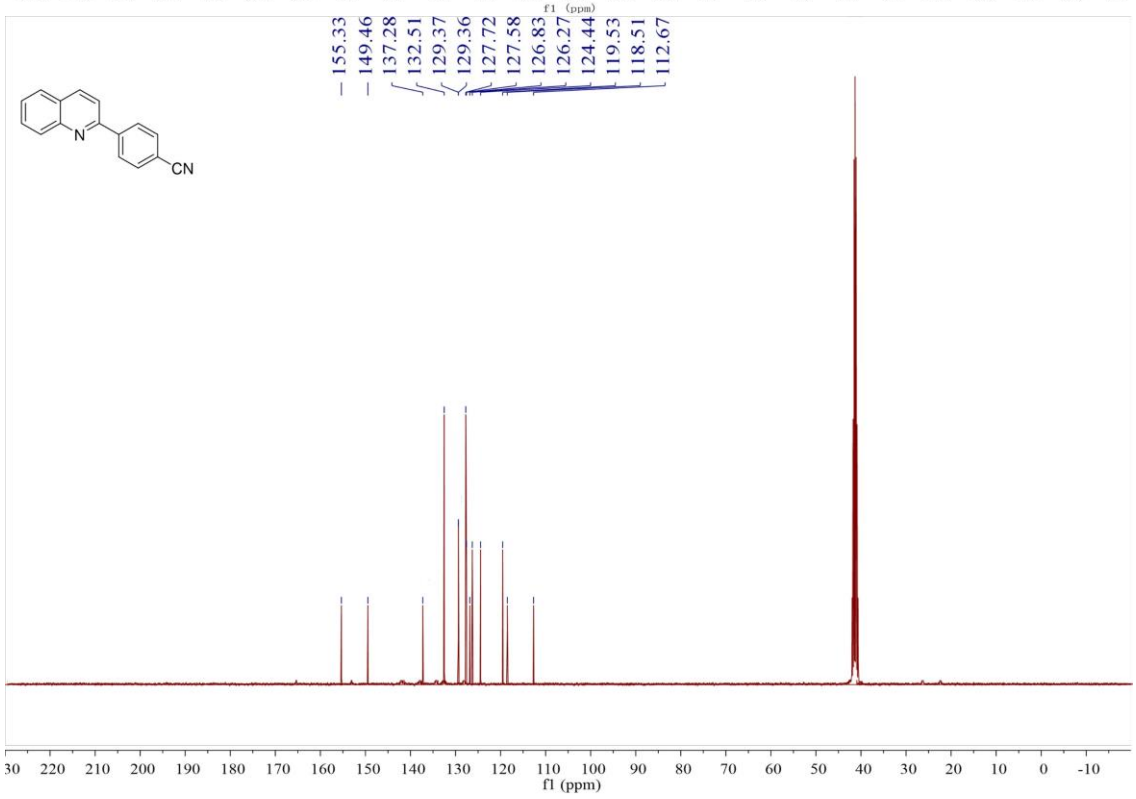
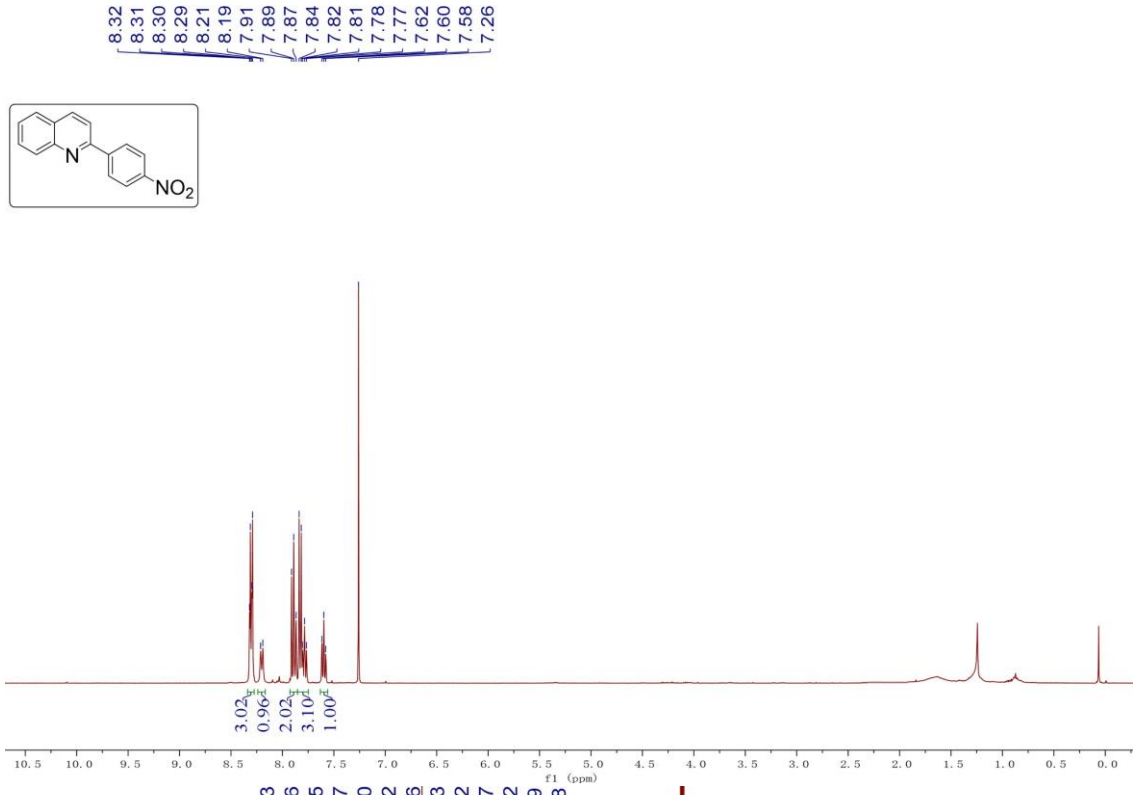
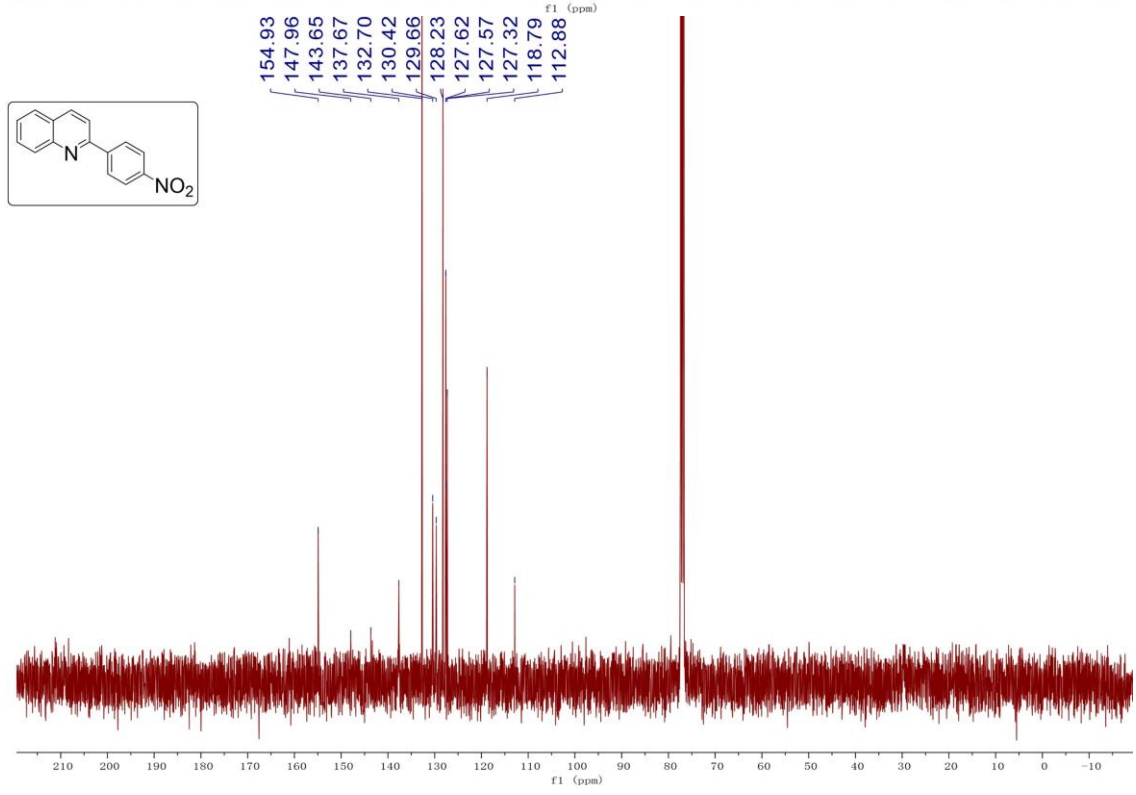
7.79
7.77
7.63
7.61
7.59
7.26

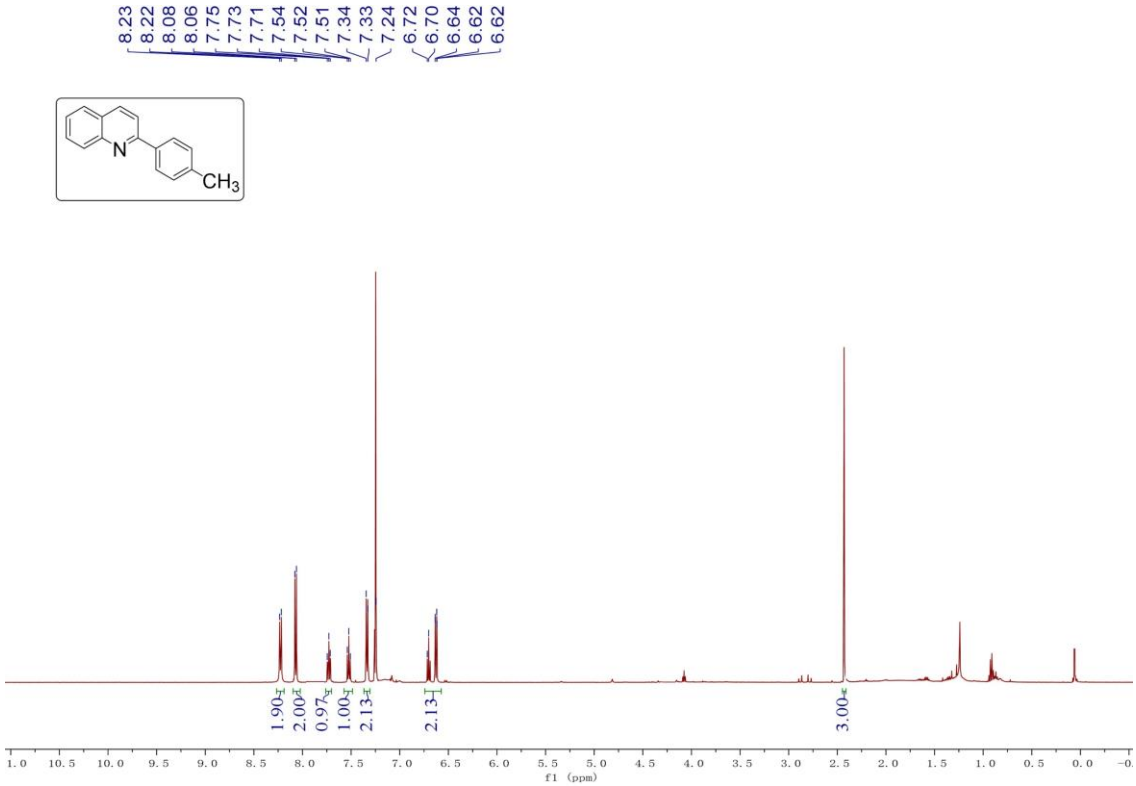

N
CN

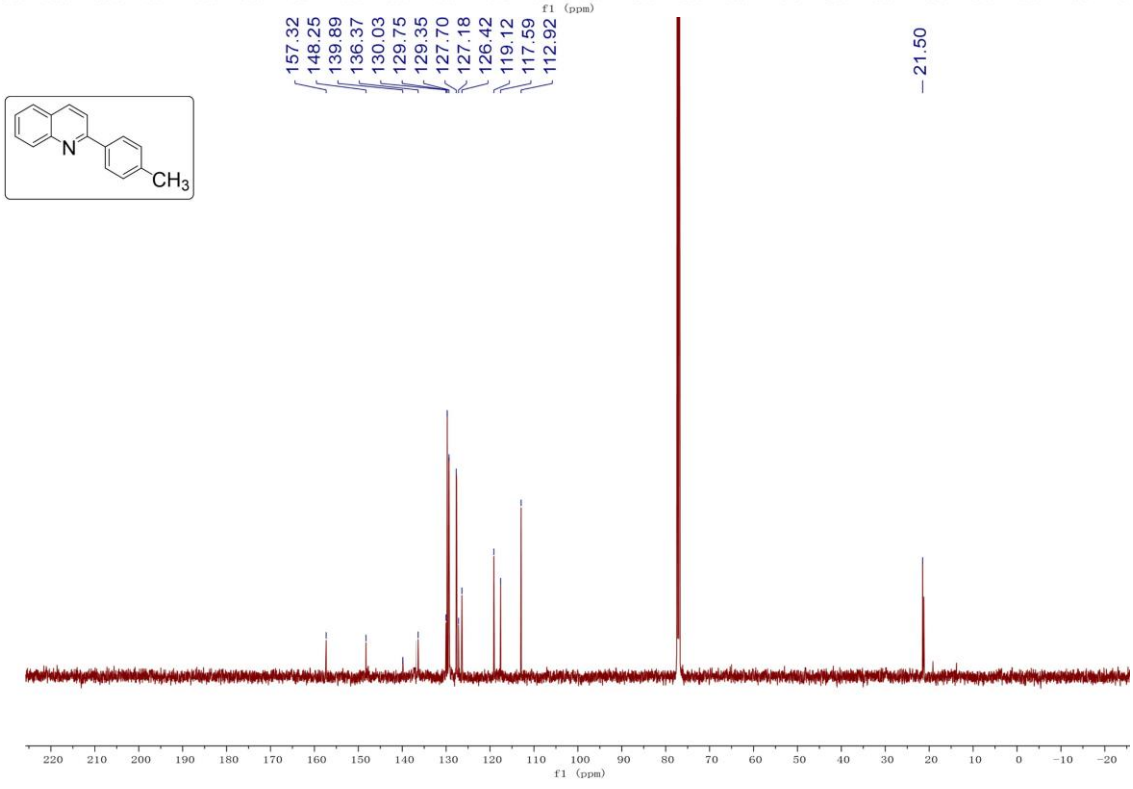

4.20
1.03
1.02
1.02
0.99
1.01
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

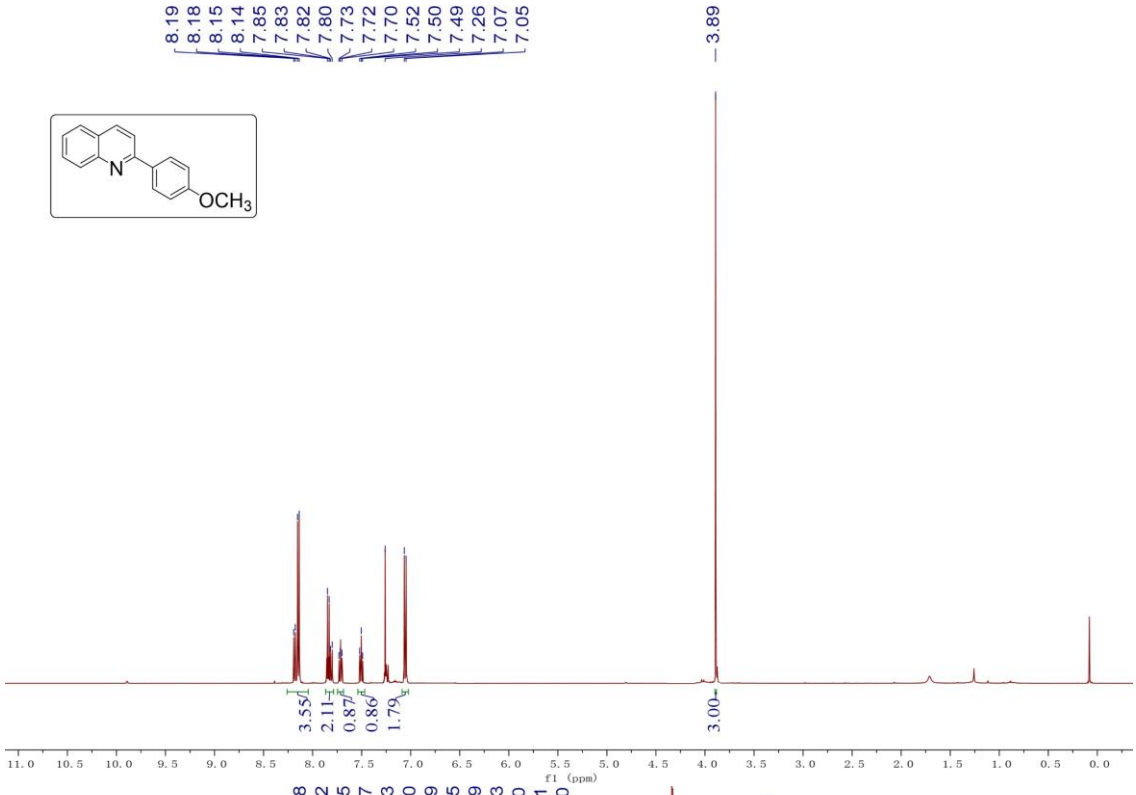

155.33
149.46
137.28
132.51
129.37
129.36
127.72
127.58
126.83
126.27
124.44
119.53
118.51
112.67
N
CN
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

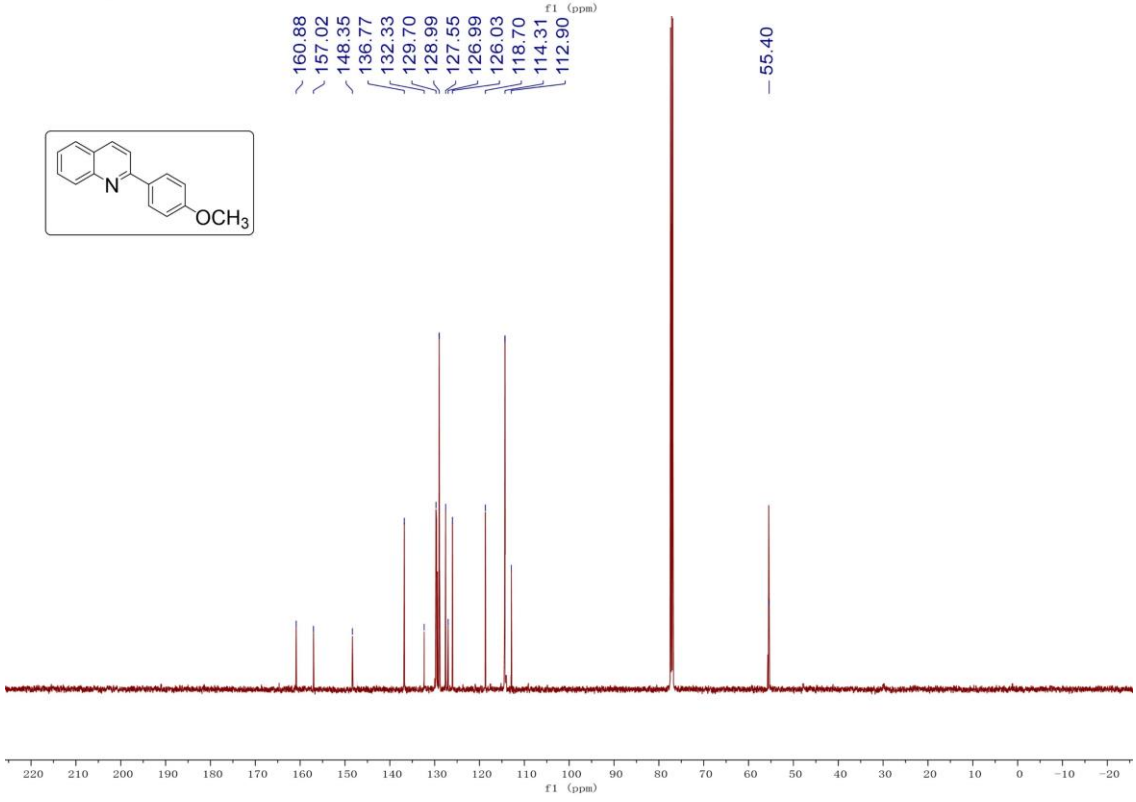

8.32
8.31
8.30
8.29
8.21
8.19
7.91
7.89
7.87
7.84
7.82
7.81
7.78
7.77
7.62
7.60
7.58
7.26
N
NO2
3.02
0.96
2.02
3.10
1.00
f1 (ppm)

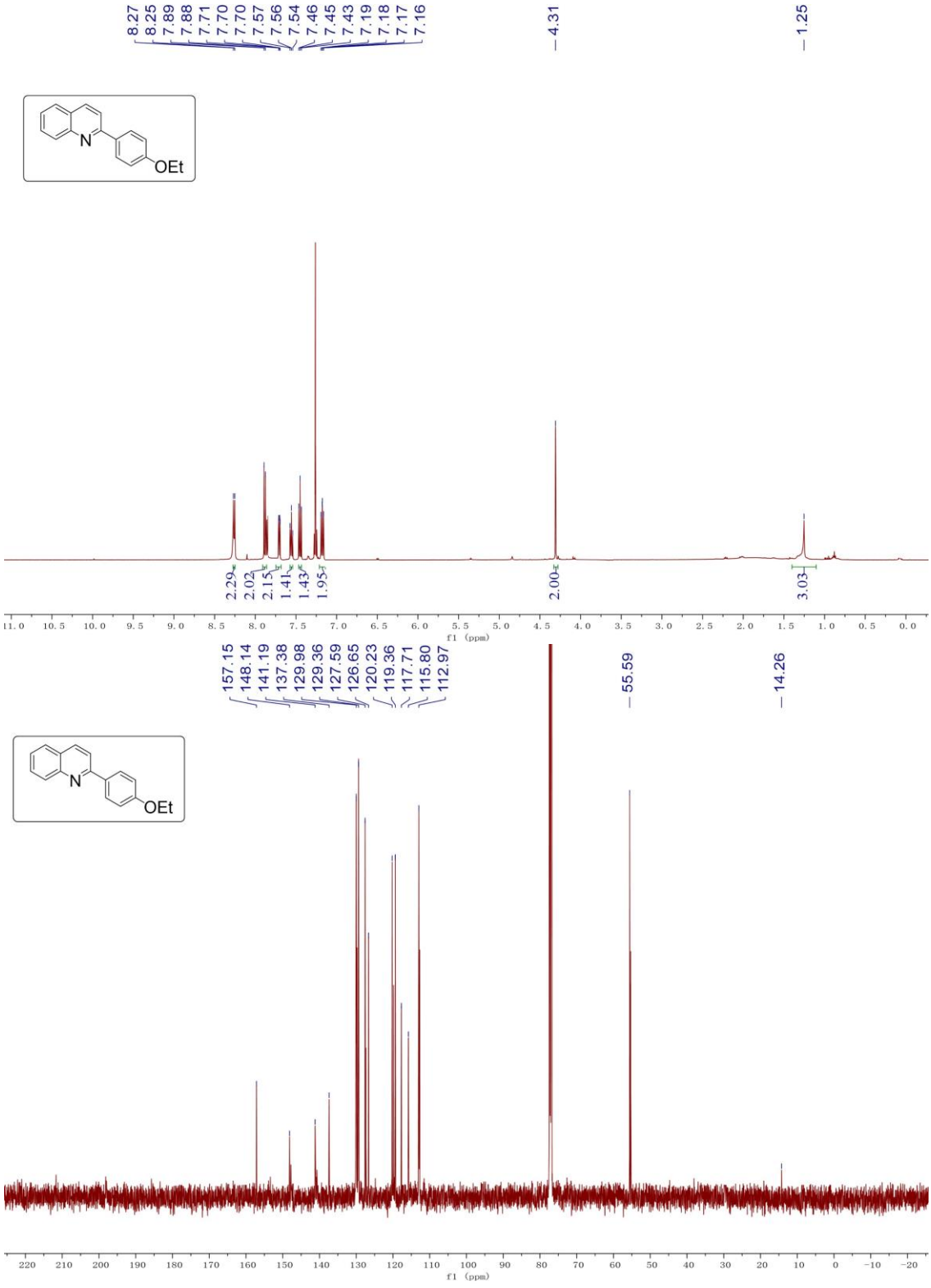

154.93
147.96
143.65
137.67
132.70
130.42
129.66
128.23
127.62
127.57
127.32
118.79
112.88
N
NO2
f1 (ppm)

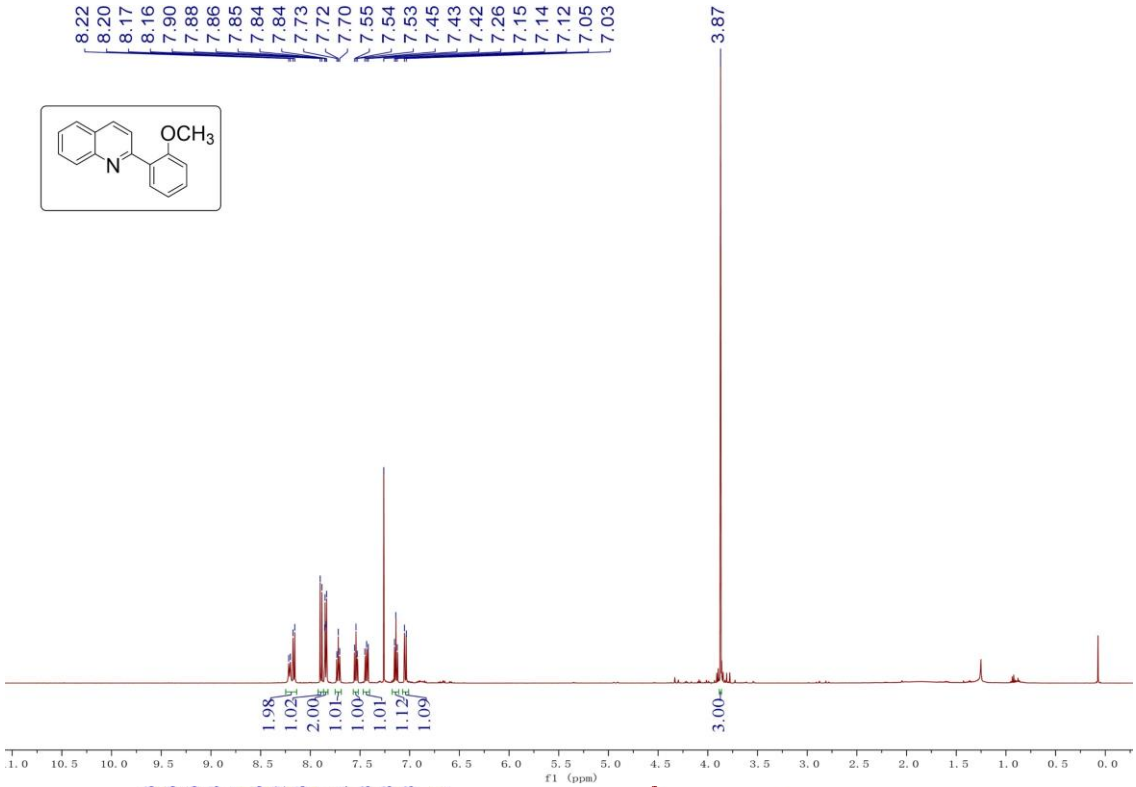

8.23
8.22
8.08
8.06
7.75
7.73
7.71
7.54
7.52
7.51
7.34
7.33
7.24
6.72
6.70
6.64
6.62
6.62
N
CH3
1.90
2.00
0.97
1.00
2.13
2.13
3.00
f1 (ppm)

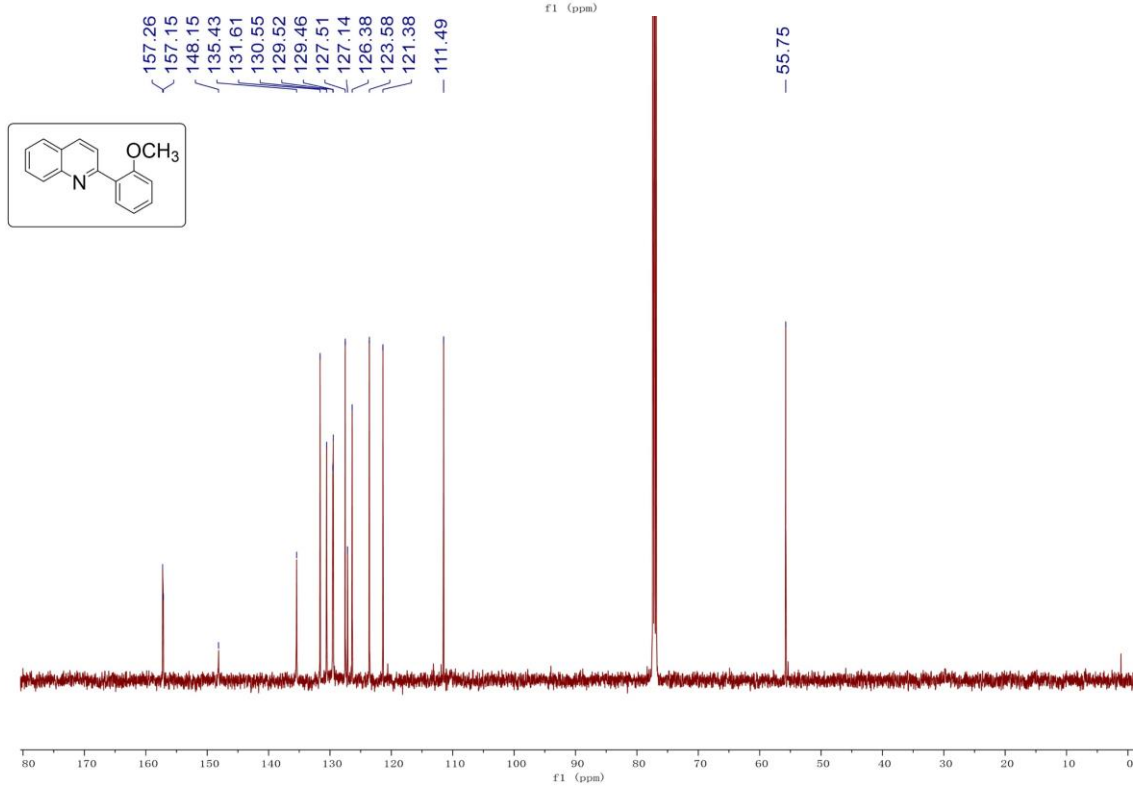

157.32
148.25
139.89
136.37
130.03
129.75
129.35
127.70
127.18
126.42
119.12
117.59
112.92
21.50
N
CH3
f1 (ppm)


8.19
8.18
8.15
8.14
7.85
7.83
7.82
7.80
7.73
7.72
7.70
7.52
7.50
7.49
7.26
7.07
7.05
3.89
N
OCH3
3.55
2.11
0.87
0.86
1.79
3.00
f1 (ppm)


160.88
157.02
148.35
136.77
132.33
129.70
128.99
127.55
126.99
126.03
118.70
114.31
112.90
55.40
N
OCH3
f1 (ppm)


8.27
8.25
7.89
7.88
7.71
7.70
7.70
7.57
7.56
7.54
7.46
7.45
7.43
7.19
7.18
7.17
7.16
4.31
1.25
OEt
2.29
2.02
2.15
1.41
1.43
1.95
2.00
3.03
f1 (ppm)
157.15
148.14
141.19
137.38
129.98
129.36
127.59
126.65
120.23
119.36
117.71
115.80
112.97
55.59
14.26
OEt
f1 (ppm)


8.22
8.20
8.17
8.16
7.90
7.88
7.86
7.85
7.84
7.84
7.73
7.72
7.70
7.55
7.54
7.53
7.45
7.43
7.42
7.26
7.15
7.14
7.12
7.05
7.03
3.87
OCH3
N
1.98
1.02
2.00
1.01
1.00
1.01
1.12
1.09
3.00
f1 (ppm)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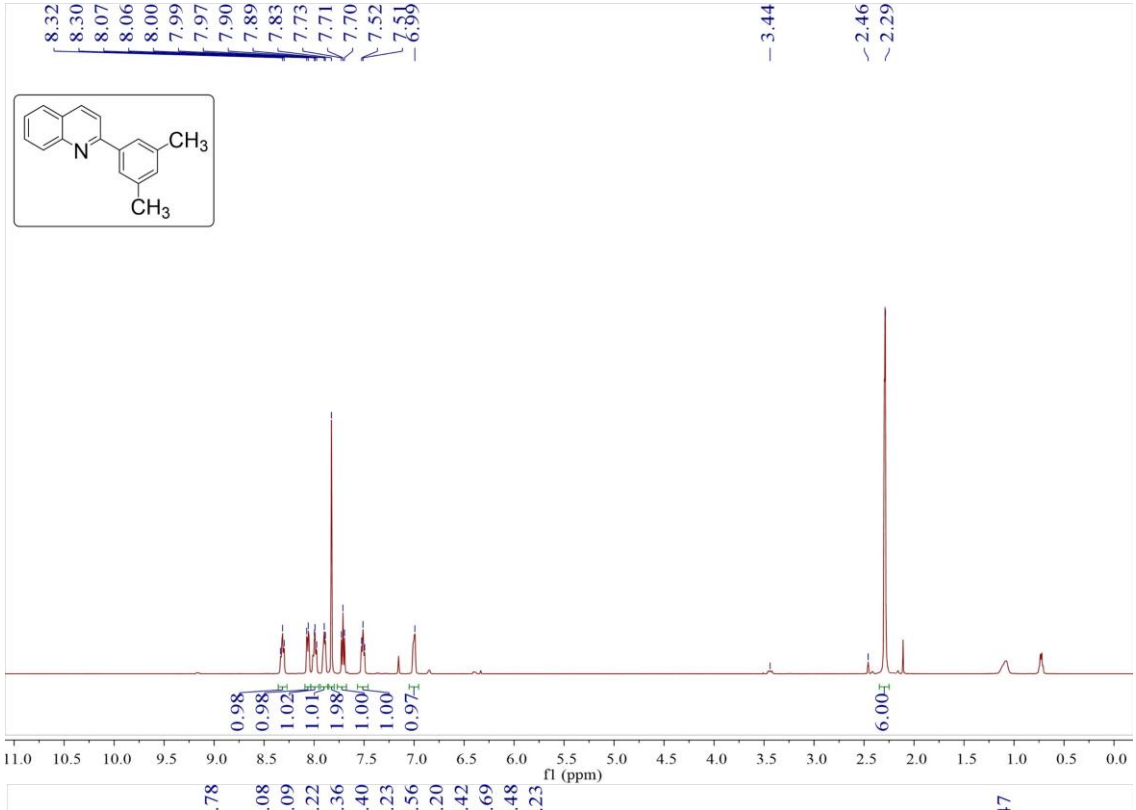
157.15
148.15
135.43
131.61
130.55
129.52
129.46
127.51
127.14
126.38
123.58
121.38
111.49
55.75
OCH3
N
f1 (ppm)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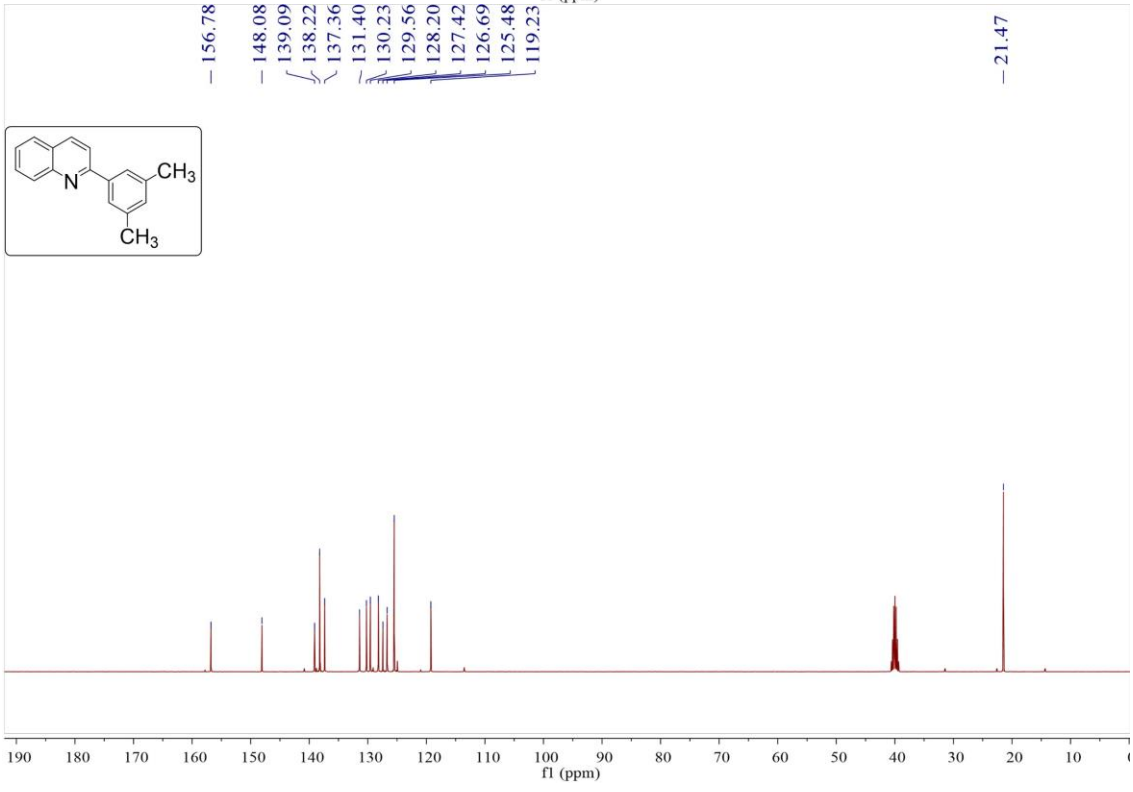
8.30
8.07
8.06
8.00
7.99
7.97
7.90
7.89
7.83
7.73
7.71
7.70
7.52
7.51
6.99
3.44
2.46
2.29
CH3
CH3
N
0.98
0.98
1.02
1.01
1.98
1.00
1.00
0.97
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.23
129.56
128.20
127.42
126.69
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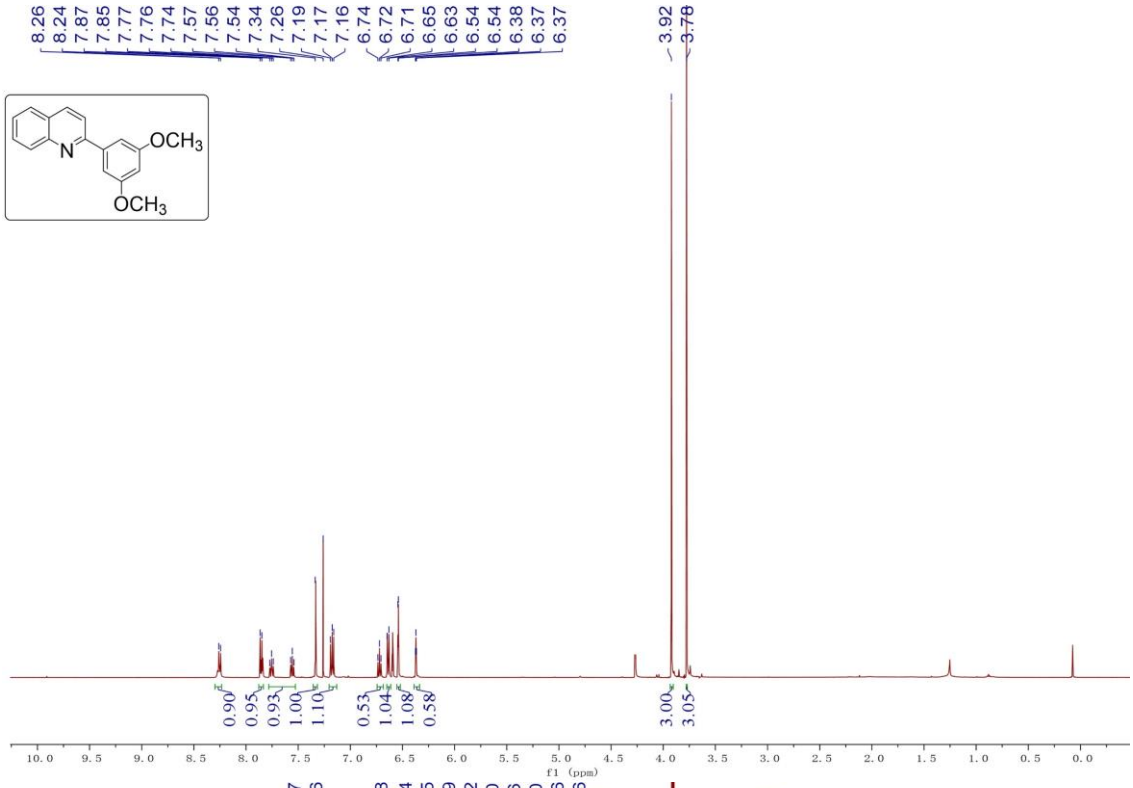
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.24
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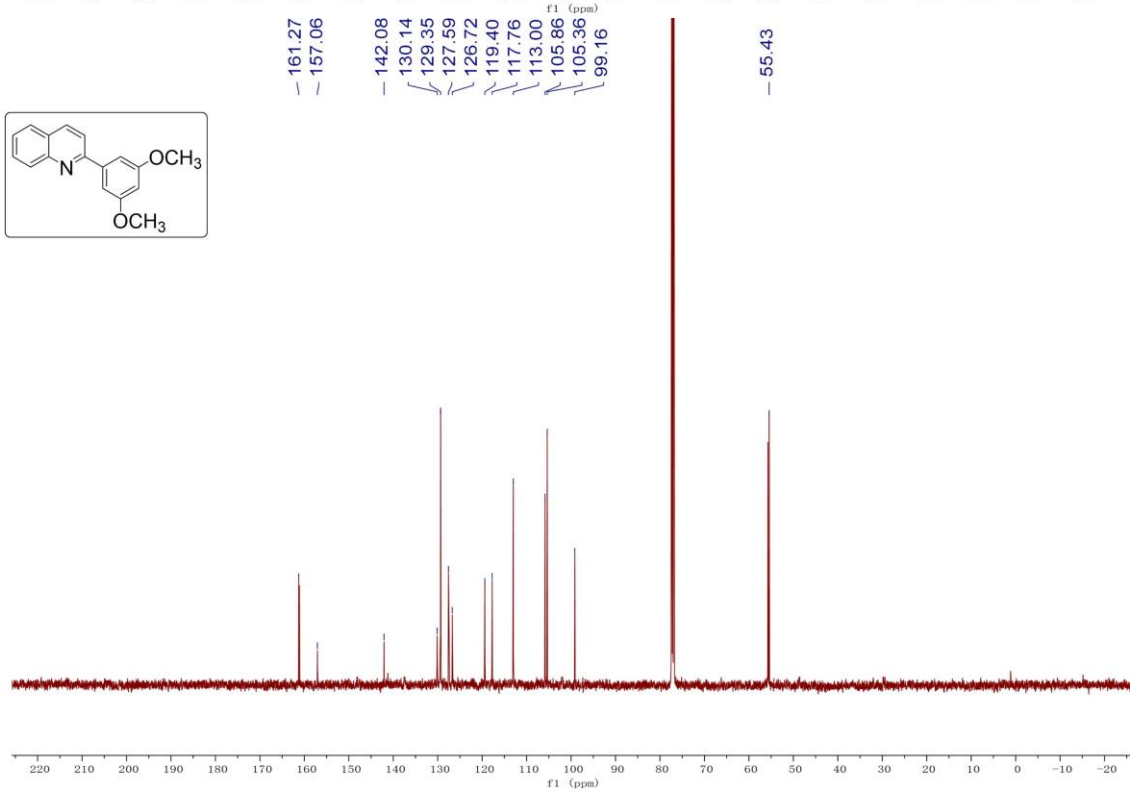
7.77
7.76
7.74
7.57
7.56
7.54
7.34
7.26
7.19
7.17
7.16
6.74
6.72
6.71
6.65
6.63
6.54
6.54
6.38
6.37
6.37
3.92
3.78
OCH3
OCH3
N
0.90
0.95
0.93
1.00
1.10
0.53
1.04
1.08
0.58
3.00
3.05
f1 (ppm)


161.27
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130.14
129.35
127.59
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117.76
113.00
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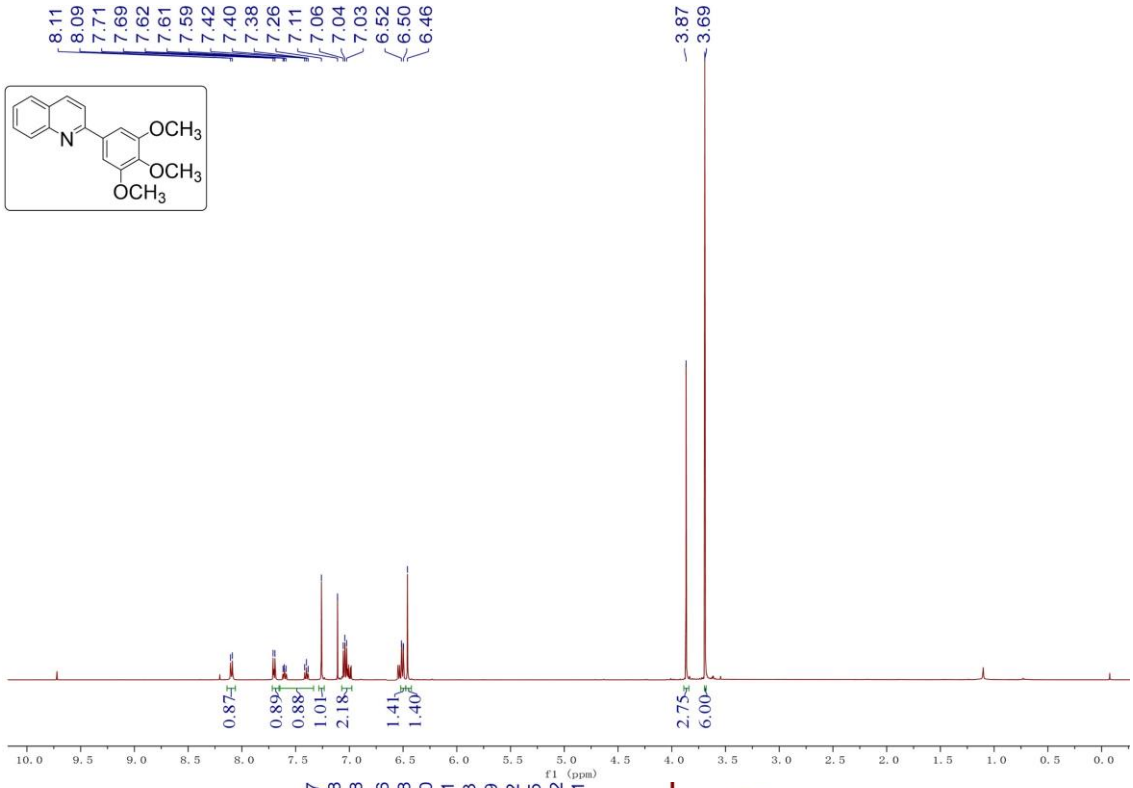
105.36
99.16
55.43
OCH3
OCH3
N
f1 (ppm)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7.69
7.62
7.61
7.59
7.42
7.40
7.38
7.26
7.11
7.06
7.04
7.03
6.52
6.50
6.46
3.87
3.69
OCH3
OCH3
OCH3
N
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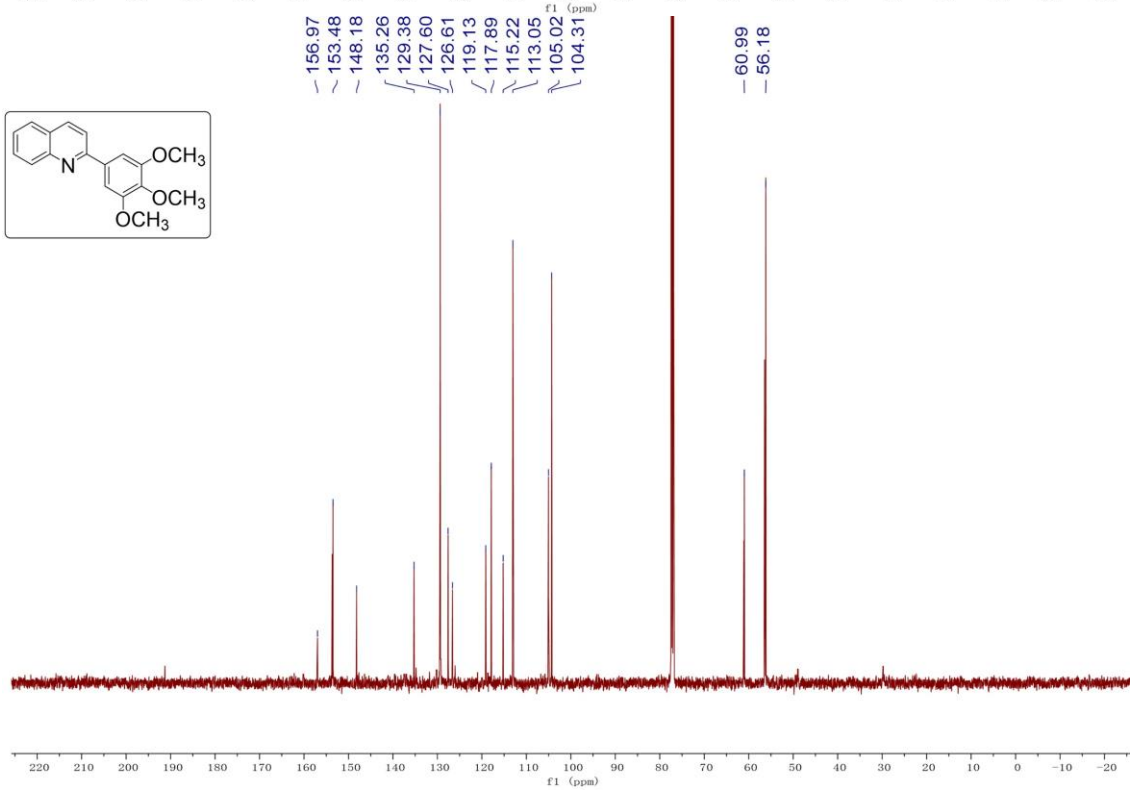
0.89
0.88
1.01
2.18
1.41
1.40
2.75
6.00
f1 (ppm)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126.61
119.13
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113.05
105.02
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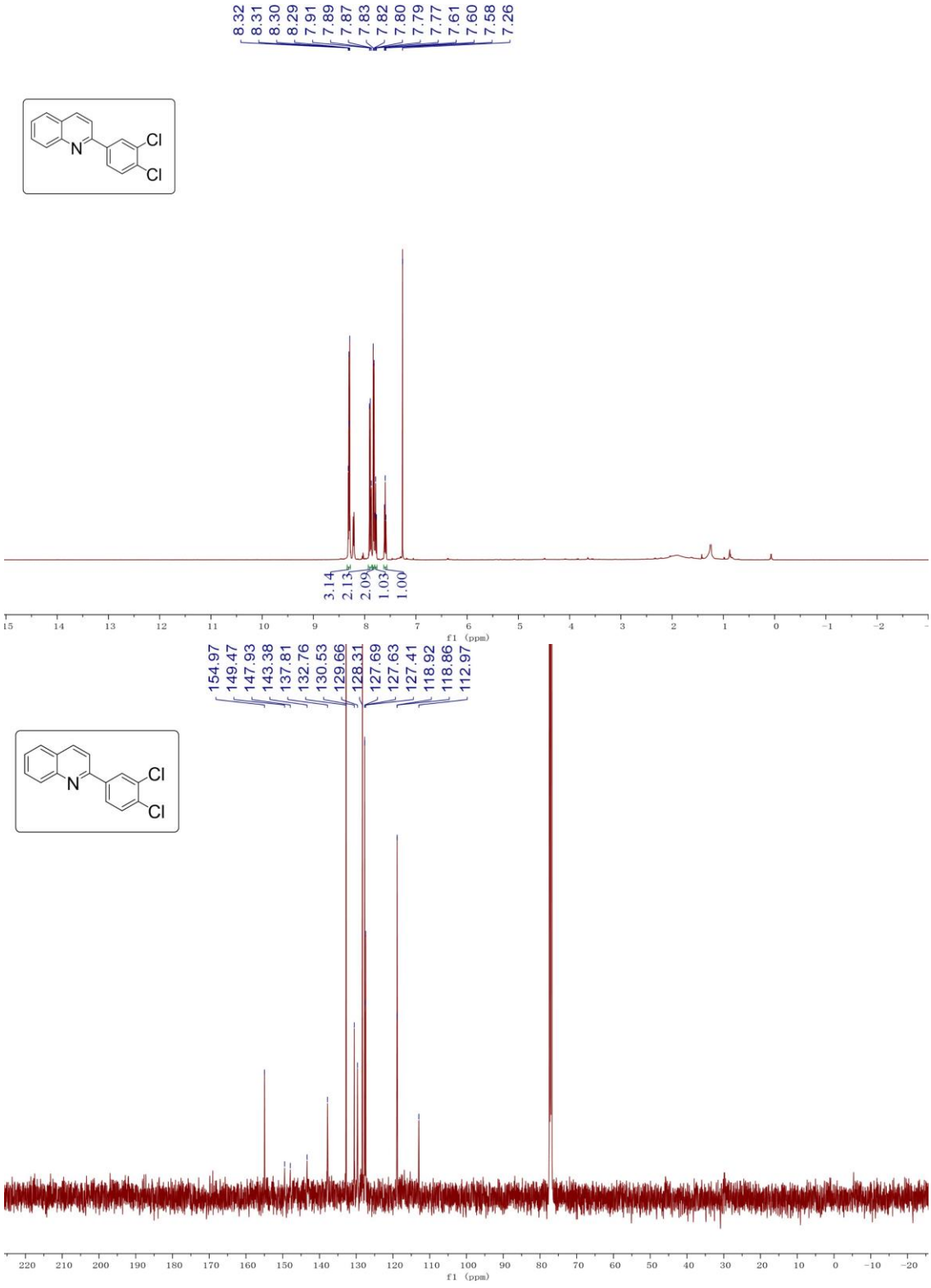
60.99
56.18
OCH3
OCH3
OCH3
N
f1 (ppm)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7.87
7.83
7.82
7.80
7.79
7.77
7.61
7.60
7.58
7.26
Cl
Cl
N
3.14
2.13
2.09
1.03
1.00
f1 (ppm)
154.97
149.47
147.93
143.38
137.81
132.76
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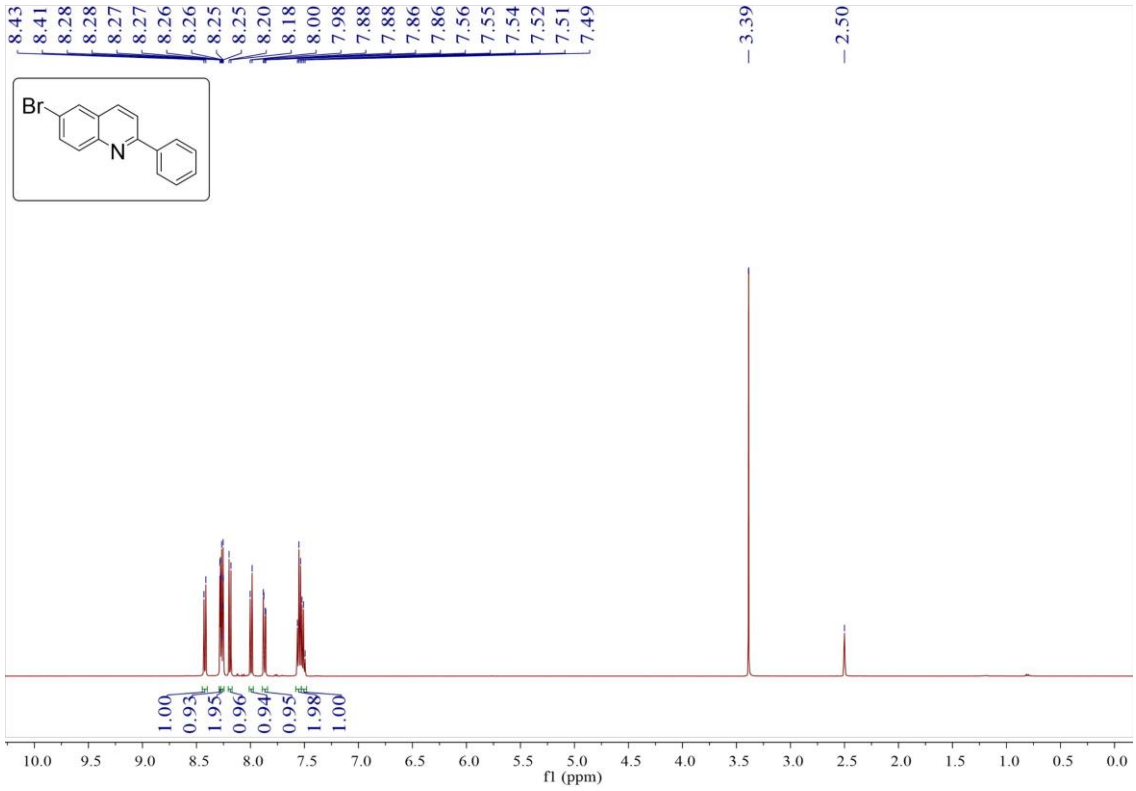
127.41
118.92
118.86
112.97
Cl
Cl
N
f1 (ppm)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8.26
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8.25
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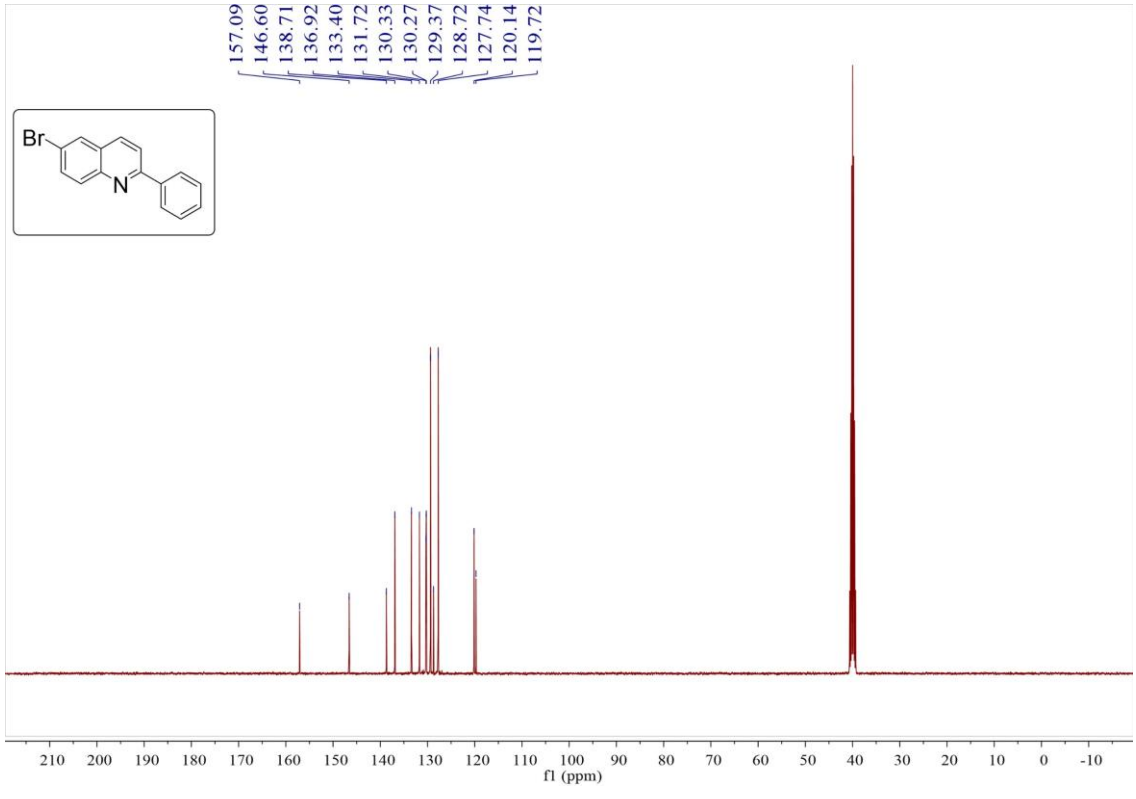
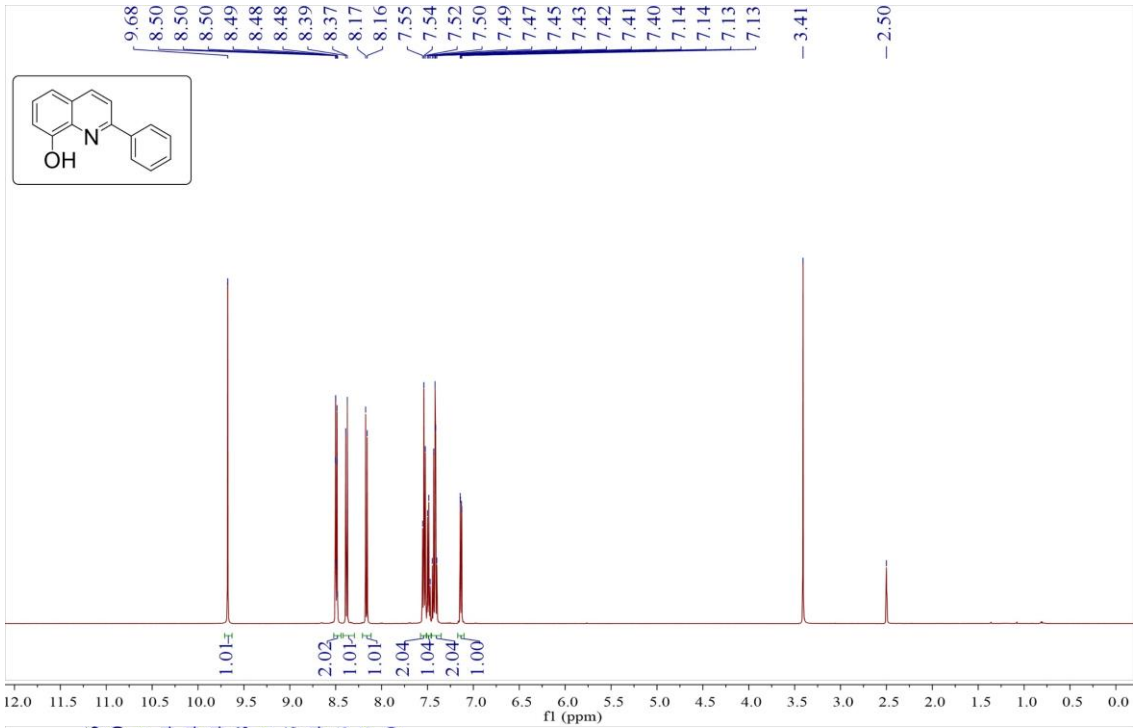
8.18
8.00
7.98
7.88
7.88
7.86
7.86
7.56
7.55
7.54
7.52
7.51
7.49
3.39
2.50
Br
N
1.00
0.93
1.95
0.96
0.94
0.95
1.98
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.09
146.60
138.71
136.92
133.40
131.72
130.33
130.27
129.37
128.72
127.74
120.14
119.72
Br
N
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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8.48
8.48
8.39
8.37
8.17
8.16
7.55
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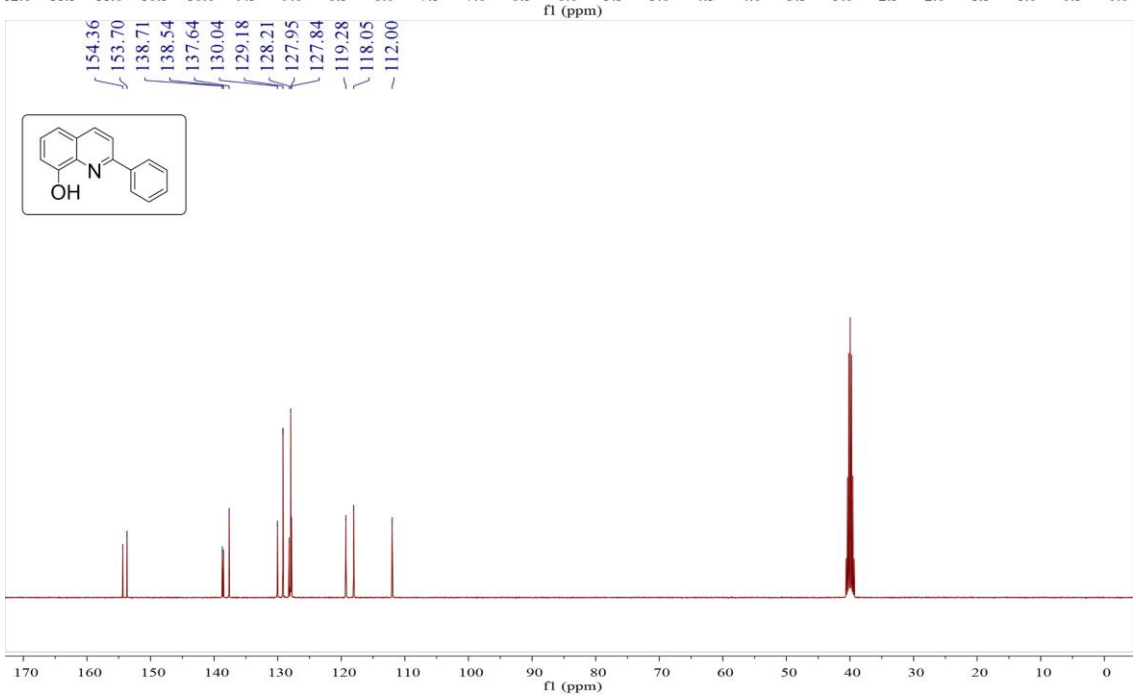
7.52
7.50
7.49
7.47
7.45
7.43
7.42
7.41
7.40
7.14
7.14
7.13
7.13
3.41
2.50
N
OH
1.01
2.02
1.01
1.01
2.04
1.04
2.04
1.00
f1 (ppm)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138.54
137.64
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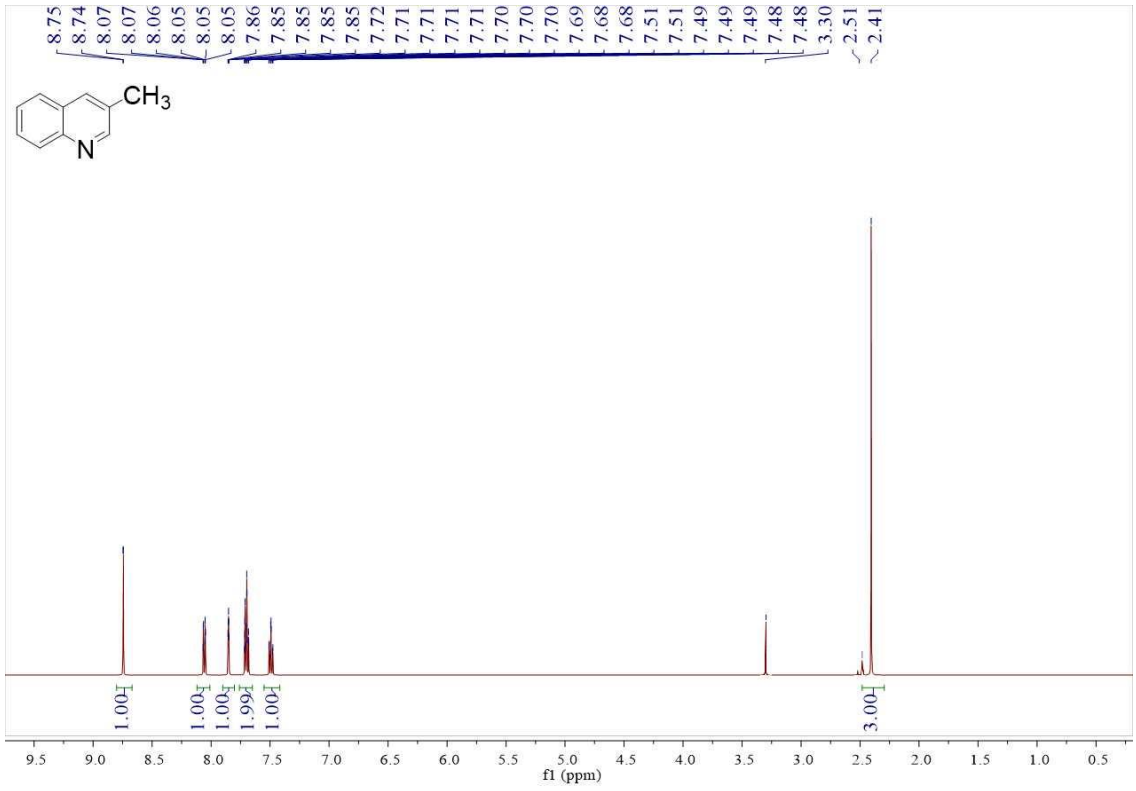
129.18
128.21
127.95
127.84
119.28
118.05
112.00
N
OH
f1 (ppm)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7.85
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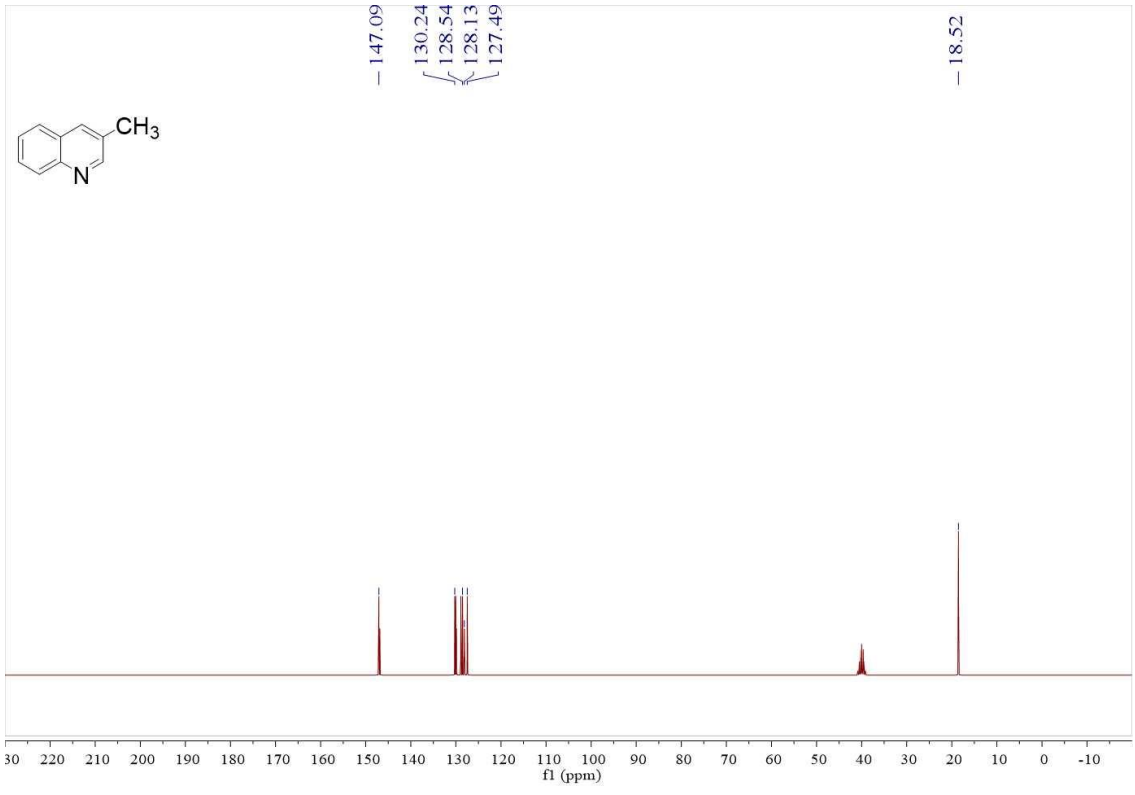
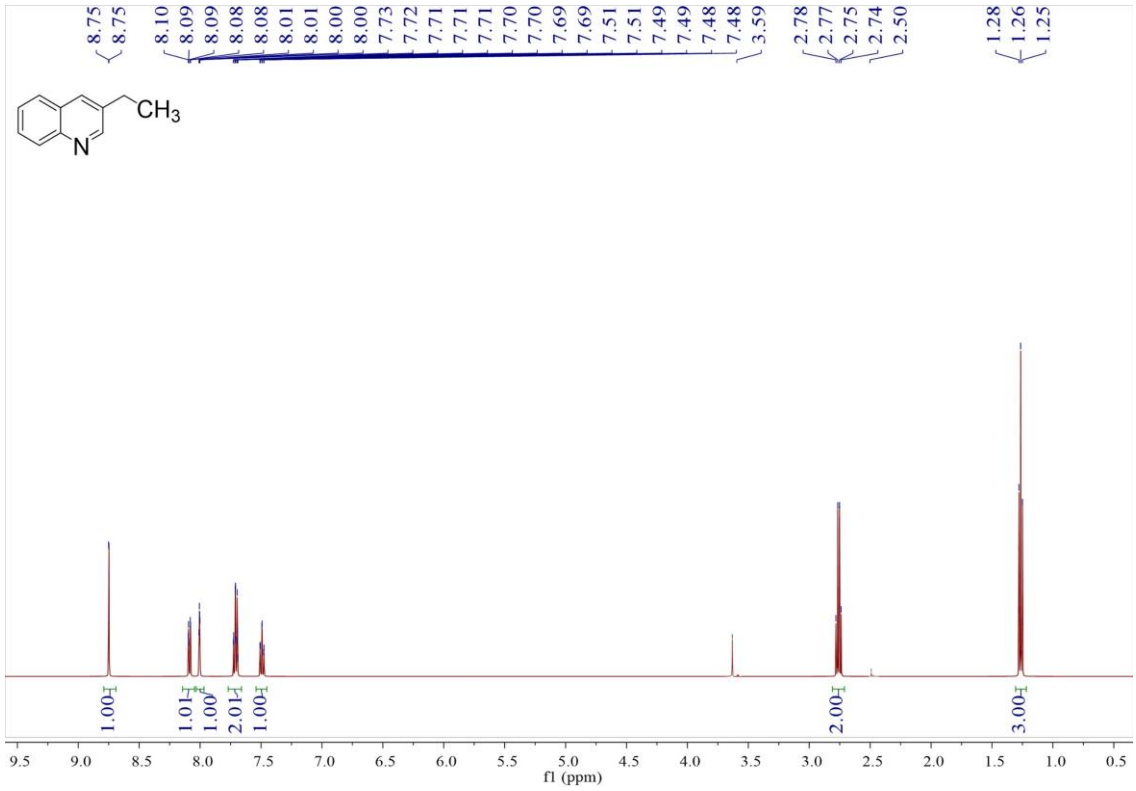
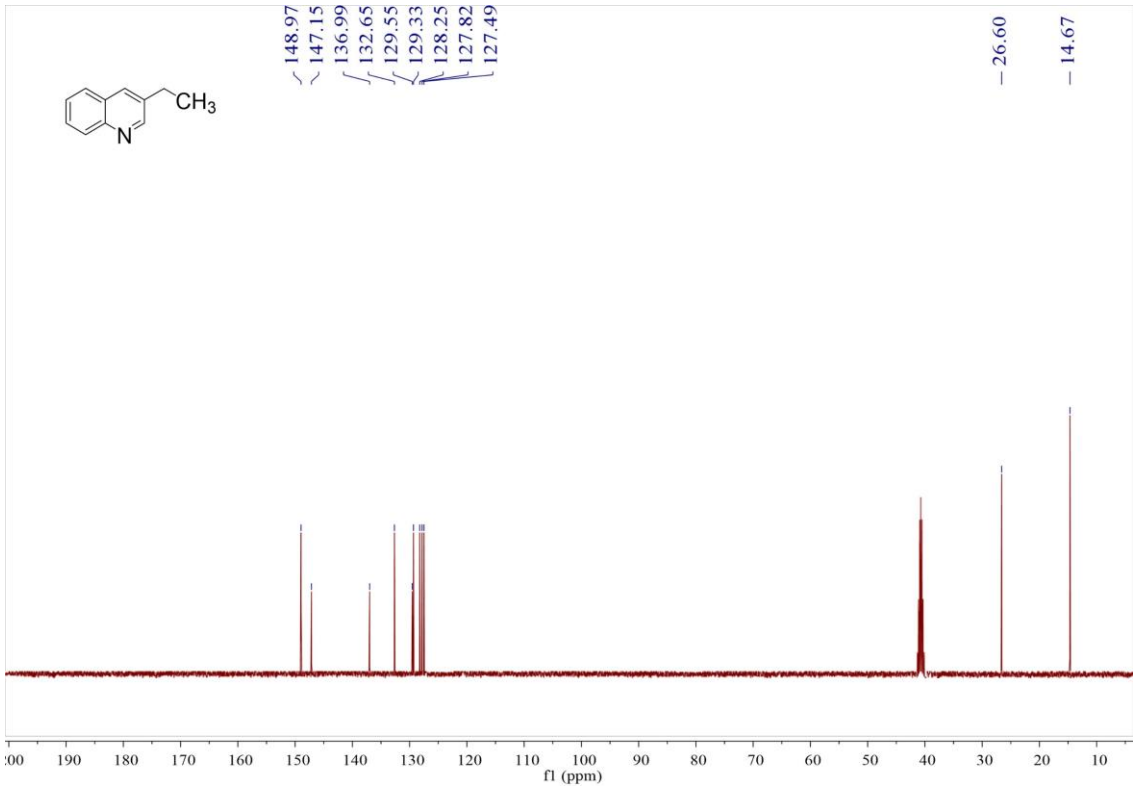
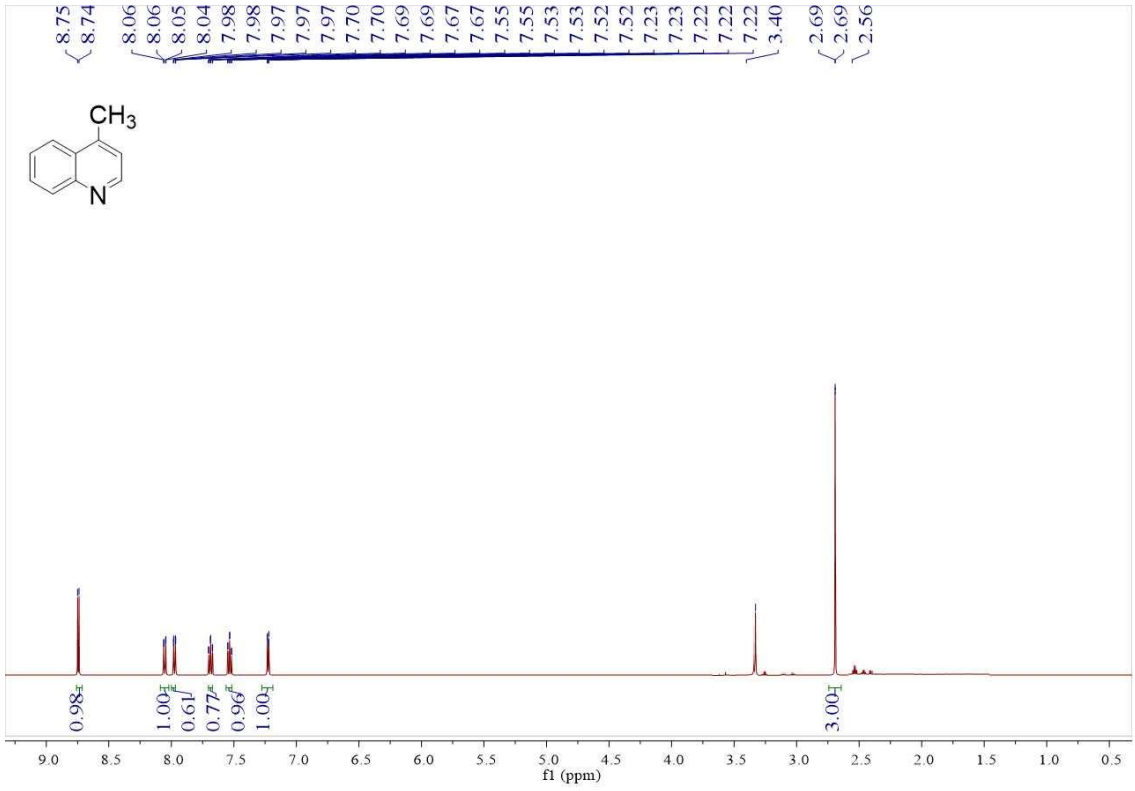
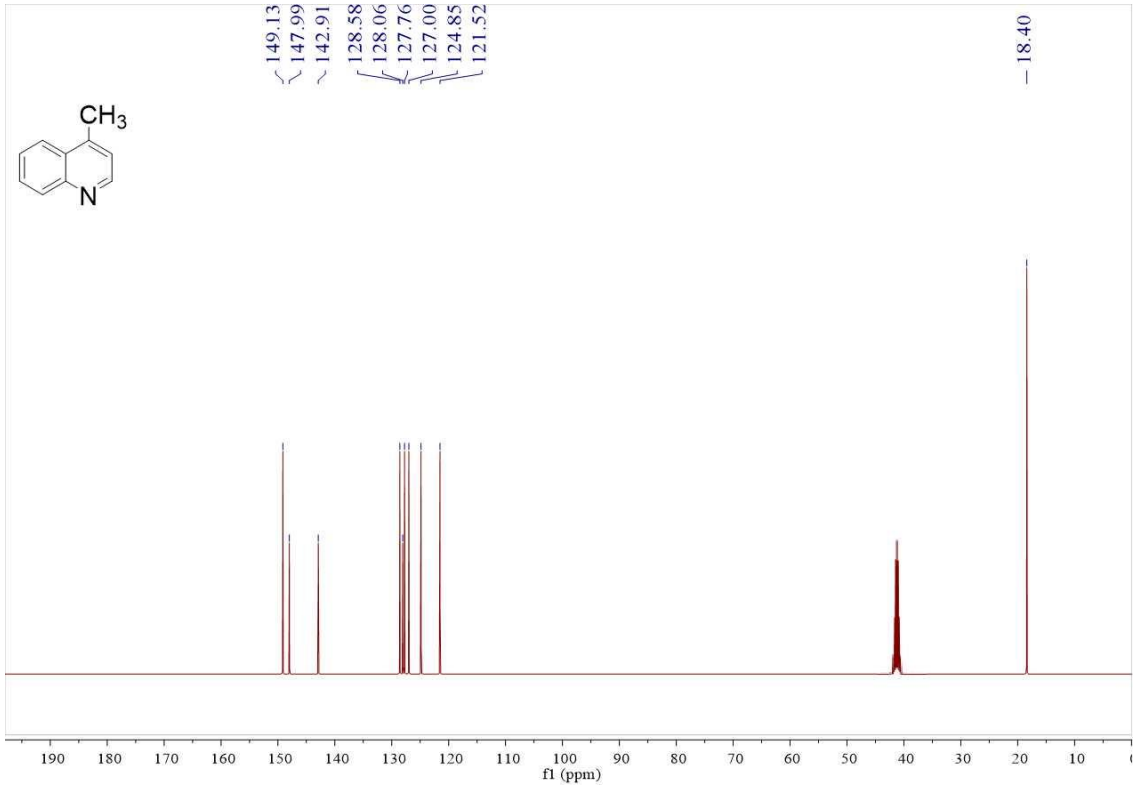
7.70
7.70
7.69
7.68
7.68
7.51
7.51
7.49
7.49
7.49
7.48
7.48
3.30
2.51
2.41
CH3
N
1.00
1.00
1.00
1.99
1.00
3.00
f1 (ppm)

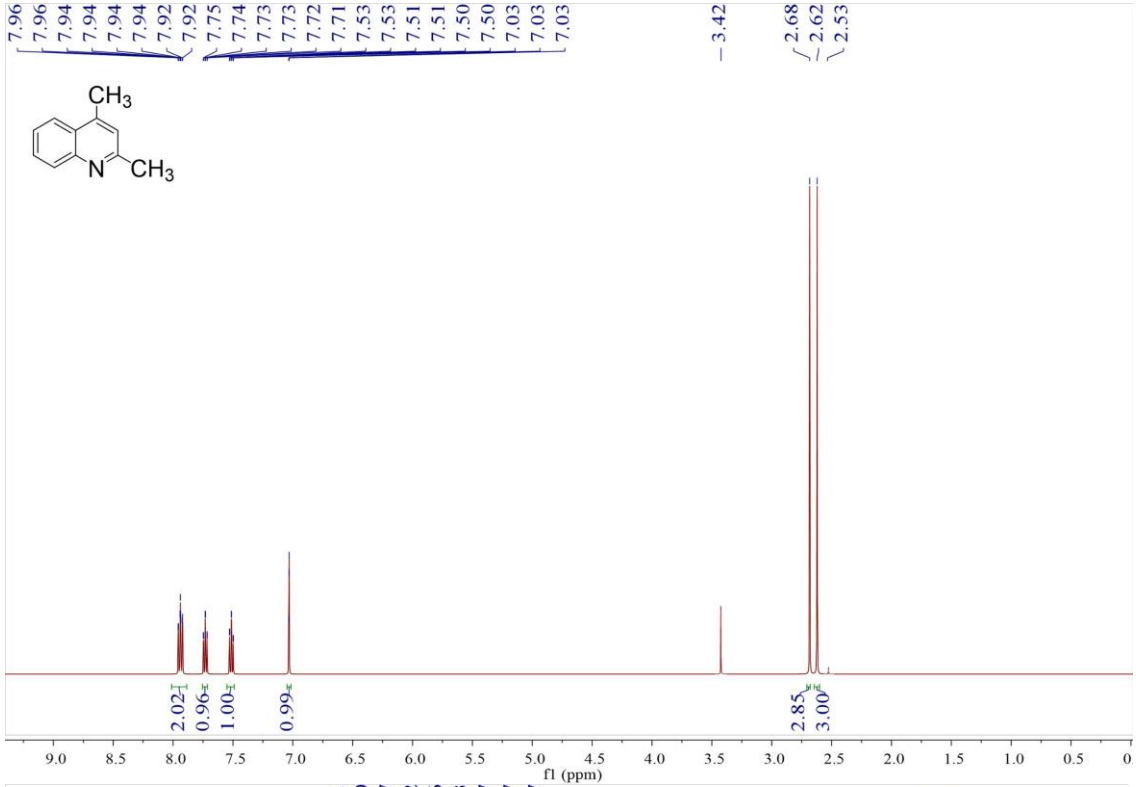

147.09
130.24
128.54
128.13
127.49
18.52
CH3
N
f1 (ppm)

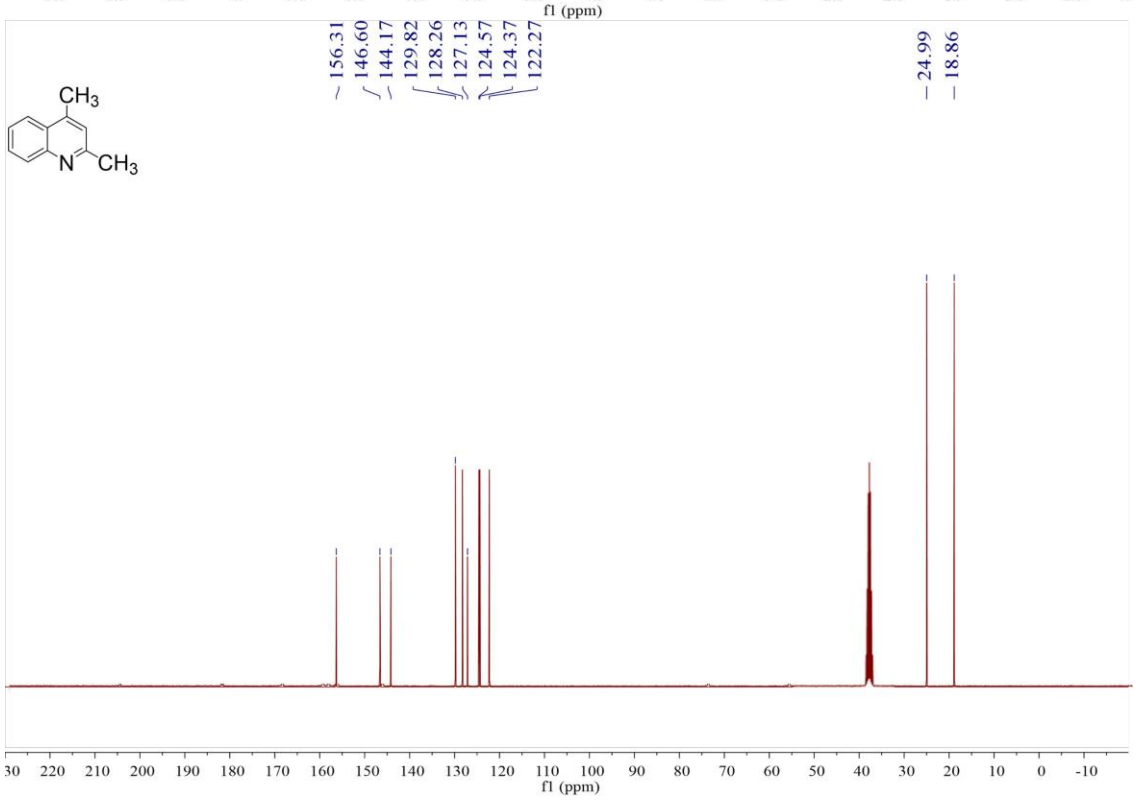

8.75
8.75
8.10
8.09
8.09
8.08
8.08
8.01
8.01
8.00
8.00
7.73
7.72
7.71
7.71
7.71
7.70
7.70
7.69
7.69
7.51
7.51
7.49
7.49
7.48
7.48
3.59
2.78
2.77
2.75
2.74
2.50
1.28
1.26
1.25
CH3
N
1.00
1.01
1.00
2.01
1.00
2.00
3.00
fl (ppm)

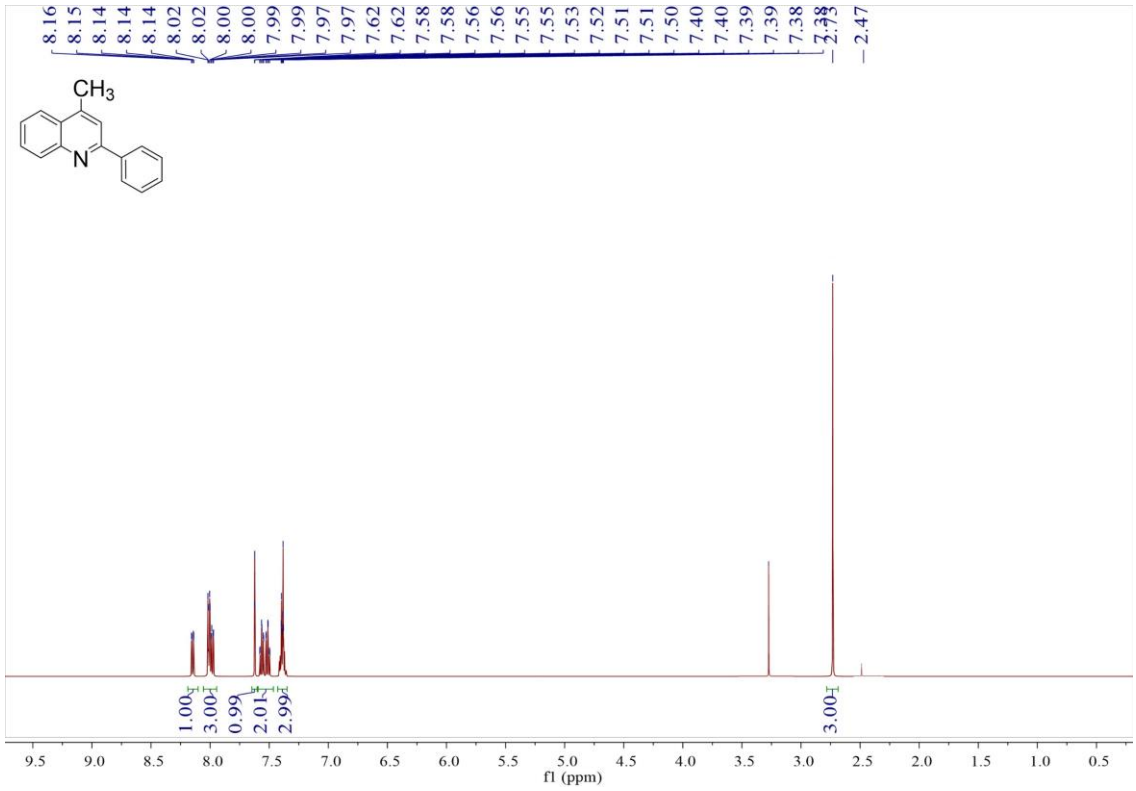

148.97
147.15
136.99
132.65
129.55
129.33
128.25
127.82
127.49
26.60
14.67
CH3
N
fl (ppm)

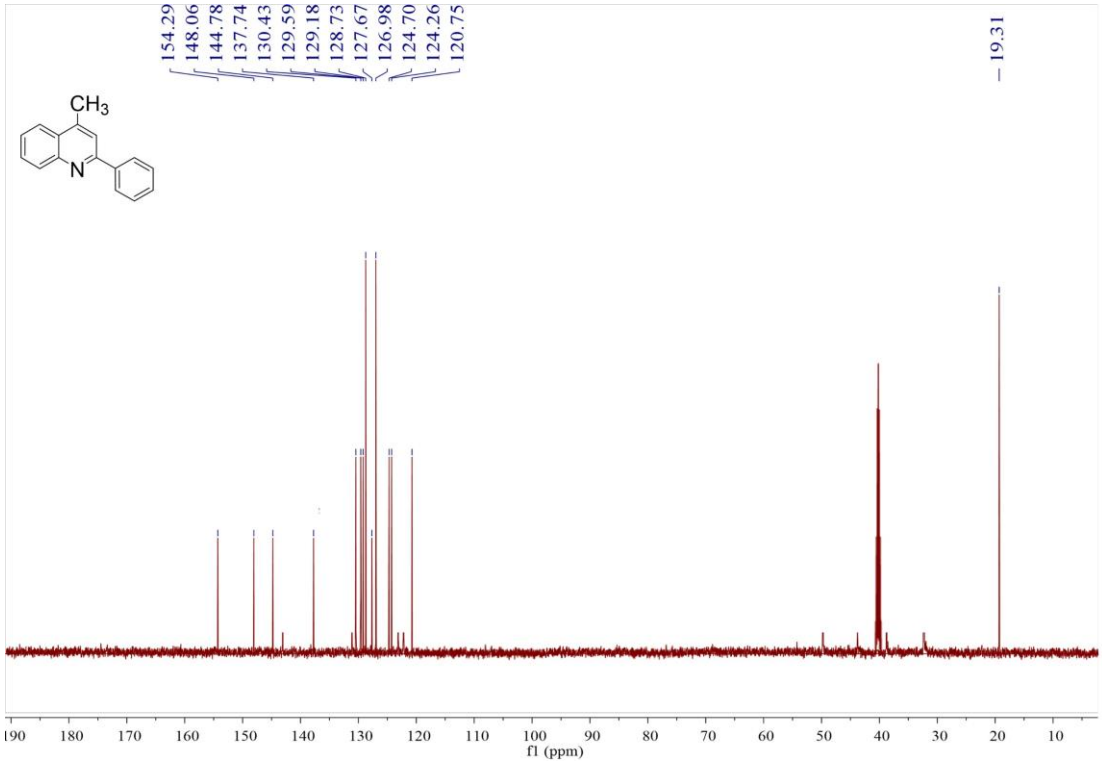

8.75
8.74
8.06
8.06
8.05
8.04
7.98
7.98
7.97
7.97
7.97
7.70
7.70
7.69
7.69
7.67
7.67
7.55
7.55
7.53
7.53
7.52
7.52
7.23
7.23
7.22
7.22
7.22
3.40
2.69
2.69
2.56
CH3
N
0.98
1.00
0.61
0.77
0.96
1.00
3.00
f1 (ppm)

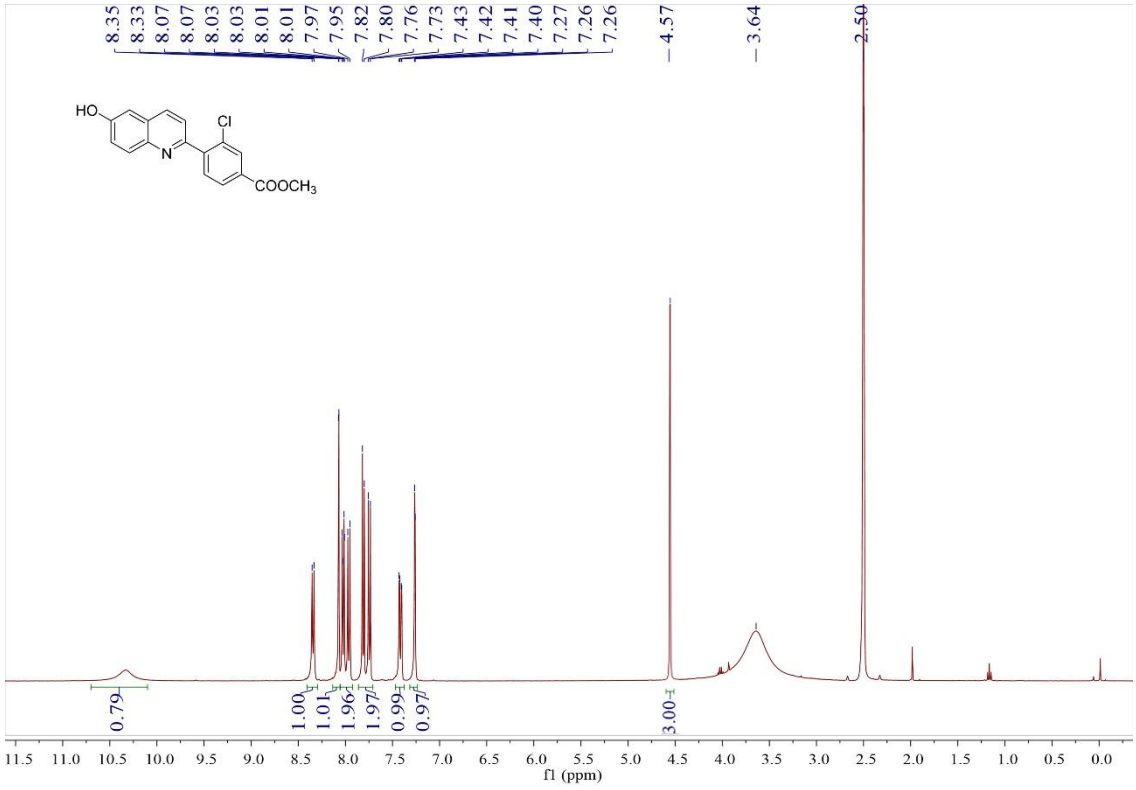

149.13
147.99
142.91
128.58
128.06
127.76
127.00
124.85
121.52
18.40
CH3
N
f1 (ppm)

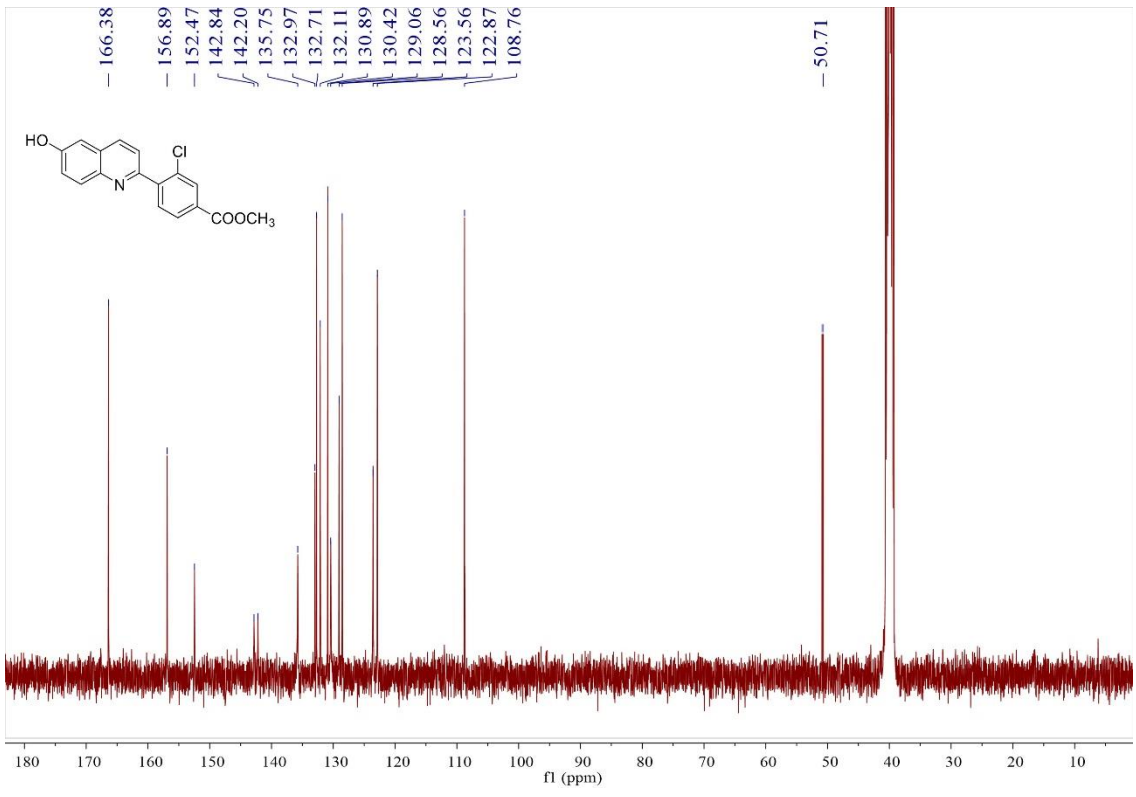

7.96
7.96
7.94
7.94
7.94
7.94
7.92
7.92
7.75
7.74
7.73
7.73
7.72
7.71
7.53
7.53
7.51
7.51
7.50
7.50
7.03
7.03
3.42
2.68
2.62
2.53
CH3
N
CH3
2.02
0.96
1.00
0.99
2.85
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

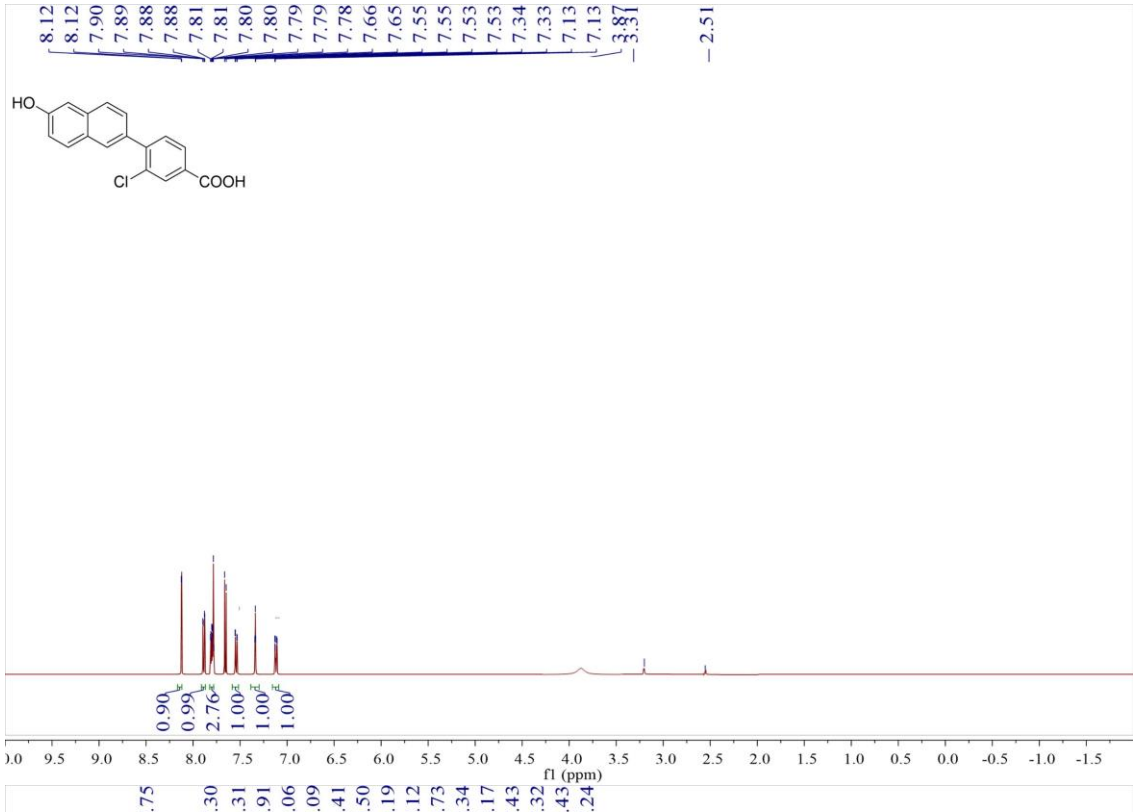

156.31
146.60
144.17
129.82
128.26
127.13
124.57
124.37
122.27
24.99
18.86
CH3
N
CH3
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

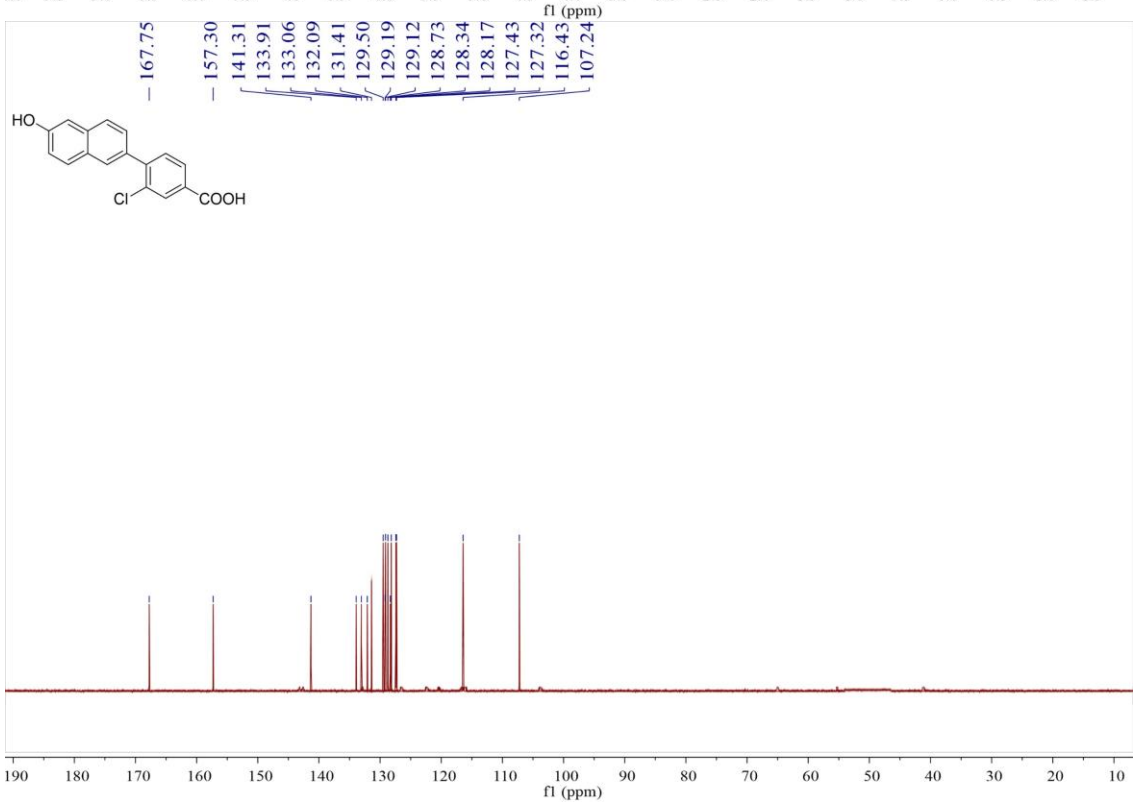

8.16
8.15
8.14
8.14
8.14
8.02
8.02
8.00
8.00
7.99
7.99
7.97
7.97
7.62
7.58
7.58
7.56
7.56
7.55
7.55
7.53
7.52
7.51
7.51
7.50
7.40
7.40
7.39
7.39
7.38
2.73
2.47
CH3
N
1.00
3.00
0.99
2.01
2.99
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


154.29
148.06
144.78
137.74
130.43
129.59
129.18
128.73
127.67
126.98
124.70
124.26
120.75
19.31
CH3
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.35
8.33
8.07
8.07
8.03
8.03
8.01
8.01
7.97
7.95
7.82
7.80
7.76
7.73
7.43
7.42
7.41
7.40
7.27
7.26
7.26
4.57
3.64
2.50
HO
N
Cl
COOCH3
0.79
1.00
1.01
1.96
1.97
0.99
0.97
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.38
156.89
152.47
142.84
142.20
135.75
132.97
132.71
132.11
130.89
130.42
129.06
128.56
123.56
122.87
108.76
50.71
HO
N
Cl
COOCH3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.12
8.12
7.90
7.89
7.88
7.88
7.81
7.81
7.80
7.80
7.79
7.79
7.78
7.66
7.65
7.55
7.55
7.53
7.53
7.34
7.33
7.13
3.87
3.31
2.51
HO
Cl
COOH
0.90
0.99
2.76
1.00
1.00
1.00
f1 (ppm)


167.75
157.30
141.31
133.91
133.06
132.09
131.41
129.50
129.19
129.12
128.73
128.34
128.17
127.43
127.32
116.43
107.24
HO
Cl
COOH
f1 (ppm)