Supporting information

Catalyst-Free Photodecarbonylation of *ortho*-Amino Benzaldehyde

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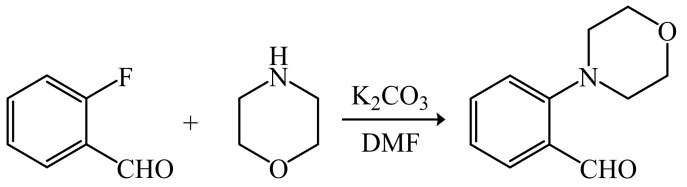
1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE 400 and 500 spectrometer. Chemical shifts of protons were reported in parts per million downfield from tetramethylsilane and were referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26). Chemical shifts of carbon were referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.0). Peaks were labeled as singlet (s), doublet (d), triplet (t), quartet (q) and multiplet (m). Melting points were measured on a WRS-2A melting point apparatus and were uncorrected. All products were further characterized by HRMS (high resolution mass spectra). Copies of their ^{1}H NMR and ^{13}C NMR spectra were provided. Substrates of **1be** and **1bf** were purchased from *J&K* and used without further purification.

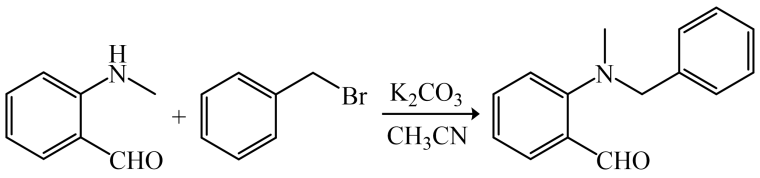
2. General Procedures

(I) Typical procedure for the preparation of substrates 1a-1f, 1i, 1p-1q, 1aa-1ar, 1bb-1bd.



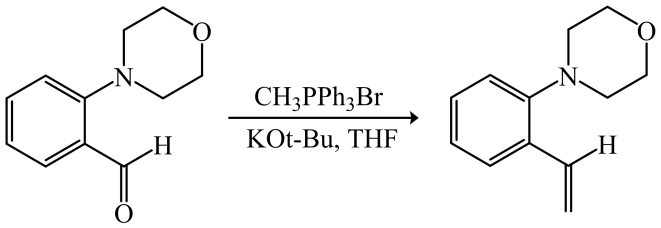
The compound was synthesized according to a known procedure.[1] To a solution of potassium carbonate (0.83 g, 6.0 mmol) in *N, N*-Dimethylformamide (10 mL), 2-fluorobenzaldehyde (0.62 g, 5.0 mmol) and morpholine (0.53 g, 6 mmol) were added. The reaction mixture was stirred at 100 °C for 15 h. After completion of the reaction as shown by TLC, water (30 mL) was used to dilute the reaction. The organic layer was extracted with ethyl acetate (20 mL × 3), the combined organic layer was washed with saturated NH_4Cl (20 mL), dried with anhydrous sodium sulfate and concentrated in vacuum. The crude production was purified by flash chromatography to give a yellow oil **1a** (0.71 g, yield: 75%).

(II) Typical procedure for the preparation of substrates 1g-1h, 1j-1o, 1bi-1bj, 1bl-1bn.



The compound was synthesized according to the similar procedures.[2] To a solution of 2-(methylamino)benzaldehyde (405 mg, 3 mmol) in acetonitrile (15 mL) was added benzyl bromide (770 mg, 4.5 mmol), K_2CO_3 (621 mg, 4.5 mmol). The reaction mixture was allowed to stir at 65 °C for 15h. After completion of the reaction as shown by TLC, the mixture was allowed to cool to room temperature, and the crude production was purified by flash chromatography, giving a yellow oil **1j** (473 mg, yield: 70%).

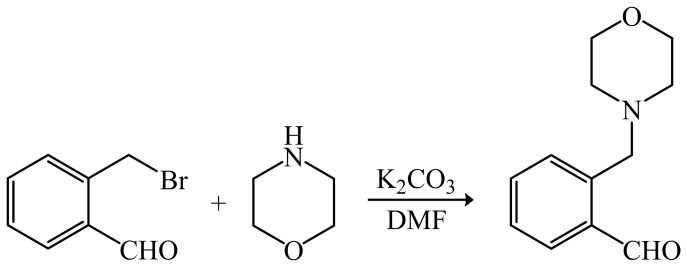
(III) Typical procedure for the preparation of substrate 1ba.



The compound was synthesized according to the similar procedures.[3] A mixture of CH_3PPh_3Br (3.6 mmol) and KOt-Bu (3.9 mmol) in dry THF (30 mL) was stirred at 0

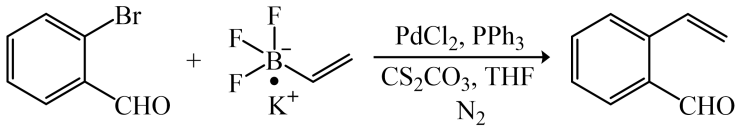
°C for 1 h. After the addition of 2-morpholinobenzaldehyde (3 mmol) at 0 °C, the reaction mixture was stirred overnight at r.t. The solvent was evaporated under reduced pressure. The residue was purified by column chromatography over silica gel, giving a colorless oil **1ba** (397 mg, yield: 70%).

(IV) Typical procedure for the preparation of substrates 1bg-1bh.



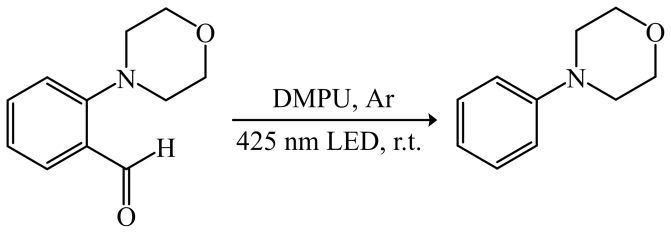
The compound was synthesized according to the similar procedures.[1] To a solution of 2-(bromomethyl)benzaldehyde (995 mg, 5 mmol) in DMF (15 mL) was added morpholine (435 mg, 5mmol), K_2CO_3 (690 mg, 5 mmol). The reaction mixture was allowed to stir at 125 °C for 12 h. After completion of the reaction as shown by TLC. The mixture was allowed to cool to room temperature, and the crude production was purified by flash chromatography, giving a yellow oil **1bg** (337 mg, yield: 32.9%).

(V) Typical procedure for the preparation of substrate 1bk.



The compound was synthesized according to the similar procedures.[4] To a solution of 2-bromobenzaldehyde (925 mg, 5 mmol) in THF (15 mL), H_2O (2 mL) was added potassium vinyltrifluoroborate (680 mg, 5 mmol), $PdCl_2$ (20 mg, 2 mol%), PPh_3 (79.8 mg, 6 mol%), CS_2CO_3 (2450 mg, 10 mmol). The reaction mixture was allowed to stir at 85 °C for 24h. After completion of the reaction as shown by TLC, water (30 mL) was used to dilute the reaction. The organic layer was extracted with ethyl acetate (20 mL × 3), the combined organic layer was washed with saturated NH_4Cl (20 mL), dried with anhydrous sodium sulfate and concentrated in vacuum. The crude production was purified by flash chromatography, giving a yellow oil **1bk** (396 mg, yield: 60%).

(VI) Typical procedure for photodecarbonylation of 2-Amine Benzaldehyde.



2-morpholinobenzaldehyde **1a** (57.3 mg, 0.3 mmol) was added to 10 mL quartz tube containing 2 mL DMPU, the reaction mixture was stirred at room temperature under irradiation of 425 nm LED in argon atmosphere condition for 6 h. After completion of the reaction as shown by TLC, water (3 mL) was used to dilute the reaction. The organic layer was extracted with ethyl acetate (5 mL × 3). The combined organic layer was washed with saturated NH_4Cl (5 mL), dried with anhydrous sodium sulfate and concentrated in vacuum. The crude product was purified by flash chromatography to give a yellow oil **2a** (36.6 mg, yield: 75%).

3. Computational Method

All the geometry optimization and vibration frequency calculation were carried out in Gaussian09 package.[5] Meanwhile, the density-functional theory (DFT)[6] and the time-dependent density-functional theory (TD-DFT)[7] were employed for the computations of ground state and the excited state, respectively. For geometry optimization, both the ground state molecules and the excited state molecules were performed at the B3LYP method[8] with 6-31+G(d, p) basis set[9]. For vibration frequency calculation, same computational method and basis set were carried out to make sure that the optimized structures were true energy minima, and obtain the absolute free energies of the optimized ground state molecules and excited state molecules. The reaction coordinate driving method (flexible scan) as well as the following restricted geometry optimization and the corresponding vibration frequency were employed to calculate the free energy profiles from O-State to H-State for the selected ground state molecules and excited state molecules also at the same computational method and basis set. The reaction coordinate from O-State to H-State was the rotation dihedral of aldehyde group. All the above calculations considered the solvation effect (DMPU) provided by the PCM solvent continuum models.[10]

4. References

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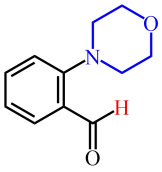
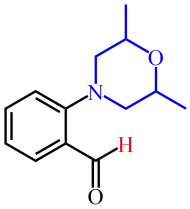
5. Characterization Data

2-morpholinobenzaldehyde (1a)



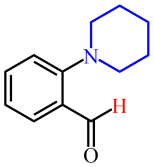
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 7.85 (dd, J = 7.6, 1.5 Hz, 1H), 7.57 (td, J = 8.0, 1.6 Hz, 1H), 7.18 (t, J = 8.7 Hz, 2H), 3.98-3.89 (m, 4H), 3.17-3.08 (m, 4H). **^{13}C NMR** (125 MHz, CDCl3) δ 191.19, 155.29, 135.12, 130.33, 128.67, 122.95, 118.87, 66.93, 54.17. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_2$ $(M+H)^+$: 192.1019, found: 192.1021.

2-(2, 6-dimethylmorpholino)benzaldehyde (1b)



Pale yellow solid. M. p. 94-95 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.33 (s, 1H), 7.82 (dd, J = 7.6, 1.1 Hz, 1H), 7.57-7.43 (m, 1H), 7.13 (dd, J = 18.2, 7.9 Hz, 2H), 4.05-3.73 (m, 2H), 3.09 (d, J = 11.4 Hz, 2H), 2.66 (t, J = 11.0 Hz, 2H), 1.24 (d, J = 6.3 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.30, 155.08, 135.09, 130.18, 128.63, 122.76, 119.00, 71.81, 59.71, 18.84. **HRMS** (ESI) calculated for $C_{13}H_{18}NO_2$ $(M+H)^+$: 220.1332, found: 220.1331.

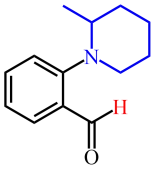
2-(piperidin-1-yl)benzaldehyde (1c)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.32 (s, 1H), 7.81 (dd, J = 7.7, 1.7 Hz, 1H), 7.58-7.40 (m, 1H), 7.12 (d, J = 8.3 Hz, 1H), 7.08 (t, J = 7.5 Hz, 1H), 3.13-3.01 (m, 4H), 1.84-1.73 (m, 4H), 1.69-1.58 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ

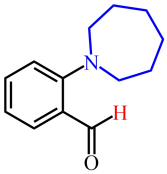
191.73, 134.84, 129.21, 128.63, 121.99, 119.01, 55.63, 26.19, 24.05. **HRMS** (ESI) calculated for $C_{12}H_{16}NO$ $(M+H)^+$: 190.1227, found: 190.1225.

2-(2-methylpiperidin-1-yl)benzaldehyde (1d)



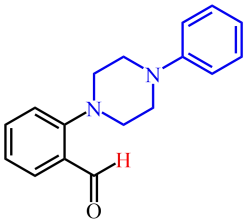
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.52 (s, 1H), 7.83 (dd, J = 7.7, 1.6 Hz, 1H), 7.53 (td, J = 8.1, 1.7 Hz, 1H), 7.23 (d, J = 8.1 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 3.19 (td, J = 6.5, 3.3 Hz, 1H), 3.14-3.01 (m, 1H), 2.83 (ddd, J = 11.8, 8.1, 3.7 Hz, 1H), 1.94-1.84 (m, 1H), 1.82-1.64 (m, 3H), 1.58-1.42 (m, 2H), 0.91 (d, J = 6.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.63, 156.46, 134.59, 131.58, 128.13, 123.54, 122.78, 56.81, 53.55, 33.60, 26.40, 22.53, 17.87. **HRMS** (ESI) calculated for $C_{13}H_{18}NO$ $(M+H)^+$: 204.1383, found: 204.1387.

2-(azepan-1-yl)benzaldehyde (1e)



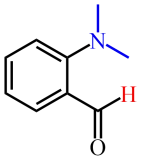
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.22 (s, 1H), 7.75 (dd, J = 7.8, 1.7 Hz, 1H), 7.43 (t, J = 8.7 Hz, 1H), 7.10 (d, J = 8.4 Hz, 1H), 6.95 (t, J = 7.4 Hz, 1H), 3.53-3.28 (m, 4H), 1.83 (s, 4H), 1.75-1.65 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.34, 156.19, 134.26, 130.61, 126.75, 119.57, 118.63, 55.98, 28.70, 27.73. **HRMS** (ESI) calculated for $C_{13}H_{18}NO$ $(M+H)^+$: 204.1383, found: 204.1381.

2-(4-phenylpiperazin-1-yl)benzaldehyde (1f)



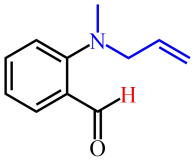
Pale yellow solid. M. p. 112-113 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.42 (s, 1H), 7.87 (dd, J = 7.6, 1.6 Hz, 1H), 7.63-7.54 (m, 1H), 7.34 (dd, J = 8.5, 7.4 Hz, 2H), 7.19 (dd, J = 12.0, 5.2 Hz, 2H), 7.03 (d, J = 8.1 Hz, 2H), 6.94 (t, J = 7.3 Hz, 1H), 3.42 (dd, J = 6.0, 3.7 Hz, 4H), 3.29 (dd, J = 6.1, 3.7 Hz, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.34, 155.44, 151.09, 135.10, 130.03, 129.26, 128.81, 122.94, 120.27, 119.06, 116.42, 54.02, 49.50. **HRMS** (ESI) calculated for $C_{17}H_{19}N_2O$ $(M+H)^+$: 267.1492, found: 267.1490.

2-(dimethylamino)benzaldehyde (1g)



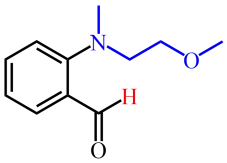
Yellow oil, **^{1}H NMR** (400 MHz, CDCl3) δ 10.22 (s, 1H), 7.76 (d, J = 7.7 Hz, 1H), 7.45 (dd, J = 11.0, 4.5 Hz, 1H), 7.04 (d, J = 8.3 Hz, 1H), 6.99 (t, J = 7.4 Hz, 1H), 2.92 (s, 3H), 2.91 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.18, 155.74, 134.61, 130.95, 127.01, 120.64, 117.65, 45.54. **HRMS** (ESI) calculated for $C_9H_{12}NO$ $(M+H)^+$: 150.0914, found: 150.0915.

2-(allyl(methyl)amino)benzaldehyde (1h)



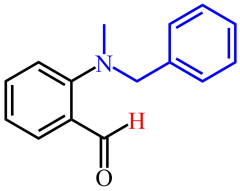
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 7.80 (dd, J = 7.7, 1.6 Hz, 1H), 7.57–7.41 (m, 1H), 7.10 (d, J = 8.3 Hz, 1H), 7.04 (t, J = 7.4 Hz, 1H), 5.93 (ddt, J = 16.2, 10.3, 5.9 Hz, 1H), 5.27 (ddd, J = 13.7, 11.5, 1.4 Hz, 2H), 3.75 (d, J = 5.8 Hz, 2H), 2.87 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 191.38, 155.52, 134.54, 134.10, 130.25, 127.82, 121.22, 118.93, 117.92, 62.02, 41.05. **HRMS** (ESI) calculated for $C_{11}H_{14}NO$ $(M+H)^+$: 176.1070, found: 176.1072.

2-((2-methoxyethyl)(methyl)amino)benzaldehyde (1i)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.32 (s, 1H), 7.78 (dd, J = 7.7, 1.7 Hz, 1H), 7.48 (ddd, J = 8.4, 7.2, 1.8 Hz, 1H), 7.15 (d, J = 8.2 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 3.58 (t, J = 5.7 Hz, 2H), 3.37-3.25 (m, 5H), 2.95 (s, 3H). **^{13}C NMR** (125 MHz, CDCl3) δ 191.69, 155.75, 134.58, 130.13, 128.41, 121.65, 119.53, 70.50, 58.81, 57.93, 42.45. HRMS (ESI) calculated for $C_{11}H_{16}NO_2$ $(M+H)^+$: 194.1176, found: 194.1179.

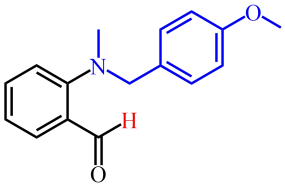
2-(benzyl(methyl)amino)benzaldehyde (1j)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.42 (s, 1H), 7.85 (dd, J = 7.7, 1.7 Hz, 1H), 7.54–7.45 (m, 1H), 7.35 (dd, J = 7.7, 6.5 Hz, 2H), 7.30 (dd, J = 7.4, 4.0 Hz, 3H), 7.10 (dd, J = 16.6, 8.0 Hz, 2H), 4.36 (s, 2H), 2.84 (s, 3H). **^{13}C NMR** (125 MHz,

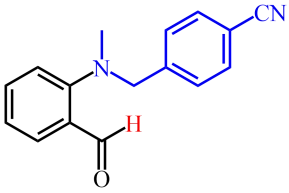
CDCl3) δ 191.33, 155.70, 137.40, 134.71, 130.20, 128.57, 128.13, 128.03, 127.48, 121.67, 119.53, 62.39, 42.37. HRMS (ESI) calculated for $C_{15}H_{16}NO$ $(M+H)^+$: 226.1227, found: 226.1226.

2-((4-methoxybenzyl)(methyl)amino)benzaldehyde (1k)



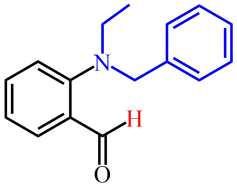
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.39 (d, J = 10.8 Hz, 1H), 7.81 (dd, J = 7.7, 1.3 Hz, 1H), 7.51-7.40 (m, 1H), 7.15 (d, J = 8.5 Hz, 2H), 7.05 (dd, J = 14.9, 7.8 Hz, 2H), 6.84 (d, J = 8.5 Hz, 2H), 4.25 (s, 2H), 3.77 (s, 3H), 2.77 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.38, 158.98, 155.73, 134.70, 130.09, 129.35, 129.32, 128.17, 121.64, 119.64, 113.90, 61.97, 55.27, 42.06. **HRMS** (ESI) calculated for $C_{16}H_{18}NO_2$ $(M+H)^+$: 256.1332, found: 256.1334.

4-(((2-formylphenyl)(methyl)amino)methyl)benzonitrile (1l)



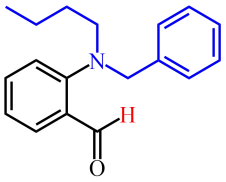
Yellow oil, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.36 (s, 1H), 7.84 (dd, J = 7.7, 1.7 Hz, 1H), 7.64 (d, J = 8.2 Hz, 2H), 7.54-7.49 (m, 1H), 7.44 (d, J = 8.2 Hz, 2H), 7.13 (dd, J = 15.2, 7.8 Hz, 2H), 4.40 (s, 2H), 2.84 (s, 3H). **^{13}C NMR** (125 MHz, CDCl3) δ 190.89, 154.75, 143.17, 134.89, 132.37, 131.16, 128.61, 128.25, 122.29, 119.52, 118.72, 111.37, 61.51, 42.82. **HRMS** (ESI) calculated for $C_{16}H_{15}N_2O$ $(M+H)^+$: 251.1179, found: 251.1175.

2-(benzyl(ethyl)amino)benzaldehyde (1m)



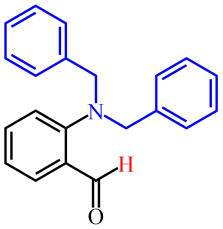
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.51 (s, 1H), 7.85 (dd, J = 7.7, 1.7 Hz, 1H), 7.53-7.46 (m, 1H), 7.34-7.26 (m, 5H), 7.18 (d, J = 8.1 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 4.35 (s, 2H), 3.21 (q, J = 7.1 Hz, 2H), 1.10 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.75, 154.50, 137.85, 134.42, 130.35, 129.16, 128.46, 128.32, 127.32, 122.69, 122.03, 58.41, 49.60, 11.87. **HRMS** (ESI) calculated for $C_{16}H_{18}NO$ $(M+H)^+$: 240.1383, found: 240.1380.

2-(benzyl(butyl)amino)benzaldehyde (1n)



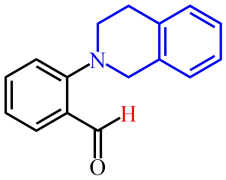
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.49 (s, 1H), 7.84 (dd, J = 7.7, 1.7 Hz, 1H), 7.49 (ddd, J = 8.3, 7.3, 1.8 Hz, 1H), 7.34-7.22 (m, 5H), 7.17 (d, J = 8.2 Hz, 1H), 7.11 (t, J = 7.5 Hz, 1H), 4.35 (s, 2H), 3.21-3.04 (m, 2H), 1.63-1.42 (m, 2H), 1.28 (dq, J = 14.7, 7.3 Hz, 2H), 0.87 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.69, 154.82, 137.71, 134.40, 130.20, 129.26, 128.42, 128.38, 127.33, 122.57, 121.98, 59.68, 54.37, 29.02, 20.28, 13.89. **HRMS** (ESI) calculated for $C_{18}H_{22}NO$ $(M+H)^+$: 268.1696, found: 268.1695.

2-(dibenzylamino)benzaldehyde (1o)



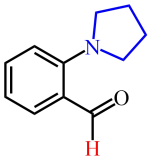
Yellow oil. **^{1}H NMR** (400 MHz, CDCl3) δ 10.40 (s, 1H), 7.87 (dd, J = 7.7, 1.4 Hz, 1H), 7.66-7.56 (m, 1H), 7.28 (s, 1H), 7.22 (t, J = 7.5 Hz, 1H), 3.38 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.36, 154.45, 137.14, 134.46, 129.85, 129.59, 128.59, 128.45, 127.46, 122.92, 122.42, 58.72. **HRMS** (ESI) calculated for $C_{21}H_{20}NO$ $(M+H)^+$: 302.1540, found: 302.1538.

2-(3, 4-dihydroisoquinolin-2(1H)-yl)benzaldehyde (1p)



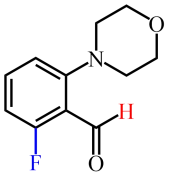
Yellow oil. **^{1}H NMR** (400 MHz, CDCl3) δ 10.35 (s, 1H), 7.87 (d, J = 7.7 Hz, 1H), 7.55 (t, J = 7.7 Hz, 1H), 7.27 – 7.17 (m, 4H), 7.13 (d, J = 7.2 Hz, 2H), 4.35 (s, 2H), 3.47 (t, J = 5.3 Hz, 2H), 3.08 (t, J = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.38, 155.20, 134.91, 134.24, 134.08, 130.04, 128.99, 128.61, 126.61, 126.37, 126.11, 122.30, 119.03, 54.80, 53.55, 29.05. **HRMS** (ESI) calculated for $C_{16}H_{16}NO$ $(M+H)^+$: 238.1227, found: 238.1225.

2-(pyrrolidin-1-yl)benzaldehyde (1q)



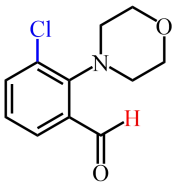
Yellow oil. **^{1}H NMR** (400 MHz, CDCl3) δ 10.11 (s, 1H), 7.72 (dd, J = 7.8, 1.7 Hz, 1H), 7.40 (ddd, J = 8.6, 7.0, 1.8 Hz, 1H), 6.86-6.81 (m, 2H), 3.41-3.35 (m, 4H), 2.03-1.98 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.14, 149.97, 134.23, 133.11, 122.98, 116.44, 114.54, 52.72, 25.97. **HRMS** (ESI) calculated for $C_{11}H_{14}NO$ $(M+H)^+$: 176.1070, found: 176.1068.

2-fluoro-6-morpholinobenzaldehyde (1aa)



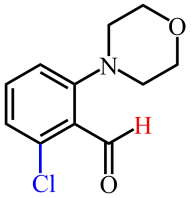
Yellow solid. M. p. 65-67 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.30 (s, 1H), 7.47 (td, J = 8.3, 6.4 Hz, 1H), 6.84 (d, J = 8.3 Hz, 1H), 6.80-6.73 (m, 1H), 3.98-3.82 (m, 4H), 3.15-2.98 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 187.04 (d, $^{3}J_{CF}$ = 7.0 Hz), 164.79 (d, $^{1}J_{CF}$ = 259.1 Hz), 155.19 (d, $^{3}J_{CF}$ = 3.8 Hz), 135.86 (d, $^{3}J_{CF}$ = 11.9 Hz), 116.79 (d, $^{2}J_{CF}$ = 7.0 Hz), 114.11 (d, $^{4}J_{CF}$ = 3.2 Hz), 109.51 (d, $^{2}J_{CF}$ = 21.8 Hz), 66.84, 53.61. **HRMS** (ESI) calculated for $C_{11}H_{13}NO_2F$ $(M+H)^+$: 210.0925, found: 210.0921.

3-chloro-2-morpholinobenzaldehyde (1ab)



Pale yellow solid. M. p. 104-105 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.59 (s, 1H), 7.74 (dd, J = 7.7, 1.6 Hz, 1H), 7.58 (dd, J = 7.9, 1.6 Hz, 1H), 7.24 (d, J = 7.9 Hz, 1H), 3.85 (t, J = 4.3 Hz, 4H), 3.33 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.82, 150.26, 136.72, 135.78, 134.09, 127.56, 126.66, 67.43, 50.85. **HRMS** (ESI) calculated for $C_{11}H_{13}NO_2Cl$ $(M+H)^+$: 226.0630, found: 226.0633.

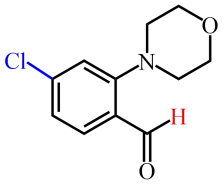
2-chloro-6-morpholinobenzaldehyde (1ac)



Pale yellow solid. M. p. 76-77 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 7.40 (t, J = 8.1 Hz, 1H), 7.10 (d, J = 7.9 Hz, 1H), 7.02 (d, J = 8.3 Hz, 1H), 4.03-3.79 (m,

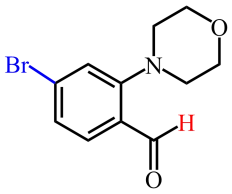
4H), 3.16-3.01 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.32, 155.63, 137.18, 134.26, 125.68, 124.56, 117.45, 66.84, 53.70. **HRMS** (ESI) calculated for $C_{11}H_{13}NO_2Cl$ $(M+H)^+$: 226.0630, found: 226.0630.

4-chloro-2-morpholinobenzaldehyde (1ad)



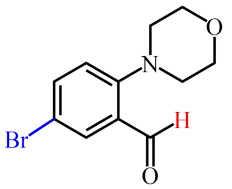
Pale yellow solid. M. p. 79-80 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 7.77 (d, J = 8.3 Hz, 1H), 7.17-7.08 (m, 2H), 3.97-3.86 (m, 4H), 3.15-3.06 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.81, 155.92, 141.32, 131.96, 126.87, 123.15, 119.32, 66.78, 53.98. **HRMS** (ESI) calculated for $C_{11}H_{13}NO_2Cl$ $(M+H)^+$: 226.0630, found: 226.0628.

4-bromo-2-morpholinobenzaldehyde (1ae)



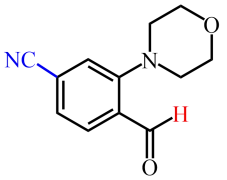
Pale yellow solid. M. p. 90-91 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 7.66 (d, J = 8.2 Hz, 1H), 7.27 (dd, J = 8.4, 1.5 Hz, 1H), 7.24 (d, J = 1.6 Hz, 1H), 3.97-3.75 (m, 4H), 3.19-2.93 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.95, 155.82, 131.90, 130.06, 127.21, 126.08, 122.33, 66.75, 53.98. **HRMS** (ESI) calculated for $C_{11}H_{13}NO_2Br$ $(M+H)^+$: 270.0124, found: 270.0122.

5-bromo-2-morpholinobenzaldehyde (1af)



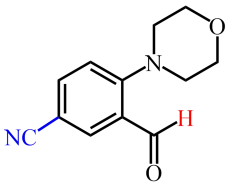
Pale yellow solid. M. p. 73-74 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 7.90 (d, J = 2.5 Hz, 1H), 7.62 (dd, J = 8.7, 2.5 Hz, 1H), 7.01 (d, J = 8.7 Hz, 1H), 4.09-3.75 (m, 4H), 3.24-2.85 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.56, 154.15, 137.62, 132.66, 130.05, 120.94, 116.14, 66.78, 54.12. HRMS (ESI) calculated for $C_{11}H_{13}NO_2Br$ $(M+H)^+$: 270.0124, found: 270.0127.

4-formyl-3-morpholinobenzonitrile (1ag)



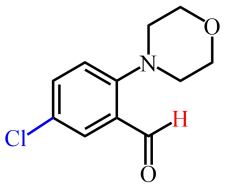
Yellow solid. M. p. 141-142 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.88 (d, J = 7.9 Hz, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.39 (s, 1H), 3.99-3.83 (m, 4H), 3.20-3.03 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.65, 154.86, 131.20, 130.99, 125.82, 122.68, 117.91, 66.65, 53.89. **HRMS** (ESI) calculated for $C_{12}H_{13}N_2O_2$ $(M+H)^+$: 217.0972, found: 217.0970.

3-formyl-4-morpholinobenzonitrile (1ah)



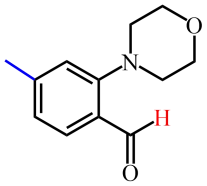
Yellow solid. M. p. 139-140 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.13 (d, J = 3.7 Hz, 1H), 8.05 (d, J = 2.1 Hz, 1H), 7.74 (dd, J = 8.6, 2.1 Hz, 1H), 7.13 (d, J = 8.6 Hz, 1H), 4.11-3.66 (m, 4H), 3.37-3.03 (m, 4H). **^{13}C NMR** (100 MHz, CDCl3) δ 188.45, 156.89, 137.61, 136.12, 127.48, 118.98, 118.22, 104.97, 66.57, 53.40. **HRMS** (ESI) calculated for $C_{12}H_{13}N_2O_2$ $(M+H)^+$: 217.0972, found: 217.0978.

5-chloro-2-morpholinobenzaldehyde (1ai)



Pale yellow solid. M. p. 82-84 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.80 (d, J = 2.6 Hz, 1H), 7.51 (dd, J = 8.7, 2.6 Hz, 1H), 7.11 (d, J = 8.7 Hz, 1H), 3.97-3.87 (m, 4H), 3.15-3.03 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.78, 153.78, 134.78, 129.81, 129.62, 128.90, 120.64, 66.83, 54.22. HRMS (ESI) calculated for $C_{11}H_{13}NO_2Cl$ $(M+H)^+$: 226.0630, found: 226.0626.

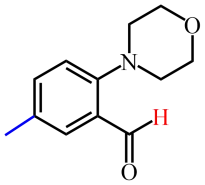
4-methyl-2-morpholinobenzaldehyde (1aj)



Pale yellow solid. M. p. 52-53 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 7.71 (d, J = 7.8 Hz, 1H), 6.95 (d, J = 7.9 Hz, 1H), 6.90 (s, 1H), 3.93-3.85 (m, 4H),

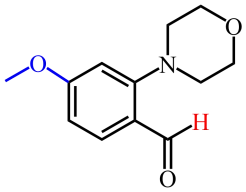
3.11-3.04 (m, 4H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.70, 155.33, 146.29, 130.65, 126.26, 123.83, 119.36, 66.94, 54.11, 22.14. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_2$ $(M+H)^+$: 206.1176, found: 206.1180.

5-methyl-2-morpholinobenzaldehyde (1ak)



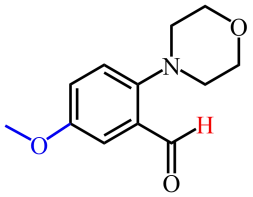
Pale yellow solid. M. p. 76-77 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.37 (s, 1H), 7.64 (d, J = 1.7 Hz, 1H), 7.37 (dd, J = 8.2, 1.9 Hz, 1H), 7.05 (d, J = 8.2 Hz, 1H), 3.96-3.82 (m, 4H), 3.11-3.00 (m, 4H), 2.35 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.50, 153.35, 135.90, 132.82, 130.09, 128.67, 119.04, 66.99, 54.34, 20.51. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_2$ $(M+H)^+$: 206.1176, found: 206.1175.

4-methoxy-2-morpholinobenzaldehyde (1al)



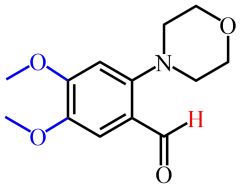
Pale yellow solid. M. p. 104-105 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.14 (s, 1H), 7.79 (d, J = 8.7 Hz, 1H), 6.66 (dd, J = 8.6, 2.3 Hz, 1H), 6.55 (d, J = 2.3 Hz, 1H), 3.93–3.85 (m, 7H), 3.11-3.04 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.49, 165.27, 157.23, 133.49, 122.23, 107.85, 104.54, 66.88, 55.54, 53.94. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_3$ $(M+H)^+$: 222.1125, found: 222.1123.

5-methoxy-2-morpholinobenzaldehyde (1am)



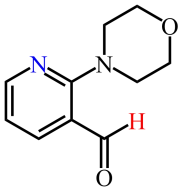
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.44 (s, 1H), 7.33 (s, 1H), 7.14 (d, J = 1.5 Hz, 2H), 3.91-3.85 (m, 4H), 3.82 (s, 3H), 3.08-2.94 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.30, 155.92, 149.85, 130.09, 122.59, 121.18, 111.34, 67.03, 55.65, 54.67. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_3$ $(M+H)^+$: 222.1125, found: 222.1121.

4, 5-dimethoxy-2-morpholinobenzaldehyde (1an)



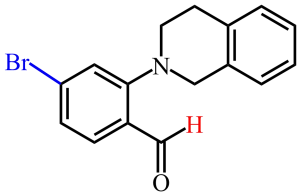
Pale yellow solid. M. p. 94-95 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.32 (s, 1H), 6.64 (s, 1H), 3.95 (s, 3H), 3.90-3.82 (m, 7H), 3.08-3.00 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.64, 154.92, 152.05, 145.66, 122.20, 109.96, 102.37, 66.95, 56.09, 56.08, 54.73. **HRMS** (ESI) calculated for $C_{13}H_{18}NO_4$ $(M+H)^+$: 252.1231, found: 252.1235.

2-morpholinonicotinaldehyde (1ao)



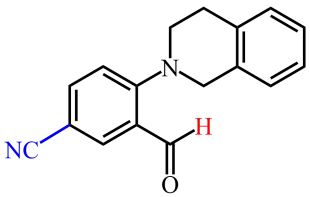
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.42 (dd, J = 4.7, 2.0 Hz, 1H), 8.03 (dd, J = 7.6, 2.0 Hz, 1H), 7.09-6.89 (m, 1H), 4.03-3.82 (m, 4H), 3.55-3.37 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.76, 161.44, 152.68, 141.17, 119.62, 116.29, 66.91, 51.41. **HRMS** (ESI) calculated for $C_{10}H_{13}N_2O_2$ $(M+H)^+$: 193.0972, found: 193.0968.

3-bromo-2-(3, 4-dihydroisoquinolin-2(1H)-yl)benzaldehyde (1ap)



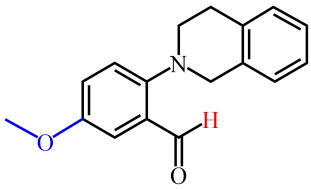
Yellow oil. **^{1}H NMR** (400 MHz, CDCl3) δ 10.21 (s, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.32 (s, 1H), 7.25 (d, J = 3.4 Hz, 1H), 7.23-7.16 (m, 3H), 7.10 (d, J = 4.6 Hz, 1H), 4.31 (s, 2H), 3.45 (t, J = 5.8 Hz, 2H), 3.07 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.15, 155.67, 133.97, 133.49, 131.66, 129.92, 128.99, 127.05, 126.80, 126.39, 126.26, 125.32, 122.19, 54.49, 53.44, 29.07. **HRMS** (ESI) calculated for $C_{16}H_{15}NOBr$ $(M+H)^+$: 316.0332, found: 316.0335.

4-(3, 4-dihydroisoquinolin-2(1H)-yl)-3-formylbenzonitrile (1aq)



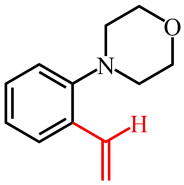
Yellow solid. M. p. 98-99 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 10.10 (s, 1H), 8.06 (d, J = 2.1 Hz, 1H), 7.68 (dd, J = 8.7, 2.2 Hz, 1H), 7.25-7.15 (m, 4H), 7.15-7.08 (m, 1H), 4.46 (s, 2H), 3.62 (t, J = 5.9 Hz, 2H), 3.08 (t, J = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 188.52, 155.98, 137.17, 136.47, 133.98, 132.94, 128.91, 127.10, 126.58, 126.43, 126.32, 118.58, 118.28, 103.23, 53.75, 52.43, 28.72. **HRMS** (ESI) calculated for $C_{17}H_{15}N_2O$ $(M+H)^+$: 263.1179, found: 263.1182.

2-(3, 4-dihydroisoquinolin-2(1H)-yl)-5-methoxybenzaldehyde (1ar)



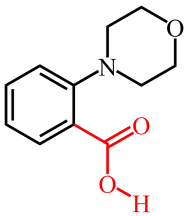
Yellow oil. **^{1}H NMR** (400 MHz, CDCl3) δ 10.15 (s, 1H), 7.82 (d, J = 9.3 Hz, 1H), 7.23-7.16 (m, 3H), 7.12-7.06 (m, 1H), 6.65-6.62 (m, 2H), 4.31 (s, 2H), 3.86 (s, 3H), 3.45 (t, J = 5.8 Hz, 2H), 3.07 (d, J = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.74, 153.33, 135.75, 134.26, 132.23, 129.78, 128.99, 128.68, 126.56, 126.38, 126.05, 119.29, 55.14, 53.67, 29.11, 20.53. **HRMS** (ESI) calculated for $C_{17}H_{18}NO_2$ $(M+H)^+$: 268.1332, found: 268.1328.

4-(2-vinylphenyl)morpholine (1ba)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.7 Hz, 1H), 7.26 (t, J = 7.7 Hz, 1H), 7.14-6.97 (m, 3H), 5.70 (dd, J = 17.8, 1.3 Hz, 1H), 5.25 (dd, J = 11.0, 1.3 Hz, 1H), 3.92-3.77 (m, 4H), 3.01-2.86 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.41, 134.16, 132.21, 128.60, 126.91, 123.25, 118.39, 113.81, 67.33, 52.59. **HRMS** (ESI) calculated for $C_{12}H_{16}NO$ $(M+H)^+$: 190.1227, found: 190.1230.

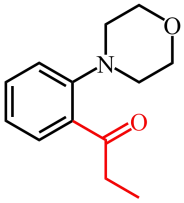
2-morpholinobenzoic acid (1bb)



Brown solid. M. p. 156-157 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.31 (dd, J = 7.8, 1.6 Hz, 1H), 7.70-7.57 (m, 1H), 7.50-7.39 (m, 2H), 4.51 (s, 1H), 3.96 (s, 4H), 3.09 (s, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.79, 150.17, 134.13, 132.56, 127.89, 125.10,

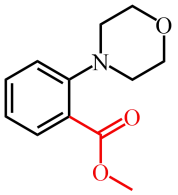
122.52, 66.91, 53.55. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0965.

1-(2-morpholinophenyl)propan-1-one (1bc)



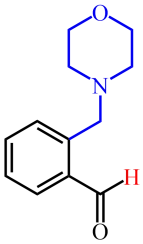
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (td, J = 8.1, 1.6 Hz, 1H), 7.31 (dd, J = 7.8, 1.6 Hz, 1H), 7.11-7.03 (m, 2H), 3.84-3.76 (m, 4H), 3.05 (q, J = 7.3 Hz, 2H), 2.99-2.92 (m, 4H), 1.16 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 208.56, 150.45, 136.02, 131.41, 128.62, 123.16, 118.68, 67.06, 53.25, 35.13, 8.70. **HRMS** (ESI) calculated for $C_{13}H_{18}NO_2$ $(M+H)^+$: 220.1332, found: 220.1337.

methyl 2-morpholinobenzoate (1bd)



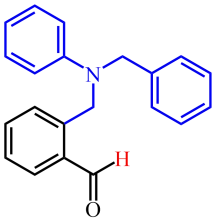
Brown oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (dd, J = 7.7, 1.6 Hz, 1H), 7.49-7.39 (m, 1H), 7.10-6.99 (m, 2H), 3.89 (s, 3H), 3.88-3.83 (m, 4H), 3.10-3.02 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 168.18, 152.20, 132.84, 131.72, 124.26, 121.88, 118.82, 67.12, 52.88, 52.05. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_3$ $(M+H)^+$: 222.1123, found: 222.1125.

2-(morpholinomethyl)benzaldehyde (1bg)



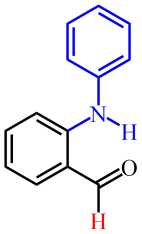
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.43 (s, 1H), 7.87 (d, J = 7.6 Hz, 1H), 7.51 (td, J = 7.4, 1.4 Hz, 1H), 7.41 (dd, J = 12.4, 7.5 Hz, 2H), 3.82 (s, 2H), 3.69-3.61 (m, 4H), 2.51-2.38 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.07, 140.40, 135.05, 133.20, 130.60, 129.41, 127.93, 66.88, 60.09, 53.29. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_2$ $(M+H)^+$: 206.1176, found: 206.1180.

2-((benzyl(phenyl)amino)methyl)benzaldehyde (1bh)



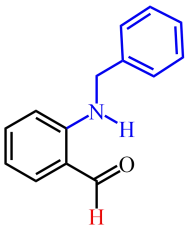
White solid. M. p. 113-114 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.17 (s, 1H), 7.88 (dd, J = 7.4, 1.4 Hz, 1H), 7.58–7.44 (m, 2H), 7.41 (d, J = 7.6 Hz, 1H), 7.36-7.29 (m, 2H), 7.26 (dd, J = 6.9, 4.8 Hz, 3H), 7.16 (dt, J = 8.7, 4.8 Hz, 2H), 6.70 (t, J = 7.3 Hz, 1H), 6.63 (d, J = 8.0 Hz, 2H), 5.10 (s, 2H), 4.66 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.57, 148.73, 141.25, 138.28, 135.35, 134.06, 133.83, 129.31, 128.74, 127.39, 127.24, 126.97, 126.59, 116.86, 112.29, 54.58, 52.98. **HRMS** (ESI) calculated for $C_{11}H_{20}NO$ $(M+H)^+$: 302.1540, found: 302.1545.

2-(cyclohex-2-en-1-ylamino)benzaldehyde (1bi)



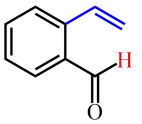
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.36 (s, 1H), 7.45 (dd, J = 7.7, 1.6 Hz, 1H), 7.36 (ddd, J = 8.6, 7.1, 1.6 Hz, 1H), 6.75 (d, J = 8.6 Hz, 1H), 6.66 (t, J = 7.4 Hz, 1H), 5.89 (dtd, J = 9.3, 3.6, 1.8 Hz, 1H), 5.74 (ddd, J = 10.0, 5.1, 2.2 Hz, 1H), 4.12 (s, 1H), 2.16-2.00 (m, 2H), 1.99-1.89 (m, 1H), 1.82-1.58 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.79, 149.80, 137.00, 135.74, 130.78, 127.34, 118.48, 114.63, 111.14, 46.90, 28.74, 25.03, 19.67. **HRMS** (ESI) calculated for $C_{13}H_{16}NO$ $(M+H)^+$: 202.1227, found: 202.1225.

2-(benzylamino)benzaldehyde (1bj)



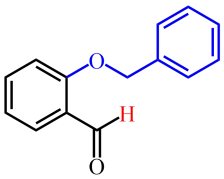
Pale yellow solid. M. p. 52-53 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.74 (s, 1H), 7.48 (dd, J = 7.7, 1.5 Hz, 1H), 7.33-7.29 (m, 5H), 7.26 (dd, J = 8.5, 4.2 Hz, 1H), 6.69 (t, J = 7.4 Hz, 1H), 6.63 (d, J = 8.5 Hz, 1H), 4.47 (d, J = 3.9 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.15, 150.60, 138.31, 136.71, 135.87, 128.77, 127.33, 127.03, 118.71, 115.33, 111.37, 46.62. **HRMS** (ESI) calculated for $C_{14}H_{14}NO$ $(M+H)^+$: 212.1070, found: 212.1072.

2-vinylbenzaldehyde (1bk)



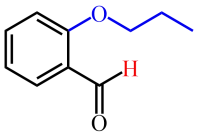
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 7.82 (d, J = 7.5 Hz, 1H), 7.60-7.49 (m, 3H), 7.45-7.41 (m, 1H), 5.70 (dd, J = 17.4 Hz, J = 1.0, 1H), 5.51 (dd, J = 11.0 Hz, J = 0.9, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.42, 140.50, 133.81, 133.37, 132.87, 131.25, 127.93, 127.44, 119.42. **HRMS** (ESI) calculated for C_9H_9O $(M+H)^+$: 133.0648, found: 133.0645.

2-(benzyloxy)benzaldehyde (1bl)



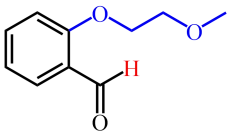
White solid. M. p. 48-49 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.59 (s, 1H), 7.89 (dd, J = 7.6, 1.8 Hz, 1H), 7.60-7.52 (m, 1H), 7.50-7.34 (m, 5H), 7.07 (t, J = 8.3 Hz, 2H), 5.22 (s, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.80, 161.08, 136.10, 135.93, 128.76, 128.49, 128.31, 127.32, 125.22, 121.05, 113.05, 70.50. **HRMS** (ESI) calculated for $C_{14}H_{13}O_2$ $(M+H)^+$: 213.0910, found: 213.0908.

2-ethoxybenzaldehyde (1bm)



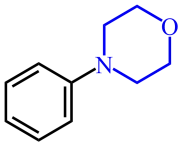
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 7.84 (dd, J = 7.7, 1.8 Hz, 1H), 7.53 (ddd, J = 9.0, 7.4, 1.8 Hz, 1H), 7.03-6.97 (m, 2H), 4.05 (t, J = 6.4 Hz, 2H), 1.95-1.82 (m, 2H), 1.09 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.78, 161.09, 136.12, 135.96, 128.77, 128.47, 128.31, 127.33, 125.22, 121.05, 113.09, 70.50. **HRMS** (ESI) calculated for $C_{10}H_{13}O_2$ $(M+H)^+$: 165.0910, found: 165.0915.

2-(2-methoxyethoxy)benzaldehyde (1bn)



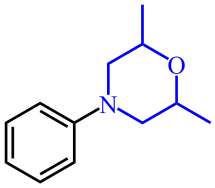
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.53 (s, 1H), 7.83 (dd, J = 7.7, 1.8 Hz, 1H), 7.53 (ddd, J = 8.4, 7.3, 1.9 Hz, 1H), 7.01 (dd, J = 16.5, 8.1 Hz, 2H), 4.25-4.23 (m, 2H), 3.87-3.75 (m, 2H), 3.45 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.79, 161.25, 135.89, 128.25, 125.09, 120.99, 112.81, 70.81, 68.17, 59.30. **HRMS** (ESI) calculated for $C_{10}H_{13}O_3$ $(M+H)^+$: 181.0859, found: 181.0855.

4-phenylmorpholine (2a)



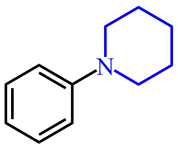
Colorless oil. Yield: 75% (36.7 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (t, J = 8.0 Hz, 2H), 6.93-6.87(m, 3H), 3.96-3.76 (m, 4H), 3.22-3.07 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.26, 129.23, 120.15, 115.79, 66.96, 49.44. **HRMS** (ESI) calculated for $C_{10}H_{14}NO$ $(M+H)^+$: 164.1070, found: 164.1073.

2, 6-dimethyl-4-phenylmorpholine (2b)



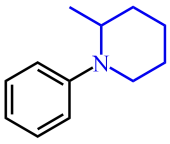
Colorless oil. Yield: 64% (36.7 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.32-7.28 (m, 2H), 6.94 (d, J = 8.0 Hz, 2H), 6.89 (t, J = 7.3 Hz, 1H), 3.92-3.77 (m, 2H), 3.48 (dd, J = 12.4, 1.8 Hz, 2H), 2.45 (dd, J = 11.8, 10.6 Hz, 2H), 1.29 (d, J = 6.3 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.99, 129.20, 119.82, 115.82, 71.68, 54.89, 19.11. **HRMS** (ESI) calculated for $C_{12}H_{18}NO$ $(M+H)^+$: 192.1383, found: 192.1387.

1-phenylpiperidine (2c)



Yellow oil. Yield: 63% (30.4 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.25 (t, J = 7.8 Hz, 2H), 6.95 (d, J = 8.2 Hz, 2H), 6.82 (t, J = 7.2 Hz, 1H), 3.26-3.06 (m, 4H), 1.78-1.66 (m, 4H), 1.63-1.51 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 129.05, 116.70, 100.00, 50.89, 25.81, 24.27. **HRMS** (ESI) calculated for $C_{11}H_{16}N$ $(M+H)^+$: 162.1277, found: 162.1270.

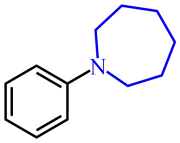
2-methyl-1-phenylpiperidine (2d)



Yellow oil. Yield: 71% (37.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (t, J = 7.9 Hz, 2H), 7.02 (d, J = 7.2 Hz, 2H), 6.89 (t, J = 7.2 Hz, 1H), 3.90 (dd, J = 10.5, 4.3 Hz, 1H), 3.24 (dt, J = 11.7, 4.3 Hz, 1H), 3.03 (t, J = 9.3 Hz, 1H), 2.00–1.80 (m, 2H), 1.73-1.58 (m, 4H), 1.04 (d, J = 6.6 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.45, 129.00,

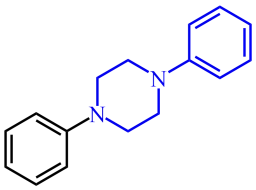
119.27, 117.73, 51.50, 45.18, 31.85, 26.15, 19.86, 13.96. **HRMS** (ESI) calculated for $C_{12}H_{18}N$ $(M+H)^+$: 176.1434, found: 176.1435.

1-phenylazepane (2e)



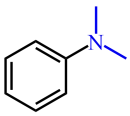
Colorless oil. Yield: 60% (31.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27-7.18 (m, 2H), 6.72 (d, J = 8.3 Hz, 2H), 6.66 (t, J = 7.2 Hz, 1H), 3.53-3.35 (m, 4H), 1.82 (s, 4H), 1.61–1.52 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.90, 129.27, 115.12, 111.16, 49.07, 27.81, 27.19. **HRMS** (ESI) calculated for $C_{12}H_{18}N$ $(M+H)^+$: 176.1434, found: 176.1432.

1, 4-diphenylpiperazine (2f)



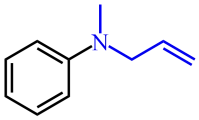
White solid. M. p. 163-164 °C. Yield: 55% (39.3 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.39–7.30 (m, 4H), 7.03 (d, J = 8.0 Hz, 4H), 6.94 (t, J = 7.3 Hz, 2H), 3.39 (s, 8H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.20, 129.23, 120.17, 116.42, 49.48. **HRMS** (ESI) calculated for $C_{16}H_{19}N_2$ $(M+H)^+$: 239.1543, found: 239.1541.

***N, N*-dimethylaniline (2g)**



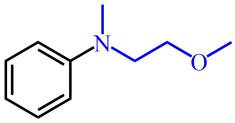
Colorless oil. Yield: 48% (17.4 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27-7.18 (m, 2H), 6.77-6.68 (m, 3H), 2.90 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.81, 129.21, 116.80, 112.82, 40.72. HRMS (ESI) calculated for $C_8H_{12}N$ $(M+H)^+$: 122.0964, found: 122.0990.

***N*-allyl-*N*-methylaniline (2h)**



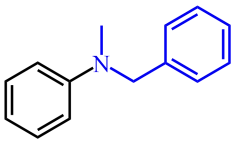
Yellow oil. Yield: 46% (20.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 (dd, J = 8.5, 7.1 Hz, 2H), 6.74-6.68 (m, 3H), 5.89-5.80 (m, 1H), 5.21-5.08 (m, 2H), 3.91 (d, J = 5.1 Hz, 2H), 2.93 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.48, 133.81, 129.13, 116.49, 116.21, 112.53, 55.33, 38.04. **HRMS** (ESI) calculated for $C_{10}H_{14}N$ $(M+H)^+$: 148.1121, found: 148.1120.

***N*-(2-methoxyethyl)-*N*-methylaniline (2i)**



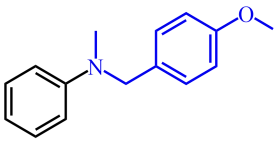
Colorless oil. Yield: 44% (21.8 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34-7.19 (m, 2H), 6.76 (d, J = 8.5 Hz, 2H), 3.61-3.58 (m, 2H), 3.56-3.51 (m, 2H), 3.39 (s, 3H), 3.01 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.30, 129.19, 116.35, 112.22, 70.19, 59.05, 52.49, 38.94. **HRMS** (ESI) calculated for $C_{10}H_{16}NO$ $(M+H)^+$: 166.1227, found: 166.1225.

***N*-benzyl-*N*-methylaniline (2j)**



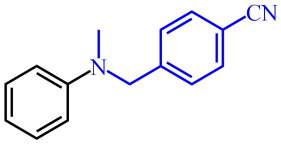
Colorless oil. Yield: 56% (33.1 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34-7.27 (m, 2H), 7.32-7.19 (m, 5H), 6.75 (d, J = 8.1 Hz, 2H), 6.71 (t, J = 7.3 Hz, 1H), 4.53 (s, 2H), 3.01 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.75, 139.03, 129.21, 128.59, 126.89, 126.78, 116.58, 112.41, 56.68, 38.55. **HRMS** (ESI) calculated for $C_{14}H_{16}N$ $(M+H)^+$: 198.1277, found : 198.1276.

***N*-(4-methoxybenzyl)-*N*-methylaniline (2k)**



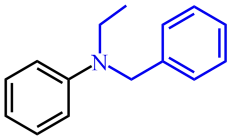
Colorless oil. Yield: 50% (34.1 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.24-7.18 (m, 2H), 7.14 (d, J = 8.6 Hz, 2H), 6.84 (d, J = 8.6 Hz, 2H), 6.76 (s, 2H), 6.70 (t, J = 7.3 Hz, 1H), 4.45 (s, 2H), 3.77 (s, 3H), 2.96 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.64, 149.86, 130.92, 129.20, 128.02, 116.59, 113.99, 112.57, 56.10, 55.31, 38.34. **HRMS** (ESI) calculated for $C_{15}H_{18}NO$ $(M+H)^+$: 228.1383, found: 228.1385.

4-((methyl(phenyl)amino)methyl)benzonitrile (2l)



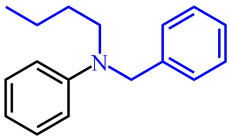
Yellow oil. Yield: 55% (36.7 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.63 (d, J = 8.3 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.32-7.22 (m, 2H), 6.80 (t, J = 7.3 Hz, 1H), 6.75 (d, J = 8.1 Hz, 2H), 4.61 (s, 2H), 3.08 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.22, 145.07, 132.50, 129.38, 127.42, 118.99, 117.26, 112.46, 110.80, 56.67, 38.92. **HRMS** (ESI) calculated for $C_{15}H_{15}N_2$ $(M+H)^+$: 223.1230, found: 223.1233.

***N*-benzyl-*N*-ethylaniline (2m)**



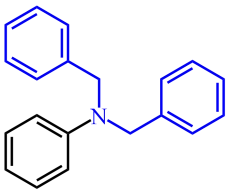
Colorless oil. Yield: 58% (36.7 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46-7.33 (m, 5H), 7.32-7.22 (m, 2H), 6.82-6.76 (m, 3H), 4.62 (s, 2H), 3.58 (q, J = 7.0 Hz, 2H), 1.31 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.51, 139.31, 129.26, 128.57, 126.77, 126.58, 116.04, 112.17, 53.93, 45.16, 12.15. **HRMS** (ESI) calculated for $C_{15}H_{18}N$ $(M+H)^+$: 212.1434, found: 212.1430.

***N*-benzyl-*N*-butylaniline (2n)**



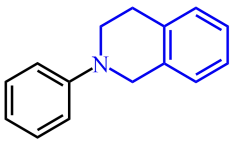
Colorless oil. Yield: 53% (38.0 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37-7.30 (m, 2H), 7.28-7.25 (m, 3H), 7.23-7.19 (m, 2H), 6.72-6.67 (m, 3H), 4.57 (s, 2H), 3.54-3.33 (m, 2H), 1.72-1.65 (m, 2H), 1.44-1.35 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 148.66, 139.22, 129.23, 128.58, 126.75, 126.57, 115.95, 112.13, 54.51, 51.11, 29.34, 20.42, 14.06. **HRMS** (ESI) calculated for $C_{17}H_{22}N$ $(M+H)^+$: 240.1747, found: 240.1743.

***N, N*-dibenzylaniline (2o)**



Colorless oil. Yield: 61% (49.9 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 4H), 7.28-7.21 (m, 6H), 7.16 (t, J = 8.0 Hz, 2H), 6.74 (d, J = 8.2 Hz, 2H), 6.70 (t, J = 7.3 Hz, 1H), 4.65 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.19, 138.62, 129.22, 128.64, 126.88, 126.66, 116.72, 112.47, 54.20. **HRMS** (ESI) calculated for $C_{20}H_{20}N$ $(M+H)^+$: 274.1590, found: 274.1595.

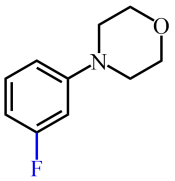
2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline (2p)



Colorless oil. Yield: 60% (37.6 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (dd, J = 8.8, 7.3 Hz, 2H), 7.20-7.13 (m, 4H), 6.98 (d, J = 7.9 Hz, 2H), 6.82 (t, J = 7.3 Hz, 1H), 4.41

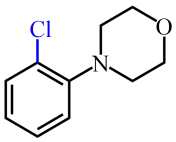
(s, 2H), 3.56 (t, J = 5.9 Hz, 2H), 2.99 (d, J = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.58, 134.90, 134.49, 129.22, 128.54, 126.56, 126.35, 126.04, 118.68, 115.16, 50.76, 46.54, 29.14. **HRMS** (ESI) calculated for $C_{15}H_{16}N$ $(M+H)^+$: 210.1277, found: 210.1275.

4-(3-fluorophenyl)morpholine (2aa)



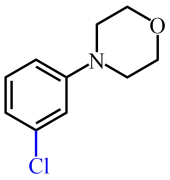
Yellow oil. Yield: 95% (51.6 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23 (dd, J = 15.2, 8.1 Hz, 1H), 6.69 (dd, J = 8.3, 2.0 Hz, 1H), 6.64-6.54 (m, 2H), 3.97-3.73 (m, 4H), 3.26-3.03 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.88 (d, $^{1}J_{CF}$ = 241.9 Hz), 152.97 (d, $^{3}J_{CF}$ = 9.5 Hz), 130.22 (d, $^{3}J_{CF}$ = 9.8 Hz), 110.82 (d, $^{4}J_{CF}$ = 2.3 Hz), 106.27 (d, $^{2}J_{CF}$ = 21.3 Hz), 102.44 (d, $^{2}J_{CF}$ = 25.0 Hz), 66.73, 48.85. **HRMS** (ESI) calculated for $C_{10}H_{13}NOF$ $(M+H)^+$: 182.0976, found: 182.0979.

4-(2-chlorophenyl)morpholine (2ab)



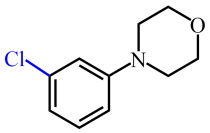
Yellow oil. Yield: 91% (53.8 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (dd, J = 7.9, 1.5 Hz, 1H), 7.30-7.22 (m, 1H), 7.06 (dd, J = 8.1, 1.5 Hz, 1H), 7.01 (td, J = 7.7, 1.5 Hz, 1H), 4.02-3.82 (m, 4H), 3.19-3.00 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.04, 130.76, 128.81, 127.68, 123.95, 120.28, 67.18, 51.69. **HRMS** (ESI) calculated for $C_{10}H_{13}ClNO$ $(M+H)^+$: 198.0680, found: 198.0681.

4-(3-chlorophenyl)morpholine (2ac)



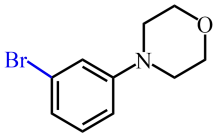
Yellow oil. Yield: 90% (53.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (t, J = 8.1 Hz, 1H), 6.89 (t, J = 2.1 Hz, 1H), 6.88-6.84 (m, 1H), 6.80 (dd, J = 8.4, 2.3 Hz, 1H), 3.96-3.77 (m, 4H), 3.24-3.06 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.36, 135.06, 130.12, 119.71, 115.53, 113.62, 66.74, 48.89. **HRMS** (ESI) calculated for $C_{10}H_{13}NOCl$ $(M+H)^+$: 198.0680, found: 198.0677.

4-(3-chlorophenyl)morpholine (2ad)



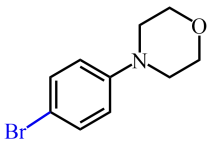
Yellow oil. Yield: 76% (44.9 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.20 (t, J = 8.1 Hz, 1H), 6.91-6.83 (m, 2H), 6.80 (dd, J = 8.4, 2.3 Hz, 1H), 3.93-3.81 (m, 4H), 3.22-3.11 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.36, 135.06, 130.11, 119.71, 115.53, 113.61, 66.75, 48.89. **HRMS** (ESI) calculated for $C_{10}H_{13}ClNO$ $(M+H)^+$: 198.0680, found: 198.0685.

4-(3-bromophenyl)morpholine (2ae)



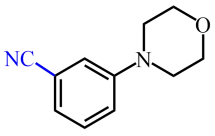
Colorless oil. Yield: 88% (63.8 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.11 (t, J = 8.1 Hz, 1H), 7.02 (s, 1H), 6.98 (d, J = 7.8 Hz, 1H), 6.81 (d, J = 8.3 Hz, 1H), 3.89-3.79 (m, 4H), 3.19-3.10 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.52, 130.41, 123.33, 122.64, 118.44, 114.10, 66.75, 48.89. **HRMS** (ESI) calculated for $C_{10}H_{13}NOBr$ $(M+H)^+$: 242.0175, found: 242.0173.

4-(4-bromophenyl)morpholine (2af)



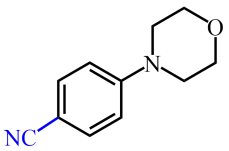
White solid. M. p. 114-115 °C. Yield: 79% (57.3 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.43-7.28 (m, 2H), 6.78 (d, J = 8.9 Hz, 2H), 4.05-3.68 (m, 4H), 3.31-2.95 (m, 4H). **^{13}C NMR** (100 MHz, CDCl3) δ 150.25, 131.97, 117.35, 112.27, 66.75, 49.19. **HRMS** (ESI) calculated for $C_{10}H_{13}NOBr$ $(M+H)^+$: 242.0175, found: 242.0170.

3-morpholinobenzonitrile (2ag)



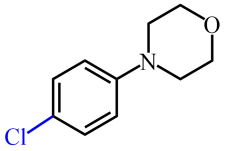
Yellow solid. M. p. 101-102 °C. Yield: 81% (45.7 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38-7.32 (m, 1H), 7.15-7.12 (m, 3H), 3.91-3.84 (m, 4H), 3.24-3.16 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.29, 129.98, 123.03, 119.65, 119.26, 118.21, 113.11, 66.58, 48.50. **HRMS** (ESI) calculated for $C_{11}H_{13}N_2O$ $(M+H)^+$: 189.1023, found: 189.1024.

4-morpholinobenzonitrile (2ah)



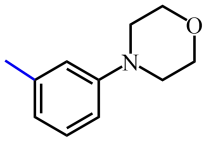
White solid. M. p. 74-75 °C. Yield: 89% (50.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (d, J = 9.1 Hz, 2H), 6.86 (d, J = 9.1 Hz, 2H), 3.94-3.69 (m, 4H), 3.32-3.12 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.52, 133.51, 119.89, 114.08, 100.87, 66.45, 47.29. **HRMS** (ESI) calculated for $C_{11}H_{13}N_2O$ $(M+H)^+$: 189.1023, found: 189.1020.

4-(4-chlorophenyl)morpholine (2ai)



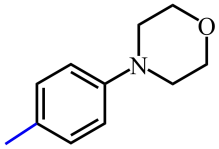
White solid. M. p. 70-71 °C. Yield: 65% (38.4 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (d, J = 9.0 Hz, 2H), 6.85 (d, J = 9.0 Hz, 2H), 3.94-3.80 (m, 4H), 3.18-3.09 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.91, 129.05, 124.92, 116.92, 66.80, 49.35. **HRMS** (ESI) calculated for $C_{10}H_{13}NOCl$ $(M+H)^+$: 198.0680, found:198.0686.

4-(m-tolyl)morpholine (2aj)



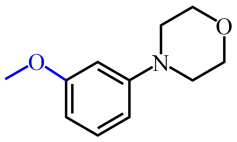
Colorless oil. Yield: 53% (28.1 mg). 138-139 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.20 (t, J = 7.7 Hz, 1H), 6.83-6.73 (m, 3H), 3.96-3.83 (m, 4H), 3.23-3.13 (m, 4H), 2.35 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 139.00, 129.09, 121.34, 116.77, 113.07, 66.89, 49.70, 21.78. **HRMS** (ESI) calculated for $C_{11}H_{16}NO$ $(M+H)^+$: 178.1227, found: 178.1225.

4-(*p*-tolyl)morpholine (2ak)



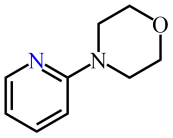
Colorless oil. Yield: 47% (25.0 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09 (d, J = 8.3 Hz, 2H), 6.83 (d, J = 8.3 Hz, 2H), 4.20-3.78 (m, 4H), 3.38-2.96 (m, 4H), 2.27 (s, 3H). **^{13}C NMR** (100MHz, $CDCl_3$) δ 149.18, 129.73, 129.65, 116.09, 66.99, 49.98, 20.43. HRMS (ESI) calculated for $C_{11}H_{16}NO$ $(M+H)^+$: 178.1227, found: 178.1223.

4-(3-methoxyphenyl)morpholine (2al)



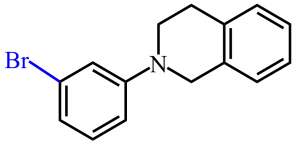
Colorless oil. Yield: 56% (32.4 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (t, J = 8.3 Hz, 1H), 6.59-6.53 (m, 1H), 6.49-6.46 (m, 2H), 3.91-3.84 (m, 4H), 3.82 (s, 3H), 3.21-3.13 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.66, 152.70, 129.90, 108.51, 104.79, 102.27, 66.90, 55.22, 49.33. HRMS (ESI) calculated for $C_{11}H_{16}NO_2$ $(M+H)^+$: 194.1177, found: 194.1175.

4-(pyridin-2-yl)morpholine (2ao)



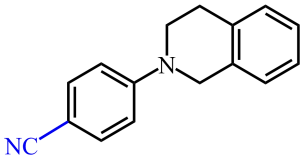
Yellow oil. Yield: 68% (33.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (dd, J = 4.8, 1.1 Hz, 1H), 7.53 (ddd, J = 8.9, 7.2, 1.9 Hz, 1H), 6.86-6.51 (m, 2H), 4.00-3.71 (m, 4H), 3.63-3.37 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.84, 137.66, 113.84, 107.04, 100.00, 66.78, 45.67. **HRMS** (ESI) calculated for $C_9H_{13}N_2O$ $(M+H)^+$: 165.1023, found: 165.1025.

2-(3-bromophenyl)-1, 2, 3, 4-tetrahydroisoquinoline (2ap)



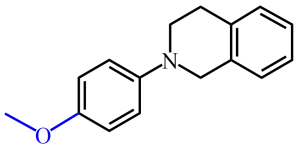
Colorless oil. Yield: 68% (58.7 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24-7.01 (m, 5H), 6.88 (t, J = 2.2 Hz, 1H), 6.82-6.66 (m, 2H), 4.34 (s, 2H), 3.48 (t, J = 5.9 Hz, 2H), 2.92 (t, J = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.46, 135.16, 134.88, 134.07, 130.21, 128.52, 126.63, 126.30, 118.04, 114.43, 112.67, 50.11, 45.95, 29.12. **HRMS** (ESI) calculated for $C_{15}H_{15}NBr$ $(M+H)^+$: 288.0383, found: 288.0385.

4-(3, 4-dihydroisoquinolin-2(1H)-yl)benzonitrile (2aq)



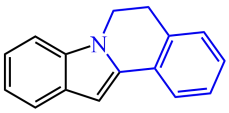
Yellow solid. M. p. 90-91 °C. Yield: 62% (43.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59-7.46 (m, 2H), 7.34-7.11 (m, 4H), 6.95-6.74 (m, 2H), 4.52 (s, 2H), 3.66 (t, J = 5.9 Hz, 2H), 3.02 (t, J = 5.9 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.21, 134.93, 133.58, 133.42, 128.21, 126.97, 126.56, 126.50, 120.45, 112.68, 98.65, 48.79, 44.62, 28.96. **HRMS** (ESI) calculated for $C_{16}H_{15}N_2$ $(M+H)^+$: 235.1230, found: 235.1226.

2-(4-methoxyphenyl)-1, 2, 3, 4-tetrahydroisoquinoline (2ar)



White solid. M. p. 93-95 °C. Yield: 50% (35.8 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.14 (dd, J = 9.9, 3.4 Hz, 4H), 6.98 (d, J = 9.0 Hz, 2H), 6.86 (d, J = 9.0 Hz, 2H), 4.29 (s, 2H), 3.77 (s, 3H), 3.44 (t, J = 5.8 Hz, 2H), 2.98 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.09, 150.61, 136.09, 129.22, 127.54, 126.68, 118.65, 115.17, 113.21, 112.37, 55.32, 50.22, 46.51, 29.43. **HRMS** (ESI) calculated for $C_{16}H_{18}NO$ $(M+H)^+$: 240.1383, found: 240.1380.

5, 6-dihydroindolo[2, 1-a]isoquinoline (3p)

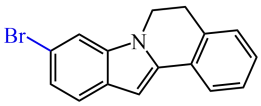


White solid. M.p. 167 – 169 °C. Yield: 60% (39.4 mg). **^{1}H NMR** (400 MHz, DMSO) δ 7.83 (d, J = 7.6 Hz, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.49 (d, J = 8.2 Hz, 1H), 7.34 (dd, J = 14.4, 7.4 Hz, 2H), 7.27 (t, J = 7.3 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 7.04 (t, J = 7.4 Hz, 1H), 6.96 (s, 1H), 4.28 (t, J = 6.5 Hz, 2H), 3.17 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 136.66, 135.62, 132.17, 129.03, 128.80, 128.31, 127.42, 127.26, 124.39, 121.68, 120.75, 119.88, 108.96, 96.43, 40.11, 29.18. **HRMS** (ESI) calculated for $C_{16}H_{14}N$ $(M+H)^+$: 220.1044, found : 220.1050.

2, 3-dihydro-1H-pyrrolo[1, 2-a]indole (3q)

White solid. M. p. 76-78 °C. Yield: 52% (24.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 (d, J = 7.8 Hz, 1H), 7.27 (d, J = 8.0 Hz, 1H), 7.14 (t, J = 7.0 Hz, 1H), 7.08 (t, J = 7.0 Hz, 1H), 6.19 (s, 1H), 4.09 (t, J = 7.0 Hz, 2H), 3.05 (t, J = 7.4 Hz, 2H), 2.71-2.55 (m, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 144.61, 133.30, 132.70, 120.33, 120.14, 119.13, 109.41, 92.31, 43.62, 27.88, 24.32. **HRMS** (ESI) calculated for $C_{11}H_{12}N$ $(M+H)^+$: 158.0964, found: 158.0969.

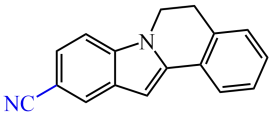
9-bromo-5, 6-dihydroindolo[2, 1-a]isoquinoline (3ap)



Pale yellow solid. M.p. 149 – 151 °C. Yield: 68% (60.7 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 (s, 2H), 7.37 - 7.21 (m, 4H), 7.17 (d, J = 8.5 Hz, 1H), 6.78 (s, 1H), 4.20 (t, J = 5.9 Hz, 2H), 3.18 (t, J = 6.2 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 137.49,

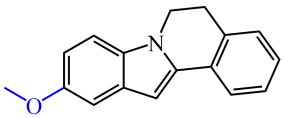
136.29, 132.09, 128.58, 128.37, 127.77, 127.64, 127.37, 124.45, 123.12, 121.86, 115.13, 112.07, 96.55, 40.24, 29.03. **HRMS** (ESI) calculated for $C_{16}H_{13}NBr$ $(M+H)^+$: 298.0149, found: 298.0153.

5, 6-dihydroindolo[2,1-a]isoquinoline-10-carbonitrile (3aq)



White solid. M.p. 203 – 205 °C. Yield: 62% (45.3 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.95 (d, J = 0.8 Hz, 1H), 7.76 (d, J = 7.4 Hz, 1H), 7.42 (dd, J = 8.5, 1.5 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.29 (d, J = 3.9 Hz, 2H), 6.91 (s, 1H), 4.29 (t, J = 6.6 Hz, 2H), 3.22 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 138.08, 137.89, 132.25, 128.49, 128.46, 127.95, 127.58, 126.07, 124.80, 124.55, 120.90, 109.74, 102.79, 97.04, 40.41, 28.87. HRMS (ESI) calcd. for $C_{17}H_{13}N_2$ $(M+H)^+$: 245.0996, found: 245.0998.

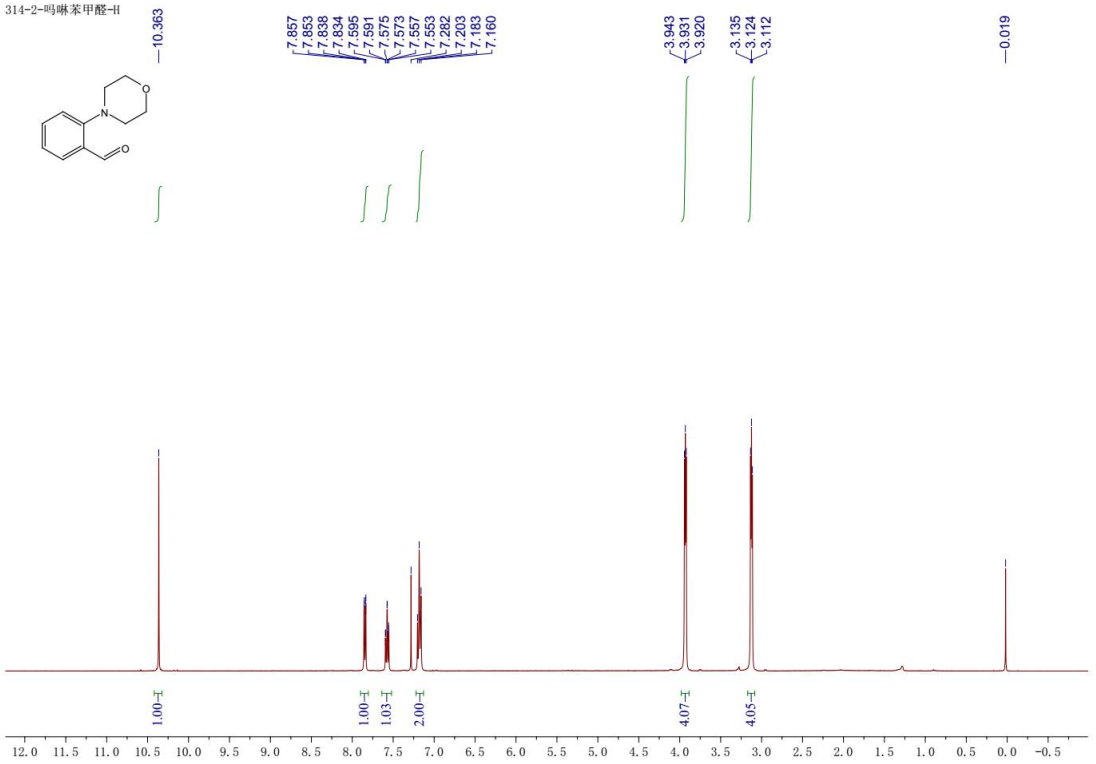
10-methoxy-5, 6-dihydroindolo[2,1-a]isoquinoline (3ar)

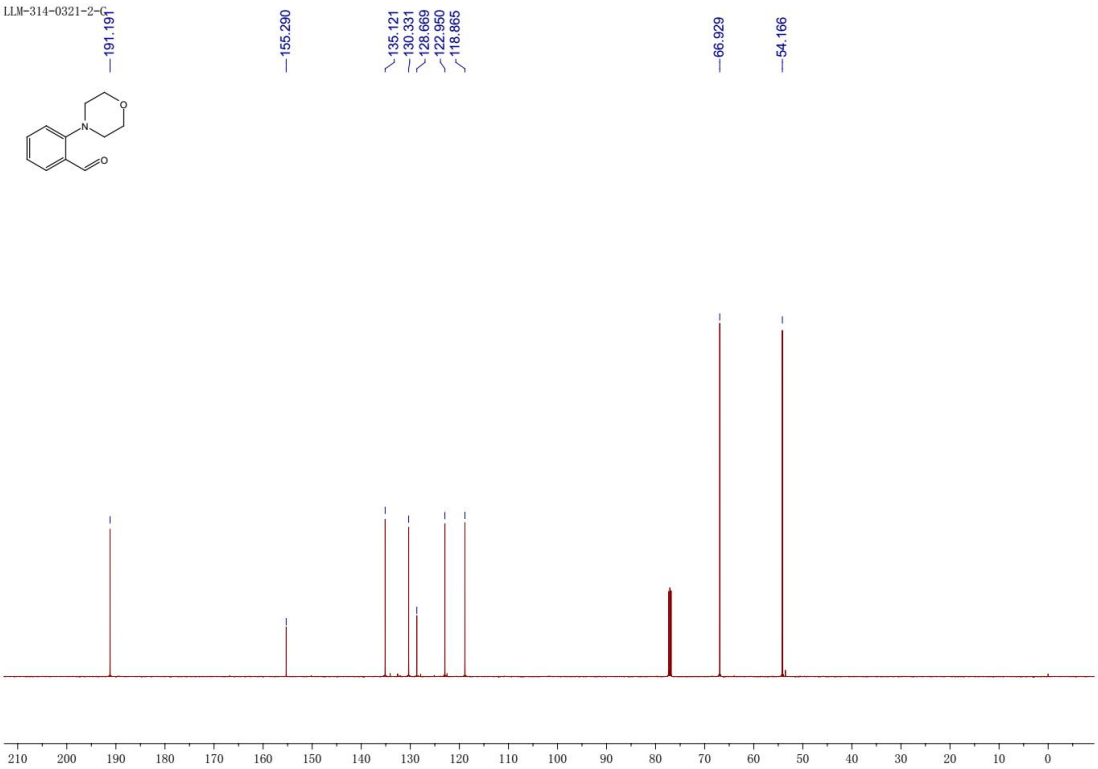


White solid. M.p. 188 – 190 °C. Yield: 50% (37.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, J = 7.7 Hz, 1H), 7.50 (d, J = 8.5 Hz, 1H), 7.32 – 7.16 (m, 3H), 6.82 – 6.75 (m, 3H), 4.20 (t, J = 6.5 Hz, 2H), 3.89 (s, 3H), 3.18 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.39, 137.41, 134.77, 131.67, 129.26, 128.27, 127.22, 126.93, 123.90, 123.11, 121.38, 109.86, 96.39, 92.63, 55.75, 40.15, 29.20. **HRMS** (ESI) calculated for $C_{17}H_{16}NO$ $(M+H)^+$: 250.1151, found: 250.1155.

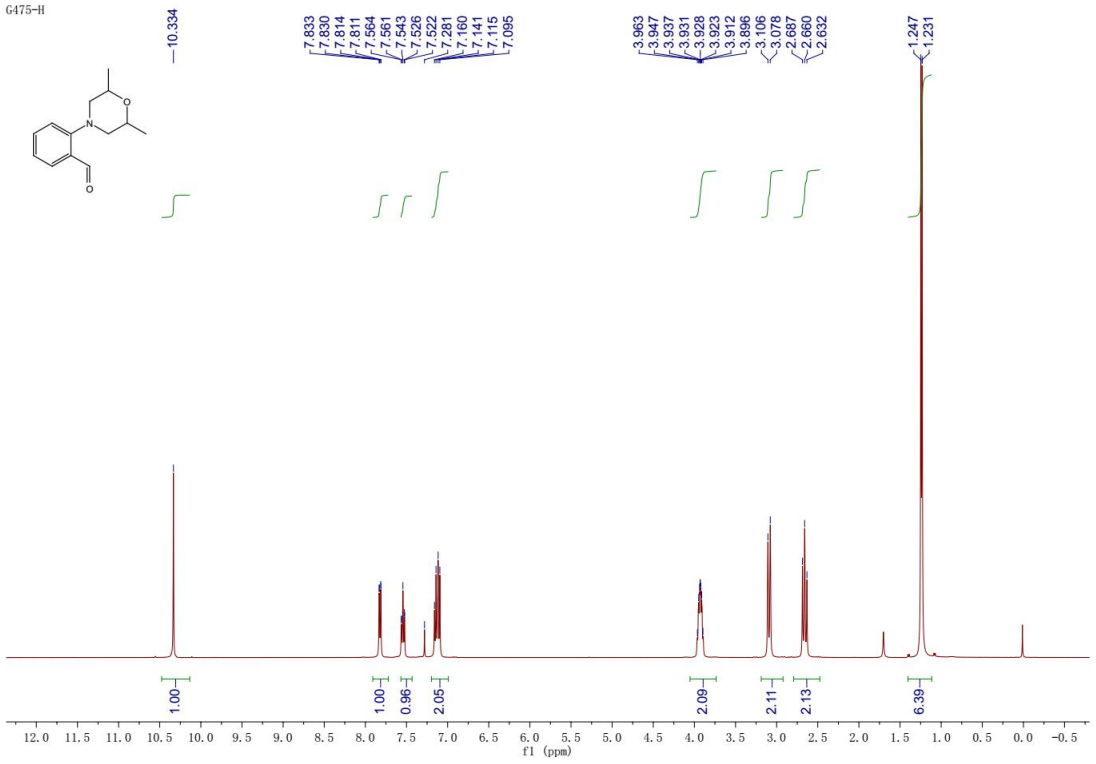
6. ^{1}H and ^{13}C NMR Spectra

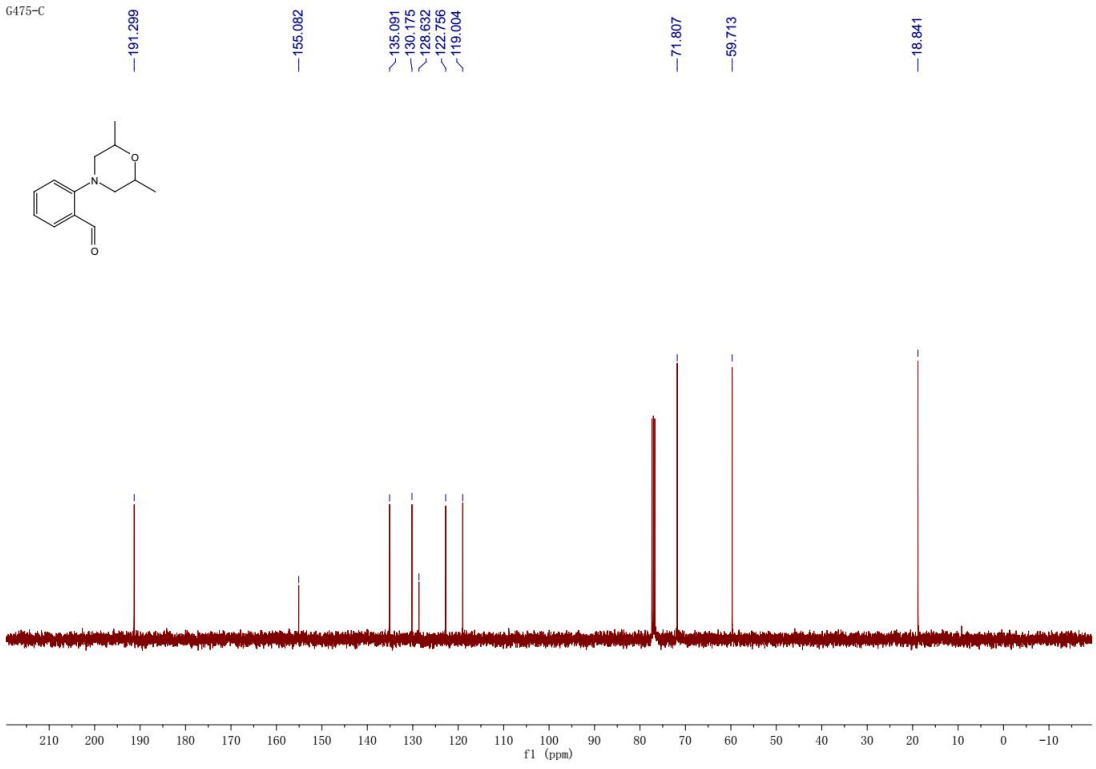
NMR of 1a



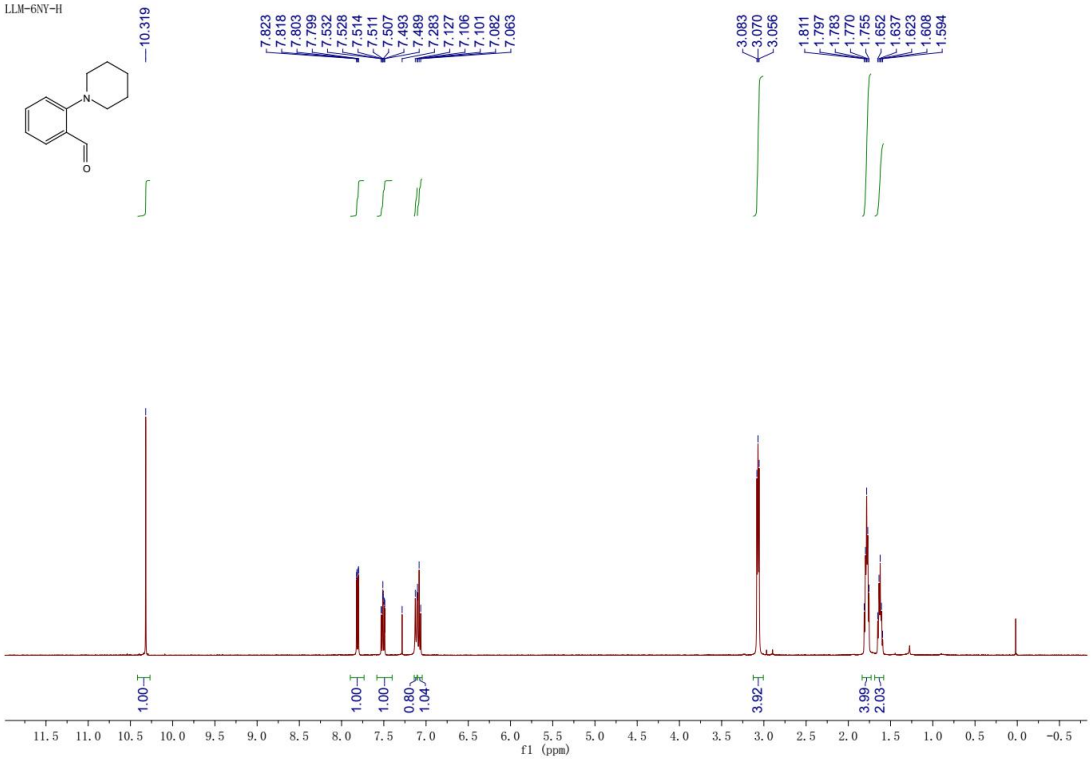


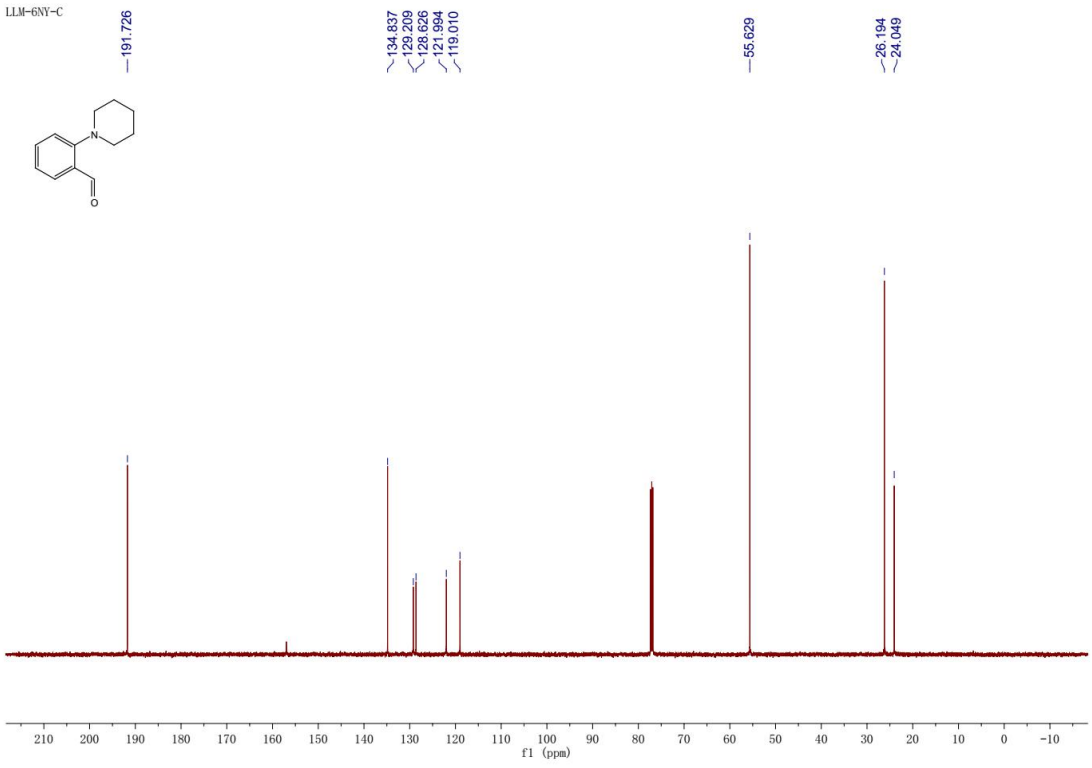
NMR of 1b


G475-H
10.334
7.833
7.830
7.814
7.811
7.564
7.561
7.543
7.526
7.522
7.281
7.160
7.141
7.115
7.095
3.963
3.947
3.937
3.931
3.928
3.923
3.912
3.896
3.106
3.078
2.687
2.660
2.632
1.247
1.231
1.00
1.00
0.96
2.05
2.09
2.11
2.13
6.39
f1 (ppm)

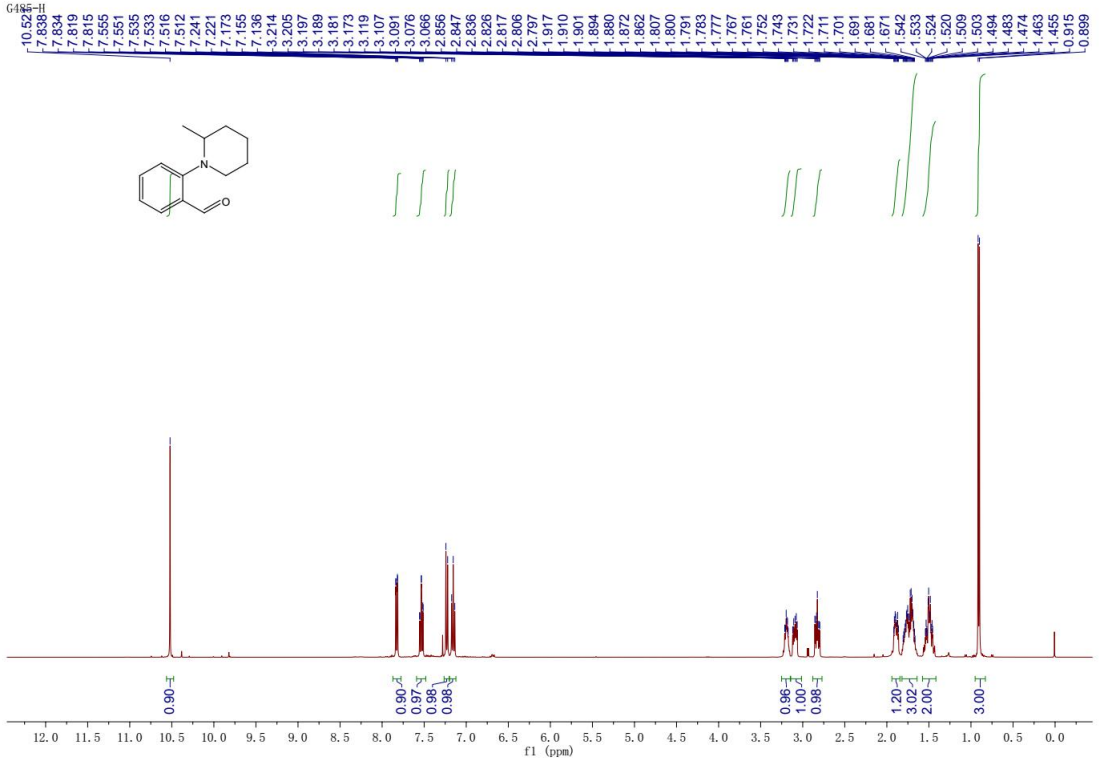

G475-C
191.299
155.082
135.091
130.175
128.632
122.756
119.004
71.807
59.713
18.841
f1 (ppm)

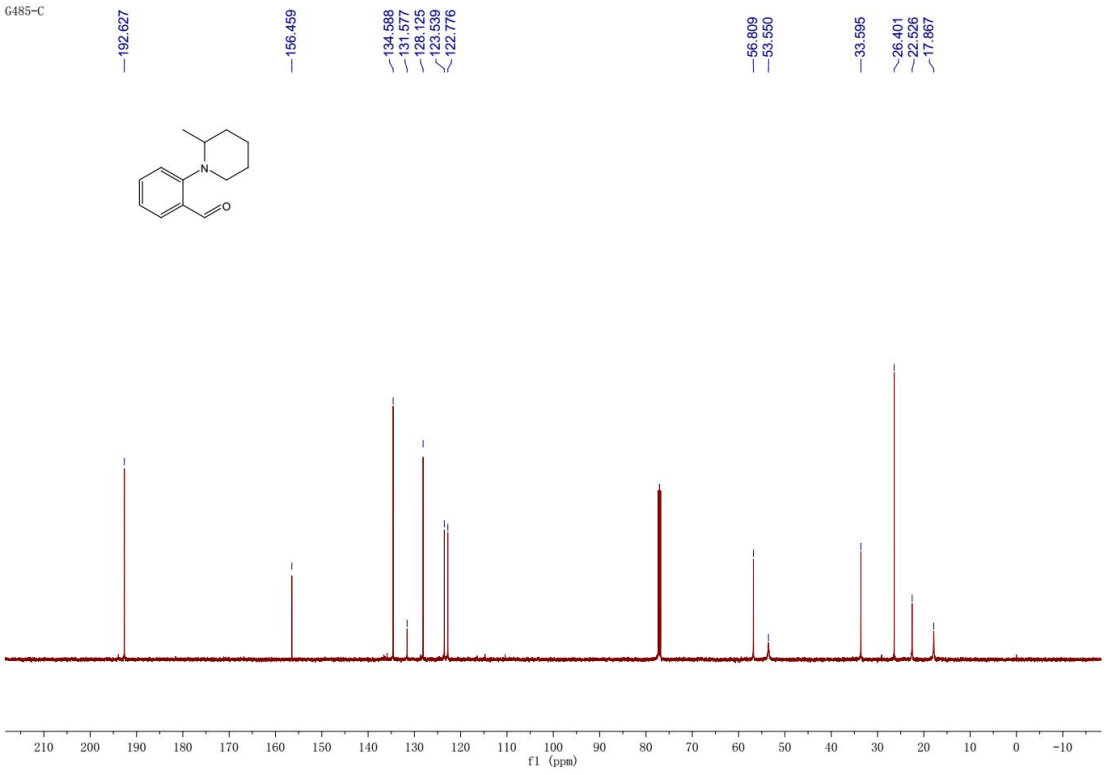
NMR of 1c


LLM-6NY-H
10.319
7.823
7.818
7.803
7.799
7.532
7.528
7.514
7.511
7.507
7.493
7.489
7.283
7.127
7.106
7.101
7.082
7.063
3.083
3.070
3.056
1.811
1.797
1.783
1.770
1.755
1.652
1.637
1.623
1.608
1.594
1.00
1.00
1.00
0.80
1.04
3.92
3.99
2.03
f1 (ppm)

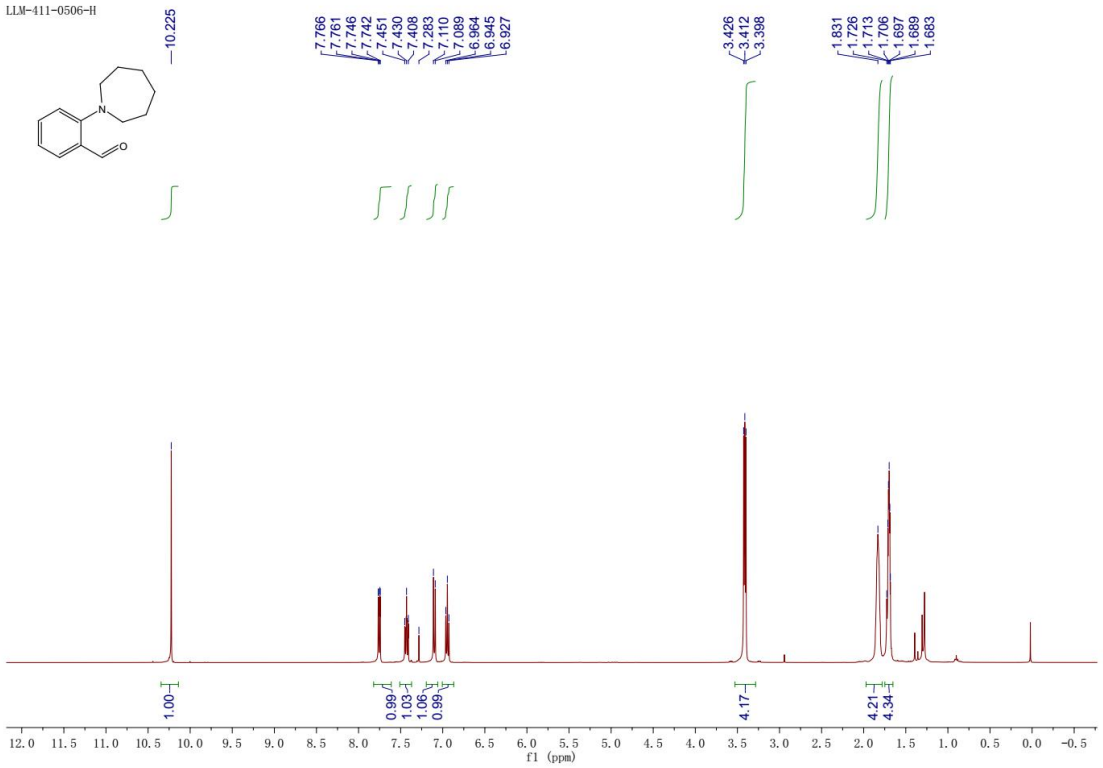

LLM-6NY-C
191.726
134.837
129.209
128.626
121.994
119.010
55.629
26.194
24.049
f1 (ppm)

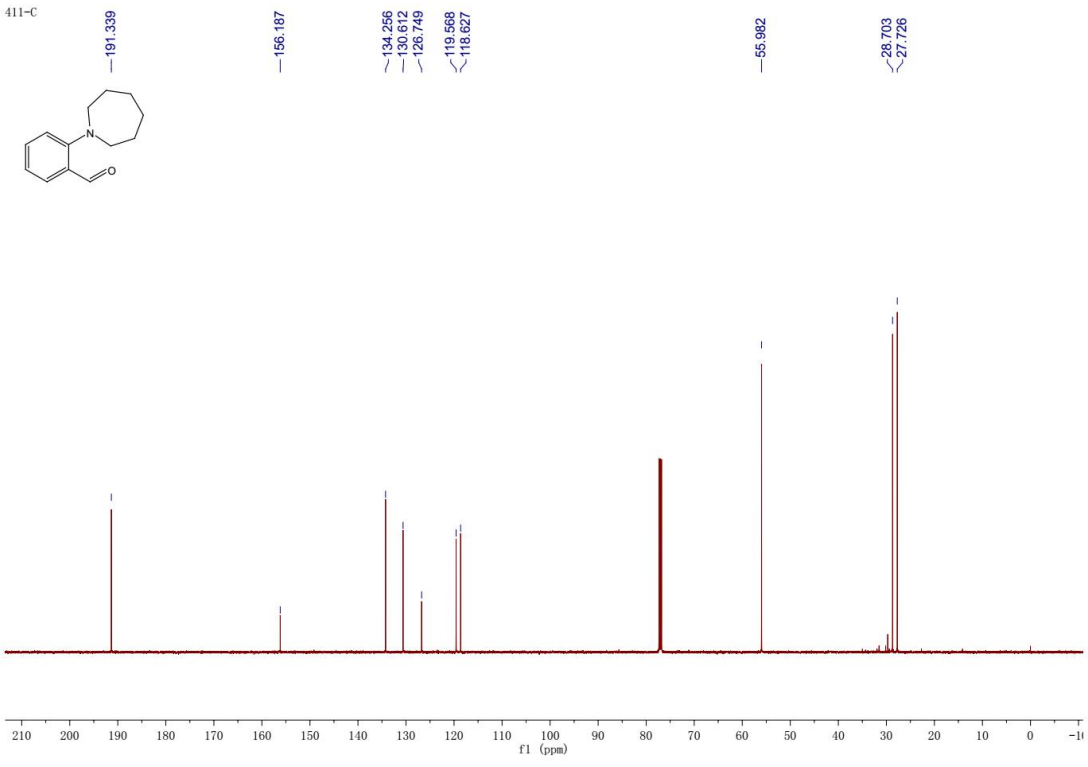
NMR of 1d


G485-H
10.522
7.838
7.834
7.819
7.815
7.555
7.551
7.535
7.533
7.516
7.512
7.241
7.221
7.173
7.155
7.136
3.214
3.205
3.197
3.189
3.181
3.173
3.119
3.107
3.091
3.076
3.066
2.856
2.847
2.836
2.826
2.817
2.806
2.797
1.917
1.910
1.901
1.894
1.880
1.872
1.862
1.807
1.800
1.791
1.783
1.777
1.767
1.761
1.752
1.743
1.731
1.722
1.711
1.701
1.691
1.681
1.671
1.542
1.533
1.524
1.520
1.509
1.503
1.494
1.483
1.474
1.463
1.455
0.915
0.899
0.90
0.90
0.97
0.98
0.98
0.96
1.00
0.98
1.20
3.02
2.00
3.00
f1 (ppm)

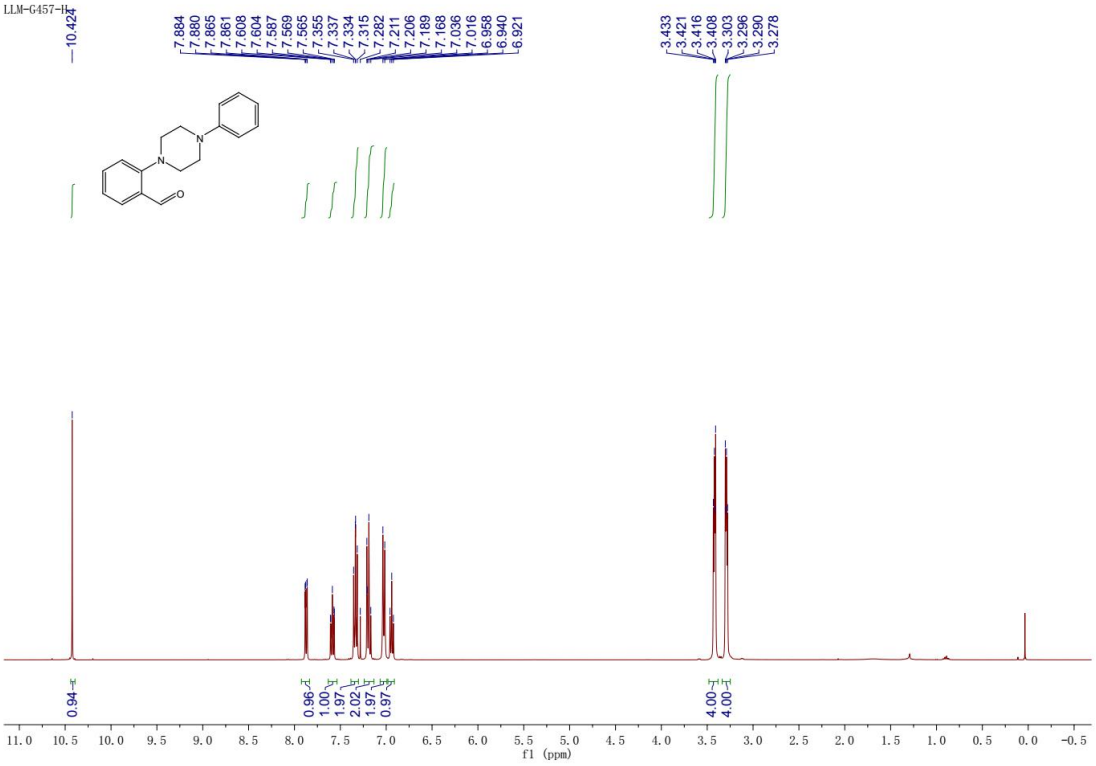

G485-C
192.627
156.459
134.588
131.577
128.125
123.539
122.776
56.809
53.550
33.595
26.401
22.526
17.867
f1 (ppm)

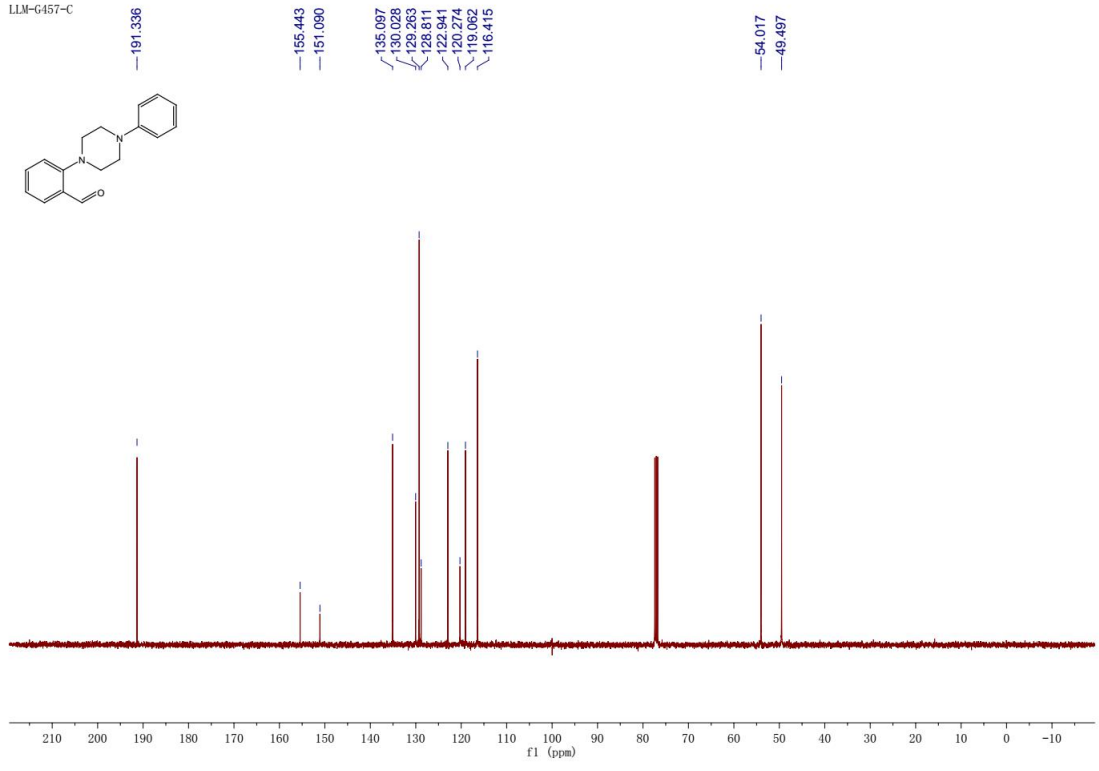
NMR of 1e


LLM-411-0506-H
10.225
7.766
7.761
7.746
7.742
7.451
7.430
7.408
7.283
7.110
7.089
6.964
6.945
6.927
3.426
3.412
3.398
1.831
1.726
1.713
1.706
1.697
1.689
1.683
1.00
0.99
1.03
1.06
0.99
4.17
4.21
4.34
f1 (ppm)

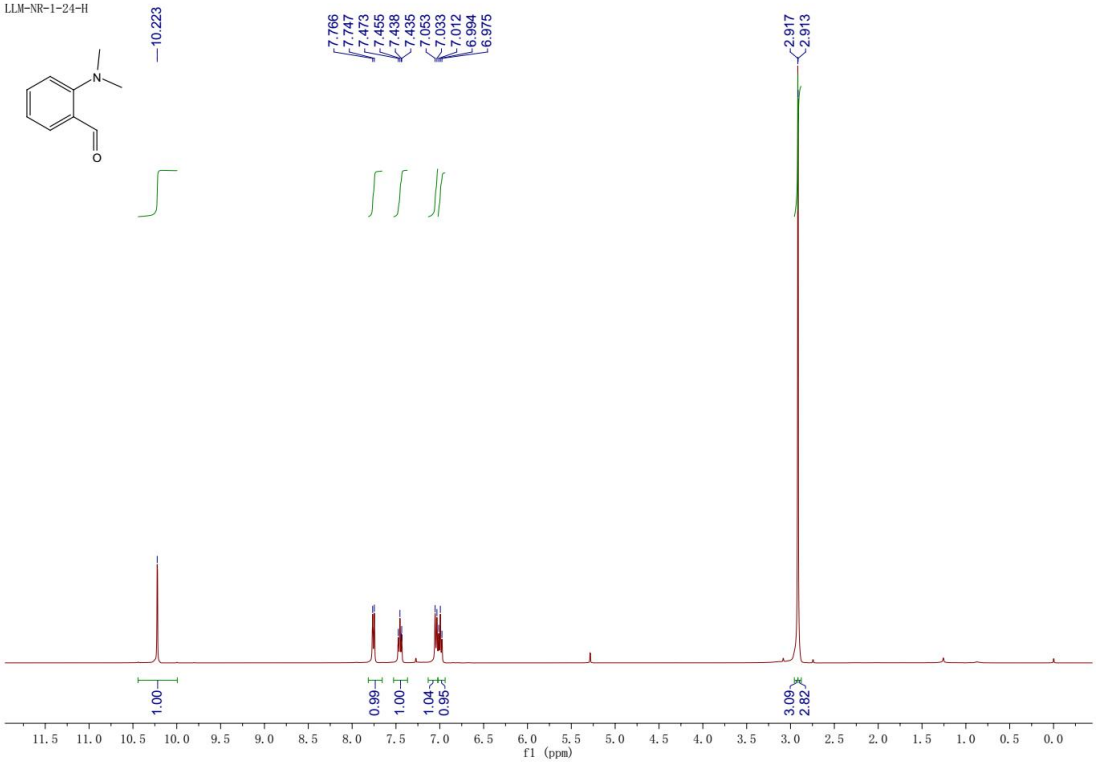

411-C
191.339
156.187
134.256
130.612
126.749
119.568
118.627
55.982
28.703
27.726
f1 (ppm)

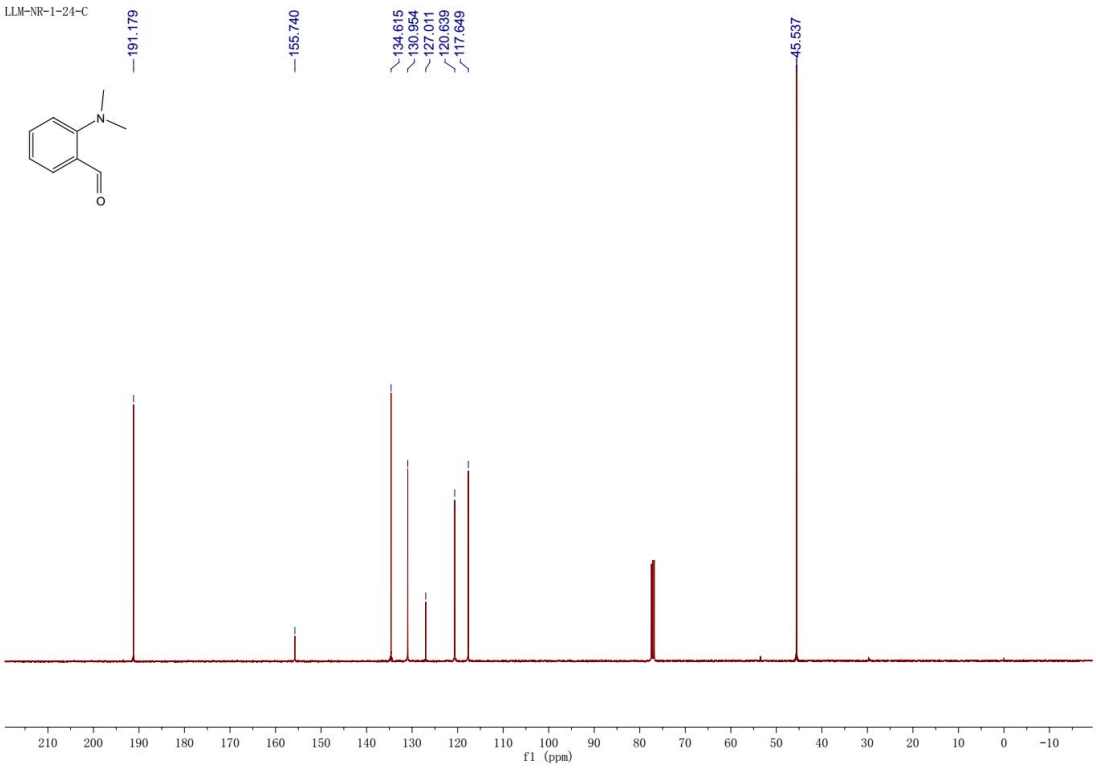
NMR of 1f


LLM-G457-H
10.424
7.884
7.880
7.865
7.861
7.608
7.604
7.587
7.569
7.565
7.355
7.337
7.334
7.315
7.282
7.211
7.206
7.189
7.168
7.036
7.016
6.958
6.940
6.921
3.433
3.421
3.416
3.408
3.303
3.296
3.290
3.278
0.94
0.96
1.00
1.97
2.02
1.97
0.97
4.00
4.00
f1 (ppm)

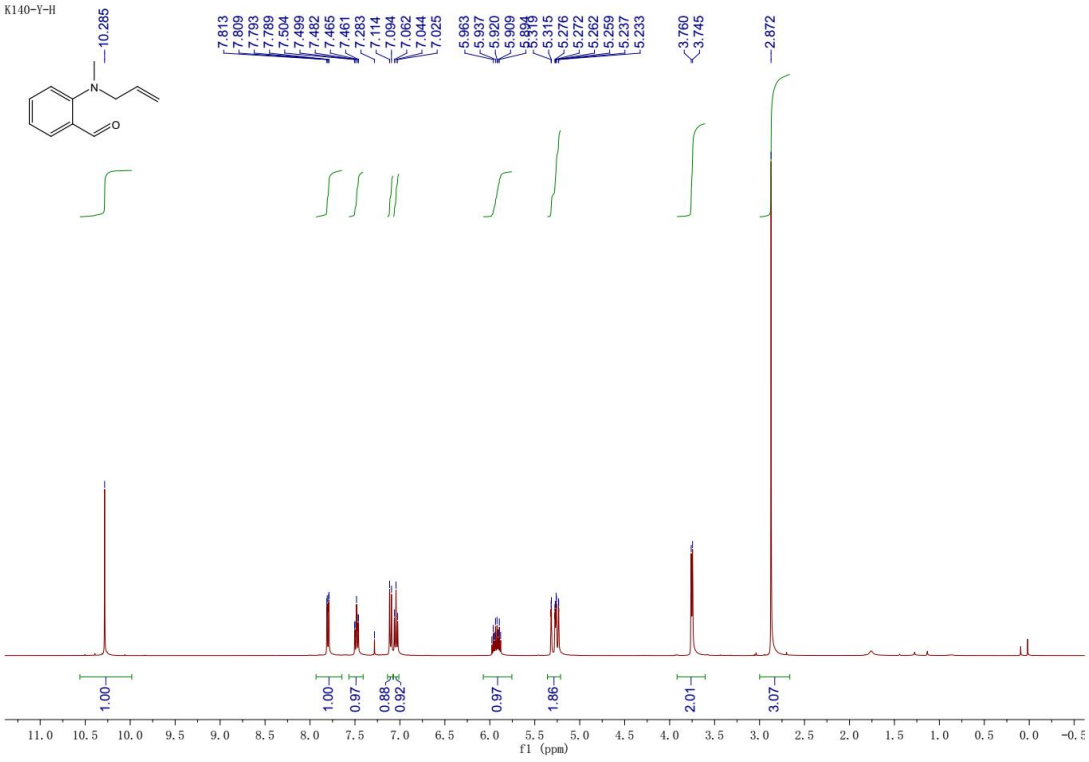

LLM-G457-C
191.336
155.443
151.090
135.097
130.028
129.263
128.811
122.941
120.274
119.062
116.415
54.017
49.497
f1 (ppm)

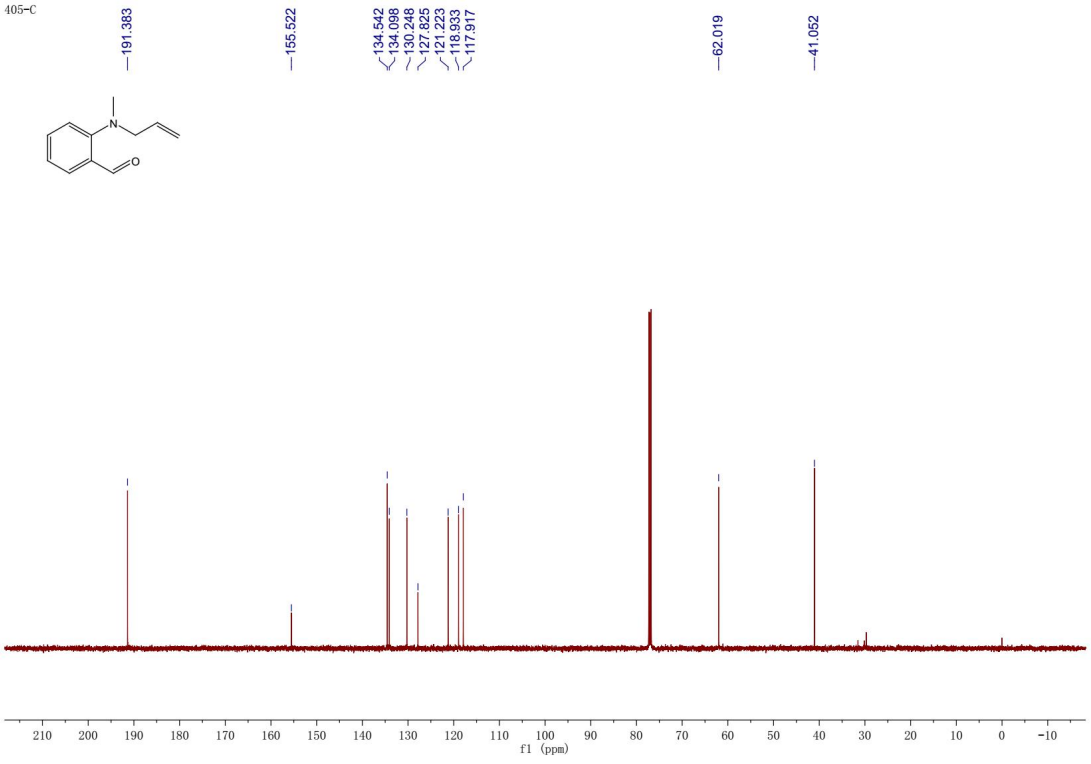
NMR of 1g


LLM-NR-1-24-H
10.223
7.766
7.747
7.473
7.455
7.438
7.435
7.053
7.033
7.012
6.994
6.975
2.917
2.913
1.00
0.99
1.00
1.04
0.95
3.09
2.82
f1 (ppm)

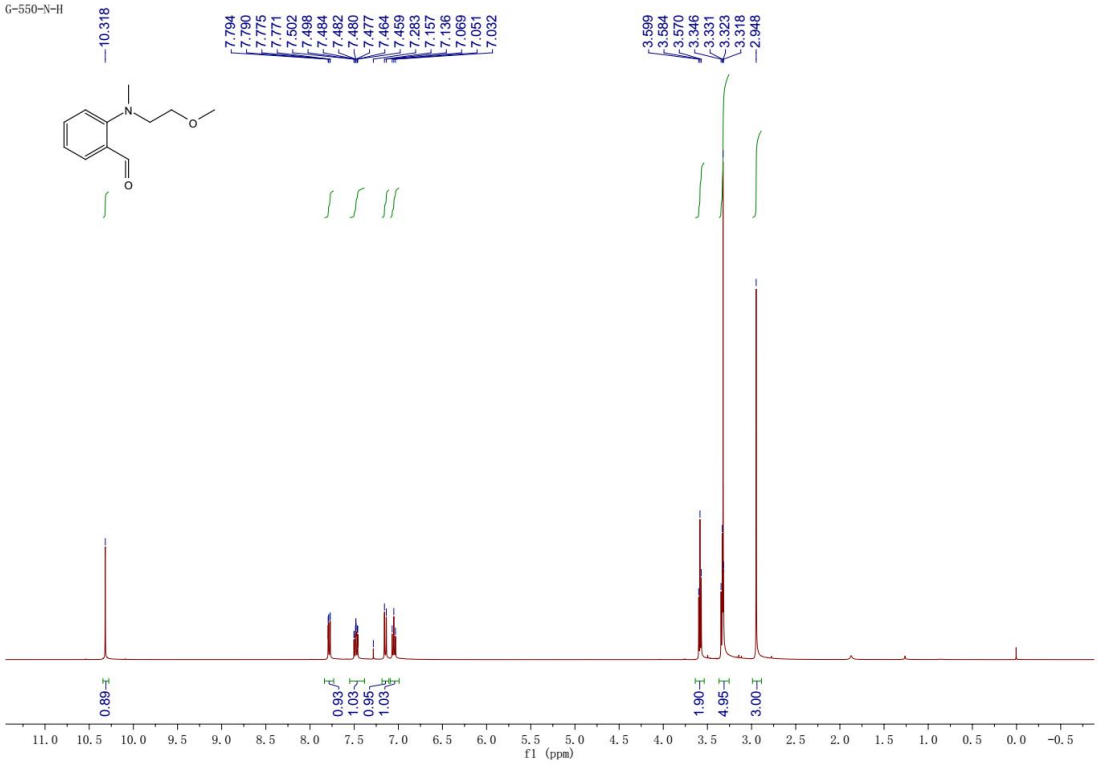

LLM-NR-1-24-C
191.179
155.740
134.615
130.964
127.011
120.639
117.649
45.537
f1 (ppm)

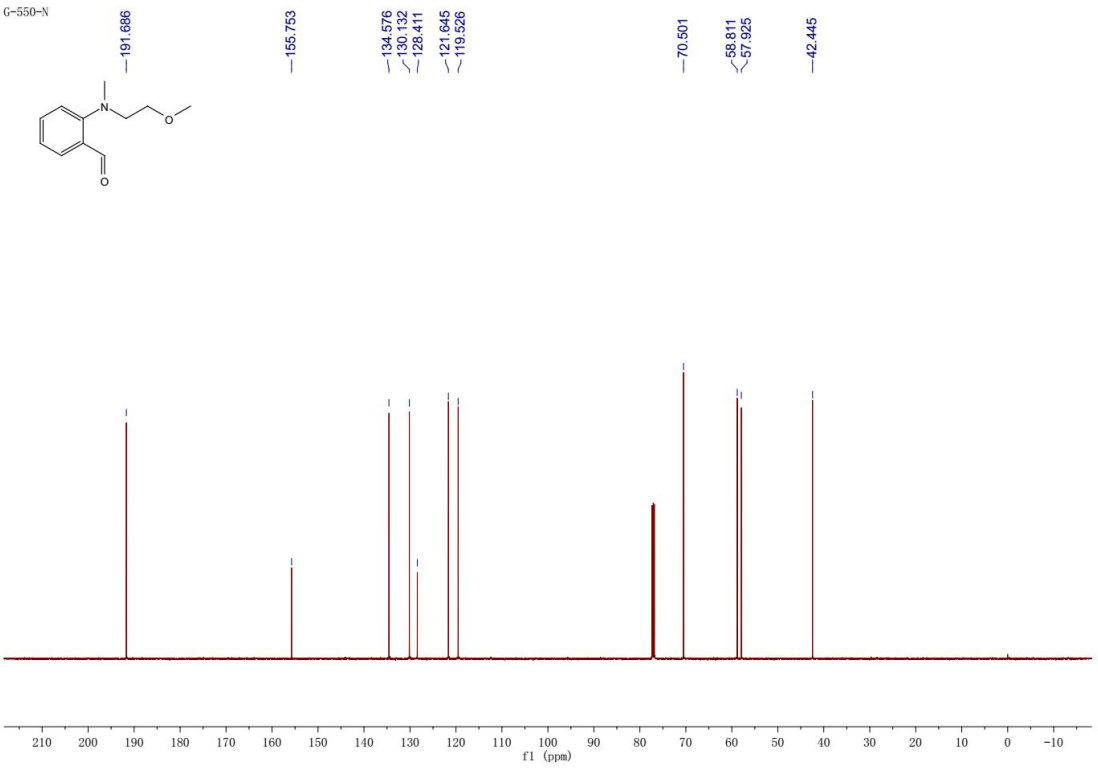
NMR of 1h


K140-Y-H
10.285
7.813
7.809
7.793
7.789
7.504
7.499
7.482
7.465
7.461
7.283
7.114
7.094
7.062
7.044
7.025
5.963
5.937
5.920
5.909
5.315
5.276
5.272
5.262
5.259
5.237
5.233
3.760
3.745
2.872
1.00
1.00
0.97
0.88
0.92
0.97
1.86
2.01
3.07
f1 (ppm)

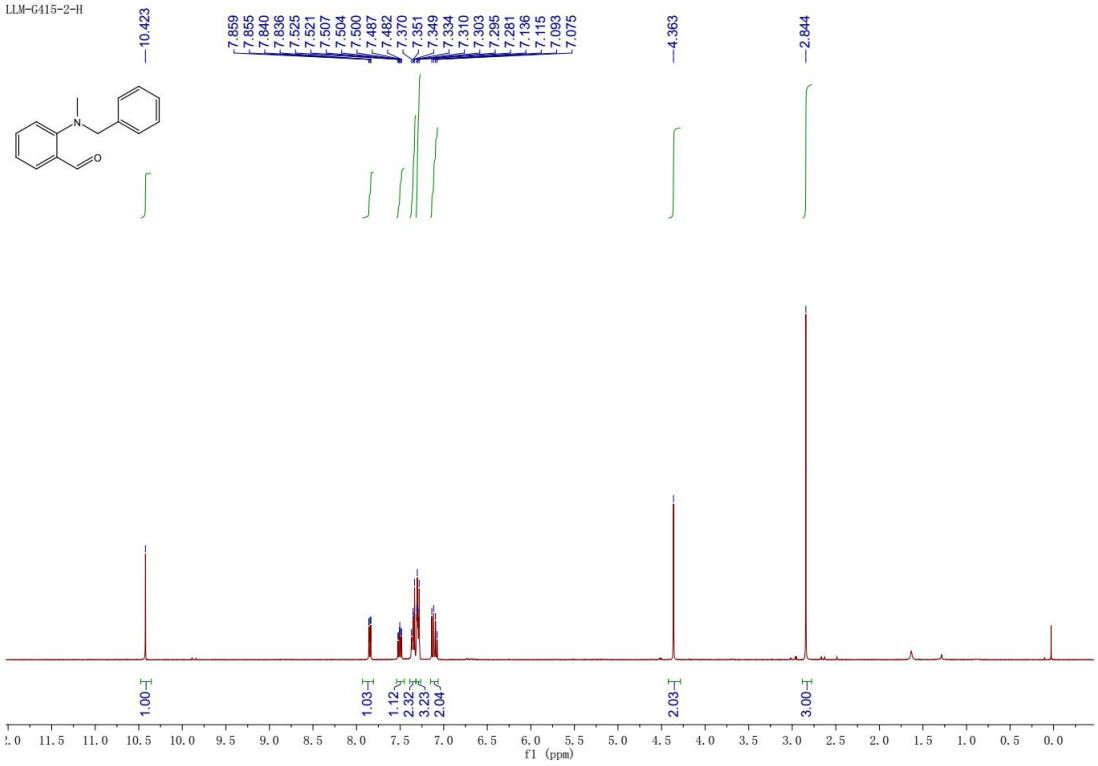

405-C
191.383
155.522
134.542
134.098
130.248
127.825
121.223
118.933
117.917
62.019
41.052
f1 (ppm)

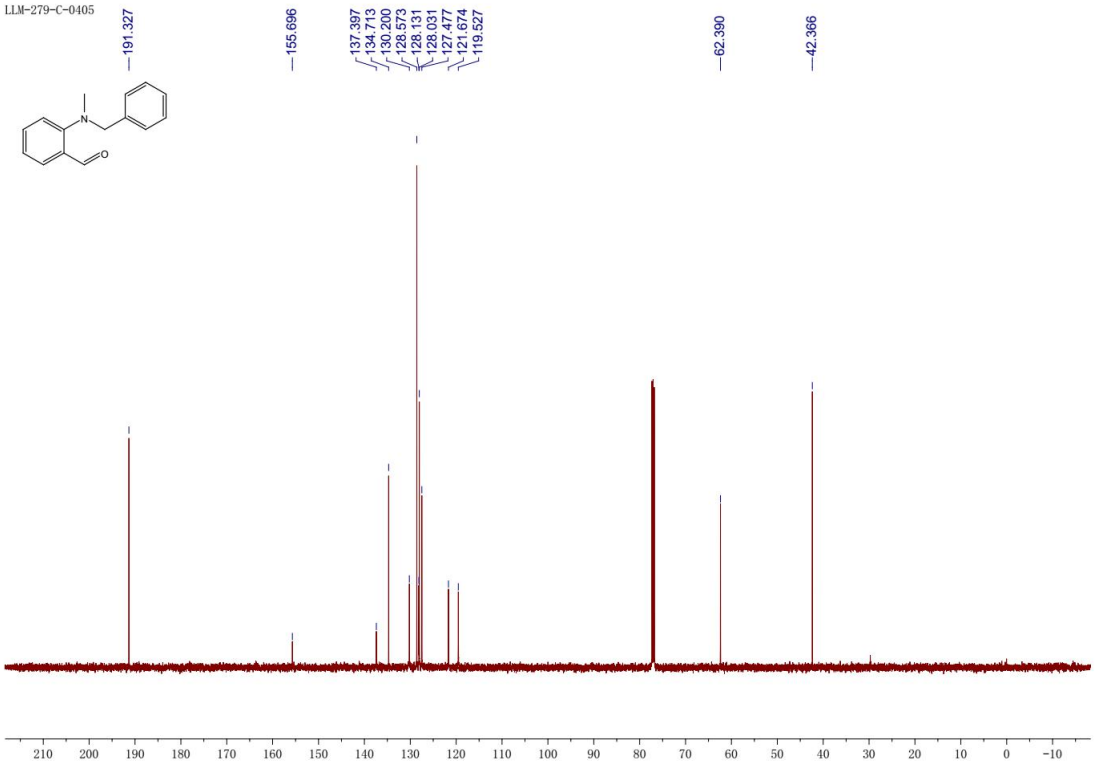
NMR of 1i


G-550-N-H
10.318
7.794
7.790
7.775
7.771
7.502
7.498
7.484
7.482
7.480
7.477
7.464
7.459
7.283
7.157
7.136
7.069
7.051
7.032
3.599
3.584
3.570
3.346
3.331
3.323
3.318
2.948
0.89
0.93
1.03
0.95
1.03
1.90
4.95
3.00
f1 (ppm)

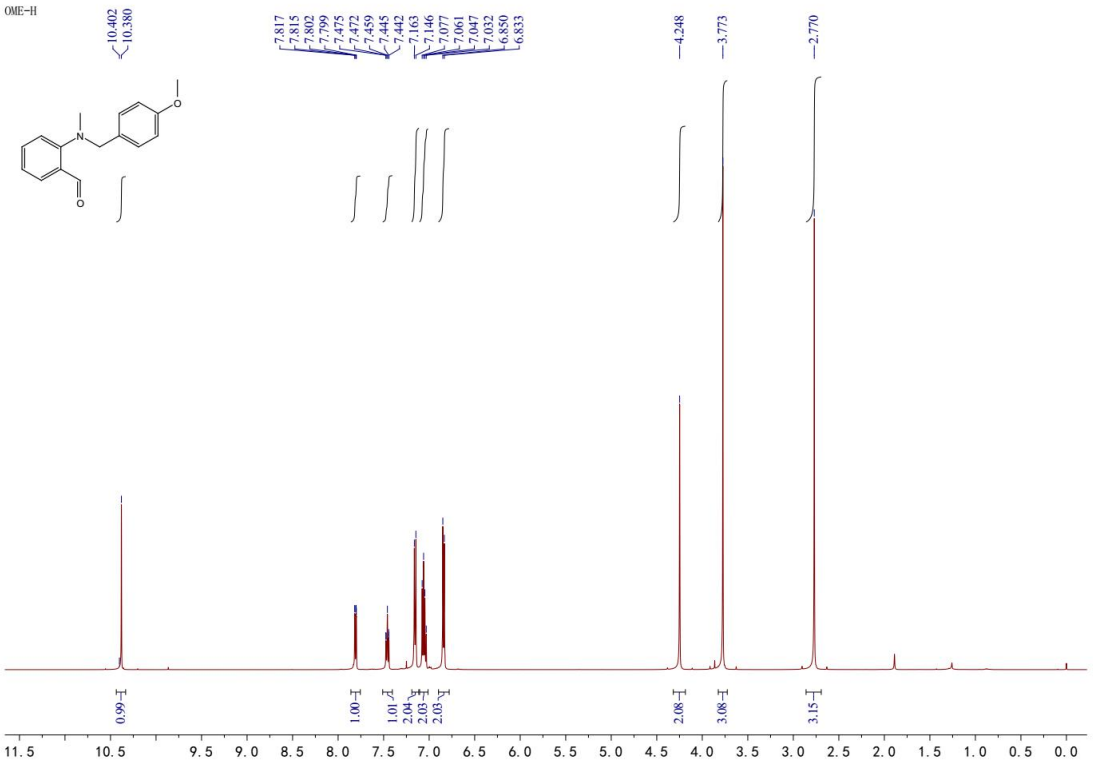

G-550-N
191.686
155.753
134.576
130.132
128.411
121.645
119.526
70.501
58.811
57.925
42.445
f1 (ppm)

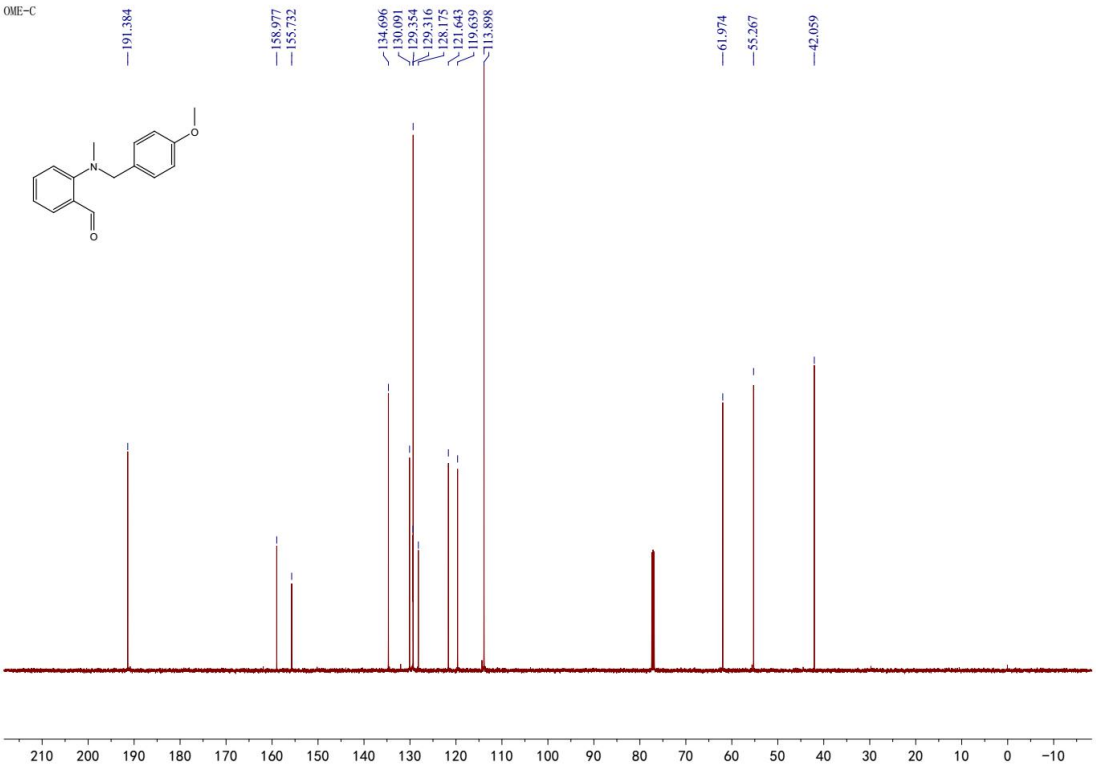
NMR of 1j


LLM-G415-2-H
10.423
7.859
7.855
7.840
7.836
7.525
7.521
7.507
7.504
7.500
7.487
7.482
7.370
7.351
7.349
7.334
7.310
7.303
7.295
7.281
7.136
7.115
7.093
7.075
4.363
2.844
1.00
1.03
1.12
2.32
3.23
2.04
2.03
3.00
f1 (ppm)

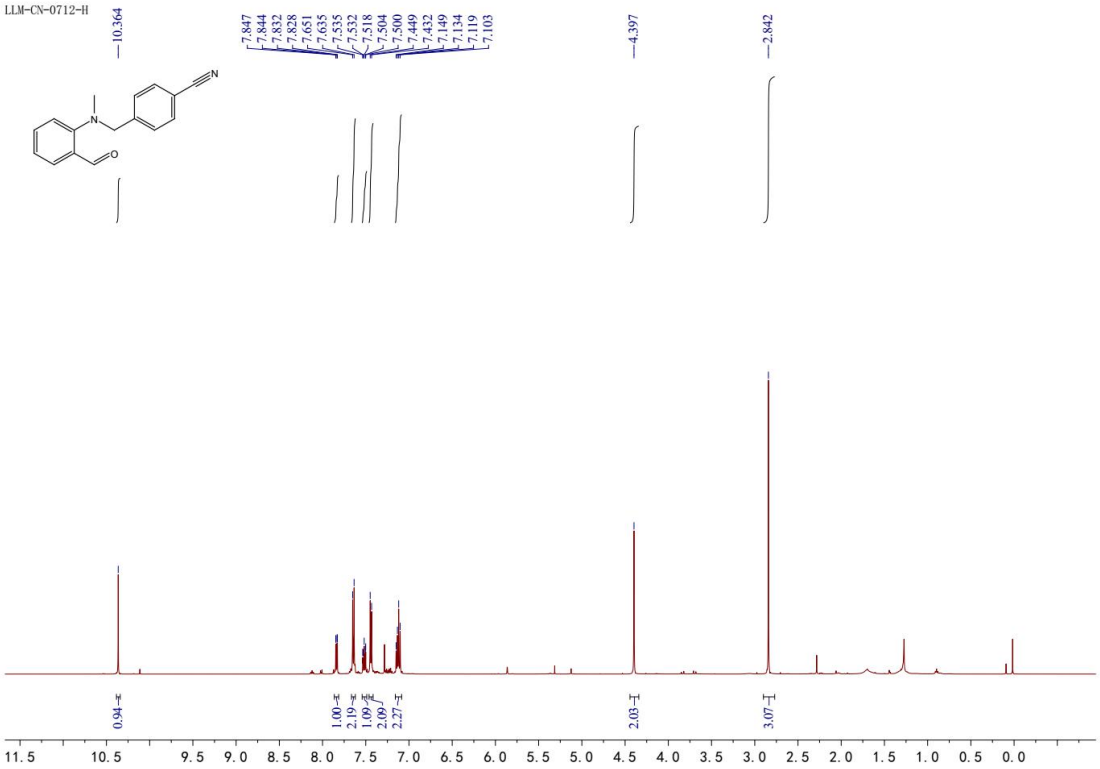

LLM-279-C-0405
191.327
155.696
137.397
134.713
130.200
128.573
128.131
128.031
127.477
121.674
119.527
62.390
42.366

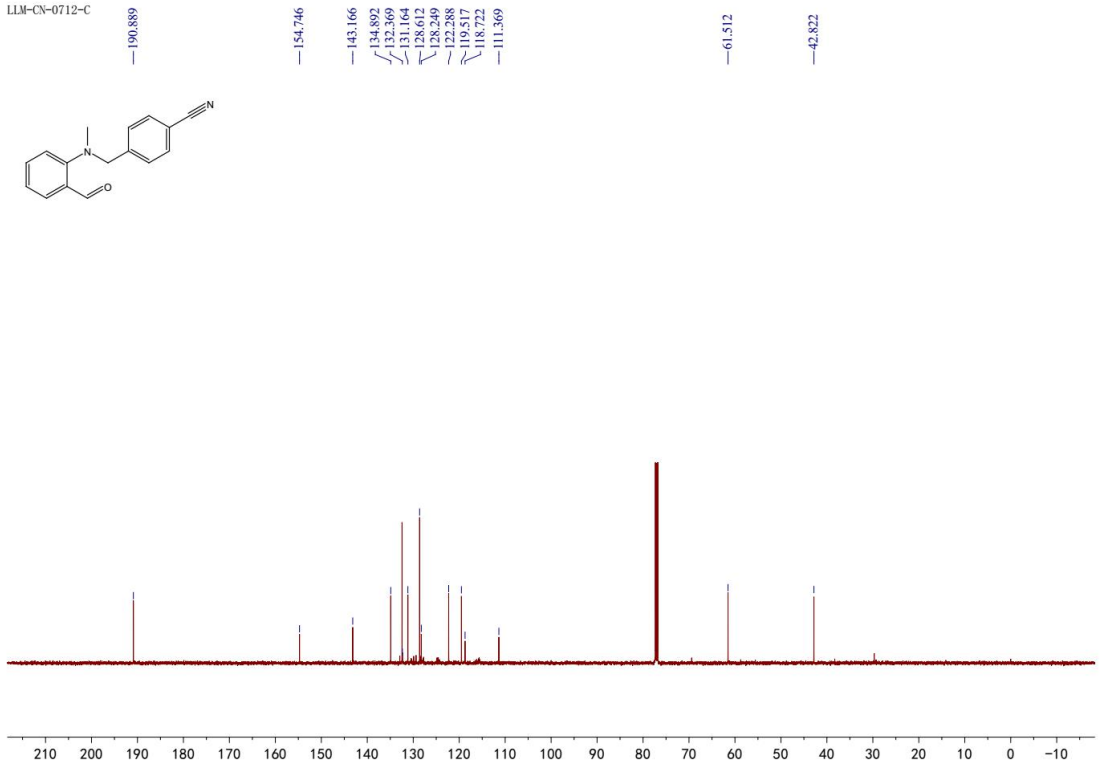
NMR of 1k


OME-H
10.402
10.380
7.817
7.815
7.802
7.799
7.475
7.472
7.459
7.445
7.442
7.163
7.146
7.077
7.061
7.047
7.032
6.850
6.833
4.248
3.773
2.770
0.99
1.00
1.01
2.04
2.03
2.03
2.08
3.08
3.15

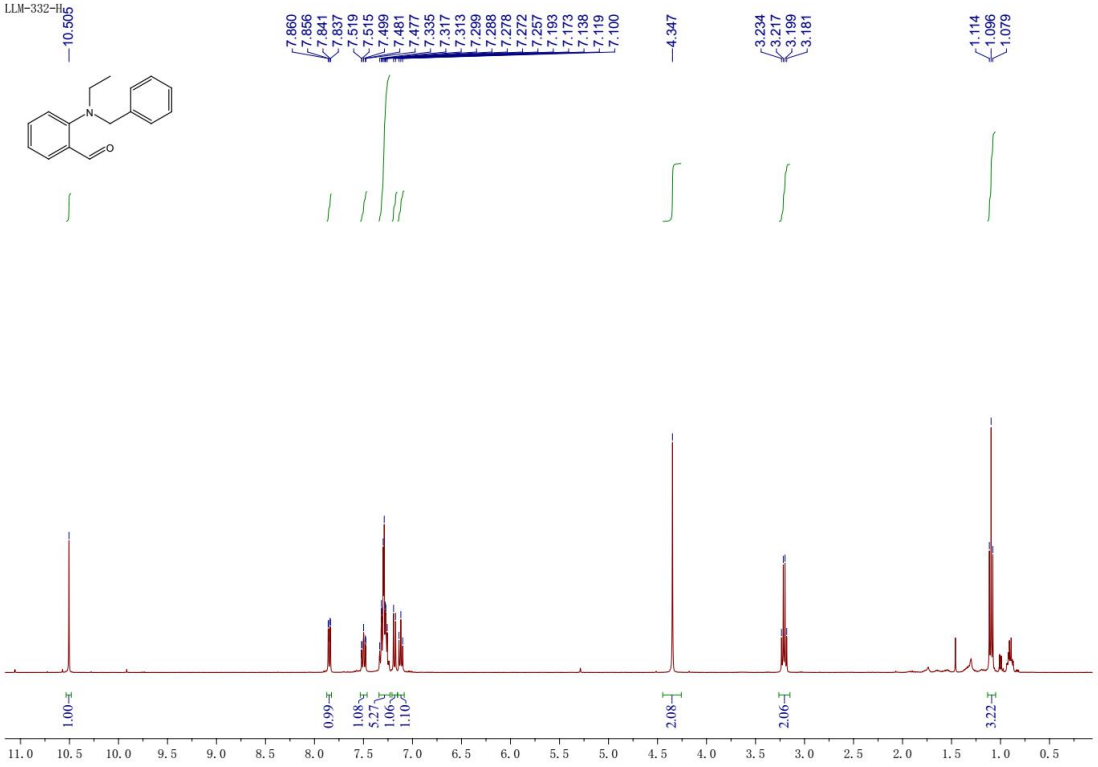

OME-C
191.384
158.977
155.732
134.696
130.091
129.354
129.316
128.175
121.643
119.639
113.898
61.974
55.267
42.059

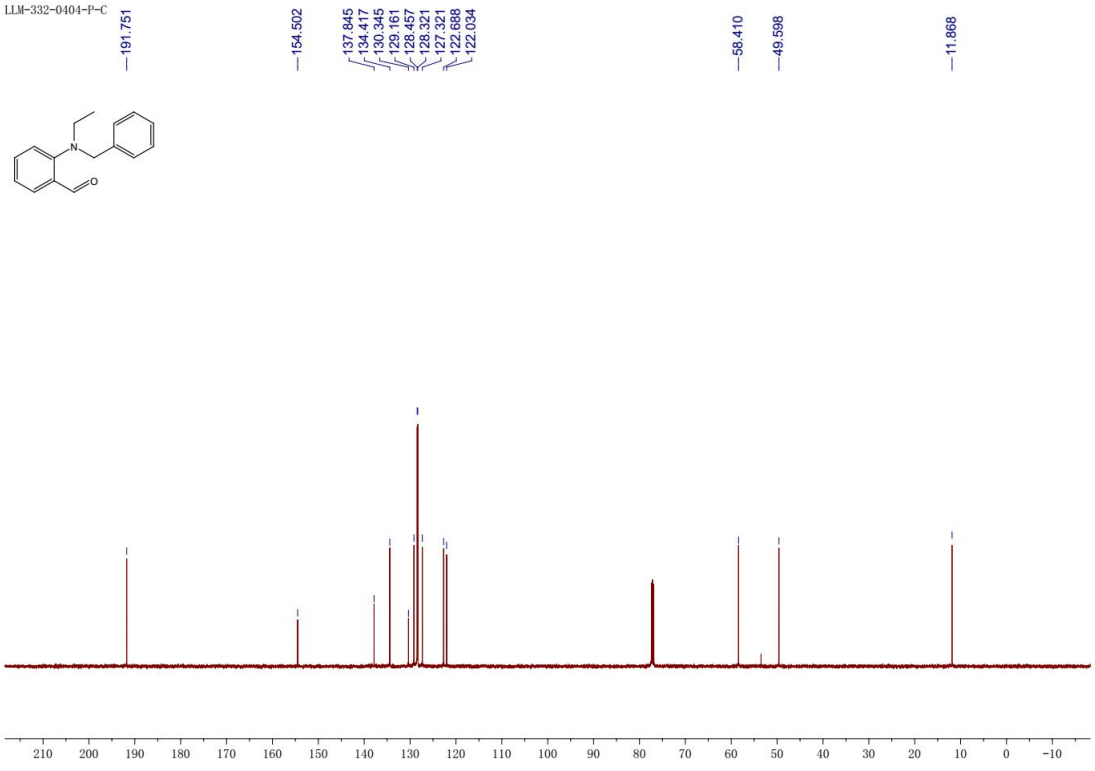
NMR of 1l


LLM-CN-0712-H
10.364
7.847
7.844
7.832
7.828
7.651
7.635
7.535
7.532
7.518
7.504
7.500
7.449
7.432
7.149
7.134
7.119
7.103
4.397
2.842
0.94
1.00
2.19
1.09
2.09
2.27
2.03
3.07

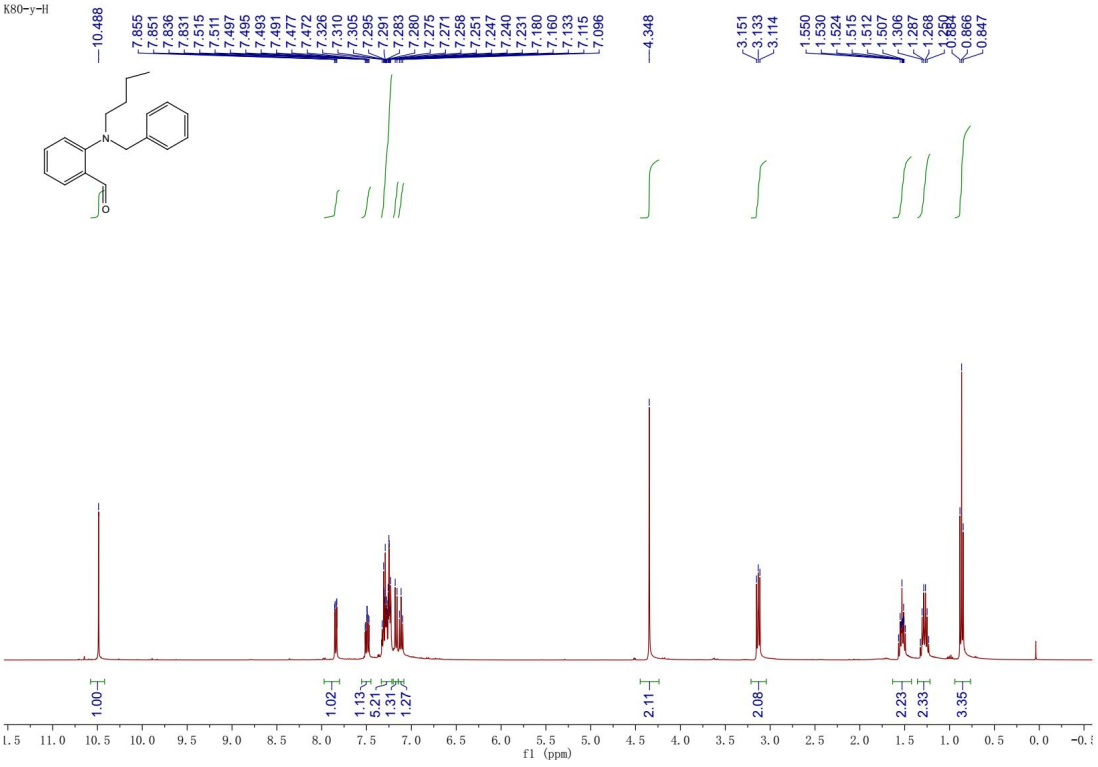

LLM-CN-0712-C
190.889
154.746
143.166
134.892
132.369
131.164
128.612
128.249
122.288
119.517
118.722
111.369
61.512
42.822

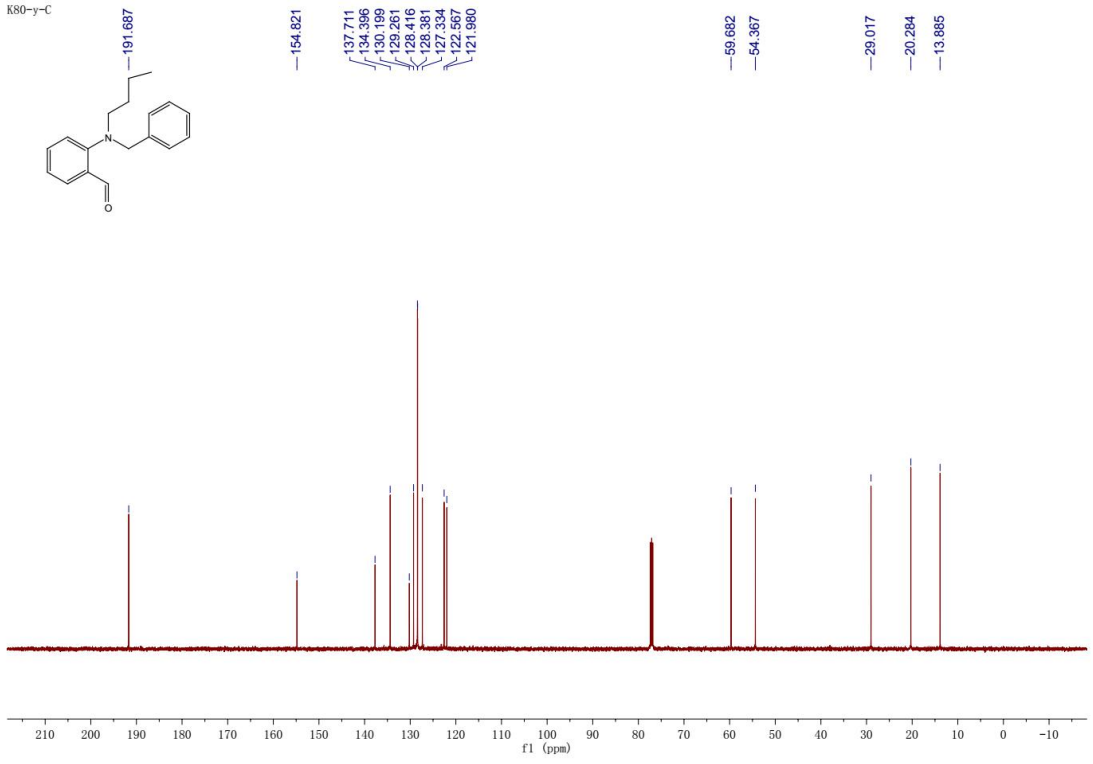
NMR of 1m


LLM-332-H
10.505
7.860
7.856
7.841
7.837
7.519
7.515
7.499
7.481
7.477
7.335
7.317
7.313
7.299
7.288
7.278
7.272
7.257
7.193
7.173
7.138
7.119
7.100
4.347
3.234
3.217
3.199
3.181
1.114
1.096
1.079
1.00
0.99
1.08
5.27
1.06
1.10
2.08
2.06
3.22

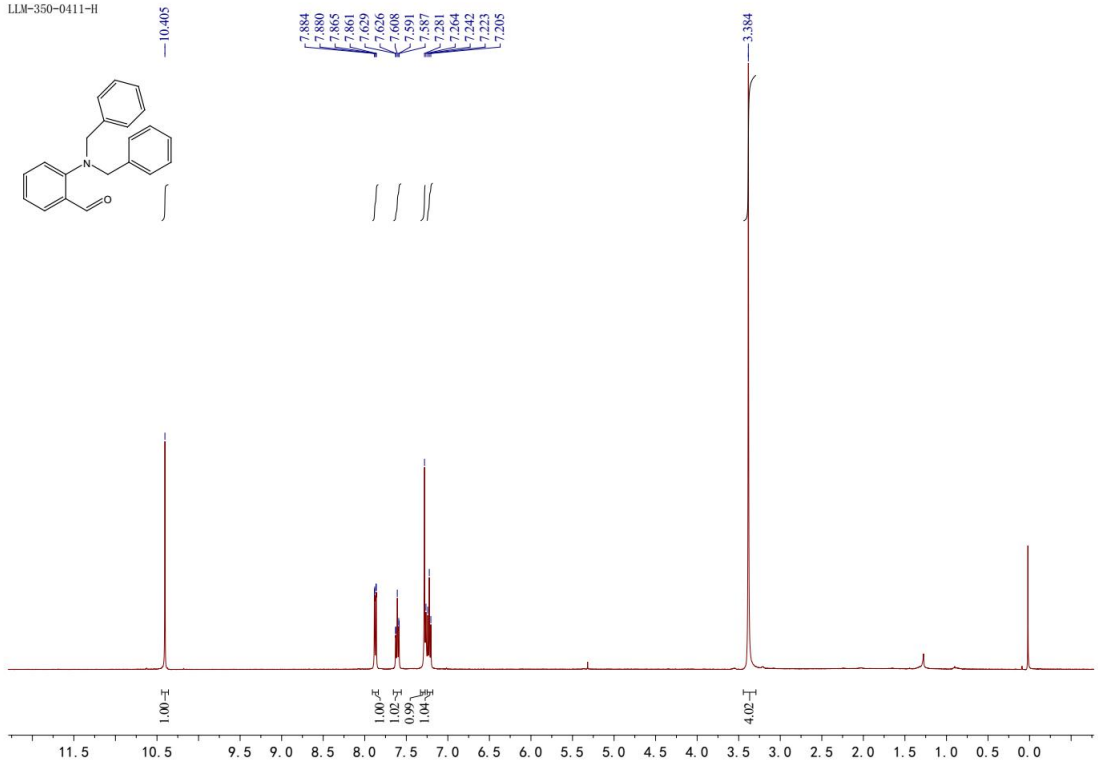

LLM-332-0404-P-C
191.751
154.502
137.845
134.417
130.345
129.161
128.457
128.321
127.321
122.688
122.034
58.410
49.598
11.868

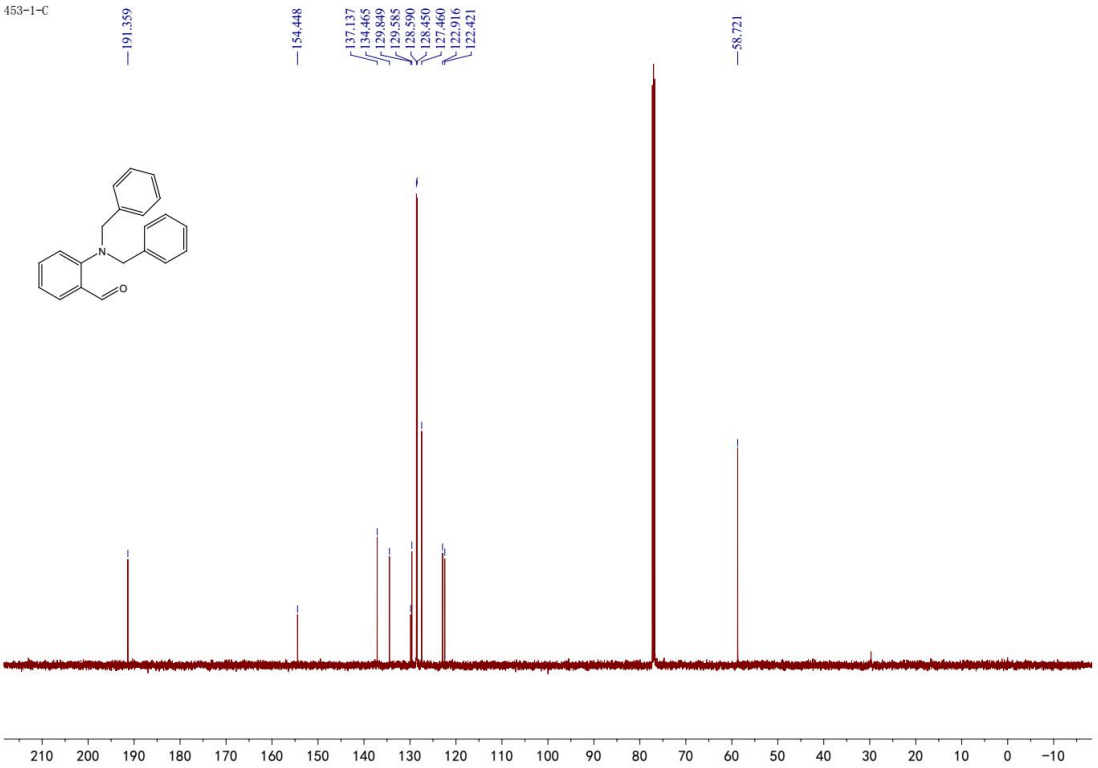
NMR of 1n


K80-y-H
10.488
7.855
7.851
7.836
7.831
7.515
7.511
7.497
7.495
7.493
7.491
7.477
7.472
7.326
7.310
7.305
7.295
7.291
7.283
7.280
7.275
7.271
7.258
7.251
7.247
7.240
7.231
7.180
7.160
7.133
7.115
7.096
4.348
3.151
3.133
3.114
1.550
1.530
1.524
1.515
1.512
1.507
1.306
1.287
1.268
0.884
0.866
0.847
1.00
1.02
1.13
5.21
1.31
1.27
2.11
2.08
2.23
2.33
3.35
f1 (ppm)

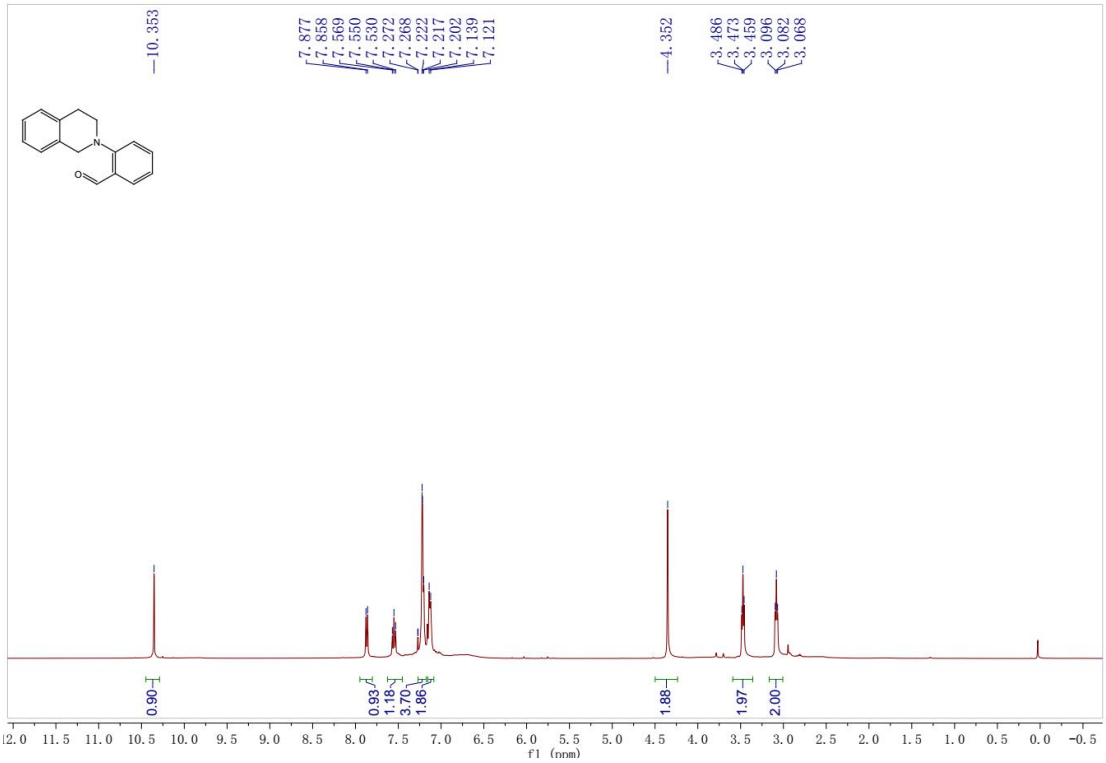

K80-y-C
191.687
154.821
137.711
134.396
130.199
129.261
128.416
128.381
127.334
122.567
121.980
59.682
54.367
29.017
20.284
13.885
f1 (ppm)

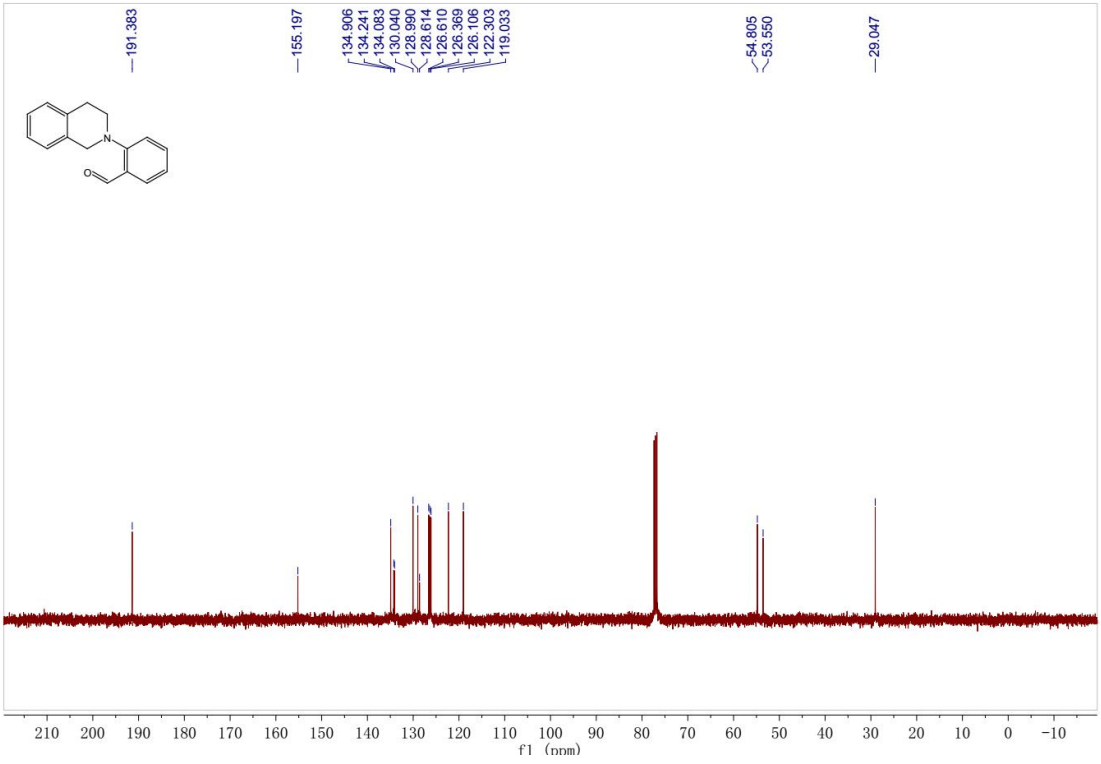
NMR of 1o


LLM-350-0411-H
10.405
7.884
7.880
7.865
7.861
7.629
7.626
7.608
7.591
7.587
7.281
7.264
7.242
7.223
7.205
3.384
1.00
1.00
1.02
0.99
1.04
4.02
11.5
10.5
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

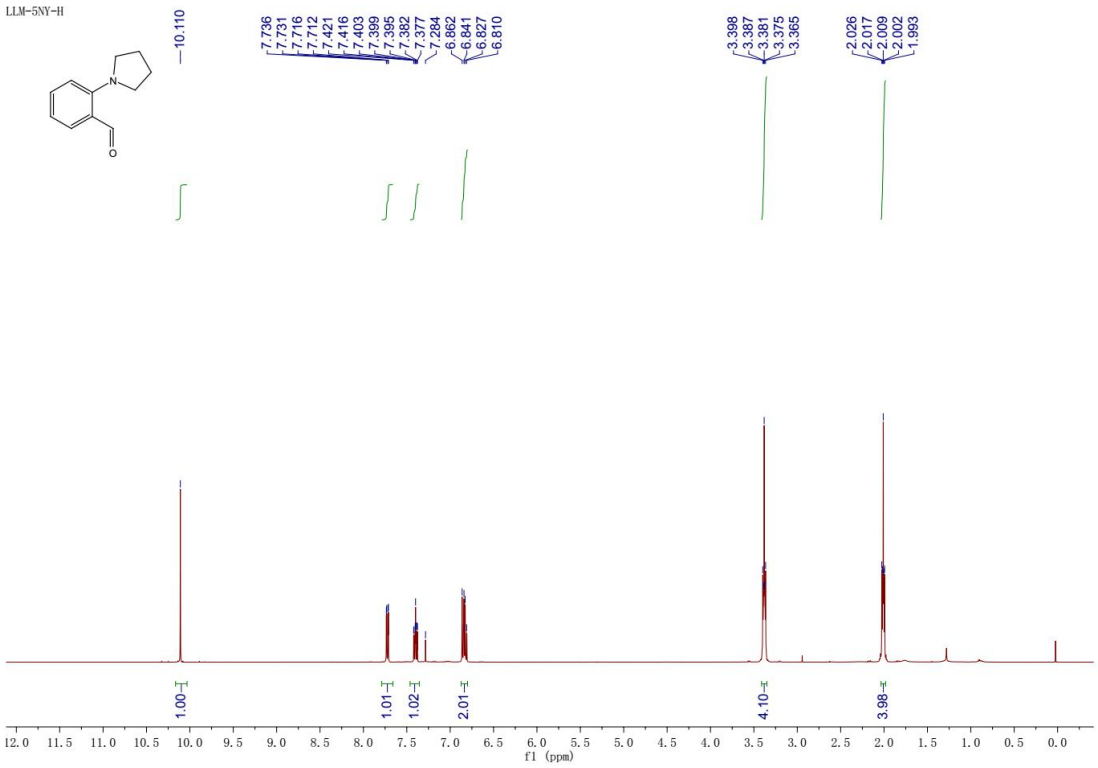

453-1-C
191.359
154.448
137.137
134.465
129.849
129.585
128.590
128.450
127.460
122.916
122.421
58.721
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

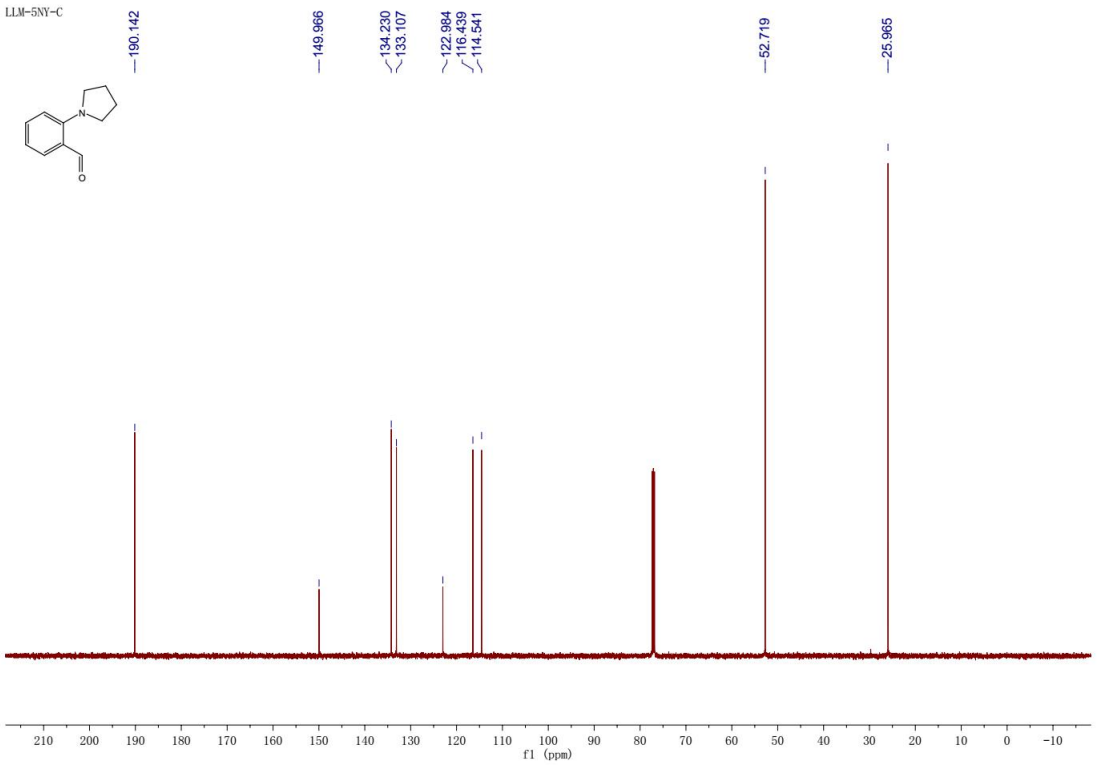
NMR of 1p


10.353
7.877
7.858
7.569
7.550
7.530
7.272
7.268
7.222
7.217
7.202
7.139
7.121
4.352
3.486
3.473
3.459
3.096
3.082
3.068
0.90
0.93
1.18
3.70
1.86
1.88
1.97
2.00
f1 (ppm)

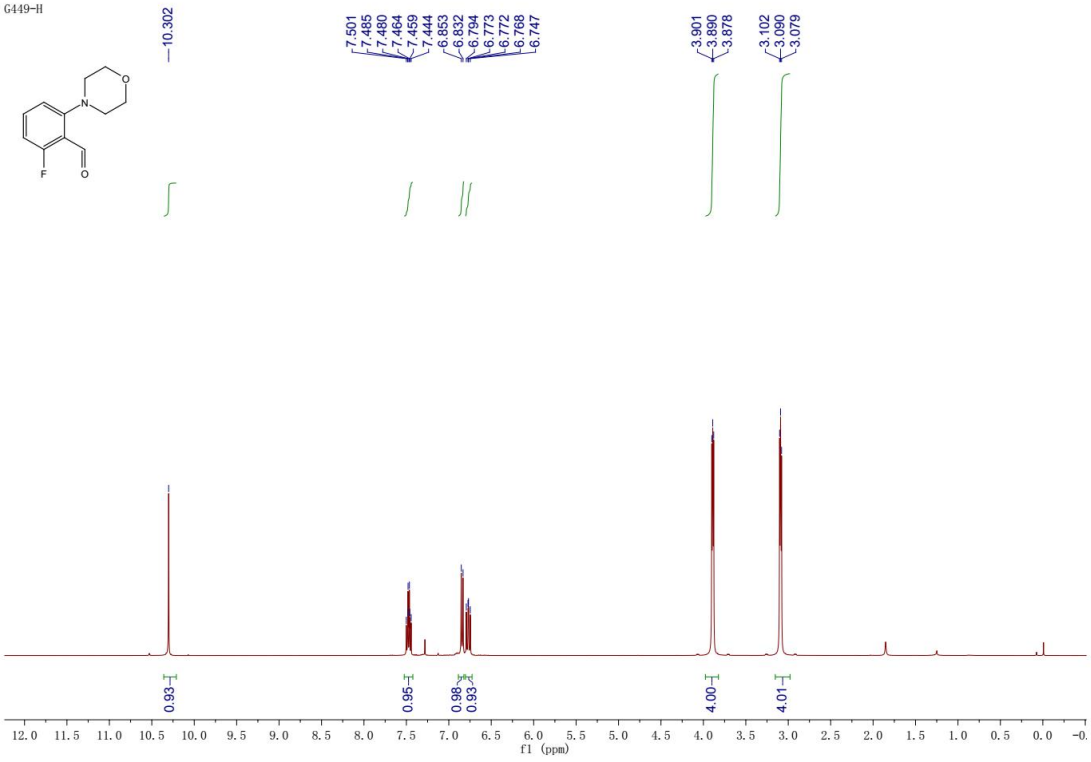

191.383
155.197
134.906
134.241
134.083
130.040
128.990
128.614
126.610
126.369
126.106
122.303
119.033
54.805
53.550
29.047
f1 (ppm)

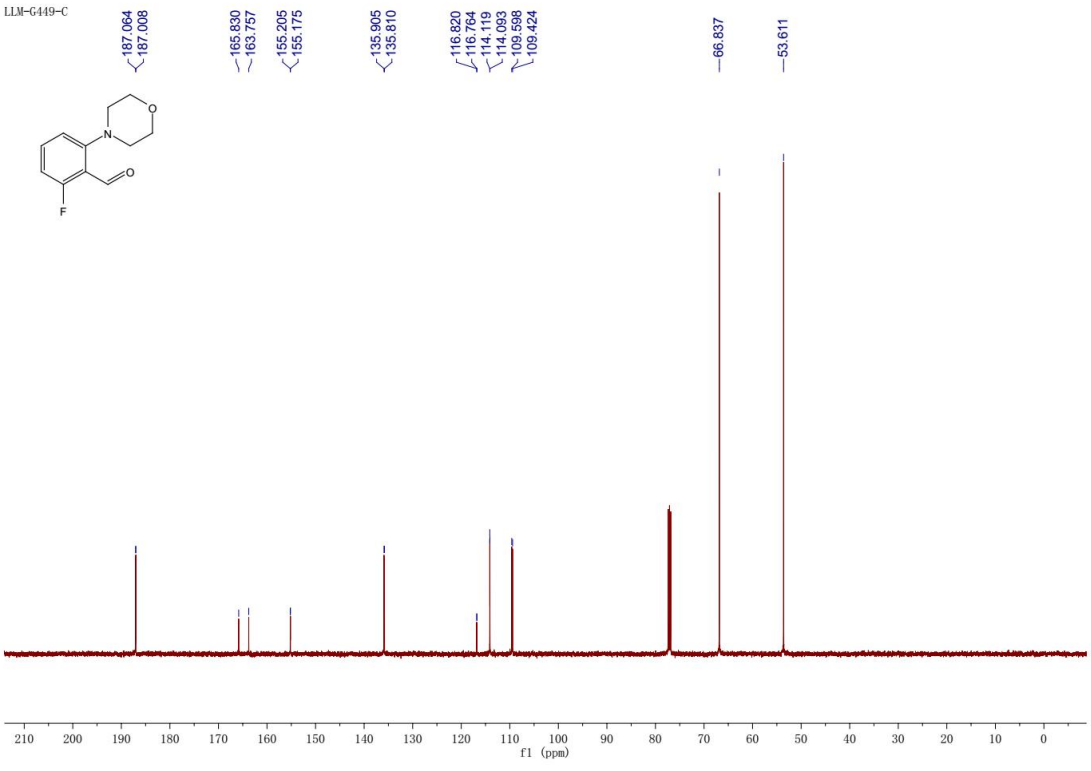
NMR of 1q


LLM-5NY-H
10.110
7.736
7.731
7.716
7.712
7.421
7.416
7.403
7.399
7.395
7.382
7.377
7.284
6.862
6.841
6.827
6.810
3.398
3.387
3.381
3.375
3.365
2.026
2.017
2.009
2.002
1.993
1.00
1.01
1.02
2.01
4.10
3.98
f1 (ppm)

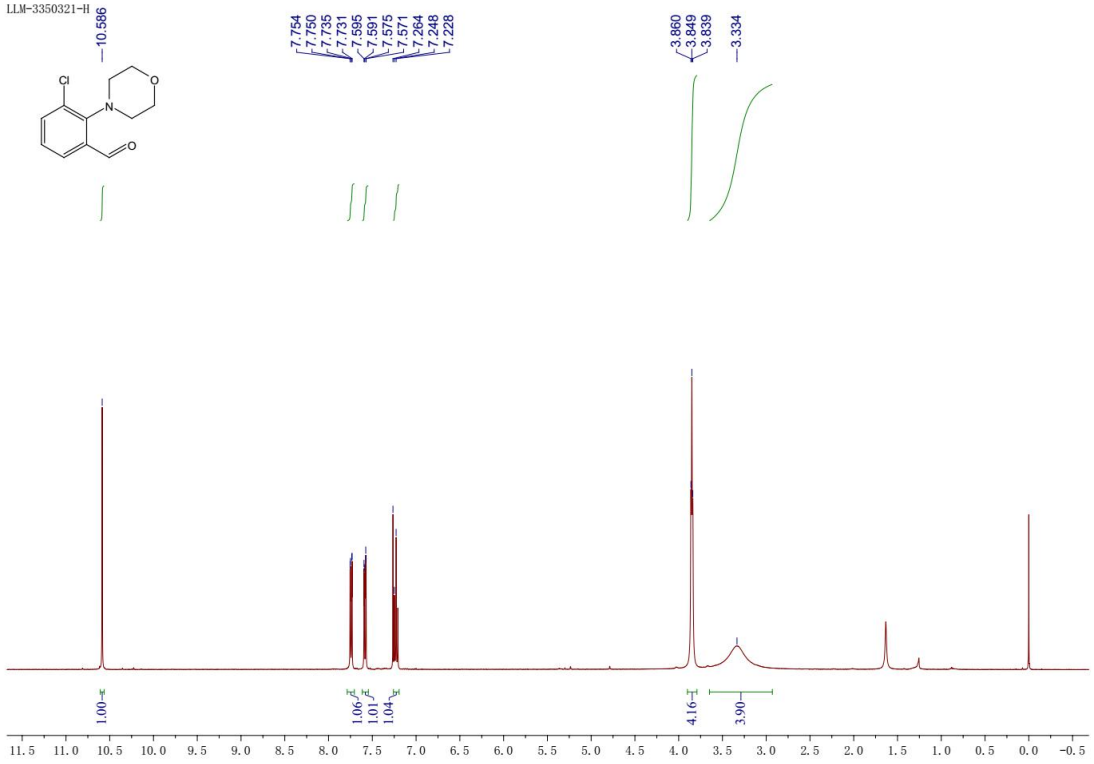

LLM-5NY-C
190.142
149.966
134.230
133.107
122.984
116.439
114.541
52.719
25.965
f1 (ppm)

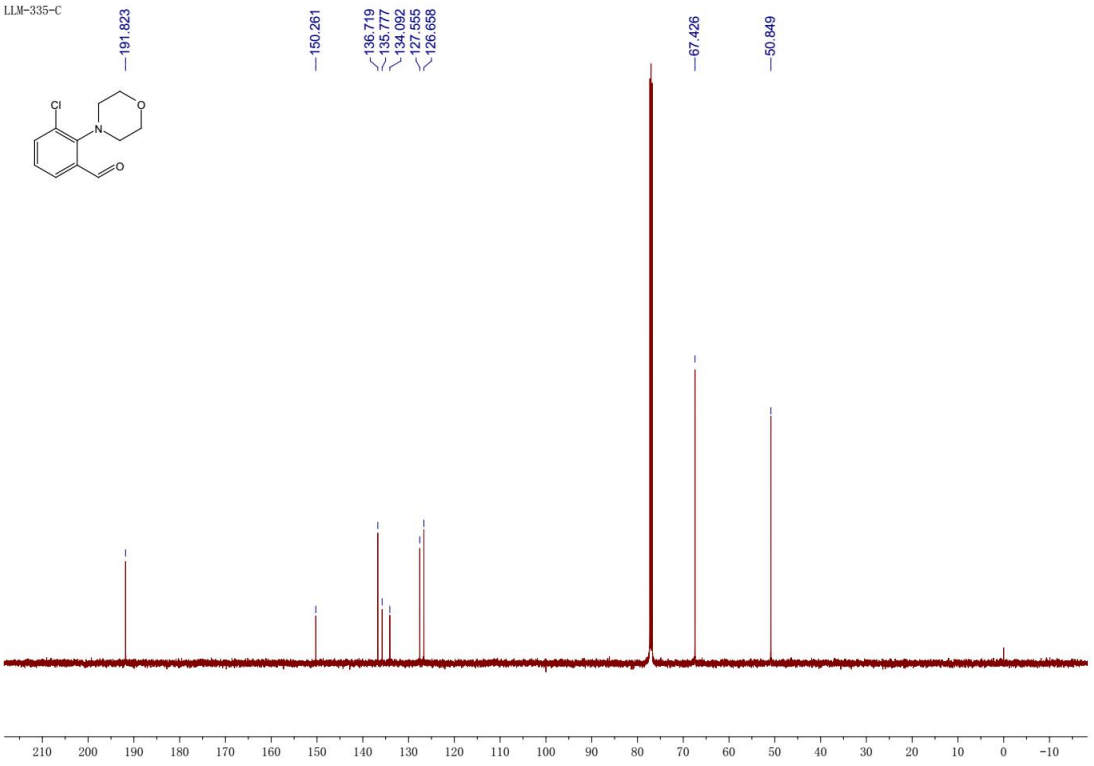
NMR of 1aa


G449-H
10.302
7.501
7.485
7.480
7.464
7.459
7.444
6.853
6.832
6.794
6.773
6.772
6.768
6.747
3.901
3.890
3.878
3.102
3.090
3.079
0.93
0.95
0.98
0.93
4.00
4.01
f1 (ppm)

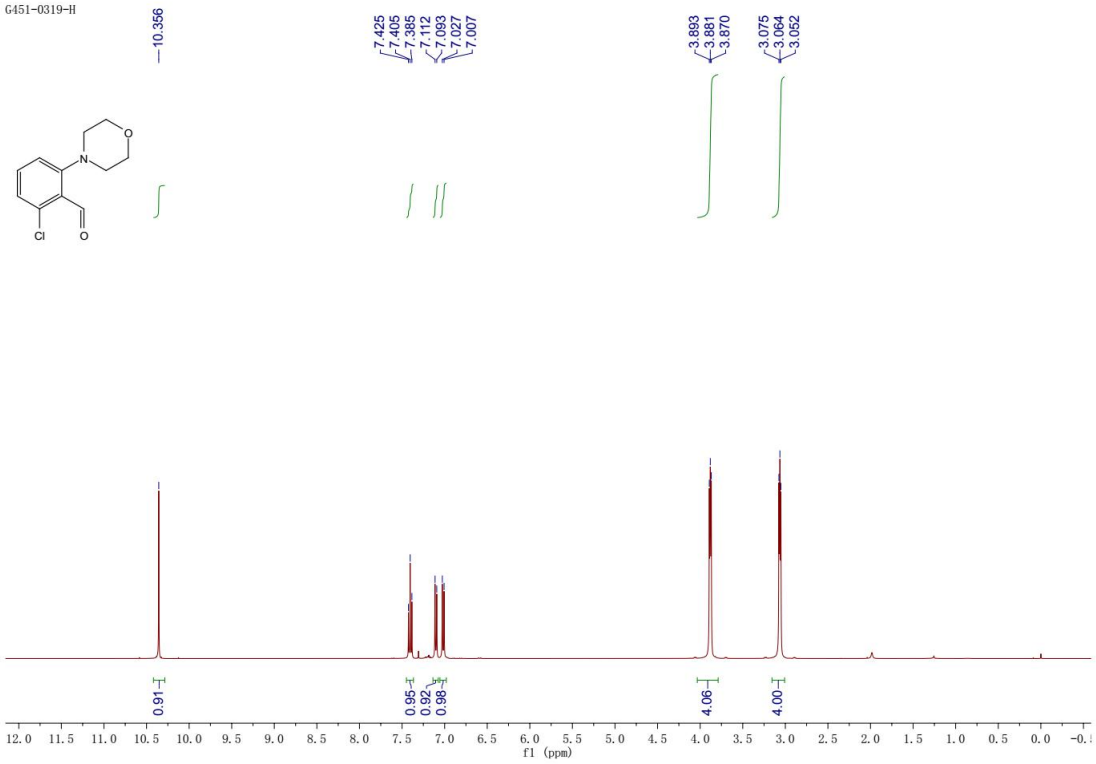

LLM-G449-C
187.064
187.008
165.830
163.757
155.205
155.175
135.905
135.810
116.820
116.764
114.119
114.093
109.598
109.424
66.837
53.611
f1 (ppm)

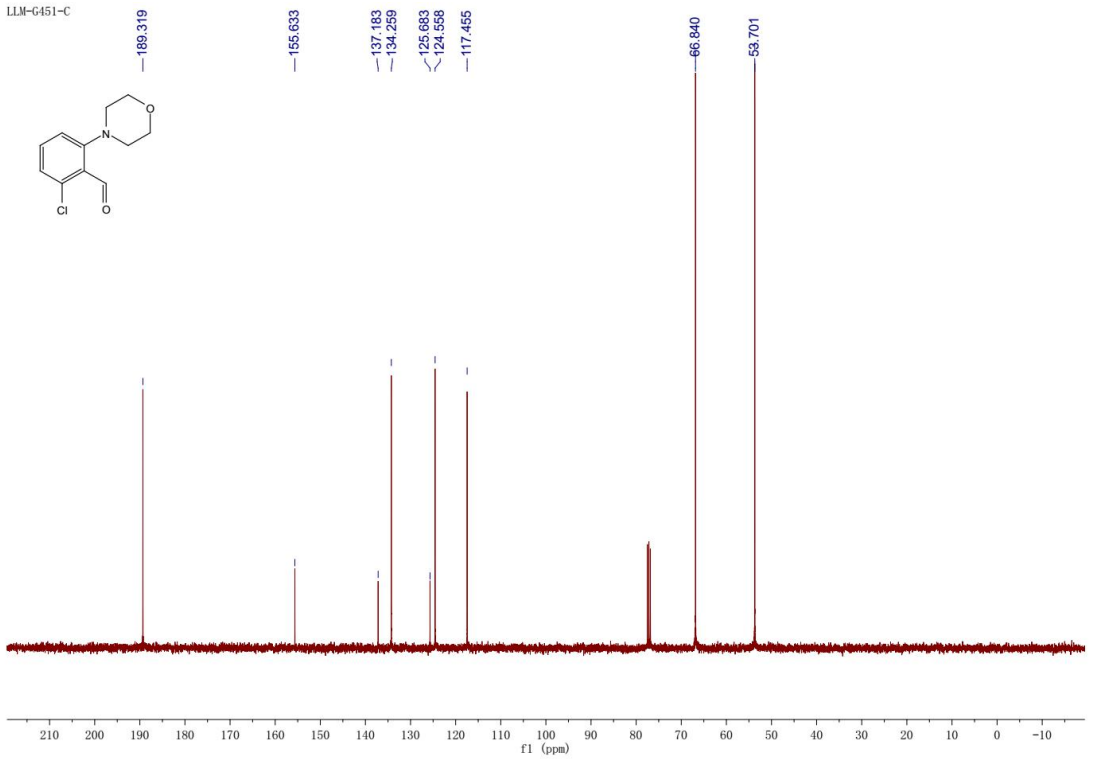
NMR of 1ab


LLM-3350321-H
10.586
7.754
7.750
7.735
7.731
7.595
7.591
7.575
7.571
7.264
7.248
7.228
3.860
3.849
3.839
3.334
Cl
N
O
O
1.00
1.06
1.01
1.04
4.16
3.90

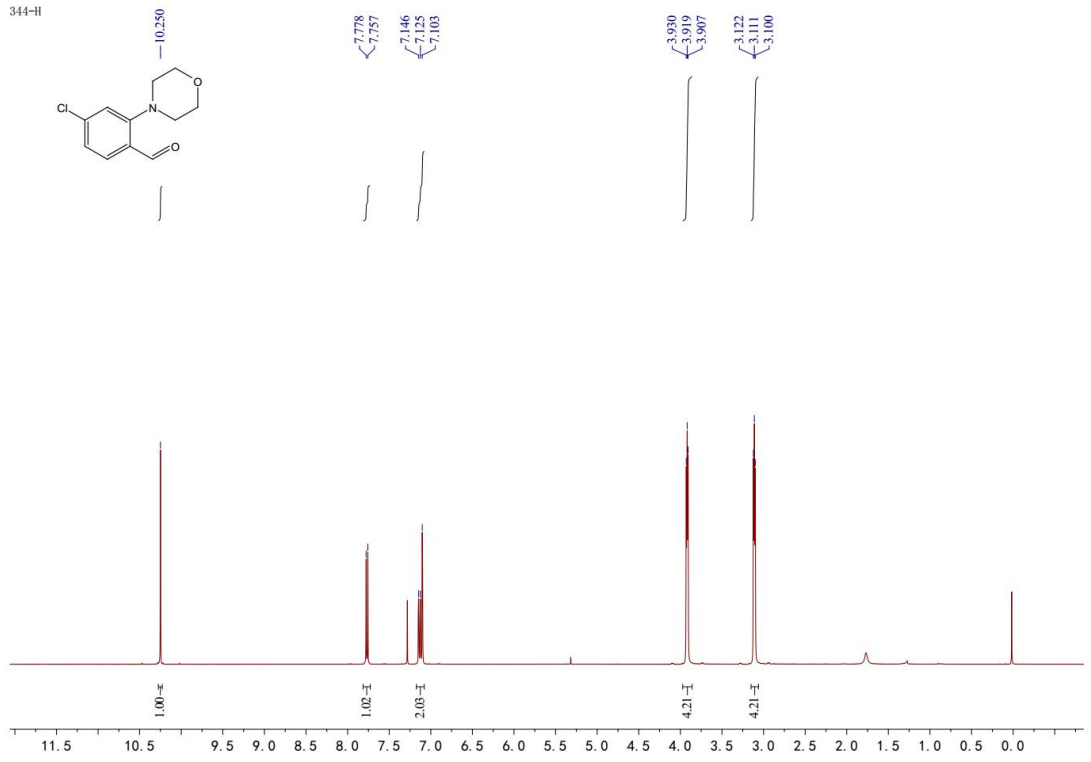

LLM-335-C
191.823
150.261
136.719
135.777
134.092
127.555
126.658
67.426
50.849
Cl
N
O
O

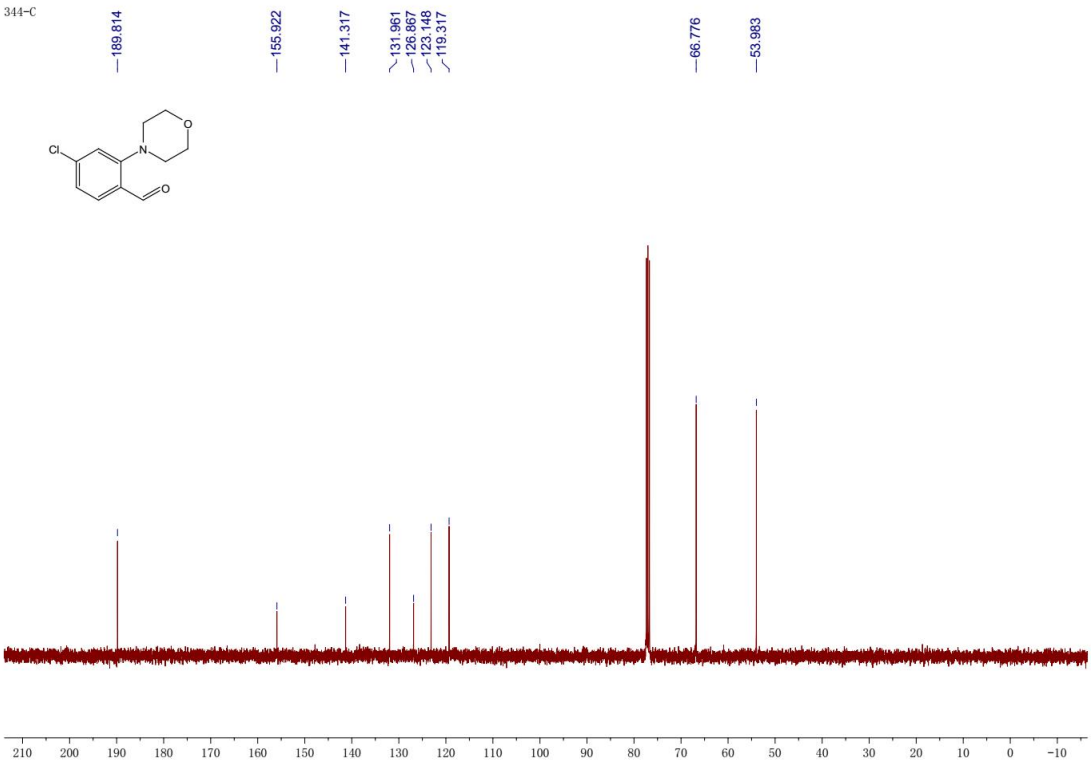
NMR of 1ac


G451-0319-H
10.356
7.425
7.405
7.385
7.112
7.093
7.027
7.007
3.893
3.881
3.870
3.075
3.064
3.052
0.91
0.95
0.92
0.98
4.06
4.00
f1 (ppm)

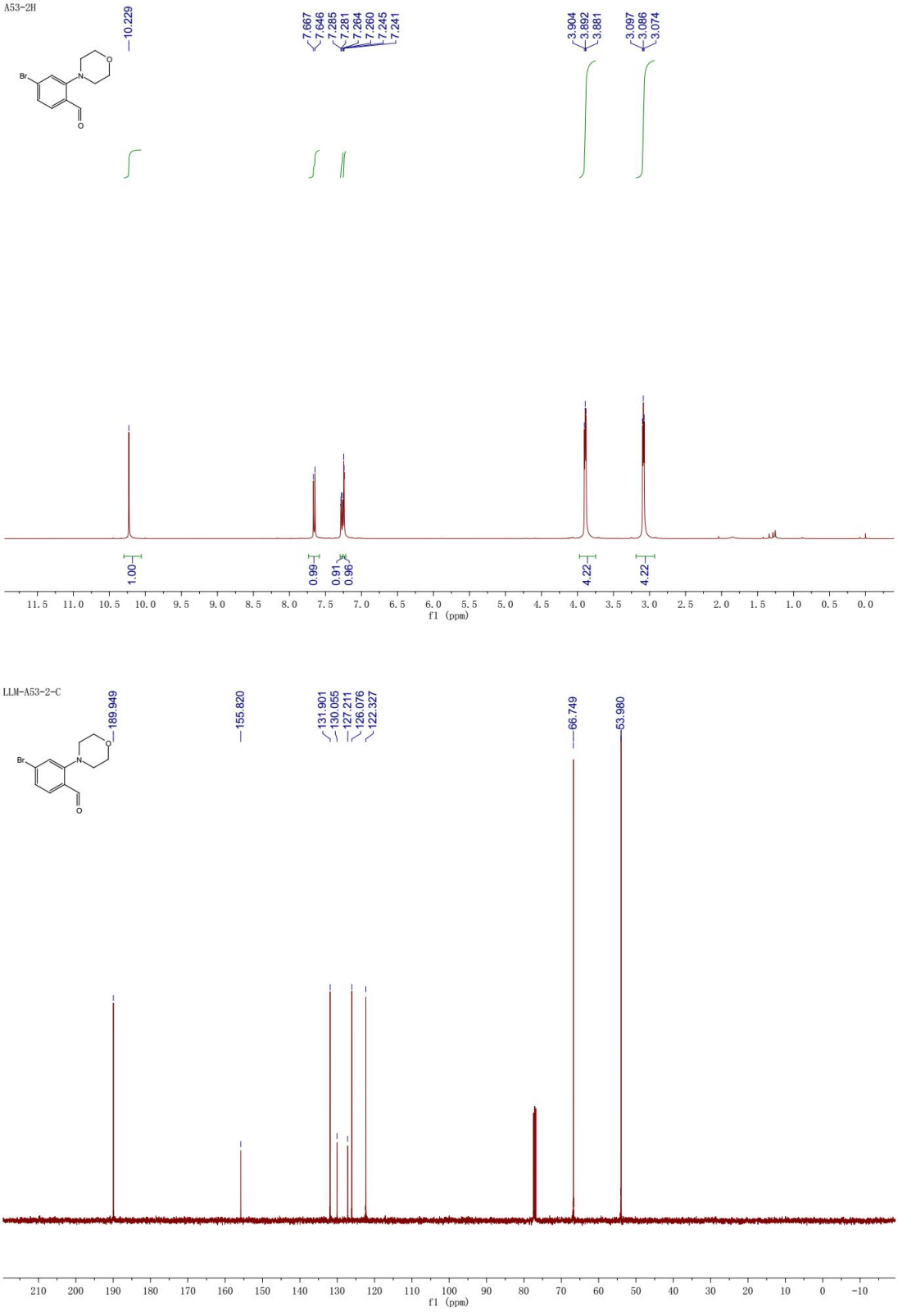

LLM-G451-C
189.319
155.633
137.183
134.259
125.683
124.558
117.455
66.840
53.701
f1 (ppm)

NMR of 1ad

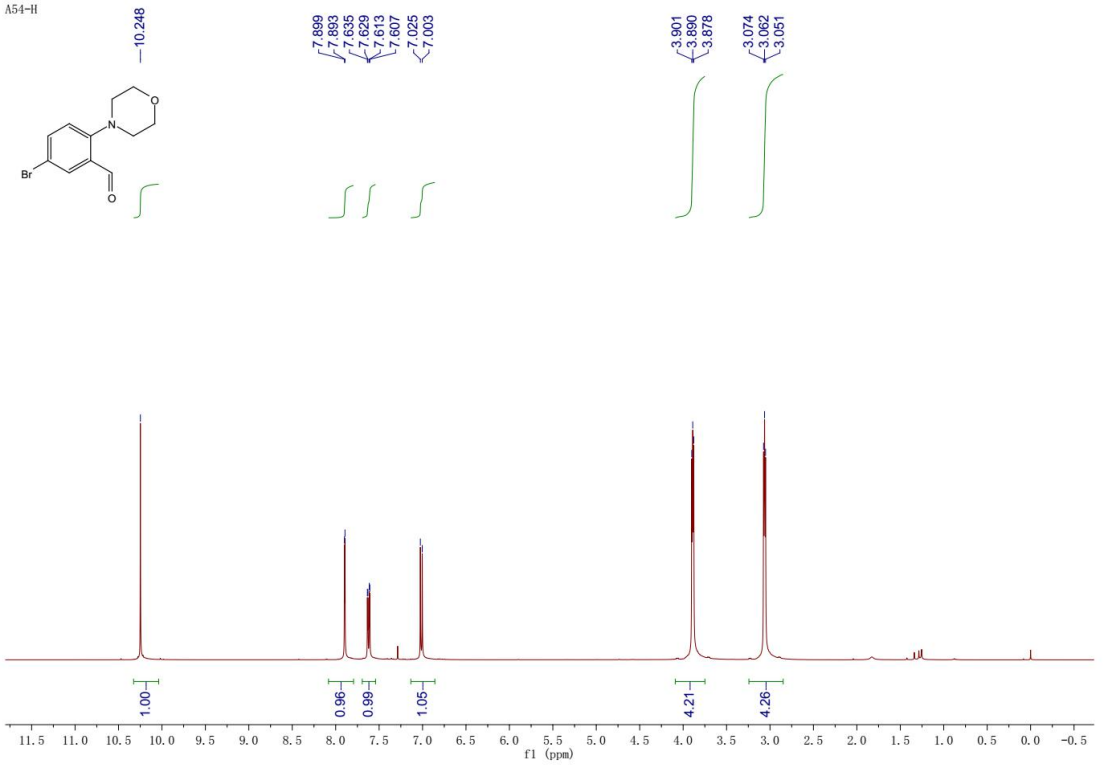

344-H
10.250
7.778
7.757
7.146
7.125
7.103
3.930
3.919
3.907
3.122
3.111
3.100
Cl
N
O
O
1.00
1.02
2.03
4.21
4.21
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

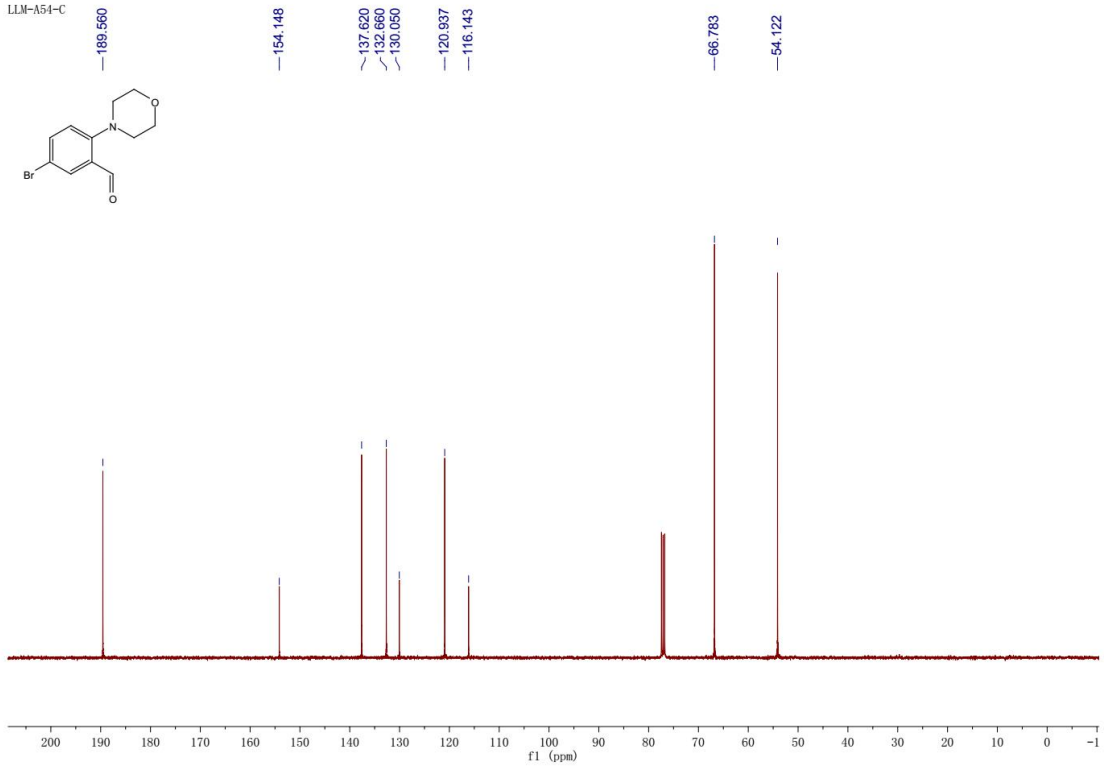

344-C
189.814
155.922
141.317
131.961
126.867
123.148
119.317
66.776
53.983
Cl
N
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

NMR of 1ae

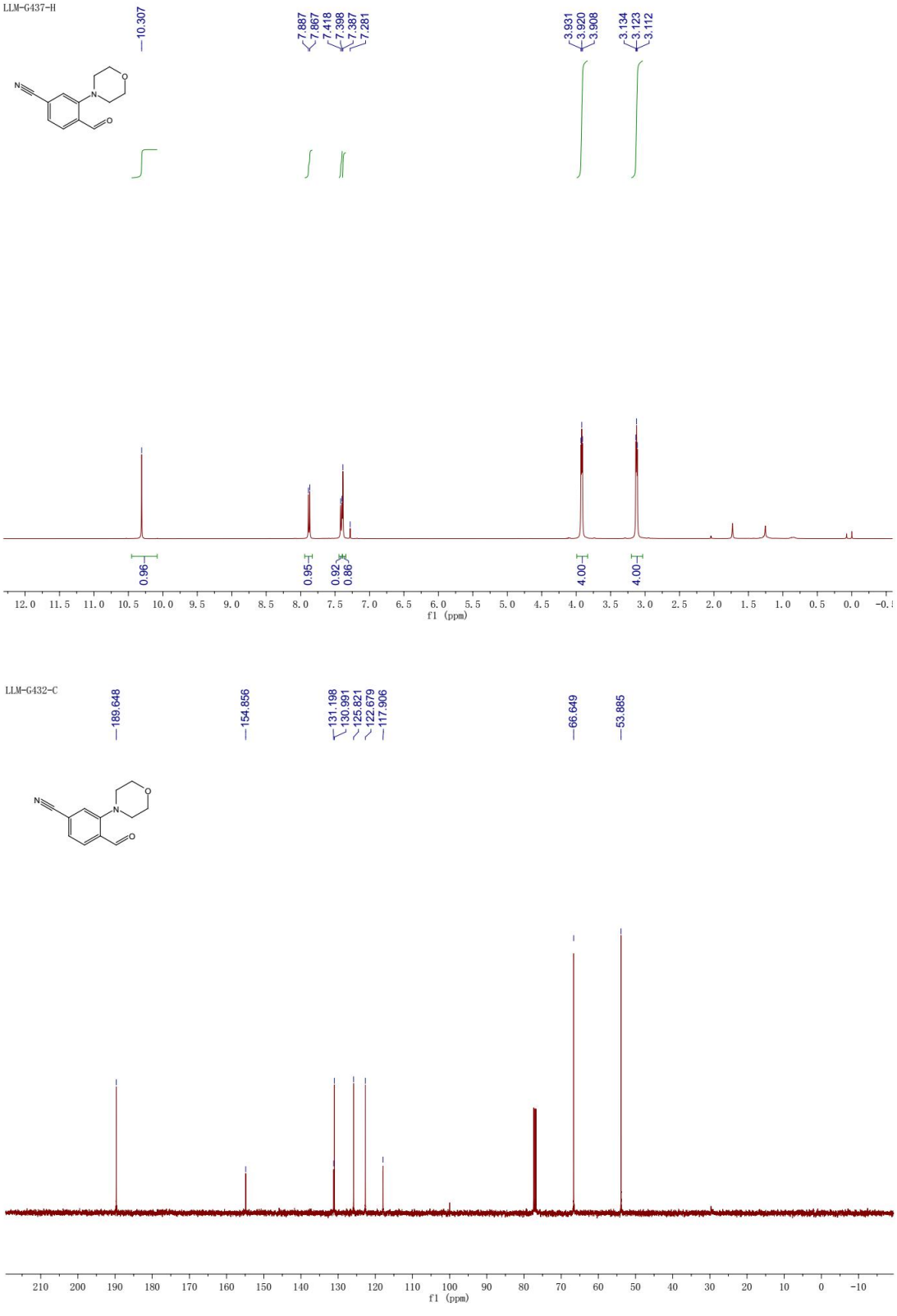

A53-2H
10.229
7.667
7.646
7.285
7.281
7.264
7.260
7.245
7.241
3.904
3.892
3.881
3.097
3.086
3.074
1.00
0.99
0.91
0.96
4.22
4.22
f1 (ppm)
LLM-A53-2-C
189.949
155.820
131.901
130.055
127.211
126.076
122.327
66.749
53.980
f1 (ppm)

NMR of 1af

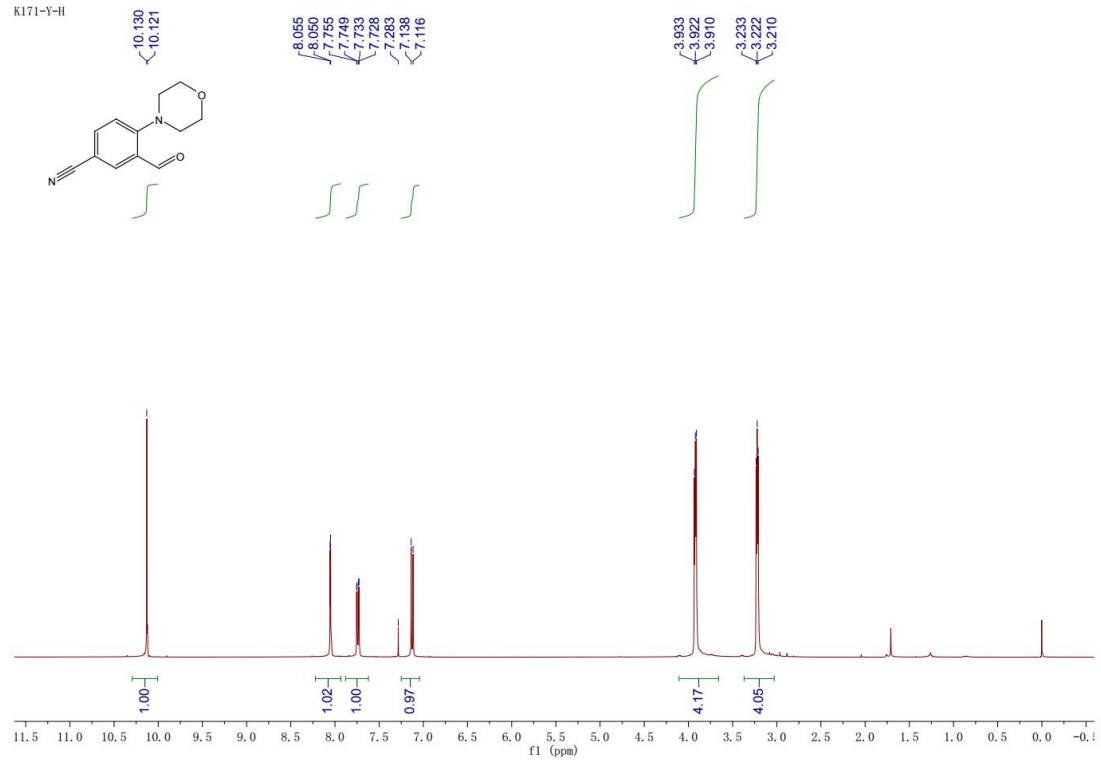

A54-H
10.248
7.899
7.893
7.635
7.629
7.613
7.607
7.025
7.003
3.901
3.890
3.878
3.074
3.062
3.051
Br
O
N
O
1.00
0.96
0.99
1.05
4.21
4.26
f1 (ppm)

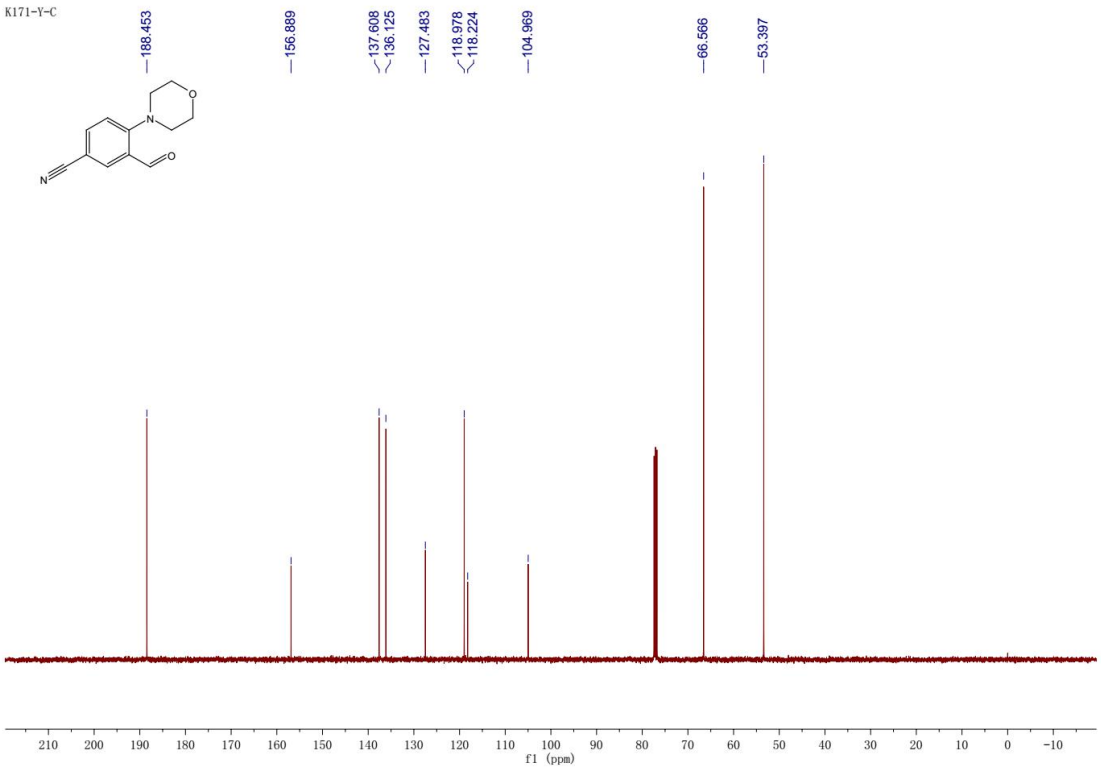

LLM-A54-C
189.560
154.148
137.620
132.660
130.050
120.937
116.143
66.783
54.122
Br
O
N
O
f1 (ppm)

NMR of 1ag

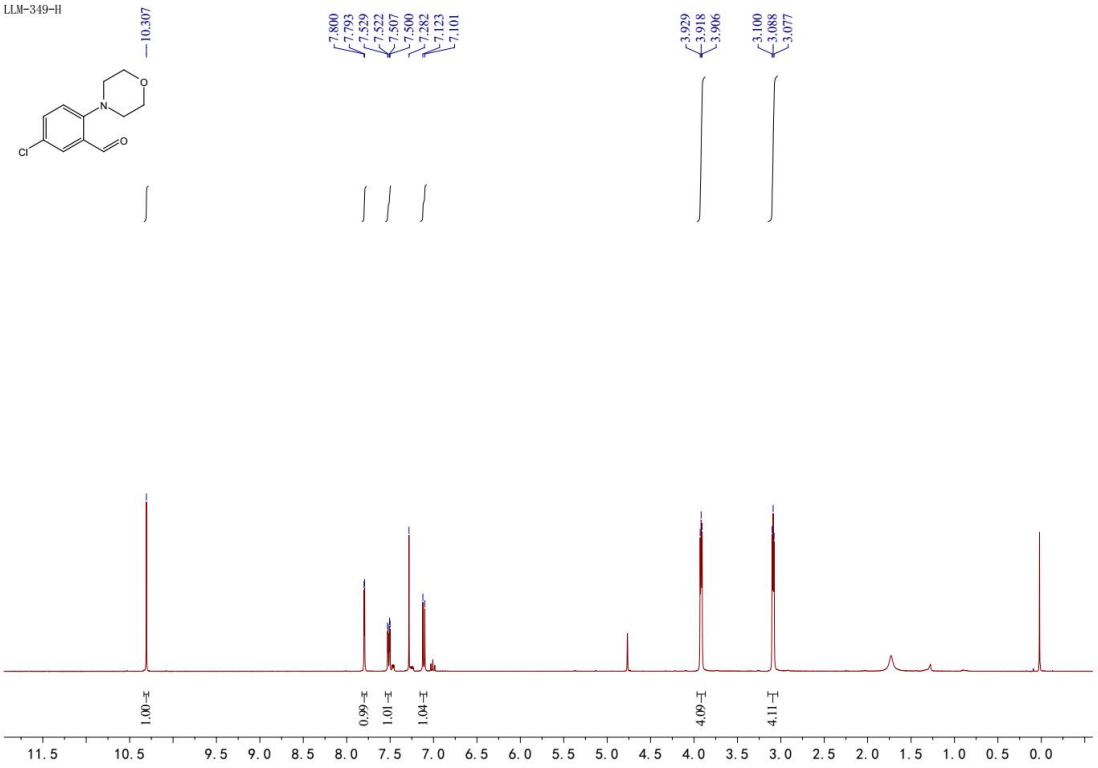

LLM-G437-H
10.307
7.887
7.867
7.418
7.398
7.387
7.281
3.931
3.920
3.908
3.134
3.123
3.112
0.96
0.95
0.92
0.86
4.00
4.00
f1 (ppm)
LLM-G432-C
189.648
154.856
131.198
130.991
125.821
122.679
117.906
66.649
53.885
f1 (ppm)

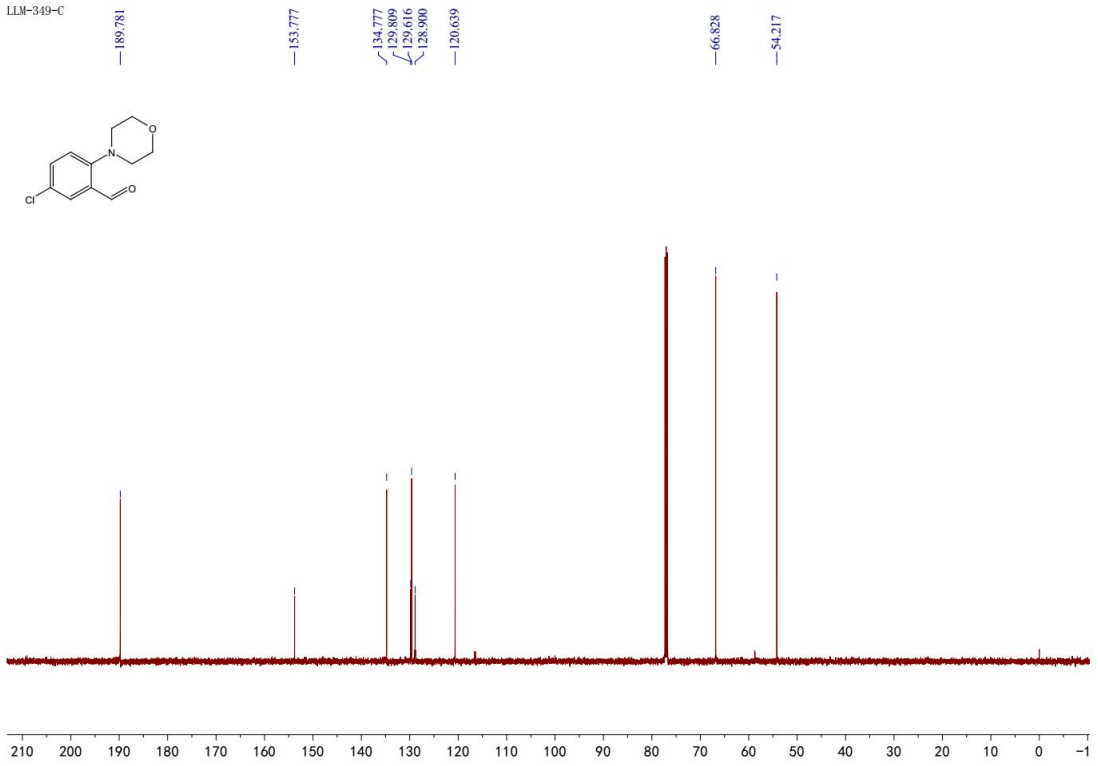
NMR of 1ah


K171-Y-H
10.130
10.121
8.055
8.050
7.755
7.749
7.733
7.728
7.283
7.138
7.116
3.933
3.922
3.910
3.233
3.222
3.210
1.00
1.02
1.00
0.97
4.17
4.05
f1 (ppm)

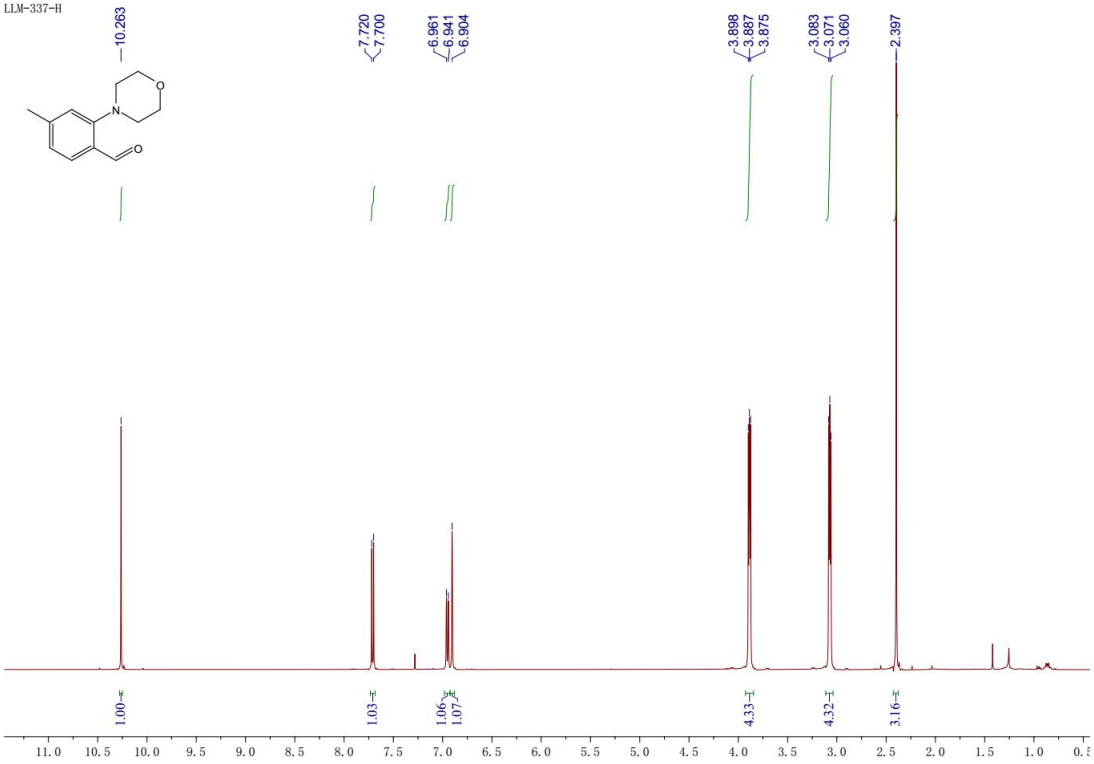

K171-Y-C
188.453
156.889
137.608
136.125
127.483
118.978
118.224
104.969
66.566
53.397
f1 (ppm)

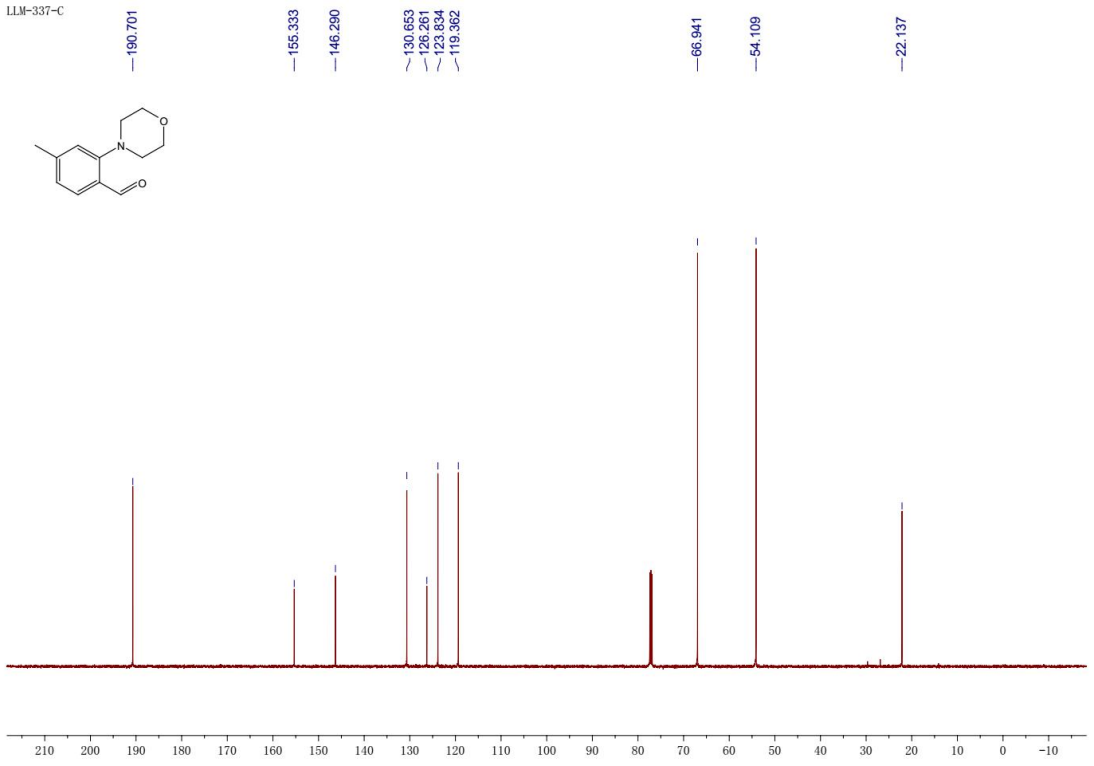
NMR of 1ai


LLM-349-H
10.307
7.800
7.793
7.529
7.522
7.507
7.500
7.282
7.123
7.101
3.929
3.918
3.906
3.100
3.088
3.077
1.00
0.99
1.01
1.04
4.09
4.11

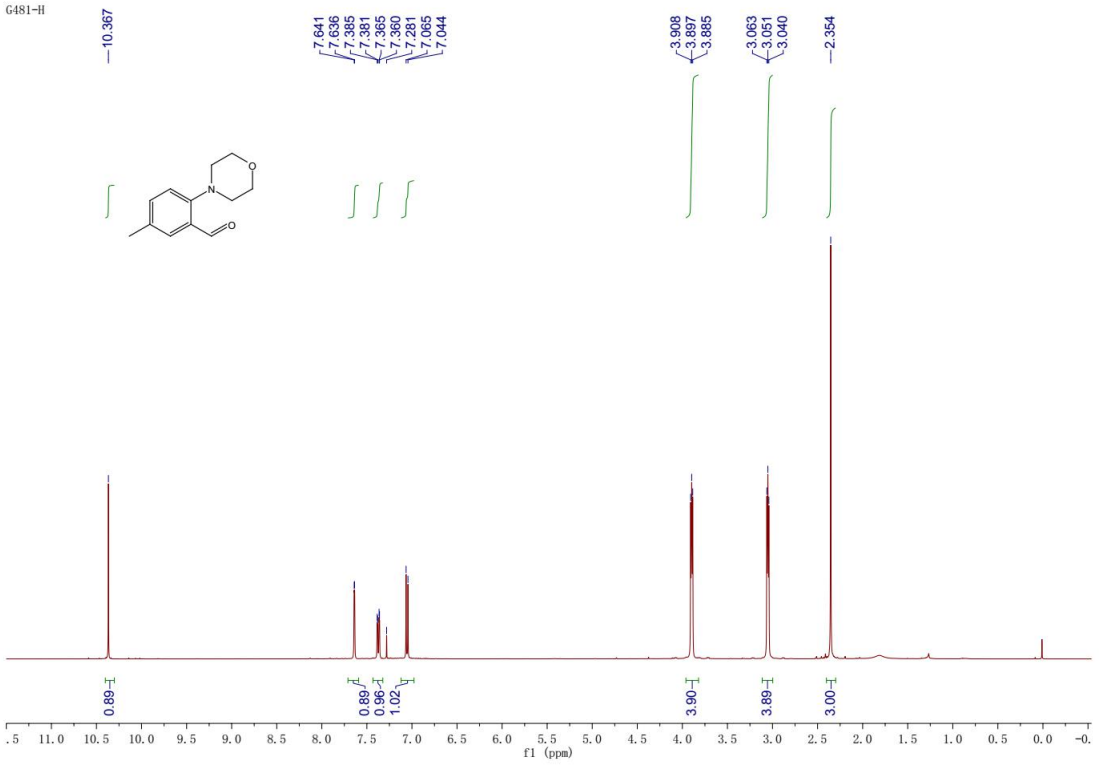

LLM-349-C
189.781
153.777
134.777
129.809
129.616
128.900
120.639
66.828
54.217

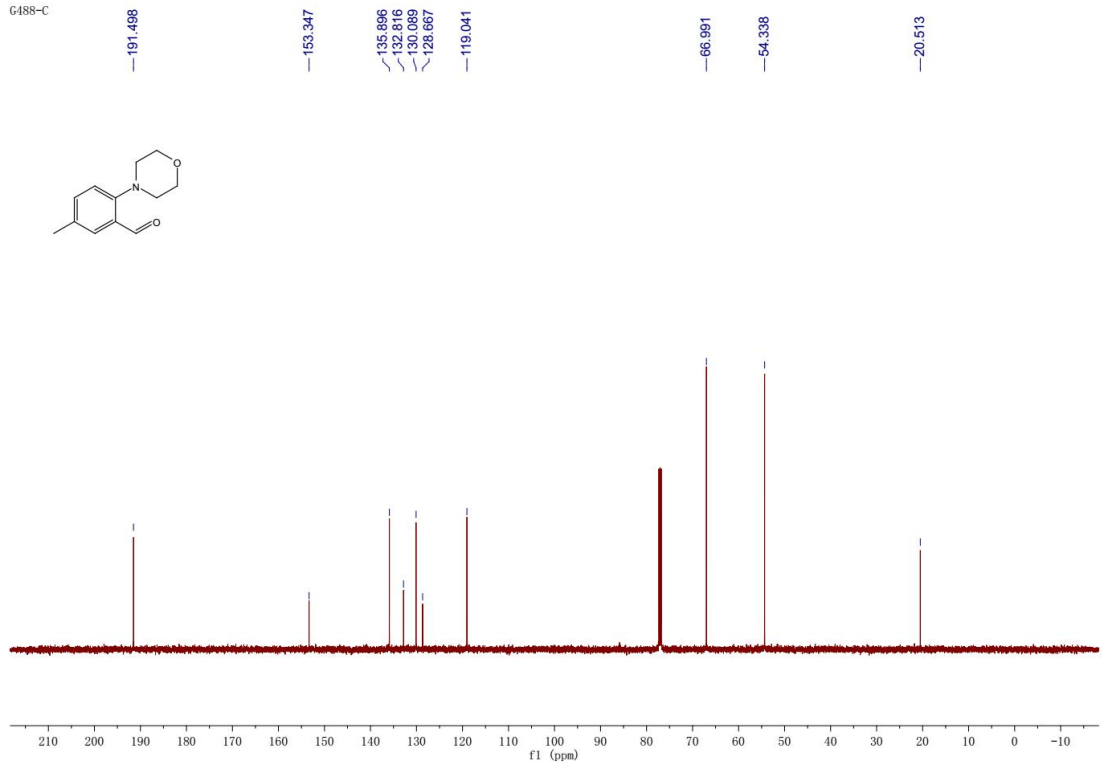
NMR of 1aj


LLM-337-H
10.263
7.720
7.700
6.961
6.941
6.904
3.898
3.887
3.875
3.083
3.071
3.060
2.397
1.00
1.03
1.06
1.07
4.33
4.32
3.16

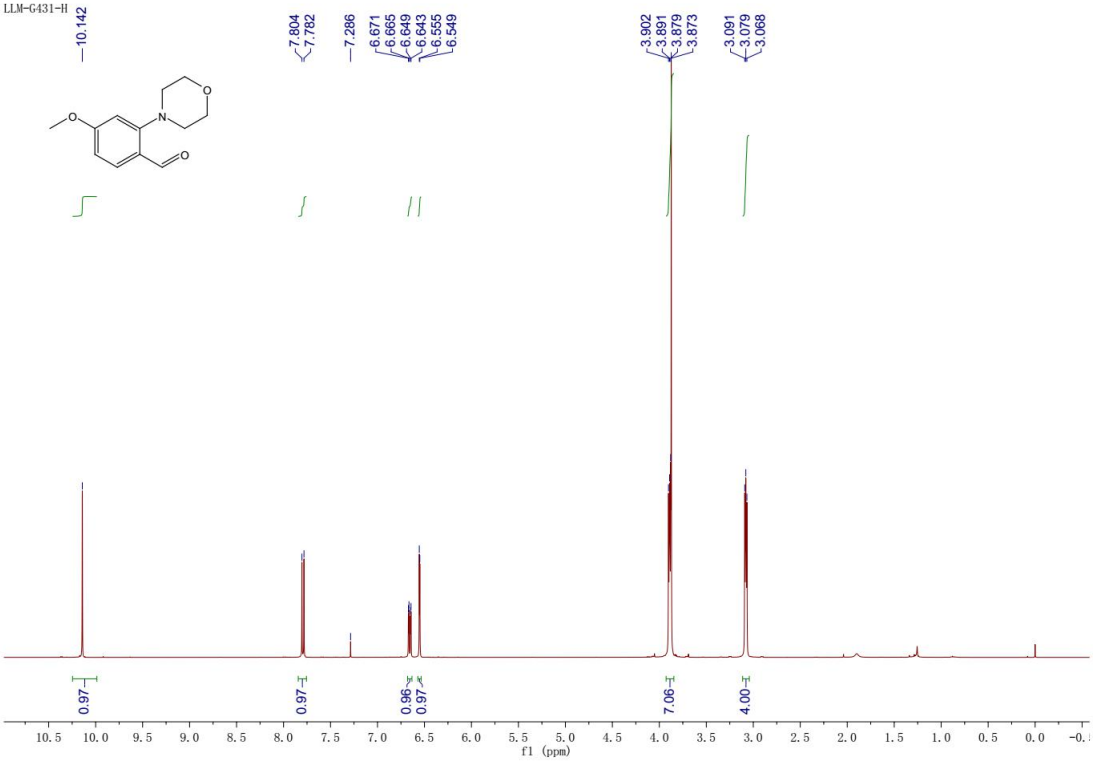

LLM-337-C
190.701
155.333
146.290
130.653
126.261
123.834
119.362
66.941
54.109
22.137

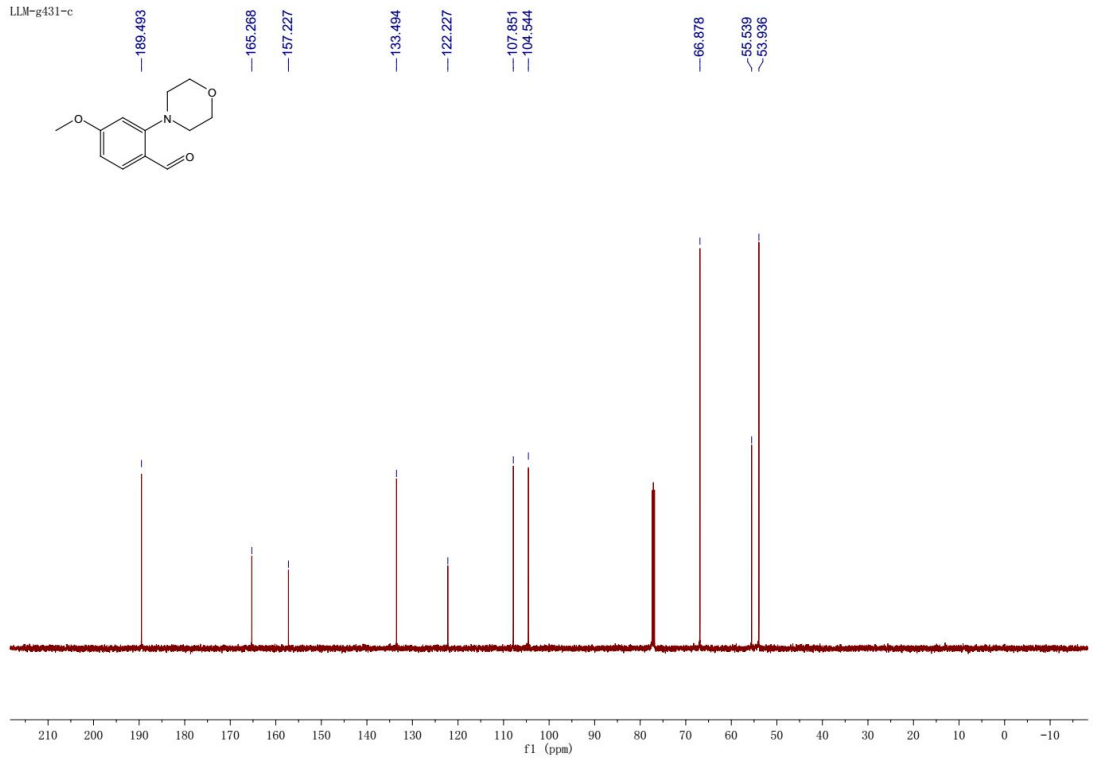
NMR of 1ak


G481-H
10.367
7.641
7.636
7.385
7.381
7.365
7.360
7.281
7.065
7.044
3.908
3.897
3.885
3.063
3.051
3.040
2.354
0.89
0.89
0.96
1.02
3.90
3.89
3.00
f1 (ppm)

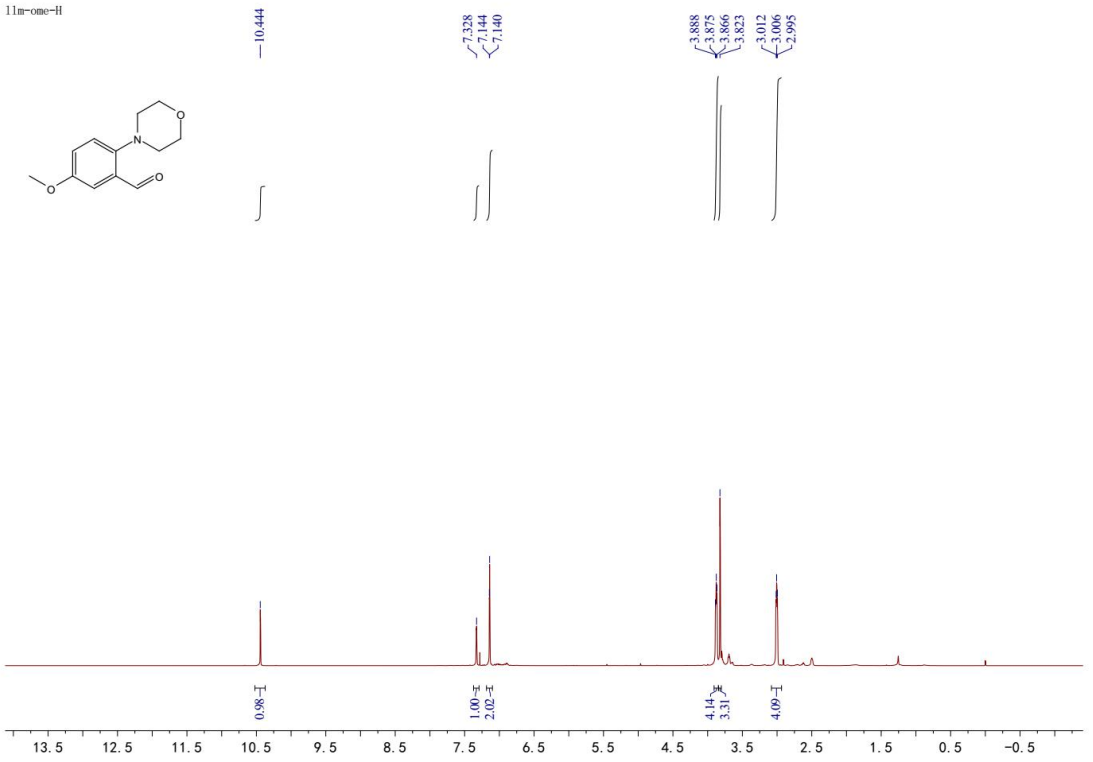

G488-C
191.498
153.347
135.896
132.816
130.089
128.867
119.041
66.991
54.338
20.513
f1 (ppm)

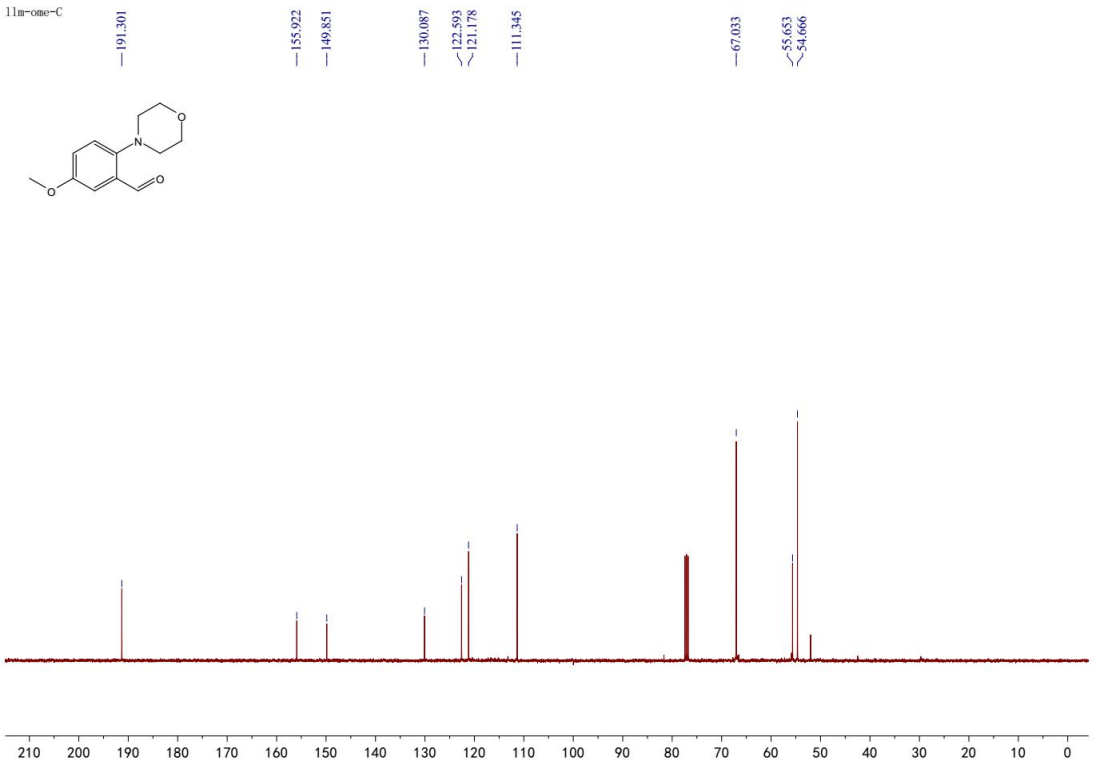
NMR of 1al


LLM-G431-H
10.142
7.804
7.782
7.286
6.671
6.665
6.649
6.643
6.555
6.549
3.902
3.891
3.879
3.873
3.091
3.079
3.068
0.97
0.97
0.96
0.97
7.06
4.00
f1 (ppm)

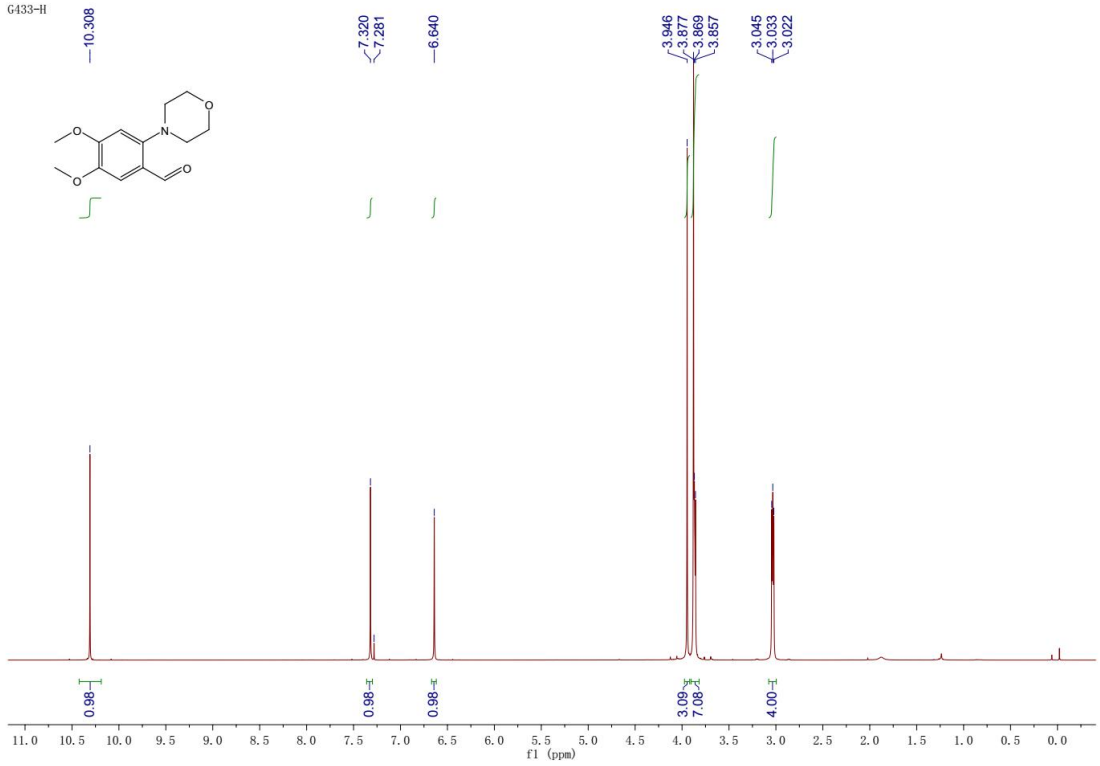

LLM-g431-c
189.493
165.268
157.227
133.494
122.227
107.851
104.544
66.878
55.539
53.936
f1 (ppm)

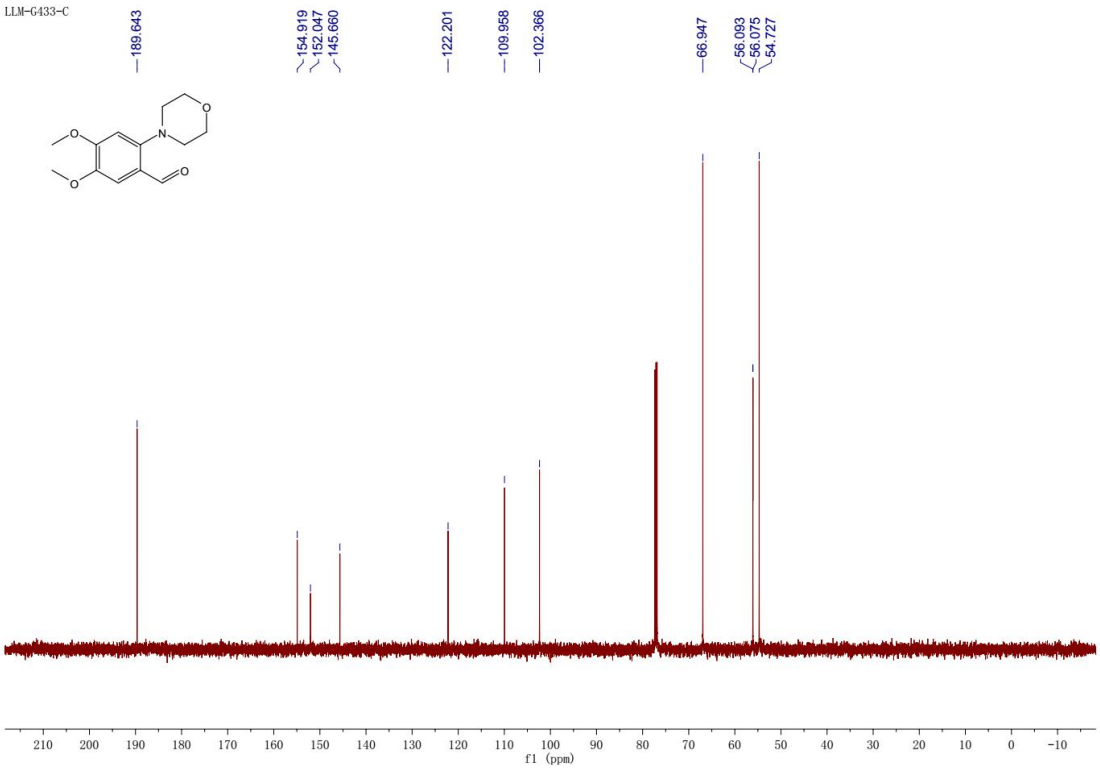
NMR of 1am


11m-ome-H
10.444
7.328
7.144
7.140
3.888
3.875
3.866
3.823
3.012
3.006
2.995
0.98
1.00
2.02
4.14
3.31
4.09
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

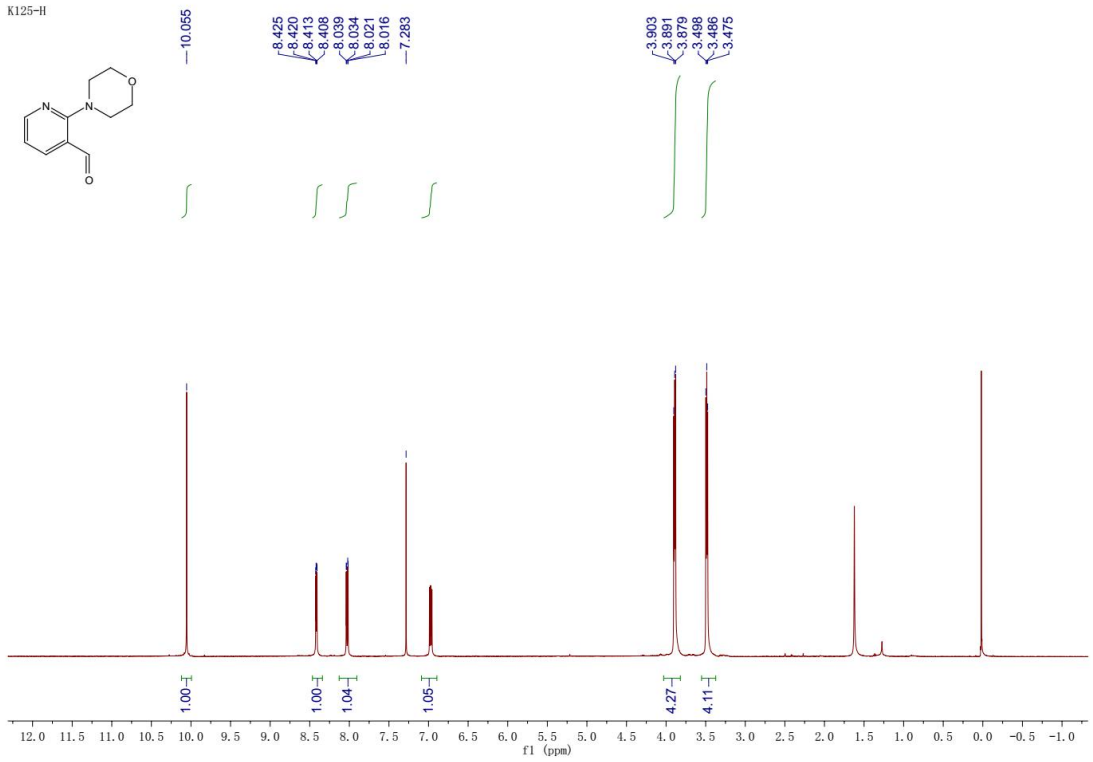

11m-ome-C
191.301
155.922
149.851
130.087
122.593
121.178
111.345
67.033
55.653
54.666
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

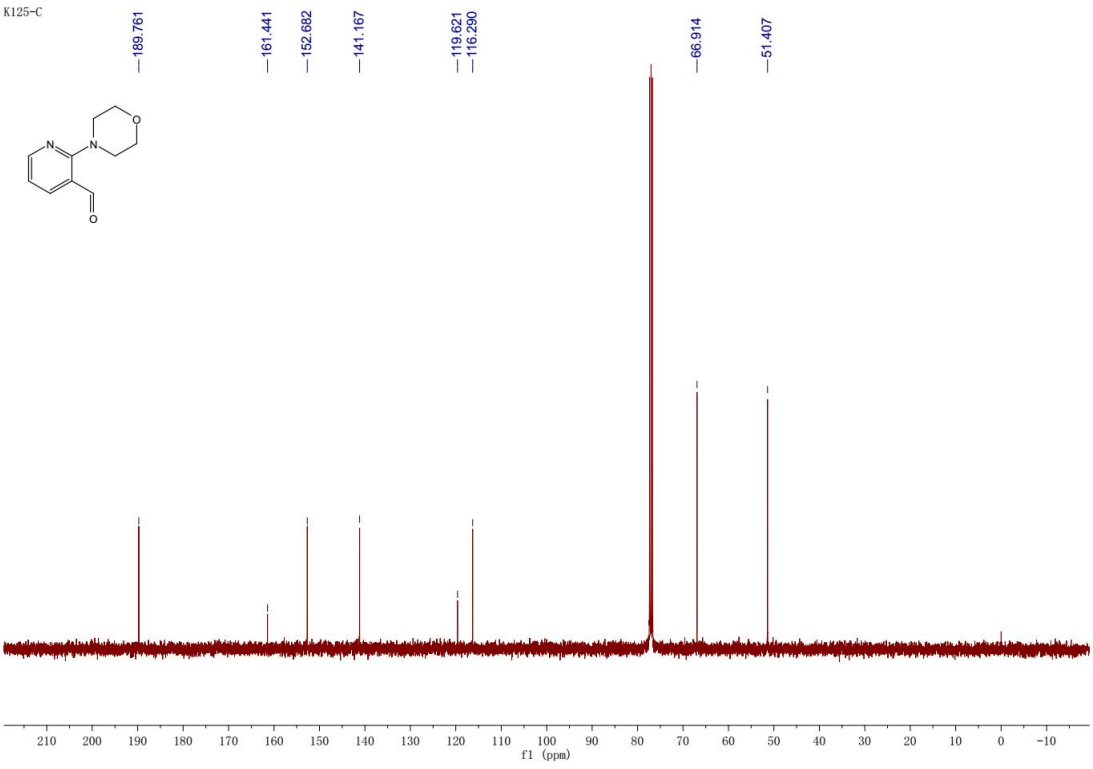
NMR of 1an


G433-H
10.308
7.320
7.281
6.640
3.946
3.877
3.869
3.857
3.045
3.033
3.022
0.98
0.98
0.98
3.09
7.08
4.00
f1 (ppm)

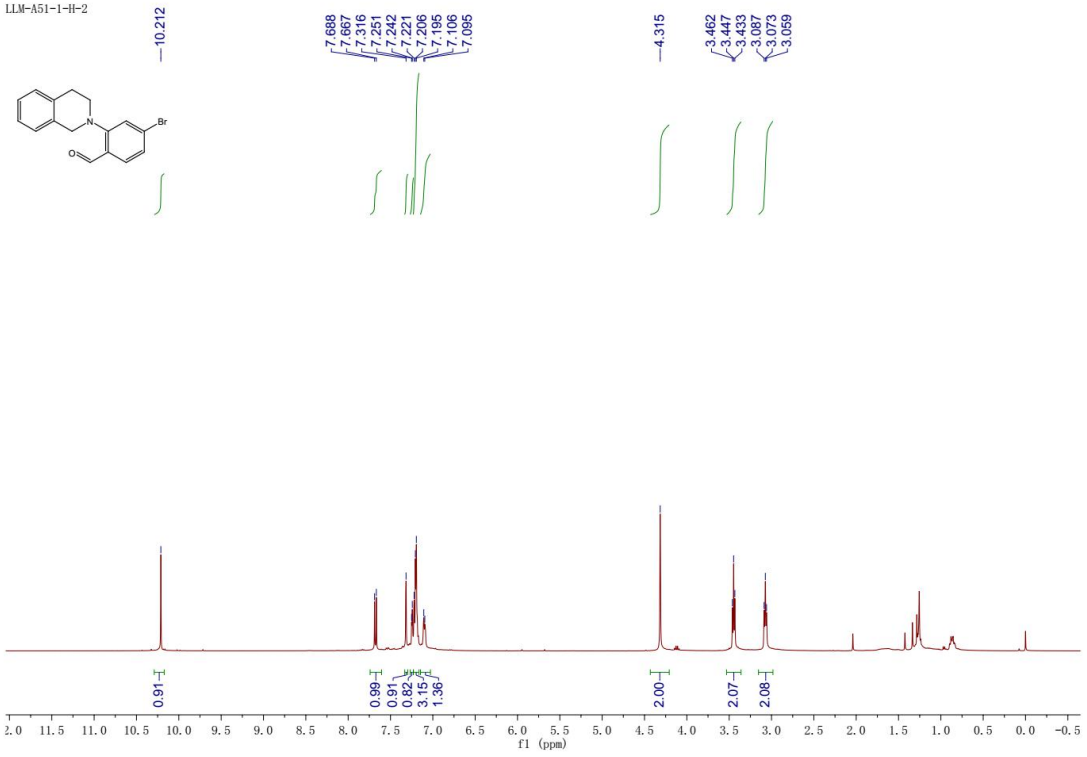

LLM-G433-C
189.643
154.919
152.047
145.660
122.201
109.958
102.366
66.947
56.093
56.075
54.727
f1 (ppm)

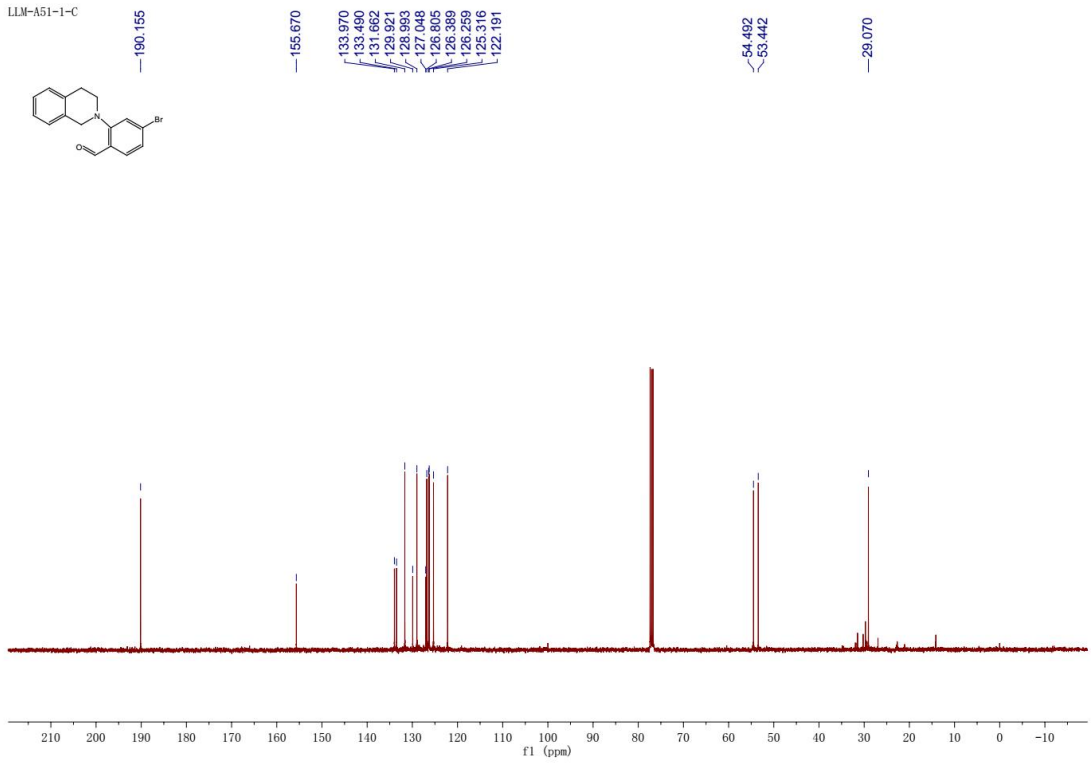
NMR of 1ao


K125-H
10.055
8.425
8.420
8.413
8.408
8.039
8.034
8.021
8.016
7.283
3.903
3.891
3.879
3.498
3.486
3.475
1.00
1.00
1.04
1.05
4.27
4.11
f1 (ppm)

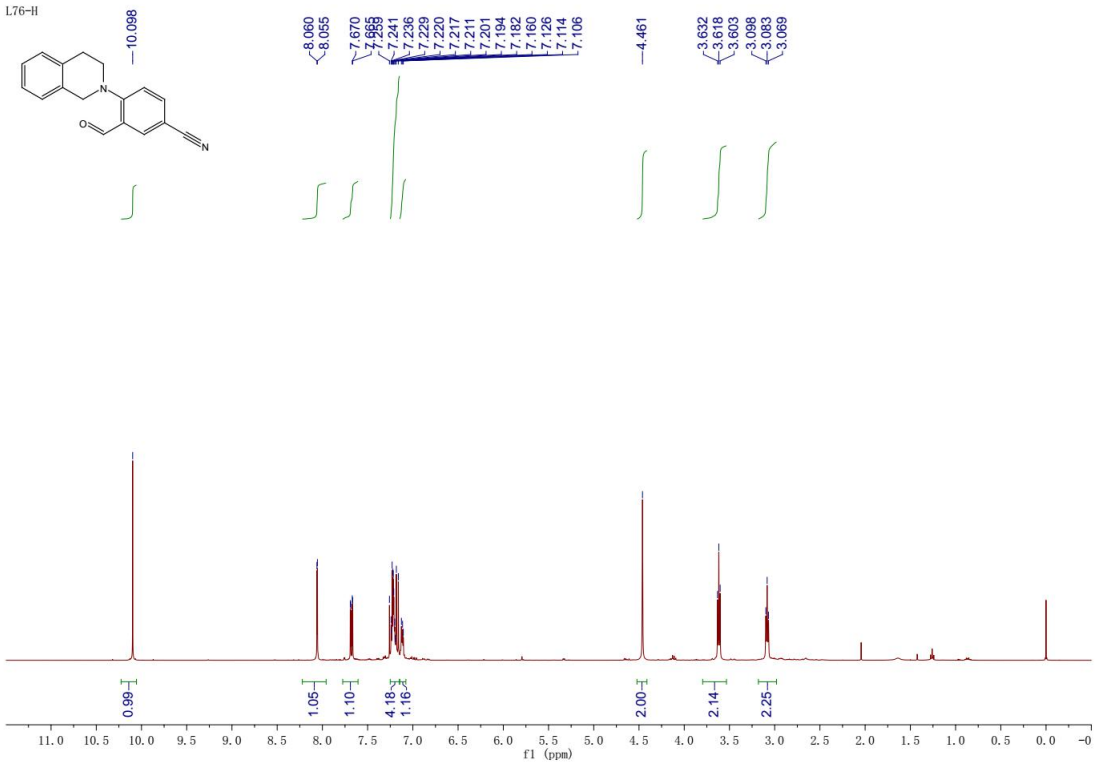

K125-C
189.761
161.441
152.682
141.167
119.621
116.290
66.914
51.407
f1 (ppm)

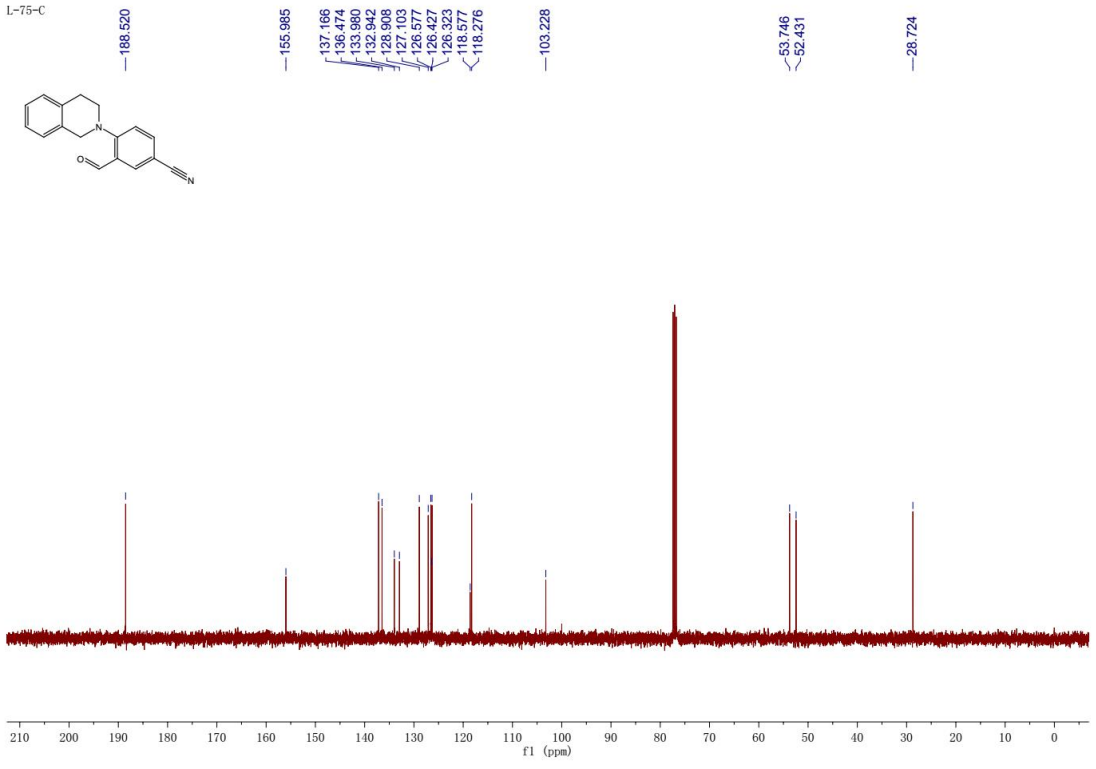
NMR of 1ap


LLM-A51-1-H-2
10.212
7.688
7.667
7.316
7.251
7.242
7.221
7.206
7.195
7.106
7.095
4.315
3.462
3.447
3.433
3.087
3.073
3.059
Br
O
0.91
0.99
0.91
0.82
3.15
1.36
2.00
2.07
2.08
f1 (ppm)

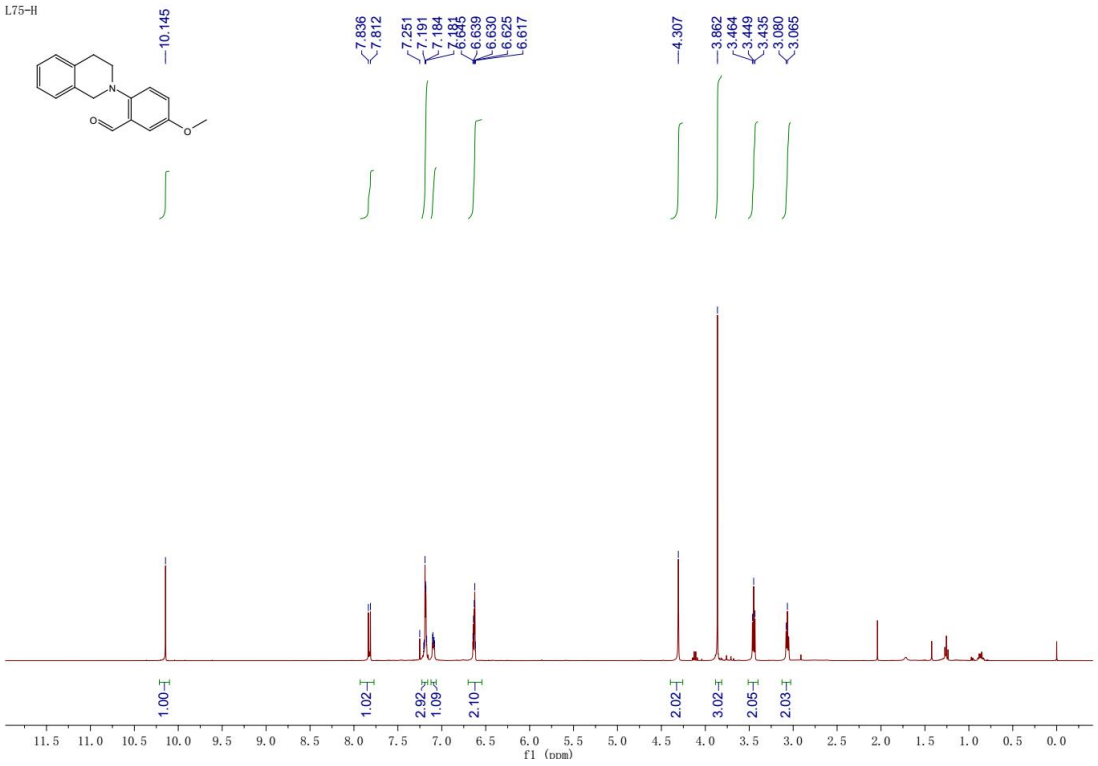

LLM-A51-1-C
190.155
155.670
133.970
133.490
131.662
129.921
128.993
127.048
126.805
126.389
126.259
125.316
122.191
54.492
53.442
29.070
Br
O
f1 (ppm)

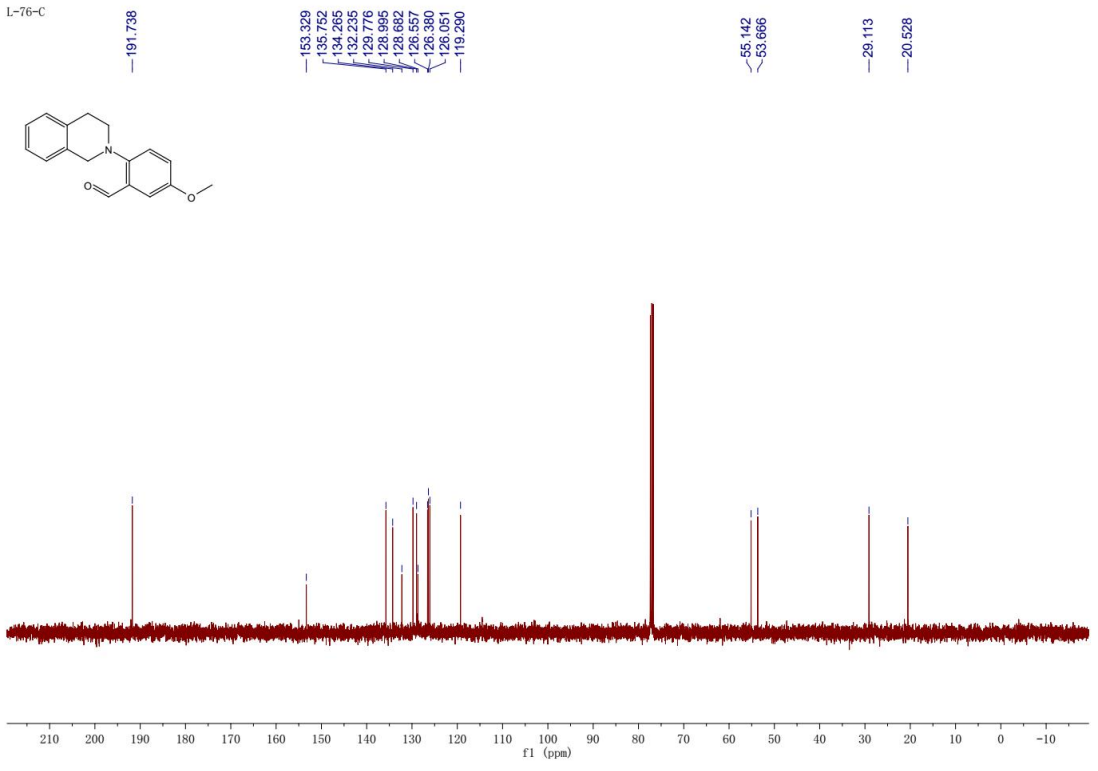
NMR of 1aq


L76-H
10.098
8.060
8.055
7.670
7.241
7.236
7.229
7.220
7.217
7.211
7.201
7.194
7.182
7.160
7.126
7.114
7.106
4.461
3.632
3.618
3.603
3.098
3.083
3.069
0.99
1.05
1.10
4.18
1.16
2.00
2.14
2.25
f1 (ppm)

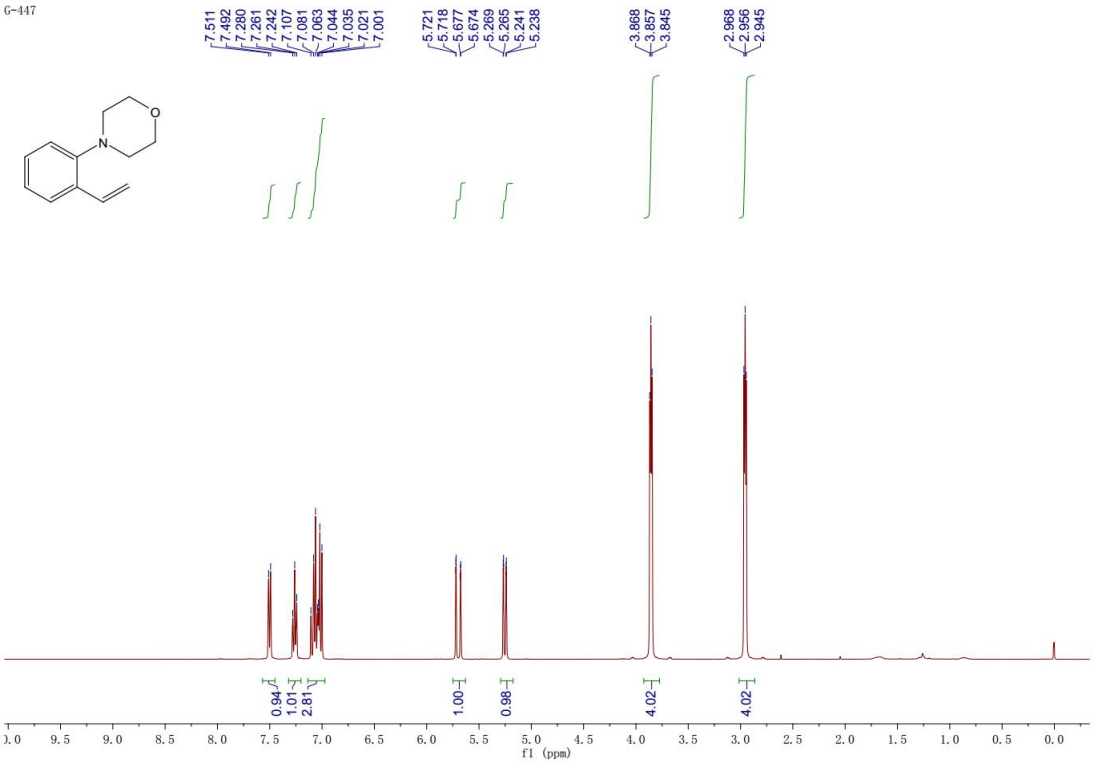

L-75-C
188.520
155.985
137.166
136.474
133.980
132.942
128.908
127.103
126.577
126.427
126.323
118.577
118.276
103.228
53.746
52.431
28.724
f1 (ppm)

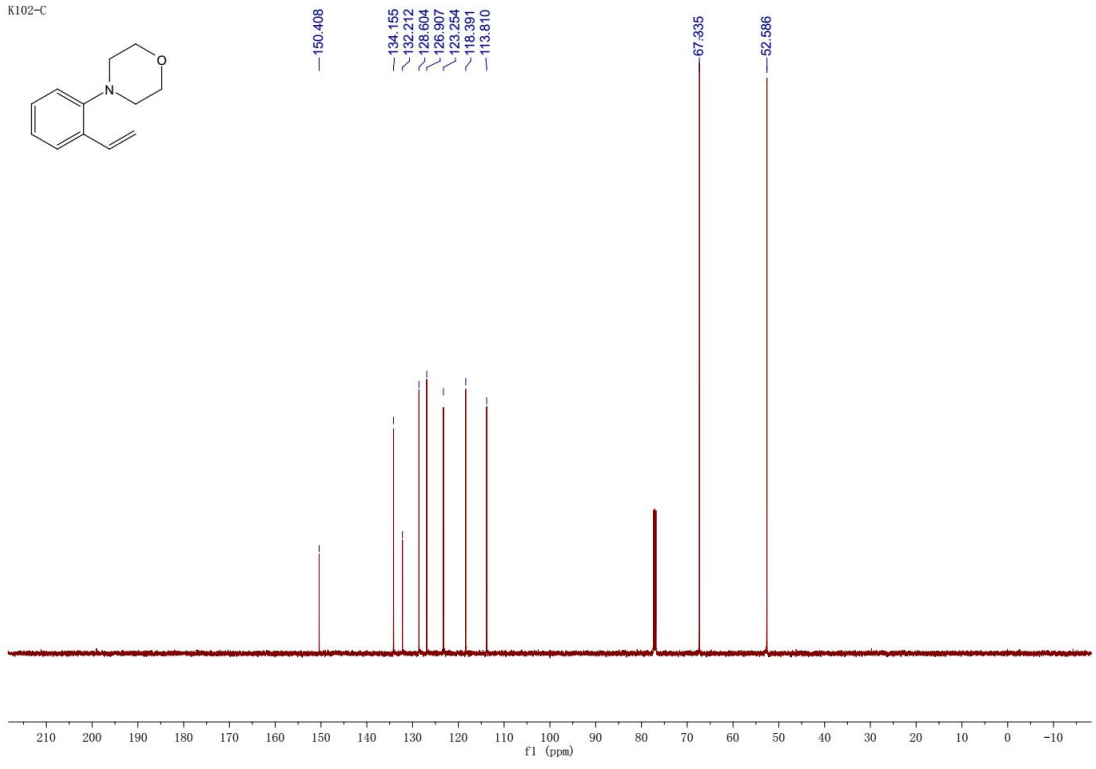
NMR of 1ar


L75-H
10.145
7.836
7.812
7.251
7.191
7.184
6.639
6.630
6.625
6.617
4.307
3.862
3.464
3.449
3.435
3.080
3.065
1.00
1.02
2.92
1.09
2.10
2.02
3.02
2.05
2.03
f1 (ppm)

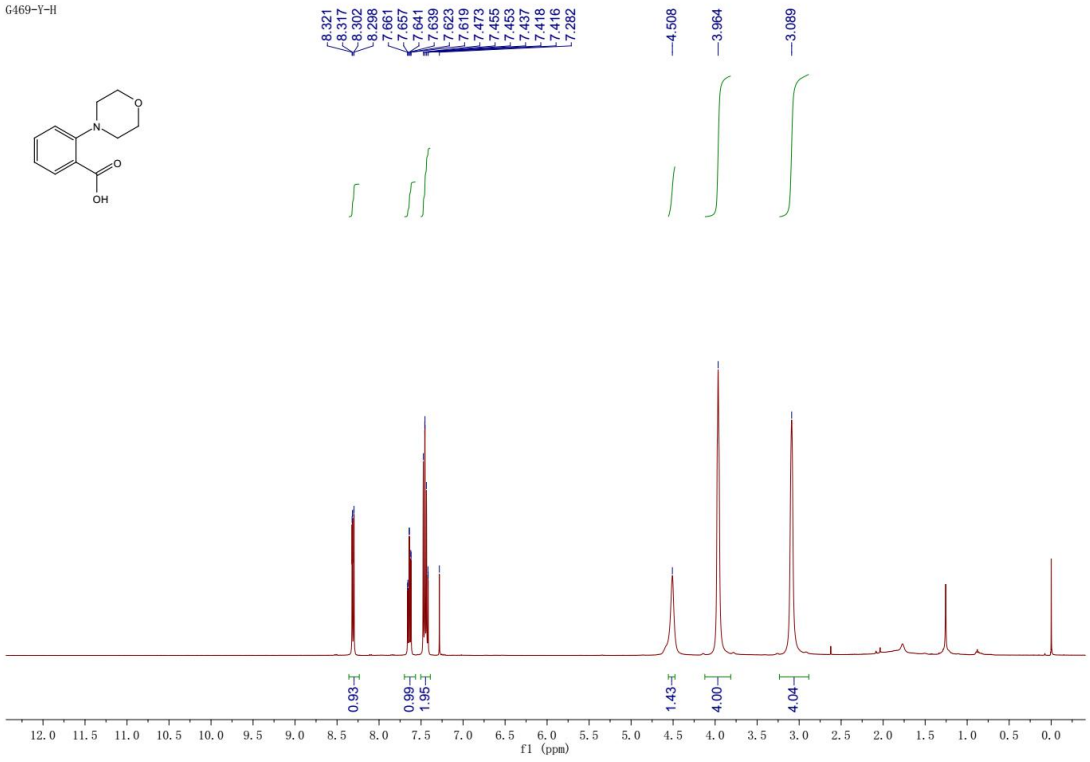

L-76-C
191.738
153.329
135.752
134.265
132.235
129.776
128.995
128.682
126.557
126.380
126.051
119.290
55.142
53.666
29.113
20.528
f1 (ppm)

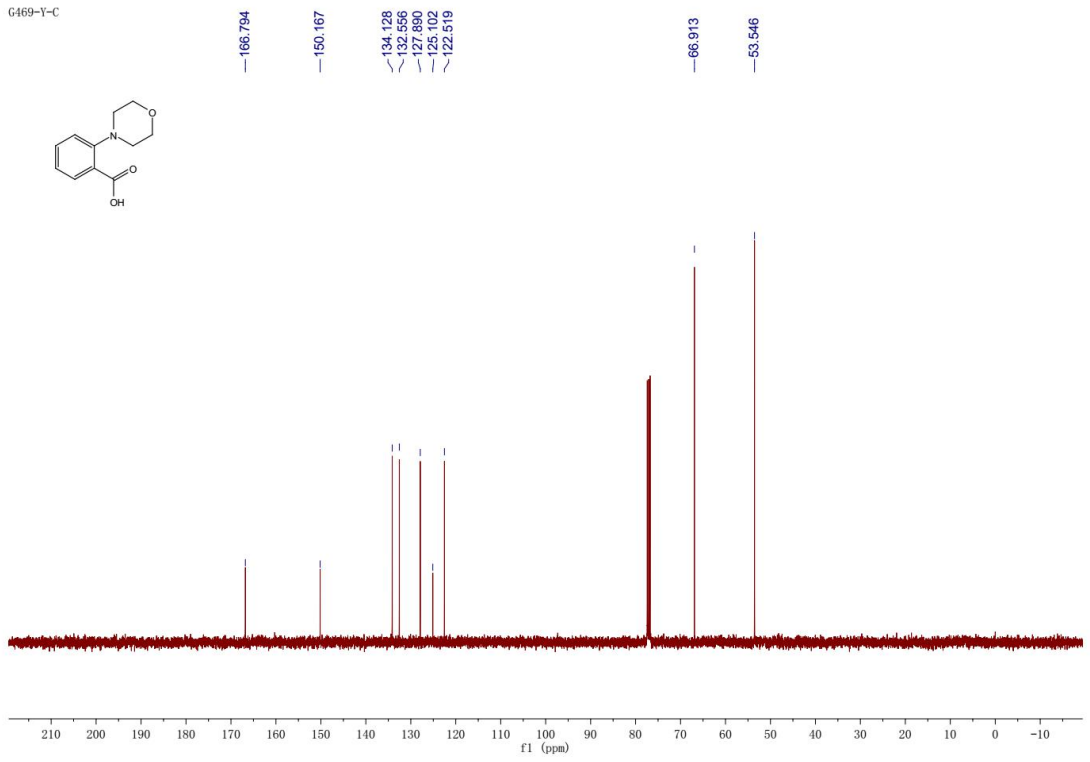
NMR of 1ba


G-447
7.511
7.492
7.280
7.261
7.242
7.107
7.081
7.063
7.044
7.035
7.021
7.001
5.721
5.718
5.677
5.674
5.269
5.265
5.241
5.238
3.868
3.857
3.845
2.968
2.956
2.945
O
N
0.94
1.01
2.81
1.00
0.98
4.02
4.02
f1 (ppm)

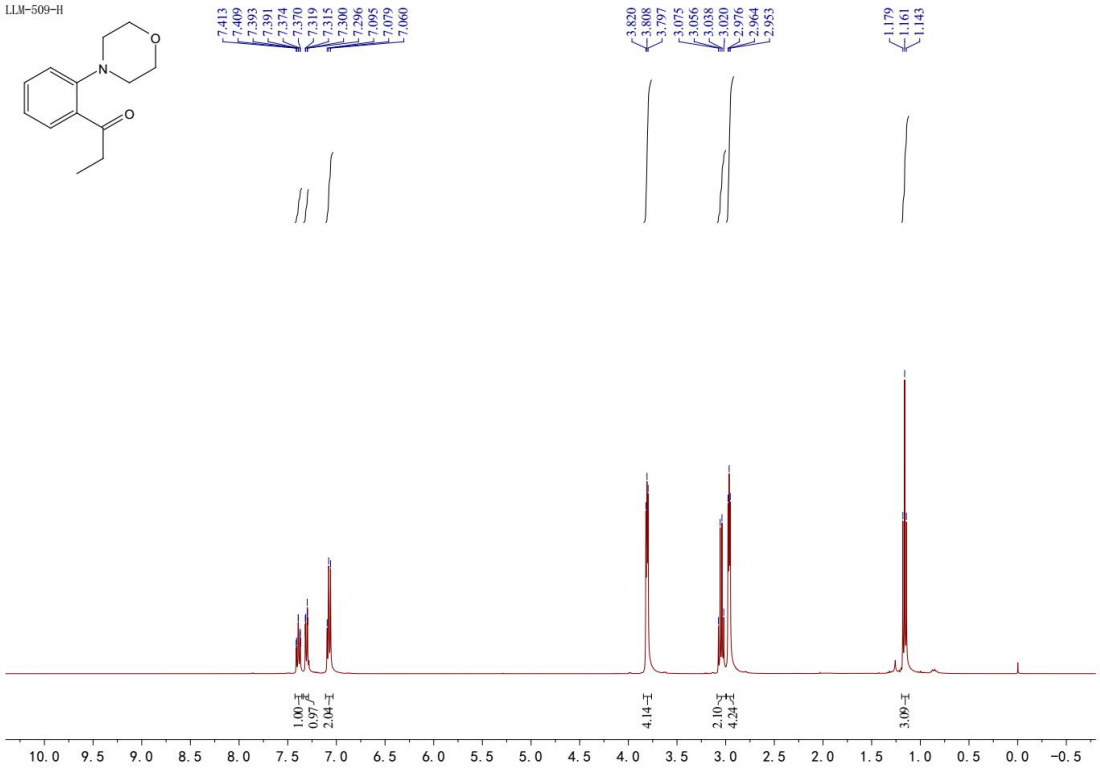

K102-C
150.408
134.155
132.212
128.604
126.907
123.254
118.391
113.810
67.335
52.586
O
N
f1 (ppm)

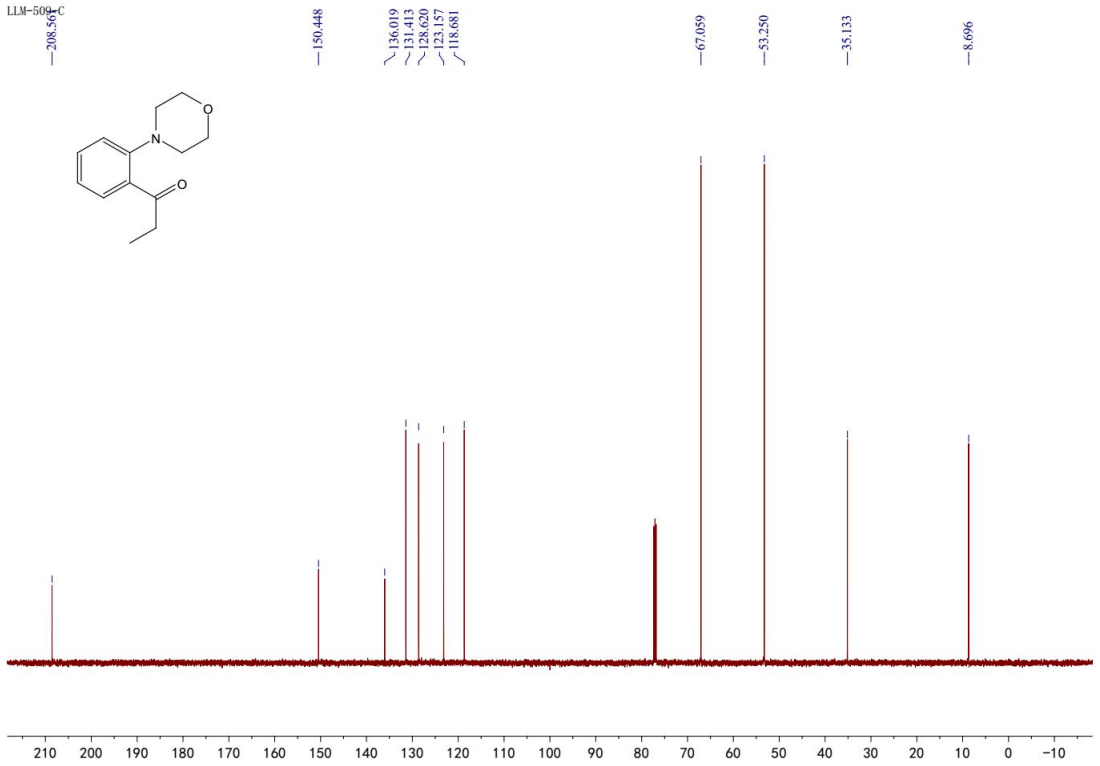
NMR of 1bb


G469-Y-H
8.321
8.317
8.302
8.298
7.661
7.657
7.641
7.639
7.623
7.619
7.473
7.455
7.453
7.437
7.418
7.416
7.282
4.508
3.964
3.089
0.93
0.99
1.95
1.43
4.00
4.04
f1 (ppm)

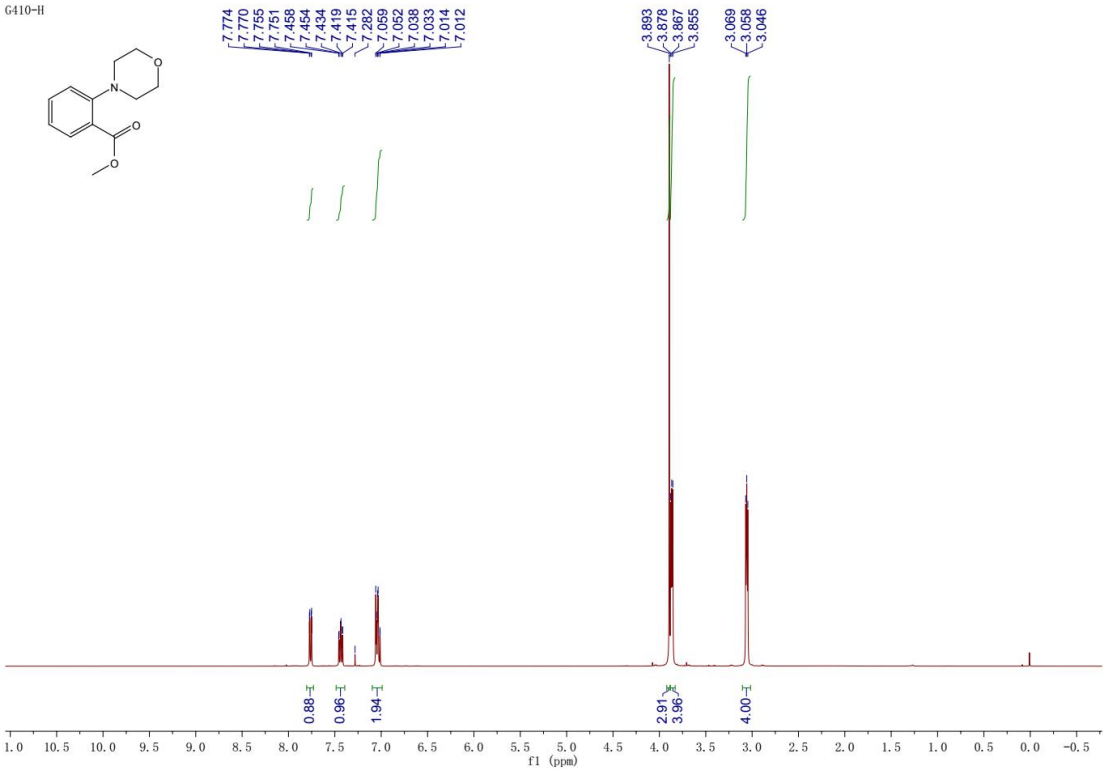

G469-Y-C
166.794
150.167
134.128
132.556
127.890
125.102
122.519
66.913
53.546
f1 (ppm)

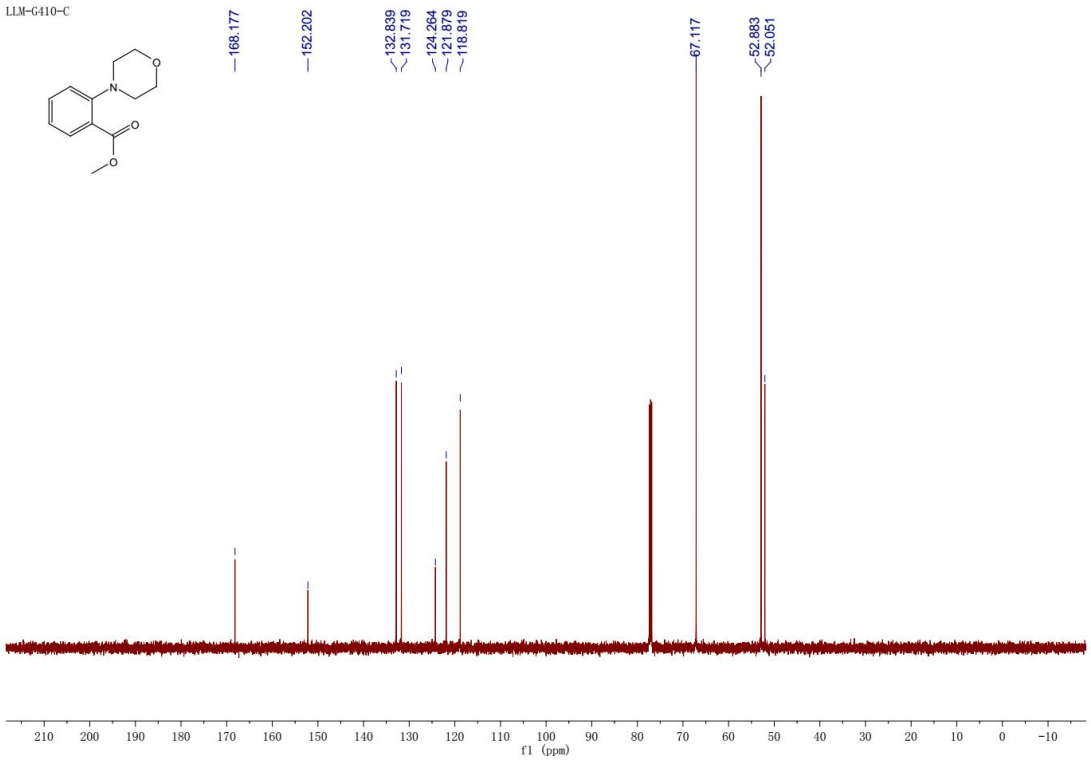
NMR of 1bc


LLM-509-H
7.413
7.409
7.393
7.391
7.374
7.370
7.319
7.315
7.300
7.296
7.095
7.079
7.060
3.820
3.808
3.797
3.075
3.056
3.038
3.020
2.976
2.964
2.953
1.179
1.161
1.143
1.00
0.97
2.04
4.14
2.10
4.24
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5

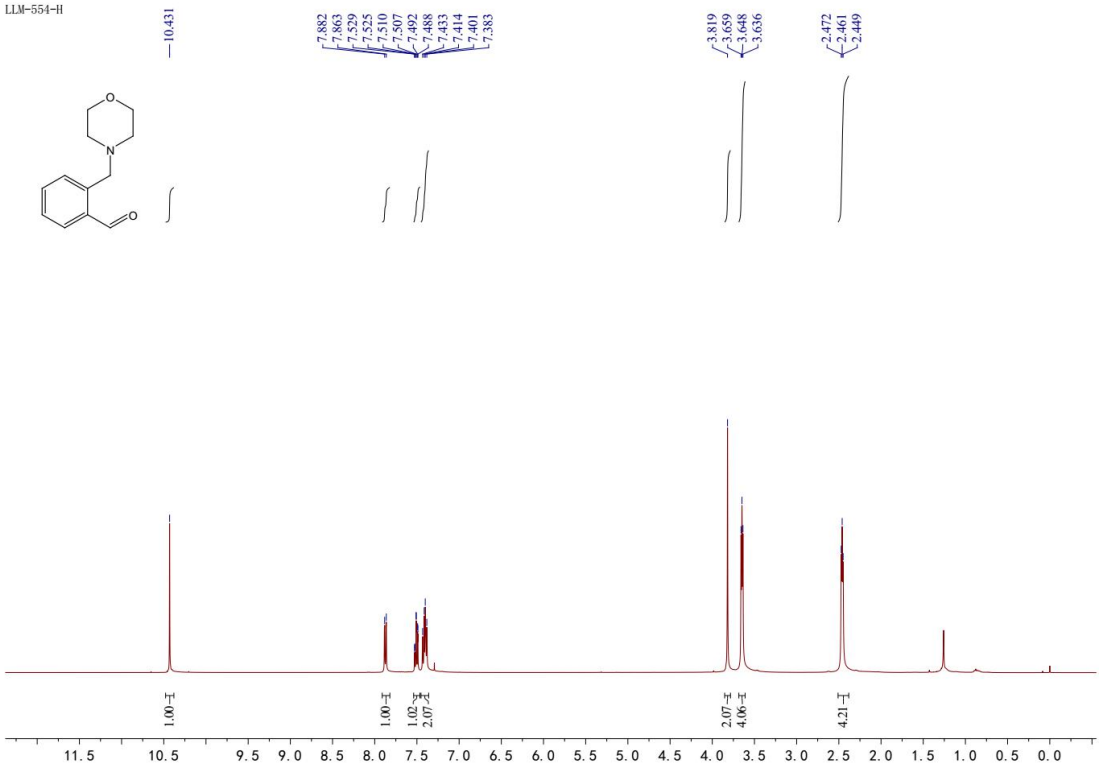

LLM-509-C
208.567
150.448
136.019
131.413
128.620
123.157
118.681
67.059
53.250
35.133
8.696
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10

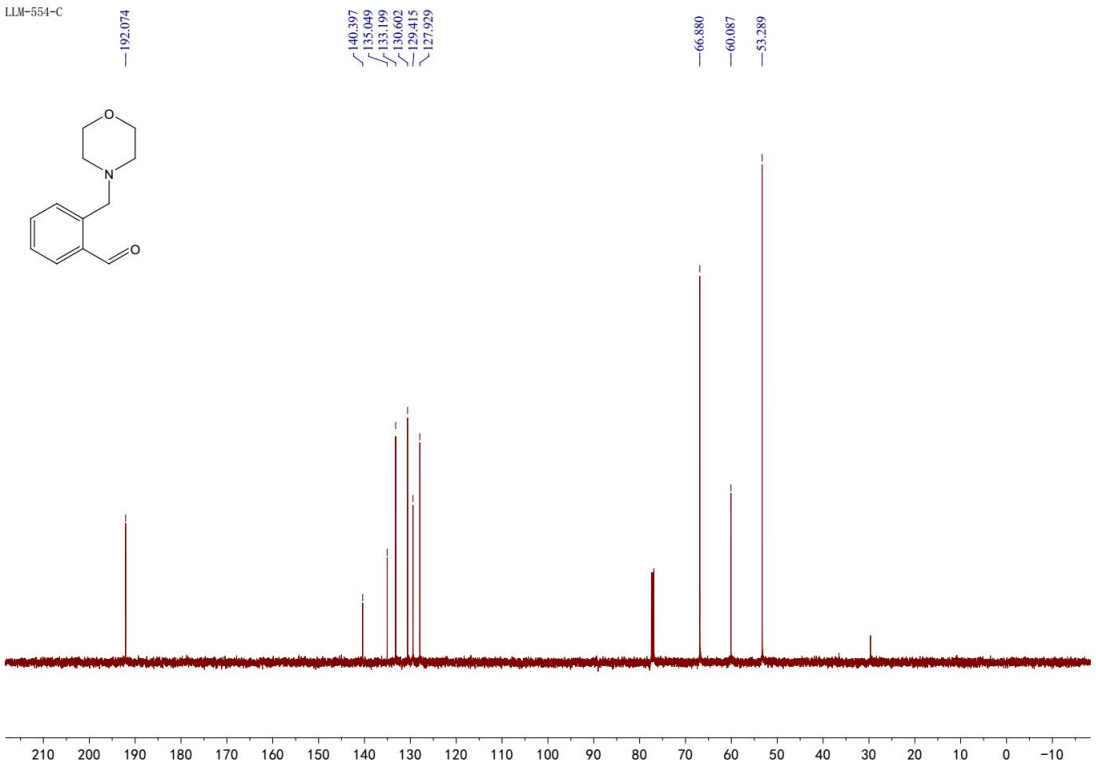
NMR of 1bd


G410-H
7.774
7.770
7.755
7.751
7.458
7.454
7.434
7.419
7.415
7.282
7.059
7.052
7.038
7.033
7.014
7.012
3.893
3.878
3.867
3.855
3.069
3.058
3.046
0.88
0.96
1.94
2.91
3.96
4.00
f1 (ppm)

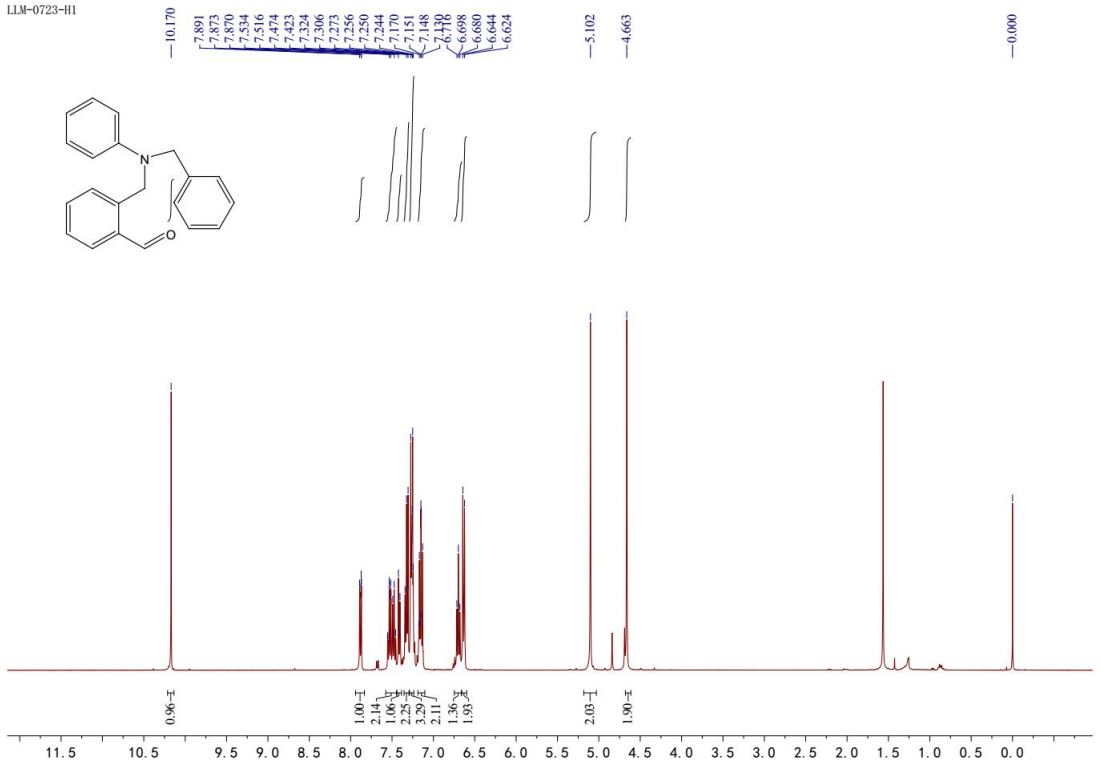

LLM-G410-C
168.177
152.202
132.839
131.719
124.264
121.879
118.819
67.117
52.883
52.051
f1 (ppm)

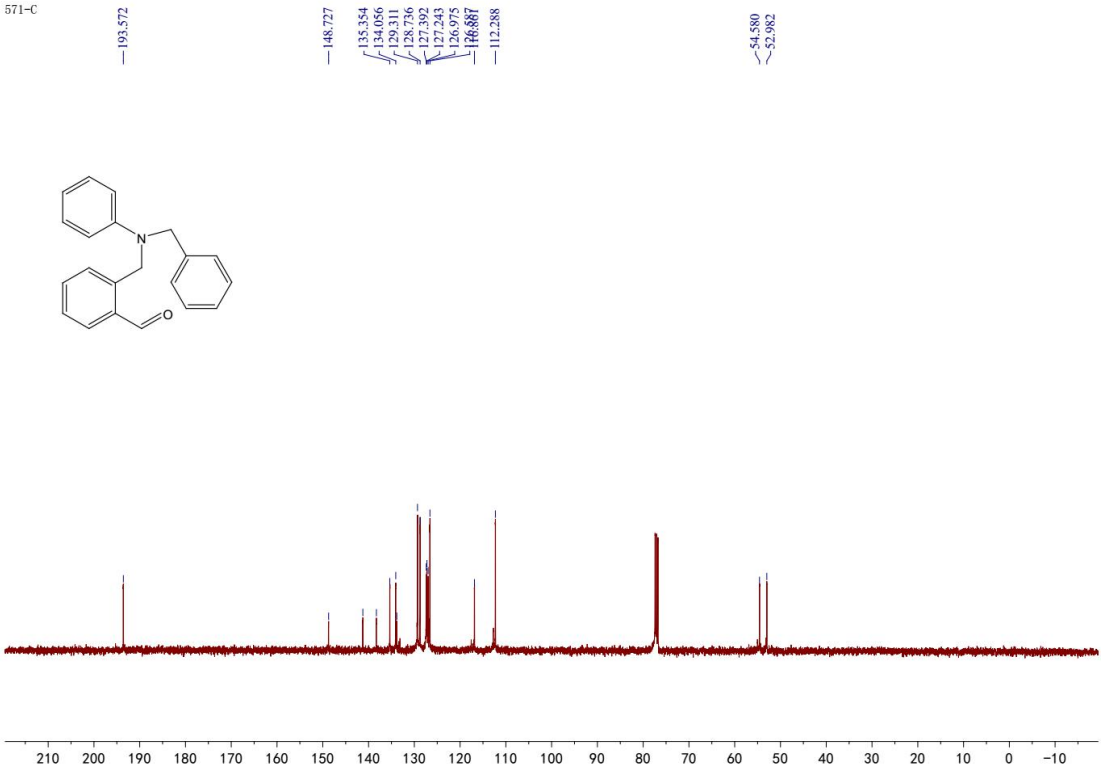
NMR of 1bg


LLM-554-H
10.431
7.882
7.863
7.529
7.525
7.510
7.507
7.492
7.488
7.433
7.414
7.401
7.383
3.819
3.659
3.648
3.636
2.472
2.461
2.449
1.00
1.00
1.02
2.07
2.07
4.06
4.21

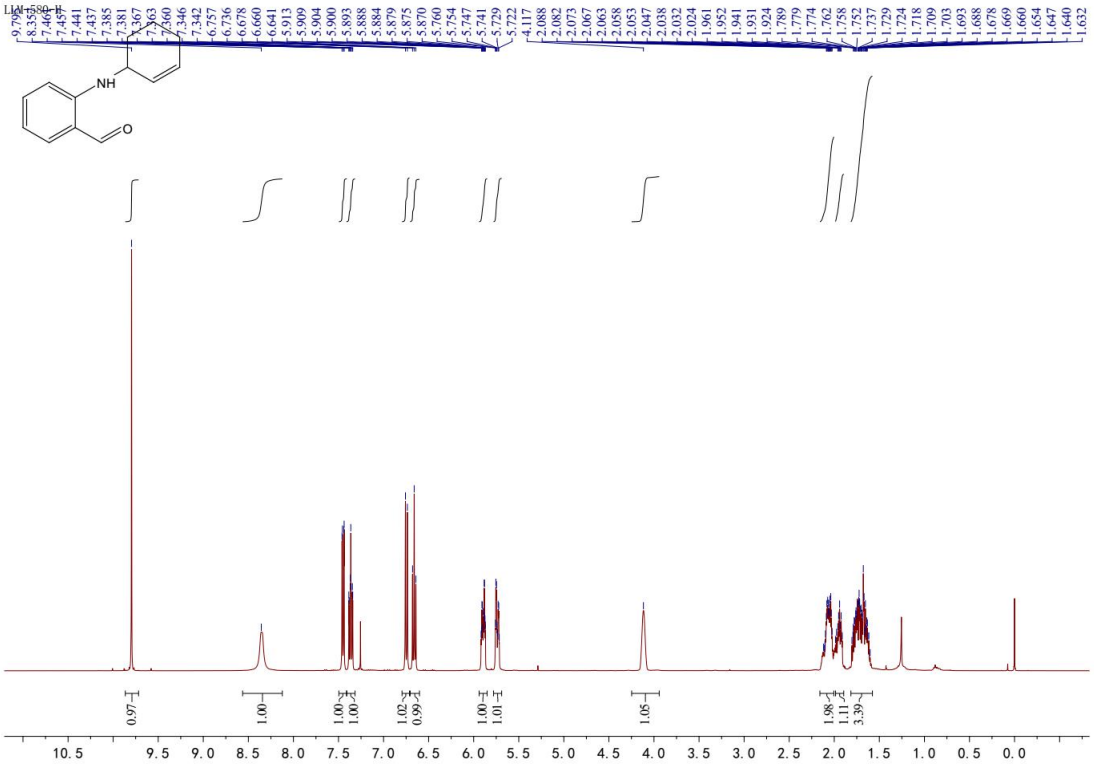

LLM-554-C
192.074
140.397
135.049
133.199
130.602
129.415
127.929
66.880
60.087
53.289

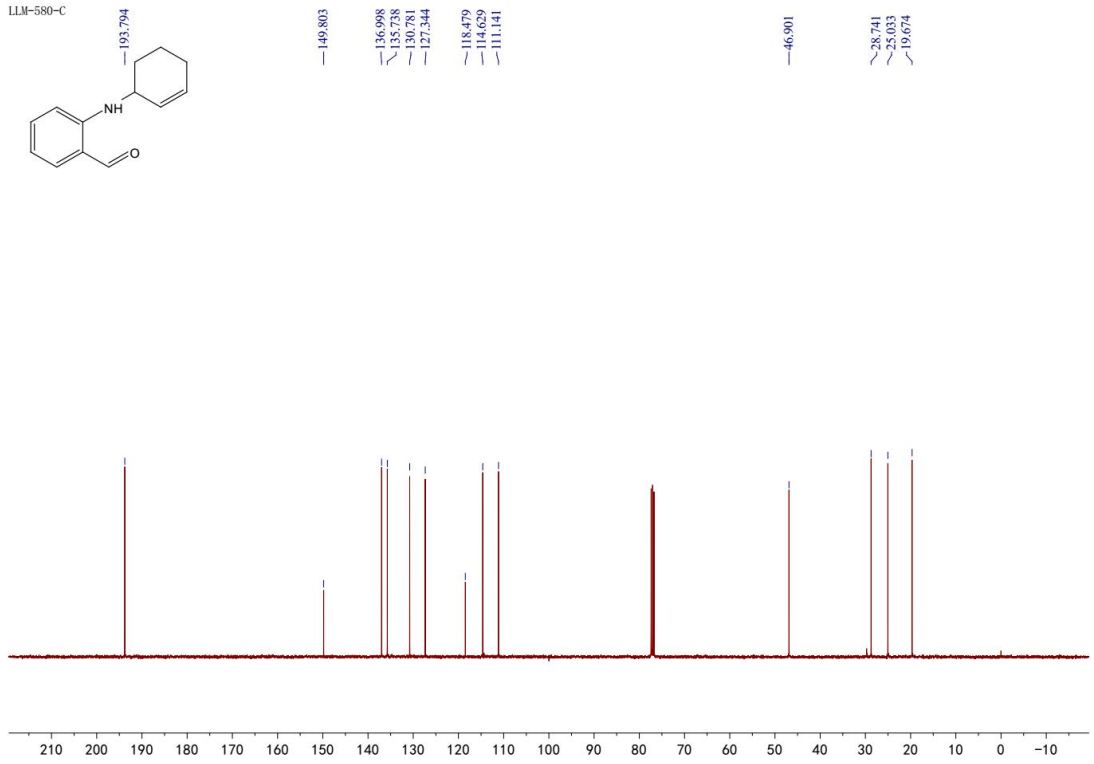
NMR of 1bh


LLM-0723-H1
10.170
7.891
7.873
7.870
7.534
7.516
7.474
7.423
7.324
7.306
7.273
7.256
7.250
7.244
7.170
7.151
7.148
6.698
6.680
6.644
6.624
5.102
4.663
0.000
0.96
1.00
2.14
1.06
2.25
3.29
2.11
1.36
1.93
2.03
1.90
11.5
10.5
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

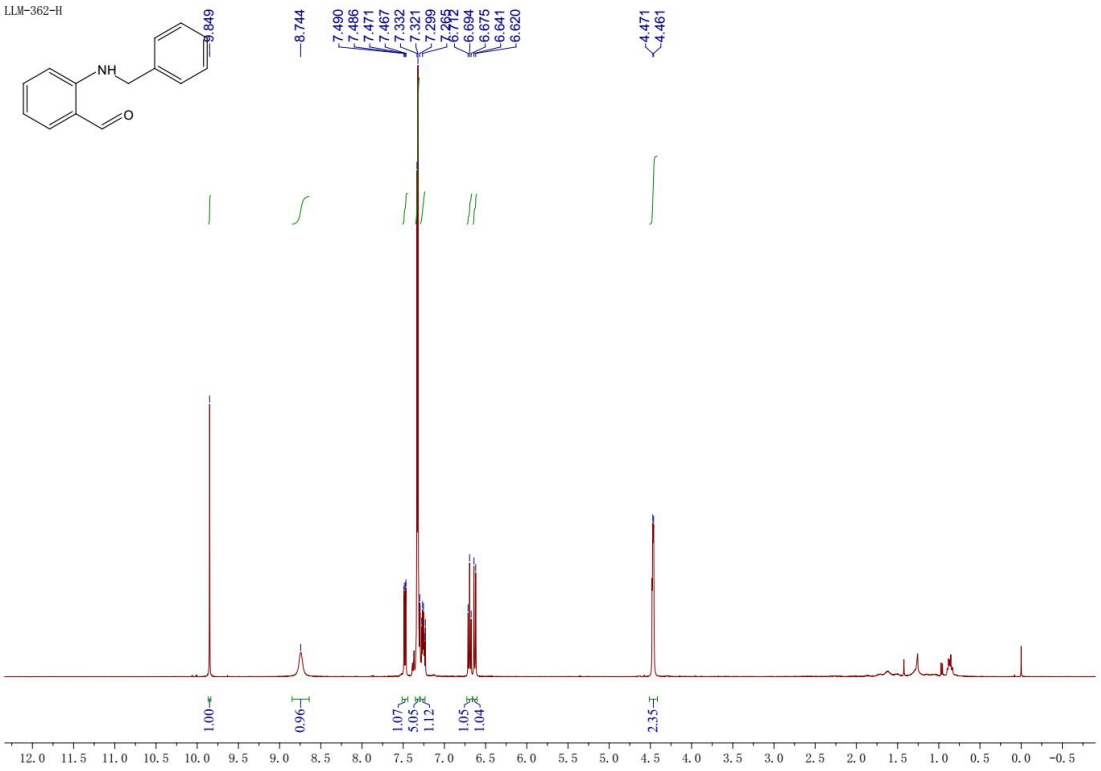

571-C
193.572
148.727
135.354
134.056
129.311
128.736
127.392
127.243
126.975
112.288
54.580
52.982
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

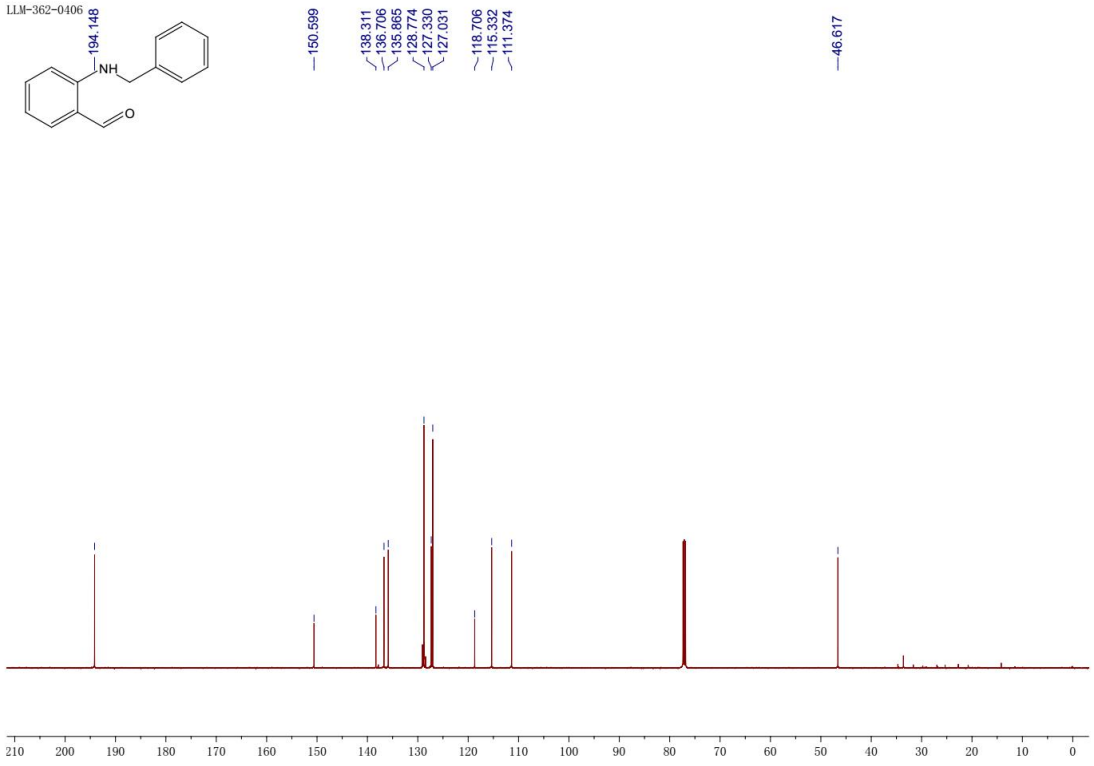
NMR of 1bi


LLM-580-H
NH
O
0.97
1.00
1.00
1.00
1.02
0.99
1.00
1.01
1.05
1.98
1.11
3.39
10.5
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

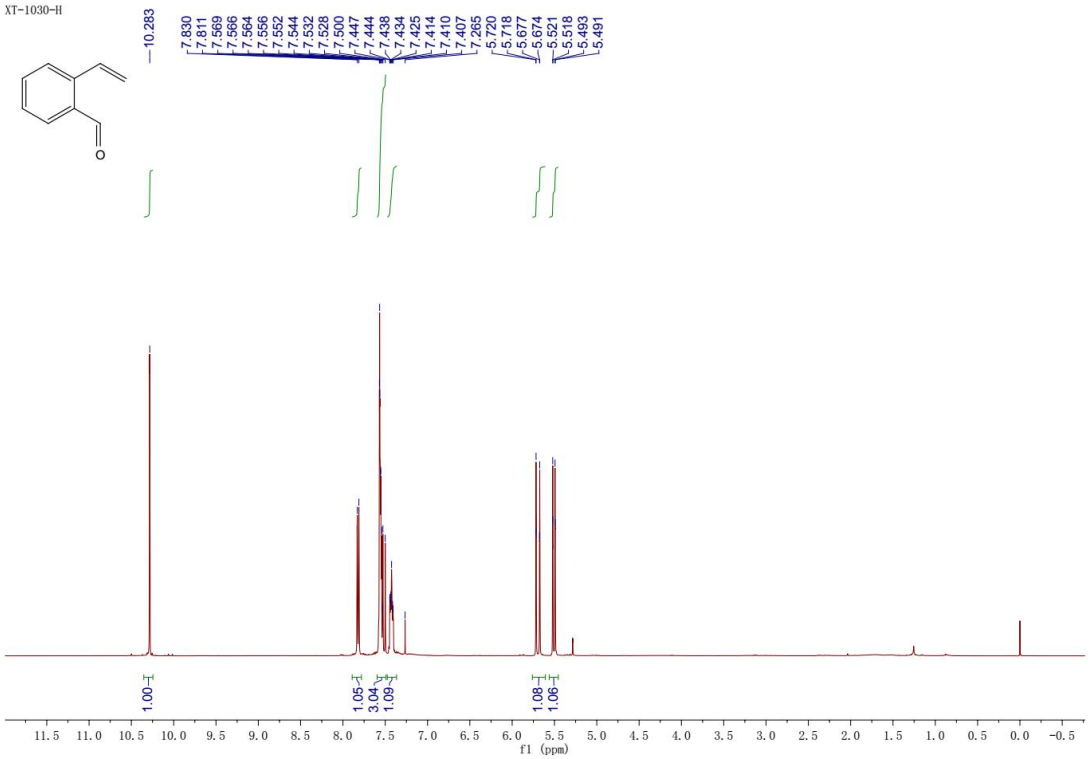

LLM-580-C
193.794
149.803
136.998
135.738
130.781
127.344
118.479
114.629
111.141
46.901
28.741
25.033
19.674
NH
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

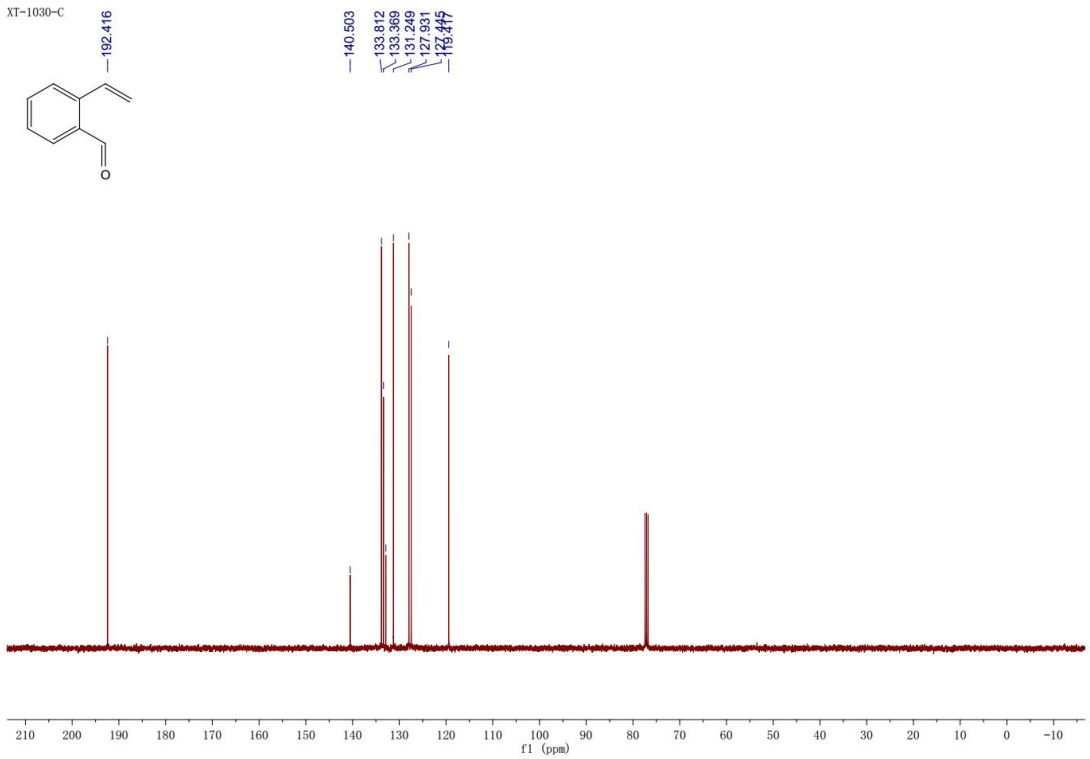
NMR of 1bj


LLM-362-H
NH
O
9.849
8.744
7.490
7.486
7.471
7.467
7.332
7.321
7.299
7.265
6.712
6.694
6.675
6.641
6.620
4.471
4.461
1.00
0.96
1.07
5.05
1.12
1.05
1.04
2.35
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 -0.5

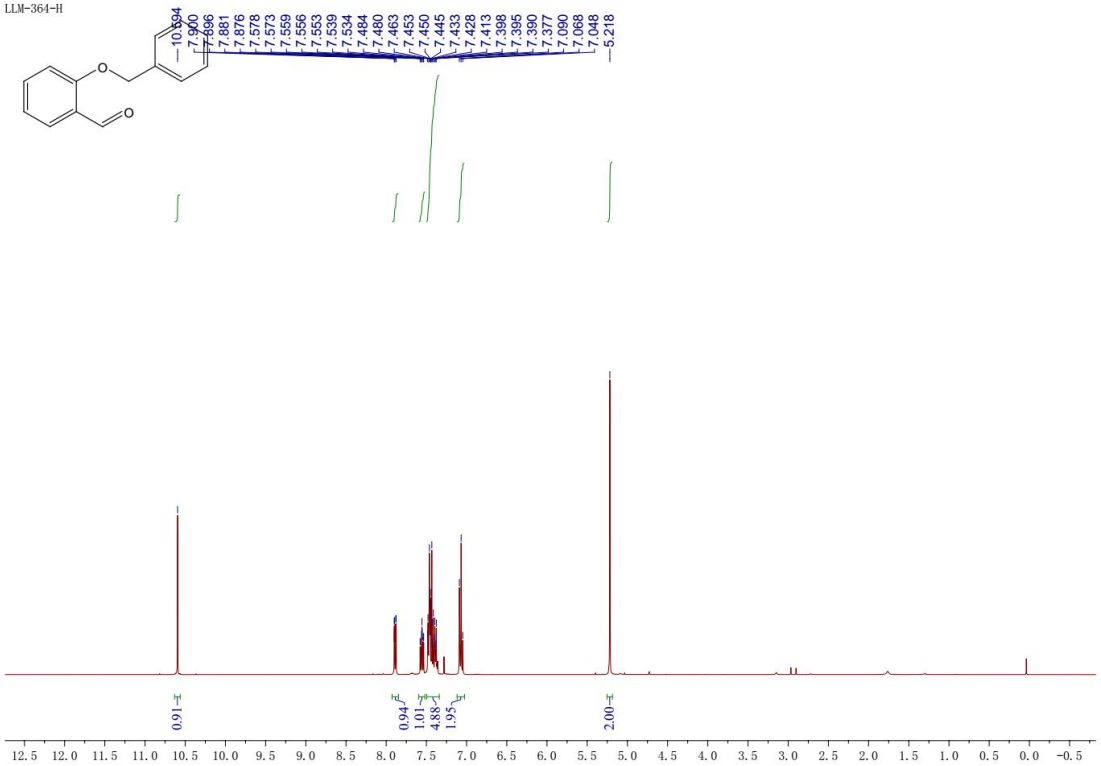

LLM-362-0406
194.148
NH
O
150.599
138.311
136.706
135.865
128.774
127.330
127.031
118.706
115.332
111.374
46.617
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

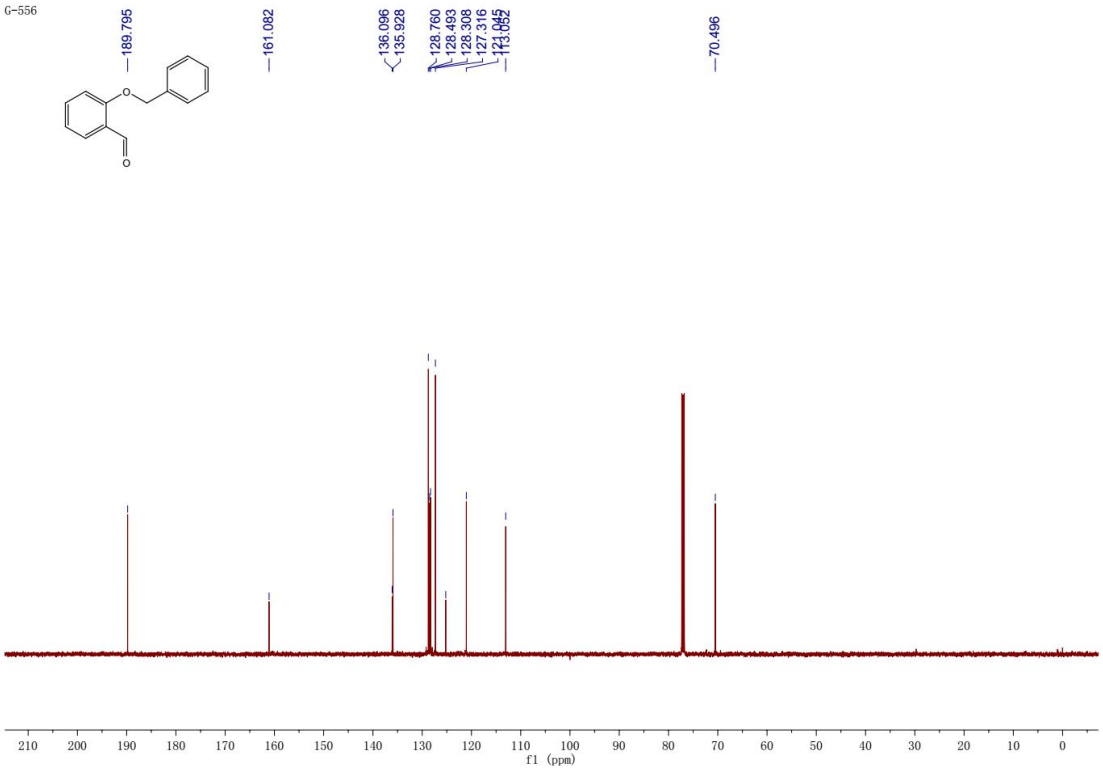
NMR of 1bk


XT-1030-H
10.283
7.830
7.811
7.569
7.566
7.564
7.556
7.552
7.544
7.532
7.528
7.500
7.447
7.444
7.438
7.434
7.425
7.414
7.410
7.407
7.265
5.720
5.718
5.677
5.674
5.521
5.518
5.493
5.491
O
1.00
1.05
3.04
1.09
1.08
1.06
f1 (ppm)

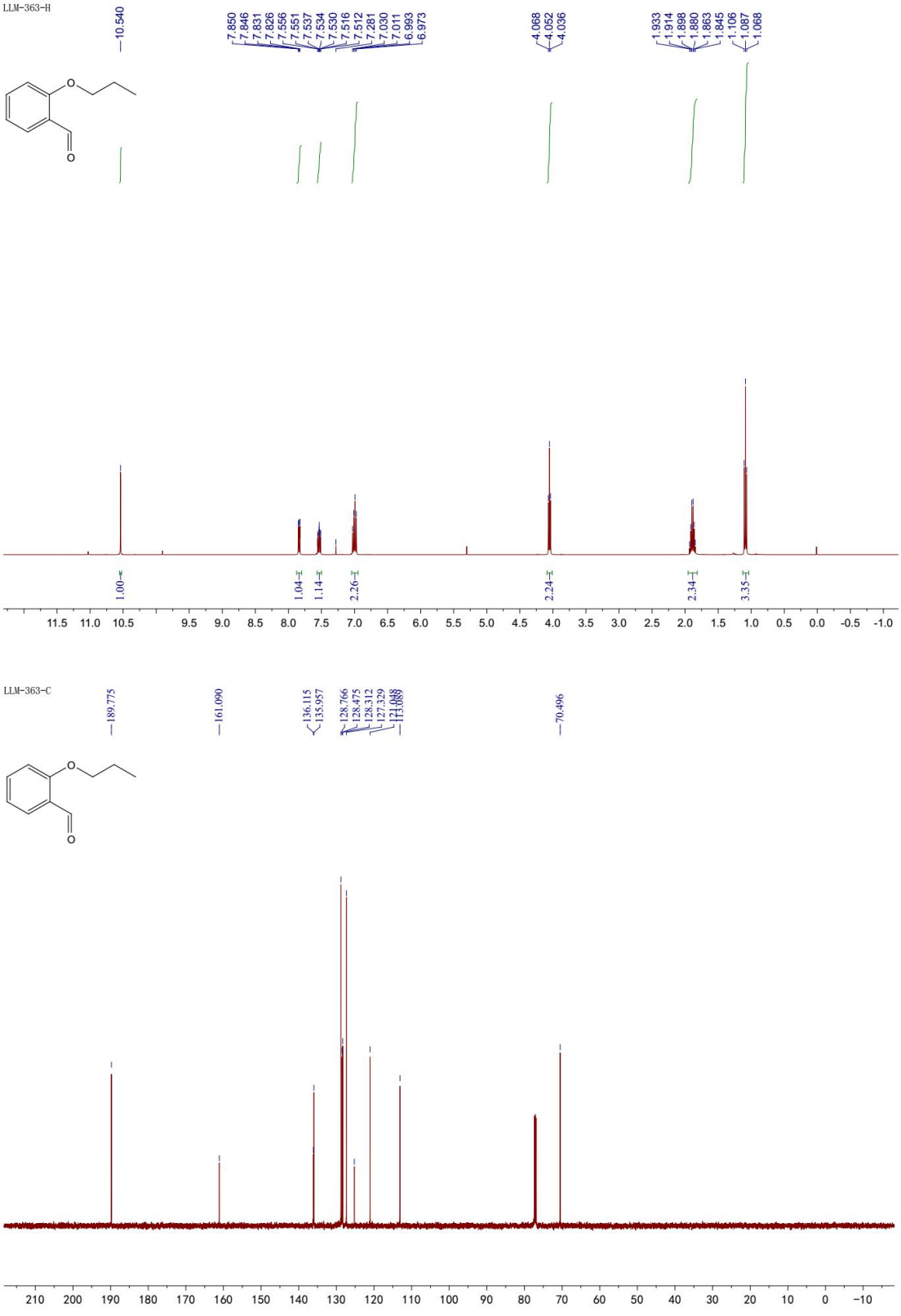

XT-1030-C
192.416
140.503
133.812
133.389
131.249
127.931
O
f1 (ppm)

NMR of 1bl

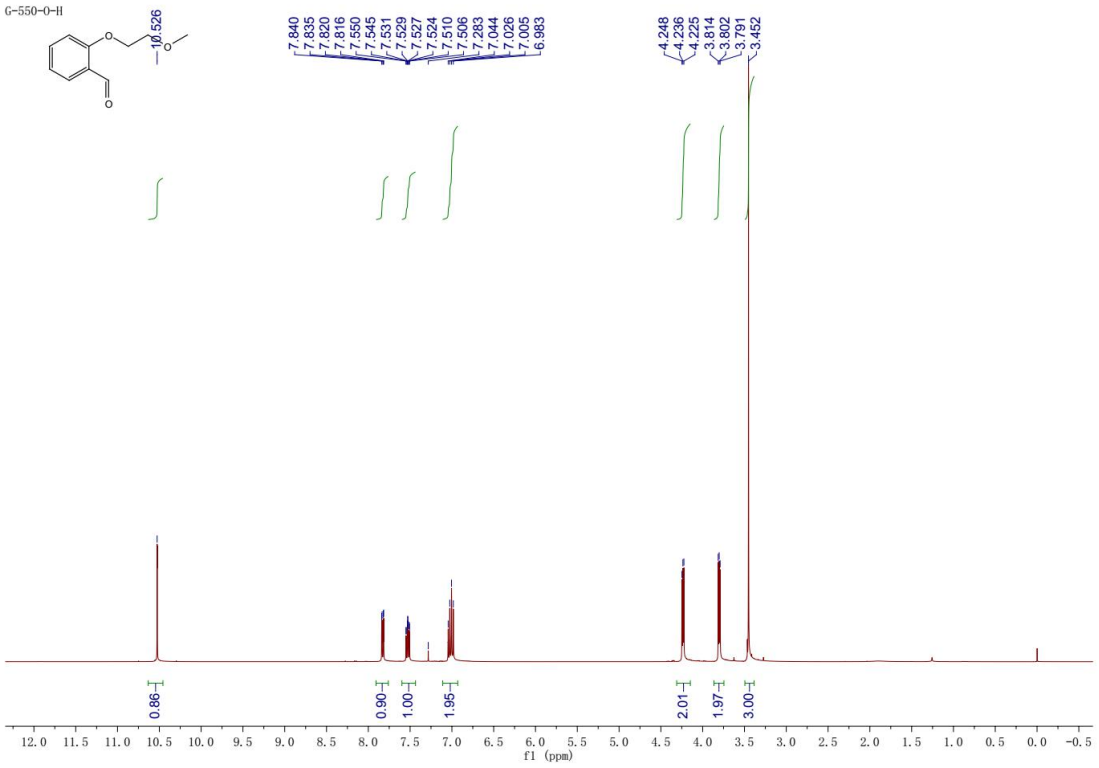

LLM-364-H
10.504
7.900
7.896
7.881
7.876
7.578
7.573
7.559
7.556
7.553
7.539
7.534
7.484
7.480
7.463
7.453
7.450
7.445
7.433
7.428
7.413
7.398
7.395
7.390
7.377
7.090
7.068
7.048
5.218
0.91
0.94
1.01
4.88
1.95
2.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

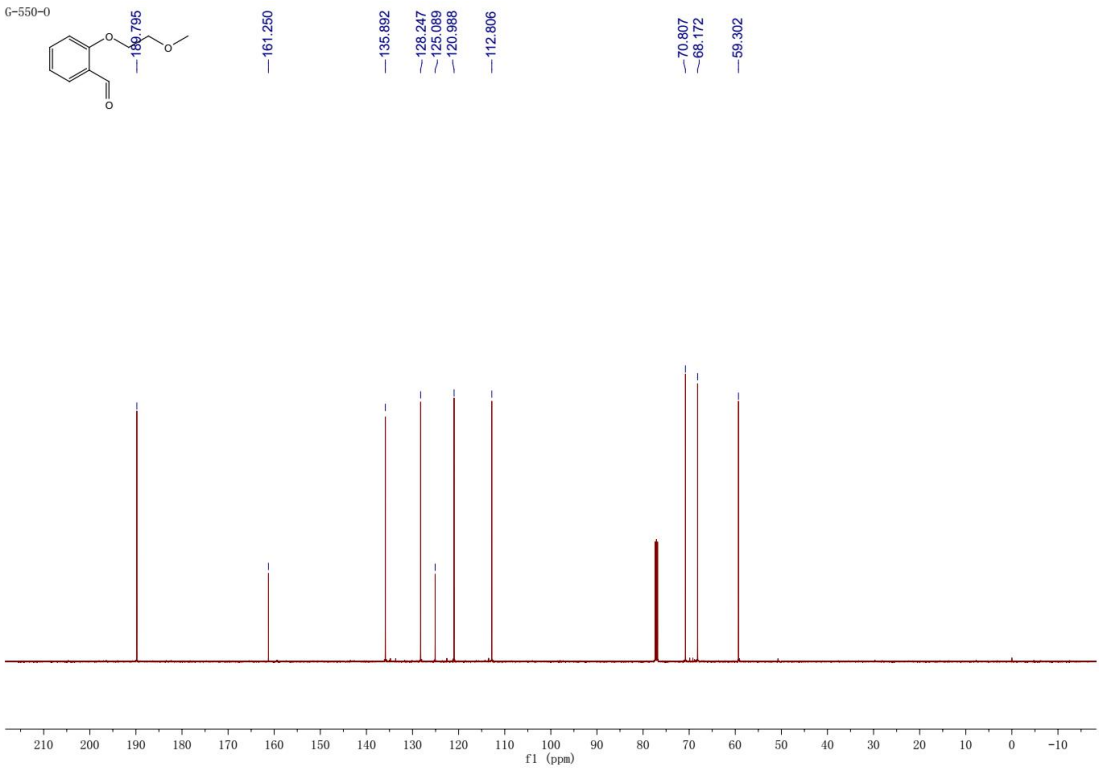

G-556
189.795
161.082
136.096
135.928
128.760
128.493
128.308
127.316
113.045
113.032
70.496
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

NMR of 1bm

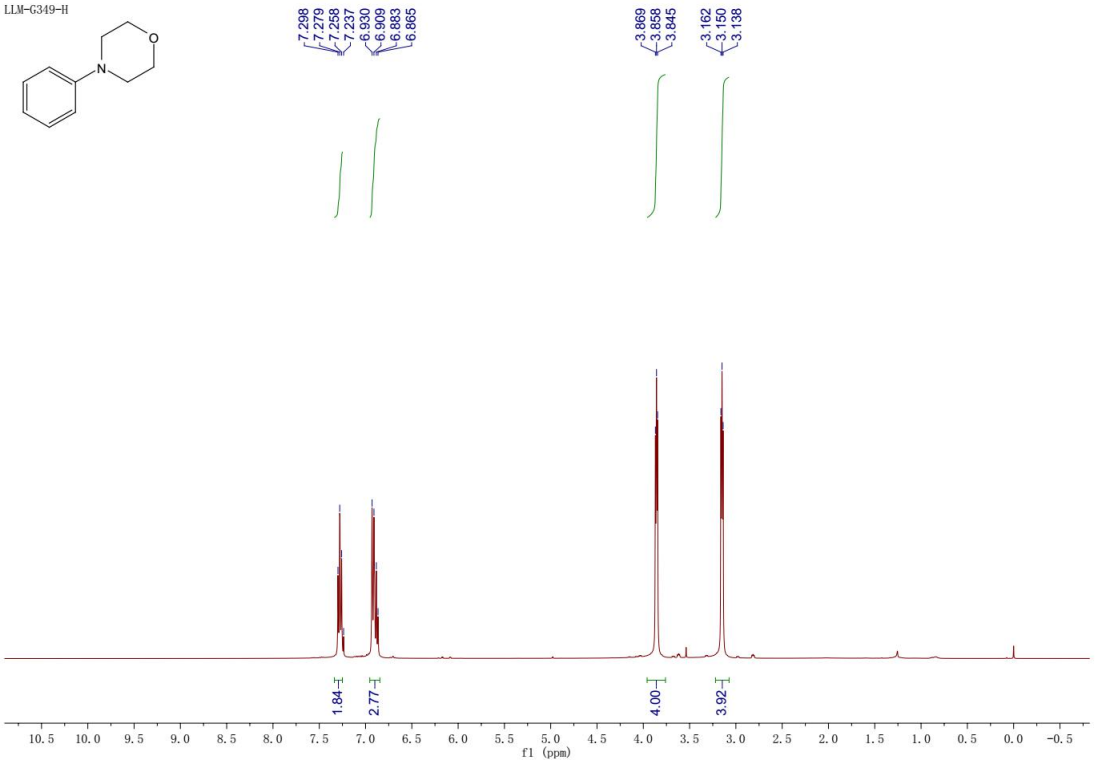

LLM-363-H
10.540
7.850
7.846
7.831
7.826
7.556
7.551
7.537
7.534
7.530
7.516
7.512
7.281
7.030
7.011
6.993
6.973
4.068
4.052
4.036
1.933
1.914
1.898
1.880
1.863
1.845
1.106
1.087
1.068
1.00
1.04
1.14
2.26
2.24
2.34
3.35
LLM-363-C
189.775
161.090
136.115
135.957
128.766
128.475
128.312
127.329
70.496

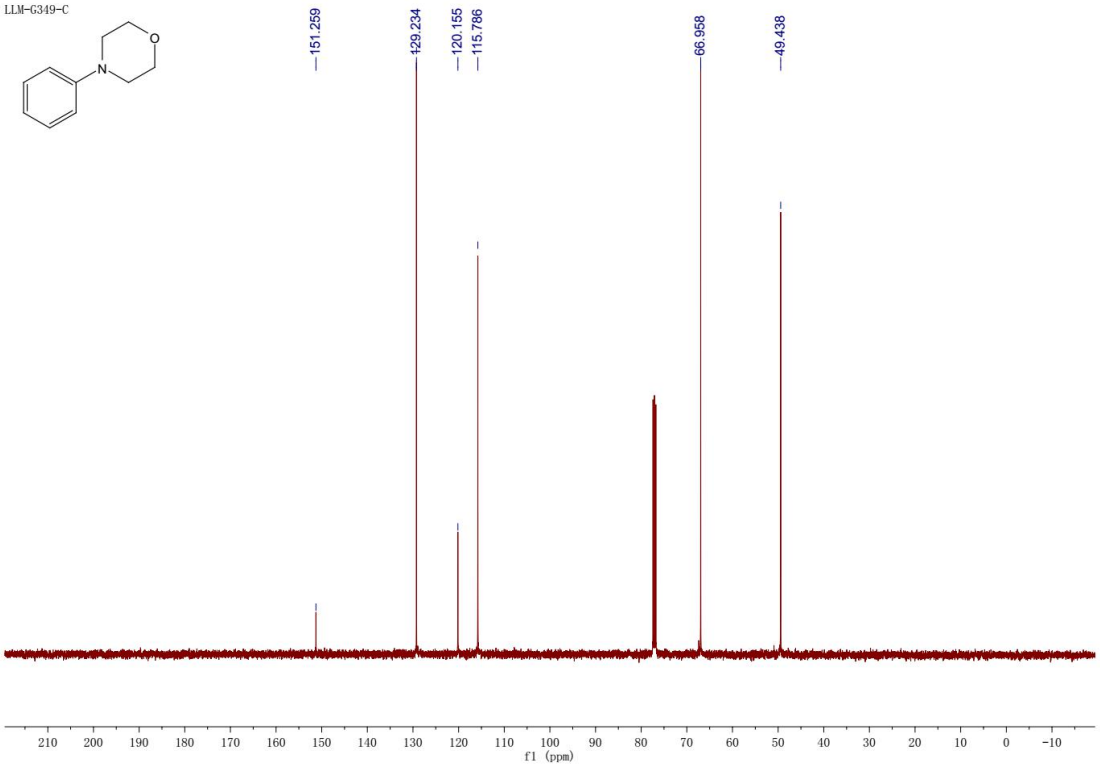
NMR of 1bn


G-550-O-H
10.526
7.840
7.835
7.820
7.816
7.550
7.545
7.531
7.529
7.527
7.524
7.510
7.506
7.283
7.044
7.026
7.005
6.983
4.248
4.236
4.225
3.814
3.802
3.791
3.452
0.86
0.90
1.00
1.95
2.01
1.97
3.00
f1 (ppm)

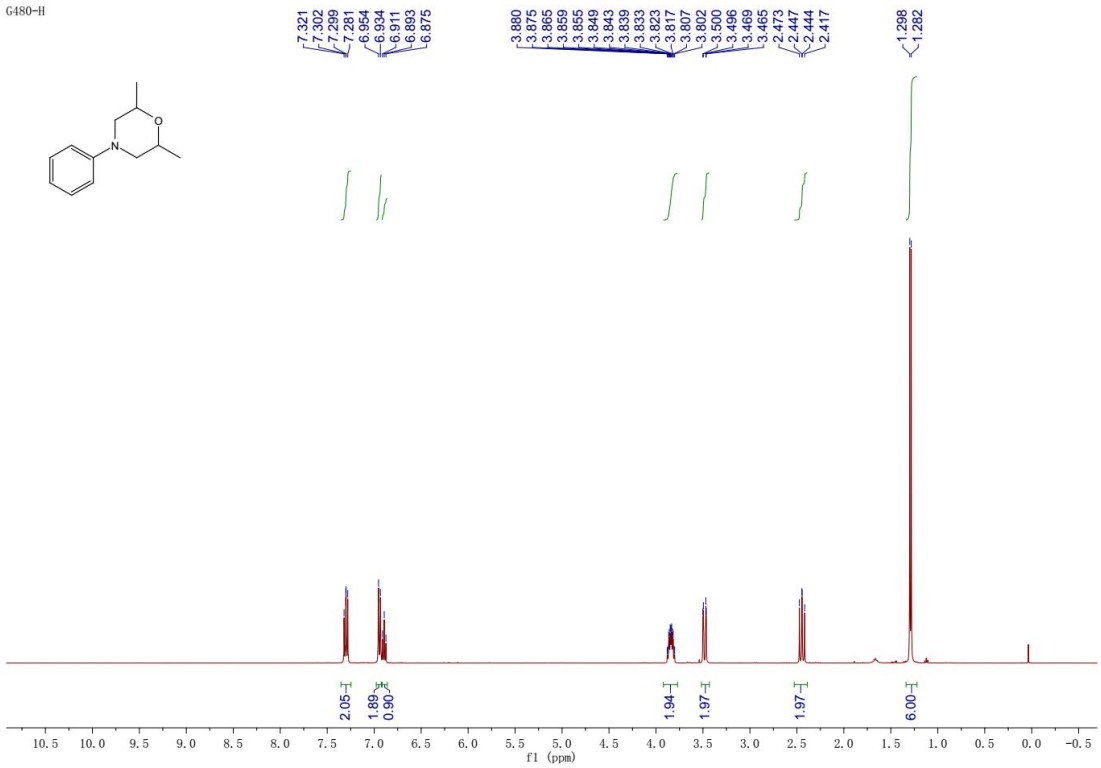

G-550-O
190.795
161.250
135.892
128.247
125.089
120.988
112.806
70.807
68.172
59.302
f1 (ppm)

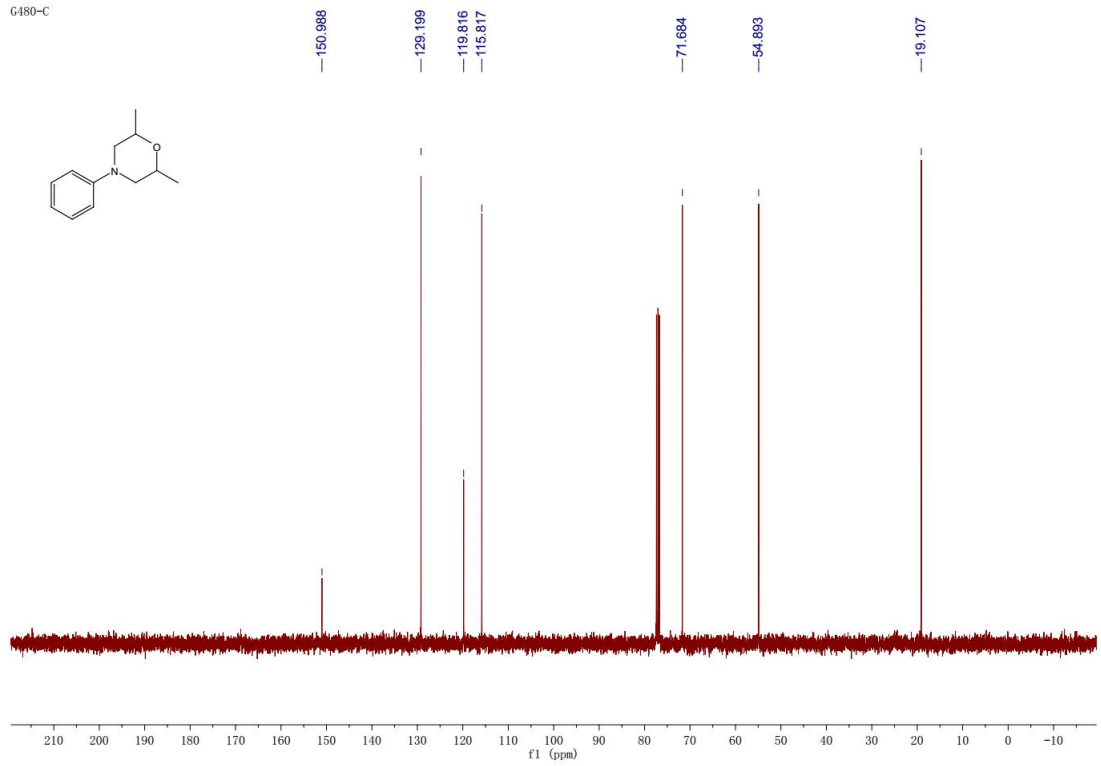
NMR of 2a


LLM-G349-H
7.298
7.279
7.258
7.237
6.930
6.909
6.883
6.865
3.869
3.858
3.845
3.162
3.150
3.138
1.84
2.77
4.00
3.92
f1 (ppm)

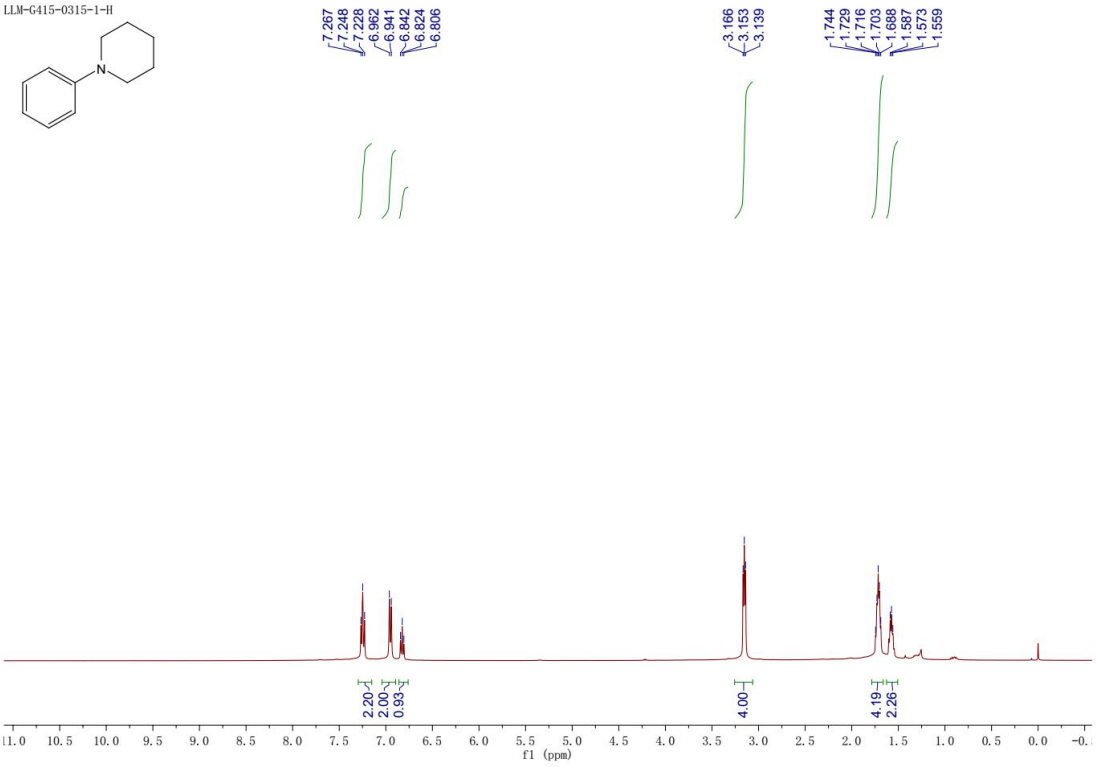

LLM-G349-C
151.259
129.234
120.155
115.786
66.958
49.438
f1 (ppm)

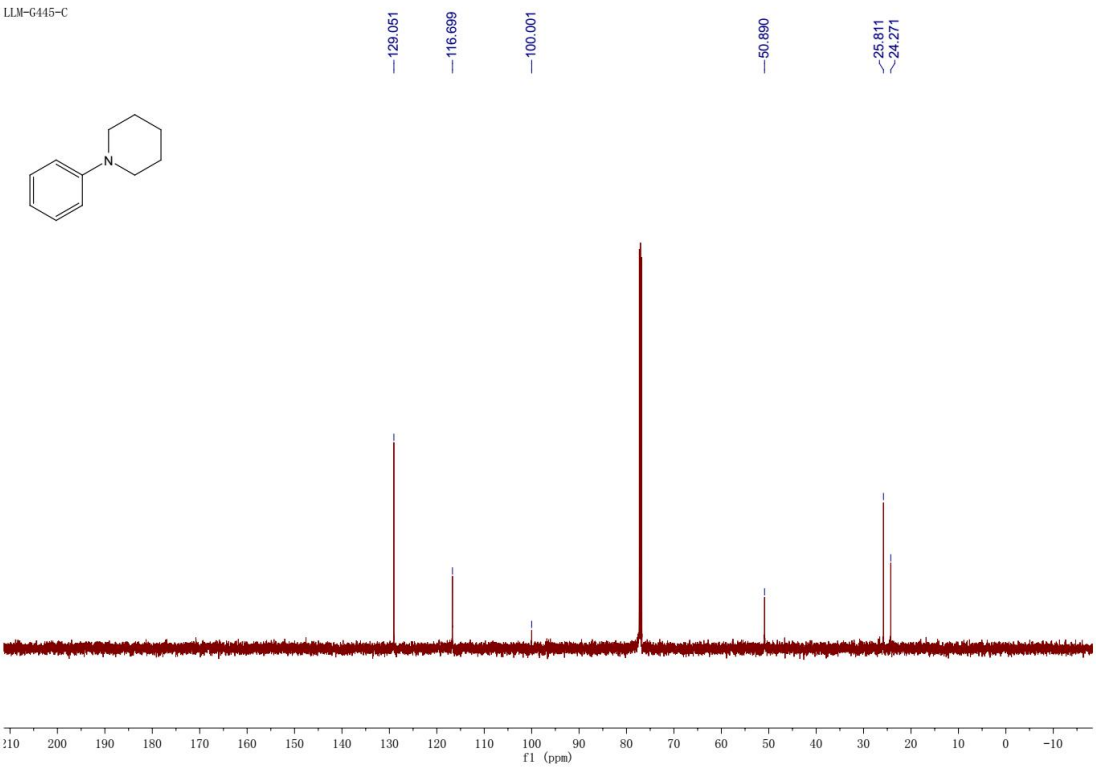
NMR of 2b


G480-H
7.321
7.302
7.299
7.281
6.954
6.934
6.911
6.893
6.875
3.880
3.875
3.865
3.859
3.855
3.849
3.843
3.839
3.833
3.823
3.817
3.807
3.802
3.500
3.496
3.469
3.465
2.473
2.447
2.444
2.417
1.298
1.282
2.05
1.89
0.90
1.94
1.97
1.97
6.00
f1 (ppm)

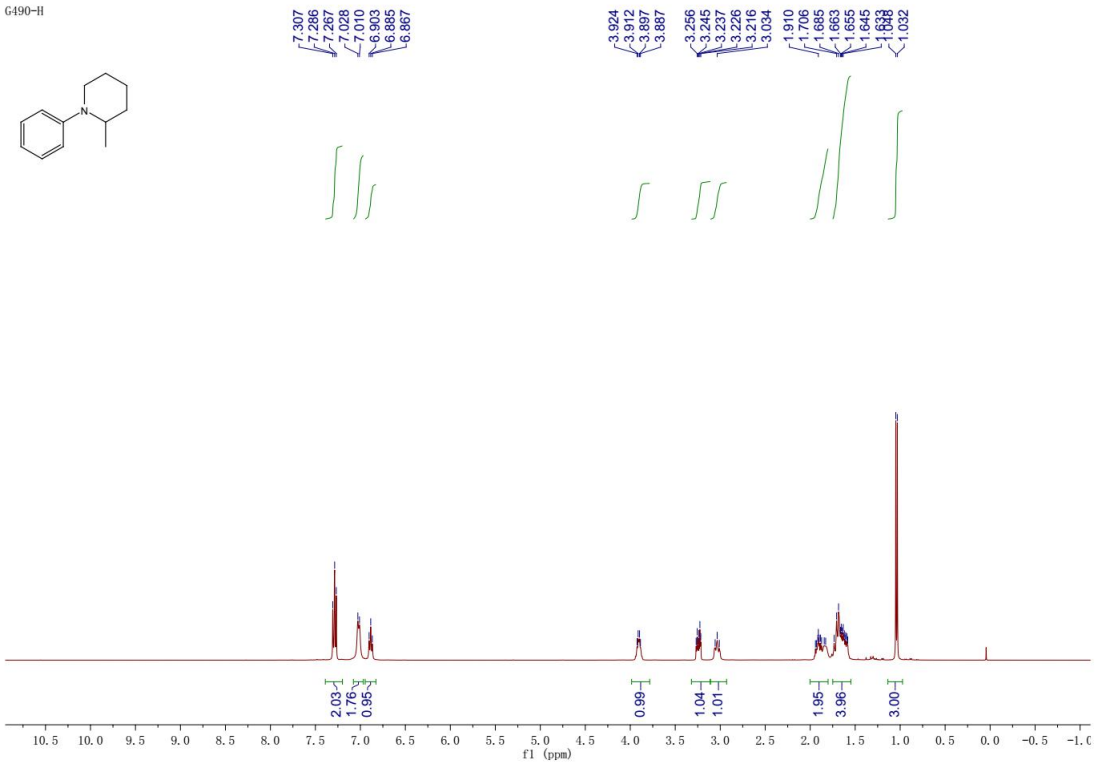

G480-C
150.988
129.199
119.816
115.817
71.684
54.893
19.107
f1 (ppm)

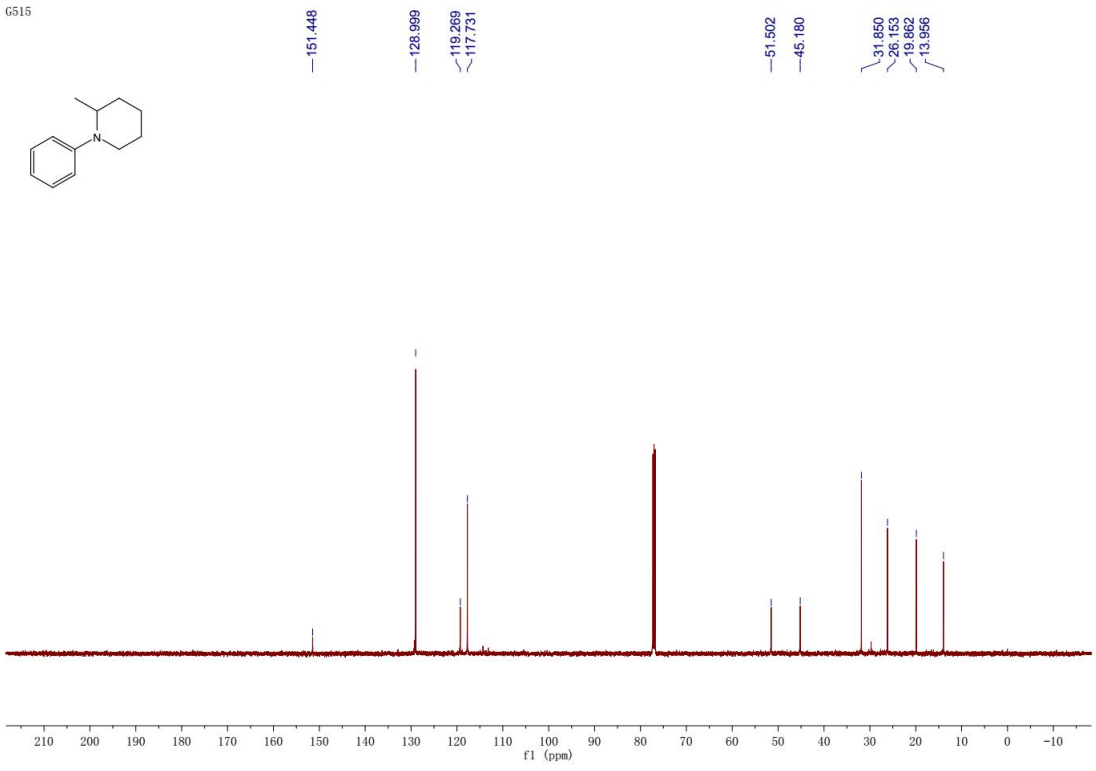
NMR of 2c


LLM-G415-0315-1-H
7.267
7.248
7.228
6.962
6.941
6.842
6.824
6.806
3.166
3.153
3.139
1.744
1.729
1.716
1.703
1.688
1.587
1.573
1.559
2.20
2.00
0.93
4.00
4.19
2.26
f1 (ppm)

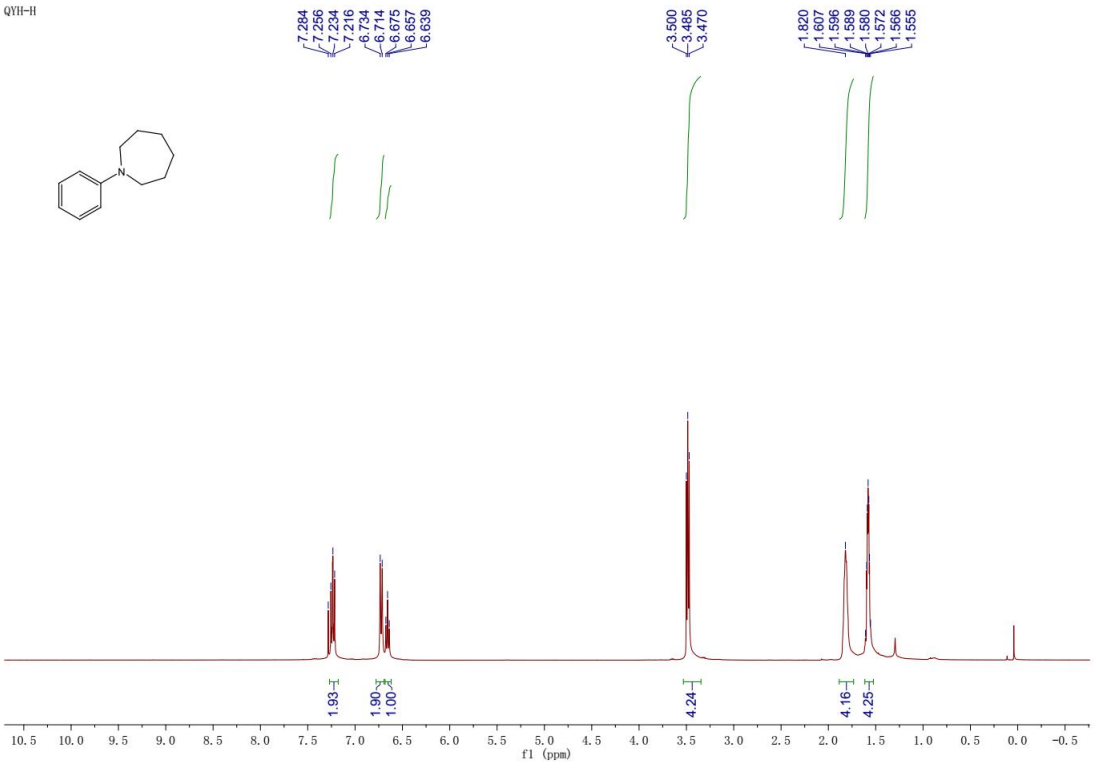

LLM-G445-C
129.051
116.699
100.001
50.890
25.811
24.271
f1 (ppm)

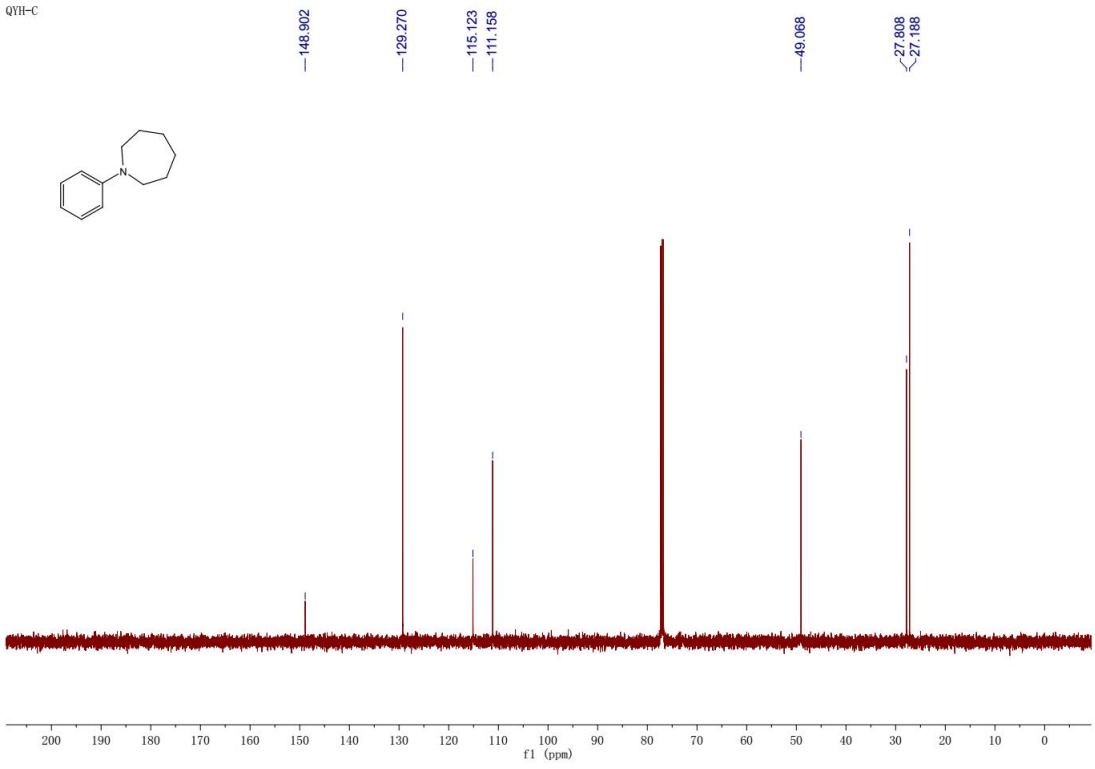
NMR of 2d


G490-H
7.307
7.286
7.267
7.028
7.010
6.903
6.885
6.867
3.924
3.912
3.897
3.887
3.256
3.245
3.237
3.226
3.216
3.034
1.910
1.706
1.685
1.663
1.655
1.645
1.633
1.048
1.032
2.03
1.76
0.95
0.99
1.04
1.01
1.95
3.96
3.00
f1 (ppm)

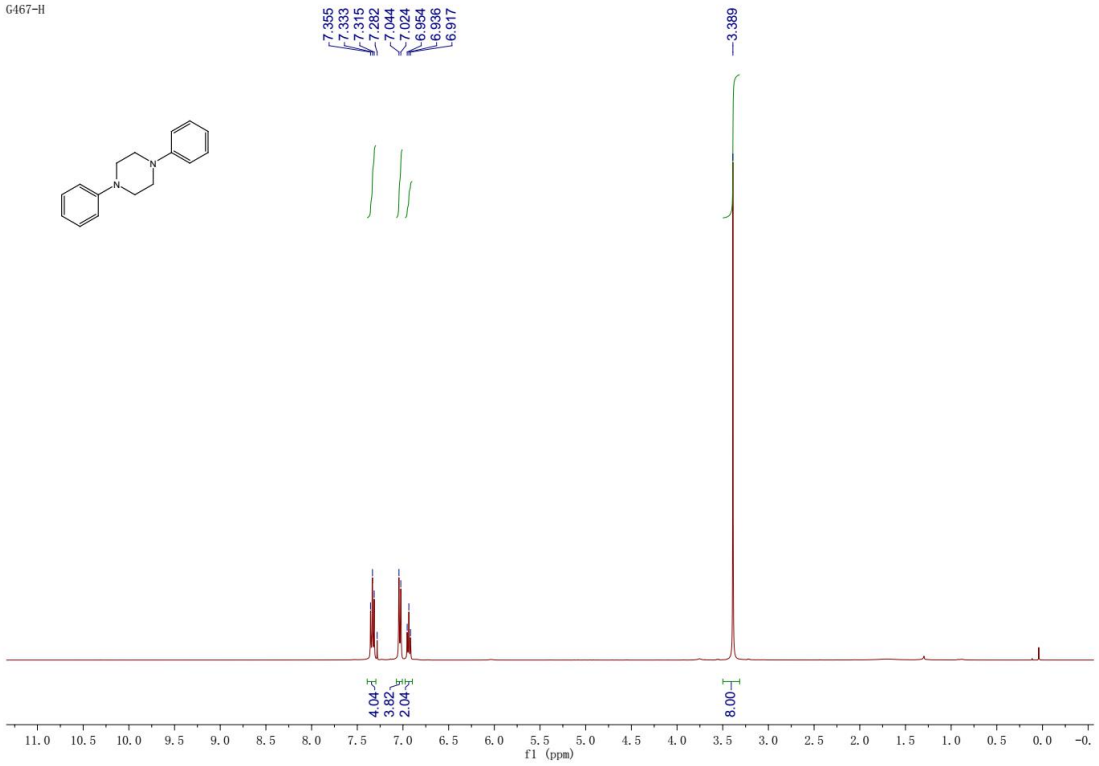

G515
151.448
128.999
119.269
117.731
51.502
45.180
31.850
26.153
19.862
13.956
f1 (ppm)

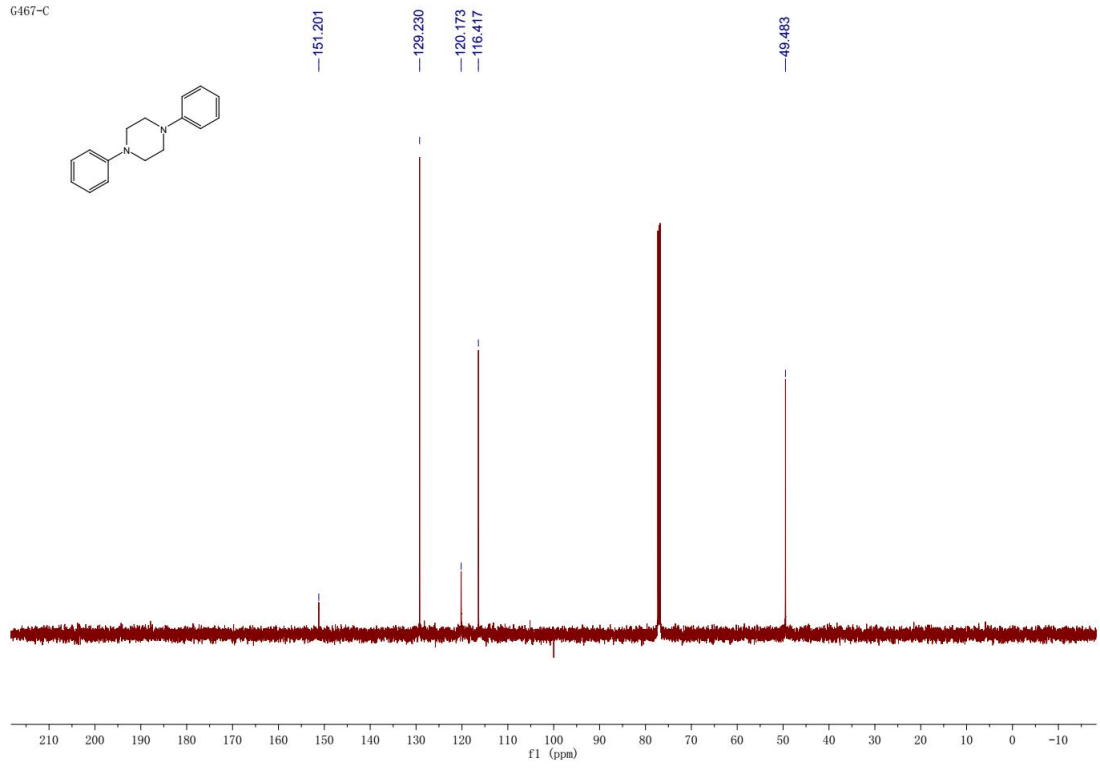
NMR of 2e


QYH-H
7.284
7.256
7.234
7.216
6.734
6.714
6.675
6.657
6.639
3.500
3.485
3.470
1.820
1.607
1.596
1.589
1.580
1.572
1.566
1.555
1.93
1.90
1.00
4.24
4.16
4.25
f1 (ppm)

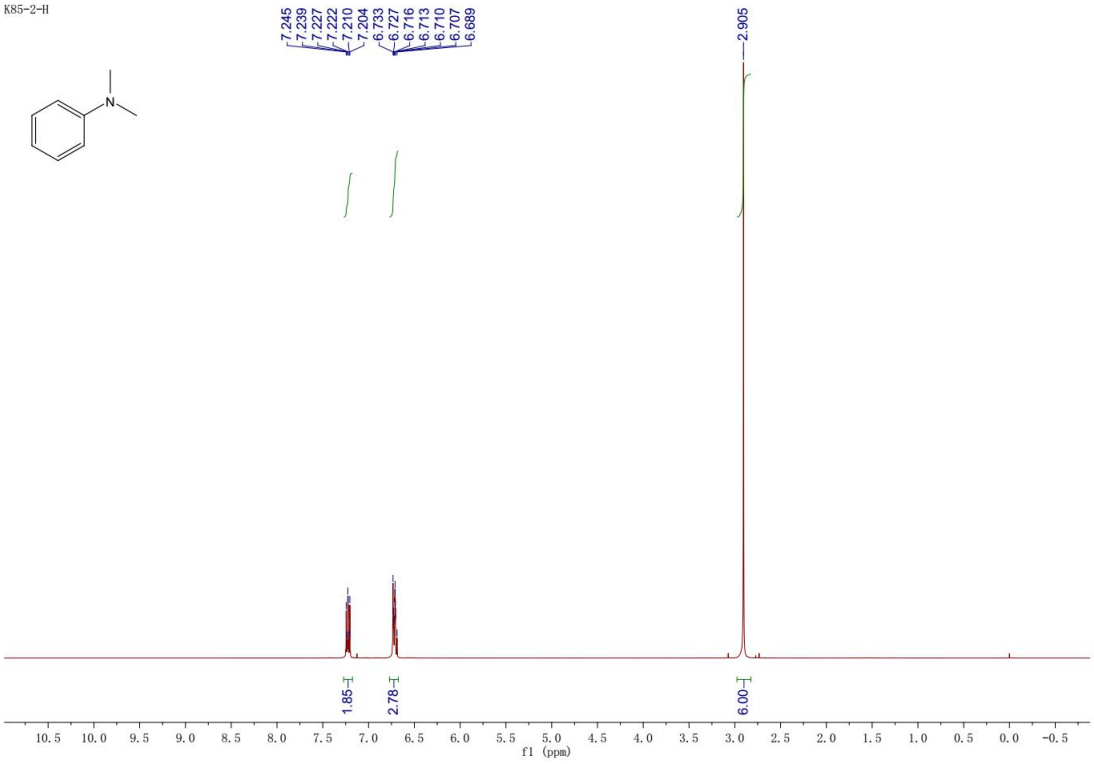

QYH-C
148.902
129.270
115.123
111.158
49.068
27.808
27.188
f1 (ppm)

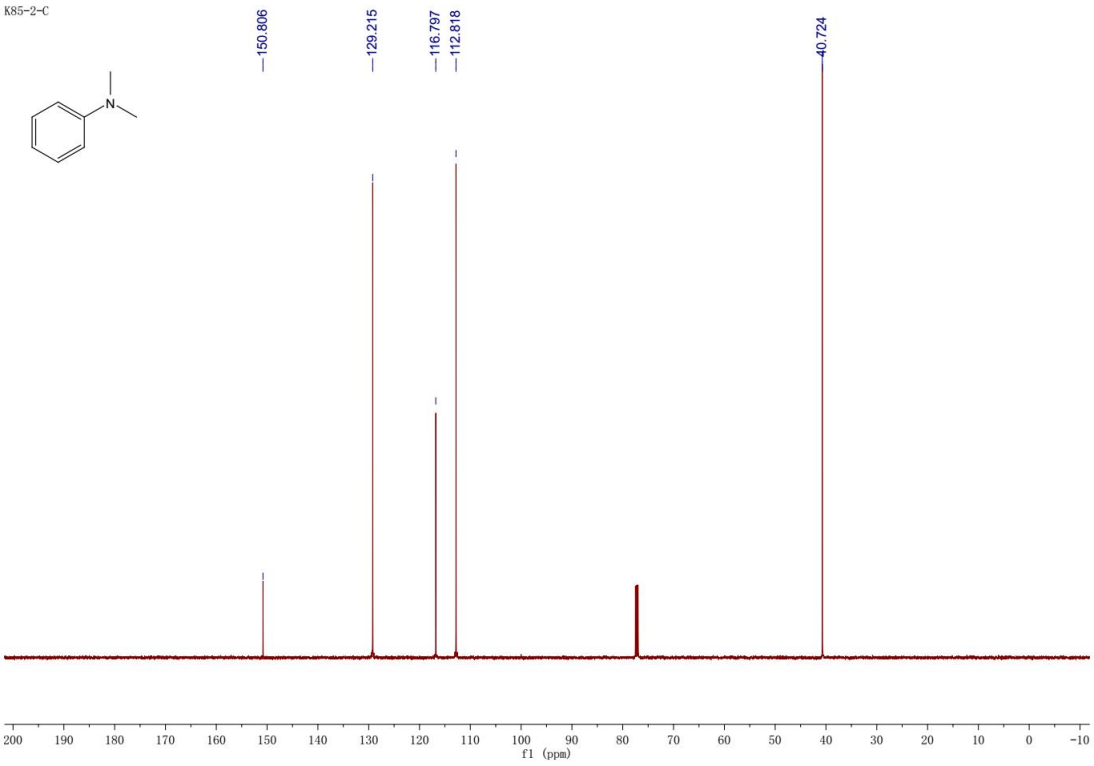
NMR of 2f


G467-H
7.355
7.333
7.315
7.282
7.044
7.024
6.954
6.936
6.917
3.389
4.04
3.82
2.04
8.00
f1 (ppm)

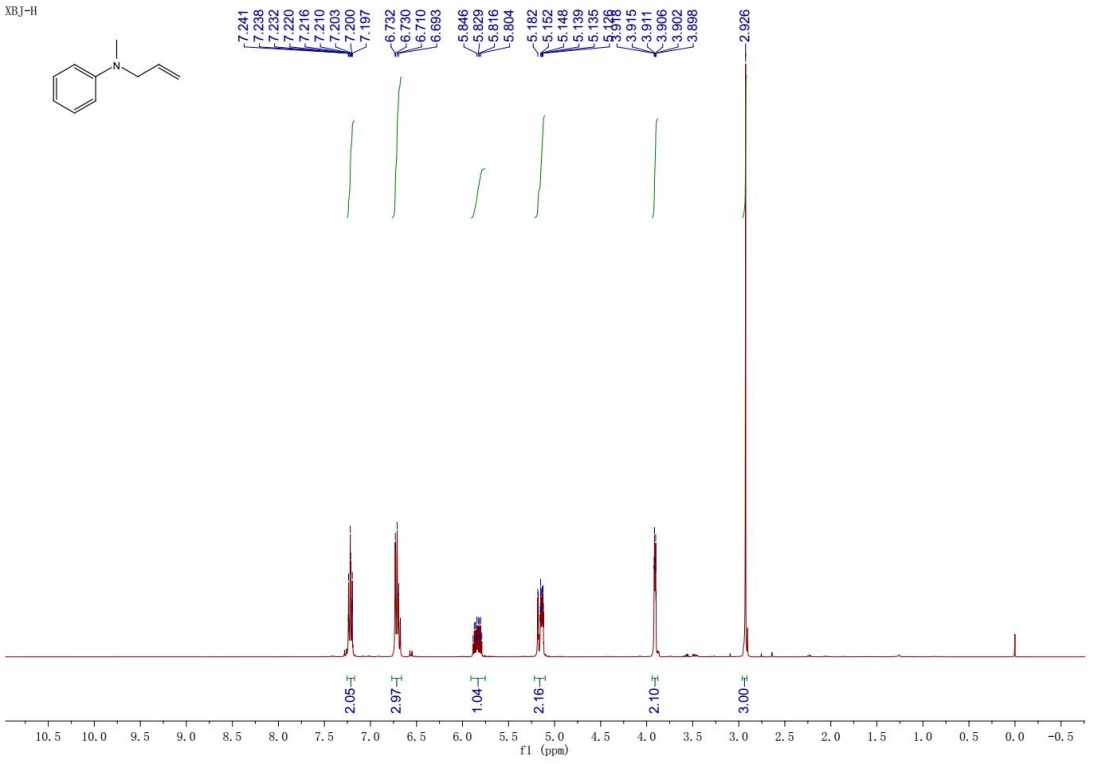

G467-C
151.201
129.230
120.173
116.417
49.483
f1 (ppm)

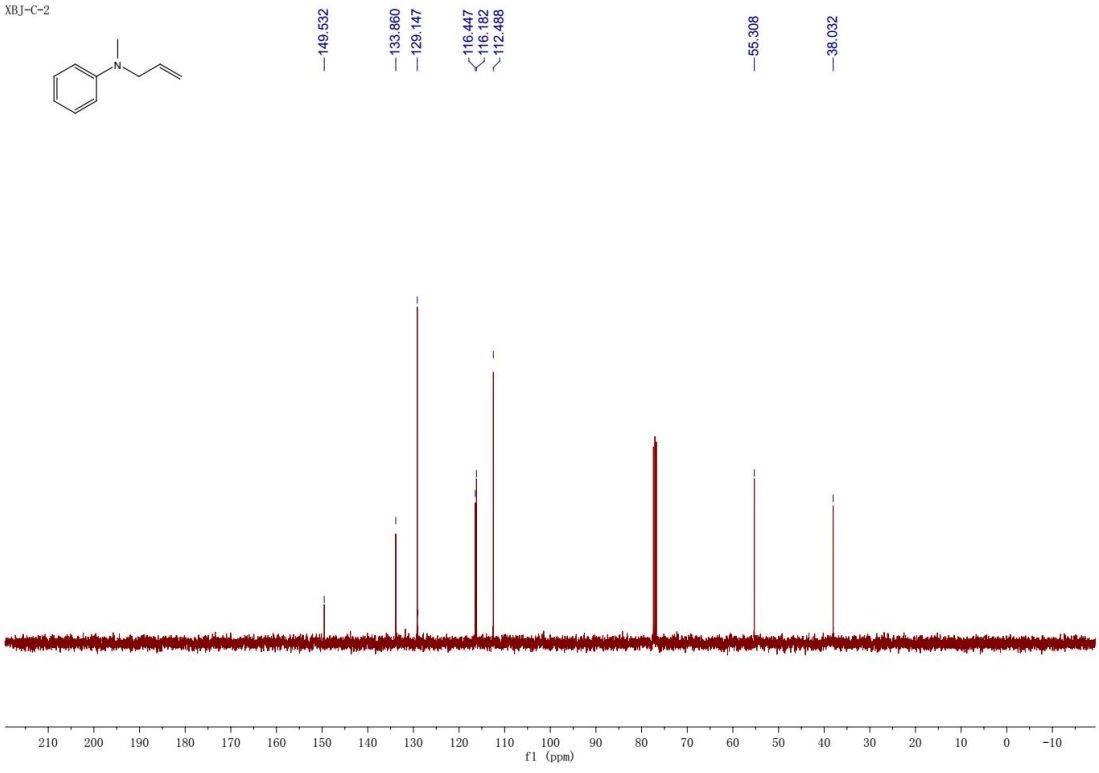
NMR of 2g


K85-2-H
7.245
7.239
7.227
7.222
7.210
7.204
6.733
6.727
6.716
6.713
6.710
6.707
6.689
2.905
1.85
2.78
6.00
f1 (ppm)

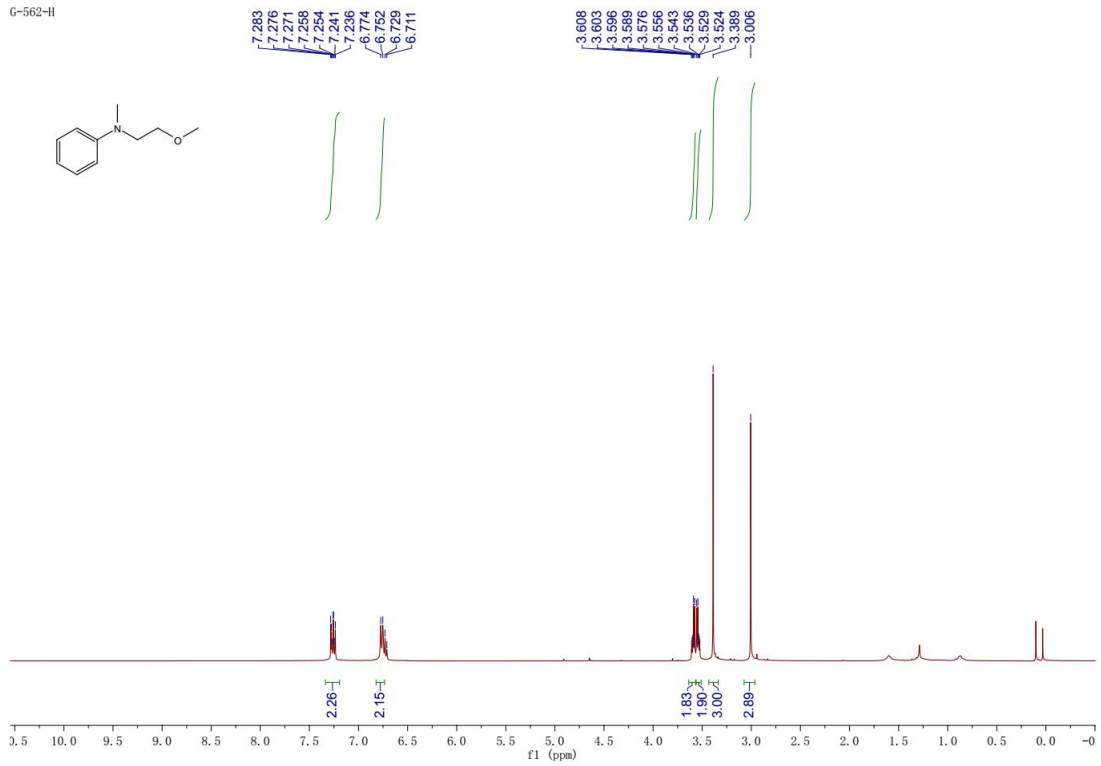

K85-2-C
150.806
129.215
116.797
112.818
40.724
f1 (ppm)

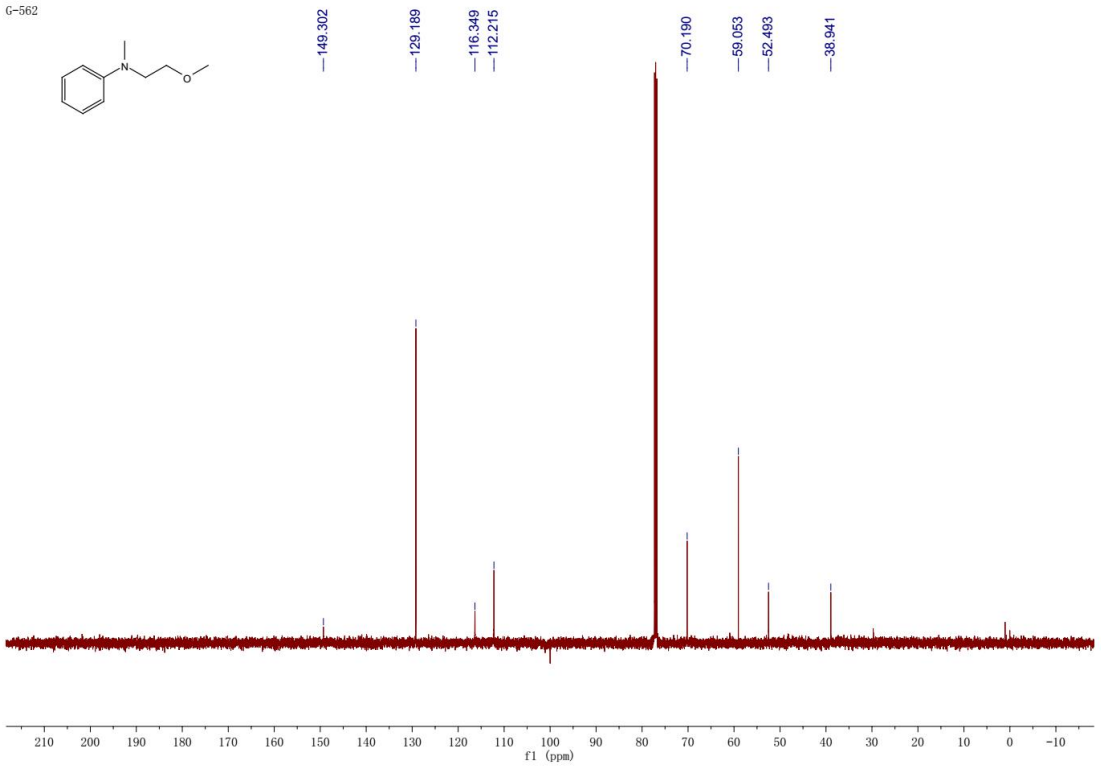
NMR of 2h


XBJ-H
7.241
7.238
7.232
7.220
7.216
7.210
7.203
7.200
7.197
6.732
6.730
6.710
6.693
5.846
5.829
5.816
5.804
5.182
5.152
5.148
5.139
5.135
3.915
3.911
3.906
3.902
3.898
2.926
2.05
2.97
1.04
2.16
2.10
3.00
f1 (ppm)

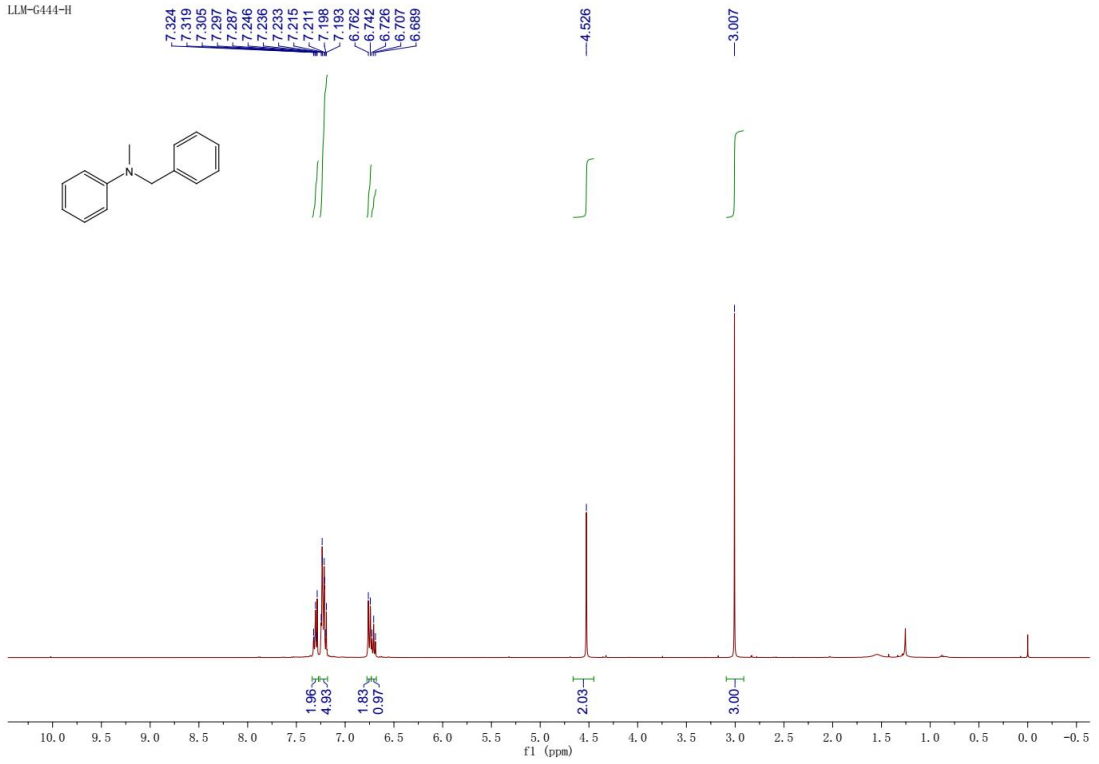

XBJ-C-2
149.532
133.860
129.147
116.447
116.182
112.488
55.308
38.032
f1 (ppm)

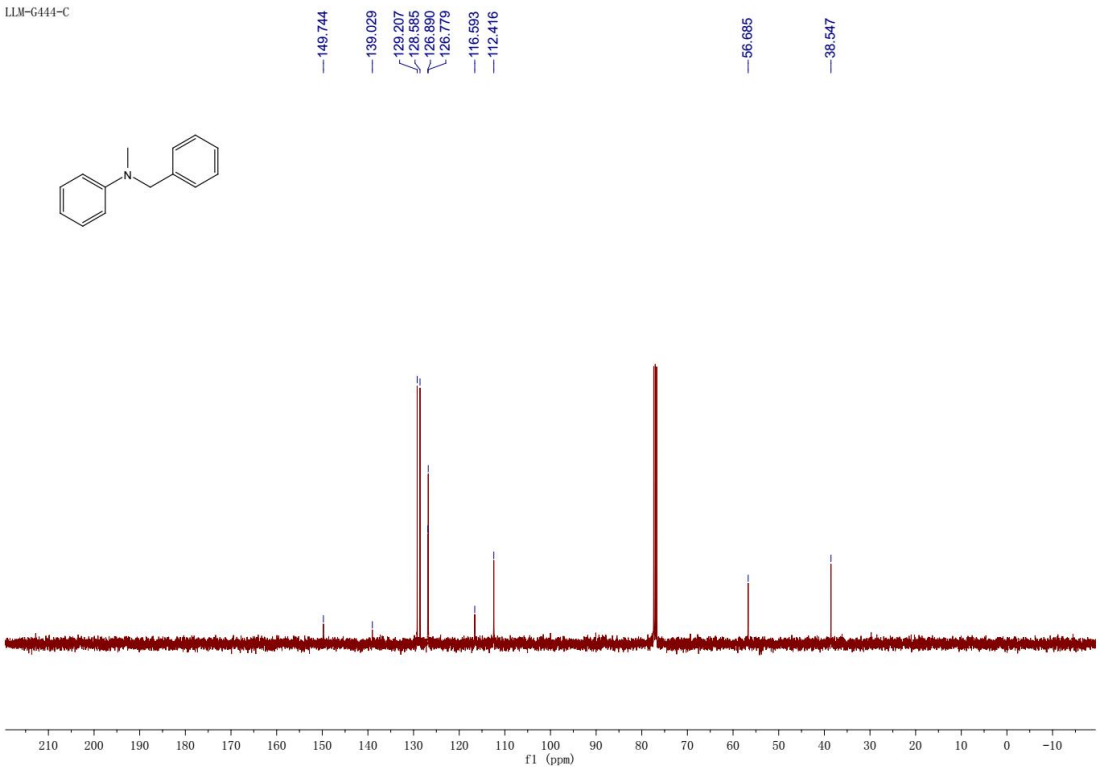
NMR of 2i


G-562-H
7.283
7.276
7.271
7.258
7.254
7.241
7.236
6.774
6.752
6.729
6.711
3.608
3.603
3.596
3.589
3.576
3.556
3.543
3.536
3.529
3.524
3.389
3.006
2.26
2.15
1.83
1.90
3.00
2.89
f1 (ppm)

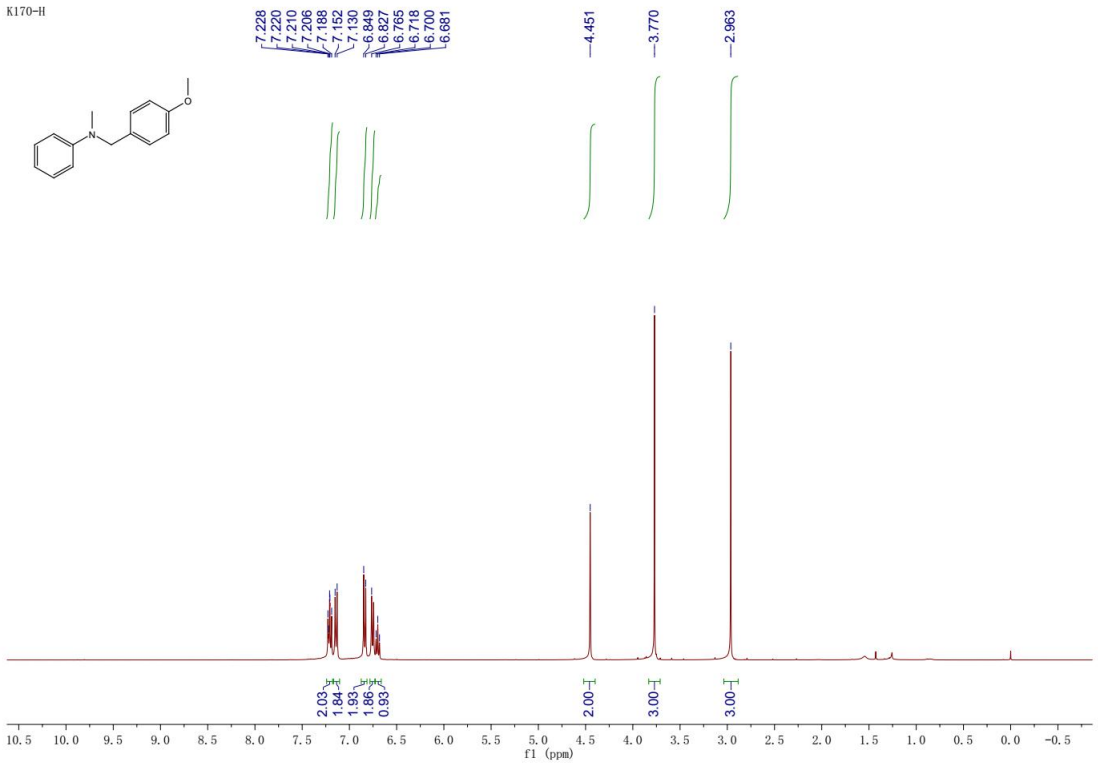

G-562
149.302
129.189
116.349
112.215
70.190
59.053
52.493
38.941
f1 (ppm)

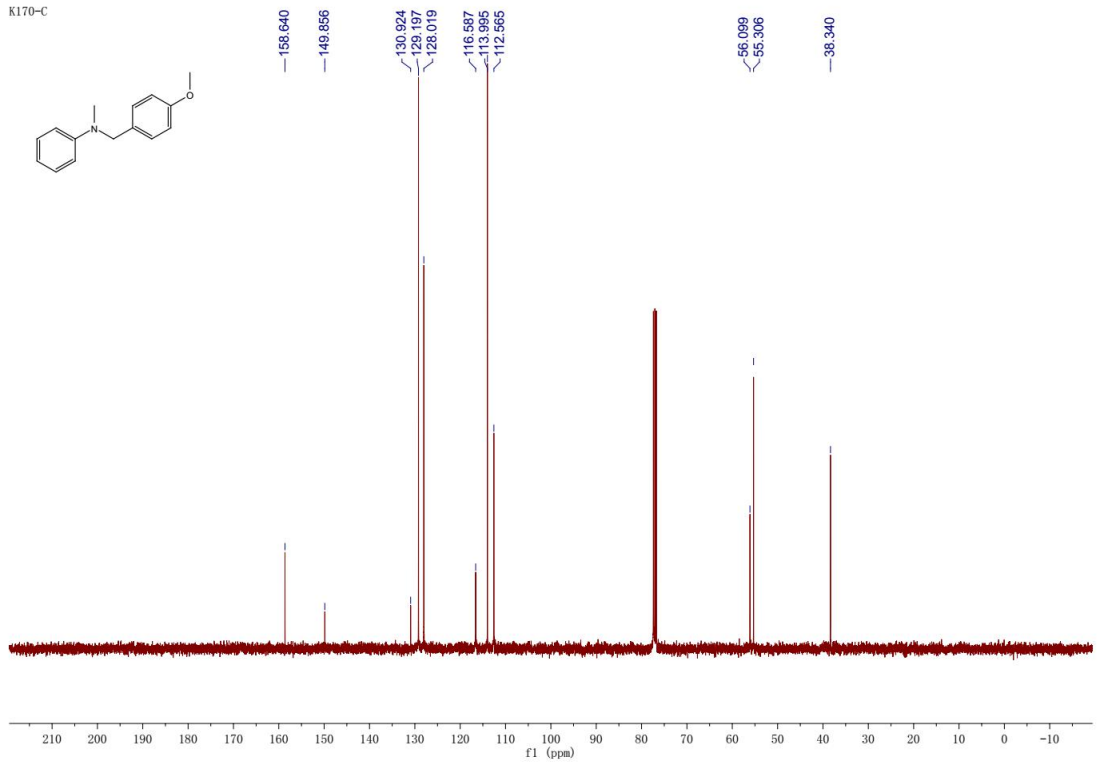
NMR of 2j


LLM-G444-H
7.324
7.319
7.305
7.297
7.287
7.246
7.236
7.233
7.215
7.211
7.198
7.193
6.762
6.742
6.726
6.707
6.689
4.526
3.007
1.96
4.93
1.83
0.97
2.03
3.00
f1 (ppm)

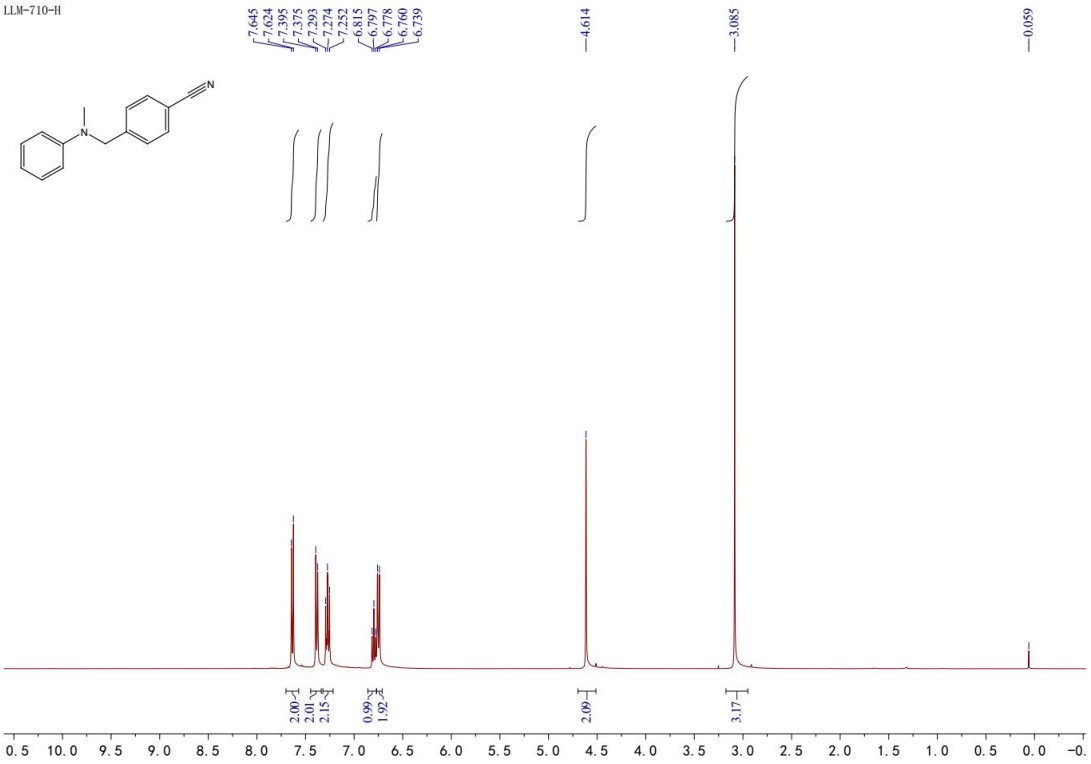

LLM-G444-C
149.744
139.029
129.207
128.585
126.890
126.779
116.593
112.416
56.685
38.547
f1 (ppm)

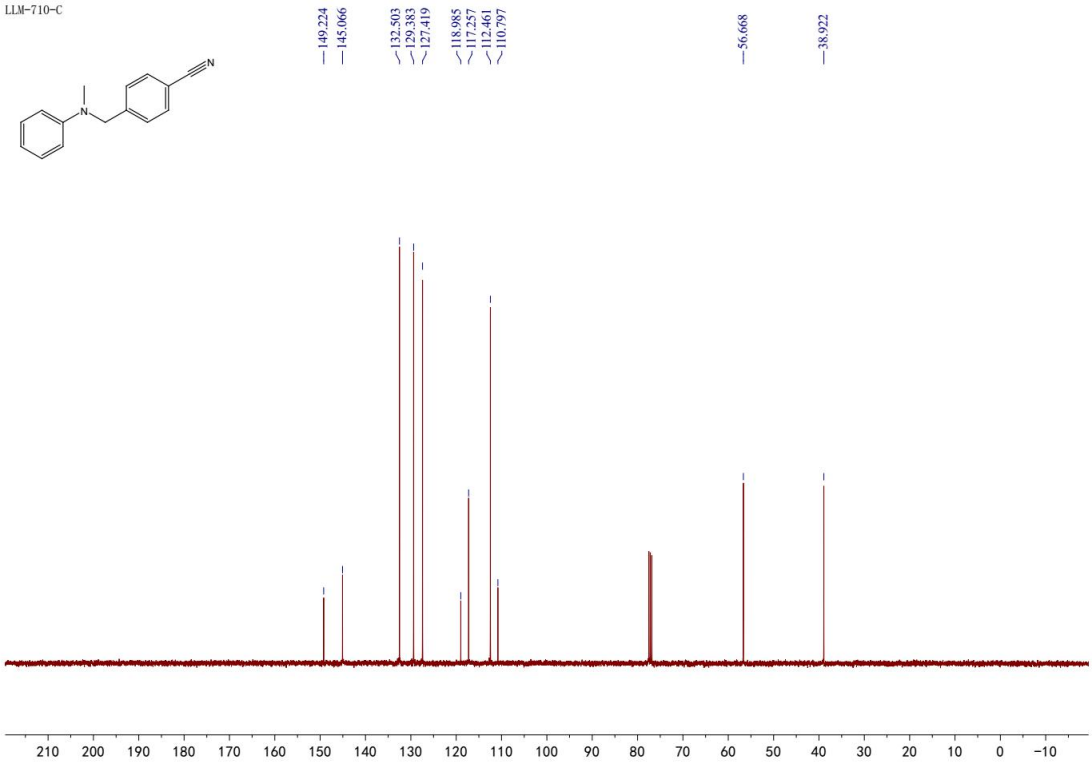
NMR of 2k


K170-H
7.228
7.220
7.210
7.206
7.188
7.152
7.130
6.849
6.827
6.765
6.718
6.700
6.681
4.451
3.770
2.963
2.03
1.84
1.93
1.86
0.93
2.00
3.00
3.00
f1 (ppm)

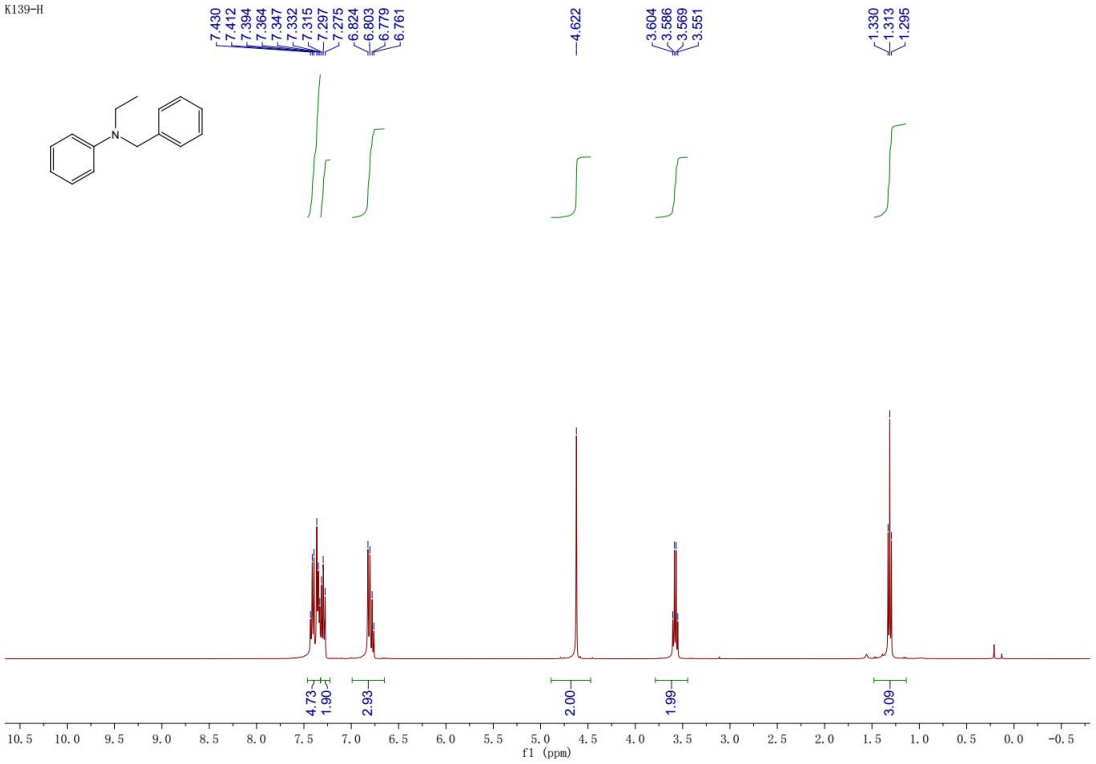

K170-C
158.640
149.856
130.924
129.197
128.019
116.587
113.995
112.565
56.099
55.306
38.340
f1 (ppm)

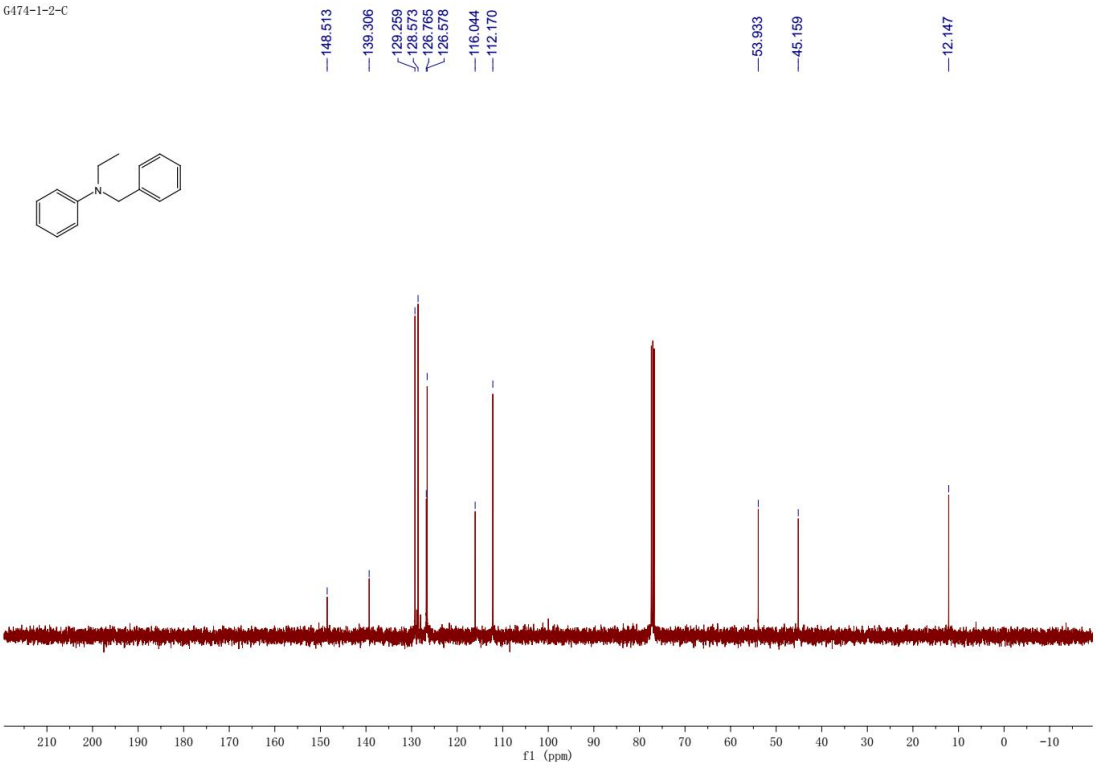
NMR of 2l


LLM-710-H
7.645
7.624
7.395
7.375
7.293
7.274
7.252
6.815
6.797
6.778
6.760
6.739
4.614
3.085
0.059
2.00
2.01
2.15
0.99
1.92
2.09
3.17

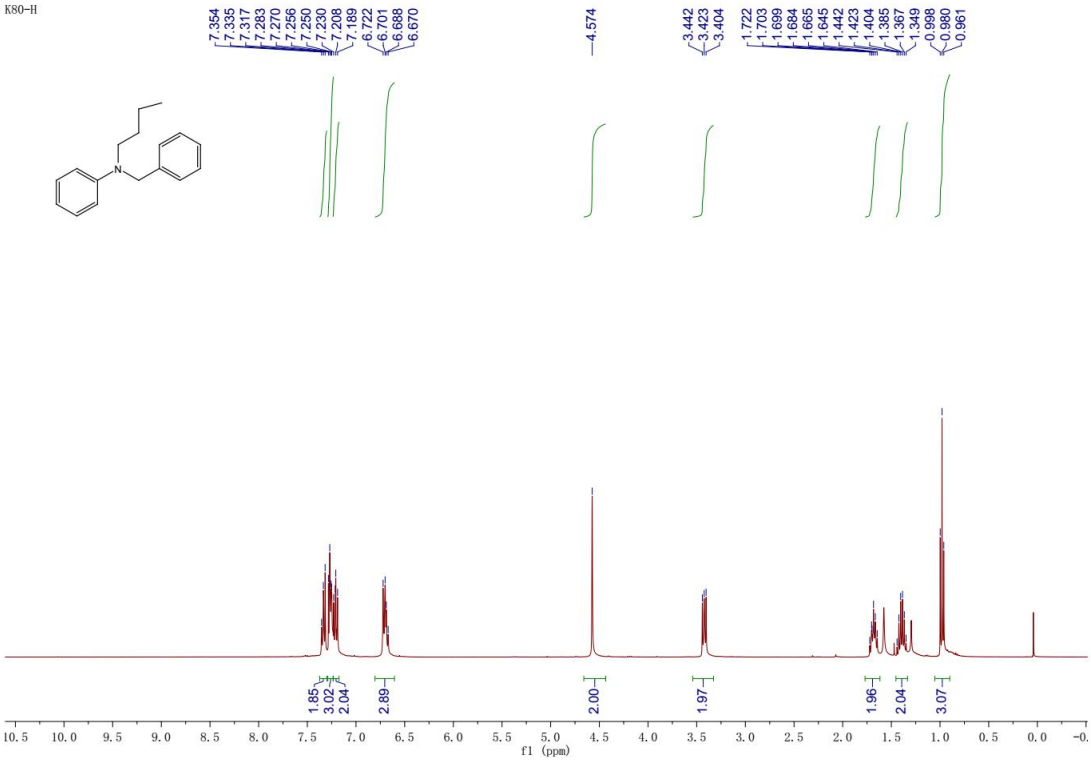

LLM-710-C
149.224
145.066
132.503
129.383
127.419
118.985
117.257
112.461
110.797
56.668
38.922

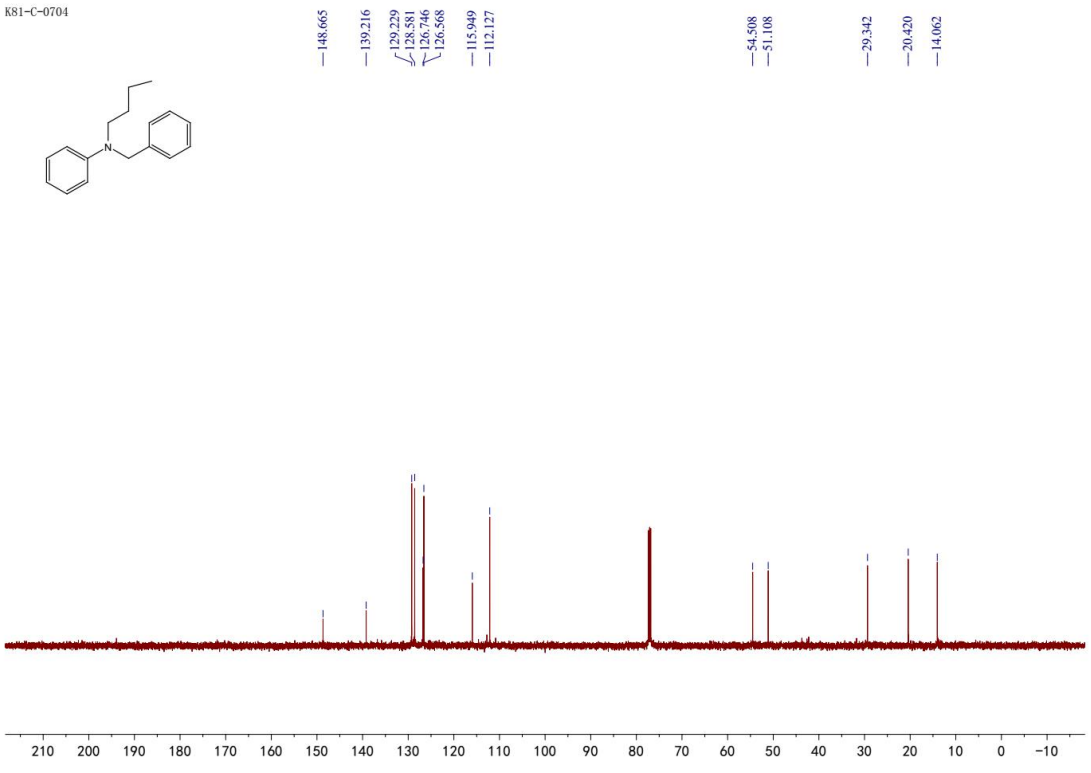
NMR of 2m


K139-H
7.430
7.412
7.394
7.364
7.347
7.332
7.315
7.297
7.275
6.824
6.803
6.779
6.761
4.622
3.604
3.586
3.569
3.551
1.330
1.313
1.295
4.73
1.90
2.93
2.00
1.99
3.09
f1 (ppm)

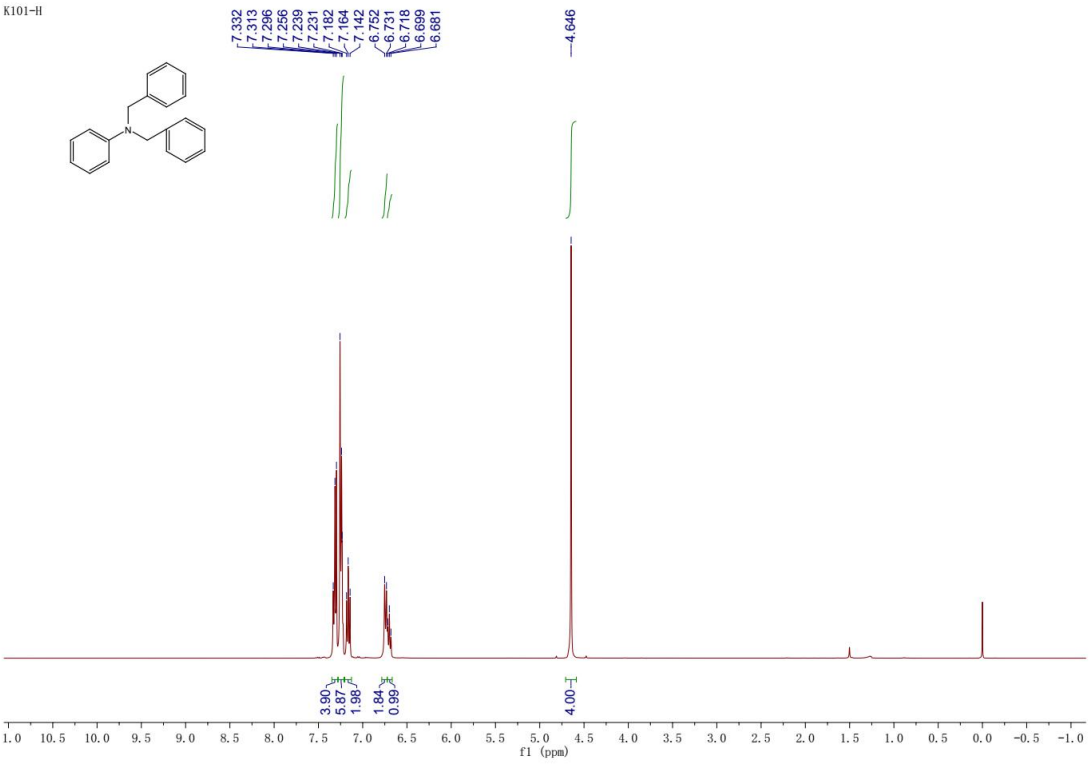

G474-1-2-C
148.513
139.306
129.259
128.573
126.765
126.578
116.044
112.170
53.933
45.159
12.147
f1 (ppm)

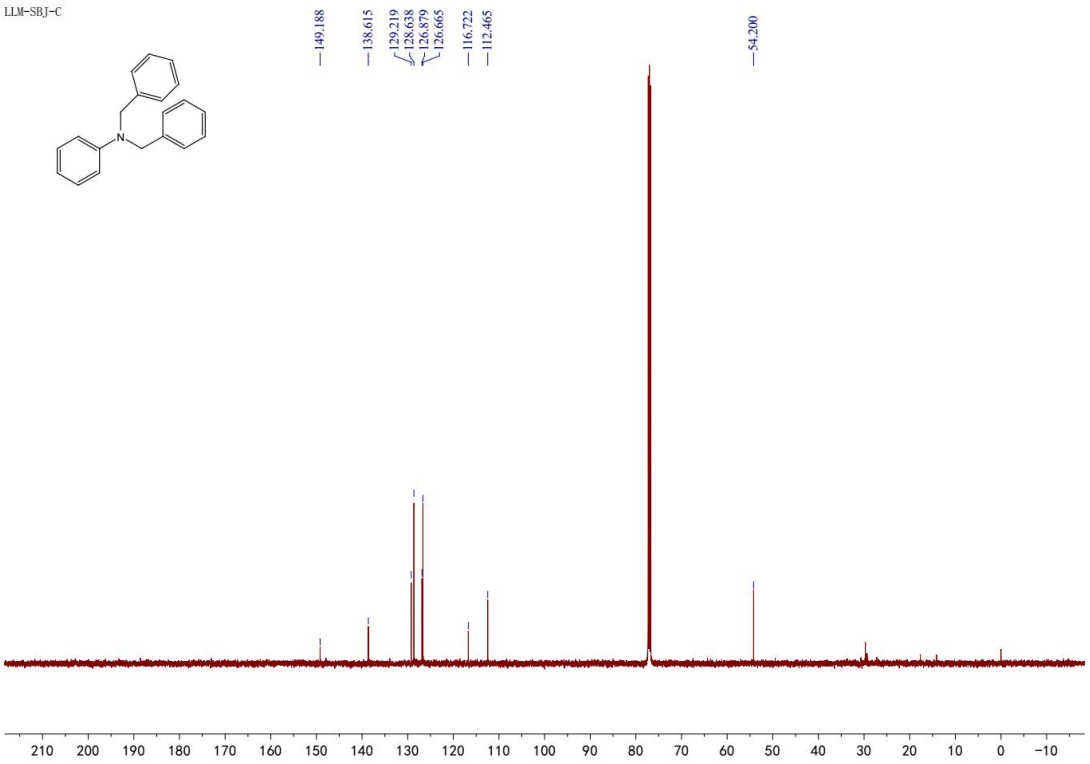
NMR of 2n


K80-H
7.354
7.335
7.317
7.283
7.270
7.256
7.250
7.230
7.208
7.189
6.722
6.701
6.688
6.670
4.574
3.442
3.423
3.404
1.722
1.703
1.699
1.684
1.665
1.645
1.442
1.423
1.404
1.385
1.367
1.349
0.998
0.980
0.961
1.85
3.02
2.04
2.89
2.00
1.97
1.96
2.04
3.07
f1 (ppm)

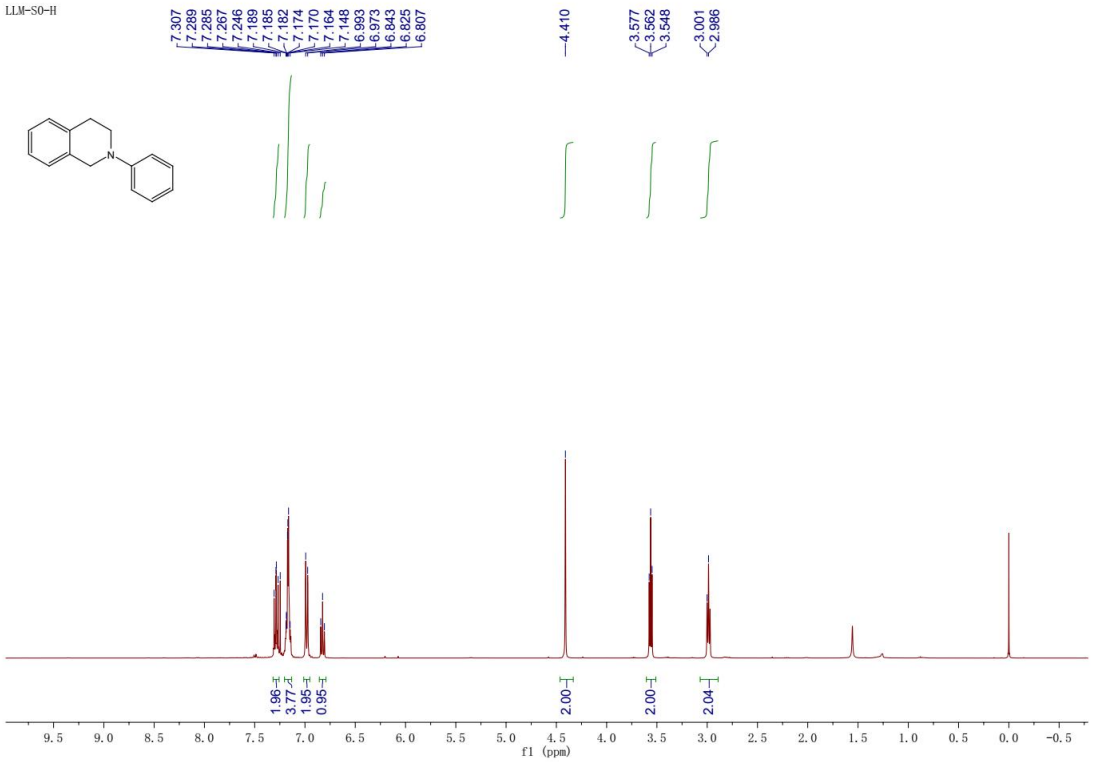

K81-C-0704
148.665
139.216
129.229
128.581
126.746
126.568
115.949
112.127
54.508
51.108
29.342
20.420
14.062

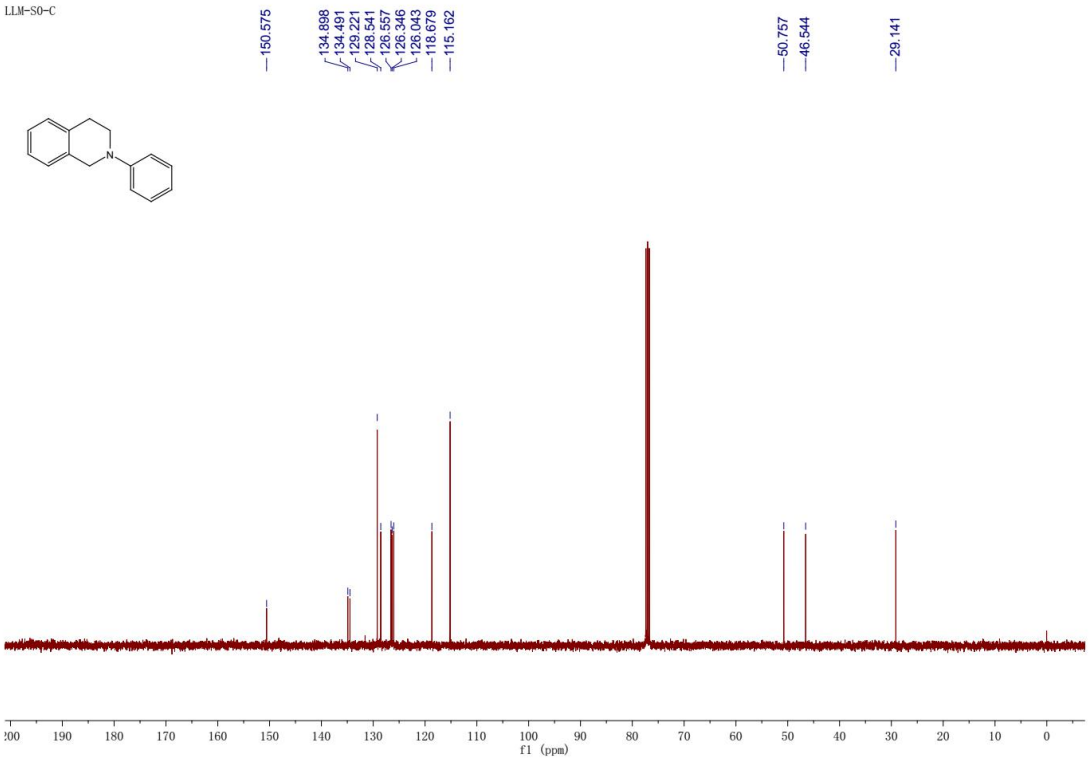
NMR of 2o


K101-H
7.332
7.313
7.296
7.256
7.239
7.231
7.182
7.164
7.142
6.752
6.731
6.718
6.699
6.681
4.646
3.90
5.87
1.98
1.84
0.99
4.00
f1 (ppm)

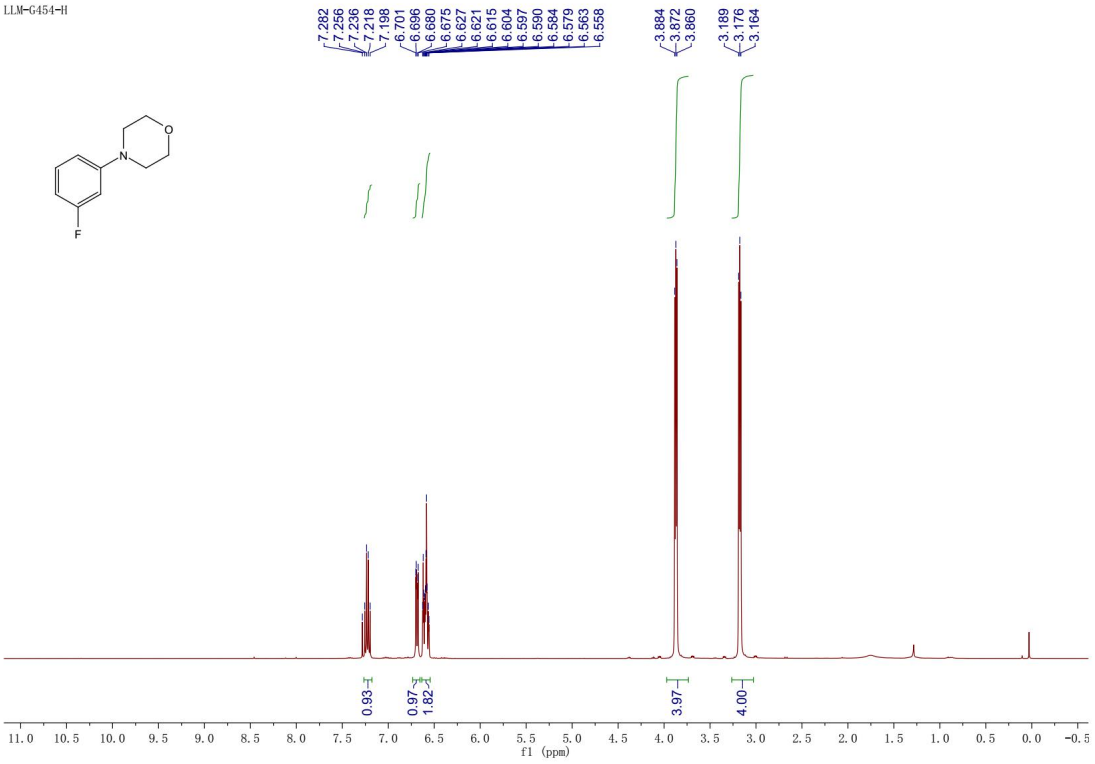

LLM-SBJ-C
149.188
138.615
129.219
128.638
126.879
126.665
116.722
112.465
54.200

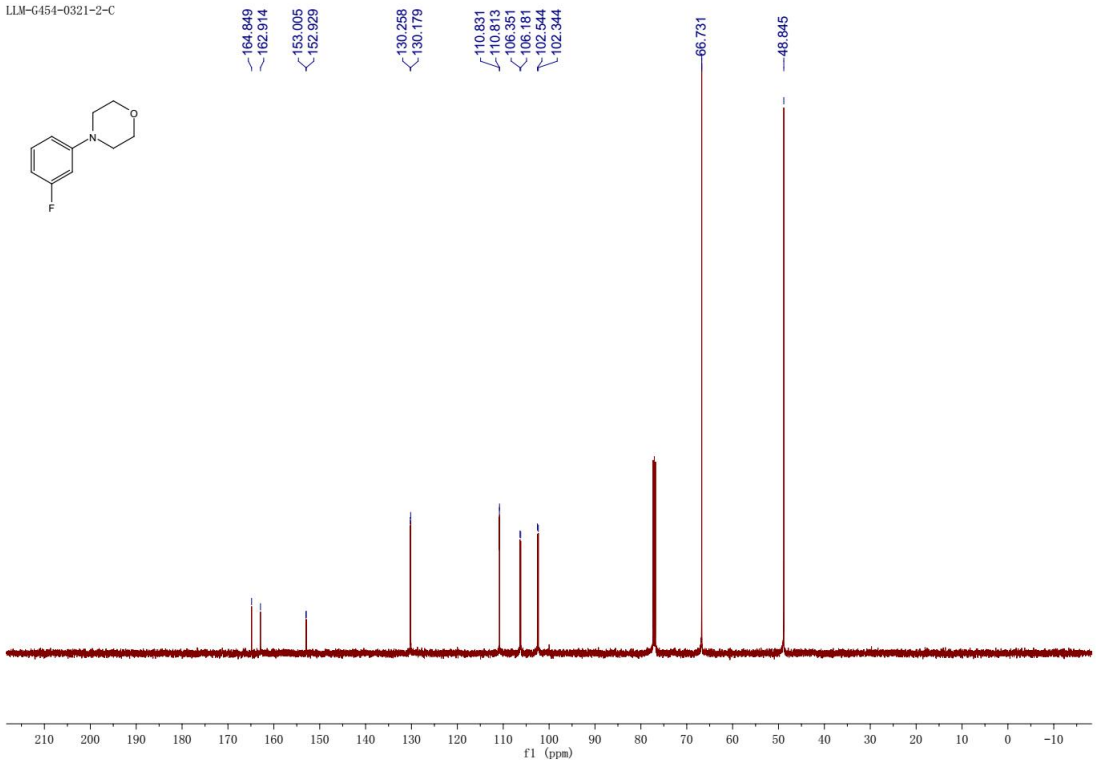
NMR of 2p


LLM-SO-H
7.307
7.289
7.285
7.267
7.246
7.189
7.185
7.182
7.174
7.170
7.164
7.148
6.993
6.973
6.843
6.825
6.807
4.410
3.577
3.562
3.548
3.001
2.986
1.96
3.77
1.95
0.95
2.00
2.00
2.04
f1 (ppm)

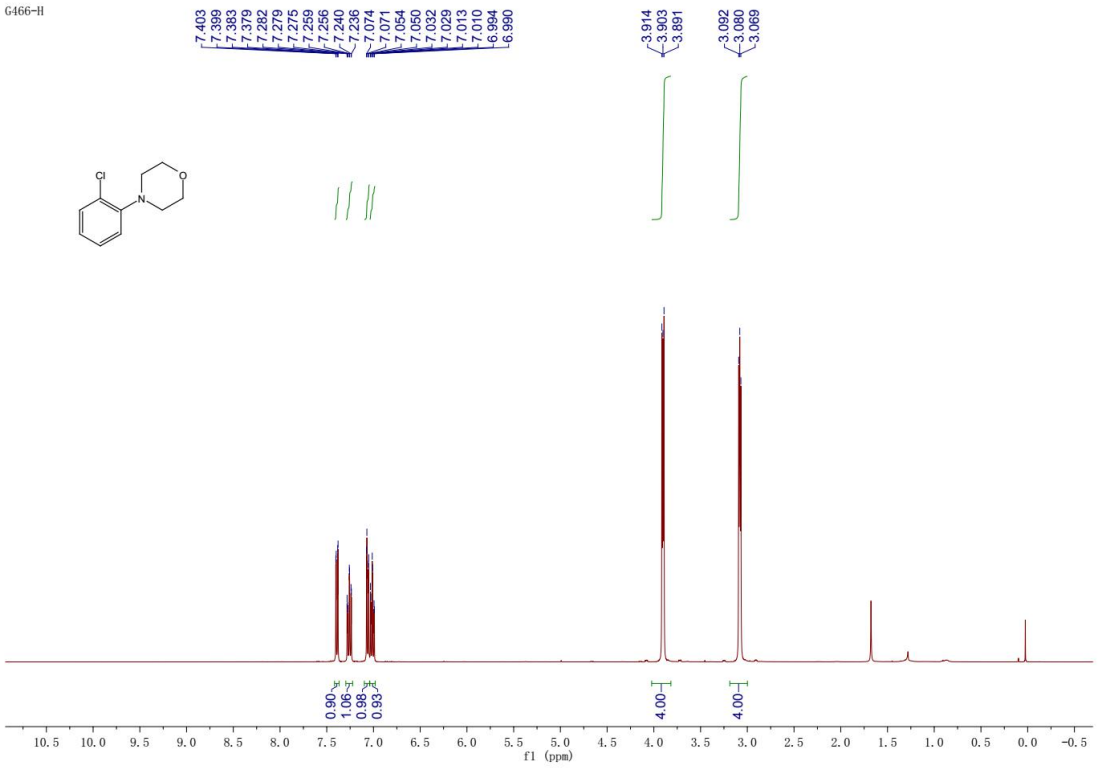

LLM-SO-C
150.575
134.898
134.491
129.221
128.541
126.557
126.346
126.043
118.679
115.162
50.757
46.544
29.141
f1 (ppm)

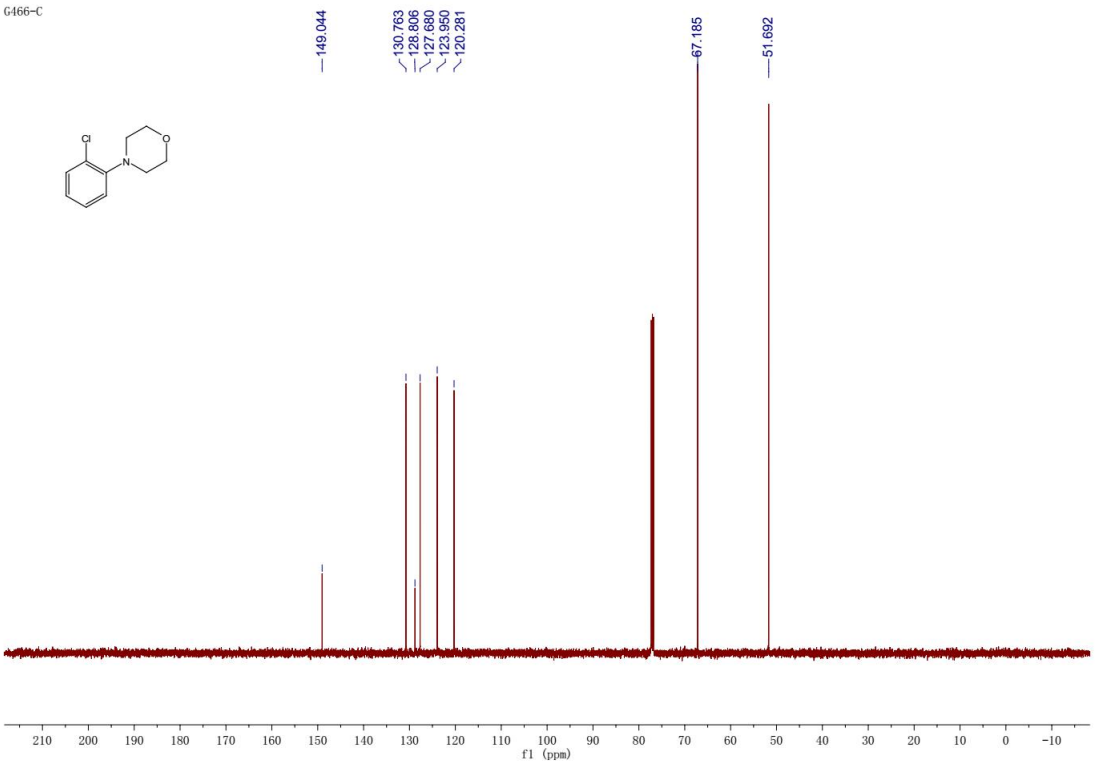
NMR of 2aa


LLM-G454-H
7.282
7.256
7.236
7.218
7.198
6.701
6.696
6.680
6.675
6.627
6.621
6.615
6.604
6.597
6.590
6.584
6.579
6.563
6.558
3.884
3.872
3.860
3.189
3.176
3.164
O
N
F
0.93
0.97
1.82
3.97
4.00
f1 (ppm)

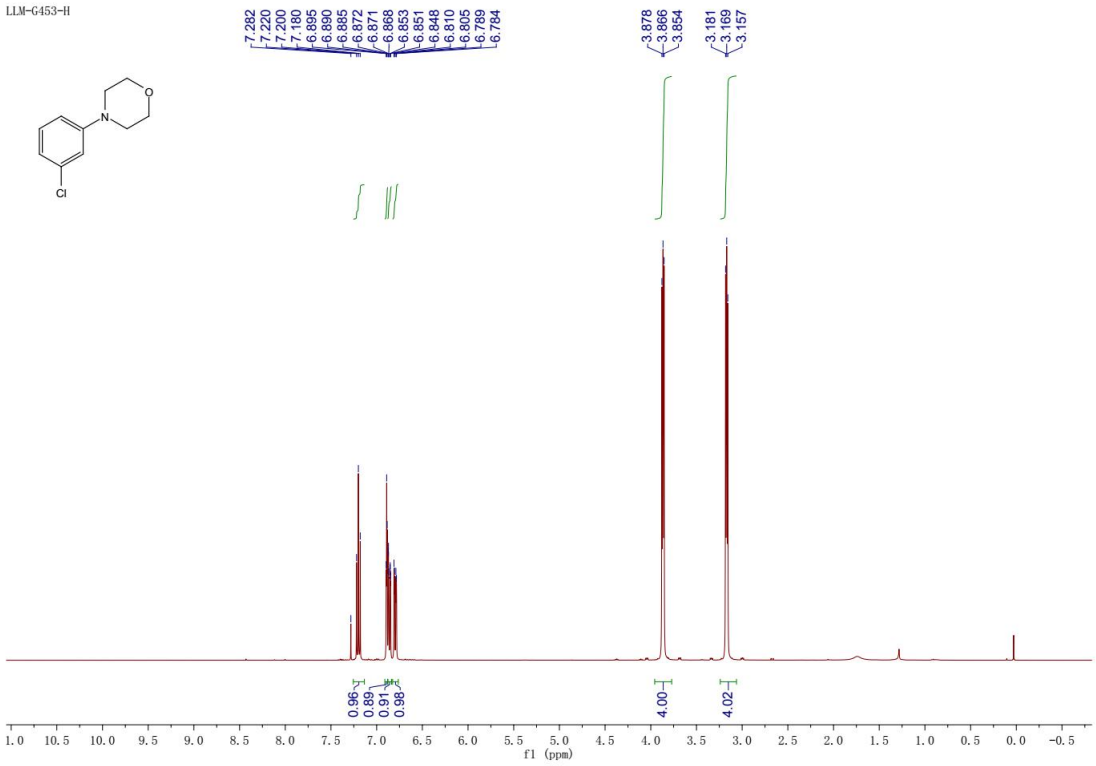

LLM-G454-0321-2-C
164.849
162.914
153.005
152.929
130.258
130.179
110.831
110.813
106.351
106.181
102.544
102.344
66.731
48.845
O
N
F
f1 (ppm)

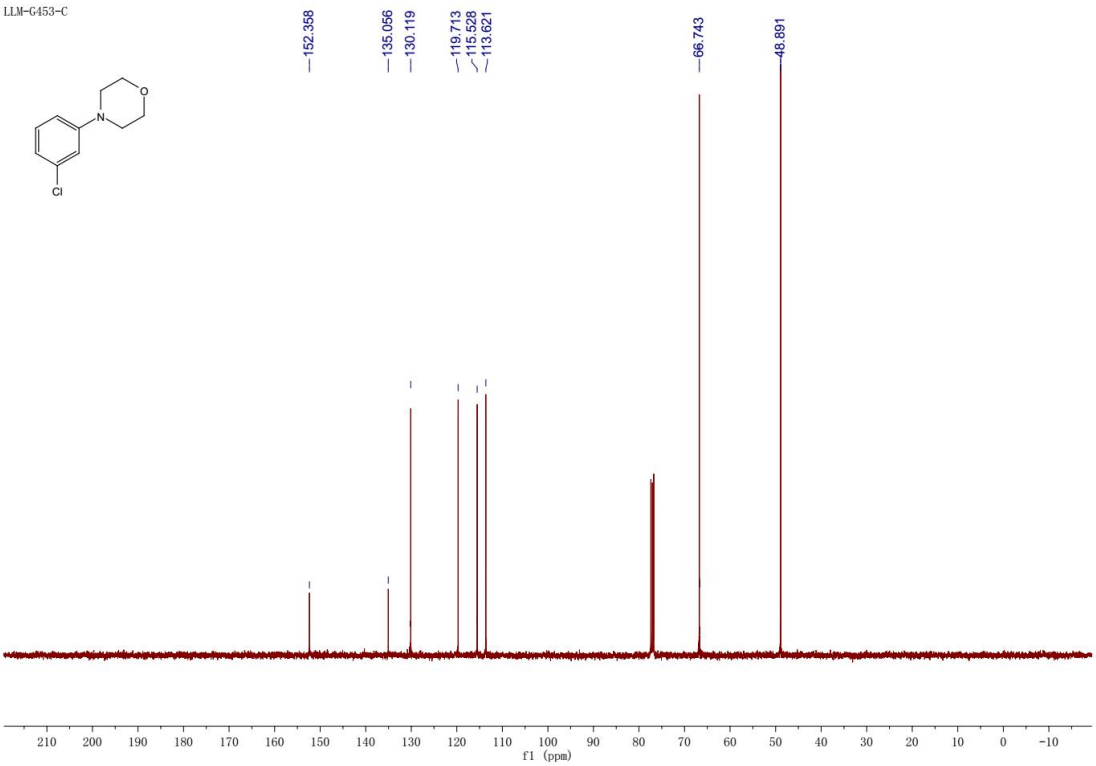
NMR of 2ab


G466-H
7.403
7.399
7.383
7.379
7.282
7.279
7.275
7.259
7.256
7.240
7.236
7.074
7.071
7.054
7.050
7.032
7.029
7.013
7.010
6.994
6.990
3.914
3.903
3.891
3.092
3.080
3.069
Cl
N
O
0.90
1.06
0.98
0.93
4.00
4.00
f1 (ppm)

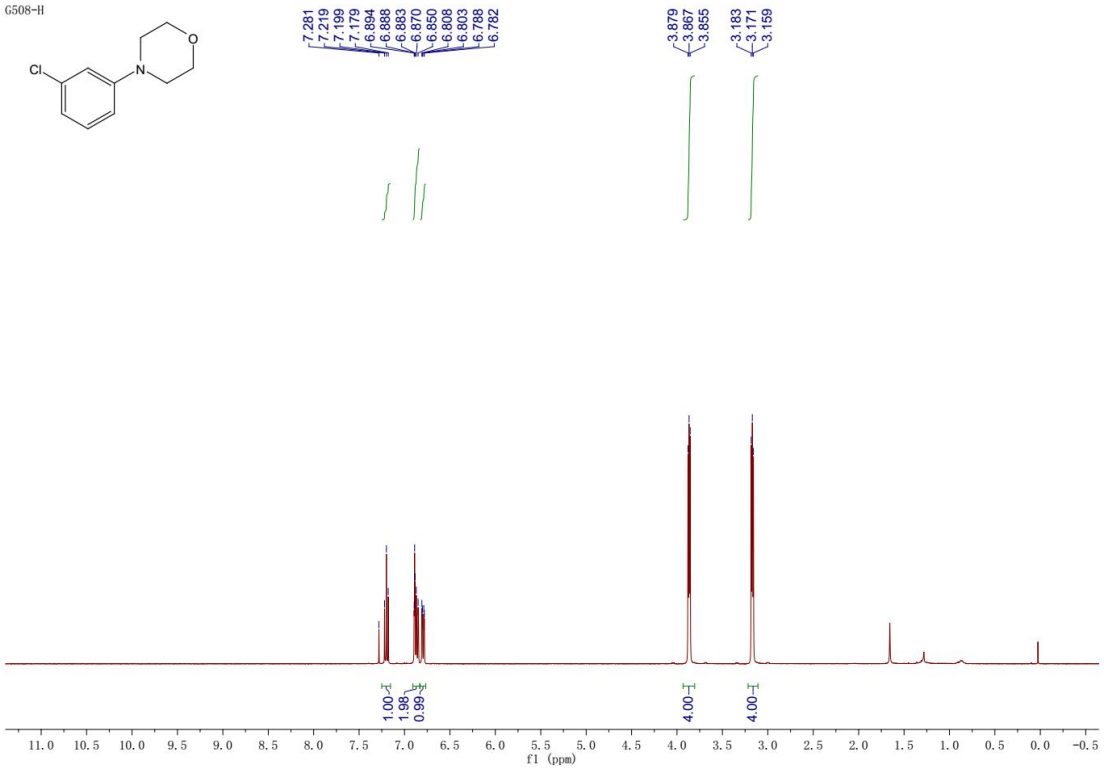

G466-C
149.044
130.763
128.806
127.680
123.950
120.281
67.185
51.692
Cl
N
O
f1 (ppm)

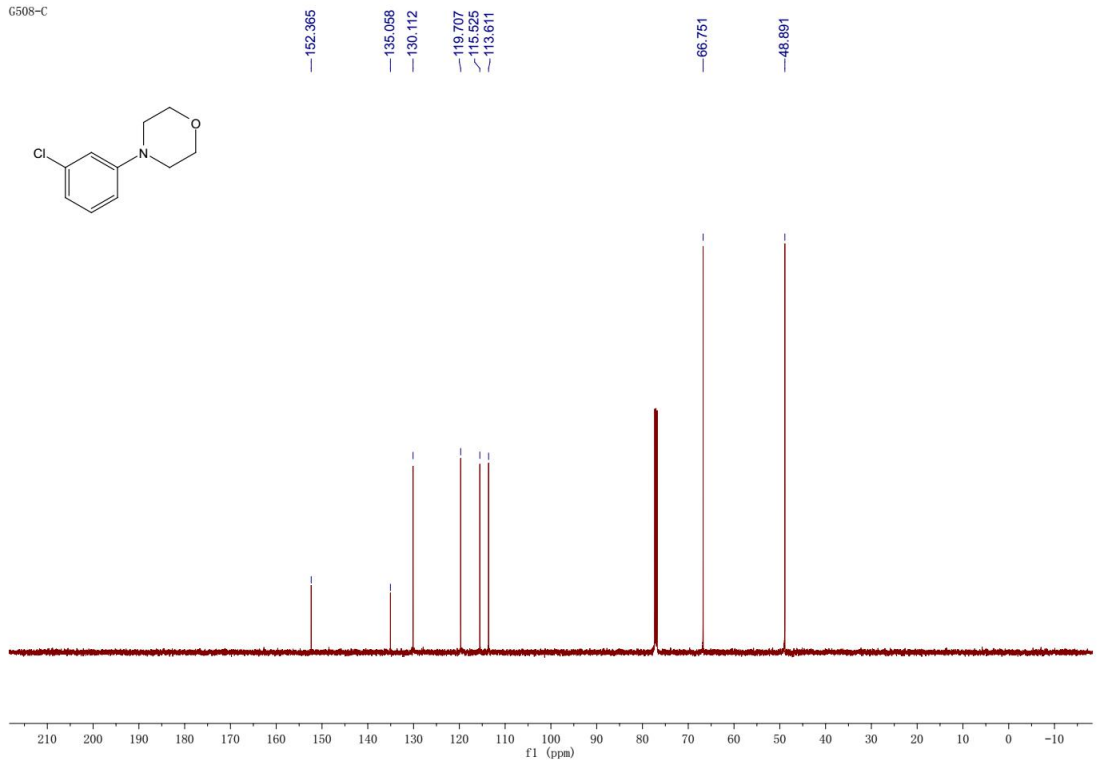
NMR of 2ac


LLM-G453-H
7.282
7.220
7.200
7.180
6.895
6.890
6.885
6.872
6.871
6.868
6.853
6.851
6.848
6.810
6.805
6.789
6.784
3.878
3.866
3.854
3.181
3.169
3.157
O
N
Cl
0.96
0.89
0.91
0.98
4.00
4.02
f1 (ppm)

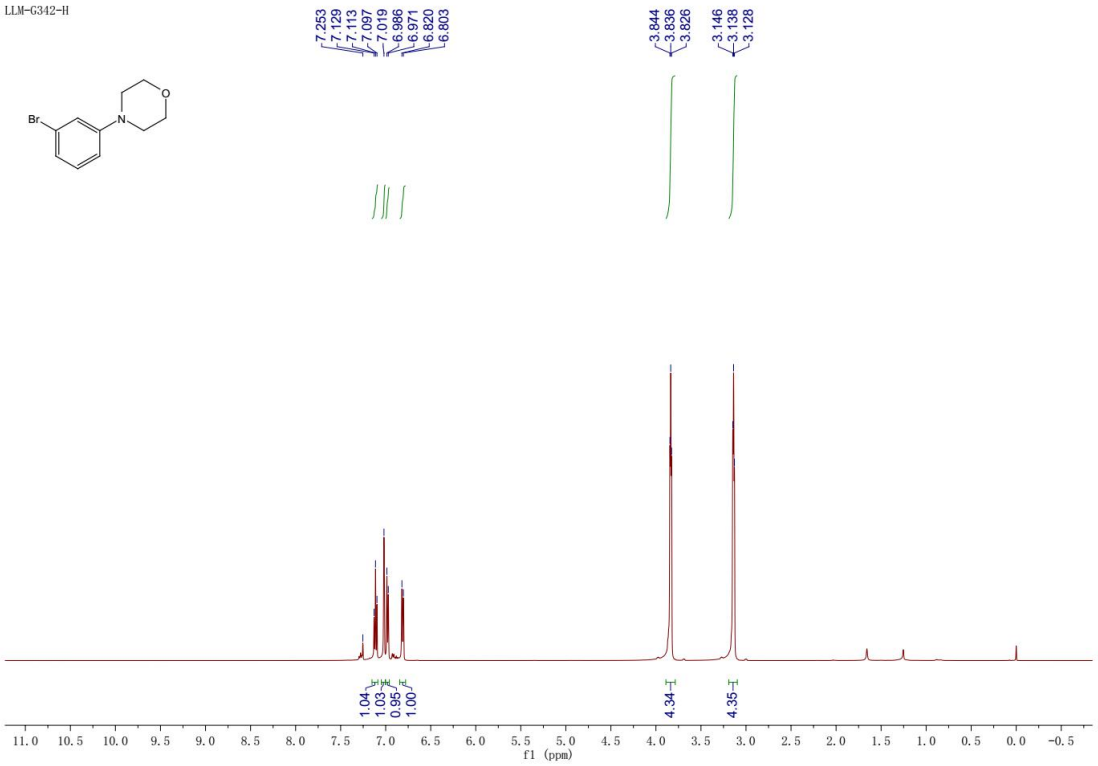

LLM-G453-C
152.358
135.056
130.119
119.713
115.528
113.621
66.743
48.891
O
N
Cl
f1 (ppm)

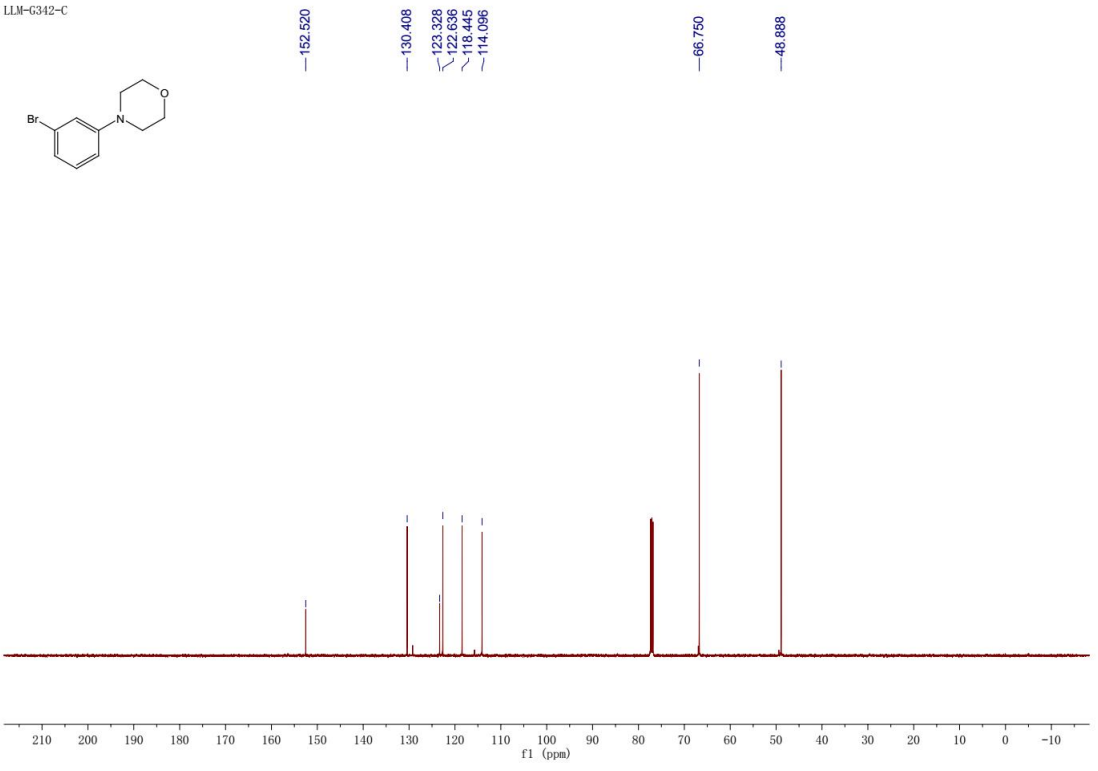
NMR of 2ad


G508-H
7.281
7.219
7.199
7.179
6.894
6.888
6.883
6.870
6.850
6.808
6.803
6.788
6.782
3.879
3.867
3.855
3.183
3.171
3.159
1.00
1.98
0.99
4.00
4.00
f1 (ppm)

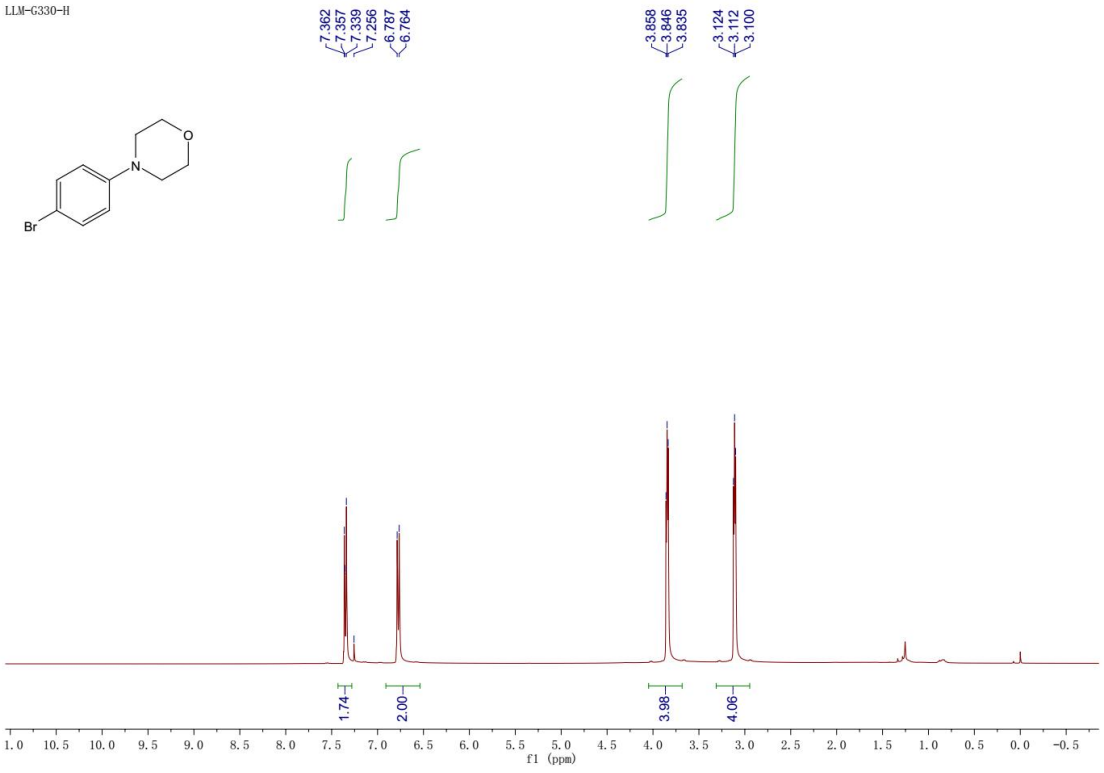

G508-C
152.365
135.058
130.112
119.707
115.525
113.611
66.751
48.891
f1 (ppm)

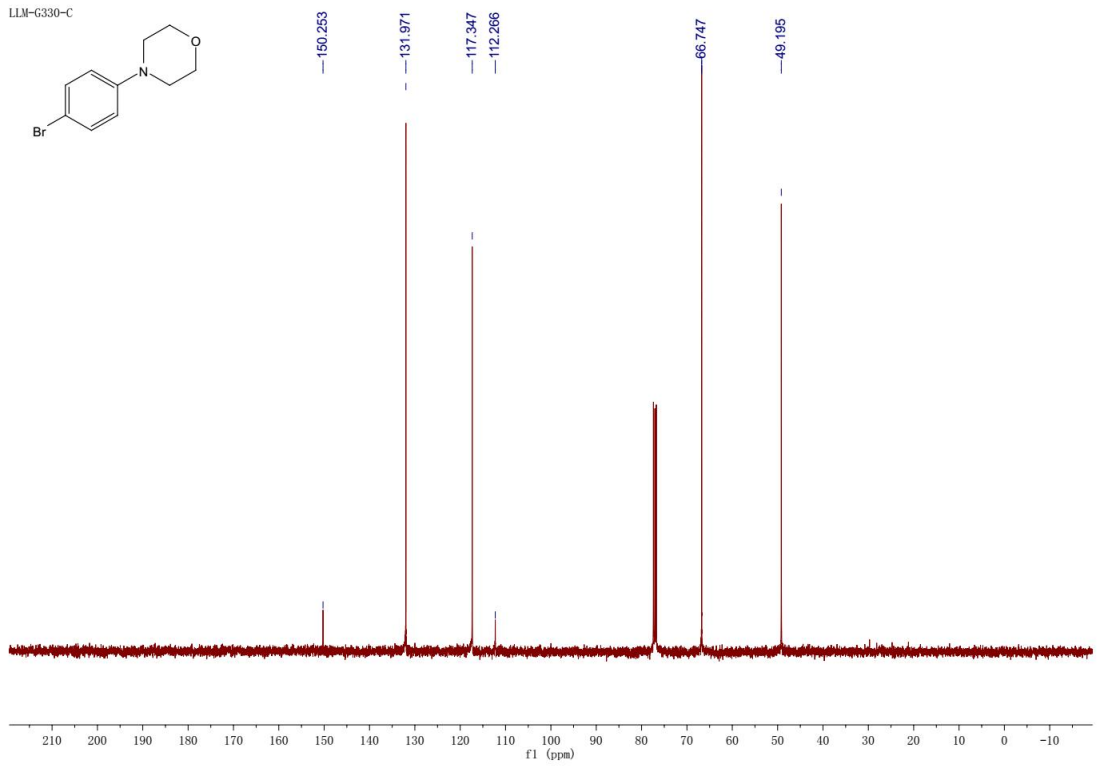
NMR of 2ae


LLM-G342-H
7.253
7.129
7.113
7.097
7.019
6.986
6.971
6.820
6.803
3.844
3.836
3.826
3.146
3.138
3.128
Br
O
N
1.04
1.03
0.95
1.00
4.34
4.35
f1 (ppm)

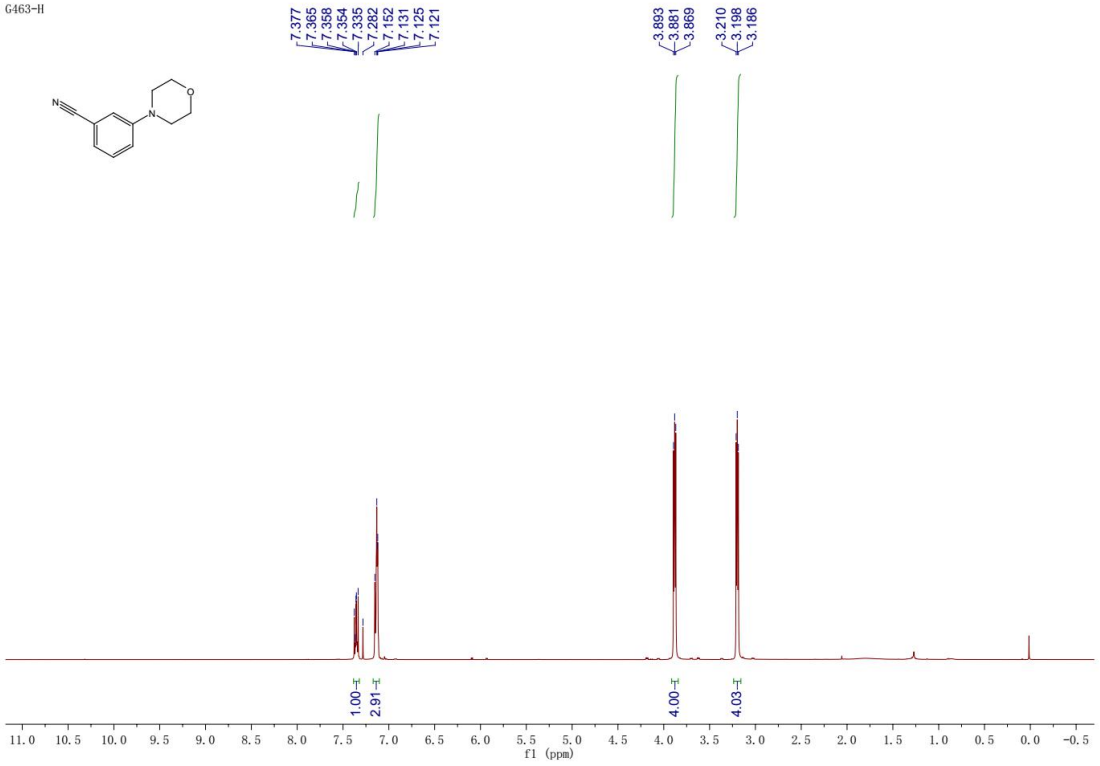

LLM-G342-C
152.520
130.408
123.328
122.636
118.445
114.096
66.750
48.888
Br
O
N
f1 (ppm)

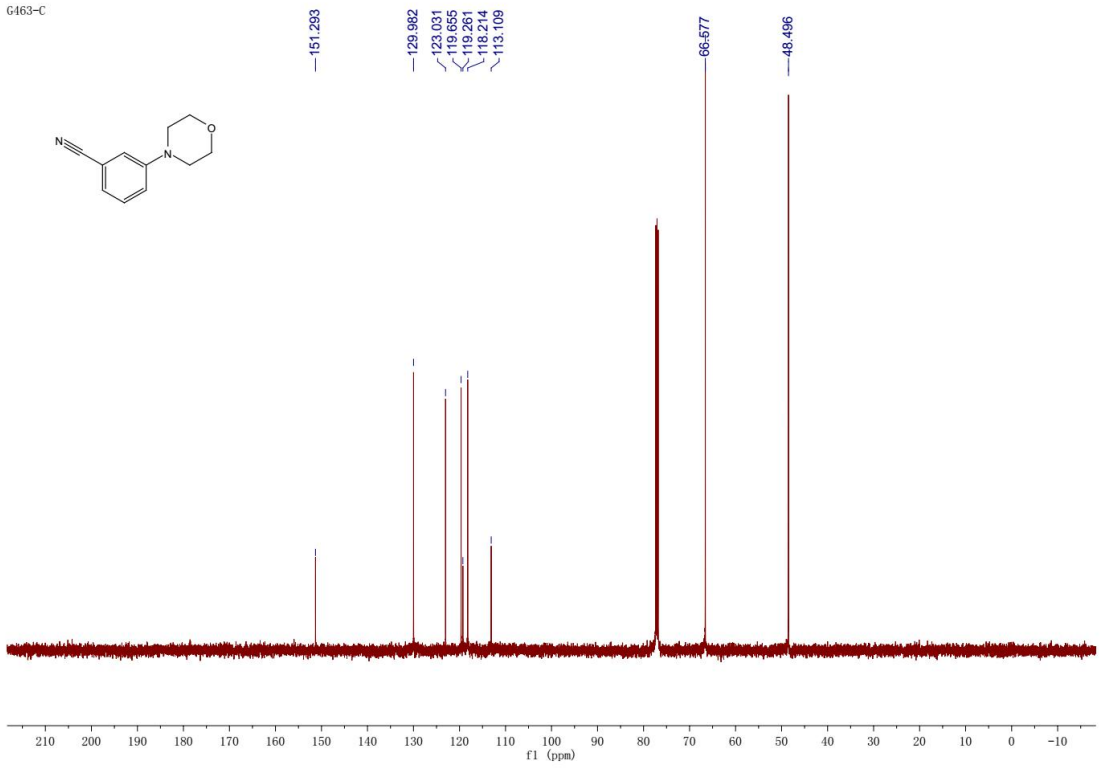
NMR of 2af


LLM-G330-H
7.362
7.357
7.339
7.256
6.787
6.764
3.858
3.846
3.835
3.124
3.112
3.100
Br
1.74
2.00
3.98
4.06
f1 (ppm)

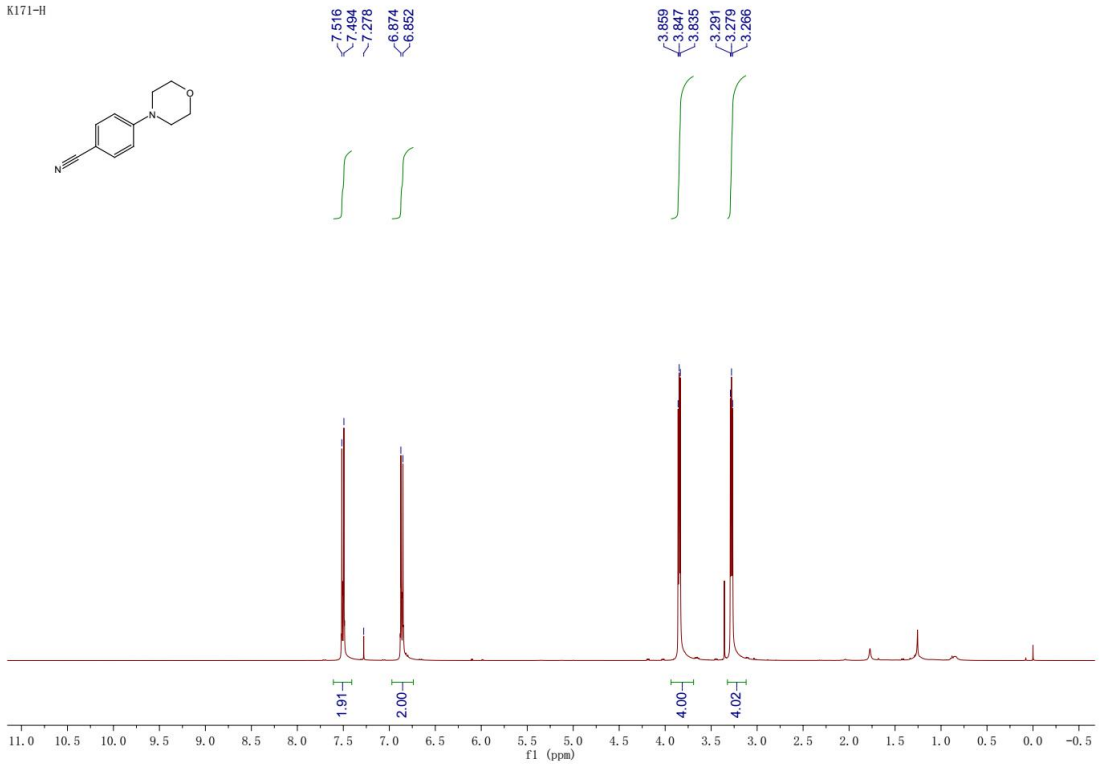

LLM-G330-C
150.253
131.971
117.347
112.266
66.747
49.195
Br
f1 (ppm)

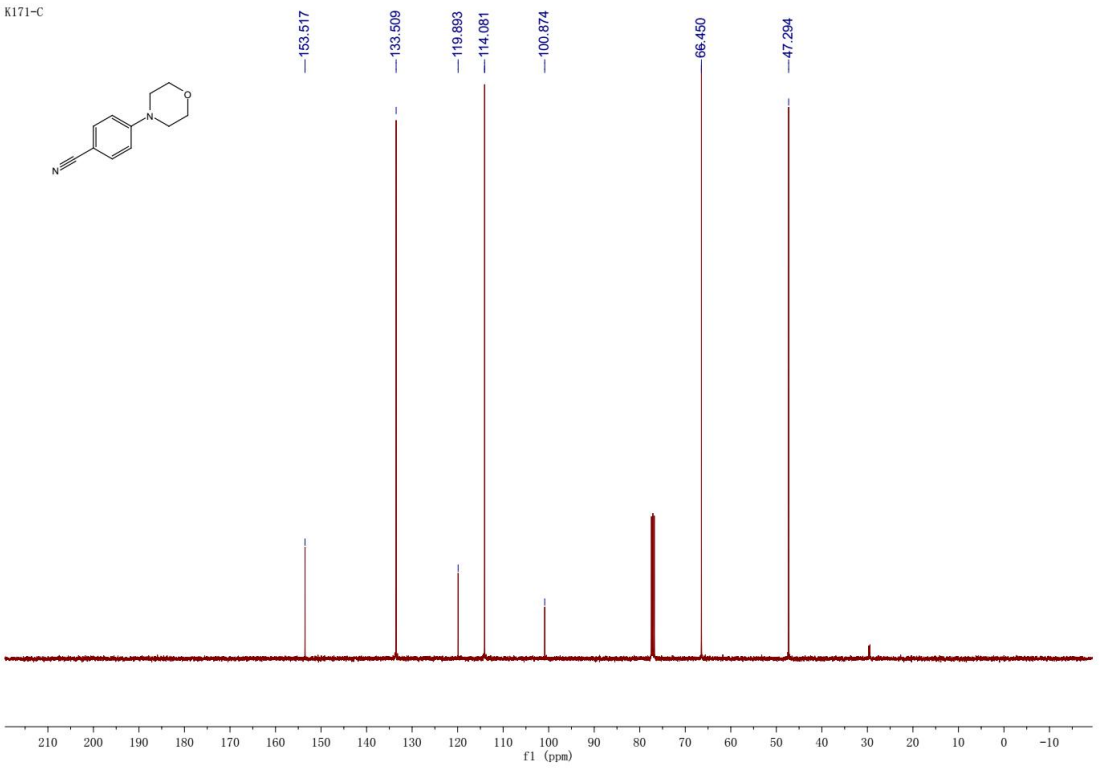
NMR of 2ag


G463-H
7.377
7.365
7.358
7.354
7.335
7.282
7.152
7.131
7.125
7.121
3.893
3.881
3.869
3.210
3.198
3.186
1.00
2.91
4.00
4.03
f1 (ppm)

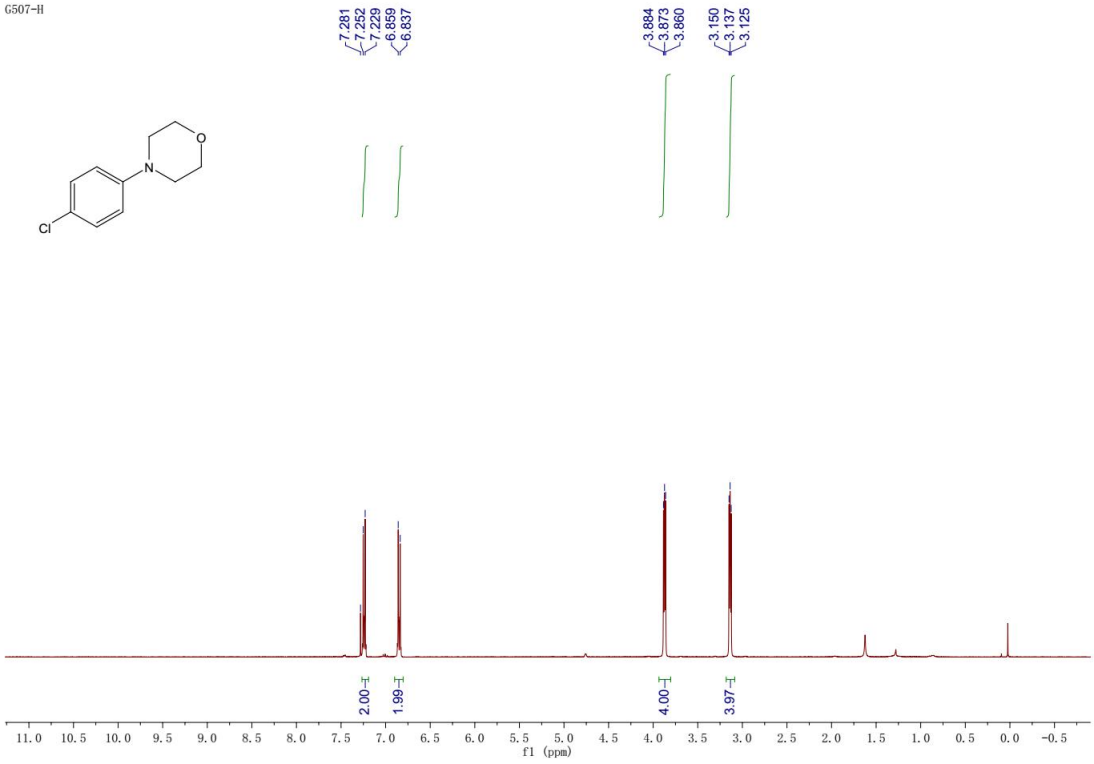

G463-C
151.293
129.982
123.031
119.655
119.261
118.214
113.109
66.577
48.496
f1 (ppm)

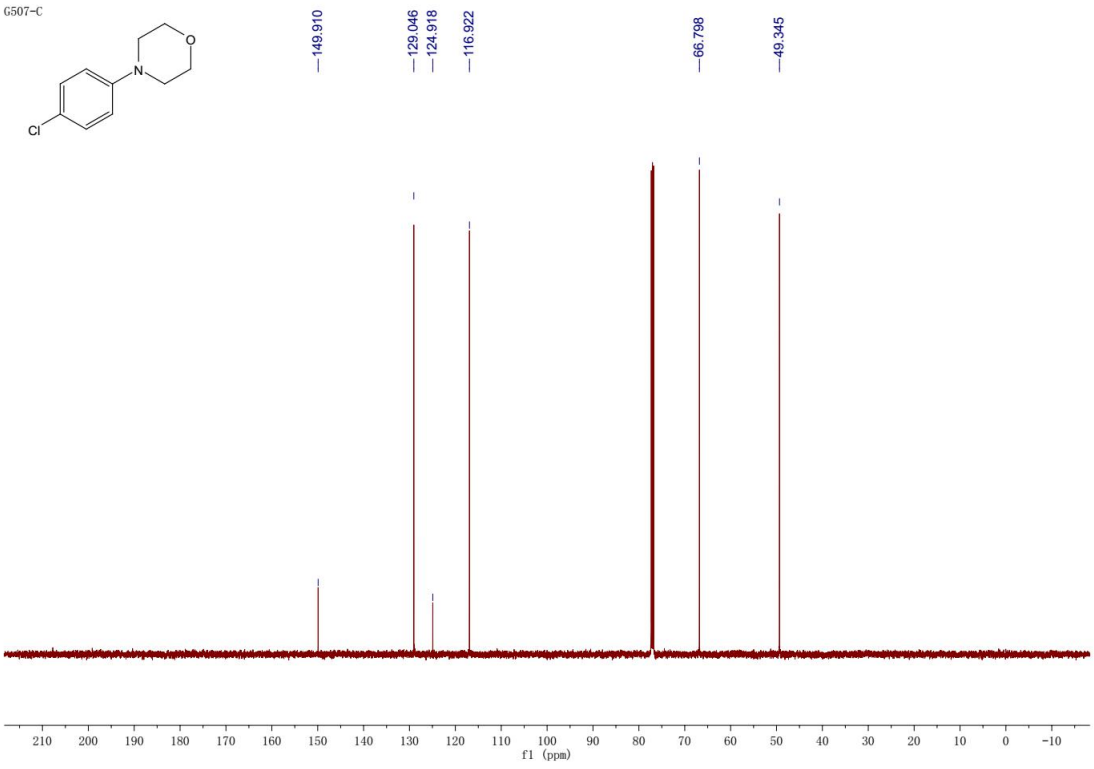
NMR of 2ah


K171-H
7.516
7.494
7.278
6.874
6.852
3.859
3.847
3.835
3.291
3.279
3.266
1.91
2.00
4.00
4.02
f1 (ppm)

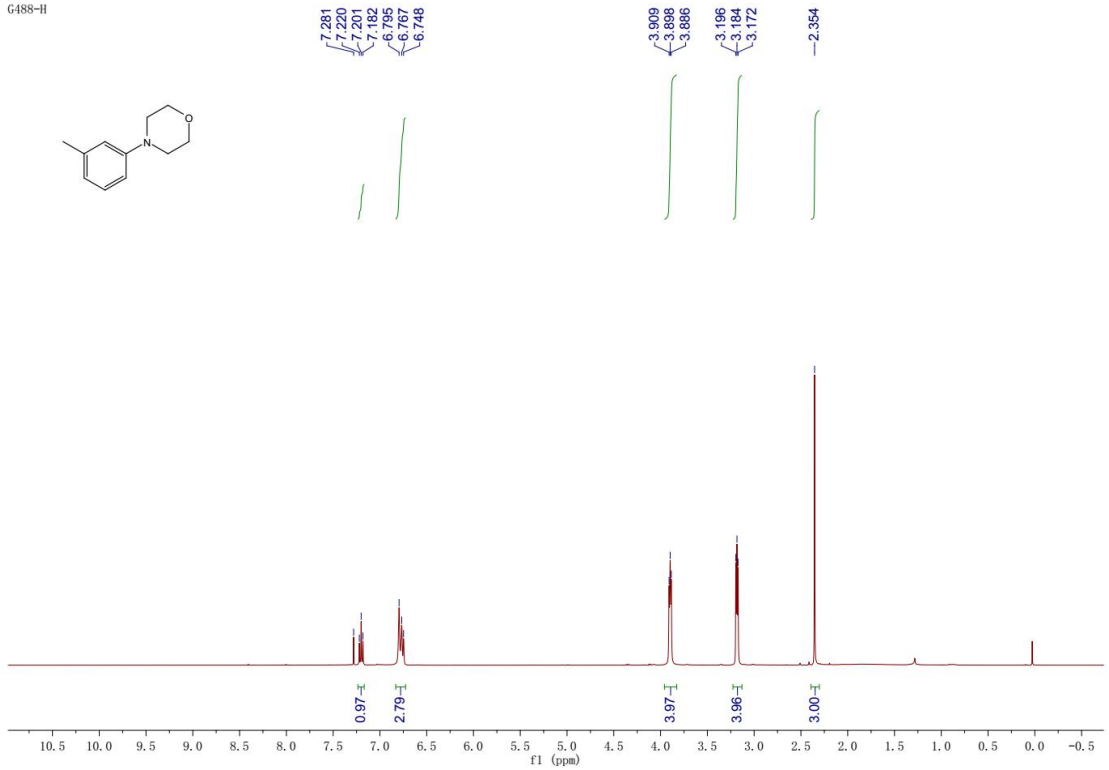

K171-C
153.517
133.509
119.893
114.081
100.874
66.450
47.294
f1 (ppm)

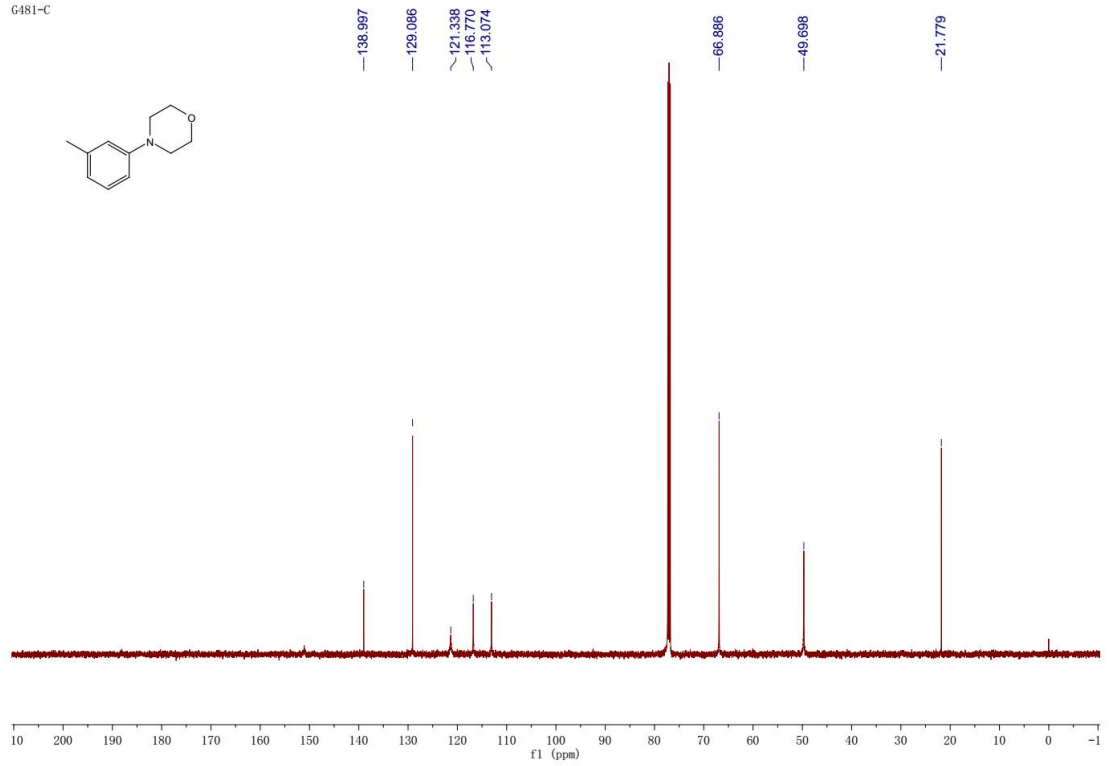
NMR of 2ai


G507-H
7.281
7.252
7.229
6.859
6.837
3.884
3.873
3.860
3.150
3.137
3.125
Cl
O
N
2.00
1.99
4.00
3.97
f1 (ppm)

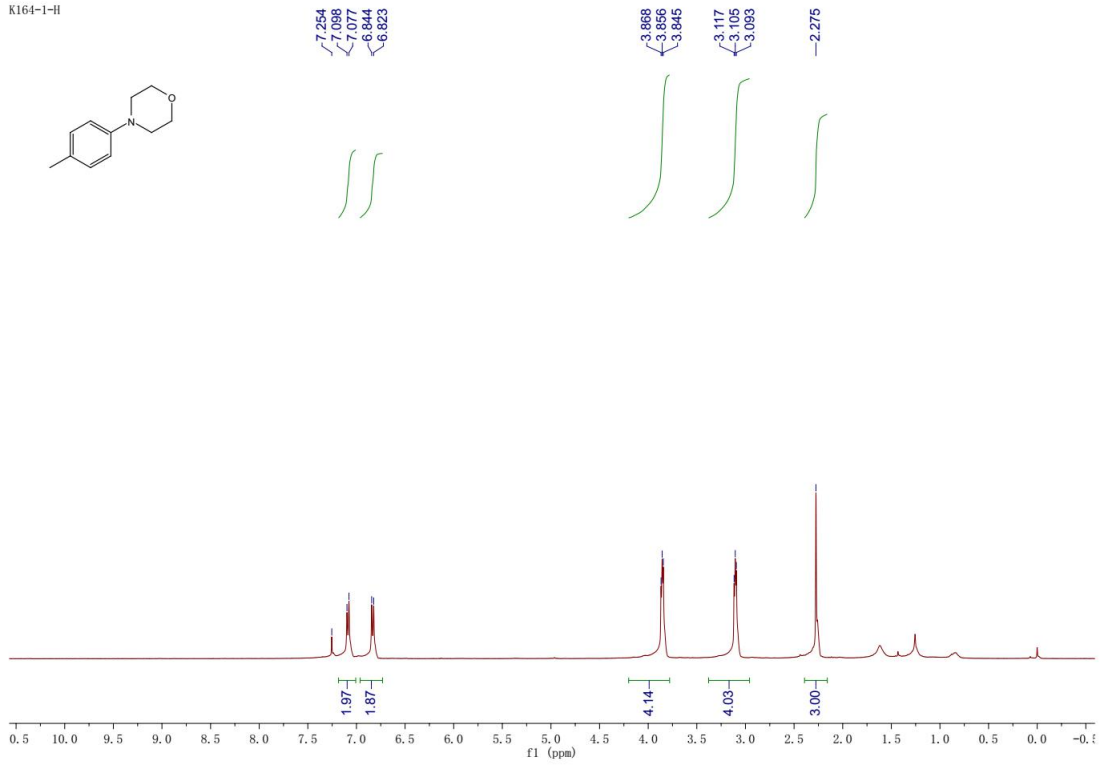

G507-C
149.910
129.046
124.918
116.922
66.798
49.345
Cl
O
N
f1 (ppm)

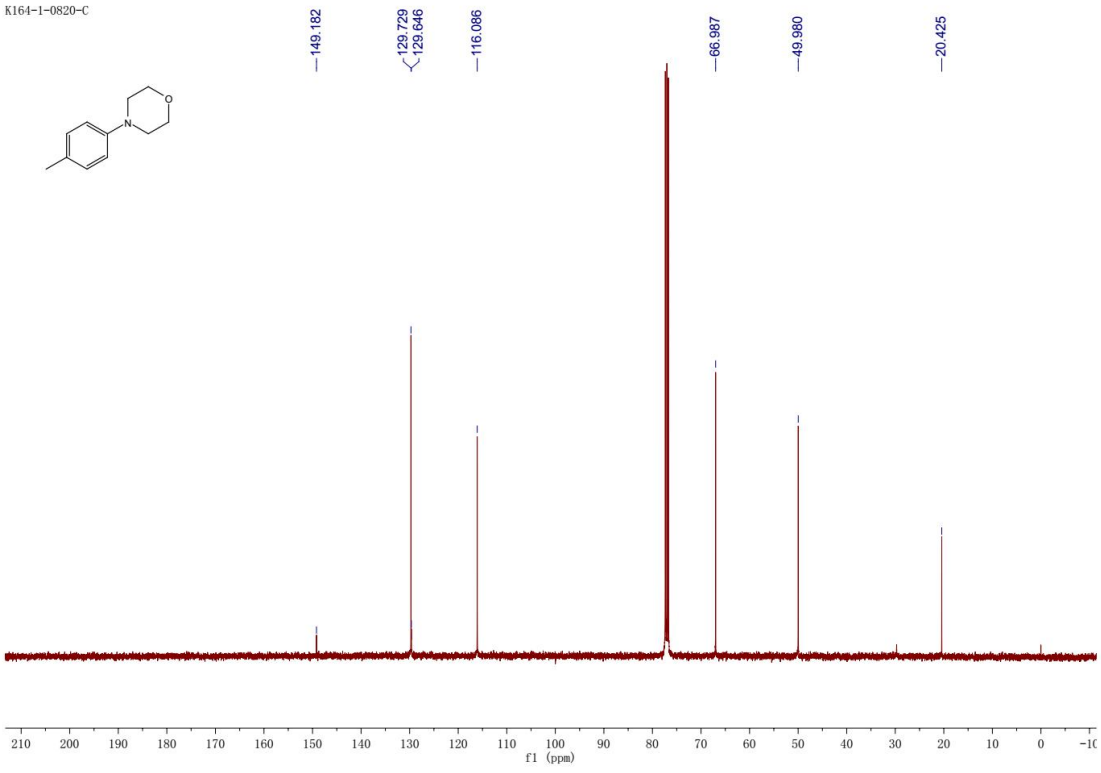
NMR of 2aj


G488-H
7.281
7.220
7.201
7.182
6.795
6.767
6.748
3.909
3.898
3.886
3.196
3.184
3.172
2.354
0.97
2.79
3.97
3.96
3.00
f1 (ppm)

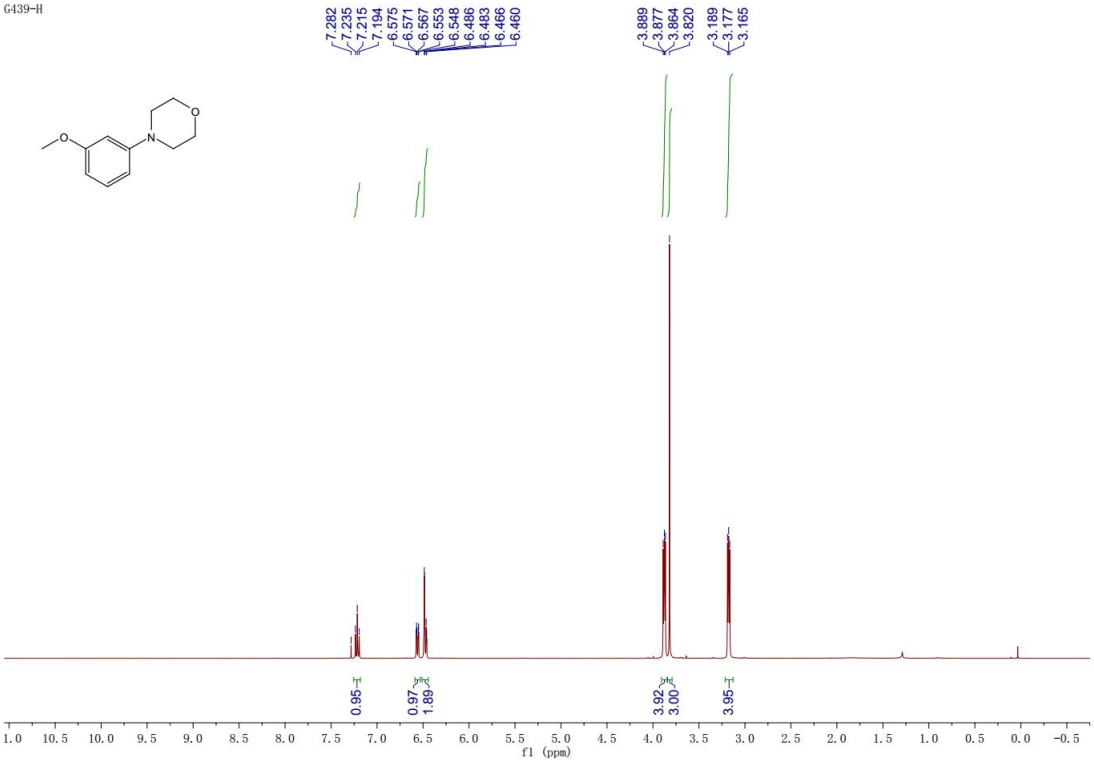

G481-C
138.997
129.086
121.338
116.770
113.074
66.886
49.698
21.779
f1 (ppm)

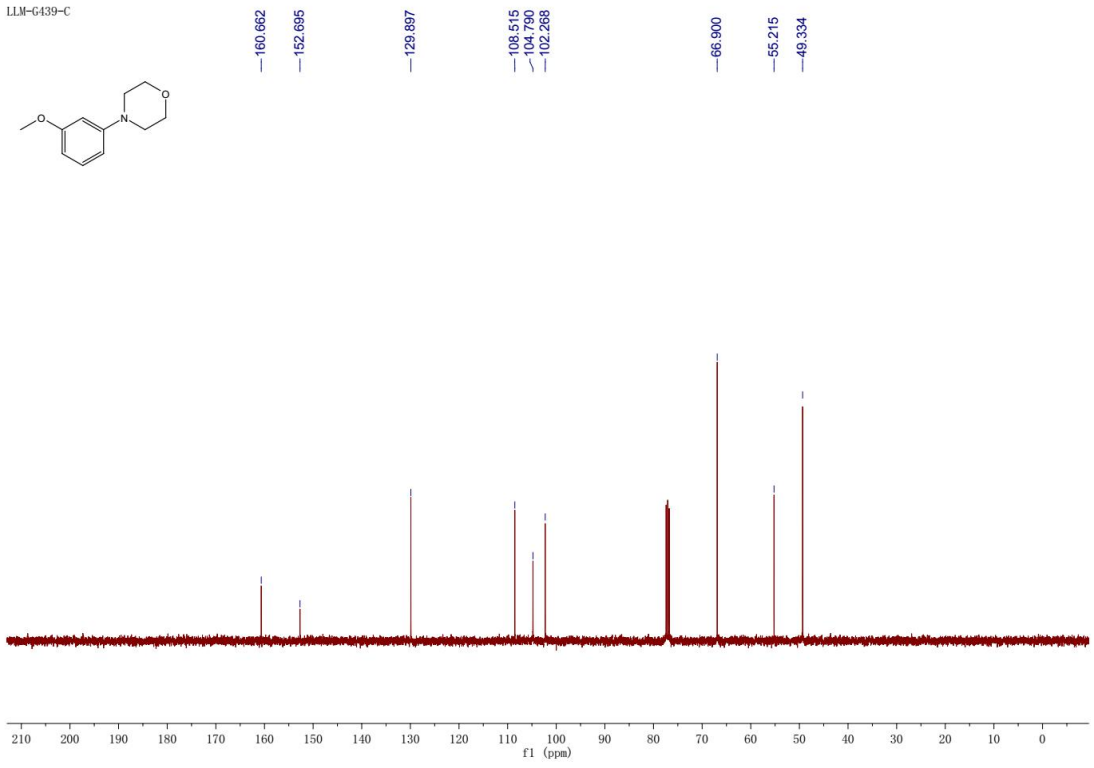
NMR of 2ak


K164-1-H
7.254
7.098
7.077
6.844
6.823
3.868
3.856
3.845
3.117
3.105
3.093
2.275
1.97
1.87
4.14
4.03
3.00
f1 (ppm)

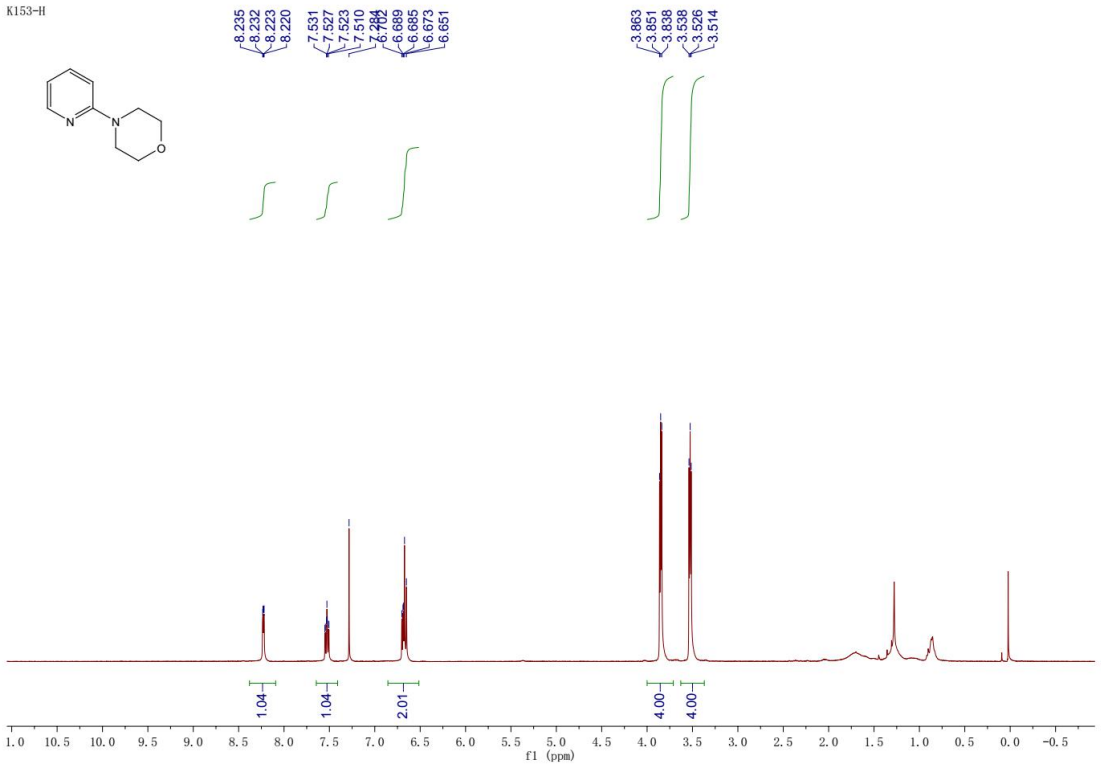

K164-1-0820-C
149.182
129.729
129.646
116.086
66.987
49.980
20.425
f1 (ppm)

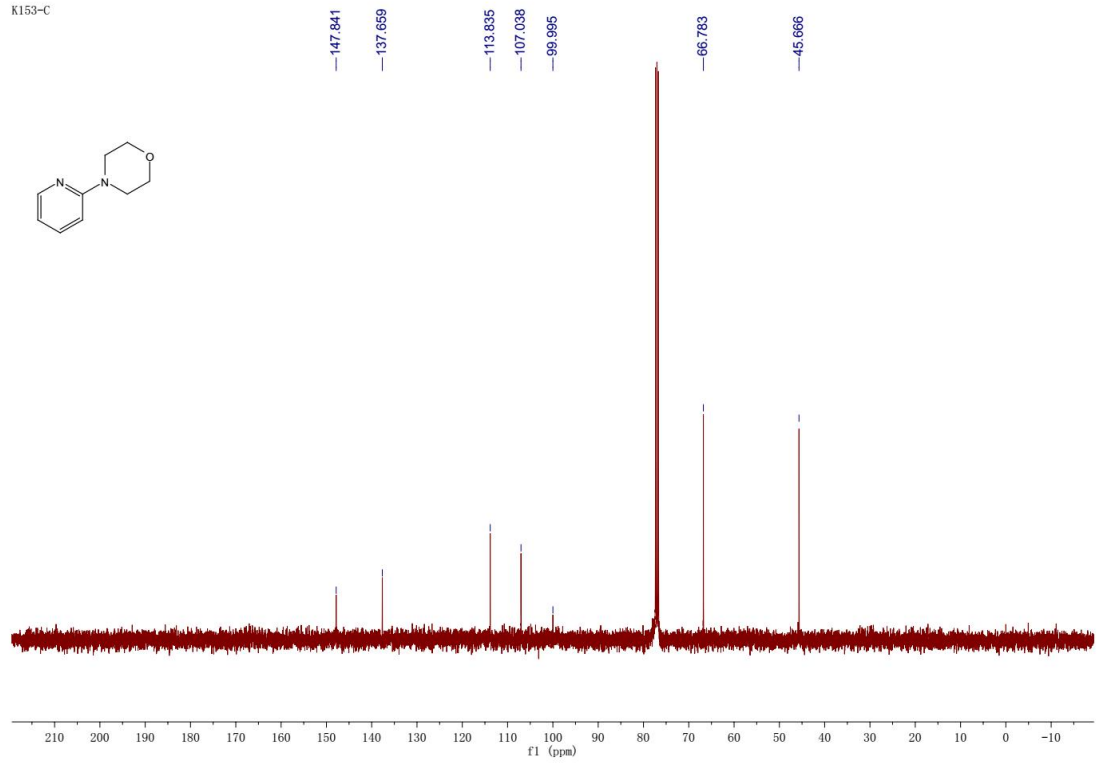
NMR of 2al


G439-H
7.282
7.235
7.215
7.194
6.575
6.571
6.567
6.553
6.548
6.486
6.483
6.466
6.460
3.889
3.877
3.864
3.820
3.189
3.177
3.165
0.95
0.97
1.89
3.92
3.00
3.95
f1 (ppm)

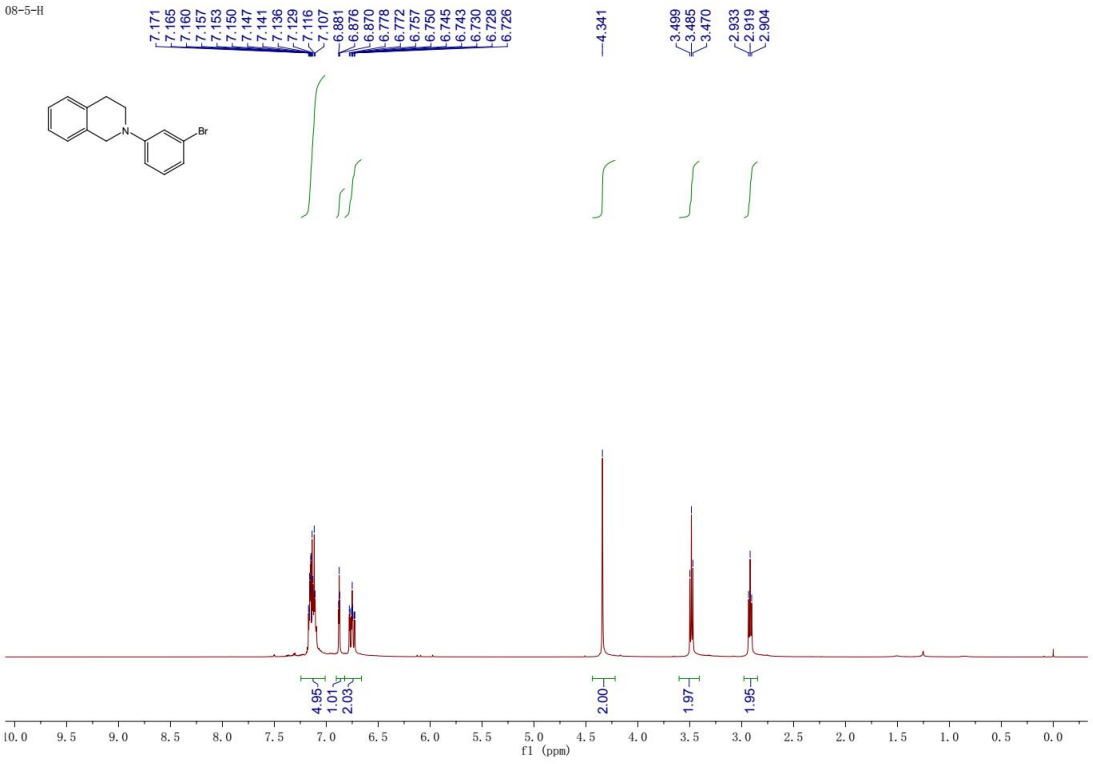

LLM-G439-C
160.662
152.695
129.897
108.515
104.790
102.268
66.900
55.215
49.334
f1 (ppm)

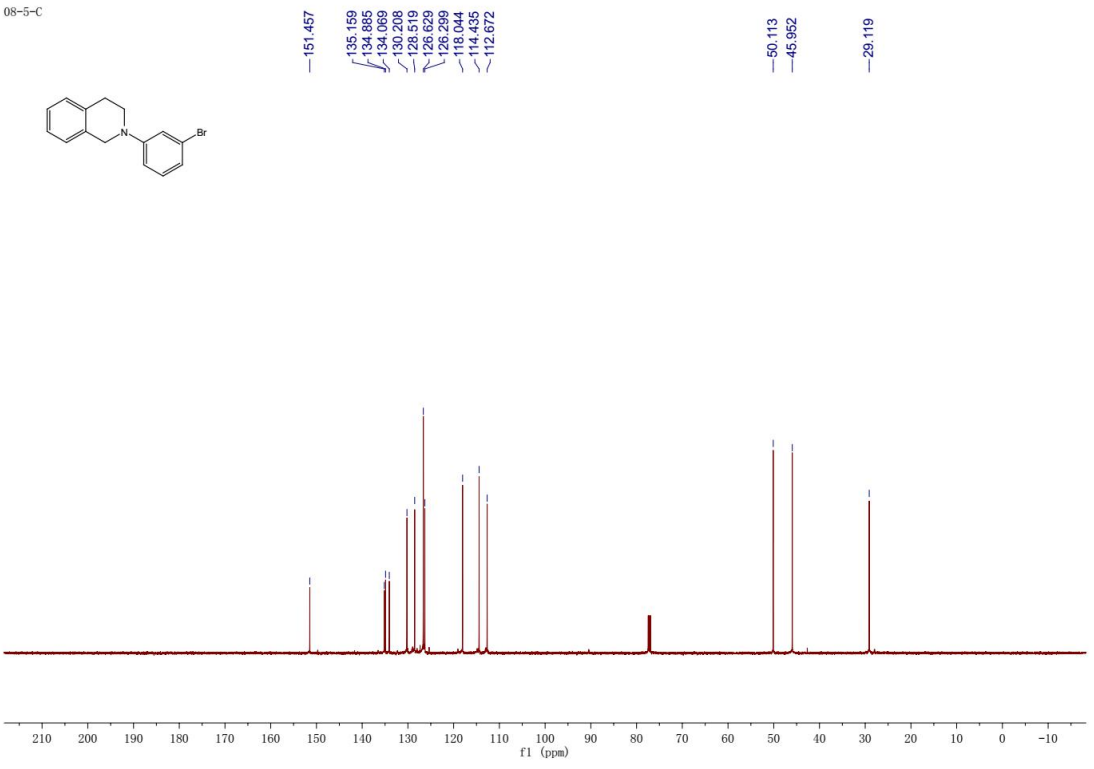
NMR of 2ao


K153-H
8.235
8.232
8.223
8.220
7.531
7.527
7.523
7.510
6.689
6.685
6.673
6.651
3.863
3.851
3.838
3.538
3.526
3.514
1.04
1.04
2.01
4.00
4.00
f1 (ppm)

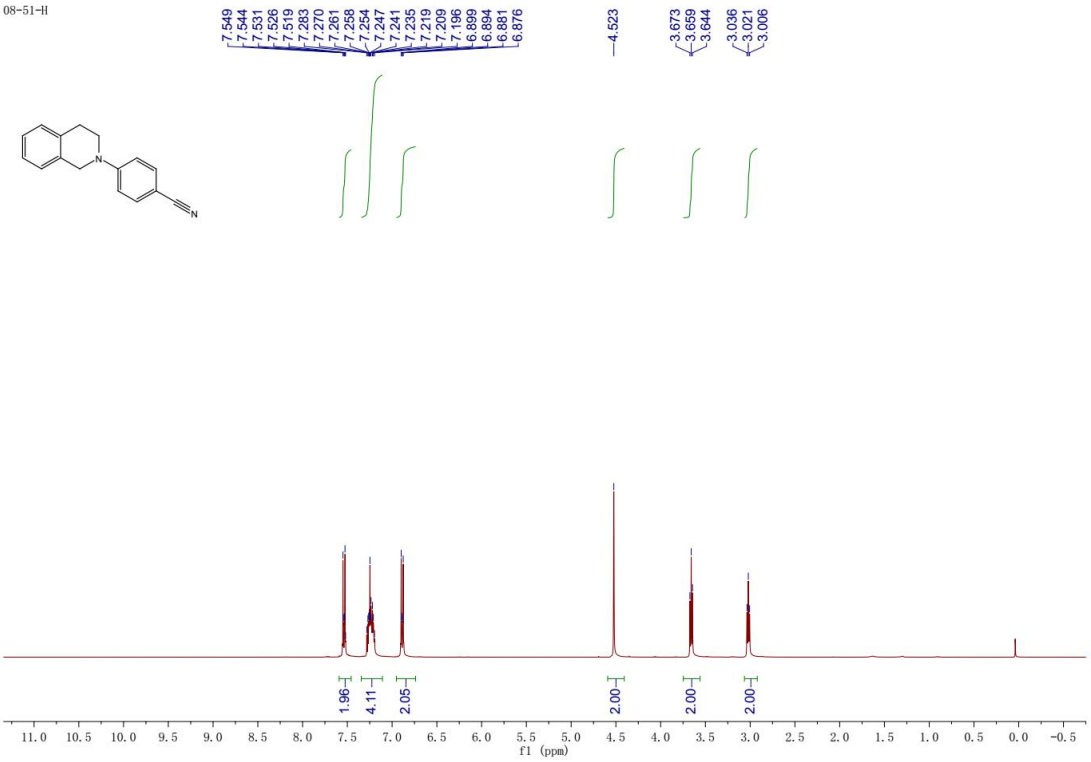

K153-C
147.841
137.659
113.835
107.038
99.995
66.783
45.666
f1 (ppm)

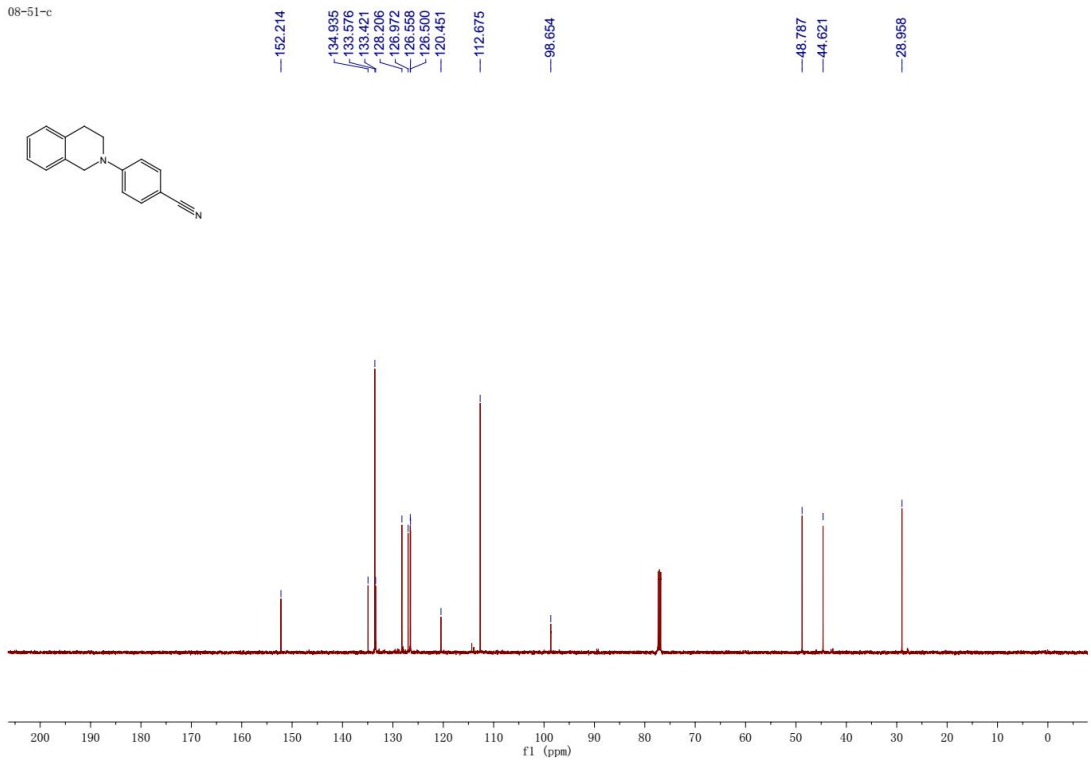
NMR of 2ap


08-5-H
7.171
7.165
7.160
7.157
7.153
7.150
7.147
7.141
7.136
7.129
7.116
7.107
6.881
6.876
6.870
6.778
6.772
6.757
6.750
6.745
6.743
6.730
6.728
6.726
4.341
3.499
3.485
3.470
2.933
2.919
2.904
Br
4.95
1.01
2.03
2.00
1.97
1.95
f1 (ppm)

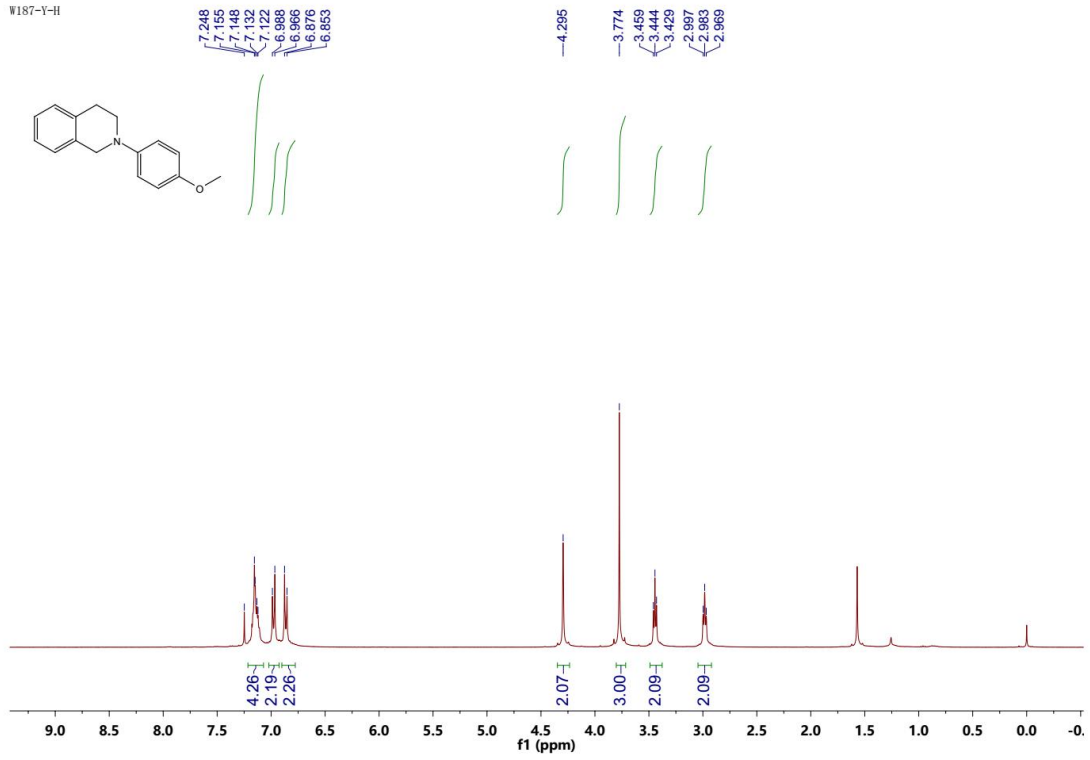

08-5-C
151.457
135.159
134.885
134.069
130.208
128.519
126.629
126.299
118.044
114.435
112.672
50.113
45.952
29.119
Br
f1 (ppm)

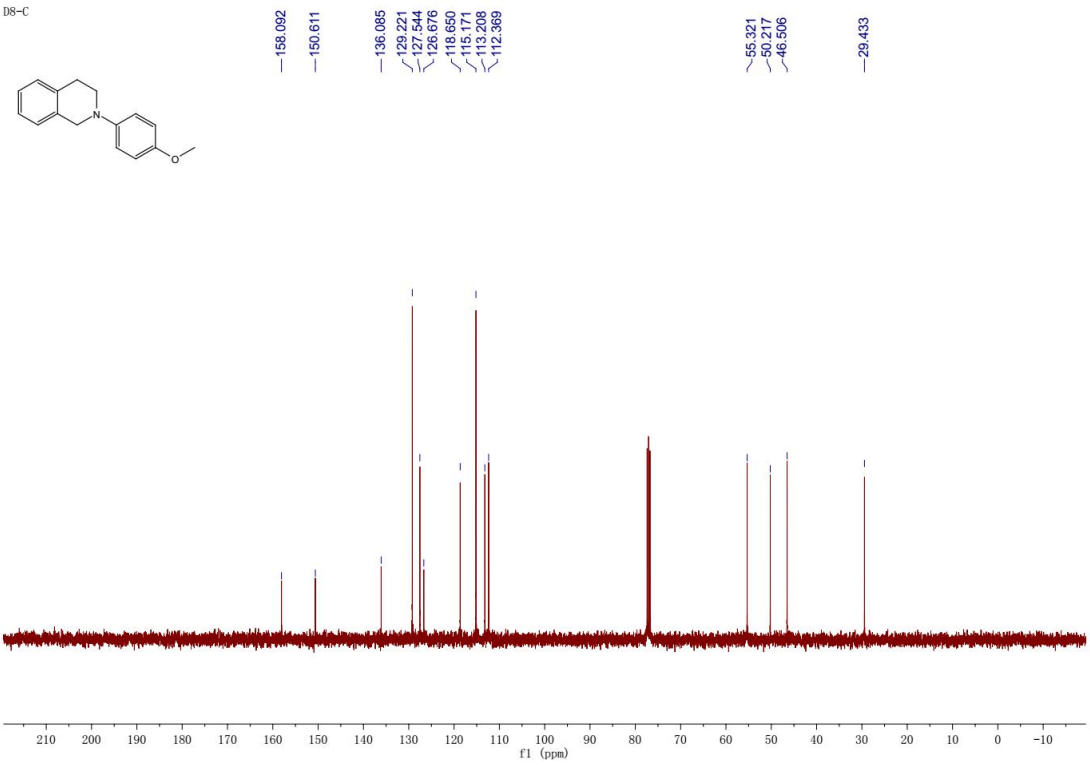
NMR of 2aq


08-51-H
7.549
7.544
7.531
7.526
7.519
7.283
7.270
7.261
7.258
7.254
7.247
7.241
7.235
7.219
7.209
7.196
6.899
6.894
6.881
6.876
4.523
3.673
3.659
3.644
3.036
3.021
3.006
1.96
4.11
2.05
2.00
2.00
2.00
f1 (ppm)

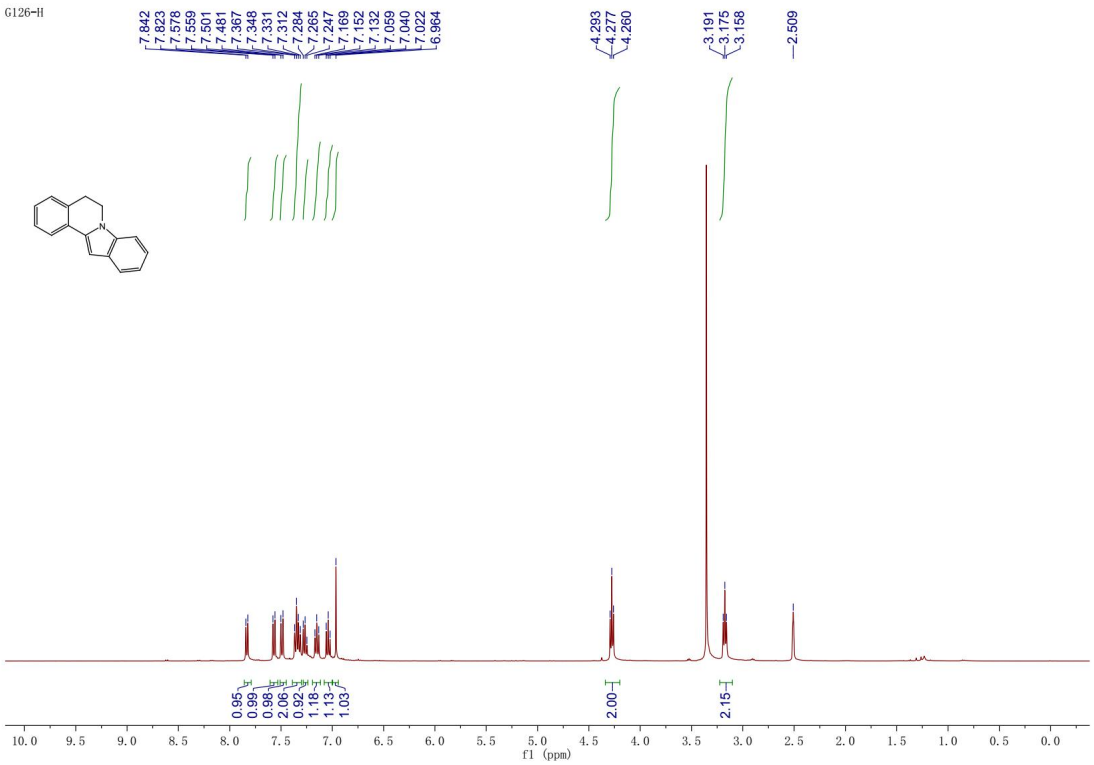

08-51-c
152.214
134.935
133.576
133.421
128.206
126.972
126.558
126.500
120.451
112.675
98.654
48.787
44.621
28.958
f1 (ppm)

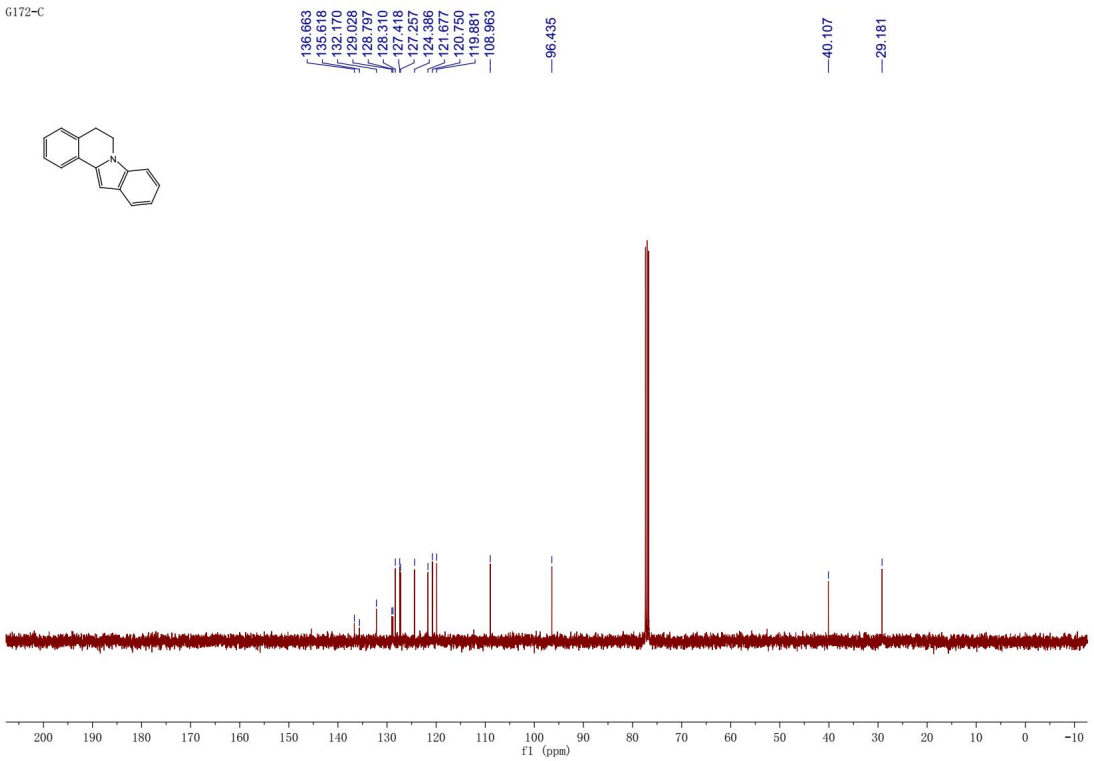
NMR of 2ar


W187-Y-H
7.248
7.155
7.148
7.132
7.122
6.988
6.966
6.876
6.853
4.295
3.774
3.459
3.444
3.429
2.997
2.983
2.969
4.26
2.19
2.26
2.07
3.00
2.09
2.09
f1 (ppm)

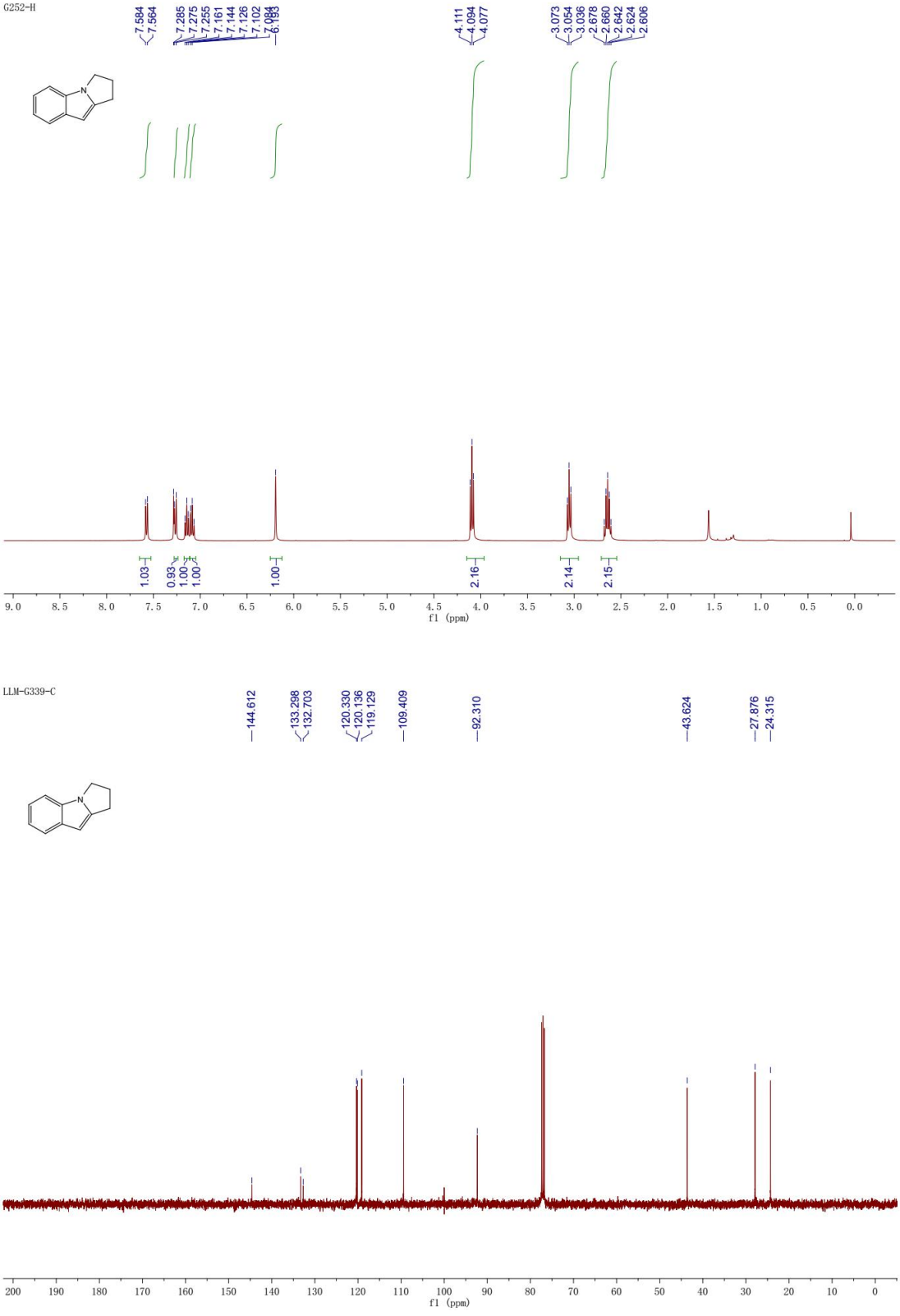

D8-C
158.092
150.611
136.085
129.221
127.544
126.676
118.650
115.171
113.208
112.369
55.321
50.217
46.506
29.433
f1 (ppm)

NMR of 3p

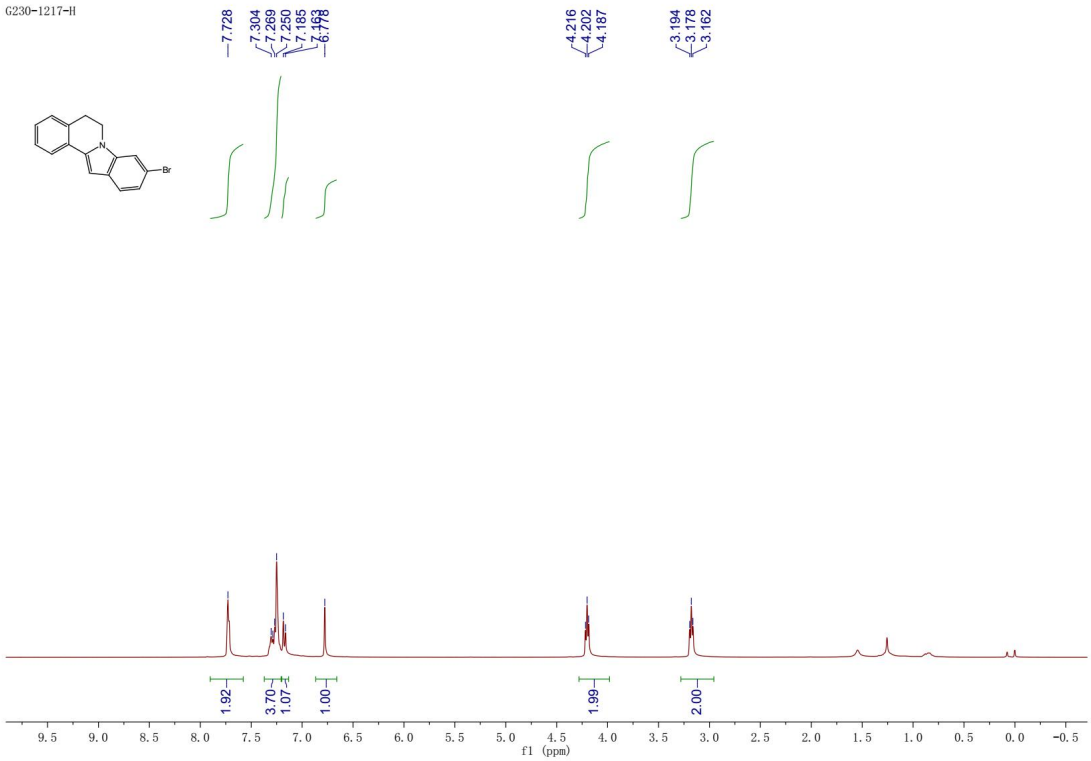

G126-H
7.842
7.823
7.578
7.559
7.501
7.481
7.367
7.348
7.331
7.312
7.284
7.265
7.247
7.169
7.152
7.132
7.059
7.040
7.022
6.964
4.293
4.277
4.260
3.191
3.175
3.158
2.509
0.95
0.99
0.98
2.06
0.92
1.18
1.13
1.03
2.00
2.15
f1 (ppm)

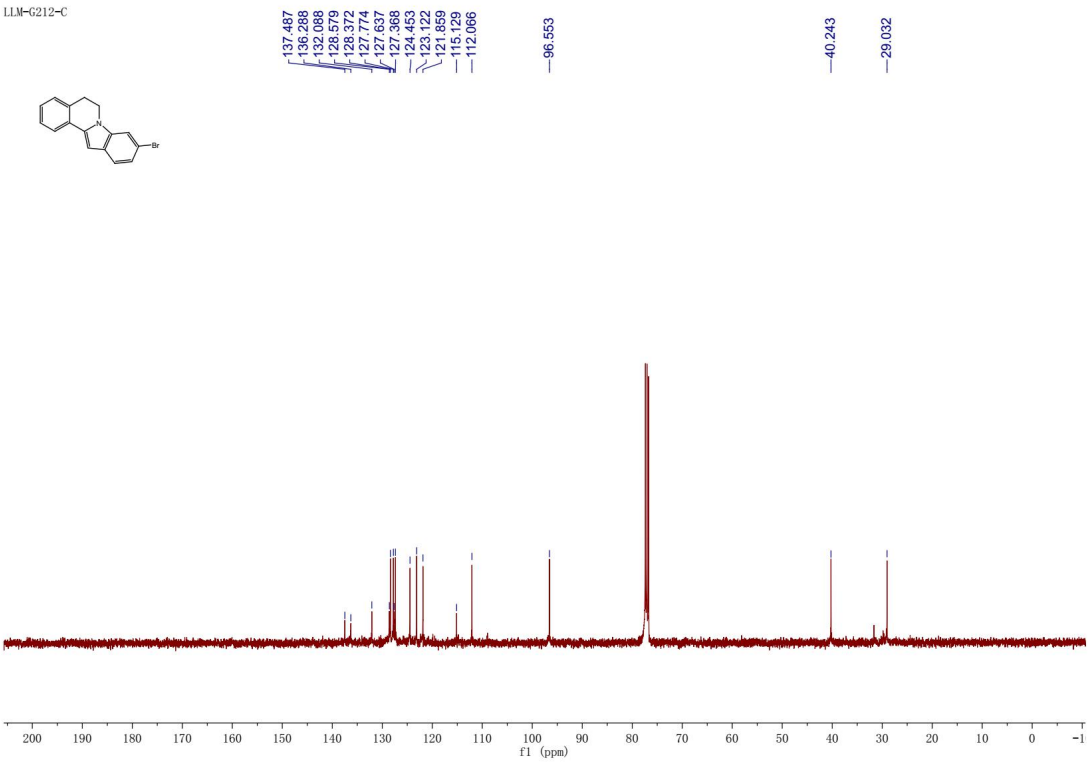

G172-C
136.663
135.618
132.170
129.028
128.797
128.310
127.418
127.257
124.386
121.677
120.750
119.881
108.963
96.435
40.107
29.181
f1 (ppm)

NMR of 3q

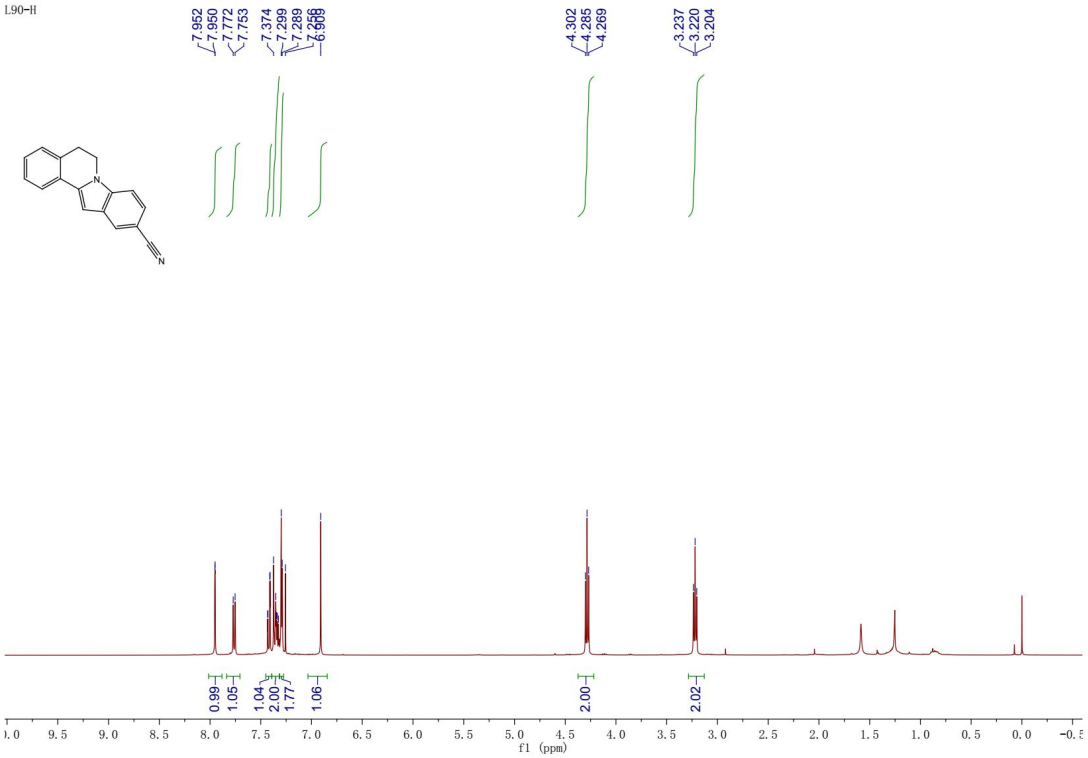

G252-H
7.584
7.564
7.285
7.275
7.255
7.161
7.144
7.126
7.102
4.111
4.094
4.077
3.073
3.054
3.036
2.678
2.660
2.642
2.624
2.606
1.03
0.93
1.00
1.00
1.00
2.16
2.14
2.15
f1 (ppm)
LLM-G339-C
144.612
133.298
132.703
120.330
120.136
119.129
109.409
92.310
43.624
27.876
24.315
f1 (ppm)

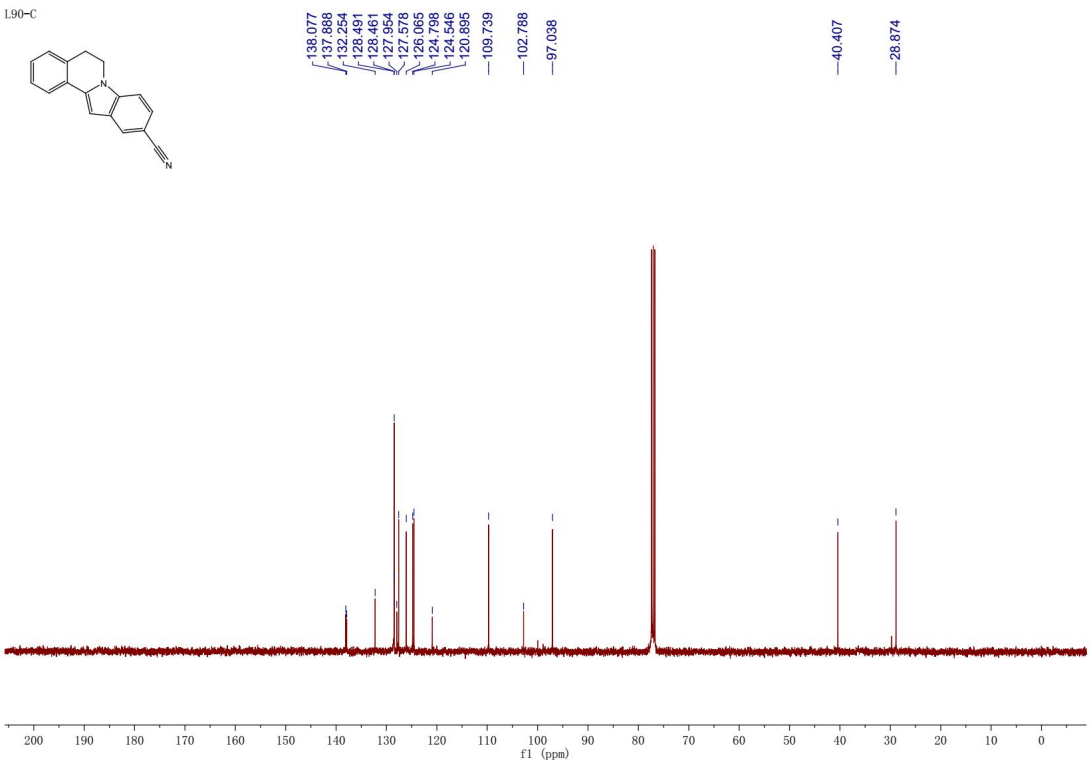
NMR of 3ap


G230-1217-H
7.728
7.304
7.269
7.250
7.185
6.778
4.216
4.202
4.187
3.194
3.178
3.162
Br
1.92
3.70
1.07
1.00
1.99
2.00
f1 (ppm)

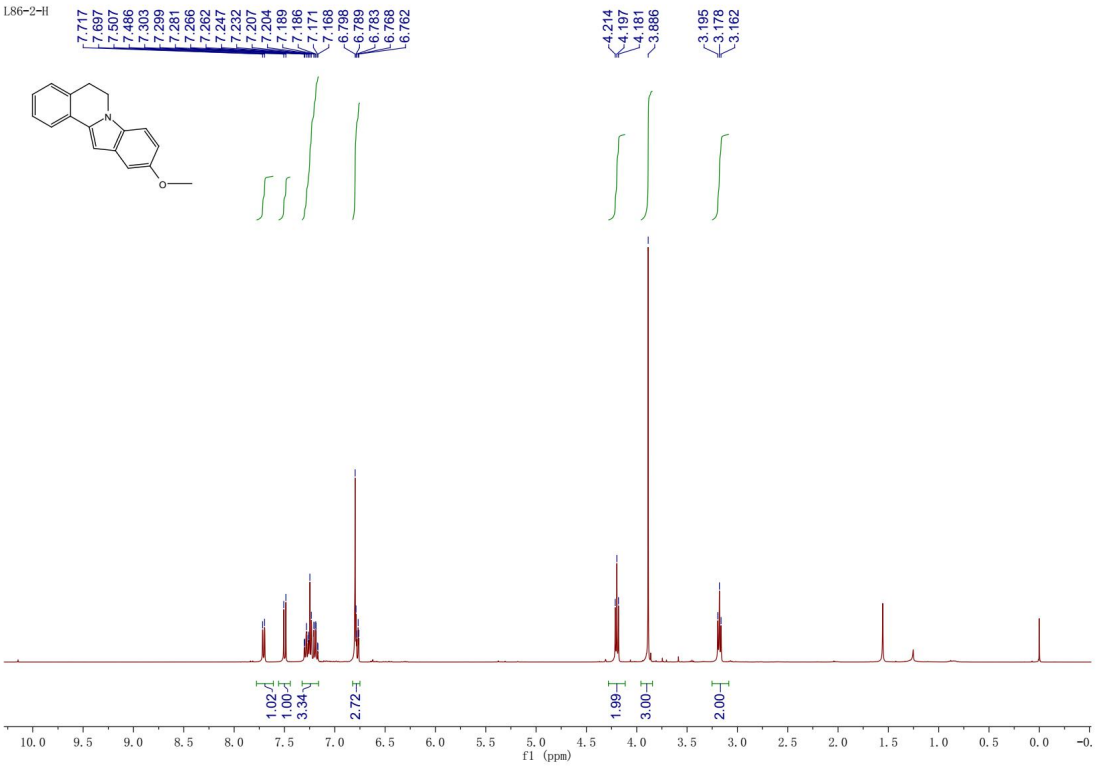

LLM-G212-C
137.487
136.288
132.088
128.579
128.372
127.774
127.637
127.368
124.453
123.122
121.859
115.129
112.066
96.553
40.243
29.032
Br
f1 (ppm)

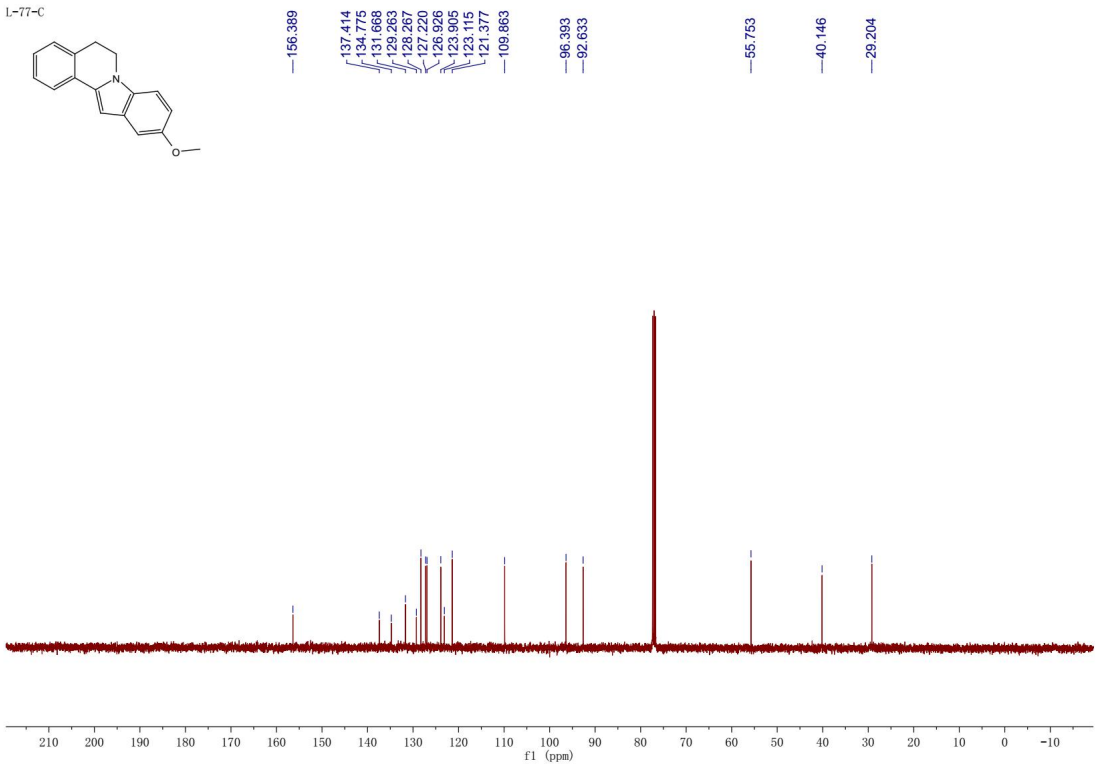
NMR of 3aq


L90-H
7.952
7.950
7.772
7.753
7.374
7.299
7.289
4.302
4.285
4.269
3.237
3.220
3.204
0.99
1.05
1.04
2.00
1.77
1.06
2.00
2.02
f1 (ppm)


L90-C
138.077
137.888
132.254
128.491
128.461
127.954
127.578
126.065
124.798
124.546
120.895
109.739
102.788
97.038
40.407
28.874
f1 (ppm)

NMR of 3ar


L86-2-H
7.717
7.697
7.507
7.486
7.303
7.299
7.281
7.266
7.262
7.247
7.232
7.207
7.204
7.189
7.186
7.171
7.168
6.798
6.789
6.783
6.768
6.762
4.214
4.197
4.181
3.886
3.195
3.178
3.162
1.02
1.00
3.34
2.72
1.99
3.00
2.00
f1 (ppm)


L-77-C
156.389
137.414
134.775
131.668
129.263
128.267
127.220
126.926
123.905
123.115
121.377
109.863
96.393
92.633
55.753
40.146
29.204
f1 (ppm)

7. Molecular Coordinates and Free Energies

1a (O-State)

ΔG = -632.028681 hartree

C	0.592002	-0.287720	-0.206205
C	0.923949	-1.665772	-0.239013
C	2.197190	-2.117960	0.084514
C	3.212344	-1.223850	0.460292
C	2.928772	0.132296	0.443066
C	1.657718	0.633951	0.076538
C	1.629925	2.076462	-0.179342
O	0.736861	2.734104	-0.712897
O	-3.383554	-0.245320	0.471326
C	-2.736196	-1.275249	-0.282155
C	-1.668609	-0.671857	-1.196410
N	-0.701077	0.136005	-0.448478
C	-1.362872	1.150023	0.379951
C	-2.439459	0.493369	1.251701
H	0.157137	-2.397175	-0.463623
H	2.392026	-3.186749	0.074164
H	4.197331	-1.583947	0.737475
H	3.712130	0.850233	0.674301
H	2.572121	2.584323	0.109264
H	-3.514179	-1.767260	-0.871685
H	-2.291653	-2.011009	0.405175
H	-2.165364	-0.006089	-1.915740
H	-1.158294	-1.446075	-1.770596
H	-1.812173	1.914777	-0.263993
H	-0.638488	1.641574	1.026440
H	-3.009629	1.259069	1.784839
H	-1.968460	-0.176131	1.988271

1a (H-State)

ΔG = -632.033918 hartree

C	-0.448154	-0.367930	0.242997
C	-0.582927	-1.771054	0.130933
C	-1.797459	-2.348731	-0.224464
C	-2.927513	-1.558505	-0.491652
C	-2.828103	-0.182777	-0.343971
C	-1.620978	0.425123	0.057802
C	-1.647206	1.840753	0.446837
O	-2.559892	2.626348	0.189796
O	3.461478	0.143216	-0.469407
C	2.940328	-0.965999	0.271577
C	1.842080	-0.499855	1.228478
N	0.775275	0.234541	0.538250
C	1.319939	1.319171	-0.297799
C	2.429594	0.795668	-1.214480
H	0.278310	-2.412177	0.276046
H	-1.857385	-3.429225	-0.320579
H	-3.865118	-2.018511	-0.786081
H	-3.694664	0.455683	-0.485506
H	-0.794278	2.180229	1.060542
H	3.780122	-1.390448	0.827905
H	2.557980	-1.725563	-0.426970
H	2.289798	0.184575	1.962023
H	1.421690	-1.340973	1.782627
H	1.721784	2.107527	0.351755
H	0.529884	1.753870	-0.911921
H	2.904687	1.625630	-1.744495
H	2.009973	0.095903	-1.953754

1a (A, O-State)

ΔG = -631.948489 hartree

C	0.665625	-0.182638	-0.000144
C	0.872413	-1.558885	-0.000159
C	2.177284	-2.078051	0.000012
C	3.275420	-1.193429	0.000227
C	3.085233	0.179562	0.000239
C	1.770591	0.732223	0.000011
C	1.468756	2.112384	-0.000154
O	0.238115	2.541821	-0.000409
O	-3.315617	-0.539004	0.000359
C	-2.524016	-0.661192	-1.180904
C	-1.446673	0.435285	-1.225914
N	-0.642687	0.406217	-0.000257
C	-1.446432	0.436112	1.225548
C	-2.523677	-0.660485	1.181468
H	0.024545	-2.236077	-0.000270
H	2.331507	-3.151948	-0.000014
H	4.286070	-1.592688	0.000361
H	3.939295	0.851530	0.000382
H	2.270596	2.858076	0.000064
H	-3.201216	-0.546527	-2.030168
H	-2.066869	-1.659634	-1.226827
H	-1.931454	1.415192	-1.284190
H	-0.791453	0.308741	-2.089000
H	-1.931271	1.416024	1.283238
H	-0.791026	0.310214	2.088588
H	-3.200648	-0.545425	2.030862
H	-2.066400	-1.658848	1.227795

1a (A, H-State)

ΔG = -631.950872 hartree

C	0.441900	-0.399504	0.225765
C	0.571081	-1.802191	0.146706
C	1.776885	-2.401577	-0.204488
C	2.891340	-1.567066	-0.494226
C	2.815265	-0.188956	-0.382634
C	1.624788	0.468072	0.050372
C	1.666866	1.851278	0.420865
O	2.693997	2.590866	0.256749

O	-3.470990	0.215556	-0.452535
C	-2.432496	0.839916	-1.197868
C	-1.300612	1.323854	-0.269514
N	-0.792579	0.173951	0.491074
C	-1.856789	-0.521428	1.214335
C	-2.995914	-0.922671	0.257288
H	-0.304733	-2.426195	0.282953
H	1.848501	-3.478628	-0.300039
H	3.832803	-2.022479	-0.790636
H	3.694012	0.424514	-0.545650
H	0.771966	2.285653	0.887849
H	-2.874078	1.700953	-1.703892
H	-2.028821	0.146069	-1.948499
H	-1.695957	2.068380	0.428973
H	-0.500027	1.761502	-0.863672
H	-2.253523	0.184333	1.953590
H	-1.454672	-1.383672	1.743845
H	-3.836189	-1.316746	0.831948
H	-2.649157	-1.691072	-0.447604

1a (TS1)

ΔG = -631.936192 hartree

C	0.772386	-0.397711	0.105250
C	1.366501	-1.657322	0.256062
C	2.751463	-1.820420	0.274721
C	3.556846	-0.672491	0.103636
C	2.984685	0.573255	-0.076224
C	1.568175	0.806441	-0.068752
C	1.167290	2.152734	-0.349374
O	-0.008825	2.692655	-0.416448
O	-3.449079	-0.080709	-0.170013
C	-2.837411	-1.296419	-0.593234
C	-1.377587	-1.058249	-0.969600
N	-0.652009	-0.364279	0.099699
C	-1.330231	0.662980	0.819570
C	-2.826542	0.400622	1.014788
H	0.720897	-2.521444	0.386175
H	3.190461	-2.801790	0.414591
H	4.639577	-0.764103	0.104467
H	3.629735	1.432789	-0.242468
H	2.009912	2.824188	-0.569568
H	-3.387204	-1.649229	-1.467621
H	-2.912504	-2.051554	0.202299
H	-1.323439	-0.426382	-1.869228
H	-0.866440	-1.996769	-1.193473
H	-1.117335	1.621027	0.231331
H	-0.831259	0.819638	1.781046
H	-3.325390	1.332654	1.286235
H	-2.973172	-0.325157	1.828952

1a (B)

ΔG = -631.950767 hartree

C	0.805657	-0.416420	0.137034
C	1.494623	-1.615829	0.305068
C	2.891384	-1.678538	0.240562
C	3.613190	-0.497216	-0.007035
C	2.950202	0.706562	-0.169303
C	1.521561	0.811782	-0.094366
C	0.980135	2.106808	-0.271093
O	-0.304352	2.507724	-0.137329
O	-3.410174	-0.049297	-0.154002
C	-2.760355	-1.025308	-0.970386
C	-1.288436	-0.677792	-1.168656
N	-0.631338	-0.482969	0.137041
C	-1.347972	0.198733	1.115985
C	-2.833487	-0.034042	1.155752
H	0.912991	-2.516567	0.480078
H	3.403499	-2.625492	0.376214
H	4.697361	-0.523812	-0.069321
H	3.520498	1.612724	-0.355967
H	1.637874	2.920198	-0.558876
H	-3.276979	-1.031185	-1.932710
H	-2.859777	-2.018944	-0.507609
H	-1.200035	0.234586	-1.777005
H	-0.779246	-1.489579	-1.695046
H	-0.848870	1.812354	0.332208
H	-0.832774	0.301651	2.069014
H	-3.331173	0.760893	1.716479
H	-3.066801	-0.995892	1.652527

1a (C)

ΔG = -632.022491 hartree

C	0.891580	-0.611618	0.297342
C	1.886741	-1.585438	0.174655
C	3.200412	-1.163848	-0.063002
C	3.517333	0.197774	-0.175941
C	2.510372	1.165950	-0.067598
C	1.200218	0.752318	0.164092
C	-0.076369	1.557119	0.239588
O	-0.441505	1.942968	-1.098341
O	-3.039452	0.032916	-0.419936
C	-2.693890	-1.353865	-0.438826
C	-1.188217	-1.517818	-0.565095
N	-0.490422	-0.831002	0.547429
C	-1.010585	0.518785	0.919488
C	-2.528497	0.648919	0.759117
H	1.652021	-2.641089	0.272273
H	3.988774	-1.906227	-0.150470
H	4.545582	0.500629	-0.349132
H	2.747115	2.221504	-0.171791
H	0.013067	2.453867	0.864538
H	-3.194016	-1.793738	-1.304597
H	-3.069816	-1.841180	0.474120
H	-0.872493	-1.111845	-1.538213
H	-0.929005	-2.581434	-0.541166
H	-1.211722	2.527650	-1.053884
H	-0.806482	0.632280	1.993520
H	-2.819243	1.702629	0.720981
H	-3.017762	0.197236	1.635119

1a (TS2)

ΔG = -631.934552 hartree

C	-0.504923	-0.300449	-0.000422
C	-0.500410	-1.679252	-0.000265
C	-1.735640	-2.368577	-0.000036
C	-2.943505	-1.644410	0.000166
C	-2.963656	-0.255025	0.000134
C	-1.725578	0.459948	-0.000158
C	-1.496986	1.851785	-0.000118
O	-2.163938	2.899101	0.000074
O	3.409578	-0.218132	0.000400
C	2.622604	-0.388362	1.180403
C	1.491184	0.636974	1.235097
N	0.651709	0.596916	-0.000296
C	1.491775	0.636859	-1.235237
C	2.623157	-0.388490	-1.179954
H	0.425211	-2.243082	-0.000369
H	-1.744445	-3.453147	0.000008
H	-3.886208	-2.185945	0.000369
H	-3.902369	0.289303	0.000329
H	-0.129586	1.675759	-0.000374
H	3.290861	-0.235707	2.030703
H	2.231633	-1.413940	1.228113
H	1.914170	1.644522	1.300096
H	0.842788	0.467895	2.096651
H	1.914871	1.644371	-1.300043
H	0.843825	0.467775	-2.097125
H	3.291811	-0.235908	-2.029956
H	2.232218	-1.414075	-1.227767

1a (D)

ΔG = -631.938166 hartree

C	0.472123	0.245111	-0.017759
C	0.341104	1.619780	-0.012889
C	1.494987	2.429927	0.007247
C	2.768034	1.819497	0.023958
C	2.907621	0.442870	0.018587
C	1.751064	-0.415577	-0.004696
C	1.812422	-1.825408	-0.016597
O	2.750619	-2.638482	-0.013701
O	-3.448695	0.091069	0.036971
C	-2.642446	0.249977	1.204149
C	-1.508681	-0.765657	1.229501
N	-0.667325	-0.704745	-0.035166
C	-1.549098	-0.687642	-1.272505
C	-2.688985	0.316025	-1.149923
H	-0.632422	2.093753	-0.025267
H	1.395011	3.509604	0.010237
H	3.658181	2.443849	0.040942
H	3.891506	-0.015435	0.030889
H	-0.141940	-1.613447	-0.067563
H	-3.289764	0.071972	2.065150
H	-2.264218	1.278181	1.268243
H	-1.916231	-1.778718	1.276008
H	-0.838761	-0.606625	2.075134
H	-1.954407	-1.697752	-1.369646
H	-0.908537	-0.471695	-2.128179
H	-3.367416	0.174921	-1.993733
H	-2.323988	1.350496	-1.176658

1a (TS3)

ΔG = -631.926948 hartree

C	0.715359	-0.736383	0.012822
C	1.679839	-1.757025	0.001664
C	3.033564	-1.423231	-0.011660
C	3.396898	-0.072797	-0.008007
C	2.400854	0.905934	0.001514
C	1.028050	0.622001	0.011596
C	0.007103	2.274713	-0.112779
O	0.796006	3.173581	0.006174
O	-3.147855	0.260603	-0.020145
C	-2.319035	0.321001	1.146237
C	-1.519110	-0.961313	1.299985
N	-0.699798	-1.283520	0.051355
C	-1.536790	-1.101796	-1.214670
C	-2.327935	0.194233	-1.194145
H	1.391284	-2.807370	0.006402
H	3.784660	-2.206967	-0.021560
H	4.447637	0.208196	-0.013509
H	2.684920	1.960434	0.002254
H	-0.551718	-2.292263	0.106617
H	-2.981709	0.420737	2.008949
H	-1.664185	1.196893	1.082117
H	-2.192629	-1.810922	1.435588
H	-0.823569	-0.911716	2.138582
H	-2.215616	-1.957749	-1.243030
H	-0.852646	-1.152000	-2.062548
H	-2.998654	0.204334	-2.056342
H	-1.667186	1.067535	-1.226574

1a (E)

ΔG = -518.615200 hartree

C	-0.804080	-0.287751	0.000006
C	-1.857257	-1.214927	0.000085
C	-3.165060	-0.725545	0.000013
C	-3.363561	0.660749	-0.000135
C	-2.259250	1.526162	-0.000206
C	-0.902924	1.102521	-0.000140
O	3.038962	0.572755	0.000015
C	2.221450	0.564687	-1.173413
C	1.403073	-0.716827	-1.253687
N	0.571691	-0.950078	0.000102
C	1.403014	-0.716583	1.253887
C	2.221385	0.564920	1.173401
H	-1.684497	-2.291297	0.000199
H	-4.005500	-1.413651	0.000070
H	-4.376941	1.059620	-0.000193

H	-2.477941	2.596995	-0.000321
H	0.372437	-1.952175	0.000195
H	2.896523	0.601012	-2.031841
H	1.563588	1.438896	-1.181089
H	2.067053	-1.580212	-1.346919
H	0.712096	-0.698059	-2.097474
H	2.066994	-1.579946	1.347315
H	0.711996	-0.697657	2.097637
H	2.896410	0.601425	2.031859
H	1.563515	1.439125	1.180862

1a (TS4)

ΔG = -518.611556 hartree

C	0.774955	-0.196251	0.000000
C	1.108967	1.155441	-0.000008
C	2.480451	1.453184	-0.000009
C	3.432211	0.424103	-0.000003
C	3.039358	-0.926073	0.000004
C	1.675978	-1.270368	0.000006
O	-3.066149	0.528658	-0.000003
C	-2.261014	0.511241	1.182230
C	-1.386001	-0.738170	1.227714
N	-0.546664	-0.869469	0.000006
C	-1.386004	-0.738192	-1.227701
C	-2.261017	0.511220	-1.182238
H	0.375730	1.955421	-0.000011
H	2.802954	2.490510	-0.000013
H	4.489226	0.681849	-0.000003
H	3.811901	-1.694096	0.000009
H	0.251370	-1.852843	0.000013
H	-2.949937	0.514193	2.030114
H	-1.649123	1.423229	1.231190
H	-2.018868	-1.630084	1.275847
H	-0.723383	-0.727591	2.096253
H	-2.018871	-1.630107	-1.275817
H	-0.723388	-0.727628	-2.096242
H	-2.949943	0.514156	-2.030119
H	-1.649126	1.423207	-1.231216

2a

ΔG = -518.710664 hartree

C	-0.723623	0.064704	0.345146
C	-1.307692	-1.183501	0.027623
C	-2.653824	-1.279516	-0.335976
C	-3.464846	-0.145343	-0.414592
C	-2.896992	1.097554	-0.109723
C	-1.559574	1.205812	0.266640
O	3.081049	-0.100474	-0.639060
C	2.299191	-1.255973	-0.307405
C	1.463937	-0.990212	0.947207
N	0.603591	0.184406	0.782692
C	1.416528	1.352537	0.416104
C	2.258506	1.056881	-0.829204
H	-0.716927	-2.090876	0.046272
H	-3.061516	-2.258705	-0.573160
H	-4.507742	-0.224501	-0.705057
H	-3.503508	1.998427	-0.152677
H	-1.172036	2.184733	0.525008
H	3.008903	-2.070840	-0.140583
H	1.651304	-1.516876	-1.157865
H	2.147420	-0.782111	1.780903
H	0.877813	-1.866749	1.225796
H	2.081621	1.587772	1.256625
H	0.791188	2.226145	0.236045
H	2.938800	1.885891	-1.043155
H	1.601484	0.902979	-1.699436

3a

ΔG = -555.638916 hartree

C	0.812283	-0.389758	0.030536
C	1.697105	-1.475757	0.005067
C	3.062778	-1.193440	-0.019498
C	3.534600	0.138000	-0.023652
C	2.650689	1.214772	-0.008860
C	1.265705	0.963011	0.012214
C	0.093098	1.794364	0.009430
O	-3.234066	0.139930	-0.418238
C	-2.891881	-1.077533	0.248057
C	-1.468318	-1.505049	-0.103630
N	-0.570395	-0.366483	0.067934
C	-0.995464	0.953192	0.033386
C	-2.469925	1.235715	0.095404
H	1.340211	-2.501146	0.006922
H	3.775502	-2.012883	-0.035491
H	4.605154	0.321798	-0.041176
H	3.024095	2.235368	-0.017648
H	0.058946	2.875486	0.002435
H	-3.603159	-1.834869	-0.086790
H	-2.999251	-0.946733	1.335008
H	-1.423716	-1.857094	-1.142082
H	-1.153947	-2.323949	0.550968
H	-2.722175	2.111043	-0.506775
H	-2.780380	1.433815	1.134274

1b (O-State)

ΔG = -710.610865 hartree

C	0.945698	-0.276188	-0.265058
C	1.159360	-1.678403	-0.302881
C	2.360786	-2.243201	0.102812
C	3.418476	-1.445688	0.572030
C	3.259096	-0.070101	0.550983
C	2.070869	0.544319	0.086267
O	-3.094781	0.416206	-0.104917
C	-2.585056	-0.710490	-0.846750
C	-2.569800	-2.011729	-0.039236
C	-1.238190	-0.351784	-1.490163
N	-0.305691	0.239824	-0.530326
C	-0.857682	1.434268	0.099107

C	-2.196791	1.106497	0.787506
C	-2.018575	0.404451	2.138502
C	2.211269	1.972754	-0.206528
O	1.477928	2.674482	-0.903349
H	0.347241	-2.335342	-0.589852
H	2.462811	-3.324762	0.087262
H	4.342508	-1.895134	0.919685
H	4.083519	0.574245	0.847320
H	-3.311555	-0.829237	-1.658484
H	-2.424426	-2.859735	-0.718036
H	-3.528379	-2.147075	0.470357
H	-1.774613	-2.036491	0.708902
H	-1.418005	0.394821	-2.278233
H	-0.795361	-1.226012	-1.967638
H	-1.002059	2.220626	-0.651578
H	-0.166582	1.815616	0.849246
H	-2.707949	2.059043	0.966703
H	-1.601774	1.114165	2.861758
H	-1.340636	-0.450656	2.080787
H	-2.984959	0.060007	2.518132
H	3.138118	2.413422	0.212533

1b (H-State)

ΔG = -710.613788 hartree

C	-0.847568	0.388477	-0.275333
C	-0.947762	1.795131	-0.123383
C	-2.127723	2.393216	0.295652
C	-3.267466	1.623831	0.593062
C	-3.209224	0.253887	0.401309
C	-2.037832	-0.377506	-0.075575
O	3.144819	-0.632519	-0.197749
C	2.725367	0.607758	-0.804645
C	2.817875	1.807067	0.143185
C	1.354416	0.431643	-1.472042
N	0.376893	-0.189897	-0.576994
C	0.839826	-1.488231	-0.090461
C	2.198251	-1.345755	0.622229
C	2.072766	-0.787139	2.043682
C	-2.151072	-1.769625	-0.524725
O	-3.096997	-2.517078	-0.269855
H	-0.072883	2.414705	-0.279694
H	-2.154164	3.472025	0.421530
H	-4.179175	2.098526	0.940593
H	-4.085568	-0.366989	0.559102
H	3.459089	0.757238	-1.604636
H	2.747403	2.734749	-0.436009
H	3.782868	1.802230	0.658460
H	2.025621	1.815988	0.894691
H	1.475864	-0.228703	-2.344535
H	0.981588	1.388224	-1.839153
H	0.946884	-2.191064	-0.929456
H	0.119954	-1.904595	0.615602
H	2.633034	-2.349198	0.690563
H	1.593570	-1.535742	2.684358
H	1.471761	0.124377	2.086818
H	3.063464	-0.572318	2.454612
H	-1.349260	-2.129914	-1.190779

1b (A, O-State)

ΔG = -710.528488 hartree

C	-0.916389	0.240948	-0.372333
C	-1.008134	1.645808	-0.498392
C	-2.126389	2.346615	-0.057187
C	-3.176696	1.620098	0.570561
C	-3.149484	0.236561	0.647259
C	-2.092951	-0.528883	0.076604
O	3.023564	-0.488192	0.120635
C	2.617174	0.509860	-0.826763
C	2.601445	1.927858	-0.250201
C	1.306289	0.081627	-1.535640
N	0.292464	-0.401131	-0.603612
C	0.795926	-1.494428	0.229925
C	2.037912	-1.022823	1.020404
C	1.700890	-0.114823	2.206310
C	-2.298559	-1.919602	-0.186835
O	-1.574134	-2.661302	-0.923286
H	-0.154924	2.204011	-0.865587
H	-2.166107	3.426474	-0.137044
H	-4.033919	2.155846	0.969324
H	-4.004516	-0.294270	1.057907
H	3.398129	0.474359	-1.593081
H	2.495958	2.652966	-1.064566
H	3.552236	2.122452	0.254139
H	1.794959	2.096528	0.465249
H	1.538273	-0.764772	-2.194392
H	0.907103	0.886471	-2.150594
H	1.079753	-2.320937	-0.425752
H	0.018417	-1.829180	0.912712
H	2.515094	-1.928293	1.409368
H	1.174551	-0.701478	2.966724
H	1.060953	0.727935	1.935098
H	2.620354	0.273766	2.652991
H	-3.185195	-2.350893	0.311722

1b (A, H-State)

ΔG = -710.530781 hartree

C	-0.783004	0.387537	-0.346886
C	-0.779955	1.795820	-0.248579
C	-1.889867	2.496699	0.213766
C	-3.039343	1.760940	0.610516
C	-3.101413	0.383708	0.475117
C	-2.029273	-0.367811	-0.092140
O	3.089590	-0.735299	-0.043289
C	2.766855	0.470137	-0.752160
C	2.846385	1.730690	0.112844
C	1.435698	0.293683	-1.524883
N	0.376162	-0.284608	-0.700218
C	0.784693	-1.560884	-0.111173
C	2.065021	-1.365417	0.738297

C	1.795691	-0.703213	2.092201
C	-2.257347	-1.719192	-0.512614
O	-3.335828	-2.356496	-0.268898
H	0.131675	2.341467	-0.459455
H	-1.854834	3.574658	0.318480
H	-3.900038	2.292654	1.008124
H	-4.013743	-0.150245	0.715094
H	3.549890	0.541423	-1.513573
H	2.800073	2.616860	-0.529198
H	3.803952	1.746685	0.641010
H	2.047015	1.801606	0.852313
H	1.609408	-0.420896	-2.339037
H	1.104225	1.231936	-1.965832
H	1.001512	-2.264877	-0.921618
H	-0.010295	-1.957839	0.516471
H	2.463651	-2.368472	0.920773
H	1.232021	-1.397254	2.724281
H	1.216813	0.219527	2.012095
H	2.742640	-0.480141	2.591235
H	-1.472045	-2.216650	-1.097976

1b (C)

ΔG = -710.610036 hartree

C	1.189923	-0.621799	0.004642
C	1.998310	-1.732340	0.275466
C	3.385689	-1.542725	0.323565
C	3.961592	-0.283958	0.105897
C	3.142045	0.821084	-0.170266
C	1.763913	0.643826	-0.228911
O	-2.817795	-0.042096	-0.872638
C	-2.498712	-1.347027	-0.340226
C	-2.986952	-1.564150	1.096095
C	-1.007546	-1.672566	-0.525914
N	-0.206162	-0.548598	-0.060264
C	-0.534489	0.708976	-0.758512
C	-1.995704	1.092659	-0.492908
C	-2.342954	1.623499	0.900581
C	0.657397	1.658452	-0.442683
O	0.506963	2.538660	0.683065
H	-0.462079	0.516944	-1.845381
H	0.512237	2.012076	1.495625
H	0.836476	2.331009	-1.283974
H	1.572437	-2.715880	0.445268
H	4.026297	-2.395905	0.529269
H	5.040204	-0.166633	0.142626
H	3.578790	1.800985	-0.344925
H	-3.065359	-2.020303	-0.991955
H	-2.994172	-2.638143	1.313204
H	-4.007521	-1.187834	1.211293
H	-2.346485	-1.075877	1.833756
H	-0.801007	-1.873245	-1.591987
H	-0.759426	-2.573329	0.041957
H	-2.279879	1.855222	-1.225946
H	-1.974319	2.645614	1.008582
H	-1.910806	1.019483	1.701412
H	-3.430680	1.629909	1.018650

2b

ΔG = -597.295263 hartree

C	-1.284342	-0.029549	-0.068519
C	-1.929300	1.168098	0.314405
C	-3.314122	1.224332	0.457373
C	-4.105166	0.089669	0.234840
C	-3.478681	-1.100233	-0.138586
C	-2.089543	-1.163898	-0.297116
O	2.909487	-0.156404	-0.684139
C	2.246692	1.122113	-0.618045
C	2.482772	1.864501	0.701470
C	0.765706	0.980896	-0.979952
N	0.124797	-0.064143	-0.168733
C	0.772627	-1.348933	-0.421237
C	2.263711	-1.281561	-0.056611
C	2.516341	-1.360282	1.453475
H	-1.340090	2.054439	0.525763
H	-3.776678	2.160282	0.758781
H	-5.183493	0.135421	0.352231
H	-4.070105	-1.993105	-0.323030
H	2.725981	1.696745	-1.418538
H	2.213555	2.919382	0.576251
H	3.539740	1.814445	0.979100
H	1.884597	1.458402	1.520270
H	0.676195	0.724361	-2.050736
H	0.268577	1.938974	-0.827711
H	0.665946	-1.644589	-1.480417
H	0.308832	-2.124234	0.192552
H	2.751331	-2.144275	-0.523867
H	2.266377	-2.365737	1.810497
H	1.911973	-0.643627	2.014036
H	3.572871	-1.176423	1.669905
H	-1.645273	-2.101152	-0.609835

1c (O-State)

ΔG = -596.113415 hartree

C	-0.586838	-0.281393	-0.214222
C	-0.895695	-1.666798	-0.257131
C	-2.152433	-2.146663	0.086876
C	-3.178741	-1.276576	0.491124
C	-2.923533	0.084737	0.476707
C	-1.669995	0.616114	0.088974
C	-1.687567	2.055933	-0.177575
O	-0.828933	2.736343	-0.739922
C	3.416992	-0.271964	0.533513
C	2.386701	0.566403	1.302582
C	1.336175	1.192383	0.367320
N	0.693475	0.164528	-0.464320
C	1.658088	-0.635633	-1.229943
C	2.713124	-1.317027	-0.344896
H	-0.118893	-2.380246	-0.503698
H	-3.717898	0.784892	0.724896

H	-2.637040	2.538954	0.130116
H	4.019775	0.389040	-0.105778
H	4.110846	-0.758349	1.228702
H	2.881480	1.372256	1.858687
H	1.872674	-0.065167	2.039768
H	1.806222	1.936773	-0.288167
H	0.581995	1.710372	0.954003
H	2.168273	0.056713	-1.915765
H	1.121547	-1.353137	-1.852545
H	3.434551	-1.839728	-0.984327
H	2.232701	-2.073617	0.288806
H	-4.150445	-1.659178	0.784751
H	-2.326311	-3.219120	0.070190

1c (H-State)

ΔG = -596.118823 hartree

C	-0.451251	-0.364805	-0.247881
C	-0.579389	-1.771043	-0.136741
C	-1.783935	-2.355108	0.237890
C	-2.915966	-1.571928	0.522538
C	-2.827925	-0.196667	0.368985
C	-1.630638	0.419090	-0.052556
C	-1.678261	1.827047	-0.461108
O	-2.593813	2.609657	-0.200117
C	3.502186	0.115190	0.524286
C	2.378516	0.869412	1.248767
C	1.293939	1.348764	0.269324
N	0.764686	0.239657	-0.549388
C	1.822697	-0.502288	-1.250735
C	2.923021	-1.030847	-0.318460
H	0.283448	-2.406619	-0.295492
H	-3.697241	0.436310	0.518708
H	-0.841365	2.163847	-1.098079
H	4.041175	0.811930	-0.133840
H	4.232844	-0.267986	1.245620
H	2.776928	1.740592	1.783011
H	1.915614	0.214040	1.998621
H	1.710090	2.112123	-0.402801
H	0.476725	1.810727	0.823861
H	2.276302	0.195806	-1.969621
H	1.367866	-1.303436	-1.836445
H	3.706426	-1.504050	-0.922600
H	2.512549	-1.805044	0.342572
H	-3.845754	-2.037932	0.832138
H	-1.835870	-3.436068	0.335152

1c (A, O-State)

ΔG = -596.033781 hartree

C	-0.624482	-0.253815	-0.234768
C	-0.876570	-1.637269	-0.319958
C	-2.121105	-2.170642	0.013753
C	-3.137063	-1.289454	0.468423
C	-2.935110	0.080660	0.511782
C	-1.714237	0.674375	0.078145
C	-1.641232	2.076101	-0.177974
O	-0.696063	2.674359	-0.792736
C	3.374935	-0.343717	0.538176
C	2.315113	0.296039	1.444173
C	1.297275	1.105044	0.615042
N	0.675367	0.227690	-0.391637
C	1.631906	-0.398936	-1.306518
C	2.715531	-1.198187	-0.552491
H	-0.062256	-2.310431	-0.565845
H	-3.754067	0.736334	0.796313
H	-2.488442	2.666312	0.213249
H	3.978443	0.446404	0.071398
H	4.060144	-0.959250	1.131315
H	2.775393	0.978903	2.166872
H	1.785204	-0.475038	2.017255
H	1.803779	1.917681	0.086435
H	0.515013	1.527864	1.242245
H	2.108042	0.421340	-1.860488
H	1.087742	-1.014826	-2.022038
H	3.453151	-1.542149	-1.285107
H	2.262210	-2.090482	-0.104653
H	-4.103365	-1.692151	0.760361
H	-2.289831	-3.240400	-0.030672

1c (A, H-State)

ΔG = -596.037839 hartree

C	-0.452713	-0.391736	-0.211069
C	-0.569517	-1.795072	-0.121311
C	-1.771226	-2.405481	0.229694
C	-2.893921	-1.580830	0.504830
C	-2.830377	-0.201894	0.381728
C	-1.643597	0.464866	-0.046093
C	-1.698468	1.845561	-0.425211
O	-2.736032	2.574852	-0.274959
C	3.538249	0.180170	0.481508
C	2.409562	0.893097	1.235625
C	1.285384	1.341919	0.277795
N	0.782409	0.179642	-0.474380
C	1.822733	-0.513966	-1.243889
C	2.984854	-0.984783	-0.348656
H	0.315808	-2.408101	-0.246574
H	-3.717068	0.403399	0.532273
H	-0.804334	2.287538	-0.886377
H	4.044467	0.895270	-0.180715
H	4.290019	-0.185938	1.189238
H	2.780476	1.785632	1.751047
H	1.981711	0.230166	1.997432
H	1.674936	2.073374	-0.439953
H	0.464495	1.788753	0.834542
H	2.200350	0.217281	-1.971113
H	1.368883	-1.331882	-1.801489
H	3.758814	-1.413205	-0.993995
H	2.631660	-1.785017	0.312712
H	-3.833182	-2.042208	0.799381
H	-1.831427	-3.482482	0.334218

1c (C)

ΔG = -596.113745 hartree

C	0.819141	-0.594780	0.037449
C	1.694038	-1.676782	0.204696
C	3.071802	-1.431175	0.123486
C	3.577013	-0.147966	-0.122723
C	2.691491	0.929127	-0.293643
C	1.323264	0.700059	-0.220997
C	0.154987	1.662985	-0.295347
O	0.024545	2.457191	0.899876
C	-1.019700	0.681380	-0.542959
N	-0.569788	-0.563825	0.113207
C	-2.419082	1.064697	-0.076491
C	-1.416983	-1.734327	-0.070088
C	-2.846630	-1.402971	0.380850
C	-3.376173	-0.123444	-0.288896
H	-1.047776	0.504807	-1.635712
H	0.231888	2.395766	-1.101107
H	0.089322	1.870333	1.667765
H	1.325830	-2.680373	0.391046
H	3.072140	1.929022	-0.486697
H	4.648896	0.011318	-0.188110
H	3.761134	-2.262089	0.247883
H	-2.766307	1.943089	-0.632663
H	-2.390066	1.338678	0.984431
H	-1.015772	-2.562943	0.520652
H	-1.417698	-2.051061	-1.129662
H	-2.851036	-1.274537	1.471019
H	-3.500077	-2.252252	0.151278
H	-3.497195	-0.301083	-1.366859
H	-4.370136	0.119741	0.103258

2c

ΔG = -482.795644 hartree

C	0.717033	0.065462	0.368742
C	1.306336	-1.184206	0.057232
C	2.644386	-1.277813	-0.333866
C	3.447681	-0.140640	-0.447608
C	2.876499	1.102795	-0.152505
C	1.545924	1.209750	0.248807
C	-3.054387	-0.113724	-0.753175
C	-2.191356	1.157644	-0.811279
C	-1.412002	1.357298	0.501043
N	-0.599125	0.176131	0.834916
C	-1.447124	-1.014834	0.967797
C	-2.219026	-1.332237	-0.324084
H	0.723065	-2.095177	0.104491
H	3.474782	2.007462	-0.225012
H	-3.865799	0.036809	-0.026274
H	-3.531181	-0.297023	-1.723156
H	-2.816542	2.039275	-0.999569
H	-1.476423	1.086351	-1.642076
H	-2.117718	1.516211	1.327513
H	-0.787114	2.247633	0.447176
H	-2.167653	-0.802946	1.769756
H	-0.849870	-1.862502	1.307242
H	-2.863399	-2.205115	-0.162354
H	-1.509234	-1.596559	-1.118580
H	4.484918	-0.218170	-0.758268
H	3.052876	-2.258583	-0.563810
H	1.159380	2.192443	0.491886

1d (O-State)

ΔG = -635.402926 hartree

C	-0.775567	-0.313982	0.074195
C	-1.161681	-1.678605	0.165940
C	-2.477276	-2.080491	-0.016775
C	-3.491589	-1.149291	-0.300143
C	-3.153725	0.192832	-0.336016
C	-1.831597	0.646292	-0.107154
C	3.249666	-0.300863	-0.942217
C	2.615970	-1.346036	-0.012620
C	1.544718	-0.730126	0.911672
C	2.147321	0.136723	2.033886
N	0.553405	0.049096	0.135324
C	1.112837	1.067117	-0.764868
C	2.157123	0.451434	-1.710788
C	-1.727998	2.086297	0.138922
O	-0.775971	2.711961	0.606547
H	-0.404288	-2.439543	0.311895
H	-2.711958	-3.140600	0.026787
H	-4.513322	-1.472700	-0.468504
H	-3.927421	0.939918	-0.497933
H	3.940027	-0.790250	-1.638827
H	3.848005	0.411730	-0.359149
H	3.379770	-1.835982	0.602616
H	2.143957	-2.127931	-0.621937
H	2.833430	-0.467141	2.637481
H	1.355269	0.514423	2.687362
H	2.706971	0.993296	1.648687
H	1.005529	-1.540442	1.403804
H	1.554551	1.886575	-0.186549
H	0.301908	1.496502	-1.350438
H	2.590832	1.254542	-2.319122
H	1.650969	-0.239126	-2.398960
H	-2.669502	2.629562	-0.081070

1d (H-State)

ΔG = -635.407383 hartree

C	-0.628428	-0.377574	0.135605
C	-0.809697	-1.782071	0.109422
C	-2.065519	-2.341636	-0.096542
C	-3.199901	-1.534349	-0.289463
C	-3.054360	-0.157043	-0.224277
C	-1.798455	0.435619	0.023919
C	3.260422	-0.053486	-1.024292
C	2.751560	-1.100559	-0.022139

C	1.721799	-0.514020	0.967395
C	2.364428	0.400899	2.025823
N	0.631538	0.203832	0.265106
C	1.086922	1.215826	-0.711535
C	2.078824	0.627131	-1.726948
C	-1.753005	1.868508	0.336433
O	-2.668748	2.666988	0.130090
H	0.046882	-2.439768	0.197191
H	-2.158935	-3.423516	-0.134937
H	-4.172334	-1.982542	-0.465833
H	-3.915583	0.498140	-0.313065
H	3.918861	-0.529994	-1.759535
H	3.866322	0.703279	-0.508606
H	3.584815	-1.535302	0.542350
H	2.280067	-1.921635	-0.577598
H	3.114314	-0.160997	2.592838
H	1.604140	0.761918	2.725096
H	2.863158	1.270369	1.587877
H	1.255797	-1.337294	1.513242
H	1.551905	2.054783	-0.178796
H	0.216941	1.612459	-1.236119
H	2.426668	1.432409	-2.385465
H	1.552859	-0.102544	-2.357355
H	-0.834194	2.214037	0.841844

1d (A, O-State)

ΔG = -635.323682 hartree

C	0.829129	-0.206842	-0.073114
C	1.121682	-1.540893	-0.345674
C	2.454034	-1.981260	-0.406304
C	3.497824	-1.062083	-0.175155
C	3.225212	0.270158	0.091846
C	1.881957	0.748955	0.131103
C	-3.039111	-1.116487	0.458889
C	-2.369828	-1.062200	-0.922486
C	-1.445810	0.174620	-1.099432
C	-2.240659	1.474393	-1.296780
N	-0.516121	0.273952	0.052392
C	-1.135357	0.256232	1.388884
C	-1.993520	-1.007714	1.576964
C	1.518548	2.100631	0.327093
O	0.282847	2.499033	0.276137
H	0.317205	-2.252802	-0.494843
H	2.669434	-3.023123	-0.619100
H	4.530229	-1.399159	-0.215057
H	4.037830	0.974106	0.251314
H	-3.599636	-2.052936	0.555074
H	-3.769449	-0.303934	0.559930
H	-3.120380	-1.036600	-1.720108
H	-1.781424	-1.973655	-1.075705
H	-2.839627	1.381965	-2.207846
H	-1.559237	2.320465	-1.396486
H	-2.922808	1.676861	-0.466674
H	-0.812968	0.022813	-1.977177
H	-1.759561	1.149392	1.483203
H	-0.336217	0.321399	2.128548
H	-2.472286	-0.953594	2.560996
H	-1.347194	-1.894046	1.581339
H	2.291551	2.847863	0.541729

1d (A, H-State)

ΔG = -635.326762 hartree

C	-0.628022	-0.407409	0.091552
C	-0.794427	-1.808245	0.089210
C	-2.044297	-2.394858	-0.095585
C	-3.167784	-1.548169	-0.283462
C	-3.050728	-0.168023	-0.246064
C	-1.802818	0.479894	-0.002428
C	3.317770	0.006021	-0.961440
C	2.819902	-1.057697	0.025826
C	1.719132	-0.524218	0.972720
C	2.253322	0.438339	2.050777
N	0.646651	0.136724	0.192105
C	1.093619	1.202403	-0.723064
C	2.137802	0.637450	-1.707822
C	-1.768760	1.884919	0.274548
O	-2.792382	2.644875	0.192143
H	0.081596	-2.444570	0.146668
H	-2.144836	-3.473179	-0.136956
H	-4.147566	-1.991578	-0.442482
H	-3.931038	0.458811	-0.331822
H	4.011470	-0.452248	-1.674746
H	3.881560	0.785609	-0.434176
H	3.640991	-1.441092	0.640759
H	2.413799	-1.908599	-0.534491
H	2.954394	-0.112190	2.684794
H	1.436360	0.805104	2.678038
H	2.782677	1.296020	1.629741
H	1.252445	-1.360321	1.493316
H	1.535353	2.014562	-0.136997
H	0.228424	1.586820	-1.259202
H	2.467635	1.461375	-2.349758
H	1.651877	-0.105276	-2.352290
H	-0.810915	2.322238	0.589108

1d (C)

ΔG = -635.402916 hartree

C	-0.876388	-0.493588	-0.152082
C	-1.652819	-1.618741	-0.468807
C	-3.045469	-1.517380	-0.349846
C	-3.665059	-0.334757	0.075370
C	-2.879865	0.787360	0.388157
C	-1.497657	0.700798	0.280217
C	3.256249	0.389981	0.037267
C	2.810840	-0.834843	-0.780055
C	1.465386	-1.422987	-0.303643
C	1.585039	-2.224022	1.007800
N	0.498252	-0.323481	-0.224632
C	0.852769	0.886712	0.546754

C	2.168321	1.478614	0.052953
C	-0.429372	1.759297	0.458857
O	-0.427494	2.713617	-0.621525
H	0.962703	0.613121	1.611615
H	-0.487448	2.230253	-1.458747
H	-0.549033	2.368724	1.356878
H	-1.197312	-2.548332	-0.794238
H	-3.656024	-2.384625	-0.587378
H	-4.745818	-0.288347	0.166632
H	-3.347904	1.713056	0.713997
H	4.183062	0.794383	-0.385413
H	3.490378	0.091612	1.067698
H	3.576561	-1.617843	-0.742085
H	2.703297	-0.539790	-1.831592
H	2.254415	-3.078772	0.863250
H	0.608608	-2.608303	1.319293
H	1.986063	-1.617864	1.825975
H	1.104304	-2.104960	-1.082535
H	2.464242	2.312166	0.700379
H	2.030246	1.882301	-0.956750

2d

ΔG = -522.082812 hartree

C	-0.909300	0.021124	0.264034
C	-1.442342	-1.090697	-0.430820
C	-2.809524	-1.185794	-0.707113
C	-3.697889	-0.179467	-0.321908
C	-3.185143	0.930337	0.360993
C	-1.826475	1.029600	0.654062
C	2.792278	0.423877	-1.133451
C	2.091936	-0.931570	-0.938407
C	1.360847	-1.019794	0.421230
C	2.328258	-1.154178	1.610877
N	0.446541	0.127554	0.613082
C	1.119476	1.432844	0.479789
C	1.813110	1.580797	-0.885096
H	-0.794524	-1.885363	-0.780018
H	-3.173720	-2.056606	-1.246308
H	-4.757665	-0.255706	-0.544601
H	-3.851549	1.725054	0.686430
H	3.208502	0.485563	-2.145829
H	3.642480	0.512022	-0.443834
H	2.812069	-1.754789	-1.021002
H	1.356436	-1.069571	-1.741631
H	2.921895	-2.067606	1.497621
H	1.767824	-1.223198	2.548441
H	3.026154	-0.316560	1.692676
H	0.748179	-1.922842	0.431444
H	1.858374	1.533572	1.283427
H	0.395792	2.233738	0.623987
H	2.333917	2.545670	-0.924111
H	1.047719	1.594241	-1.673165
H	-1.479067	1.887025	1.219749

1e (O-State)

ΔG = -635.391921 hartree

C	-1.022231	-0.373617	0.032096
C	-1.613373	-1.643346	0.221692
C	-2.993832	-1.810155	0.306123
C	-3.857711	-0.713136	0.204581
C	-3.304052	0.541599	-0.009184
C	-1.910413	0.744506	-0.113678
C	-1.531005	2.106556	-0.515072
O	-0.406720	2.551469	-0.730441
C	3.695024	-0.697023	-0.443928
C	2.415988	-1.024978	-1.238735
C	1.163776	-1.401670	-0.424173
N	0.370769	-0.224847	-0.028359
C	0.957903	0.602223	1.045905
C	2.356501	1.172049	0.776764
C	3.492943	0.138033	0.836985
H	-0.979632	-2.512691	0.346677
H	-3.956340	1.403578	-0.126512
H	-2.407844	2.770507	-0.657163
H	-4.932462	-0.840319	0.280406
H	-3.395320	-2.805443	0.475449
H	4.378992	-0.167934	-1.119823
H	4.203692	-1.631215	-0.173100
H	2.639590	-1.860928	-1.912966
H	2.143425	-0.180241	-1.881819
H	1.437965	-2.018732	0.449210
H	0.528790	-2.015683	-1.064703
H	1.002243	-0.004358	1.969582
H	0.276789	1.428639	1.236059
H	2.528130	1.920031	1.561412
H	2.359868	1.714866	-0.175490
H	3.297595	-0.530751	1.686406
H	4.435796	0.646597	1.072155

1e (H-State)

ΔG = -635.395108 hartree

C	0.905536	-0.489585	-0.009505
C	1.401699	-1.788703	-0.235672
C	2.771720	-2.024300	-0.347570
C	3.693980	-0.973029	-0.247424
C	3.224829	0.312088	-0.004034
C	1.848211	0.566971	0.140189
C	1.414245	1.907704	0.565333
O	2.133818	2.905937	0.573696
C	-3.814176	-0.381332	0.525268
C	-2.560654	-0.779399	1.332346
C	-1.351057	-1.299392	0.534396
N	-0.479638	-0.207850	0.061229
C	-1.000595	0.546209	-1.101216
C	-2.347777	1.248515	-0.887542
C	-3.559374	0.302444	-0.833072
H	0.712566	-2.616595	-0.356791
H	3.913940	1.142446	0.115677

H	0.374443	1.974129	0.928071
H	4.757989	-1.162952	-0.345780
H	3.121308	-3.035719	-0.535155
H	-4.420271	0.280824	1.156703
H	-4.429843	-1.272542	0.348587
H	-2.850017	-1.556716	2.050122
H	-2.210386	0.070679	1.929380
H	-1.679619	-1.946414	-0.297226
H	-0.750671	-1.918234	1.204287
H	-1.094904	-0.135979	-1.966662
H	-0.251557	1.291999	-1.374802
H	-2.473379	1.923450	-1.743468
H	-2.302701	1.884921	0.005713
H	-3.426391	-0.461317	-1.611382
H	-4.463101	0.856320	-1.114425

1e (A, O-State)

ΔG = -635.312574 hartree

C	-0.816277	-0.153495	-0.052005
C	-0.828693	-1.539167	-0.176316
C	-2.046451	-2.238558	-0.209917
C	-3.258183	-1.523560	-0.114715
C	-3.263419	-0.143057	0.007277
C	-2.041125	0.591886	0.038970
C	-1.944099	1.997460	0.145379
O	-0.794764	2.606706	0.154198
C	2.851337	-1.169362	0.635963
C	1.938809	-0.499888	1.693327
C	1.131322	0.740521	1.252998
N	0.400111	0.603987	-0.010003
C	1.121502	0.925091	-1.247332
C	2.236725	-0.069165	-1.618777
C	3.315428	-0.297121	-0.545702
H	0.106765	-2.083596	-0.247231
H	-4.203921	0.397257	0.076813
H	-2.851298	2.607088	0.223415
H	-4.202292	-2.061306	-0.138497
H	-2.046825	-3.319270	-0.305744
H	2.342379	-2.048083	0.219196
H	3.733016	-1.562046	1.154914
H	2.545612	-0.150605	2.537552
H	1.251191	-1.247712	2.102674
H	1.795273	1.600235	1.131996
H	0.404727	0.988871	2.030303
H	1.552988	1.921505	-1.106899
H	0.384703	0.984156	-2.050873
H	2.702356	0.336378	-2.525602
H	1.795265	-1.032859	-1.901887
H	3.708119	0.665800	-0.191082
H	4.158027	-0.806882	-1.027507

1e (A, H-State)

ΔG = -635.317021 hartree

C	0.912874	-0.548527	-0.122608
C	1.520435	-1.817800	-0.222698
C	2.904832	-1.965288	-0.217091
C	3.711024	-0.801132	-0.105361
C	3.150972	0.457593	0.032522
C	1.738627	0.654396	0.090059
C	1.207288	1.928011	0.471862
O	1.926519	2.966394	0.658178
C	-3.695253	-0.371354	0.700492
C	-2.380887	-0.903952	1.301924
C	-1.359609	-1.480236	0.292770
N	-0.470704	-0.434006	-0.234998
C	-1.037790	0.524520	-1.200815
C	-2.319445	1.257823	-0.783683
C	-3.564952	0.366910	-0.646588
H	0.897343	-2.687945	-0.398681
H	3.783062	1.327444	0.170694
H	0.120876	2.003748	0.620358
H	4.793499	-0.900997	-0.110940
H	3.353714	-2.944124	-0.340051
H	-4.150594	0.299249	1.439249
H	-4.396846	-1.204054	0.570013
H	-2.613544	-1.704433	2.012566
H	-1.874723	-0.123882	1.880788
H	-1.868080	-1.978397	-0.541838
H	-0.736341	-2.211811	0.801984
H	-1.237417	-0.059636	-2.113149
H	-0.251208	1.236742	-1.450197
H	-2.492913	1.993222	-1.577814
H	-2.145831	1.832376	0.134235
H	-3.566155	-0.357454	-1.471908
H	-4.460767	0.981063	-0.790468

1e (C)

ΔG = -635.392973 hartree

C	-0.866878	-0.610725	0.401557
C	-1.507119	-1.830905	0.138671
C	-2.816034	-1.799784	-0.366007
C	-3.478923	-0.592898	-0.614565
C	-2.828345	0.625548	-0.345779
C	-1.534859	0.605398	0.151732
C	-0.637581	1.733326	0.596723
O	-0.714098	2.847384	-0.291416
C	3.194601	-0.840056	-0.805471
C	2.057709	-1.780160	-0.345599
C	1.409832	-1.421968	1.006876
N	0.394314	-0.375003	0.937416
C	0.765400	1.040123	0.694866
C	1.651012	1.259453	-0.547220
C	3.058237	0.646370	-0.413525
H	-0.935228	2.062682	1.603595
H	-0.366805	3.629748	0.158442
H	1.310813	1.412457	1.570873
H	-1.011594	-2.781052	0.307946
H	-3.329406	1.572028	-0.530053
H	-4.488783	-0.596483	-1.013136

H	-3.318683	-2.740361	-0.575860
H	3.279390	-0.916645	-1.896964
H	4.148586	-1.205126	-0.403694
H	2.448850	-2.803716	-0.288150
H	1.262240	-1.804220	-1.100138
H	2.170460	-1.105674	1.730497
H	0.931840	-2.309579	1.434349
H	1.746766	2.341763	-0.685338
H	1.142452	0.880621	-1.443226
H	3.401888	0.787100	0.620492
H	3.757485	1.220083	-1.033774

2e

ΔG = -522.070371 hartree

C	1.171639	-0.005663	0.073241
C	1.862128	-1.087736	-0.507699
C	3.261503	-1.103399	-0.558053
C	4.008200	-0.039249	-0.050391
C	3.331891	1.047441	0.520401
C	1.940290	1.062606	0.586848
C	-3.540691	-0.716999	0.213571
C	-2.265232	-1.266788	0.881598
C	-0.966763	-1.228822	0.054490
N	-0.244025	0.045824	0.185065
C	-0.853372	1.191216	-0.519640
C	-2.293160	1.544805	-0.120782
C	-3.358167	0.559950	-0.631606
H	1.315933	-1.920200	-0.936014
H	3.892387	1.881988	0.933143
H	5.093048	-0.053488	-0.093776
H	3.763503	-1.953809	-1.011934
H	-4.276031	-0.527285	1.006138
H	-3.981179	-1.494292	-0.424114
H	-2.453752	-2.309933	1.164553
H	-2.067203	-0.729265	1.816432
H	-1.169286	-1.478778	-1.003047
H	-0.308545	-2.008054	0.443354
H	-0.832744	1.007493	-1.611367
H	-0.221068	2.061473	-0.337653
H	-2.492789	2.529490	-0.562010
H	-2.361225	1.672708	0.967320
H	-3.094631	0.285584	-1.662072
H	-4.325286	1.072784	-0.699889
H	1.437453	1.898649	1.063613

1f (O-State)

ΔG = -843.142997 hartree

C	-2.337692	-0.309216	0.211359
C	-2.456917	-1.721600	0.184215
C	-3.534941	-2.352858	-0.424101
C	-4.556021	-1.613332	-1.040943
C	-4.491257	-0.230612	-0.977630
C	-3.431906	0.448418	-0.331019
C	-3.682297	1.874959	-0.105360
O	-3.043520	2.655999	0.599029
N	1.648349	0.227982	0.412290
C	0.961070	-0.886150	1.066373
C	-0.341988	-0.387714	1.702843
N	-1.221777	0.299012	0.757283
C	-0.523741	1.397054	0.083513
C	0.773764	0.898767	-0.563855
C	5.741242	-0.247596	-0.642442
C	5.091742	0.983674	-0.799543
C	3.747979	1.130319	-0.462131
C	2.999156	0.041169	0.038090
C	3.660144	-1.195277	0.186667
C	5.013652	-1.328863	-0.143721
H	-1.664614	-2.334839	0.595779
H	-5.297117	0.366506	-1.397813
H	-4.601867	2.235177	-0.608930
H	1.596978	-1.284754	1.861268
H	0.750268	-1.705516	0.356690
H	-0.084401	0.334996	2.488601
H	-0.871508	-1.211677	2.181961
H	-0.302392	2.186115	0.811329
H	-1.155697	1.824949	-0.690712
H	1.289583	1.756637	-0.995824
H	0.525936	0.207057	-1.388928
H	-5.383045	-2.110651	-1.536288
H	-3.563514	-3.438773	-0.443347
H	6.789781	-0.356985	-0.901774
H	5.638764	1.843921	-1.175721
H	3.283384	2.105291	-0.563621
H	3.127281	-2.065086	0.551132
H	5.492395	-2.296180	-0.016928

1f (H-State)

ΔG = -843.148617 hartree

C	-2.261284	-0.383284	0.266895
C	-2.310291	-1.781871	0.063171
C	-3.382914	-2.373766	-0.595508
C	-4.448978	-1.602653	-1.087256
C	-4.442241	-0.234739	-0.857761
C	-3.388957	0.384811	-0.154075
C	-3.566244	1.775786	0.282021
O	-4.421476	2.547576	-0.153264
N	1.703863	0.234793	0.454353
C	1.046073	-0.933351	1.042299
C	-0.252282	-0.506318	1.738666
N	-1.167050	0.236898	0.870457
C	-0.487117	1.378912	0.240705
C	0.802695	0.947351	-0.465430
C	5.785755	-0.094187	-0.694224
C	5.114845	1.134345	-0.749869
C	3.774620	1.232754	-0.382156
C	3.051823	0.097032	0.047032
C	3.733770	-1.135671	0.093766
C	5.083674	-1.221621	-0.266283
H	-1.483211	-2.405572	0.380381

H	-5.276139	0.385817	-1.171052
H	-2.902557	2.106289	1.100483
H	1.704079	-1.375726	1.794760
H	0.834889	-1.703931	0.280361
H	0.008561	0.153480	2.577037
H	-0.761270	-1.376172	2.156545
H	-0.250721	2.123569	1.011395
H	-1.142756	1.845603	-0.494752
H	1.295155	1.839903	-0.852258
H	0.551131	0.303662	-1.327428
H	-5.271796	-2.072461	-1.616085
H	-3.375437	-3.448941	-0.751177
H	6.831545	-0.166337	-0.976663
H	5.642203	2.029064	-1.069421
H	3.292352	2.204318	-0.403707
H	3.220679	-2.038837	0.401097
H	5.579730	-2.187339	-0.219027

1f (A, O-State)

ΔG = -843.062624 hartree

C	2.323968	-0.247464	-0.243843
C	2.725177	-1.589163	-0.157121
C	4.026352	-1.941685	0.215075
C	4.940668	-0.907813	0.536721
C	4.580158	0.423448	0.420142
C	3.290248	0.828170	-0.045140
C	3.069262	2.193785	-0.403200
O	2.064346	2.670180	-1.030768
N	-1.557004	-0.759240	0.592330
C	-0.853316	-1.619433	-0.339162
C	0.094805	-0.761462	-1.256761
N	0.970250	0.076753	-0.470838
C	0.259346	0.931056	0.466833
C	-0.633265	0.028400	1.382896
C	-5.523872	0.510395	-0.198862
C	-4.611869	1.383902	0.399068
C	-3.298856	0.985789	0.655907
C	-2.864269	-0.313865	0.317196
C	-3.797923	-1.195476	-0.272808
C	-5.103227	-0.782554	-0.530196
H	1.998551	-2.377380	-0.324533
H	5.317254	1.198534	0.616641
H	3.878517	2.880002	-0.091506
H	-1.543200	-2.158883	-0.984559
H	-0.254893	-2.346529	0.217596
H	-0.543992	-0.114559	-1.869770
H	0.676984	-1.406928	-1.913877
H	-0.375024	1.628624	-0.085186
H	0.972680	1.487751	1.072148
H	-1.161768	0.647203	2.106888
H	0.021352	-0.652084	1.937854
H	5.948502	-1.160653	0.855874
H	4.311423	-2.985169	0.288881
H	-6.542851	0.827087	-0.397045
H	-4.915382	2.392819	0.662734
H	-2.620630	1.701618	1.103576
H	-3.515661	-2.216762	-0.501853
H	-5.799677	-1.484894	-0.978637

1f (A, H-State)

ΔG = -843.068590 hartree

C	2.232608	-0.377558	-0.226472
C	2.584885	-1.721895	-0.050194
C	3.888638	-2.095018	0.299181
C	4.855644	-1.079825	0.486273
C	4.544065	0.254253	0.282750
C	3.241848	0.675102	-0.139092
C	3.022334	2.028097	-0.549907
O	3.902675	2.955025	-0.469644
N	-1.672637	-0.622101	0.603517
C	-0.998776	-1.616983	-0.206853
C	-0.009339	-0.907175	-1.205957
N	0.899027	-0.020209	-0.515873
C	0.214696	0.963509	0.306029
C	-0.728775	0.211032	1.311516
C	-5.629924	0.612212	-0.263896
C	-4.703584	1.525941	0.246870
C	-3.393893	1.137444	0.527849
C	-2.977155	-0.192879	0.301650
C	-3.924213	-1.113593	-0.202393
C	-5.226901	-0.709625	-0.483802
H	1.826172	-2.492194	-0.135944
H	5.308017	1.018005	0.380075
H	2.042531	2.271743	-0.987483
H	-1.704073	-2.200318	-0.793989
H	-0.434850	-2.294423	0.440841
H	-0.618400	-0.312344	-1.896334
H	0.545909	-1.649118	-1.778318
H	-0.390966	1.621955	-0.324868
H	0.938455	1.552064	0.868139
H	-1.234219	0.932520	1.951109
H	-0.102614	-0.424920	1.946287
H	5.867553	-1.351602	0.777250
H	4.135647	-3.139558	0.453512
H	-6.647391	0.921478	-0.480240
H	-4.994584	2.557209	0.422607
H	-2.704196	1.881779	0.905235
H	-3.657102	-2.154337	-0.342355
H	-5.934974	-1.440190	-0.863184

1f (C)

ΔG = -843.146829 hartree

C	2.613195	-0.576239	-0.053272
C	3.557691	-1.609360	-0.067212
C	4.913975	-1.260079	-0.133377
C	5.326741	0.077336	-0.188632
C	4.369690	1.105529	-0.179695
C	3.021797	0.774611	-0.120770
C	1.791191	1.657929	-0.030404

O	1.638053	2.259895	1.268619
N	-1.557344	-0.316744	-0.214658
C	-1.001274	-1.589423	0.255657
C	0.419308	-1.802896	-0.279730
N	1.226883	-0.646428	0.056608
C	0.682360	0.640097	-0.400714
C	-0.716151	0.839363	0.160979
C	-5.770409	0.245208	-0.031538
C	-4.943862	1.167970	-0.685706
C	-3.564034	0.981532	-0.733378
C	-2.957231	-0.134930	-0.115037
C	-3.796917	-1.054062	0.546083
C	-5.183473	-0.864597	0.577479
H	1.797336	1.584346	1.944381
H	1.797782	2.501202	-0.723504
H	0.614333	0.626171	-1.503851
H	3.258594	-2.651911	-0.028786
H	4.679549	2.146513	-0.224414
H	-1.629686	-2.405079	-0.108670
H	-0.980387	-1.638804	1.358470
H	0.387044	-1.963132	-1.371576
H	0.842224	-2.698677	0.183814
H	-1.145138	1.755208	-0.244793
H	-0.671536	0.942060	1.256743
H	6.383788	0.317662	-0.246219
H	5.659438	-2.050539	-0.148657
H	-6.845918	0.390210	-0.001518
H	-5.377309	2.034632	-1.177414
H	-2.954626	1.695266	-1.277841
H	-3.380640	-1.917405	1.050811
H	-5.801612	-1.592597	1.096027

2f

ΔG = -729.824819 hartree

C	2.637641	-0.158148	0.275917
C	2.985180	1.210067	0.198283
C	4.115217	1.628753	-0.509857
C	4.931599	0.712536	-1.176426
C	4.595843	-0.645006	-1.111231
C	3.478825	-1.076735	-0.398271
N	-1.288790	-0.304378	0.538752
C	-0.490036	0.823277	1.028900
C	0.722990	0.303136	1.812300
N	1.551022	-0.617495	1.036860
C	0.732507	-1.741902	0.571560
C	-0.477632	-1.259496	-0.237043
C	-5.243852	0.462940	-0.827986
C	-4.751218	-0.845155	-0.735843
C	-3.451088	-1.090249	-0.299062
C	-2.587742	-0.028352	0.055989
C	-3.091509	1.285153	-0.047341
C	-4.402645	1.519575	-0.476825
H	2.371404	1.963758	0.675881
H	5.216907	-1.384303	-1.610185
H	-1.102829	1.426587	1.704063
H	-0.155893	1.473155	0.201302
H	0.357391	-0.246665	2.689034
H	1.319957	1.136559	2.183779
H	0.383235	-2.299553	1.449548
H	1.320958	-2.424406	-0.039570
H	-1.083357	-2.124558	-0.507615
H	-0.127972	-0.790044	-1.173824
H	5.804165	1.043741	-1.730737
H	4.344646	2.690504	-0.546498
H	-6.259038	0.649792	-1.164341
H	-5.388535	-1.686664	-0.993837
H	-3.113224	-2.116988	-0.208651
H	-2.466574	2.135764	0.195349
H	-4.757433	2.544555	-0.544834
H	3.276094	-2.140489	-0.346543

1g (O-State)

ΔG = -479.429876 hartree

C	0.031904	-0.448497	-0.024264
C	-0.873015	-1.536596	-0.137259
C	-2.246857	-1.351882	-0.045105
C	-2.798917	-0.076840	0.158570
C	-1.938650	1.008685	0.204615
C	-0.537386	0.868710	0.068469
C	0.170749	2.124880	-0.185988
O	1.312319	2.274453	-0.622592
C	2.275335	0.082148	0.885414
N	1.390993	-0.669422	-0.006487
C	1.927373	-1.963228	-0.416767
H	-0.490445	-2.543990	-0.242907
H	-2.342944	2.013741	0.300122
H	-0.459373	3.020378	-0.011792
H	3.009347	0.670832	0.327946
H	1.699619	0.758815	1.516280
H	2.801496	-0.624849	1.538808
H	2.992739	-1.842057	-0.626357
H	1.441813	-2.309836	-1.331379
H	1.817240	-2.733784	0.361544
H	-3.871190	0.057170	0.253513
H	-2.897010	-2.220374	-0.105739

1g (H-State)

ΔG = -479.432890 hartree

C	0.364414	-0.387759	-0.069007
C	0.115489	-1.775832	-0.028230
C	-1.182890	-2.267009	0.096460
C	-2.279973	-1.398176	0.187496
C	-2.057927	-0.029292	0.107235
C	-0.759310	0.490641	-0.052531
C	-0.607897	1.920804	-0.359249
O	-1.488036	2.768240	-0.210343
C	2.116674	1.020284	0.938988
N	1.666427	0.132040	-0.143840
C	2.734036	-0.763894	-0.581948

H	0.941492	-2.476057	-0.058027
H	-2.888017	0.670269	0.120486
H	0.362699	2.211714	-0.797712
H	2.878906	1.708267	0.561035
H	1.289092	1.605274	1.337780
H	2.551632	0.438411	1.767412
H	3.609243	-0.158749	-0.833889
H	2.427653	-1.310804	-1.476166
H	3.034790	-1.485902	0.194569
H	-3.286075	-1.789867	0.296718
H	-1.337818	-3.341366	0.142133

1g (A, O-State)

ΔG = -479.348905 hartree

C	0.070791	-0.378541	-0.000046
C	0.912530	-1.483957	-0.000020
C	2.305899	-1.304084	-0.000002
C	2.834513	0.003698	0.000007
C	2.002998	1.113752	0.000010
C	0.585303	0.957291	-0.000023
C	-0.360173	2.007638	-0.000078
O	-1.644319	1.772905	-0.000232
C	-2.011721	-0.898922	1.243070
N	-1.358061	-0.507025	0.000008
C	-2.011911	-0.899462	-1.242787
H	0.489446	-2.485034	0.000013
H	2.424894	2.115215	0.000014
H	-0.034834	3.052836	-0.000060
H	-3.070172	-0.634348	1.194611
H	-1.921632	-1.983988	1.395938
H	-1.540025	-0.380886	2.078318
H	-1.540621	-0.381448	-2.078281
H	-3.070438	-0.635249	-1.194088
H	-1.921525	-1.984539	-1.395450
H	3.912012	0.145223	0.000003
H	2.964494	-2.166335	-0.000003

1g (A, H-State)

ΔG = -479.351428 hartree

C	0.391019	-0.402402	-0.025683
C	0.195915	-1.800263	-0.059701
C	-1.074757	-2.358219	0.042622
C	-2.188994	-1.486742	0.193602
C	-2.043044	-0.109510	0.178768
C	-0.772577	0.510288	-0.015164
C	-0.698427	1.906931	-0.325612
O	-1.710497	2.684130	-0.304543
C	2.792372	-0.664971	-0.567146
N	1.675908	0.107634	-0.028569
C	2.078376	1.211319	0.847201
H	1.061322	-2.453118	-0.078536
H	-2.913047	0.535064	0.228473
H	0.279069	2.319465	-0.611128
H	3.580564	0.033085	-0.857446
H	3.201198	-1.347326	0.189448
H	2.470443	-1.233445	-1.438636
H	1.209677	1.682134	1.298987
H	2.661751	1.944681	0.284152
H	2.710538	0.799646	1.644147
H	-3.183738	-1.911305	0.302848
H	-1.204449	-3.433948	0.060698

1g (C)

ΔG = -479.431326 hartree

C	0.138566	0.615726	-0.087593
C	1.256736	1.439896	-0.279023
C	2.529613	0.863561	-0.170068
C	2.698907	-0.494585	0.128872
C	1.572236	-1.309279	0.327127
C	0.305474	-0.749505	0.224235
C	-1.057630	-1.386696	0.343457
O	-1.306008	-2.157540	-0.852414
C	-1.970956	-0.145370	0.459749
N	-1.212808	0.943083	-0.177863
C	-1.673370	2.304337	0.034821
H	-1.158451	-2.041333	1.215922
H	-2.146722	-2.625062	-0.741606
H	-2.939707	-0.293913	-0.026965
H	-2.146260	0.084704	1.523799
H	1.150754	2.495783	-0.505202
H	1.689784	-2.363243	0.565805
H	-2.739702	2.362349	-0.198233
H	-1.147320	2.990498	-0.633585
H	-1.523350	2.641167	1.074478
H	3.696950	-0.913019	0.214345
H	3.404289	1.492303	-0.313859

2g

ΔG = -366.109628 hartree

C	-0.185923	-0.000041	-0.073017
C	0.551756	1.210408	-0.031675
C	1.946375	1.200662	0.017107
C	2.663391	-0.000005	0.039020
C	1.946415	-1.200660	0.017229
C	0.551766	-1.210434	-0.031557
C	-2.299146	-1.243540	0.063520
N	-1.573082	0.000004	-0.166873
C	-2.299025	1.243586	0.063733
H	0.039981	2.164692	-0.039871
H	2.474789	-2.150237	0.044206
H	-3.365268	-1.061852	-0.076625
H	-1.999191	-2.012177	-0.655568
H	-2.145714	-1.643592	1.078455
H	-3.365234	1.061840	-0.075644
H	-1.999554	2.012098	-0.655712
H	-2.144923	1.643829	1.078482
H	3.748183	0.000047	0.079839
H	2.474782	2.150224	0.044000

H	0.040066	-2.164762	-0.039616

1h (O-State)

ΔG = -556.799567 hartree

C	0.443019	-0.323614	0.326488
C	1.020174	-1.616195	0.340379
C	2.298420	-1.855834	-0.154465
C	3.073036	-0.816650	-0.686868
C	2.552857	0.468836	-0.657893
C	1.271866	0.757225	-0.133898
C	1.020273	2.189660	0.060056
O	0.077623	2.726367	0.640296
C	-2.484825	-0.282407	-1.094602
C	-1.828501	0.597709	-0.056359
N	-0.857431	-0.131932	0.783012
C	-1.468249	-1.169980	1.612293
C	-3.804557	-0.453391	-1.218411
H	0.440620	-2.455437	0.703621
H	-1.808218	-0.788240	-1.784477
H	3.156940	1.300398	-1.012452
H	1.833792	2.825938	-0.341792
H	-4.227933	-1.076445	-2.001408
H	-4.506627	0.032741	-0.543667
H	-2.586742	1.037140	0.600881
H	-1.316167	1.425428	-0.542822
H	-2.358419	-0.746846	2.085080
H	-0.774505	-1.473238	2.399598
H	-1.778313	-2.061675	1.048693
H	4.061961	-1.007620	-1.089755
H	2.683557	-2.871707	-0.145270

1h (H-State)

ΔG = -556.803470 hartree

C	0.303958	-0.435964	0.355490
C	0.657433	-1.792048	0.192811
C	1.896816	-2.151143	-0.333389
C	2.828213	-1.176326	-0.720109
C	2.515844	0.162990	-0.524776
C	1.284755	0.549946	0.038874
C	1.108661	1.952602	0.444256
O	1.819069	2.886319	0.072612
C	-2.602478	0.065806	-1.051723
C	-1.806040	0.817130	-0.010668
N	-0.958565	-0.053002	0.837614
C	-1.723144	-1.035271	1.606582
C	-3.930764	0.136586	-1.180086
H	-0.053161	-2.569996	0.445264
H	-2.025259	-0.553498	-1.738926
H	3.235791	0.941136	-0.758871
H	0.302190	2.136614	1.175897
H	-4.457264	-0.400734	-1.963973
H	-4.535434	0.742270	-0.507775
H	-2.479856	1.382174	0.643298
H	-1.161134	1.540913	-0.514473
H	-2.535839	-0.512555	2.118832
H	-1.079303	-1.490855	2.362264
H	-2.169053	-1.831495	0.993396
H	3.785728	-1.464951	-1.141397
H	2.130469	-3.204414	-0.461302

1h (A, O-State)

ΔG = -556.716782 hartree

C	-0.664610	-0.329835	0.136779
C	-1.314020	-1.558075	0.102891
C	-2.692869	-1.616660	-0.159184
C	-3.405016	-0.420828	-0.386996
C	-2.767754	0.810459	-0.353311
C	-1.369387	0.896268	-0.085308
C	-0.619156	2.091084	-0.011525
O	0.660057	2.085900	0.249853
C	3.018977	0.067695	-0.571589
C	1.654955	-0.550565	-0.715446
N	0.742907	-0.218760	0.393639
C	1.199533	-0.478237	1.754750
C	4.159583	-0.623320	-0.648472
H	-0.751966	-2.471518	0.277450
H	3.029861	1.147079	-0.436262
H	-3.330389	1.723794	-0.526912
H	-1.096885	3.062334	-0.175112
H	5.124462	-0.128292	-0.588551
H	4.167716	-1.703094	-0.780505
H	1.736009	-1.645935	-0.791272
H	1.170042	-0.190126	-1.627811
H	2.208651	-0.084964	1.885722
H	1.212201	-1.559788	1.953574
H	0.519589	0.005499	2.456247
H	-4.471716	-0.463230	-0.590315
H	-3.199795	-2.575553	-0.186098

1h (A, H-State)

ΔG = -556.721348 hartree

C	0.510215	-0.608025	-0.081547
C	1.356619	-1.739561	-0.062565
C	2.727210	-1.618591	0.136725
C	3.274646	-0.319764	0.339209
C	2.487975	0.817298	0.276192
C	1.095911	0.751257	-0.029471
C	0.392233	1.944677	-0.394349
O	0.908489	3.109093	-0.329620
C	-3.010345	0.487564	-0.029364
C	-1.780794	0.002201	0.690736
N	-0.859816	-0.777305	-0.168898
C	-1.420782	-2.019146	-0.698025
C	-4.257034	0.259907	0.392491
H	0.917490	-2.728913	-0.116581
H	-2.839608	1.088186	-0.921712
H	2.934664	1.800613	0.367800
H	-0.637571	1.843349	-0.761876

H	-5.113109	0.672608	-0.132602
H	-4.462320	-0.337622	1.277752
H	-2.061547	-0.651104	1.528609
H	-1.215720	0.836757	1.109549
H	-2.450434	-1.828596	-1.002325
H	-1.428873	-2.805031	0.068912
H	-0.842649	-2.352597	-1.558945
H	4.340231	-0.216152	0.527235
H	3.355118	-2.500013	0.193234

1h (C)

ΔG = -556.800946 hartree

C	0.787969	0.615912	-0.103896
C	1.959561	1.371642	-0.249235
C	3.190514	0.721679	-0.086414
C	3.265893	-0.642645	0.221888
C	2.085713	-1.387825	0.374800
C	0.860112	-0.753028	0.218499
C	-0.538070	-1.310406	0.280987
O	-0.773914	-2.075696	-0.915151
C	-2.753311	-0.095092	-0.259332
C	-1.395264	-0.004019	0.376705
N	-0.537235	1.028349	-0.248978
C	-0.897075	2.422718	-0.040530
C	-3.904032	-0.044110	0.419210
H	-0.720226	-1.946206	1.154019
H	-1.636825	-2.508420	-0.835437
H	-1.511072	0.222920	1.450648
H	1.926118	2.430626	-0.482573
H	-2.763244	-0.218196	-1.341089
H	2.129435	-2.445769	0.620278
H	-4.862656	-0.137115	-0.082879
H	-3.924231	0.090009	1.498692
H	-1.956242	2.558103	-0.269601
H	-0.323605	3.063436	-0.714962
H	-0.716496	2.751360	0.996584
H	4.232800	-1.119328	0.349697
H	4.106143	1.296733	-0.195421

2h

ΔG = -443.478761 hartree

C	0.521245	0.242632	-0.243083
C	1.489680	1.137114	0.279003
C	2.797790	0.718739	0.530360
C	3.196541	-0.598751	0.288464
C	2.245777	-1.496329	-0.209259
C	0.935029	-1.095477	-0.467078
C	-2.433712	-0.877945	0.462352
C	-1.848649	-0.277917	-0.795840
N	-0.766296	0.680256	-0.545502
C	-1.181439	2.013977	-0.124774
C	-3.728964	-0.829173	0.789532
H	1.226999	2.166074	0.489830
H	-1.727224	-1.370646	1.130183
H	2.520730	-2.530904	-0.397773
H	-4.103137	-1.279713	1.704700
H	-4.460394	-0.341176	0.148032
H	-2.631792	0.242004	-1.356155
H	-1.476785	-1.066971	-1.456546
H	-2.203283	2.186560	-0.465307
H	-0.545389	2.781040	-0.578292
H	-1.156552	2.146495	0.967292
H	4.213779	-0.919757	0.489718
H	3.508797	1.438809	0.927186
H	0.238532	-1.834831	-0.842419

1i (O-State)

ΔG = -633.215492 hartree

C	0.942288	-0.349975	0.392705
C	1.594053	-1.590551	0.190478
C	2.694054	-1.714536	-0.652444
C	3.208069	-0.605176	-1.336887
C	2.625789	0.632331	-1.106993
C	1.529854	0.804902	-0.230249
C	1.253417	2.208473	0.096187
O	0.499680	2.656405	0.958946
C	-2.238303	-0.440883	-0.238040
C	-1.393301	0.413055	0.715247
N	-0.192144	-0.280292	1.195548
C	-0.462985	-1.380170	2.122367
O	-3.344212	0.354591	-0.648146
C	-4.226387	-0.333122	-1.527487
H	1.204058	-2.482344	0.664517
H	3.042877	1.517922	-1.580163
H	1.862943	2.915186	-0.501360
H	-5.036039	0.356208	-1.775941
H	-4.647416	-1.228078	-1.047614
H	-3.711589	-0.634442	-2.450882
H	-1.638742	-0.739862	-1.112203
H	-2.599162	-1.356089	0.254377
H	-1.996584	0.693778	1.584968
H	-1.116176	1.335797	0.213105
H	-1.228294	-1.048585	2.828498
H	0.440074	-1.623323	2.687322
H	-0.825997	-2.296400	1.634733
H	4.052857	-0.706326	-2.009801
H	3.139160	-2.695464	-0.794106

1i (H-State)

ΔG = -633.218267 hartree

C	0.838227	-0.529449	0.393997
C	1.289134	-1.778415	-0.081922
C	2.371044	-1.863575	-0.956103
C	3.042673	-0.711360	-1.390037
C	2.643975	0.522920	-0.892920
C	1.577525	0.631099	0.020097
C	1.365187	1.917563	0.700924
O	1.840158	2.992560	0.336680

C	-2.350016	-0.257281	-0.207012
C	-1.411246	0.423422	0.797275
N	-0.285311	-0.419660	1.231134
C	-0.682128	-1.599754	2.001471
O	-3.335482	0.699596	-0.576264
C	-4.295746	0.180260	-1.489324
H	0.769387	-2.685628	0.202386
H	3.179127	1.428929	-1.160047
H	0.775031	1.867780	1.632917
H	-5.000492	0.985108	-1.708063
H	-4.839622	-0.668971	-1.052083
H	-3.818067	-0.146802	-2.423674
H	-1.784885	-0.585214	-1.093617
H	-2.835013	-1.141141	0.232492
H	-1.980420	0.722193	1.684300
H	-1.033937	1.335801	0.333680
H	-1.403047	-1.286549	2.761563
H	0.190572	-2.016948	2.509636
H	-1.146765	-2.394950	1.400984
H	3.875385	-0.786022	-2.081850
H	2.680739	-2.839794	-1.318571

1i (A, O-State)

ΔG = -633.127146 hartree

C	0.909883	-0.122624	0.327722
C	0.937826	-1.431008	0.797948
C	2.002695	-2.280041	0.454424
C	3.037217	-1.793711	-0.371303
C	3.029122	-0.486754	-0.834398
C	1.969872	0.400827	-0.482890
C	1.890384	1.764658	-0.843471
O	0.911514	2.524405	-0.435301
C	-2.367550	-0.306682	0.106179
C	-1.345552	0.785905	-0.240284
N	-0.165179	0.779063	0.626348
C	-0.308672	1.260560	1.995924
O	-3.447789	-0.150595	-0.801812
C	-4.474561	-1.119212	-0.608683
H	0.131533	-1.798364	1.426364
H	3.841411	-0.120647	-1.456480
H	2.654273	2.219528	-1.482105
H	-5.251548	-0.912546	-1.347089
H	-4.903394	-1.045167	0.400293
H	-4.091193	-2.137764	-0.760237
H	-1.919688	-1.304964	-0.001269
H	-2.722537	-0.198119	1.142075
H	-1.820614	1.766971	-0.155217
H	-1.007069	0.653654	-1.269925
H	-0.970999	2.128589	2.006064
H	0.672651	1.542612	2.379307
H	-0.730407	0.482577	2.646581
H	3.859461	-2.450355	-0.642668
H	2.020590	-3.301437	0.819756

1i (A, H-State)

ΔG = -633.131363 hartree

C	-1.112038	-0.611600	0.077738
C	-2.213531	-1.490005	-0.031662
C	-3.498907	-1.018328	-0.270750
C	-3.694031	0.384895	-0.421255
C	-2.651393	1.281942	-0.271680
C	-1.335450	0.853112	0.075448
C	-0.370777	1.813205	0.520155
O	-0.575471	3.071923	0.501012
C	2.581263	-0.376750	0.189831
C	1.279094	-0.579167	-0.591142
N	0.167984	-1.126014	0.206060
C	0.358339	-2.494936	0.688607
O	3.473661	0.268974	-0.703883
C	4.754079	0.512586	-0.127079
H	-2.040901	-2.559720	-0.018145
H	-2.832108	2.349207	-0.327195
H	0.586365	1.439754	0.906796
H	5.356486	1.010044	-0.889166
H	5.241403	-0.427632	0.165390
H	4.672677	1.163409	0.754178
H	2.405468	0.244607	1.080668
H	3.010189	-1.332076	0.522166
H	1.456123	-1.277928	-1.420352
H	0.966626	0.369089	-1.025682
H	1.370374	-2.597115	1.079443
H	0.230977	-3.220069	-0.125694
H	-0.351293	-2.709086	1.486283
H	-4.689850	0.762144	-0.639270
H	-4.323820	-1.709428	-0.398148

1i (C)

ΔG = -633.216826 hartree

C	1.025219	-0.684183	-0.290320
C	1.945407	-1.631017	0.178421
C	3.155968	-1.166148	0.717075
C	3.445256	0.199902	0.799580
C	2.511290	1.141624	0.327353
C	1.312845	0.692706	-0.203391
C	0.167940	1.448801	-0.834192
O	-0.124145	2.651338	-0.126427
C	-1.903113	0.506087	0.369155
C	-0.977631	0.377391	-0.845905
N	-0.210273	-0.887348	-0.892065
C	-0.862389	-2.185198	-0.874316
O	-3.036295	-0.336801	0.179773
C	-3.960511	-0.255050	1.257021
H	0.419154	1.697385	-1.875610
H	-0.617117	3.246468	-0.707858
H	-1.591315	0.462319	-1.749347
H	1.735575	-2.694650	0.136372
H	2.721740	2.205992	0.385532
H	-4.794281	-0.919004	1.018850

H	-4.338110	0.770484	1.379683
H	-3.500456	-0.577424	2.202199
H	-1.370694	0.228493	1.292435
H	-2.229816	1.549568	0.472152
H	-1.760558	-2.142979	-1.492427
H	-1.155195	-2.508566	0.135591
H	-0.187959	-2.936022	-1.298243
H	4.384941	0.533394	1.229046
H	3.877832	-1.889812	1.086435

2i

ΔG = -519.896985 hartree

C	-1.100412	0.292501	0.067558
C	-2.355154	0.888673	-0.214583
C	-3.514056	0.115290	-0.306217
C	-3.478759	-1.269574	-0.119257
C	-2.245361	-1.869530	0.159096
C	-1.076654	-1.114160	0.247952
C	2.251887	-0.017202	-0.303376
C	1.277946	0.531636	0.743375
N	0.054885	1.058597	0.147831
C	-0.004892	2.494127	-0.094324
O	3.409124	-0.487236	0.376443
C	4.391483	-1.020763	-0.503624
H	-2.432799	1.959825	-0.354139
H	-2.183728	-2.945304	0.301938
H	5.230727	-1.351788	0.111627
H	4.742363	-0.259760	-1.215064
H	3.995887	-1.877758	-1.067051
H	1.784586	-0.835043	-0.872775
H	2.524241	0.775428	-1.017613
H	1.772718	1.333543	1.301292
H	1.040053	-0.251077	1.470328
H	1.010229	2.892742	-0.113636
H	-0.570128	3.029274	0.684070
H	-0.464697	2.712522	-1.063982
H	-4.383674	-1.864837	-0.190731
H	-4.457011	0.611478	-0.521243
H	-0.142126	-1.627537	0.441024

1j (O-State)

ΔG = -710.421777 hartree

C	1.376577	-0.073653	0.529279
C	1.654944	-1.342356	1.093739
C	2.673634	-2.154131	0.605467
C	3.474715	-1.742436	-0.468872
C	3.263639	-0.476771	-0.995624
C	2.262922	0.391826	-0.502712
C	2.387259	1.773868	-0.978037
O	1.787999	2.772274	-0.580783
C	-0.643443	1.305689	0.066019
N	0.311896	0.681532	1.000527
C	-0.255365	0.366119	2.309671
C	-4.183720	-1.094176	-0.682784
C	-2.931405	-1.524216	-1.138091
C	-1.793316	-0.751743	-0.895166
C	-1.884386	0.460061	-0.190649
C	-3.142992	0.880324	0.259634
C	-4.287099	0.111862	0.015231
H	1.031402	-1.718040	1.895291
H	3.911122	-0.109373	-1.788155
H	3.168974	1.891454	-1.755001
H	-0.939378	2.277163	0.475474
H	-0.133605	1.501628	-0.873473
H	-0.860448	1.217055	2.633617
H	0.546092	0.221188	3.037456
H	-0.899026	-0.524938	2.307579
H	4.254477	-2.385966	-0.862032
H	2.826860	-3.131625	1.054383
H	-5.069330	-1.693276	-0.873879
H	-2.843295	-2.457251	-1.687556
H	-0.827180	-1.091248	-1.259161
H	-3.231382	1.817269	0.804331
H	-5.254329	0.455436	0.371071

1j (H-State)

ΔG = -710.423862 hartree

C	-1.229362	0.078317	0.679226
C	-1.262274	1.398765	1.172970
C	-2.192211	2.319686	0.693396
C	-3.119529	1.961825	-0.295910
C	-3.131589	0.652760	-0.761122
C	-2.226097	-0.304728	-0.265698
C	-2.436282	-1.717947	-0.614283
O	-3.158262	-2.116560	-1.527726
C	0.642832	-1.452914	0.107349
N	-0.268598	-0.851481	1.113100
C	0.366491	-0.616244	2.409338
C	4.104213	0.979644	-0.860736
C	2.857180	1.272132	-1.424726
C	1.745393	0.484512	-1.114937
C	1.859054	-0.604338	-0.234968
C	3.114767	-0.890173	0.319724
C	4.231175	-0.105433	0.011230
H	-0.534001	1.719064	1.908477
H	-3.872966	0.326950	-1.484260
H	-1.932666	-2.447698	0.043746
H	0.968097	-2.422366	0.499294
H	0.074447	-1.646387	-0.803148
H	0.865286	-1.538616	2.720579
H	-0.396892	-0.373380	3.151937
H	1.117717	0.186470	2.398452
H	-3.831156	2.689001	-0.673326
H	-2.179213	3.334140	1.082032
H	4.969667	1.589162	-1.104140
H	2.752465	2.108069	-2.110555
H	0.783866	0.713383	-1.566848
H	3.222492	-1.736317	0.994171
H	5.196563	-0.343807	0.448574

1j (A, O-State)

ΔG = -710.337300 hartree

C	-1.306852	0.072784	0.338950
C	-0.969296	1.296607	0.906600
C	-1.848246	2.386938	0.801475
C	-3.068190	2.229819	0.111320
C	-3.423315	1.010799	-0.446315
C	-2.559753	-0.118018	-0.331825
C	-2.851813	-1.422317	-0.791017
O	-2.037965	-2.420108	-0.583190
C	0.559919	-1.244082	-0.692380
N	-0.436259	-1.063776	0.386167
C	-0.161218	-1.675759	1.679770
C	4.199097	1.029981	-0.089860
C	3.142636	1.576868	-0.825278
C	1.969906	0.841769	-1.020182
C	1.837710	-0.447915	-0.483356
C	2.907897	-0.992291	0.243121
C	4.080608	-0.258287	0.441801
H	-0.018083	1.410108	1.417469
H	-4.375299	0.898557	-0.958251
H	-3.777968	-1.626504	-1.338122
H	0.778746	-2.313613	-0.743674
H	0.072124	-0.950059	-1.623029
H	0.213182	-2.690628	1.527521
H	-1.082915	-1.707307	2.261510
H	0.591072	-1.100044	2.235435
H	-3.746564	3.074234	0.023158
H	-1.581482	3.342184	1.241444
H	5.111257	1.600009	0.060417
H	3.232146	2.572358	-1.250329
H	1.155255	1.269599	-1.597751
H	2.829986	-1.998648	0.646117
H	4.901556	-0.694332	1.003484

1j (A, H-State)

ΔG = -710.341070 hartree

C	1.639092	-0.608772	-0.062342
C	2.664572	-1.568532	-0.227952
C	4.007770	-1.221903	-0.152361
C	4.348070	0.134336	0.120162
C	3.378320	1.113606	0.240401
C	1.991813	0.827697	0.060339
C	1.071675	1.912528	-0.118329
O	1.405978	3.136770	0.009147
C	-0.629532	-0.452177	0.946072
N	0.318205	-1.018220	-0.031767
C	-0.053310	-2.340594	-0.539613
C	-4.632608	0.384032	-0.474905
C	-3.548478	0.516155	-1.347561
C	-2.251834	0.233630	-0.907893
C	-2.023887	-0.192687	0.408647
C	-3.118285	-0.334466	1.274192
C	-4.413415	-0.042465	0.838938
H	2.399959	-2.613533	-0.333572
H	3.659216	2.150296	0.385086
H	0.035810	1.677138	-0.390884
H	-0.684606	-1.166439	1.779568
H	-0.190958	0.461115	1.353256
H	-1.132489	-2.364545	-0.686633
H	0.215871	-3.124397	0.179926
H	0.443869	-2.529852	-1.490626
H	5.394924	0.410634	0.216466
H	4.777292	-1.979772	-0.240586
H	-5.639162	0.606131	-0.816598
H	-3.708765	0.840738	-2.371492
H	-1.419389	0.334388	-1.598252
H	-2.957269	-0.675115	2.293840
H	-5.249341	-0.155734	1.522924

1j (C)

ΔG = -710.422106 hartree

C	-1.813421	0.600995	0.019507
C	-2.994520	1.320174	0.246736
C	-4.204382	0.613185	0.278472
C	-4.250656	-0.772536	0.080370
C	-3.062435	-1.481856	-0.157271
C	-1.858599	-0.790078	-0.195050
C	-0.450858	-1.296243	-0.374430
O	-0.052802	-1.940254	0.846310
C	0.317507	0.035311	-0.680669
N	-0.499899	1.074753	-0.022651
C	-0.240956	2.459652	-0.389792
C	4.504082	-0.054026	0.421145
C	3.539357	0.282403	1.376722
C	2.186710	0.325979	1.027047
C	1.778747	0.039586	-0.284971
C	2.755067	-0.288568	-1.238015
C	4.107824	-0.340367	-0.888948
H	-0.334028	-1.998072	-1.207637
H	0.877146	-2.201079	0.766626
H	0.254197	0.172869	-1.774206
H	-2.985028	2.394597	0.396667
H	-3.084517	-2.556490	-0.318618
H	0.826267	2.666234	-0.285330
H	-0.779147	3.132623	0.281901
H	-0.542888	2.679928	-1.427164
H	-5.202435	-1.294177	0.102142
H	-5.127220	1.159729	0.453140
H	5.554996	-0.086521	0.693606
H	3.839252	0.511387	2.395422
H	1.439919	0.592204	1.768263
H	2.454904	-0.500897	-2.261391
H	4.849498	-0.595243	-1.640470

2j

ΔG = -597.102969 hartree

C	1.614140	0.322818	-0.143883
C	2.863061	0.640218	0.446593
C	3.859731	-0.328172	0.580499
C	3.661261	-1.639333	0.137526
C	2.429857	-1.965063	-0.441837
C	1.420425	-1.012541	-0.579876
C	-0.552203	1.028776	-1.104540
N	0.620693	1.281520	-0.280942
C	0.840390	2.635316	0.210822
C	-3.926520	-0.919070	0.818044
C	-2.876513	-0.421523	1.594648
C	-1.778302	0.195682	0.984252
C	-1.714665	0.323506	-0.407938
C	-2.771092	-0.182650	-1.181076
C	-3.869565	-0.797746	-0.575460
H	3.064191	1.645727	0.795299
H	2.242594	-2.978505	-0.787358
H	-0.907178	1.994889	-1.479143
H	-0.266476	0.456048	-1.996090
H	-0.081356	3.207016	0.099444
H	1.638034	3.156994	-0.338896
H	1.103659	2.633924	1.274876
H	4.441109	-2.386960	0.243802
H	4.805623	-0.044750	1.034954
H	-4.778332	-1.399274	1.290879
H	-2.908512	-0.514010	2.676751
H	-0.961128	0.574854	1.590540
H	-2.733123	-0.097019	-2.265062
H	-4.677545	-1.185293	-1.189808
H	0.473569	-1.315590	-1.010225

1k (O-State)

ΔG = -824.924016 hartree

C	-2.042625	0.055926	0.529821
C	-2.064330	1.157791	1.418871
C	-2.776578	2.318366	1.132494
C	-3.511363	2.441256	-0.054637
C	-3.557610	1.351367	-0.911433
C	-2.876085	0.143295	-0.638804
C	-3.274825	-0.972005	-1.504097
O	-2.987153	-2.162959	-1.392783
C	-0.365132	-1.629295	-0.200542
N	-1.274019	-1.064025	0.820228
C	-0.814898	-1.263014	2.192918
C	3.629930	0.086189	-0.133136
C	2.562992	0.808938	-0.685538
C	1.283427	0.243124	-0.702843
C	1.033171	-1.030761	-0.177185
C	2.117675	-1.737521	0.367608
C	3.400245	-1.194525	0.391921
O	4.919339	0.538917	-0.067712
C	5.216197	1.834164	-0.595854
H	-1.475472	1.122604	2.326855
H	-4.169940	1.399136	-1.808667
H	-3.962234	-0.660310	-2.315756
H	-0.305818	-2.709582	-0.032149
H	-0.814581	-1.488568	-1.179347
H	-1.640732	-1.100735	2.889147
H	-0.482360	-2.299517	2.294411
H	0.023087	-0.610462	2.477023
H	-4.049401	3.354314	-0.286142
H	-2.736363	3.146015	1.835277
H	2.712764	1.795885	-1.106466
H	0.470051	0.813616	-1.143697
H	1.958876	-2.732767	0.775791
H	4.234093	-1.749052	0.811370
H	6.284393	1.981212	-0.436293
H	4.656808	2.614807	-0.068212
H	4.996339	1.884142	-1.668164

1k (H-State)

ΔG = -824.927021 hartree

C	-1.944511	-0.054416	0.653741
C	-1.770143	1.005311	1.567712
C	-2.425389	2.222146	1.387119
C	-3.273892	2.430187	0.289994
C	-3.491734	1.383045	-0.596793
C	-2.869084	0.133387	-0.415331
C	-3.311339	-0.999692	-1.241953
O	-3.972933	-0.899820	-2.274978
C	-0.354361	-1.701068	-0.313375
N	-1.255076	-1.271599	0.789121
C	-0.754945	-1.621605	2.117987
C	3.610940	0.074254	-0.195990
C	2.533402	0.793626	-0.731539
C	1.263914	0.206457	-0.768388
C	1.035100	-1.086212	-0.280174
C	2.131197	-1.791023	0.245199
C	3.403093	-1.226008	0.289982
O	4.891074	0.547859	-0.111758
C	5.166018	1.864662	-0.597433
H	-1.091113	0.890914	2.404338
H	-4.184609	1.491361	-1.425603
H	-3.054404	-1.999759	-0.850730
H	-0.276393	-2.792214	-0.260333
H	-0.833424	-1.457390	-1.262423
H	-1.540228	-1.458600	2.859615
H	-0.498254	-2.684981	2.119858
H	0.139508	-1.057861	2.419676
H	-3.769464	3.385382	0.149707
H	-2.255520	3.024141	2.100072
H	2.666969	1.794519	-1.123865
H	0.441734	0.774381	-1.195830
H	1.989855	-2.801369	0.621139
H	4.246037	-1.777849	0.694402
H	6.230290	2.026701	-0.426805
H	4.588769	2.617248	-0.048830
H	4.951062	1.943954	-1.668908

1k (A, O-State)

ΔG = -824.839976 hartree

C	-1.951045	0.193707	0.347921
C	-1.352794	1.279603	0.978084
C	-1.945619	2.550656	0.903921
C	-3.144844	2.714686	0.179967
C	-3.759233	1.637491	-0.440736
C	-3.192194	0.331687	-0.357152
C	-3.773015	-0.846894	-0.878260
O	-3.232013	-2.018644	-0.693568
C	-0.421635	-1.488414	-0.709582
N	-1.374093	-1.116897	0.362235
C	-1.281928	-1.822679	1.633550
C	3.611446	-0.040362	-0.026137
C	2.714960	0.713924	-0.795419
C	1.418162	0.233451	-1.008256
C	0.990251	-0.986741	-0.472845
C	1.908465	-1.733905	0.286437
C	3.200642	-1.271765	0.511502
O	4.897277	0.328972	0.246017
C	5.378893	1.570840	-0.276733
H	-0.417988	1.144269	1.513368
H	-4.693894	1.774460	-0.978022
H	-4.701357	-0.799537	-1.457242
H	-0.439570	-2.579161	-0.779075
H	-0.823451	-1.081311	-1.638836
H	-2.197899	-1.655614	2.200989
H	-1.154439	-2.891042	1.444735
H	-0.427871	-1.462895	2.222853
H	-3.601638	3.698692	0.115693
H	-1.475455	3.397083	1.393615
H	3.008601	1.660492	-1.232583
H	0.734980	0.825295	-1.611218
H	1.614847	-2.695746	0.698128
H	3.908406	-1.854032	1.093117
H	6.410089	1.655188	0.065742
H	4.794837	2.414102	0.107950
H	5.355264	1.573710	-1.372018

1k (A, H-State)

ΔG = -824.845892 hartree

C	2.402609	-0.551150	-0.176137
C	3.454067	-1.423881	-0.539910
C	4.780129	-1.008022	-0.541938
C	5.076901	0.327126	-0.145220
C	4.075180	1.227573	0.170222
C	2.693595	0.881149	0.077669
C	1.709057	1.923121	0.098664
O	1.992777	3.145289	0.328318
C	0.240007	-0.642704	1.048593
N	1.112467	-1.040710	-0.072820
C	0.757321	-2.314512	-0.701650
C	-3.943202	0.010366	0.112709
C	-2.962687	0.367031	-0.822449
C	-1.612802	0.144842	-0.527704
C	-1.214794	-0.437818	0.680267
C	-2.212860	-0.800551	1.600410
C	-3.558264	-0.576328	1.329444
O	-5.285155	0.186080	-0.068087
C	-5.739064	0.779368	-1.288552
H	3.232884	-2.465139	-0.740646
H	4.316268	2.256977	0.408529
H	0.664957	1.656450	-0.105356
H	0.317973	-1.439087	1.802410
H	0.668910	0.252079	1.504736
H	1.133803	-3.159812	-0.111499
H	-0.328497	-2.385308	-0.750425
H	1.167334	-2.360728	-1.710288
H	6.113232	0.653036	-0.108522
H	5.574506	-1.704456	-0.783469
H	-3.229101	0.813792	-1.772464
H	-0.869294	0.421772	-1.269420
H	-1.934346	-1.264892	2.542912
H	-4.324834	-0.856915	2.044797
H	-6.825302	0.821038	-1.210502
H	-5.457034	0.168352	-2.153123
H	-5.340857	1.793189	-1.406295

1k (C)

ΔG = -824.923872 hartree

C	2.541113	0.605334	-0.080563
C	3.691875	1.336457	-0.405407
C	4.897511	0.638796	-0.561938
C	4.970163	-0.749414	-0.391816
C	3.813193	-1.470936	-0.055899
C	2.614117	-0.789029	0.105455
C	1.232138	-1.306433	0.409351
O	0.720114	-1.931260	-0.778755
C	0.488169	0.013571	0.809455
N	1.235542	1.068760	0.093125
C	1.004617	2.447033	0.500787
C	-3.791924	-0.070235	0.114311
C	-2.923873	0.265704	-0.933509
C	-1.543872	0.302901	-0.703051
C	-1.003232	0.018866	0.556579
C	-1.891815	-0.305992	1.596281
C	-3.266254	-0.355828	1.384513
O	-5.152580	-0.138520	0.000734
C	-5.747212	0.140729	-1.269815
H	1.198249	-2.023442	1.237462
H	-0.208856	-2.161617	-0.625042
H	0.655471	0.134867	1.894139
H	3.662476	2.413167	-0.535473
H	3.856712	-2.547782	0.085312
H	1.459535	3.132655	-0.218239
H	-0.069736	2.641585	0.515813
H	1.416127	2.660831	1.501235
H	5.918721	-1.263801	-0.510654
H	5.796874	1.194826	-0.812745

H	-3.302013	0.498204	-1.921708
H	-0.879043	0.570215	-1.518291
H	-1.502305	-0.519706	2.588701
H	-3.946968	-0.605492	2.192425
H	-6.821336	0.024858	-1.125555
H	-5.401726	-0.566742	-2.031783
H	-5.529526	1.165153	-1.591703

2k

ΔG = -711.602081 hartree

C	2.346869	0.330650	-0.012353
C	2.855072	-0.073723	1.244079
C	3.655295	-1.213859	1.367064
C	3.968312	-1.999027	0.256152
C	3.464032	-1.614236	-0.992706
C	2.672149	-0.476399	-1.130698
C	0.525391	1.593509	-1.157823
N	1.604925	1.511406	-0.155006
C	1.401051	2.348855	1.020579
C	-3.228106	-0.190712	0.126806
C	-2.246530	-0.984068	-0.481895
C	-1.047414	-0.395989	-0.902116
C	-0.794712	0.970647	-0.727936
C	-1.798688	1.747877	-0.124442
C	-2.998506	1.183121	0.300003
O	-4.434195	-0.657488	0.573988
C	-4.728453	-2.048059	0.418083
H	2.623992	0.494135	2.136631
H	3.694325	-2.202526	-1.877134
H	0.373003	2.655811	-1.374184
H	0.867370	1.136131	-2.086612
H	2.360104	2.568992	1.497371
H	0.961038	3.296628	0.701546
H	0.734123	1.899518	1.773008
H	4.585992	-2.886062	0.356636
H	4.025768	-1.489318	2.351093
H	-2.400955	-2.044706	-0.639757
H	-0.300946	-1.024798	-1.379027
H	-1.643802	2.815419	0.010957
H	-3.769592	1.791555	0.762668
H	-5.722468	-2.189791	0.842369
H	-4.007116	-2.668819	0.961219
H	-4.738194	-2.334531	-0.639549
H	2.321876	-0.209102	-2.120869

1l (O-State)

ΔG = -802.673725 hartree

C	-1.925548	0.104546	0.518292
C	-1.989329	1.314315	1.248956
C	-2.798967	2.372112	0.845612
C	-3.591456	2.276319	-0.305830
C	-3.591343	1.077567	-1.004432
C	-2.808694	-0.029911	-0.606755
C	-3.147508	-1.279748	-1.296975
O	-2.754815	-2.417523	-1.044033
C	-0.162590	-1.559114	-0.043188
N	-1.065360	-0.911693	0.922906
C	-0.560314	-0.904956	2.294775
C	3.729916	0.329781	-0.298339
C	2.588191	1.003059	-0.772987
C	1.342945	0.388641	-0.687396
C	1.205546	-0.894254	-0.130500
C	2.351574	-1.552421	0.337455
C	3.608527	-0.954997	0.257525
C	5.017290	0.954359	-0.385514
N	6.063282	1.462542	-0.455834
H	-1.359902	1.445146	2.120349
H	-4.241649	0.957995	-1.867576
H	-3.889698	-1.135339	-2.107125
H	-0.041717	-2.607020	0.248613
H	-0.631153	-1.556805	-1.023914
H	-1.377323	-0.701272	2.990142
H	-0.163808	-1.899376	2.516848
H	0.242417	-0.173811	2.466926
H	-4.206674	3.108748	-0.630241
H	-2.791299	3.290566	1.425821
H	2.684155	1.992145	-1.207882
H	0.469050	0.911803	-1.063123
H	2.262925	-2.545586	0.768198
H	4.488314	-1.474743	0.621522

1l (H-State)

ΔG = -802.67708 hartree

C	-1.804126	0.022550	0.655848
C	-1.646019	1.203506	1.407854
C	-2.371221	2.352777	1.096136
C	-3.273306	2.367416	0.022979
C	-3.471790	1.199574	-0.703475
C	-2.777542	0.017253	-0.384663
C	-3.189619	-1.238179	-1.032451
O	-3.897057	-1.309720	-2.036223
C	-0.165697	-1.668686	-0.134505
N	-1.049112	-1.135269	0.927288
C	-0.506182	-1.290789	2.277120
C	3.689875	0.293723	-0.363614
C	2.551037	0.913328	-0.910991
C	1.318207	0.271678	-0.837760
C	1.192107	-0.985097	-0.222451
C	2.337000	-1.592114	0.314076
C	3.580459	-0.966260	0.249468
C	4.964543	0.945971	-0.437575
N	5.999997	1.476457	-0.496703
H	-0.927667	1.235951	2.218398
H	-4.202507	1.161454	-1.505455
H	-2.861297	-2.162945	-0.526273
H	-0.025957	-2.737734	0.055378
H	-0.673256	-1.572649	-1.095051
H	-1.283803	-1.066428	3.010422
H	-0.203393	-2.333573	2.408791

H	0.366916	-0.655342	2.483792
H	-3.823959	3.269955	-0.221567
H	-2.214992	3.252055	1.685218
H	2.639043	1.881492	-1.392088
H	0.446261	0.751396	-1.271509
H	2.258656	-2.568270	0.783951
H	4.459858	-1.445818	0.665715

1l (A, O-State)

ΔG = -802.591637 hartree

C	-2.383406	-0.309813	0.134172
C	-3.095880	-1.499391	0.036403
C	-4.472567	-1.473744	-0.239257
C	-5.119968	-0.233217	-0.414970
C	-4.419937	0.959734	-0.317972
C	-3.021449	0.959179	-0.037900
C	-2.211970	2.109141	0.090156
O	-0.935343	2.023787	0.352680
C	-0.096499	-0.727248	-0.686383
N	-0.974115	-0.288305	0.417035
C	-0.568516	-0.590509	1.787553
C	4.126253	-0.010920	-0.133337
C	3.249801	1.074796	-0.318391
C	1.888423	0.841065	-0.486433
C	1.379779	-0.467715	-0.467382
C	2.262055	-1.541595	-0.284469
C	3.628760	-1.324572	-0.117829
C	5.530724	0.224050	0.037720
N	6.671208	0.415167	0.177197
H	-2.585495	-2.448375	0.176572
H	-4.931466	1.908657	-0.454576
H	-2.636928	3.111200	-0.022640
H	-0.259521	-1.803138	-0.844469
H	-0.446264	-0.209765	-1.583414
H	-0.599203	-1.674837	1.966800
H	0.446322	-0.231004	1.961686
H	-1.255334	-0.095046	2.473470
H	-6.184921	-0.210427	-0.629875
H	-5.027783	-2.402727	-0.315576
H	3.638336	2.087388	-0.333011
H	1.206021	1.673725	-0.616634
H	1.881188	-2.558387	-0.272536
H	4.304525	-2.161045	0.023058

1l (A, H-State)

ΔG = -802.596015 hartree

C	2.269588	-0.567301	-0.118103
C	3.341013	-1.454749	-0.374364
C	4.661198	-1.025512	-0.359819
C	4.932588	0.341081	-0.056258
C	3.913457	1.252502	0.152772
C	2.540157	0.884973	0.035810
C	1.545954	1.913868	-0.055458
O	1.808580	3.150823	0.104408
C	0.065251	-0.582854	1.026006
N	0.979638	-1.057633	-0.027182
C	0.661603	-2.389476	-0.548271
C	-4.041832	0.111542	-0.120652
C	-3.022850	0.277419	-1.074292
C	-1.697818	0.038820	-0.717607
C	-1.368556	-0.372929	0.582113
C	-2.394936	-0.546044	1.523074
C	-3.722575	-0.302569	1.185084
C	-5.407587	0.359418	-0.480068
N	-6.517361	0.560122	-0.771277
H	3.135751	-2.510604	-0.501352
H	4.137828	2.299489	0.319939
H	0.514606	1.622342	-0.289292
H	0.093058	-1.325992	1.834728
H	0.472406	0.340875	1.443614
H	1.018246	-3.171858	0.133612
H	-0.420711	-2.480114	-0.636761
H	1.113455	-2.524216	-1.530581
H	5.964308	0.679453	-0.007553
H	5.470342	-1.728938	-0.516867
H	-3.268389	0.591794	-2.082768
H	-0.919585	0.166284	-1.463059
H	-2.155483	-0.874122	2.530281
H	-4.508326	-0.437527	1.920211

1l (C)

ΔG = -802.674829 hartree

C	2.408195	0.594588	-0.058912
C	3.578749	1.302838	-0.361066
C	4.776072	0.583440	-0.474242
C	4.820185	-0.803675	-0.284872
C	3.643093	-1.501630	0.027265
C	2.452048	-0.796594	0.147243
C	1.056016	-1.292923	0.421397
O	0.570680	-1.938851	-0.764476
C	0.320148	0.050408	0.772271
N	1.104463	1.083772	0.071378
C	0.889528	2.468405	0.471020
C	-3.902371	-0.011256	-0.137720
C	-2.980671	0.362950	-1.132505
C	-1.620923	0.395218	-0.835943
C	-1.156701	0.064161	0.446444
C	-2.086781	-0.300042	1.432410
C	-3.449884	-0.344826	1.151164
C	-5.304283	-0.045884	-0.435888
N	-6.443360	-0.075307	-0.678433
H	0.990794	-1.987642	1.265292
H	-0.296886	-2.325942	-0.575710
H	0.437194	0.185637	1.861027
H	3.570872	2.377804	-0.506698
H	3.663702	-2.577092	0.182492
H	1.388339	3.141599	-0.229866
H	-0.179191	2.691327	0.443117
H	1.266223	2.671876	1.486740

H	5.762788	-1.335094	-0.371122
H	5.691275	1.120975	-0.706981
H	-3.331181	0.623540	-2.125457
H	-0.908646	0.687830	-1.599383
H	-1.742611	-0.547618	2.432649
H	-4.160353	-0.626717	1.920689

2l

ΔG = -689.357963 hartree

C	-2.275635	0.231292	0.005967
C	-3.501673	0.279122	-0.701637
C	-4.397734	-0.790558	-0.654849
C	-4.117745	-1.938513	0.092293
C	-2.908229	-1.996982	0.793093
C	-1.998186	-0.940682	0.752927
C	-0.300928	1.397238	0.928693
N	-1.374379	1.288856	-0.044367
C	-1.667920	2.460584	-0.860646
C	3.511060	-0.345481	-0.173789
C	2.447719	-0.366353	-1.092260
C	1.217987	0.187060	-0.738496
C	1.027135	0.765844	0.521611
C	2.096448	0.780384	1.432627
C	3.329945	0.233112	1.097365
C	4.778258	-0.912839	-0.528444
N	5.809084	-1.373947	-0.815847
H	-3.765536	1.154277	-1.282598
H	-2.659077	-2.879828	1.375975
H	-0.125875	2.460330	1.128064
H	-0.618091	0.969733	1.887925
H	-2.519623	3.040602	-0.474351
H	-0.791170	3.109159	-0.879189
H	-1.888155	2.173289	-1.894056
H	-4.820021	-2.765553	0.125643
H	-5.330176	-0.715619	-1.208290
H	2.586029	-0.813120	-2.071165
H	0.395182	0.169627	-1.445351
H	1.962589	1.224998	2.415337
H	4.149817	0.249171	1.807537
H	-1.061841	-1.040789	1.289285

1m (O-State)

ΔG = -749.712748 hartree

C	-1.371055	0.050506	0.276368
C	-1.702514	1.030704	1.244118
C	-2.724156	1.949733	1.033834
C	-3.481297	1.935317	-0.147213
C	-3.223353	0.940732	-1.078012
C	-2.216475	-0.033092	-0.882953
C	-2.288061	-1.165012	-1.812762
O	-1.678184	-2.232365	-1.759817
C	0.682027	-1.020381	-0.618920
N	-0.286551	-0.793041	0.467495
C	0.226074	-1.047771	1.822791
C	-0.774021	-1.786868	2.715147
C	4.363567	1.250288	-0.236726
C	3.132805	1.913426	-0.318289
C	1.947987	1.183021	-0.432251
C	1.970289	-0.220973	-0.463796
C	3.207196	-0.873918	-0.380138
C	4.397924	-0.145988	-0.269713
H	-1.117423	1.105452	2.152063
H	-3.835589	0.868694	-1.973886
H	-3.039044	-1.015422	-2.614471
H	0.916614	-2.088334	-0.673851
H	0.209863	-0.754356	-1.562283
H	1.115835	-1.669693	1.700759
H	-0.323046	-1.974550	3.695232
H	-1.046905	-2.749099	2.270460
H	-1.690786	-1.211768	2.872906
H	0.570879	-0.123737	2.308650
H	-4.264181	2.666991	-0.316187
H	-2.916406	2.703226	1.792691
H	5.285098	1.818493	-0.149099
H	3.097527	2.999066	-0.297280
H	0.998767	1.707863	-0.499205
H	3.241250	-1.960583	-0.402896
H	5.347255	-0.670375	-0.206437

1m (H-State)

ΔG = -749.714847 hartree

C	-1.192737	0.229017	-0.351217
C	-1.171938	-0.203070	-1.692345
C	-2.056609	-1.180413	-2.144501
C	-2.990633	-1.765471	-1.276979
C	-3.051799	-1.325230	0.039135
C	-2.190653	-0.314661	0.507858
C	-2.432955	0.257320	1.841733
O	-3.157661	-0.246511	2.699220
C	0.662683	0.717391	1.212105
N	-0.270985	1.171555	0.150681
C	0.316730	2.145327	-0.783570
C	-0.722104	3.090469	-1.389337
C	4.219917	-1.302042	-0.243679
C	2.996771	-1.980220	-0.190570
C	1.854140	-1.330472	0.283105
C	1.911621	0.007638	0.707506
C	3.144779	0.673475	0.656272
C	4.291989	0.026674	0.184130
H	-0.439290	0.202243	-2.380040
H	-3.794204	-1.722539	0.724472
H	-1.947622	1.229696	2.035335
H	0.951441	1.597877	1.795336
H	0.118724	0.050383	1.883195
H	1.029381	2.734900	-0.199767
H	-0.221914	3.819256	-2.035557
H	-1.253617	3.635022	-0.602346
H	-1.461140	2.558931	-1.995612
H	0.905104	1.660630	-1.577527

H	-3.667453	-2.534923	-1.634193
H	-2.003239	-1.503205	-3.180489
H	5.109166	-1.807871	-0.608583
H	2.934755	-3.016426	-0.510932
H	0.912484	-1.870696	0.330945
H	3.211863	1.704591	0.994790
H	5.238527	0.558939	0.154587

1m (A, O-State)

ΔG = -749.628054 hartree

C	-1.204002	0.197074	0.197902
C	-0.840465	1.205358	1.084338
C	-1.623035	2.366389	1.191018
C	-2.771334	2.504257	0.383641
C	-3.152625	1.501396	-0.494764
C	-2.392817	0.298907	-0.597414
C	-2.738299	-0.817551	-1.393237
O	-2.043070	-1.919525	-1.375603
C	0.615433	-0.968712	-1.050107
N	-0.416312	-0.984261	0.012983
C	-0.207405	-1.903491	1.138795
C	-1.486619	-2.242124	1.898425
C	4.314078	0.955567	0.134515
C	3.305309	1.694921	-0.491215
C	2.113858	1.071627	-0.873070
C	1.914267	-0.296660	-0.634735
C	2.937234	-1.031976	-0.016315
C	4.128782	-0.410937	0.368466
H	0.059709	1.098486	1.682157
H	-4.051889	1.611143	-1.095050
H	-3.608257	-0.775583	-2.057329
H	0.794313	-2.009050	-1.332854
H	0.177225	-0.453195	-1.906143
H	0.241395	-2.810294	0.723561
H	-1.245655	-2.955230	2.692413
H	-2.221923	-2.694613	1.228831
H	-1.929333	-1.356733	2.361921
H	0.533581	-1.460492	1.821413
H	-3.374261	3.405302	0.458848
H	-1.335936	3.151741	1.882449
H	5.241028	1.438464	0.429669
H	3.446760	2.753962	-0.686472
H	1.336789	1.649522	-1.365481
H	2.808439	-2.097280	0.155911
H	4.912598	-0.994389	0.842643

1m (A, H-State)

ΔG = -749.633281 hartree

C	1.646629	0.395346	0.121636
C	2.663733	1.352701	0.351460
C	4.011390	1.030576	0.247797
C	4.367854	-0.295188	-0.124728
C	3.408906	-1.277416	-0.303755
C	2.021414	-1.025816	-0.089649
C	1.126309	-2.139125	0.043164
O	1.481907	-3.347257	-0.159554
C	-0.618359	0.234371	-0.891760
N	0.319753	0.792621	0.100316
C	-0.105568	2.057360	0.730458
C	-0.150537	3.264004	-0.219851
C	-4.634089	-0.658581	0.457973
C	-3.551305	-0.885180	1.313366
C	-2.251277	-0.583429	0.898792
C	-2.016698	-0.042977	-0.374784
C	-3.109417	0.190268	-1.222104
C	-4.409102	-0.120329	-0.812657
H	2.392869	2.385301	0.530583
H	3.702736	-2.298284	-0.518691
H	0.092893	-1.941649	0.352333
H	-0.671101	0.947516	-1.724054
H	-0.168282	-0.671369	-1.303131
H	-1.105619	1.880303	1.133772
H	-0.436983	4.147425	0.358316
H	-0.892701	3.129484	-1.010868
H	0.819702	3.456366	-0.684794
H	0.554206	2.244760	1.577388
H	5.417229	-0.549818	-0.249225
H	4.769962	1.791214	0.390221
H	-5.643648	-0.895427	0.780377
H	-3.716057	-1.298186	2.304202
H	-1.421220	-0.758388	1.577024
H	-2.943554	0.615844	-2.208506
H	-5.243264	0.065106	-1.482878

1m (C)

ΔG = -749.712601 hartree

C	-1.804629	0.360207	-0.094353
C	-2.994060	1.094381	0.019528
C	-4.200747	0.389566	0.130770
C	-4.238045	-1.010064	0.125416
C	-3.042245	-1.736518	0.002969
C	-1.842030	-1.048486	-0.113829
C	-0.431083	-1.566023	-0.216661
O	-0.030070	-2.022542	1.085047
C	0.329180	-0.288252	-0.712566
N	-0.497434	0.830611	-0.211646
C	-0.231124	2.182967	-0.711688
C	-0.197104	3.243660	0.392889
C	4.519219	-0.191939	0.380125
C	3.550134	0.224131	1.299289
C	2.196571	0.208905	0.951184
C	1.790603	-0.219273	-0.322633
C	2.771496	-0.628016	-1.239194
C	4.125668	-0.619355	-0.891646
H	-0.308355	-2.380839	-0.938889
H	0.901773	-2.285577	1.043809
H	0.267548	-0.312579	-1.813796
H	-2.994340	2.178770	0.023970
H	-3.056093	-2.823296	-0.010726

H	0.739335	2.160539	-1.215578
H	-0.006140	4.230657	-0.042462
H	0.596696	3.024771	1.113588
H	-1.144323	3.293784	0.938136
H	-0.979006	2.451739	-1.473796
H	-5.187138	-1.530426	0.208356
H	-5.128227	0.949204	0.217928
H	5.571008	-0.177701	0.650740
H	3.847281	0.561977	2.288063
H	1.447503	0.537868	1.663831
H	2.473896	-0.950849	-2.233983
H	4.870354	-0.937332	-1.615644

2m

ΔG = -636.394538 hartree

C	1.517856	-0.048112	-0.088811
C	2.771346	0.076532	0.562568
C	3.676592	-0.984787	0.590806
C	3.385095	-2.205546	-0.026487
C	2.152414	-2.341124	-0.673180
C	1.231803	-1.293220	-0.704844
C	-0.578950	0.935798	-0.963345
N	0.601862	0.995272	-0.116109
C	0.838468	2.252098	0.596916
C	1.653726	3.285193	-0.193646
C	-4.121479	-0.940109	0.715101
C	-2.999321	-0.731239	1.521043
C	-1.848098	-0.138343	0.988550
C	-1.803632	0.254143	-0.353831
C	-2.934383	0.038547	-1.157362
C	-4.084744	-0.552529	-0.629830
H	3.053322	1.007661	1.038307
H	1.891152	-3.279608	-1.155469
H	-0.850351	1.965399	-1.223021
H	-0.332447	0.451972	-1.916082
H	-0.140723	2.673805	0.846442
H	1.775112	4.200382	0.396502
H	1.147562	3.550089	-1.128051
H	2.648842	2.904651	-0.443143
H	1.323122	2.034911	1.553814
H	4.095809	-3.025687	-0.003207
H	4.627573	-0.845127	1.098490
H	-5.014345	-1.401309	1.127250
H	-3.015507	-1.031204	2.565216
H	-0.976470	0.016365	1.617103
H	-2.913888	0.335298	-2.203956
H	-4.950169	-0.712484	-1.266932
H	0.278217	-1.455822	-1.192391

1n (O-State)

ΔG = -828.296420 hartree

C	-1.156037	-0.690988	-0.154023
C	-1.568998	-0.466793	-1.491156
C	-2.390185	-1.364442	-2.163271
C	-2.858436	-2.529481	-1.536848
C	-2.529789	-2.733140	-0.205731
C	-1.726353	-1.824378	0.521930
C	-1.739738	-2.041718	1.971991
O	-1.302800	-1.304725	2.855372
C	0.885039	-0.370734	1.222650
N	-0.255711	0.165905	0.460535
C	-0.086876	1.542177	-0.028936
C	-1.331751	2.415869	0.172444
C	-1.123747	3.848481	-0.336547
C	-2.350742	4.742387	-0.122570
C	4.656472	-0.305570	-0.928478
C	3.569311	-1.028882	-1.434590
C	2.353844	-1.042009	-0.747028
C	2.201116	-0.331863	0.455162
C	3.294974	0.389553	0.951340
C	4.516699	0.402545	0.267730
H	-1.200083	0.398390	-2.027253
H	-2.930860	-3.594751	0.322748
H	-2.270210	-2.970865	2.262306
H	0.987219	0.188224	2.158408
H	0.663668	-1.400171	1.495098
H	0.738875	1.973808	0.542679
H	-3.227094	4.342368	-0.646243
H	-2.173036	5.756898	-0.495390
H	-2.604404	4.816912	0.941495
H	-0.874080	3.821177	-1.406020
H	-0.256014	4.292495	0.170419
H	-1.577380	2.432620	1.242236
H	-2.193620	1.971044	-0.339689
H	0.234614	1.564660	-1.080772
H	-3.482141	-3.237804	-2.071683
H	-2.649304	-1.163620	-3.199201
H	5.602295	-0.296477	-1.462429
H	3.670792	-1.585689	-2.361941
H	1.517842	-1.610555	-1.145678
H	3.192808	0.944572	1.880897
H	5.353671	0.967149	0.668877

1n (H-State)

ΔG = -828.298143 hartree

C	0.910364	-0.675381	0.178031
C	0.960181	-0.485120	1.573298
C	1.474111	-1.471024	2.413537
C	1.952973	-2.683287	1.895222
C	1.947016	-2.873885	0.519232
C	1.463612	-1.877087	-0.349876
C	1.668544	-2.040602	-1.797772
O	1.991377	-3.094111	-2.345733
C	-0.871818	-0.128066	-1.448389
N	0.341483	0.278009	-0.693290
C	0.345164	1.691468	-0.284076
C	1.756854	2.278048	-0.172306
C	1.743124	3.766893	0.200645
C	3.148874	4.371941	0.290103

C	-4.587856	0.191899	0.773474
C	-3.742927	-0.906863	0.967146
C	-2.549711	-1.009574	0.247471
C	-2.177861	-0.016871	-0.674323
C	-3.036719	1.075502	-0.864414
C	-4.233096	1.182298	-0.147064
H	0.566434	0.425232	2.009407
H	2.354137	-3.780104	0.081446
H	1.557583	-1.120464	-2.397296
H	-0.922088	0.495636	-2.346663
H	-0.740210	-1.159676	-1.779577
H	-0.197066	2.237008	-1.062673
H	3.751333	3.861279	1.050685
H	3.108286	5.434280	0.553911
H	3.677375	4.284735	-0.666614
H	1.227878	3.897051	1.162055
H	1.153742	4.322281	-0.541813
H	2.269089	2.141385	-1.133652
H	2.339379	1.724540	0.574390
H	-0.215216	1.860511	0.648904
H	2.340219	-3.450756	2.557641
H	1.482980	-1.299414	3.486277
H	-5.517259	0.270566	1.330073
H	-4.016588	-1.686383	1.672625
H	-1.906506	-1.872702	0.396199
H	-2.773195	1.845624	-1.585376
H	-4.886681	2.034461	-0.310684

1n (A, O-State)

ΔG = -828.211475 hartree

C	0.651273	0.965731	-0.084920
C	0.216057	1.211675	-1.382781
C	0.555915	2.413050	-2.025387
C	1.330340	3.370689	-1.337846
C	1.780442	3.133751	-0.047842
C	1.476541	1.907488	0.613932
C	1.954749	1.531985	1.890496
O	1.707820	0.360775	2.404186
C	-0.922637	-0.167714	1.483573
N	0.289716	-0.219535	0.632743
C	0.694151	-1.531446	0.114547
C	2.178258	-1.625351	-0.246888
C	2.550240	-3.028190	-0.746776
C	4.034122	-3.149267	-1.112169
C	-4.616827	-0.700940	-0.719285
C	-4.098623	0.581809	-0.514311
C	-2.908104	0.750979	0.198136
C	-2.219278	-0.357678	0.713266
C	-2.753072	-1.639679	0.511202
C	-3.943091	-1.811938	-0.201458
H	-0.402025	0.477792	-1.891222
H	2.394170	3.871128	0.462719
H	2.544805	2.235693	2.487636
H	-0.809723	-0.943927	2.244158
H	-0.914980	0.802614	1.982311
H	0.445978	-2.266553	0.886196
H	4.304377	-2.443586	-1.906472
H	4.273147	-4.157991	-1.465440
H	4.672797	-2.937577	-0.246623
H	1.937004	-3.279402	-1.622787
H	2.303357	-3.768760	0.025853
H	2.769893	-1.370491	0.639063
H	2.418798	-0.886740	-1.020162
H	0.077164	-1.768046	-0.766688
H	1.588400	4.304850	-1.829575
H	0.212977	2.602378	-3.037202
H	-5.543071	-0.833168	-1.270786
H	-4.622257	1.450031	-0.903832
H	-2.514213	1.750330	0.360679
H	-2.244054	-2.507505	0.922247
H	-4.345850	-2.810251	-0.345701

1n (A, H-State)

ΔG = -828.215780 hartree

C	-1.739565	0.169288	-0.103922
C	-2.521505	1.332393	-0.298929
C	-3.906280	1.312554	-0.184856
C	-4.543608	0.088421	0.159243
C	-3.823092	-1.084443	0.304822
C	-2.414754	-1.138095	0.084652
C	-1.785695	-2.417166	-0.078158
O	-2.395545	-3.522584	0.103936
C	0.435945	-0.488207	0.897956
N	-0.356202	0.263740	-0.095127
C	0.331921	1.395881	-0.738672
C	0.696347	2.557984	0.206209
C	1.337919	3.718305	-0.567546
C	1.744482	4.881512	0.344330
C	4.223899	-2.120814	-0.416083
C	3.114182	-2.177112	-1.265450
C	1.890445	-1.636981	-0.861545
C	1.760717	-1.026035	0.395311
C	2.880946	-0.966309	1.236436
C	4.103663	-1.513575	0.837351
H	-2.029364	2.283429	-0.458793
H	-4.332359	-2.021363	0.498714
H	-0.735790	-2.443155	-0.394403
H	0.611287	0.184358	1.747284
H	-0.193584	-1.294331	1.280727
H	1.249426	0.994353	-1.178100
H	0.877347	5.287846	0.877606
H	2.192652	5.695605	-0.234909
H	2.477583	4.559896	1.092979
H	0.635690	4.079173	-1.330637
H	2.220207	3.349741	-1.107325
H	1.395460	2.205233	0.973061
H	-0.199719	2.909777	0.730913
H	-0.294459	1.741918	-1.561492
H	-5.622675	0.067306	0.288313
H	-4.479633	2.224889	-0.300004

H	5.173947	-2.542611	-0.730286
H	3.198743	-2.642343	-2.243126
H	1.039572	-1.682357	-1.535220
H	2.797221	-0.489554	2.209760
H	4.960421	-1.458919	1.502456

1n (C)

ΔG = -828.297140 hartree

C	-1.830561	-0.154271	-0.125694
C	-2.982363	0.641927	-0.047728
C	-4.220476	0.004107	0.111501
C	-4.324842	-1.390108	0.187998
C	-3.166202	-2.179305	0.101945
C	-1.935376	-1.558146	-0.061956
C	-0.551744	-2.148592	-0.139064
O	-0.167566	-2.552142	1.185218
C	0.267843	-0.939272	-0.708039
N	-0.503759	0.245721	-0.276494
C	-0.177940	1.550228	-0.859926
C	-0.058618	2.675181	0.177635
C	0.249948	4.034570	-0.462785
C	0.394605	5.161656	0.566587
C	4.458081	-0.978107	0.387580
C	3.510091	-0.463017	1.278113
C	2.157383	-0.433788	0.927604
C	1.731314	-0.916667	-0.319825
C	2.691204	-1.426434	-1.207450
C	4.044422	-1.461130	-0.857633
H	-0.472424	-3.007328	-0.815022
H	0.749240	-2.864861	1.156297
H	0.204338	-1.025690	-1.805988
H	-2.929942	1.723632	-0.105031
H	-3.232213	-3.263098	0.152257
H	0.777400	1.448640	-1.384725
H	-0.526160	5.284224	1.149200
H	0.612572	6.119014	0.080925
H	1.208161	4.950961	1.270780
H	-0.546455	4.290787	-1.174922
H	1.174654	3.956464	-1.051262
H	0.732970	2.412253	0.890700
H	-0.987834	2.746352	0.757145
H	-0.930367	1.816921	-1.619347
H	-5.297013	-1.858359	0.306631
H	-5.119257	0.612075	0.171441
H	5.509442	-0.997630	0.659572
H	3.823227	-0.082070	2.246077
H	1.424776	-0.027683	1.617106
H	2.378150	-1.793751	-2.181830
H	4.772975	-1.856753	-1.559447

2n

ΔG = -714.977339 hartree

C	-0.627712	1.234927	-0.090202
C	-1.732042	1.834315	0.567312
C	-1.883351	3.220810	0.602587
C	-0.957384	4.069284	-0.013074
C	0.135902	3.490830	-0.665645
C	0.307286	2.106704	-0.704726
C	0.562825	-0.747943	-0.967749
N	-0.457196	-0.142823	-0.125085
C	-1.379023	-1.053965	0.555072
C	-2.626403	-1.426531	-0.264123
C	-3.556055	-2.392166	0.482244
C	-4.799734	-2.774348	-0.328762
C	4.559723	-1.078227	0.705914
C	3.494760	-0.689852	1.523168
C	2.205161	-0.568839	0.991991
C	1.962798	-0.833883	-0.360650
C	3.038314	-1.220905	-1.175277
C	4.326403	-1.343786	-0.648763
H	-2.487079	1.221053	1.043370
H	0.878111	4.121854	-1.147917
H	0.228167	-1.762614	-1.210243
H	0.617814	-0.222656	-1.929293
H	-0.819074	-1.963750	0.798630
H	-5.395567	-1.888359	-0.578155
H	-5.442943	-3.463409	0.229326
H	-4.522197	-3.264007	-1.269772
H	-3.866301	-1.935564	1.432290
H	-2.998462	-3.301399	0.746334
H	-2.307321	-1.882556	-1.211265
H	-3.176055	-0.513974	-0.527621
H	-1.673678	-0.618517	1.516140
H	-1.083651	5.147024	0.015440
H	-2.746718	3.637767	1.114815
H	5.560865	-1.170602	1.116946
H	3.665008	-0.477483	2.575050
H	1.381712	-0.259993	1.628826
H	2.866860	-1.426251	-2.229921
H	5.147206	-1.642960	-1.294711
H	1.184866	1.707615	-1.198579

1o (O-State)

ΔG = -941.409679 hartree

C	-1.067929	-1.085463	0.476732
C	-1.492483	-0.687580	1.749631
C	-2.665633	-1.179520	2.331472
C	-3.456713	-2.097574	1.639433
C	-3.054826	-2.509510	0.371703
C	-1.875823	-2.025131	-0.231358
C	-1.616202	-2.584153	-1.575735
O	-0.673718	-2.347468	-2.320659
C	0.036622	0.456849	-1.102078
N	0.160511	-0.504350	0.010583
C	1.297993	-1.437608	-0.108006
C	-2.247400	4.005269	-0.104358
C	-2.704361	3.130647	-1.093190
C	-1.968918	1.980593	-1.406015
C	-0.771875	1.688380	-0.739512

C	-0.321949	2.575929	0.251446
C	-1.051009	3.723918	0.567918
C	5.148886	0.473565	0.476342
C	4.873282	-0.202923	-0.714406
C	3.624771	-0.808565	-0.903369
C	2.638009	-0.748935	0.089572
C	2.927568	-0.067603	1.282980
C	4.170304	0.538829	1.476668
H	-0.874966	0.025852	2.284381
H	-3.661136	-3.227021	-0.175434
H	-2.397395	-3.299069	-1.902634
H	1.058546	0.764566	-1.348816
H	-0.382205	-0.009169	-2.004194
H	1.168188	-2.192924	0.674852
H	1.297649	-1.965995	-1.070466
H	-4.369051	-2.487373	2.079241
H	-2.955831	-0.843092	3.322504
H	-2.814477	4.898840	0.140571
H	-3.630804	3.339450	-1.620944
H	-2.329342	1.304300	-2.177347
H	0.605072	2.361012	0.776264
H	-0.686207	4.401900	1.334704
H	6.115764	0.945362	0.626564
H	5.624345	-0.257933	-1.497488
H	3.415450	-1.332333	-1.833050
H	2.169970	-0.012130	2.059886
H	4.378708	1.059463	2.407367

1o (H-State)

ΔG = -941.411571 hartree

C	-1.071340	-0.938538	0.506809
C	-1.437684	-0.403901	1.749663
C	-2.615705	-0.792032	2.390637
C	-3.462280	-1.736557	1.797462
C	-3.119469	-2.277331	0.563738
C	-1.937445	-1.888359	-0.096809
C	-1.647580	-2.486453	-1.417313
O	-2.359920	-3.321902	-1.966324
C	0.084481	0.468189	-1.177226
N	0.171536	-0.486889	-0.058544
C	1.244696	-1.487988	-0.184640
C	-1.885125	4.197537	-0.179212
C	-2.451317	3.336052	-1.121897
C	-1.817716	2.127597	-1.436613
C	-0.615634	1.764568	-0.816550
C	-0.054302	2.638698	0.128009
C	-0.681824	3.844824	0.445308
C	5.221202	0.137421	0.415566
C	4.919401	-0.569061	-0.751120
C	3.630337	-1.079528	-0.947087
C	2.630018	-0.894208	0.015928
C	2.944116	-0.182687	1.184680
C	4.227781	0.329049	1.384432
H	-0.774231	0.320352	2.209243
H	-3.758549	-3.010721	0.082504
H	-0.734228	-2.142306	-1.926197
H	1.117010	0.689755	-1.467723
H	-0.405440	0.031280	-2.063393
H	1.064778	-2.248193	0.582686
H	1.229894	-2.009547	-1.155749
H	-4.376448	-2.044389	2.295240
H	-2.869890	-0.361245	3.354667
H	-2.373277	5.136153	0.066942
H	-3.383914	3.600309	-1.612403
H	-2.263005	1.462079	-2.172058
H	0.878667	2.367863	0.614925
H	-0.232574	4.511986	1.175756
H	6.219452	0.536509	0.570807
H	5.681261	-0.720281	-1.510640
H	3.400766	-1.626447	-1.858540
H	2.174920	-0.028749	1.936161
H	4.455746	0.875278	2.295582

1o (A, O-State)

ΔG = -941.327476 hartree

C	-0.977578	-1.284574	-0.316344
C	-1.607501	-1.587946	-1.518308
C	-2.756197	-2.394566	-1.529565
C	-3.256141	-2.903155	-0.312739
C	-2.634096	-2.613172	0.891720
C	-1.475553	-1.782050	0.929374
C	-0.784971	-1.405954	2.102780
O	0.249687	-0.612202	2.071559
C	0.195803	0.889814	-0.752798
N	0.227498	-0.503306	-0.265312
C	1.464984	-1.274205	-0.549234
C	-3.270977	3.238910	0.333247
C	-3.065211	2.859954	-0.995957
C	-1.952668	2.084030	-1.337667
C	-1.034961	1.677755	-0.359277
C	-1.245046	2.069082	0.972082
C	-2.357317	2.840922	1.316042
C	5.227507	0.769137	0.082458
C	4.782001	0.496235	-1.213649
C	3.558506	-0.152619	-1.409981
C	2.766680	-0.535603	-0.317621
C	3.225877	-0.264728	0.981597
C	4.445930	0.386220	1.178770
H	-1.204873	-1.204646	-2.451808
H	-3.032015	-3.007063	1.823073
H	-1.099152	-1.785348	3.080469
H	1.098175	1.372777	-0.369333
H	0.287777	0.872189	-1.849566
H	1.409415	-2.170170	0.073581
H	1.412371	-1.600635	-1.597931
H	-4.143923	-3.529854	-0.317683
H	-3.247746	-2.625128	-2.468956
H	-4.133551	3.841870	0.601991
H	-3.766743	3.166144	-1.766550
H	-1.798113	1.793690	-2.373558

H	-0.541289	1.753425	1.735574
H	-2.508809	3.135990	2.350513
H	6.177455	1.272074	0.238612
H	5.383446	0.784820	-2.070748
H	3.218917	-0.364827	-2.420661
H	2.614618	-0.556064	1.829281
H	4.789643	0.590583	2.188831

1o (A, H-State)

ΔG = -941.330100 hartree

C	1.764867	-0.801458	0.053990
C	1.713545	-1.510994	1.276970
C	2.775185	-1.500239	2.171174
C	3.932418	-0.736379	1.845323
C	4.050544	-0.085631	0.629960
C	3.035908	-0.166717	-0.368967
C	3.352423	0.186544	-1.724069
O	4.439278	0.756643	-2.063511
C	-0.309235	-1.842406	-0.865542
N	0.626738	-0.709293	-0.733576
C	0.259769	0.549699	-1.409732
C	-4.400971	-1.368937	0.479119
C	-4.122157	-1.711615	-0.845993
C	-2.795778	-1.835265	-1.272388
C	-1.734189	-1.622819	-0.382616
C	-2.024266	-1.280630	0.947149
C	-3.347107	-1.153197	1.374325
C	-1.935050	3.421222	0.981307
C	-2.496780	2.898097	-0.187162
C	-1.795009	1.952216	-0.940236
C	-0.522328	1.524943	-0.539641
C	0.041823	2.063723	0.626084
C	-0.663373	3.000887	1.385725
H	0.791198	-2.002068	1.564751
H	4.972236	0.420522	0.365753
H	2.629455	-0.087649	-2.506265
H	-0.333579	-2.079709	-1.936589
H	0.145982	-2.699415	-0.367034
H	1.184954	1.035227	-1.727205
H	-0.317060	0.293200	-2.300690
H	4.754024	-0.687032	2.555104
H	2.698600	-2.014352	3.122013
H	-5.429423	-1.269662	0.813441
H	-4.932054	-1.881082	-1.549365
H	-2.586520	-2.101446	-2.305237
H	-1.221831	-1.099676	1.654971
H	-3.554665	-0.885285	2.406094
H	-2.480778	4.152873	1.569796
H	-3.481424	3.221421	-0.512216
H	-2.240912	1.544316	-1.843075
H	1.034737	1.757142	0.942634
H	-0.215761	3.408315	2.287569

1o (C)

ΔG = -941.409996 hartree

C	-0.220286	1.335580	-0.185762
C	-1.029108	1.952831	-1.148936
C	-0.824761	3.317723	-1.405245
C	0.151621	4.053769	-0.725511
C	0.949553	3.423119	0.246984
C	0.759050	2.074544	0.505702
C	1.425812	1.163976	1.515352
O	2.826359	1.339736	1.680976
C	-0.959594	-1.032520	-0.455455
N	-0.226978	0.013057	0.235900
C	0.977914	-0.275600	1.038716
C	-5.200814	-1.269531	0.439381
C	-4.310929	-0.777707	1.400150
C	-2.946107	-0.680254	1.112058
C	-2.450887	-1.071794	-0.138965
C	-3.350323	-1.557233	-1.098662
C	-4.715349	-1.659603	-0.813013
C	4.117760	-2.410513	-1.069441
C	3.403713	-1.400939	-1.723245
C	2.384566	-0.714779	-1.056132
C	2.064014	-1.026383	0.275458
C	2.784069	-2.043284	0.918824
C	3.804037	-2.731220	0.254677
H	1.013642	1.340586	2.515061
H	3.262054	1.193316	0.827461
H	0.701530	-0.875880	1.910849
H	-1.790888	1.399186	-1.687261
H	1.710772	3.982484	0.784444
H	-0.826349	-0.949217	-1.544636
H	-0.510209	-1.989008	-0.167007
H	0.291631	5.107574	-0.945433
H	-1.441395	3.808373	-2.153589
H	-6.261369	-1.342733	0.662154
H	-4.678950	-0.467686	2.374313
H	-2.258934	-0.290794	1.857484
H	-2.981786	-1.854640	-2.077952
H	-5.398135	-2.035925	-1.569635
H	4.906948	-2.945679	-1.589362
H	3.636664	-1.148826	-2.753795
H	1.829795	0.058209	-1.579539
H	2.541923	-2.300768	1.947008
H	4.347333	-3.518953	0.768717

2o

ΔG = -828.090919 hartree

C	-1.037105	-1.426982	0.106963
C	-1.743664	-1.309309	1.310226
C	-2.893955	-2.072109	1.537542
C	-3.348686	-2.965355	0.562601
C	-2.647623	-3.088783	-0.641887
C	-1.501667	-2.321347	-0.870707
C	-0.036225	0.469907	-1.060240
N	0.151026	-0.624906	-0.084450
C	1.348673	-1.434051	-0.391566

C	-2.839837	3.513799	0.226677
C	-3.105984	2.753582	-0.914880
C	-2.203625	1.764298	-1.324688
C	-1.027409	1.521399	-0.603817
C	-0.769025	2.293405	0.540238
C	-1.665662	3.280567	0.953866
C	5.086449	0.612449	0.413499
C	4.837392	0.078409	-0.853235
C	3.623542	-0.568784	-1.114581
C	2.646271	-0.693973	-0.118428
C	2.907669	-0.154119	1.151217
C	4.115679	0.494328	1.416276
H	-1.379363	-0.618299	2.063786
H	-2.993070	-3.781115	-1.404708
H	0.944656	0.938624	-1.193658
H	-0.341794	0.082017	-2.047227
H	1.301946	-2.323414	0.245864
H	1.354786	-1.790168	-1.435957
H	-4.239401	-3.561260	0.739303
H	-3.430888	-1.970184	2.476443
H	-3.537841	4.281705	0.547779
H	-4.013954	2.925891	-1.486027
H	-2.417160	1.175246	-2.213223
H	0.140111	2.115460	1.108013
H	-1.449024	3.870366	1.840329
H	6.026339	1.116397	0.619857
H	5.582031	0.167089	-1.639291
H	3.434316	-0.978723	-2.103828
H	2.155612	-0.241692	1.930201
H	4.302748	0.904702	2.404818
H	-0.968471	-2.422295	-1.811793

1p (O-State)

ΔG = -748.526650 hartree

C	2.561731	-0.546958	0.494217
C	3.901154	-0.829227	0.206620
C	4.596553	-0.067217	-0.738391
C	3.945982	0.972119	-1.411191
C	2.603109	1.249980	-1.134723
C	1.910068	0.498211	-0.179333
C	1.721191	-1.334884	1.465352
C	0.487351	0.831028	0.210856
N	-0.337560	-0.364979	0.478959
C	0.351042	-1.615077	0.839451
C	-4.252496	-0.561999	-1.117713
C	-3.489765	-1.720843	-0.899146
C	-2.228325	-1.657400	-0.322032
C	-1.649184	-0.418251	0.066031
C	-2.488943	0.746955	-0.024472
C	-2.298411	2.004437	0.699756
O	-1.524749	2.227274	1.632934
C	-3.744736	0.646745	-0.671084
H	4.400178	-1.647007	0.720745
H	5.637404	-0.289990	-0.954856
H	4.478380	1.559631	-2.153558
H	2.096020	2.054360	-1.661992
H	1.586407	-0.777914	2.402979
H	2.196329	-2.286603	1.720524
H	0.009099	1.404743	-0.588354
H	0.491530	1.480901	1.094716
H	-0.278450	-2.165309	1.545774
H	0.496423	-2.250961	-0.046575
H	-5.224781	-0.616375	-1.595638
H	-3.873127	-2.688765	-1.210260
H	-1.661979	-2.573802	-0.222642
H	-4.343117	1.550191	-0.762143
H	-3.007342	2.797839	0.389896

1p (H-State)

ΔG = -748.526676 hartree

C	2.537123	-0.687291	0.399480
C	3.913880	-0.629315	0.668203
C	4.729272	0.322568	0.055103
C	4.170226	1.239028	-0.843663
C	2.803038	1.189471	-1.117330
C	1.980166	0.233331	-0.503096
C	1.656370	-1.710600	1.086295
C	0.507578	0.183280	-0.857841
N	-0.282126	-0.563173	0.139971
C	0.307707	-1.885421	0.384793
C	-4.480928	-0.272894	-0.445000
C	-3.819445	-1.490317	-0.654691
C	-2.442446	-1.600306	-0.458112
C	-1.684624	-0.493670	-0.032829
C	-2.365764	0.727948	0.227534
C	-1.668859	1.862286	0.858237
O	-2.140126	2.991983	0.976187
C	-3.749994	0.824613	-0.004947
H	4.347072	-1.342247	1.366031
H	5.792618	0.350382	0.275205
H	4.794072	1.986909	-1.324415
H	2.365616	1.901013	-1.814054
H	1.478247	-1.399041	2.123999
H	2.169178	-2.678368	1.132714
H	0.389283	-0.287893	-1.851873
H	0.116641	1.198881	-0.948935
H	-0.365597	-2.462311	1.022308
H	0.442334	-2.445249	-0.557214
H	-5.550564	-0.192528	-0.609829
H	-4.377157	-2.359296	-0.992156
H	-1.953694	-2.545779	-0.662575
H	-4.239129	1.771052	0.203752
H	-0.672825	1.634544	1.274932

1p (A, O-State)

ΔG = -748.450381 hartree

C	2.405056	0.364570	0.596970
C	3.785210	0.604235	0.691640
C	4.691561	-0.065223	-0.130252

C	4.223166	-0.996604	-1.064844
C	2.854660	-1.245443	-1.163957
C	1.940511	-0.570059	-0.341137
C	1.427817	1.115935	1.473071
C	0.467986	-0.898350	-0.482499
N	-0.410347	-0.059401	0.331857
C	0.106638	0.366622	1.635775
C	-4.576092	-0.588405	-0.138863
C	-3.841998	-1.547208	0.590078
C	-2.456903	-1.378436	0.749003
C	-1.821769	-0.273942	0.192543
C	-2.548121	0.711319	-0.549668
C	-1.811885	1.796765	-1.074088
O	-0.525156	1.910667	-0.889084
C	-3.953275	0.516562	-0.698955
H	4.146943	1.324852	1.421094
H	5.755601	0.133410	-0.041042
H	4.919072	-1.525702	-1.709094
H	2.488856	-1.970864	-1.886913
H	1.216116	2.096258	1.031871
H	1.860158	1.288358	2.464145
H	0.296209	-1.950127	-0.199662
H	0.145092	-0.796112	-1.522893
H	-0.651094	0.994448	2.106902
H	0.246143	-0.527601	2.264365
H	-5.647910	-0.716514	-0.264438
H	-4.337067	-2.409010	1.025181
H	-1.879218	-2.109906	1.307740
H	-4.531869	1.247179	-1.257812
H	-2.308725	2.577782	-1.658684

1p (A, H-State)

ΔG = -748.449844 hartree

C	-2.442431	-0.654543	0.201698
C	-3.721260	-0.895486	-0.325757
C	-4.444741	0.119222	-0.951232
C	-3.892260	1.400851	-1.060955
C	-2.621708	1.651252	-0.543753
C	-1.894502	0.632508	0.089123
C	-1.660643	-1.776543	0.852554
C	-0.530430	0.979304	0.678310
N	0.272839	-0.226023	0.920009
C	-0.466358	-1.249210	1.663744
C	3.717893	-1.037604	-1.318892
C	2.857333	-2.104230	-0.941694
C	1.736208	-1.811517	-0.171386
C	1.451136	-0.492755	0.248012
C	2.423975	0.591970	-0.010716
C	2.417297	1.858225	0.660430
O	3.261333	2.783776	0.415306
C	3.502087	0.260177	-0.882985
H	-4.148739	-1.891438	-0.241123
H	-5.433226	-0.086598	-1.351015
H	-4.445960	2.197866	-1.548032
H	-2.188920	2.644774	-0.629618
H	-1.304551	-2.471251	0.082006
H	-2.305943	-2.355883	1.521342
H	-0.665079	1.503641	1.633604
H	0.007394	1.639235	0.000479
H	0.212043	-2.047272	1.961216
H	-0.828952	-0.759595	2.575367
H	4.579682	-1.247281	-1.947389
H	3.037596	-3.114451	-1.289625
H	1.024239	-2.601124	0.038060
H	4.209447	1.044837	-1.125575
H	1.660868	2.026758	1.438794

1p (TS1)

ΔG = -748.440655 hartree

C	2.472570	-0.680189	0.483988
C	3.856795	-0.852737	0.597738
C	4.736697	-0.047418	-0.130394
C	4.231501	0.933954	-0.990738
C	2.851950	1.106235	-1.115331
C	1.966459	0.305367	-0.378302
C	1.478638	-1.525992	1.240746
C	0.490377	0.566278	-0.468865
N	-0.373371	-0.506326	-0.033839
C	0.230288	-1.777305	0.389796
C	-4.570983	-0.332686	-0.408570
C	-3.868112	-1.518849	-0.717045
C	-2.483211	-1.512621	-0.563107
C	-1.771013	-0.373574	-0.140789
C	-2.476756	0.872495	0.185833
C	-2.004293	2.105418	0.749338
O	-0.809731	2.514034	1.002219
C	-3.899720	0.794184	0.032994
H	4.245716	-1.624784	1.256835
H	5.808893	-0.190548	-0.034367
H	4.908635	1.558086	-1.566164
H	2.458756	1.865639	-1.786423
H	1.184557	-1.036211	2.178509
H	1.911345	-2.494812	1.507809
H	0.194903	0.864829	-1.484045
H	0.199766	1.452868	0.173278
H	-0.515006	-2.338699	0.951084
H	0.505661	-2.353315	-0.505674
H	-5.652359	-0.299089	-0.509985
H	-4.381282	-2.407346	-1.065963
H	-1.927674	-2.411035	-0.809457
H	-4.476292	1.676966	0.296849
H	-2.821303	2.794100	1.013084

1p (B)

ΔG = -748.474154 hartree

C	2.506995	0.448353	0.558929
C	3.879790	0.508616	0.781378
C	4.775812	-0.262250	0.024243
C	4.279827	-1.111908	-0.980807

C	2.914827	-1.197885	-1.216415
C	1.991828	-0.429553	-0.447749
C	1.520202	1.311569	1.310854
C	0.599326	-0.524376	-0.671374
N	-0.331091	0.203958	0.086249
C	0.154538	0.632760	1.427373
C	-4.335770	-1.245674	0.202294
C	-3.271665	-2.080159	0.591902
C	-1.962044	-1.588395	0.532994
C	-1.695952	-0.296388	0.085760
C	-2.762028	0.563007	-0.339434
C	-2.579047	1.864494	-0.855307
O	-1.373364	2.447755	-1.057438
C	-4.090334	0.039788	-0.250149
H	4.261940	1.172557	1.553836
H	5.843133	-0.200403	0.213374
H	4.966958	-1.708431	-1.574647
H	2.533700	-1.861244	-1.988775
H	1.400837	2.275722	0.795522
H	1.890061	1.540346	2.315956
H	0.192225	-1.120222	-1.479380
H	-0.692025	1.794131	-0.761998
H	-0.586907	1.314736	1.850022
H	0.220456	-0.246959	2.083618
H	-5.357497	-1.611306	0.250088
H	-3.459618	-3.090836	0.939488
H	-1.130248	-2.215661	0.842243
H	-4.916992	0.672816	-0.561439
H	-3.419287	2.483007	-1.149100

1p (C)

ΔG = -748.534700 hartree

C	-2.291893	0.914640	0.115949
C	-3.678313	0.929640	0.339710
C	-4.454901	-0.215468	0.160889
C	-3.848282	-1.405614	-0.256302
C	-2.472607	-1.434164	-0.485353
C	-1.684933	-0.289014	-0.294234
C	-1.482779	2.183454	0.336156
C	-0.207773	-0.312718	-0.616156
N	0.492288	0.848255	-0.050327
C	-0.101222	2.142031	-0.328668
C	4.422465	-0.542766	0.006338
C	4.232872	0.843263	0.075600
C	2.952508	1.414271	0.047392
C	1.851846	0.554490	-0.050209
C	2.036549	-0.844126	-0.128603
C	0.671343	-1.508120	-0.147702
O	0.309520	-2.045061	1.134225
C	3.310382	-1.395710	-0.092676
H	-0.094770	-0.284869	-1.718626
H	-4.151502	1.856826	0.654777
H	-5.525817	-0.179001	0.339133
H	-4.442009	-2.303200	-0.402727
H	-2.003214	-2.357672	-0.812060
H	-1.346523	2.334554	1.415215
H	-2.044228	3.049220	-0.032594
H	0.408231	-1.346474	1.798287
H	0.534709	2.932328	0.077056
H	-0.187407	2.307900	-1.417021
H	5.426360	-0.955493	0.022342
H	5.097348	1.497953	0.145722
H	2.830175	2.491350	0.096650
H	3.445286	-2.473064	-0.145281
H	0.599624	-2.352195	-0.835165

1p (TS2)

ΔG = -748.432369 hartree

C	2.235084	-0.163910	0.736055
C	3.502213	0.376530	1.007255
C	4.414407	0.625278	-0.017652
C	4.065704	0.338068	-1.342788
C	2.808875	-0.196033	-1.624787
C	1.890980	-0.452577	-0.595094
C	1.245468	-0.385801	1.863259
C	0.558384	-1.089990	-0.945063
N	-0.464185	-0.929419	0.120933
C	0.081779	-1.291873	1.461604
C	-3.240723	2.253492	-0.131688
C	-1.885356	2.594151	0.043543
C	-0.908892	1.574966	0.136327
C	-1.311944	0.259283	0.052708
C	-2.684785	-0.112968	-0.150398
C	-2.854011	-1.509548	-0.260233
O	-3.779681	-2.317890	-0.441873
C	-3.657937	0.931049	-0.230163
H	3.770541	0.602512	2.036378
H	5.390533	1.041339	0.213622
H	4.766354	0.532296	-2.149308
H	2.534008	-0.417198	-2.653260
H	0.857297	0.580644	2.207908
H	1.748792	-0.835815	2.725888
H	0.688072	-2.168543	-1.097718
H	0.148895	-0.672087	-1.866965
H	-0.736978	-1.238503	2.181418
H	0.409426	-2.333724	1.386407
H	-3.981848	3.046204	-0.197986
H	-1.584495	3.634259	0.108803
H	0.136583	1.834669	0.263439
H	-4.704903	0.686069	-0.376299
H	-1.511006	-1.743778	-0.111196

1p (D)

ΔG = -748.437074 hartree

C	2.197364	-0.302362	0.735478
C	3.434728	0.190565	1.178241
C	4.421528	0.576352	0.272131
C	4.179531	0.477737	-1.103265
C	2.952805	-0.005735	-1.554946

C	1.959784	-0.398815	-0.644746
C	1.120102	-0.674825	1.733510
C	0.673135	-0.971022	-1.201009
N	-0.449764	-1.022076	-0.194095
C	0.046828	-1.569788	1.135331
C	-3.052484	2.332975	0.123800
C	-1.658720	2.562348	0.123322
C	-0.781624	1.464724	0.016720
C	-1.298008	0.188377	-0.086546
C	-2.708717	-0.089213	-0.113941
C	-3.170901	-1.413826	-0.274492
O	-4.307991	-1.907169	-0.363175
C	-3.574310	1.056348	0.008356
H	3.620004	0.269328	2.246468
H	5.373674	0.952287	0.634372
H	4.939699	0.778723	-1.817585
H	2.760065	-0.079964	-2.622144
H	0.660278	0.233986	2.140651
H	1.558238	-1.204128	2.585874
H	0.827810	-2.003647	-1.530339
H	0.310886	-0.395257	-2.054062
H	-0.826578	-1.659322	1.781690
H	0.432915	-2.569737	0.919302
H	-3.731460	3.178003	0.210681
H	-1.259651	3.567397	0.204057
H	0.290053	1.631424	0.008848
H	-4.647889	0.895612	-0.000791
H	-1.142017	-1.725856	-0.530623

1p (TS3)

ΔG = -748.434211 hartree

C	2.492737	0.465396	0.551056
C	3.858543	0.464022	0.848896
C	4.762838	-0.178493	-0.003946
C	4.304615	-0.834107	-1.151267
C	2.937553	-0.852186	-1.445522
C	2.036245	-0.196728	-0.601512
C	1.446647	1.166370	1.381416
C	0.552738	-0.181139	-0.846821
N	-0.161568	-0.594253	0.433301
C	0.188718	0.310533	1.618882
C	-4.346446	-1.034556	-0.134815
C	-3.577834	-2.148203	0.227401
C	-2.198881	-1.998436	0.413540
C	-1.653119	-0.724522	0.228926
C	-2.354421	0.417630	-0.128580
C	-1.746362	2.577773	-0.604775
O	-2.769267	3.098111	-0.842550
C	-3.730111	0.214295	-0.308266
H	4.216200	0.968284	1.742676
H	5.823231	-0.171644	0.230531
H	5.006607	-1.337343	-1.809151
H	2.574605	-1.372334	-2.327958
H	1.144999	2.088150	0.868506
H	1.844019	1.463341	2.355773
H	0.247743	-0.886005	-1.620909
H	0.159799	0.808558	-1.091856
H	-0.681579	0.944126	1.777197
H	0.311382	-0.355465	2.474210
H	-5.419337	-1.147114	-0.280417
H	-4.040199	-3.121194	0.364668
H	-1.587557	-2.854932	0.694969
H	-4.350662	1.068559	-0.596778
H	0.195117	-1.525990	0.658159

1p (E)

ΔG = -635.122376 hartree

C	1.757822	0.385054	-0.666393
C	2.875473	-0.162727	-1.315315
C	3.807000	-0.931648	-0.619199
C	3.628145	-1.168385	0.749090
C	2.520403	-0.631779	1.403440
C	1.583420	0.146349	0.706161
C	0.732666	1.180435	-1.447440
C	0.432650	0.748590	1.485367
N	-0.687279	1.258226	0.615809
C	-0.138474	2.049642	-0.554246
C	-3.838164	-1.407487	-0.355304
C	-2.521274	-1.854846	-0.521950
C	-1.461048	-0.997529	-0.211806
C	-1.786309	0.279792	0.257163
C	-3.061950	0.805102	0.465720
C	-4.086881	-0.112503	0.124611
H	3.010539	0.020051	-2.378420
H	4.666515	-1.344743	-1.138606
H	4.345162	-1.768914	1.300530
H	2.378098	-0.816937	2.465195
H	0.101499	0.500060	-2.032163
H	1.230834	1.834016	-2.170733
H	0.780712	1.606966	2.068938
H	-0.003937	0.026973	2.178373
H	-1.000484	2.455767	-1.084549
H	0.435007	2.874070	-0.121580
H	-4.665344	-2.073761	-0.594706
H	-2.316707	-2.857522	-0.886307
H	-0.436924	-1.339550	-0.328612
H	-5.131514	0.182262	0.243688
H	-1.243383	1.925320	1.168903

1p (TS4)

ΔG = -635.109871 hartree

C	1.836557	0.420568	-0.615064
C	2.978383	-0.113090	-1.233732
C	3.857543	-0.941115	-0.535968
C	3.600182	-1.254331	0.804048
C	2.466625	-0.733493	1.427701
C	1.582568	0.104274	0.730945
C	0.877094	1.290363	-1.406443
C	0.389530	0.692763	1.460712

N	-0.678371	1.173541	0.547352
C	-0.107449	2.047729	-0.515444
C	-3.971557	-1.253060	-0.309829
C	-2.751401	-1.712983	-0.825401
C	-1.569412	-0.987100	-0.611834
C	-1.698588	0.186747	0.124991
C	-2.881734	0.694162	0.677986
C	-4.042250	-0.062064	0.435170
H	3.176364	0.128280	-2.275412
H	4.736830	-1.340712	-1.032735
H	4.275235	-1.901581	1.356087
H	2.261806	-0.977957	2.467355
H	0.322994	0.666629	-2.119420
H	1.435642	2.014877	-2.009439
H	0.702983	1.556402	2.059811
H	-0.055009	-0.036233	2.142657
H	-0.939609	2.455249	-1.094100
H	0.390841	2.874840	0.000697
H	-4.873237	-1.835275	-0.488238
H	-2.717145	-2.638655	-1.393000
H	-0.620771	-1.345059	-1.000331
H	-5.009993	0.253095	0.823642
H	-1.734885	1.635089	1.083933

2p

ΔG = -635.208605 hartree

C	1.774074	0.681214	-0.440551
C	2.851876	0.489218	-1.318924
C	3.765020	-0.549274	-1.127466
C	3.608653	-1.419653	-0.042628
C	2.540579	-1.237401	0.837825
C	1.620433	-0.196363	0.649250
C	0.777980	1.802985	-0.679845
C	0.490376	0.025626	1.647385
N	-0.622063	0.806381	1.107655
C	-0.106597	2.067531	0.548246
C	-3.879066	-1.124262	-0.835633
C	-2.797630	-1.870451	-0.363438
C	-1.704379	-1.250246	0.249596
C	-1.668465	0.150161	0.427623
C	-3.848954	0.266588	-0.676368
H	2.974441	1.165903	-2.161748
H	4.592888	-0.679059	-1.818746
H	4.310221	-2.234196	0.113335
H	2.414989	-1.912544	1.681696
H	0.136623	1.540129	-1.532540
H	1.305227	2.721820	-0.963262
H	0.883557	0.583562	2.508621
H	0.127875	-0.922961	2.047357
H	-0.923782	2.743471	0.296665
H	0.476325	2.555174	1.337702
H	-4.722628	-1.610047	-1.316137
H	-2.788046	-2.950856	-0.480972
H	-0.877519	-1.869566	0.574592
H	-4.678766	0.873352	-1.029008
C	-2.770527	0.894401	-0.055834
H	-2.797205	1.970709	0.073420

3p

ΔG = -672.148338 hartree

C	-2.284402	0.789213	0.156401
C	-3.681845	0.845755	0.120199
C	-4.444882	-0.312609	-0.051273
C	-3.806158	-1.550184	-0.195065
C	-2.414405	-1.621748	-0.171862
C	-1.640329	-0.460995	0.007681
C	-1.444137	2.025904	0.398181
C	-0.178447	-0.509993	0.037272
N	0.537255	0.679081	-0.062286
C	-0.104035	1.960846	-0.339521
C	4.426778	-0.724900	0.057706
C	4.262644	0.670398	-0.100094
C	2.995579	1.248318	-0.158999
C	1.887247	0.395444	-0.055572
C	2.030311	-1.018576	0.092449
C	0.709096	-1.566524	0.146980
C	3.325613	-1.570511	0.154807
H	-4.176846	1.807355	0.231114
H	-5.528735	-0.249929	-0.077510
H	-4.391007	-2.454512	-0.334734
H	-1.921417	-2.580300	-0.302887
H	-1.248796	2.126757	1.475027
H	-1.985603	2.924191	0.087091
H	0.555792	2.763960	-0.004861
H	-0.253088	2.073515	-1.422158
H	5.429678	-1.140025	0.100896
H	5.140318	1.305560	-0.177223
H	2.880109	2.320641	-0.281514
H	3.460579	-2.642392	0.272534
H	0.446466	-2.607418	0.274498

1q (O-State)

ΔG = -556.832140 hartree

C	0.424218	-0.364898	-0.117608
C	1.018630	-1.652594	-0.253058
C	2.373381	-1.853539	-0.033047
C	3.221986	-0.791356	0.325029
C	2.683786	0.483391	0.376047
C	1.319099	0.742929	0.098154
C	-3.040688	0.189672	0.857295
C	-1.689734	0.836482	0.525527
N	-0.935393	-0.233274	-0.161481
C	-1.812637	-1.383122	-0.458375
C	-3.225547	-0.820839	-0.283985
C	1.026766	2.151804	-0.156323
O	0.087551	2.622257	-0.802615
H	0.399882	-2.507615	-0.492668
H	2.772910	-2.860289	-0.120225
H	4.274730	-0.961326	0.523886

H	3.329596	1.333999	0.581310
H	-3.843295	0.929754	0.915383
H	-2.990250	-0.334450	1.818811
H	-1.138995	1.167721	1.413429
H	-1.807285	1.704295	-0.129207
H	-1.635668	-2.199541	0.257052
H	-1.619324	-1.766392	-1.465496
H	-3.951781	-1.605797	-0.057825
H	-3.547820	-0.309983	-1.198517
H	1.809066	2.836909	0.227415

1q (H-State)

ΔG = -556.825058 hartree

C	0.257063	-0.448349	-0.128011
C	0.655028	-1.818608	-0.108993
C	1.973061	-2.193029	0.094989
C	2.983726	-1.232929	0.284578
C	2.636707	0.103231	0.205879
C	1.309328	0.529334	-0.040007
C	-3.104848	0.703565	0.697701
C	-1.703535	1.118761	0.235946
N	-1.078799	-0.145569	-0.209366
C	-2.099904	-1.208177	-0.333576
C	-3.433394	-0.460481	-0.246865
C	1.131802	1.952992	-0.338618
O	1.989787	2.821242	-0.148384
H	-0.087845	-2.595352	-0.230084
H	2.218212	-3.251473	0.116076
H	4.012396	-1.533719	0.453597
H	3.394344	0.876406	0.283841
H	-3.817111	1.530385	0.635019
H	-3.074938	0.354019	1.736040
H	-1.105156	1.578171	1.030322
H	-1.781801	1.833672	-0.591946
H	-2.009518	-1.925478	0.494528
H	-1.976263	-1.756626	-1.273037
H	-4.236700	-1.104877	0.119123
H	-3.723621	-0.080029	-1.232833
H	0.191108	2.246084	-0.826151

1q (A, O-State)

ΔG = -556.749558 hartree

C	-0.580338	-0.313990	-0.004708
C	-1.196136	-1.560374	0.044954
C	-2.596752	-1.653917	0.071877
C	-3.368552	-0.472439	0.049689
C	-2.766798	0.775224	-0.002908
C	-1.345626	0.897716	-0.038161
C	3.067788	-0.075620	0.740357
C	1.629629	-0.258579	1.226564
N	0.841151	-0.185417	-0.011789
C	1.658267	-0.537016	-1.189318
C	3.067797	-0.794309	-0.624813
C	-0.629009	2.113654	-0.113239
O	0.671636	2.139639	-0.160280
H	-0.587107	-2.460279	0.068601
H	-3.075388	-2.626789	0.111840
H	-4.453001	-0.540819	0.070962
H	-3.374700	1.675845	-0.025083
H	3.794954	-0.495299	1.439453
H	3.280578	0.990360	0.615946
H	1.279683	0.499413	1.929967
H	1.478037	-1.250604	1.679520
H	1.626512	0.303591	-1.890009
H	1.221428	-1.409600	-1.686836
H	3.847933	-0.427453	-1.295711
H	3.222928	-1.869068	-0.484535
H	-1.164626	3.069403	-0.131110

1q (A, H-State)

ΔG = -556.742423 hartree

C	0.265300	-0.473649	-0.105713
C	0.637697	-1.839667	-0.115048
C	1.958738	-2.243157	0.066193
C	2.939781	-1.248138	0.308063
C	2.626637	0.103518	0.271681
C	1.315864	0.569722	-0.042381
C	-3.121565	0.652749	0.752437
C	-1.688031	1.079381	0.419097
N	-1.070577	-0.150925	-0.138881
C	-2.119854	-1.147228	-0.455984
C	-3.432068	-0.366417	-0.351080
C	1.135475	1.950109	-0.381579
O	2.059790	2.824139	-0.260929
H	-0.130484	-2.598464	-0.194656
H	2.214576	-3.295976	0.085051
H	3.965157	-1.547628	0.510286
H	3.403639	0.849474	0.391778
H	-3.799312	1.509313	0.758665
H	-3.158221	0.176254	1.738022
H	-1.112303	1.437774	1.272108
H	-1.702314	1.858866	-0.350039
H	-2.092456	-1.949540	0.291894
H	-1.926950	-1.583852	-1.439110
H	-4.270448	-1.023897	-0.111607
H	-3.652876	0.142469	-1.295363
H	0.169865	2.265243	-0.791542

1q (TS1)

ΔG = -556.740586 hartree

C	0.547820	-0.416191	0.138613
C	1.262587	-1.613174	0.229008
C	2.659999	-1.646261	0.160753
C	3.349322	-0.432931	-0.018788
C	2.655990	0.760672	-0.129334
C	1.226207	0.850507	-0.051582
C	-3.126746	0.029607	0.568119
C	-1.681933	0.464722	0.801506

N	-0.866360	-0.492462	0.167579
C	-1.645287	-1.479947	-0.599556
C	-3.028261	-0.821841	-0.713419
C	0.676811	2.151795	-0.269928
O	-0.561698	2.584052	-0.192284
H	0.710829	-2.539155	0.360673
H	3.191208	-2.588206	0.243778
H	4.434326	-0.425966	-0.077541
H	3.208504	1.682426	-0.294261
H	-3.804638	0.880422	0.463002
H	-3.479849	-0.575556	1.412648
H	-1.376808	0.661813	1.837630
H	-1.366326	1.523235	0.280285
H	-1.696165	-2.420669	-0.033592
H	-1.158564	-1.681060	-1.557006
H	-3.827254	-1.561576	-0.799393
H	-3.059556	-0.178531	-1.598857
H	1.403342	2.915898	-0.564501

1q (B)

ΔG = -556.749064 hartree

C	0.526380	-0.395115	0.081943
C	1.189919	-1.618921	0.186012
C	2.588193	-1.710448	0.159222
C	3.345108	-0.534663	0.040259
C	2.709753	0.692642	-0.061732
C	1.282434	0.827144	-0.058876
C	-3.127663	-0.068219	0.722539
C	-1.695213	0.366860	0.910598
N	-0.890888	-0.391727	0.058670
C	-1.687210	-1.321547	-0.761742
C	-3.100384	-0.724363	-0.675832
C	0.789363	2.141503	-0.252595
O	-0.485641	2.592391	-0.246553
H	0.597893	-2.523192	0.288531
H	3.071155	-2.679216	0.237053
H	4.430263	-0.580492	0.021622
H	3.305040	1.595489	-0.170350
H	-3.842088	0.758609	0.789893
H	-3.416534	-0.805272	1.488778
H	-1.283367	0.624324	1.886637
H	-1.109508	1.896646	0.116439
H	-1.662454	-2.333454	-0.331599
H	-1.287764	-1.372011	-1.778688
H	-3.876638	-1.481454	-0.810416
H	-3.227900	0.039198	-1.450600
H	1.499166	2.934551	-0.464347

1q (C)

ΔG = -556.841860 hartree

C	-0.577515	-0.660405	0.254343
C	-1.518274	-1.664871	-0.021488
C	-2.849480	-1.287640	-0.231905
C	-3.247592	0.056185	-0.174630
C	-2.295423	1.055208	0.075907
C	-0.966338	0.693595	0.280379
C	2.603591	0.499546	-0.259461
C	1.399874	0.531989	0.691668
N	0.774147	-0.815633	0.534024
C	1.641952	-1.721083	-0.242251
C	2.996860	-0.990012	-0.258641
C	0.252853	1.574700	0.452712
O	0.449275	2.469416	-0.655929
H	1.748652	0.636209	1.726374
H	0.177430	2.243042	1.314152
H	-1.225555	-2.709751	-0.059106
H	-3.589466	-2.056345	-0.438195
H	-4.288503	0.321928	-0.331336
H	-2.588384	2.102033	0.093420
H	3.413490	1.158101	0.065697
H	2.306280	0.808969	-1.267278
H	0.263703	1.990419	-1.476720
H	1.249473	-1.847969	-1.262605
H	1.705536	-2.710994	0.221117
H	3.604996	-1.272816	-1.122336
H	3.566075	-1.231995	0.646285

1q (TS2)

ΔG = -556.726991 hartree

C	-0.460804	-0.437560	0.007156
C	-0.926594	-1.733240	0.040417
C	-2.323577	-1.953996	0.050211
C	-3.204850	-0.854629	0.025251
C	-2.744974	0.457582	-0.007601
C	-1.335940	0.698877	-0.017640
C	3.210796	-0.504277	-0.695103
C	1.763095	-0.376224	-1.215260
N	0.934654	-0.029226	-0.008141
C	1.757856	-0.292682	1.208947
C	3.170120	0.052982	0.743604
C	-0.619927	1.914746	-0.048329
O	-0.864641	3.133460	-0.078584
H	-0.238325	-2.573711	0.057181
H	-2.710266	-2.967159	0.075676
H	-4.276850	-1.036183	0.031339
H	-3.439957	1.290769	-0.027017
H	3.918499	0.033517	-1.329926
H	3.507960	-1.557069	-0.681453
H	1.386797	-1.305880	-1.647638
H	1.635343	0.420567	-1.952848
H	1.667276	-1.351828	1.476825
H	1.381378	0.314774	2.035124
H	3.933104	-0.387589	1.389502
H	3.308963	1.139539	0.746069
H	0.589425	1.287683	-0.037088

1q (D)

ΔG = -556.733188 hartree

C	-0.390802	-0.396652	0.000046
C	-0.699307	-1.741884	0.025528
C	-2.048779	-2.146114	0.038800
C	-3.060516	-1.159185	0.025242
C	-2.755375	0.190486	0.000097
C	-1.385420	0.639977	-0.013656
C	3.319239	-0.147676	-0.734945
C	1.857946	-0.309102	-1.207022
N	1.003101	0.084261	-0.010317
C	1.849957	-0.231119	1.204679
C	3.242038	0.217863	0.771690
C	-0.996913	1.996405	-0.039520
O	-1.637705	3.061650	-0.058179
H	0.086413	-2.492316	0.034059
H	-2.300024	-3.200801	0.058212
H	-4.103632	-1.466777	0.034650
H	-3.544434	0.935945	-0.009972
H	3.838644	0.625983	-1.303814
H	3.857652	-1.086630	-0.882817
H	1.609308	-1.340872	-1.451825
H	1.573888	0.331197	-2.042562
H	1.790930	-1.307994	1.372172
H	1.434726	0.295157	2.064791
H	4.018848	-0.271916	1.362326
H	3.346369	1.298187	0.913120
H	0.878830	1.119808	-0.036314

1q (TS3)

ΔG = -556.729460 hartree

C	-0.477982	-0.744806	0.000526
C	-1.190769	-1.948349	0.000759
C	-2.588136	-1.882512	0.000457
C	-3.215110	-0.629993	-0.000072
C	-2.439345	0.539139	-0.000293
C	-1.037606	0.527095	0.000005
C	3.186117	-0.139080	0.779158
C	1.709355	-0.214378	1.190254
N	1.020379	-0.854922	0.000667
C	1.709466	-0.216536	-1.189848
C	3.186320	-0.146333	-0.779730
C	-0.207151	2.642574	-0.000764
O	-1.172625	3.310115	-0.001190
H	-0.688775	-2.915028	0.001147
H	-3.173761	-2.797089	0.000628
H	-4.302201	-0.573077	-0.000306
H	-2.950219	1.507194	-0.000726
H	3.741065	-0.997304	1.166917
H	3.645988	0.762473	1.189349
H	1.248856	0.768576	1.290599
H	1.504883	-0.812405	2.078762
H	1.251963	0.767917	-1.289671
H	1.502266	-0.813933	-2.078162
H	3.652379	0.747987	-1.198669
H	3.735298	-1.012179	-1.159157
H	1.259649	-1.850527	0.001430

1q (E)

ΔG = -443.416469 hartree

C	0.649930	-0.191665	-0.016718
C	1.146903	1.113204	0.080222
C	2.534588	1.273812	0.095449
C	3.355333	0.140029	0.013448
C	2.785537	-1.138206	-0.082512
C	1.386562	-1.374181	-0.102451
C	-3.084627	0.163856	-0.755124
C	-1.605784	0.202261	-1.189407
N	-0.836198	-0.397369	-0.031135
C	-1.609001	0.024500	1.195871
C	-3.070196	-0.135846	0.772131
H	0.500338	1.986098	0.142509
H	2.965763	2.268016	0.170007
H	4.437439	0.260478	0.024720
H	3.472210	-1.985048	-0.143772
H	-3.634187	-0.608683	-1.297490
H	-3.560772	1.122196	-0.973861
H	-1.238800	1.220946	-1.317413
H	-1.374732	-0.371819	-2.086999
H	-1.346575	1.064621	1.398265
H	-1.297741	-0.595221	2.037357
H	-3.718035	0.537274	1.337523
H	-3.406659	-1.158622	0.965230
H	-0.880338	-1.425236	-0.103579

1q (TS4)

ΔG = -443.402328 hartree

C	0.618990	0.027845	-0.000056
C	1.287329	1.234211	0.181108
C	2.688767	1.166769	0.175217
C	3.339761	-0.063151	-0.005514
C	2.611820	-1.253638	-0.184590
C	1.205399	-1.229970	-0.186459
C	-3.095220	0.261848	-0.702211
C	-1.622036	0.319019	-1.173282
N	-0.821899	-0.249498	-0.041474
C	-1.626977	-0.056719	1.196077
C	-3.047590	-0.355980	0.717070
H	0.772451	2.181504	0.320566
H	3.272335	2.072940	0.311694
H	4.427563	-0.088599	-0.006565
H	3.160573	-2.184708	-0.321374
H	-3.716061	-0.328463	-1.380472
H	-3.513795	1.271569	-0.668232
H	-1.295069	1.345276	-1.363990
H	-1.418790	-0.276954	-2.067027
H	-1.523678	0.978265	1.544578
H	-1.256285	-0.729785	1.973306
H	-3.804777	0.061565	1.385155
H	-3.198550	-1.439595	0.671553
H	-0.314079	-1.417924	-0.213022

2q

ΔG = -443.496625 hartree

C	-0.527263	0.000018	-0.000361
C	-1.263328	-1.210313	0.088301
C	-2.658148	-1.199241	0.086301
C	-3.375070	0.000004	0.000139
C	-2.658194	1.199176	-0.086075
C	3.078126	0.705885	0.304275
C	1.660018	1.218925	0.013316
N	0.846469	-0.000029	-0.000655
C	1.660027	-1.218872	-0.012799
C	3.078082	-0.705918	-0.304243
H	-0.741736	-2.157431	0.167212
H	-3.189231	-2.145195	0.157403
H	-4.460634	-0.000059	0.000244
H	-3.189204	2.145198	-0.157000
H	3.238287	0.649819	1.387128
H	3.848471	1.357083	-0.117387
H	1.610995	1.739096	-0.956340
H	1.308256	1.918329	0.781277
H	1.308490	-1.919357	-0.779863
H	1.611111	-1.737756	0.957590
H	3.237783	-0.649902	-1.387165
H	3.848530	-1.357148	0.117174
C	-1.263326	1.210334	-0.088541
H	-0.741940	2.157542	-0.167571

3q

ΔG = -480.434320 hartree

C	0.540291	-0.420480	0.013549
C	1.455304	-1.481355	0.016400
C	2.813221	-1.162994	-0.005327
C	3.247953	0.181008	-0.031472
C	2.335570	1.234855	-0.034382
C	0.956476	0.951522	-0.008153
C	-2.798749	0.876331	0.110608
C	-1.298677	0.887683	0.027959
N	-0.835456	-0.412779	0.019577
C	-1.887379	-1.421021	0.122699
C	-3.148194	-0.598117	-0.243391
C	-0.235837	1.762724	0.003405
H	-0.287102	2.842826	-0.005673
H	1.121661	-2.514657	0.037186
H	3.548461	-1.962609	-0.001383
H	4.313275	0.393858	-0.048102
H	2.684567	2.264207	-0.052808
H	-3.271727	1.591723	-0.567718
H	-3.126964	1.125970	1.127921
H	-1.934973	-1.820534	1.143829
H	-1.708125	-2.251764	-0.565165
H	-4.035551	-0.957940	0.281864
H	-3.335212	-0.682556	-1.318367

H_2O

ΔG = -76.438547 hartree

O	0.000000	0.000000	0.117718
H	0.000000	0.766916	-0.470872
H	0.000000	-0.766916	-0.470872

CO

ΔG = -113.332229 hartree

C	0.000000	0.000000	-0.649817
O	0.000000	0.000000	0.487363