

# Supporting Information

For

## Metal-free C-H methylation and acetylation of Heteroarenes with PEG-400.

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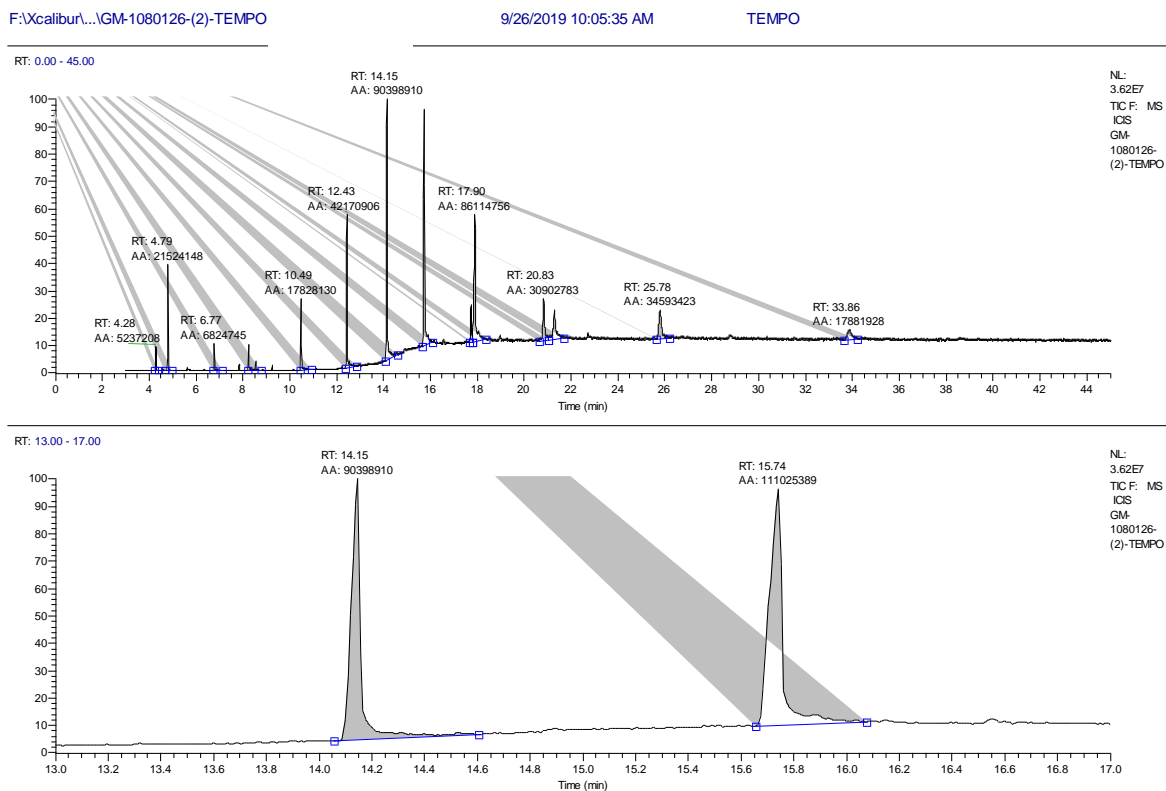
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## (1) General Information

$^1\text{H}$ ,  $^{13}\text{C}$  and DEPT NMR spectra were recorded on a 400 MHz Varian Unity Plus or Varian Mercury plus spectrometer. The chemical shift ( $\delta$ ) values are reported in parts per million (ppm), and the coupling constants ( $J$ ) are given in Hz. The spectra were recorded using  $\text{CDCl}_3$  as a solvent.  $^1\text{H}$  NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm).  $^{13}\text{C}$  NMR was referenced to  $\text{CDCl}_3$  (77.0 ppm) or  $\text{DMSO-d}_6$  (39.51 ppm). The abbreviations used are as follows: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublet; ddd, doublet of doublet of doublet; dt, doublet of triplets; td, triplet of doublet; m, multiplet. Mass spectra and high resolution mass spectra (HRMS) were measured using the ESI (FT-MS solarix) at National Sun Yat-Sen University, Kaohsiung, Taiwan. Melting points were determined on an EZ-Melt (Automated melting point apparatus). All products reported showed  $^1\text{H}$  NMR spectra in agreement with the assigned structures. Reaction progress and product mixtures were routinely monitored by TLC using Merck TLC aluminum sheets (silica gel 60 F254). Column chromatography was carried out with 230–400 mesh silica gel 60 (Merck) and a mixture of hexane/ethyl acetate or hexane as an eluent. Preparative TLC was run on a Merck TLC aluminum sheets (silica gel 60 F254).

## (2) Mechanistic studies:



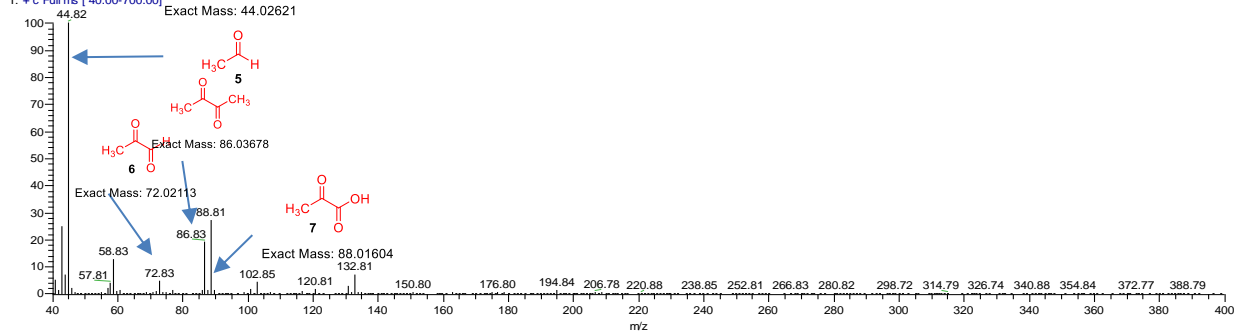
**Fig S1:** GC-MS with different retention time generated from PEG-400 in presence of oxidant & radical scavenger.

GM-1080126-(2)-TEMPO #908-911 RT: 12.41-12.4

L: 5.38E6

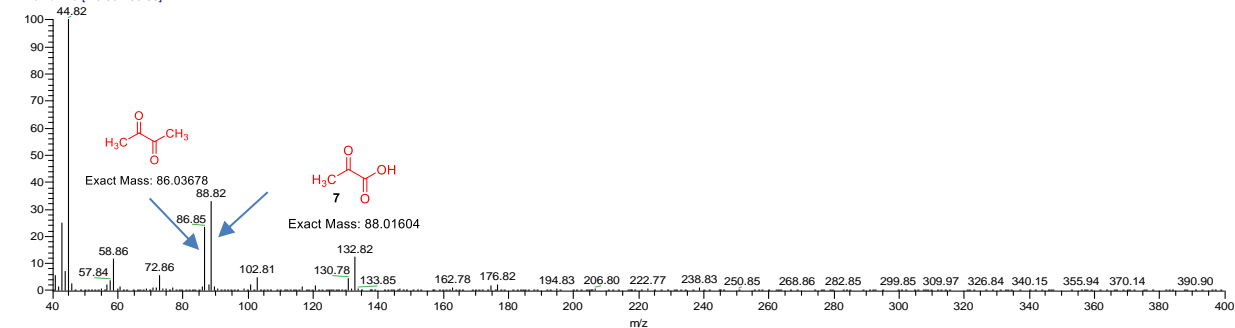
T: + c Full ms [ 40.00-700.00]

Exact Mass: 44.02621



GM-1080126-(2)-TEMPO #1073-1077 RT: 14.12-14.16 AV: 5 SB: 11 14.20-14.30 NL: 8.18E6

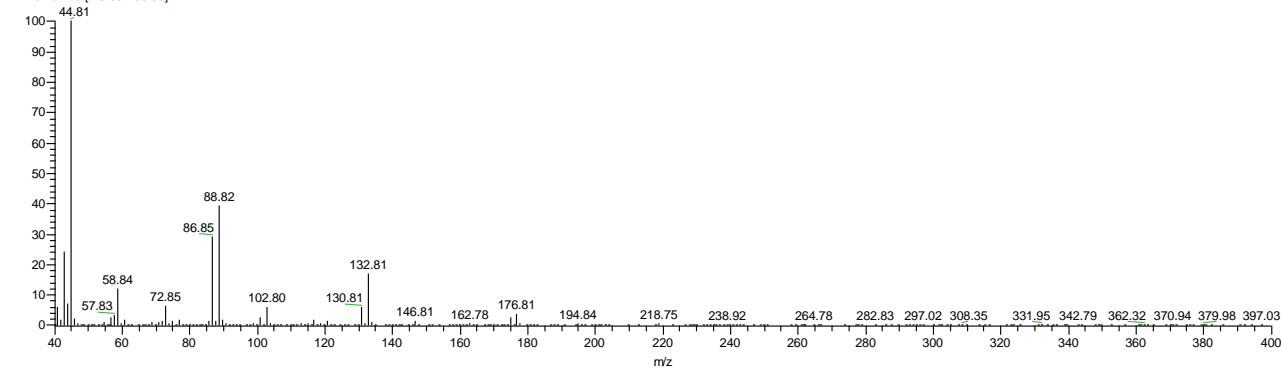
T: + c Full ms [ 40.00-700.00]



GM-1080126-(2)-TEMPO #1229-1234 RT: 15.70-16

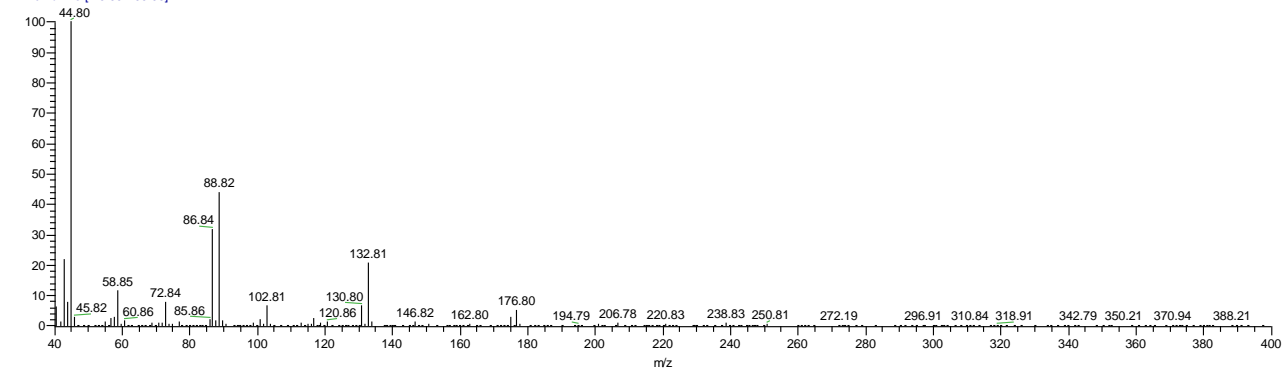
I: 90 NL: 7.28E6

T: + c Full ms [ 40.00-700.00]

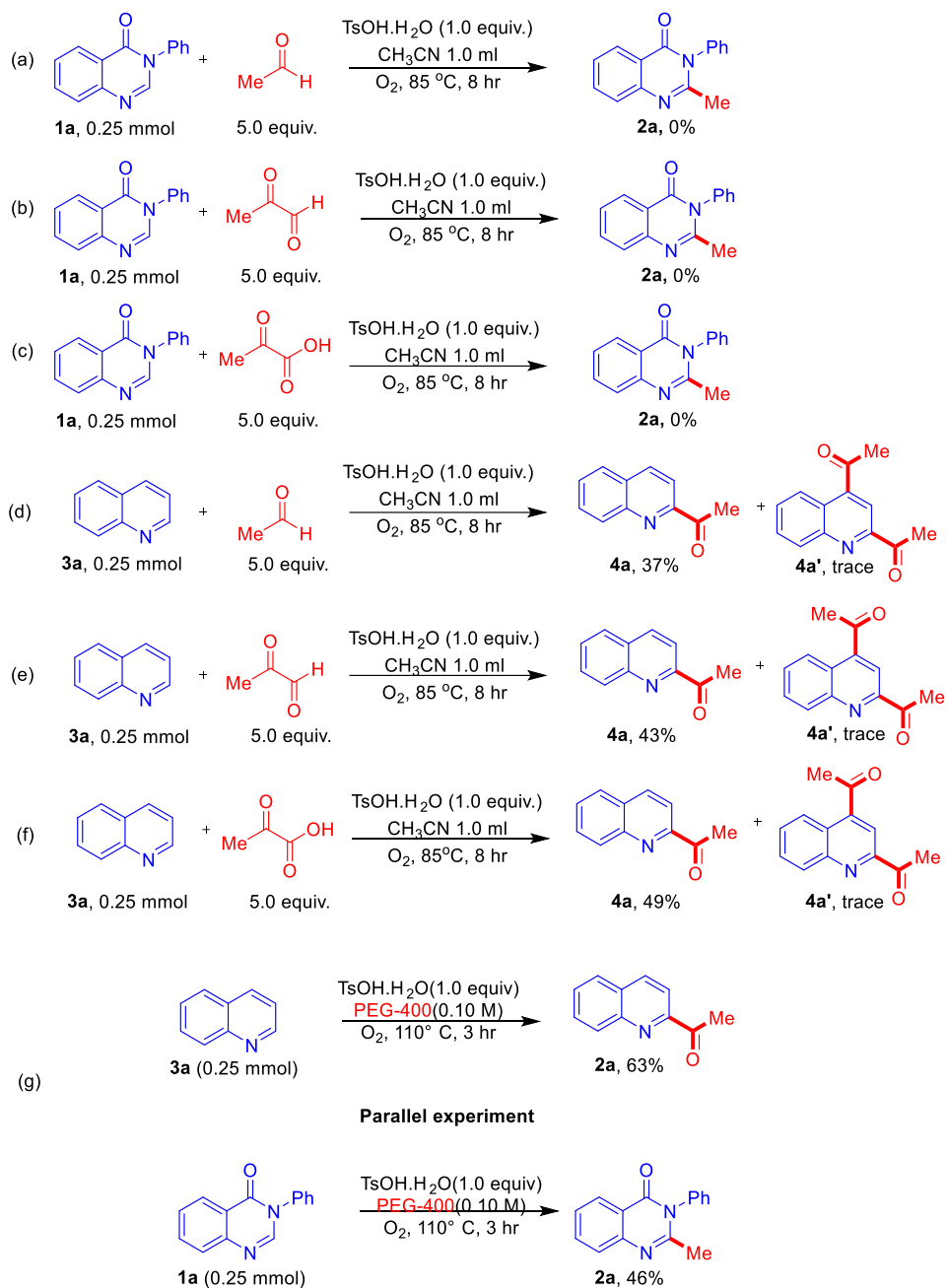


GM-1080126-(2)-TEMPO #1443-1449 RT: 17.86-17.92 AV: 7 SB: 11 18.00-18.10 NL: 3.65E6

T: + c Full ms [ 40.00-700.00]

**Fig S2:** GC-MS observed fragments acetaldehyde, 2-oxopropanal, 2-oxopropanoic acid from PEG-400.

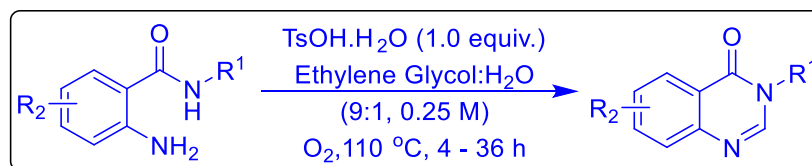
## Scheme S1 Control Experiments:



S

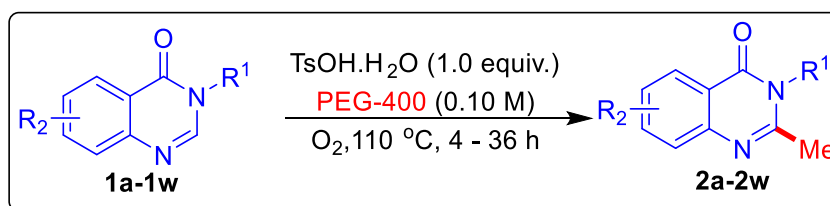
## (3) Experimental Procedures

### (i) General Experimental Procedure for the synthesis of quinazolinone.<sup>1</sup>



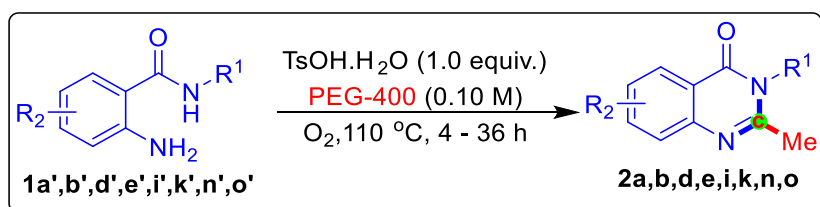
To an oven dried sealed tube was charged with **1a'-y'** (0.5 mmol), ethylene glycol (EG): H<sub>2</sub>O (9:1) (0.25 M) and TsOH. H<sub>2</sub>O (0.5 mmol) and allowed to stir at 110° C until the completion of reaction (4 ~ 36 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 20 mL of water. The water layer was extracted with (3X20 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X20 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from hexane to 20% ethyl acetate/hexane to afford pure quinazolin-4(3*H*)-ones **1a-1y** in 75%-90% yields.

**(ii) General Experimental Procedure (B) and Spectral Characterization for the Synthesis of 2-methyl-3-phenylquinazolin-4(3*H*)-one with PEG-400 as “-CH<sub>3</sub>-” Source**



To an oven dried sealed tube was charged with **1a-1w** (0.25 mmol), PEG-400 (0.10 M) and TsOH. H<sub>2</sub>O (0.25 mmol) and allowed to stir at 110° C until the completion of reaction (4 ~ 36 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X20 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X20 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from hexane to 15-25% ethyl acetate/hexane to afford pure 2-methyl-3-arylquinazolin-4(3*H*)-one **2a-2w** in 66%-82% yields.

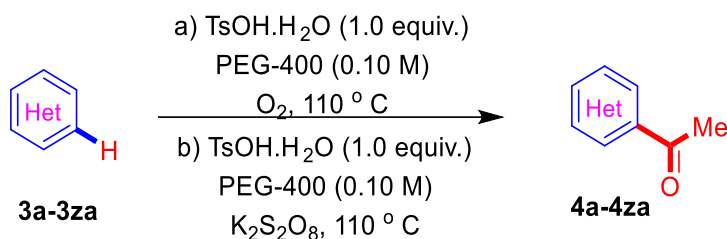
**(iii) General Experimental Procedure (A) and Spectral Characterization for the Synthesis of 2-methyl-3-phenylquinazolin-4(3*H*)-one with PEG-400 as “-CH- & -CH<sub>3</sub>-” Source**



To an oven dried sealed tube was charged with **1a',b',d',e',i',k',n',o'** (0.25 mmol), PEG-400 (0.10 M) and TsOH. H<sub>2</sub>O (0.15 mmol) and allowed to stir at 110° C until the completion of reaction (4 ~ 36 h) by TLC.

After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X20 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X20 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from hexane to 15-25% ethyl acetate/hexane to afford pure 2-methyl-3-arylquinazolin-4(3*H*)-one **2a,b,d,e,i,k,n,o** in 67%-81% yields.

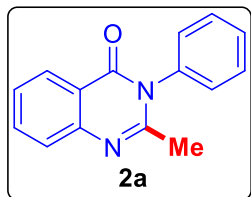
#### (iv) General Experimental Procedure (C) and Spectral Characterization for the Synthesis of heteroaryl acetylation with PEG-400 as “CH<sub>3</sub>CO” Source



To an oven dried sealed tube was charged with **3a-3za** (0.25 mmol), PEG-400 (0.10 M) and TsOH. H<sub>2</sub>O (0.25 mmol) and allowed to stir at 110° C until the completion of reaction (4 ~ 24 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 5.0 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from hexane to 10- 20% ethyl acetate/hexane to afford pure heteroaryl acetylation **4a-4za** in 48%-85% yields

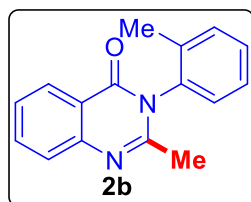
#### (4) Spectral Characterization

**2-methyl-3-phenylquinazolin-4(3*H*)-one (2a):**<sup>2</sup> The title compound was prepared according to the general



procedure B on a 0.25 mmol scale to obtain as a white solid (46 mg, yield = 80%); Mp.144-146 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.27 (ddd, *J* = 8.0, 1.6, 0.4 Hz, 1H), 7.79-7.75 (m, 1H), 7.69 (dd, *J* = 8.4, 0.8, 1H), 7.58-7.54 (m, 2H), 7.53-7.51 (m, 1H), 7.47 (ddd, *J* = 9.2, 2.0, 0.8 Hz, 1H), 7.28-7.26 (m, 2H), 2.25 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.22, 154.16, 147.41, 137.70, 134.54, 129.95, 129.24, 127.97, 127.00, 126.71, 126.59, 120.72, 77.31, 76.99, 76.67, 24.35.

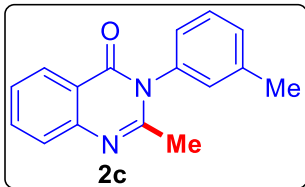
**2-methyl-3-(*o*-tolyl)quinazolin-4(3*H*)-one (2b):**<sup>2</sup> The title compound was prepared according to the general



procedure B on a 0.25 mmol scale to obtain as a white solid (44 mg, yield = 71 %); Mp.

117-119 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.29 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.78 (ddd, *J* = 8.4, 7.2, 1.6 Hz, 1H), 7.70 (d, *J* = 8.8, 1H), 7.50 - 7.46 (m, 1H), 7.42-7.36 (m, 3H), 7.17 (d, 7.2 Hz, 1H), 2.19 (s, 3H), 2.13 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 161.63, 154.30, 147.61, 136.76, 135.32, 134.57, 131.51, 129.56, 127.88, 127.62, 127.09, 126.74, 126.57, 120.70, 23.85, 17.37.

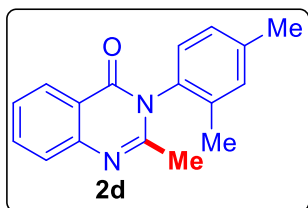
**2-methyl-3-(*m*-tolyl)quinazolin-4(3*H*)-one (2c):**<sup>3</sup> The title compound was prepared according to the general



procedure B on a 0.25 mmol scale to obtain as a white solid (41 mg, yield = 66 %); Mp. 126-128 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.27 (ddd, *J* = 8.0, 1.6, 0.4 Hz, 1H), 7.78-7.74 (m, 1H), 7.68 (ddd, *J* = 8.0, 1.2, 0.4, 1H), 7.48-7.41 (m, 2H), 7.32-7.29 (m, 1H), 7.08-7.04 (m, 2H), 2.42 (s, 3H), 2.25 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100

MHz) δ 162.28, 154.29, 147.43, 140.11, 137.60, 134.49, 130.05, 129.73, 128.42, 127.01, 126.68, 126.54, 124.87, 120.74, 24.31, 21.31.

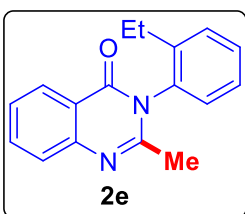
**3-(2,4-dimethylphenyl)-2-methylquinazolin-4(3*H*)-one (2d):**<sup>4</sup> The title compound was prepared according



to the general procedure B on a 0.25 mmol scale to obtain as a white solid (48 mg, yield = 73 %); Mp. 133-135 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.29 (ddd, *J* = 8.0, 1.6, 0.4 Hz 1H), 7.79-7.75 (m, 1H), 7.69 (dd, *J* = 7.6, 0.8 Hz 1H), 7.47 (ddd, *J* = 8.0, 3.2, 1.2 Hz, 1H), 7.18 (ddd, *J* = 7.6, 1.2, 0.4 Hz, 2H), 7.03 (d, *J* = 8.0 Hz 1H),

2.40 (s, 3H), 2.19 (s, 3H), 2.08 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 161.76, 154.62, 147.58, 139.52, 134.83, 134.51, 134.09, 132.22, 128.30, 127.54, 127.12, 126.68, 126.51, 120.71, 77.31, 76.99, 76.68, 23.84, 21.16, 17.29.

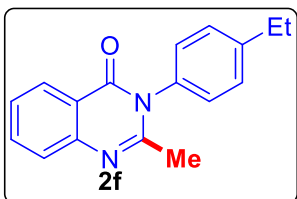
**3-(2-ethylphenyl)-2-methylquinazolin-4(3*H*)-one (2e):**<sup>5</sup> The title compound was prepared according to the



general procedure B on a 0.25 mmol scale to obtain as a white solid (45 mg, yield = 69 %); Mp. 88-90 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.29 (ddd, *J* = 8.0, 1.2, 0.4 Hz, 1H), 7.80-7.76 (m, 1H), 7.71-7.68 (m, 1H), 7.49-7.45 (m, 3H), 7.40-7.35 (m, 1H), 7.15-7.13 (m, 1H), 2.46-2.39 (m, 2H), 2.19 (s, 3H), 1.18 (t, *J* = 7.6, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100

MHz) δ 161.89, 154.50, 147.59, 140.69, 136.18, 134.54, 129.72, 129.46, 128.00, 127.46, 127.11, 126.73, 126.56, 120.71, 77.31, 76.99, 76.67, 24.01, 23.56, 13.59.

**3-(4-ethylphenyl)-2-methylquinazolin-4(3*H*)-one (2f):**<sup>6</sup> The title compound was prepared according to the

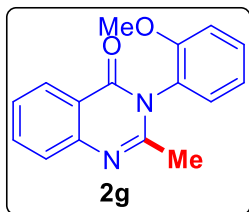


general procedure B on a 0.25 mmol scale to obtain as a white solid (45 mg, yield = 68 %); Mp. 145-147 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.27 (ddd, *J* = 8.0, 1.6, 0.4 Hz, 1H), 7.78-7.73 (m, 1H), 7.67 (dd, *J* = 8.4, 0.8, 1H), 7.46 (ddd, *J* = 8.4, 7.2, 1.2, 1H), 7.39-7.35 (m, 2H), 7.18-7.15 (m, 2H), 2.75 (q, *J* = 8.4, 2H), 2.25 (s, 3H), 1.30



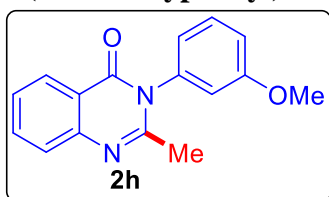
(t,  $J = 8.4$ , 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  162.33, 154.50, 147.41, 145.40, 135.15, 134.46, 129.37, 127.66, 127.03, 126.66, 126.51, 120, 28.51, 24.37, 15.23.

**3-(2-methoxyphenyl)-2-methylquinazolin-4(3H)-one (2g):**<sup>3</sup> The title compound was prepared according to



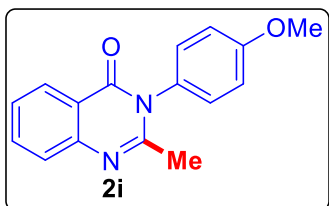
the general procedure B on a 0.25 mmol scale to obtain as a white solid (47 mg, yield = 70 %); Mp. 126-128 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.28 (ddd,  $J = 8.0$ , 1.6, 0.4 Hz 1H), 7.76 (ddd,  $J = 8.0$ , 6.8, 1.2 Hz 1H), 7.68 (ddd,  $J = 8.4$ , 1.2, 0.8 Hz 1H), 7.50-7.43(m, 2H), 7.21(dd,  $J = 7.6$ , 1.6 Hz 1H), 7.11 (ddd,  $J = 8.8$ , 7.6, 1.2 Hz 2H), 3.79 (s, 3H), 2.22 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  161.92, 154.98, 154.50, 147.59, 134.37, 130.82, 129.23, 127.05, 126.60, 126.32, 126.12, 121.32, 120.78, 112.17, 55.69, 23.45.

**3-(3-methoxyphenyl)-2-methylquinazolin-4(3H)-one (2h):**<sup>7</sup> The title compound was prepared according to



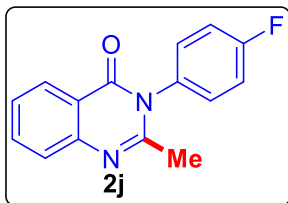
the general procedure B on a 0.25 mmol scale to obtain as a white solid (48 mg, yield = 71 %); Mp. 152-154 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.28 (dd,  $J = 8.0$ , 1.2 Hz 1H), 7.77 (ddd,  $J = 8.4$ , 7.2, 1.6 Hz 1H), 7.68 (dd,  $J = 8.0$ , 0.4 Hz 1H), 7.48-7.43(m, 2H), 7.05(ddd,  $J = 8.4$ , 2.4, 0.8 Hz 1H), 6.86 (ddd,  $J = 7.6$ , 1.6, 0.8 Hz 1H), 6.80 (t,  $J = 2.0$  Hz 1H), 3.84 (s, 3H), 2.28 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  162.16, 160.78, 154.19, 147.42, 138.74, 134.57, 130.68, 127.03, 126.72, 126.61, 120.74, 120.09, 115.04, 113.70, , 55.47, 24.14.

**3-(4-methoxyphenyl)-2-methylquinazolin-4(3H)-one (2i):**<sup>2</sup> The title compound was prepared according to



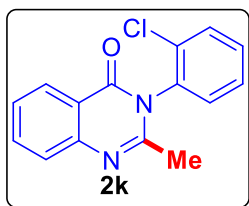
the general procedure B on a 0.25 mmol scale to obtain as a white solid (49 mg, yield = 73 %); Mp. 167-169 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.27 (ddd,  $J = 8.0$ , 1.2, 0.4 Hz, 1H), 7.78-7.75 (m, 1H), 7.67 (dd,  $J = 8.4$ , 0.8, 1H), 7.46 (ddd,  $J = 8.0$ , 7.2, 1.2, 1H), 7.18-7.15 (m, 2H), 7.07-7.04 (m, 2H), 3.87 (s, 3H), 2.26 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  162.49, 159.90, 154.75, 147.39, 134.49, 130.20, 128.94, 127.04, 126.67, 126.54, 120.73, 115.17, 55.51, 24.37.

**3-(4-fluorophenyl)-2-methylquinazolin-4(3H)-one (2j):**<sup>2</sup> The title compound was prepared according to the



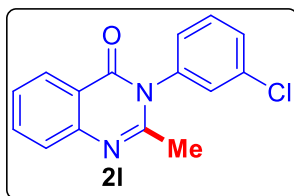
general procedure B on a 0.25 mmol scale to obtain as a white solid (39 mg, yield = 62 %); Mp. 132-134°C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.26 (ddd,  $J = 8.0$ , 1.6, 0.4 Hz, 1H), 7.79-7.75 (m, 1H), 7.68-7.63 (m, 1H), 7.47 (ddd,  $J = 8.4$ , 7.2, 1.2, 1H), 7.26 (d,  $J = 0.8$ , 2H), 7.24 (s, 2H), 2.24 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  13C NMR (101 MHz,  $\text{cdCl}_3$ )  $\delta$  163.95, 161.47(d,  $J_F = 280$  Hz), 153.97, 147.36, 145.80, 134.70, 129.90 (d,  $J_F = 22.9$  Hz), 129.82, 127.02, 126.81, 126.76 (d,  $J_F = 9$  Hz), 120.62, 117.18 (d,  $J_F = 5.5$  Hz), 116.95, 24.39.

**3-(2-chlorophenyl)-2-methylquinazolin-4(3H)-one (2k):**<sup>2</sup> The title compound was prepared according to the



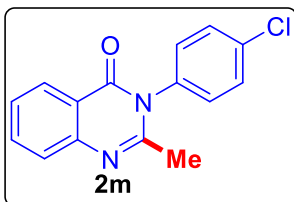
general procedure B on a 0.25 mmol scale to obtain as a white solid (50 mg, yield = 74 %); Mp. 124-126 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.29-8.27 (m, 1H), 7.79 (ddd, *J* = 8.8, 7.2, 1.6 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.63-7.61 (m, 1H), 7.50-7.45 (m, 3H), 7.36 -7.33 (m, 1H), 2.23 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 161.45, 153.66, 147.49, 135.41, 134.73, 132.55, 130.78, 130.73, 129.81, 128.35, 127.11, 126.85, 126.70, 120.54, 23.51.

**3-(3-chlorophenyl)-2-methylquinazolin-4(3H)-one (2l):**<sup>2</sup> The title compound was prepared according to the



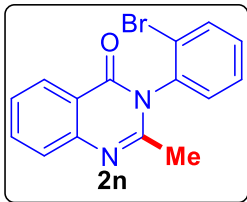
general procedure B on a 0.25 mmol scale to obtain as a white solid (46 mg, yield = 68 %); Mp. 129-131 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.27 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.79 (ddd, *J* = 8.4, 7.2, 1.6 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.51-7.46 (m, 3H), 7.31 (s, 1H), 7.20 -7.17 (m, 1H), 2.27 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.07, 153.51, 147.35, 138.79, 135.61, 134.79, 130.93, 129.70, 128.55, 127.04, 126.87, 126.85, 126.47, 120.59, 24.33.

**3-(4-chlorophenyl)-2-methylquinazolin-4(3H)-one (2m):**<sup>2</sup> The title compound was prepared according to



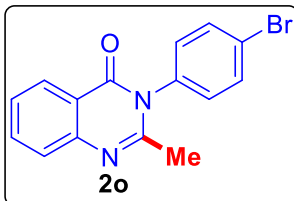
the general procedure B on a 0.25 mmol scale to obtain as a white solid (51 mg, yield = 76 %); Mp. 153-155 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.26 (ddd, *J* = 8.0, 1.6, 0.4 Hz, 1H), 7.80-7.75 (m, 1H), 7.68 (dd, *J* = 8.4, 0.8, 1H), 7.55-7.52 (m, 2H), 7.48 (ddd, *J* = 8.0, 7.2, 1.2, 1H), 7.23-7.22 (m, 1H), 7.21-7.20 (m, 1H), 2.25 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.14, 153.66, 147.34, 136.15, 135.38, 134.74, 130.27, 129.45, 127.02, 126.83, 126.79, 120.56, 24.36.

**3-(2-bromophenyl)-2-methylquinazolin-4(3H)-one (2n):**<sup>8</sup> The title compound was prepared according to



the general procedure B on a 0.25 mmol scale to obtain as a white solid (53 mg, yield = 67 %); Mp. 149-151 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.29 (ddd, *J* = 8.0, 1.6, 0.8 Hz, 1H), 7.79 (ddd, *J* = 8.4, 2.0, 0.8 Hz, 2H), 7.70 (m, ddd, *J* = 7.6, 1.2, 0.8 Hz, 1H), 7.54-7.46 (m, 2H), 7.42-7.34 (m, 2H), 2.22(s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 161.42, 153.60, 147.50, 137.10, 134.76, 133.95, 130.92, 129.82, 129.08, 127.16, 126.88, 126.72, 122.87, 120.61, 23.70.

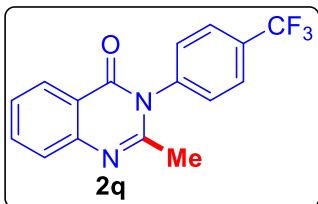
**3-(4-bromophenyl)-2-methylquinazolin-4(3H)-one (2o):**<sup>2</sup> The title compound was prepared according to the



general procedure B on a 0.25 mmol scale to obtain as a white solid (59 mg, yield = 75 %); Mp. 166-168 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.26 (ddd, *J* = 8.0, 1.6, 0.4 Hz 1H), 7.78 (ddd, *J* = 8.0, 6.8, 1.6 Hz 1H), 7.71-7.67 (m, 3H), 7.48 (ddd, *J* =

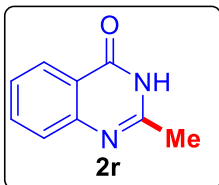
8.4, 7.2, 1.2 Hz 1H), 7.17-7.14 (m, 2H), 2.25(s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.09, 153.58, 147.32, 136.68, 134.76, 133.26, 129.76, 127.02, 126.81, 123.45, 120.54, 77.31, 76.99, 76.67, 24.36.

**2-methyl-3-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (2q):**<sup>9</sup> The title compound was prepared



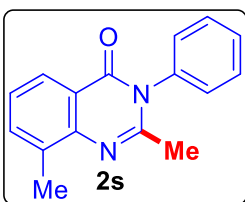
according to the general procedure B on a 0.25 mmol scale to obtain as a white solid (55 mg, yield = 72 %); Mp. 147-149 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.26 (ddd, *J* = 8.0, 1.6, 0.4 Hz, 1H), 7.85-7.83 (m, 2H), 7.79 (ddd, *J* = 8.4, 7.2, 1.6, 1H), 7.69 (ddd, *J* = 8.4, 1.2, 0.4, 1H), 7.49 (ddd, *J* = 8.0, 7.2, 1.2, 1H), 7.44-7.42 (m, 2H), 2.24 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.02, 153.10, 147.32, 140.90, 134.87, 131.76, 131.43, 128.86, 127.24 (q, *J<sub>F</sub>* = 3.6 Hz), 127.20, 127.17, 127.13, 127.01, 126.93, 126.91, 124.89, 122.18, 120.50, 24.37.

**2-methylquinazolin-4(3H)-one (2r):**<sup>8</sup> The title compound was prepared according to the general procedure B



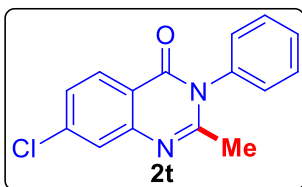
on a 0.25 mmol scale to obtain as a white solid (30 mg, yield = 75%); Mp. 230-232 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 12.15 (*bs*, 1H), 8.31-8.28 (m, 1H), 7.78 (ddd, *J* = 8.4, 2.8, 1.2 Hz 1H), 7.71-7.68 (m, 1H), 7.49 (ddd, *J* = 8.0, 6.8, 0.8 Hz 1H), 2.62(s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 164.31, 153.35, 149.34, 134.89, 126.94, 126.40, 126.17, 120.19, 77.31, 76.99, 76.68, 22.03.

**2,8-dimethyl-3-phenylquinazolin-4(3H)-one (2t):** The title compound was prepared according to the general



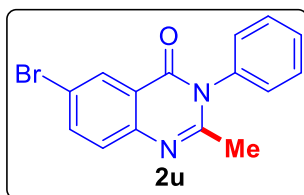
procedure B on a 0.25 mmol scale to obtain as a white solid (52 mg, yield = 83 %); Mp. 146-148 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.12 (ddd, *J* = 8.0, 1.6, 0.8 Hz, 1H), 7.61 (ddd, *J* = 7.6, 1.6, 0.8 Hz, 1H), 7.57-7.53 (m, 2H), 7.51-7.49 (m, 1H), 7.34 (t, *J* = 7.6, 1H), 7.27-7.24 (m, 2H), 2.63 (s, 3H), 2.25 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.72, 152.71, 146.07, 137.99, 135.33, 135.10, 129.93, 129.13, 128.02, 126.08, 124.67, 120.72, 24.61, 17.33. HRMS (ESI) calcd for C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 250.1106; found: 250.1109.

**7-chloro-2-methyl-3-phenylquinazolin-4(3H)-one (2u):**<sup>10</sup> The title compound was prepared according to the



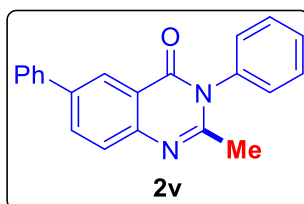
general procedure B on a 0.25 mmol scale to obtain as a white solid (46 mg, yield = 68 %); Mp. 173-175 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.27 (ddd, *J* = 8.0, 1.2, 0.4 Hz 1H), 7.80-7.76 (m, 1H), 7.69 (dd, *J* = 7.6, 0.8 Hz 1H), 7.51-7.50 (m, 2H), 7.48-7.46 (m, 1H), 7.31 (td, *J* = 2.8, 1.2 Hz, 1H), 7.20-7.17 (m, 1H), 2.27 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.04, 153.48, 147.32, 138.76, 135.57, 134.77, 130.91, 129.67, 128.53, 127.01, 126.85, 126.82, 126.45, 120.56, 24.31.

**6-bromo-2-methyl-3-phenylquinazolin-4(3H)-one (2v):**<sup>9</sup> The title compound was prepared according to the



general procedure B on a 0.25 mmol scale to obtain as a white solid (60 mg, yield = 76 %); Mp. 178-180 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.25 (ddd, *J* = 8.0, 1.2, 0.4 Hz 1H), 7.79-7.74 (m, 1H), 7.70-7.65 (m, 3H), 7.47 (ddd, *J* = 8.0, 3.2, 1.2 Hz 1H), 7.19-7.14 (m, 2 H), 2.24 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 162.06, 153.54, 147.31, 136.67, 134.73, 133.24, 129.75, 126.99, 126.80, 126.78, 123.42, 120.53, 24.35.

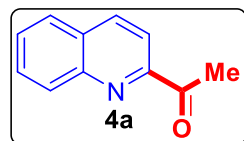
**2-methyl-3,6-diphenylquinazolin-4(3H)-one (2w):** The title compound was prepared according to the



general procedure B on a 0.25 mmol scale to obtain as a white solid (61 mg, yield = 79 %); Mp. 173-175 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.49 (d, *J* = 2.4 Hz, 1H), 8.02 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.75 (d, *J* = 8.4, 1H), 7.70-7.67 (m, 2H), 7.59-7.45 (m, 5H), 7.40-7.35 (m, 1H), 7.30-7.27 (m, 2H), 2.26 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>,

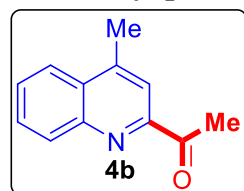
100 MHz) δ 162.30, 154.12, 146.64, 139.59, 139.52, 137.74, 133.48, 129.99, 129.29, 128.93, 128.00, 127.76, 127.27, 127.13, 124.88, 120.98, 24.40. HRMS (ESI) calcd for C<sub>21</sub>H<sub>16</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 312.1263; found: 312.1257.

**1-(quinolin-2-yl)ethan-1-one (4a):**<sup>11</sup> The title compound was prepared according to the general procedure C



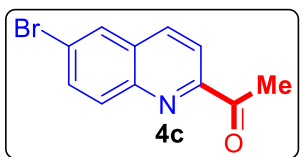
on a 0.25 mmol scale to obtain as a white solid (28 mg, yield = 66 %) Mp. 51-53 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.26 (d, *J* = 8.8 Hz, 1H), 8.20 (d, *J* = 8.8 Hz, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.80-7.76 (m, 1H), 7.66-6.4- (m, 1H), 2.87 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 200.64, 153.20, 147.20, 136.82, 130.53, 129.94, 129.54, 128.51, 127.60, 117.92, 25.53.

**1-(4-methylquinolin-2-yl)ethan-1-one (4b):**<sup>11</sup> The title compound was prepared according to the general



procedure C on a 0.15 mmol scale to obtain as a white solid (30 mg, yield = 65 %) Mp. 66-68 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.19 (ddd, *J* = 8.4, 0.8, 0.4 Hz, 1H), 8.03(ddd, *J* = 8.0, 0.8, 0.4 Hz, 1H), 7.96 (d, *J* = 1.2 Hz, 1H), 7.76 (ddd, *J* = 8.4, 6.8, 1.6 Hz, 1H), 7.66 (ddd, *J* = 8.4, 6.8, 1.2 Hz, 1H), 2.85 (s, 3H), 2.75 (d, *J* = 0.8 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 201.03, 152.81, 147.07, 145.24, 131.13, 129.55, 128.25, 123.74, 118.43, 25.47, 18.84.

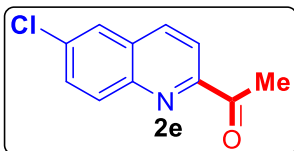
**1-(6-bromoquinolin-2-yl)ethan-1-one (4c):**<sup>12</sup> The title compound was prepared according to the general



procedure C on a 0.15 mmol scale to obtain as a white solid (38 mg, yield = 60%) Mp. 62-64 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.18 (dd, *J* = 8.4, 0.4 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 8.08-8.05 (m, 1H), 7.05 (d, *J* = 2.4 Hz, 1H), 7.85 (dd, *J* = 9.2, 2.4

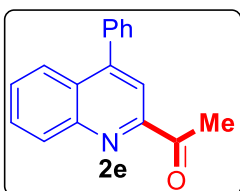
Hz, 1H), 2.85 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  200.20, 153.41, 145.76, 135.85, 133.57, 132.14, 130.52, 129.73, 122.81, 118.84, 25.49.

**1-(4-phenylquinolin-2-yl)ethan-1-one (4d):**<sup>17</sup> The title compound was prepared according to the general



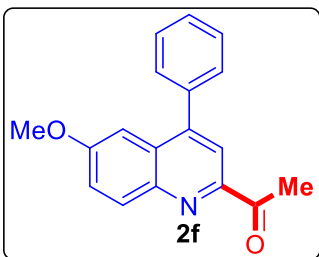
procedure C on a 0.15 mmol scale to obtain as a white solid (31 mg, yield = 61 %) Mp. 68-70 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.18-8.12 (m, 3H), 7.85 (d,  $J$  = 2.4 Hz, 1H), 7.71 (dd,  $J$  = 8.8, 2.0 Hz, 1H), 2.85 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  200.16, 153.30, 145.53, 135.91, 134.47, 132.07, 131.00, 130.05, 126.32, 118.83, 25.48.

**1-(4-phenylquinolin-2-yl)ethan-1-one (4e):**<sup>11</sup> The title compound was prepared according to the general



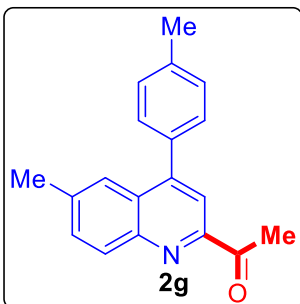
procedure C on a 0.15 mmol scale to obtain as a white solid (36 mg, yield = 58 %) Mp. 58-60 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.27 (dd,  $J$  = 8.8, 0.8 Hz, 1H), 8.08 (s, 1H), 7.98 (dd,  $J$  = 8.4, 0.8 Hz, 1H), 7.78 (ddd,  $J$  = 8.4, 6.8, 0.4 Hz, 1H), 7.59 (ddd,  $J$  = 8.4, 6.8, 1.2 Hz, 1H), 7.53-7.49 (m, 5H), 2.90 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  200.79, 152.69, 149.34, 147.81, 137.70, 130.92, 129.74, 129.52, 128.58, 128.57, 128.54, 128.01, 125.80, 118.12, 25.57.

**1-(6-methyl-4-(p-tolyl)quinolin-2-yl)ethan-1-one (4f):** The title compound was prepared according to the



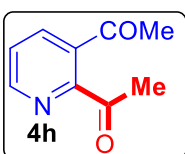
general procedure C on a 0.15 mmol scale to obtain as a white solid (40 mg, yield = 59 %) Mp. 176-178 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.17 (d,  $J$  = 9.2 Hz, 1H), 8.04 (s, 1H), 7.54-7.49 (m, 5H), 7.44 (dd,  $J$  = 8.2, 2.8 Hz, 1H), 7.24 (d,  $J$  = 2.8 Hz, 1H), 3.81 (s, 3H), 2.87 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  200.65, 159.60, 150.78, 147.69, 143.80, 138.08, 132.47, 129.43, 129.31, 128.72, 128.53, 122.50, 118.72, 103.57, 55.54, 25.52. HRMS (ESI) calcd for  $\text{C}_8\text{H}_6\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 277.1702 found: 277.1105.

**1-(6-methyl-4-(p-tolyl)quinolin-2-yl)ethan-1-one (4g):** The title compound was prepared according to the



general procedure C on a 0.15 mmol scale to obtain as a white solid (39 mg, yield = 56 %) Mp. 185-187 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.14 (d,  $J$  = 8.8 Hz, 1H), 8.02 (s, 1H), 7.747-7.743 (m, 1H), 7.60 (dd,  $J$  = 8.8, 2.0 Hz, 1H), 7.41-7.39 (m, 2H), 7.34 (d,  $J$  = 8.0 Hz, 1H), 2.88 (s, 3H), 2.49 (s, 3H), 2.47 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $^{13}\text{C}$  NMR (101 MHz,  $\text{cdCl}_3$ )  $\delta$  200.88, 152.00, 148.55, 146.40, 138.81, 138.37, 134.99, 131.98, 130.60, 129.42, 129.28, 128.13, 124.63, 118.22, 25.54, 22.01, 21.29. HRMS (ESI) calcd for  $\text{C}_8\text{H}_6\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 275.1310 found: 275.1312.

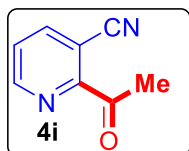
**1,1'-(pyridine-2,3-diyl)bis(ethan-1-one) (4h):**<sup>13</sup> The title compound was prepared according to the general



procedure C on a 0.15 mmol scale to obtain as a white solid (29 mg, yield = 70 %); Mp. 77-

78 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  9.21 (dd,  $J = 2.4, 1.2$ , 1H), 8.34 (dd,  $J = 8.4, 2.4$ , 1H), 8.13 (dd,  $J = 8.4, 1.2$ , 1H), 2.76 (s, 3H), 2.69 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  199.31, 196.18, 155.78, 149.17, 136.48, 134.22, 121.48, 27.02, 25.99.

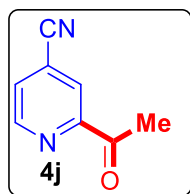
**2-acetylnicotinonitrile (4i):** The title compound was prepared according to the general procedure C on a 0.15



mmol scale to obtain as a white solid (20 mg, yield = 55 %); Mp. 112-114 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.95 (dd,  $J = 1.6, 1.2$ , 1H), 8.16-8.10 (m, 2H), 2.75 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  198.51, 167.70, 155.05, 151.75, 140.35, 121.21, 116.01, 112.88, 25.81.

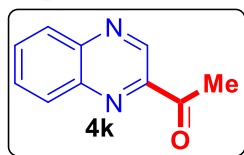
HRMS (ESI) calcd for  $\text{C}_8\text{H}_6\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 146.0480; found: 146.0485.

**3-acetylnicotinonitrile (4j):**<sup>14</sup> The title compound was prepared according to the general procedure C on a 0.15



mmol scale to obtain as a white solid (26 mg, yield = 72 %); Mp. 88-90 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.88 (dd,  $J = 4.8, 0.8$ , 1H), 8.26 (dd,  $J = 1.6, 1.2$ , 1H), 7.70 (dd,  $J = 3.2, 1.6$ , 1H), 2.74 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  198.14, 150.01, 128.06, 126.20, 123.40, 121.64, 115.86, 25.62.

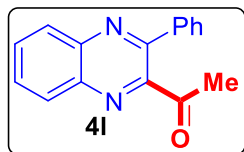
**1-(quinoxalin-2-yl)ethan-1-one (4k):**<sup>11</sup> The title compound was prepared according to the general procedure C



on a 0.15 mmol scale to obtain as a white solid (34 mg, yield = 81 %); Mp. 77-79 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  9.50 (s, 1H), 8.22-8.16 (m, 2H), 7.92-7.84 (m, 2H), 2.86 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  199.77, 146.54, 143.84, 143.02, 141.04, 132.17,

130.69, 130.45, 129.39, 25.52.

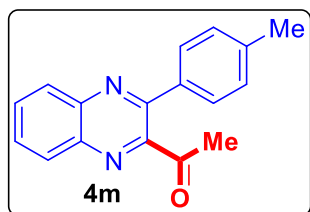
**1-(3-phenylquinoxalin-2-yl)ethan-1-one (4l):**<sup>15</sup> The title compound was prepared according to the general



procedure C on a 0.25 mmol scale to obtain as a white solid (47 mg, yield = 77 %); Mp. 107-109 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.19-8.16 (m, 2H), 7.89-7.80 (m, 2H), 7.65-7.63 (m, 2H), 7.52-7.48 (m, 3H), 2.76 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  201.17,

152.44, 150.03, 142.32, 139.72, 137.97, 131.82, 130.41, 129.57, 129.39, 129.32, 128.90, 128.62, 28.48.

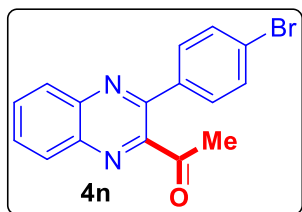
**1-(3-(p-tolyl)quinoxalin-2-yl)ethan-1-one (4m):** The title compound was prepared according to the general



procedure C on a 0.25 mmol scale to obtain as a white solid (48 mg, yield = 74%); Mp. 114-116 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.17-8.15(m, 2H), 7.88-7.85 (m, 2H), 7.56-7.35 (m, 2H), 7.32 (d,  $J = 8.0$ , 2H), 2.74 (s, 3H), 2.43 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  201.42, 152.33, 150.23, 142.37, 139.60, 135.03, 132.61,

132.02, 131.68, 130.60, 130.21, 129.53, 129.40, 129.27, 128.86, 28.58, 21.40. HRMS (ESI) calcd for  $\text{C}_{17}\text{H}_{14}\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 262.1106; found: 262.1107.

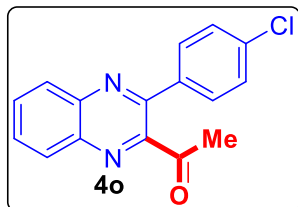
**1-(3-(naphthalen-2-yl)quinoxalin-2-yl)ethan-1-one (4n):** The title compound was prepared according to the



general procedure C on a 0.25 mmol scale to obtain as a white solid (57 mg, yield = 70 %); Mp. 182-184 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.17 (dddd,  $J = 8.5, 7.0, 1.6, 0.6$  Hz, 2H), 7.86 (dddd,  $J = 16.8, 8.0, 6.9, 1.6$  Hz, 2H), 7.65-7.61 (m, 2H), 7.52-7.48 (m, 2H), 2.81 (s, 3H), 2.81 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$

200.83, 151.49, 149.19, 142.29, 139.75, 137.01, 132.09, 131.71, 130.65, 130.53, 129.63, 129.27, 123.97, 28.28. HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{11}\text{BrON}_2$   $[\text{M}+\text{H}]^+$ : 326.0055; found: 326.0056.

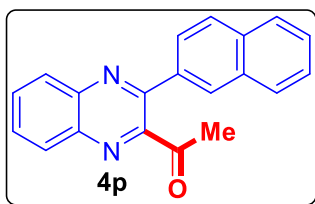
**1-(3-(4-chlorophenyl)quinoxalin-2-yl)ethan-1-one (4o):** The title compound was prepared according to the



general procedure C on a 0.25 mmol scale to obtain as a white solid (59 mg, yield = 85 %) Mp. 167-169 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.19-8.14 (m, 2H), 7.85 (dddd,  $J = 16.7, 8.0, 6.9, 1.6$  Hz, 2H), 7.60-7.56 (m, 2H), 7.49-7.45 (m, 2H), 2.81 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  200.84, 151.39, 149.23, 142.26, 139.72,

136.52, 135.61, 132.06, 130.62, 130.28, 129.60, 129.25, 128.76, 28.28. HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{11}\text{ClON}_2$   $[\text{M}+\text{H}]^+$ : 282.0560; found: 282.0562.

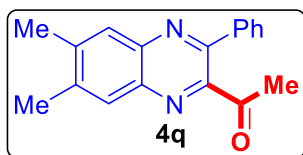
**1-(3-(naphthalen-2-yl)quinoxalin-2-yl)ethan-1-one (4p):** The title compound was prepared according to the



general procedure C on a 0.25 mmol scale to obtain as a white solid (54 mg, yield = 73 %); Mp. 160-162 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.22-8.16 (m, 3H), 7.96-7.80 (m, 5H), 7.71 (dd,  $J = 8.4, 2.0$  Hz, 1H), 7.56-7.51 (m, 2H), 2.78 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  201.20, 152.34, 150.12, 142.38, 139.70, 135.35, 133.53,

133.14, 131.85, 130.42, 129.59, 129.29, 128.82, 128.66, 128.26, 127.73, 126.98, 126.48, 126.11, 28.47. HRMS (ESI) calcd for  $\text{C}_{20}\text{H}_{14}\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 298.1106; found: 298.1112.

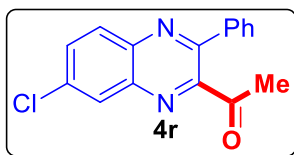
**1-(6,7-dimethyl-3-phenylquinoxalin-2-yl)ethan-1-one (4q):** The title compound was prepared according to the



general procedure C on a 0.25 mmol scale to obtain as a white solid (49 mg, yield = 71%); Mp. 102-104 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  7.92 (d,  $J = 0.8$  Hz, 2H), 7.62-7.59 (m, 2H), 7.48-7.47 (m, 3H), 2.74 (s, 3H), 2.53 (s, 6H);  $^{13}\text{C}$  NMR

( $\text{CDCl}_3$ , 100 MHz)  $\delta$  201.36, 151.65, 149.03, 142.88, 141.33, 141.19, 138.69, 138.35, 129.08, 128.86, 128.50, 128.45, 128.28, 28.44, 20.61, 20.38. HRMS (ESI) calcd for  $\text{C}_{18}\text{H}_{16}\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 276.1263; found: 276.1265.

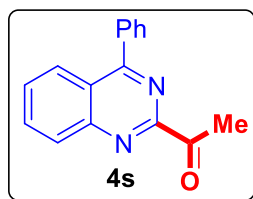
**1-(7-chloro-3-phenylquinoxalin-2-yl)ethan-1-one (4r):** The title compound was prepared according to the



general procedure C on a 0.25 mmol scale to obtain as a white solid (51 mg, yield = 73 %) Mp. 137-139 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.17 (d,  $J = 2.0$  Hz, 1H), 8.11 (d,  $J = 9.2$  Hz, 1H), 7.76 (dd,  $J = 8.8, 2.4$  Hz, 1H), 7.64 -7.61 (m, 2H), 7.52 -

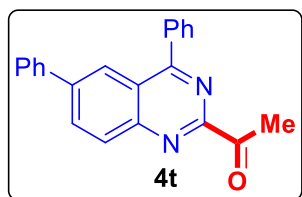
7.49 (m, 3H), 2.75 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  200.78, 153.34, 150.03, 142.57, 138.17, 137.84, 137.50, 131.51, 130.74, 129.69, 128.92, 128.65, 128.21, 28.41. HRMS (ESI) calcd for  $\text{C}_{17}\text{H}_{14}\text{ON}_2$   $[\text{M}+\text{H}]^+$ : 282.0560; found: 282.0556.

**1-(4-phenylquinazolin-2-yl)ethan-1-one (4s):**<sup>15</sup> The title compound was prepared according to the general



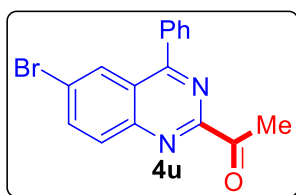
procedure C on a 0.25 mmol scale to obtain as a white solid (43 mg, yield = 69%); Mp. 106-108 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.31 (ddd,  $J$  = 8.4, 0.8, 0.4 Hz, 1H), 8.21 (ddd,  $J$  = 8.4, 1.2, 0.8 Hz, 1H), 8.00 (ddd,  $J$  = 8.4, 7.2, 1.6 Hz, 1H), 7.85-7.82 (m, 2H), 7.73 (ddd,  $J$  = 8.4, 7.2, 1.2 Hz, 1H), 7.60-7.59 (m, 3H), 2.94 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  198.77, 169.27, 155.87, 151.12, 136.79, 134.20, 130.30, 130.25, 130.21, 129.50, 128.65, 127.12, 123.22, 27.20.

**1-(4,6-diphenylquinazolin-2-yl)ethan-1-one (4t):**<sup>16</sup> The title compound was prepared according to the general



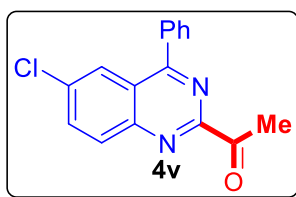
procedure C on a 0.25 mmol scale to obtain as a white solid (34 mg, yield = 42%); Mp. 106-108 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.39-8.35 (m, 2H), 8.26 (dd,  $J$  = 8.8, 2.0 Hz, 1H), 7.89-7.87 (m, 2H), 7.65-7.60 (m, 5H), 7.51-7.47 (m, 2H), 7.44-7.43 (m, 1H), 2.96 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  198.69, 169.22, 155.69, 150.47, 142.44, 139.40, 136.84, 133.94, 130.70, 130.36, 130.20, 129.16, 128.76, 128.47, 127.50, 124.48, 123.46, 27.20.

**1-(6-bromo-4-phenylquinazolin-2-yl)ethan-1-one (4u):** The title compound was prepared according to the



general procedure C on a 0.25 mmol scale to obtain as a white solid (47 mg, yield = 42 %) Mp. 127-29 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.35 (dd,  $J$  = 2.0, 0.4 Hz, 1H), 8.18 (dd,  $J$  = 8.8, 0.4 Hz, 1H), 8.06 (dd,  $J$  = 9.2, 2.4 Hz, 1H), 7.83-7.80 (m, 2H), 7.63-7.16 (m, 3H), 2.92 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz)  $\delta$  198.31, 168.41, 155.89, 149.82, 137.87, 136.17, 131.87, 130.64, 130.09, 130.04, 129.97, 129.24, 128.88, 124.14, 123.80, 27.15. HRMS (ESI) calcd for  $\text{C}_{16}\text{H}_{11}\text{BrON}_2$   $[\text{M}+\text{H}]^+$ : 326.0055; found: 326.0056.

**1-(6-chloro-4-phenylquinazolin-2-yl)ethan-1-one (4v):**<sup>16</sup> The title compound was prepared according to the

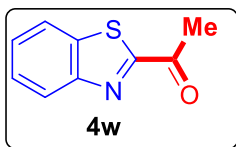


general procedure C on a 0.25 mmol scale to obtain as a white solid (42 mg, yield = 59%) Mp. 102-104 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$  8.25 (d,  $J$  = 9.2 Hz, 1H), 8.17 (d,  $J$  = 2.0 Hz, 1H), 7.93 (dd,  $J$  = 9.2, 2.4 Hz, 1H), 7.82 (dd,  $J$  = 6.0, 2.0 Hz, 2H), 7.62 (dd,  $J$  = 5.6, 2.4 Hz, 1H), 2.92 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) 198.32,

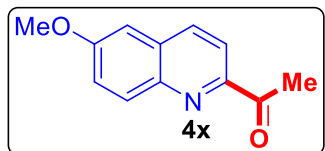
168.53, 155.92, 149.64, 136.22, 135.57, 135.31, 131.89, 130.64, 130.09, 128.89, 125.92, 123.77, 102.92, 27.16



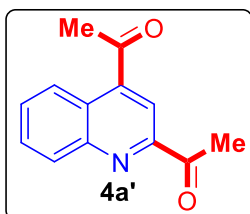
**1-(benzo[d]thiazol-2-yl)ethan-1-one (4w):**<sup>17</sup> The title compound was prepared according to the general procedure C on a 0.25 mmol scale to obtain as a white solid (31 mg, yield = 70 %) Mp. 105-107 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.19 (ddd, *J* = 7.6, 1.2, 0.4, 1H), 7.98 (ddd, *J* = 8.0, 1.6, 0.8, 1H), 7.60-7.55 (m, 1H), 7.55-7.50 (m, 1H), 2.83 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 198.51, 167.70, 155.05, 151.75, 140.35, 121.21, 116.01, 112.88, 25.81.



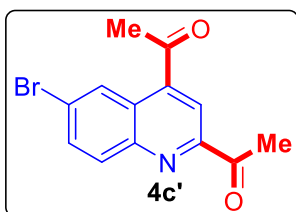
**1-(quinolin-2-yl)ethan-1-one (4x):**<sup>17</sup> The title compound was prepared according to the general procedure C on a 0.25 mmol scale to obtain as a white solid (22 mg, yield = 42 %) Mp. 94-96 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.14-8.07 (m, 3H), 8.43 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.11 (d, *J* = 2.8 Hz, 1H), 2.96 (s, 3H), 2.84 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 200.49, 159.44, 151.23, 143.19, 135.27, 132.02, 131.00, 123.06, 118.46, 104.86.



**1,1'-(quinoline-2,4-diyl)bis(ethan-1-one) (4a'):**<sup>11</sup> The title compound was prepared according to the general procedure C on a 0.25 mmol scale to obtain as a white solid (14 mg, yield = 26%) Mp. 67-69 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.57-8.54 (m, 1H), 8.37 (s, 1H), 8.25 (ddd, *J* = 8.4, 1.5, 0.8 Hz, 1H), 7.83 (ddd, *J* = 8.4, 6.8, 2.4 Hz, 1H), 7.76-7.72 (m, 1H), 2.89 (s, 3H), 2.79 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 200.99, 199.99, 152.64, 148.31, 142.94, 131.01, 130.38, 130.31, 125.64, 124.99, 116.97, 29.94, 25.38.



**1,1'-(6-bromoquinoline-2,4-diyl)bis(ethan-1-one) (4c'):** The title compound was prepared according to the general procedure C on a 0.25 mmol scale to obtain as a white solid (15 mg, yield = 21%) Mp. 68-70 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) δ 8.85 (d, *J* = 2.0 Hz, 1H), 8.24 (s, 1H), 8.11 (d, *J* = 6.8 Hz, 1H), 7.91 (dd, *J* = 7.2, 2.0 Hz, 1H), 2.87 (s, 3H), 2.79 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) δ 200.27, 199.60, 152.86, 146.98, 141.39, 134.07, 132.37, 128.28, 125.97, 125.59, 118.10, 29.71, 25.35. HRMS (ESI) calcd for C<sub>13</sub>H<sub>10</sub>BrNO<sub>2</sub> [M+H]<sup>+</sup>: 290.9895; found: 290.9893



## (5) X-ray Analysis

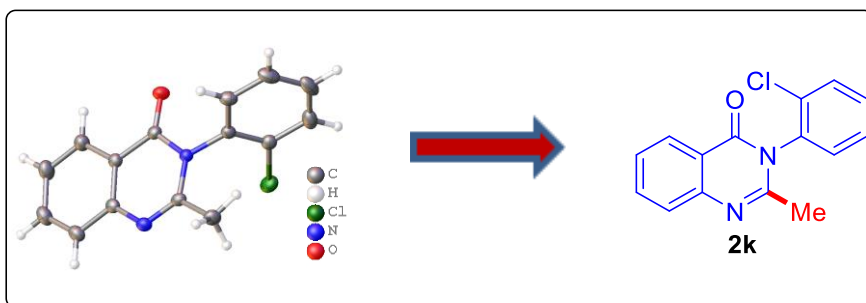


Table S1. Crystal data and structure refinement for **2k**.

Identification code	<b>2k</b>	
Empirical formula	C <sub>15</sub> H <sub>11</sub> Cl N <sub>2</sub> O	
Formula weight	270.71	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /c	
Unit cell dimensions	a = 17.6237(6) Å	a = 90°.
	b = 5.6260(2) Å	b = 98.1143(15)°.
	c = 12.7950(5) Å	g = 90°.
Volume	1255.94(8) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.432 Mg/m <sup>3</sup>	
Absorption coefficient	0.296 mm <sup>-1</sup>	
F(000)	560	
Crystal size	0.390 x 0.230 x 0.200 mm <sup>3</sup>	
Theta range for data collection	3.263 to 27.916°.	
Index ranges	-23 ≤ h ≤ 23, -7 ≤ k ≤ 7, -16 ≤ l ≤ 16	
Reflections collected	24365	
Independent reflections	2977 [R(int) = 0.0299]	
Completeness to theta = 25.242°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9281 and 0.8677	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2977 / 0 / 172	
Goodness-of-fit on F <sup>2</sup>	1.038	
Final R indices [I > 2σ(I)]	R1 = 0.0459, wR2 = 0.1444	

R indices (all data)	R1 = 0.0501, wR2 = 0.1508
Extinction coefficient	n/a
Largest diff. peak and hole	0.728 and -0.682 e.Å <sup>-3</sup>

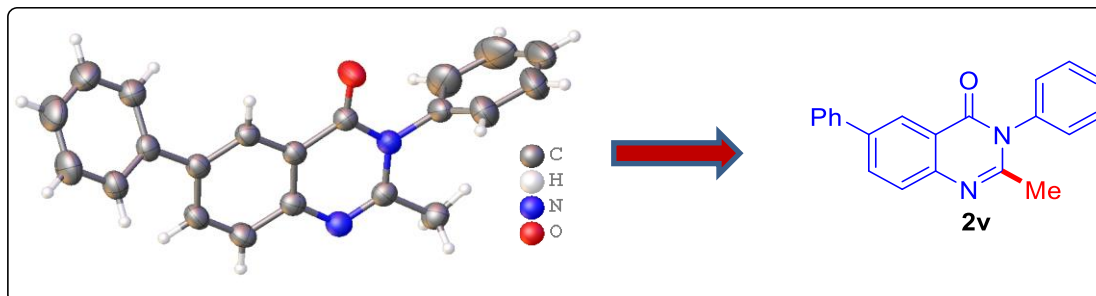


Table S1. Crystal data and structure refinement for **2v**.

Identification code	<b>2v</b>	
Empirical formula	C <sub>21</sub> H <sub>16</sub> N <sub>2</sub> O	
Formula weight	312.36	
Temperature	301(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /c	
Unit cell dimensions	a = 14.5419(6) Å	a = 90°.
	b = 15.7313(6) Å	b = 91.8219(17)°.
	c = 7.0669(3) Å	g = 90°.
Volume	1615.83(11) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.284 Mg/m <sup>3</sup>	
Absorption coefficient	0.080 mm <sup>-1</sup>	
F(000)	656	
Crystal size	0.520 x 0.410 x 0.130 mm <sup>3</sup>	
Theta range for data collection	2.945 to 27.093°.	
Index ranges	-18 ≤ h ≤ 18, -20 ≤ k ≤ 20, -9 ≤ l ≤ 9	
Reflections collected	29530	
Independent reflections	3531 [R(int) = 0.0482]	
Completeness to theta = 25.242°	99.0 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9281 and 0.8374
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3531 / 0 / 217
Goodness-of-fit on F <sup>2</sup>	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0703, wR2 = 0.2011
R indices (all data)	R1 = 0.0964, wR2 = 0.2456
Extinction coefficient	n/a
Largest diff. peak and hole	0.522 and -0.423 e.Å <sup>-3</sup>

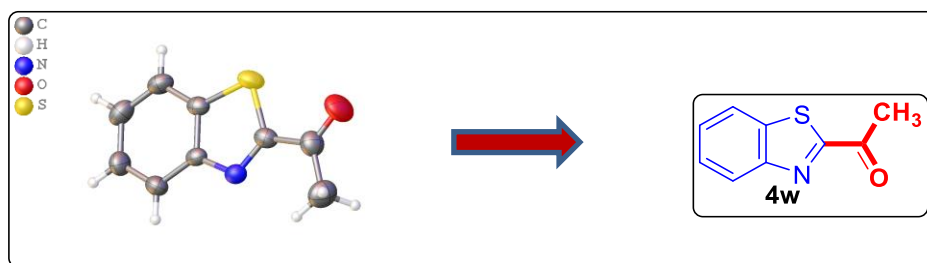


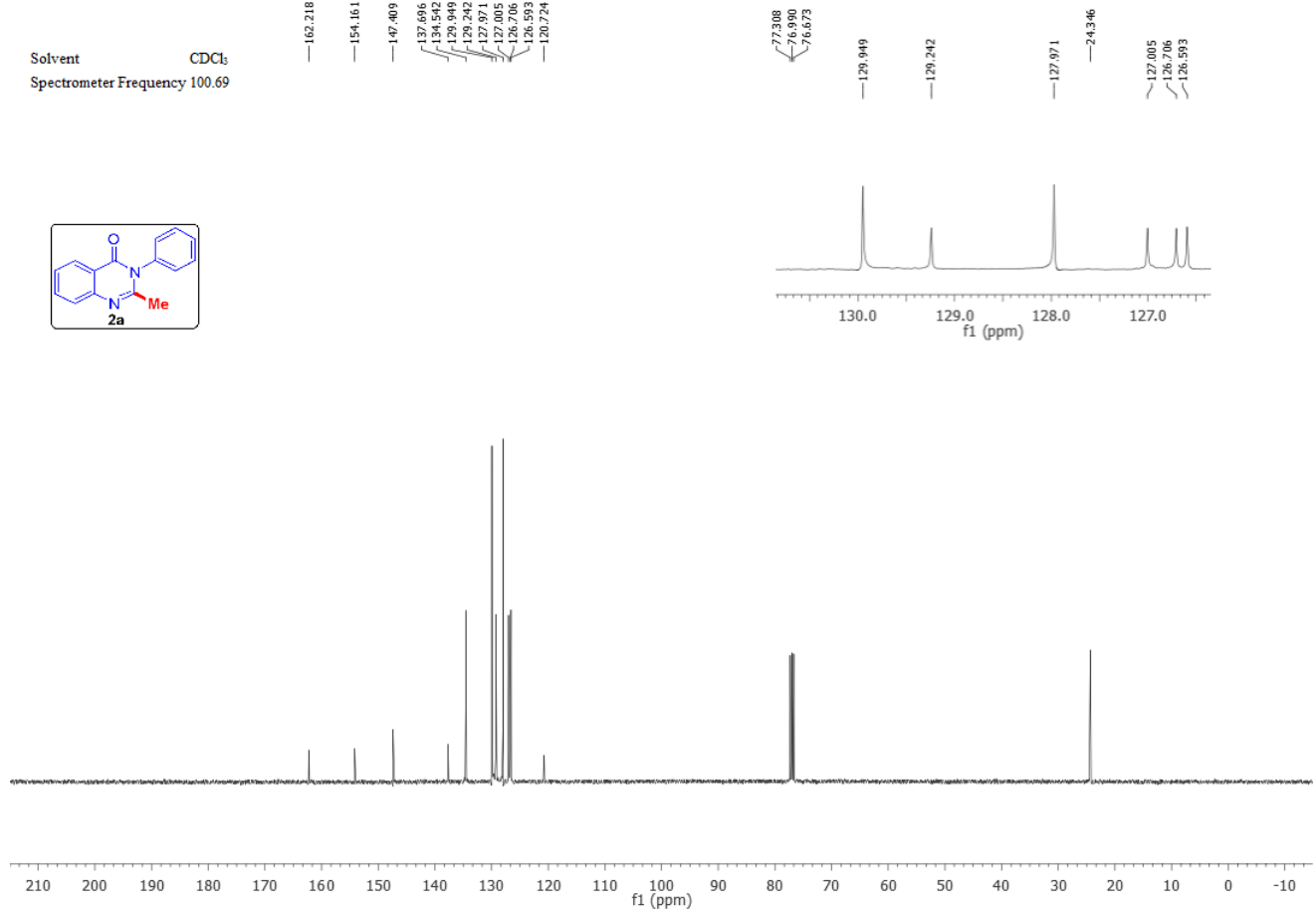
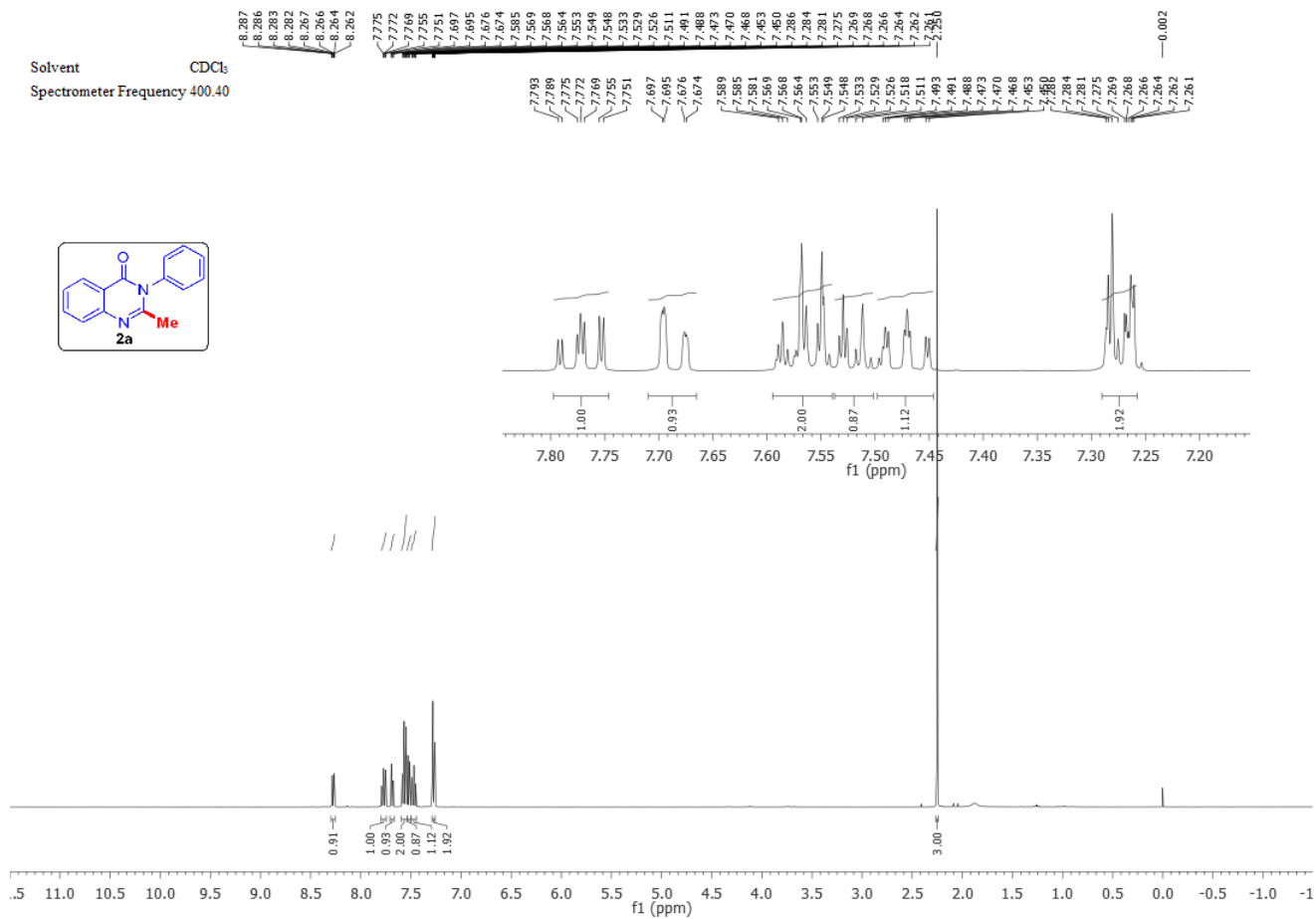
Table S1. Crystal data and structure refinement for **4w**.

Identification code	<b>4x</b>	
Empirical formula	C <sub>9</sub> H <sub>7</sub> N O S	
Formula weight	177.22	
Temperature	285(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /n	
Unit cell dimensions	a = 5.7146(8) Å	a = 90°.
	b = 10.4692(19) Å	b = 97.873(6)°.
	c = 13.978(3) Å	g = 90°.
Volume	828.4(2) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.421 Mg/m <sup>3</sup>	
Absorption coefficient	0.334 mm <sup>-1</sup>	
F(000)	368	

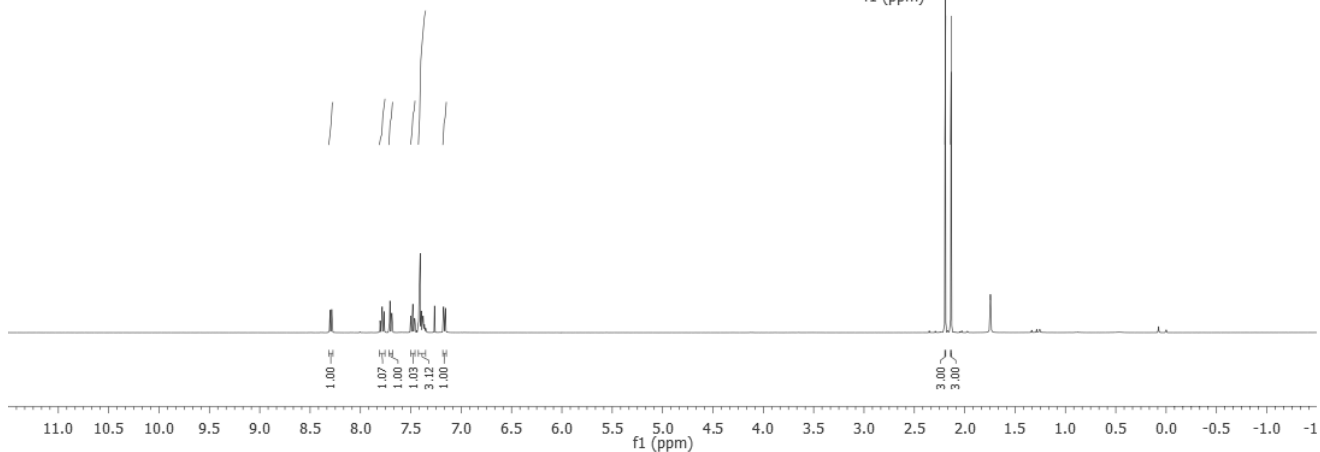
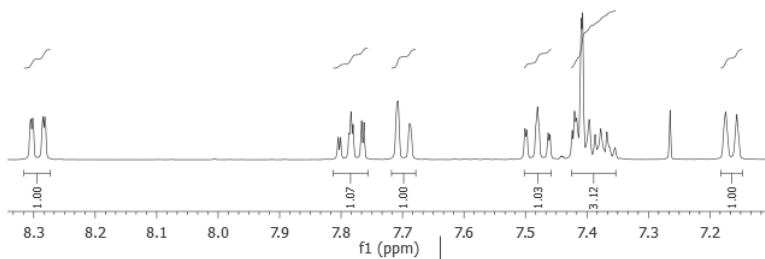
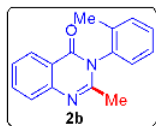
Crystal size	0.600 x 0.320 x 0.160 mm <sup>3</sup>
Theta range for data collection	3.528 to 26.721°.
Index ranges	-7<=h<=7, -13<=k<=13, -17<=l<=17
Reflections collected	11618
Independent reflections	1644 [R (int) = 0.0463]
Completeness to theta = 25.242°	96.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9268 and 0.7078
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	1644 / 0 / 109
Goodness-of-fit on F <sup>2</sup>	1.102
Final R indices [I>2sigma(I)]	R1 = 0.0616, wR2 = 0.1553
R indices (all data)	R1 = 0.0853, wR2 = 0.1754
Extinction coefficient	n/a
Largest diff. peak and hole	0.314 and -0.394 e.Å <sup>-3</sup>

**(6) References:**

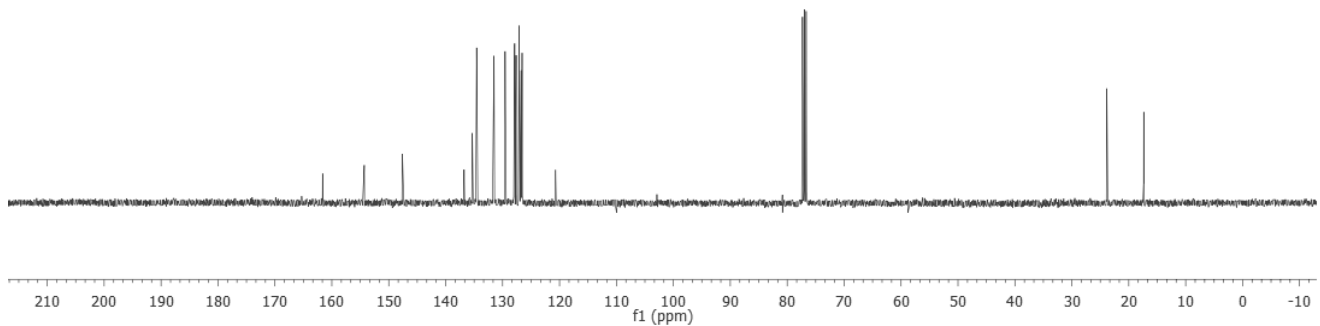
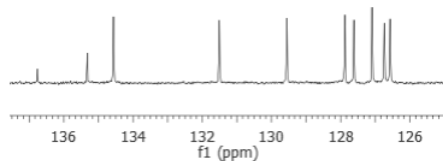
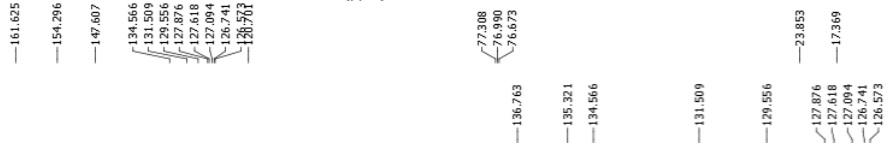
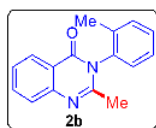
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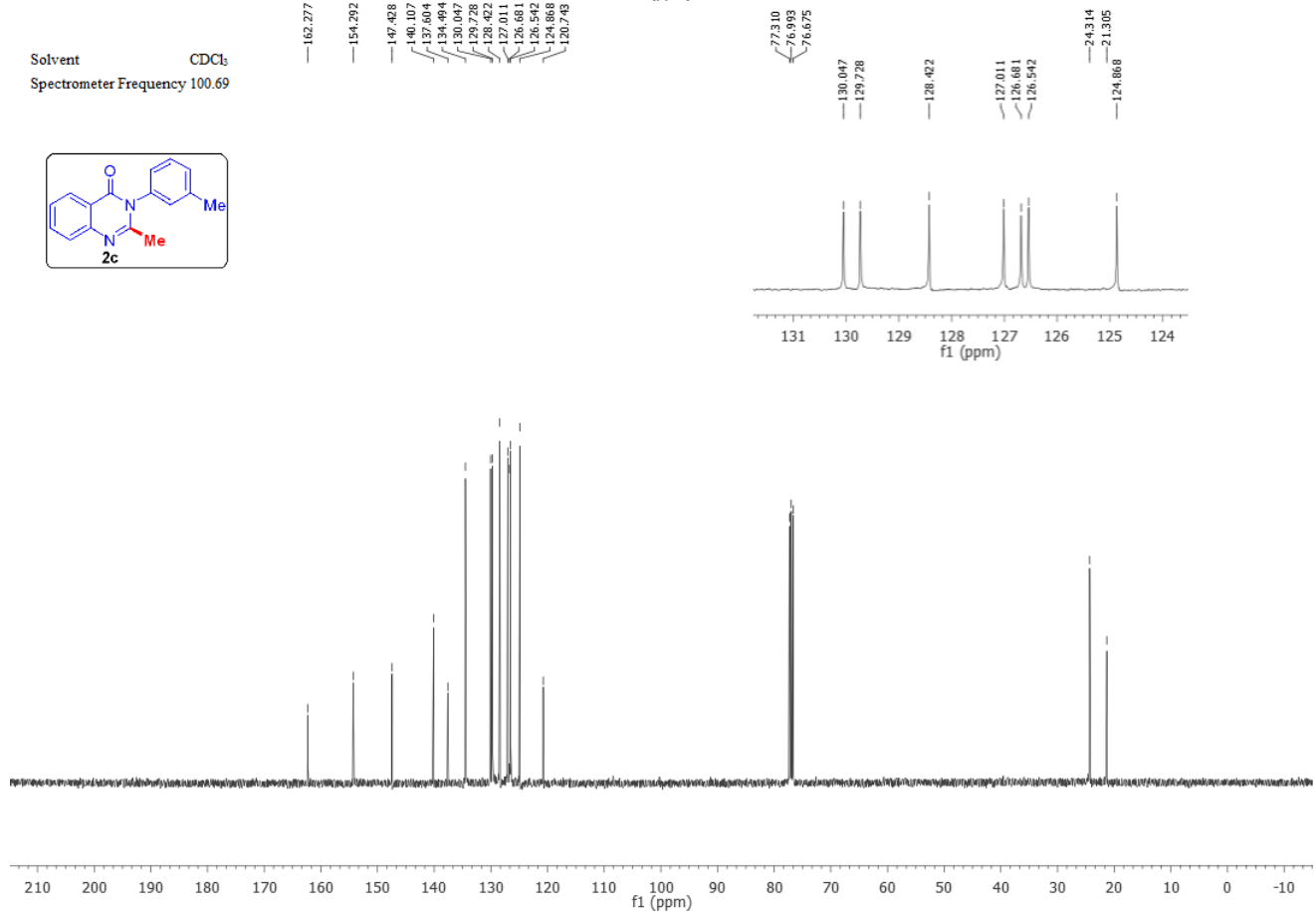
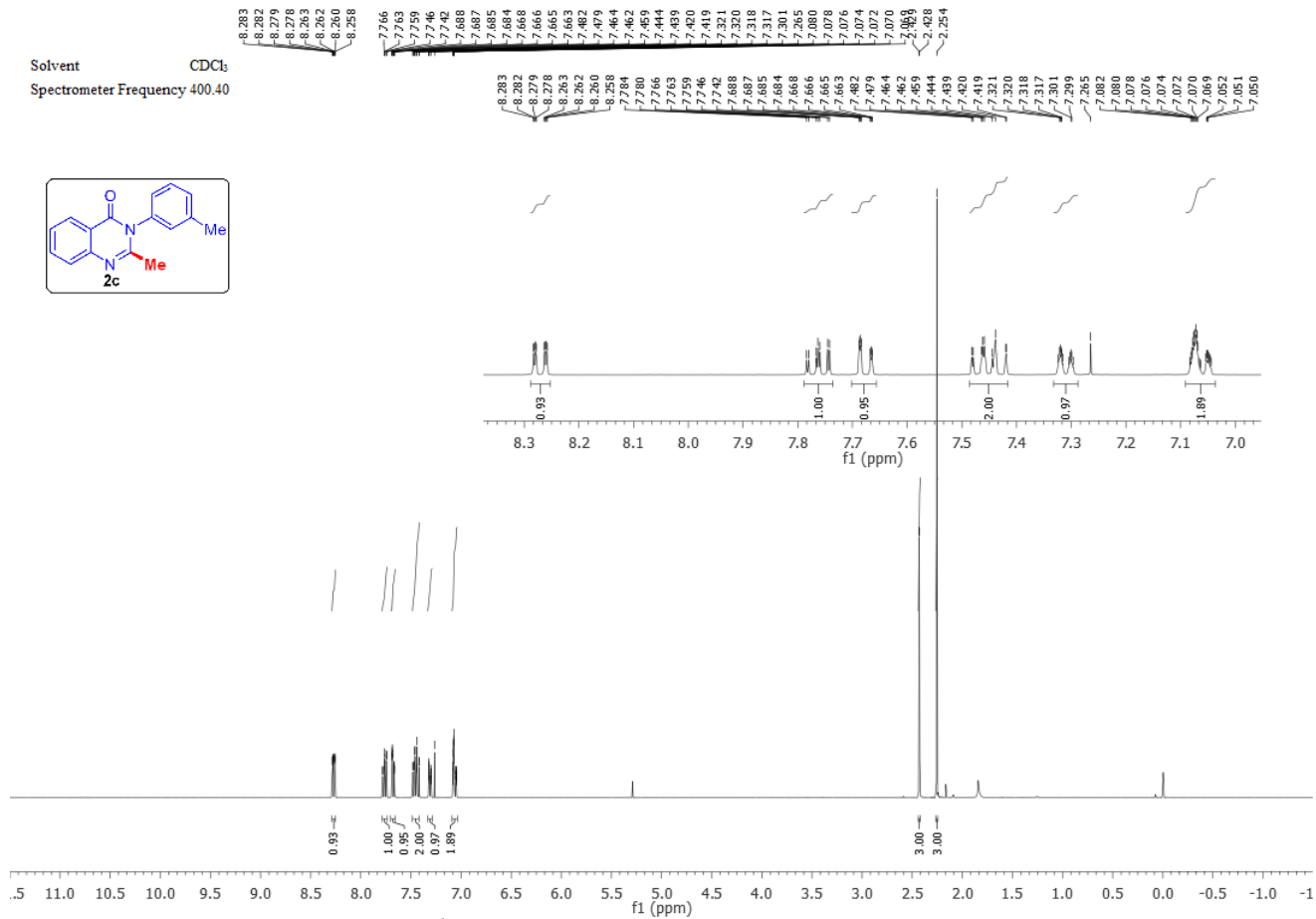
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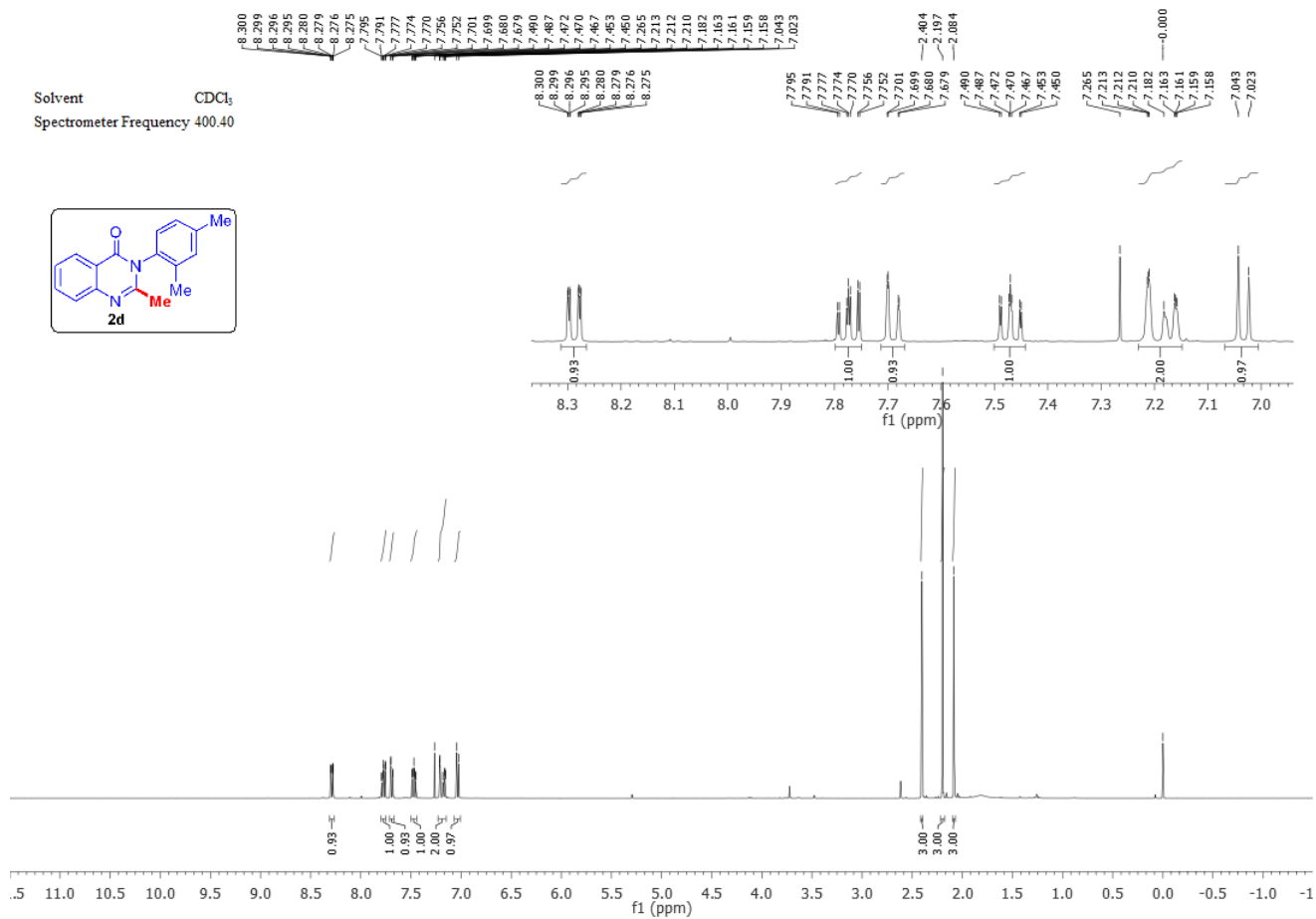
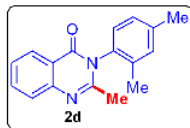
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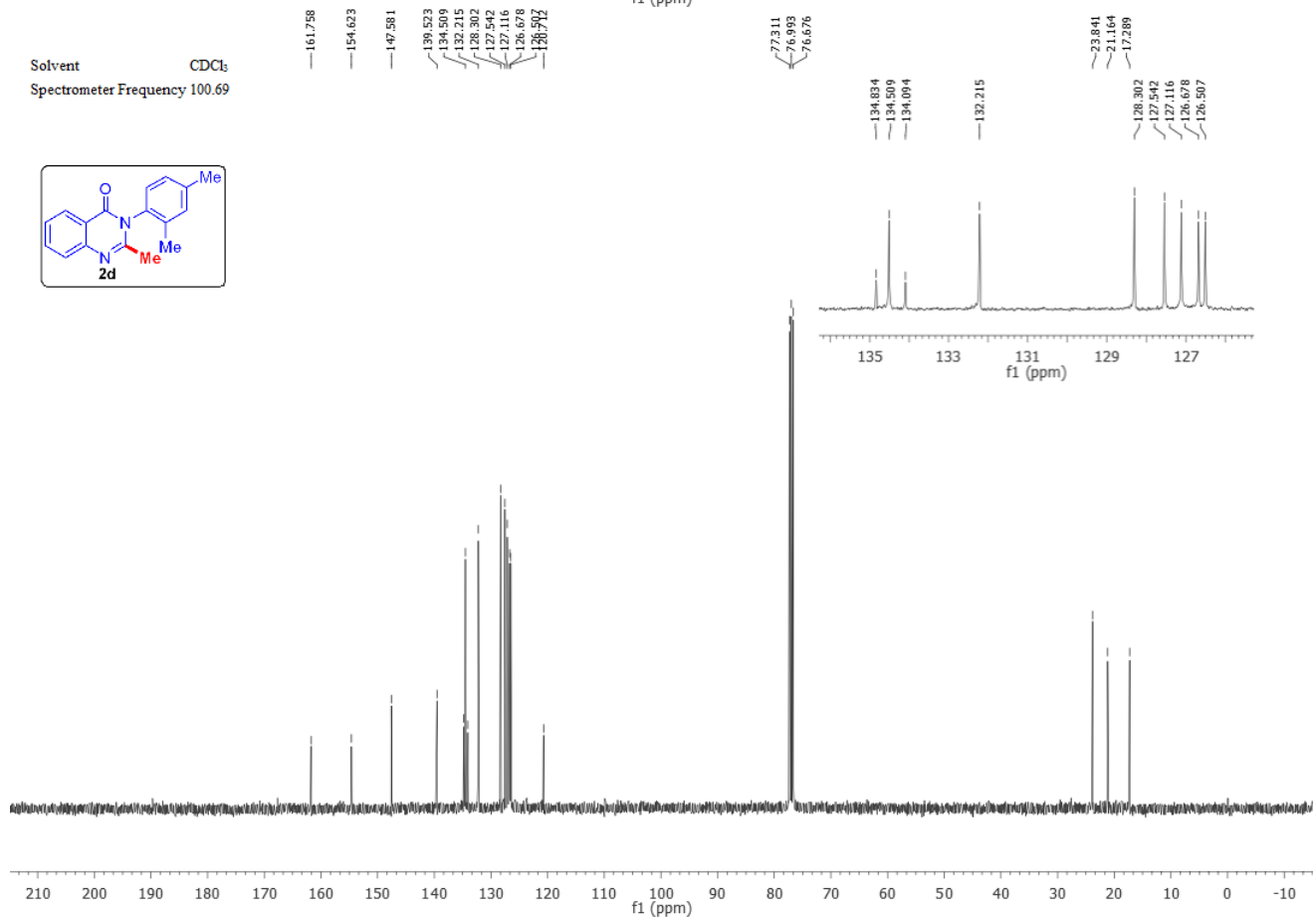
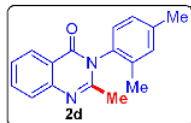




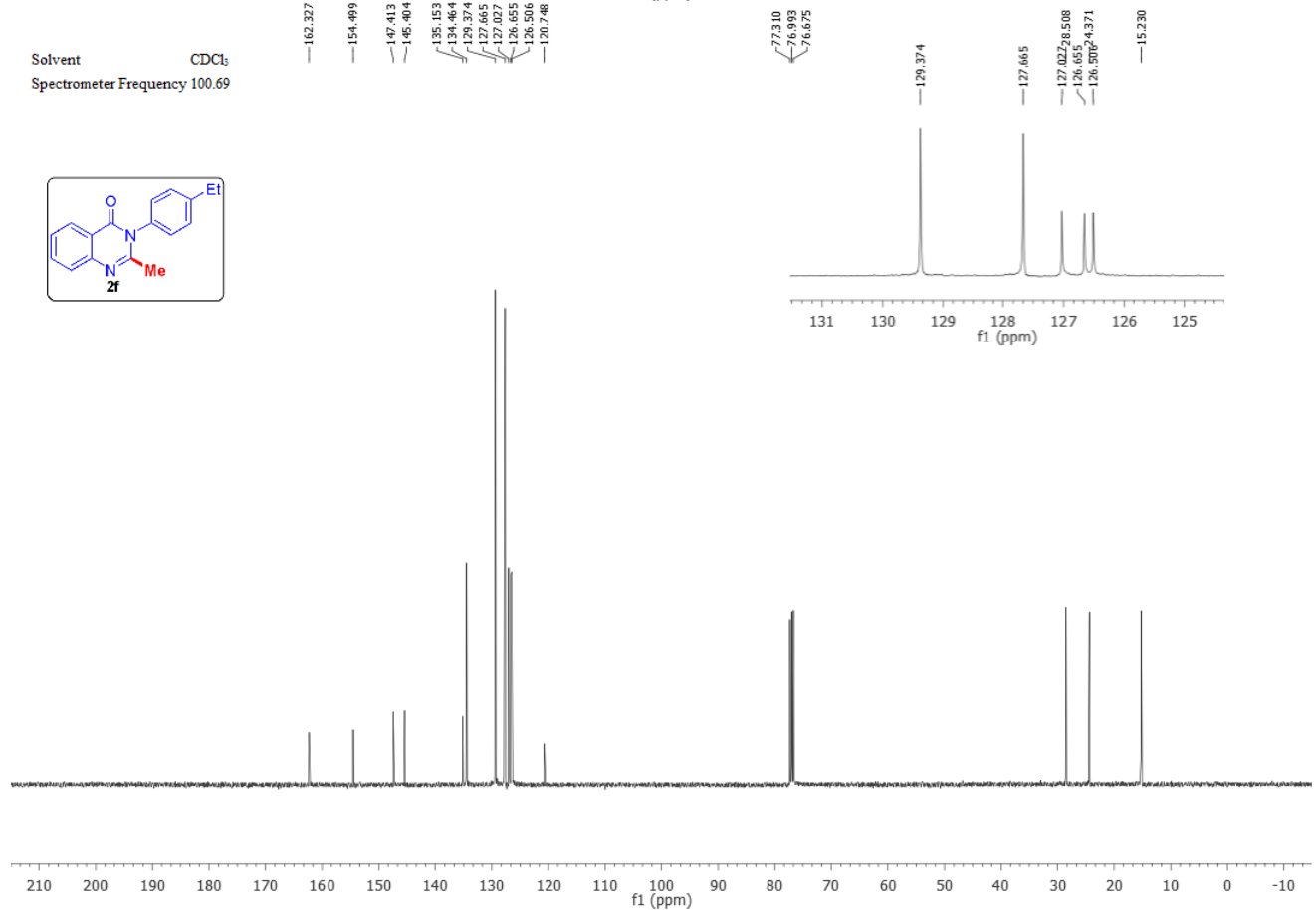
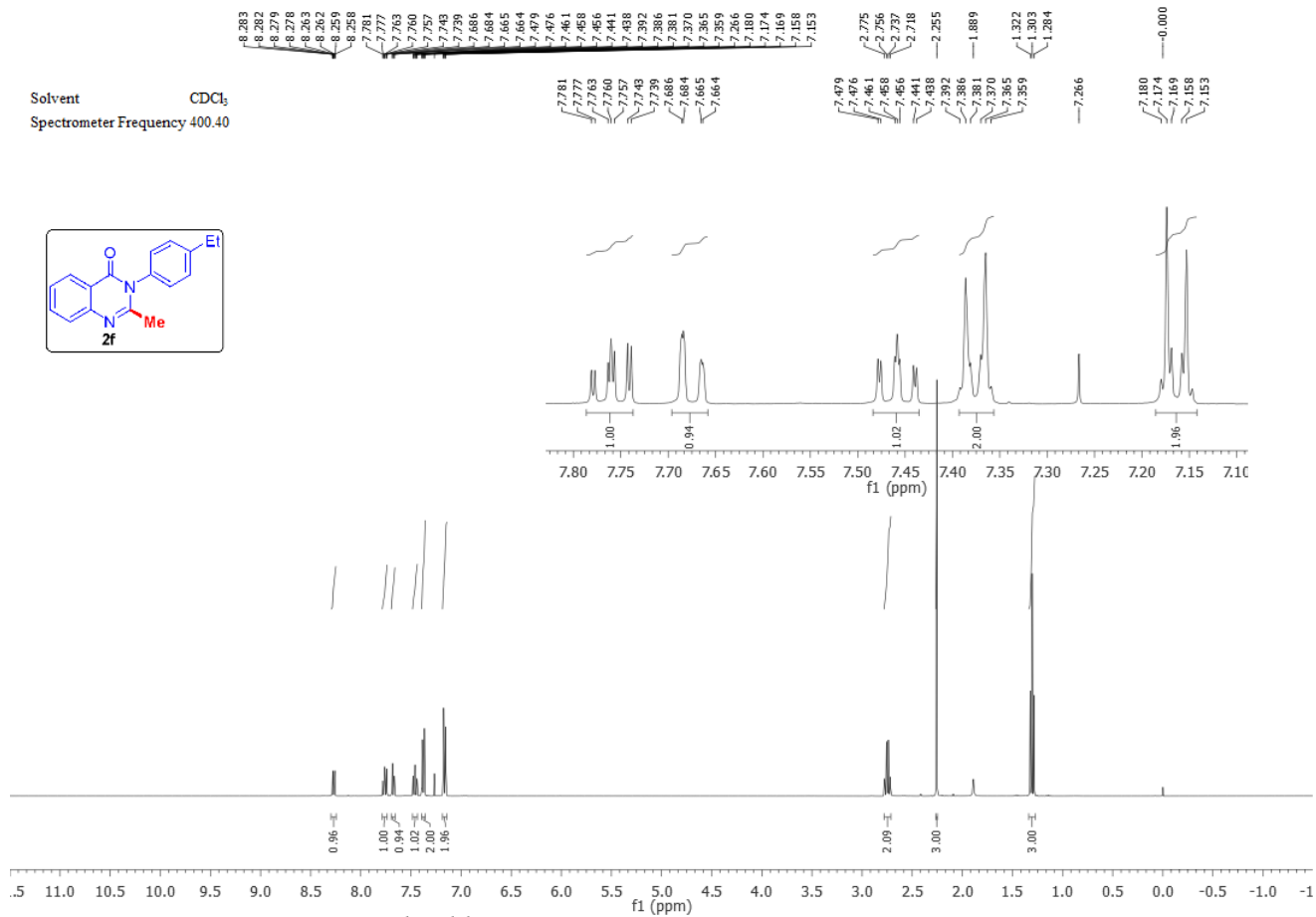
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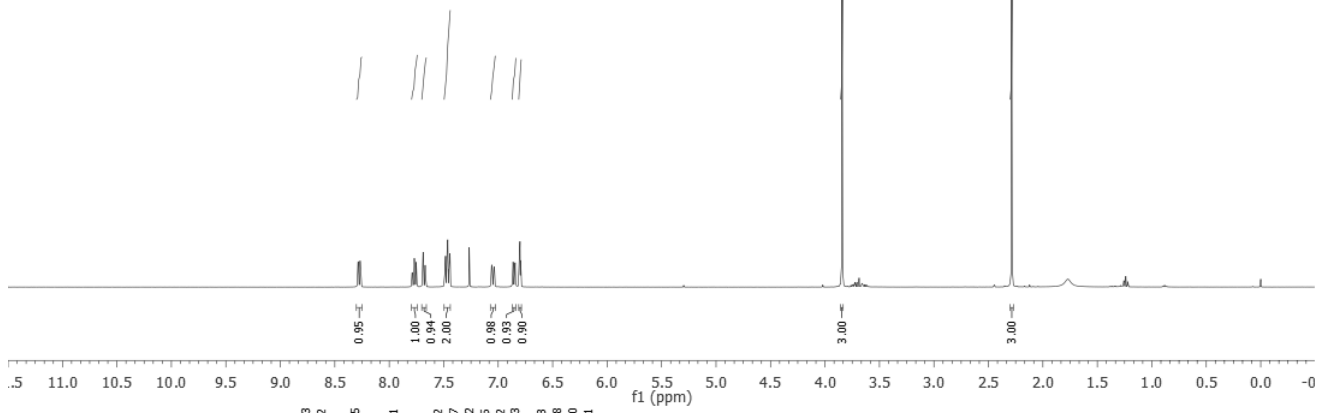
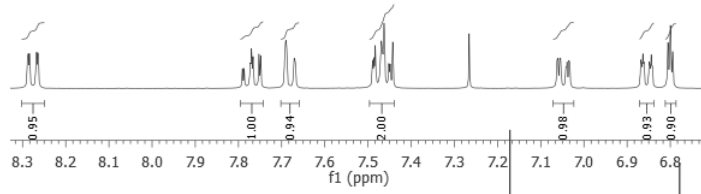
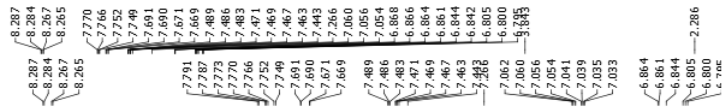
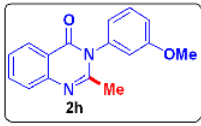




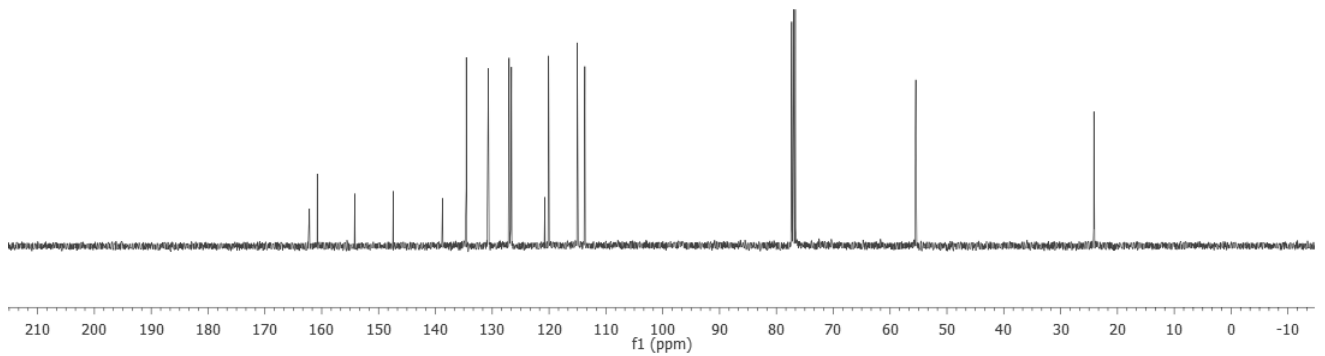
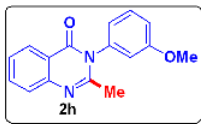


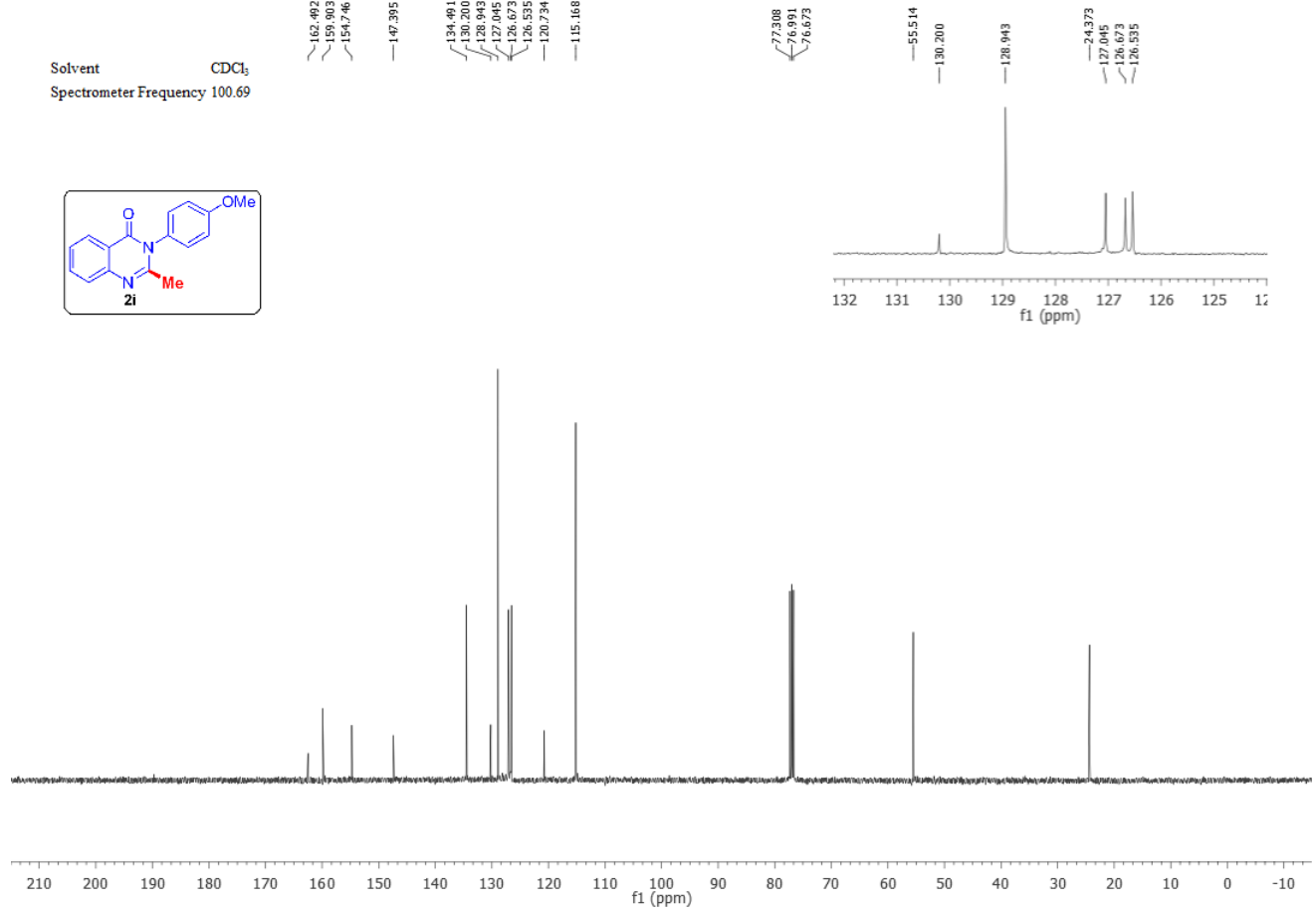
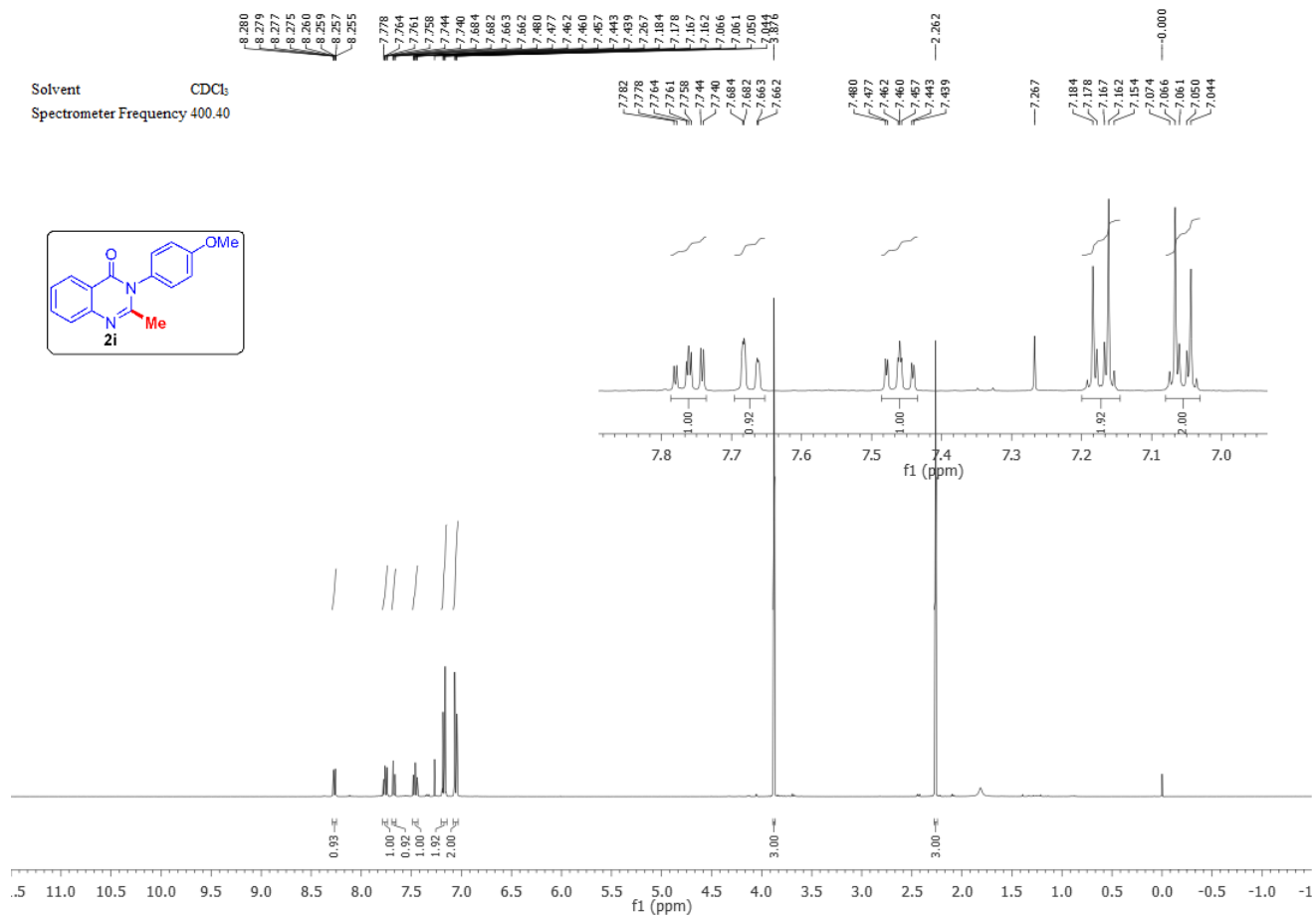


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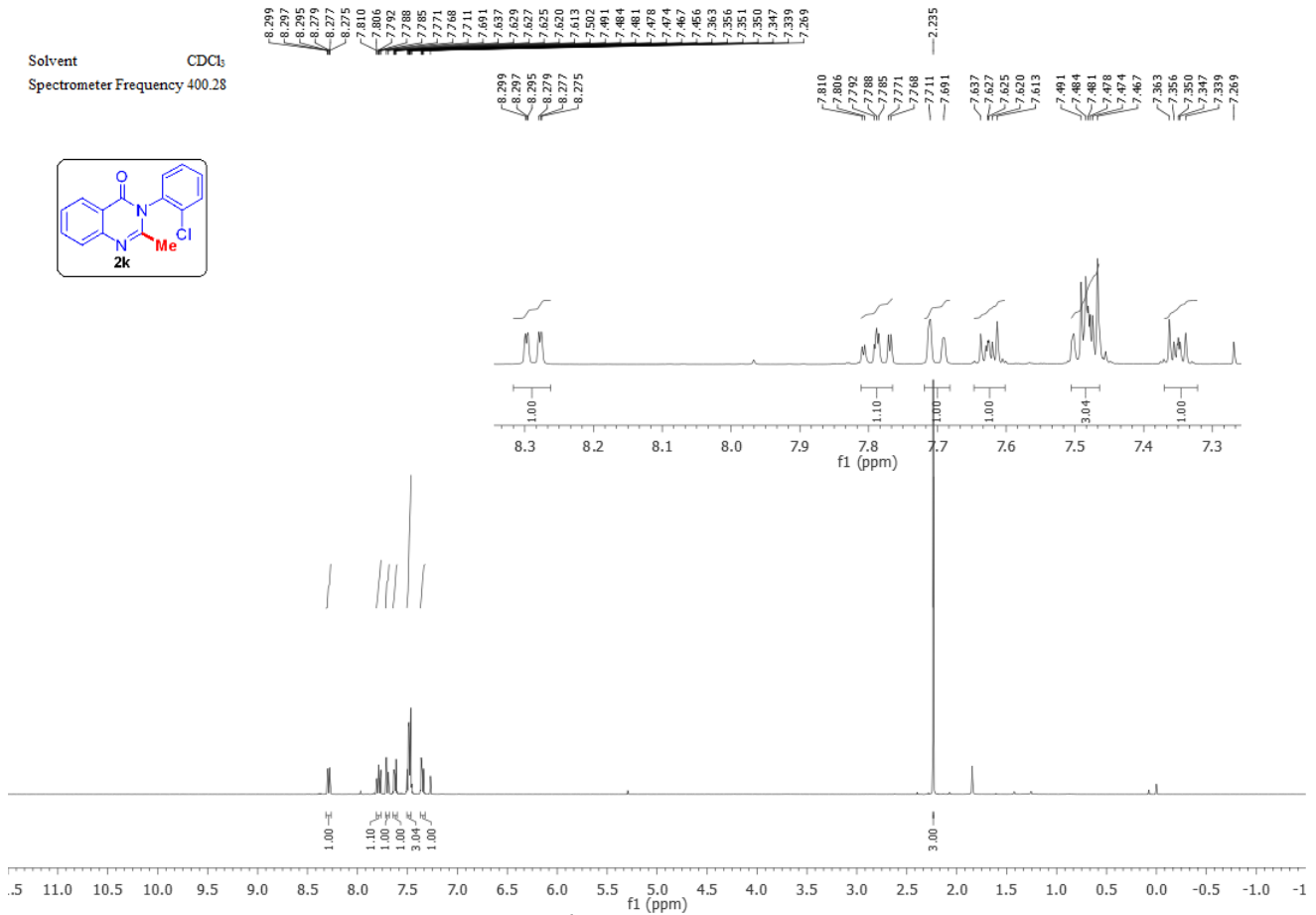
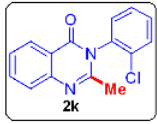




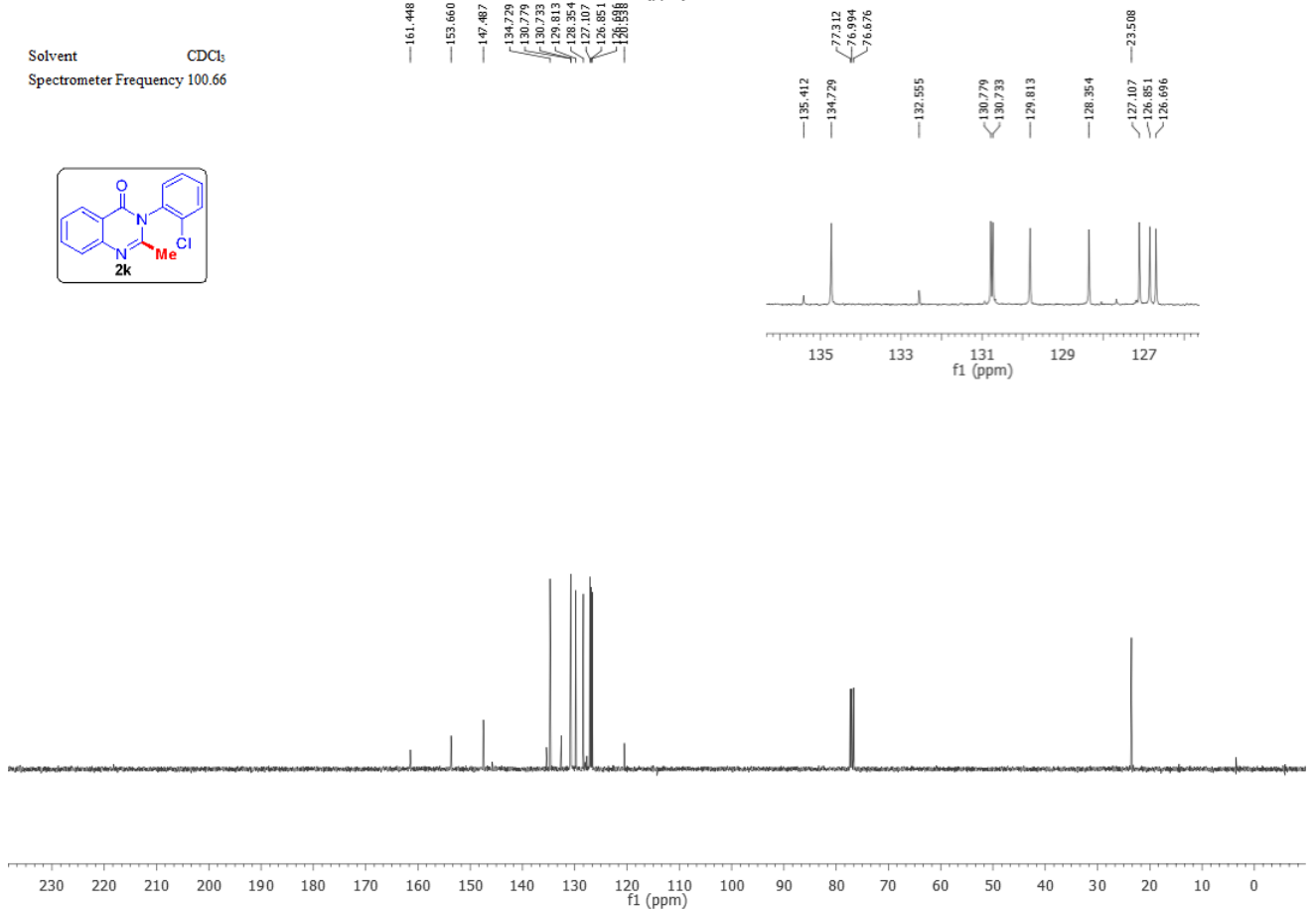
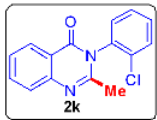




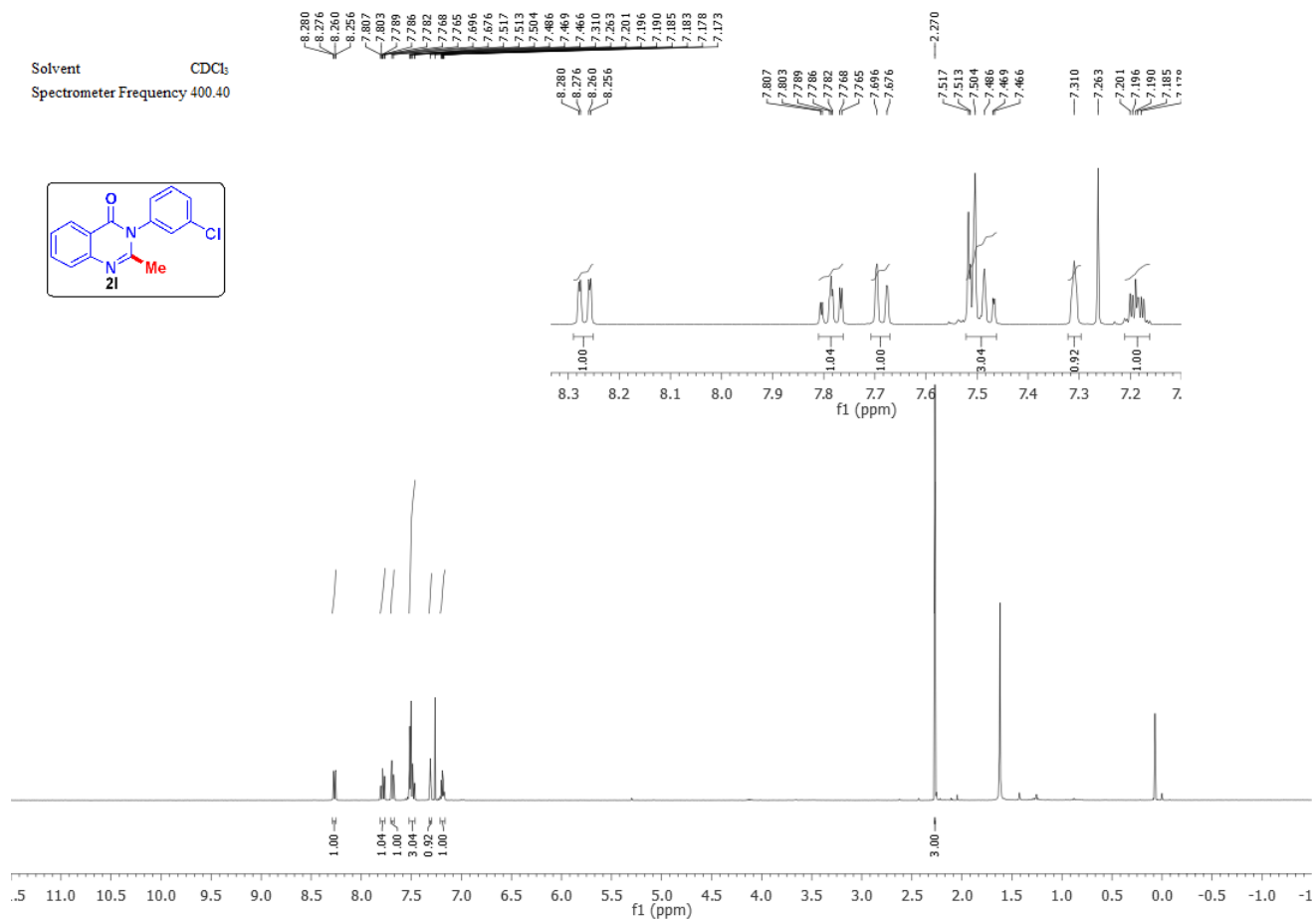
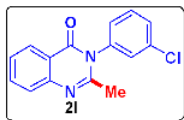
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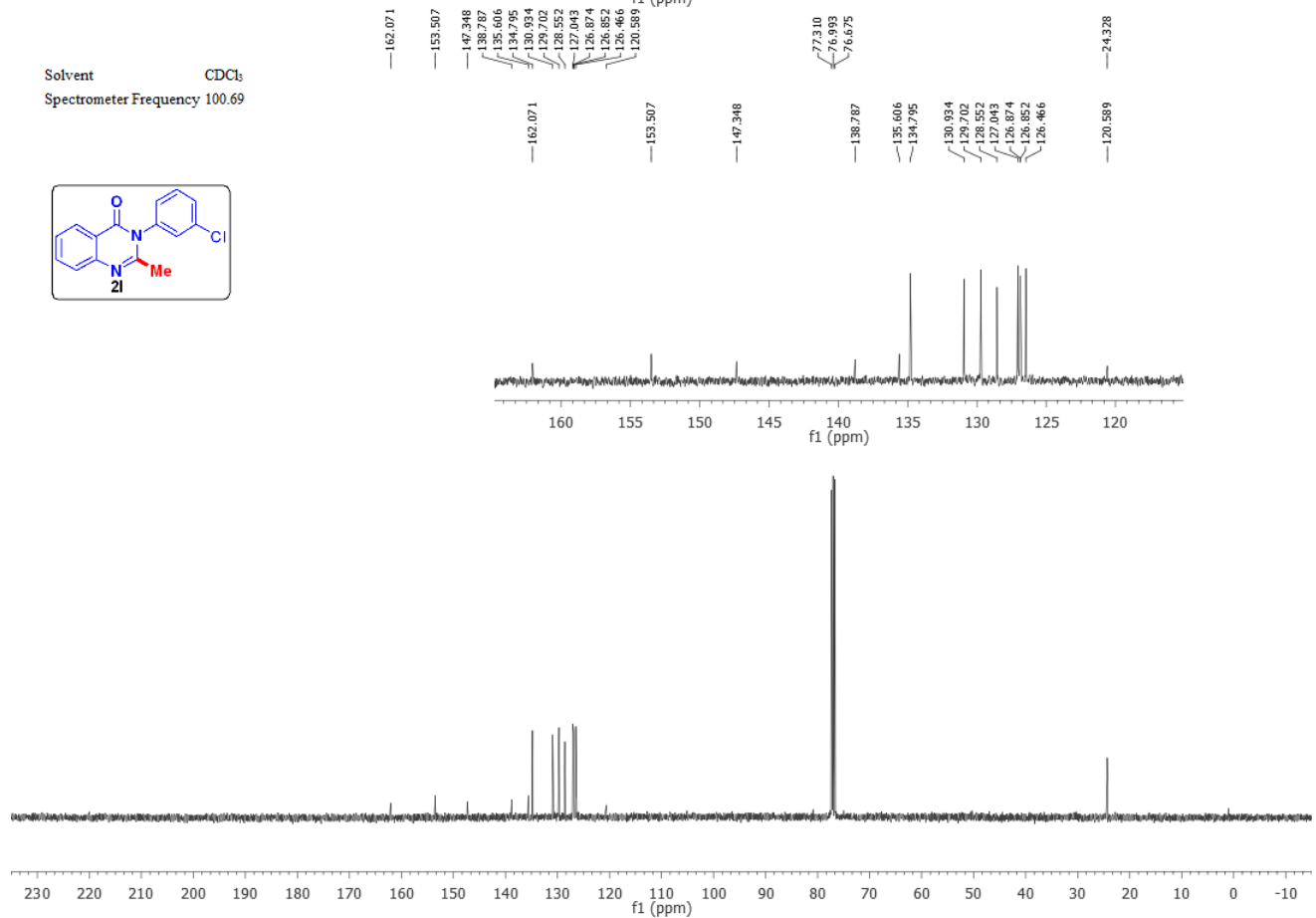
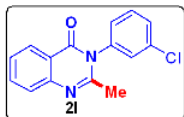
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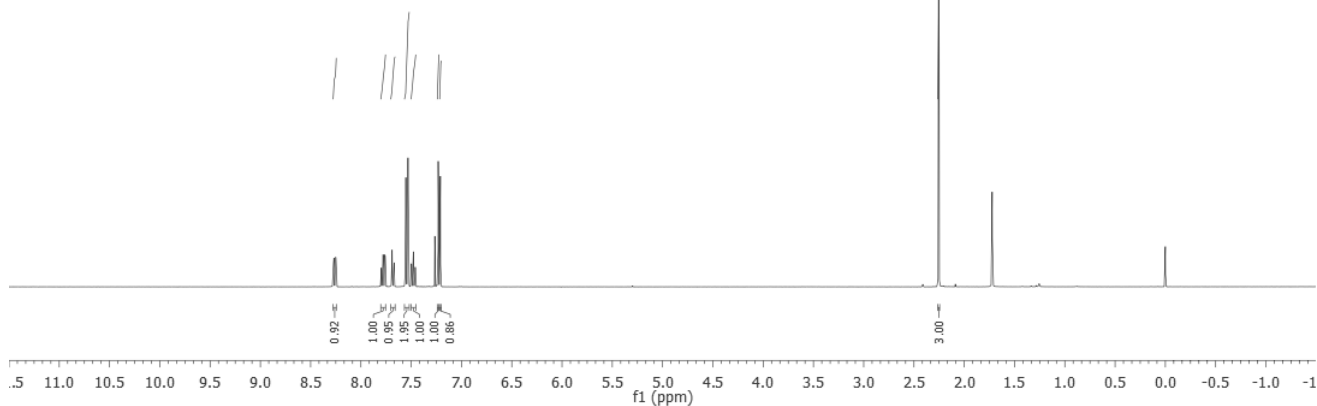
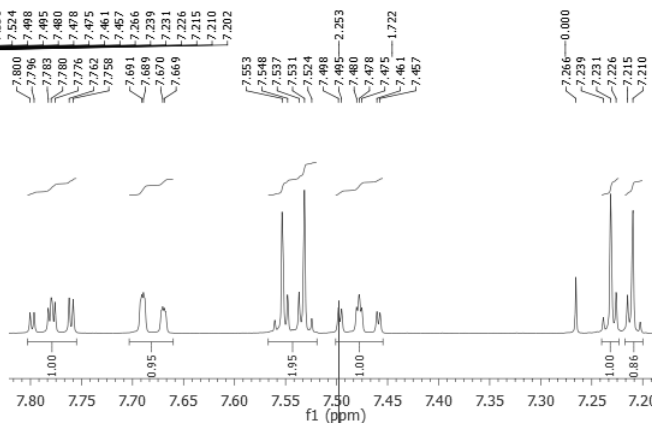
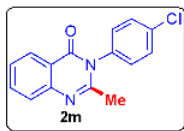
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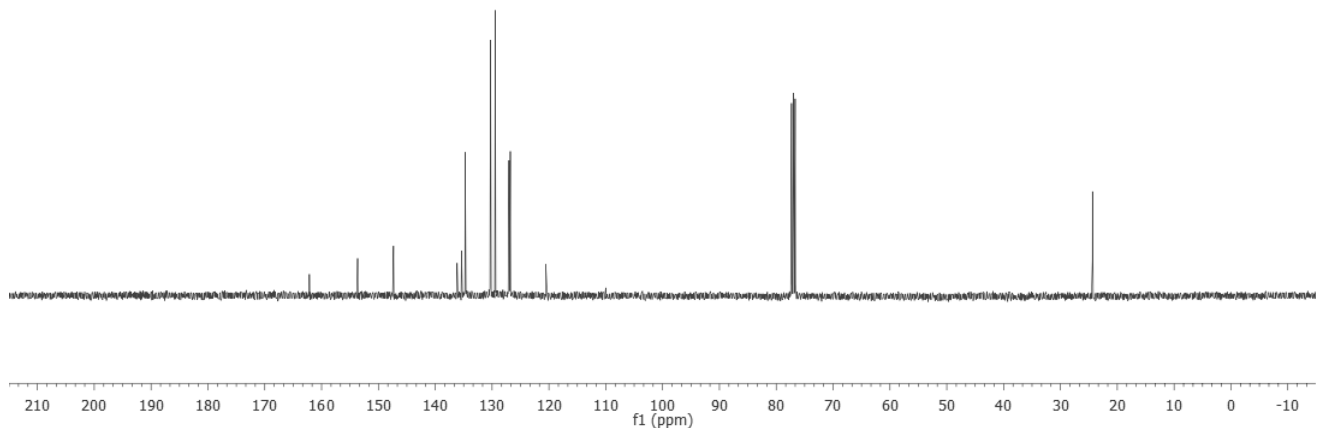
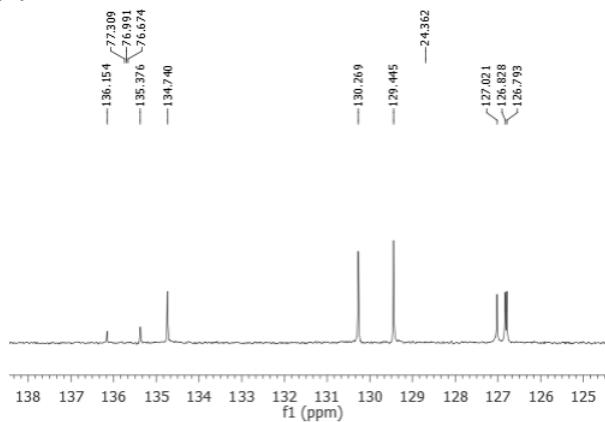
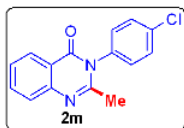
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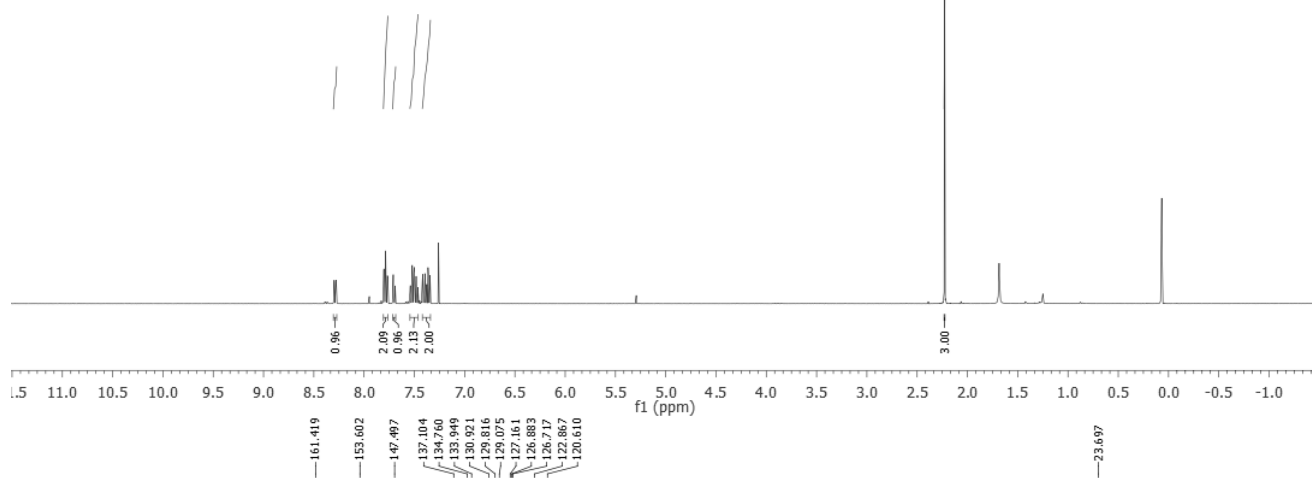
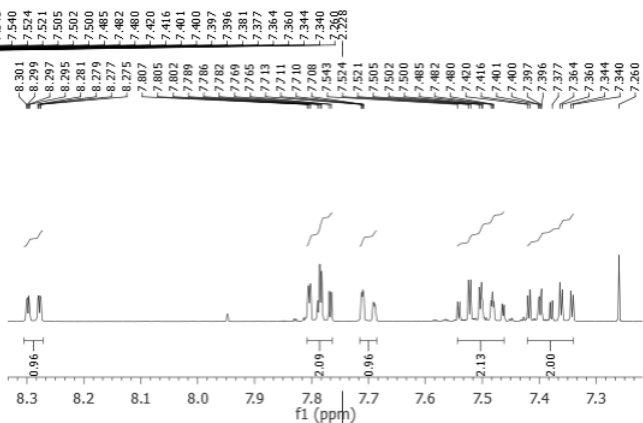
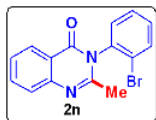
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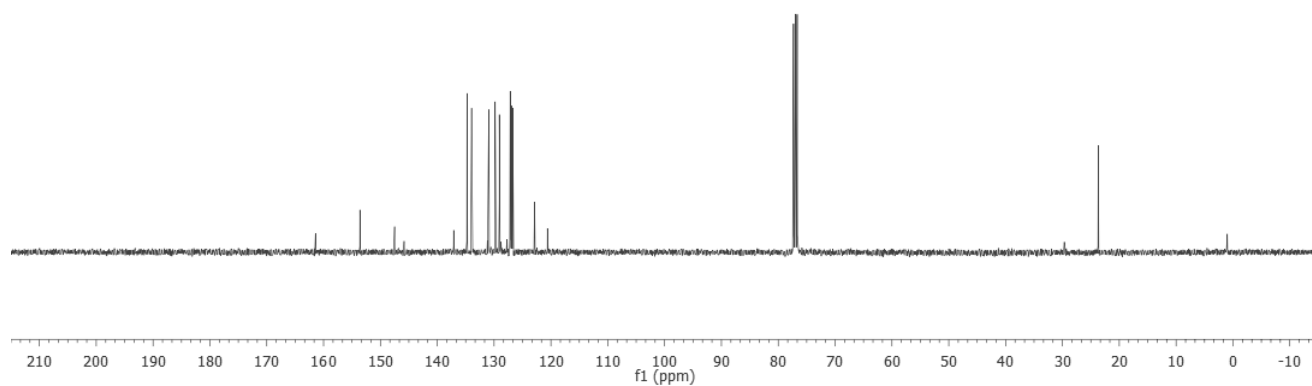
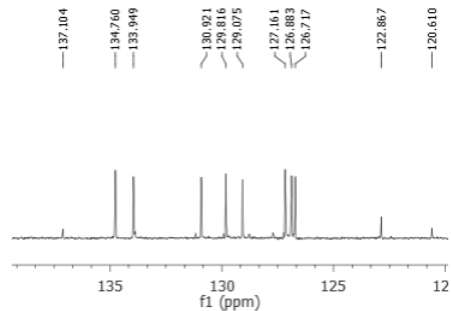
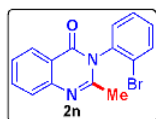
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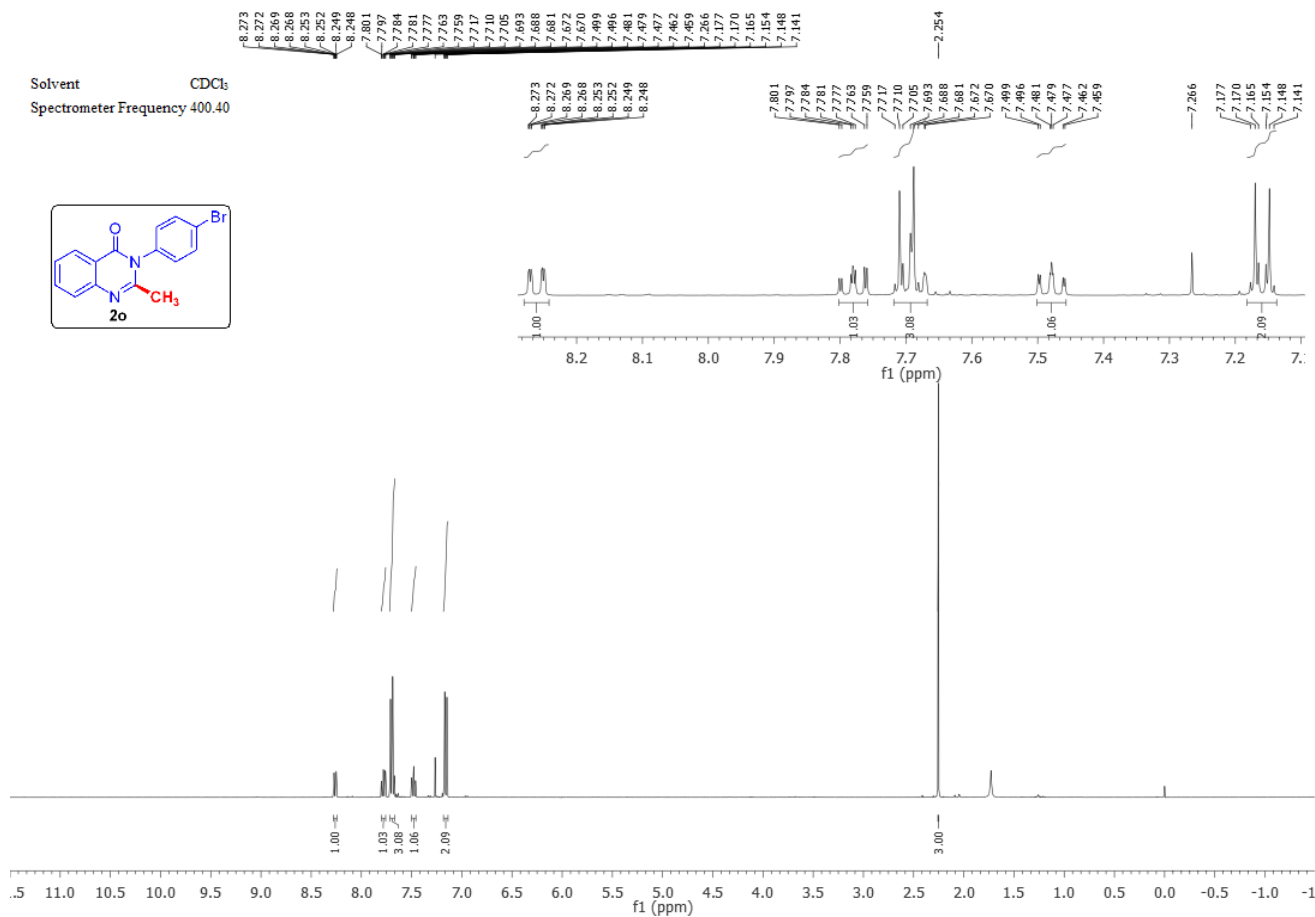
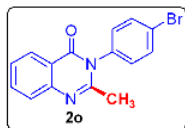
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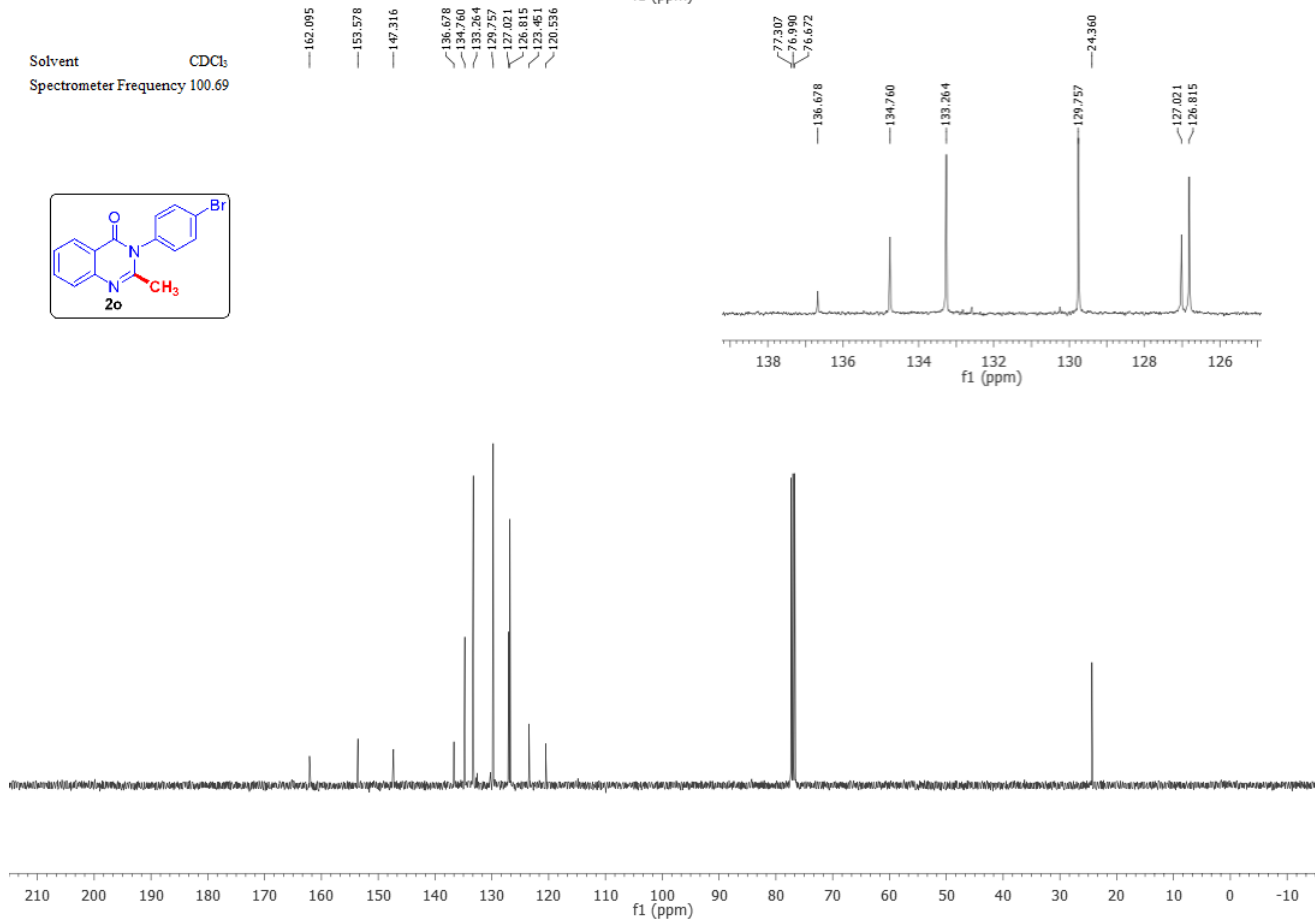
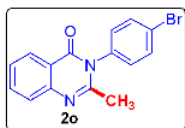
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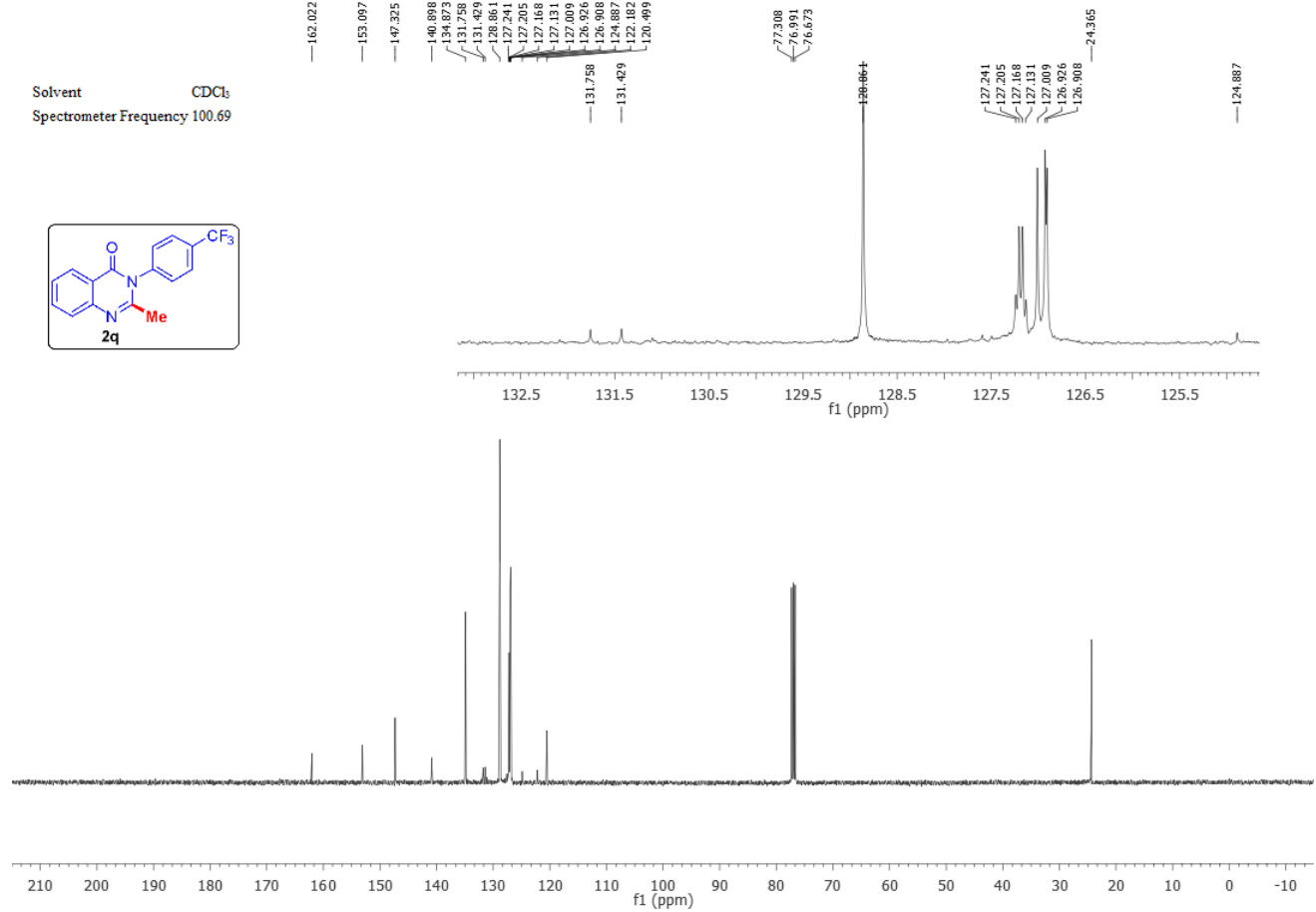
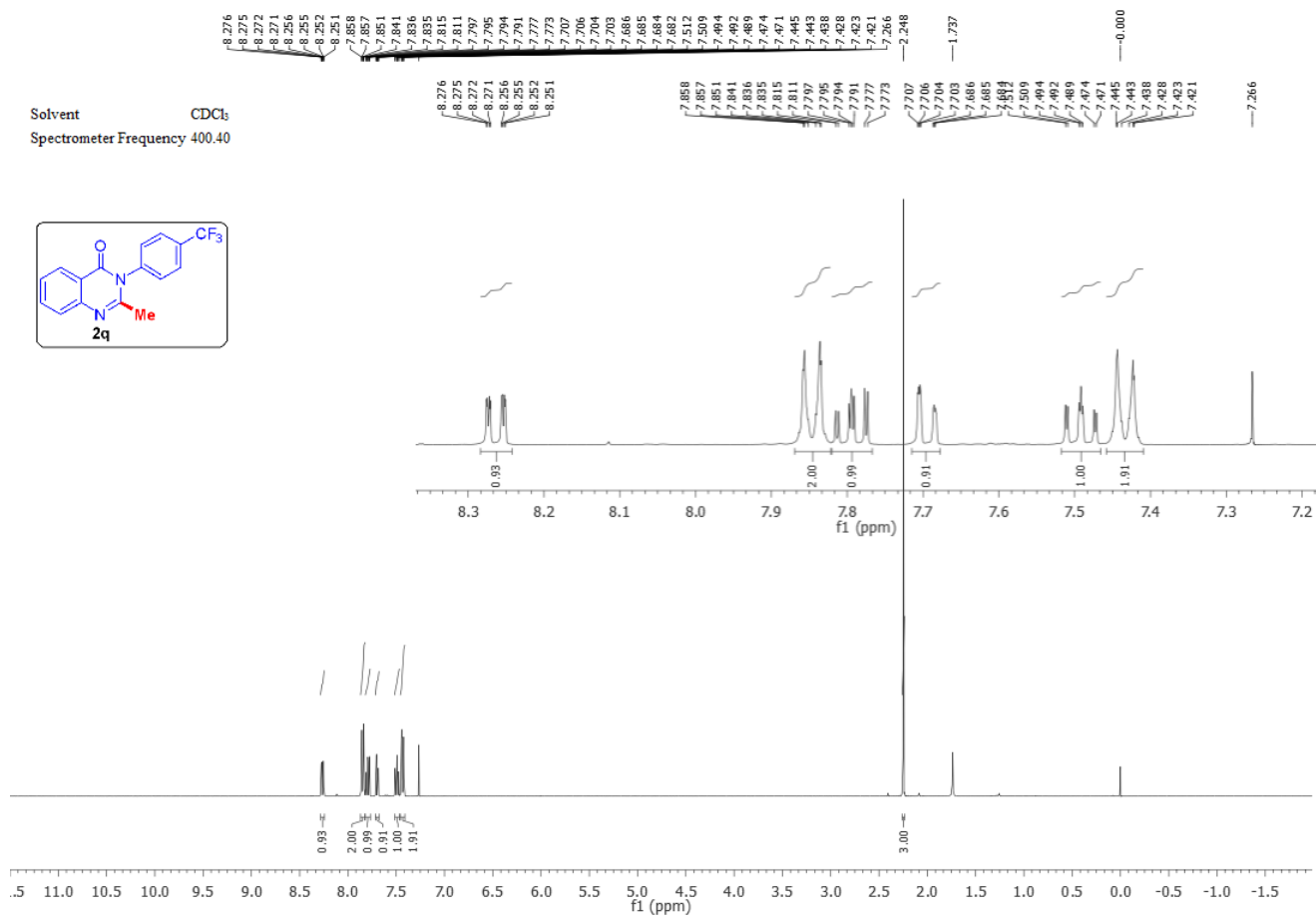


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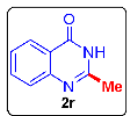


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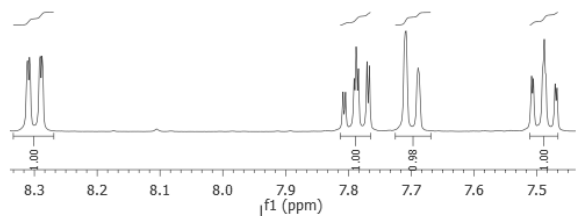




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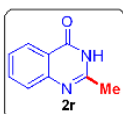


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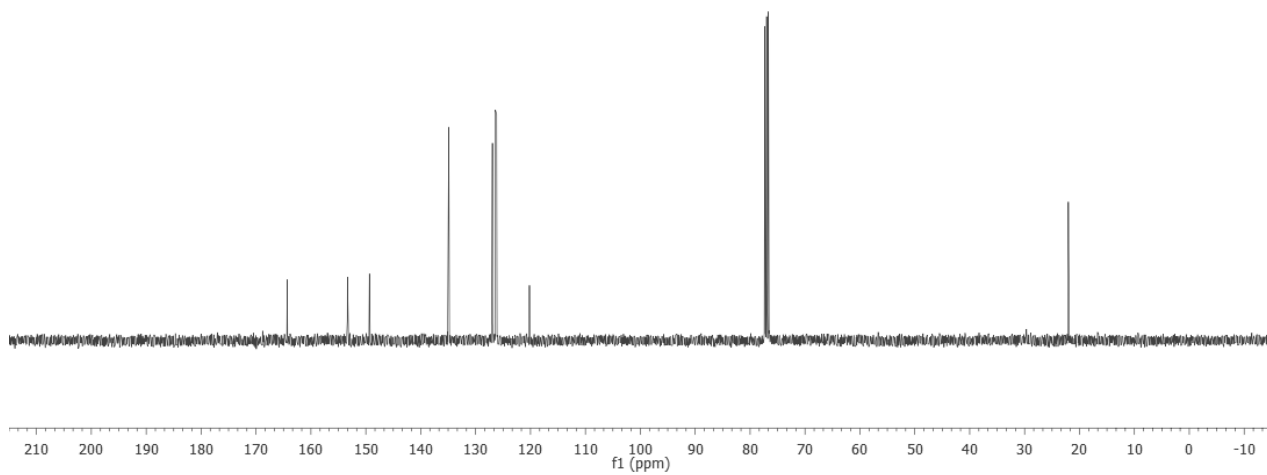
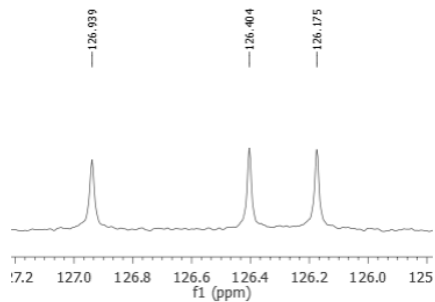


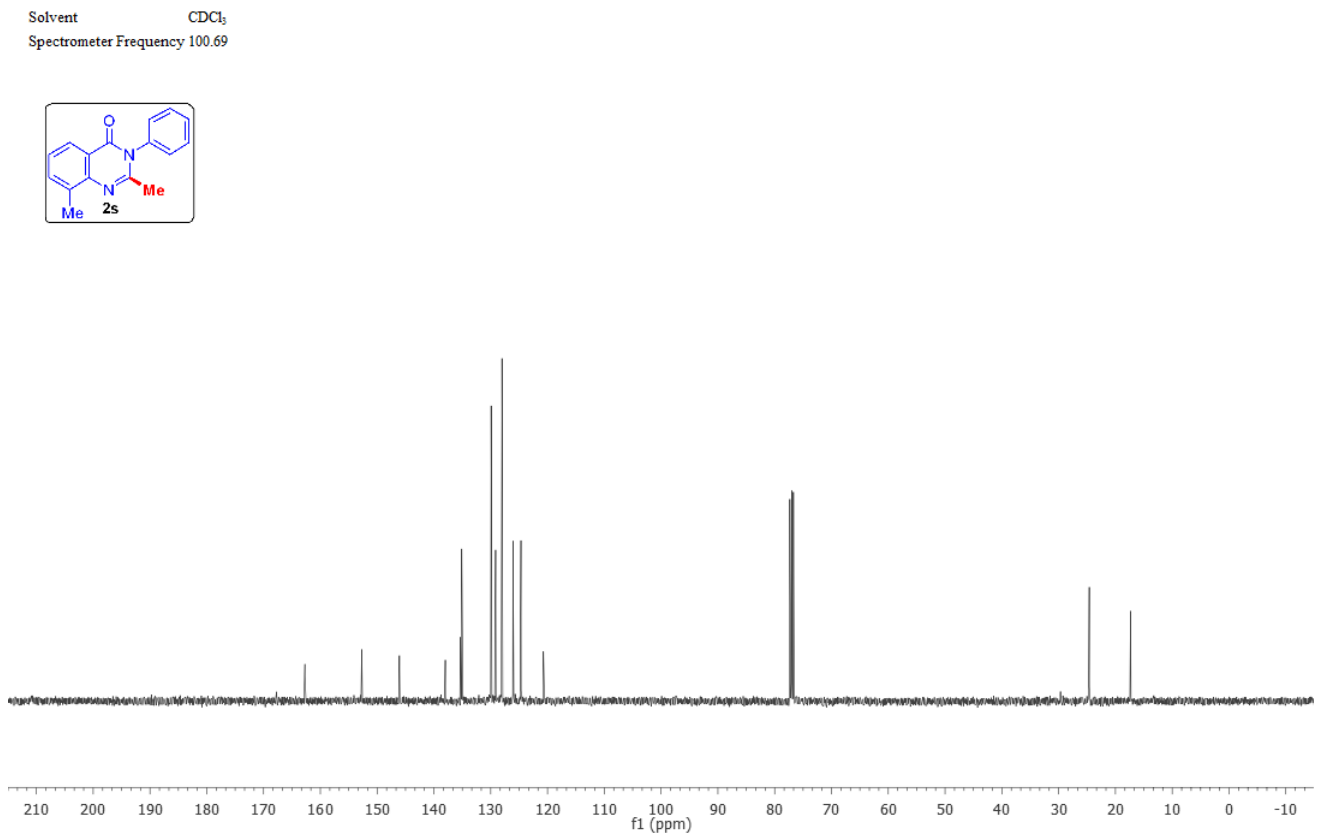
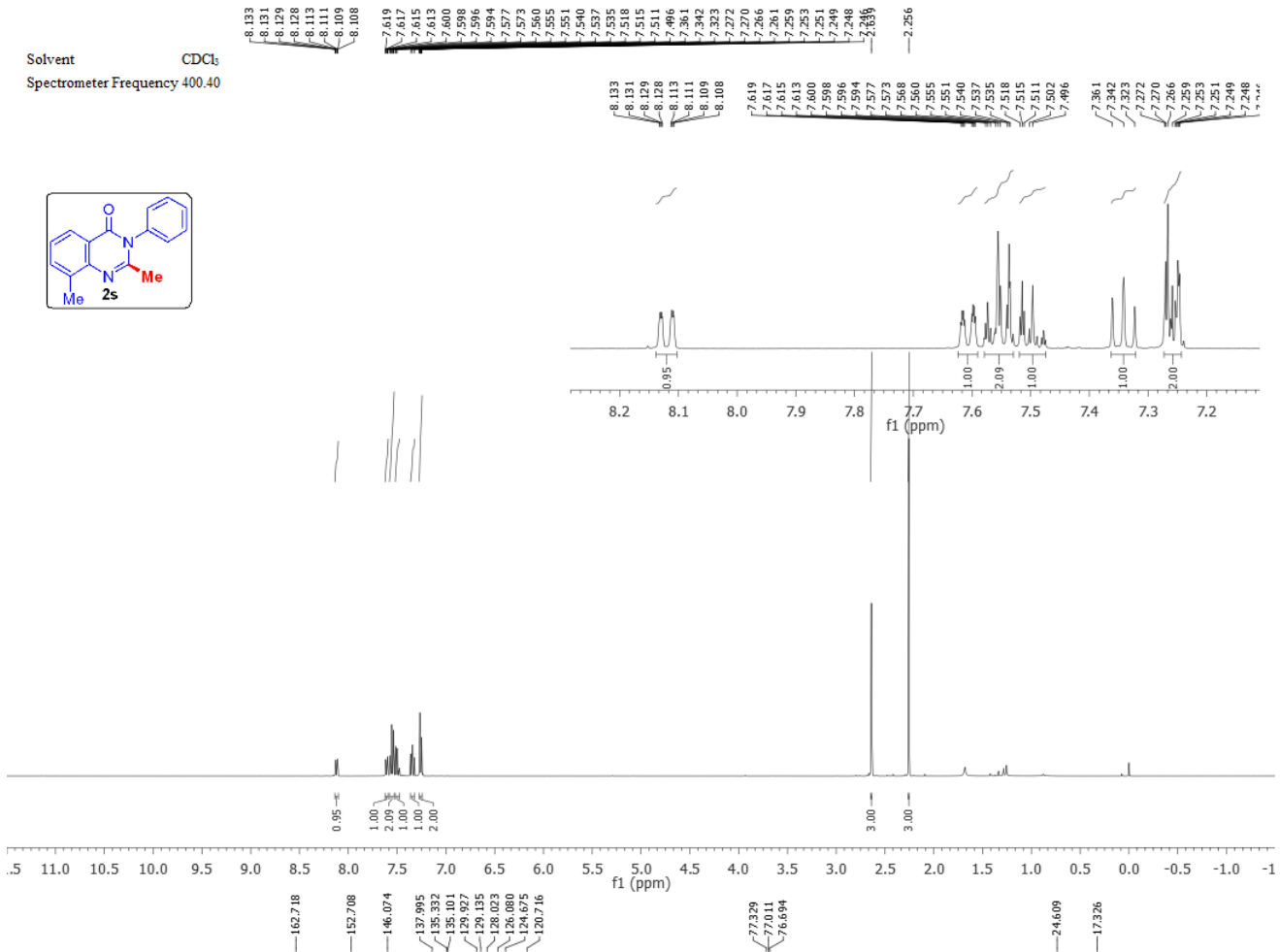
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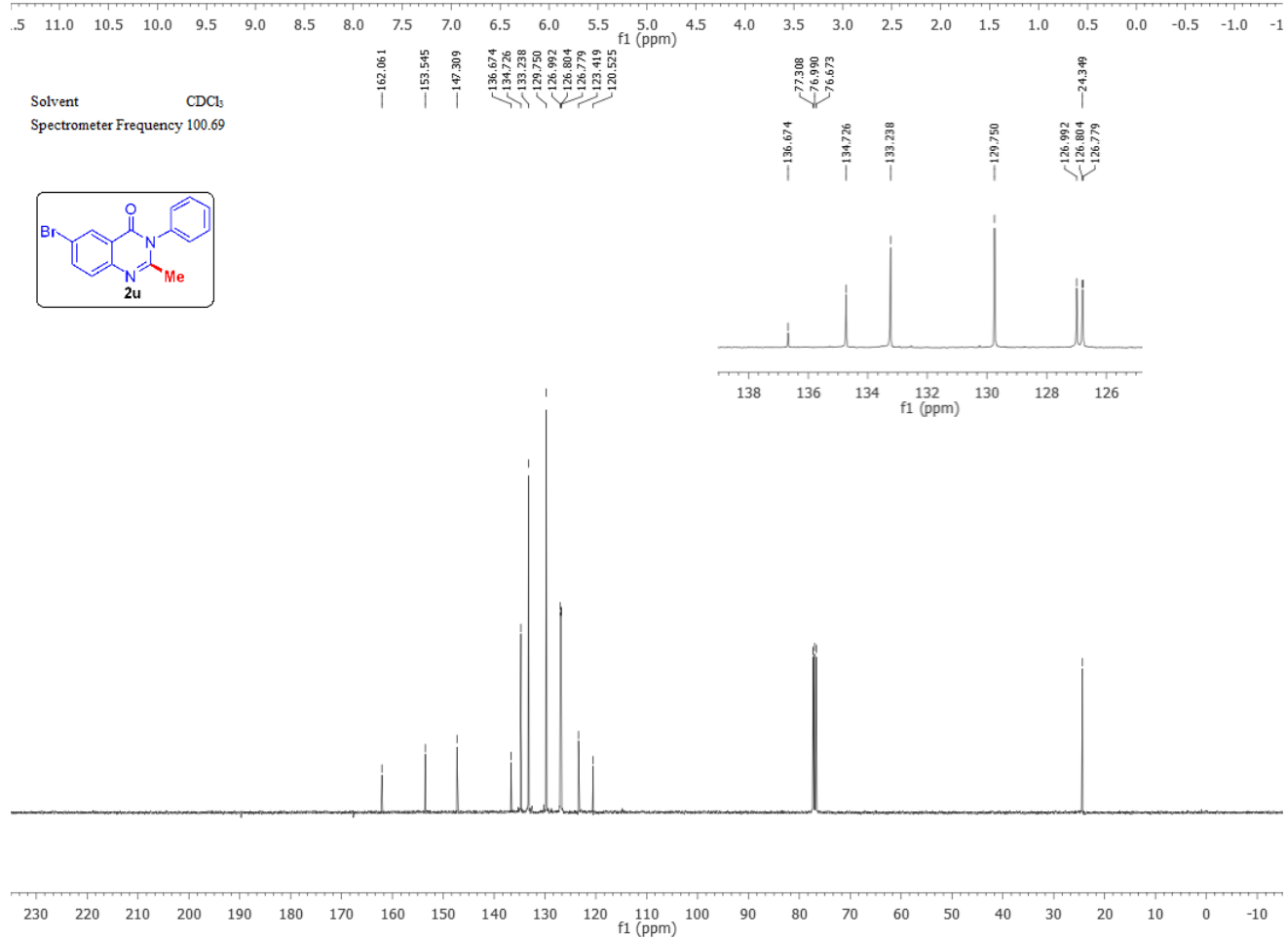
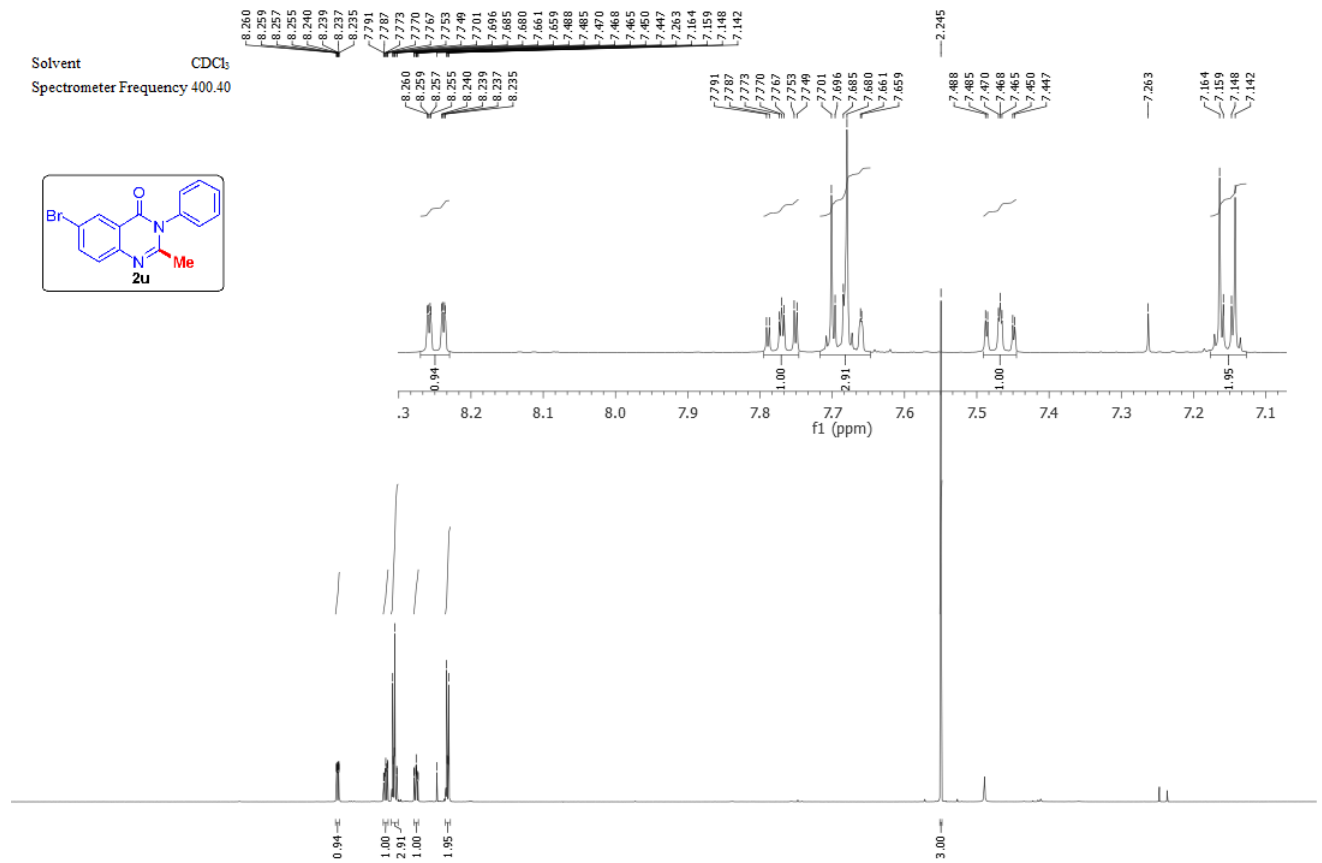
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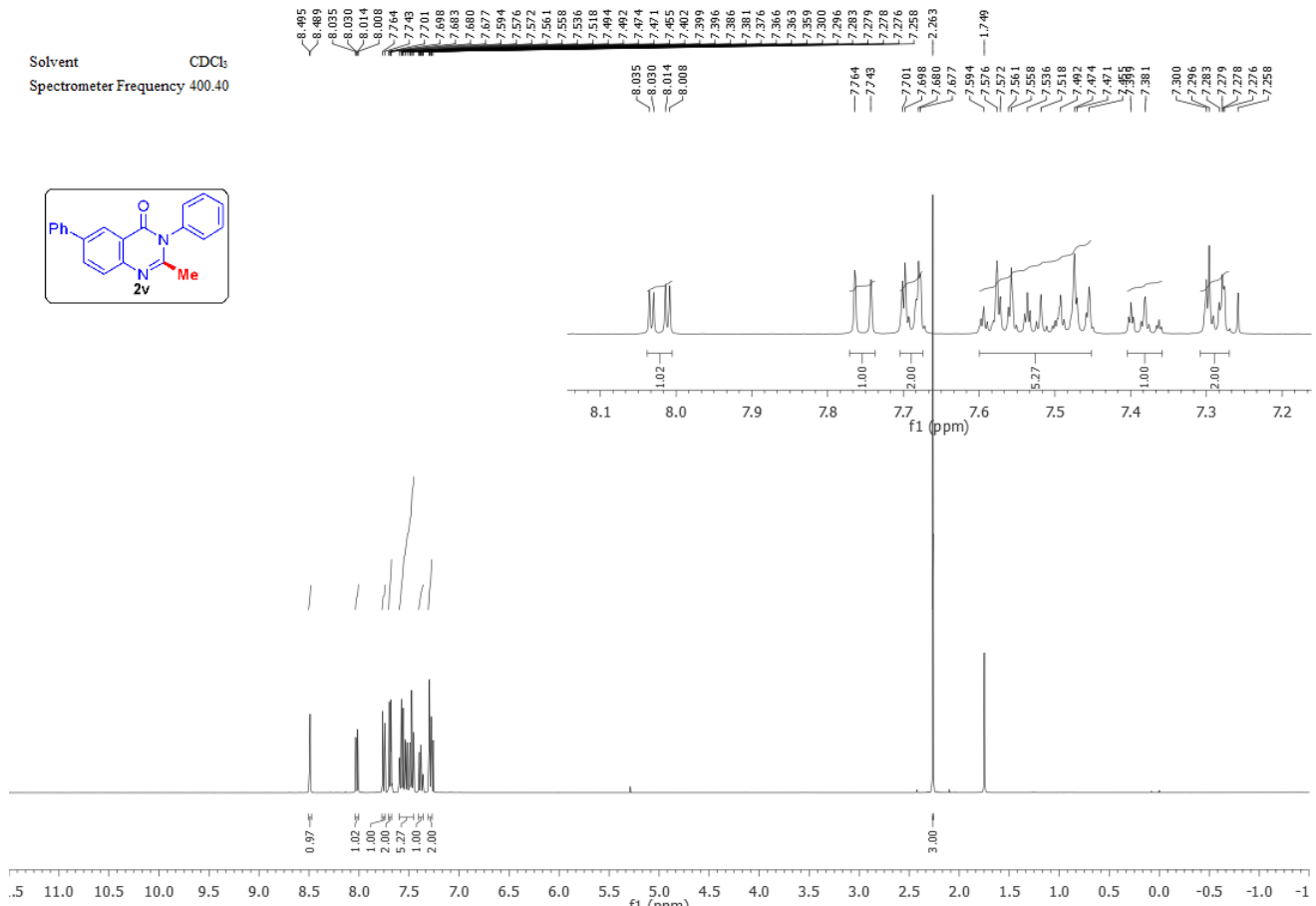
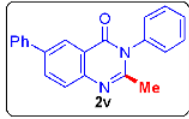




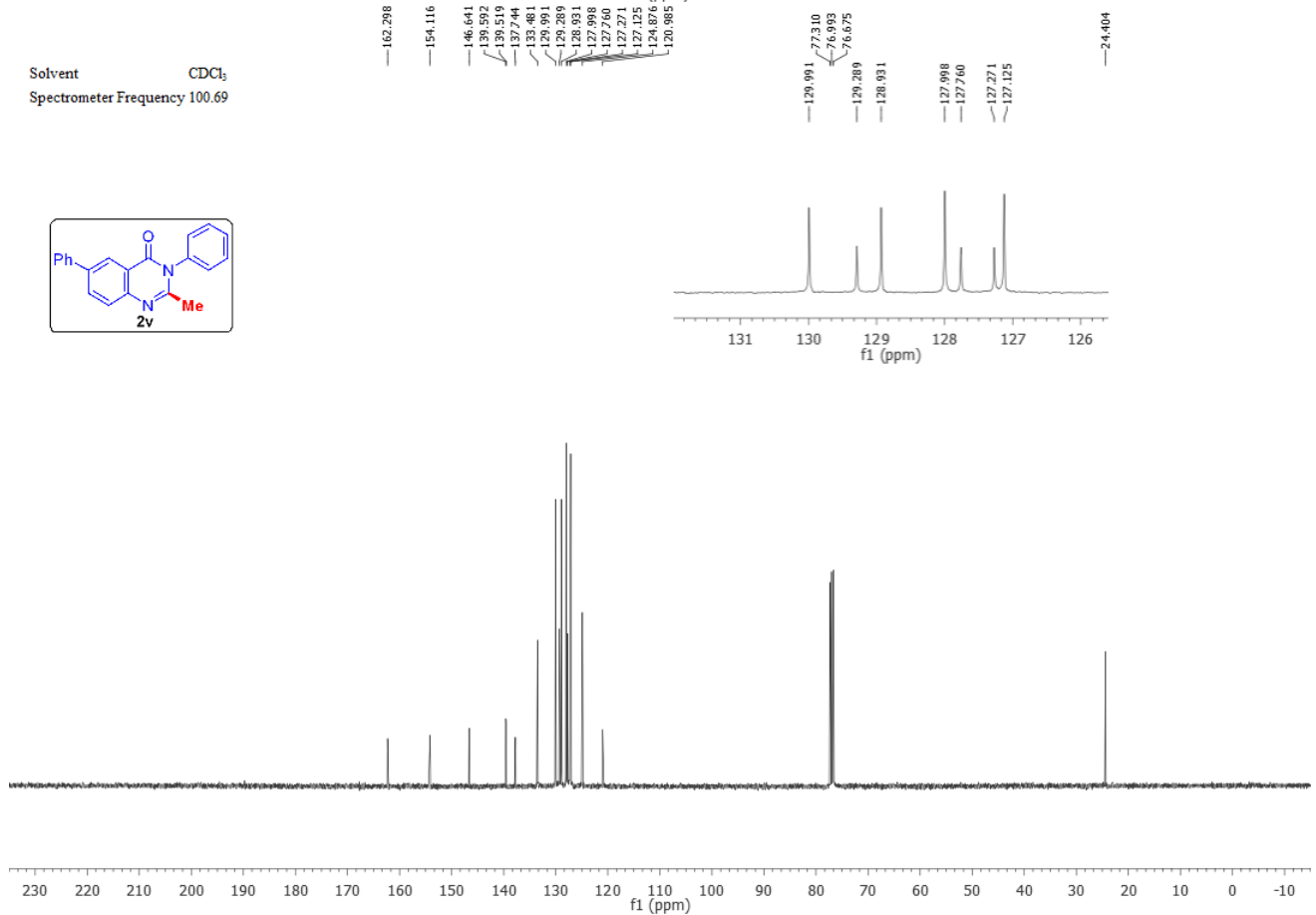
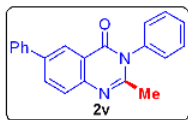


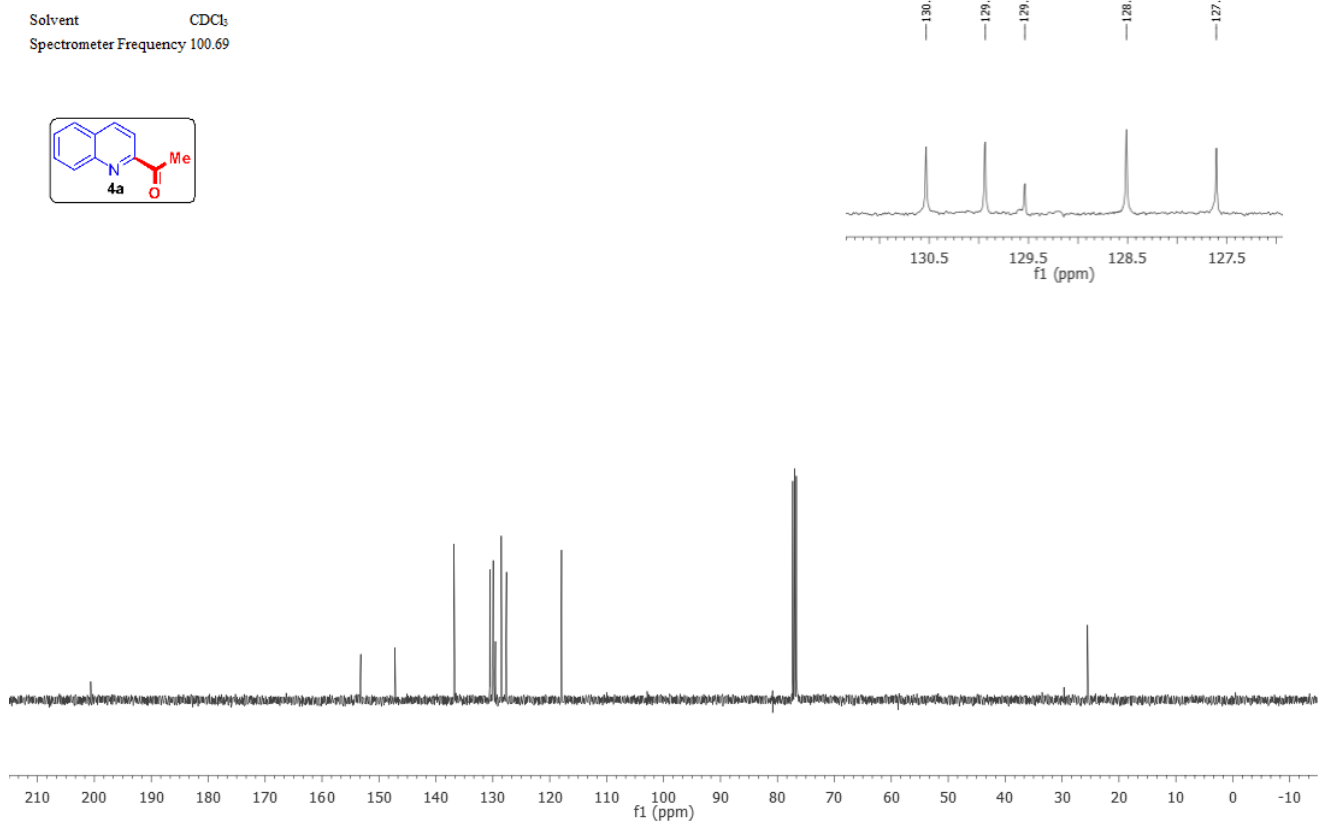
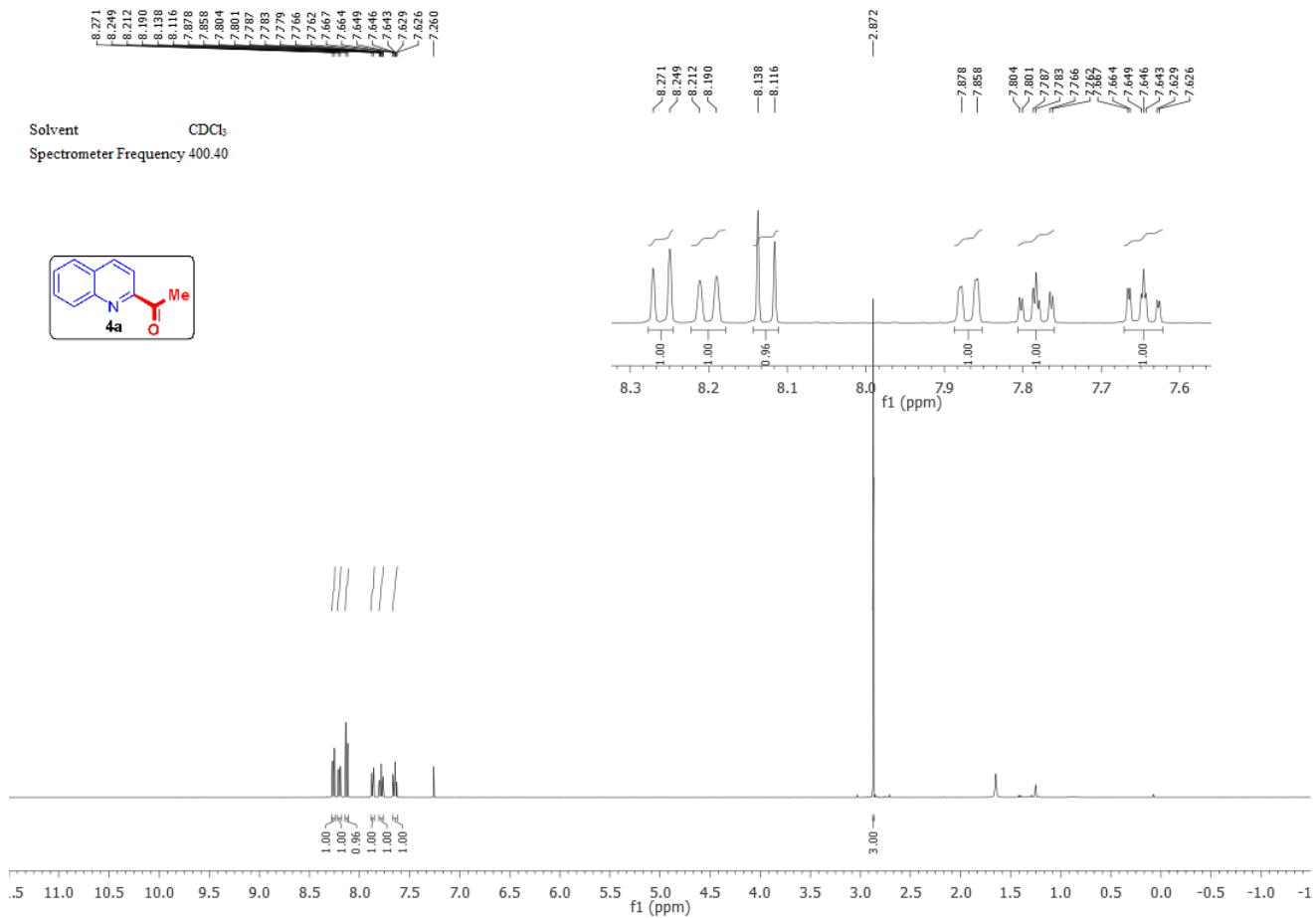


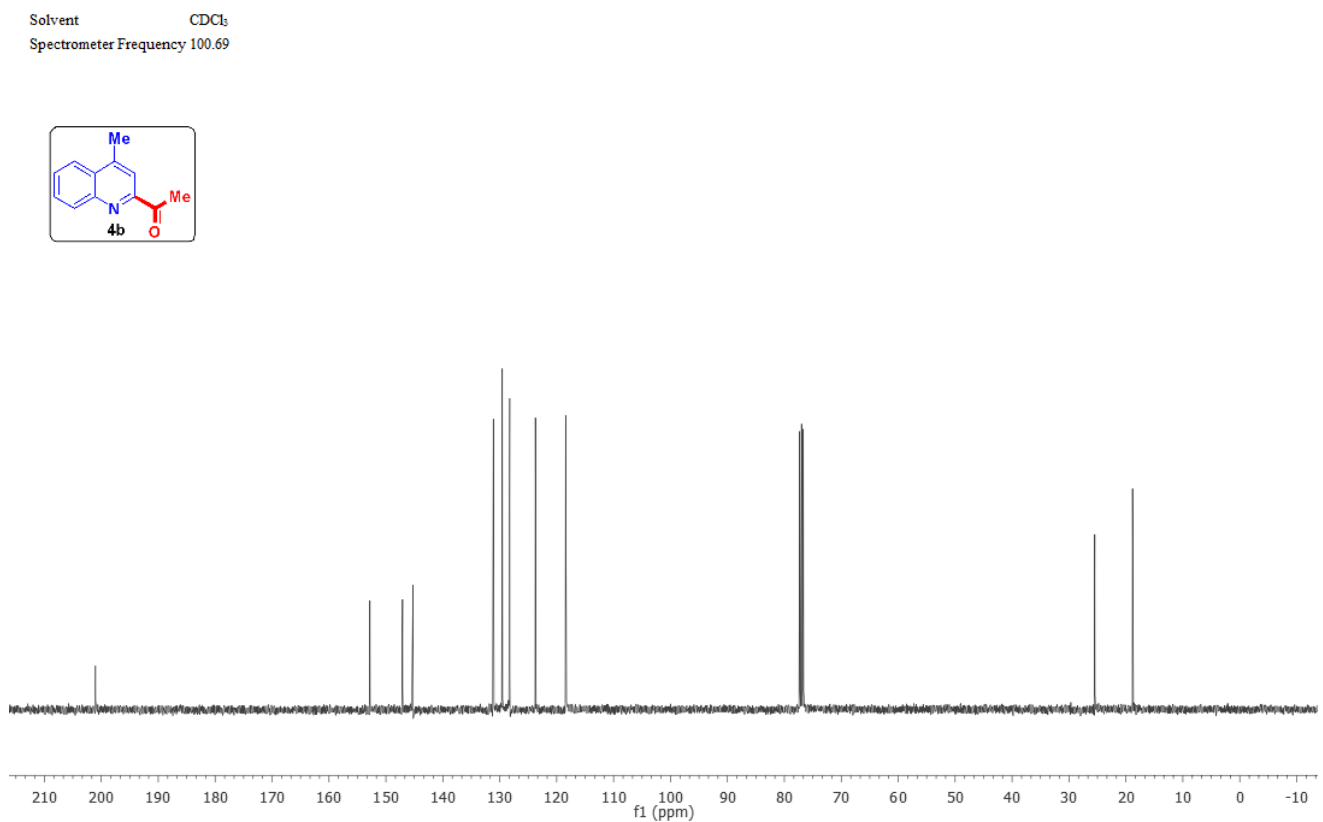
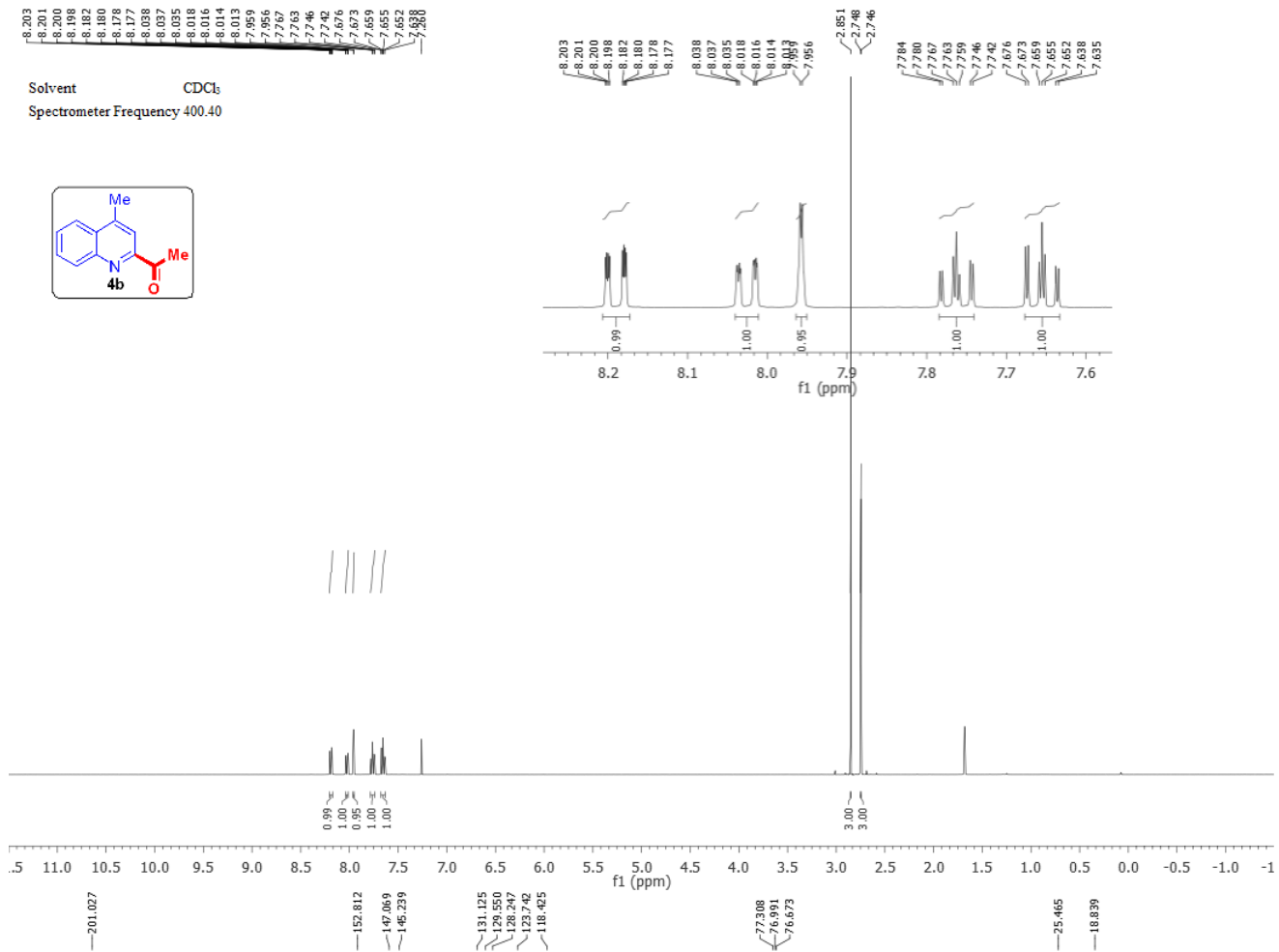
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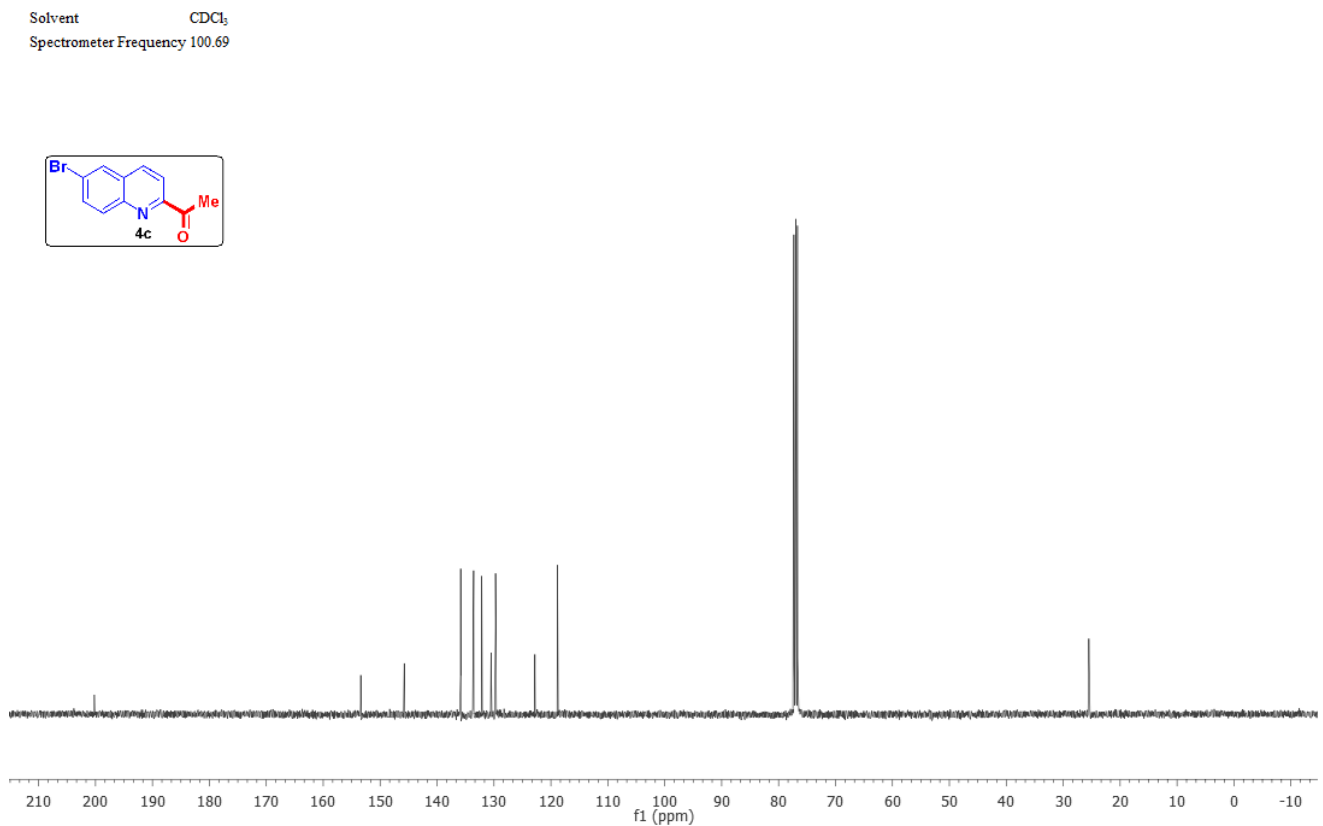
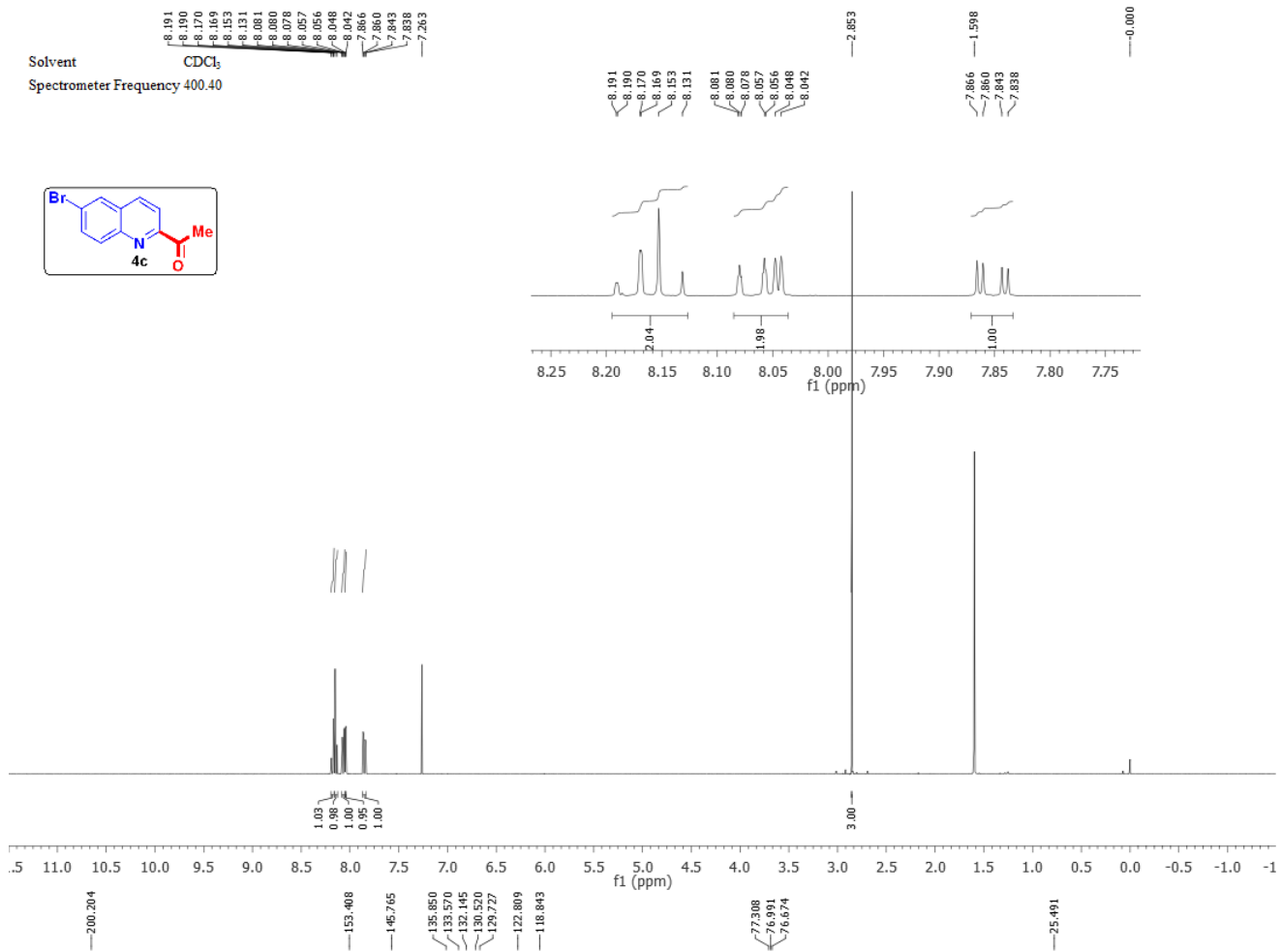


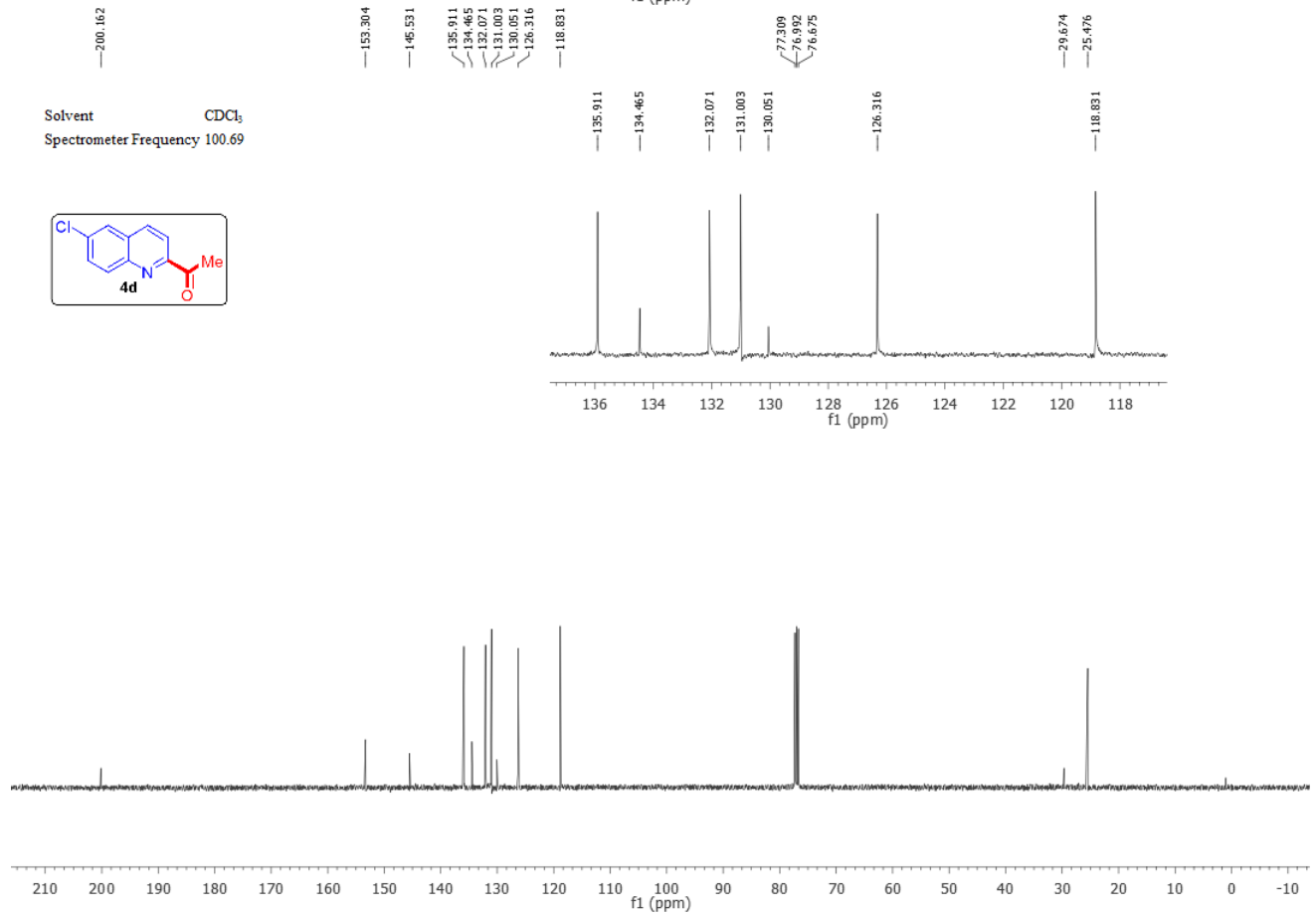
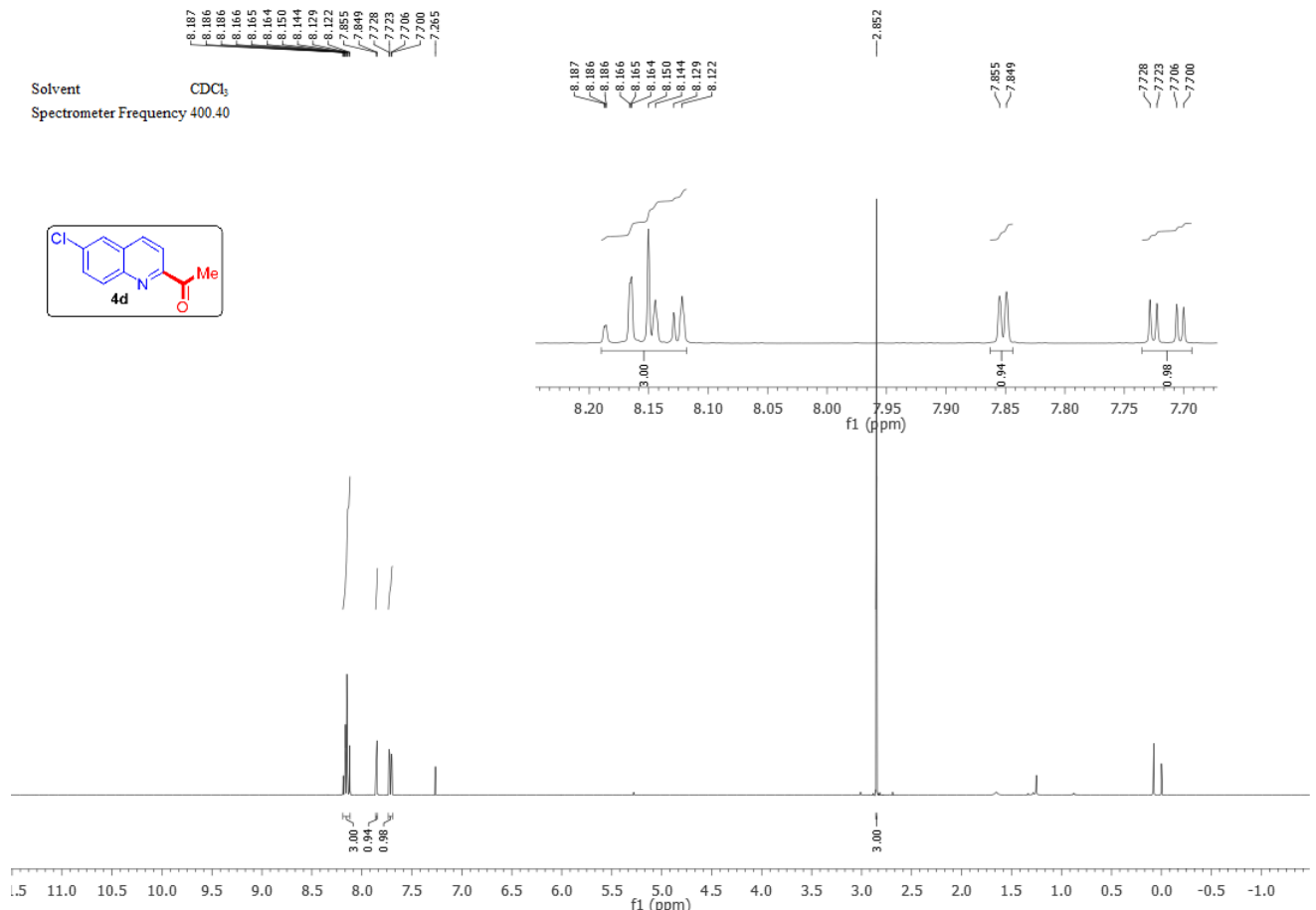
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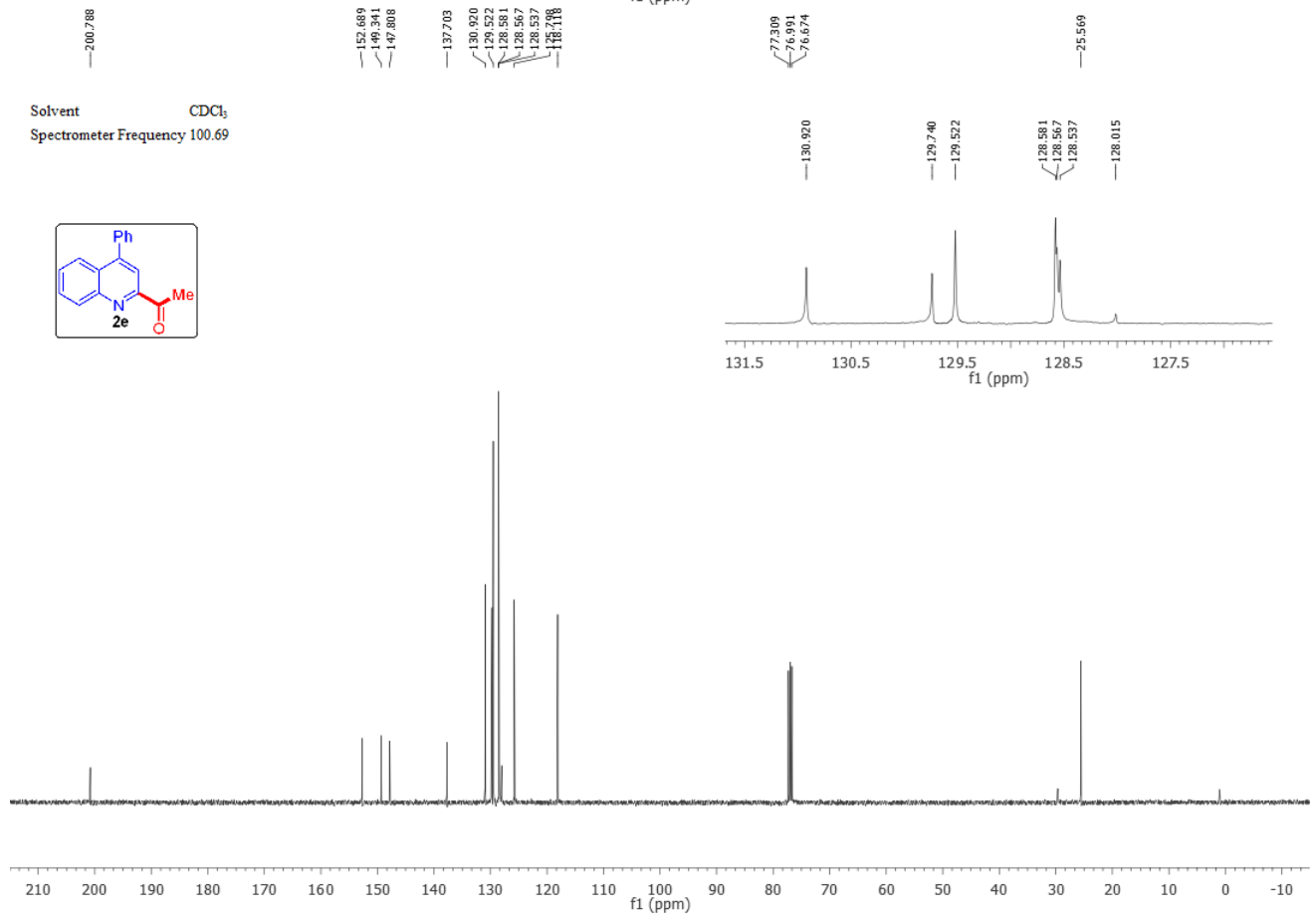
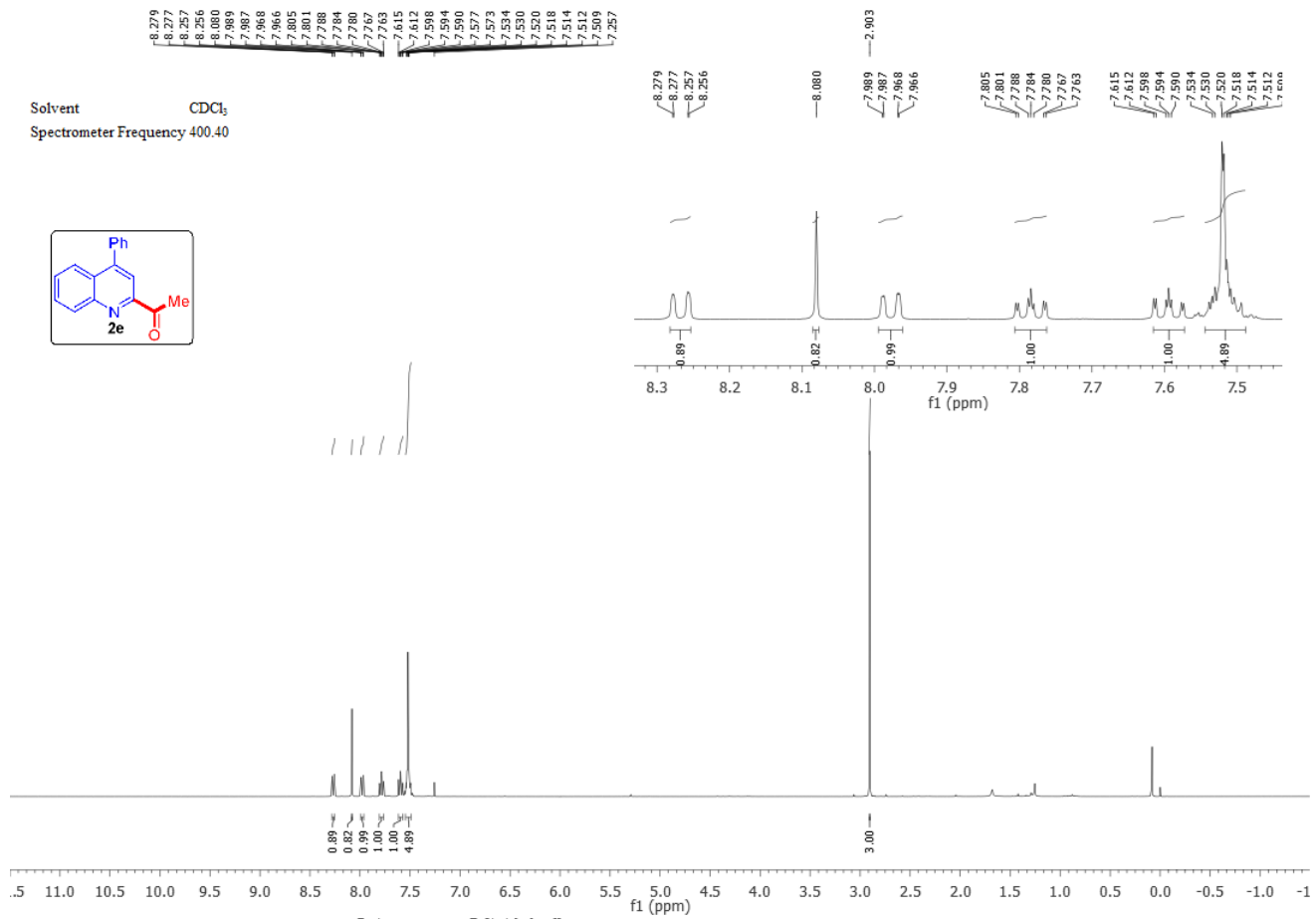






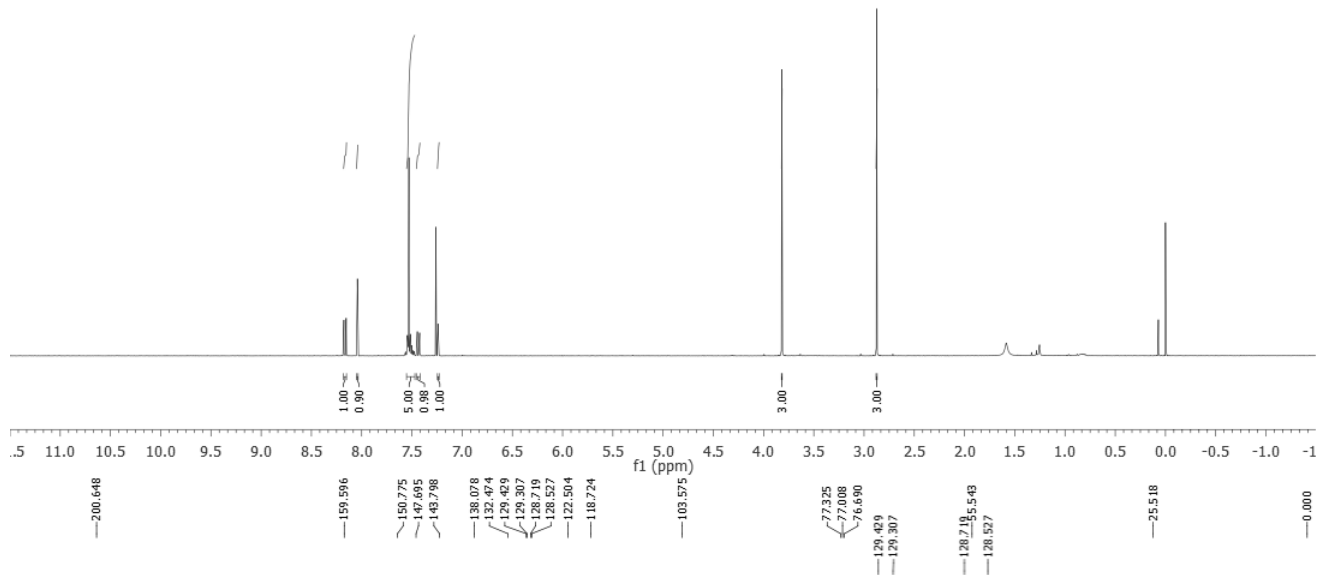
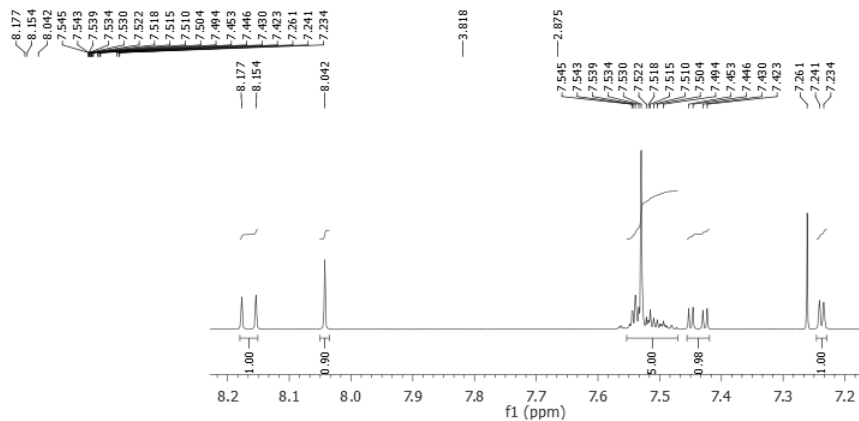
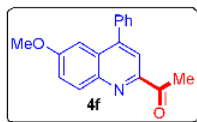




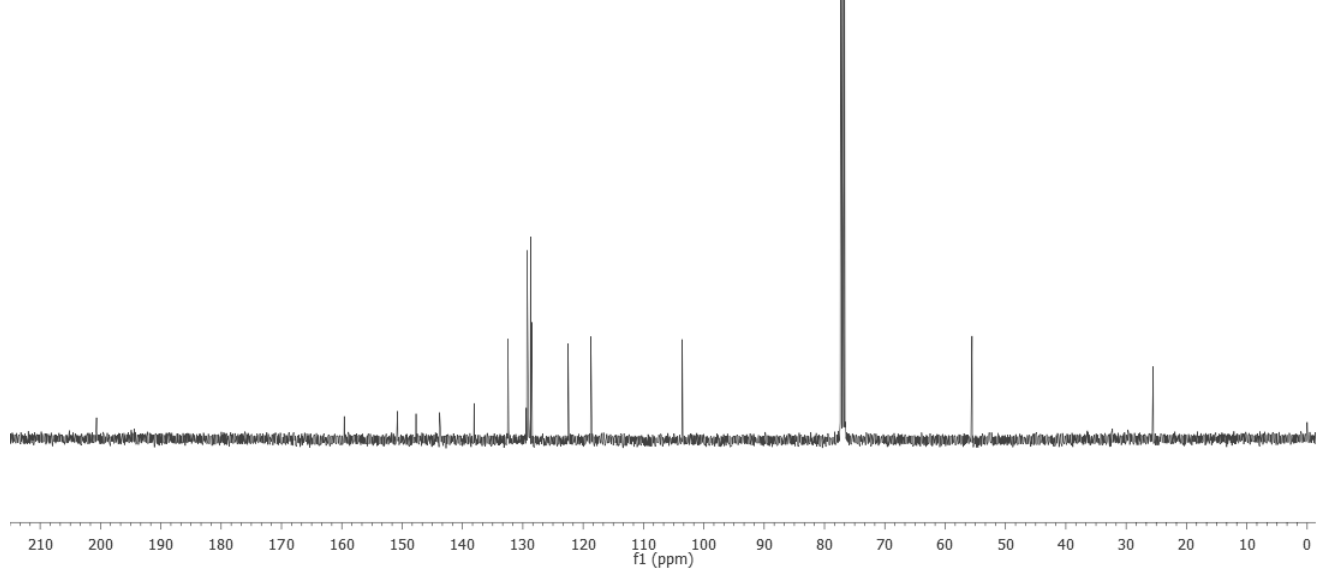
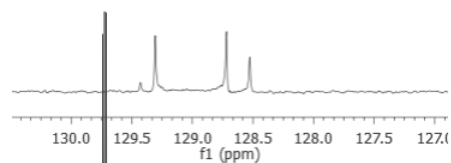
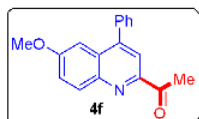


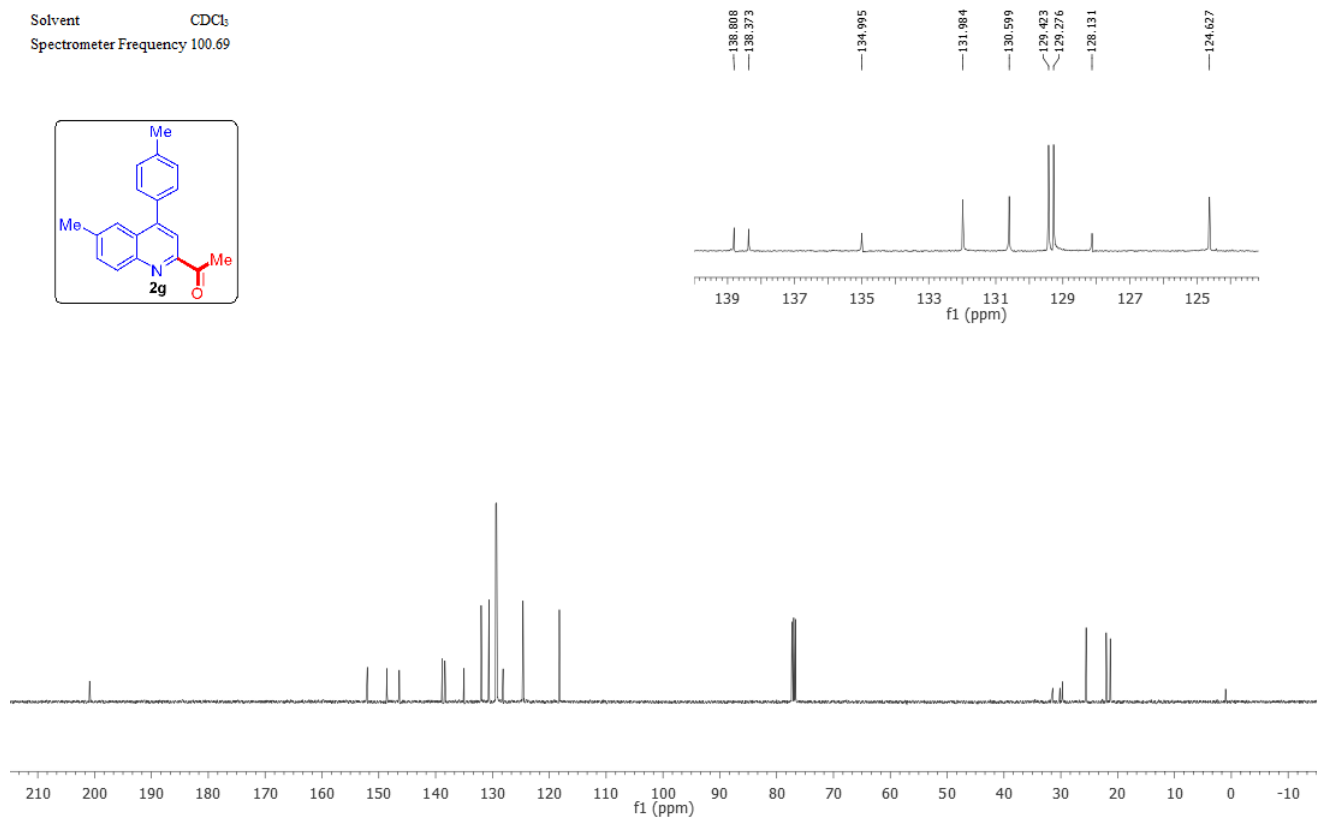
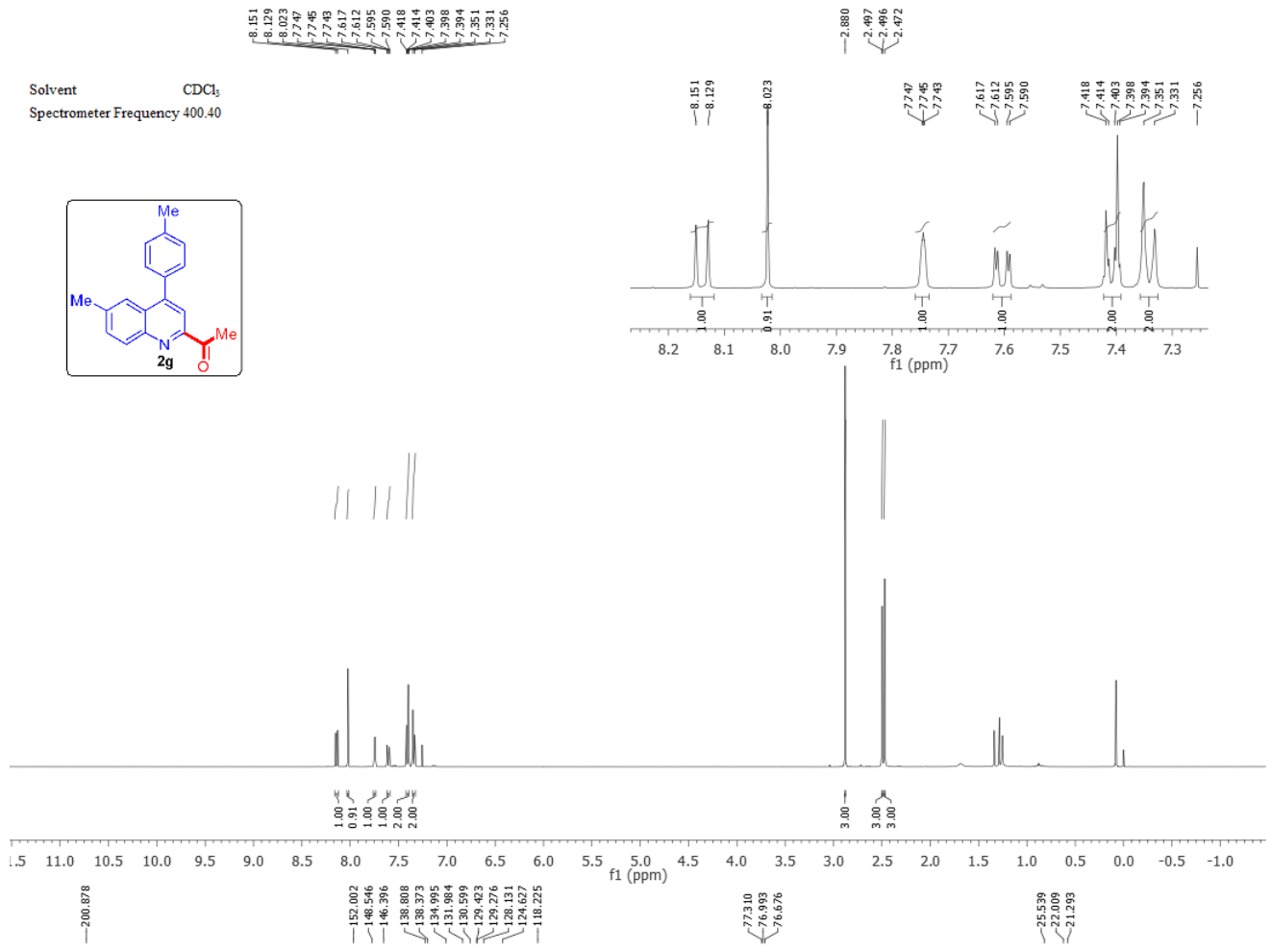


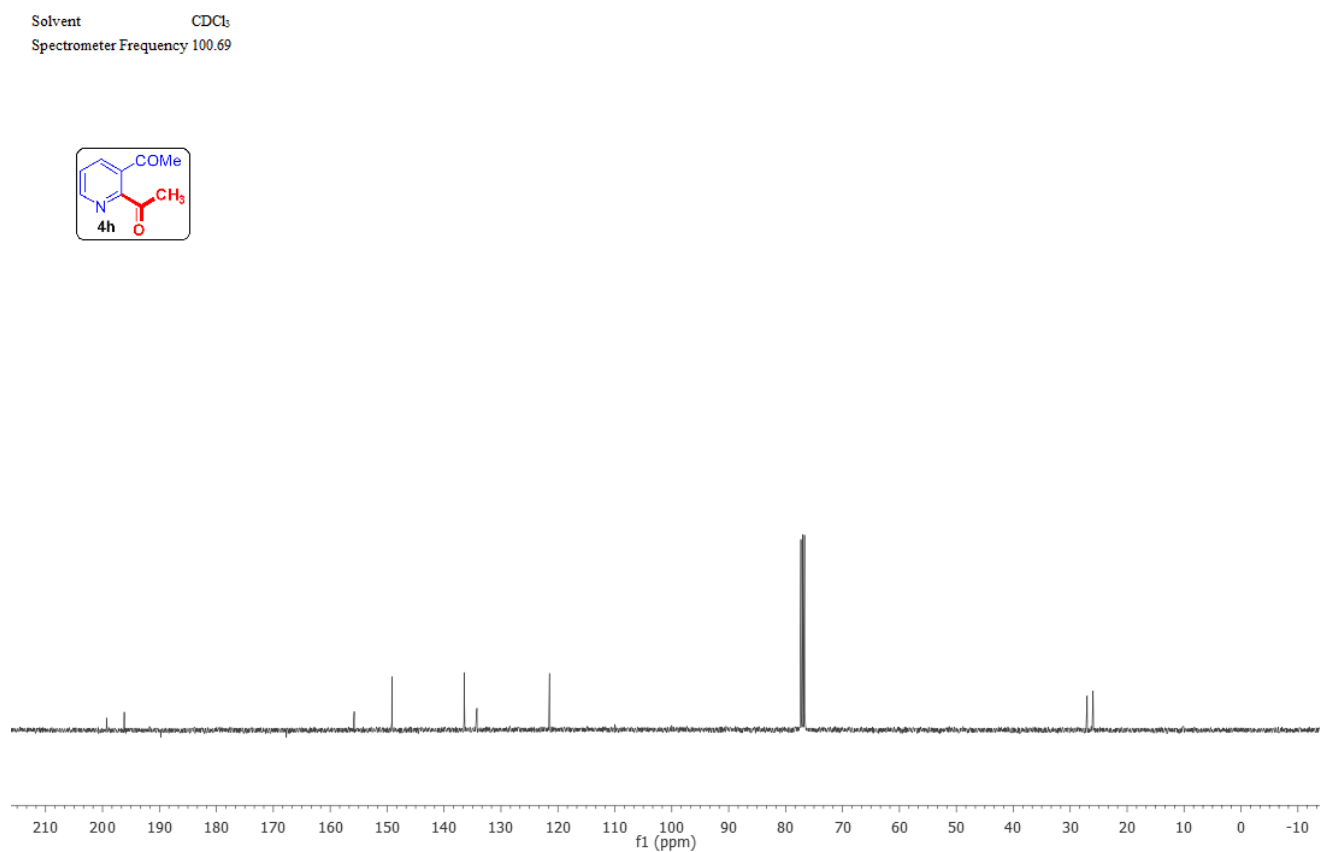
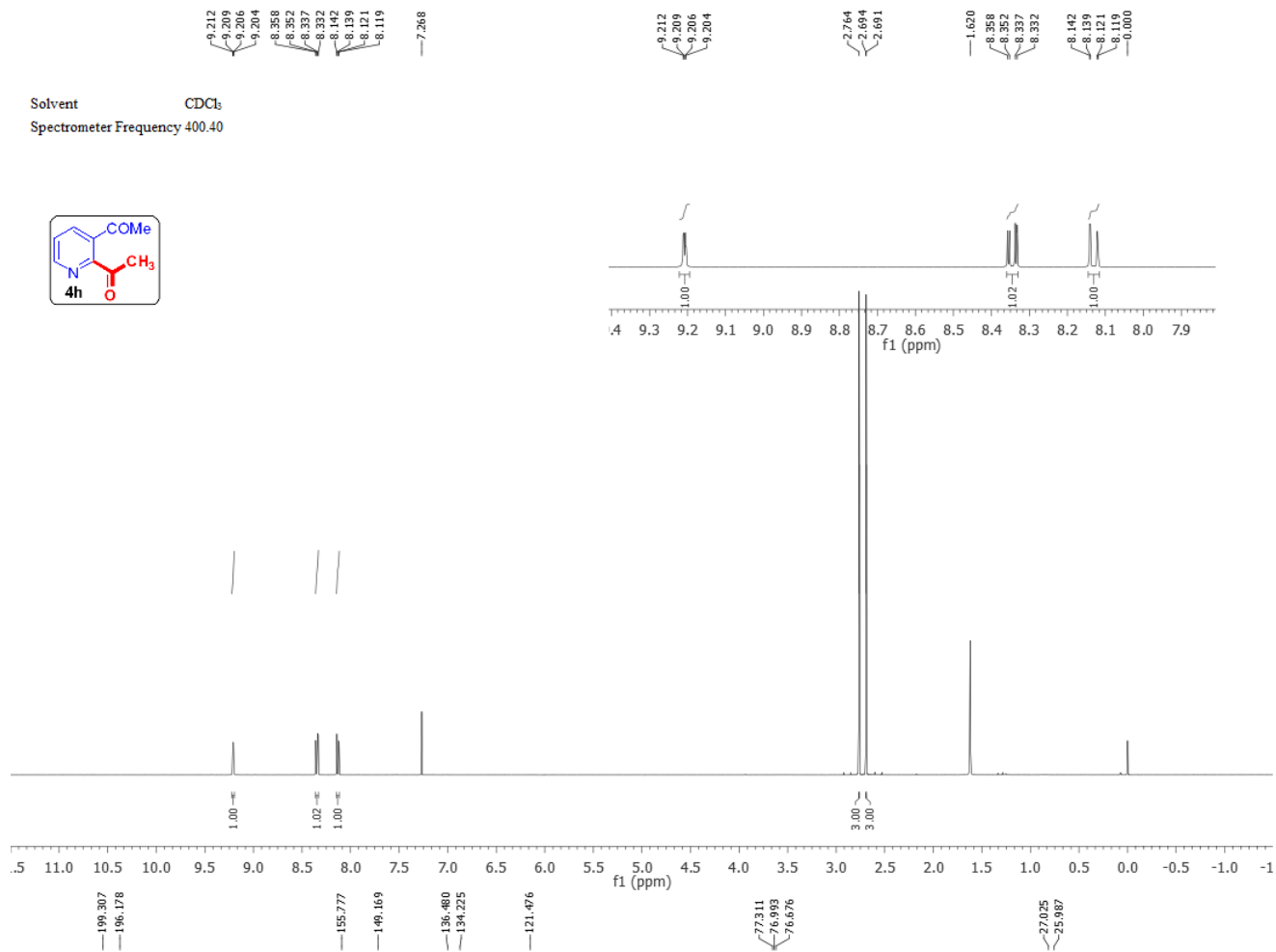
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.40

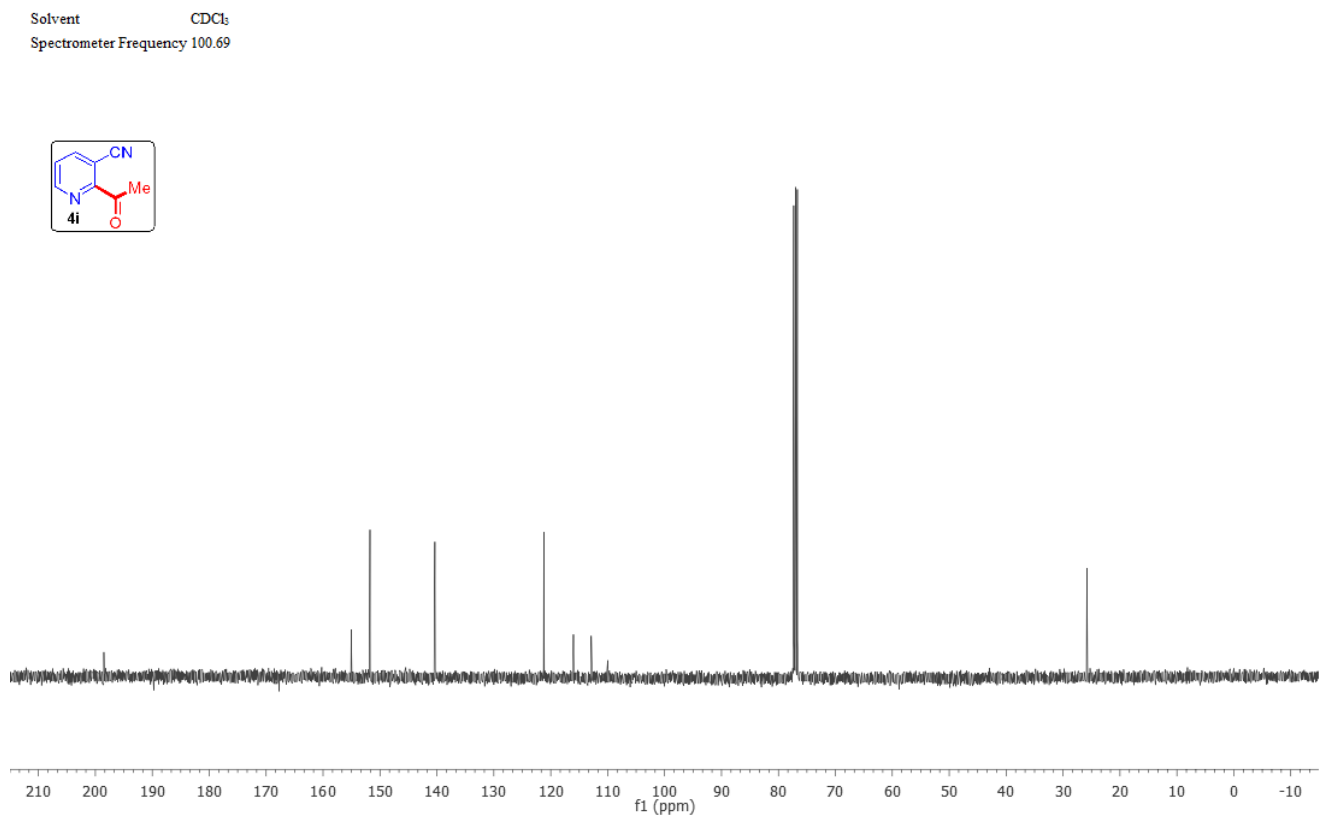
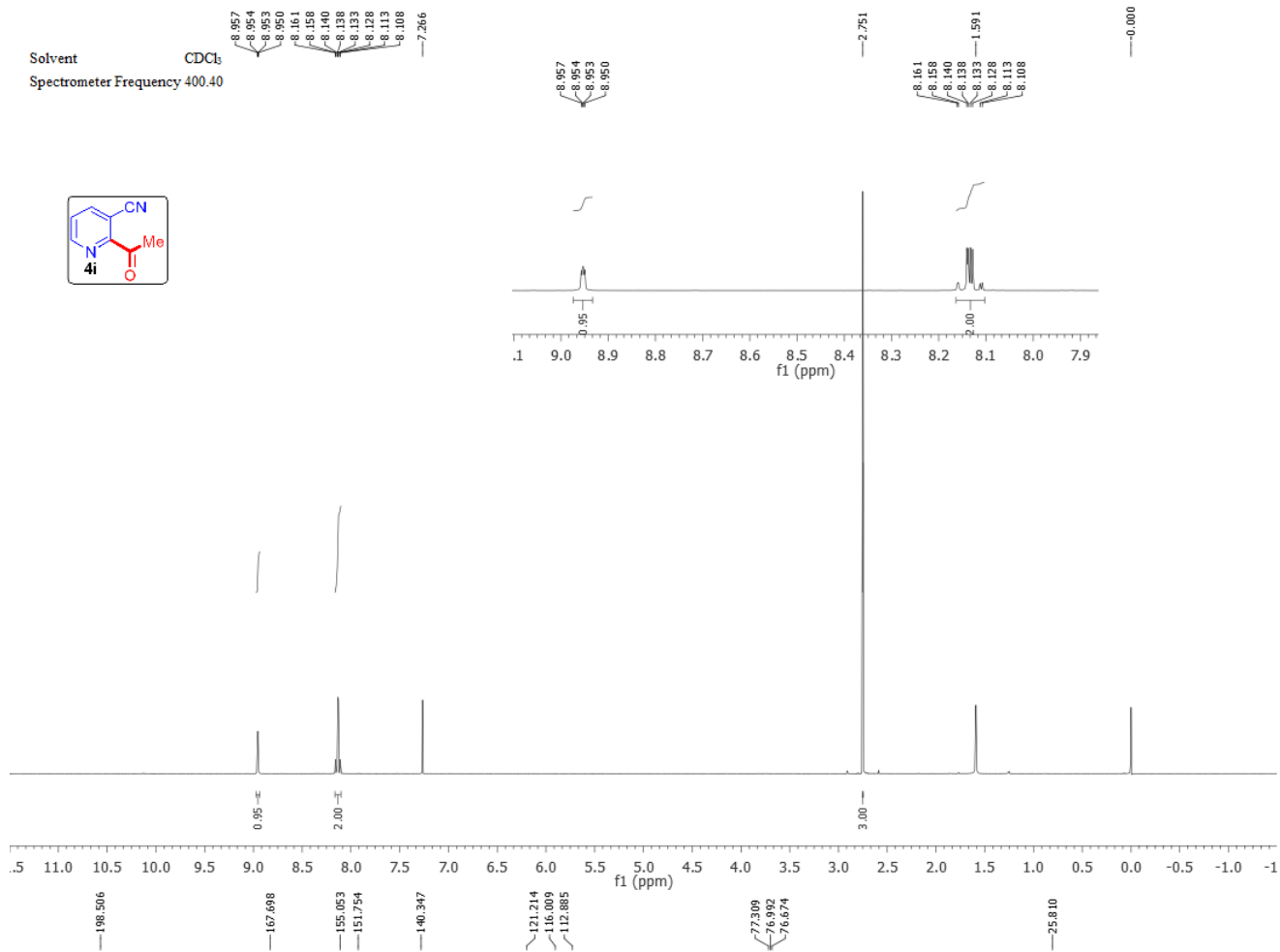


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69

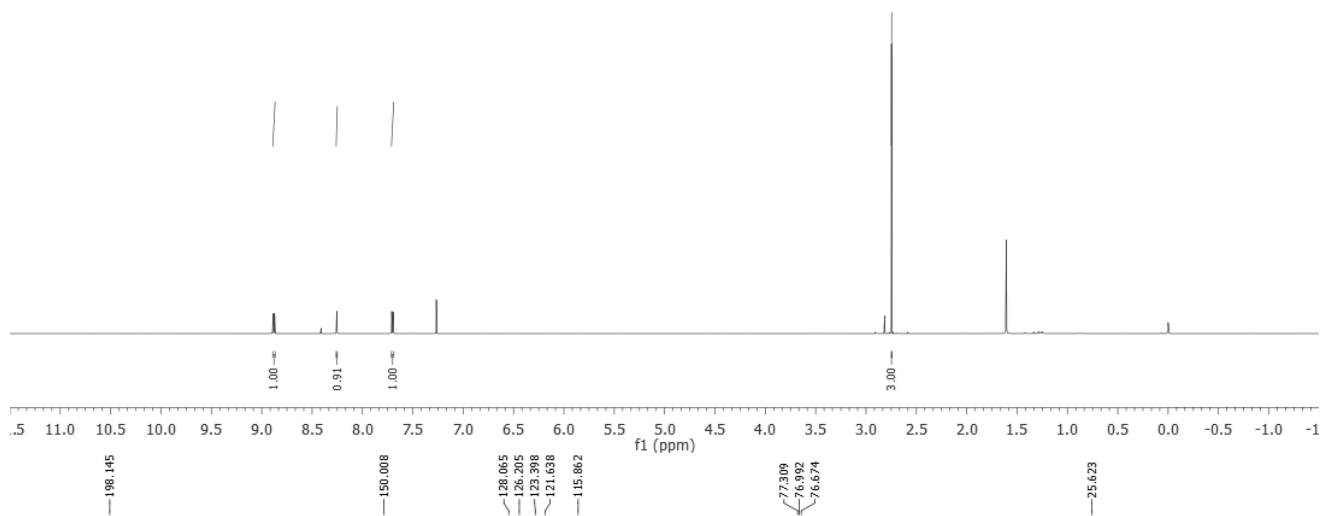
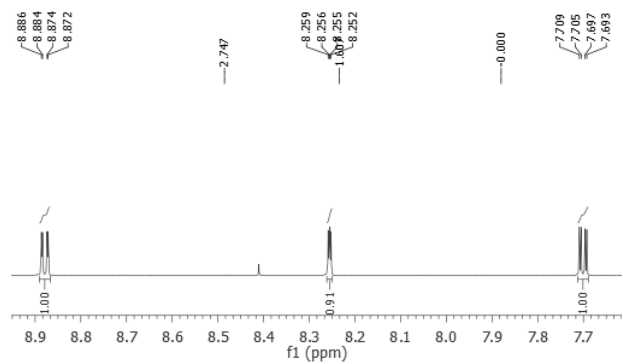
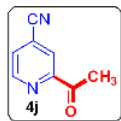




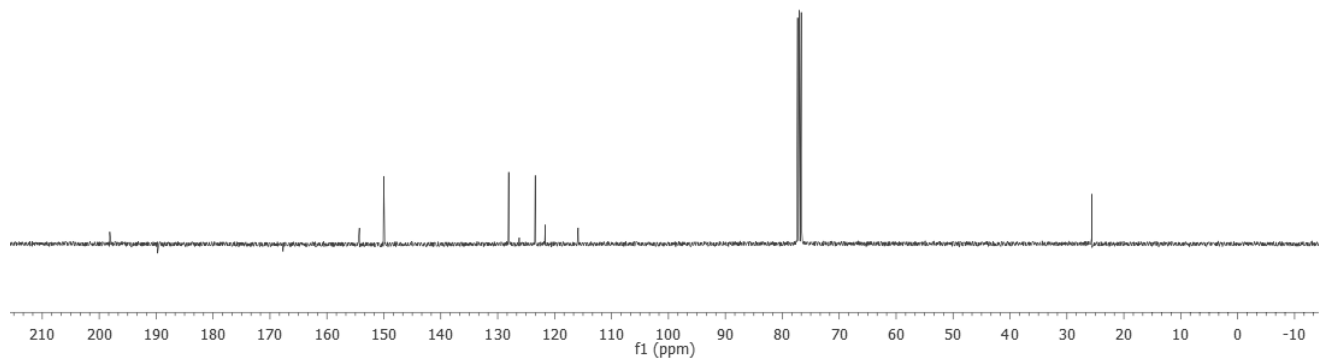
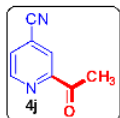


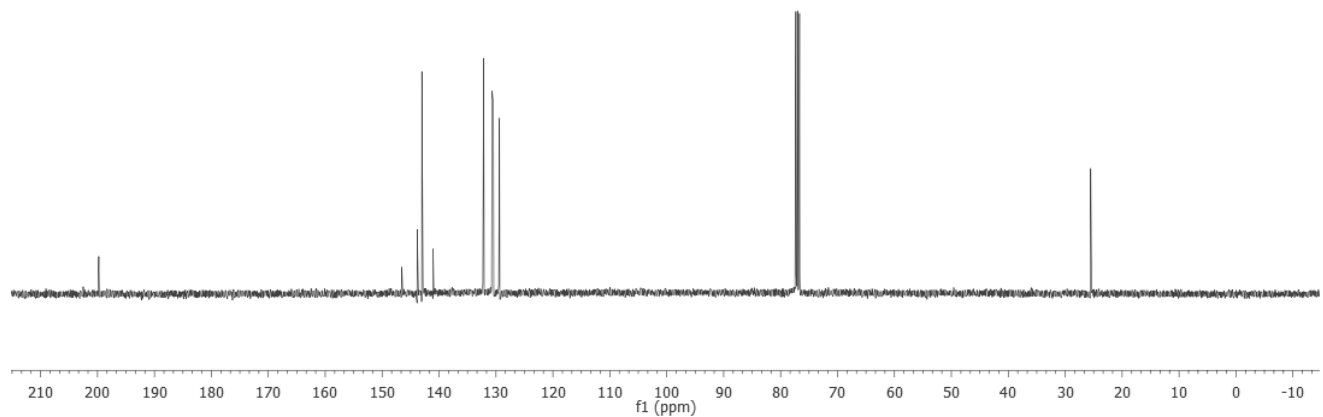
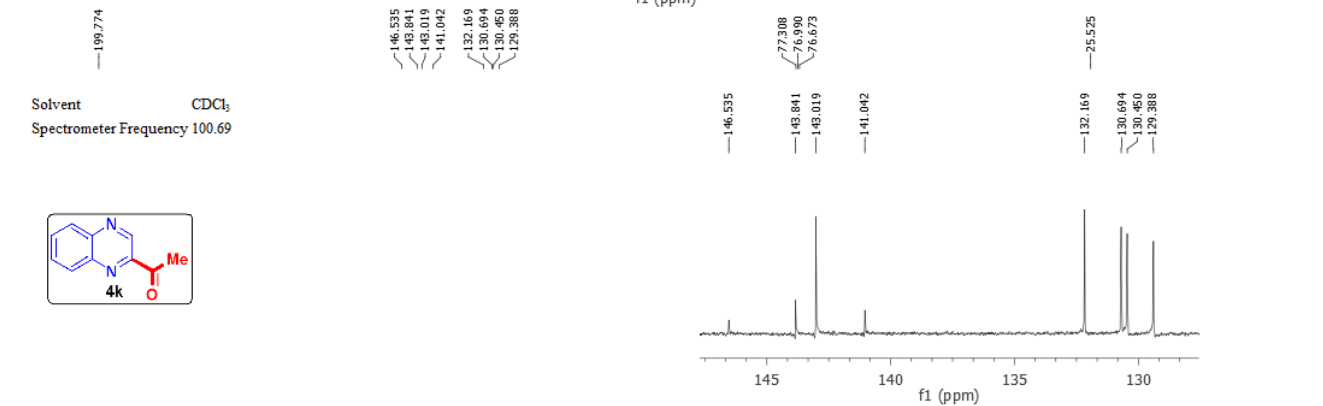
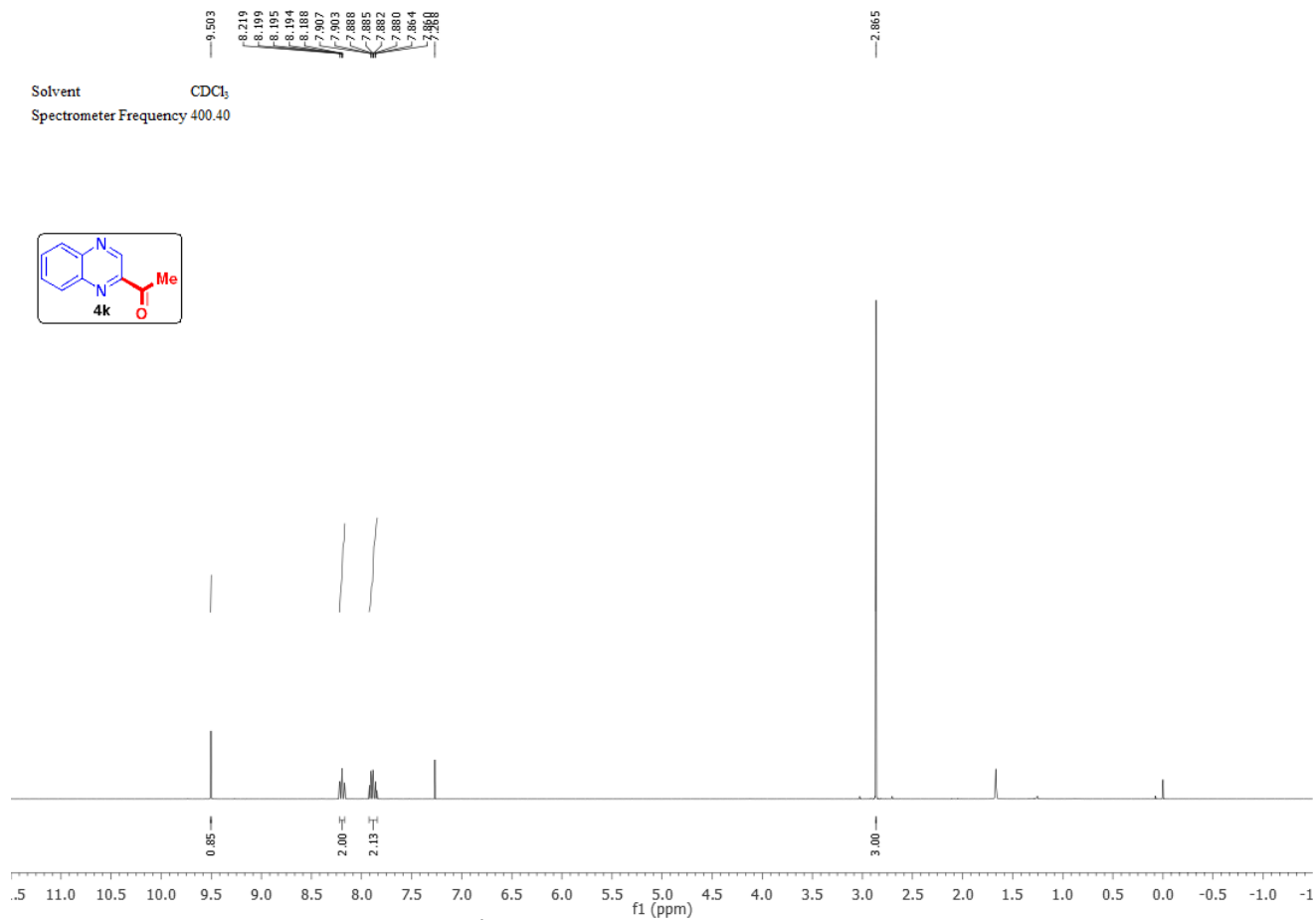


Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 400.40



Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 100.69



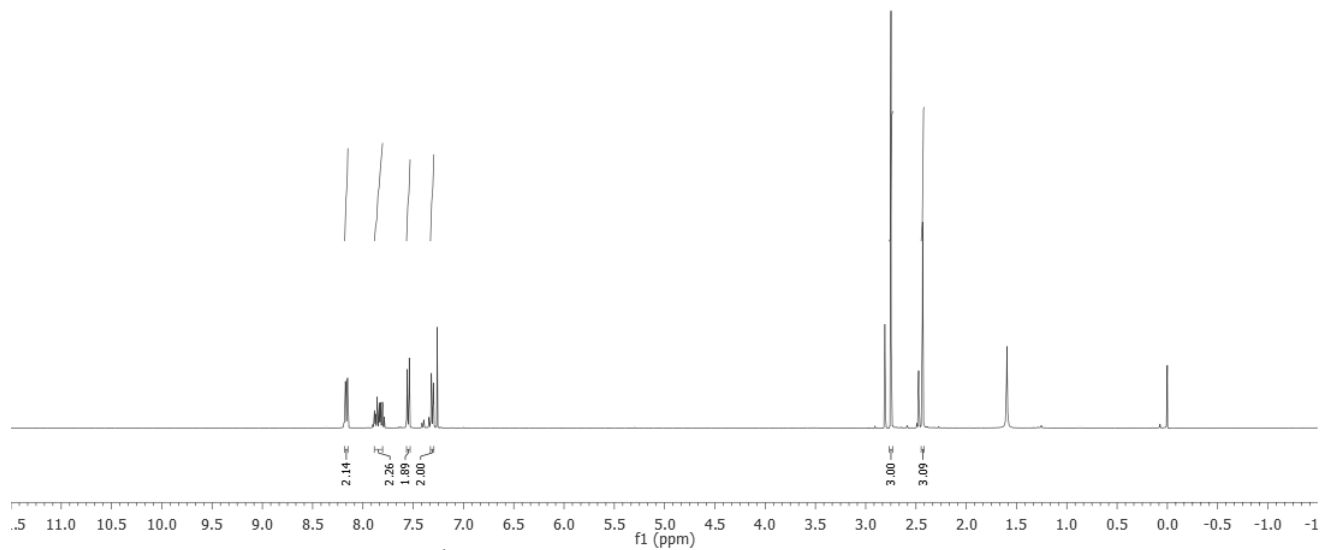
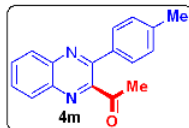




8.174  
8.169  
8.166  
8.157  
8.153  
8.150  
7.886  
7.885  
7.881  
7.877  
7.873  
7.864  
7.860  
7.855  
7.852  
7.839  
7.835  
7.830  
7.826  
7.822  
7.809  
7.806  
7.802  
7.788  
7.785  
7.565  
7.560  
7.555  
7.544  
7.539  
7.535  
7.519  
7.299  
7.282

— 2.748  
— 2.484

Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 400.40



201.418

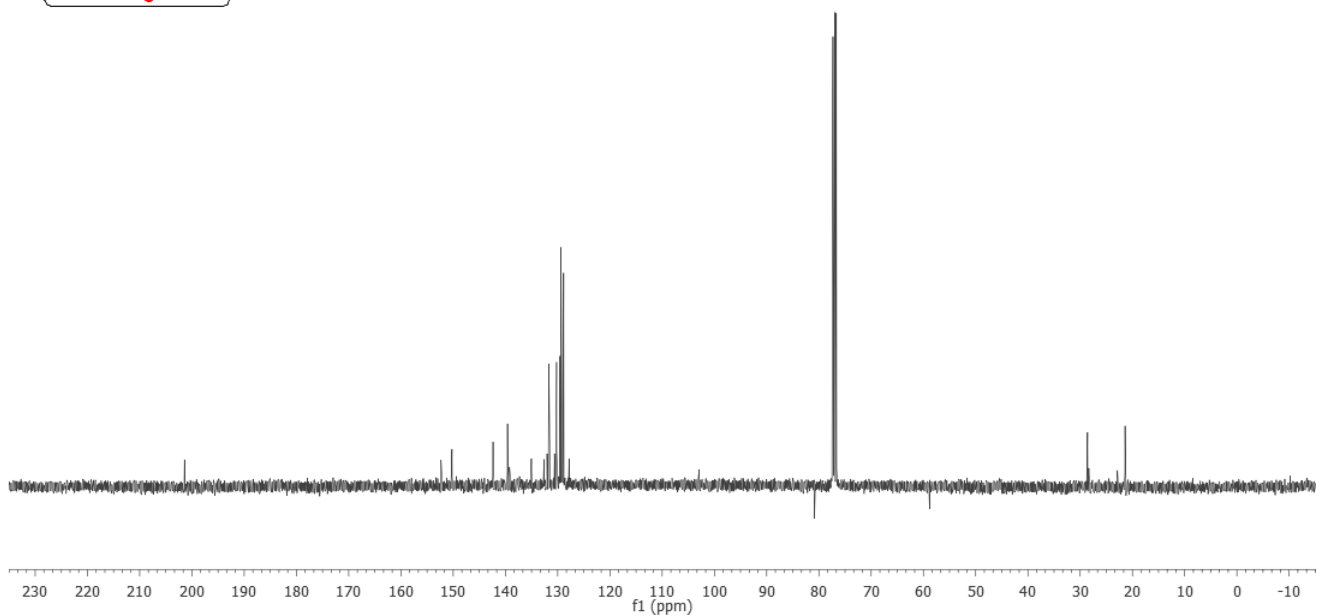
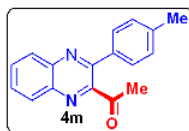
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142.367  
139.599  
135.029  
132.605  
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129.351  
129.268  
128.860

77.310  
76.993  
76.675

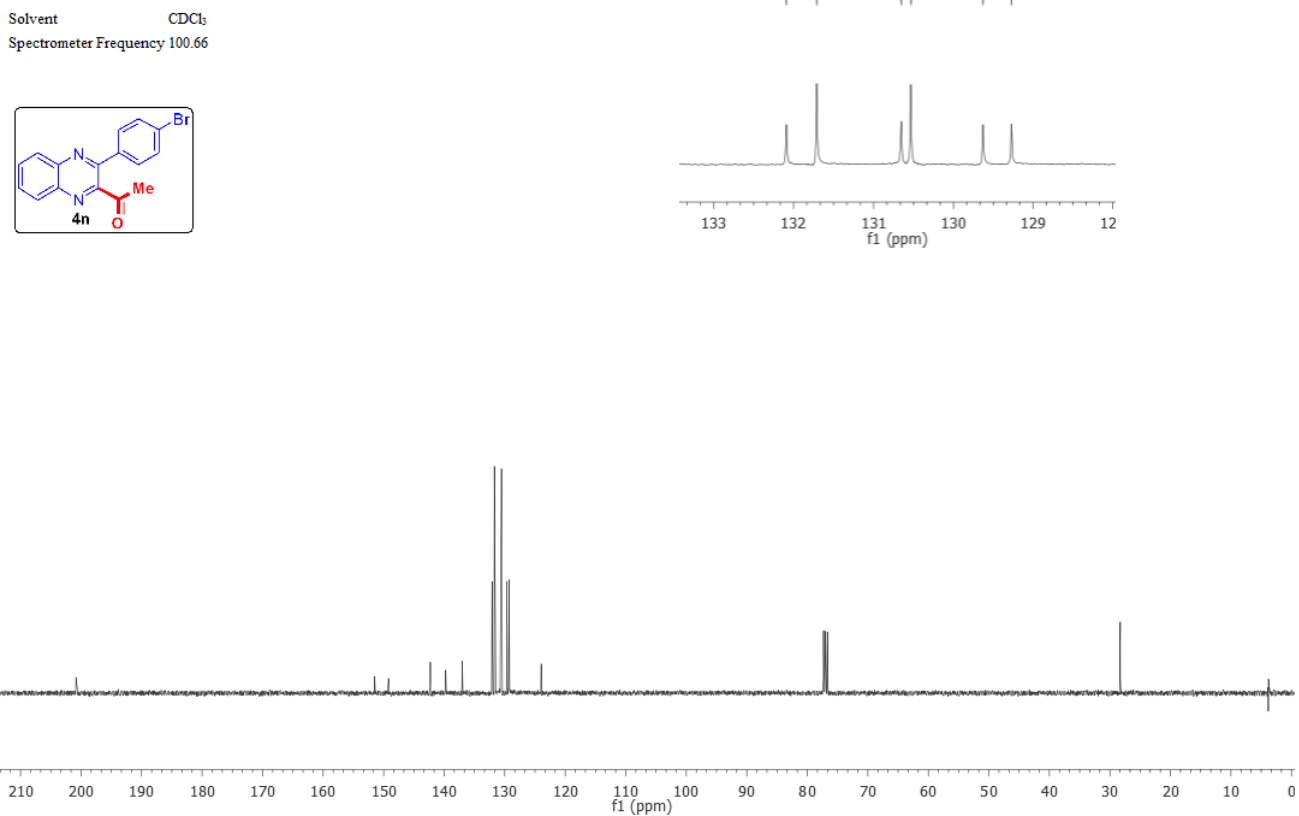
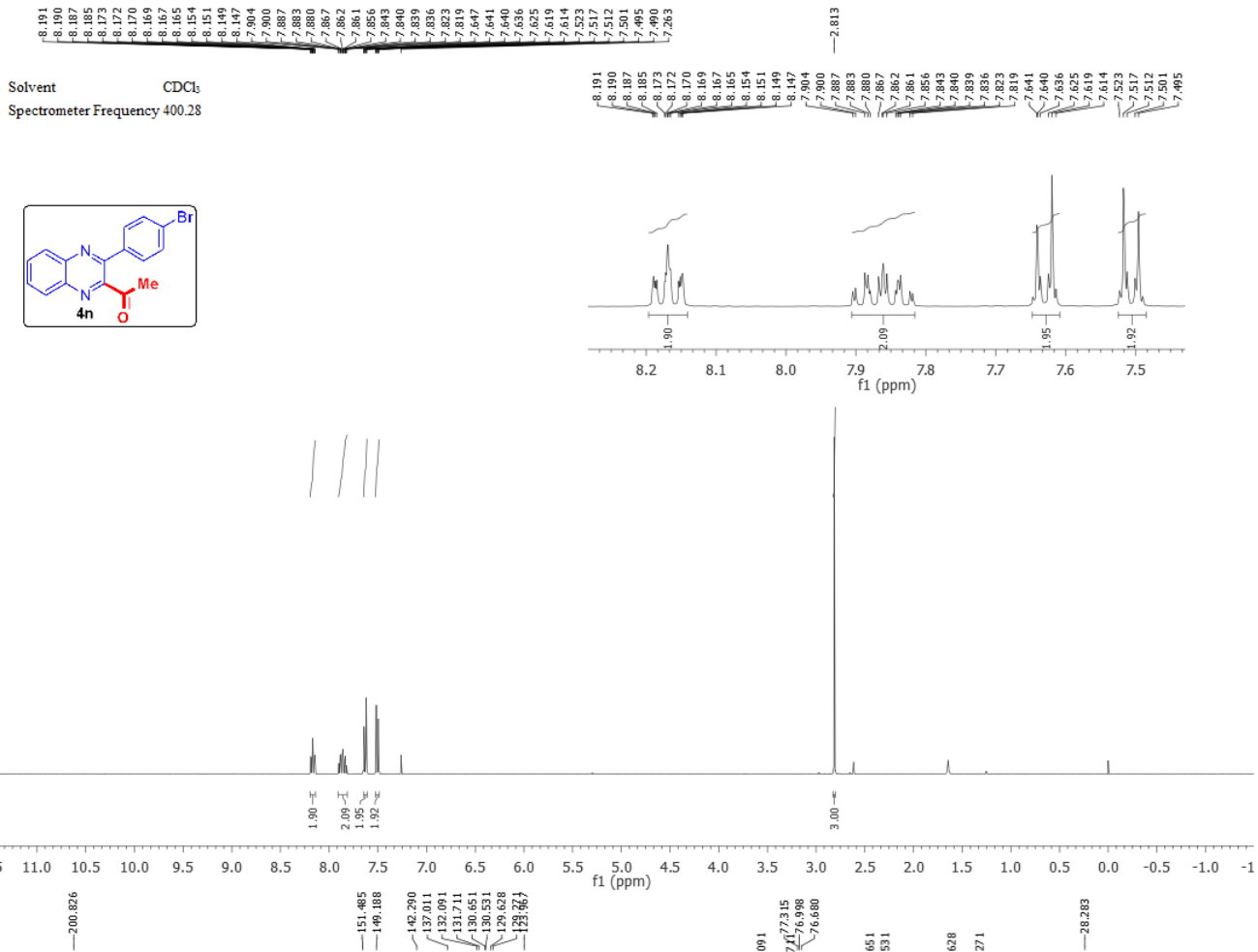
28.583

21.404

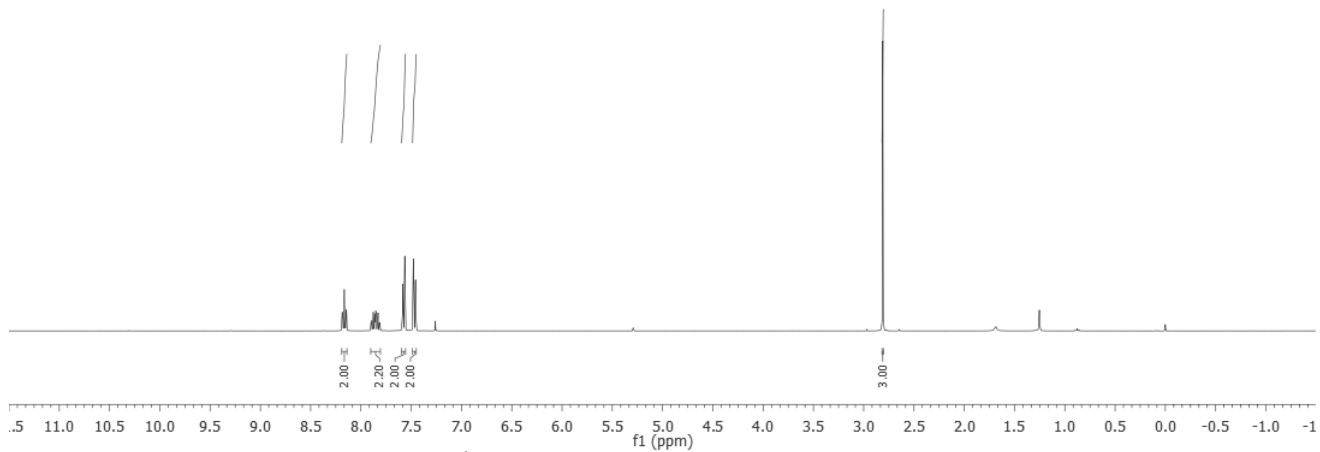
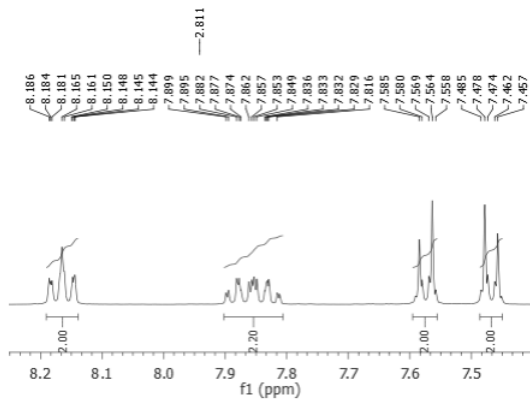
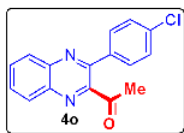
Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 100.69



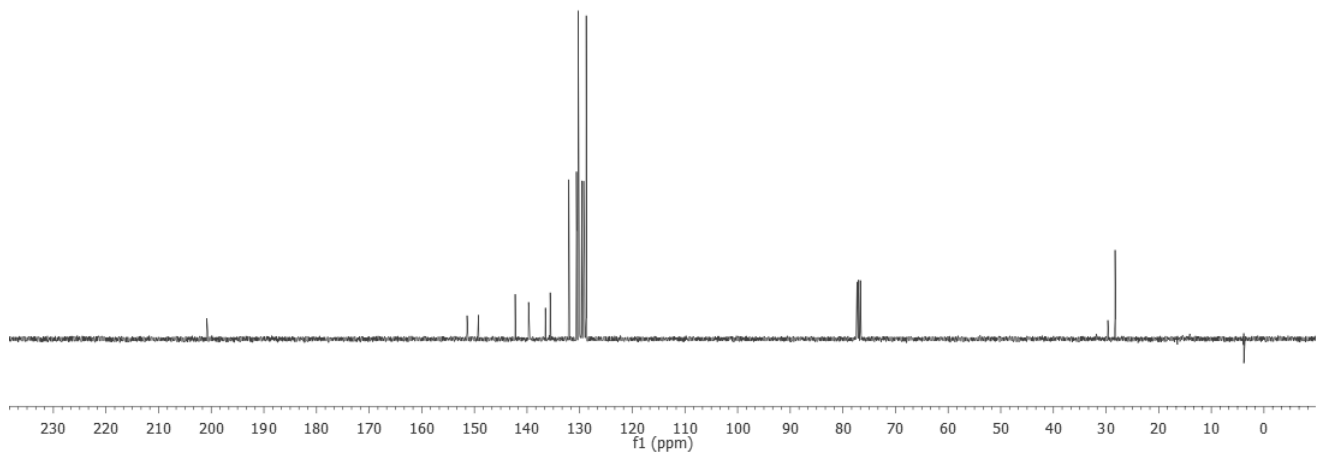
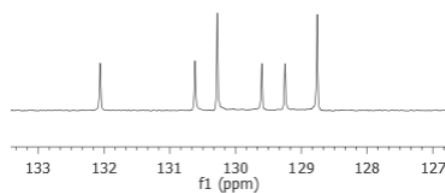
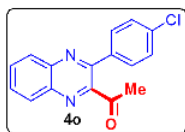


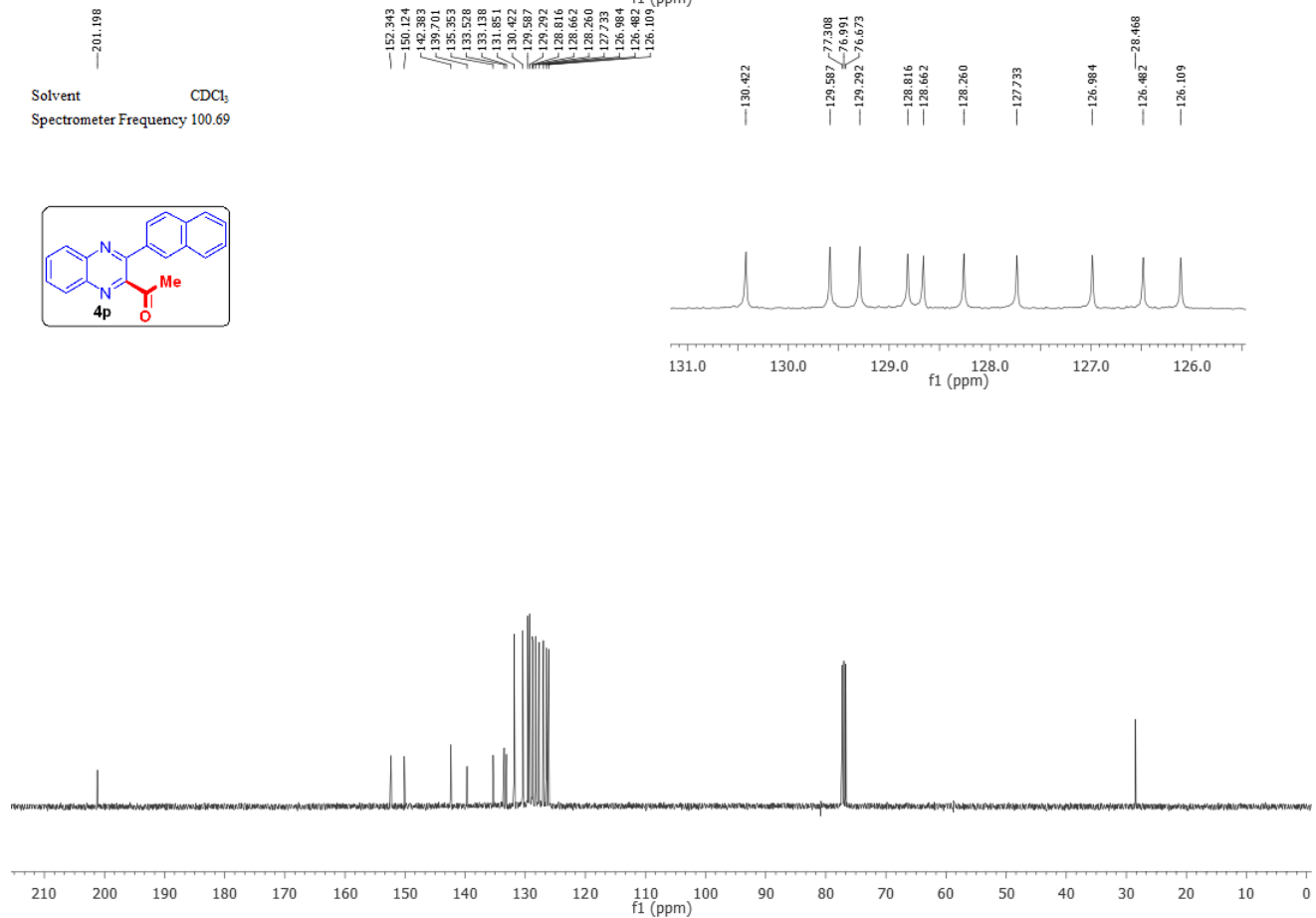
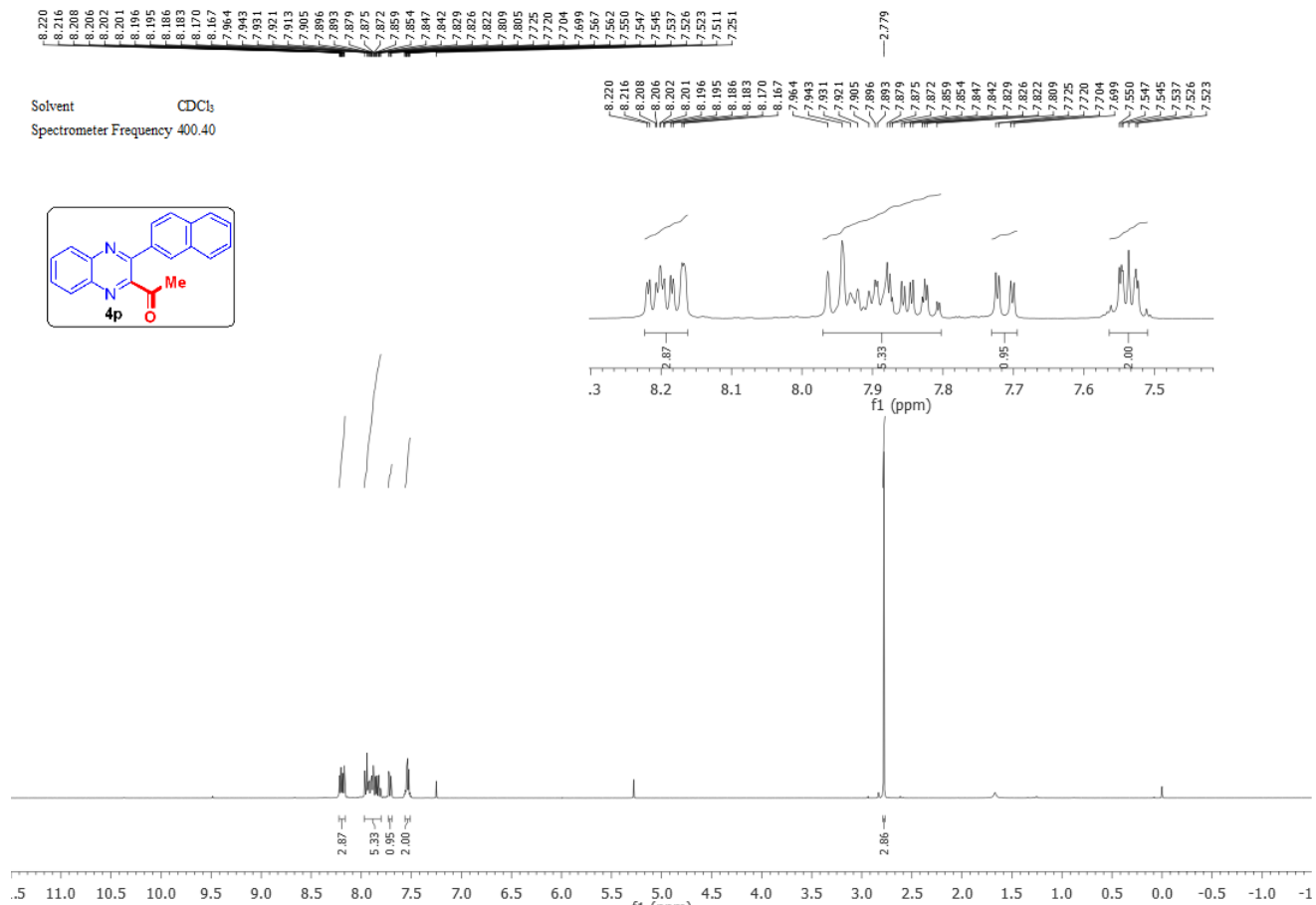


Solvent  $\text{CDCl}_3$   
 Spectrometer Frequency 400.28



Solvent  $\text{CDCl}_3$   
 Spectrometer Frequency 100.66

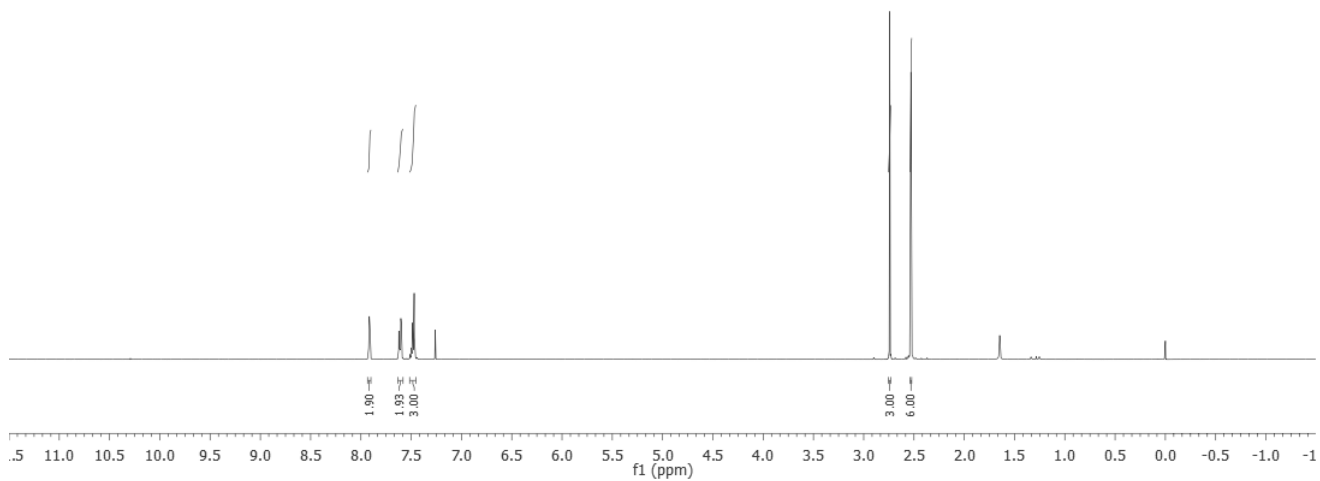
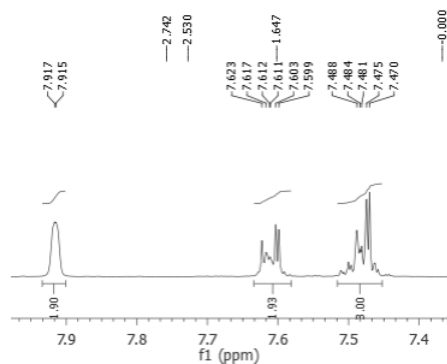




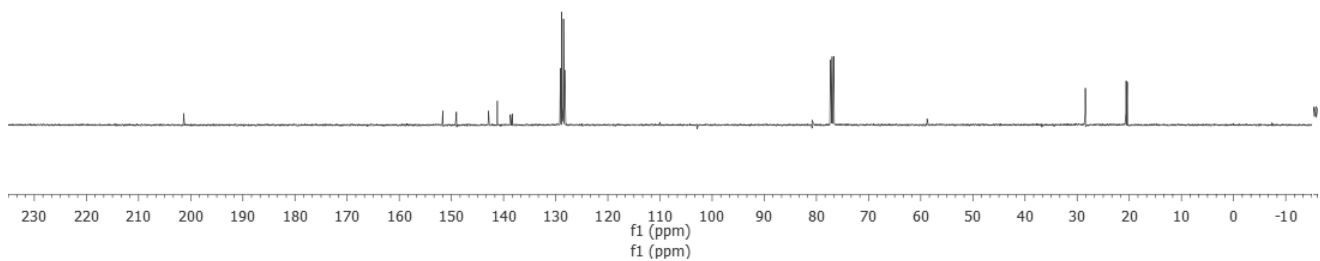
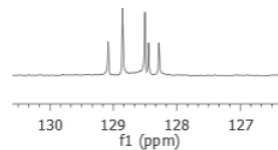
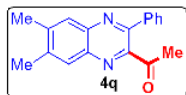
Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 400.40



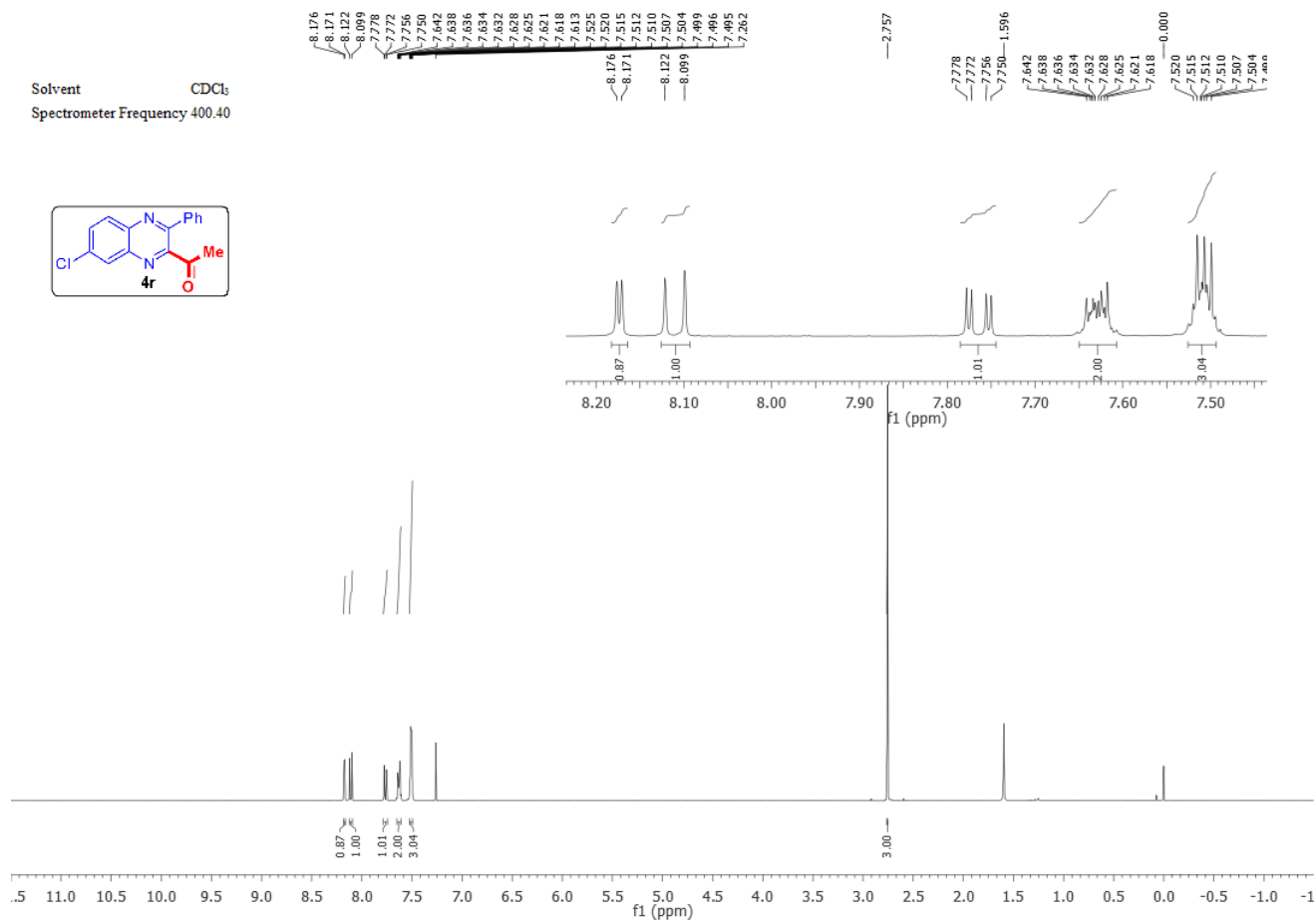
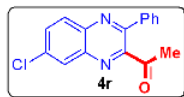
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7.623  
7.617  
7.612  
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7.603  
7.599  
7.488  
7.484  
7.481  
7.475  
7.470  
7.261



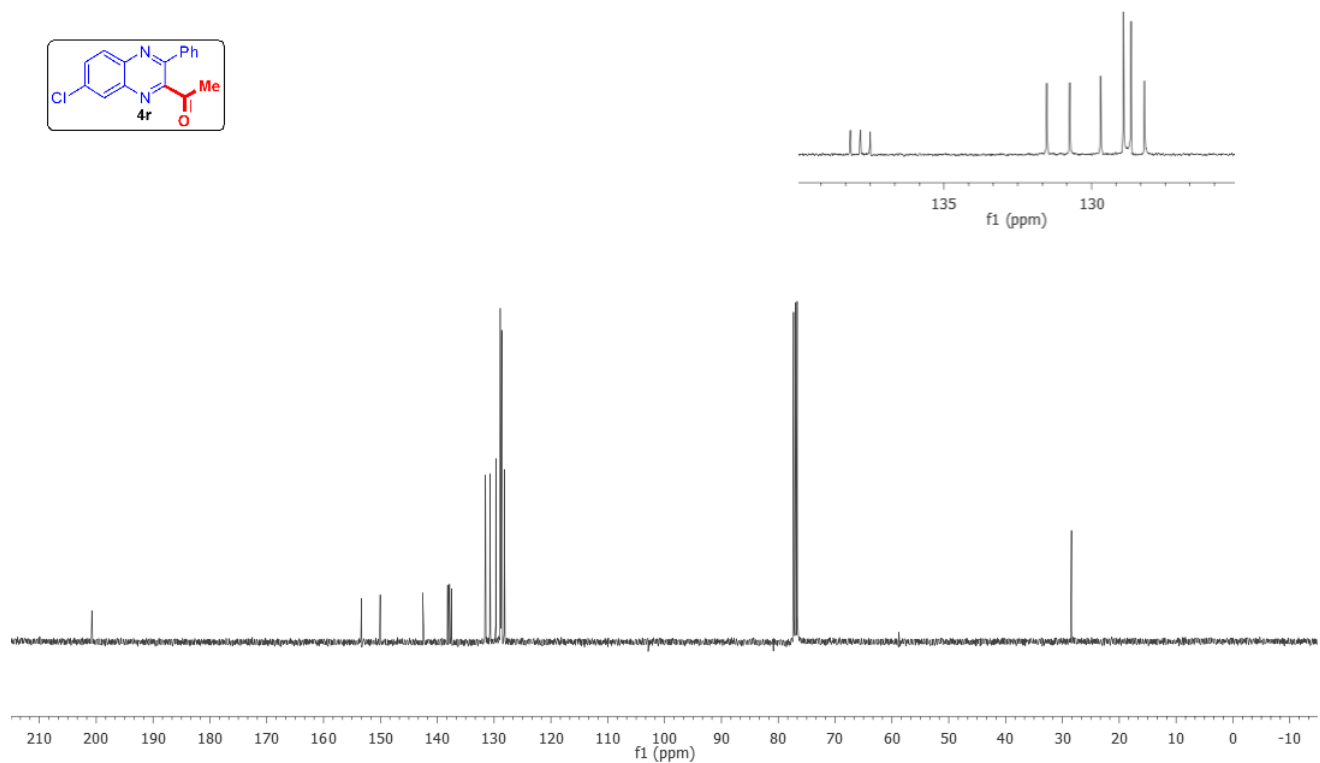
Solvent CDCl<sub>3</sub>  
Spectrometer Frequency 100.69



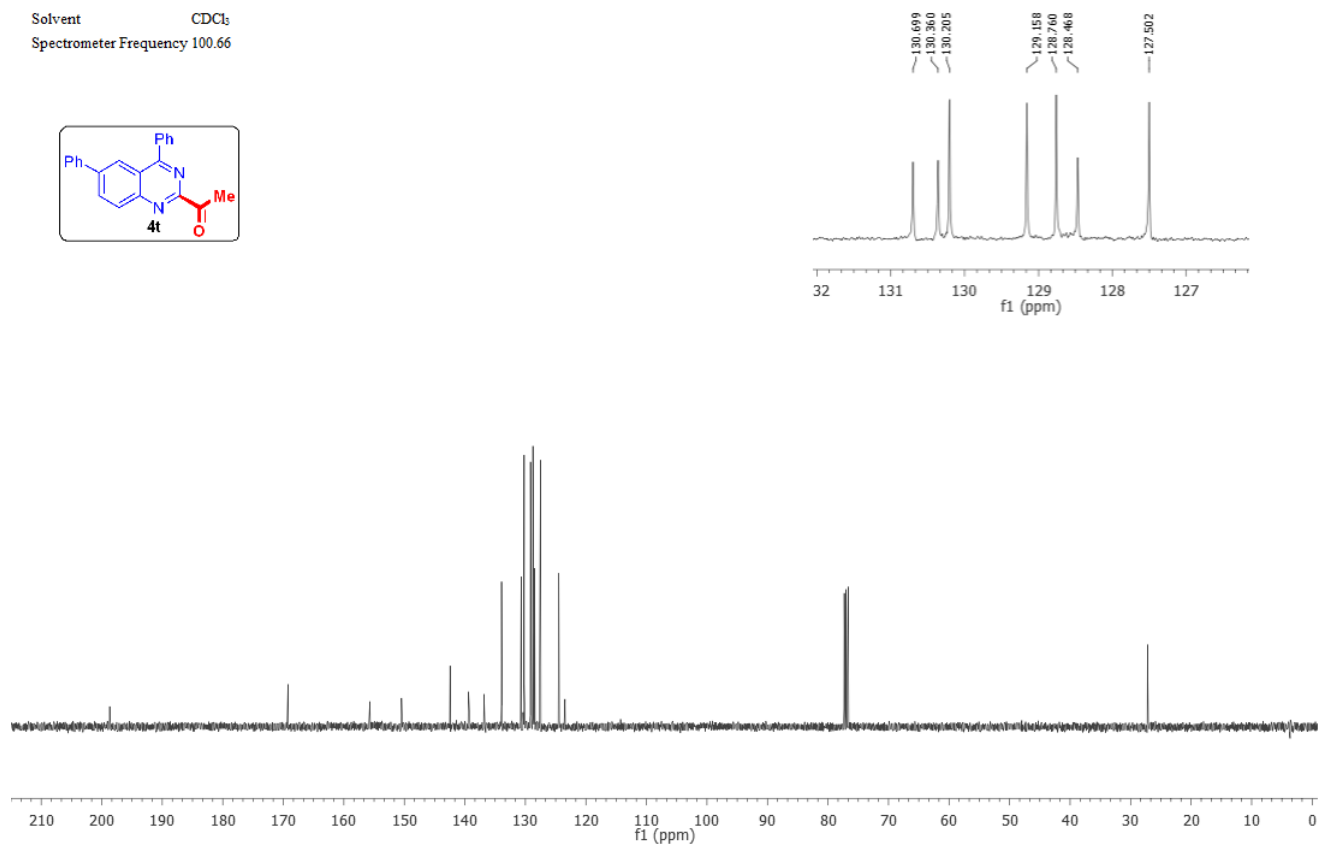
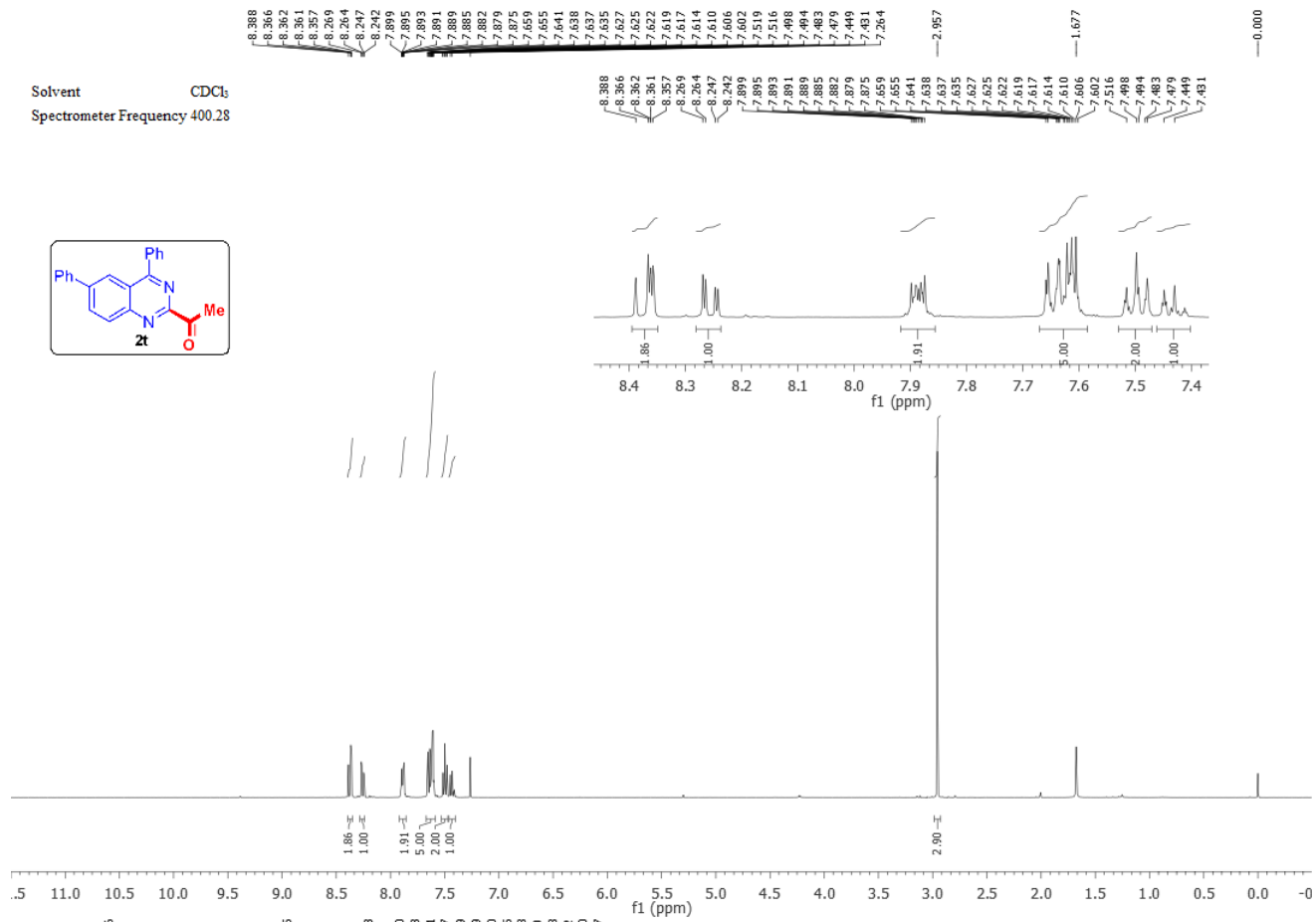
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.40

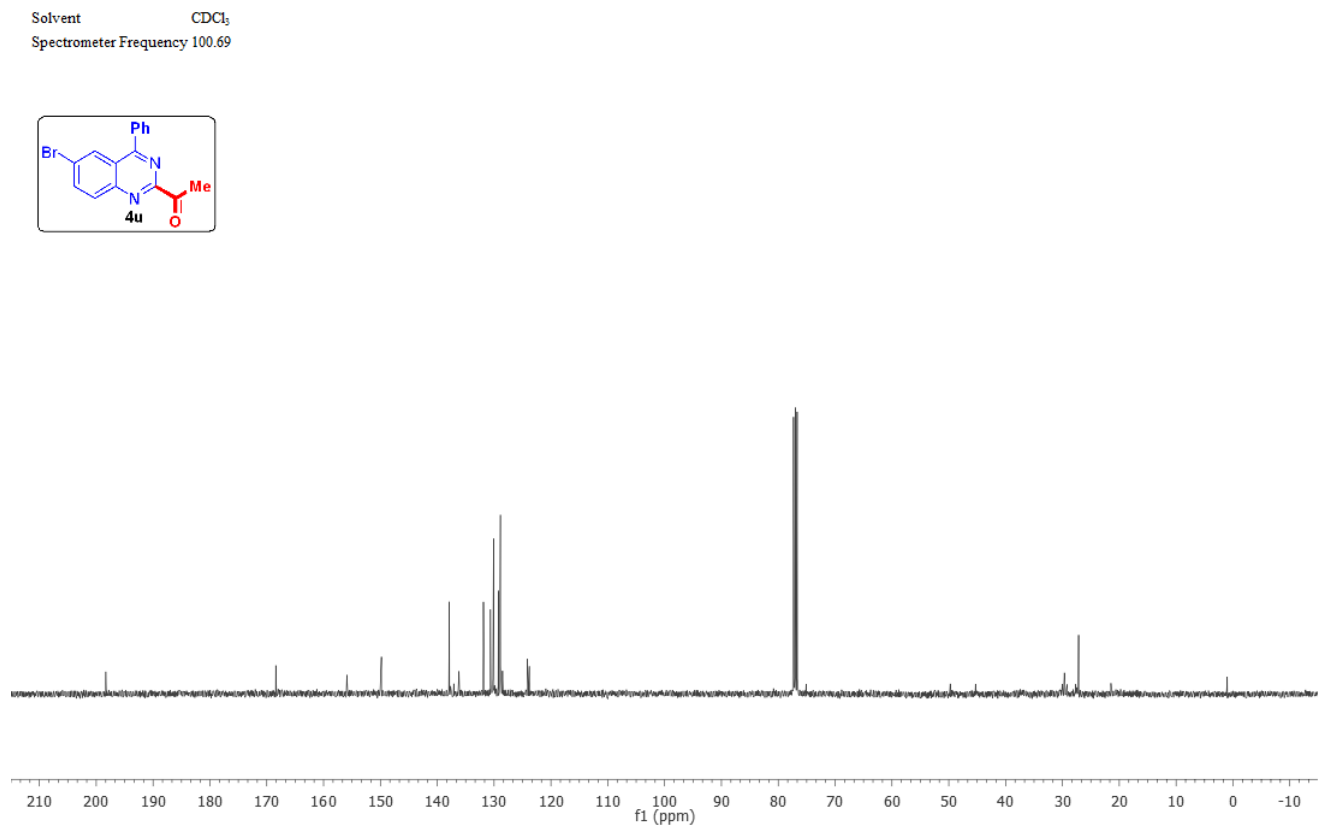
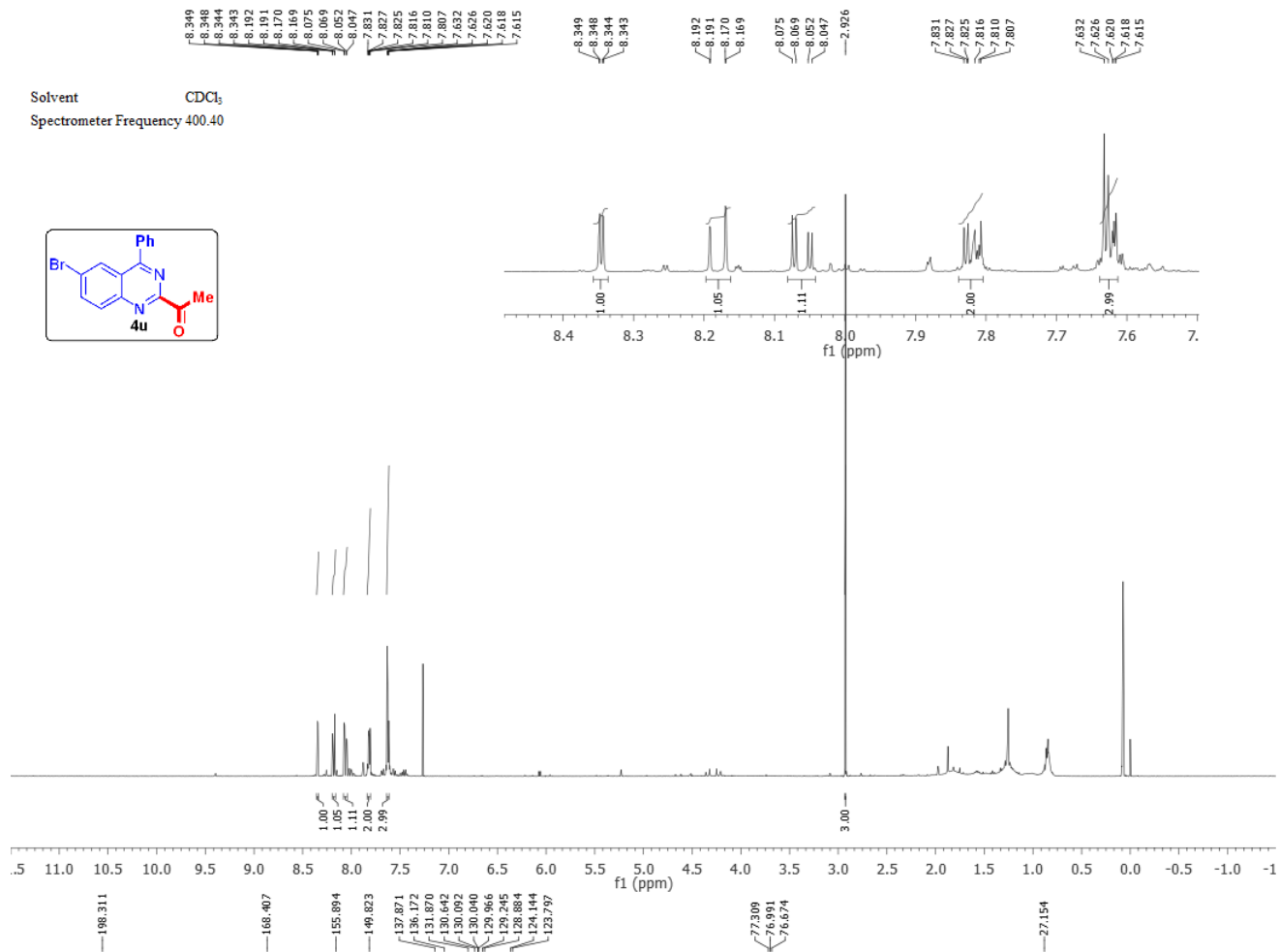


Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69

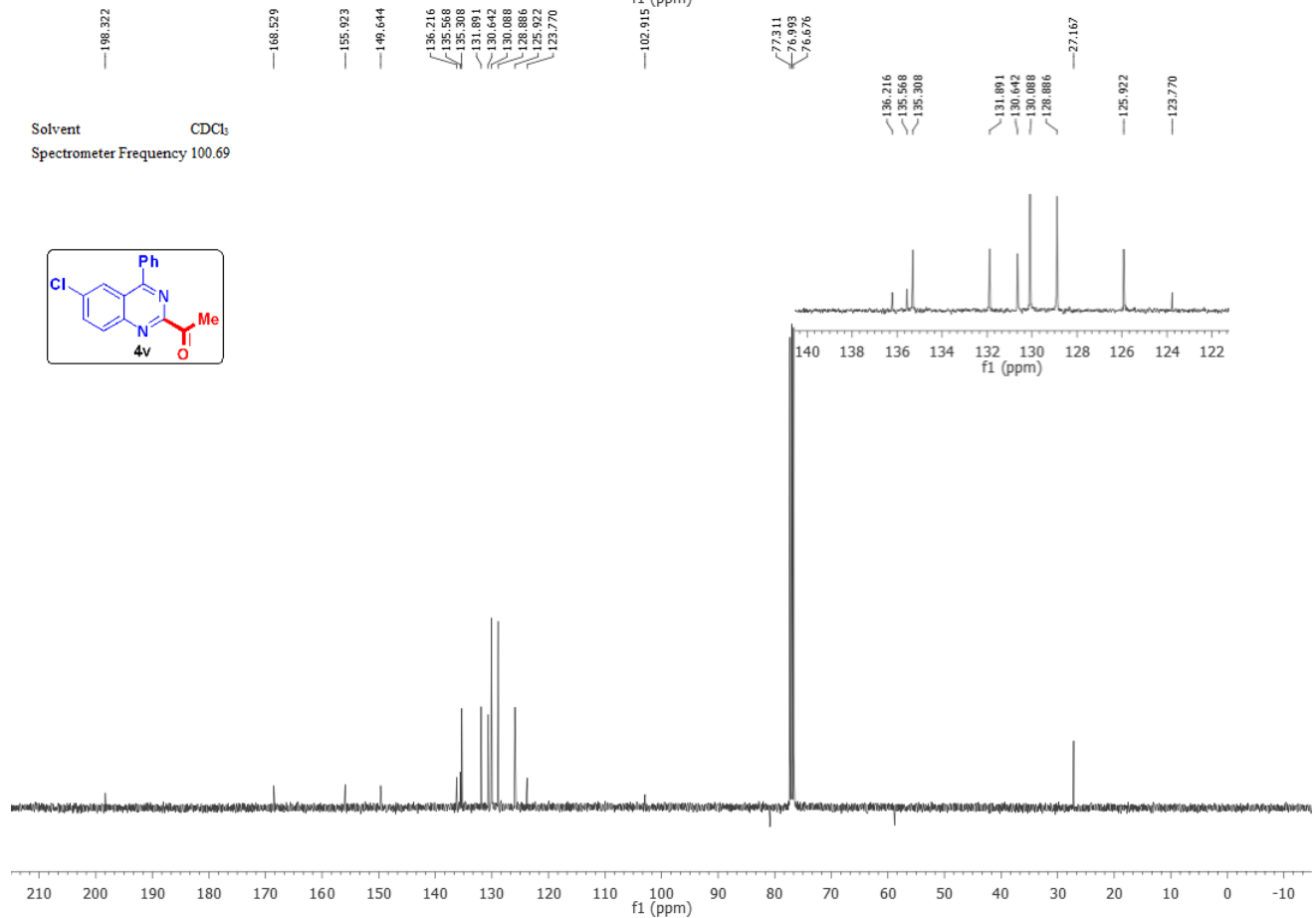
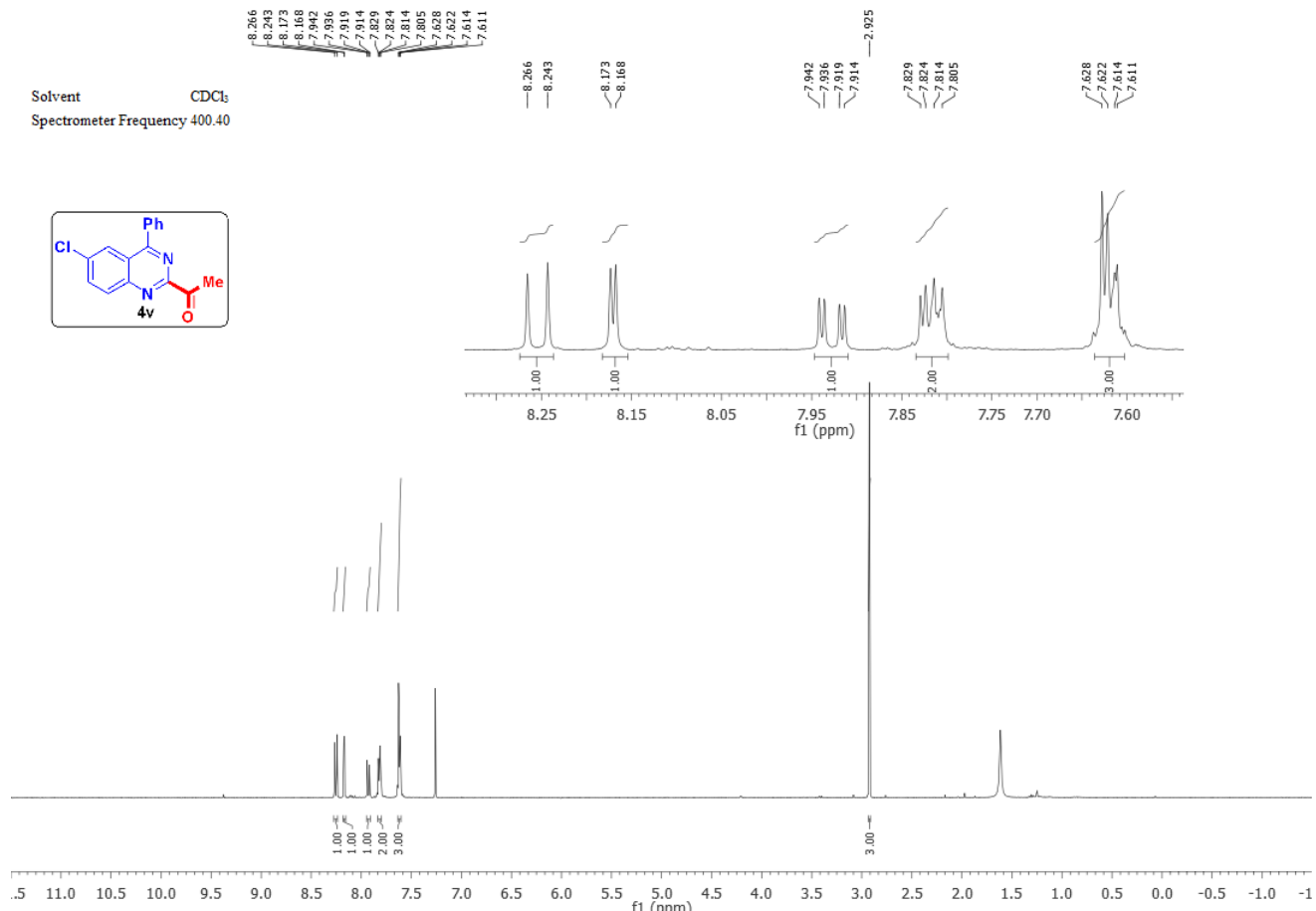


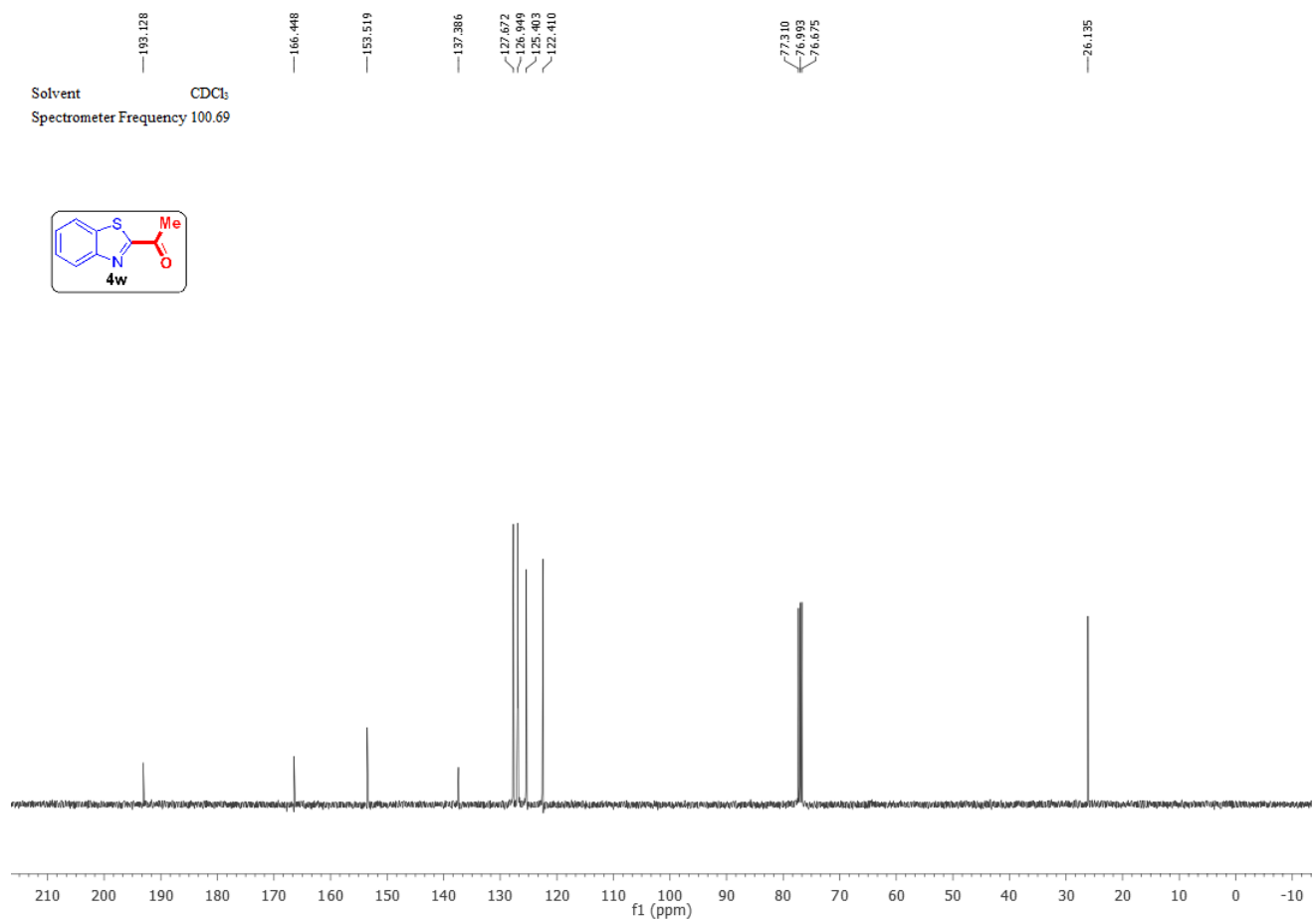
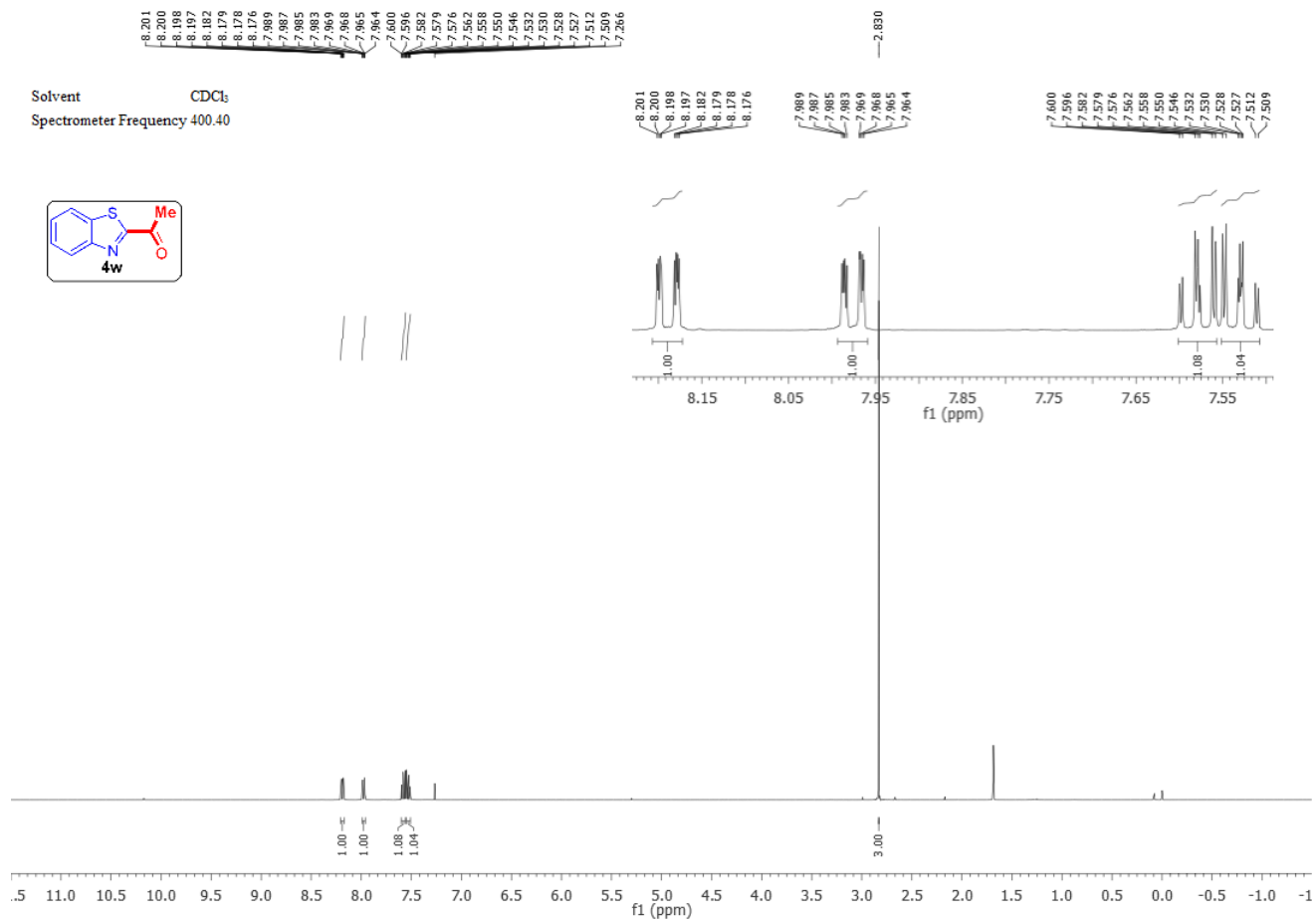




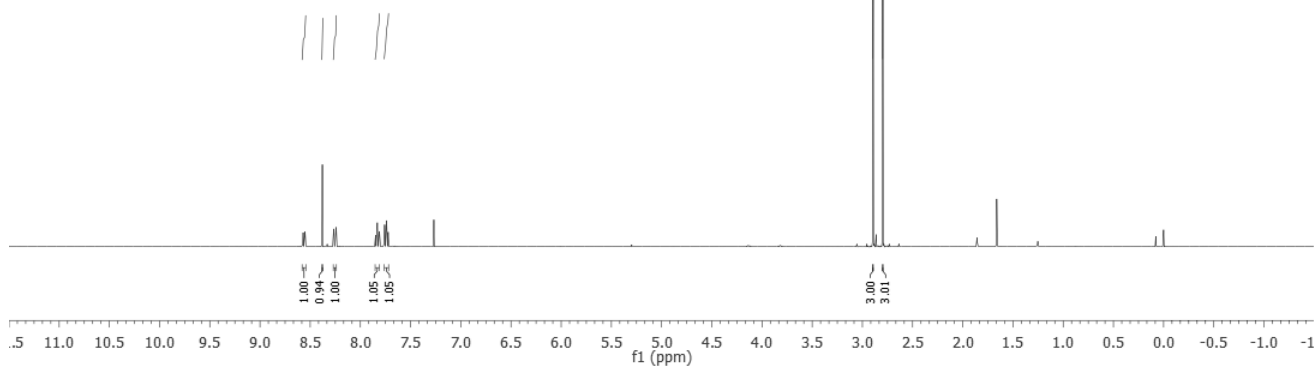
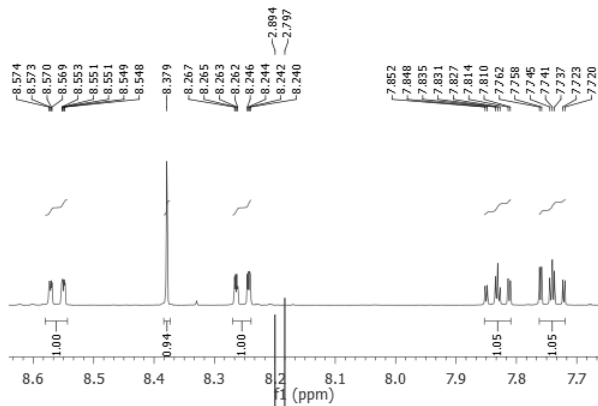
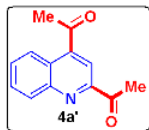




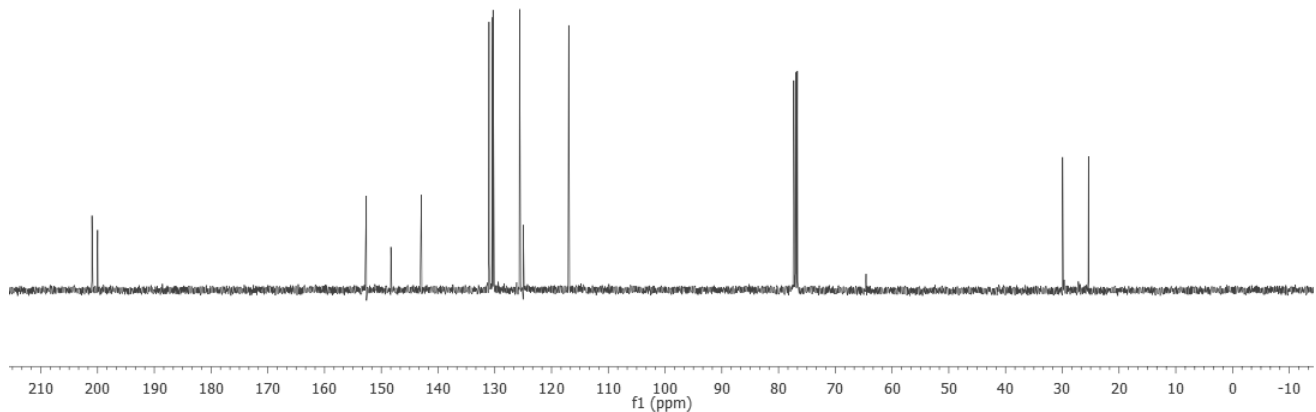
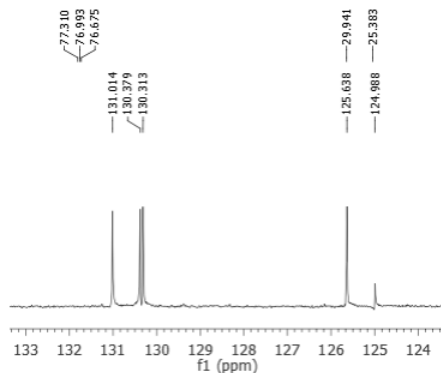
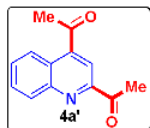




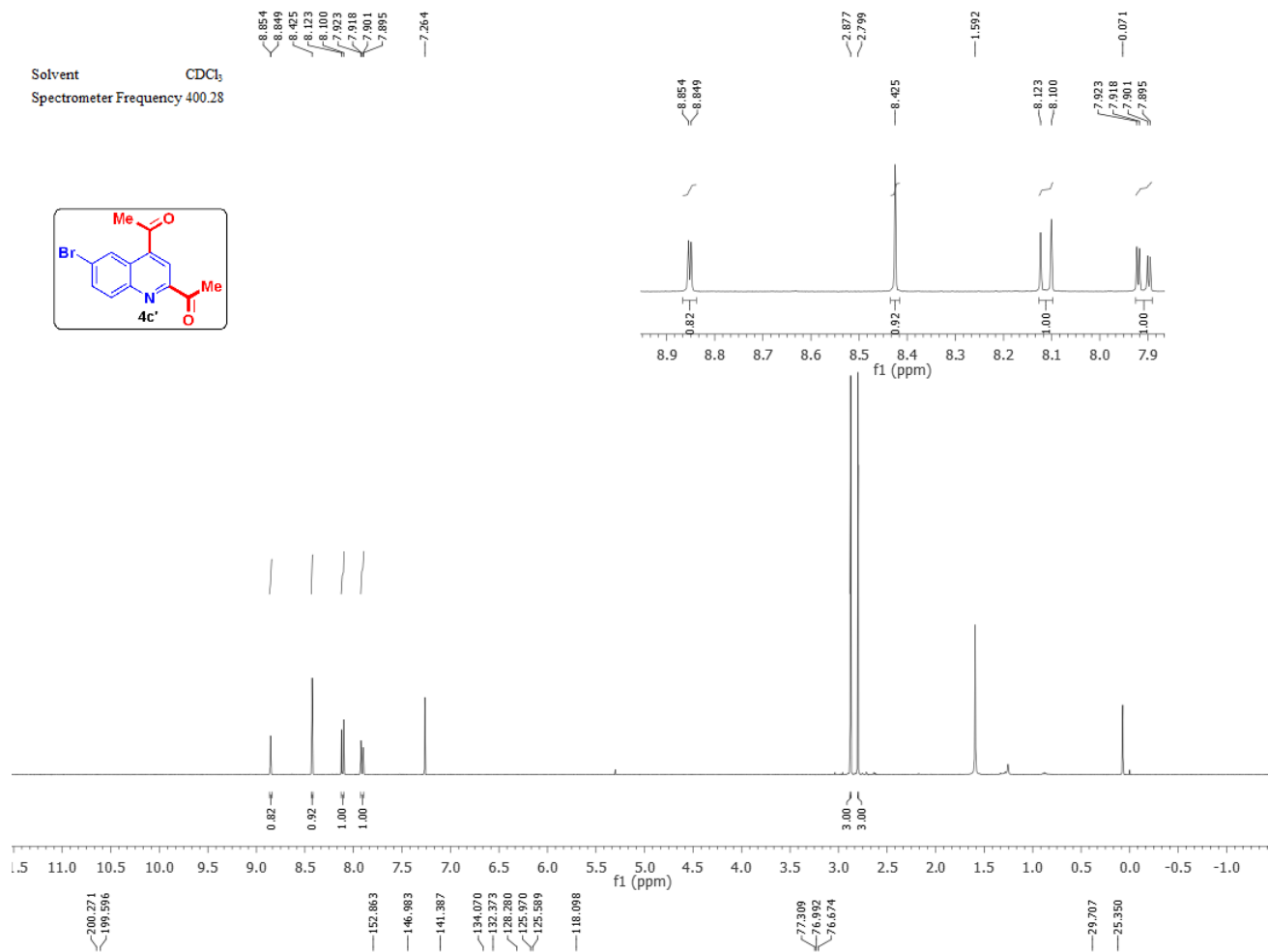
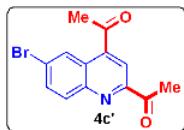
Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.40



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.69



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 400.28



Solvent  $\text{CDCl}_3$   
Spectrometer Frequency 100.66

