

## Electronic Supplementary Information

### **Green light-mediated dual eosin Y/Pd<sup>II</sup>-catalyzed C(sp<sup>2</sup>)-H arylation of N-H unprotected 2-arylquinazolinone**

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### General Information:

All manipulations with air-sensitive reagents were carried out under a dry nitrogen atmosphere. Unless otherwise stated, all commercial reagents were used without additional purification. Solvents were dried using standard methods and distilled before use. TLC was performed on silica gel plates (Merck silica gel 60, f254), and the spots were visualized with UV light (254 and 365 nm).  $^1\text{H}$  NMR was recorded at 400 MHz (JEOL-JNM-ECZ400S/L1) and 600 MHz (Bruker-Avance 600) frequency and  $^{13}\text{C}$  NMR spectra were recorded at 100 MHz (JEOL-JNM-ECZ400S/L1) and 150 MHz (Bruker-Avance) frequency in  $\text{CDCl}_3$  solvent using TMS as the internal standard.  $^{19}\text{F}$  NMR was recorded at 376 MHz frequency (JEOL-JNM-ECZ400S/L1). Chemical shifts were measured in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br. = broad. Coupling constants,  $J$  were reported in Hertz unit (Hz). HRMS ( $m/z$ ) were measured using ESI techniques Q-ToF Micro mass spectrometer respectively. Crystals were grown in dichloromethane-hexane and crystal data was recorded in Bruker Kappa Apex-2 (CCD Area Detector) or Bruker D8 Venture (Photon-III detector). Kessil PR160-456 nm, Kessil PR160L-440 nm and PR160L-525 nm were used as a source of blue LEDs and green LEDs light for the reaction.

### Synthesis of the starting materials:

The starting material substituted anthranilamide,<sup>1</sup> 2-phenylquinazolin-4(3H)-one,<sup>2,3</sup> and Isoquinolin-1(2H)-one<sup>4</sup> substrates were prepared using literature-reported methods. Aryl diazonium salts<sup>5</sup> were prepared on a 5 mmol scale according to the literature.

### Synthesis of the Aryl triflate Diazonium Salt:

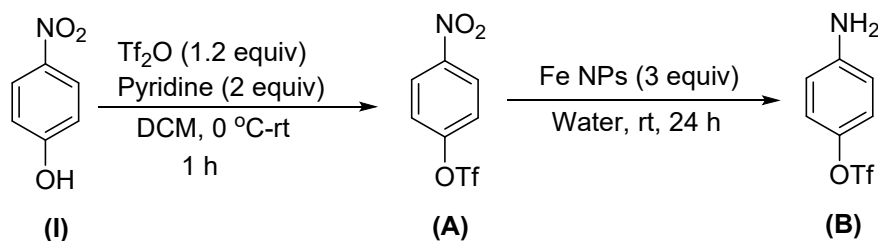
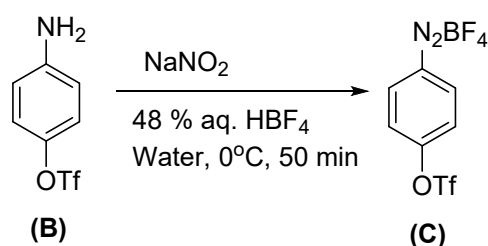


Figure 1: Preparation of 4-aminophenyl trifluoromethanesulfonate.

4-Nitro phenyl trifluoromethanesulfonate (A) was prepared as per the reported procedure.<sup>6</sup> Then 4-aminophenyl trifluoromethanesulfonate was synthesized from (A) with a modified process.<sup>7</sup>

**Preparation of Fe Nanoparticles and Nitro reduction<sup>7</sup>:** In a 500 mL round bottom flask, ferrous sulphate hepta-hydrate [ $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ ] (3.4 g, 12 mmol) and citric acid (220 mg, 1 mmol) were taken in distilled water (250 mL) and stirring to dissolve the solid. Then, Sodium borohydride ( $\text{NaBH}_4$ ) (800 mg, 20 mmol) was added to it portion-wise, and vigorous stirring was continued for 5 minutes. Thereafter, the solution was settled down and the water layer was decanted. The residual black solid material of Fe nanoparticles was further washed with distilled water two times to be ready for use in nitro reduction. The nitro compound (A) (4 mmol) was added to these Fe nanoparticles in distilled water (10 mL) in the same pot under constant stirring for 24 h at room temperature under argon atmosphere. The reaction mixture is filtered through celite pad and washed with ethyl acetate thoroughly. Then collected filtrate is poured into a separatory funnel to eliminate the water part. The

ethyl acetate part is concentrated under reduced pressure and product (B) is isolated by column chromatography. (Yield 83%).



**Figure 2: Diazonium salt Preparation.**

Aniline (**B**) (2.5 mmol) was taken in a 50 mL round bottom flask and cooled in an ice bath, and tetrafluoroboric acid solution (48 wt % in H<sub>2</sub>O, 0.85 mL) was added at 0 °C. To the precipitate, 1 mL of distilled water was added. Then, Sodium nitrite (173 mg, 2.5 mmol) in distilled water (2 mL) was added dropwise to the reaction mixture and allowed to stir for 50 min at 0 °C. A thick precipitate was formed and collected by filtration. The precipitate was washed with diethyl ether (10 mL) three times. The resulting precipitate was recrystallized with acetonitrile/diethyl ether to give the desired aryldiazonium tetrafluoroborate as a brown solid.

#### **General procedure for dual palladium-photoredox catalyzed C–H arylation of quinazoline scaffold:**

To an oven-dried Schlenk tube equipped with a magnetic stir bar, 2-phenyl quinazoline derivative (0.3 mmol, 1 equiv), freshly prepared aryldiazonium salt (1.2 mmol, 4 equiv), Pd(OAc)<sub>2</sub> (10 mol%, 6.7 mg), Eosin Y (1 mol%, 2.1 mg), and MeOH (4.5 mL), were sequentially added. Then the tube was frozen in liquid N<sub>2</sub>, degassed by the freeze-pump-thaw procedure refilled with argon gas. This freeze-pump-thaw procedure was performed three times. Then the schlenk tube was placed on a magnetic stirrer with Kessil Green LED light (40 W) kept about 4 cm away from it. After 30 h, the solvent was evaporated under reduced pressure, and work up with DCM-water. Then, the residue was purified by silica gel column chromatography (eluting with Ethyl Acetate/Hexane) to isolate the desired product. During the photoirradiation, the reaction temperature was probed to be in the range of 33 °C - 35 °C.

#### **Mechanistic Study:**

##### **Intermolecular Kinetic Experiment:**

A mixture of 2-phenylquinazolin-4(3H)-one (0.15 mmol), *d*<sub>5</sub>-2-phenylquinazolin-4(3H)-one (0.15 mmol), freshly prepared aryldiazonium salt (1.2 mmol, 4 equiv), Pd(OAc)<sub>2</sub> (10 mol%, 6.7 mg), Eosin Y (1 mol%, 2.1 mg), and MeOH (4.5 mL), were taken in an oven-dried schlenk tube equipped with a magnetic stir bar. Then the tube was frozen in liquid N<sub>2</sub> and degassed by the freeze-pump-thaw procedure refilling with argon gas (three times). Then the reaction tube was placed on a magnetic stirrer with Kessil Green LED light (40 W) kept about 4 cm away from it and irradiated at room temperature with constant stirring for 12 h. Thereafter, the solvent was evaporated under reduced pressure and worked up with DCM-water. Then, the residue was purified by silica gel column chromatography (eluting with Ethyl Acetate/Hexane) to isolate the desired product. The K<sub>H</sub>/K<sub>D</sub> value was determined by <sup>1</sup>H NMR analysis.



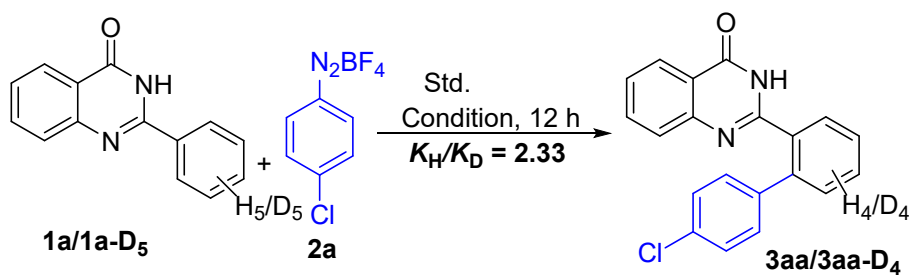


Figure 3: Primary kinetic isotope effect experiment.

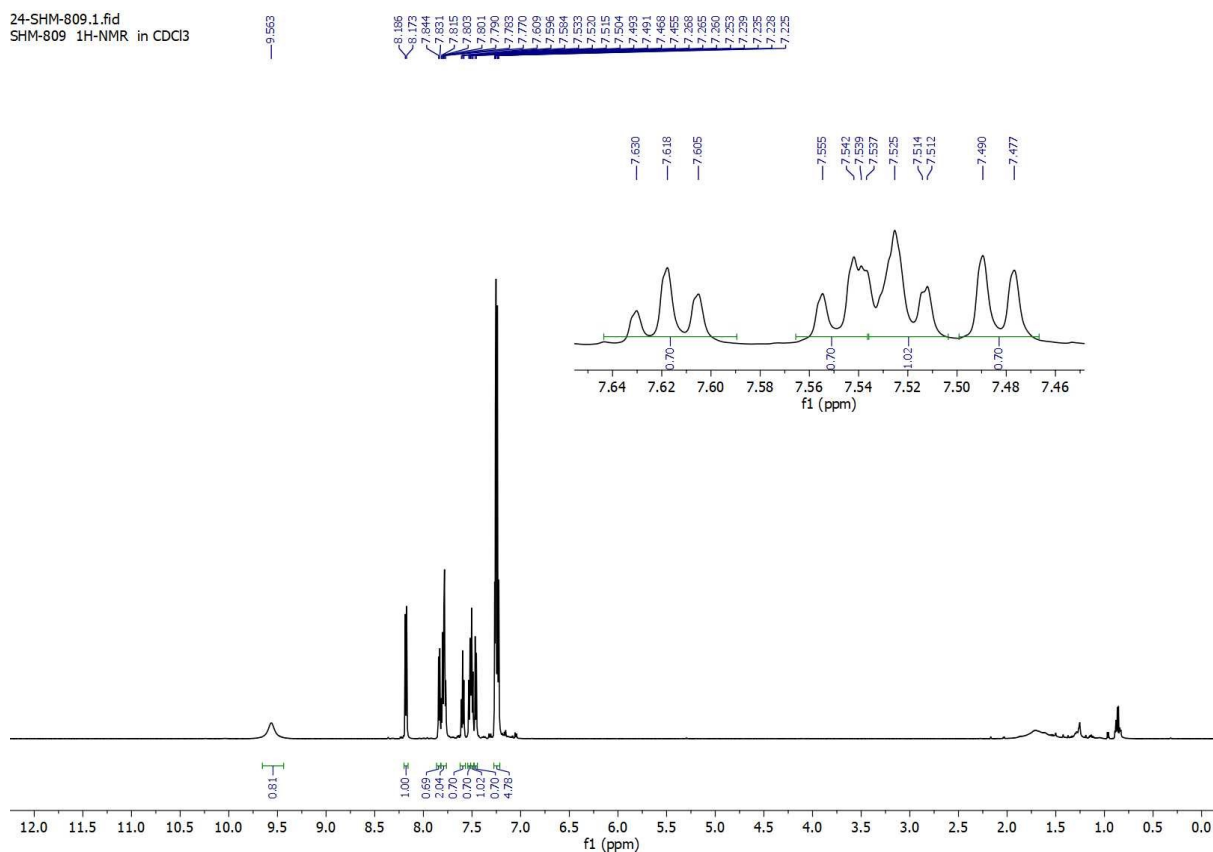


Figure 4:  $^1\text{H-NMR}$  of Primary kinetic isotope effect experiment.

#### Free radical-trapping experiment for arylation:

2-phenylquinazolin-4(3H)-one **1a** (0.3 mmol), phenyl diazonium trifluoroborate **2e** (1.2 mmol), Eosin Y (1.0 mol%),  $\text{Pd}(\text{OAc})_2$  (10 mol%) and, TEMPO (79.5 mg, 0.5 mmol) were taken in MeOH (4.5 mL) in an oven-dried Schlenk tube and after performing freeze-thaw-pump it was placed magnetic stirring, irradiated with 40 W green LED at room temperature for 30 h. The reaction was concentrated under reduced pressure and worked up with DCM-Water. Phenyl-TEMPO adduct was detected by HRMS which confirms the presence of free radical formation during the reaction.

HRMS of TEMPO-adduct product  $\text{C}_{15}\text{H}_{23}\text{NO}$   $[\text{M}+\text{H}]^+$  : Exact Mass: 234.1858; found: 234.1853.

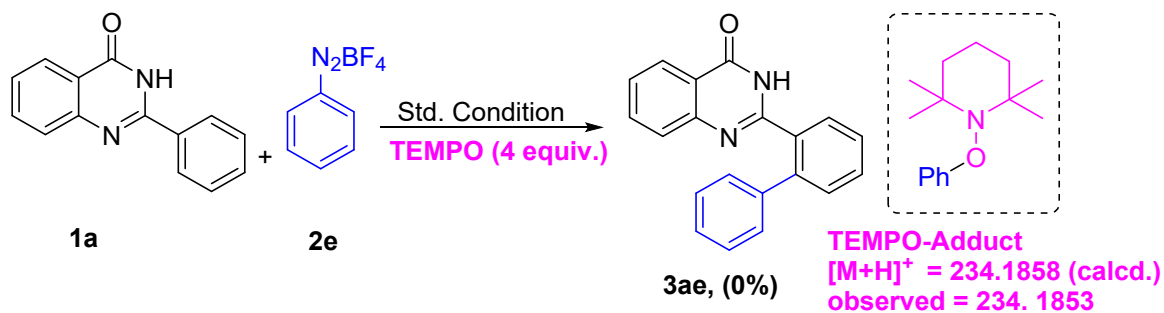


Figure 5: Free radical-trapping experiment using TEMPO (radical scavenger).

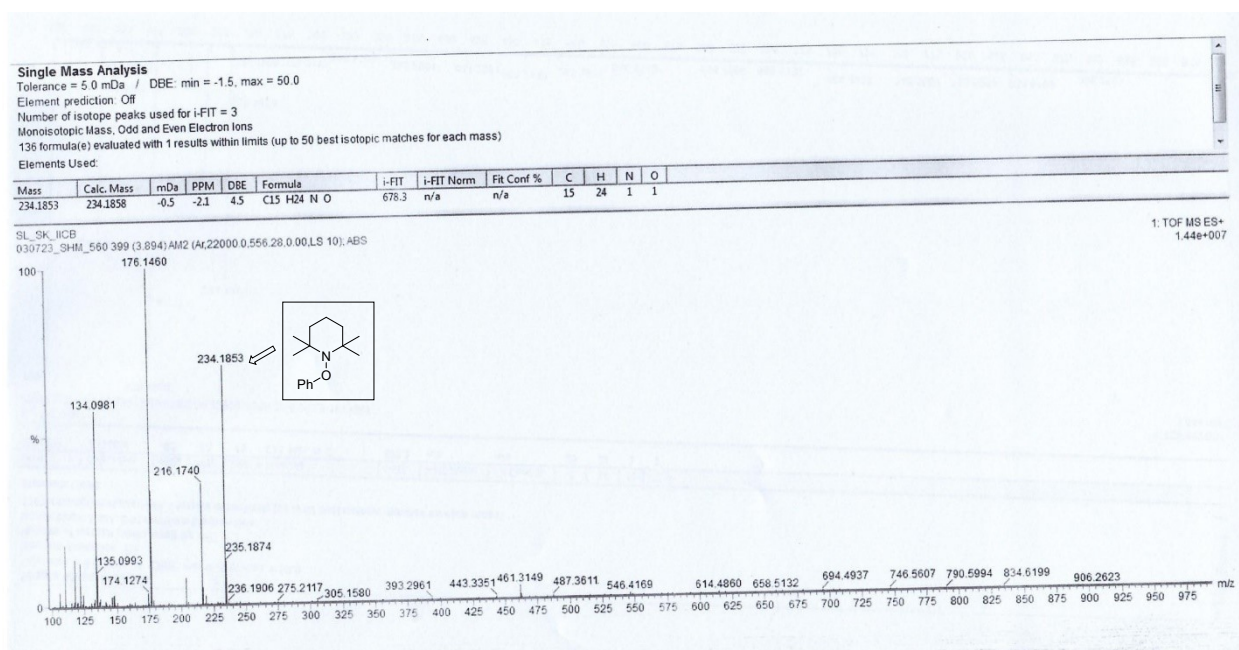


Figure 6: HRMS analysis of the reaction mixture.

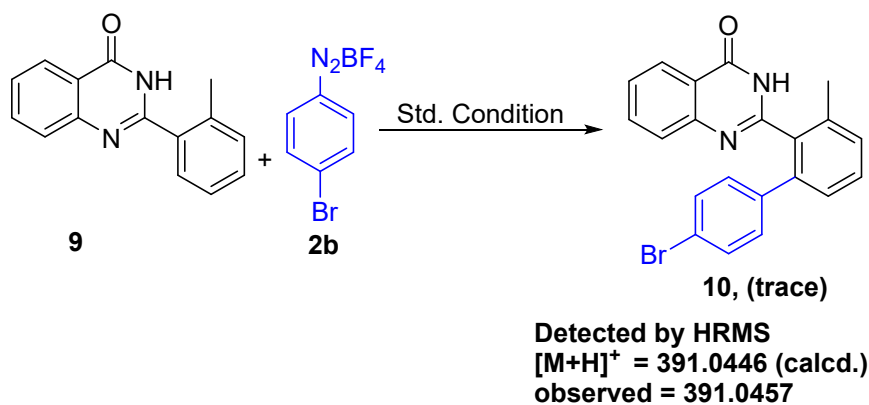


Figure 7: Arylation reaction of 2-(o-tolyl)quinazolin-4(3H)-one (9).

HRMS of arylated product  $C_{21}H_{15}BrN_2O$   $[M+H]^+$  : Exact Mass: 391.0446; found: 391.0457.

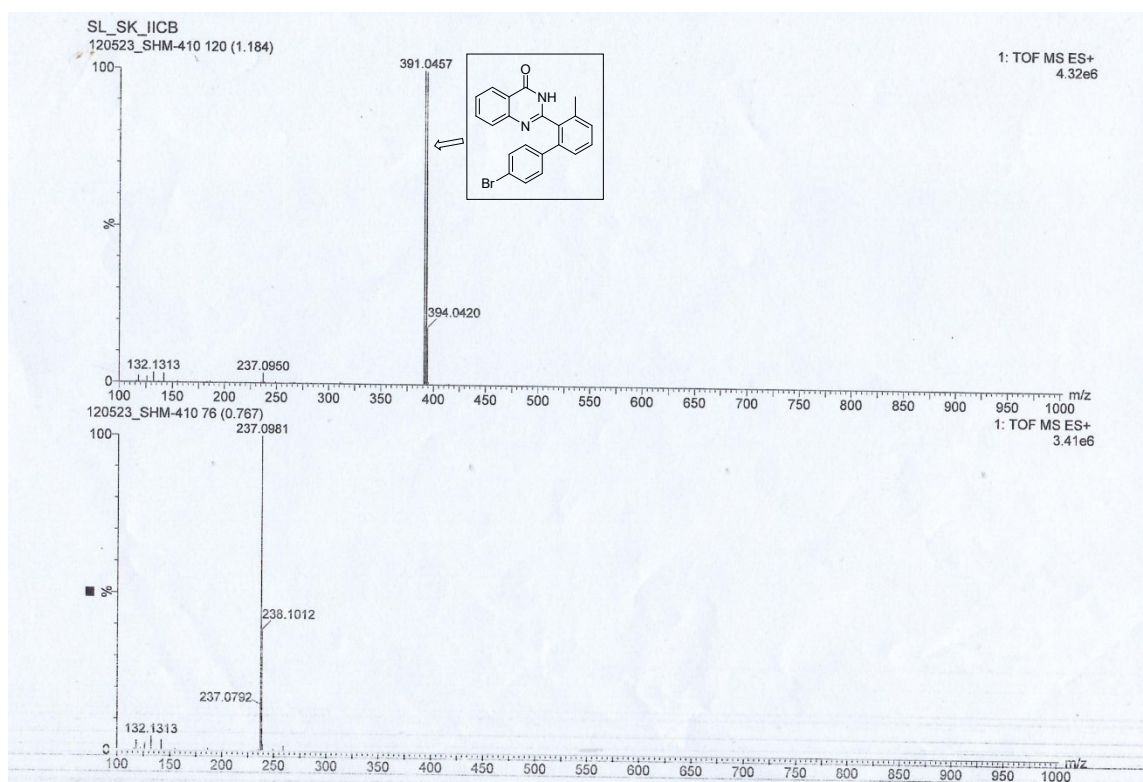
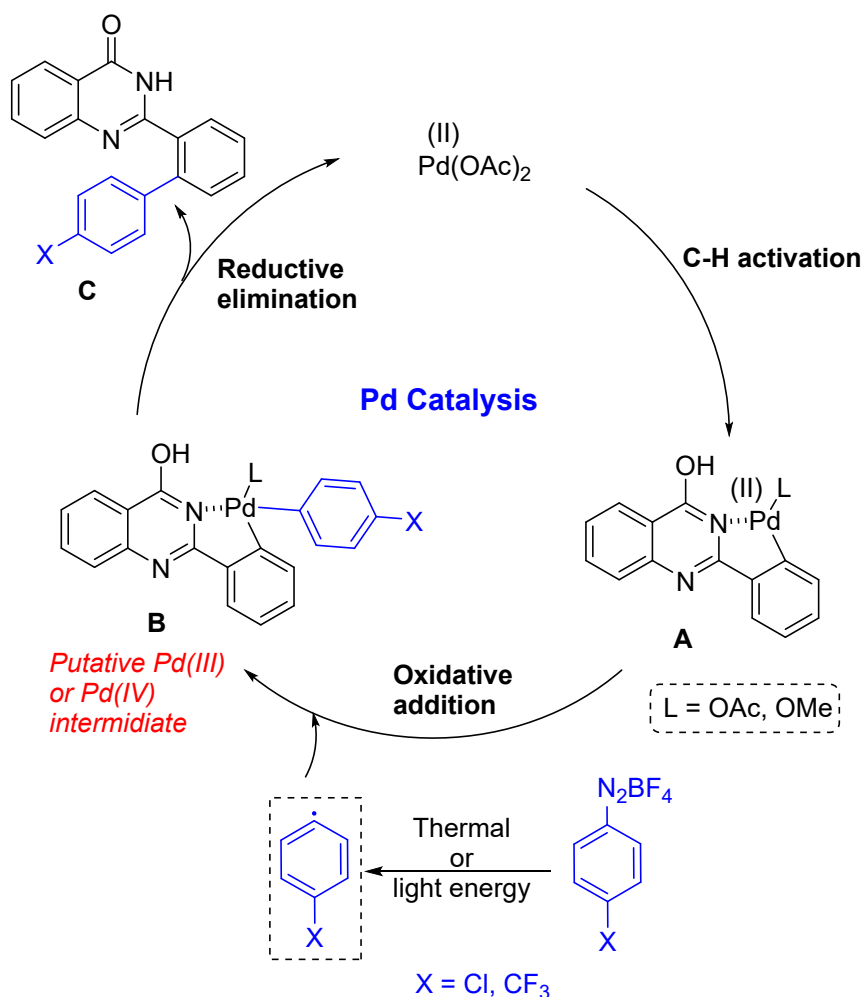


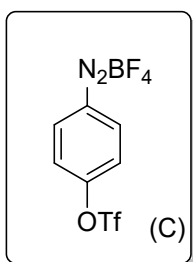
Figure 8: MS analysis of the reaction mixture of 2-(o-tolyl)quinazolin-4(3H)-one (9).

**Plausible mechanism for C–H arylation under thermal condition (no light irradiation) and green light irradiation in the absence of a photocatalyst:**



An anticipated mechanism is drawn here for the aryl reaction occurring in thermal conditions and light irradiation without any photocatalyst. Certain thermal or photonic energy may induce aryl radical formation<sup>8,9</sup> in methanol, which coupled with the Pd-complex (**A**) and results in the formation of either cationic Pd(III) [via 1e transfer] or Pd(IV) [via 2e transfer] complex. Again, the presence of excess aryl diazonium salt may be considered to be involved in electronic transfer. Thereafter, reductive elimination from high valent Pd complex (**B**) afforded product (**C**).

## Spectral data

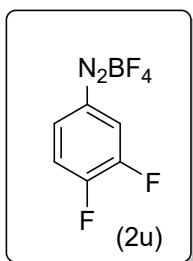


### **Aryl triflate diazonium salt (C).**

$^1H$  NMR (400 MHz, Acetone- $d_6$ )  $\delta$  9.18 – 9.11 (m, 2H), 8.28 – 8.23 (m, 2H).

$^{19}F$  NMR (376 MHz, Acetone- $d_6$ )  $\delta$  -73.63, -150.87, -150.92.

$^{13}C$  NMR (100 MHz, Acetone- $d_6$ )  $\delta$  157.6, 137.2, 126.2, 119.5 (q,  $J = 318$  Hz), 117.3.

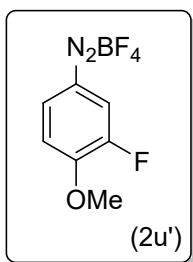


### **3,4-difluoro phenyl diazonium salt (2u):**

$^1H$  NMR (400 MHz, Acetone- $d_6$ )  $\delta$  8.96 (ddd,  $J = 9.0, 6.6, 2.6$  Hz, 1H), 8.90 – 8.85 (m, 1H), 8.11 (td,  $J = 9.5, 7.5$  Hz, 1H).

$^{19}F$  NMR (376 MHz, Acetone- $d_6$ )  $\delta$  -111.49 – -111.54 (m, 1F), -129.52 (dt,  $J = 19.4, 8.2$  Hz, 1F), -150.65 (s, 1F), -150.70 (s, 3F).

$^{13}C$  NMR (100 MHz, Acetone- $d_6$ )  $\delta$  159.7 (dd,  $J = 270.8, 11.9$  Hz), 151.0 (dd,  $J = 257.3, 14.4$  Hz), 134.1 (dd,  $J = 10.6, 3.9$  Hz), 123.9 (dd,  $J = 25.2, 3.7$  Hz), 122.3 (d,  $J = 21.1$  Hz), 112.5 – 112.4 (m).

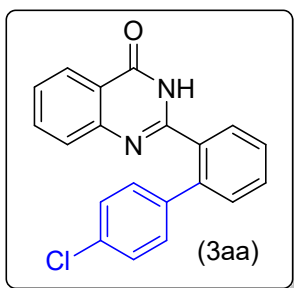


### **3-fluoro-4-methoxy phenyl diazonium salt (2u'):**

$^1H$  NMR (400 MHz, Acetone- $d_6$ )  $\delta$  8.77 (ddd,  $J = 9.3, 2.6, 1.4$  Hz, 1H), 8.63 (dd,  $J = 9.7, 2.6$  Hz, 1H), 7.81 (dd,  $J = 9.3, 7.9$  Hz, 1H), 4.27 (s, 3H).

$^{19}F$  NMR (376 MHz, Acetone- $d_6$ )  $\delta$  -128.21 (t,  $J = 9.4$  Hz, 1H), -150.77 (s, 1H), -150.82 (s, 3H).

$^{13}C$  NMR (100 MHz, Acetone- $d_6$ )  $\delta$  160.7 (d,  $J = 10.0$  Hz), 151.8 (d,  $J = 254.8$  Hz), 135.0 (d,  $J = 2.8$  Hz), 120.5 (d,  $J = 26.1$  Hz), 117.1 (d,  $J = 2.5$  Hz), 103.8 (d,  $J = 10.8$  Hz), 58.8.

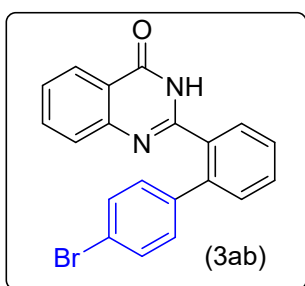


**2-(4'-chloro-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3aa):** Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a white solid (80 mg, 80%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.89 (s, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.85 – 7.73 (m, 3H), 7.58 (td, *J* = 7.6, 1.3 Hz, 1H), 7.51 (dd, *J* = 7.7, 1.2 Hz, 2H), 7.46 (td, *J* = 7.3, 1.2 Hz, 1H), 7.27 – 7.17 (m, 4H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.5, 153.6, 149.2, 139.5, 137.9, 134.9, 134.1, 132.8, 131.1, 130.9, 130.5, 130.4, 128.9, 128.3, 127.9, 127.2, 126.4, 120.7.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup> : 333.0795; found: 333.0783.



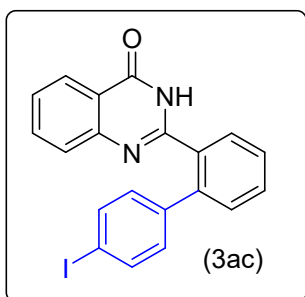
**2-(4'-bromo-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ab):**

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (87.1 mg, 77%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.45 (s, 1H), 8.19 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.84 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.82 – 7.74 (m, 2H), 7.60 (td, *J* = 7.5, 1.5 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.49 – 7.44 (m, 1H), 7.42 – 7.37 (m, 2H), 7.23 – 7.18 (m, 2H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.9, 153.4, 149.1, 139.4, 138.3, 135.0, 132.7, 132.1, 131.3, 130.9, 130.6, 130.6, 128.5, 128.0, 127.3, 126.6, 122.6, 120.8.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> : 377.0290; found: 377.0274.



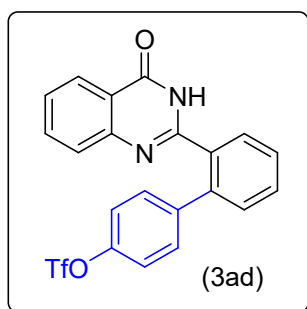
### 2-(4'-iodo-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ac):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (44.5 mg, 35%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.11 (s, 1H), 8.20 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.85 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.83 – 7.74 (m, 2H), 7.66 – 7.61 (m, 2H), 7.61 – 7.47 (m, 3H), 7.46 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.11 – 7.05 (m, 2H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.8, 153.4, 149.1, 139.5, 138.8, 138.1, 135.0, 132.7, 131.3, 130.9, 130.8, 130.6, 128.5, 128.0, 127.3, 126.6, 120.8, 94.3.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>IN<sub>2</sub>O [M+H]<sup>+</sup> : 425.0151; found: 425.0158.



### 2'--(4-oxo-3,4-dihydroquinazolin-2-yl)-[1,1'-biphenyl]-4-yl trifluoromethanesulfonate (3ad):

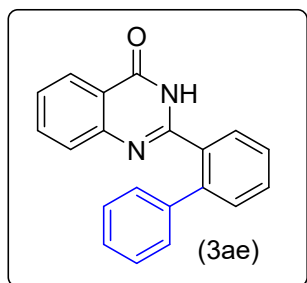
Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (73.6 mg, 55%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.62 (s, 1H), 8.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.82 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.80 – 7.75 (m, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.62 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.56 (td, *J* = 7.5, 1.4 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.42 – 7.37 (m, 2H), 7.15 – 7.10 (m, 2H).

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -72.69.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.8, 153.2, 149.1, 140.3, 139.2, 135.1, 133.0, 131.2, 131.0, 130.9, 130.3, 128.7, 128.0, 127.3, 126.4, 121.4, 120.5, δ 118.8 (q, *J* = 319.2 Hz).

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>14</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>S [M+H]<sup>+</sup> : 447.0626 ; found: 447.0624.



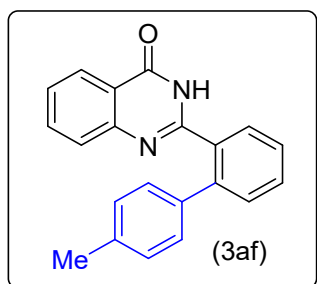
### 2-([1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ae):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a white solid (35.7 mg, 40%).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  9.16 (s, 1H), 8.17 (d,  $J = 7.8$  Hz, 1H), 7.89 (d,  $J = 7.5$  Hz, 1H), 7.82 – 7.76 (m, 2H), 7.59 (t,  $J = 7.5$  Hz, 1H), 7.54 – 7.46 (m, 3H), 7.34 – 7.31 (m, 2H), 7.27-7.30 (m, 3H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.7, 153.7, 149.1, 140.6, 139.2, 134.9, 132.6, 131.2, 131.0, 130.6, 129.0, 128.4, 128.2, 127.9, 127.2, 126.6, 120.8.

HRMS (ESI,  $m/z$ ) calcd. for  $\text{C}_{20}\text{H}_{15}\text{N}_2\text{O}$   $[\text{M}+\text{H}]^+$  : 299.1184; found: 299.1177.



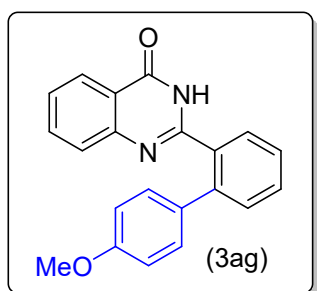
### 2-(4'-methyl-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3af):

Column chromatography ( $\text{SiO}_2$ , eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a white solid (57 mg, 61%).

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.76 (s, 1H), 8.19 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.91 (dd,  $J = 7.6, 1.4$  Hz, 1H), 7.83 (d,  $J = 8.1$  Hz, 1H), 7.81 – 7.77 (m, 1H), 7.58 (td,  $J = 7.6, 1.4$  Hz, 1H), 7.52 – 7.42 (m, 3H), 7.23 (d,  $J = 8.0$  Hz, 2H), 7.13 (d,  $J = 7.8$  Hz, 2H), 2.33 (s, 3H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.6, 153.8, 149.2, 140.5, 138.3, 136.1, 134.8, 132.6, 131.1, 131.0, 130.6, 129.8, 128.9, 128.0, 127.1, 126.6, 120.8, 21.3.

HRMS (ESI,  $m/z$ ) calcd. for  $\text{C}_{21}\text{H}_{17}\text{N}_2\text{O}$   $[\text{M}+\text{H}]^+$  : 313.1341; found: 313.1327.



### 2-(4'-methoxy-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ag):

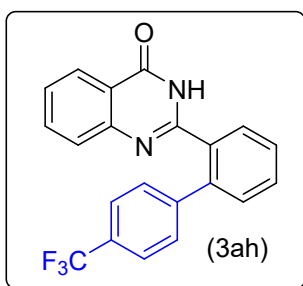
Column chromatography ( $\text{SiO}_2$ , eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (69.8 mg, 71%).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.04 (s, 1H), 8.19 (d,  $J = 7.8$  Hz, 1H), 7.87 (dd,  $J = 8.0, 1.3$  Hz, 1H), 7.86 – 7.74 (m, 2H), 7.61 – 7.51 (m, 1H), 7.54 – 7.41 (m, 3H), 7.31 – 7.19 (m, 2H), 6.87 – 6.75 (m, 2H), 3.76 (s, 3H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.7, 159.6, 153.9, 149.3, 140.1, 134.8, 132.5, 131.2, 131.1, 131.0, 130.6, 130.2, 128.0, 127.7, 127.1, 126.6, 120.9, 114.5, 55.3.

HRMS (ESI,  $m/z$ ) calcd. for  $\text{C}_{21}\text{H}_{17}\text{N}_2\text{O}_2$   $[\text{M}+\text{H}]^+$  : 329.1290; found: 329.1275.





### 2-(4'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ah):

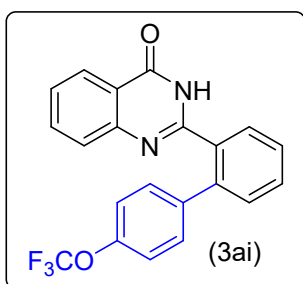
Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (95.5 mg, 87%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 10.22 (s, 1H), 8.16 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.82 – 7.77 (m, 2H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.62 (td, *J* = 7.6, 1.4 Hz, 1H), 7.54 (td, *J* = 7.6, 1.3 Hz, 1H), 7.52 – 7.46 (m, 4H), 7.44 (d, *J* = 8.2 Hz, 2H).

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.46.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.5, 153.3, 149.1, 143.3, 139.5, 135.1, 133.0, 131.2, 131.0, 130.5, 130.0 (q, *J* = 32 Hz), 129.5, 128.8, 124.1 (q, *J* = 271 Hz), 128.0, 127.3, 126.5, 125.6 (q, *J* = 4.0 Hz), 120.7.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>14</sub>F<sub>3</sub>N<sub>2</sub>O [M+H]<sup>+</sup> : 367.1058; found: 367.1043.



### 2-(4'-(trifluoromethoxy)-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ai):

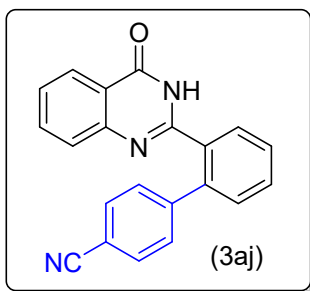
Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (98.5 mg, 86%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.85 (s, 1H), 8.18 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.84 – 7.76 (m, 2H), 7.72 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.61 (td, *J* = 7.6, 1.5 Hz, 1H), 7.56 – 7.46 (m, 3H), 7.38 – 7.33 (m, 2H), 7.13 – 7.07 (m, 2H).

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -57.71.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.2, 153.4, 149.1, 149.0, 139.4, 138.2, 135.0, 132.9, 131.2, 131.0, 130.6, 130.5, 128.5, 128.0, 127.3, 126.5, 121.1, 120.7, 120.5 (q, *J* = 255.5 Hz).

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>14</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 383.1007; found: 383.1014.



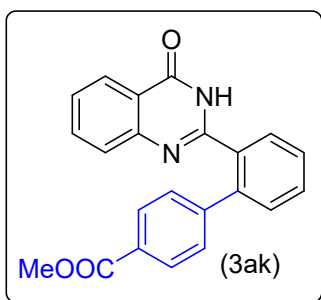
**2'-(4-oxo-3,4-dihydroquinazolin-2-yl)-[1,1'-biphenyl]-4-carbonitrile (3aj):**

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (53.3 mg, 55%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.49 (s, 1H), 8.16 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.84 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.82 – 7.76 (m, 1H), 7.65 (td, *J* = 8.1, 7.6, 1.3 Hz, 2H), 7.59 (td, *J* = 7.5, 1.5 Hz, 1H), 7.54 – 7.48 (m, 4H), 7.45 – 7.41 (m, 2H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.7, 152.9, 149.0, 144.6, 139.2, 135.2, 132.9, 132.3, 131.3, 130.9, 130.4, 129.9, 129.2, 128.0, 127.5, 126.4, 120.5, 118.6, 111.6.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>14</sub>N<sub>3</sub>O [M+H]<sup>+</sup> : 324.1137; found: 324.1124.



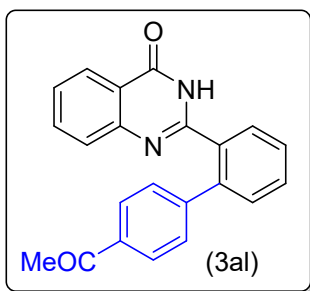
**methyl 2'-(4-oxo-3,4-dihydroquinazolin-2-yl)-[1,1'-biphenyl]-4-carboxylate (3ak):**

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (52.3 mg, 49%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.63 (s, 1H), 8.17 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.95 – 7.90 (m, 2H), 7.84 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.73 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.62 (td, *J* = 7.5, 1.5 Hz, 1H), 7.55 (td, *J* = 7.6, 1.4 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.42 – 7.37 (m, 2H), 3.87 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 166.7, 162.1, 153.3, 149.1, 144.1, 139.8, 135.0, 133.0, 131.2, 130.9, 130.4, 130.0, 129.6, 129.1, 128.7, 128.0, 127.3, 126.5, 120.7, 52.3.

HRMS (ESI, *m/z*) calcd. for C<sub>22</sub>H<sub>17</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> : 357.1239; found: 357.1237.



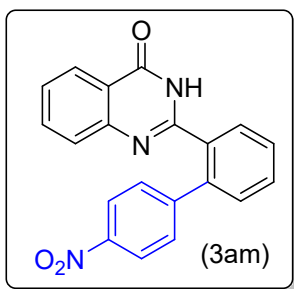
### 2-(4'-acetyl-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3al):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (50 mg, 49%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.97 (s, 1H), 8.16 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.84 – 7.76 (m, 4H), 7.73 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.61 (td, *J* = 7.5, 1.5 Hz, 1H), 7.56 – 7.47 (m, 3H), 7.44 – 7.38 (m, 2H), 2.52 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 197.6, 162.3, 153.3, 149.1, 144.3, 139.7, 136.2, 135.0, 132.9, 131.2, 130.9, 130.5, 129.3, 128.7, 128.0, 127.3, 126.5, 120.7, 26.7.

HRMS (ESI, *m/z*) calcd. for C<sub>22</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 341.1290; found: 341.1279.



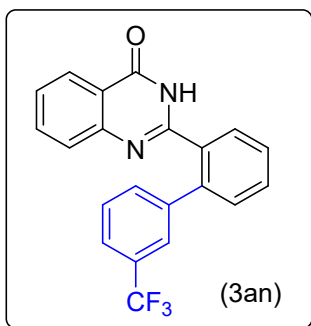
### 2-(4'-nitro-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3am):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (70 mg, 68%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.40 (s, 1H), 8.16 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.12 – 8.07 (m, 2H), 7.83 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.81 – 7.76 (m, 1H), 7.69 – 7.64 (m, 2H), 7.61 (td, *J* = 7.5, 1.5 Hz, 1H), 7.54 – 7.46 (m, 4H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 163.0, 152.9, 149.0, 147.2, 146.7, 139.0, 135.3, 133.0, 131.3, 130.9, 130.4, 130.0, 129.3, 128.0, 127.5, 126.4, 123.7, 120.5.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup> : 344.1035; found: 344.1024.



### 2-(3'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3an):

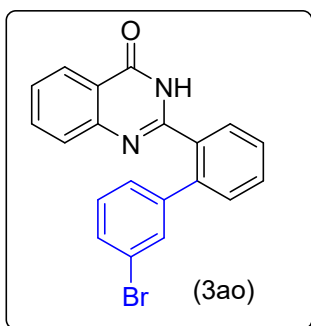
Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (87.8 mg, 80%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.54 (s, 1H), 8.14 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.83 – 7.75 (m, 2H), 7.72 – 7.66 (m, 2H), 7.63 (td, *J* = 7.6, 1.4 Hz, 1H), 7.58 – 7.46 (m, 4H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.27 (t, *J* = 7.8 Hz, 1H).

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.72.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.8, 153.3, 149.0, 140.4, 139.5, 135.0, 133.1, 132.4, 131.2, 130.9, 131.0 (q, *J* = 32 Hz), 130.3, 128.9, 128.7, 127.9, 127.3, 126.4, 126.1 (q, *J* = 3.7 Hz), 123.9 (q, *J* = 271 Hz), 124.5 (q, *J* = 3.7 Hz), 120.5.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>14</sub>F<sub>3</sub>N<sub>2</sub>O [M+H]<sup>+</sup> : 367.1058; found: 367.1060.



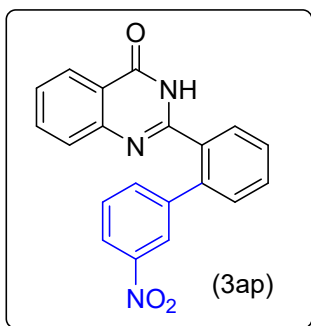
### 2-(3'-bromo-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ao):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (73.5 mg, 65%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 10.19 (s, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.80 (dd, *J* = 15.4, 7.5 Hz, 2H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.56 (s, 1H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.37 (dd, *J* = 8.0, 1.9 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.5, 153.4, 149.1, 141.5, 139.3, 135.0, 132.8, 132.1, 131.2, 131.0, 130.9, 130.5, 130.0, 128.6, 127.9, 127.8, 127.3, 126.5, 122.8, 120.7.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> : 377.0290; found: 377.0289.



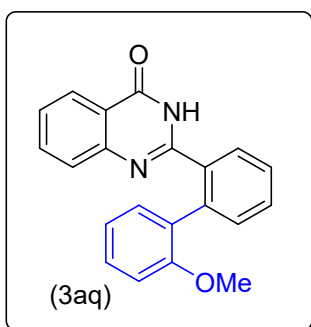
### 2-(3'-nitro-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ap):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (62.7 mg, 61%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.59 (s, 1H), 8.32 (t, *J* = 1.9 Hz, 1H), 8.15 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.10 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.83 (d, *J* = 7.4 Hz, 1H), 7.81 – 7.76 (m, 1H), 7.66 (t, *J* = 7.9 Hz, 2H), 7.62 – 7.53 (m, 3H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.8, 152.8, 148.9, 148.3, 141.5, 138.7, 135.2, 135.2, 133.1, 131.4, 131.0, 130.4, 129.3, 129.1, 128.0, 127.5, 126.4, 124.3, 122.6, 120.5.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 344.1035; found: 344.1029.



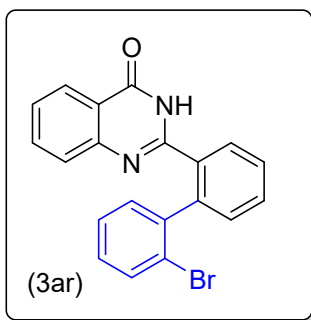
### 2-(2'-methoxy-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3aq):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (64 mg, 65%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.35 (s, 1H), 8.18 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.93 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.74 (d, *J* = 1.1 Hz, 1H), 7.73 (t, *J* = 1.2 Hz, 1H), 7.58 (td, *J* = 7.5, 1.7 Hz, 1H), 7.53 (td, *J* = 7.5, 1.6 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.40 – 7.32 (m, 2H), 7.23 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.00 (td, *J* = 7.5, 1.0 Hz, 1H), 6.92 (dd, *J* = 8.4, 1.1 Hz, 1H), 3.67 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.5, 155.9, 153.8, 149.4, 137.1, 134.7, 133.7, 131.7, 131.3, 130.9, 130.3, 129.7, 128.4, 128.3, 127.9, 126.8, 126.5, 121.6, 120.9, 111.1, 55.5.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 329.1290; found: 329.1277.



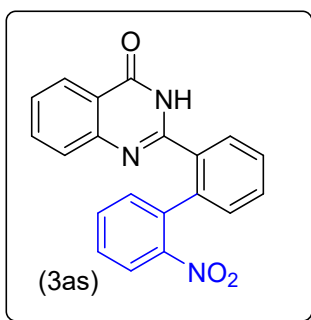
### 2-(2'-bromo-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3ar):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (38.5 mg, 34%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.10 (s, 1H), 8.18 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.98 (d, *J* = 4.9 Hz, 1H), 7.73 (t, *J* = 7.3 Hz, 1H), 7.68 – 7.58 (m, 4H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.40 (dd, *J* = 6.5, 2.1 Hz, 1H), 7.37 – 7.29 (m, 2H), 7.22 (t, *J* = 7.3 Hz, 1H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.6, 152.4, 149.0, 140.5, 139.9, 134.8, 133.2, 133.1, 131.5, 131.3, 130.9, 130.0, 129.7, 129.0, 128.0, 127.1, 126.5, 123.2, 120.8.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> : 377.0290; found: 377.0283.



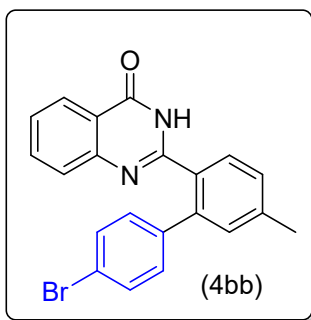
### 2-(2'-nitro-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3as):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (18.5 mg, 18%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 9.73 (s, 1H), 8.18 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.02 – 7.94 (m, 1H), 7.89 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.73 (t, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.62–7.55 (m, 2H), 7.50 – 7.47 (m, 2H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.30 – 7.25 (m, 2H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.8, 152.2, 149.6, 148.8, 137.0, 135.0, 134.9, 133.0, 132.7, 132.0, 131.0, 129.7, 129.5, 129.2, 129.2, 127.9, 127.2, 126.5, 124.2, 120.9.

HRMS (ESI, *m/z*) calcd. for C<sub>20</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup> : 344.1035; found: 344.1041.



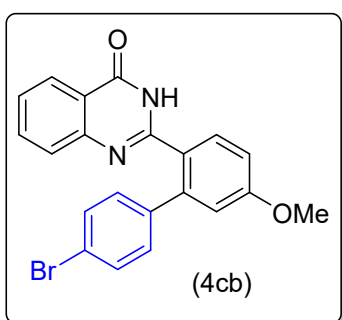
### 2-(4'-bromo-5-methyl-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (4bb):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (91.5 mg, 78%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.71 (s, 1H), 8.18 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.82 – 7.76 (m, 1H), 7.76 – 7.70 (m, 2H), 7.52 – 7.45 (m, 1H), 7.37 – 7.33 (m, 2H), 7.29 – 7.26 (m, 1H), 7.24 (s, 1H), 7.18 – 7.14 (m, 2H), 2.44 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.2, 153.5, 149.2, 141.5, 139.3, 138.5, 134.9, 131.9, 131.6, 130.7, 130.6, 123.0, 129.1, 127.9, 127.1, 126.5, 122.4, 120.7, 21.6.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> : 391.0446; found: 391.0445.



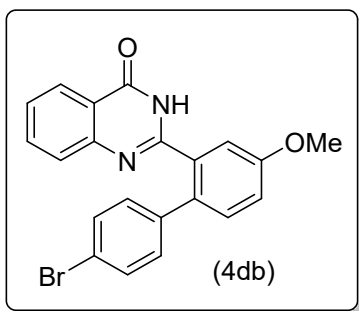
### 2-(4'-bromo-5-methoxy-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (4cb):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (91.6 mg, 75%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.52 (s, 1H), 8.18 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.81 (d, *J* = 8.6 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.50 – 7.45 (m, 1H), 7.41 – 7.36 (m, 2H), 7.22 – 7.16 (m, 2H), 7.01 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.93 (d, *J* = 2.6 Hz, 1H), 3.88 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.2, 161.6, 153.2, 149.3, 141.2, 138.3, 134.9, 132.4, 132.0, 130.6, 127.9, 127.0, 126.5, 125.3, 122.7, 120.6, 116.4, 113.7, 55.7.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 407.0395; found: 407.0385.



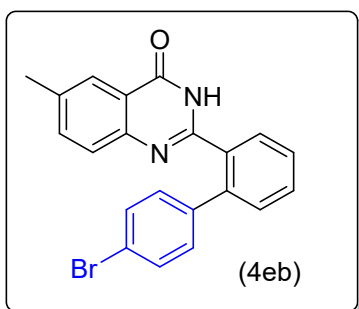
### 2-(4'-bromo-6-methoxy-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (4db):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (62.1 mg, 51%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 9.17 (s, 1H), 8.21 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.83 – 7.77 (m, 2H), 7.53 – 7.49 (m, 1H), 7.42 – 7.34 (m, 4H), 7.19 – 7.15 (m, 2H), 7.13 (dd, *J* = 8.6, 2.8 Hz, 1H), 3.91 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.6, 159.6, 153.5, 148.3, 137.8, 135.2, 132.3, 132.1, 131.8, 130.7, 127.7, 127.6, 126.7, 124.7, 122.3, 120.7, 118.1, 115.3, 55.9.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 407.0395; found: 407.0383.



### 2-(4'-bromo-[1,1'-biphenyl]-2-yl)-6-methylquinazolin-4(3H)-one (4eb):

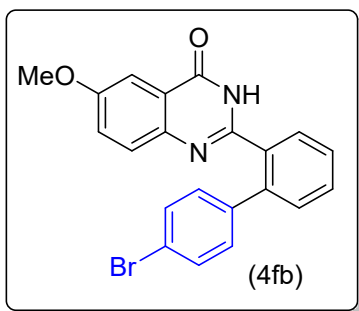
Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (83.3 mg, 71%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.46 (s, 1H), 7.91 (s, 1H), 7.74 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.59 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.50 (td, *J* = 7.5, 1.4 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.29 – 7.23 (m, 2H), 7.14 – 7.08 (m, 2H), 2.48 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.5, 152.7, 147.1, 139.5, 138.5, 137.5, 136.4, 132.8, 131.7, 131.0, 130.7, 130.7, 130.4, 128.3, 127.7, 125.8, 122.2, 120.4, 21.5.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> : 391.0446; found: 391.0433.





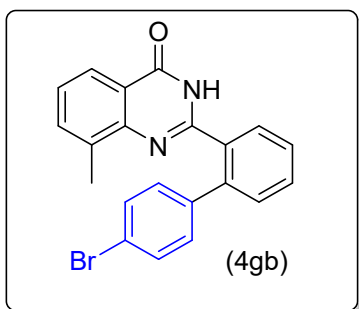
### 2-(4'-bromo-[1,1'-biphenyl]-2-yl)-6-methoxyquinazolin-4(3H)-one (4fb):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (85.5 mg, 70%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 9.21 (s, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.9 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 2.8 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.37-7.43 (m, 3H), 7.19 (d, *J* = 8.1 Hz, 2H), 3.91 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.6, 158.9, 151.1, 143.3, 139.4, 138.2, 132.5, 132.2, 131.5, 131.2, 130.9, 130.6, 129.4, 128.5, 125.3, 122.7, 121.5, 106.1, 56.0.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 407.0395; found: 407.0386.



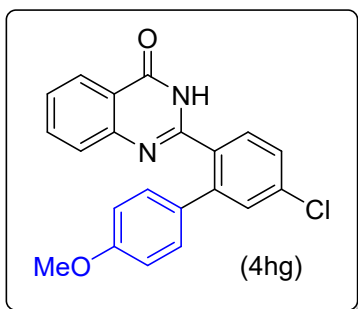
### 2-(4'-bromo-[1,1'-biphenyl]-2-yl)-8-methylquinazolin-4(3H)-one (4gb):

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (46.9 mg, 40%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.15 (s, 1H), 8.06 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.88 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.63 – 7.58 (m, 2H), 7.55 (td, *J* = 7.5, 1.5 Hz, 1H), 7.49 – 7.42 (m, 3H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.19 (m, 2H), 2.49 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.6, 151.4, 147.6, 140.0, 139.0, 136.7, 135.6, 132.9, 131.9, 131.1, 130.8, 130.6, 128.5, 126.8, 124.1, 122.3, 120.7, 17.6.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup> : 391.0446; found: 391.0448.



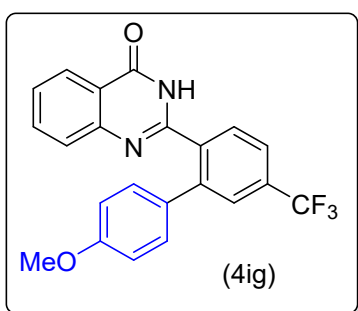
**2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (4hg):**

Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (41.4 mg, 38%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.17 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.89 – 7.78 (m, 3H), 7.55 – 7.50 (m, 1H), 7.44 (d, *J* = 2.1 Hz, 1H), 7.40 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.23 – 7.15 (m, 2H), 6.80 – 6.73 (m, 2H), 3.74 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 161.7, 160.0, 153.4, 148.1, 142.1, 137.5, 135.3, 132.1, 130.9, 130.3, 130.1, 129.9, 127.8, 127.6, 127.4, 126.7, 120.6, 114.6, 55.4.

HRMS (ESI, *m/z*) calcd. for C<sub>21</sub>H<sub>16</sub>ClN<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 363.0900; found: 363.0891.



**2-(4'-methoxy-5-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (4ig):**

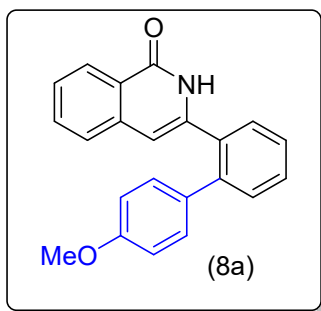
Column chromatography (SiO<sub>2</sub>, eluting with 5:1 hexane/ethyl acetate) afforded the desired product as a brown solid (41.6 mg, 35%).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.65 (s, 1H), 8.17 (d, *J* = 7.7 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.86 – 7.78 (m, 2H), 7.72 (d, *J* = 4.3 Hz, 2H), 7.55 – 7.50 (m, 1H), 7.28 – 7.20 (m, 2H), 6.85 – 6.75 (m, 2H), 3.75 (s, 3H).

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.76.

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 162.1, 160.1, 152.7, 149.0, 141.2, 135.7, 135.1, 133.0 (q, *J* = 32.8 Hz), 131.3, 130.3, 130.0, 128.1, 127.8 (q, *J* = 3.7 Hz), 127.5, 126.6, 124.3 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 271.2 Hz), 120.9, 114.6, 55.3.

HRMS (ESI, *m/z*) calcd. for C<sub>22</sub>H<sub>16</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 397.1164; found: 397.1165.



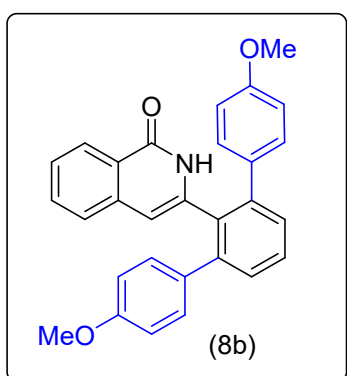
### 3-(4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinolin-1(2H)-one (8a):

Column chromatography (SiO<sub>2</sub>, eluting with 4:1 hexane/ethyl acetate) afforded the desired product as a brown solid (27.5 mg, 28%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.46 (s, 1H), 8.31 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.53 – 7.49 (m, 2H), 7.47 – 7.41 (m, 3H), 7.24 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 8.3 Hz, 2H), 6.52 (s, 1H), 3.76 (s, 3H).

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 159.4, 140.2, 140.1, 138.3, 133.3, 132.9, 131.8, 131.2, 130.3, 130.2, 130.0, 127.7, 127.6, 126.8, 126.5, 114.3, 107.2, 55.3.

HRMS (ESI, *m/z*) calcd. for C<sub>22</sub>H<sub>18</sub>NO<sub>2</sub> [M+H]<sup>+</sup> : 328.1338 ; found: 328.1330.



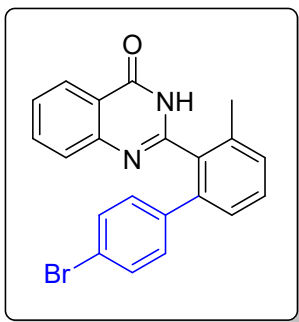
### 3-(4,4''-dimethoxy-[1,1':3',1''-terphenyl]-2'-yl)isoquinolin-1(2H)-one (8b):

Column chromatography (SiO<sub>2</sub>, eluting with 4:1 hexane/ethyl acetate) afforded the desired product as a brown solid (23.4 mg, 18%).

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.27 (s, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 7.52 (q, *J* = 7.1 Hz, 2H), 7.41 (d, *J* = 7.7 Hz, 2H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 8.3 Hz, 4H), 6.74 (d, *J* = 8.4 Hz, 4H), 6.09 (s, 1H), 3.72 (s, 6H).

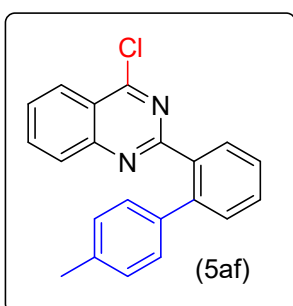
<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 158.9, 142.2, 137.8, 137.7, 132.8, 132.6, 131.8, 130.0, 129.8, 129.6, 127.4, 126.6, 126.4, 113.9, 110.4, 55.3.

HRMS (ESI, *m/z*) calcd. for C<sub>29</sub>H<sub>24</sub>NO<sub>3</sub> [M+H]<sup>+</sup> : 434.1756; found: 434.1751.



**2-(4'-bromo-3-methyl-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one-** Detected by LC-MS.

HRMS (ESI, m/z) calcd. for  $C_{21}H_{16}BrN_2O$   $[M+H]^+$  : 391.0446; found: 391.0457.



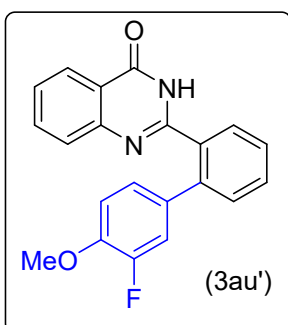
**4-chloro-2-(4'-methyl-[1,1'-biphenyl]-2-yl)quinazoline (5af):**

Column chromatography ( $SiO_2$ , eluting with 19:1 hexane/ethyl acetate) afforded the desired product as a white solid (52 mg, 80%).

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.20 (d,  $J = 8.2$  Hz, 1H), 7.98 – 7.85 (m, 3H), 7.71-7.63 (m, 1H), 7.57 – 7.45 (m, 3H), 7.09 (d,  $J = 8.1$  Hz, 2H), 7.02 (d,  $J = 7.8$  Hz, 2H), 2.30 (s, 3H).

$^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  163.3, 161.9, 151.4, 142.2, 138.7, 137.2, 136.3, 134.9, 131.0, 131.0, 129.9, 129.2, 128.9, 128.8, 128.6, 127.4, 125.8, 121.9, 21.2.

HRMS (ESI, m/z) calcd. for  $C_{21}H_{16}ClN_2$   $[M+H]^+$  : 331.1002; found: 331.0992.



**2-(3'-fluoro-4'-methoxy-[1,1'-biphenyl]-2-yl)quinazolin-4(3H)-one (3au'):**

Column chromatography ( $SiO_2$ , eluting with 19:1 hexane/ethyl acetate) afforded the desired product as a white solid (67 mg, 64%).

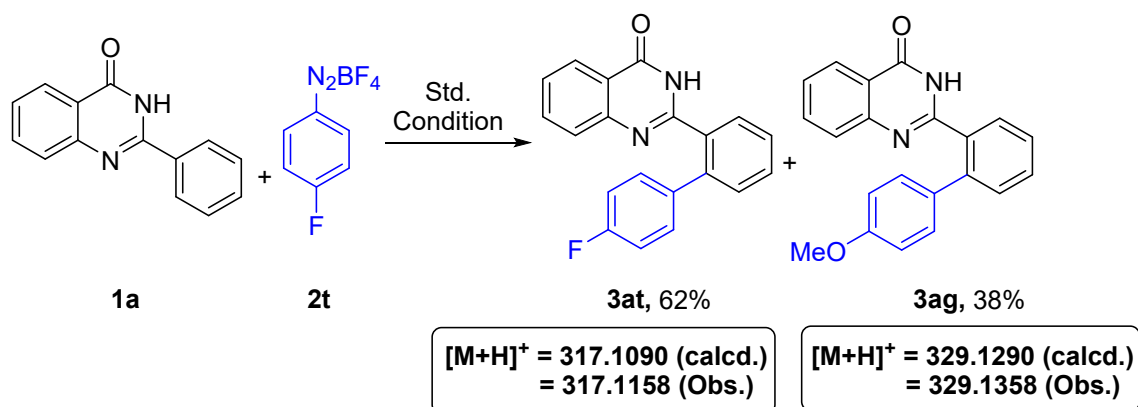
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  9.94 (s, 1H), 8.17 (d,  $J = 7.8$  Hz, 1H), 7.82 – 7.76 (m, 3H), 7.55 – 7.48 (m, 2H), 7.42 (t,  $J = 7.0$  Hz, 2H), 7.07 (dd,  $J = 12.0, 2.1$  Hz, 1H), 6.76 (t,  $J = 8.5$  Hz, 1H), 3.79 (s, 3H).

$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -134.16.

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  152.2 (d,  $J = 247.2$  Hz), 147.5 (d,  $J = 10.6$  Hz), 132.1 (d,  $J = 6.6$  Hz), 125.1 (d,  $J = 3.4$  Hz), 116.9 (d,  $J = 19.1$  Hz), 113.4 (d,  $J = 2.2$  Hz).

HRMS (ESI,  $m/z$ ) calcd. for  $\text{C}_{21}\text{H}_{16}\text{FN}_2\text{O}_2$   $[\text{M}+\text{H}]^+$  : 347.1196; found: 347.1124.

#### Nuisance effect and C–H arylation for 4-fluoro aryl diazonium salt:



SHM-559  
single\_pulse

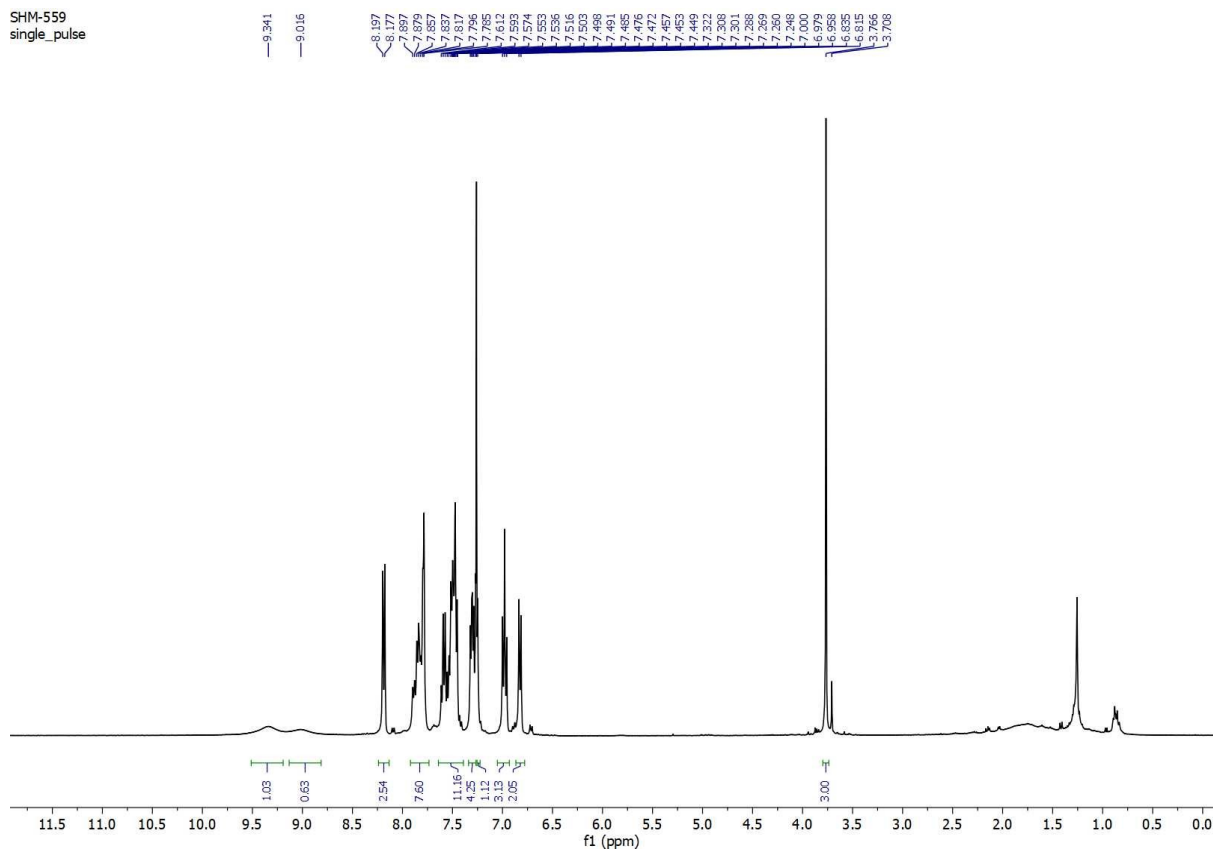
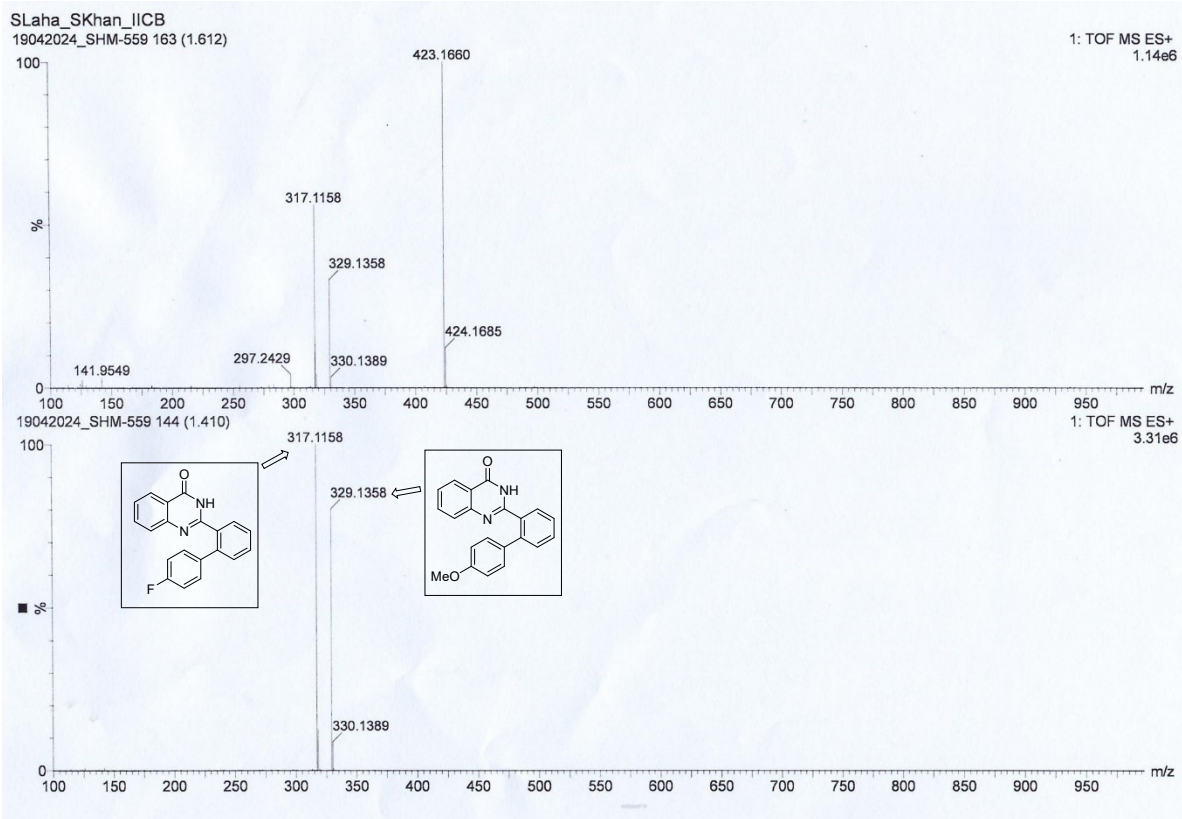


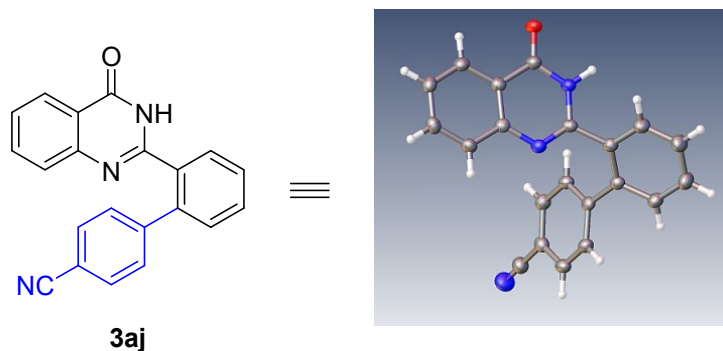
Figure 9:  $^1\text{H}$ NMR of the products mixture derived from the arylation reaction of 4-fluoro aryl diazonium salt with 2-phenyl quinazolinone.



**Figure 10: MS analysis of the arylation reaction of 4-fluoro aryl diazonium salt with 2-phenyl quinazolinone.**

### Crystal structure of 3aj:

The crystals of **3aj** were grown in dichloromethane-hexane solvent system. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



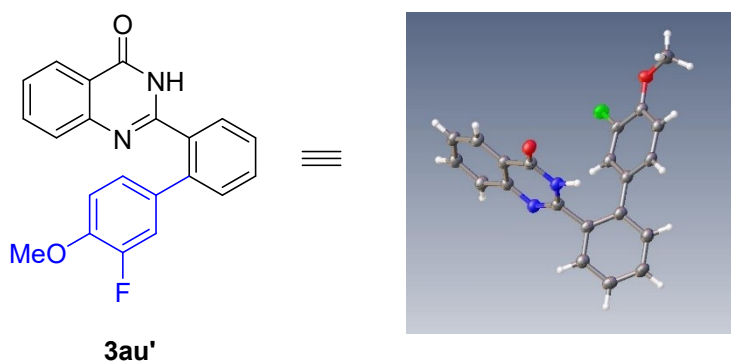
Thermal ellipsoid plot of **3aj**. Ellipsoids are represented with 50% probability. X-ray determined molecular structure of **3aj**, **CCDC: 2333220**

Identification code	SHM_305_0m_a
Empirical formula	C <sub>21</sub> H <sub>13</sub> N <sub>3</sub> O
Formula weight	323.34
Temperature/K	122
Crystal system	monoclinic
Space group	P21/c
a/Å	4.7332(2)
b/Å	20.9652(8)
c/Å	16.2410(6)
α/°	90
β/°	94.249(10)
γ/°	90
Volume/Å <sup>3</sup>	1607.21(11)
Z	4
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.336
μ/mm <sup>-1</sup>	0.677
F(000)	672.0
Crystal size/mm <sup>3</sup>	0.32 x 0.12 x 0.1

Radiation	CuK $\alpha$ ( $\lambda = 1.54178$ )
2 $\theta$ range for data collection/ $^\circ$	8.434 to 133.312
Index ranges	$-5 \leq h \leq 5, -24 \leq k \leq 24, -19 \leq l \leq 19$
Reflections collected	22992
Independent reflections	2803 [ $R_{\text{int}} = 0.0597, R_{\text{sigma}} = 0.0358$ ]
Data/restraints/parameters	2803/0/230
Goodness-of-fit on $F^2$	1.065
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0451, wR_2 = 0.1200$
Final R indexes [all data]	$R_1 = 0.0465, wR_2 = 0.12014$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.18/-0.24

### Crystal structure of 3au':

The crystals of **3au'** were grown in chloroform-hexane solvent system. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.



Thermal ellipsoid plot of **3au'**. Ellipsoids are represented with 50% probability. X-ray determined molecular structure of **3au'**, **CCDC: 2353282**

Identification code	SHM_420_0m_a
Empirical formula	$C_{84}H_{60}F_4N_8O_8$
Formula weight	1385.40
Temperature/K	100.00
Crystal system	monoclinic
Space group	P21/c
a/ $\text{\AA}$	7.4997(6)



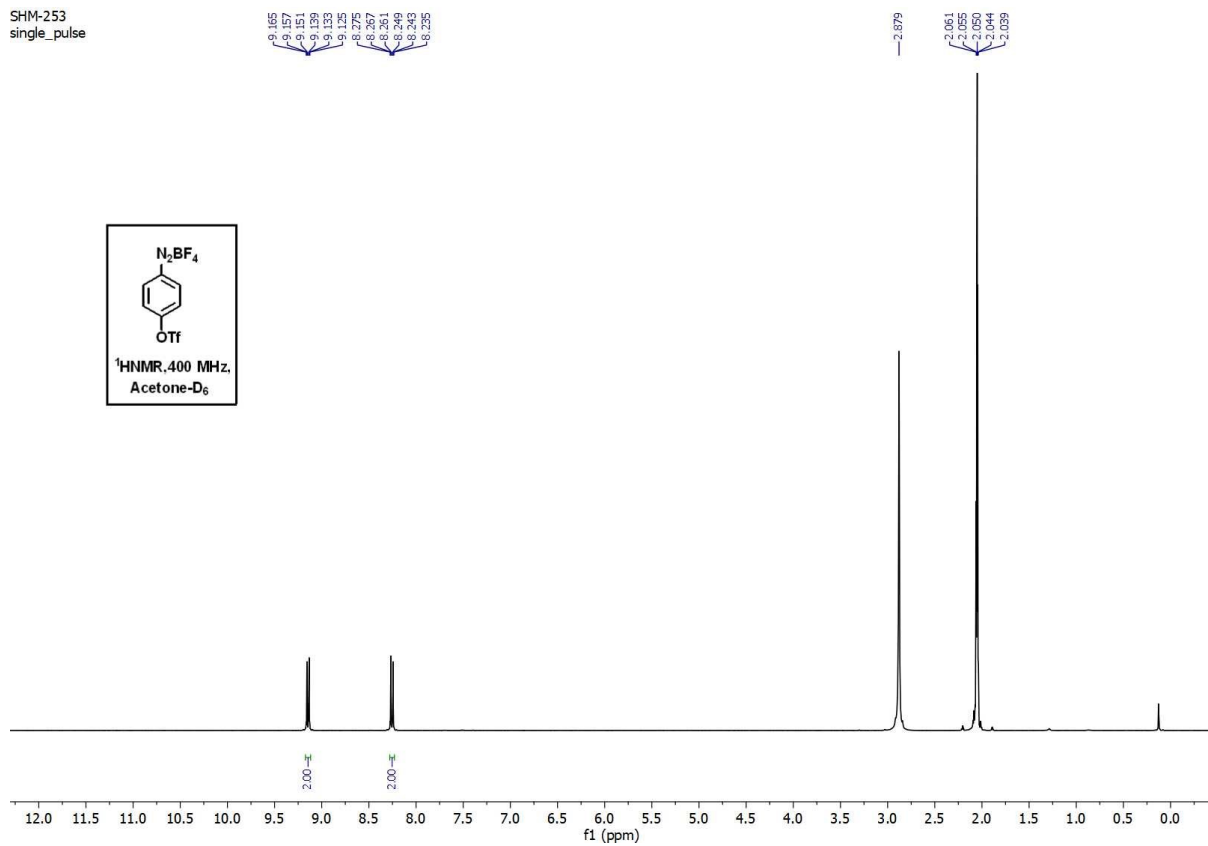
b/Å	13.6212(11)
c/Å	16.1797(12)
$\alpha$ /°	90
$\beta$ /°	93.812(4)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	1649.2(2)
Z	1
$\rho_{\text{calc}}$ g/cm <sup>3</sup>	1.395
$\mu$ /mm <sup>-1</sup>	0.812
F(000)	720.0
Crystal size/mm <sup>3</sup>	0.2 × 0.1 × 0.09
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54178)
2 $\theta$ range for data collection/°	8.494 to 137.322
Index ranges	-8 ≤ h ≤ 8, -15 ≤ k ≤ 16, -19 ≤ l ≤ 19
Reflections collected	24330
Independent reflections	2914 [R <sub>int</sub> = 0.0776, R <sub>sigma</sub> = 0.0433]
Data/restraints/parameters	2914/0/241
Goodness-of-fit on F <sup>2</sup>	1.071
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0682, wR <sub>2</sub> = 0.1471
Final R indexes [all data]	R <sub>1</sub> = 0.0729, wR <sub>2</sub> = 0.1533
Largest diff. peak/hole / e Å <sup>-3</sup>	0.25/-0.28

## References:

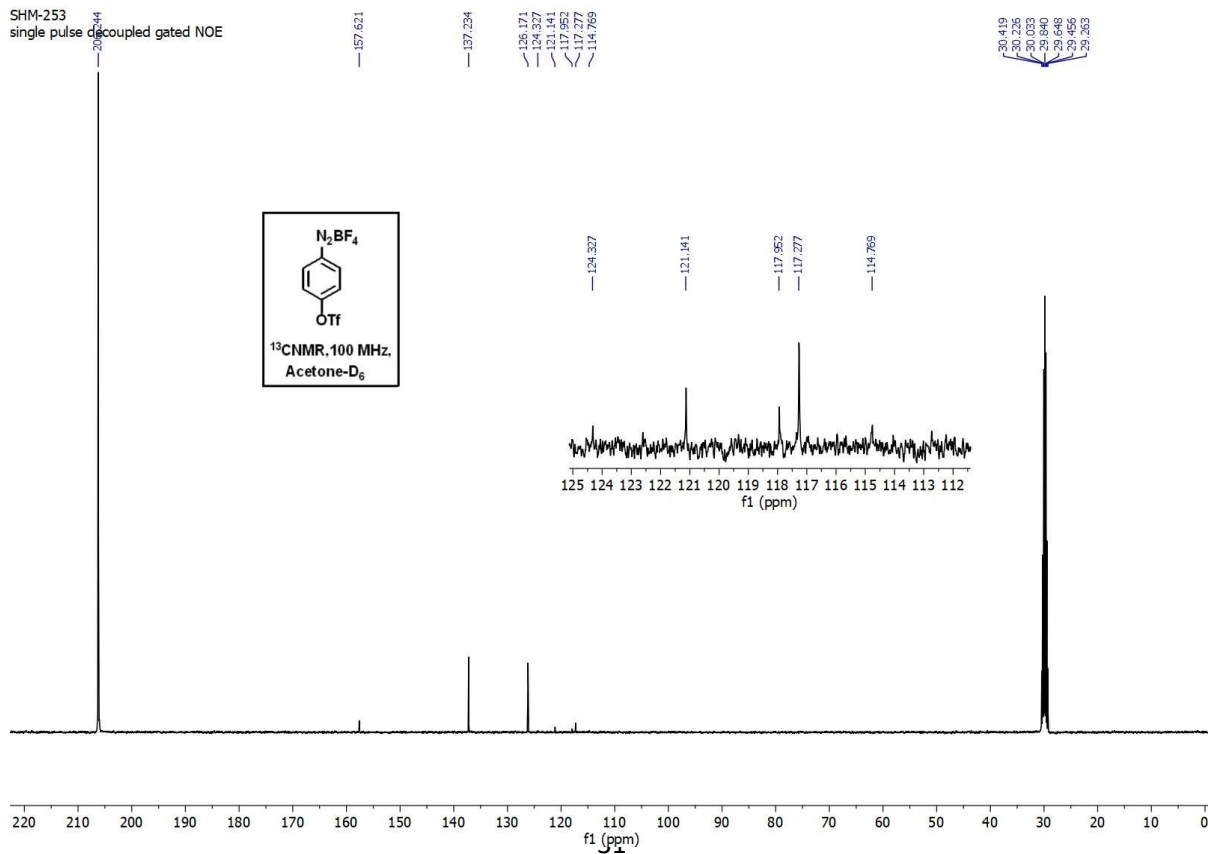
1. R. Cheng, T. Guo, D. Zhang-Negrerie, Y. Du and K. Zhao, *Synthesis*, 2013, **45**, 2998-3006.
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8. A. Polley, K. Varalaxmi and R. Jana, *ACS Omega*, 2018, **3**, 14503-14516.
9. S. Witzel, M. Hoffmann, M. Rudolph, M. Kerscher, P. Comba, A. Dreuw and A. S. K. Hashmi, *Cell Rep. Phys. Sci.*, 2021, **2**, 100325.

# NMR spectra

SHM-253  
single\_pulse



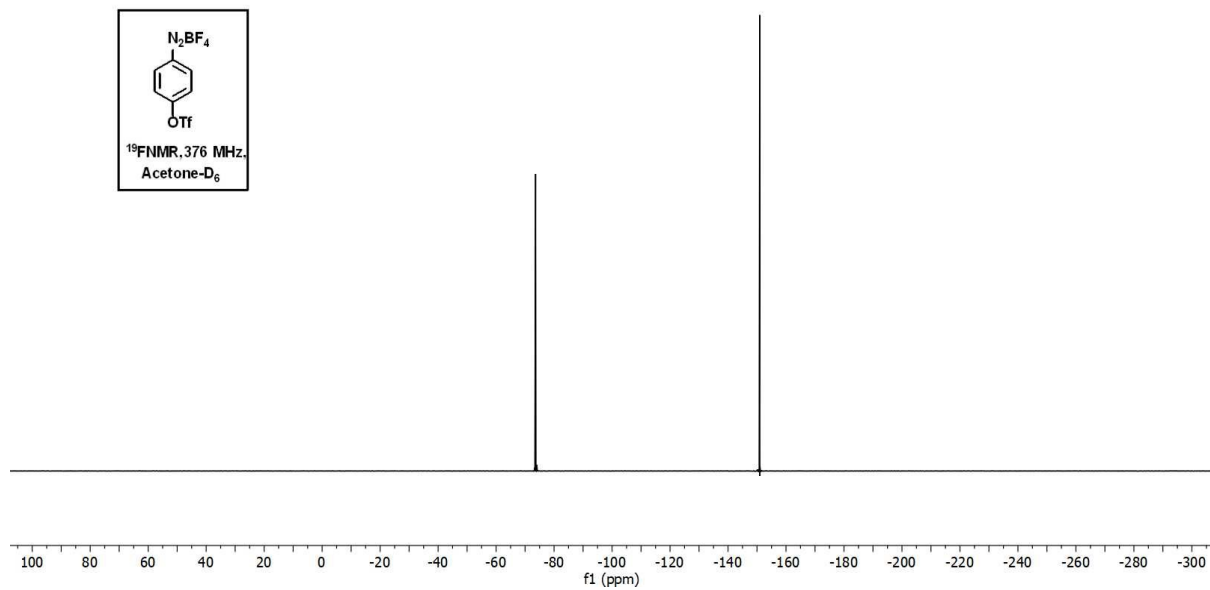
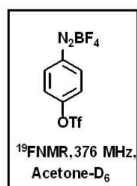
SHM-253  
single\_pulse decoupled gated NOE



SHM-253  
single pulse decoupled gated NOE

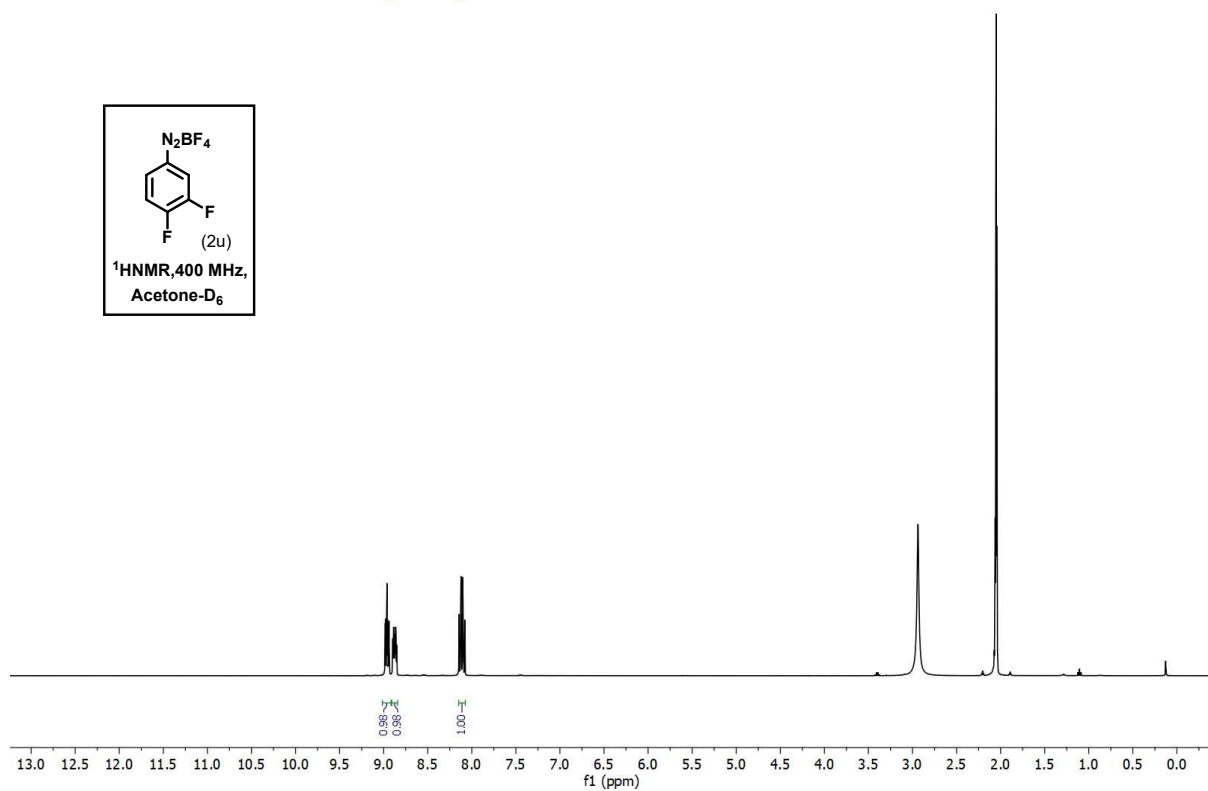
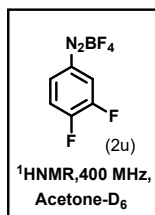
-73.626

150.872  
150.925



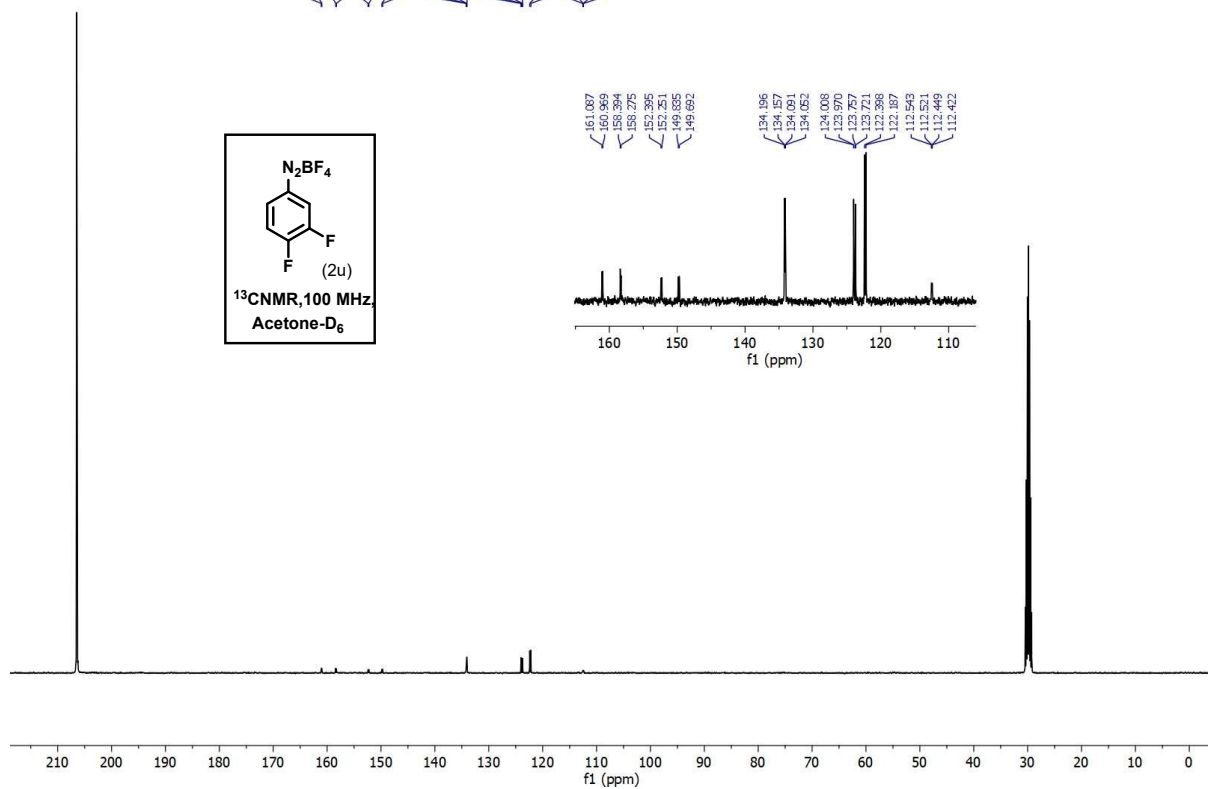
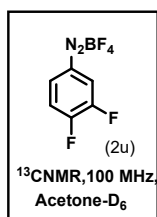
SHM-894S  
single\_pulse

8.984  
8.978  
8.968  
8.962  
8.956  
8.946  
8.937  
8.932  
8.890  
8.888  
8.886  
8.883  
8.871  
8.873  
8.869  
8.867  
8.864  
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8.858  
8.853  
8.146  
8.127  
8.122  
8.103  
8.098  
8.079



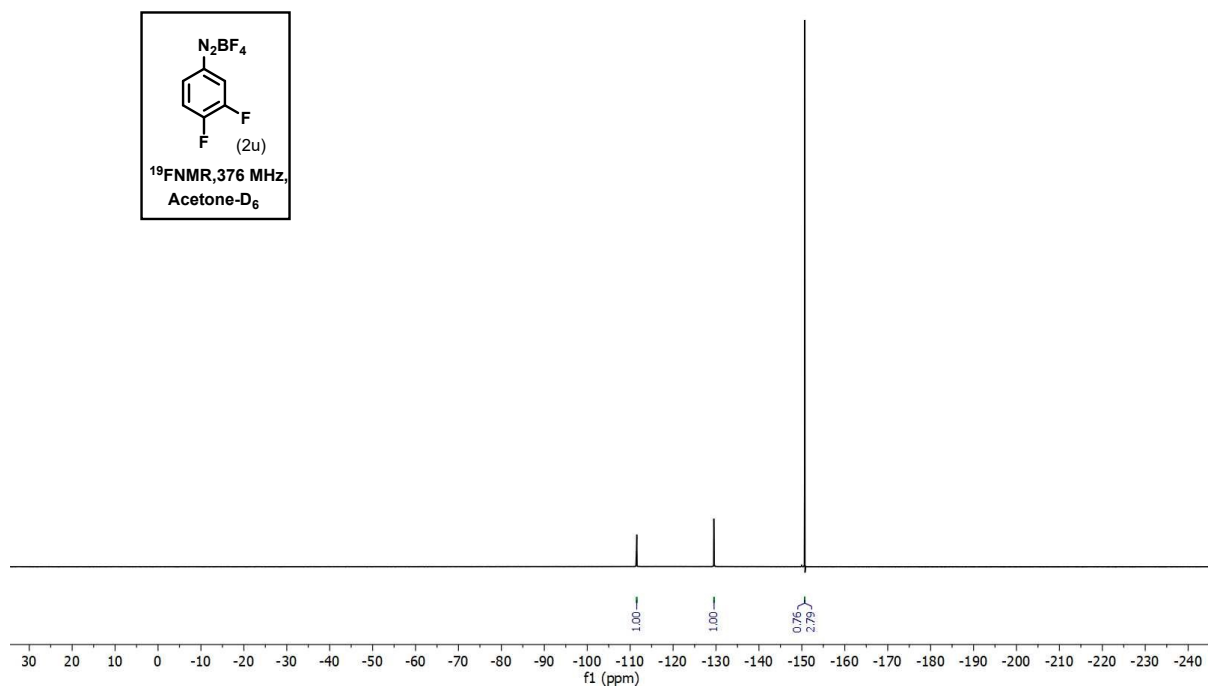
SHM-894S  
single pulse decoupled gated NOE

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160.969  
158.394  
158.275  
152.251  
149.855  
149.692  
134.196  
134.157  
134.091  
134.052  
124.008  
123.970  
123.757  
123.721  
122.996  
112.548  
112.521  
112.449  
112.422



SHM-894S  
single pulse decoupled gated NOE

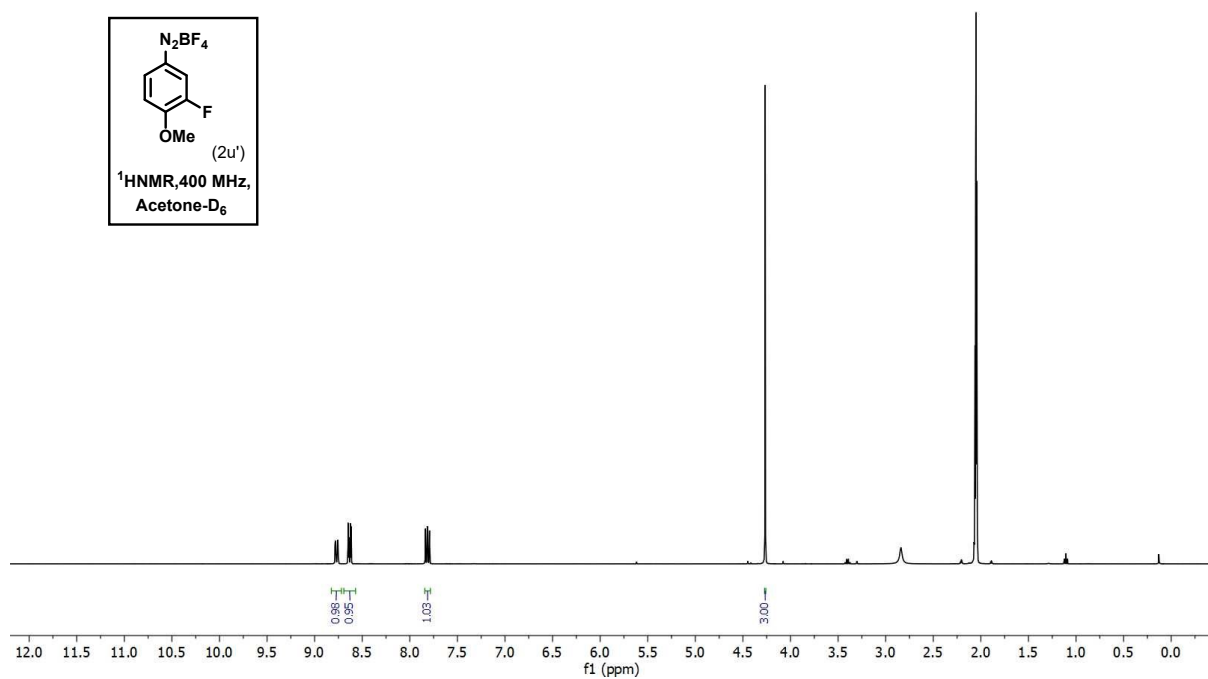
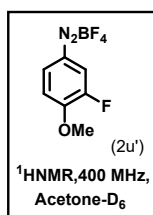
111.486  
111.515  
111.541  
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129.491  
129.517  
129.546  
129.569  
150.651  
150.705



SHM-890  
single\_pulse

8.786  
8.782  
8.779  
8.776  
8.775  
8.769  
8.756  
8.753  
8.648  
8.642  
8.624  
8.617  
8.586  
7.816  
7.813  
7.793

4.356



SHM-890  
single pulse decoupled gated NOE

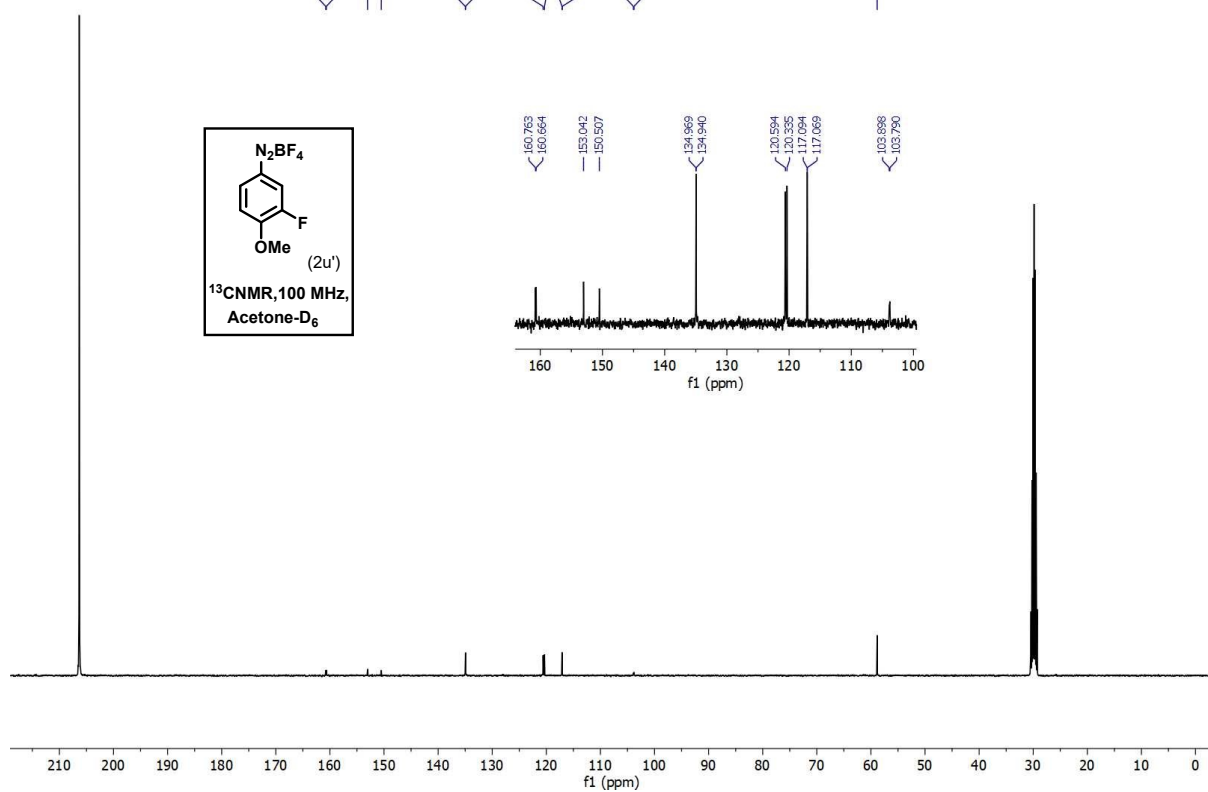
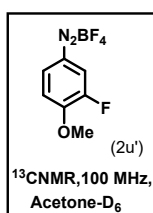
160.763  
160.664  
153.042  
150.507

134.969  
134.940

120.594  
120.335  
117.094  
117.069

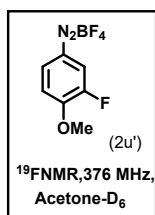
103.898  
103.790

58.845

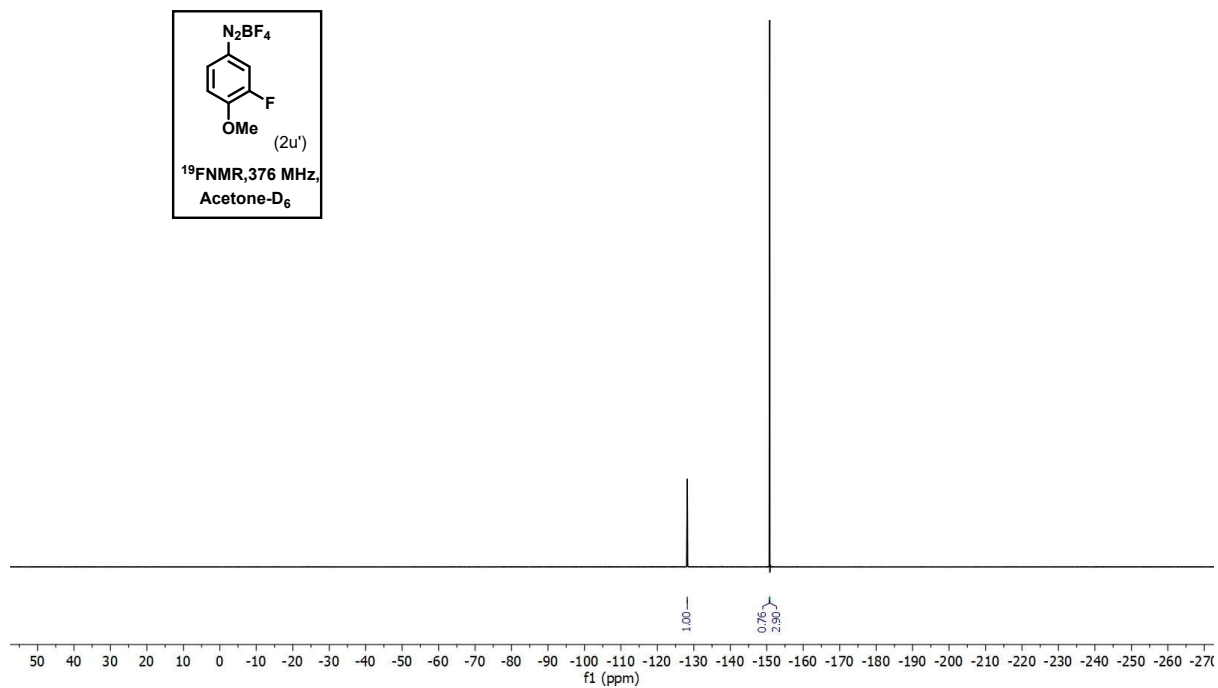


SHM-890  
single pulse decoupled gated NOE

128.189  
128.215  
128.238  
150.768  
150.823



<sup>19</sup>F NMR, 376 MHz,  
Acetone-D<sub>6</sub>

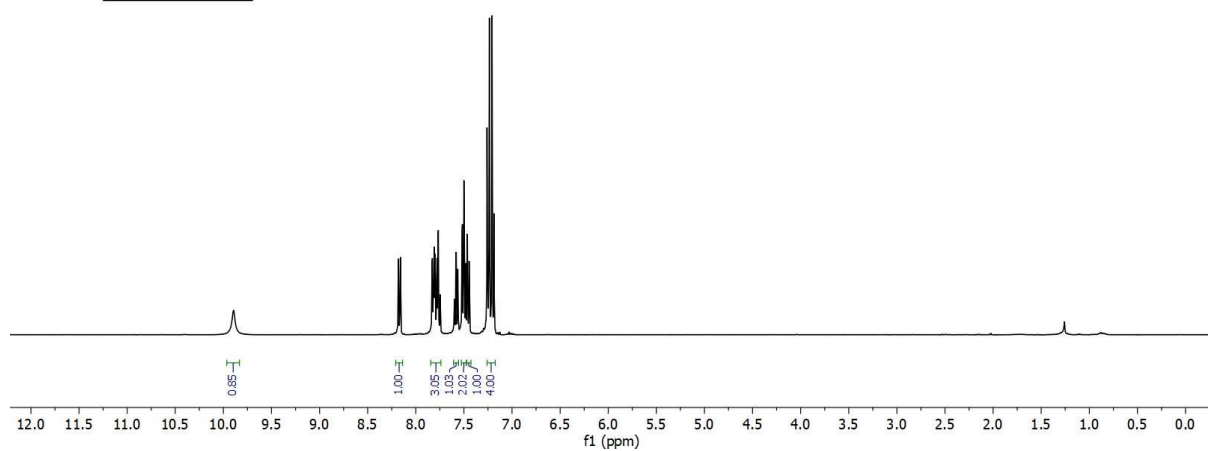
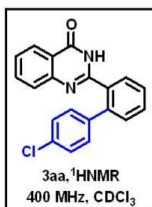




SHM-212  
single\_pulse

—9.894

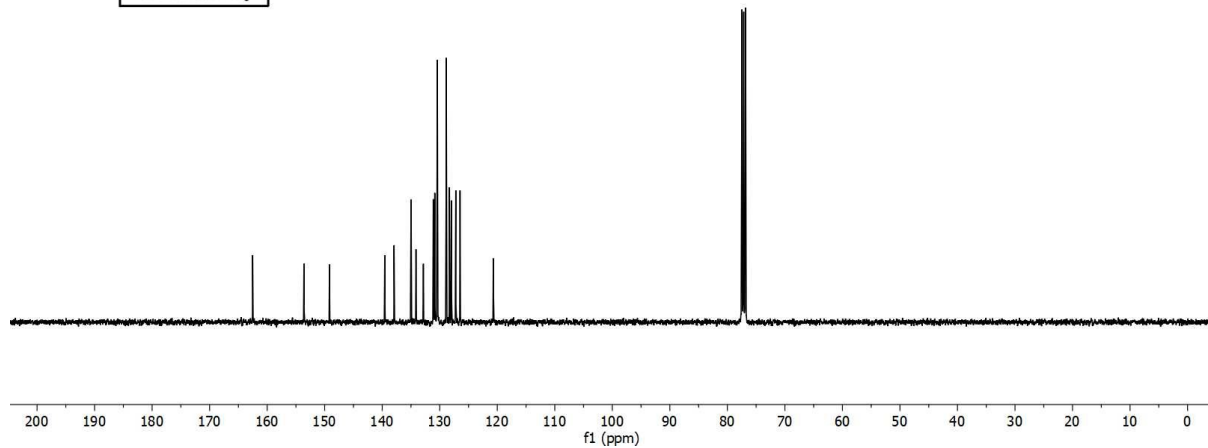
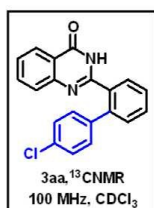
8.181  
7.818  
7.830  
7.828  
7.820  
7.816  
7.811  
7.808  
7.796  
7.794  
7.779  
7.768  
7.766  
7.748  
7.602  
7.588  
7.586  
7.580  
7.564  
7.561  
7.519  
7.516  
7.500  
7.482  
7.479  
7.465  
7.462  
7.445  
7.443  
7.430  
7.352  
7.241  
7.235  
7.230  
7.213  
7.208  
7.192  
7.186  
7.182



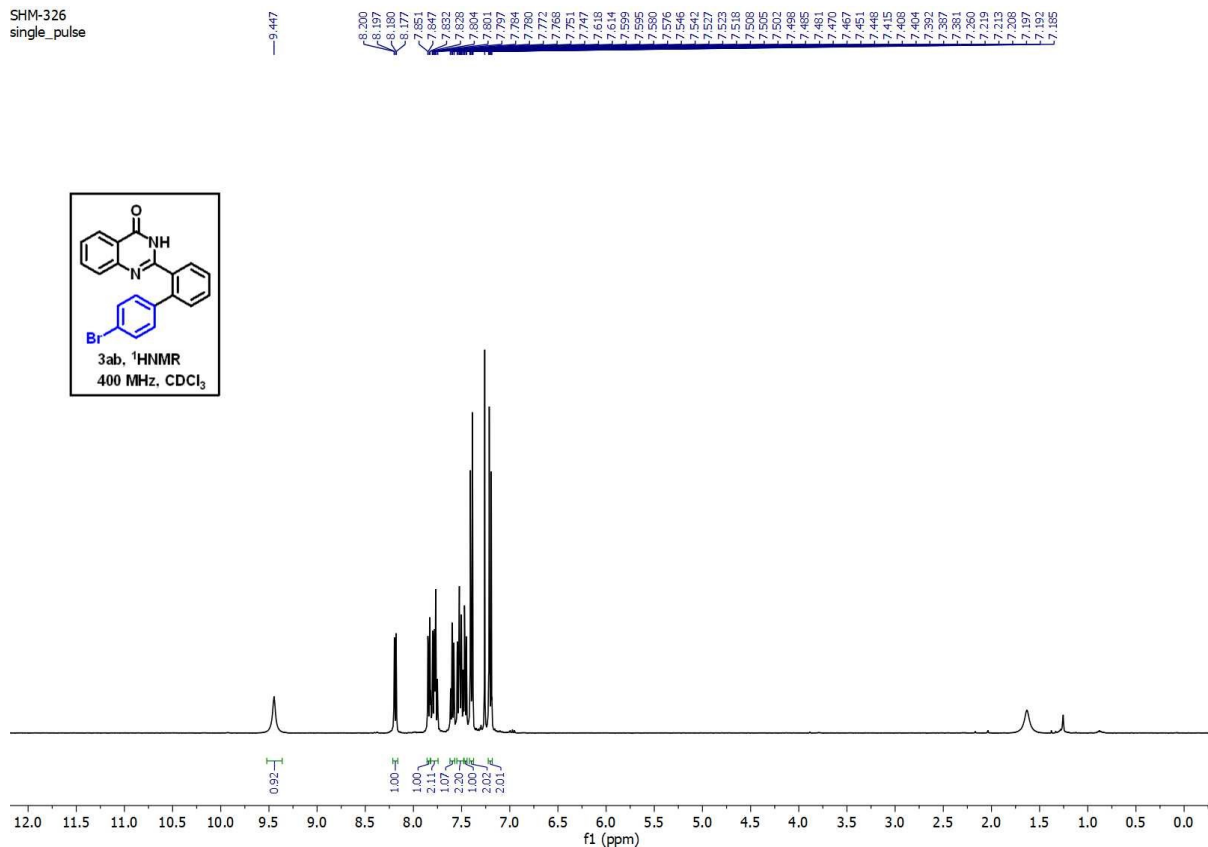
SHM-212  
single pulse decoupled gated NOE

162.523  
153.604  
149.164  
139.853  
137.942  
134.328  
134.126  
132.841  
131.117  
130.859  
130.467  
130.417  
128.865  
127.884  
127.209  
126.471  
120.683

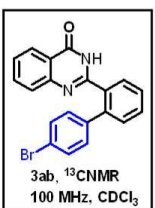
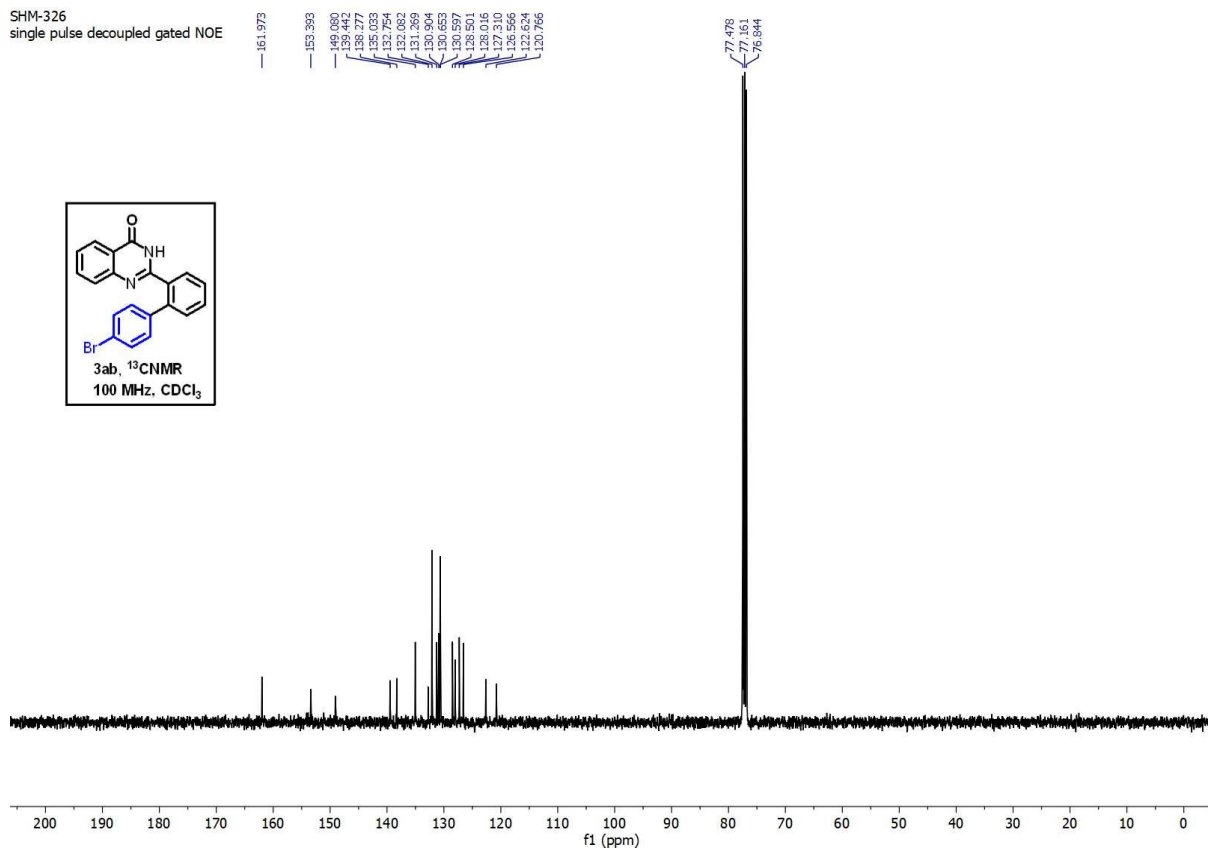
77.480  
77.180  
76.841



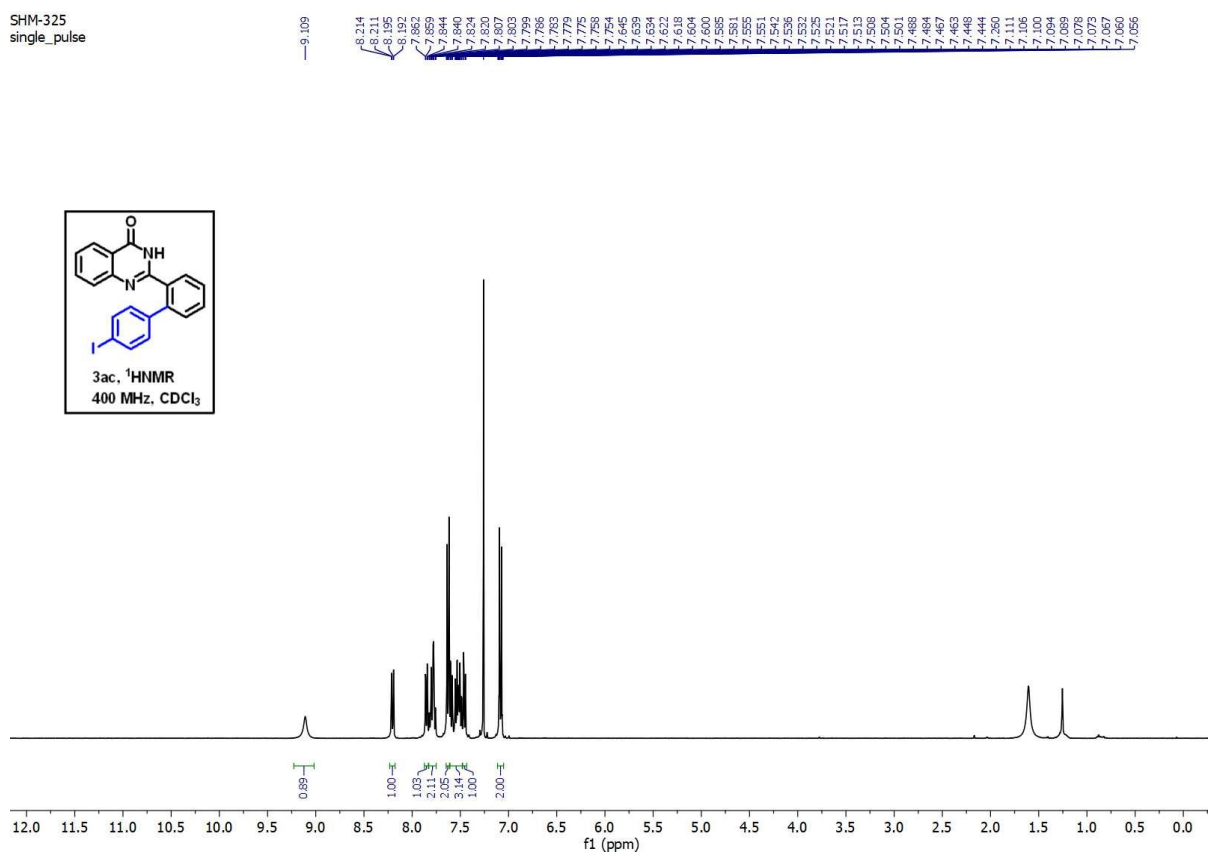
SHM-326  
single\_pulse



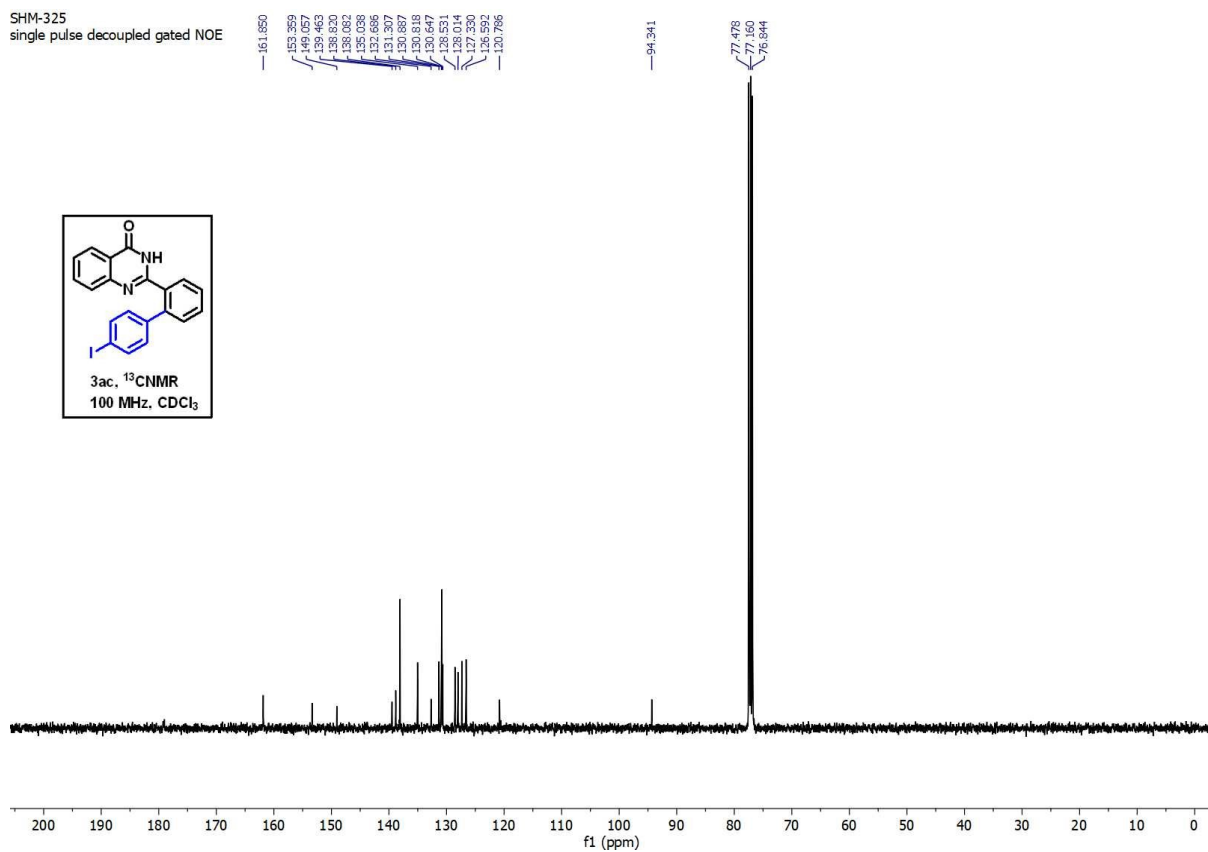
SHM-326  
single\_pulse decoupled gated NOE



SHM-325  
single\_pulse



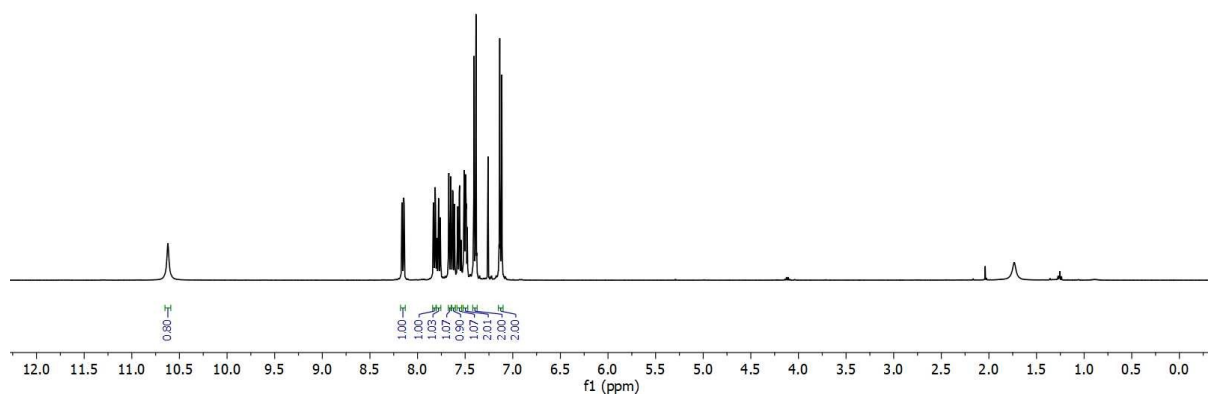
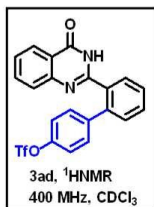
SHM-325  
single pulse decoupled gated NOE



SHM-421  
single\_pulse

—10.621

8.165  
8.161  
8.144  
8.141  
7.854  
7.850  
7.815  
7.811  
7.800  
7.796  
7.782  
7.779  
7.776  
7.762  
7.758  
7.671  
7.651  
7.632  
7.628  
7.613  
7.599  
7.594  
7.578  
7.562  
7.559  
7.543  
7.540  
7.516  
7.510  
7.510  
7.506  
7.498  
7.496  
7.493  
7.490  
7.487  
7.485  
7.475  
7.415  
7.408  
7.403  
7.391  
7.386  
7.379  
7.379  
7.364  
7.144  
7.137  
7.131  
7.120  
7.115  
7.107

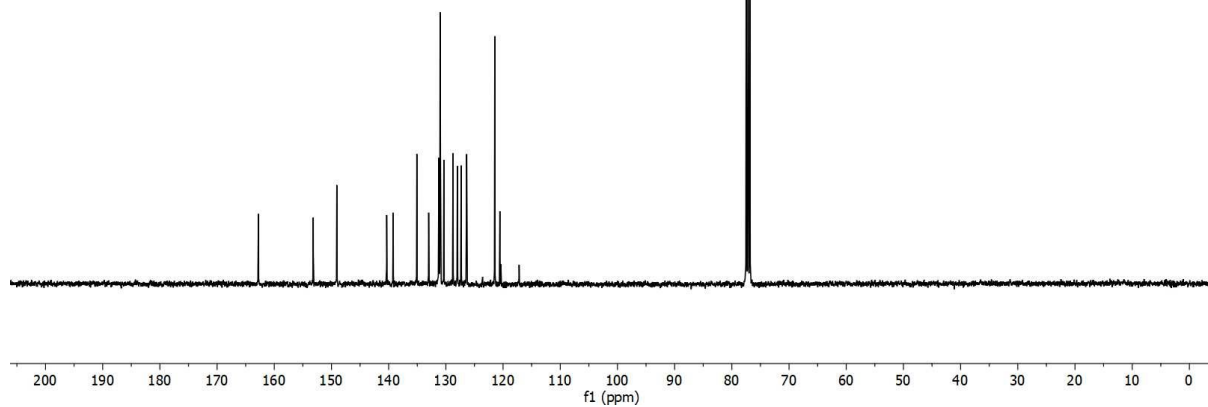
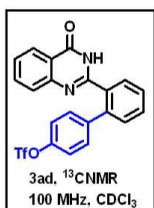


SHM-421  
single pulse decoupled gated NOE

—162.771

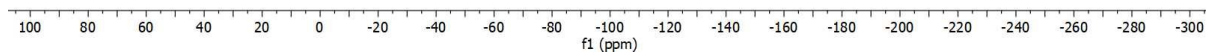
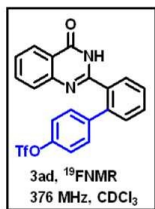
151.187  
149.056  
140.345  
137.025  
136.072  
133.004  
131.224  
131.000  
130.831  
130.348  
128.749  
127.324  
126.364  
123.575  
121.446  
120.383  
117.951  
113.955

77.478  
77.160  
76.842

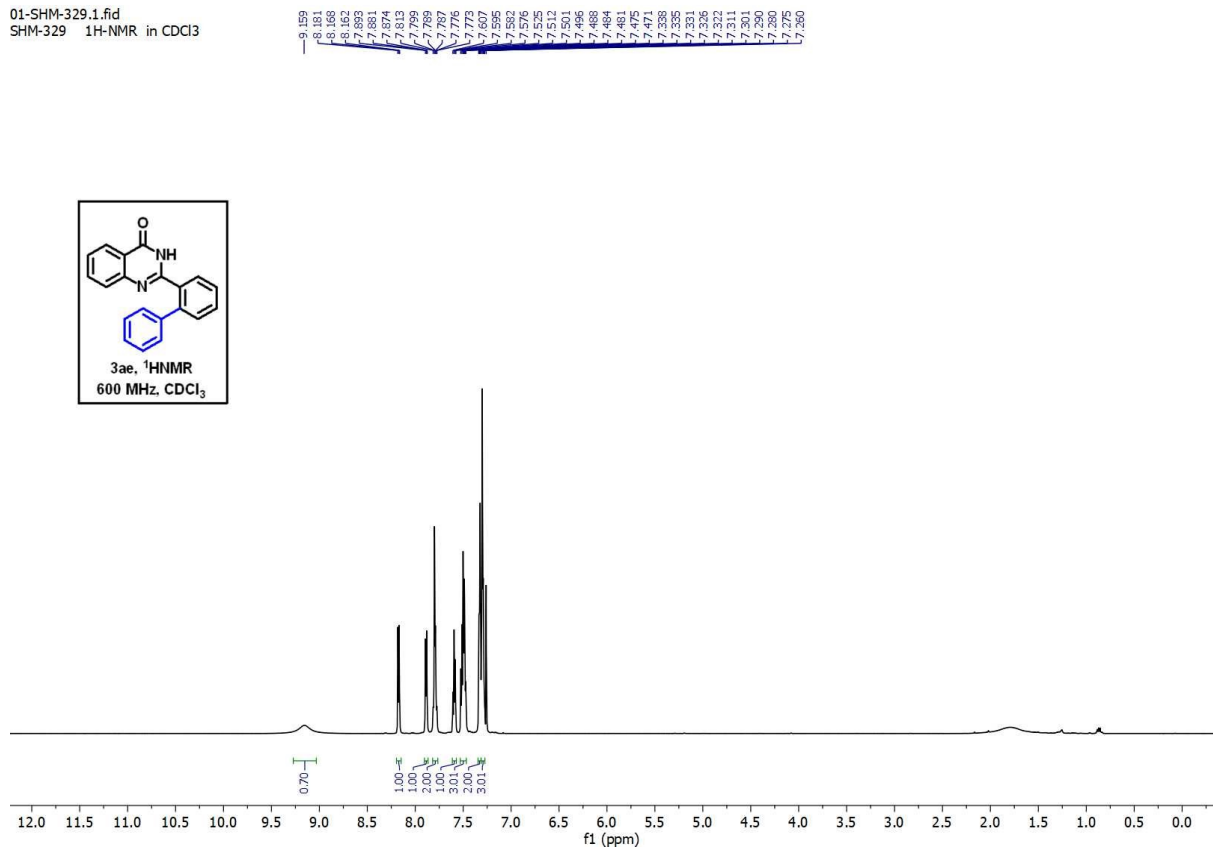
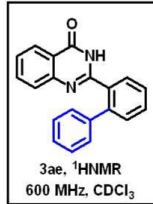


SHM-421  
single pulse decoupled gated NOE

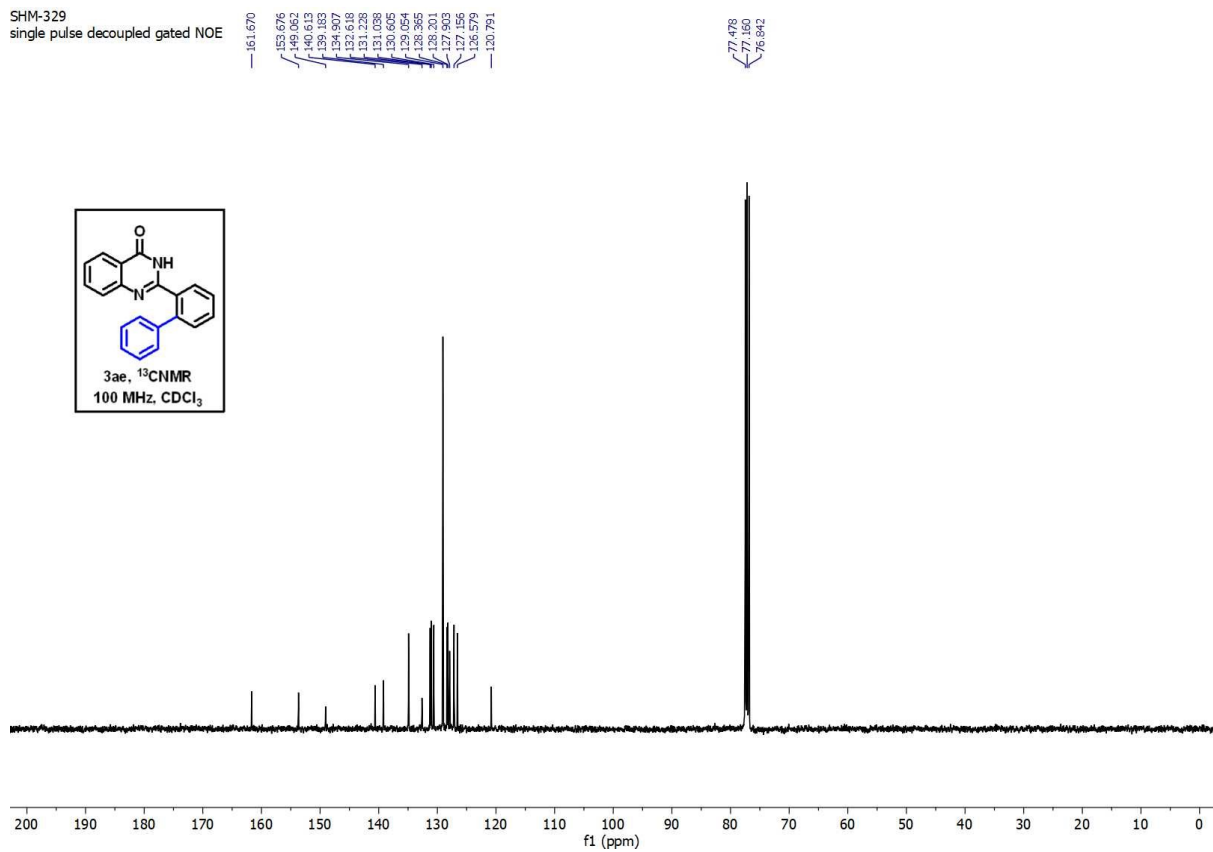
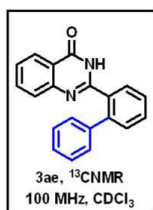
—72.694



01-SHM-329.1.fid  
SHM-329 <sup>1</sup>H-NMR in CDCl<sub>3</sub>



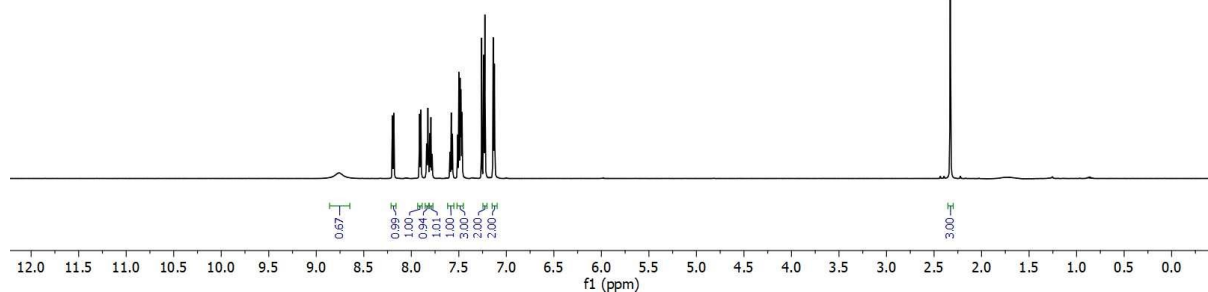
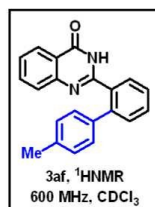
SHM-329  
single pulse decoupled gated NOE



13-SHM-275.1.fid  
SHM-275 1H-NMR in CDCl<sub>3</sub>

8.761  
8.199  
8.186  
8.184  
7.912  
7.900  
7.839  
7.835  
7.805  
7.794  
7.792  
7.783  
7.780  
7.594  
7.592  
7.582  
7.579  
7.569  
7.567  
7.513  
7.511  
7.501  
7.498  
7.487  
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7.477  
7.474  
7.467  
7.465  
7.239  
7.138  
7.125

2.330

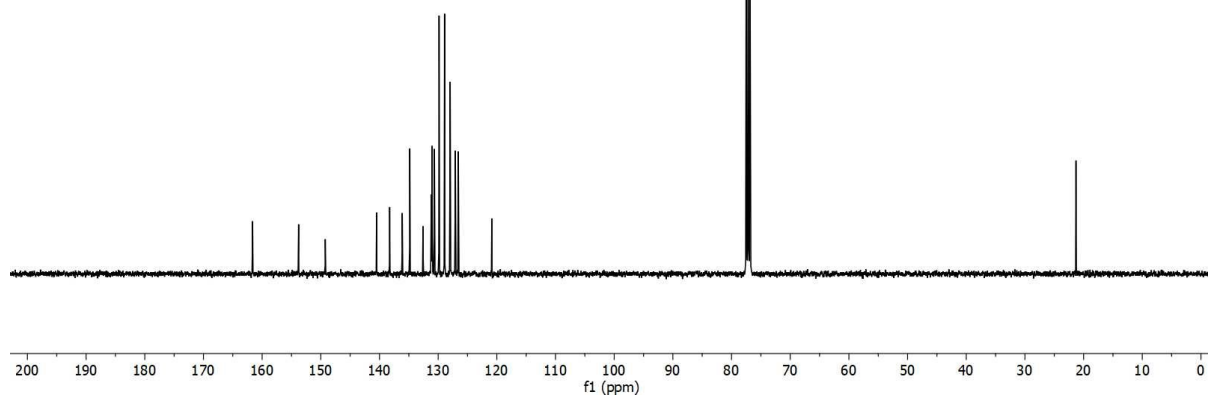
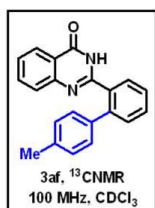


SHM-275  
single pulse decoupled gated NOE

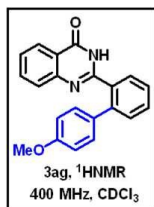
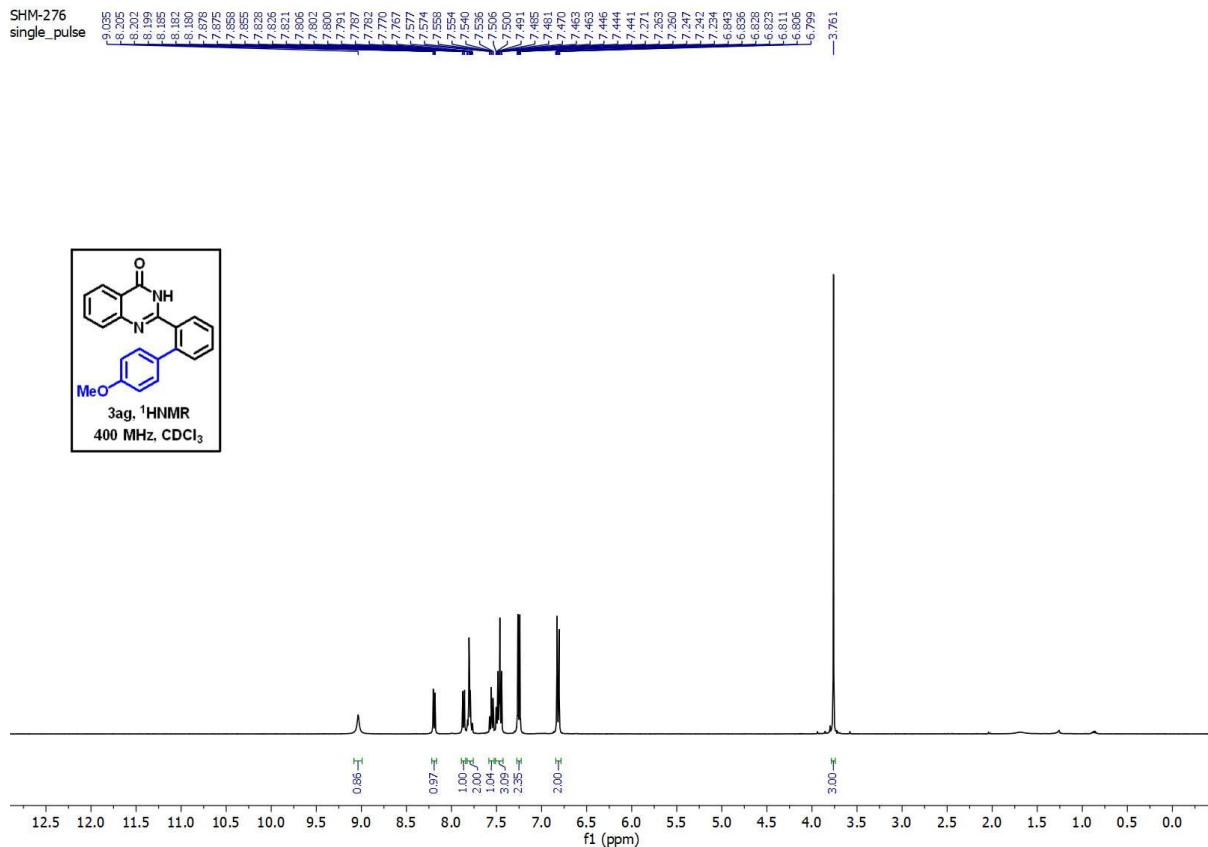
161.630  
153.781  
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140.480  
138.269  
136.121  
134.835  
132.574  
131.195  
131.074  
129.843  
128.913  
127.973  
126.567  
120.653

77.478  
77.160  
76.842

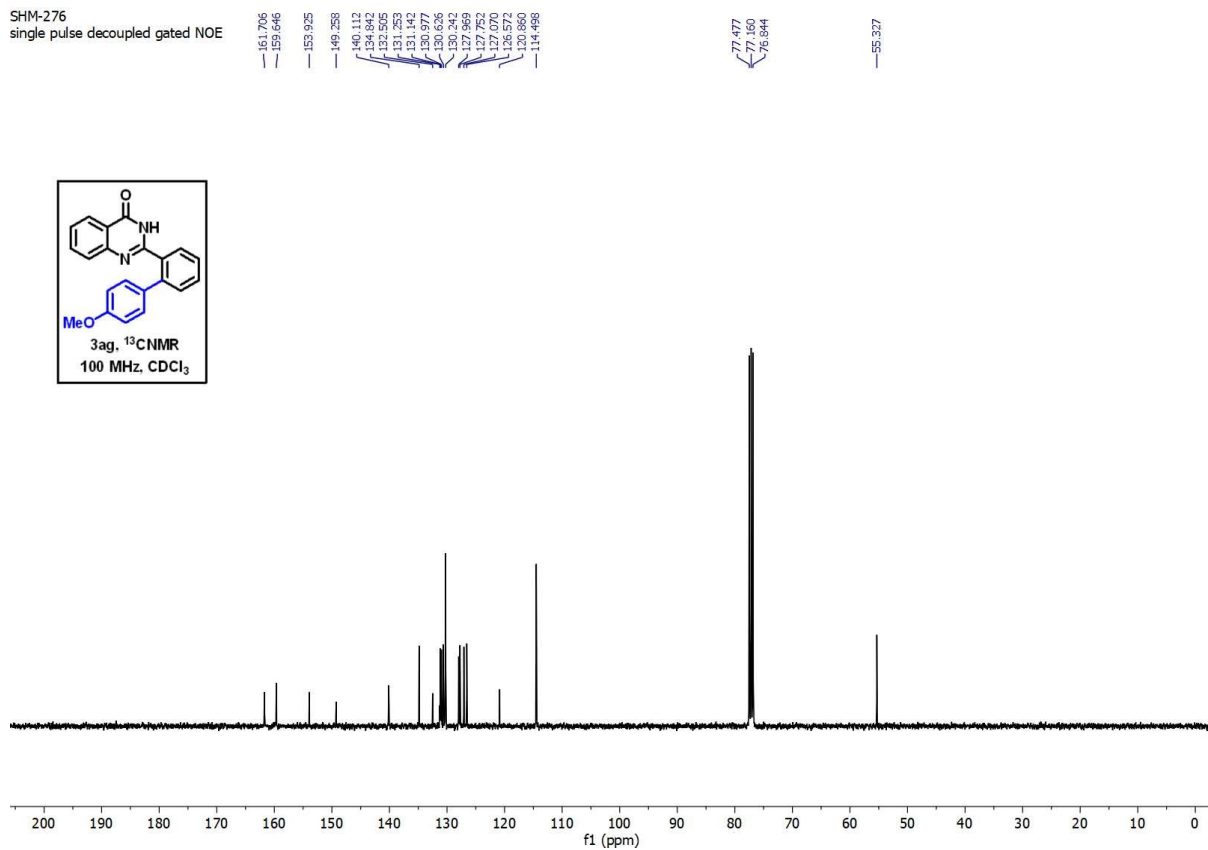
21.301



SHM-276  
single\_pulse



SHM-276  
single\_pulse decoupled gated NOE

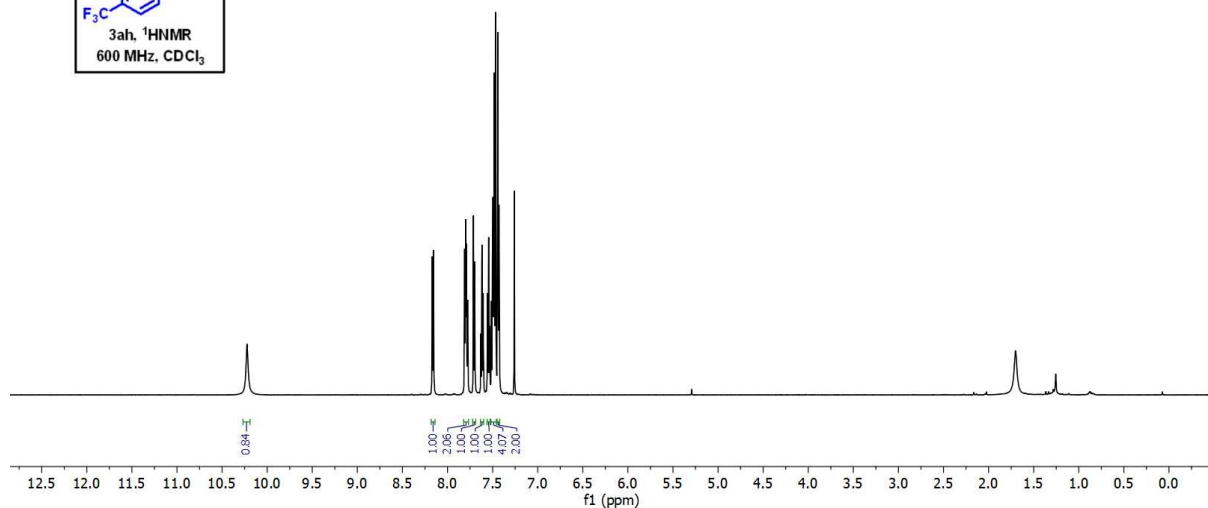
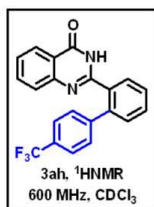




03-SHM-332.1.fid  
 SHM-332 1H-NMR in CDCl<sub>3</sub>

10.223

8.171  
 8.169  
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 7.000

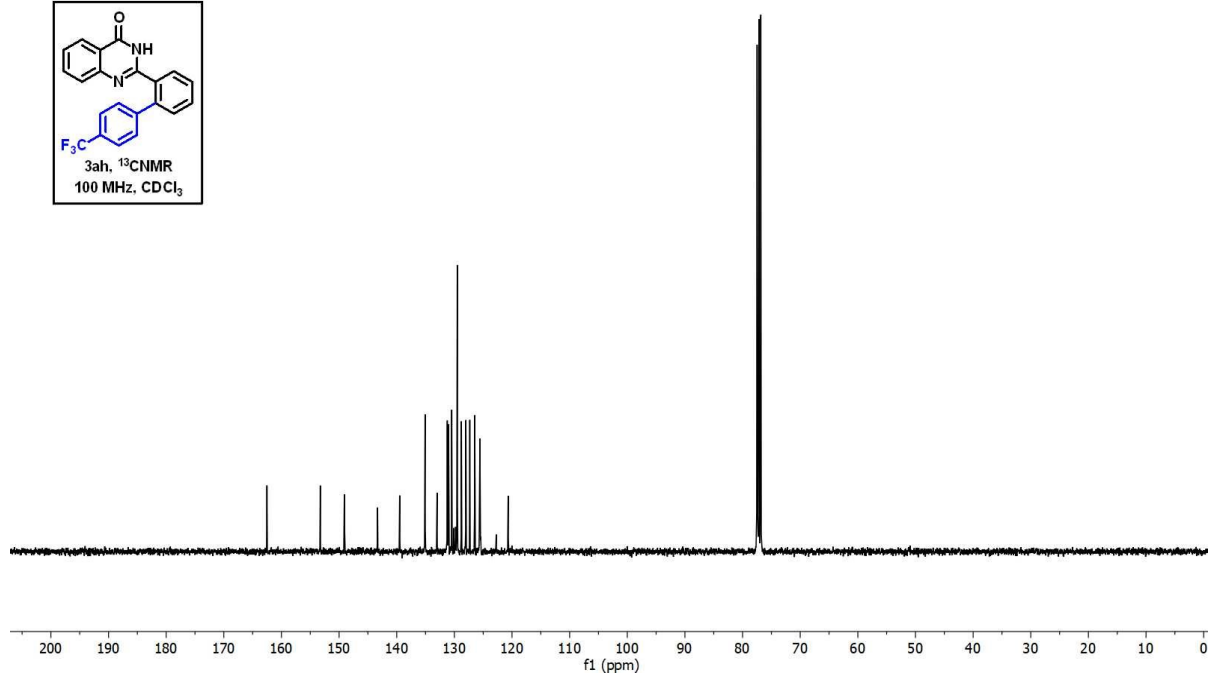
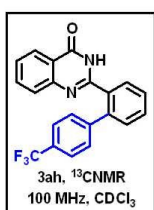


SHM-332  
 single pulse decoupled gated NOE

162.519

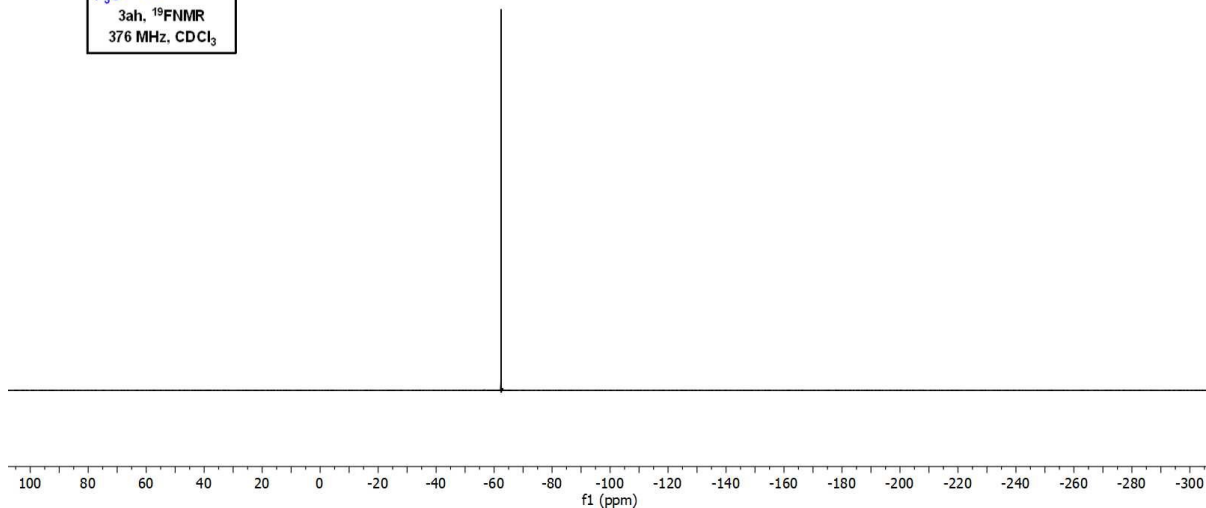
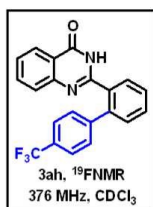
153.259  
 149.336  
 148.336  
 139.486  
 135.079  
 133.007  
 131.225  
 130.461  
 130.118  
 129.796  
 129.492  
 128.782  
 128.153  
 127.927  
 127.324  
 126.473  
 125.618  
 125.578  
 125.540  
 125.501  
 125.447  
 125.264  
 120.664  
 120.025

77.479  
 77.160  
 76.842

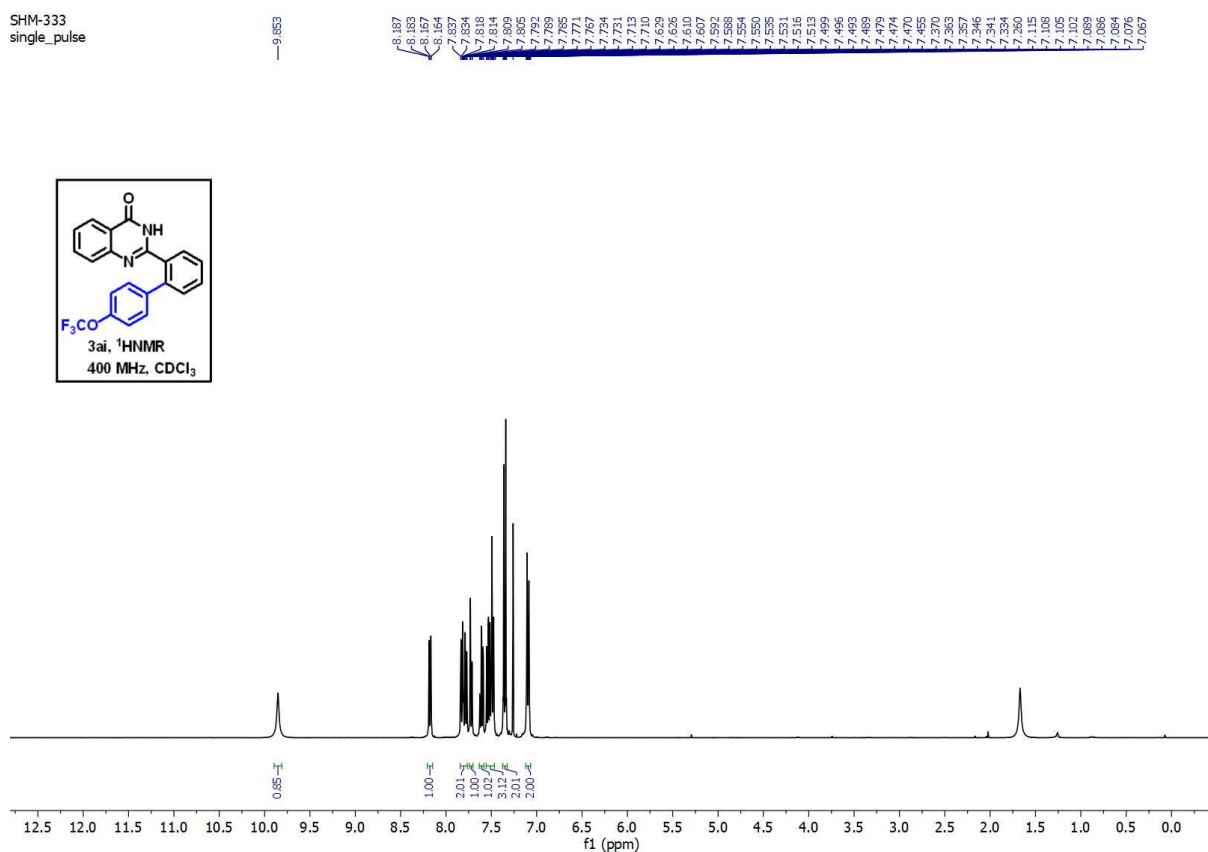
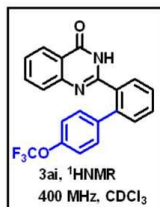


SHM-332  
single pulse decoupled gated NOE

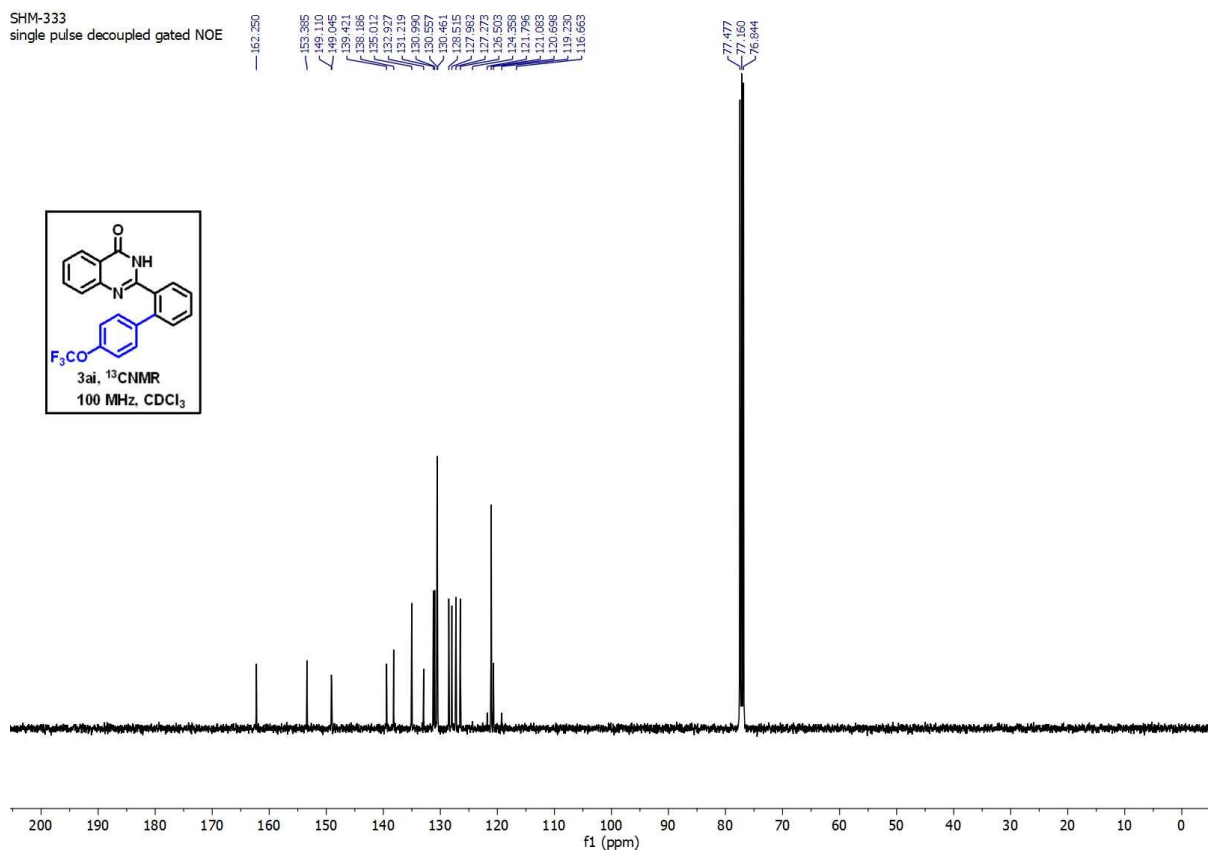
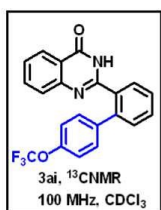
— 62.463



SHM-333  
single\_pulse

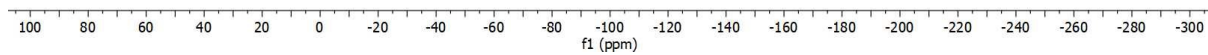
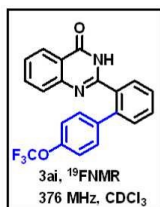


SHM-333  
single pulse decoupled gated NOE

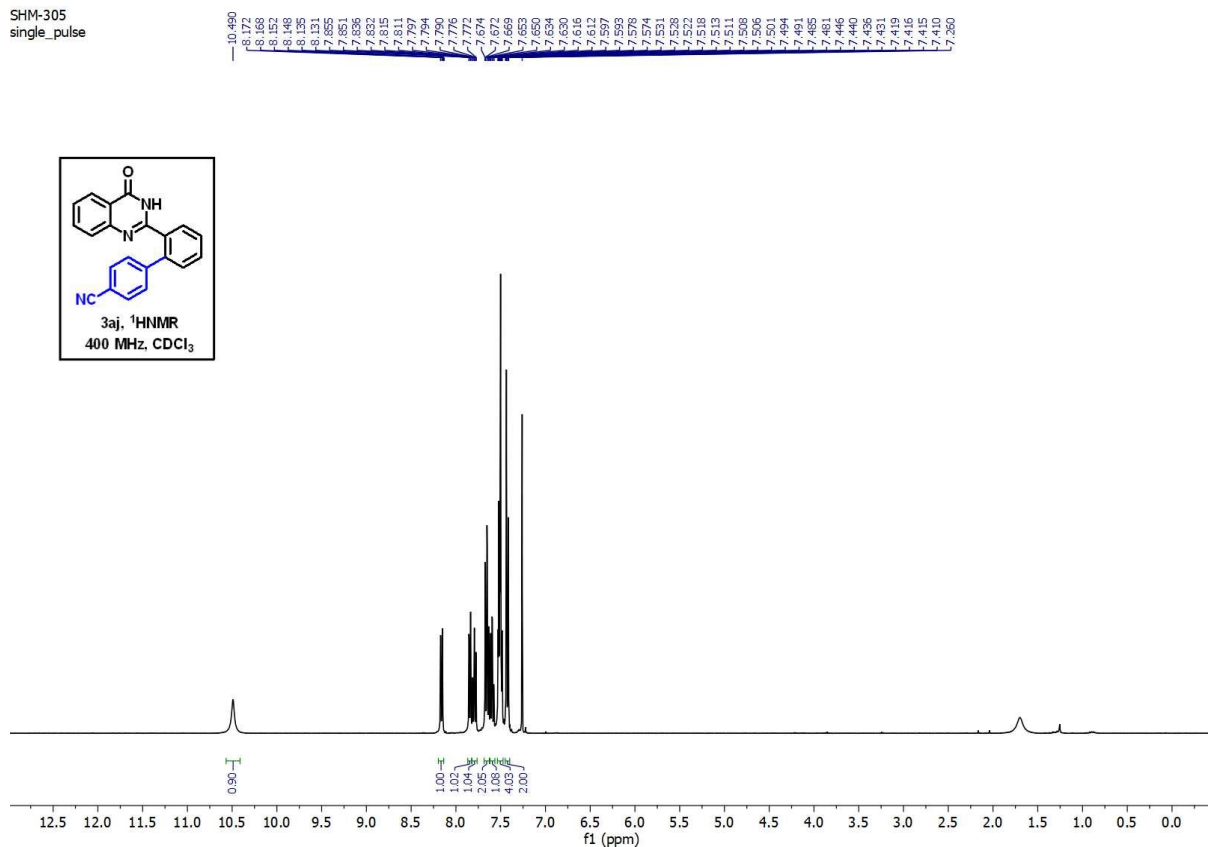


SHM-333  
single pulse decoupled gated NOE

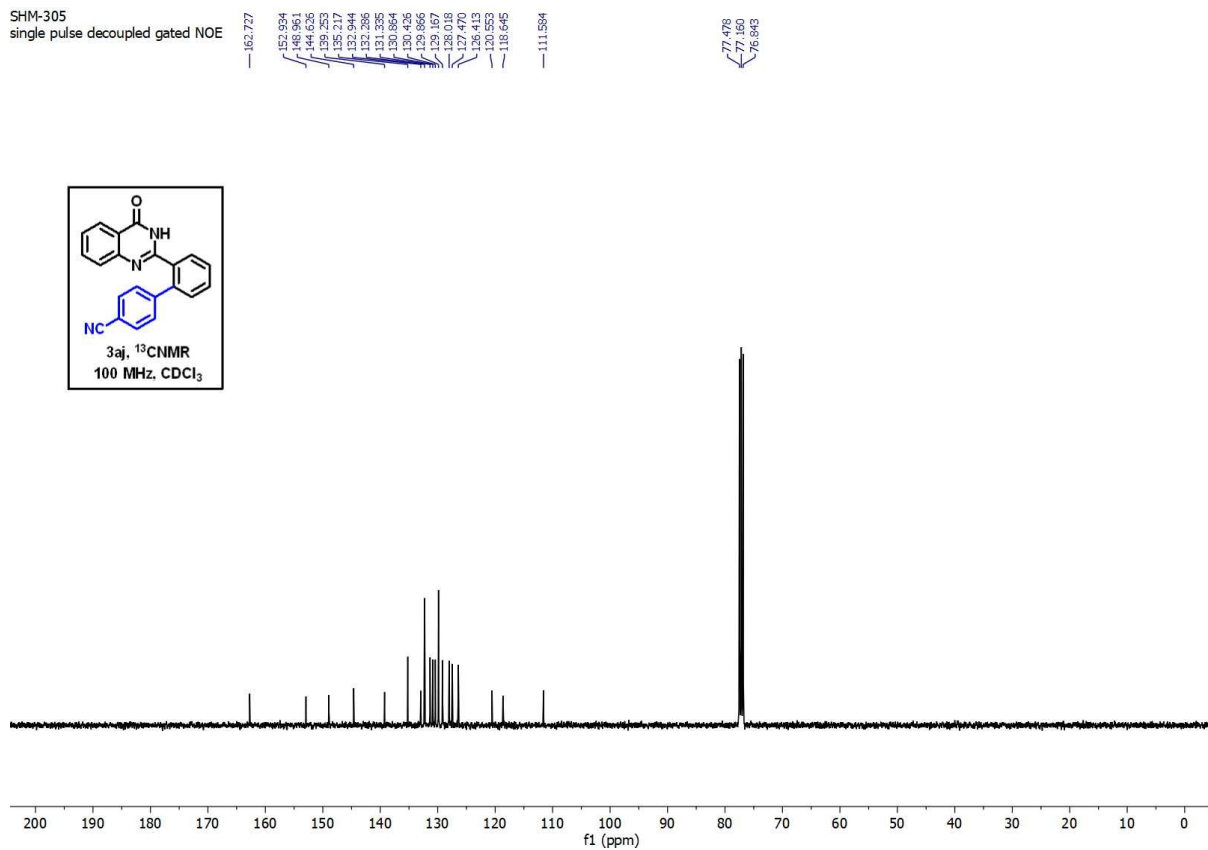
—57.705

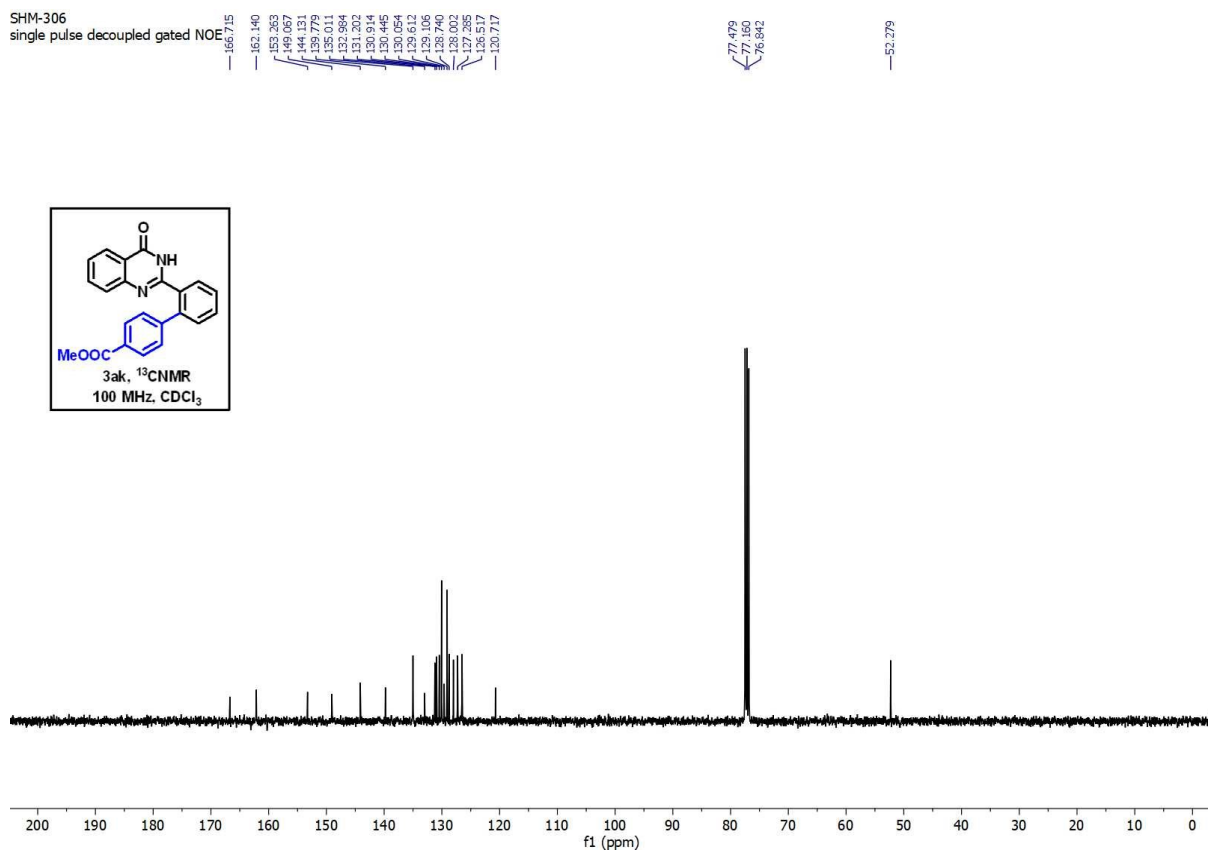
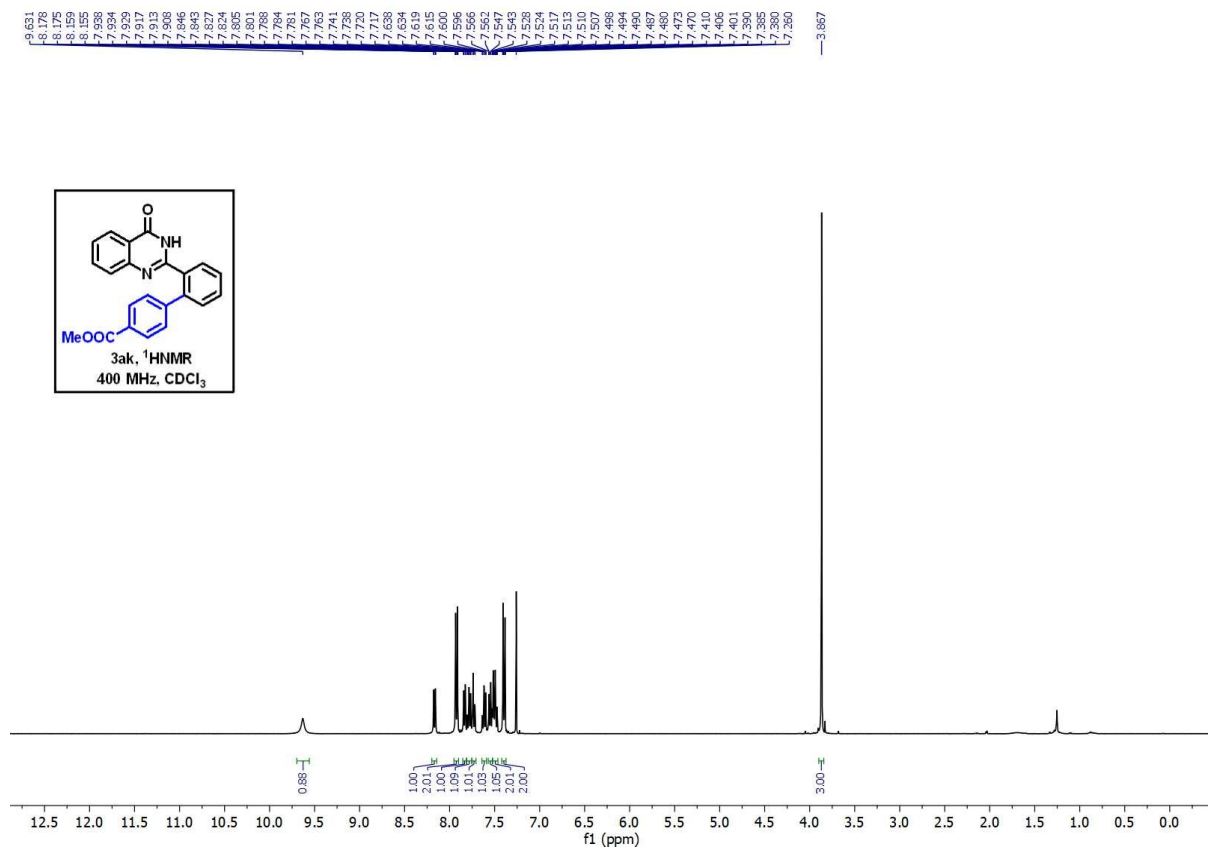


SHM-305  
single\_pulse



SHM-305  
single pulse decoupled gated NOE

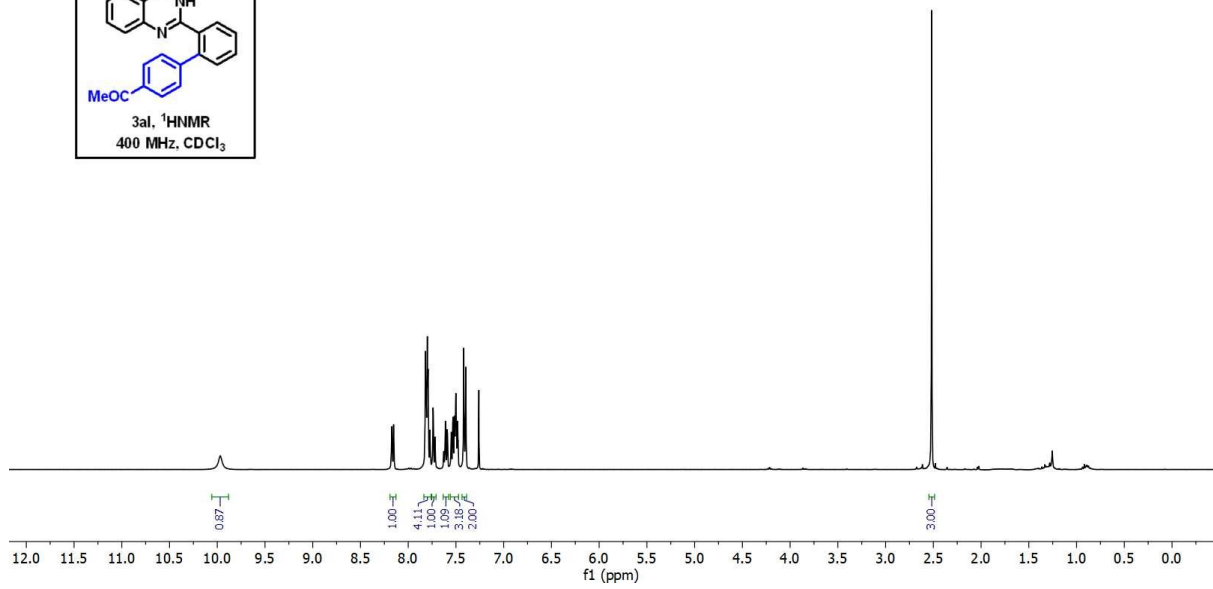
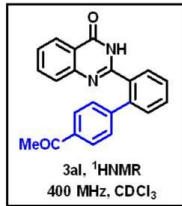




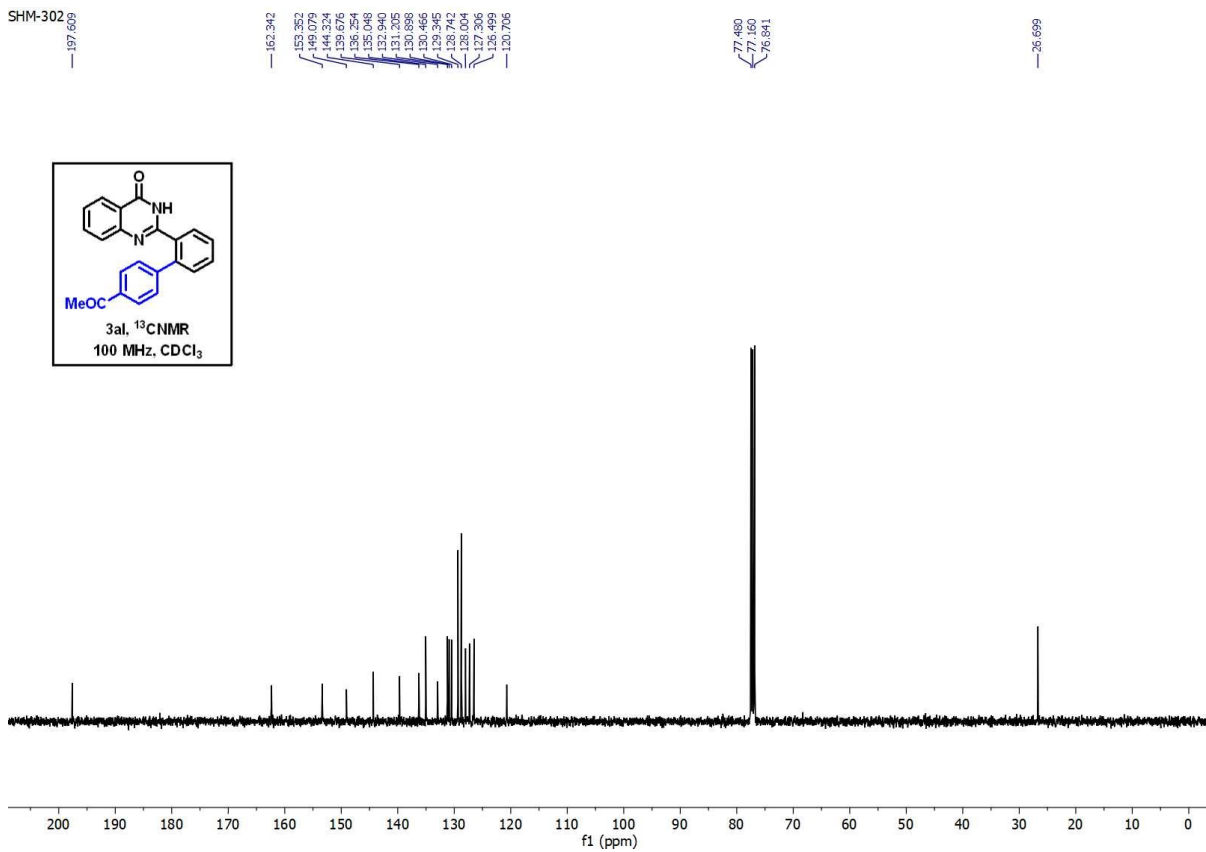
SHM-302  
single\_pulse

— 9.966

8.174  
8.170  
8.154  
8.150  
7.825  
7.821  
7.815  
7.811  
7.804  
7.800  
7.794  
7.791  
7.787  
7.774  
7.771  
7.741  
7.738  
7.730  
7.717  
7.630  
7.626  
7.611  
7.601  
7.592  
7.588  
7.552  
7.549  
7.530  
7.533  
7.516  
7.511  
7.505  
7.501  
7.498  
7.495  
7.486  
7.483  
7.483  
7.477  
7.442  
7.418  
7.413  
7.401  
7.397  
7.387  
7.366  
2.518

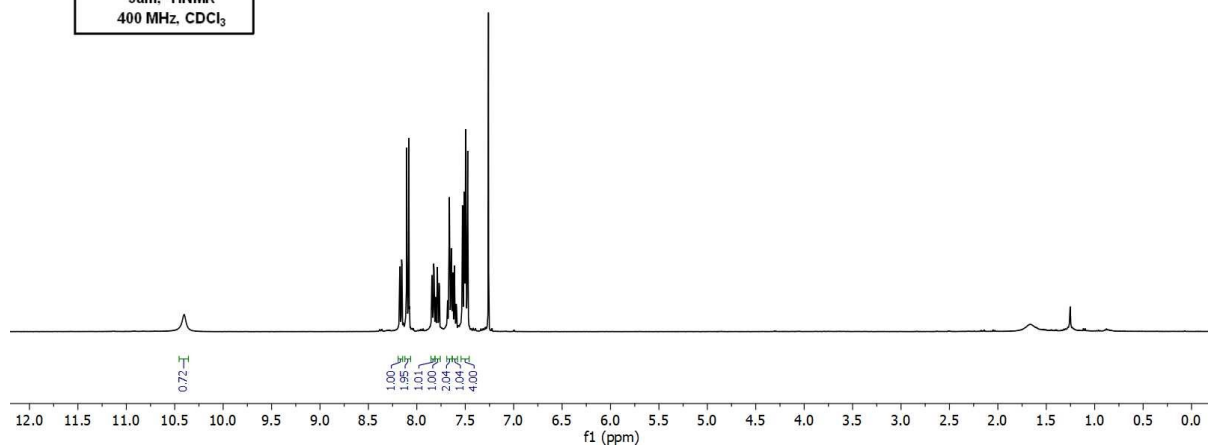
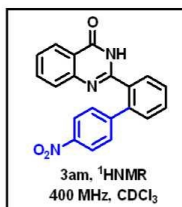


SHM-302.69



SHM-213  
single\_pulse

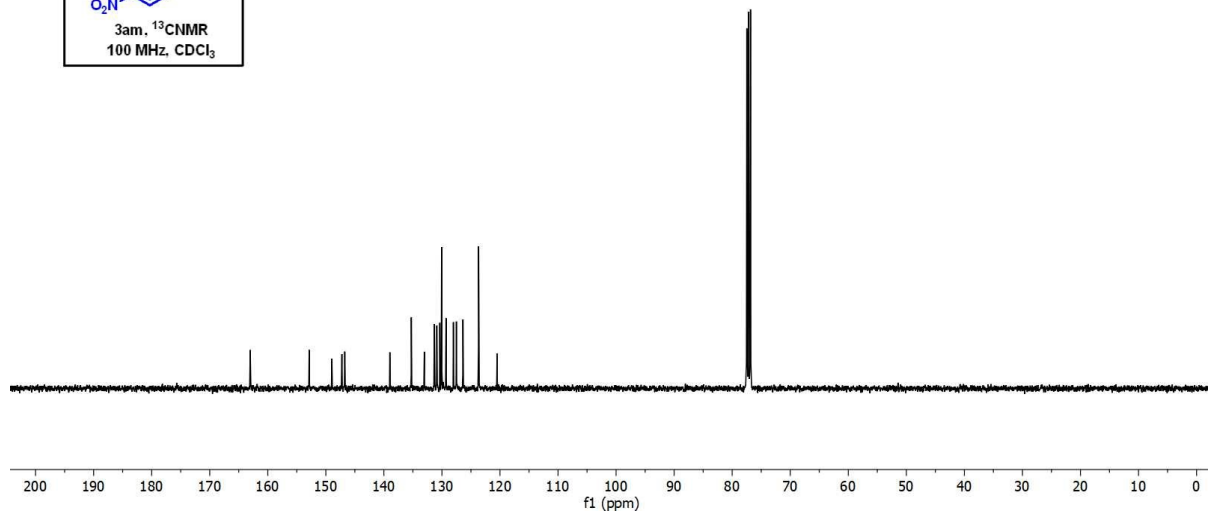
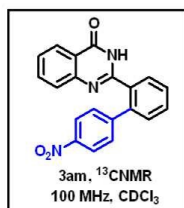
10.404  
8.177  
8.157  
8.153  
8.120  
8.115  
8.111  
8.105  
8.100  
8.088  
8.083  
8.076  
7.845  
7.841  
7.832  
7.809  
7.805  
7.791  
7.788  
7.784  
7.765  
7.762  
7.686  
7.683  
7.668  
7.664  
7.660  
7.649  
7.644  
7.641  
7.631  
7.627  
7.612  
7.609  
7.593  
7.590  
7.582  
7.528  
7.525  
7.519  
7.513  
7.511  
7.507  
7.499  
7.493  
7.482  
7.480  
7.475  
7.469  
7.260



SHM-213  
single pulse decoupled gated NOE

163.014  
152.866  
148.965  
147.231  
146.731  
138.972  
138.704  
133.025  
131.302  
130.880  
130.363  
130.047  
129.252  
128.027  
126.375  
125.684  
120.493

77.478  
77.160  
76.842

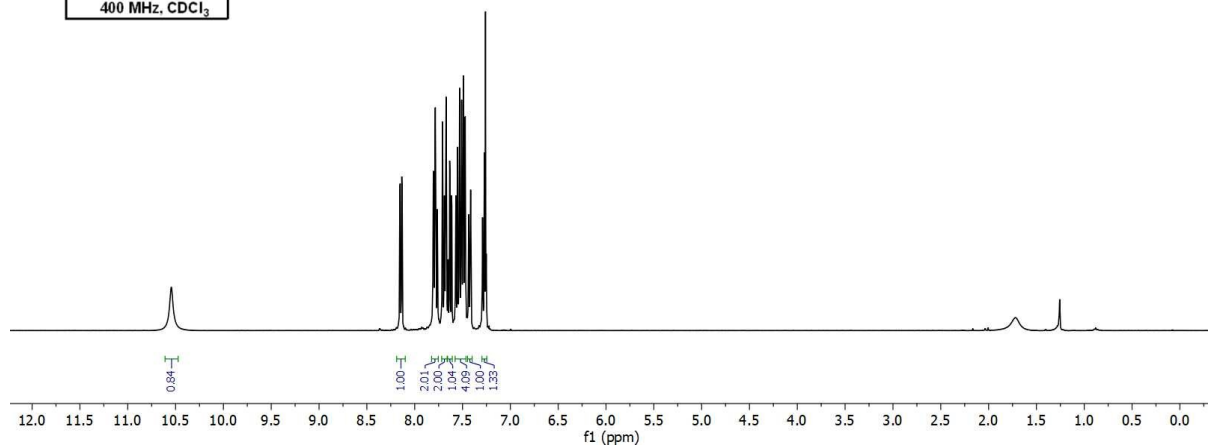
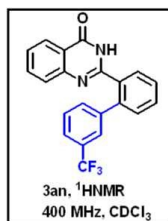




SHM-356  
single\_pulse

— 10.544

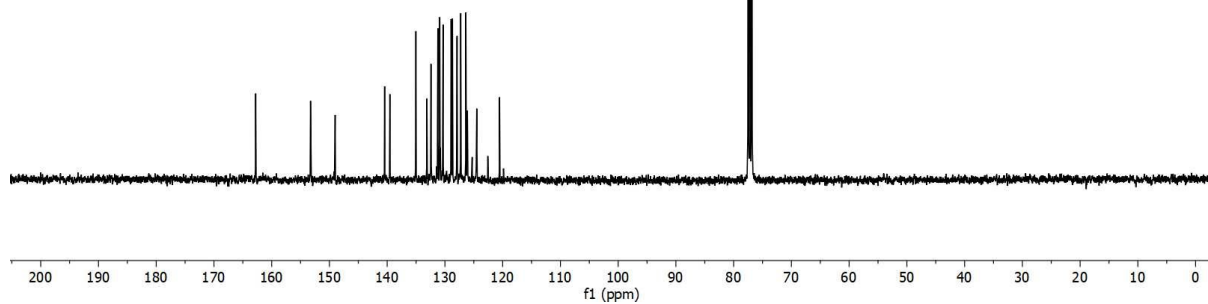
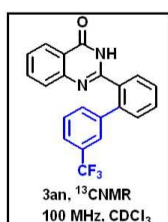
8.156  
8.152  
8.135  
8.132  
7.898  
7.894  
7.882  
7.798  
7.789  
7.785  
7.781  
7.777  
7.763  
7.758  
7.711  
7.708  
7.690  
7.687  
7.677  
7.672  
7.667  
7.653  
7.650  
7.650  
7.634  
7.631  
7.616  
7.612  
7.573  
7.573  
7.554  
7.551  
7.535  
7.531  
7.527  
7.512  
7.506  
7.507  
7.496  
7.492  
7.489  
7.486  
7.476  
7.472  
7.456  
7.456  
7.415  
7.291  
7.271  
7.260  
7.252



SHM-356  
single pulse decoupled gated NOE

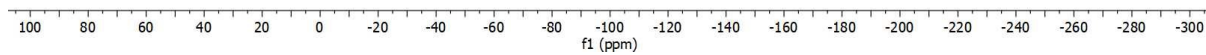
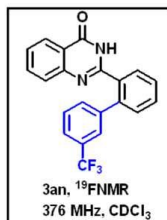
— 162.774

153.276  
149.013  
140.445  
139.535  
135.028  
133.123  
132.413  
131.514  
131.323  
131.121  
130.898  
130.803  
130.478  
130.329  
128.924  
128.824  
127.925  
127.895  
127.903  
127.257  
126.376  
126.194  
126.145  
126.102  
126.002  
125.294  
125.264  
124.525  
124.489  
124.453  
122.571  
122.559  
120.559  
119.829  
77.489  
77.160  
76.842



SHM-356  
single pulse decoupled gated NOE

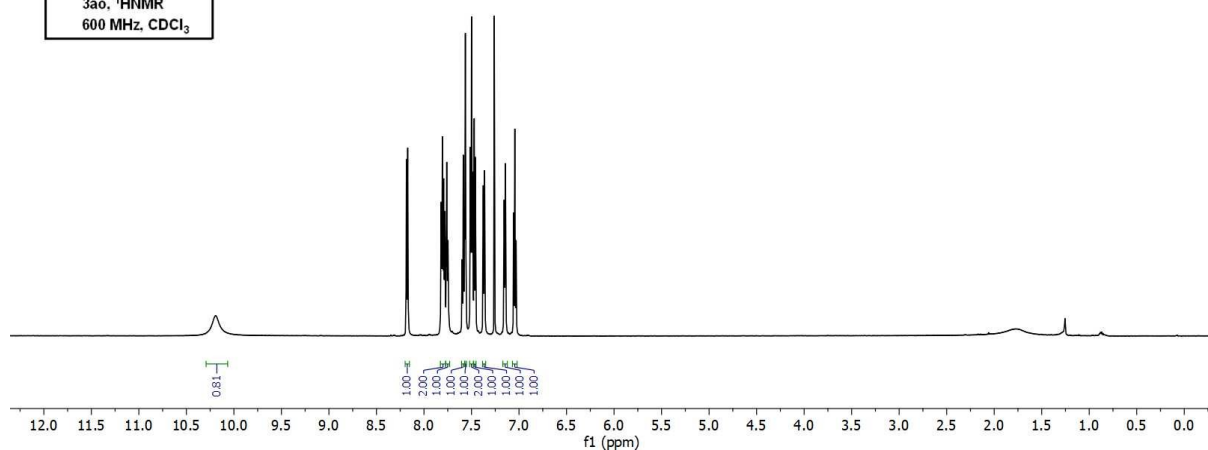
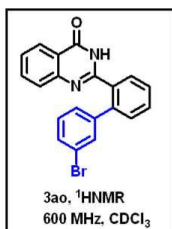
—62.717



12-SHM-374.1.fid  
SHM-374 1H-NMR in CDCl<sub>3</sub>

10.192

8.184  
8.171  
7.819  
7.806  
7.793  
7.760  
7.747  
7.599  
7.586  
7.574  
7.565  
7.550  
7.530  
7.487  
7.471  
7.459  
7.378  
7.375  
7.365  
7.352  
7.360  
7.156  
7.143  
7.057  
7.044  
7.031

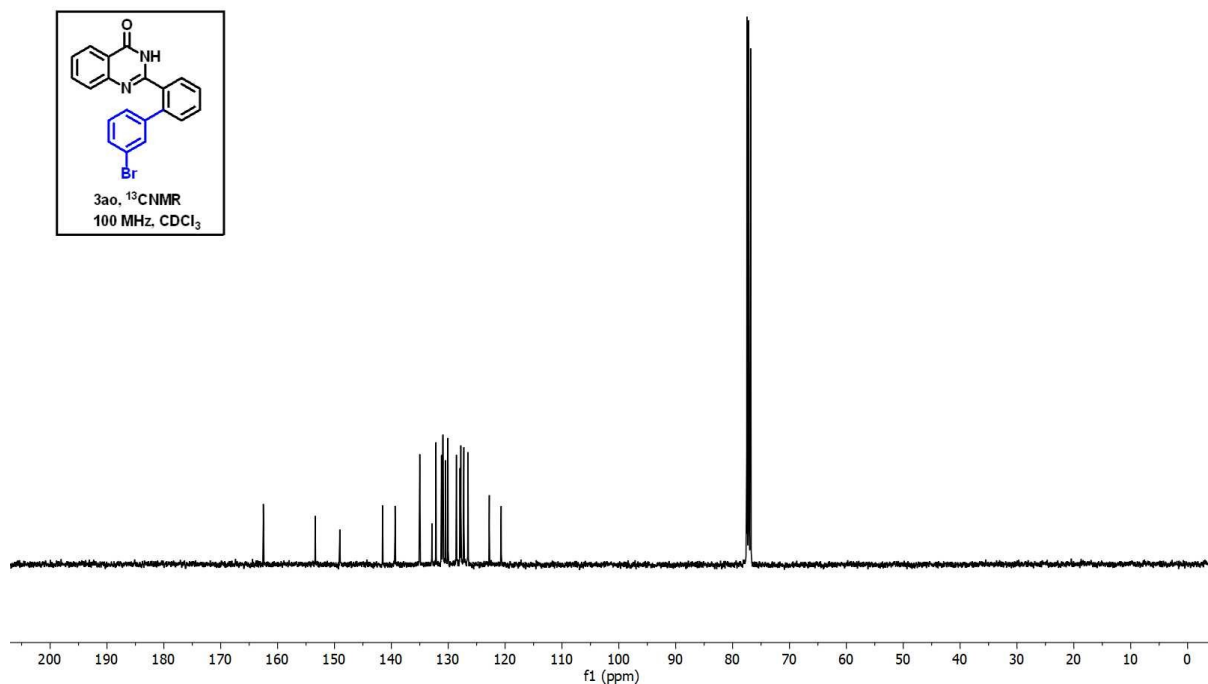
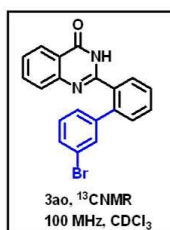


SHM-374  
single pulse decoupled gated NOE

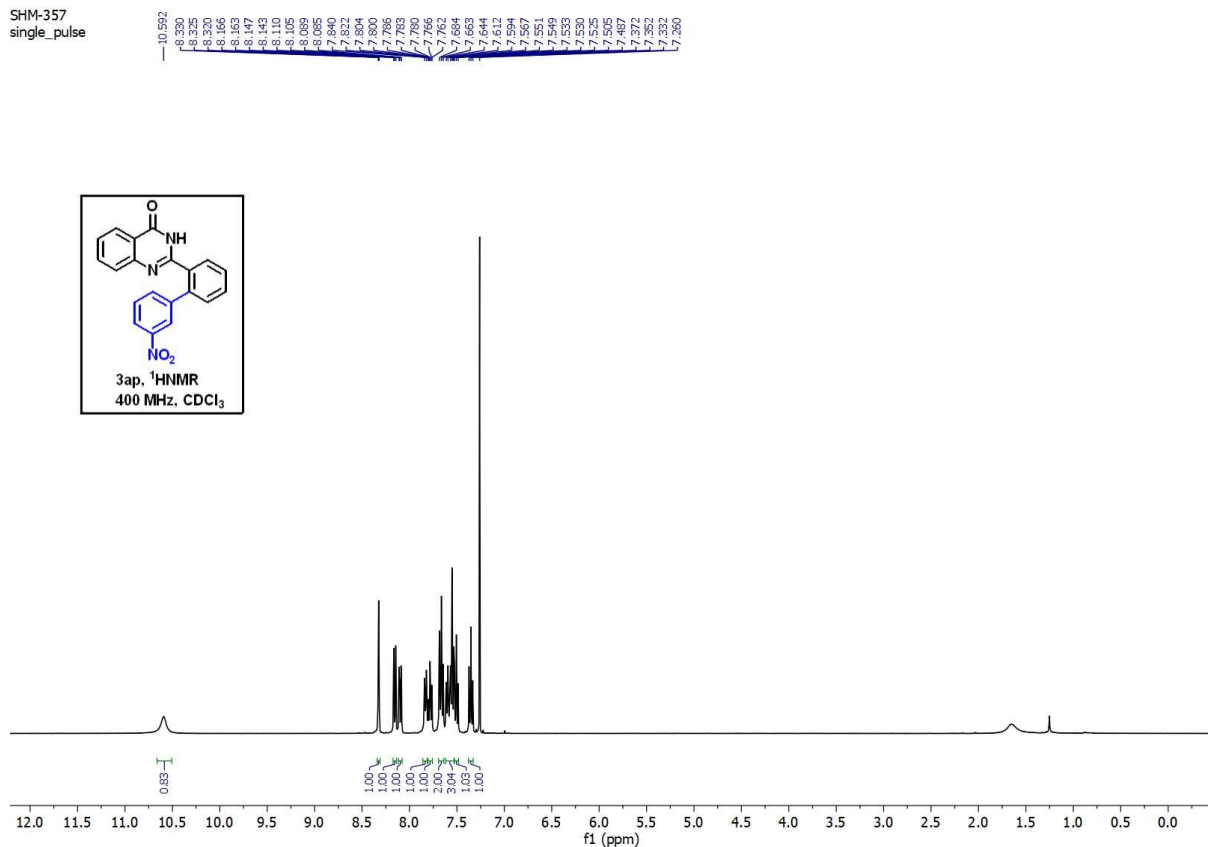
162.503

153.362  
149.073  
141.547  
139.338  
137.581  
133.852  
133.154  
131.186  
130.976  
130.896  
130.462  
130.044  
129.921  
127.921  
127.780  
127.256  
126.521  
122.780  
120.690

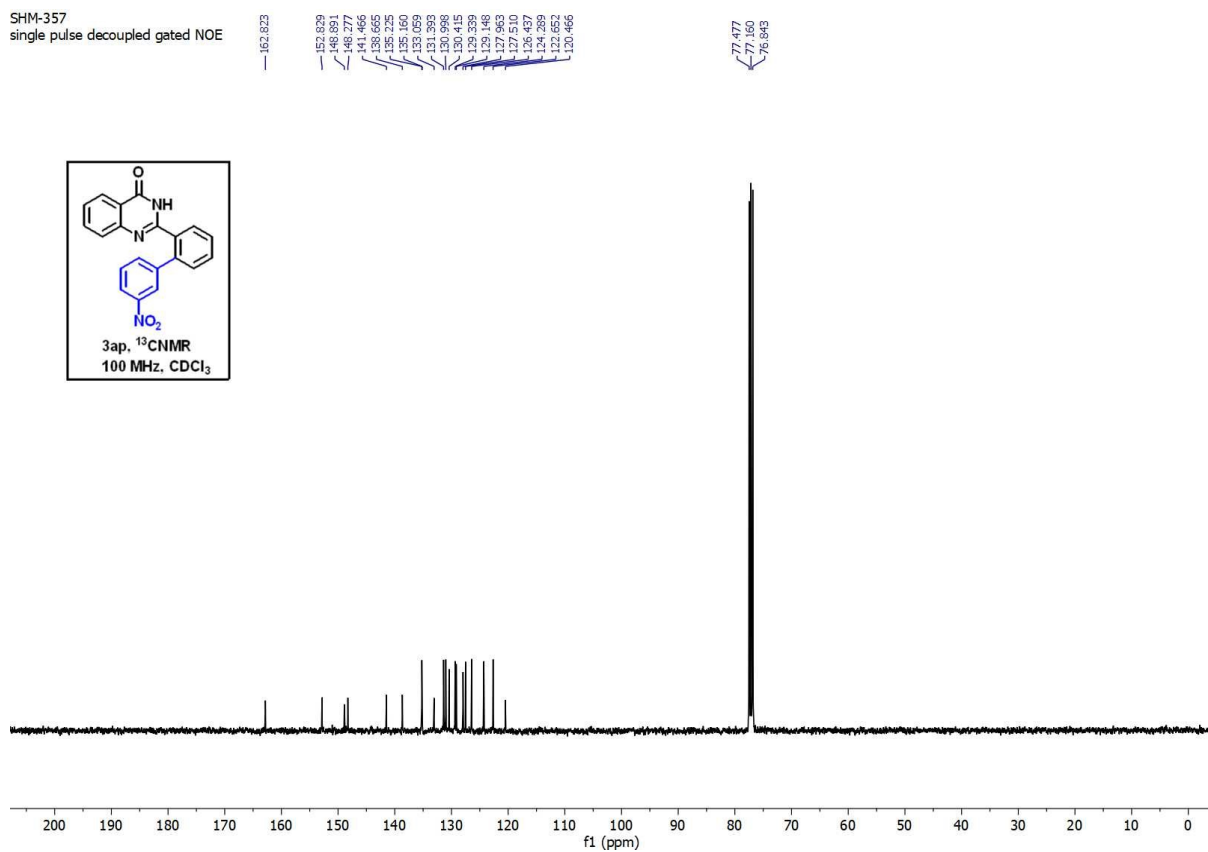
77.479  
77.162  
76.843



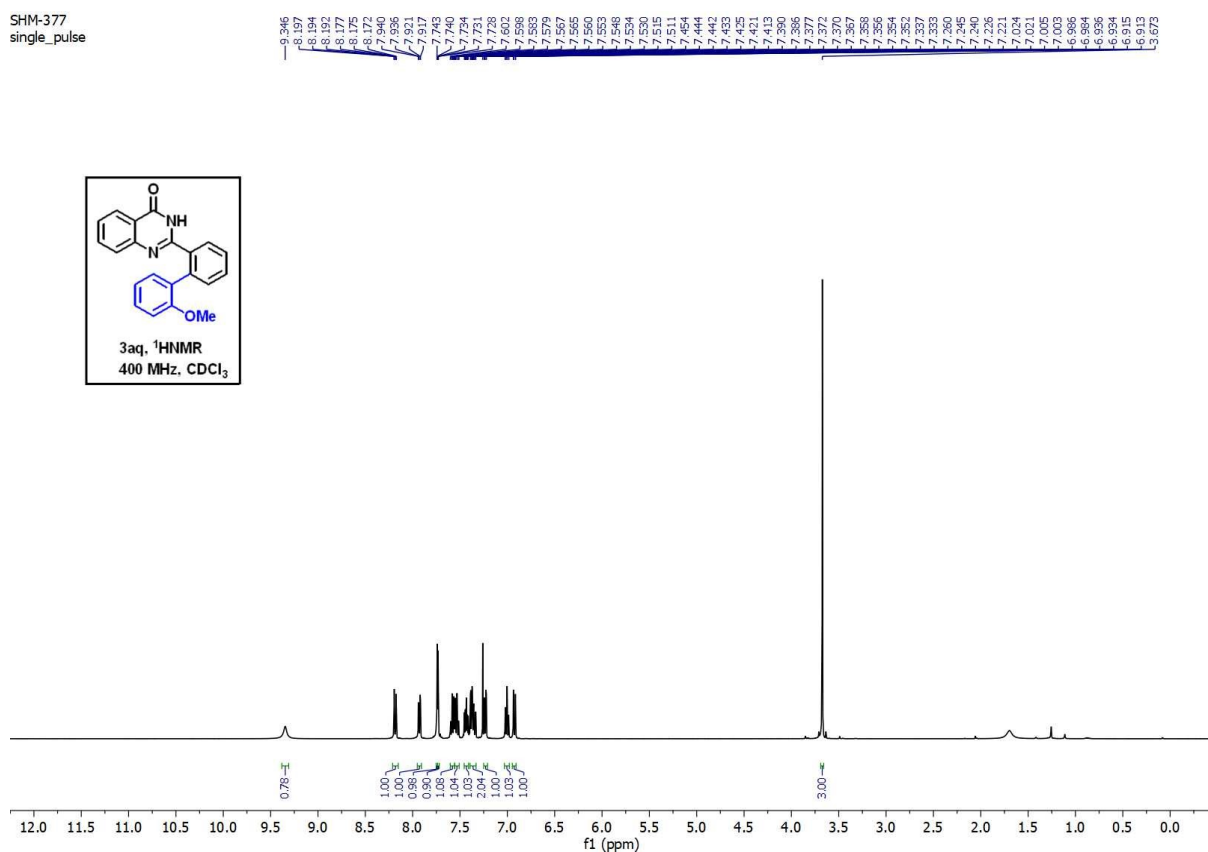
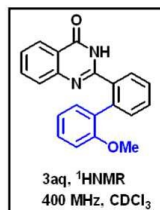
SHM-357  
single\_pulse



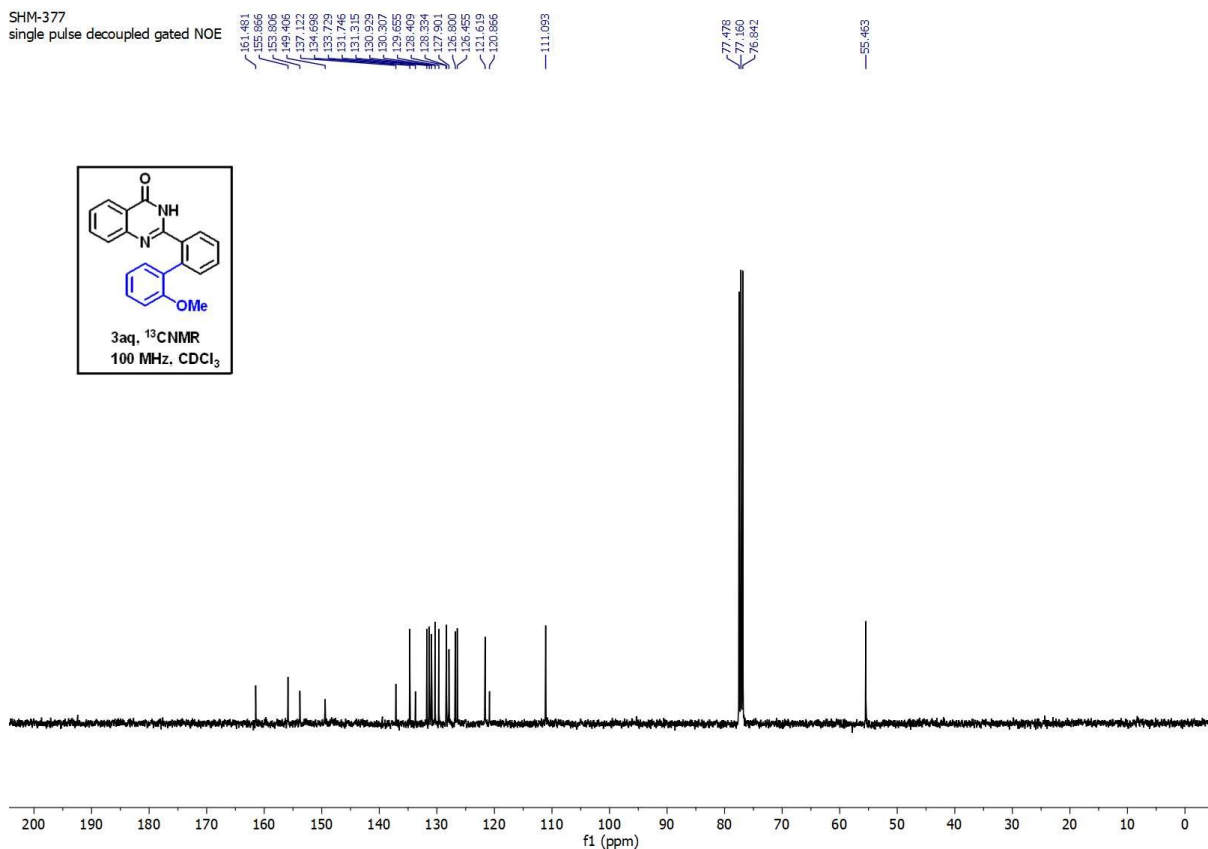
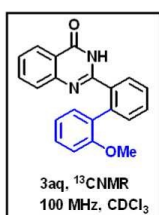
SHM-357  
single pulse decoupled gated NOE



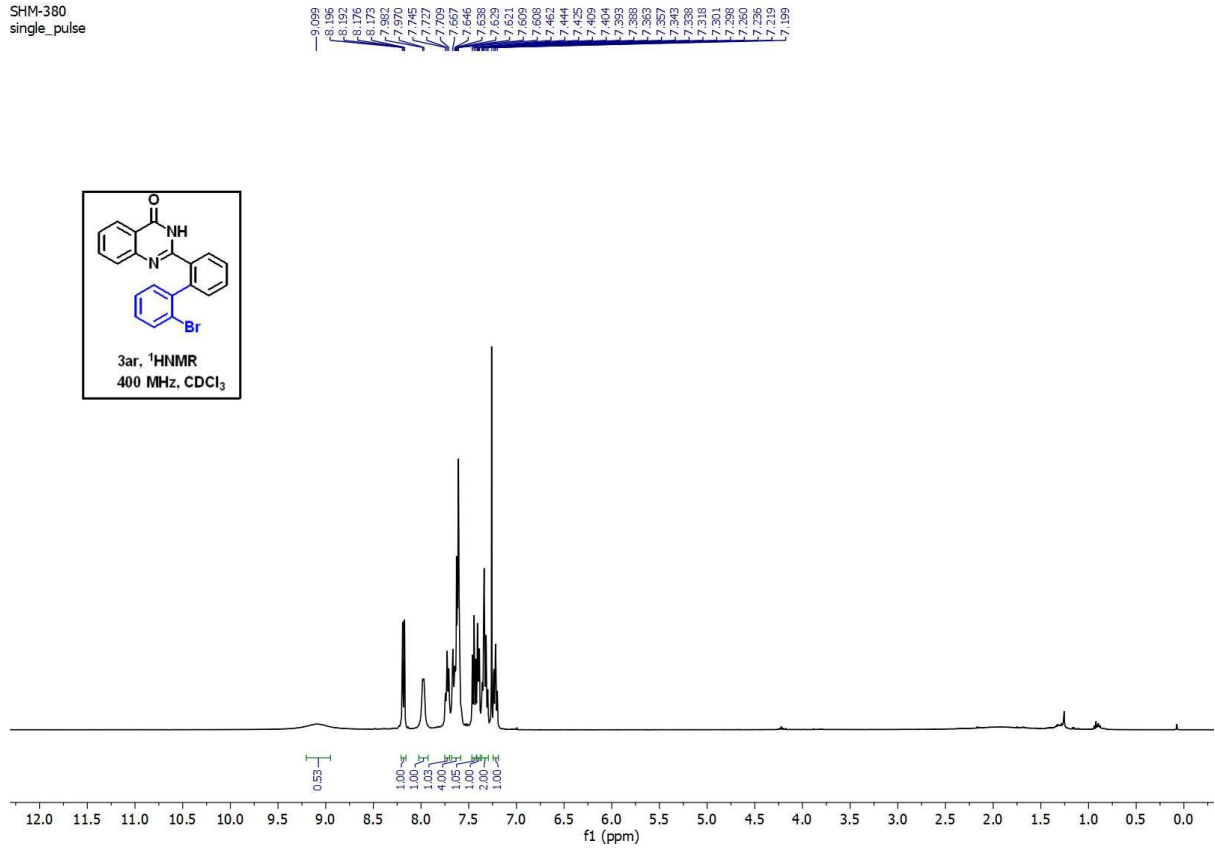
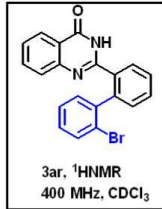
SHM-377  
single\_pulse



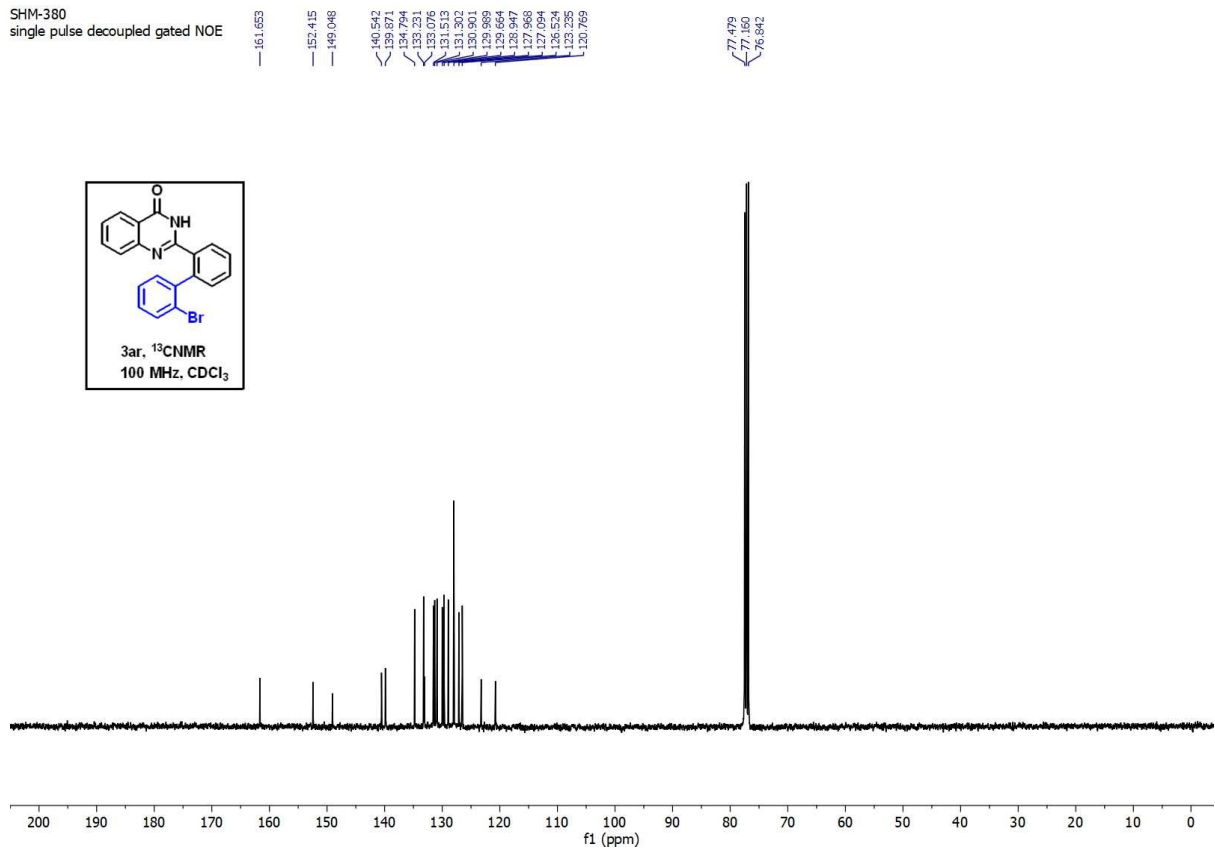
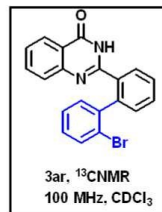
SHM-377  
single\_pulse decoupled gated NOE



SHM-380  
single\_pulse

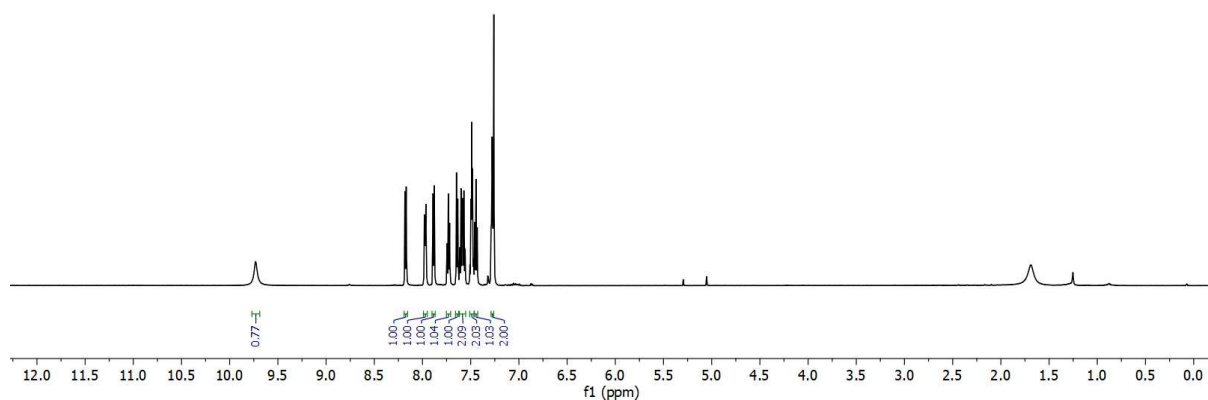
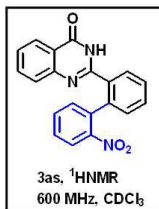


SHM-380  
single pulse decoupled gated NOE



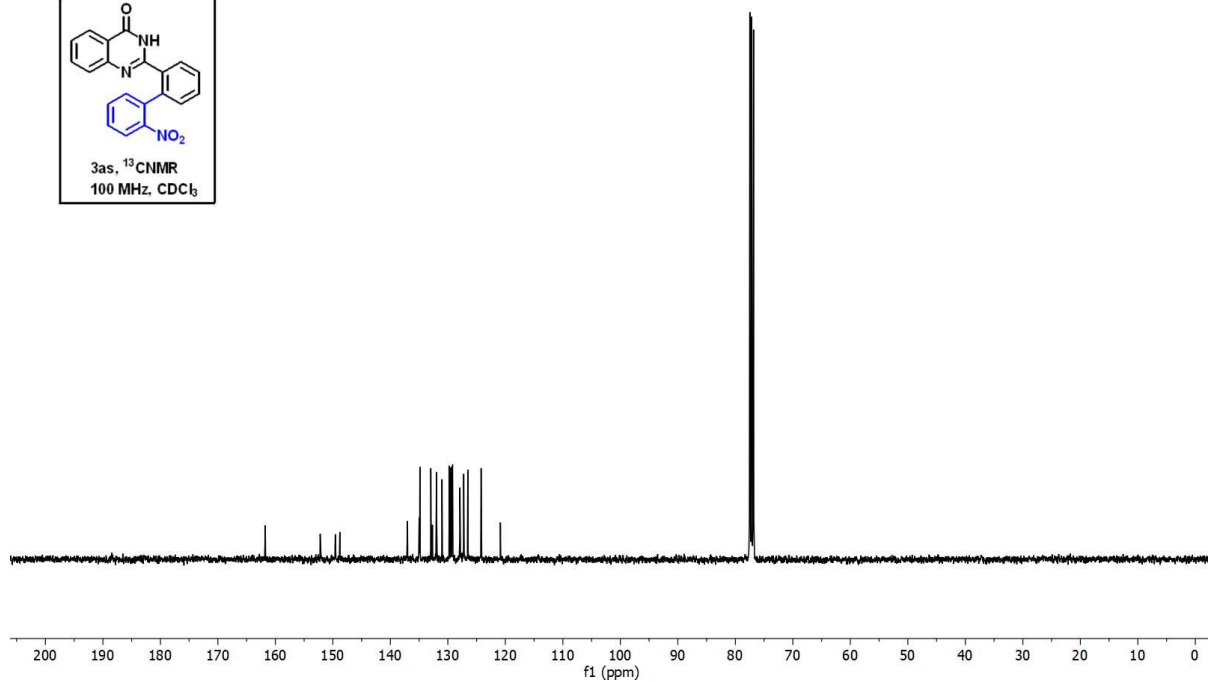
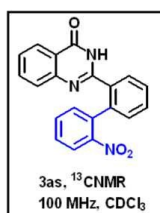
13-SHM-378.1.fid  
SHM-378 1H-NMR in CDCl<sub>3</sub>

9.731, 8.184, 8.182, 8.181, 8.169, 7.980, 7.978, 7.974, 7.969, 7.965, 7.953, 7.950, 7.900, 7.878, 7.744, 7.732, 7.719, 7.698, 7.684, 7.681, 7.613, 7.603, 7.600, 7.590, 7.588, 7.586, 7.582, 7.570, 7.560, 7.558, 7.499, 7.495, 7.490, 7.486, 7.480, 7.468, 7.445, 7.433, 7.287, 7.283, 7.279, 7.275, 7.272, 7.267, 7.265, 7.261, 7.260

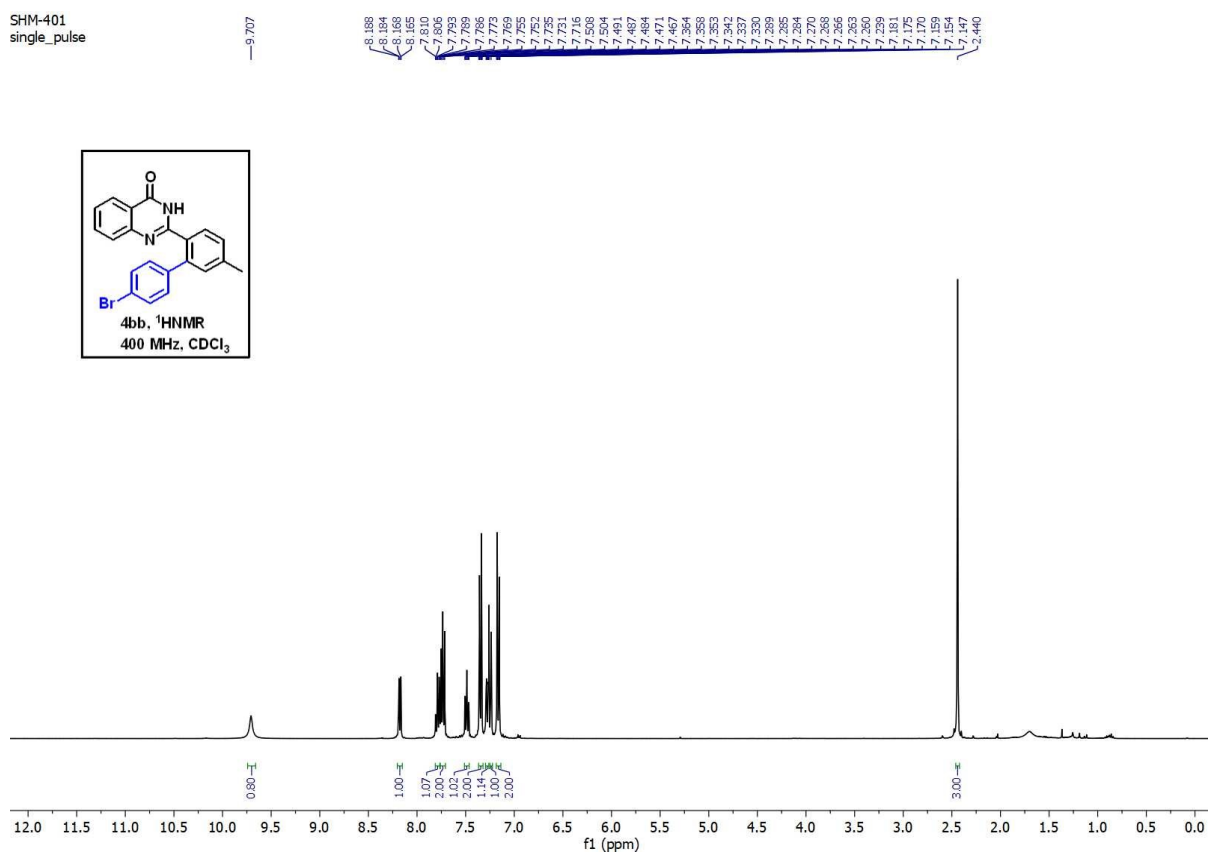
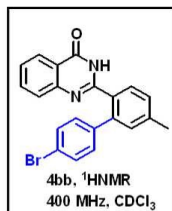


SHM-378  
single pulse decoupled gated NOE

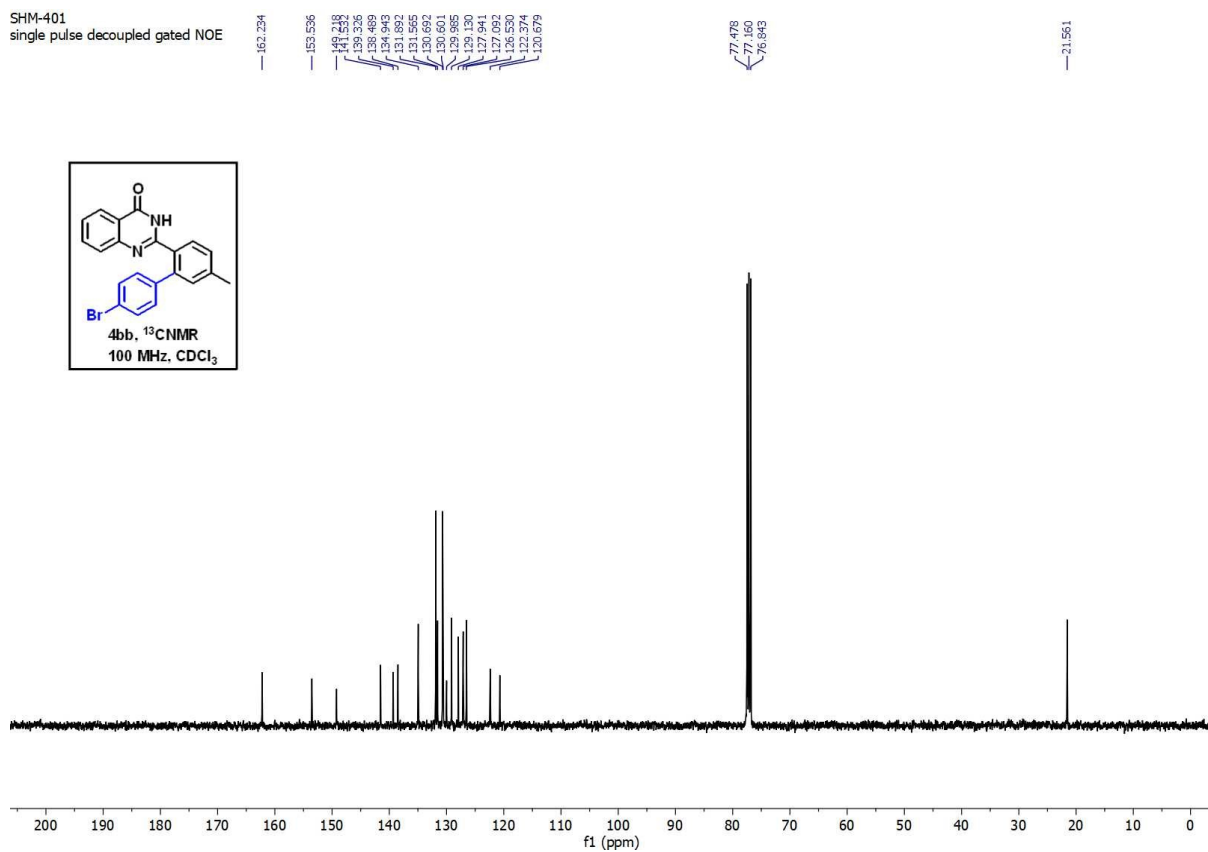
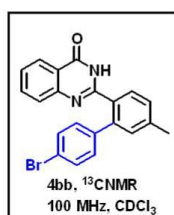
161.764, 152.213, 149.574, 147.713, 137.081, 134.969, 134.864, 132.968, 132.693, 131.972, 131.000, 129.527, 129.250, 129.172, 127.907, 127.244, 126.525, 124.627, 123.853, 77.479, 77.162, 76.843



SHM-401  
single\_pulse

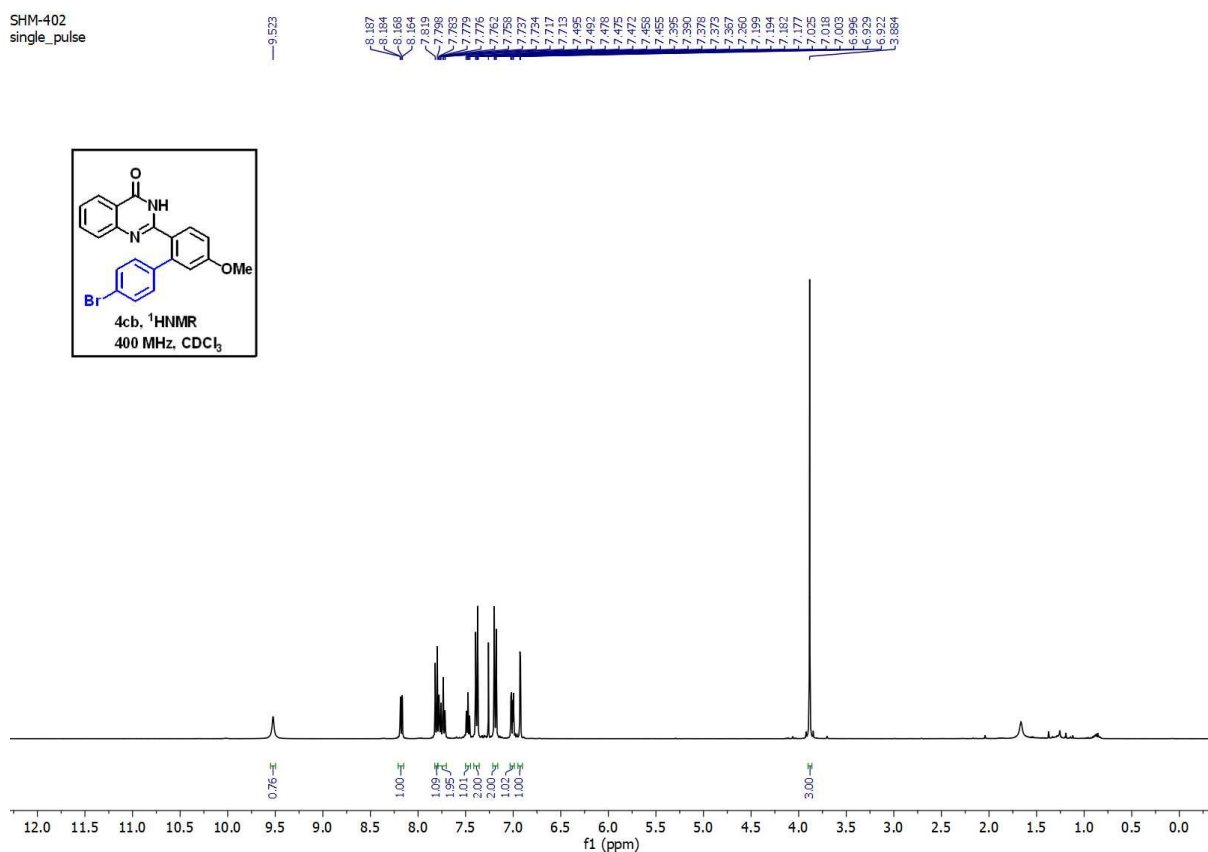


SHM-401  
single pulse decoupled gated NOE

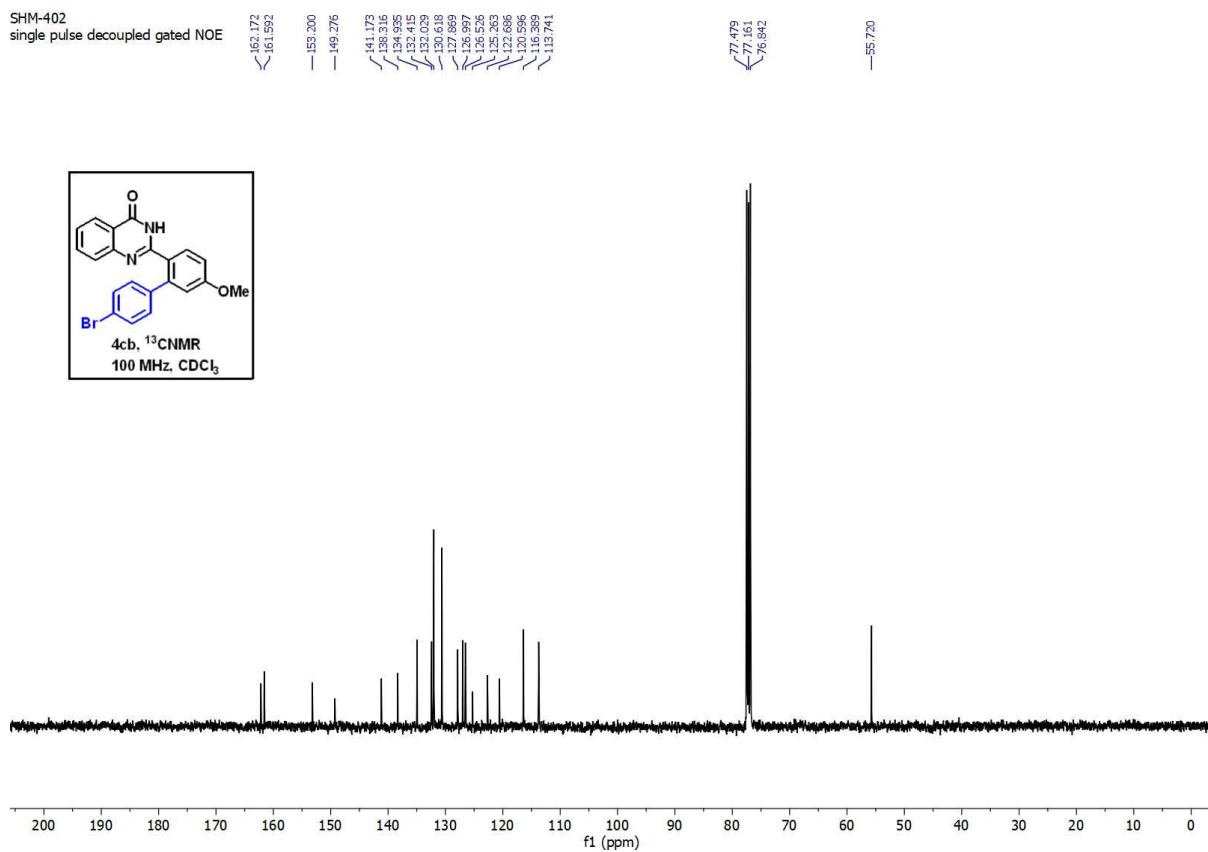




SHM-402  
single\_pulse

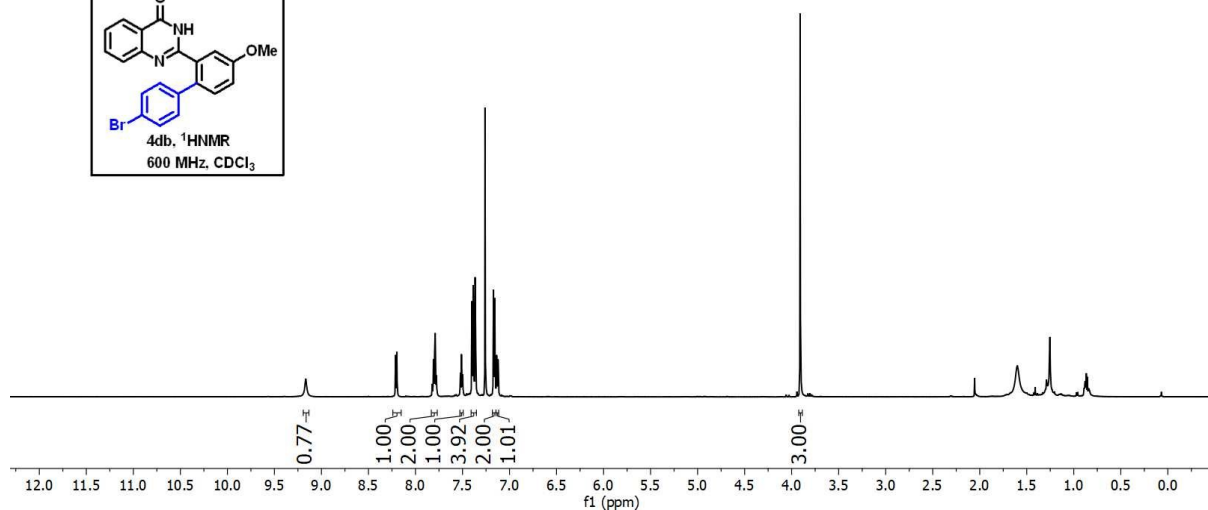
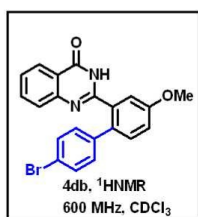


SHM-402  
single pulse decoupled gated NOE



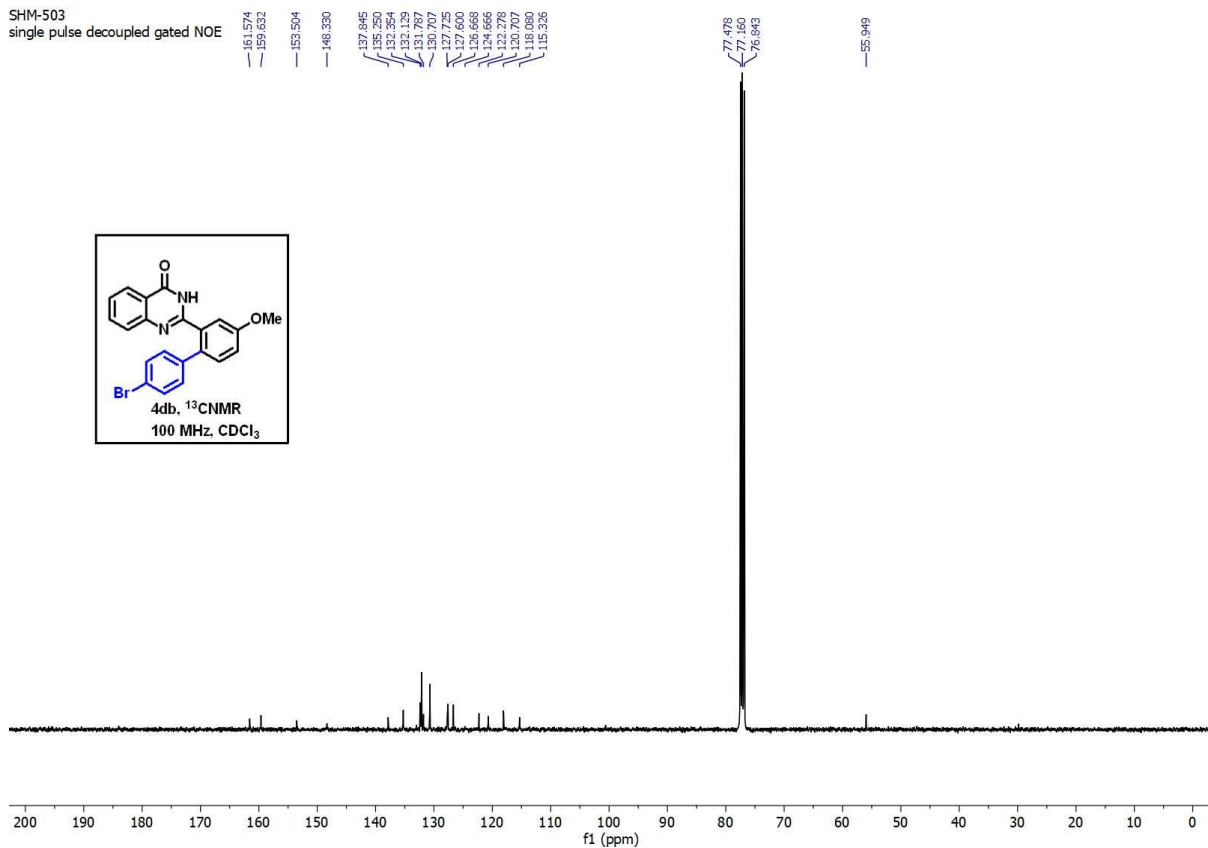
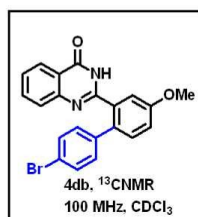
04-SHM-503/1  
 SHM-503 <sup>1</sup>H-NMR in CDCl<sub>3</sub>

9.167  
 8.213  
 8.211  
 8.200  
 8.198  
 7.823  
 7.821  
 7.809  
 7.807  
 7.798  
 7.796  
 7.792  
 7.789  
 7.778  
 7.775  
 7.524  
 7.522  
 7.513  
 7.511  
 7.508  
 7.500  
 7.497  
 7.400  
 7.387  
 7.381  
 7.366  
 7.361  
 7.260  
 7.171  
 7.167  
 7.160  
 7.157  
 7.139  
 7.134  
 7.125  
 7.120  
 3.910

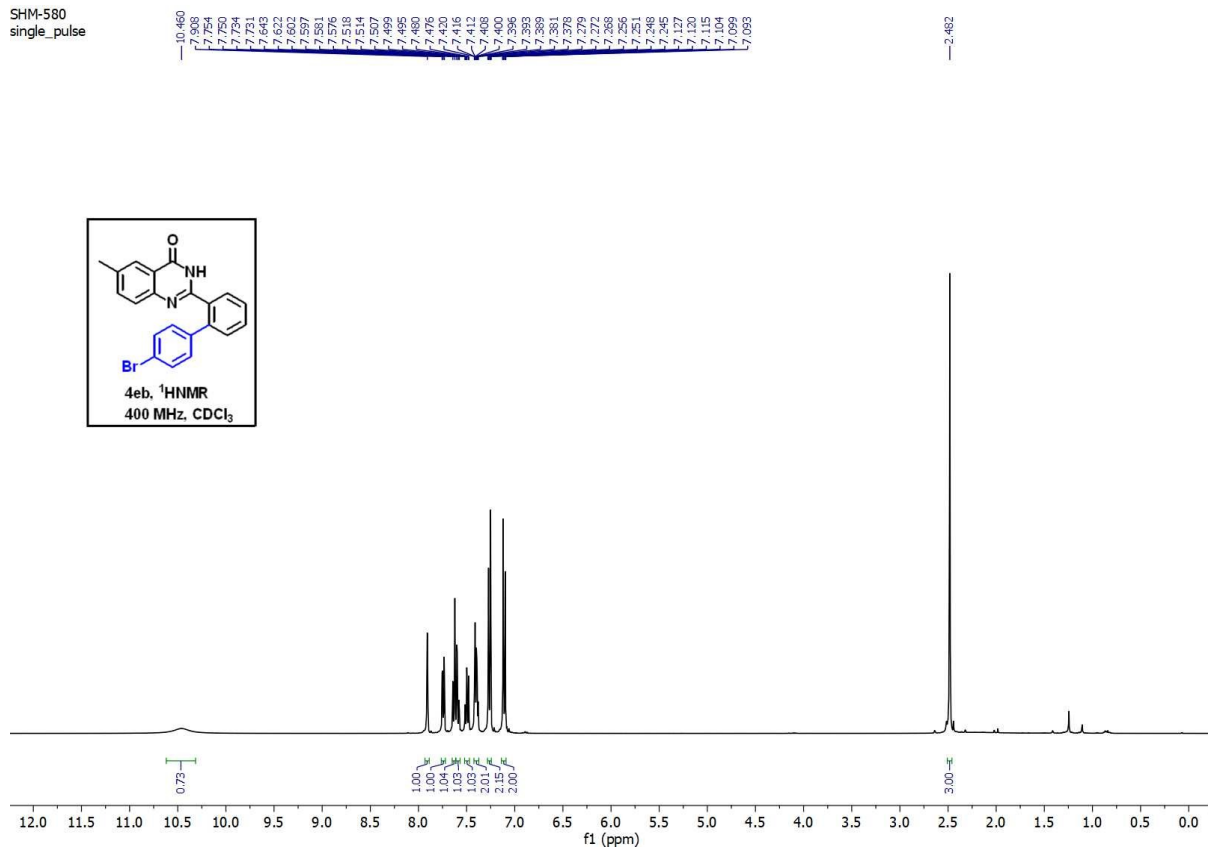


SHM-503  
 single pulse decoupled gated NOE

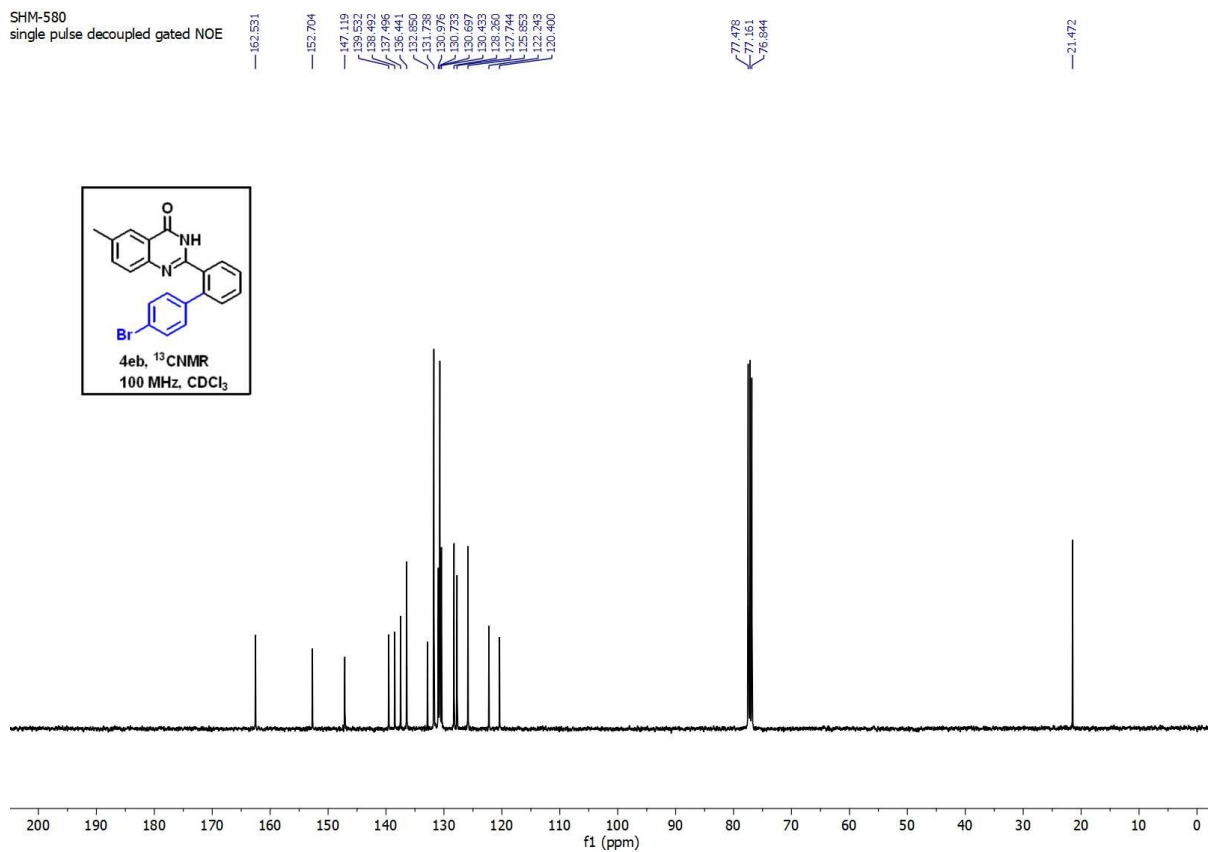
151.574  
 150.552  
 153.504  
 148.330  
 137.845  
 135.250  
 134.254  
 133.129  
 131.787  
 130.707  
 127.725  
 127.600  
 126.668  
 124.686  
 120.775  
 120.707  
 118.080  
 115.326  
 77.478  
 77.160  
 76.845  
 55.949



SHM-580  
single\_pulse



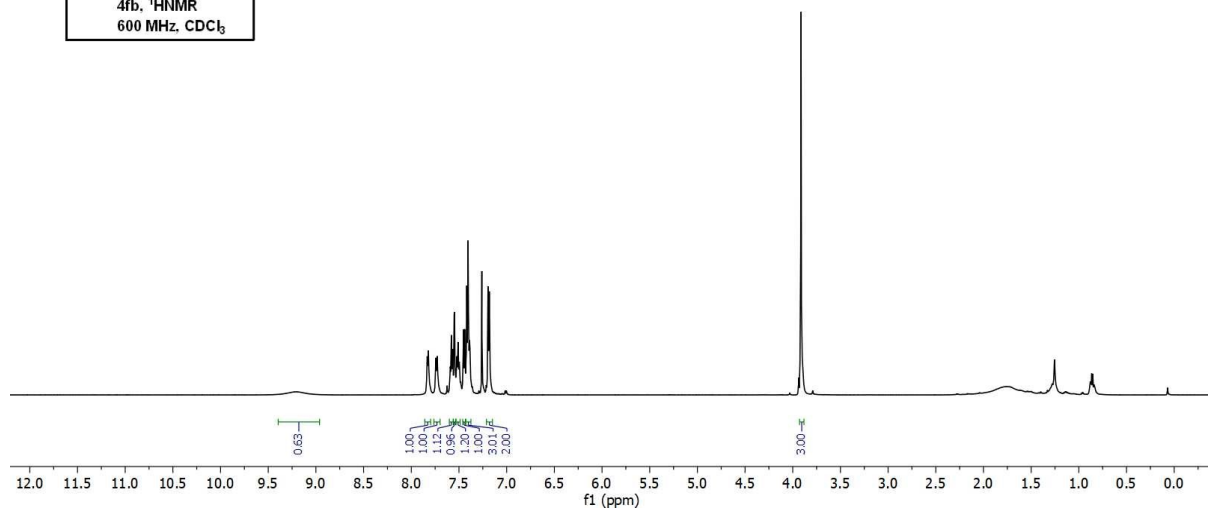
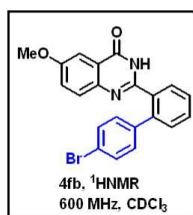
SHM-580  
single pulse decoupled gated NOE



24-SHM-608.1.fid  
SHM-608 1H-NMR in CDCl<sub>3</sub>

9.207  
7.833  
7.814  
7.742  
7.728  
7.592  
7.579  
7.567  
7.551  
7.546  
7.510  
7.510  
7.466  
7.463  
7.440  
7.419  
7.405  
7.386  
7.386  
7.314  
7.185  
7.182  
7.170

3.913

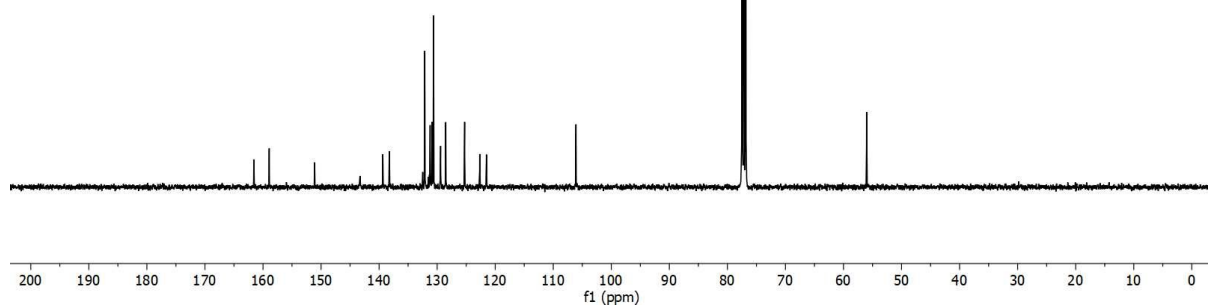
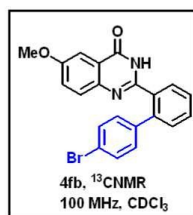


SHM-608  
single pulse decoupled gated NOE

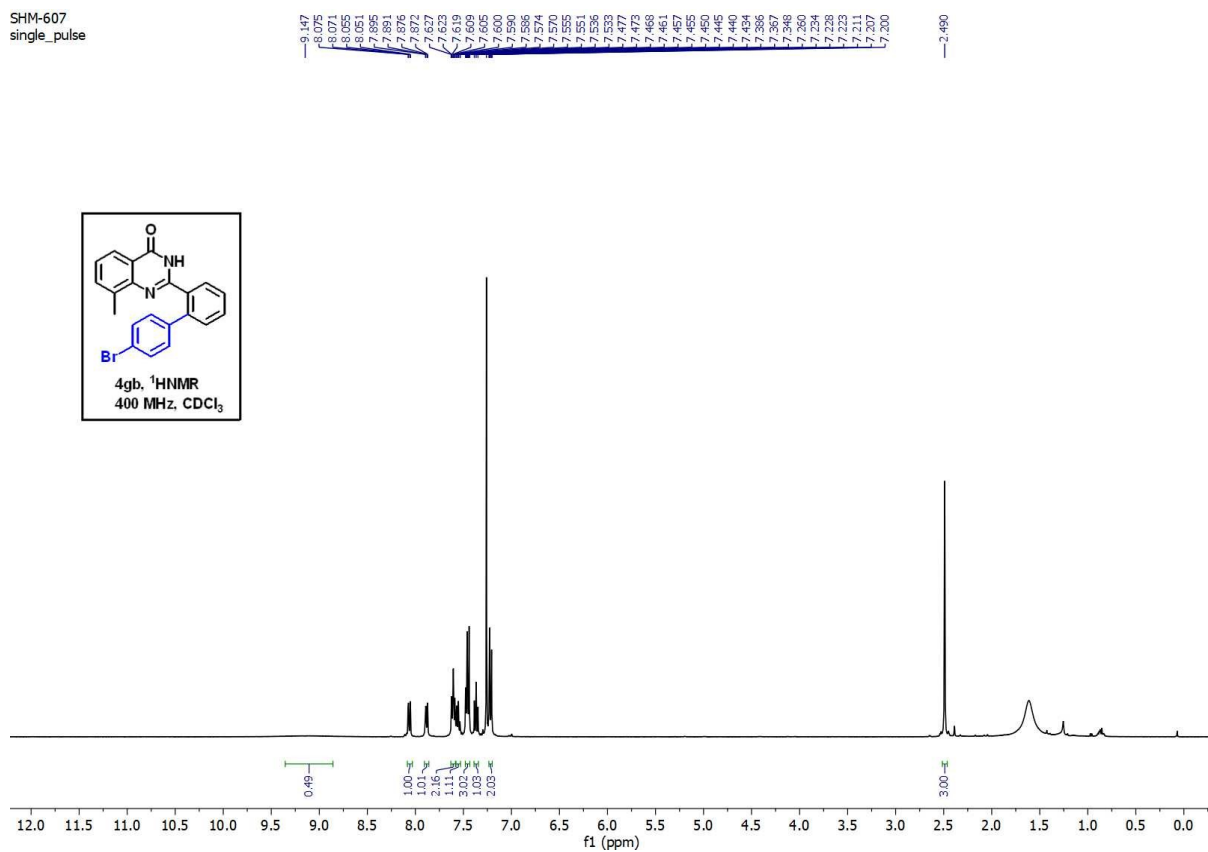
161.580  
158.931  
151.112  
143.285  
138.269  
138.237  
132.463  
132.189  
131.550  
131.208  
130.877  
130.664  
128.928  
128.523  
122.666  
121.510  
106.092

77.478  
77.160  
76.842

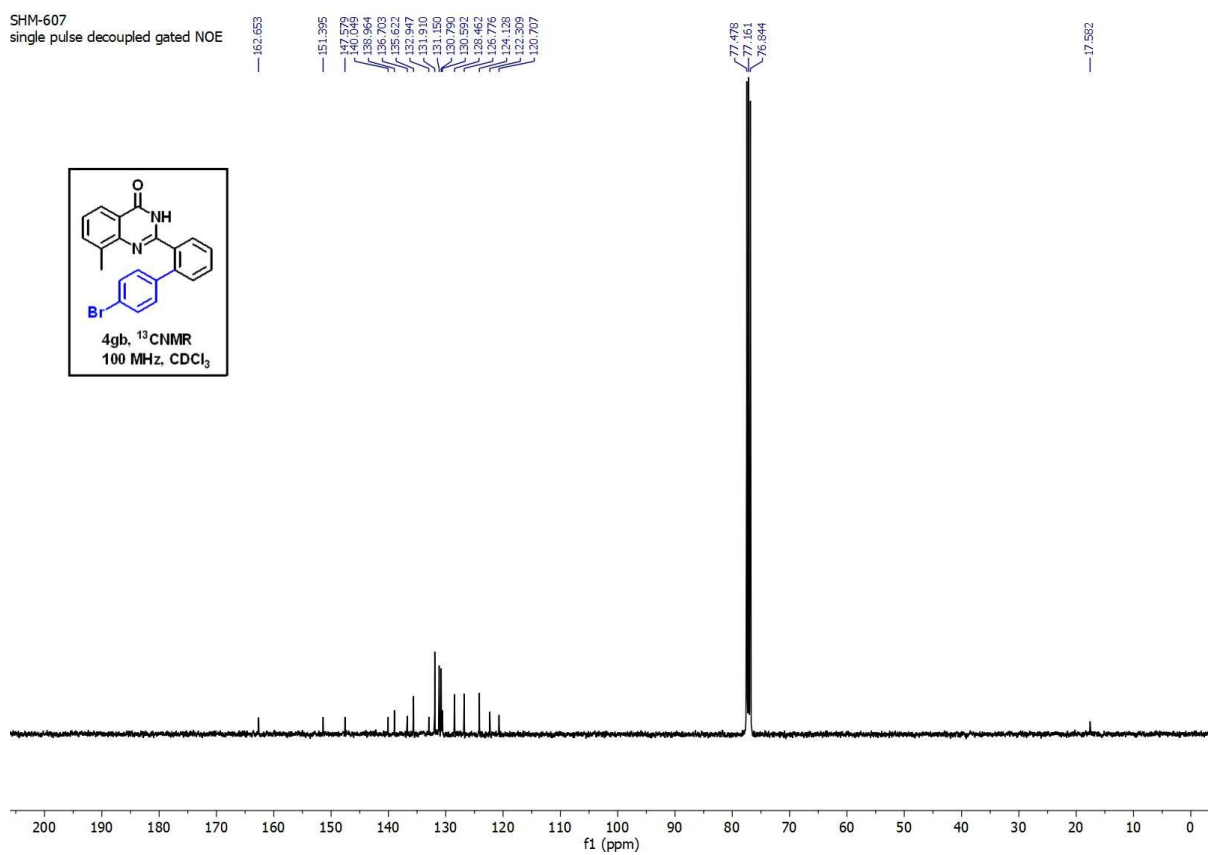
56.023



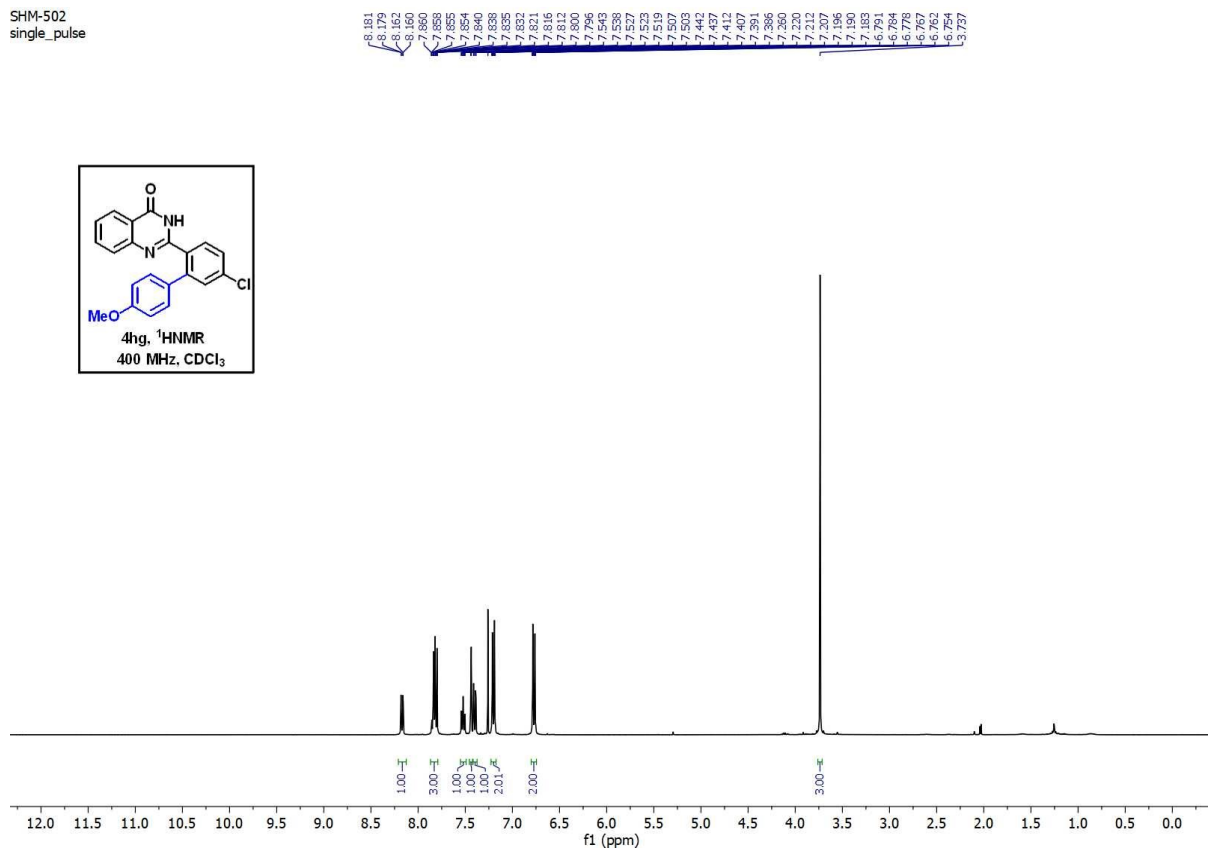
SHM-607  
single\_pulse



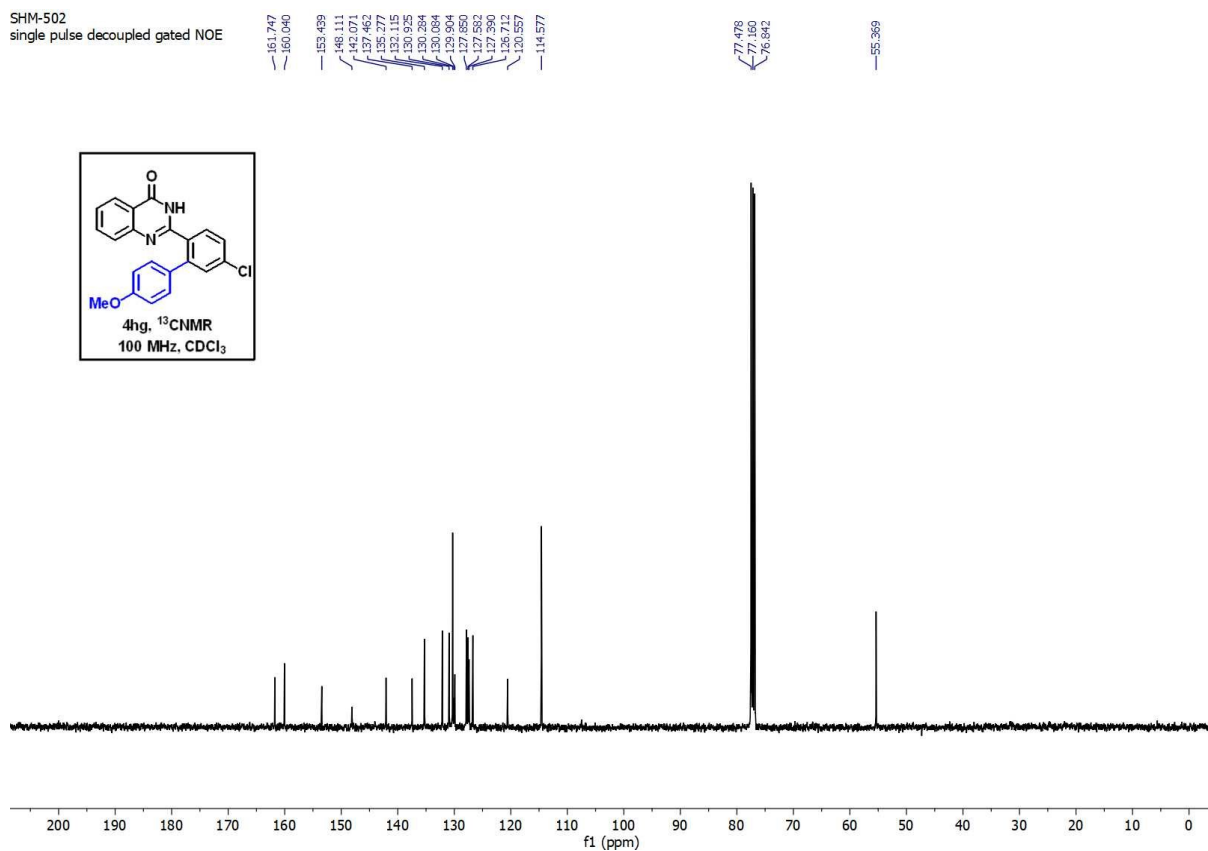
SHM-607  
single pulse decoupled gated NOE



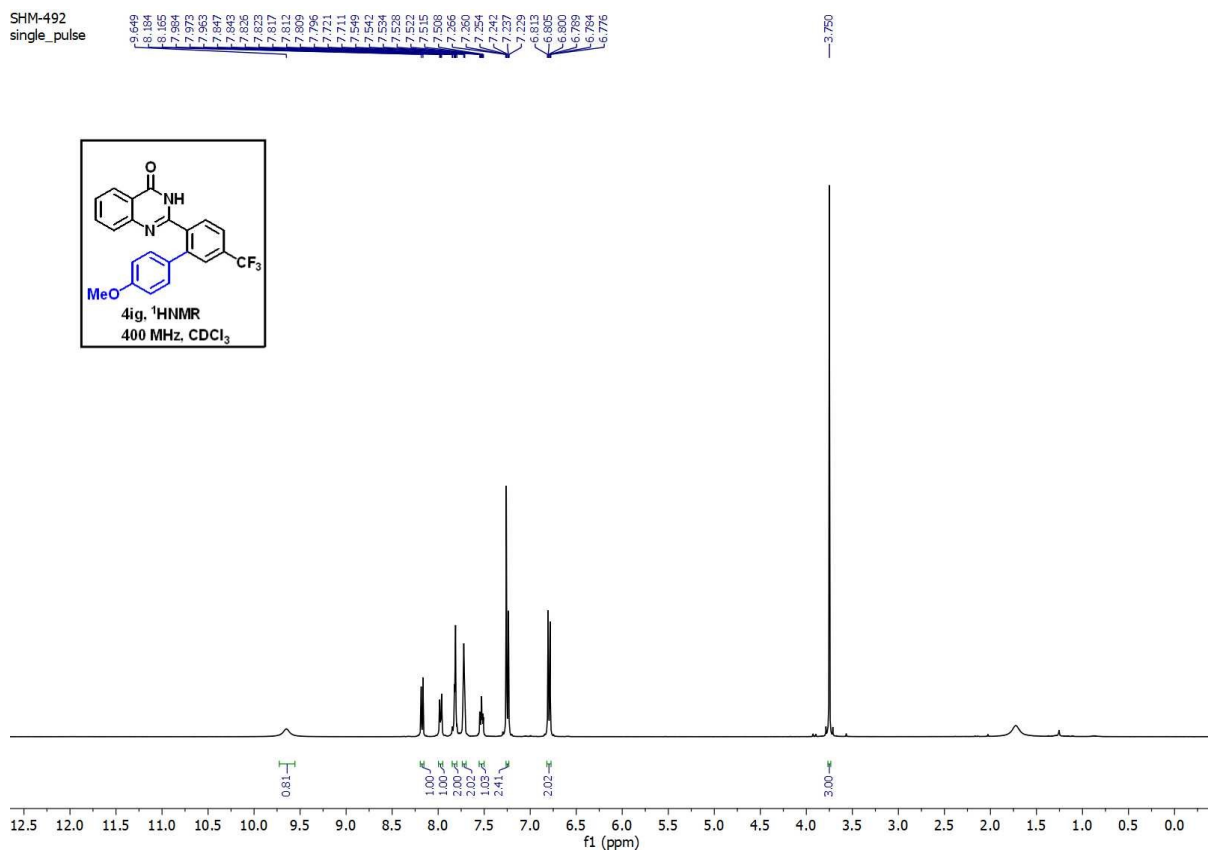
SHM-502  
single\_pulse



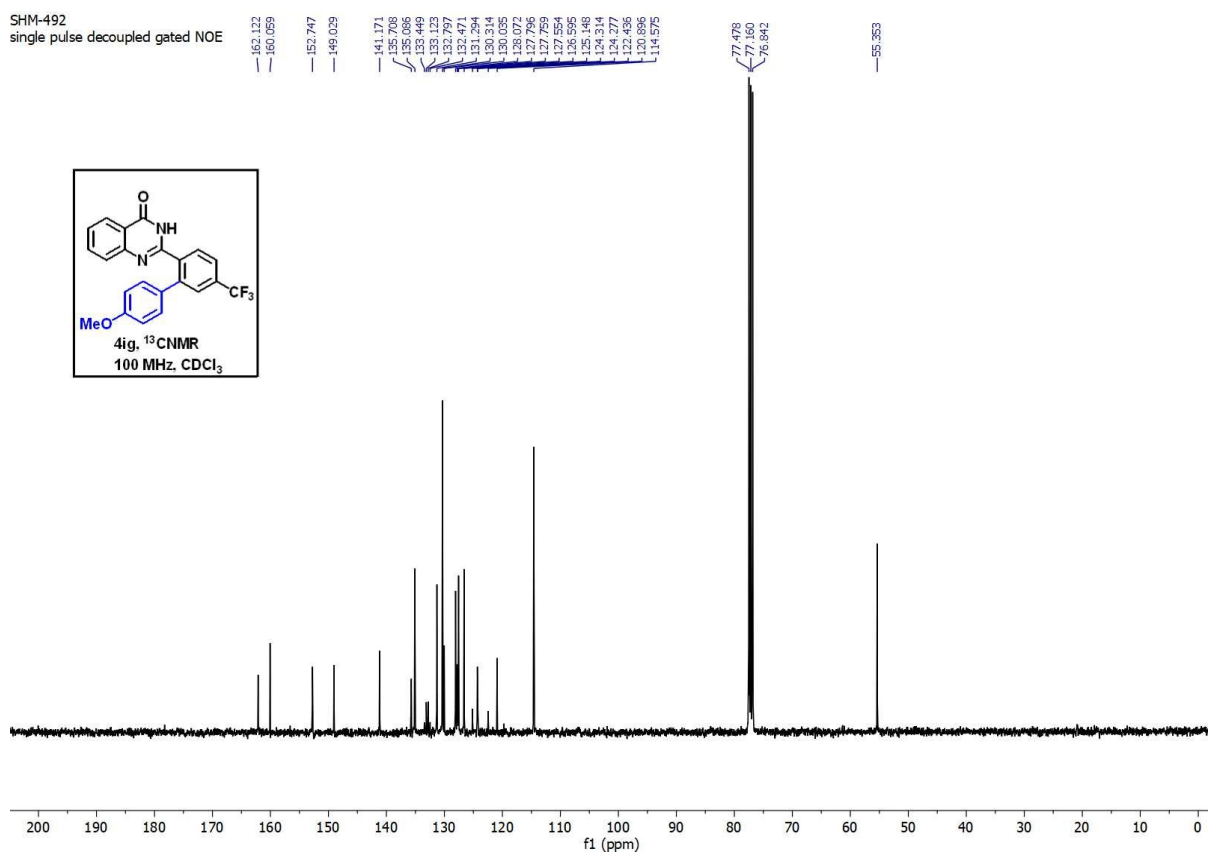
SHM-502  
single pulse decoupled gated NOE



SHM-492  
single\_pulse

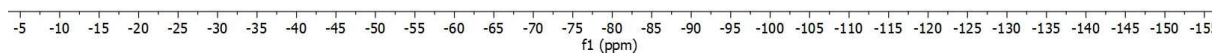
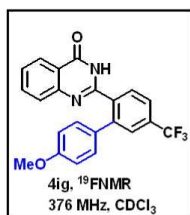


SHM-492  
single pulse decoupled gated NOE



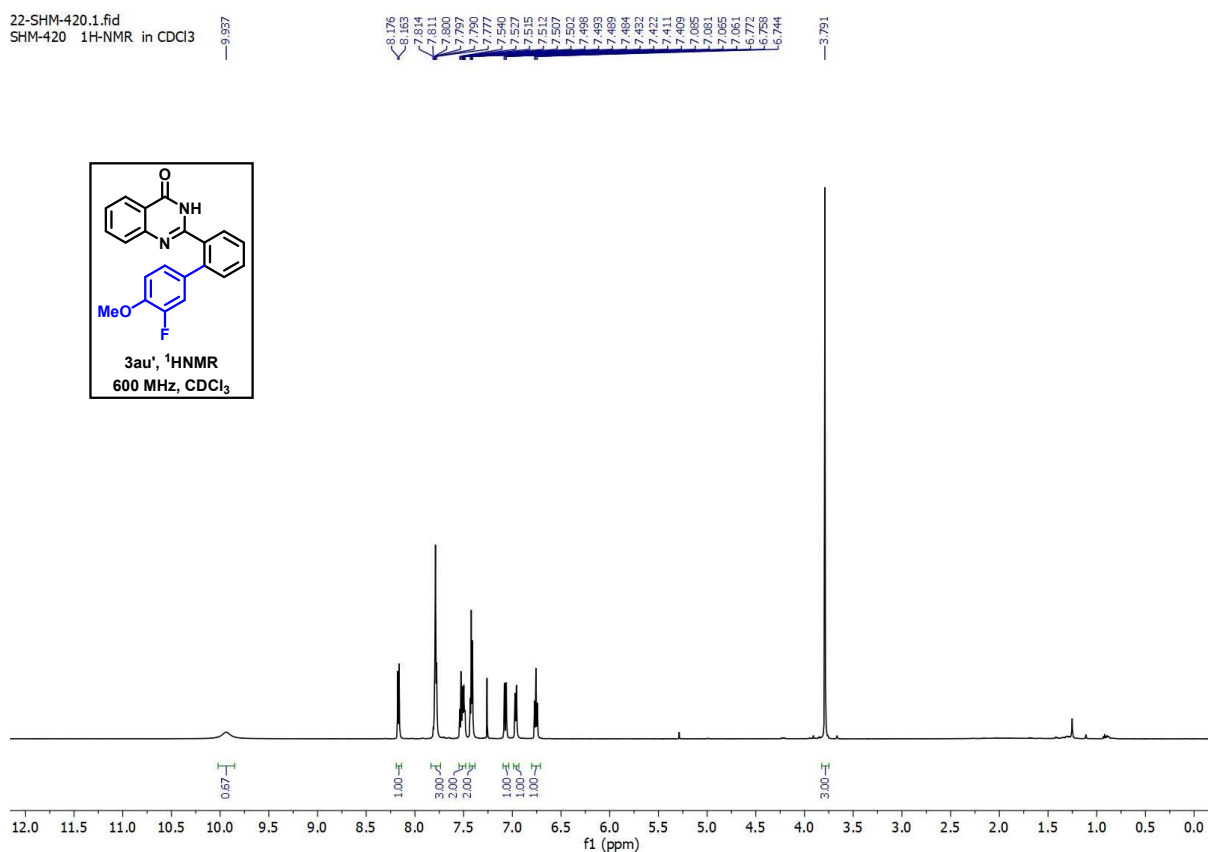
SHM-492  
single pulse decoupled gated NOE

—63.759

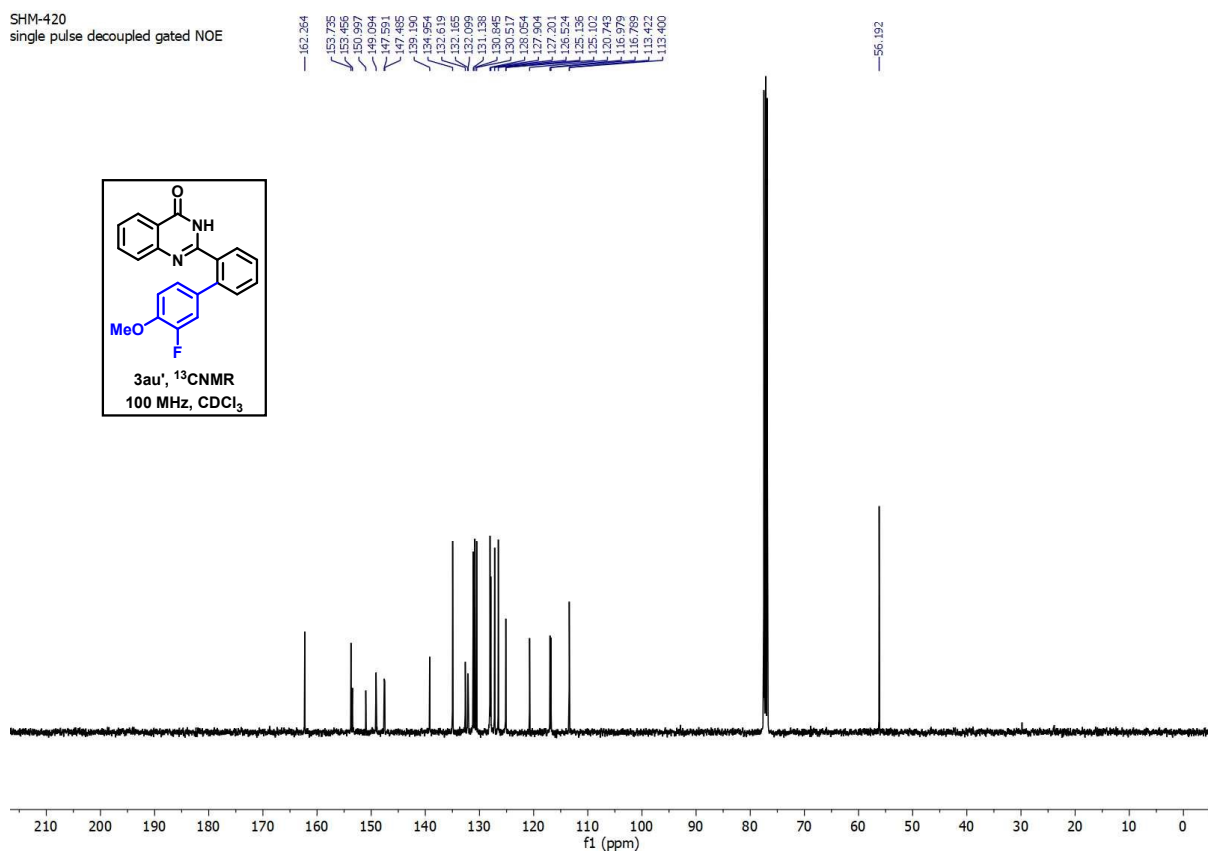




22-SHM-420.1.fid  
SHM-420 1H-NMR in CDCl<sub>3</sub>

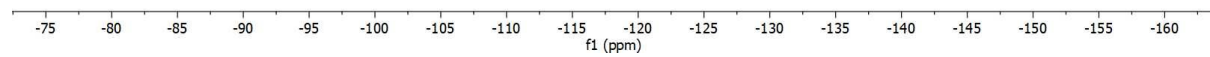
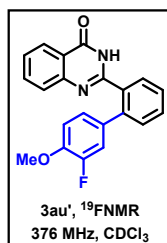


SHM-420  
single pulse decoupled gated NOE



SHM-420  
1D 19F experiment

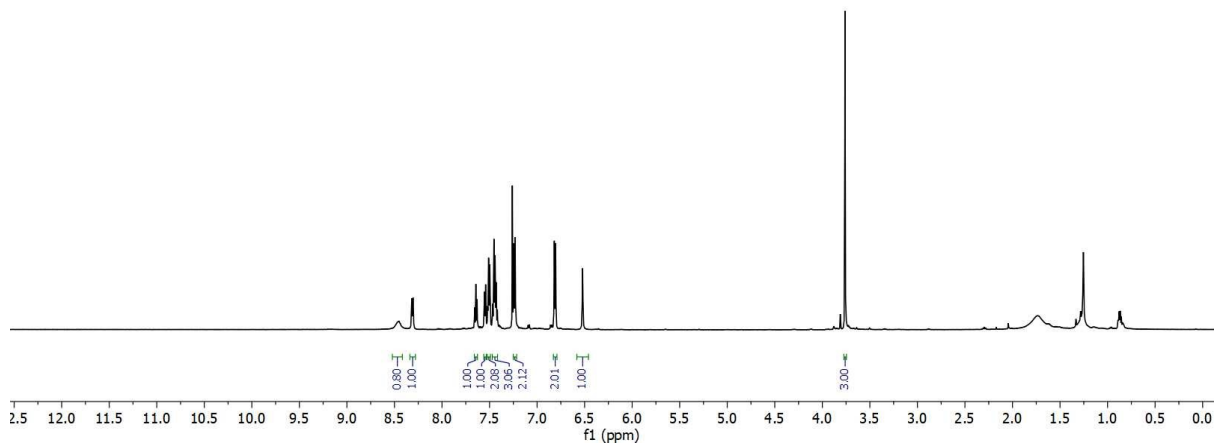
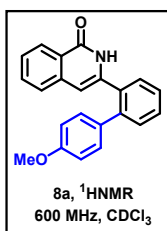
— 134.160



06-SHM-400M.1.fid

8.459  
8.318  
8.304  
7.656  
7.644  
7.511  
7.504  
7.541  
7.532  
7.520  
7.511  
7.498  
7.486  
7.474  
7.467  
7.455  
7.453  
7.444  
7.442  
7.439  
7.432  
7.426  
7.420  
7.418  
7.350  
7.256  
7.244  
7.233  
7.226  
6.819  
6.809  
6.805  
6.521

3.762



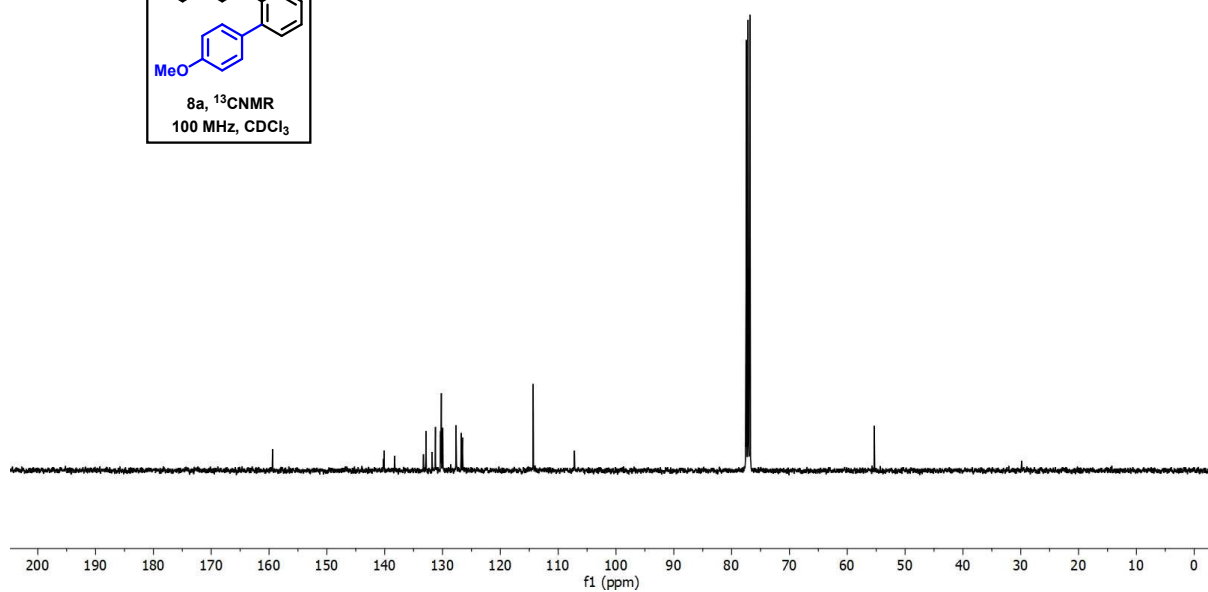
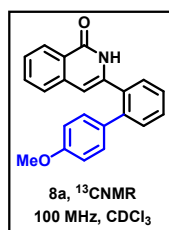
SHM-400M  
single pulse decoupled gated NOE

159.381

140.236  
140.122  
138.237  
133.294  
132.864  
131.817  
131.227  
130.533  
129.961  
129.961  
127.672  
127.613  
126.779  
126.553  
114.322  
107.161

77.478  
77.160  
76.842

55.325

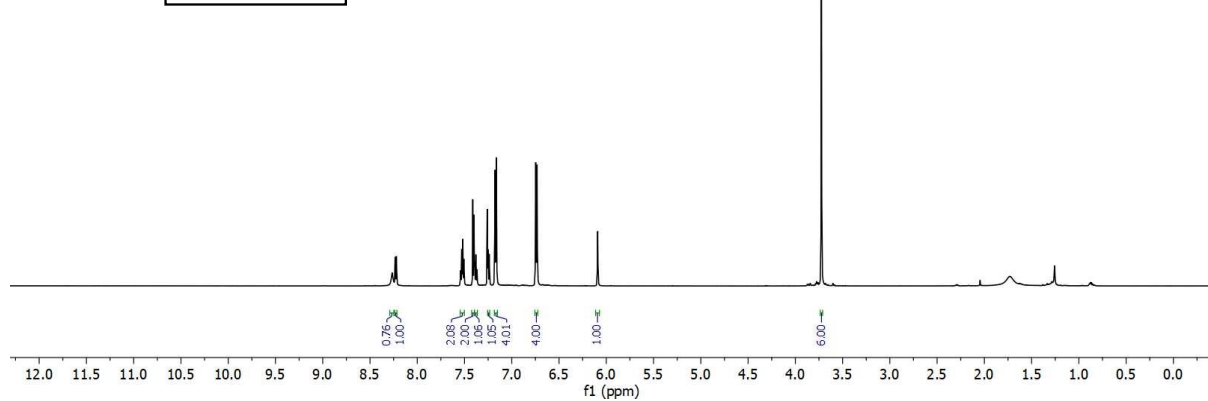
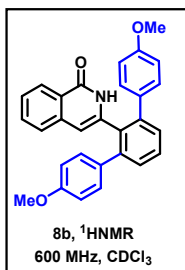


01-SHM-400D.1.fid  
SHM-400D 1H-NMR in CDCl3

8.365  
8.234  
8.220  
7.541  
7.530  
7.519  
7.507  
7.485  
7.480  
7.393  
7.380  
7.367  
7.260  
7.252  
7.238  
7.164  
6.747  
6.733

6.091

3.724



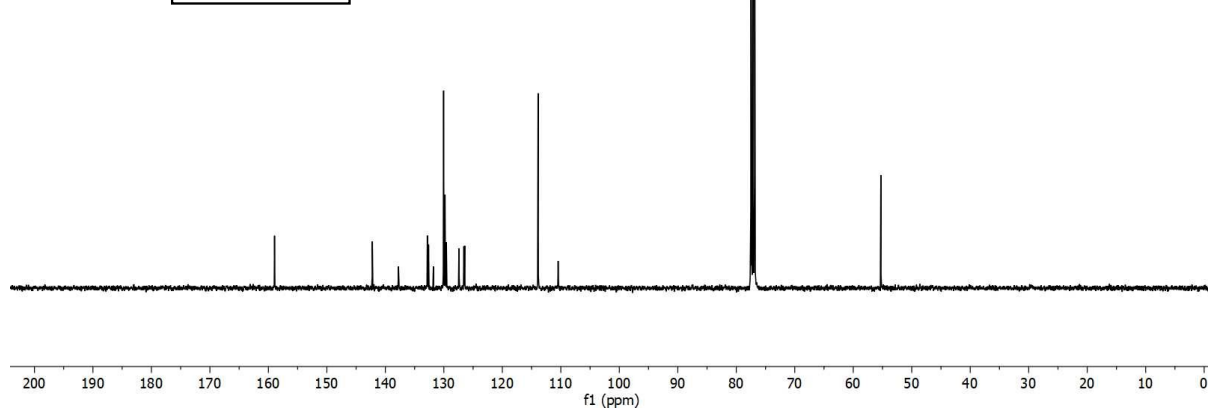
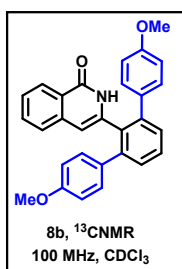
SHM-400D  
single pulse decoupled gated NOE

158.946

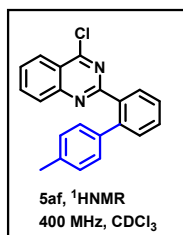
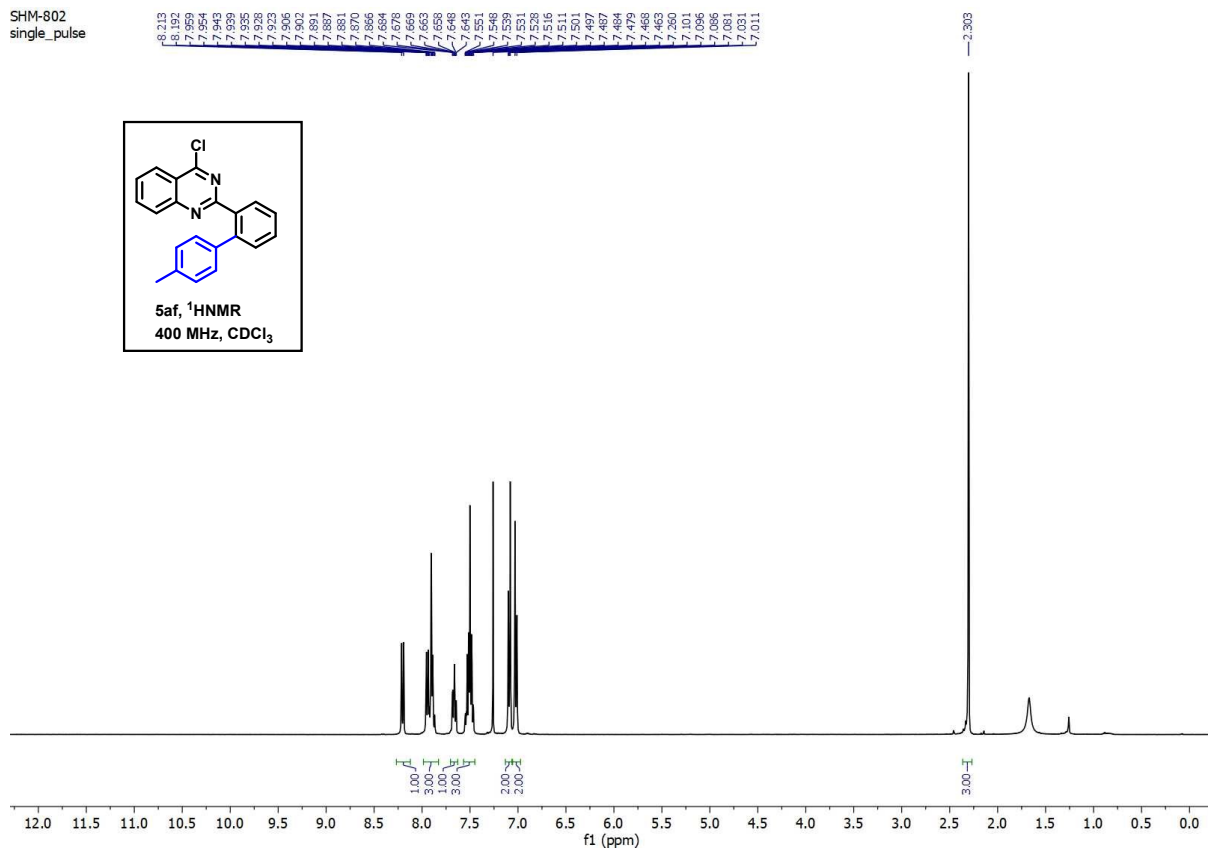
142.235  
137.760  
137.699  
132.623  
132.615  
131.787  
129.524  
129.563  
127.417  
126.573  
126.490  
113.687  
110.461

77.478  
77.160  
76.842

55.263



SHM-802  
single\_pulse



SHM-802  
single pulse decoupled gated NOE

