Supporting Information

Iridium Supported on Porous Polypyridine-Oxadiazole as High Active and Recyclable Catalyst for Borrowing Hydrogen Reaction

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Table of contents

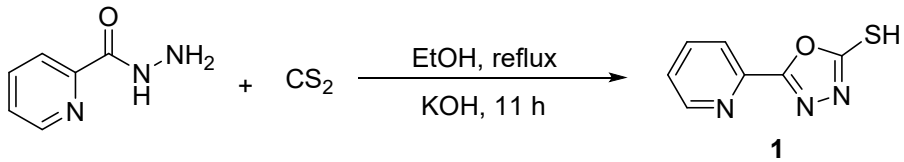
1. General methods and materials……S2
2. Preparation of **PPO-Ir**…… S2-S4
3. Characterization of catalyst **PPO-Ir**……S4-S5
4. General procedure for **5**……S5
5. General procedure for **7**……S5-S6
6. General procedure for **9**……S6
7. Hammett plot and mechanism studies ……S6-S7
8. Analytical data of the obtained compounds……S7-S21
9. NMR spectra of obtained compounds…… S22-S79
10. Reference……S80

1. General Methods and Materials

All the reactions dealing with air were carried out in a high purity argon or nitrogen atmosphere using standard Schlenk techniques or glovebox techniques. Unless the special instructions, all the reagents were provided from commercial suppliers (TCI, Acros, J&K, Energy Chemical, etc.) and used without further purification. All the obtained products were characterized by ^{1}H-NMR, ^{13}C-NMR and referenced to $CDCl_3$ (7.26 ppm for ^{1}H, and 77.1 ppm for ^{13}C) or DMSO-d_6 (2.50 ppm for ^{1}H, and 39.5 ppm for ^{13}C) with tetramethylsilane as internal standard (0 ppm). ^{1}H-NMR and ^{13}C-NMR spectra were obtained on Varian 400 or 101 MHz respectively on Bruker Advance III HD 400 MHz spectrometer. TEM was recorded on a transmission electron microscope (JEM–2100, JEOL, Japan), operating at 200 kV. SEM image and EDS spectra was performed on a HITACHI S-4800 field-emission scanning electron microscope. XPS data were recorded with electron energy analyzer (ESCALAB 250Xi, Thermo Fisher Co, USA). The nitrogen sorption isotherms and pore-size distribution curves were measured at the temperature of liquid nitrogen (77 K) by using an automatic volumetric adsorption equipment (Mircomeritics, ASAP2010). Thermogravimetric analysis was carried out using a TGA/DSC 1/1100SF instrument in dry nitrogen atmosphere at a heating rate of 10 ^{o}C/min from 50 to 650 ^{o}C. Inductively coupled plasma atomic emission spectroscopy (ICP-AES) analysis for Ir loading amount was determined by a Jarrell-Ash 1100 ICP-AES spectrometer.

2. Preparation of PPO-Ir

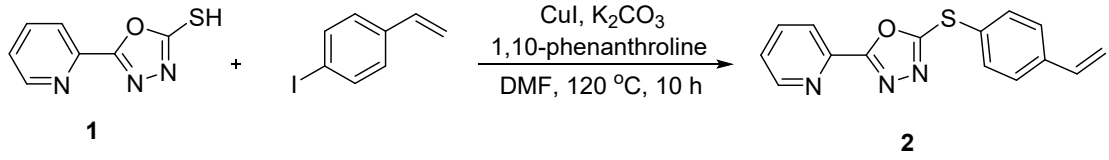
2.1 Procedure for synthesis of monomer 2[1]



1

First, KOH (18 mmol) dissolved in ethanol (30 mL), and picolinohydrazide (18 mmol) was added until cooled to room temperature. Then CS_2 (27 mmol) was added into the mixture with a constant pressure dropping funnel. The resulting mixture was stirred at 80 °C for 11 h and

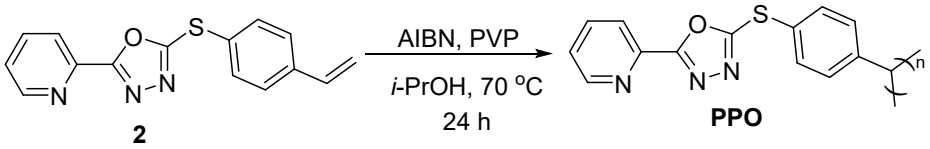
monitored by TLC until complete disappearance of picolinohydrazide. After completion of the reaction, the solution was removed under vacuum. Remaining mixture was added deionized water (40 mL) and was adjusted to pH=3 with hydrochloric acid. At this point, a great deal of yellow solids (**1**) was precipitated with a Brinell funnel (56% yield).



1 **2**

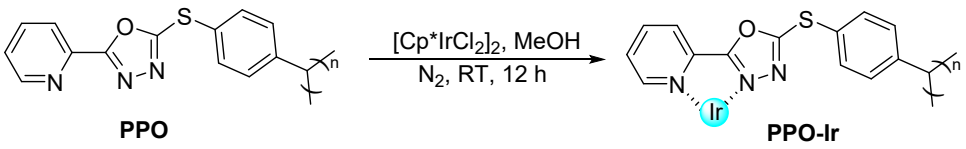
1 (3 mmol) and 1-iodo-4-vinylbenzene (3.6 mmol) were dissolved in DMF (9 mL) and added a mixture of CuI (0.15 mmol), 1,10-phenanthroline (0.3 mmol) and K_2CO_3 (3.9 mmol) were dissoved in DMF (9 mL) in advance. The mixture was stirred at 120 °C for 10 h, the reaction mixture was added water and extracted with ethyl acetate (3×50 mL). The organic phases were concentrated by removing the solvent under vacuum. Finally, the residue was purified by column chromatography with petroleum ether/ethyl acetate (petroleum ether /ethyl acetate = 5:1) as eluent to give the monomer **2** (78% yield).

2.2 Procedure for synthesis of PPO-Ir



2 **PPO**

The PVP (33.4 mg), and isopropanol (12 mL) were separately weighed into a 50 mL Schlenk bottle, fully dissolved, and heated to 70 ° C under nitrogen. Then the monomer **2** (645 mg) and AIBN (2.5 mg) were added to the Schlenk tube sequentially under vigorous stirring. Before cooling to ambient temperature, the polymerization was allowed to proceed for 24 h. The desired supported (PPO) was synthesized as a yellowish solid by centrifugal suspension and washed with EtOH in ultrasonic vibration for several times.



PPO **PPO-Ir**

Under N_2 atmosphere, PPO (1.0 g), $[Cp^*IrCl_2]_2$ (80 mg, 0.1 mmol) and dry methanol (5 mL) was added to an oven-dried 25 mL Schlenk tube equipped with a stir bar. Then, the tube was closed and the resulting mixture was stirred at room temperature for 12 h. After the reaction, the solid changed from white to yellow and the volume became clear. Solids were obtained by centrifugation and washed with methanol and dichloromethane three times each before dried to give the desired product **PPO-Ir**.

3. Characterization of catalyst PPO-Ir

Figure S1 showed SEM EDS image of **PPO-Ir** (a), and corresponding elemental mapping images of (b) C, (c) N, (d) O, (e) S, (f) Ir, which revealed iridium complex was supported on PPO successfully.

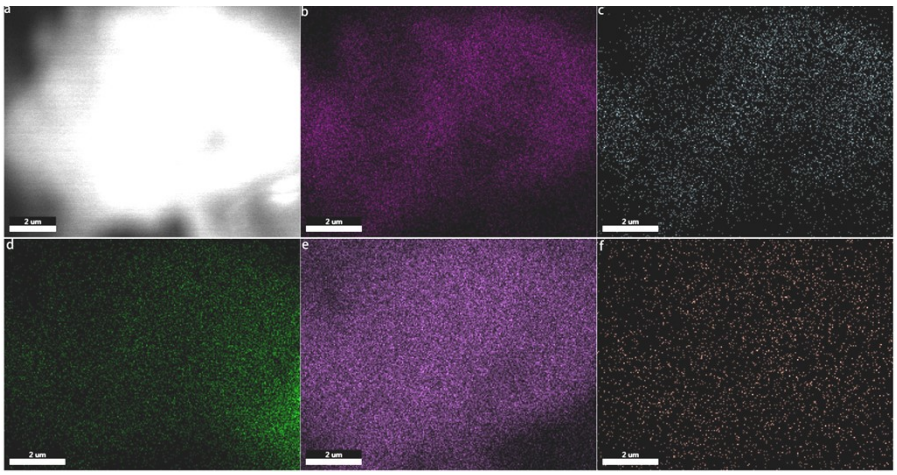


Figure S1. SEM EDS image of **PPO-Ir** (a), and corresponding elemental mapping images of (b) C, (c) N, (d) O, (e) S, (f) Ir.

Table.S1. Quantitative elemental composition of C, O, N and Ir from the PPO-Ir XPS data.

Name	Start BE	Peak BE	End BE	Height CPS	FWHM eV	Area (P) CPS.eV	Area (N) TPP-2M	Atomic %
N1s	408	399.37	394	20297.54	1.42	34617.76	312.72	12.81
Ir4f	70	62.2	58	3858.18	1.51	11797.73	10.4	0.43
O1s	540	534.48	526	10326.78	1.51	29631.38	172.25	7.05
C1s	296	284.56	281	70796.11	1.52	138836.17	1946.52	79.71

Thermogravimetric results showed that the synthesized heterogeneous iridium catalyst was very stable below 300 °C (Figure S2).

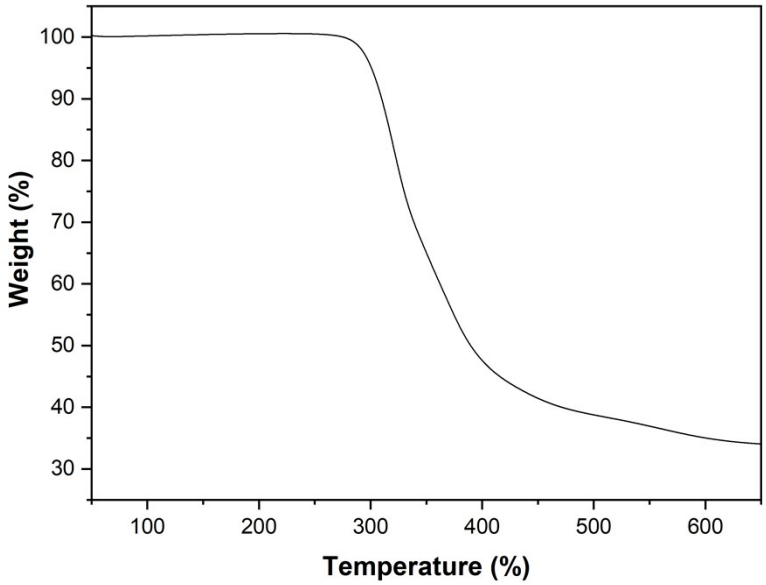
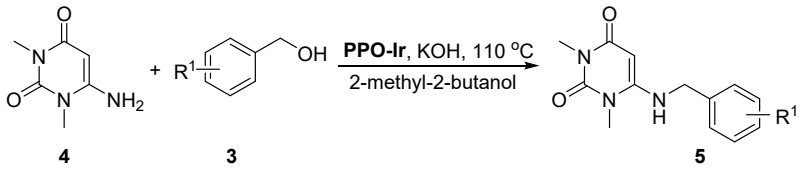


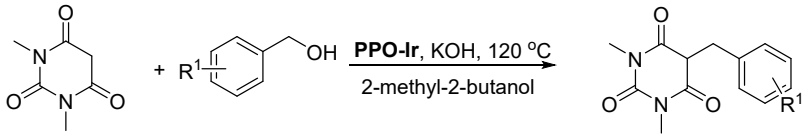
Figure S2. TG pattern of **PPO-Ir**.

4. General procedure for 5



To 25 mL Schlenk tube was added PPO-Ir (10 mg, 4.35% loading, *w/w*), 2-methyl-2-butanol (1.0 mL) and KOH (0.5 equiv.). Then **4** (0.5 mmol), **3** (0.75 mmol) were added and the mixture was stirred at 110 °C for 12 h. After the reaction mixture was cooled to room temperature, the reaction mixture was extracted with ethyl acetate three times. The organic phases were dried over anhydrous $MgSO_4$ and concentrated by removing the solvent under vacuum to give a crude product. The crude product was purified by column chromatography, eluting with petroleum ether/ethyl acetate to afford the desired product **5**.

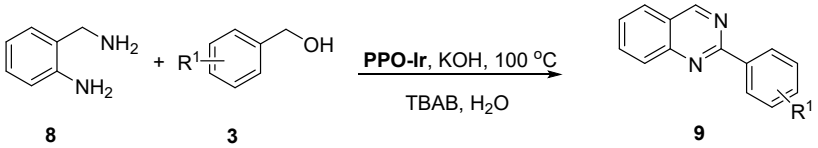
5. General procedure for 7



6 **3** **7**

To 25 mL Schlenk tube was added PPO-Ir (10 mg, 4.35% loading, *w/w*), 2-methyl-2-butanol (1.0 mL) and KOH (0.5 equiv.). Then **6** (0.5 mmol), **3** (0.75 mmol) were added and the mixture was stirred at 120 °C for 12 h. After the reaction mixture was cooled to room temperature, the reaction mixture was extracted with ethyl acetate three times. The organic phases were dried over anhydrous $MgSO_4$ and concentrated by removing the solvent under vacuum to give a crude product. The crude product was purified by column chromatography, eluting with petroleum ether/ethyl acetate to afford the desired product **7**.

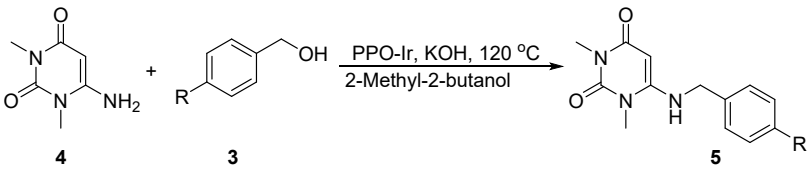
6. General procedure for 9



8 **3** **9**

To 25 mL Schlenk tube was added PPO-Ir (10 mg, 4.35% loading, *w/w*), TBAB (0.1 equiv.), water (1.0 mL) and KOH (0.5 equiv.). Then **8** (0.5 mmol), **3** (0.75 mmol) were added and the mixture was stirred at 100 °C for 16 h. After the reaction mixture was cooled to room temperature, the reaction mixture was extracted with ethyl acetate three times. The organic phases were dried over anhydrous $MgSO_4$ and concentrated by removing the solvent under vacuum to give a crude product. The crude product was purified by column chromatography, eluting with petroleum ether/ethyl acetate to afford the desired product **9**.

7. Hammett plot and mechanism studies

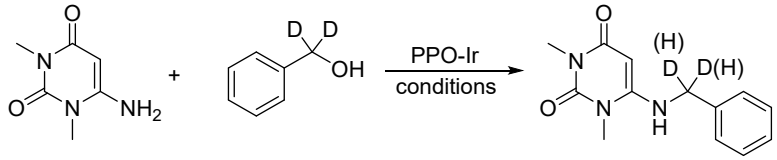


4 **3** **5**

Experimental procedure: To 25 mL reaction tube was added dimethyl-6-aminouracil (0.5 mmol), corresponding benzyl alcohol (0.75 mmol), catalyst **PPO-Ir** (10 mg, 4% loading, w/w), KOH (0.75 equiv.). Then, 2-methyl-2-butanol (1.0 mL) were added and the mixture was stirred at 110 °C for 0.1 h. The solvent was removed under reduced pressure carefully and purification of the crude product by column chromatography on silica-gel (petroleum ether/ethyl acetate = 1:1) afforded the compound **5**. Next, the yield of product **5** was determined by GC.

R	OMe	Me	H	F	CF_3
Yield	28%	20%	18%	12%	8%

Kinetic plot of benzyl alcohol and benzyl alcohol -d_2.



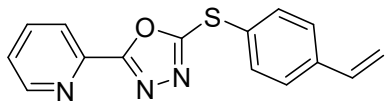
4 **3a-*d*2** **5a-*d*2**

Experimental procedure: To 25 mL reaction tube was added dimethyl-6-aminouracil (0.5 mmol), benzyl alcohol-*d*2 or benzyl alcohol (0.75 mmol), catalyst **1a** (10 mg, 4% loading, w/w), KOH (0. 5 equiv.). Then, 2-methyl-2-butanol (1.1 mL) were added and the mixture was stirred at 110 °C. The yield of **3a**-*d*2 or **3a** was determined by NMR.

Time	0 h	1.5 h	3.0 h	4.5 h	6.0 h	7.5 h
Concentration of **3a** (mol/L)	0.50	0.41	0.33	0.26	0.19	0.15
Concentration of **3a-*d*$_2$** (mol/L)	0.50	0.46	0.42	0.37	0.32	0.28

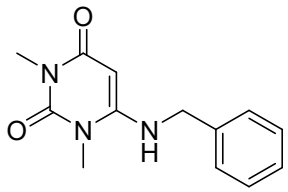
8. Analytical data of the obtained compounds

(1)2-(pyridin-2-yl)-5-((4-vinylphenyl) thio)-1,3,4-oxadiazole (2).



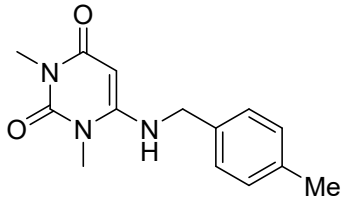
Light yellow solid; Mp. 62-64 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 8.14 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.84 (td, *J* = 7.8, 1.7 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.5 Hz, 3H), 6.69 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.79 (d, *J* = 17.6 Hz, 1H), 5.32 (d, *J* = 10.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.38, 164.70, 150.29, 143.18, 139.31, 137.24, 135.66, 134.07, 127.50, 125.91, 125.40, 123.00, 115.99. HRMS Calculated for $C_{15}H_{12}N_3OS$ $[M+H]^+$ 282.0701, found 282.0700.

(2)6-(benzylamino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5a)[2].



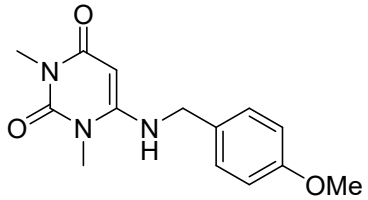
White solid; Mp. 149-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.24 (m, 5H), 5.61 (s, 1H), 4.79 (s, 1H), 4.22 (d, *J* = 5.2 Hz, 2H), 3.40 (s, 3H), 3.25 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.12, 153.06, 151.86, 136.11, 129.00, 128.14, 127.40, 76.11, 47.19, 28.85, 27.78.

(3)1,3-dimethyl-6-((4-methylbenzyl) amino) pyrimidine-2,4(1H,3H)-dione (5b)[2].



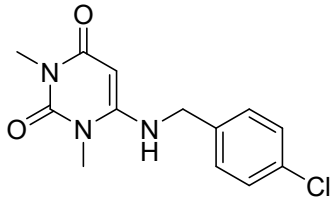
White solid; Mp. 136-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (s, 4H), 5.36 (s, 1H), 4.83 (s, 1H), 4.18 (d, *J* = 5.0 Hz, 2H), 3.40 (s, 3H), 3.26 (s, 3H), 2.33 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.11, 152.92, 151.88, 138.09, 132.95, 129.69, 127.56, 76.10, 47.06, 28.78, 27.80, 21.12.

(4)6-((4-methoxybenzyl) amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5c)[2].



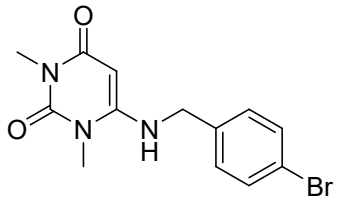
Light red solid; Mp. 176-177 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.16 (m, 2H), 6.96 – 6.81 (m, 2H), 5.20 (t, *J* = 5.0 Hz, 1H), 4.85 (s, 1H), 4.16 (d, *J* = 4.9 Hz, 2H), 3.79 (s, 3H), 3.40 (s, 3H), 3.27 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.08, 159.54, 152.85, 151.88, 129.02, 127.92, 114.39, 76.08, 55.35, 46.83, 28.77, 27.79.

(5)6-((4-chlorobenzyl) amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5d)[2].



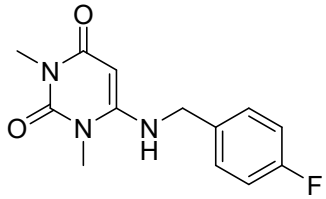
White solid; Mp. 201-202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 5.92 (s, 1H), 4.68 (s, 1H), 4.19 (d, *J* = 5.3 Hz, 2H), 3.43 (s, 3H), 3.24 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.15, 153.21, 151.75, 134.75, 133.80, 129.06, 128.60, 75.92, 46.35, 29.05, 27.80.

(6)6-((4-bromobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5e).



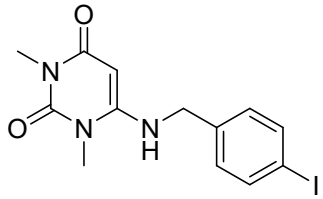
Light yellow solid; Mp. 209-210 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.3 Hz, 2H), 5.37 (s, 1H), 4.77 (s, 1H), 4.20 (d, *J* = 5.2 Hz, 2H), 3.42 (s, 3H), 3.27 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.03, 152.83, 151.78, 134.99, 132.18, 129.14, 122.17, 76.39, 46.66, 28.83, 27.86. HRMS Calculated for $C_{13}H_{15}N_3O_2Br$ $[M+H]^+$ 324.0348, found 324.0346.

(7)6-((4-fluorobenzyl) amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5f).



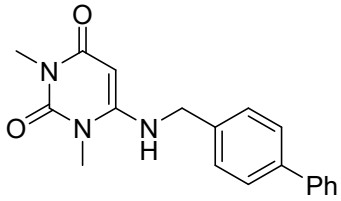
White solid; Mp. 167-168 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.51 (s, 1H), 7.40 (dd, *J* = 8.2, 5.7 Hz, 2H), 7.17 (t, *J* = 8.8 Hz, 2H), 4.53 (s, 1H), 4.32 (d, *J* = 5.6 Hz, 2H), 3.37 (s, 3H), 3.07 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.92, 161.75 (d, *J* = 242.6 Hz), 153.56, 151.91, 134.51 (d, *J* = 2.9 Hz), 129.27 (d, *J* = 8.1 Hz), 115.61 (d, *J* = 21.3 Hz), 74.88, 45.08, 29.79, 27.52. HRMS Calculated for $C_{13}H_{15}N_3O_2F$ $[M+H]^+$ 264.1148, found 264.1149.

(8) 6-((4-iodobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5g).



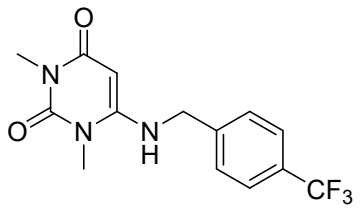
Light yellow solid; Mp. 181-183 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.50 (s, 1H), 7.17 (d, *J* = 8.2 Hz, 2H), 4.49 (s, 1H), 4.29 (d, *J* = 5.7 Hz, 2H), 3.36 (s, 3H), 3.06 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.89, 153.52, 151.90, 138.31, 137.60, 129.69, 93.26, 74.95, 45.29, 29.81, 27.55. HRMS Calculated for $C_{13}H_{15}N_3O_2I$ $[M+H]^+$ 372.0209, found 372.0207.

(9) 6-(([1,1'-biphenyl]-4-ylmethyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5h).



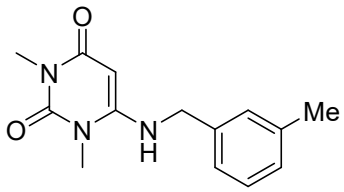
White solid; Mp. 199-200 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.53 (m, 4H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.35 (dd, *J* = 15.7, 7.7 Hz, 3H), 5.29 (s, 1H), 4.86 (s, 1H), 4.25 (d, *J* = 4.9 Hz, 2H), 3.42 (s, 3H), 3.28 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.11, 152.96, 151.87, 141.20, 140.28, 134.96, 128.90, 127.99, 127.70, 127.63, 127.04, 76.25, 46.98, 28.85, 27.83. HRMS Calculated for $C_{19}H_{20}N_3O_2$ $[M+H]^+$ 322.1556, found 322.1554.

(10) 1,3-dimethyl-6-((4-(trifluoromethyl) benzyl) amino) pyrimidine-2,4(1H,3H)-dione (5i)[2].



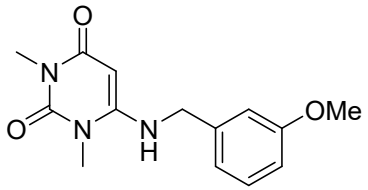
White liquid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (d, J = 8.1 Hz, 2H), 7.58 (d, J = 8.1 Hz, 3H), 4.51 (s, 1H), 4.44 (d, J = 5.6 Hz, 2H), 3.39 (s, 3H), 3.07 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.91, 153.58, 151.91, 143.42, 128.37, 128.03, 125.73 (q, J = 3.7 Hz), 124.76 (d, J = 271.9 Hz), 74.97, 45.37, 29.82, 27.52.

(11) 1,3-dimethyl-6-((3-methylbenzyl) amino) pyrimidine-2,4(1H,3H)-dione (5j)[2].



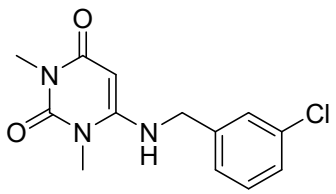
White solid; Mp. 176-177 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (t, J = 7.5 Hz, 1H), 7.12 – 7.02 (m, 3H), 5.78 (s, 1H), 4.77 (s, 1H), 4.17 (d, J = 5.2 Hz, 2H), 3.41 (s, 3H), 3.24 (s, 3H), 2.32 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.19, 153.22, 151.87, 138.71, 136.14, 128.82, 128.79, 128.03, 124.36, 75.86, 47.07, 28.95, 27.76, 21.41.

(12) 6-((3-methoxybenzyl) amino) -1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5k).



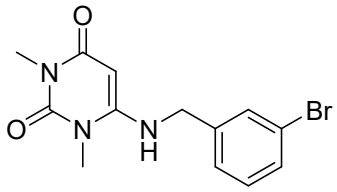
Light yellow solid; Mp. 164-165 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, J = 14.1 Hz, 1H), 6.90 – 6.79 (m, 3H), 5.50 (s, 1H), 4.80 (s, 1H), 4.20 (d, J = 4.9 Hz, 2H), 3.78 (s, 3H), 3.41 (s, 3H), 3.26 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.16, 160.08, 153.08, 151.84, 137.71, 130.09, 119.55, 113.49, 112.92, 76.08, 55.28, 47.08, 28.86, 27.78. HRMS Calculated for $C_{14}H_{18}N_3O_3$ $[M+H]^+$ 276.1348, found 276.1349.

(13) 6-((3-chlorobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5l).



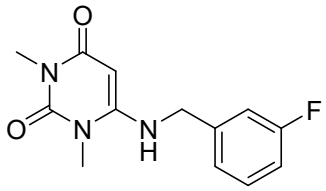
Light red solid; Mp. 176-177 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 3H), 7.20 – 7.13 (m, 1H), 5.36 (s, 1H), 4.79 (s, 1H), 4.24 (d, *J* = 5.3 Hz, 2H), 3.44 (s, 3H), 3.27 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.05, 152.84, 151.78, 138.07, 134.99, 130.36, 128.43, 127.42, 125.55, 76.45, 46.67, 28.84, 27.86. HRMS Calculated for $C_{13}H_{15}N_3O_2Cl$ $[M+H]^+$ 280.0853, found 280.0852.

(14) 6-((3-bromobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5m).



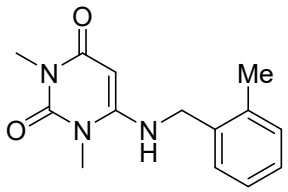
White solid; Mp. 184-185 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 9.0 Hz, 2H), 7.24 (d, *J* = 6.8 Hz, 2H), 5.10 (s, 1H), 4.81 (s, 1H), 4.25 (d, *J* = 5.2 Hz, 2H), 3.44 (s, 3H), 3.29 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 162.94, 152.72, 151.80, 138.28, 131.42, 130.65, 130.39, 126.06, 123.17, 76.59, 46.68, 28.80, 27.86. HRMS Calculated for $C_{13}H_{15}N_3O_2Br$ $[M+H]^+$ 324.0348, found 324.0350.

(15) 6-((3-fluorobenzyl) amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5n).



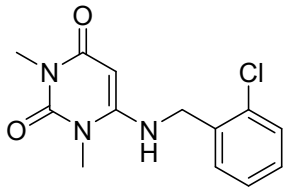
White solid; Mp. 158-160 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.53 (s, 1H), 7.39 (q, *J* = 7.4 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.09 (t, *J* = 8.2 Hz, 1H), 4.52 (s, 1H), 4.36 (d, *J* = 5.7 Hz, 2H), 3.38 (s, 3H), 3.07 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 162.86 (d, *J* = 243.5 Hz), 161.94, 153.60, 151.91, 141.58 (d, *J* = 7.1 Hz), 130.83 (d, *J* = 8.3 Hz), 123.29 (d, *J* = 2.6 Hz), 114.27 (d, *J* = 21.1 Hz), 114.03 (d, *J* = 21.8 Hz), 74.90, 45.29, 29.80, 27.53. HRMS Calculated for $C_{13}H_{15}N_3O_2F$ $[M+H]^+$ 264.1148, found 264.1146.

(16) 1,3-dimethyl-6-((2-methylbenzyl)amino)pyrimidine-2,4(1H,3H)-dione (5o)[2].



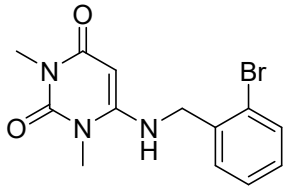
Light red solid; Mp. 188-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.17 (m, *J* = 4.1 Hz, 4H), 4.88 (s, 1H), 4.86 (s, 1H), 4.19 (d, *J* = 4.7 Hz, 2H), 3.39 (s, 3H), 3.28 (s, 3H), 2.33 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.04, 152.82, 151.86, 136.40, 133.60, 130.91, 128.51, 128.32, 126.51, 76.11, 45.55, 28.77, 27.81, 18.95.

(17) 6-((2-chlorobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5p).



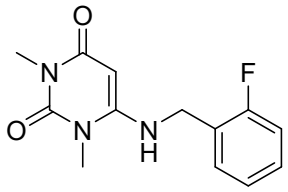
Light red solid; Mp. 209-210 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 1H), 7.35 – 7.28 (m, 3H), 4.98 (s, 1H), 4.89 (s, 1H), 4.38 (s, 2H), 3.44 (s, 3H), 3.29 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 162.94, 152.58, 151.84, 133.64, 133.24, 130.12, 129.79, 129.74, 127.36, 76.44, 45.35, 28.63, 27.85. HRMS Calculated for $C_{13}H_{15}N_3O_2Cl$ $[M+H]^+$ 280.0853, found 280.0855.

(18) 6-((2-bromobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5q).



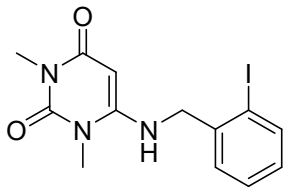
White solid; Mp. 210-211 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.9 Hz, 1H), 7.32 (d, J = 4.3 Hz, 2H), 7.22 (dt, J = 8.9, 4.5 Hz, 1H), 5.04 (s, 1H), 4.88 (s, 1H), 4.35 (d, J = 5.5 Hz, 2H), 3.44 (s, 3H), 3.29 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 162.99, 152.57, 151.84, 134.83, 133.39, 130.03, 129.92, 127.97, 123.62, 76.45, 47.62, 28.67, 27.86. HRMS Calculated for $C_{13}H_{15}N_3O_2Br$ $[M+H]^+$ 324.0348, found 324.0347.

(19) 6-((2-fluorobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5r).



White Liquid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.46 (s, 1H), 7.43 – 7.30 (m, 2H), 7.26 – 7.16 (m, 2H), 4.54 (s, 1H), 4.37 (d, J = 5.7 Hz, 2H), 3.37 (s, 3H), 3.07 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 161.94, 160.51 (d, J = 244.3 Hz), 153.57, 151.89, 129.63 (d, J = 8.2 Hz), 129.49 (d, J = 4.1 Hz), 124.95 (d, J = 3.4 Hz), 124.90, 124.76, 115.68 (d, J = 21.1 Hz), 74.48, 29.83, 27.54. HRMS Calculated for $C_{13}H_{15}N_3O_2F$ $[M+H]^+$ 264.1148, found 264.1147.

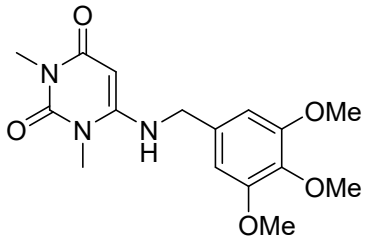
(20) 6-((2-iodobenzyl)amino)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (5s).



Light yellow solid; Mp. 184-185 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.92 – 7.87 (m, 1H), 7.53 (s, 1H), 7.42 – 7.37 (m, 1H), 7.35 – 7.28 (m, 1H), 7.11 – 7.00 (m, 1H), 4.32 (s, 1H), 4.24 (d, J = 5.5 Hz, 2H), 3.40 (s, 3H), 3.08 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.92, 153.57, 151.89, 139.61,

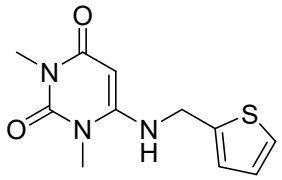
139.09, 129.80, 128.95, 128.36, 98.85, 74.96, 51.36, 29.92, 27.59. HRMS Calculated for $C_{13}H_{15}N_3O_2I$ $[M+H]^+$ 372.0209, found 372.0208.

(21) 1,3-dimethyl-6-((3,4,5-trimethoxybenzyl)amino)pyrimidine-2,4(1H,3H)-dione (5t).



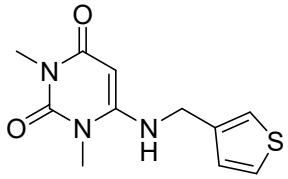
Light yellow solid; Mp. 185-186 °C;^{1}H NMR (400 MHz, DMSO-d_6) δ 7.44 (s, 1H), 6.70 (s, 2H), 4.60 (s, 1H), 4.24 (d, J = 5.7 Hz, 2H), 3.77 (s, 6H), 3.64 (s, 3H), 3.38 (s, 3H), 3.07 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.99, 153.72, 153.44, 151.95, 136.95, 134.14, 104.75, 74.88, 60.41, 56.36, 46.13, 29.83, 27.53. HRMS Calculated for $C_{16}H_{22}N_3O_5$ $[M+H]^+$ 336.1559, found 336.1558.

(22) 1,3-dimethyl-6-((thiophen-2-ylmethyl)amino)pyrimidine-2,4(1H,3H)-dione (5u).



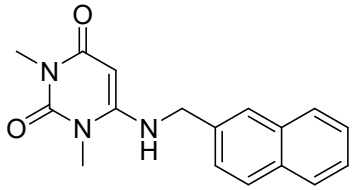
Light red solid; Mp. 181-182 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.54 (t, J = 5.7 Hz, 1H), 7.46 – 7.39 (m, 1H), 7.10 (d, J = 2.9 Hz, 1H), 6.98 (dd, J = 5.0, 3.5 Hz, 1H), 4.73 (s, 1H), 4.51 (d, J = 5.7 Hz, 2H), 3.31 (s, 3H), 3.07 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.96, 153.42, 151.91, 141.84, 127.26, 126.19, 125.60, 75.01, 41.45, 29.83, 27.56. HRMS Calculated for $C_{11}H_{14}N_3O_2S$ $[M+H]^+$ 252.0807, found 252.0808.

(23) 1,3-dimethyl-6-((thiophen-3-ylmethyl)amino)pyrimidine-2,4(1H,3H)-dione (5v).



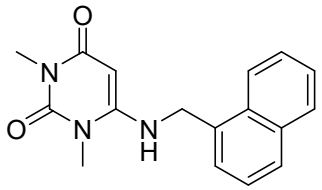
Red oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (dd, J = 4.9, 3.0 Hz, 1H), 7.23 – 7.17 (m, 1H), 7.08 – 7.00 (m, 1H), 5.33 (s, 1H), 4.89 (s, 1H), 4.27 (d, J = 5.1 Hz, 2H), 3.41 (s, 3H), 3.28 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.24, 152.96, 151.84, 136.83, 127.14, 126.79, 123.11, 75.98, 42.57, 28.84, 27.85. HRMS Calculated for $C_{11}H_{14}N_3O_2S$ $[M+H]^+$ 252.0807, found 252.0809.

(24) 1,3-dimethyl-6-((naphthalen-2-ylmethyl)amino)pyrimidine-2,4(1H,3H)-dione (5w)[2].



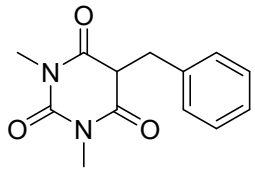
White solid; Mp. 201-202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 14.0, 8.7 Hz, 3H), 7.68 (s, 1H), 7.53 – 7.46 (m, 2H), 7.38 – 7.31 (m, 1H), 5.20 (s, 1H), 4.86 (s, 1H), 4.32 (d, *J* = 5.0 Hz, 2H), 3.39 (s, 3H), 3.27 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.03, 152.86, 151.83, 133.28, 133.01, 129.01, 127.79, 127.74, 126.69, 126.60, 126.45, 125.18, 76.30, 47.49, 28.78, 27.82.

(25) 1,3-dimethyl-6-((naphthalen-1-ylmethyl)amino)pyrimidine-2,4(1H,3H)-dione (5x)[2].



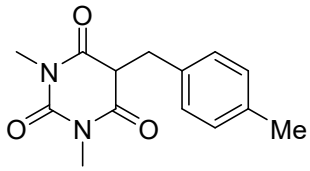
White solid; Mp. 209-210 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.17 (d, *J* = 8.0 Hz, 1H), 8.04 – 7.94 (m, 1H), 7.91 – 7.82 (m, 1H), 7.64 – 7.51 (m, 3H), 7.52 – 7.46 (m, 2H), 4.80 (d, *J* = 5.5 Hz, 2H), 4.54 (s, 1H), 3.40 (s, 3H), 3.07 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 161.96, 153.82, 151.97, 133.83, 132.91, 131.11, 129.10, 128.10, 126.77, 126.35, 125.89, 124.83, 123.68, 74.92, 44.16, 29.94, 27.55.

(26) 5-benzyl-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7a)[3].



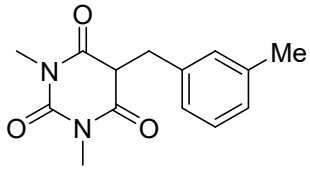
Light yellow solid; Mp. 93-94 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.21 (m, 3H), 7.06 – 7.00 (m, 2H), 3.78 (t, *J* = 4.7 Hz, 1H), 3.47 (d, *J* = 4.8 Hz, 2H), 3.13 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.32, 151.01, 135.12, 128.87, 128.64, 127.87, 50.72, 37.93, 28.21.

(27) 1,3-dimethyl-5-(4-methylbenzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7b)[3].



White Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (d, *J* = 7.9 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 2H), 3.75 (t, *J* = 4.8 Hz, 1H), 3.42 (d, *J* = 4.8 Hz, 2H), 3.12 (s, 6H), 2.28 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.42, 151.08, 137.50, 131.93, 129.30, 128.74, 50.79, 37.63, 28.20, 21.10.

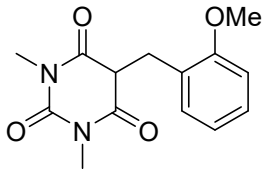
(28) 1,3-dimethyl-5-(3-methylbenzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7c)[3].



White solid; Mp. 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (t, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.86 – 6.78 (m, 2H), 3.75 (t, *J* = 4.8 Hz, 1H), 3.41 (d, *J* = 4.8 Hz, 2H), 3.11 (s, 6H), 2.27 (s, 3H).

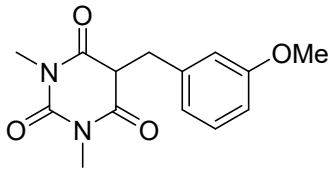
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.43, 151.04, 138.33, 134.97, 129.52, 128.55, 128.45, 125.81, 50.77, 38.10, 28.11, 21.24.

(29) 5-(2-methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7d).



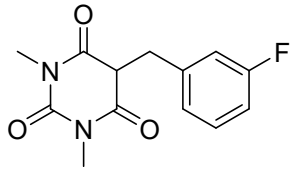
White solid; Mp.126-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (td, *J* = 7.8, 1.8 Hz, 1H), 6.99 (dd, *J* = 7.5, 1.8 Hz, 1H), 6.86 – 6.74 (m, 2H), 3.74 (d, *J* = 5.6 Hz, 1H), 3.72 (s, 3H), 3.37 (d, *J* = 5.7 Hz, 2H), 3.07 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.51, 157.27, 151.55, 131.12, 129.03, 123.50, 120.36, 110.10, 55.14, 50.10, 33.31, 28.06. HRMS Calculated for $C_{14}H_{17}N_2O_4$ $[M+H]^+$ 277.1188, found 277.1186.

(30) 5-(3-methoxybenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7e)[4].



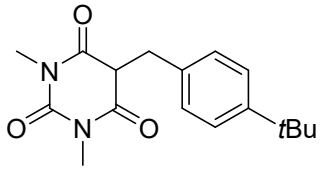
Yellow Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (dd, *J* = 8.3, 7.5 Hz, 1H), 6.77 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 1H), 6.63 – 6.56 (m, 2H), 3.76 (t, *J* = 4.7 Hz, 1H), 3.74 (s, 3H), 3.43 (d, *J* = 4.8 Hz, 2H), 3.14 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.28, 159.73, 151.04, 136.66, 129.61, 121.12, 114.39, 113.30, 55.17, 50.60, 37.75, 28.22.

(31) 5-(3-fluorobenzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7f)[4].



Yellow Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.15 (m, 2H), 7.09 (t, *J* = 1.8 Hz, 1H), 6.96 (dt, *J* = 7.3, 1.5 Hz, 1H), 3.78 (t, *J* = 4.8 Hz, 1H), 3.45 (d, *J* = 4.8 Hz, 2H), 3.18 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.90, 162.72 (d, *J* = 247.0 Hz), 150.96, 137.92 (d, *J* = 7.3 Hz), 130.17 (d, *J* = 8.3 Hz), 124.71 (d, *J* = 2.9 Hz), 116.02 (d, *J* = 21.5 Hz), 114.74 (d, *J* = 21.1 Hz), 50.37, 36.57 (d, *J* = 1.9 Hz), 28.35.

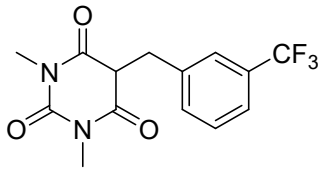
(32) 5-(4-(tert-butyl)benzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7g).



White Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.3 Hz, 2H), 6.90 (d, *J* = 8.3 Hz, 2H), 4.03 (s, 1H), 3.25 (s, 2H), 3.11 (s, 6H), 1.28 (s, 9H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.98, 151.66, 149.78,

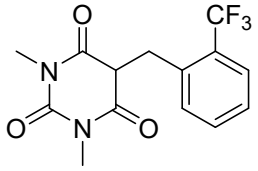
128.92, 128.79, 125.41, 49.36, 34.55, 31.22, 28.53. HRMS Calculated for $C_{17}H_{23}N_2O_3$ $[M+H]^+$ 303.1709, found 303.1707.

(33) 1,3-dimethyl-5-(3-(trifluoromethyl)benzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7h).



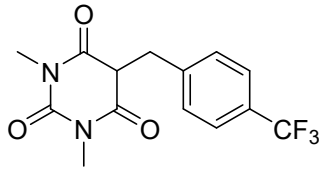
White solid; Mp.115-116 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.49 (m, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 1.9 Hz, 1H), 7.28 (dd, *J* = 7.0, 2.1 Hz, 1H), 3.82 (t, *J* = 4.7 Hz, 1H), 3.54 (d, *J* = 4.8 Hz, 2H), 3.15 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.82, 150.80, 136.56, 132.51, 131.06 (q, *J* = 32.5 Hz), 129.11, 127.87 (q, *J* = 271.0 Hz), 125.82 (q, *J* = 3.7 Hz), 124.56 (q, *J* = 3.9 Hz), 50.37, 36.63, 28.28. HRMS Calculated for $C_{14}H_{14}F_3N_2O_3$ $[M+H]^+$ 315.0907, found 315.0906.

(34) 1,3-dimethyl-5-(2-(trifluoromethyl)benzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7i).



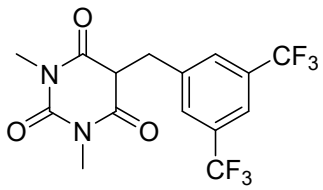
Yellow Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.62 (m, 1H), 7.55 – 7.48 (m, 1H), 7.41 – 7.34 (m, 2H), 3.80 (t, *J* = 7.0 Hz, 1H), 3.53 (dd, *J* = 7.1, 1.4 Hz, 2H), 3.27 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.55, 151.52, 135.14, 131.88, 131.15, 128.89 (q, *J* = 29.9 Hz), 128.40 (q, *J* = 272.0 Hz), 127.42, 126.36 (q, *J* = 5.9 Hz), 50.73, 33.01 (q, *J* = 2.0 Hz), 28.66. HRMS Calculated for $C_{14}H_{14}F_3N_2O_3$ [M+H]+ 315.0907, found 315.0908.

(35) 1,3-dimethyl-5-(4-(trifluoromethyl)benzyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7j)[3].



Yellow Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.6 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 3.82 (t, *J* = 4.9 Hz, 1H), 3.55 (d, *J* = 4.9 Hz, 2H), 3.19 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.58, 150.87, 140.03, 130.38(q, *J* = 32.0 Hz), 129.64, 128.01 (q, *J* = 270.8 Hz), 125.54 (q, *J* = 3.7 Hz), 50.22, 35.58, 28.47.

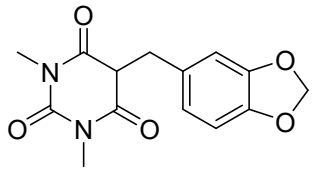
(36) 5-(3,5-bis(trifluoromethyl)benzyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7k).



White solid; Mp.137-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.64 – 7.61 (m, 2H), 3.85 (t, *J* = 4.8 Hz, 1H), 3.62 (d, *J* = 4.8 Hz, 2H), 3.20 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.23, 150.67,

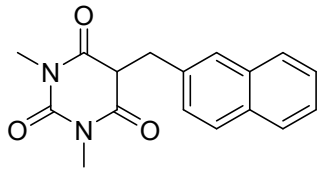
138.67, 131.95 (q, *J* = 33.4 Hz), 129.68, 127.11 (q, *J* = 271.0 Hz), 121.59 (q, *J* =4.0 Hz), 50.16, 35.07, 28.47. HRMS Calculated for $C_{15}H_{13}F_6N_2O_3$ $[M+H]^+$ 383.0830, found 383.0827.

(37) 5-(benzo[d][1,3]dioxol-5-ylmethyl)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7l)[3].



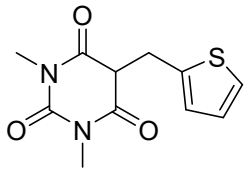
Yellow Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.66 (d, *J* = 7.8 Hz, 1H), 6.55 – 6.48 (m, 2H), 5.92 (s, 2H), 3.73 (t, *J* = 4.7 Hz, 1H), 3.39 (d, *J* = 4.7 Hz, 2H), 3.17 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.26, 151.12, 147.80, 147.09, 128.76, 122.24, 109.15, 108.33, 101.10, 50.79, 37.33, 28.28.

(38) 1,3-dimethyl-5-(naphthalen-2-ylmethyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7m)[3].



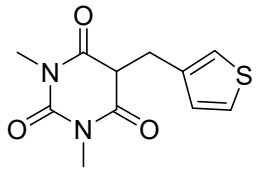
Green Oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.77 (m, 1H), 7.73 (dd, *J* = 9.0, 5.9 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.48 – 7.43 (m, 2H), 7.15 (dd, *J* = 8.4, 1.9 Hz, 1H), 3.86 (t, *J* = 4.8 Hz, 1H), 3.64 (d, *J* = 4.8 Hz, 2H), 3.10 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.29, 150.90, 133.32, 132.74, 132.64, 128.34, 127.99, 127.72, 127.60, 126.75, 126.42, 126.12, 50.74, 37.65, 28.28.

(39) 1,3-dimethyl-5-(thiophen-2-ylmethyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7n)[5].



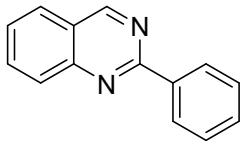
Orange solid; Mp.100-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.88 (dd, *J* = 5.2, 3.4 Hz, 1H), 6.78 (dd, *J* = 3.6, 1.2 Hz, 1H), 3.73 (q, *J* = 3.2 Hz, 3H), 3.21 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.82, 151.12, 136.57, 127.34, 127.07, 125.33, 50.52, 30.88, 28.48.

(40) 1,3-dimethyl-5-(thiophen-3-ylmethyl)pyrimidine-2,4,6(1H,3H,5H)-trione (7o)[5].



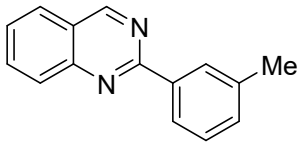
Yellow solid; Mp.128-129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 4.9, 3.0 Hz, 1H), 6.97 (dd, *J* = 3.1, 1.3 Hz, 1H), 6.77 (dd, *J* = 4.9, 1.3 Hz, 1H), 3.72 (t, *J* = 4.6 Hz, 1H), 3.52 (d, *J* = 4.6 Hz, 2H), 3.17 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.26, 151.07, 135.34, 127.93, 126.30, 123.37, 50.27, 31.65, 28.34.

(41) 2-phenylquinazoline (9a)[6].



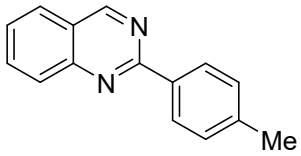
White solid; Mp.237-238 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 8.54 (dd, *J* = 8.0, 1.8 Hz, 2H), 8.02 (d, *J* = 9.4 Hz, 1H), 7.87 – 7.80 (m, 2H), 7.56 – 7.51 (m, 1H), 7.49 – 7.39 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 161.08, 160.55, 150.78, 138.03, 134.19, 130.66, 128.69, 128.66, 128.60, 127.33, 127.17, 123.62.

(42) 2-(m-tolyl)quinazoline (9b)[6].



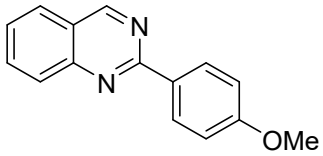
Yellow solid; Mp.99-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.42 (d, *J* = 11.4 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.89 (t, *J* = 8.0 Hz, 2H), 7.63 – 7.56 (m, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.5 Hz, 1H), 2.49 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 161.21, 160.50, 150.77, 138.33, 137.93, 134.17, 131.50, 129.15, 128.63, 128.61, 127.26, 127.17, 125.83, 123.59, 21.58.

(43) 2-(m-tolyl)quinazoline (9c)[6].



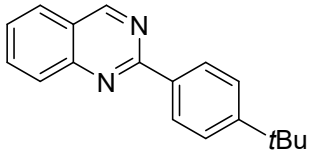
White solid; Mp.98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.44 (d, *J* = 8.2 Hz, 2H), 8.00 (s, 1H), 7.86 – 7.79 (m, 2H), 7.52 (t, *J* = 7.0 Hz, 1H), 7.27 (d, *J* = 7.9 Hz, 2H), 2.37 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 161.13, 160.50, 150.78, 140.95, 135.26, 134.14, 129.46, 128.55, 128.54, 127.17, 127.10, 123.52, 21.56.

(44) 2-(4-methoxyphenyl)quinazoline (9d)[6].



White solid; Mp.87-88 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 8.60 – 8.54 (m, 2H), 8.02 (d, *J* = 8.9 Hz, 1H), 7.87 – 7.82 (m, 2H), 7.53 (t, *J* = 8.1 Hz, 1H), 7.06 – 7.01 (m, 2H), 3.88 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 161.85, 160.85, 160.41, 150.83, 134.03, 130.73, 130.24, 128.40, 127.14, 126.79, 123.32, 113.99, 55.40.

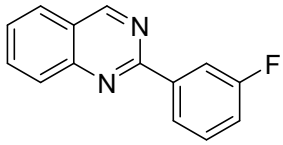
(45) 2-(4-(tert-butyl)phenyl)quinazoline (9e)[6].



White solid; Mp.82-84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.57 – 8.51 (m, 2H), 8.07 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.90 – 7.84 (m, 2H), 7.59 – 7.54 (m, 3H), 1.38 (s, 9H).^{13}C NMR (101 MHz, $CDCl_3$)

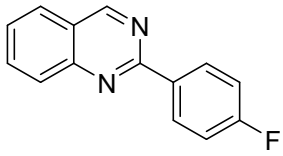
δ 161.15, 160.04, 153.97, 150.84, 135.33, 134.03, 128.62, 128.39, 127.13, 127.05, 125.65, 123.53, 34.91, 31.31.

(46) 2-(3-fluorophenyl)quinazoline (9f)[7].



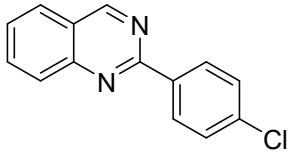
Yellow solid; Mp.95-97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.41 (d, *J* = 7.8 Hz, 1H), 8.32 (d, *J* = 10.4 Hz, 1H), 8.07 (d, *J* = 8.1 Hz, 1H), 7.90 (t, *J* = 7.3 Hz, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.18 (dd, *J* = 8.3, 2.7 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 163.29 (d, *J* = 244.8 Hz), 160.56, 159.82 (d, *J* = 3.0 Hz), 150.64, 140.45 (d, *J* = 7.9 Hz), 134.30, 130.09 (d, *J* = 7.9 Hz), 128.68, 127.63, 127.16, 124.19 (d, *J* = 2.9 Hz), 123.75, 117.48 (d, *J* = 21.4 Hz), 115.41 (d, *J* = 23.4 Hz).

(47) 2-(4-fluorophenyl)quinazoline (9g)[6].



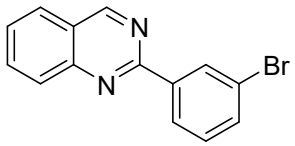
Yellow solid; Mp.69-70 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.57 – 8.48 (m, 2H), 7.95 (d, *J* = 8.8 Hz, 1H), 7.85 – 7.74 (m, 2H), 7.49 (t, *J* = 7.0 Hz, 1H), 7.10 (t, *J* = 8.7 Hz, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 164.69 (d, *J* = 250.4 Hz), 160.52, 160.10, 150.71, 134.21, 130.73, 130.65, 128.55, 127.29, 127.15, 123.49, 115.57 (d, *J* = 21.6 Hz).

(48) 2-(4-chlorophenyl)quinazoline (9h)[6].



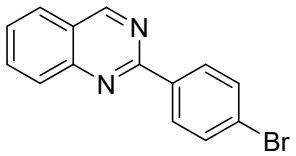
White solid; Mp.133-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 – 9.31 (m, 1H), 8.52 – 8.44 (m, 2H), 7.98 (dt, *J* = 9.1, 1.0 Hz, 1H), 7.86 – 7.79 (m, 2H), 7.53 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.45 – 7.38 (m, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.56, 160.01, 150.67, 136.86, 136.49, 134.32, 129.92, 128.85, 128.59, 127.51, 127.19, 123.62.

(49) 2-(3-bromophenyl)quinazoline (9i)[6].



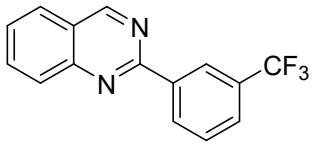
White solid; Mp.153-154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.77 (t, *J* = 1.8 Hz, 1H), 8.54 (dt, *J* = 7.8, 1.3 Hz, 1H), 8.06 (d, *J* = 8.9 Hz, 1H), 7.95 – 7.85 (m, 2H), 7.61 (td, *J* = 7.1, 1.1 Hz, 2H), 7.38 (t, *J* = 7.9 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.57, 159.52, 150.62, 140.07, 134.35, 133.48, 131.58, 130.16, 128.67, 127.68, 127.17, 127.11, 123.74, 122.96.

(50) 2-(4-bromophenyl)quinazoline (9j)[6].



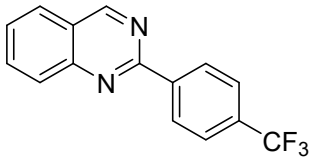
White solid; Mp.120-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.39 (d, *J* = 8.6 Hz, 2H), 7.96 (d, *J* = 8.8 Hz, 1H), 7.81 (ddd, *J* = 7.3, 4.0, 2.3 Hz, 2H), 7.58 – 7.48 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.55, 160.06, 150.65, 136.94, 134.31, 131.80, 130.16, 128.60, 127.52, 127.18, 125.44, 123.63.

(51) 2-(3-(trifluoromethyl)phenyl)quinazoline (9k)[7].



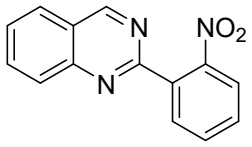
Yellow solid; Mp.126-128 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.80 (s, 1H), 8.68 (d, *J* = 7.9 Hz, 1H), 7.95 (d, *J* = 9.1 Hz, 1H), 7.78 (ddd, *J* = 8.4, 6.2, 1.6 Hz, 2H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.50 (q, *J* = 7.6 Hz, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.58, 159.44, 150.59, 138.80, 134.34, 131.68, 131.05 (q, *J* = 32.4 Hz), 129.06, 128.68, 128.36 (q, *J* = 271.0 Hz), 127.74, 127.14, 127.01 (q, *J* = 3.7 Hz), 125.47 (q, *J* = 3.9 Hz), 123.77.

(52) 2-(3-(trifluoromethyl)phenyl)quinazoline (9l)[6].



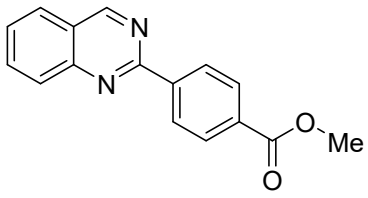
White solid; Mp.146-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.50 (s, 1H), 8.98 – 8.78 (m, 2H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.00 – 7.93 (m, 2H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.69 – 7.64 (m, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.64, 159.61, 150.66, 141.31, 134.41, 132.12 (q, *J* = 32.3 Hz), 129.09 128.84, 128.78, 127.89, 127.19, 125.53 (q, *J* = 3.9 Hz), 123.85.

(53) 2-(2-nitrophenyl)quinazoline (9m)[8].



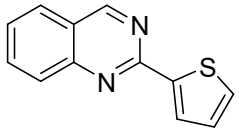
Yellow solid; Mp.91-92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.13 (dd, *J* = 7.7, 1.5 Hz, 1H), 8.08 (d, *J* = 7.4 Hz, 1H), 8.00 – 7.93 (m, 2H), 7.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.61 (td, *J* = 7.8, 1.5 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.55, 159.70, 150.43, 150.01, 134.61, 133.68, 132.31, 131.85, 130.18, 128.64, 128.34, 127.27, 124.17, 123.49.

(54) methyl 4-(quinazolin-2-yl)benzoate (9n)[8].



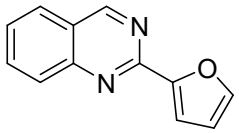
Pale brown solid; Mp.120-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.62 – 8.57 (m, 2H), 8.14 – 8.08 (m, 2H), 8.01 (d, *J* = 9.3 Hz, 1H), 7.87 – 7.79 (m, 2H), 7.55 (td, *J* = 7.4, 1.1 Hz, 1H), 3.87 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 166.96, 160.57, 159.98, 150.66, 142.12, 134.35, 132.25, 129.86, 128.77, 128.49, 127.82, 127.17, 123.75, 52.25.

(55) 2-(thiophen-2-yl)quinazoline (9o)[6].



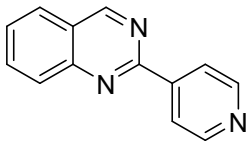
White solid; Mp.137-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.15 (dd, *J* = 3.7, 1.2 Hz, 1H), 8.00 (d, *J* = 8.6 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.58 – 7.53 (m, 1H), 7.52 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.19 (dd, *J* = 5.0, 3.7 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.56, 157.88, 150.64, 143.86, 134.39, 129.98, 129.26, 128.42, 128.21, 127.30, 127.03, 123.39.

(56) 2-(furan-2-yl)quinazoline (9p)[8].



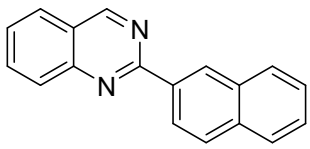
Yellow solid; Mp.127-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.37 (d, *J* = 0.9 Hz, 1H), 8.13 – 8.07 (m, 1H), 7.91 – 7.85 (m, 2H), 7.69 (dd, *J* = 1.7, 0.9 Hz, 1H), 7.58 (td, *J* = 7.4, 1.1 Hz, 1H), 7.46 (dd, *J* = 3.4, 0.9 Hz, 1H), 6.62 (dd, *J* = 3.4, 1.7 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.74, 154.08, 152.50, 150.41, 145.36, 134.53, 128.36, 127.28, 123.36, 114.12, 112.35.

(57) 2-(pyridin-4-yl)quinazoline (9q)[6].



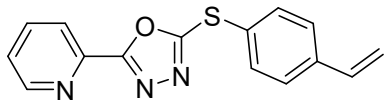
Gray solid; Mp.134-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.35 (s, 1H), 8.69 (d, *J* = 6.1 Hz, 2H), 8.32 (d, *J* = 6.1 Hz, 2H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.82 (ddd, *J* = 7.3, 4.0, 2.3 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.68, 158.82, 150.48, 150.45, 145.23, 134.48, 128.82, 128.27, 127.15, 124.10, 122.30.

(58) 2-(naphthalen-2-yl)quinazoline (9r)[8].



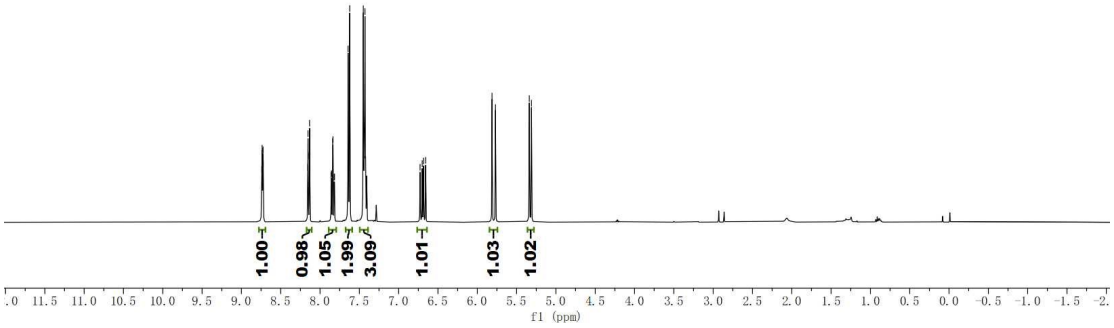
Yellow solid; Mp.133-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.35 (s, 1H), 9.04 (s, 1H), 8.62 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.87 (d, *J* = 8.7 Hz, 1H), 7.81 – 7.74 (m, 3H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.39 (m, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 161.00, 160.53, 150.83, 135.41, 134.72, 134.19, 133.45, 129.32, 129.00, 128.65, 128.33, 127.77, 127.32, 127.19, 127.14, 126.27, 125.47, 123.64.

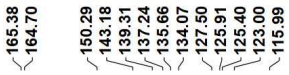
9. NMR spectra of obtained compounds

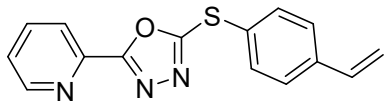


2

^{1}H NMR, 400 Hz

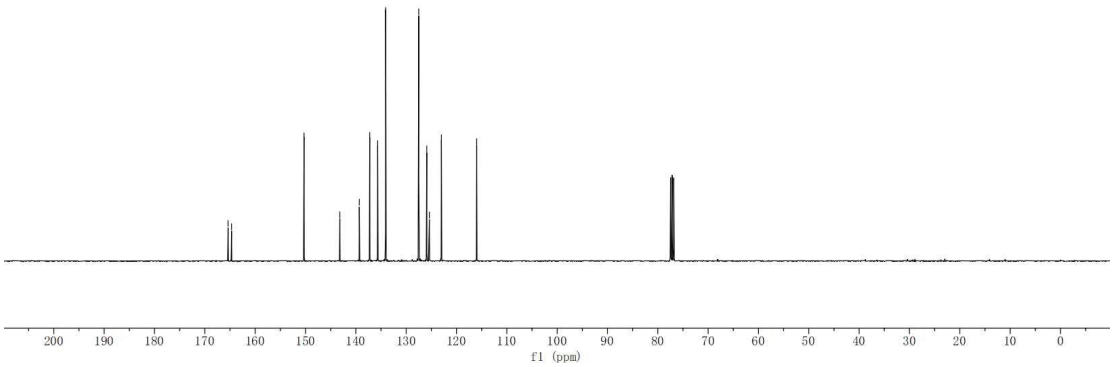


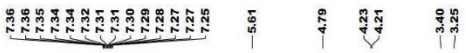


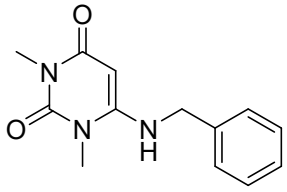


2

^{13}C NMR, 101Hz

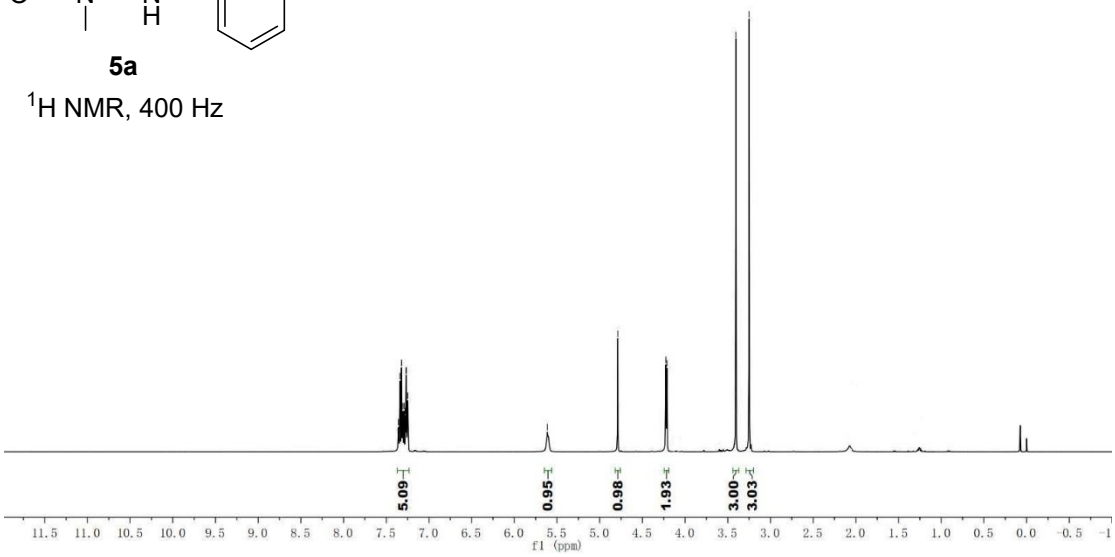


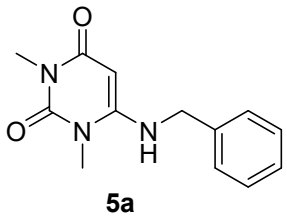




5a

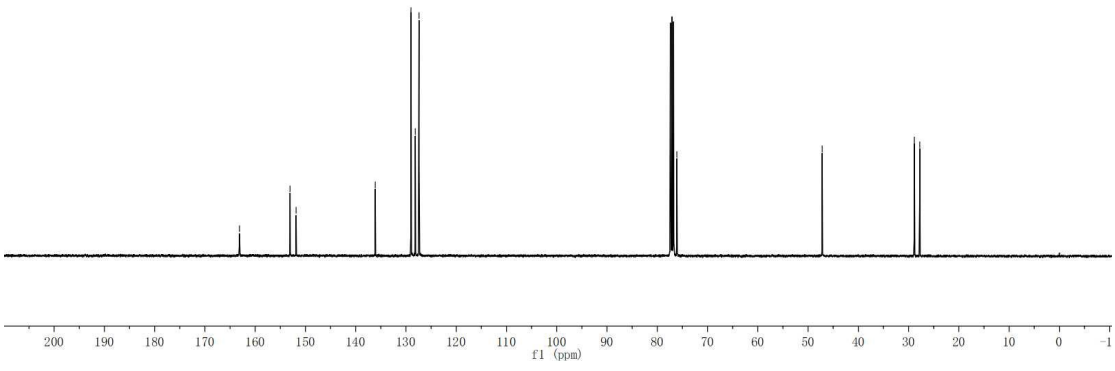
^{1}H NMR, 400 Hz

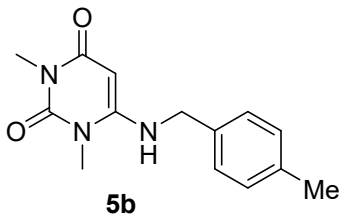




5a

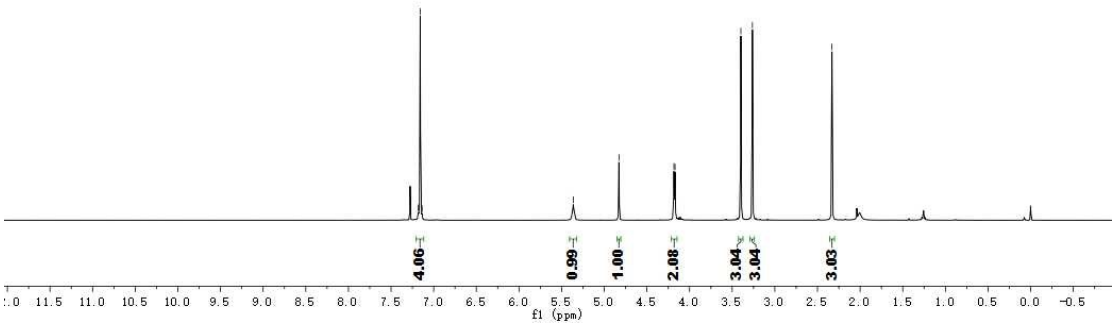
^{13}C NMR, 101 Hz

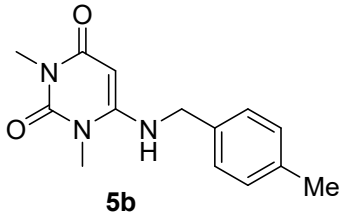




5b

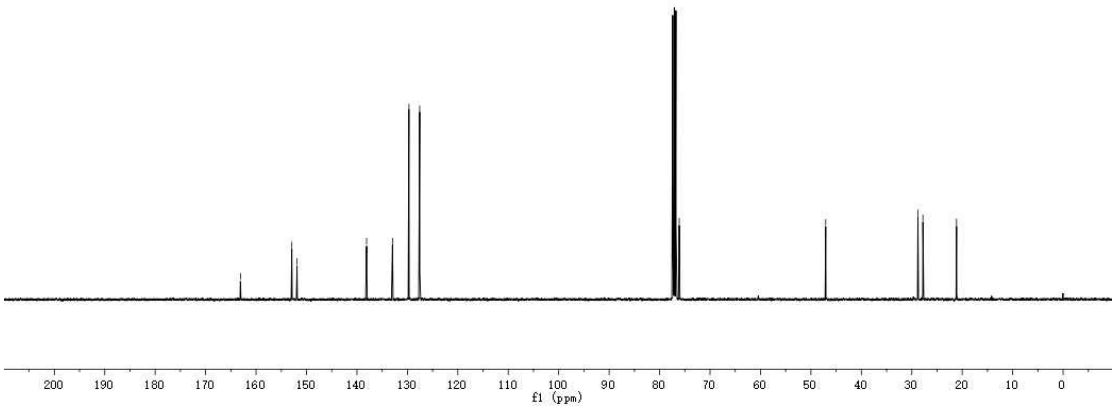
^{1}H NMR, 400 Hz

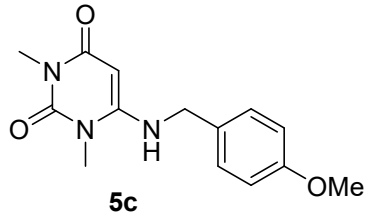




5b

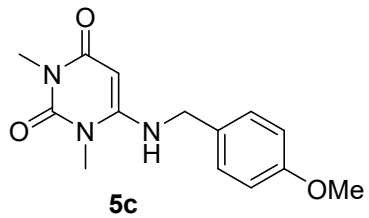
^{13}C NMR, 101 Hz





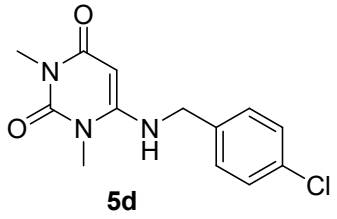
5c

^{1}H NMR, 400 Hz



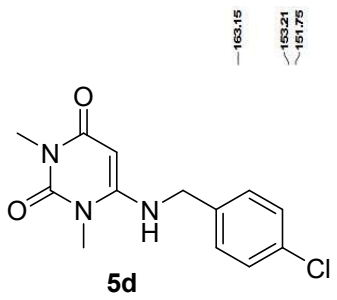
5c

^{13}C NMR, 101 Hz



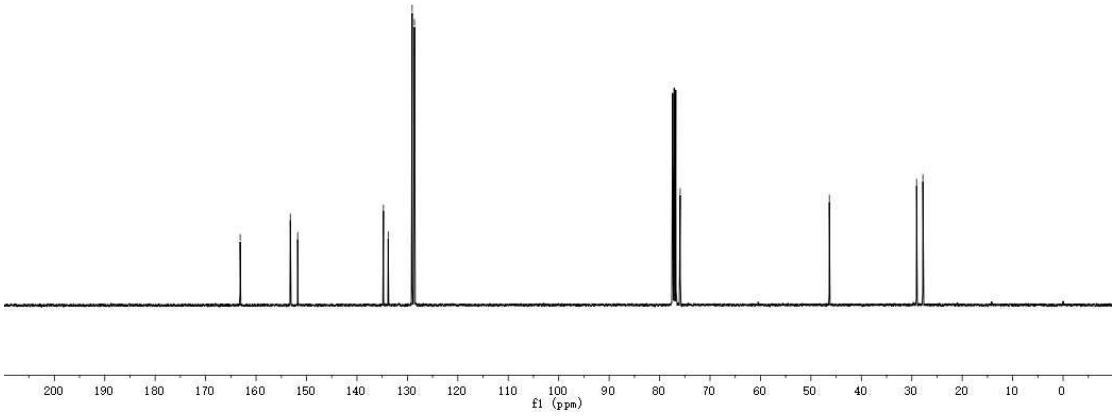
5d

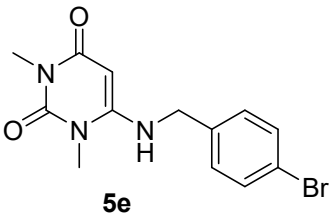
^{1}H NMR, 400 Hz



5d

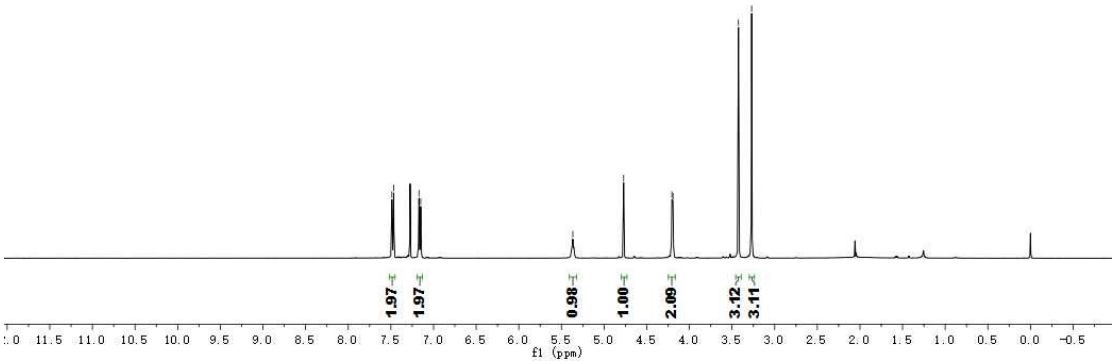
^{13}C NMR, 101 Hz

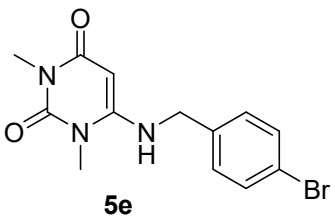




5e

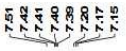
^{1}H NMR, 400 Hz

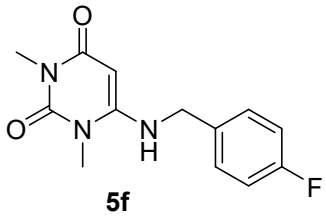




5e

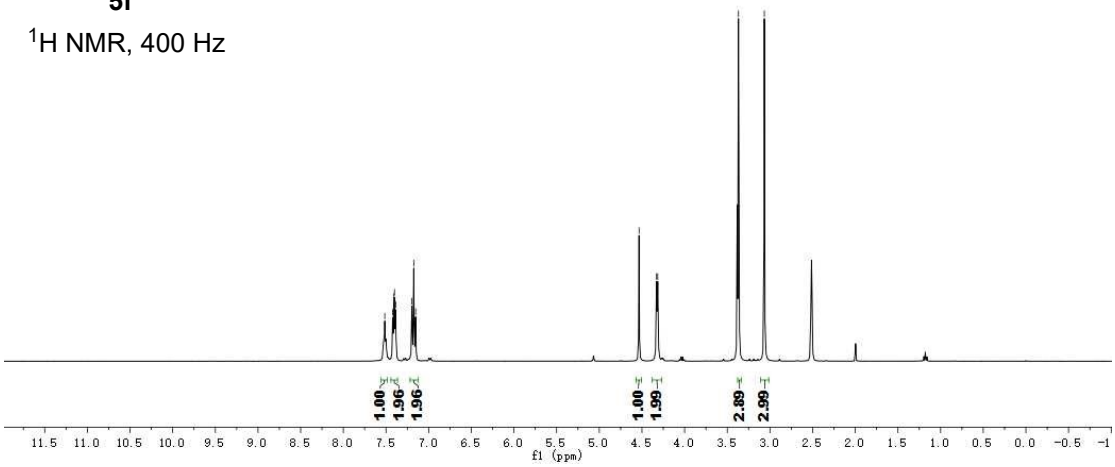
^{13}C NMR, 101 Hz

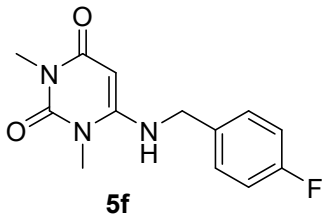




5f

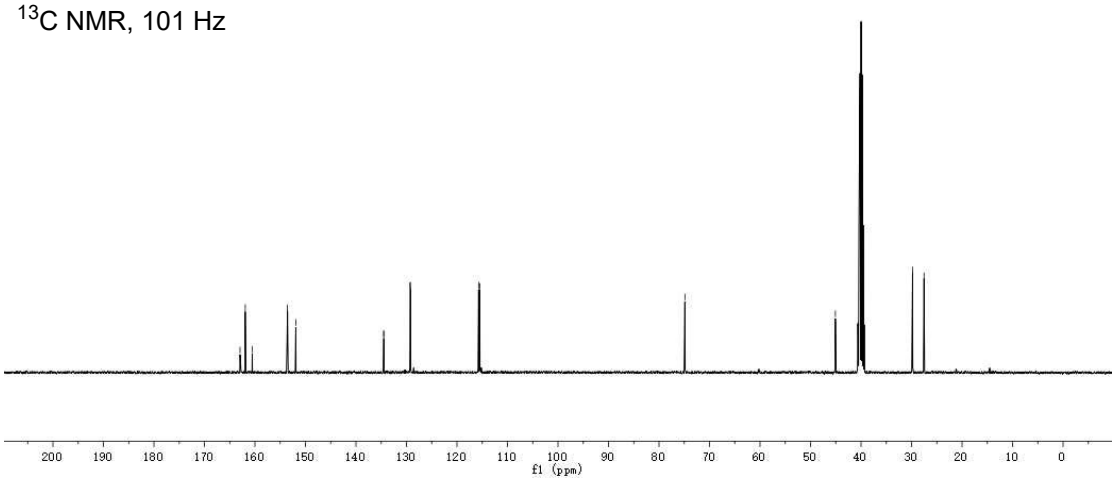
^{1}H NMR, 400 Hz

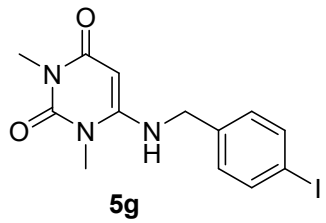




5f

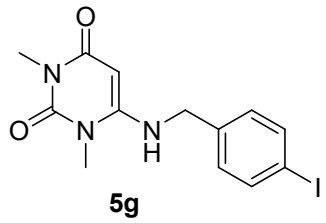
^{13}C NMR, 101 Hz





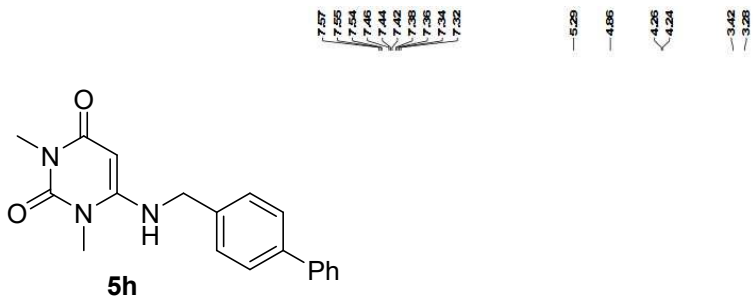
5g

^{1}H NMR, 400 Hz



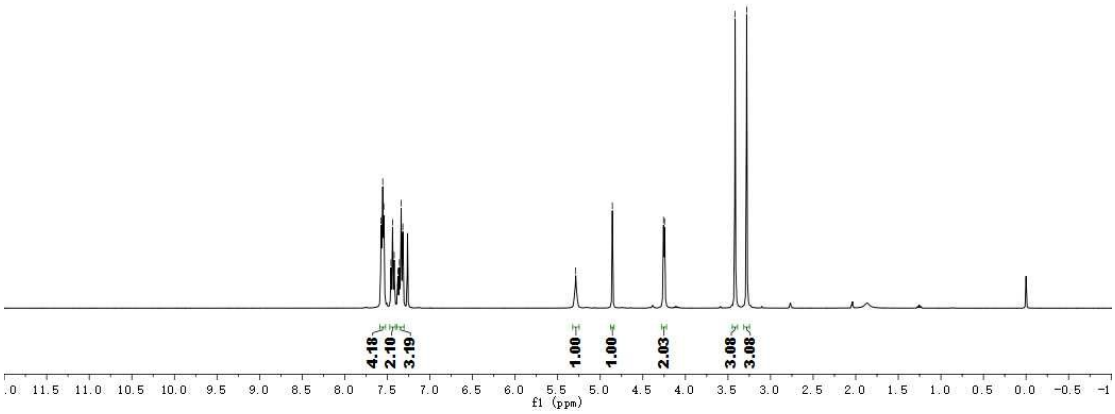
5g

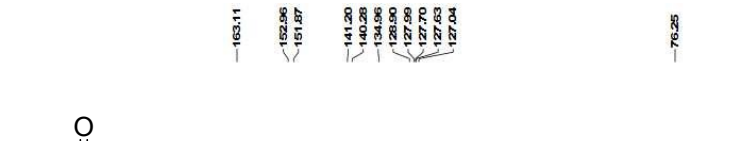
^{13}C NMR, 101 Hz



5h

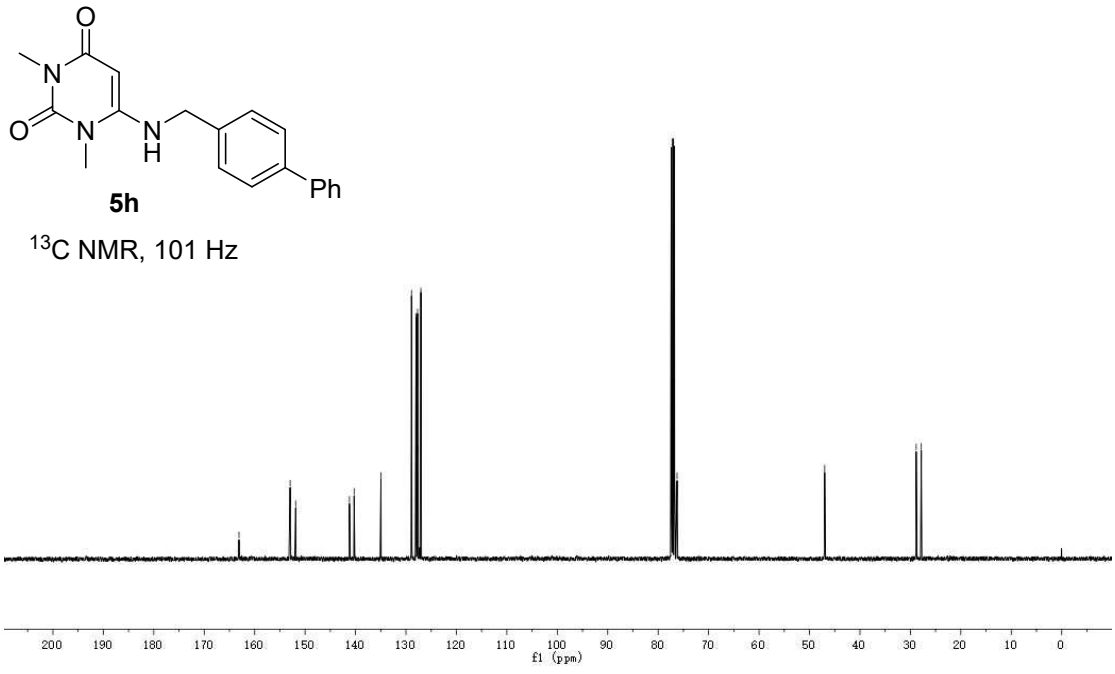
^{1}H NMR, 400 Hz

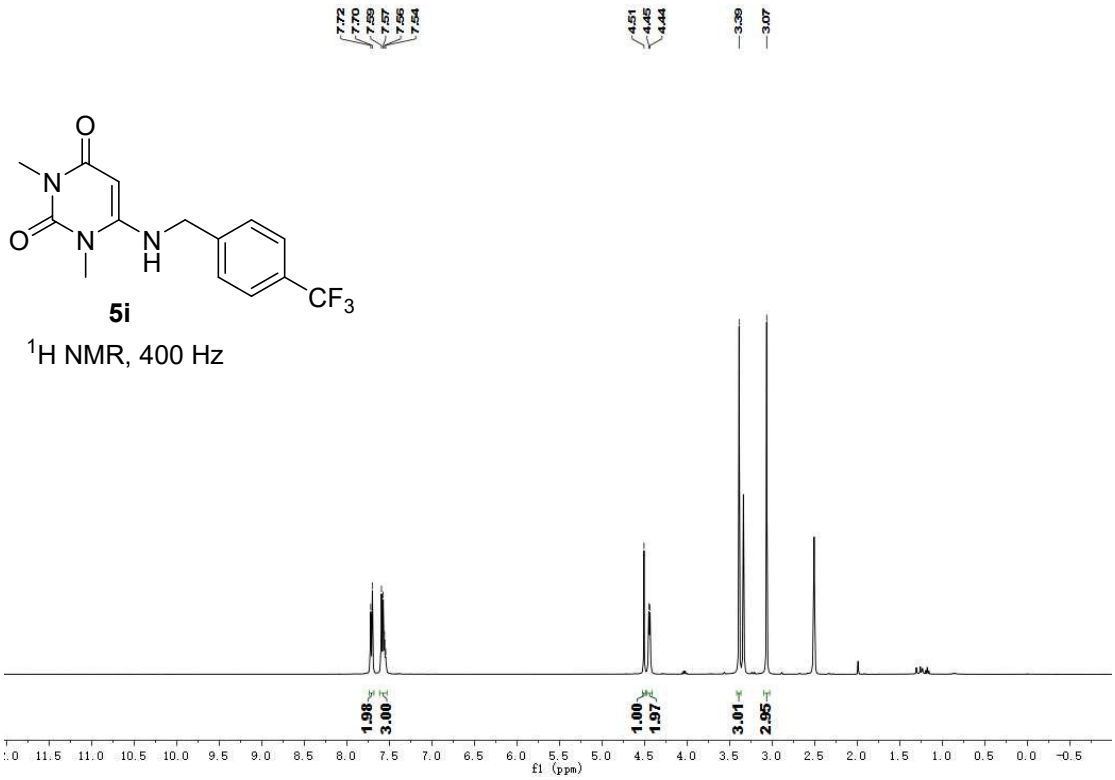




5h

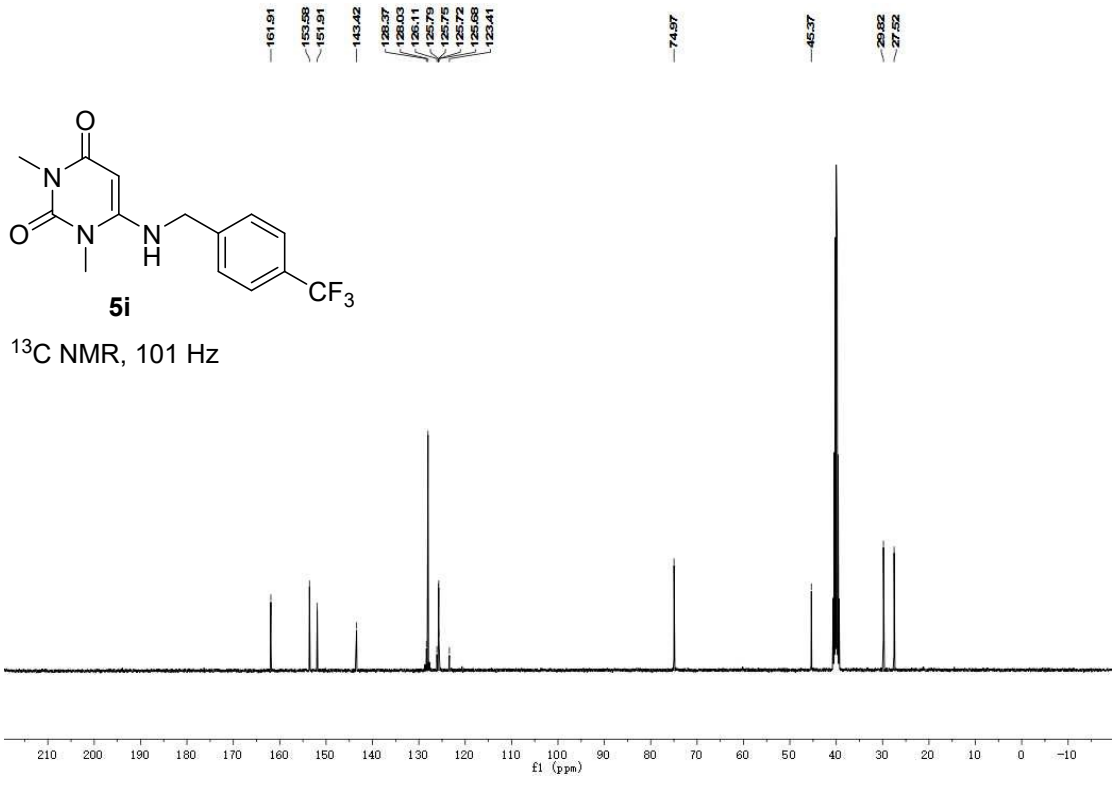
^{13}C NMR, 101 Hz





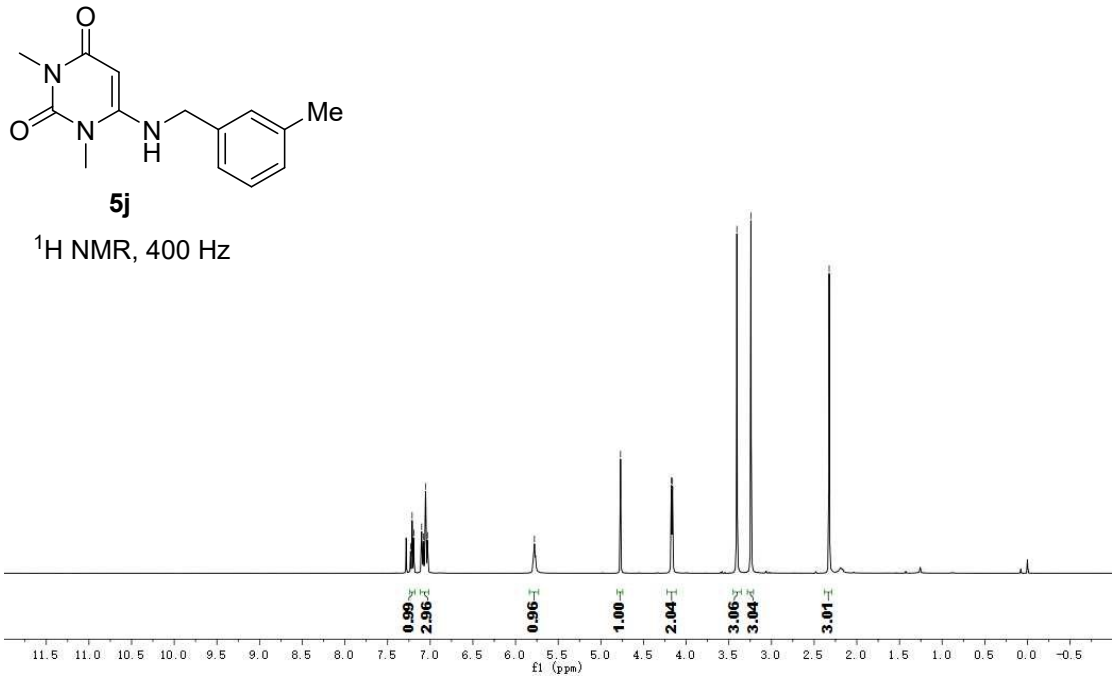
5i

^{1}H NMR, 400 Hz



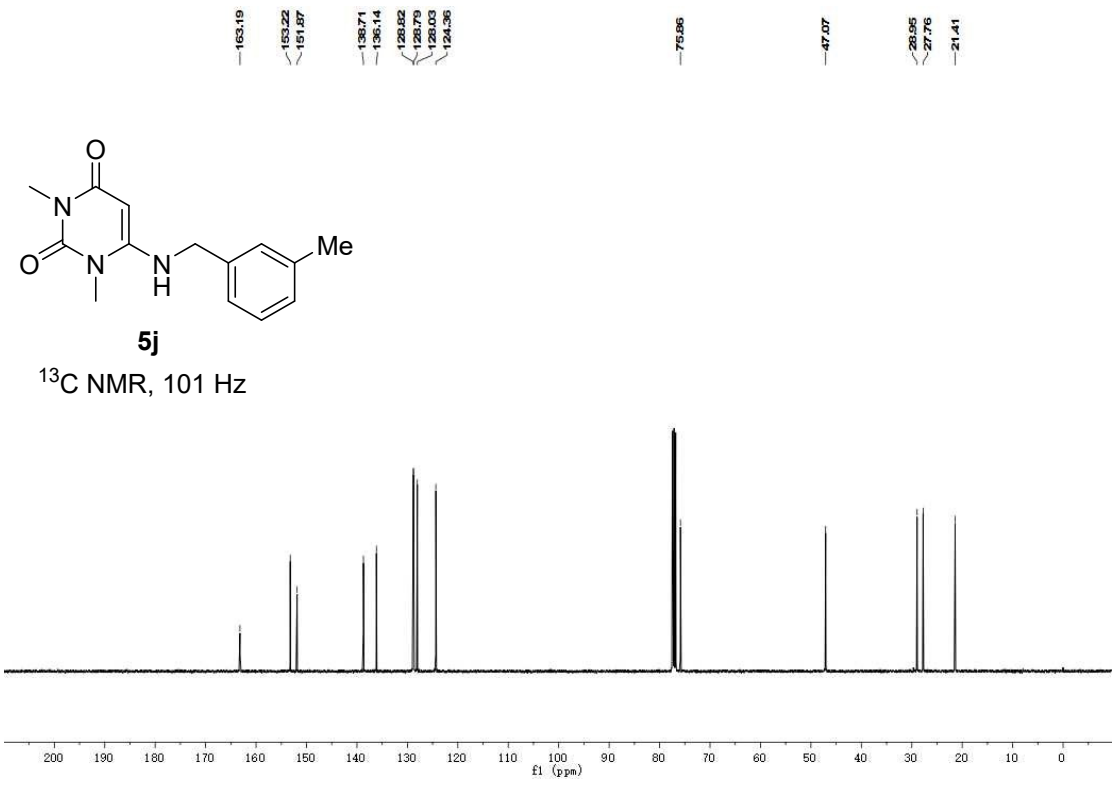
5i

^{13}C NMR, 101 Hz



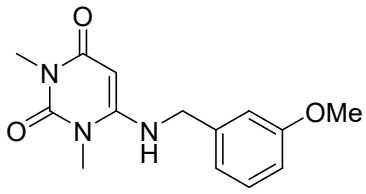
5j

^{1}H NMR, 400 Hz



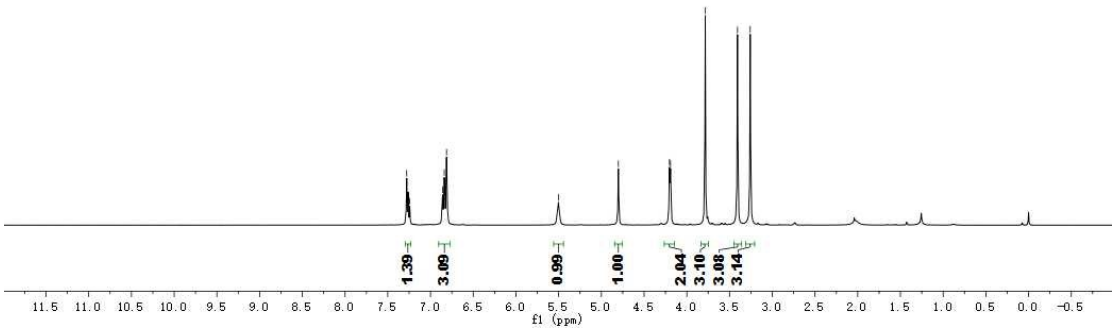
5j

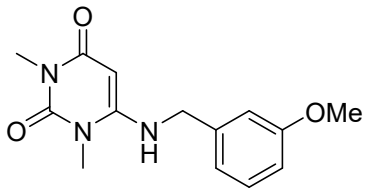
^{13}C NMR, 101 Hz



5k

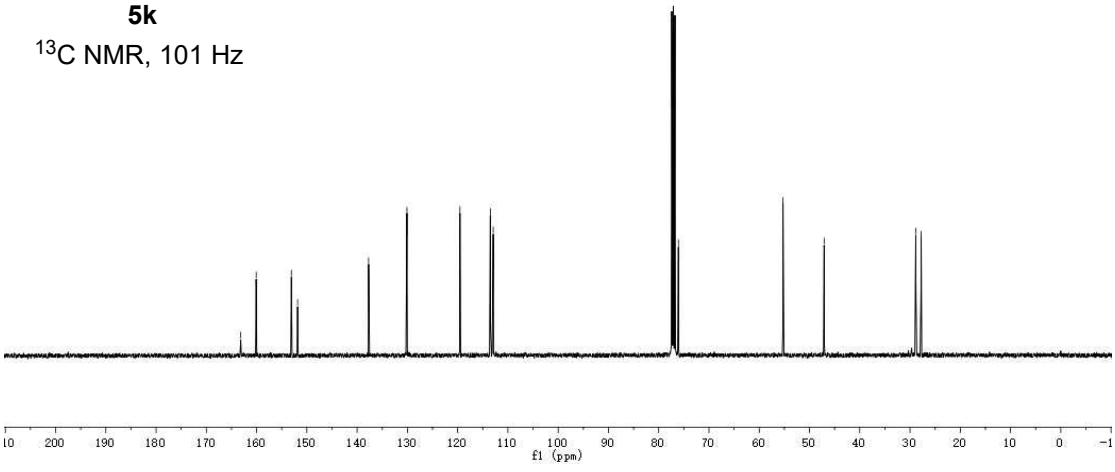
^{1}H NMR, 400 Hz

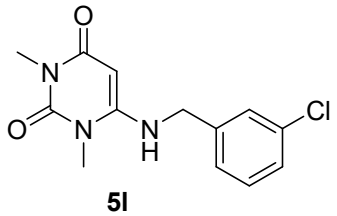




5k

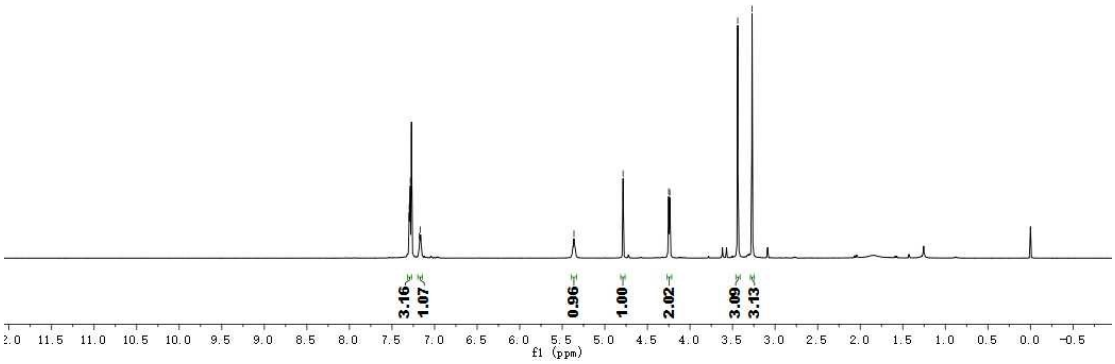
^{13}C NMR, 101 Hz

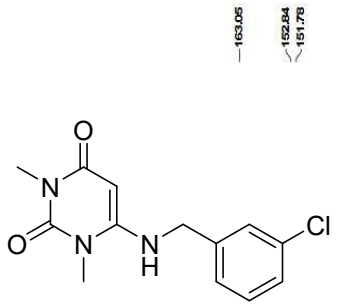




5l

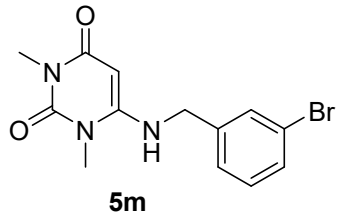
^{1}H NMR, 400 Hz





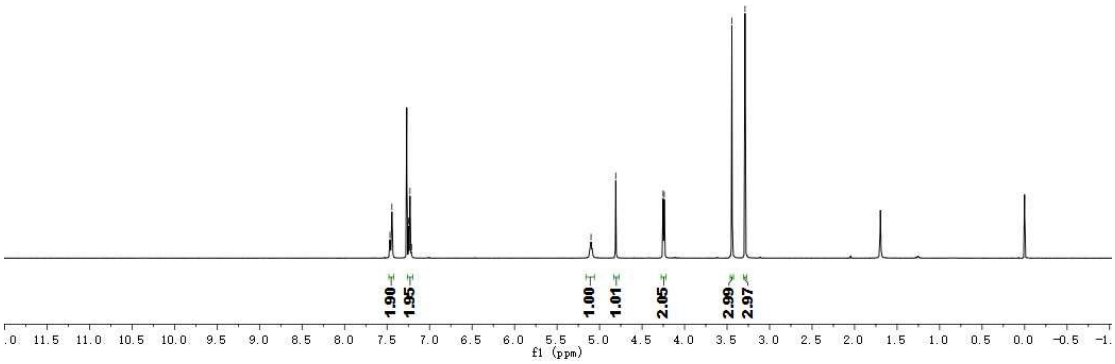
5l

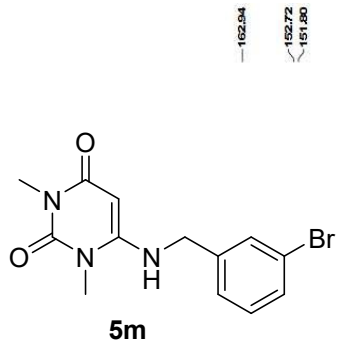
^{13}C NMR, 101 Hz



5m

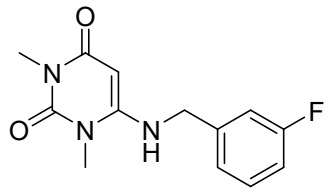
^{1}H NMR, 400 Hz





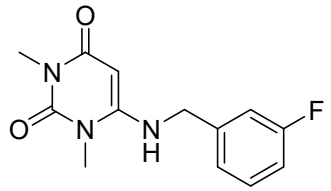
5m

^{13}C NMR, 101 Hz



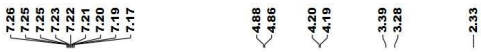
5n

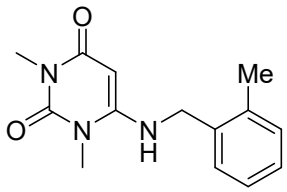
^{1}H NMR, 400 Hz



5n

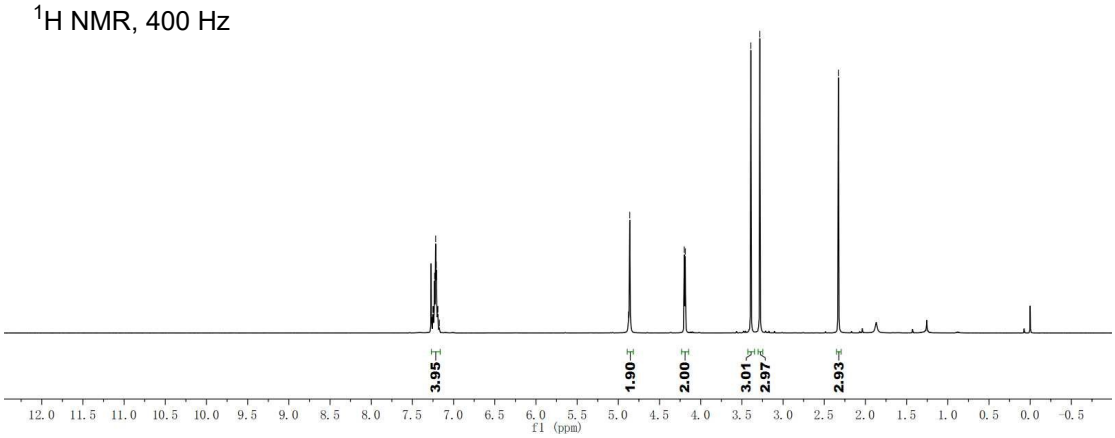
^{13}C NMR, 101 Hz

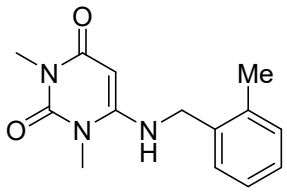




5o

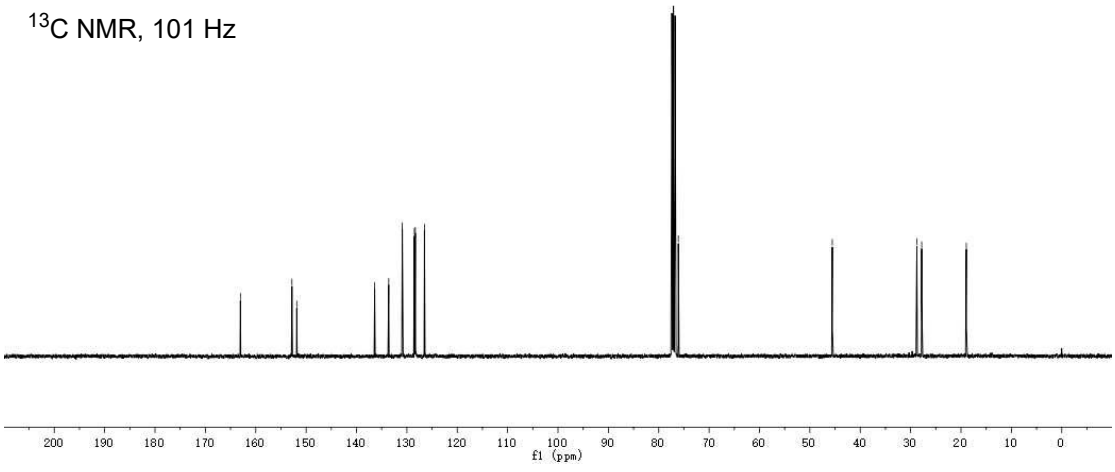
^{1}H NMR, 400 Hz

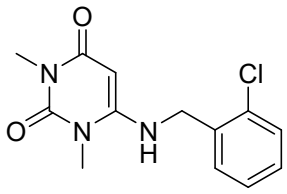




5o

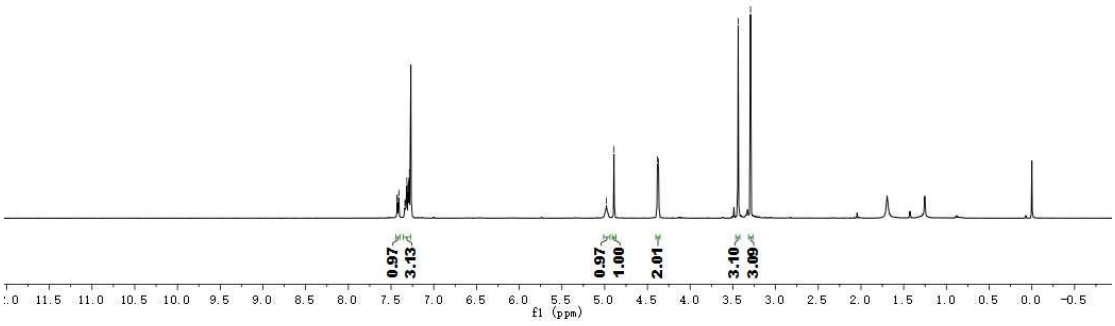
^{13}C NMR, 101 Hz

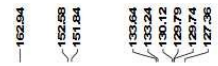


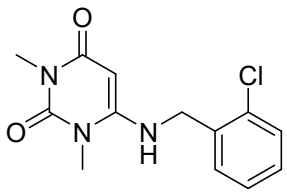


5p

^{1}H NMR, 400 Hz

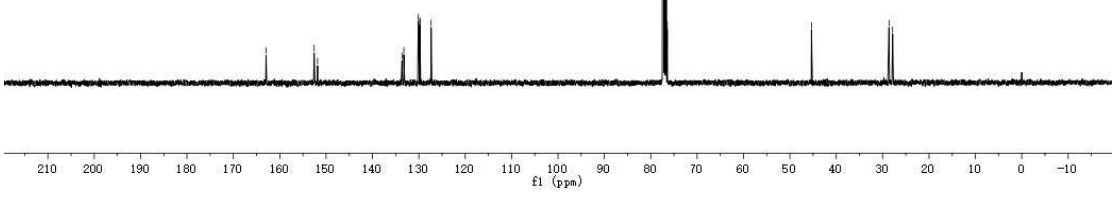


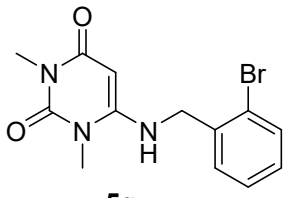




5p

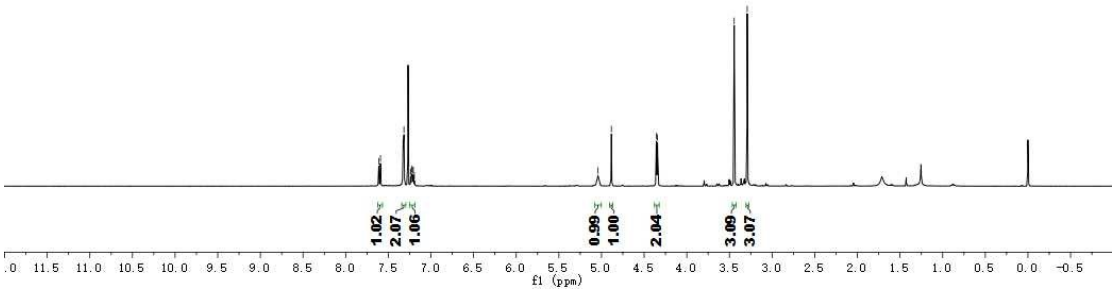
^{13}C NMR, 101 Hz

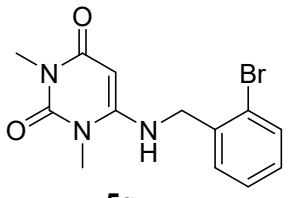




5q

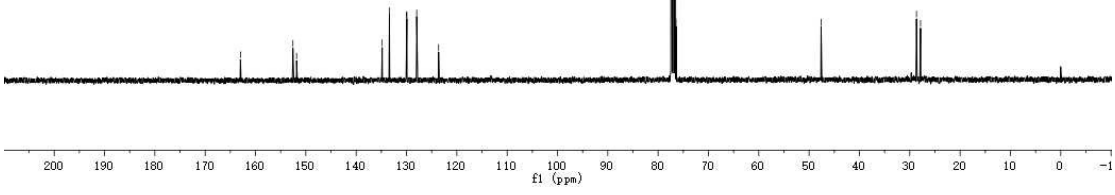
^{1}H NMR, 400 Hz

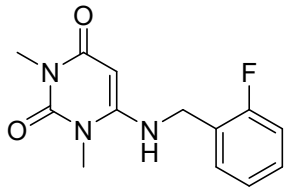




5q

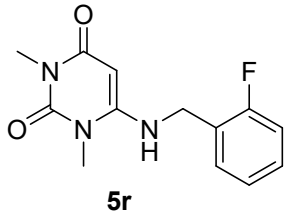
^{13}C NMR, 101 Hz





5r

^{1}H NMR, 400 Hz



5r

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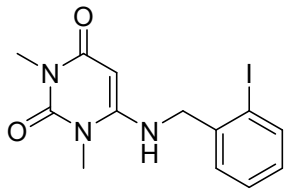
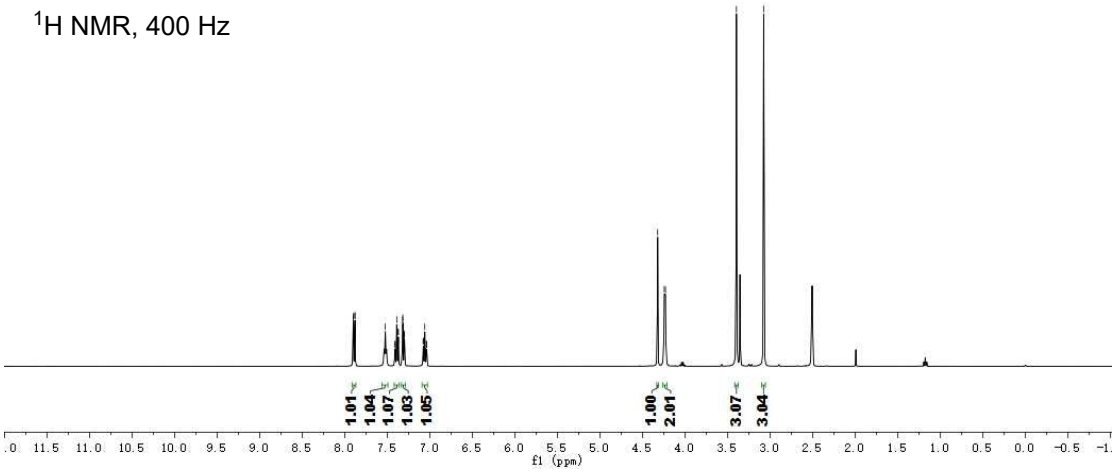
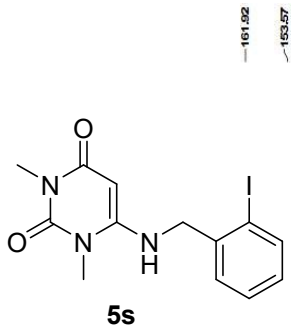


5s

^{1}H NMR, 400 Hz





5s

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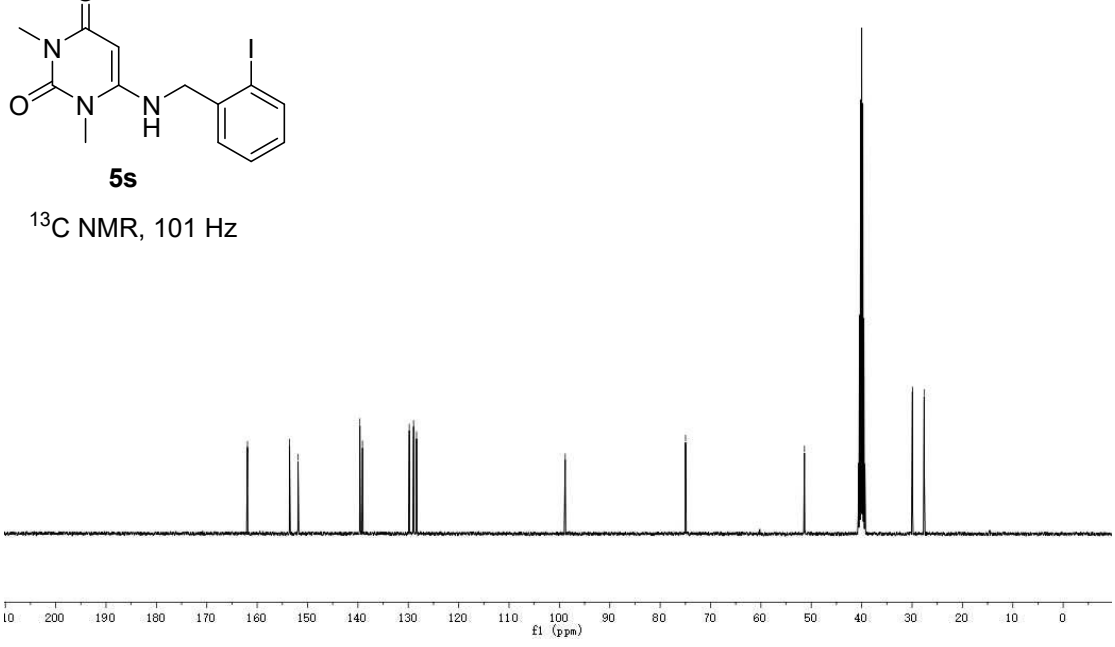
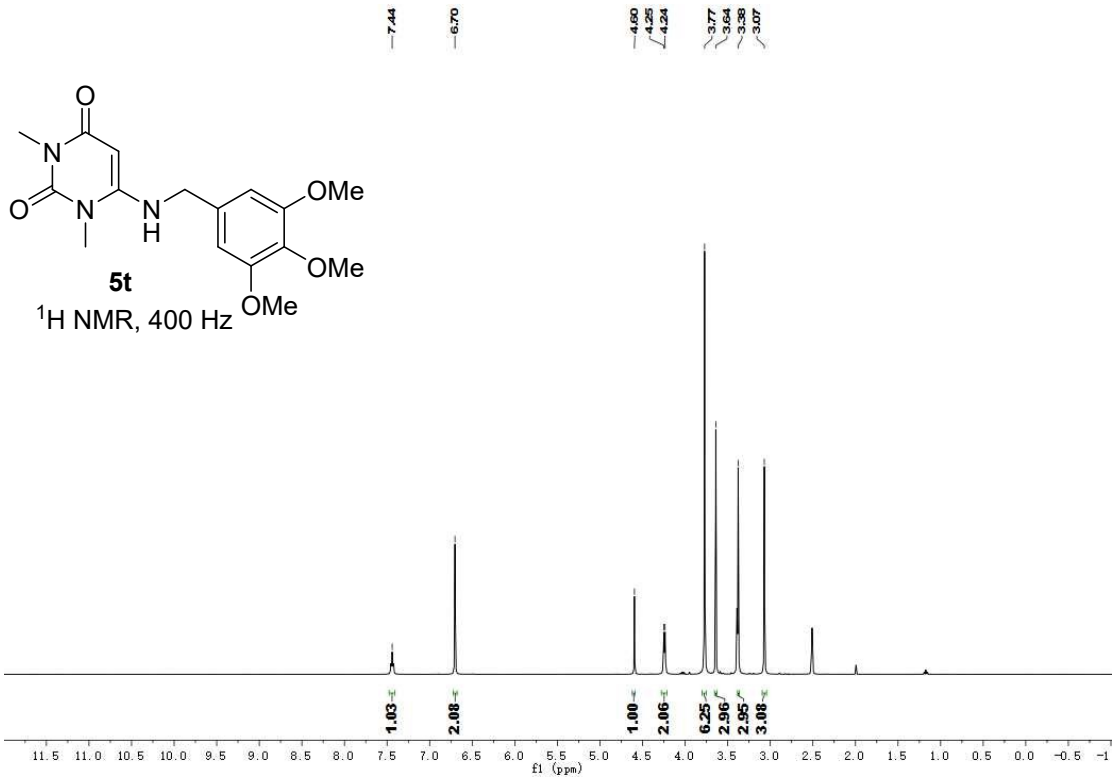
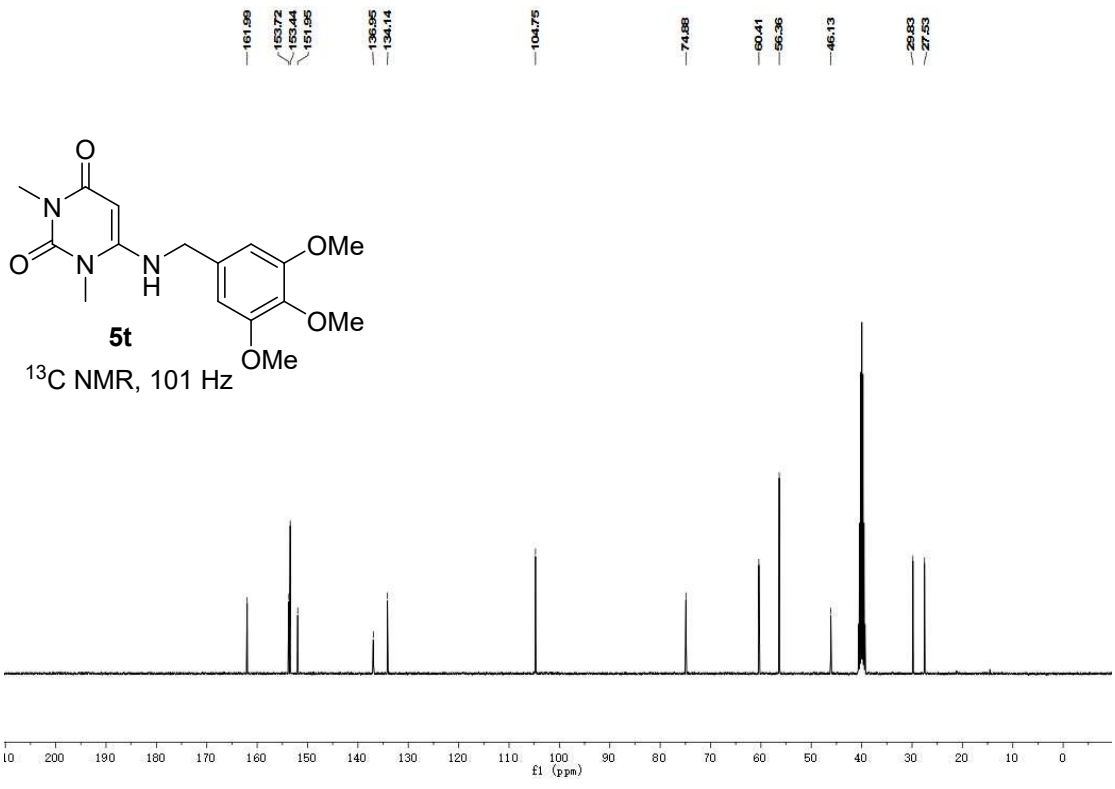




5t

^{1}H NMR, 400 Hz



5t

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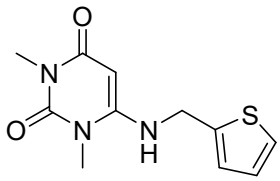
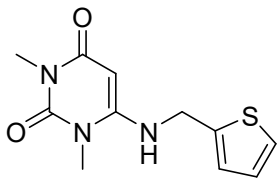


5u

^{1}H NMR, 400 Hz



5u

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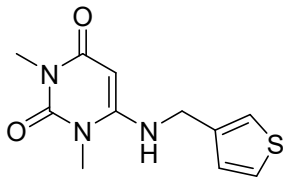
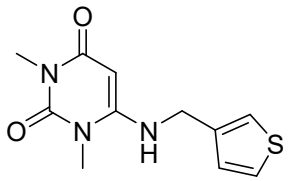


5v

^{1}H NMR, 400 Hz



5v

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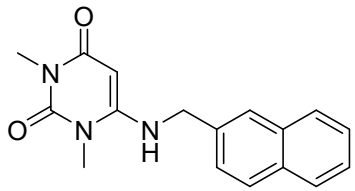

5w

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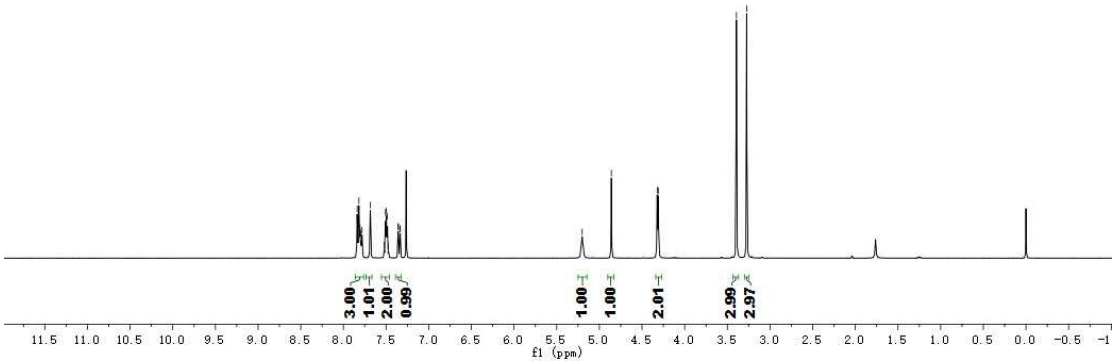

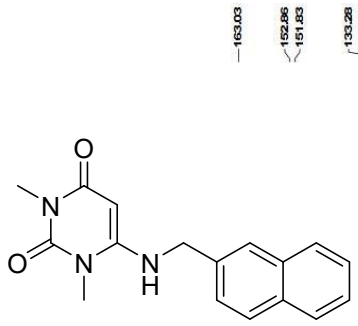

5w

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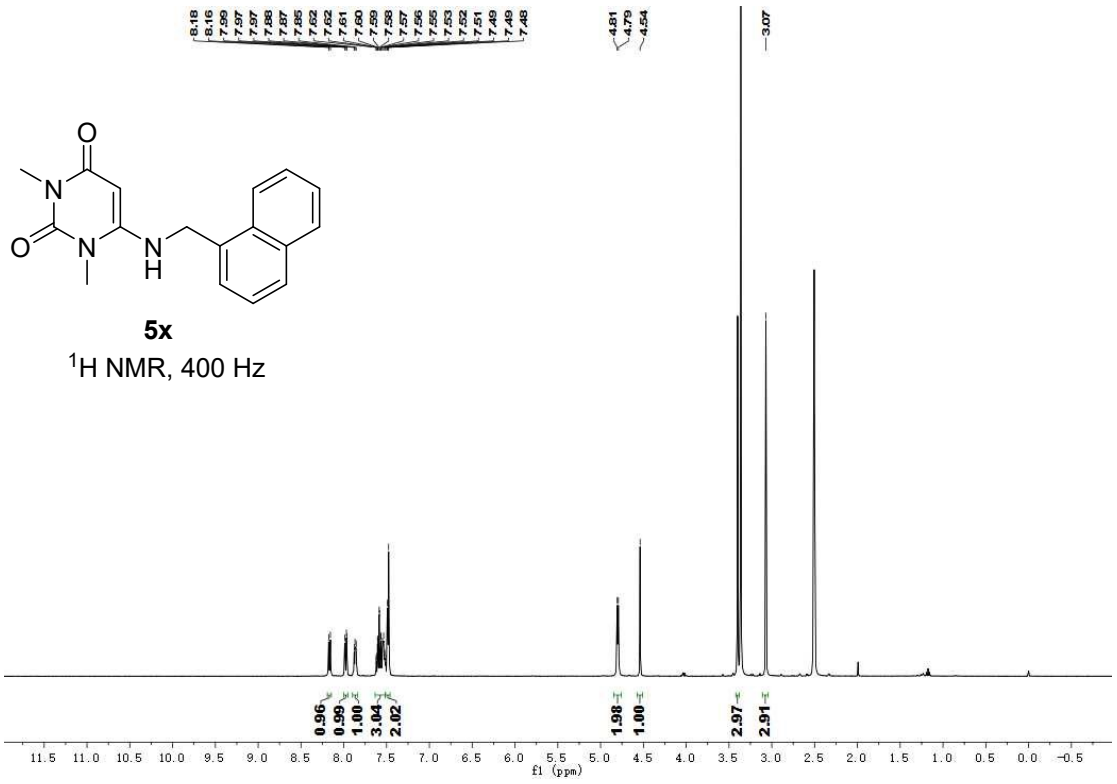
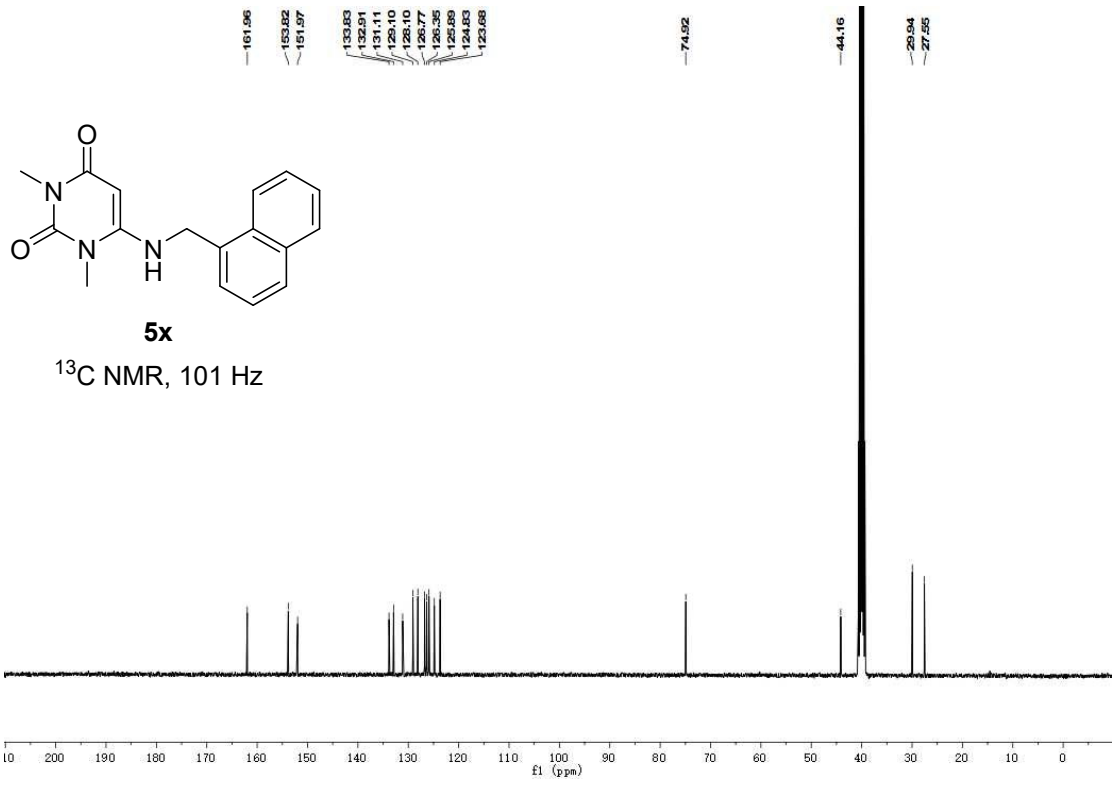


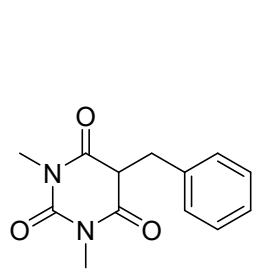
5x

^{1}H NMR, 400 Hz



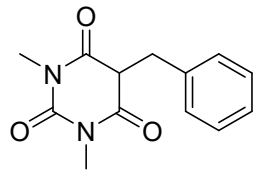
5x

^{13}C NMR, 101 Hz



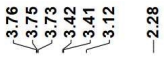
7a

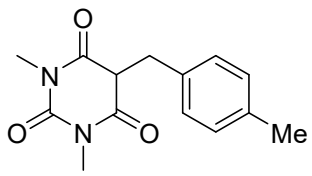
^{1}H NMR, 400 Hz



7a

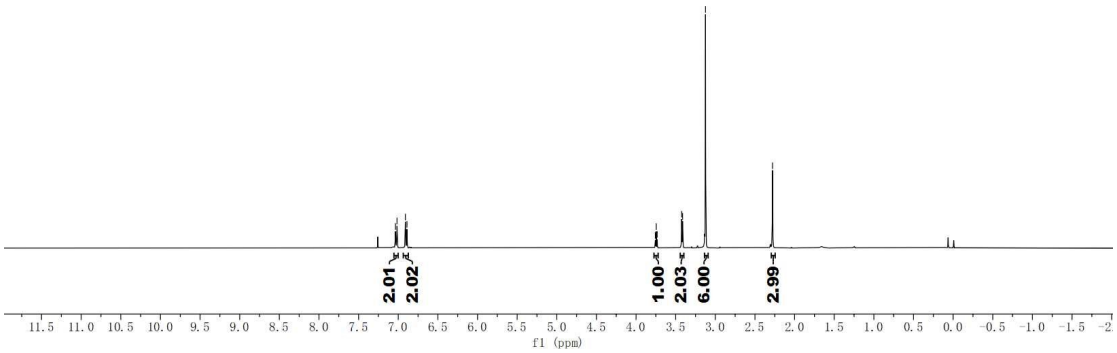
^{13}C NMR, 101 Hz

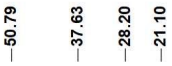


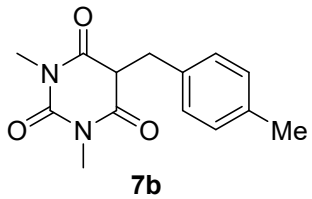


7b

^{1}H NMR, 400 Hz

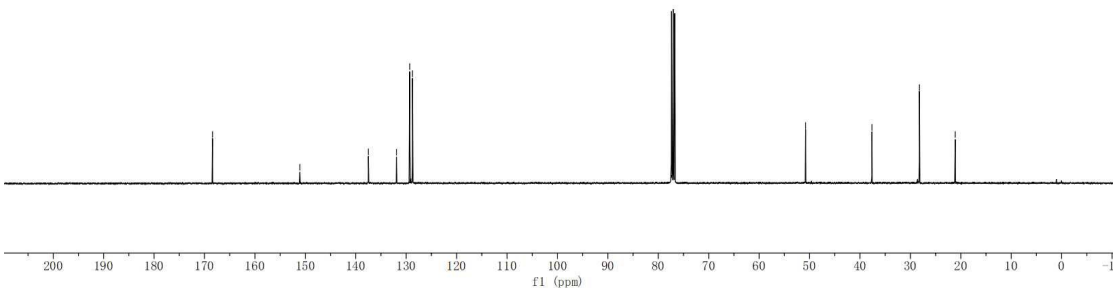


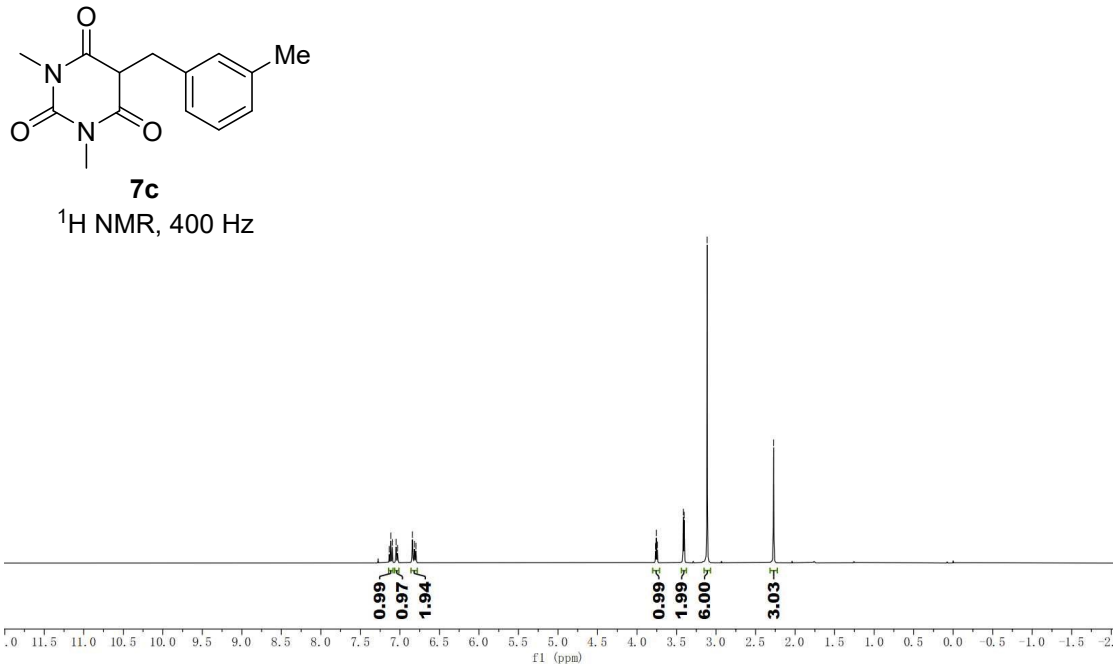




7b

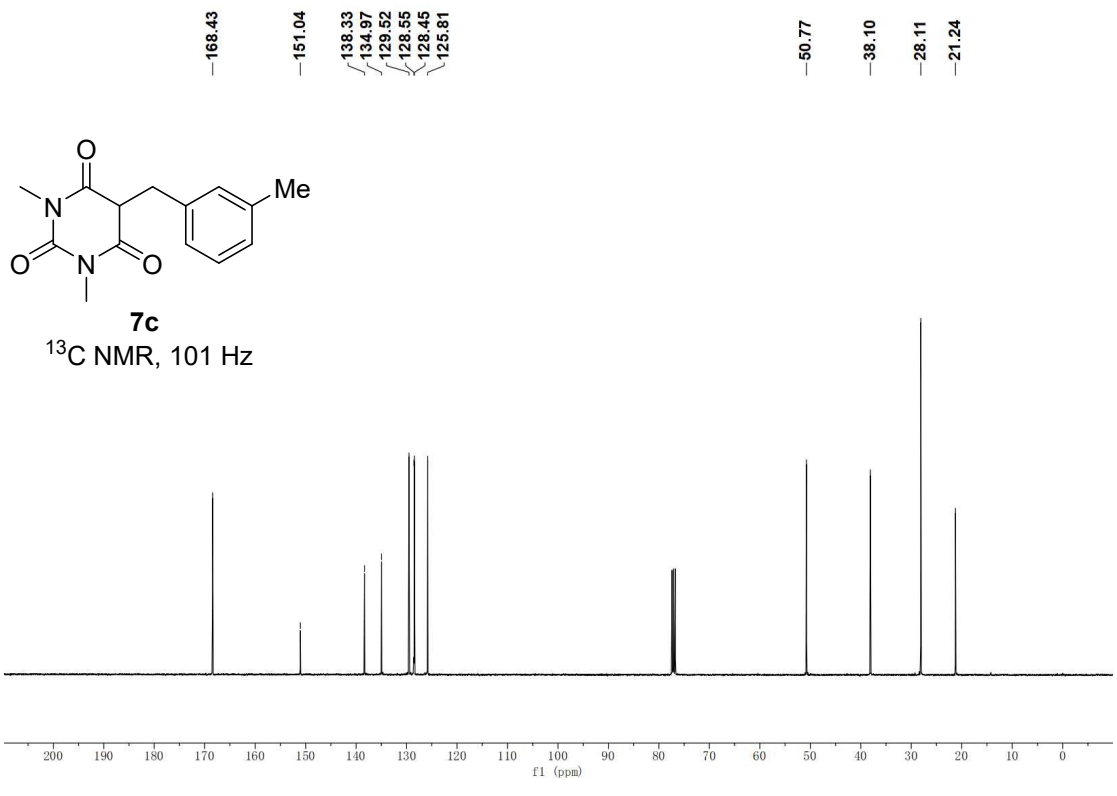
^{13}C NMR, 101 Hz





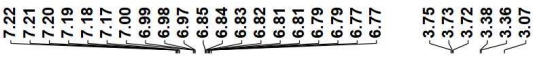
7c

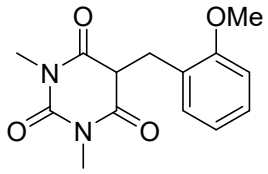
^{1}H NMR, 400 Hz



7c

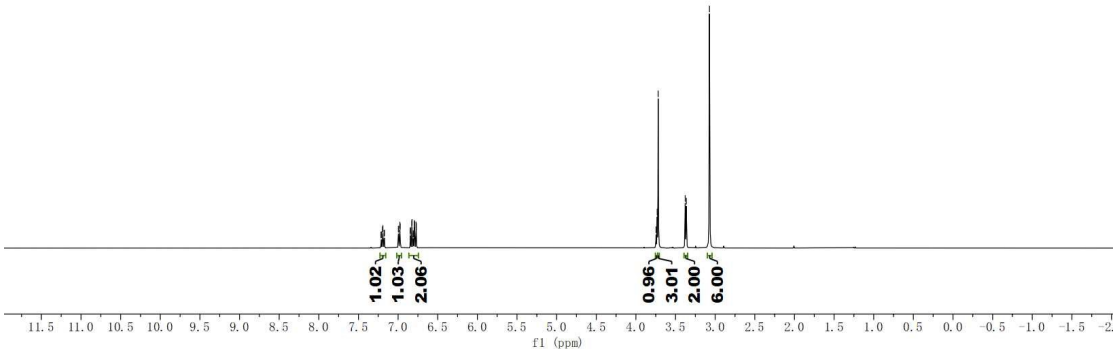
^{13}C NMR, 101 Hz

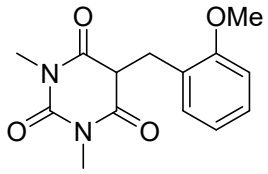




7d

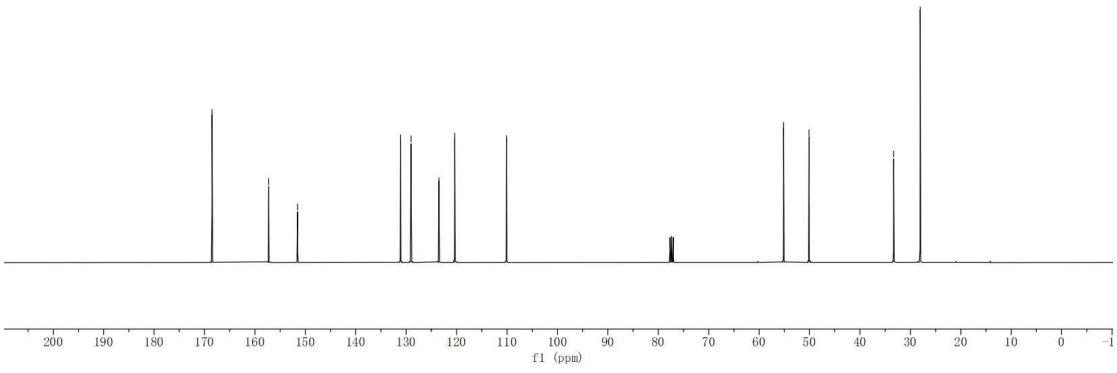
^{1}H NMR, 400 Hz

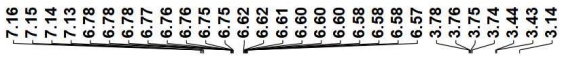


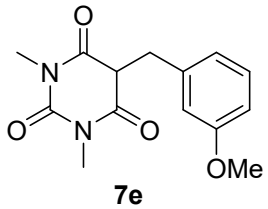


7d

^{13}C NMR, 101 Hz

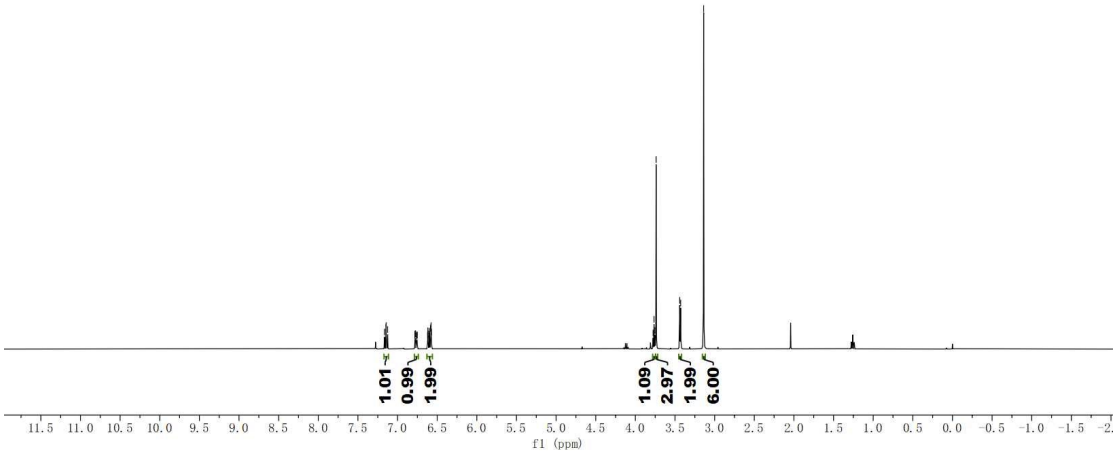


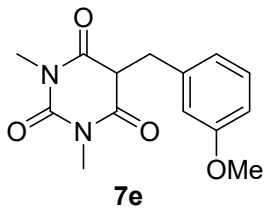




7e

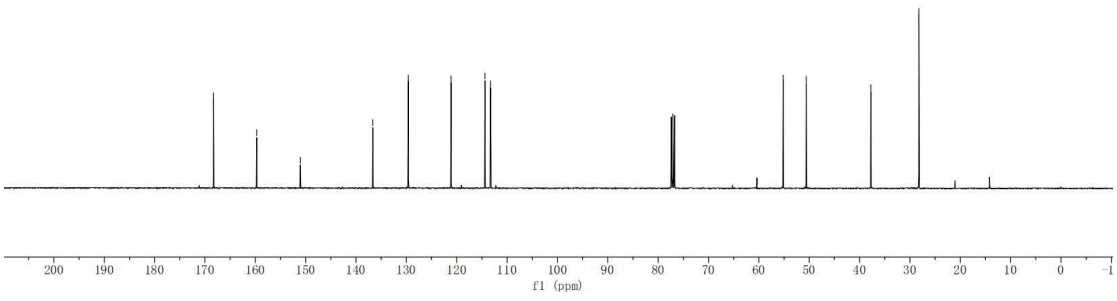
^{1}H NMR, 400 Hz

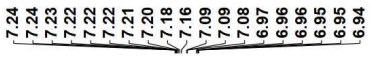


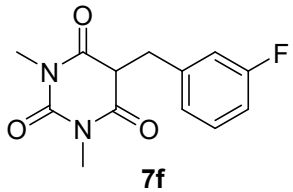


7e

^{13}C NMR, 101 Hz

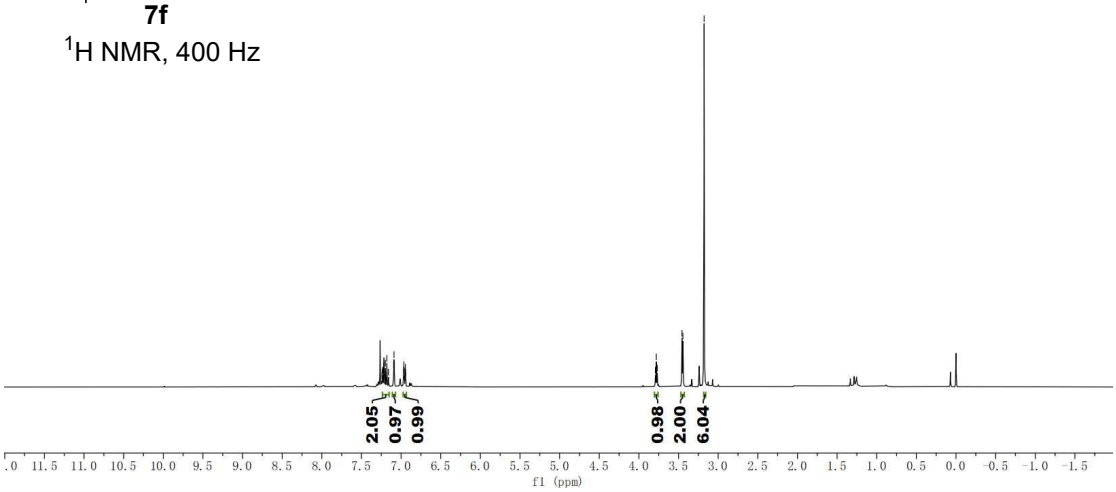


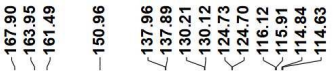


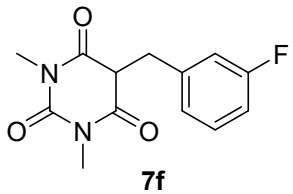


7f

^{1}H NMR, 400 Hz

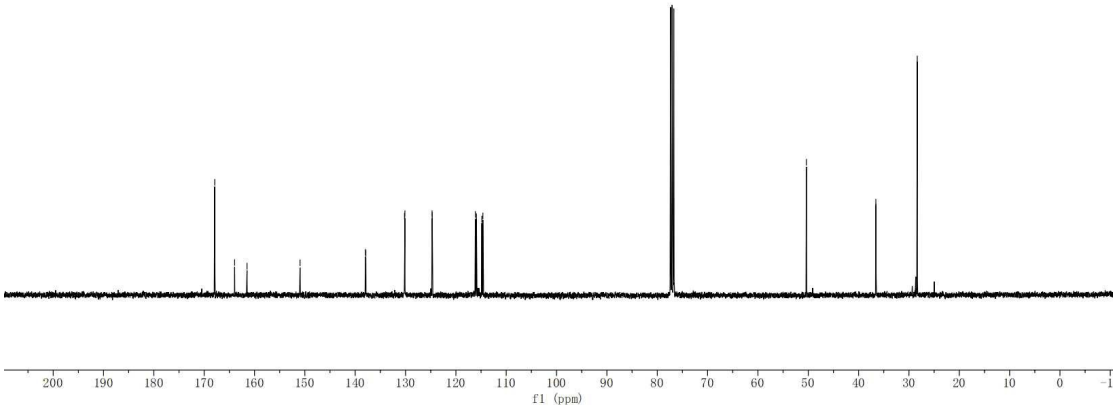


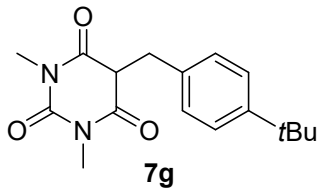




7f

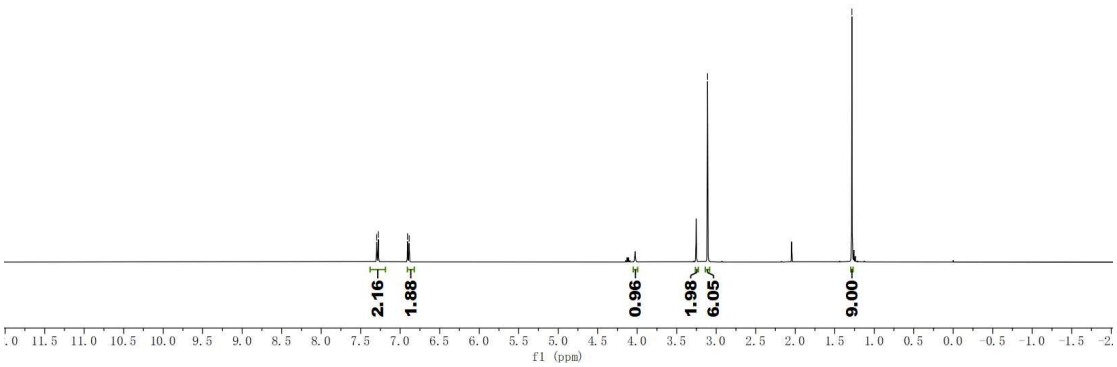
^{13}C NMR, 101 Hz

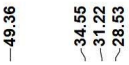


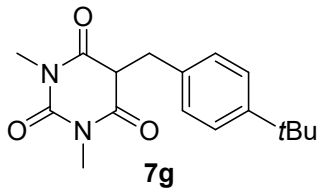


7g

^{1}H NMR, 400 Hz

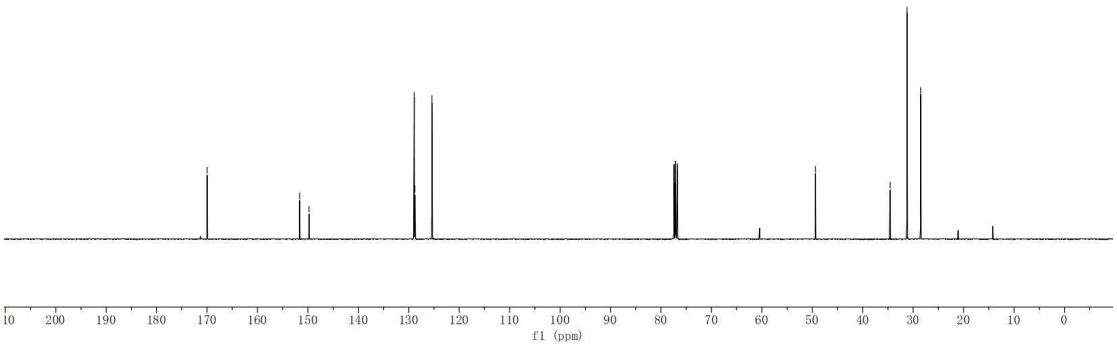


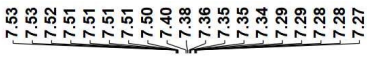


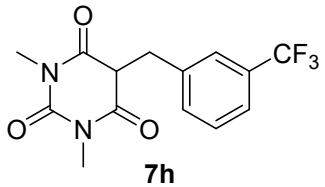


7g

^{13}C NMR, 101 Hz

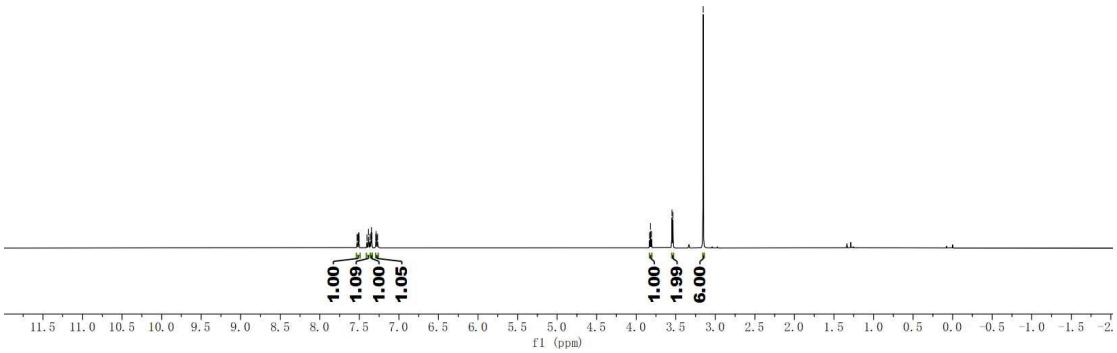


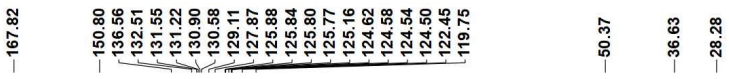


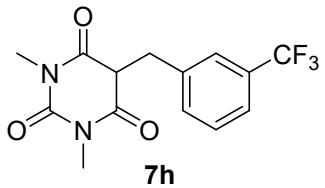


7h

^{1}H NMR, 400 Hz

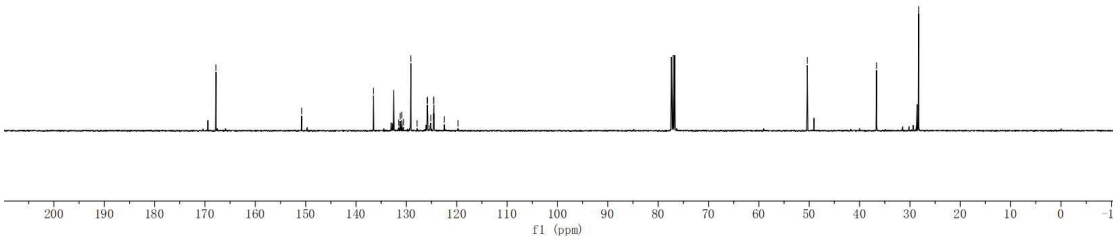


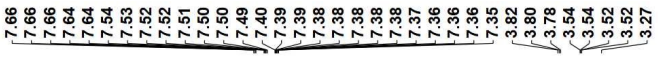


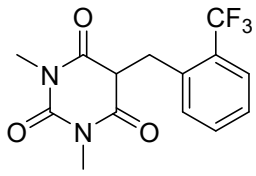


7h

^{13}C NMR, 101 Hz

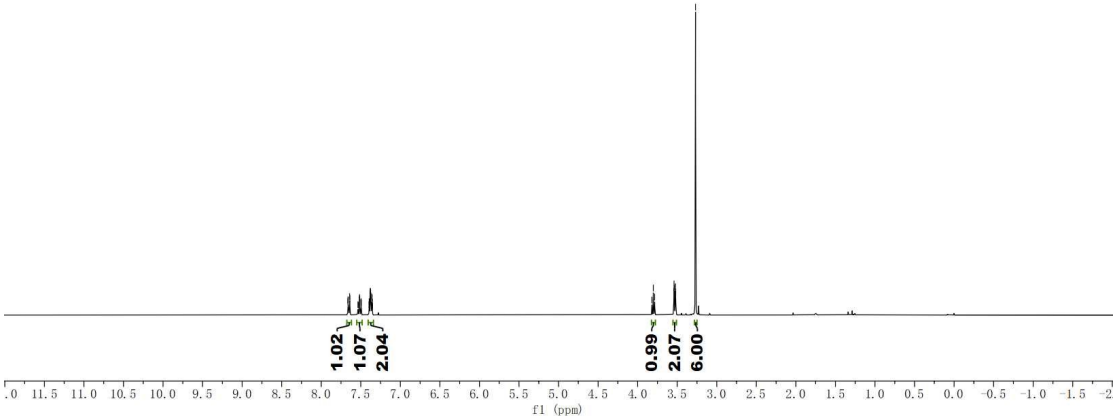


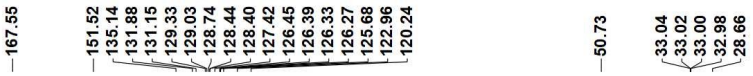


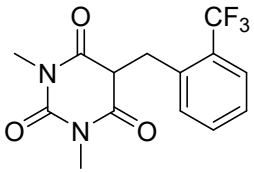


7i

^{1}H NMR, 400 Hz

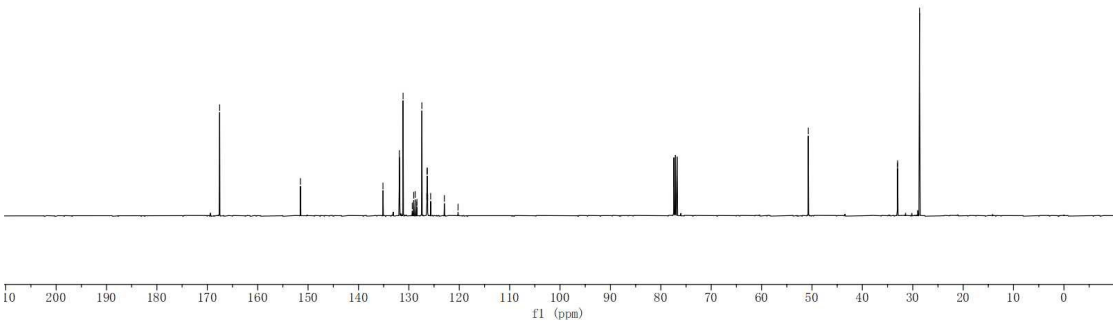


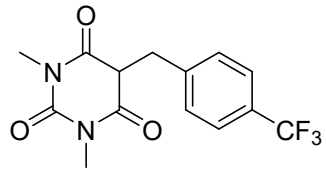




7i

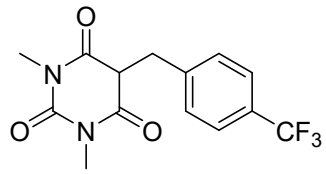
^{13}C NMR, 101 Hz





7j

^{1}H NMR, 400 Hz



7j

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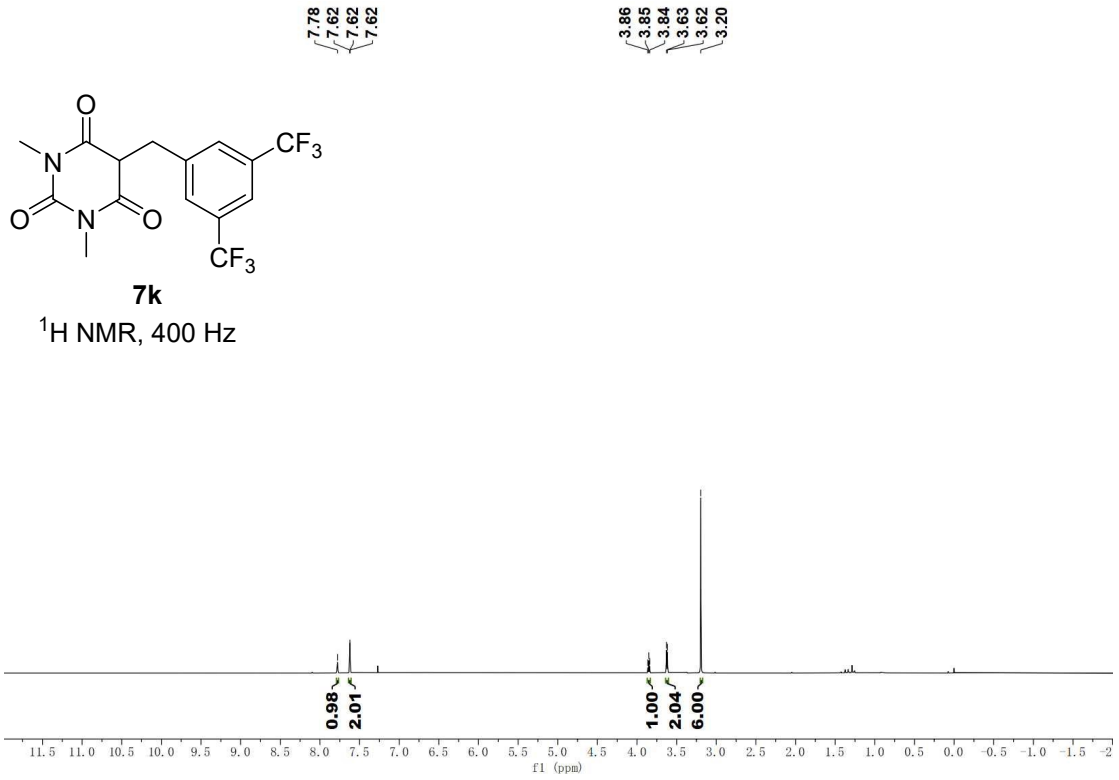

7k

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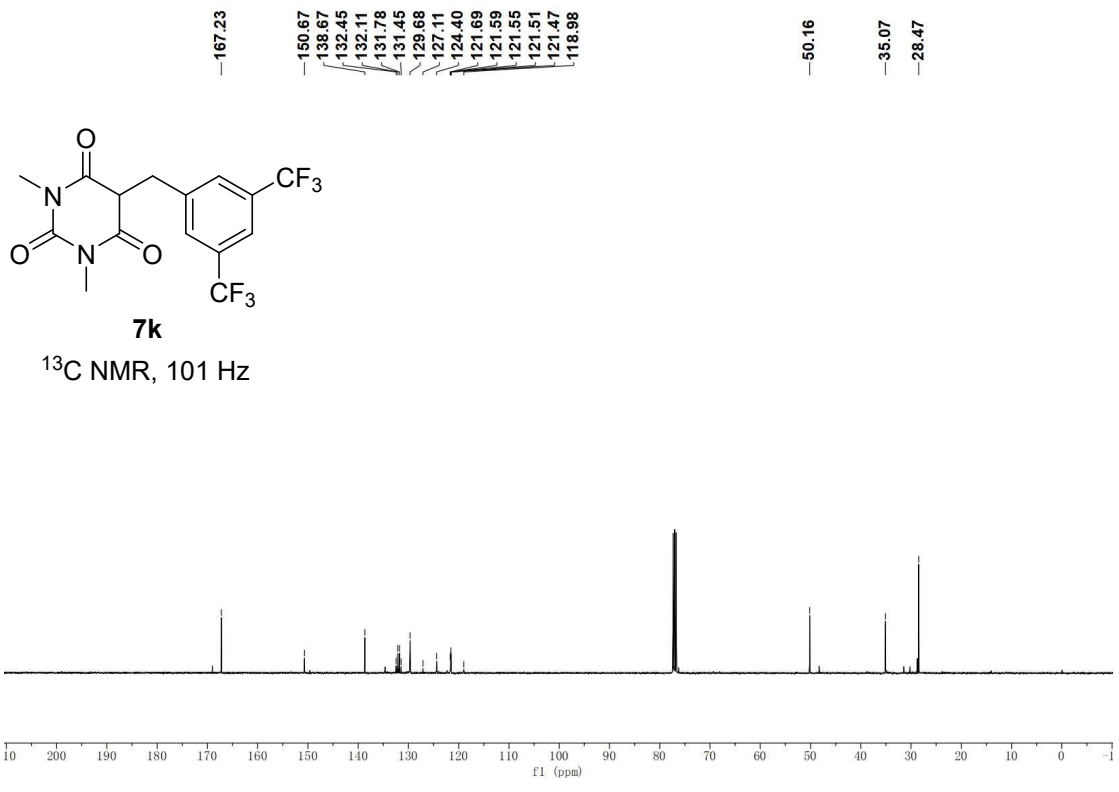
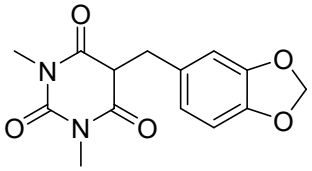


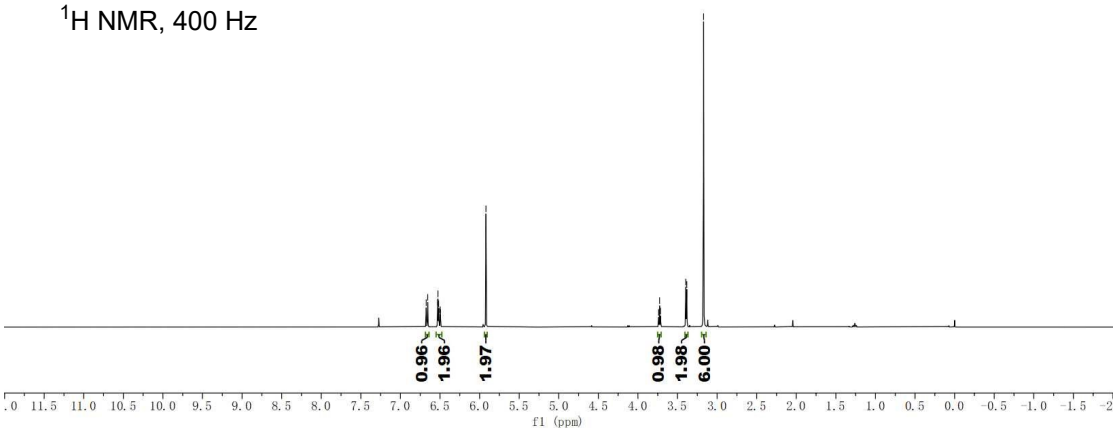
7k

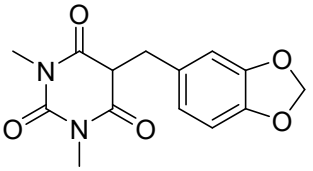
^{13}C NMR, 101 Hz



7l

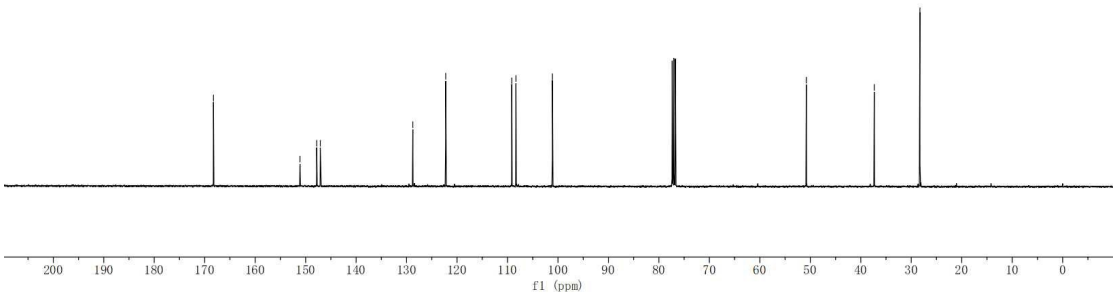
^{1}H NMR, 400 Hz

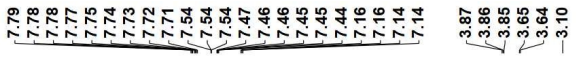


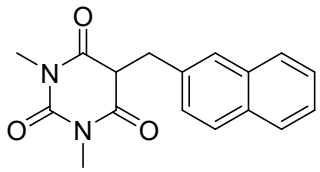


7l

^{13}C NMR, 101 Hz

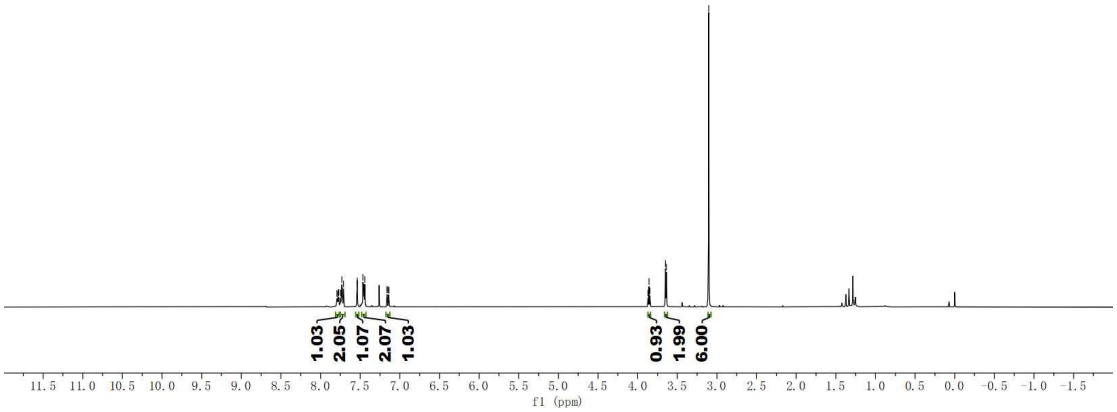


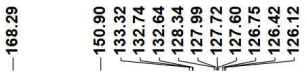


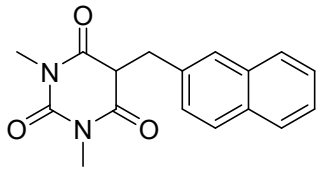


7m

^{1}H NMR, 400 Hz

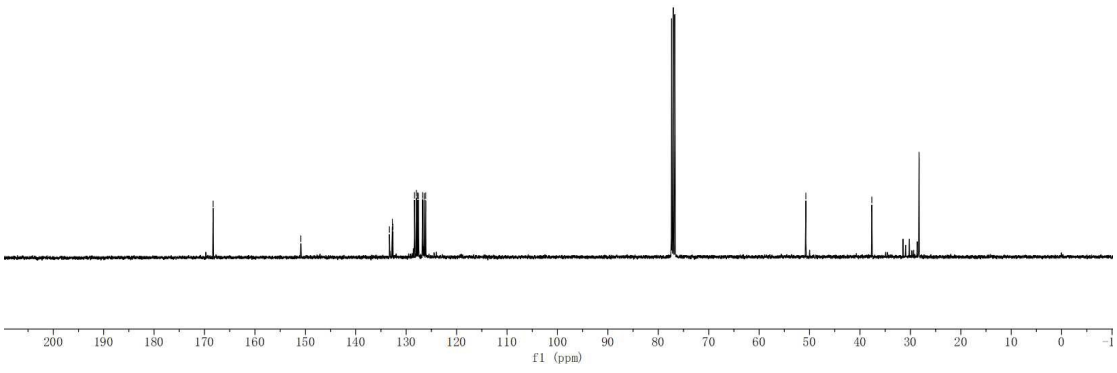


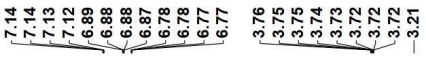


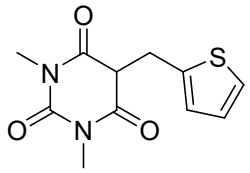


7m

^{13}C NMR, 101 Hz

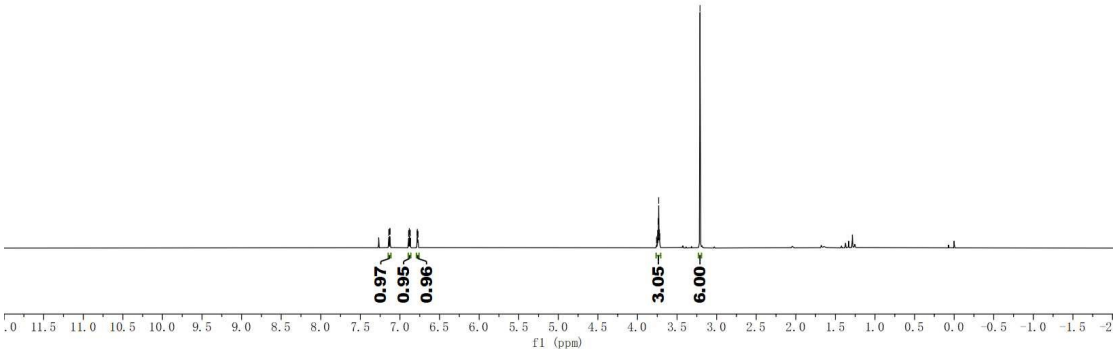


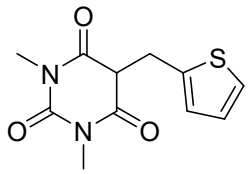




7n

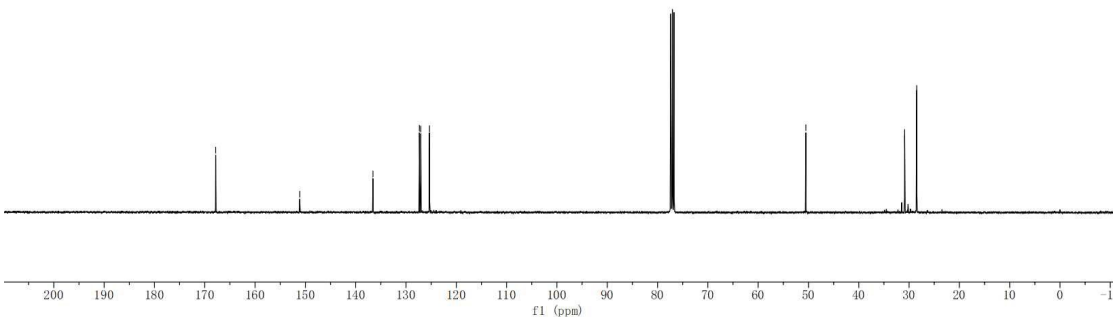
^{1}H NMR, 400 Hz

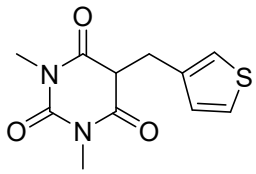




7n

^{13}C NMR, 101 Hz





7o

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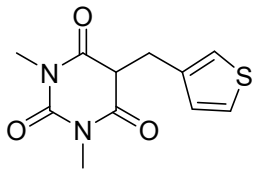

7o

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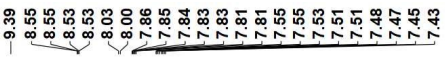
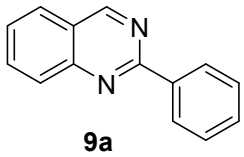
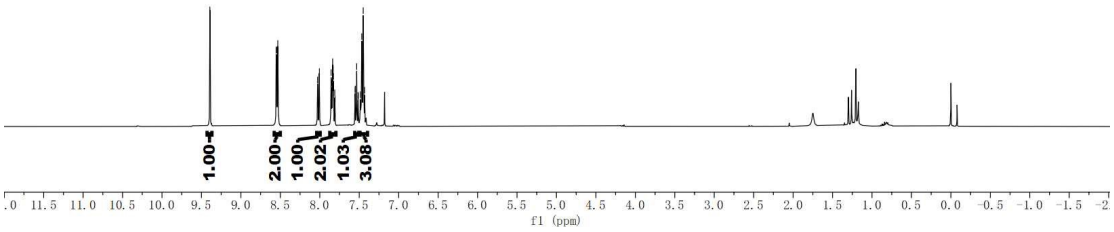
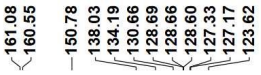


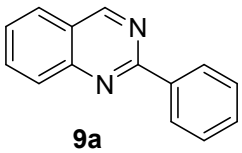


9a

^{1}H NMR 400 Hz

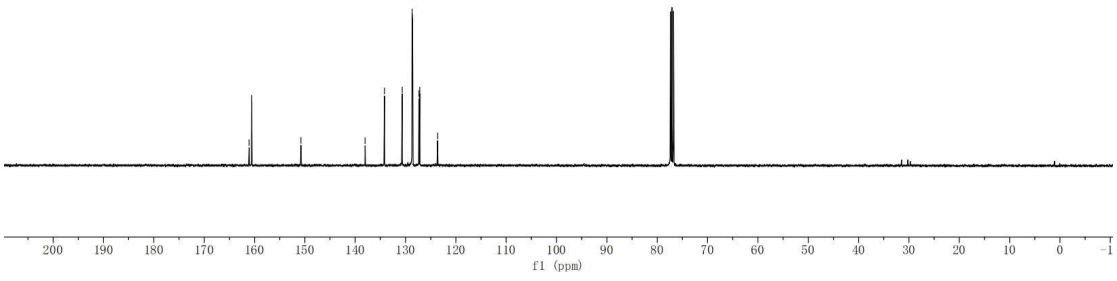


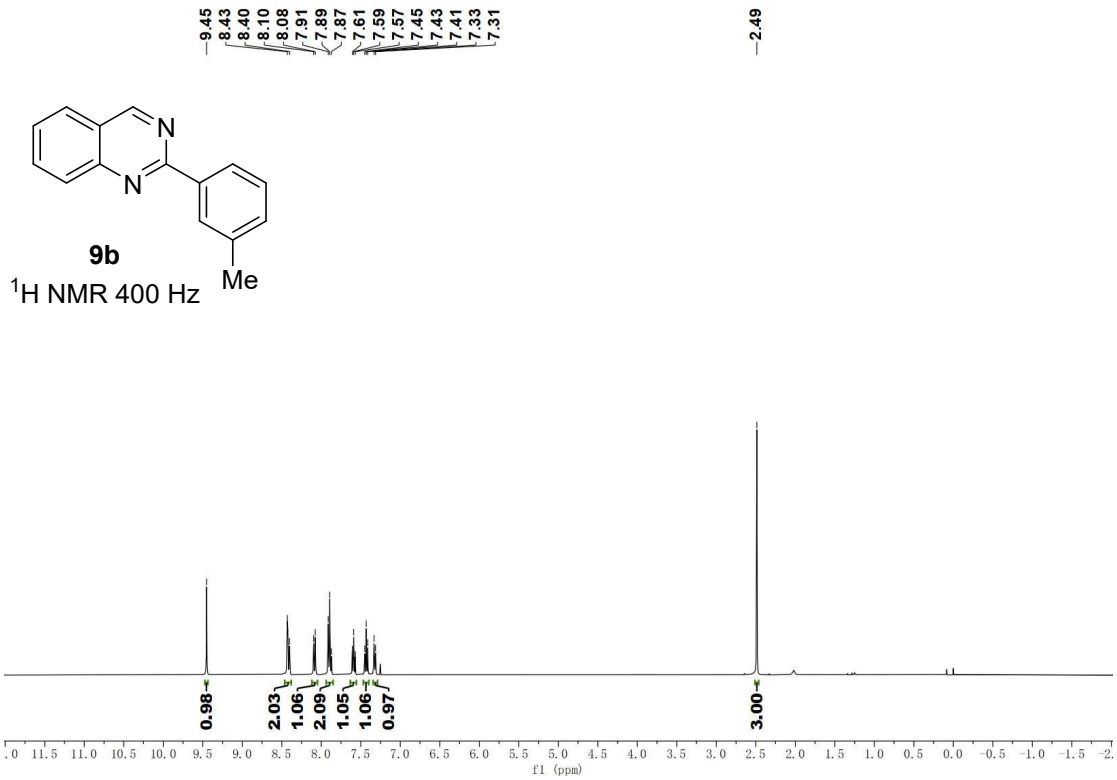




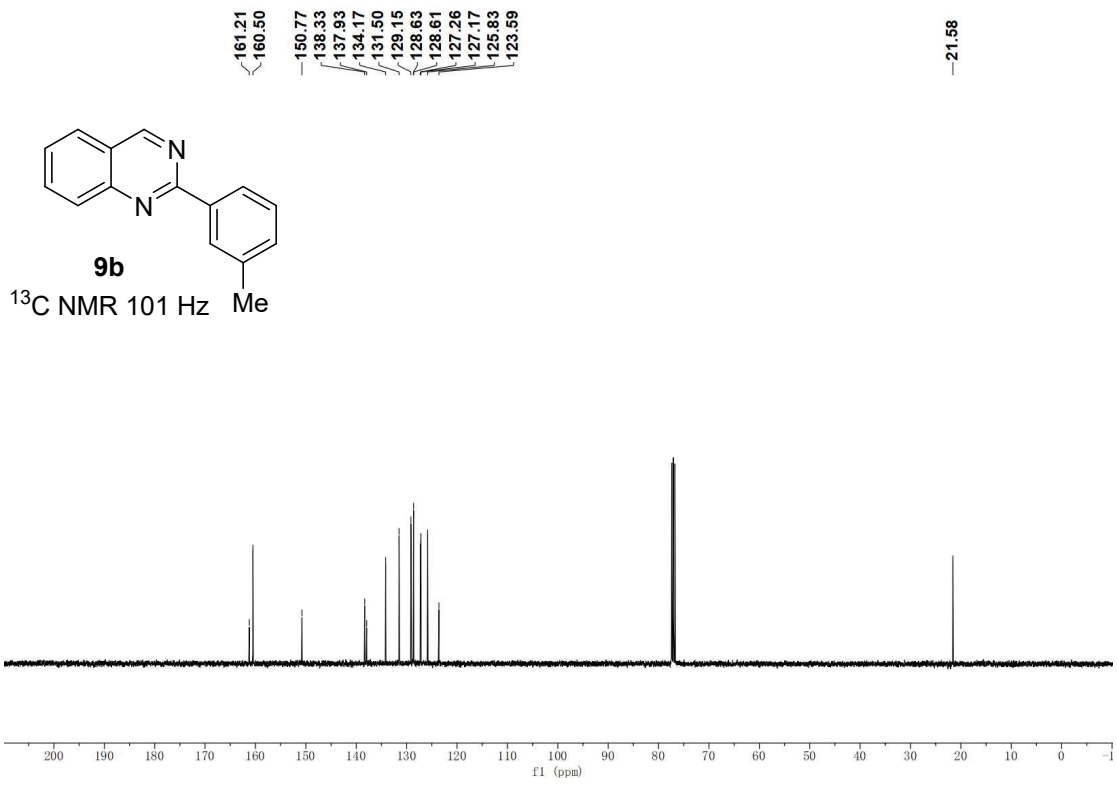
9a

^{13}C NMR 101 Hz

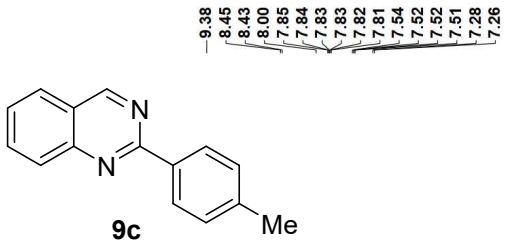




^{1}H NMR 400 Hz

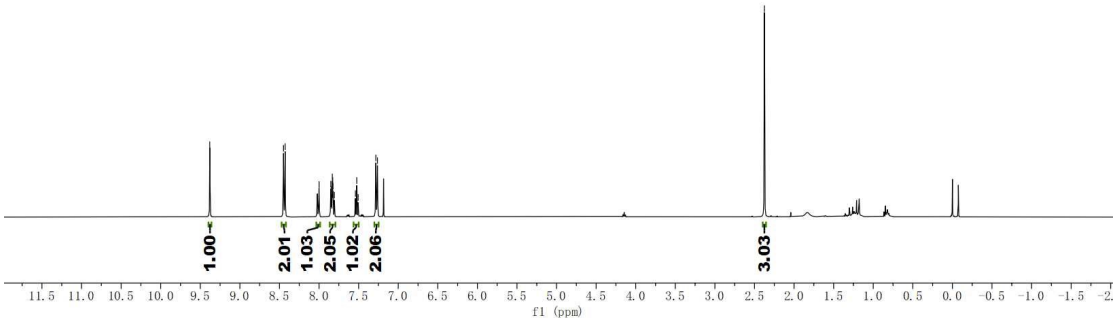


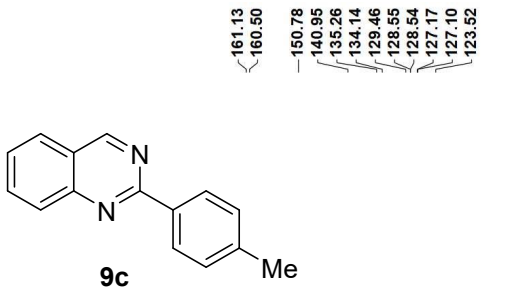
^{13}C NMR 101 Hz



9c

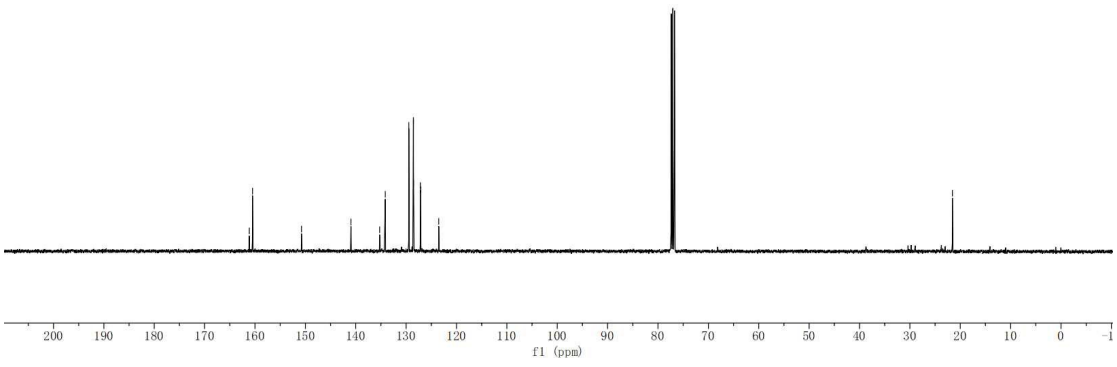
^{1}H NMR 400 Hz

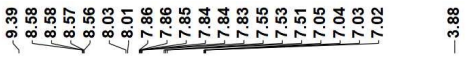


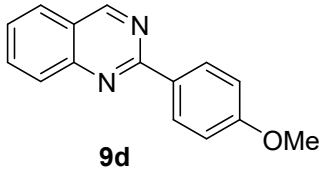


9c

^{13}C NMR 101 Hz

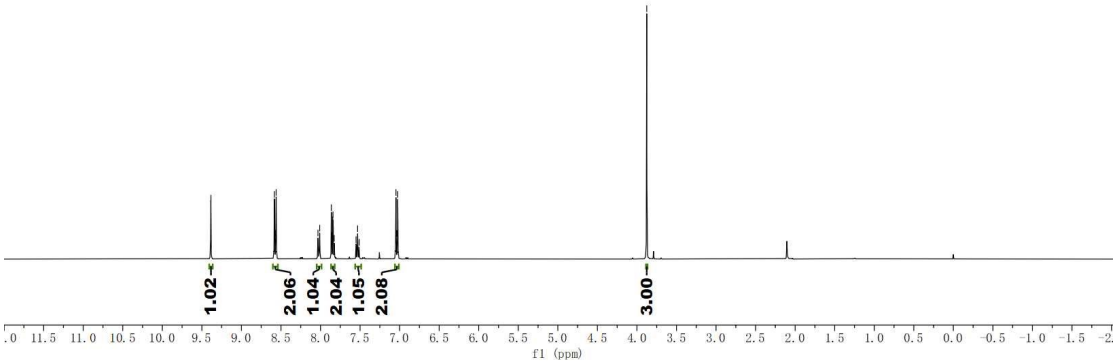


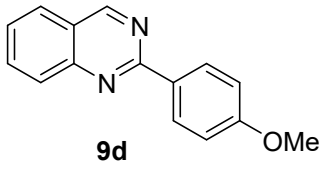




9d

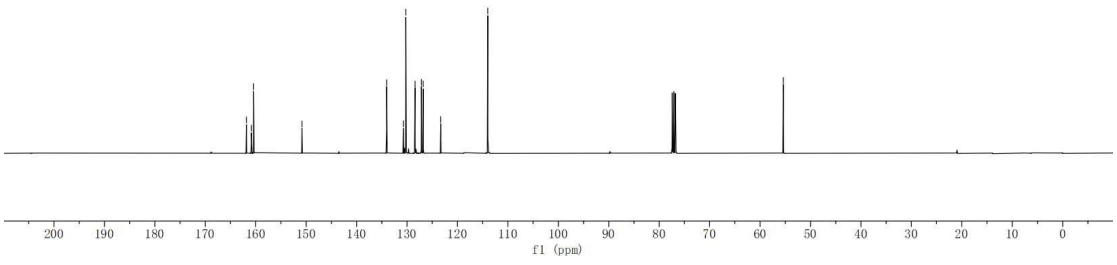
^{1}H NMR 400 Hz

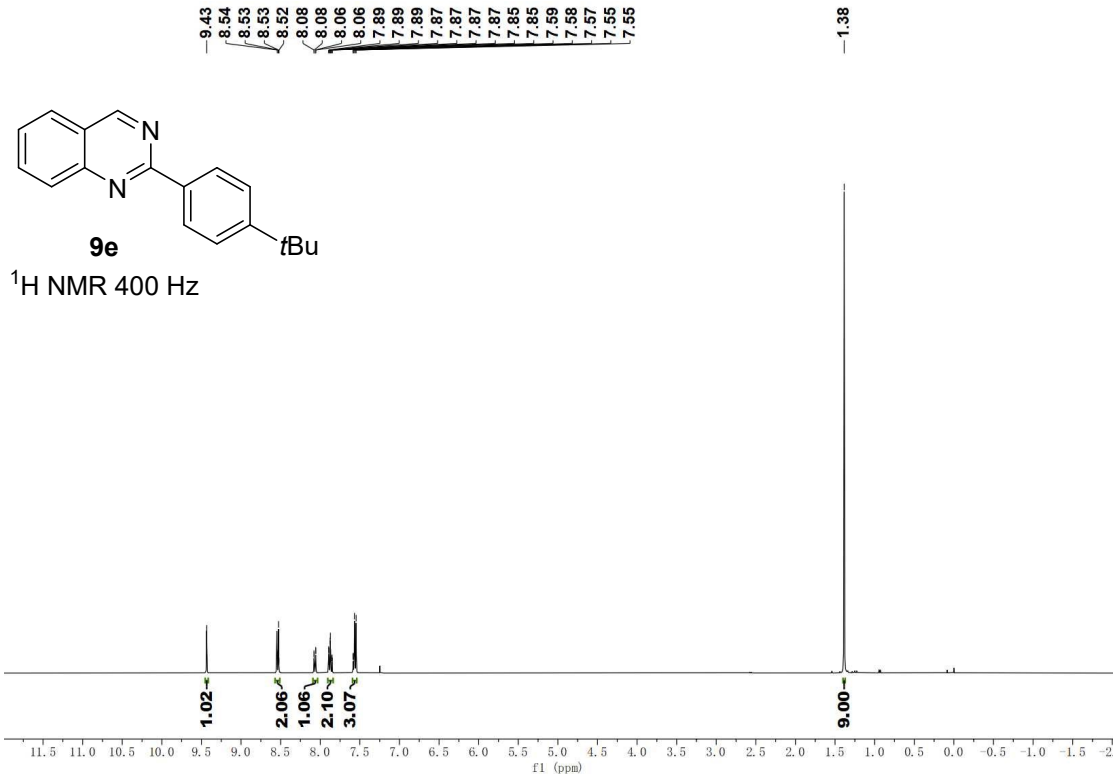




9d

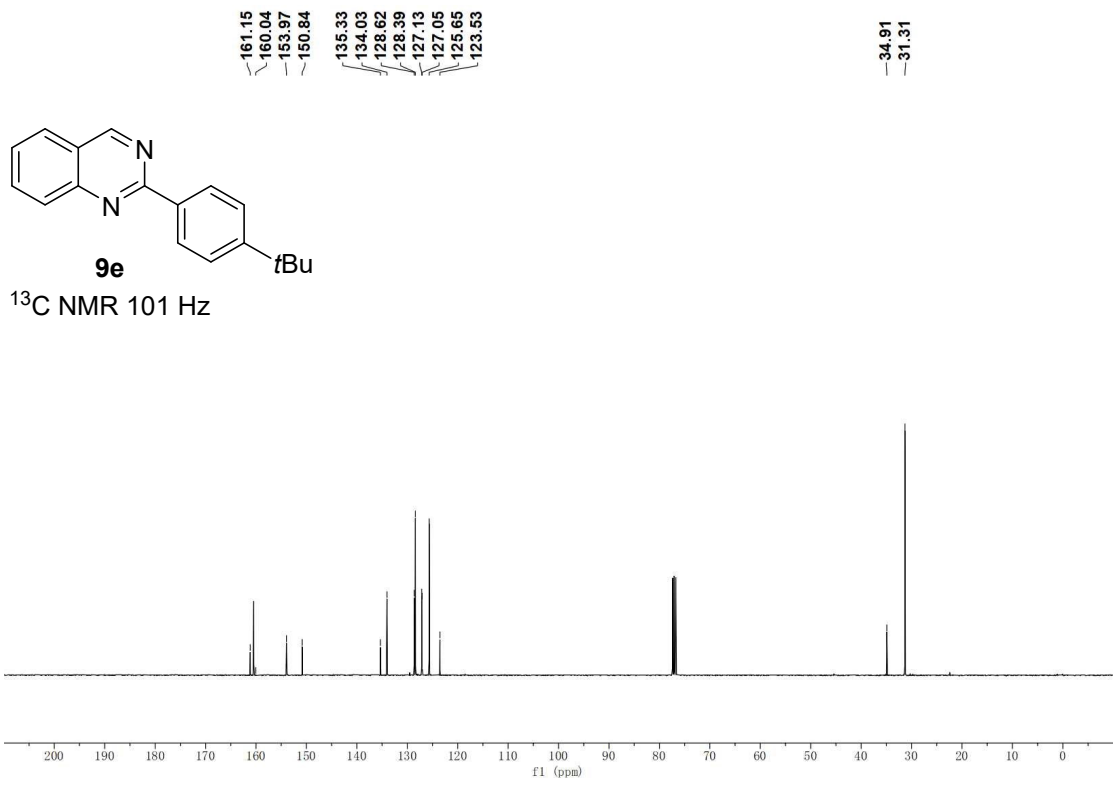
^{13}C NMR 101 Hz





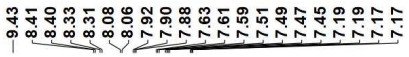
9e *t*Bu

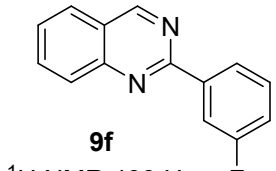
^{1}H NMR 400 Hz



9e *t*Bu

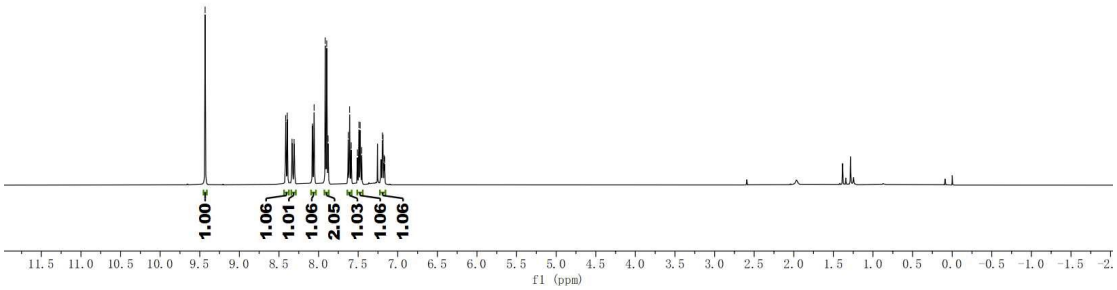
^{13}C NMR 101 Hz

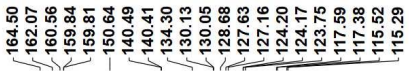


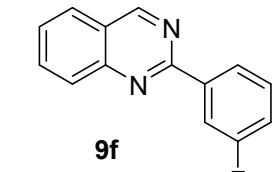


9f

^{1}H NMR 400 Hz F

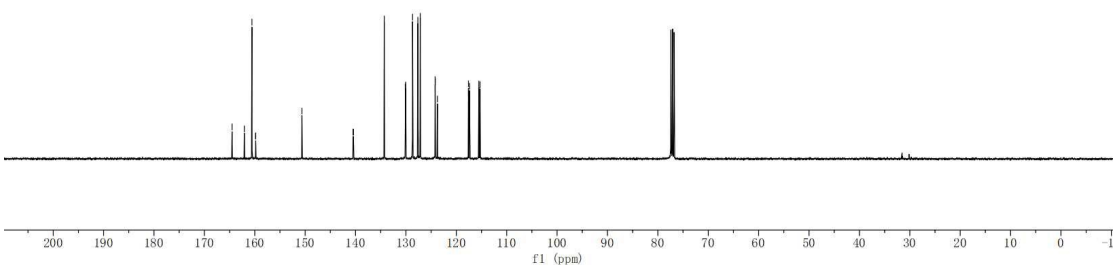


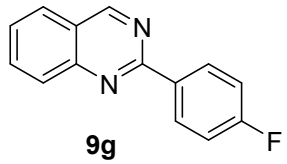




9f

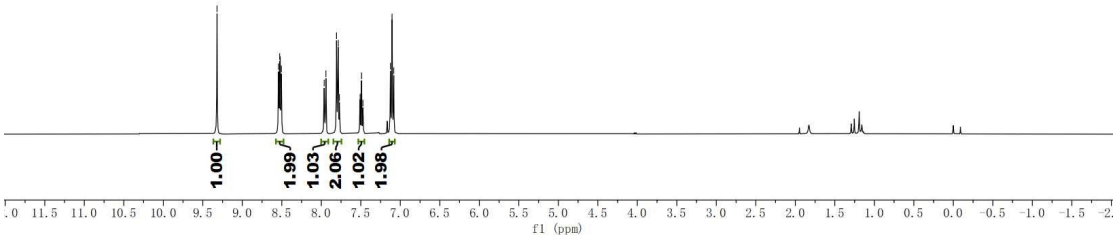
^{13}C NMR 101 Hz F

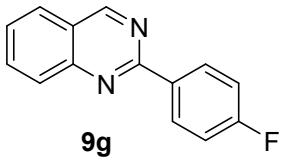




9g

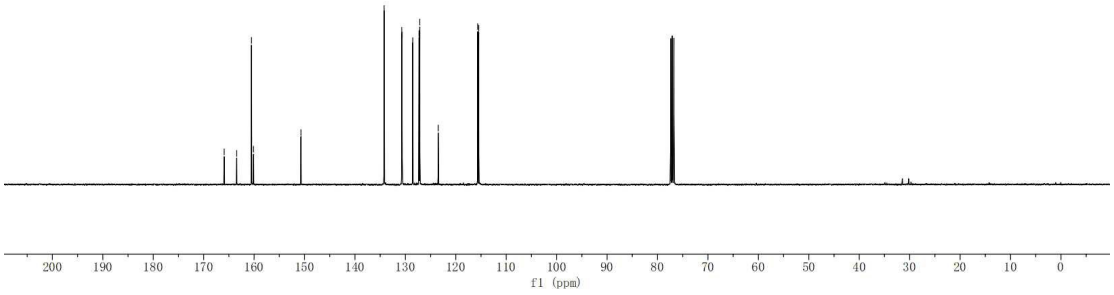
^{1}H NMR 400 Hz

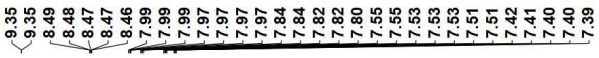


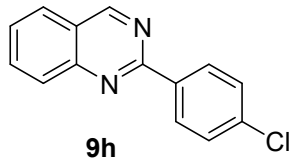


9g

^{13}C NMR 101 Hz

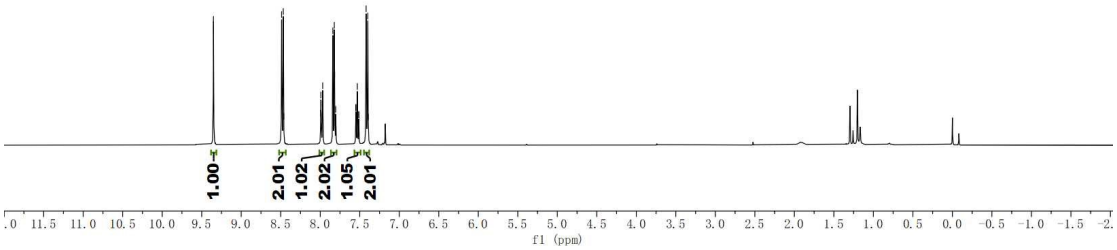


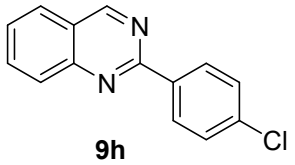




9h

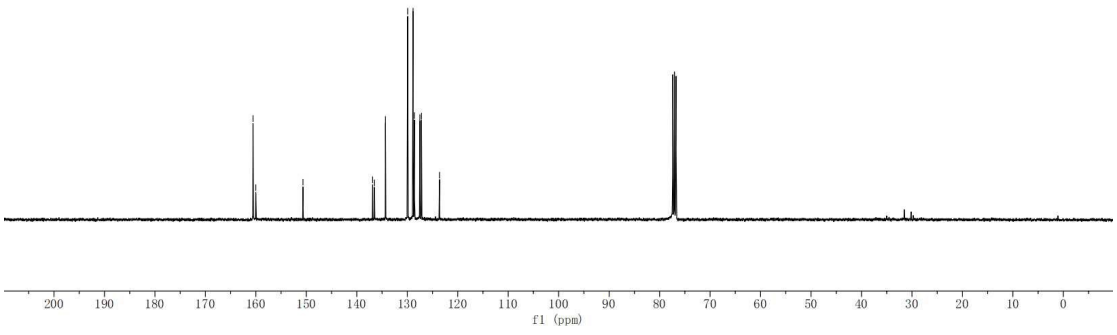
^{1}H NMR 400 Hz

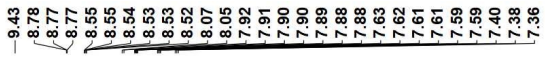


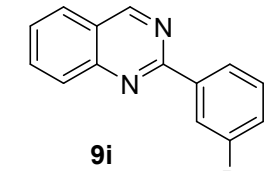


9h

^{13}C NMR 101 Hz

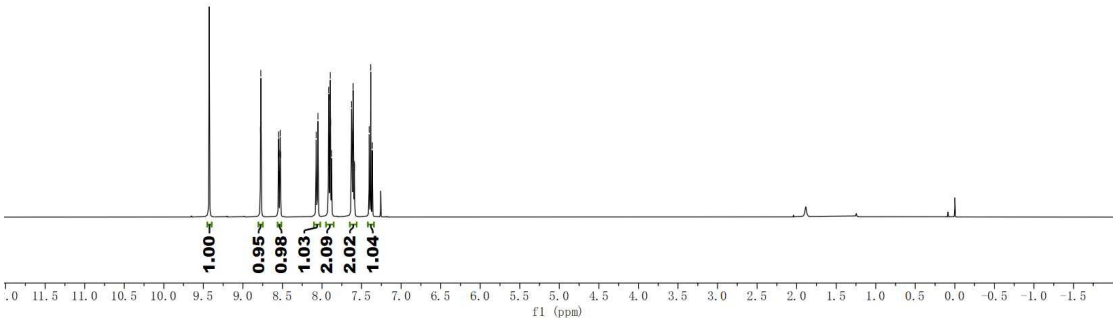


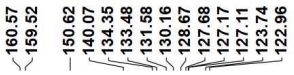


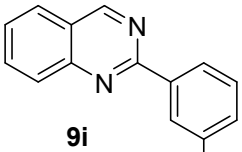


9i

^{1}H NMR 400 Hz

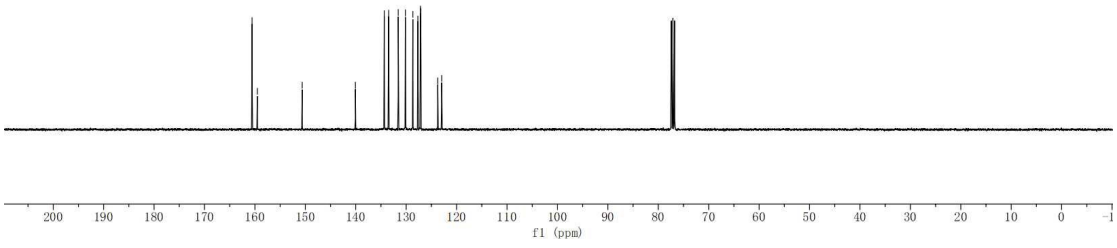


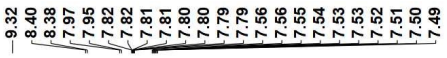


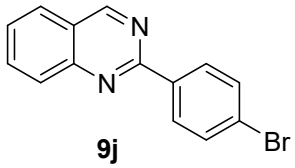


9i

^{13}C NMR 101 Hz

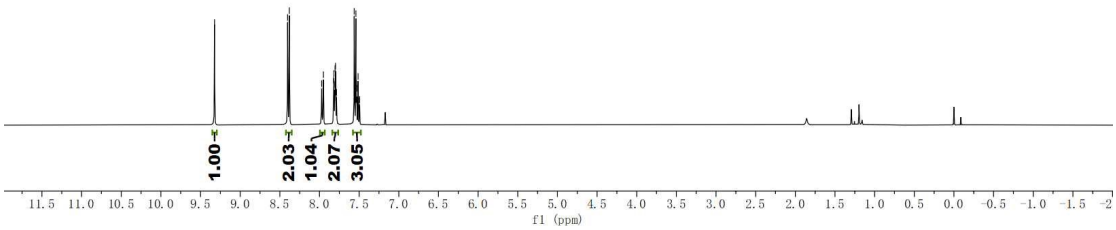


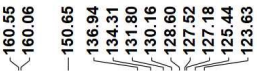


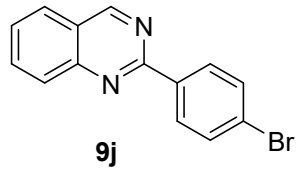


9j

^{1}H NMR 400 Hz

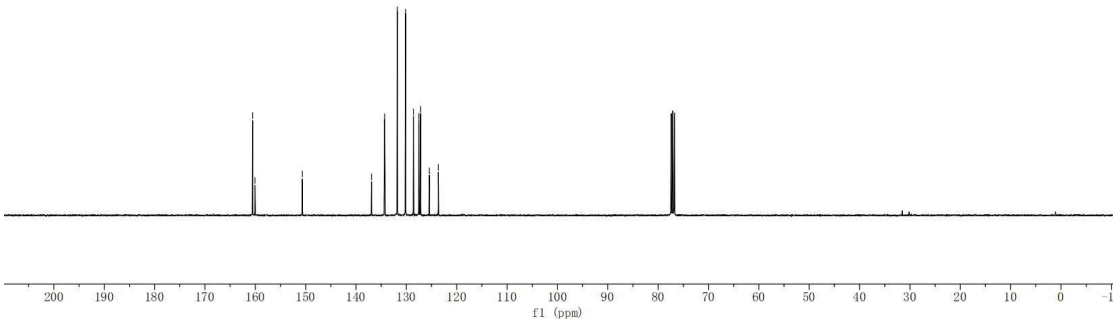


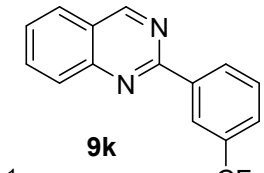




9j

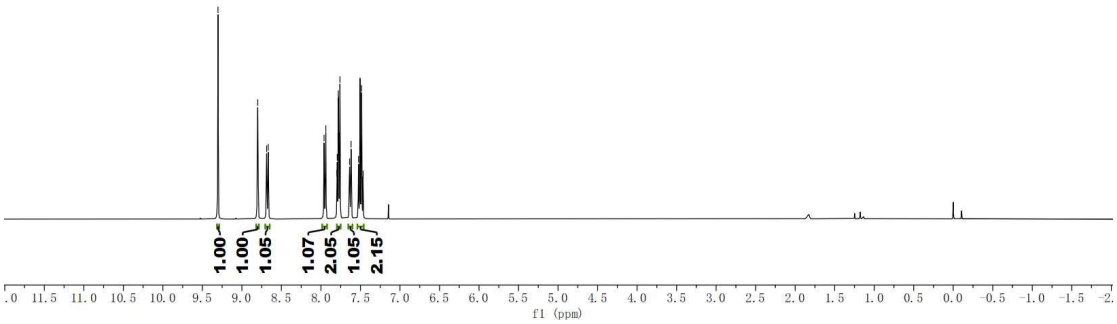
^{13}C NMR 101 Hz

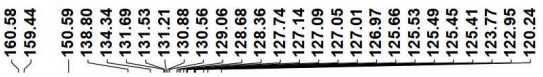


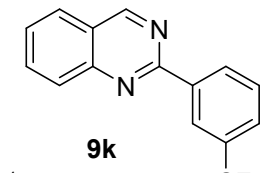


9k

^{1}H NMR 400 Hz

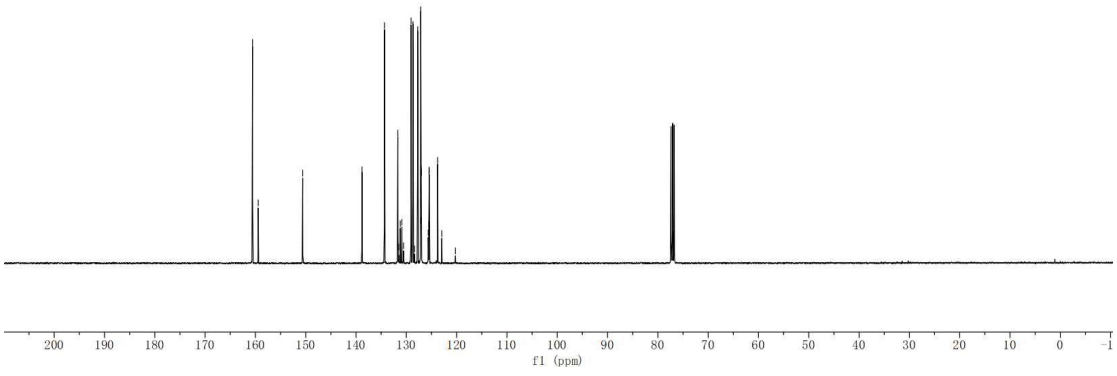


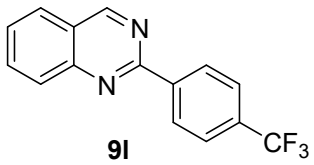




9k

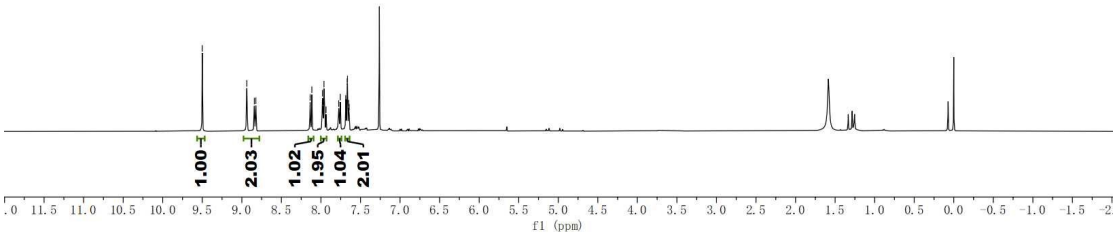
^{1}H NMR 400 Hz

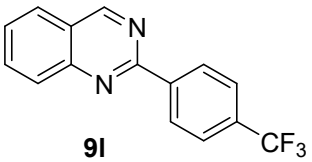




9l

^{1}H NMR 400 Hz





9l

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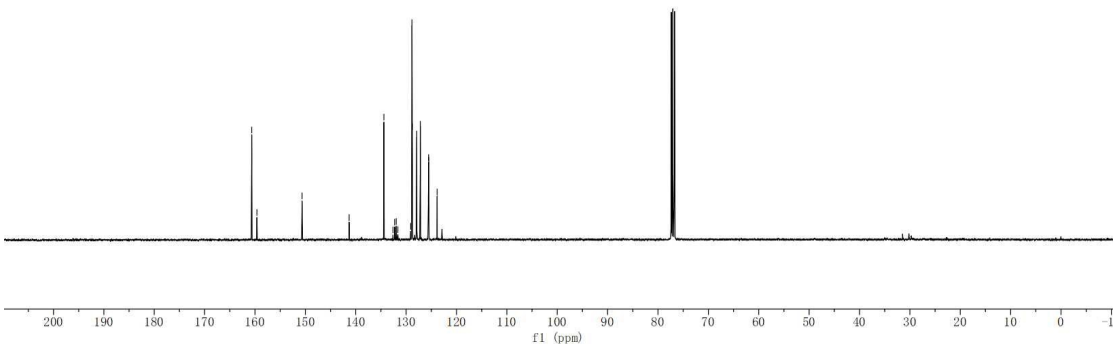
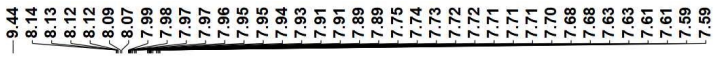
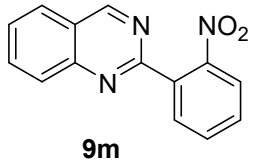
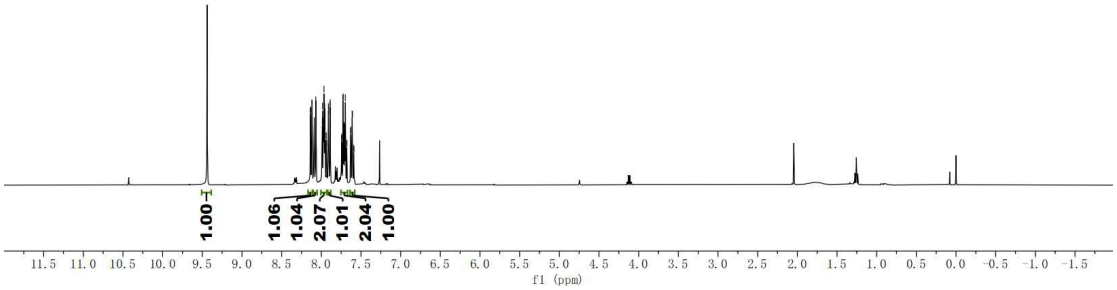


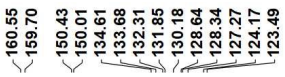


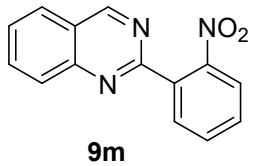


9m

^{1}H NMR 400 Hz

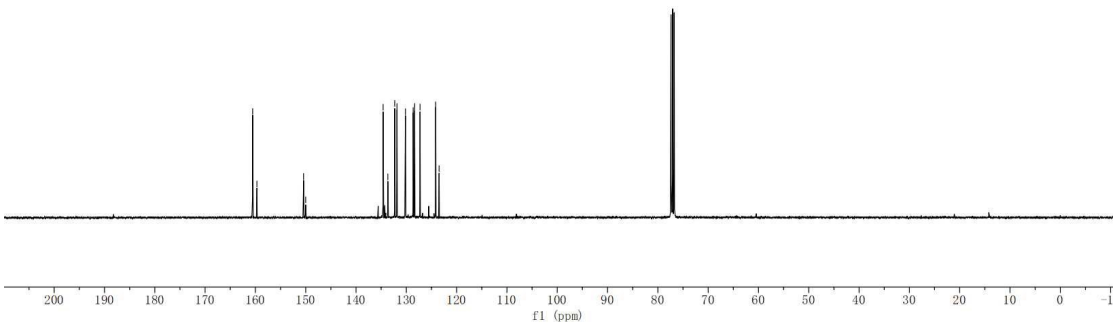


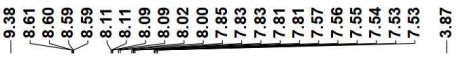


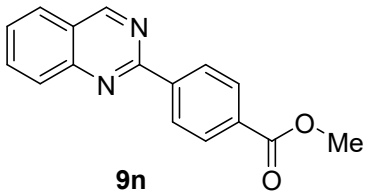


9m

^{13}C NMR 101 Hz

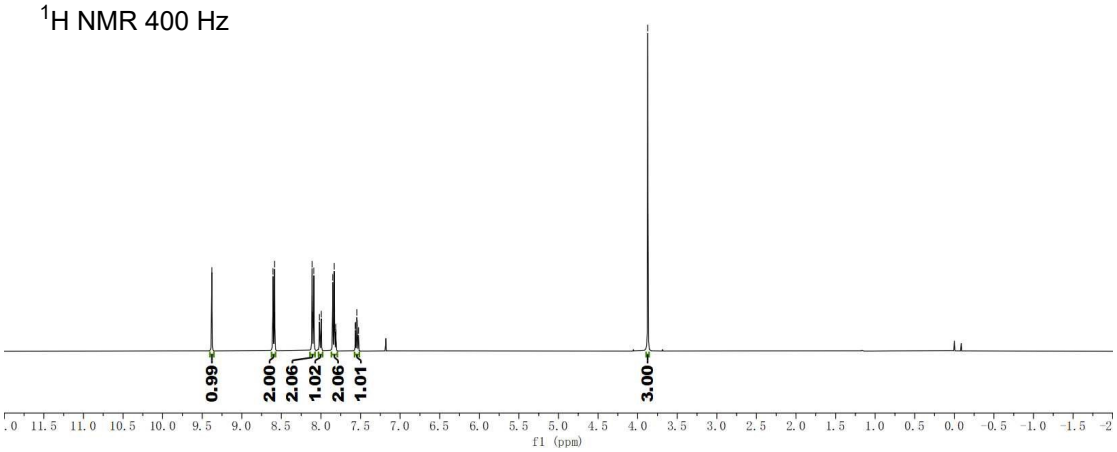


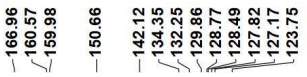


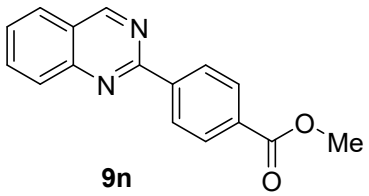


9n

^{1}H NMR 400 Hz

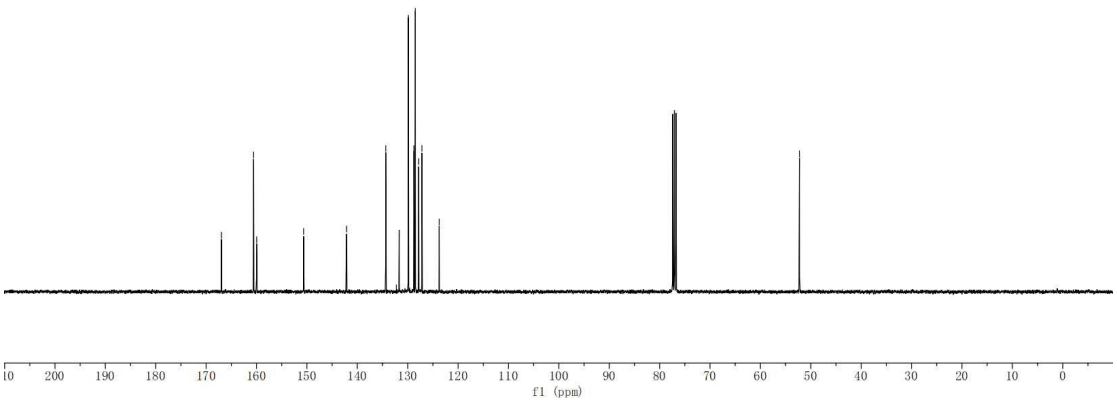


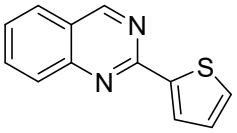




9n

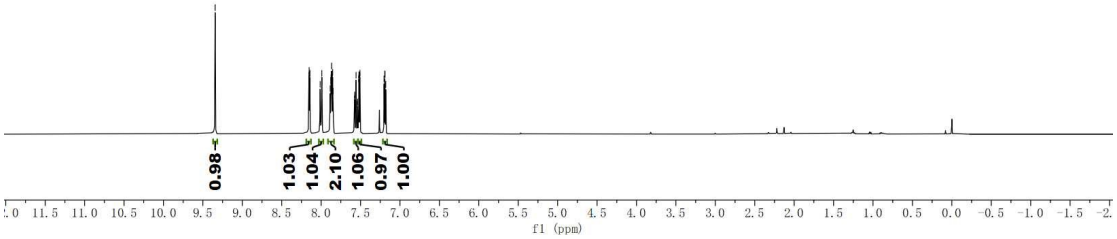
^{13}C NMR 101 Hz

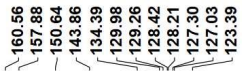


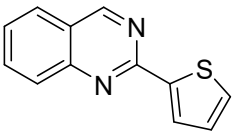


9o

^{1}H NMR 400 Hz

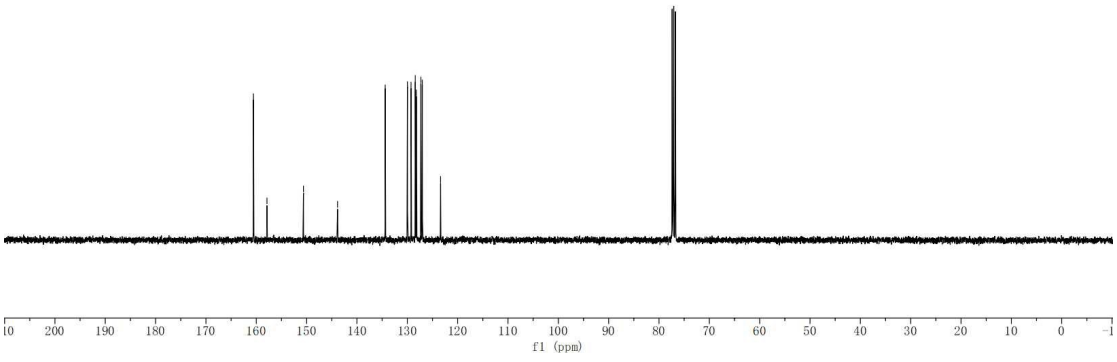


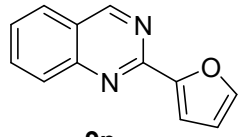




9o

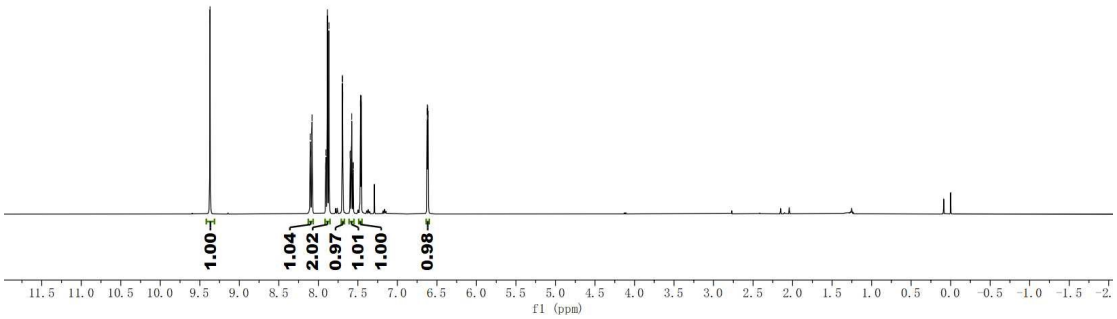
^{13}C NMR 101 Hz

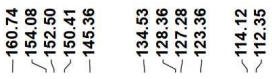


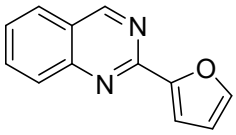


9p

^{1}H NMR 400 Hz

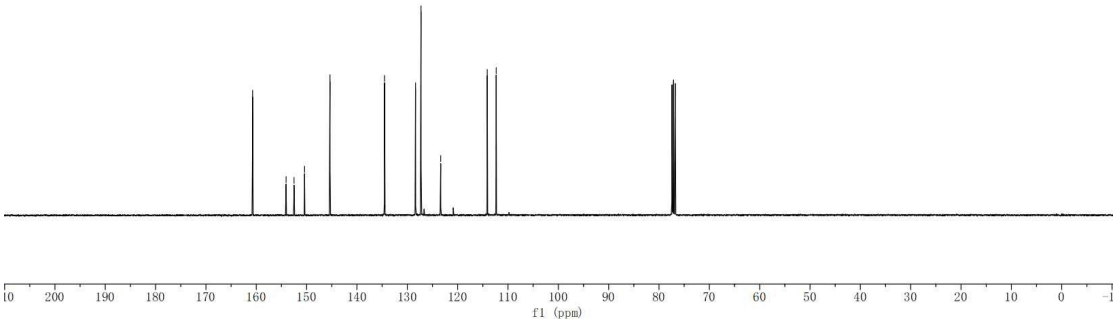


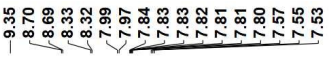


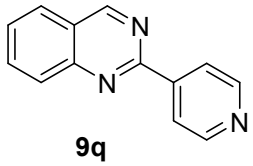


9p

^{13}C NMR 101 Hz

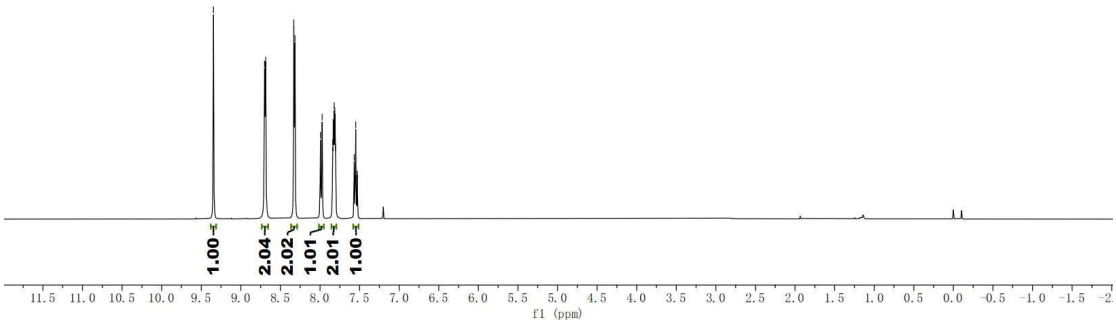


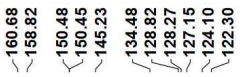


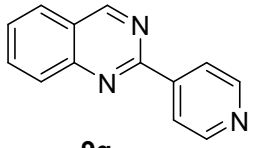


9q

^{1}H NMR 400 Hz

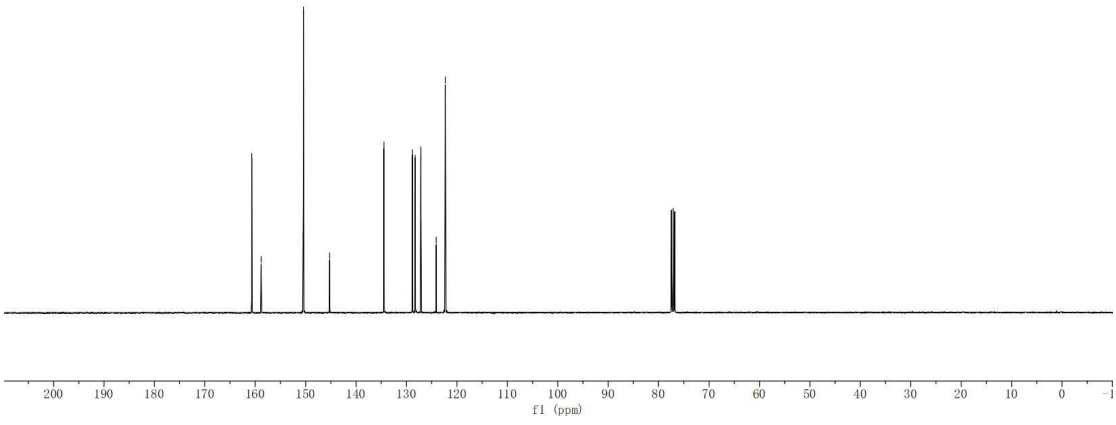


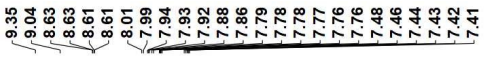


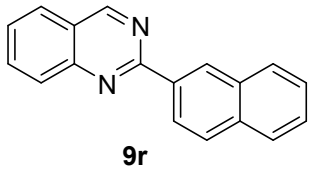


9q

^{13}C NMR 101 Hz

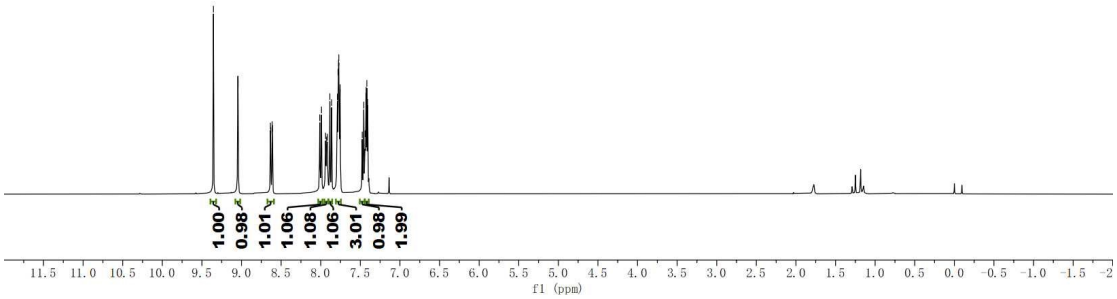


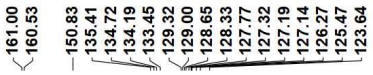


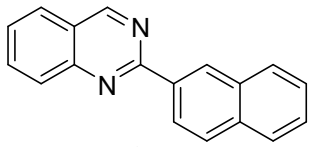


9r

^{1}H NMR 400 Hz

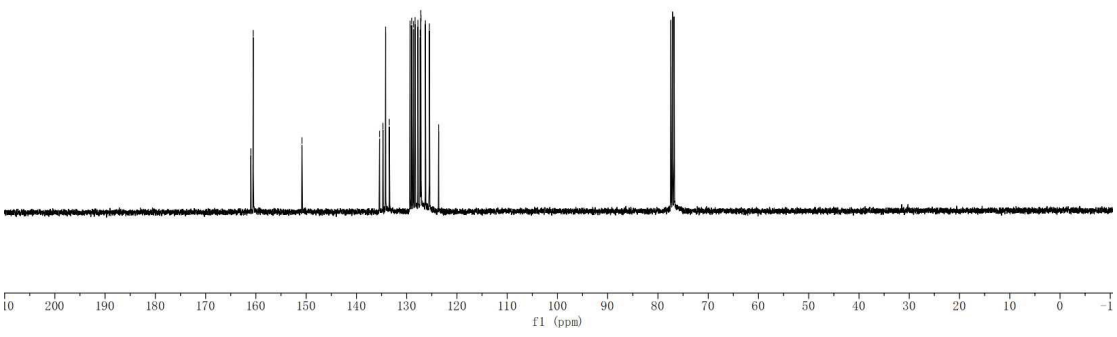






9r

^{13}C NMR 101 Hz



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