Supporting Information

Decatungstate-Photocatalyzed Direct Acylation of *N*-Heterocycles with Aldehydes

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1. General Information

1.1 Materials and instruments

All reagents were purchased from commercial suppliers and used without further purification unless otherwise stated. TLC was performed on silica gel plates (GF254, 200-300 mesh) using UV light (254/366 nm) for detection. Products were purified by column chromatography using silica gel (200-300 mesh) purchased from Qing Dao Hai Yang Chemical Industry Co. The ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on Bruker Avance 400 MHz or 600 MHz spectrometer. Proton chemical shifts (δ) were reported in parts per million (ppm) using tetramethylsilane as an internal standard. All NMR spectra were recorded in $CDCl_3$ at room temperature (20 ± 3°C). High-resolution mass spectra (HRMS) were acquired using an Agilent Infinity II Q-TOF G6545 equipped with electrospray ionization (ESI) technique.

1.2 The spectrum of our lamp and the visible-light irradiation instrument

The photochemical reaction was carried out under visible light irradiation by a blue LED at 25 ºC. RLH-18 8-position Photo Reaction System manufactured by Beijing Roger Tech Ltd. was used in this system. Eight 10 W purple LEDs were equipped in this Photo reactor. The purple LED's energy peak wavelength is 390 nm, peak width at half-height is 17.8 nm, and irradiance @7 W is 61.69 mW/cm^2. The reaction vessels are borosilicate glass test tubes and the distance between them and the lamp is 15 mm, no filter is applied.

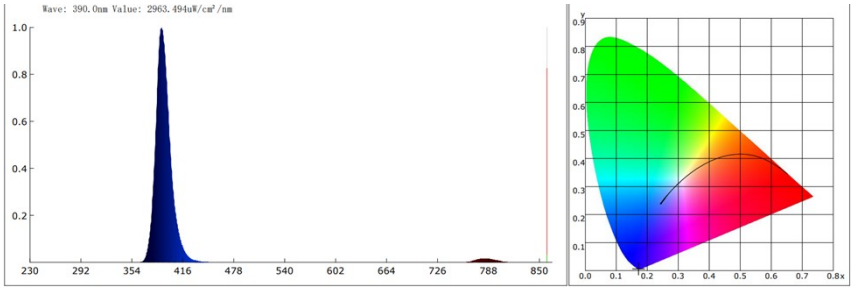


Figure S1. The spectrum of our lamp (390 nm LED)

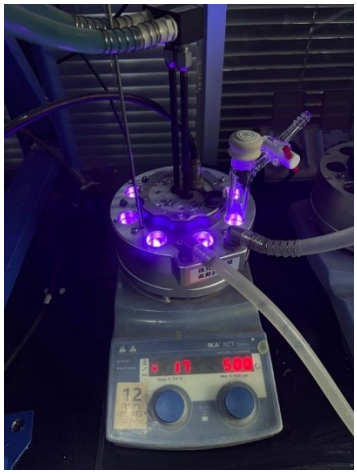
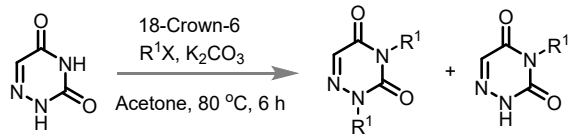


Figure S2. The 390 nm irradiation instrument

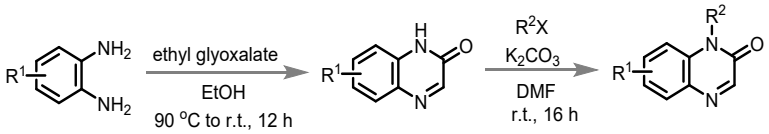
1.3 General procedure for the synthesis of azauracil substrates[1]



Scheme S1. General experimental procedures for azauracil substrates

A solution of 1,2,4-triazin-3,5(2*H*,4*H*)-dione (5 mmol, 1 equiv.) in dry acetone (30 mL) was mixed with anhydrous potassium carbonate (5 mmol, 1 equiv.) and a catalytic amount of 18-crown-6-ether (0.5 mmol, 0.1 equiv). Then benzyl bromide (5 mmol, 1 equiv.) was added and the mixture was refluxed for 6 h (monitored by TLC). The solvent was evaporated to afford a crude product which was then applied to a silica gel column. The column was eluted with a mixture of petroleum ether and ethyl acetate (50:1) and the appropriate fractions were combined and evaporated.

1.4 General procedure for the synthesis of quinoxalinone substrates[2]



Scheme S2. General experimental procedures for quinoxalinone substrates

Ethyl glyoxalate (5.5 mmol, 1.1 equiv.) was added dropwise to a stirring solution of *o*-arylenediamine (5 mmol, 1 equiv.) in ethanol (30 ml). The reaction mixture was allowed to stir at 80 °C for 1 h, then stirred at room temperature overnight. After the reaction, the precipitated solid was filtered, washed with ethanol, and then dried to obtain quinoxalin-2(1*H*)-one. The crude product did not need to be further purified and could be directly used in the next step. To a suspension of quinoxalinone (5 mmol, 1 equiv.) in DMF (30 ml) was added potassium carbonate (6 mmol, 1.2 equiv.) and the corresponding alkyl halides (8 mmol, 1.6 equiv.). The mixture was stirred at room temperature overnight. Ethyl acetate and water were added. The aqueous layer was extracted twice with EtOAc. The combined organic layers were washed with a saturated solution of NaCl, dried over $MgSO_4$, filtered, and evaporated under reduced pressure. The residue was purified by flash chromatography over silica gel to afford the desired product *N*-alkyl quinoxalinone.

1.5 Preparation of photocatalyst tetrabutylammonium decatungstate (TBADT)[3]

In a 250 mL round-bottom flask, 16 g of sodium tungstate dihydrate (approximately 48.5 mmol) was solubilized in 100 mL of deionized water. The solution's pH was meticulously brought down to 2 by the careful addition of approximately 30 mL of 3.0 M HCl, introduced drop by drop while maintaining vigorous agitation. During this process, the solution acquired a subtle green hue. After the pH adjustment, the flask containing the tungstate solution was

positioned in an oil bath preheated to 85 °C and maintained under these conditions for 20 minutes. In a separate vessel, 6 g of tetrabutylammonium bromide was dissolved in 10 mL of deionized water. This solution was then gradually transferred into the preheated flask within the oil bath, which was kept at a steady 85 °C, with continuous stirring for an additional 30 minutes. This procedure resulted in the formation of a white suspension, indicative of tetrabutylammonium decatungstate (TBADT). Once the reaction was complete, the flask was removed from the oil bath and allowed to reach room temperature. The suspension was then subjected to filtration to separate the solid phase. The recovered solid was thoroughly washed, first with water and then with ethanol, to eliminate any impurities. The final step involved drying the solid under a vacuum at 60 °C for 12 hours, yielding a pale yellow solid. The synthesized TBADT was of sufficient purity to be utilized directly in subsequent applications without the need for additional purification steps.

1.6 UV-vis absorption spectrum of TBADT

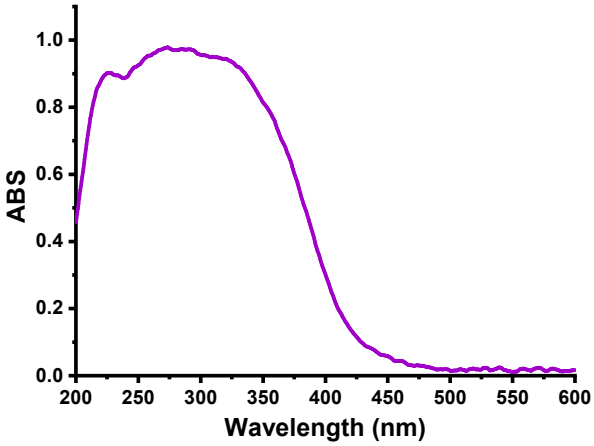
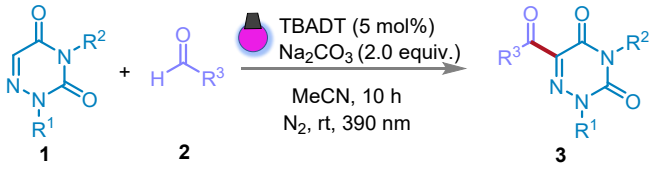


Figure S3. Absorbance spectra of TBADT

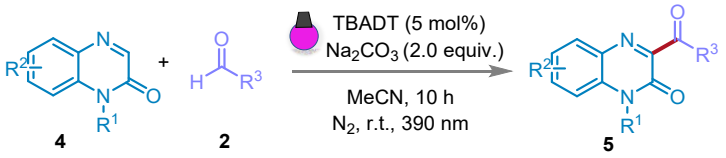
2. Experimental Procedures

2.1 General experimental procedures for the desired product



Scheme S3. General experimental procedures for acylated azauracils

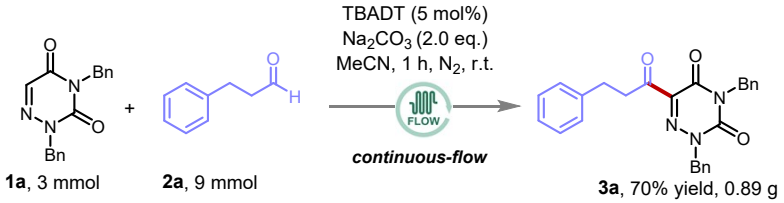
The mixture of azauracil **1** (0.2 mmol), aldehyde **2** (0.6 mmol), TBADT (5 mol%), Na_2CO_3 (2.0 equiv.) and MeCN (2.0 mL) were sequentially added in a 25 mL reaction vessel. Then the reaction vessel was irradiated with 10 W purple LED (390 nm) at room temperature under an N_2 atmosphere for 10 h. After the reaction, the solvent was evaporated under vacuum. The residue was purified by chromatography on silica gel using petroleum ether/ethyl acetate as eluent to afford the desired product **3**.



Scheme S4. General experimental procedures for acylated quinoxalinones

The mixture of quinoxalinone **4** (0.2 mmol) aldehyde **2** (0.6 mmol), TBADT (5 mol%), Na_2CO_3 (2.0 equiv.) and MeCN (2.0 mL) were sequentially added in a 25 mL reaction vessel. Then the reaction vessel was irradiated with 10 W purple LED (390 nm) at room temperature under an N_2 atmosphere for 10 h. After the reaction, the solvent was evaporated under vacuum. The residue was purified by chromatography on silica gel using petroleum ether/ethyl acetate as eluent to afford the desired product **5**.

2.2 Synthesis applications



Scheme S5. Scale-up synthesis of **3a** by continuous-flow instrument

The scale-up synthesis of **3a** by continuous flow (PFA tubing, flow rate 4.0 mL/min): **1a** (3 mmol, 1 equiv), **2a** (9 mmol, 3.0 eq), TBADT (5 mol%), Na_2CO_3 (2.0 equiv.) and MeCN (30 mL) were sequentially added into the reaction flask. Then a continuous-flow instrument was connected, and the reaction system was replaced with an N_2 atmosphere. The reaction system was pushed into the continuous-flow instrument by a peristaltic pump and reacted under purple LED (8 × 10 W) irradiation for 1 h. The isolated yield of **3a** (70%, 0.89 g) was given. The continuous-flow instrument is shown in Figure S4.

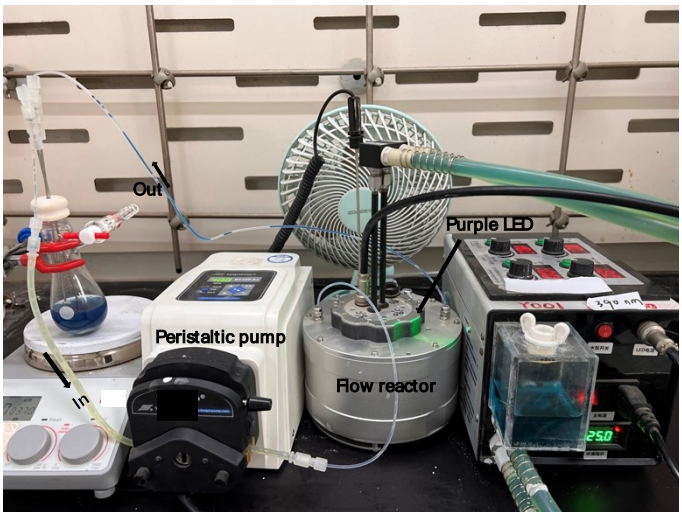
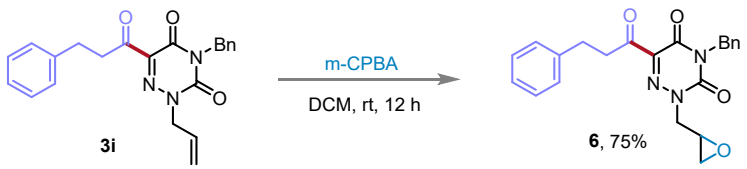
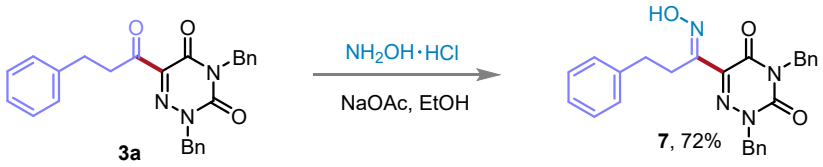


Figure S4. The continuous-flow instrument



Scheme S6. Epoxidation reaction of **3i**

A mixture of **3i** (0.2 mmol) and an excess of m-CPBA (0.4 mmol) was stirred at room temperature for 10 h.[2] The mixture was poured into saturated $NaHCO_3$ (aq.) and extracted with ethyl acetate. The combined extracts were dried over anhydrous Na_2SO_4, filtered, and evaporated. The residue was purified by column chromatography to afford **6** as colorless oil in 75% yield.



Scheme S7. Oximation reaction of **3a**

The reaction was carried out following a modified procedure from Wang et al.[4] To a solution of hydroxylamine hydrochloride (69.5 mg, 1.0 mmol, 5 equiv) in water was added a solution of sodium acetate (114.8 mg, 1.4 mmol, 7 equiv) in ethanol. The mixture was stirred at room temperature while **3a** (88.1 mg, 0.2 mmol, 1 equiv) was added as a solution in ethanol. The mixture was stirred overnight and concentrated in vacuo. Then, the mixture was extracted with ethyl acetate 3 times and the combined extracts were washed with water and brine, dried ($MgSO_4$), filtered, and concentrated in vacuo. The crude material was purified by flash chromatography on silica gel to afford title compound **7** as a white solid (66.5 mg, 72%).

2.3 Catalyst recycling experiments

The mixture of **1a** (0.2 mmol), **2a** (3 equiv.), Na_2CO_3 (2.0 equiv.), TBADT (5 mol%) and MeCN (2 mL) were sequentially added in a 20 mL reaction vial. The vessel was then evacuated and filled with N_2 through a Freeze-Pump-Thaw degassing procedure. After being stirred for 10 hours at room temperature under irradiation of 390 nm (10 W). After the reaction, 15 mL diethyl ether was added to the reaction mixture to ensure that TBADT was completely precipitated from the reaction solution. The resulting suspension was filtered through Celite and then washed with EA (10 mL). The residue was purified by flash chromatography (petroleum ether/ethyl acetate = 10:1) to provide product **3a** in 77% yield. Then the residual TBADT in Celite was washed by MeCN (10 mL) to give a TBADT solution as filtrate, which was evaporated to afford the recycled TBADT. Then, the recycled TBADT can be directly used for the next run. (The mass of the initial catalyst is 33 mg. After each recovery, the catalyst mass was 29 mg, 24 mg, and 20 mg, respectively). Figure S5 illustrates that the mass loss rate

of TBADT reached 39.3% upon the catalyst's fourth usage. The diminished catalytic performance could primarily be attributed to the progressive loss of the catalyst during the recovery process.

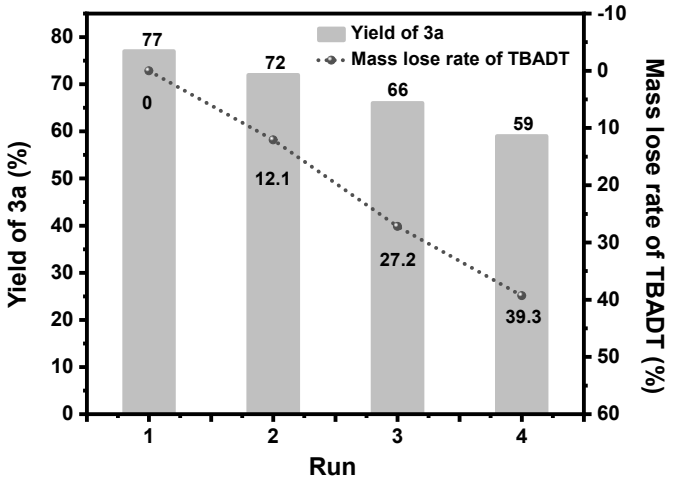
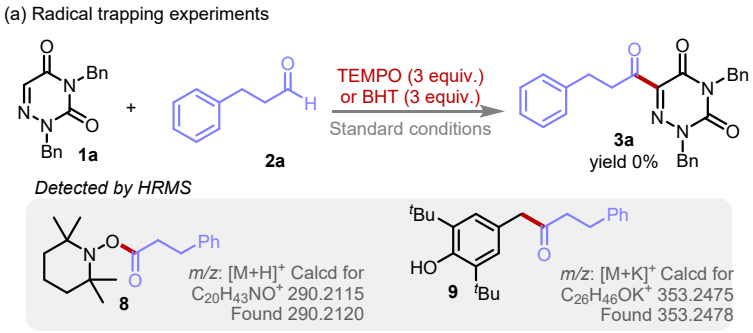


Figure S5. Catalyst recycling experiments.

2.4 Control experiments



Scheme S8. Control experiments

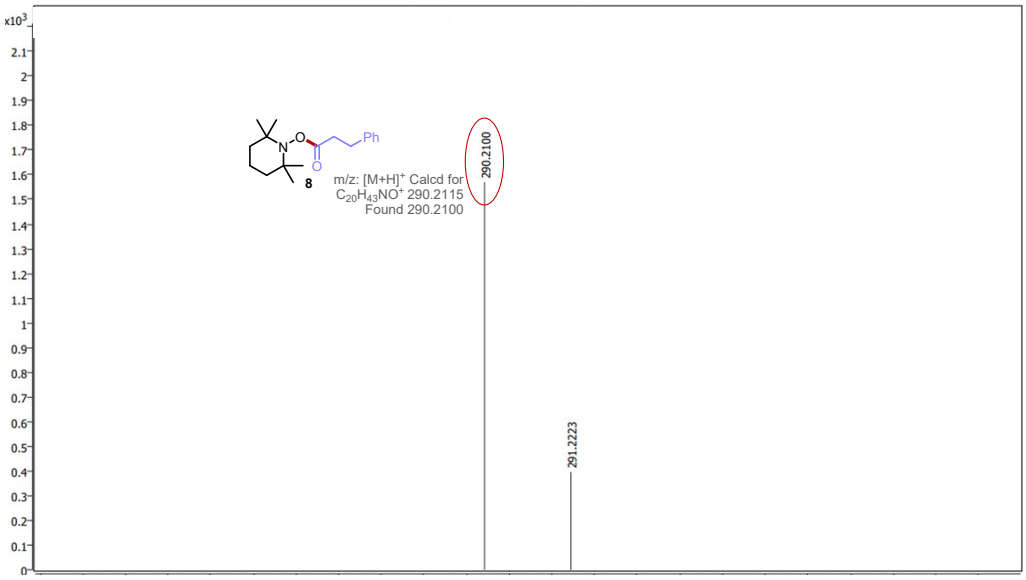


Figure S6. The HRMS analysis of compound **8**

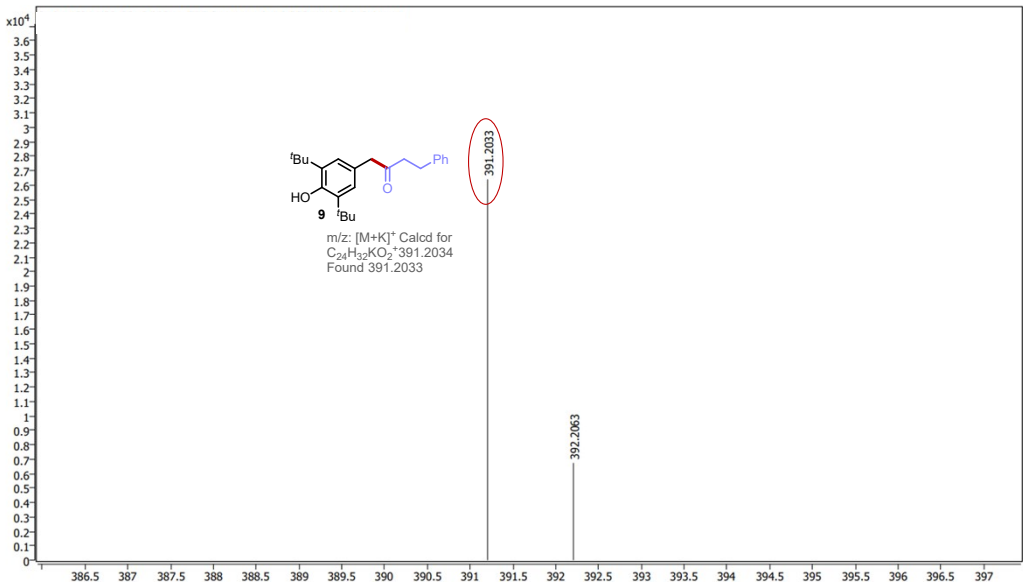


Figure S7. The HRMS analysis of compound **9**

2.5 Detection of H_2 generation

To confirm the generation of H_2 in our experimental system, a mixture of azauracil **1a** (2 mmol), aldehyde **2a** (6 mmol), TBADT (5 mol%), Na_2CO_3 (2.0 equiv.), and CH_3CN (15 mL) were sequentially added in a 50 mL reaction vessel. The Freeze-Pump-Thaw technique was employed for the degassing process. After the reaction reached completion, the evolved gas phase was captured for subsequent analysis. Gas chromatographic assessment, employing a thermal conductivity detector (TCD), facilitated the detection of H_2. As delineated in Figure S7, a distinct peak at a retention time of 1.3 minutes was indicative of H_2 production, providing conclusive evidence for its presence.

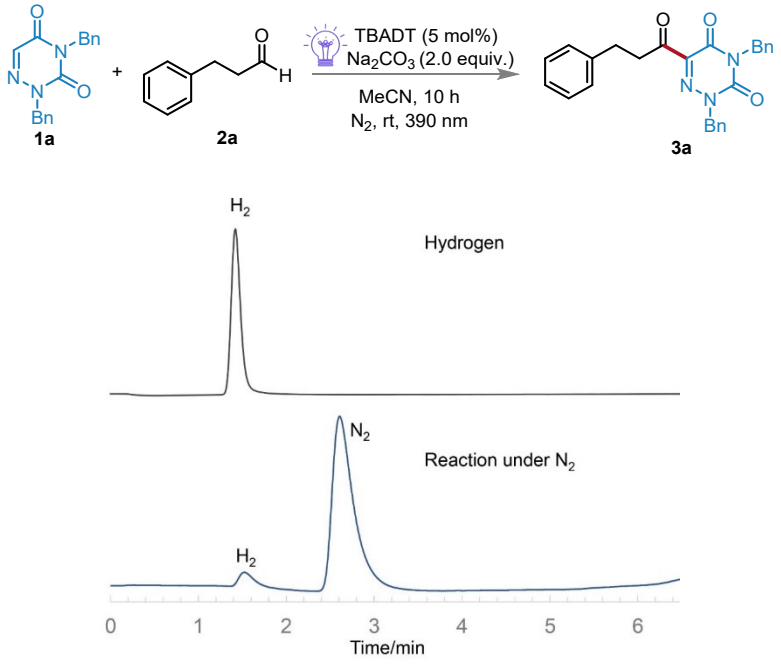
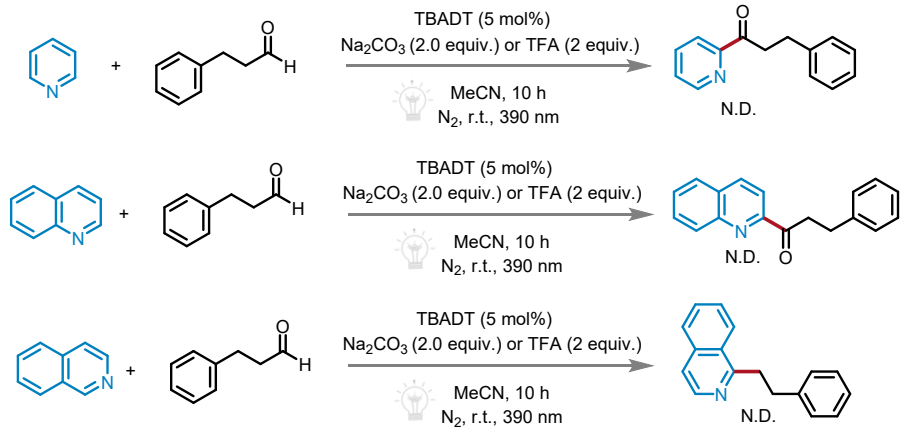


Figure S8. Detection of H_2 Generation

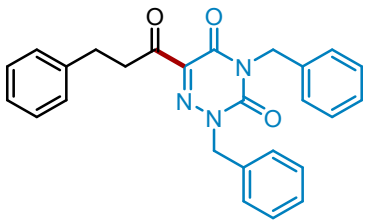
2.6 Ineffective transformations



Scheme S9. Ineffective heterocyclic substrates

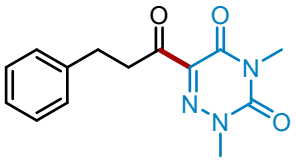
3. Characterization Data for Products

2,4-dibenzyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3a)



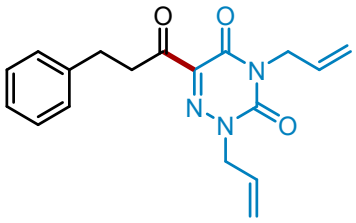
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (62.9 mg, 74% yield), mp 97 – 99 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.45 (m, 2H), 7.38 – 7.31 (m, 5H), 7.29 – 7.21 (m, 5H), 7.19 – 7.14 (m, 3H), 5.11 (s, 2H), 5.03 (s, 2H), 3.19 (t, *J* = 7.6 Hz, 2H), 2.95 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 186.5, 154.0, 148.5, 145.4, 139.7, 135.2, 135.0, 132.6, 130.4, 129.8, 129.3, 129.1, 128.9, 128.68, 128.66, 128.3, 55.8, 44.5, 21.9. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{26}H_{24}N_3O_3^+$, 426.1812; Found: 426.1814.

2,4-dimethyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3b)



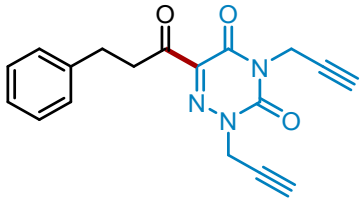
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (41.0 mg, 75% yield), mp 90 – 92 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 2H), 7.23 – 7.17 (m, 3H), 3.69 (s, 3H), 3.34 (s, 3H), 3.25 (t, *J* = 7.6 Hz, 2H), 2.99 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.1, 153.5, 148.8, 140.7, 136.8, 128.5, 126.2, 41.5, 40.4, 29.7, 27.4. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{14}H_{16}N_3O_3^+$, 274.1186; Found: 274.1189.

2,4-diallyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3c)



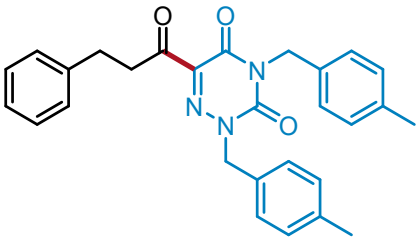
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow oil (46.2 mg, 71% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 2H), 7.23 – 7.16 (m, 3H), 5.93 (ddt, *J* = 16.1, 8.8, 5.5 Hz, 1H), 5.88 – 5.76 (m, 1H), 5.36 – 5.30 (m, 2H), 5.30 – 5.21 (m, 2H), 4.61 (dt, *J* = 6.2, 1.4 Hz, 2H), 4.52 (dt, *J* = 6.2, 1.3 Hz, 2H), 3.28 – 3.18 (t, *J* = 7.6 Hz, 2H), 2.99 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.1, 152.8, 148.0, 140.7, 137.1, 130.5, 129.8, 128.5, 126.2, 120.2, 120.1, 55.0, 43.2, 41.5, 29.8. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{18}H_{20}N_3O_3^+$, 326.1499; Found: 326.1505.

6-(3-phenylpropanoyl)-2,4-di(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (3d)



Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (41.7 mg, 65% yield), mp 97 – 99 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 (dd, *J* = 8.0, 6.7 Hz, 2H), 7.24 – 7.19 (m, 3H), 4.81 (d, *J* = 2.5 Hz, 2H), 4.68 (d, *J* = 2.5 Hz, 2H), 3.27 (t, *J* = 7.6 Hz, 2H), 3.01 (t, *J* = 7.6 Hz, 2H), 2.44 (t, *J* = 2.5 Hz, 1H), 2.23 (t, *J* = 2.5 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.6, 152.0, 147.1, 140.6, 137.5, 128.6, 128.5, 126.3, 75.7, 74.8, 72.2, 42.3, 41.5, 30.3, 29.7. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{18}H_{16}N_3O_3^+$, 322.1186; Found: 322.1189.

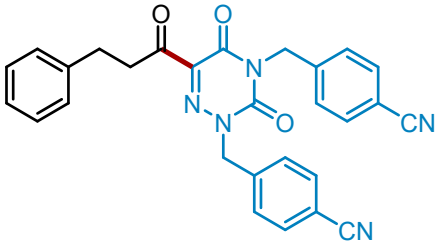
2,4-bis(4-methylbenzyl)-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3e)



Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (63.5 mg, 70% yield), mp 129 – 131 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.1 Hz, 2H), 7.35 – 7.29 (m, 4H), 7.23 (dd, *J* = 13.0, 7.5 Hz, 5H), 7.16 (d, *J* = 7.8 Hz, 2H), 5.15 (s, 2H), 5.07 (s,

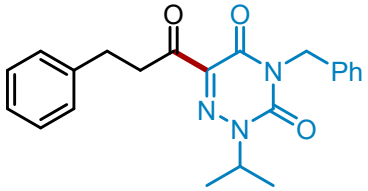
2H), 3.26 (t, *J* = 7.6 Hz, 2H), 3.02 (t, *J* = 7.6 Hz, 2H), 2.39 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.1, 153.0, 148.5, 140.8, 138.6, 138.2, 137.0, 132.2, 131.6, 129.8, 129.6, 129.3, 128.9, 128.54, 128.52, 126.2, 56.0, 44.2, 41.3, 29.9, 21.3, 21.2. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{28}H_{28}N_3O_3^+$, 454.2125; Found: 454.2125.

4,4'-((3,5-dioxo-6-(3-phenylpropanoyl)-1,2,4-triazine 2,4(3H,5H)diyl)bis(methylene))dibenzonitrile (3f)



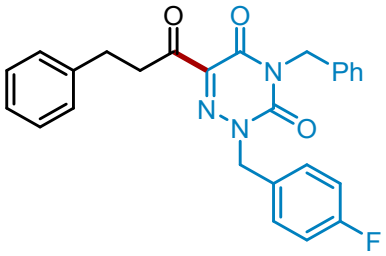
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (62.6 mg, 63% yield), mp 141 – 143 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.64 (m, 2H), 7.62 – 7.57 (m, 4H), 7.52 – 7.47 (m, 2H), 7.31 – 7.26 (m, 2H), 7.24 – 7.18 (m, 3H), 5.20 (s, 2H), 5.10 (s, 2H), 3.23 (t, *J* = 7.5 Hz, 2H), 3.00 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.6, 152.7, 148.3, 140.5, 139.7, 139.2, 137.7, 132.8, 132.5, 130.4, 129.5, 128.6, 128.5, 126.3, 118.4, 118.2, 112.9, 112.4, 55.8, 44.1, 41.4, 29.6. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{28}H_{21}N_5O_3Na^+$, 498.1537; Found: 498.1540.

4-benzyl-2-isopropyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3g)



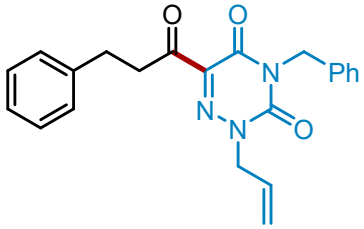
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow oil (54.3 mg, 71% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.48 (m, 2H), 7.32 – 7.17 (m, 8H), 5.08 (s, 2H), 5.00 (q, *J* = 6.7 Hz, 1H), 3.25 – 3.19 (t, *J* = 7.6 Hz, 2H), 2.99 (t, *J* = 7.6 Hz, 2H), 1.34 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.3, 152.7, 148.3, 140.8, 136.6, 135.2, 129.9, 128.62, 128.55, 128.5, 128.3, 126.2, 52.1, 44.4, 41.2, 30.0, 20.8. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{24}N_3O_3^+$, 378.1812; Found: 378.1828.

4-benzyl-2-(4-fluorobenzyl)-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3h)



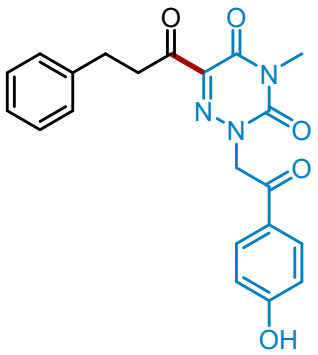
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (54.1 mg, 61% yield), mp 102 – 104 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.44 (m, 2H), 7.39 – 7.34 (m, 2H), 7.33 – 7.23 (m, 5H), 7.21 – 7.15 (m, 3H), 7.06 – 7.00 (m, 2H), 5.09 (s, 2H), 5.05 (s, 2H), 3.21 (t, *J* = 7.6 Hz, 2H), 2.97 (t, *J* = 7.6 Hz, 2H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -112.6. HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{23}FN_3O_3^+$, 444.1718; Found: 444.1720.

2-allyl-4-benzyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3i)



Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (53.5 mg, 71% yield), , mp 80 – 82 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.44 (m, 2H), 7.26 – 7.13 (m, 8H), 6.00 – 5.77 (m, 1H), 5.36 – 5.21 (m, 2H), 5.01 (s, 2H), 4.55 (d, *J* = 6.2 Hz, 2H), 3.18 (t, *J* = 7.6 Hz, 2H), 2.94 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.1, 153.0, 148.3, 140.9, 137.1, 135.2, 130.7, 129.8, 128.7, 128.57, 128.55, 128.3, 126.2, 120.2, 55.0, 44.4, 41.4, 29.9. HRMS (ESI-TOF) *m/z*: $[M + NH_4]^+$ Calcd for $C_{22}H_{25}N_4O_3^+$, 393.1921; Found: 393.1917.

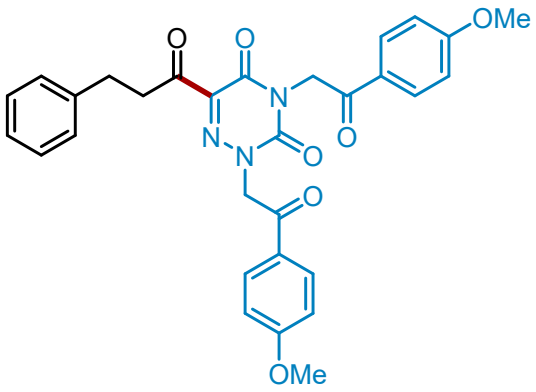
2-(2-(4-hydroxyphenyl)-2-oxoethyl)-4-methyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3j)



Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow oil (39.3 mg, 50% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.23 (m, 2H), 7.21

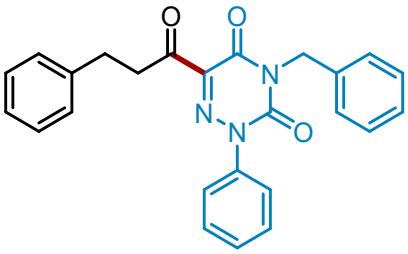
– 7.16 (m, 3H), 6.86 (d, J = 8.4 Hz, 2H), 5.34 (s, 2H), 3.34 (s, 3H), 3.29 (t, J = 7.6 Hz, 2H), 2.98 (t, J = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.0, 189.3, 162.3, 153.8, 148.9, 140.5, 137.2, 130.8, 128.53, 128.47, 126.3, 116.0, 57.8, 42.0, 29.5, 27.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{20}N_3O_5^+$, 394.1397; Found: 394.1401.

2,4-bis(2-(4-methoxyphenyl)-2-oxoethyl)-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3k)



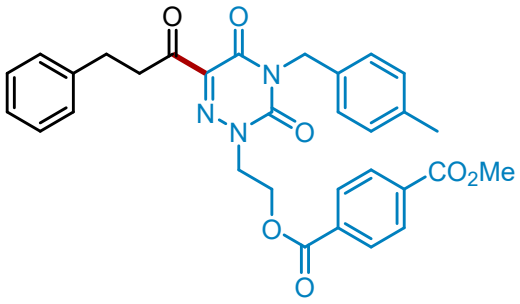
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow oil (75.7 mg, 70% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (t, J = 8.6 Hz, 4H), 7.26 – 7.23 (m, 2H), 7.20 – 7.16 (m, 3H), 6.98 – 6.93 (m, 4H), 5.43 (s, 2H), 5.33 (s, 2H), 3.87 (s, 3H), 3.86 (s, 3H), 3.24 (t, J = 7.7 Hz, 2H), 2.97 (t, J = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.8, 189.1, 188.3, 164.5, 164.3, 153.0, 148.6, 140.8, 137.5, 130.53, 130.48, 128.5, 127.4, 127.1, 126.1, 114.3, 114.1, 57.8, 55.6, 55.6, 46.4, 41.7, 29.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{28}N_3O_7^+$, 542.1922; Found: 542.1918.

4-benzyl-2-phenyl-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3l)



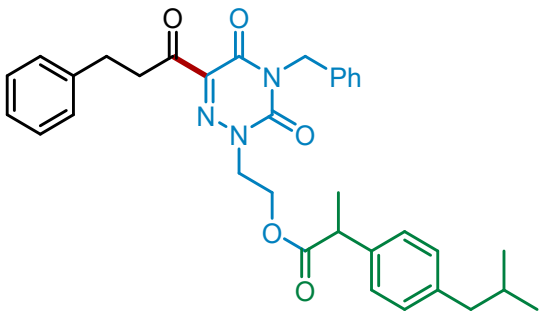
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow oil (49.2 mg, 60% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.45 (m, 2H), 7.36 – 7.21 (m, 11H), 6.95 (d, J = 7.0 Hz, 2H), 4.88 – 4.75 (m, 2H), 2.78 (t, J = 7.6 Hz, 2H), 2.49 (t, J = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.6, 169.3, 154.2, 139.5, 135.2, 134.2, 129.4, 128.91, 128.88, 128.5, 128.4, 128.3, 126.8, 126.4, 123.7, 43.3, 38.2, 29.1. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{21}N_3O_3Na^+$, 434.1475; Found: 434.1472.

methyl (2-(4-(4-methylbenzyl)-3,5-dioxo-6-(3-phenylpropanoyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl) terephthalate (3m)



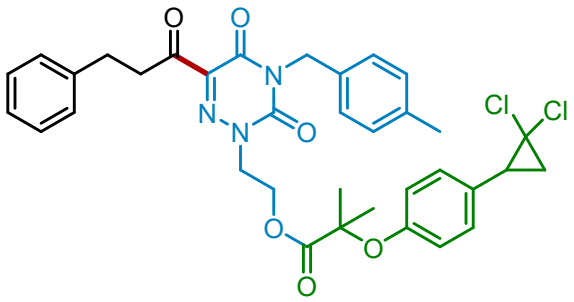
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (40.3 mg, 38% yield), mp 110 – 112 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 8.00 (m, 2H), 7.98 – 7.94 (m, 2H), 7.37 – 7.33 (m, 2H), 7.25 – 7.21 (m, 2H), 7.18 – 7.14 (m, 1H), 7.11 – 7.06 (m, 4H), 5.04 (s, 2H), 4.65 (t, *J* = 4.5 Hz, 2H), 4.42 (t, *J* = 4.5 Hz, 2H), 3.95 (s, 3H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.87 (t, *J* = 7.6 Hz, 2H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.8, 166.1, 165.4, 152.9, 148.6, 140.6, 138.2, 137.6, 134.3, 133.0, 131.9, 129.7, 129.6, 129.3, 128.5, 128.4, 126.2, 62.1, 52.5, 51.3, 44.2, 41.4, 29.5, 21.2. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{31}H_{30}N_3O_7^+$, 556.2078; Found: 556.2077.

2-(4-benzyl-3,5-dioxo-6-(3-phenylpropanoyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl 2-(4-isobutylphenyl)propanoate (3n)



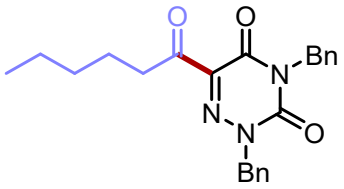
Purification by flash column chromatography (PE:EA, 8:1 v/v). Yellow oil (65.8 mg, 58% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.46 (m, 2H), 7.31 – 7.15 (m, 8H), 7.04 – 6.98 (m, 2H), 6.93 (d, *J* = 8.2 Hz, 2H), 5.02 (s, 2H), 4.43 – 4.24 (m, 3H), 4.19 – 4.10 (m, 1H), 3.53 (q, *J* = 7.1 Hz, 1H), 3.12 (t, *J* = 7.9 Hz, 2H), 2.94 (t, *J* = 7.5 Hz, 2H), 2.39 (d, *J* = 7.1 Hz, 2H), 1.83 – 1.74 (m, 1H), 1.36 (d, *J* = 7.1 Hz, 3H), 0.88 (s, 3H), 0.86 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.7, 174.4, 152.8, 148.6, 140.82, 140.80, 137.2, 137.0, 135.1, 129.8, 129.4, 128.7, 128.6, 128.4, 127.0, 126.2, 61.0, 51.2, 45.0, 44.9, 44.4, 41.4, 30.2, 29.7, 22.4, 18.4. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{34}H_{38}N_3O_5^+$, 568.2806; Found: 568.2805.

2-(4-(4-methylbenzyl)-3,5-dioxo-6-(3-phenylpropanoyl)-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl 2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropanoate (3o)



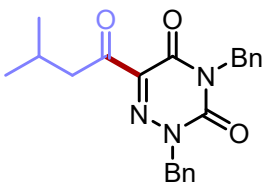
Purification by flash column chromatography (PE:EA, 8:1 v/v).Yellow oil (58.3 mg, 44% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.34 (m, 2H), 7.27 – 7.24 (m, 2H), 7.22 – 7.18 (m, 3H), 7.10 (d, *J* = 7.8 Hz, 2H), 6.97 – 6.93 (m, 2H), 6.65 – 6.60 (m, 2H), 4.96 (s, 2H), 4.46 (t, *J* = 5.1 Hz, 2H), 4.25 (t, *J* = 5.3, 2.2 Hz, 2H), 3.15 (t, *J* = 7.5 Hz, 2H), 2.95 (t, *J* = 7.5 Hz, 2H), 2.78 (dd, *J* = 10.7, 8.4 Hz, 1H), 2.30 (s, 3H), 1.93 (dd, *J* = 10.7, 7.4 Hz, 1H), 1.72 (dd, *J* = 8.3, 7.4 Hz, 1H), 1.49 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.7, 174.1, 154.6, 152.7, 148.4, 140.7, 138.2, 137.1, 132.0, 129.7, 129.7, 129.3, 128.5, 128.3, 126.3, 118.1, 61.9, 60.9, 51.2, 44.2, 41.4, 34.7, 29.6, 25.9, 25.3, 25.2, 21.2. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{35}H_{35}Cl_2N_3O_6^+$, 664.1976; Found: 664.1968.

2,4-dibenzyl-6-pentanoyl-1,2,4-triazine-3,5(2H,4H)-dione (3p)



Purification by flash column chromatography (PE:EA, 15:1 v/v). Yellow oil (62.5 mg, 80% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.45 (m, 2H), 7.44 – 7.36 (m, 3H), 7.39 – 7.30 (m, 4H), 7.32 – 7.23 (m, 4H), 5.16 (t, *J* = 7.0 Hz, 2H), 5.06 (s, 2H), 2.85 (t, *J* = 7.4 Hz, 2H), 1.63 (dd, *J* = 8.6, 6.1 Hz, 2H), 1.35 – 1.26 (m, 5H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.3, 153.1, 148.5, 137.4, 135.1, 134.7, 129.8, 128.9, 128.7, 128.6, 128.3, 56.2, 44.4, 39.7, 31.4, 23.5, 22.5, 14.0. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{26}N_3O_3^+$, 392.1969; Found: 392.1975.

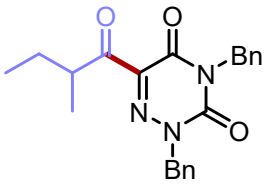
2,4-dibenzyl-6-(3-methylbutanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3q)



Purification by flash column chromatography (PE:EA, 15:1 v/v). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 – 7.50 (m, 2H), 7.46 – 7.36 (m, 5H), 7.36 – 7.30 (m, 3H), 5.20 (s, 2H), 5.10 (s, 2H), 2.78 (d, *J* = 7.0 Hz, 2H), 2.26 – 2.14 (m, 1H), 0.97 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR

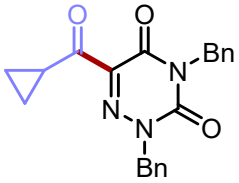
(101 MHz, Chloroform-*d*) δ 194.9, 153.0, 148.5, 137.5, 135.1, 134.6, 129.8, 128.94, 128.93, 128.7, 128.6, 128.3, 56.2, 48.4, 44.4, 24.8, 22.6. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{23}H_{25}N_3O_3Na^+$, 414.1788; Found: 414.1788.

2,4-dibenzyl-6-(2-methylbutanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3r)



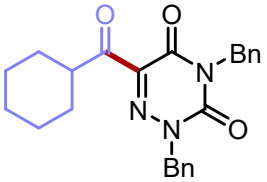
Purification by flash column chromatography (PE:EA, 15:1 v/v). Yellow oil (48.5 mg, 65% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 – 7.49 (m, 2H), 7.46 – 7.30 (m, 9H), 5.19 (s, 2H), 5.11 (s, 2H), 3.44 – 3.32 (m, 1H), 1.81 – 1.71 (m, 1H), 1.50 – 1.40 (m, 1H), 1.14 (d, J = 6.9 Hz, 3H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 198.8, 153.1, 148.5, 137.5, 135.1, 134.7, 129.8, 128.9, 128.7, 128.6, 128.3, 56.1, 44.4, 43.5, 25.9, 15.6, 11.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{24}N_3O_3^+$, 378.1812; Found: 378.1825.

2,4-dibenzyl-6-(cyclopropanecarbonyl)-1,2,4-triazine-3,5(2H,4H)-dione (3s)



Purification by flash column chromatography (PE:EA, 12:1 v/v). Yellow oil (65.0 mg, 90% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.50 (m, 2H), 7.48 – 7.44 (m, 2H), 7.43 – 7.36 (m, 3H), 7.35 – 7.29 (m, 3H), 5.24 (s, 2H), 5.11 (s, 2H), 2.86 – 2.77 (m, 1H), 1.29 – 1.24 (m, 2H), 1.11 – 1.05 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 153.1, 148.6, 137.9, 135.1, 134.7, 129.7, 128.93, 128.87, 128.7, 128.6, 128.3, 56.3, 44.4, 18.4, 12.8. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{20}N_3O_3^+$, 362.1499; Found: 362.1507.

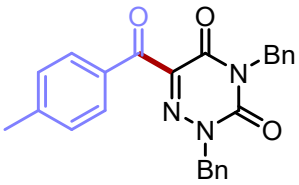
2,4-dibenzyl-6-(cyclohexanecarbonyl)-1,2,4-triazine-3,5(2H,4H)-dione (3t)



Purification by flash column chromatography (PE:EA, 13:1 v/v). Yellow oil (44.5 mg, 55% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 – 7.50 (m, 2H), 7.46 – 7.37 (m, 5H), 7.35 – 7.31 (m, 3H), 5.20 (s, 2H), 5.10 (s, 2H), 3.23 (tt, J = 11.3, 3.0 Hz, 1H), 1.85 – 1.80 (m, 3H), 1.74 – 1.70 (m, 1H), 1.48 – 1.27 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 198.1, 153.2,

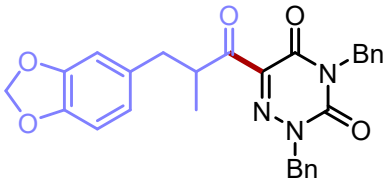
148.5, 137.2, 135.1, 134.7, 129.8, 129.0, 128.9, 128.7, 128.6, 128.3, 56.0, 46.8, 44.4, 28.4, 25.8, 25.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{26}N_3O_3^+$, 404.1969; Found: 404.1971.

2,4-dibenzyl-6-(4-methylbenzoyl)-1,2,4-triazine-3,5(2H,4H)-dione (3u)



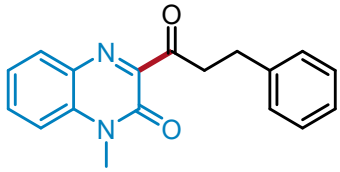
Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow solid (64.9 mg, 79% yield), mp 120 – 122 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.77 (m, 2H), 7.59 – 7.54 (m, 2H), 7.45 – 7.34 (m, 8H), 7.30 – 7.26 (m, 2H), 5.17 (s, 2H), 5.15 (s, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 186.5, 153.9, 148.5, 145.4, 139.7, 135.1, 135.0, 132.6, 130.4, 129.8, 129.3, 129.0, 128.9, 128.7, 128.6, 128.3, 55.8, 44.5, 21.9. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{22}N_3O_3^+$, 412.1656; Found: 412.1655.

6-(3-(benzo[d][1,3]dioxol-5-yl)-2-methylpropanoyl)-2,4-dibenzyl-1,2,4-triazine-3,5(2H,4H)-dione (3v)



Purification by flash column chromatography (PE:EA, 10:1 v/v). Yellow oil (38.4 mg, 40% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.46 (m, 2H), 7.41 – 7.31 (m, 8H), 6.66 – 6.58 (m, 2H), 6.58 – 6.52 (m, 1H), 5.90 (s, 2H), 5.16 (s, 2H), 5.08 (s, 2H), 3.80 – 3.68 (m, 1H), 2.94 (dd, *J* = 13.7, 7.4 Hz, 1H), 2.57 (dd, *J* = 13.7, 7.4 Hz, 1H), 1.14 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 198.0, 152.9, 148.4, 147.5, 145.9, 137.1, 135.0, 134.6, 133.1, 129.8, 129.0, 128.9, 128.7, 128.6, 128.3, 122.1, 109.4, 108.1, 100.8, 56.1, 44.4, 44.0, 39.0, 16.3. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{28}H_{25}N_3O_5Na^+$, 506.1686; Found: 506.1689.

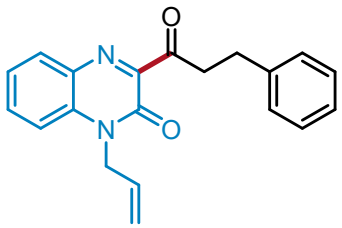
1-methyl-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one (5a)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow oil (42.0 mg, 72% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.68 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.46 – 7.33 (m, 2H), 7.29 (d, *J* = 6.1 Hz, 4H), 7.20 (td, *J* = 6.0, 2.7 Hz, 1H),

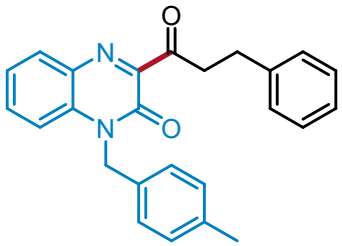
3.72 (s, 3H), 3.45 (t, J = 8.2, 7.4, 2.0 Hz, 2H), 3.11 (t, J = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 199.7, 152.9, 152.1, 140.9, 134.4, 132.7, 131.9, 131.4, 128.49, 128.47, 126.1, 124.2, 113.9, 42.4, 29.5, 29.1.HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{18}H_{17}N_2O_2^+$, 293.1285; Found: 293.1288.

1-allyl-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one (5b)



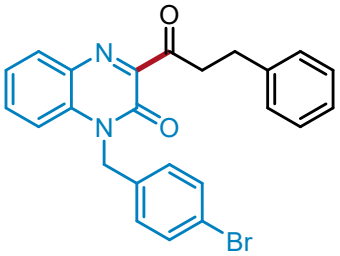
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (38.2 mg, 60% yield), mp 87 – 89 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.96 – 7.90 (m, 1H), 7.65 – 7.61 (m, 1H), 7.40 – 7.36 (m, 1H), 7.34 – 7.31 (m, 1H), 7.30 – 7.25 (m, 4H), 7.20 – 7.16 (m, 1H), 5.97 – 5.87 (m, 1H), 5.29 (dd, J = 10.4, 1.8 Hz, 1H), 5.22 – 5.17 (m, 1H), 4.94 – 4.89 (m, 2H), 3.45 (t, J = 7.6 Hz, 2H), 3.09 (t, J = 7.9 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.5, 152.4, 152.1, 141.0, 133.7, 132.6, 132.1, 131.5, 130.3, 128.50, 128.47, 126.1, 124.2, 118.7, 114.5, 44.5, 42.5, 29.5. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{19}N_2O_2^+$, 319.1441; Found: 319.1444.

1-(4-methylbenzyl)-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one (5c)



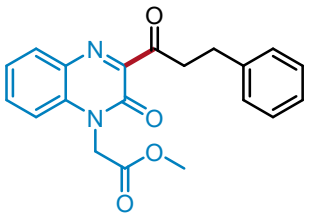
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (48.9 mg, 64% yield), mp 126 – 128 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 – 7.92 (m, 1H), 7.59 – 7.53 (m, 1H), 7.39 – 7.31 (m, 6H), 7.20 – 7.13 (m, 5H), 5.49 (s, 2H), 3.51 (t, J = 7.4 Hz, 2H), 3.14 (t, J = 8.0 Hz, 2H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.6, 153.0, 152.1, 141.0, 137.7, 133.8, 132.7, 132.2, 131.8, 131.5, 129.7, 128.53, 128.50, 127.1, 126.1, 124.2, 114.7, 45.7, 42.5, 29.6, 21.1. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{25}H_{23}N_2O_2^+$, 383.1754; Found:383.1756.

1-(4-bromobenzyl)-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one (5d)



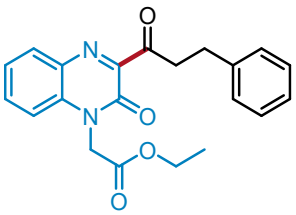
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (51.7 mg, 58% yield), mp 141 – 143 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.48 – 7.45 (m, 2H), 7.41 – 7.37 (m, 1H), 7.35 – 7.30 (m, 4H), 7.26 – 7.15 (m, 4H), 5.46 (s, 2H), 3.50 (t, *J* = 7.4 Hz, 2H), 3.14 (t, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.4, 152.8, 151.9, 140.9, 133.9, 133.6, 132.8, 132.19, 132.17, 131.7, 128.9, 128.5, 128.5, 126.1, 124.4, 121.9, 114.4, 45.3, 42.4, 29.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{20}BrN_2O_2^+$, 447.0703; Found: 447.0702.

methyl 2-(2-oxo-3-(3-phenylpropanoyl)quinoxalin-1(2H)-yl)acetate (5e)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (39.9 mg, 57% yield), mp 120 – 122 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.42 – 7.38 (m, 1H), 7.30 – 7.25 (m, 4H), 7.21 – 7.17 (m, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 5.04 (s, 2H), 3.78 (s, 3H), 3.45 (t, *J* = 7.8 Hz, 2H), 3.08 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 201.0, 153.0, 152.9, 134.3, 132.4, 132.0, 131.3, 124.1, 113.9, 42.7, 29.0, 17.0, 13.7. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{19}N_2O_4^+$, 351.1339; Found: 351.1341.

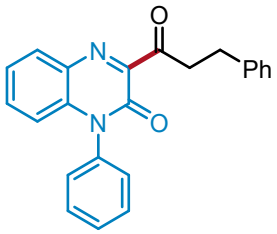
ethyl 2-(2-oxo-3-(3-phenylpropanoyl)quinoxalin-1(2H)-yl)acetate (5f)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (43.7 mg, 60% yield), mp 76 – 78 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.67 – 7.60 (m, 1H), 7.43 – 7.37 (m, 1H), 7.29 – 7.27 (m, 3H), 7.23 – 7.15 (m, 2H), 7.11 (dd, *J* = 8.5, 1.2 Hz, 1H), 5.03 (s, 2H), 4.25 (q, *J* = 7.1 Hz, 3H), 3.45 (t, *J* = 7.3 Hz, 2H), 3.09 (t, *J* =

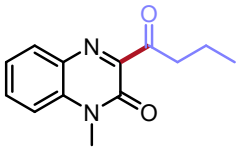
8.0, 4.5 Hz, 2H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.0, 166.7, 152.4, 151.5, 140.9, 133.6, 133.0, 132.0, 131.8, 128.5, 126.1, 124.5, 113.4, 62.3, 43.4, 42.3, 29.5, 14.1. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{21}N_2O_4^+$, 365.1496; Found: 365.1486.

1-phenyl-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one (5g)



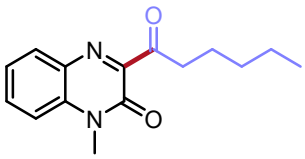
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (35.6 mg, 48% yield), mp 94 – 96 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.97 (dd, J = 8.1, 1.5 Hz, 1H), 7.64 – 7.60 (m, 2H), 7.58 – 7.56 (m, 1H), 7.46 – 7.43 (m, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.30 – 7.25 (m, 6H), 7.20 – 7.16 (m, 1H), 6.71 (d, J = 8.4 Hz, 1H), 3.47 (t, J = 7.8 Hz, 2H), 3.10 (t, J = 7.8 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.4, 153.1, 152.7, 140.9, 135.2, 135.1, 132.3, 132.0, 131.0, 130.4, 129.8, 128.5, 128.5, 128.2, 126.1, 124.4, 115.7, 42.7, 29.5. HRMS (ESI-TOF) *m/z*: $[M + NH_4]^+$ Calcd for $C_{23}H_{22}N_3O_2^+$, 372.1707; Found: 372.1668.

3-butyryl-1-methylquinoxalin-2(1H)-one (5h)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow soild (30.4 mg, 66% yield), mp 93 – 95 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 (d, J = 8.0 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.43 – 7.37 (m, 1H), 7.36 (d, J = 8.5 Hz, 1H), 3.72 (s, 3H), 3.06 (t, J = 7.3 Hz, 2H), 1.83 – 1.75 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 201.0, 153.0, 152.9, 134.3, 132.4, 132.0, 131.3, 124.1, 113.9, 42.7, 29.0, 17.0, 13.7. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{15}N_2O_2^+$, 231.1128; Found: 231.1131.

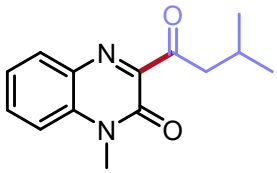
3-hexanoyl-1-methylquinoxalin-2(1H)-one (5i)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow soild (35.0 mg, 68% yield), mp 87 – 89 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.93 (dd, J = 8.0, 1.7 Hz, 1H),

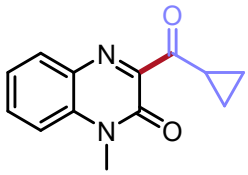
7.69 – 7.64 (m, 1H), 7.40 (t, J = 7.7 Hz, 1H), 7.36 (d, J = 8.5 Hz, 1H), 3.72 (s, 3H), 3.07 (t, J = 7.4 Hz, 2H), 1.80 – 1.73 (m, 2H), 1.42 – 1.33 (m, 4H), 0.91 (t, J = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 201.1, 153.1, 152.9, 134.2, 132.4, 132.0, 131.3, 124.1, 113.9, 40.8, 31.3, 29.0, 23.1, 22.5, 13.9. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{18}N_2NaO_2^+$, 281.1260; Found: 281.1264.

1-methyl-3-(3-methylbutanoyl)quinoxalin-2(1H)-one (5j)



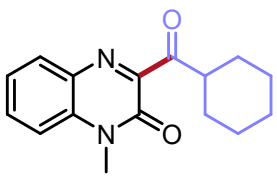
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (34.3 mg, 70% yield), mp 82 – 84 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 (dd, J = 8.0, 1.5 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.42 – 7.38 (m, 1H), 7.36 (dd, J = 8.5, 1.1 Hz, 1H), 3.72 (s, 3H), 2.97 (d, J = 6.9 Hz, 2H), 2.37 – 2.27 (m, 1H), 1.03 (d, J = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 200.7, 153.1, 152.9, 134.3, 132.4, 132.0, 131.3, 124.1, 113.9, 49.6, 29.0, 24.5, 22.7. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{17}N_2O_2^+$, 245.1285; Found: 245.1287.

3-(cyclopropanecarbonyl)-1-methylquinoxalin-2(1H)-one (5k)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (32.5 mg, 71% yield), mp 123 – 125 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.98 (dd, J = 8.0, 1.5 Hz, 1H), 7.70 – 7.65 (m, 1H), 7.44 – 7.35 (m, 2H), 3.74 (s, 3H), 2.89 – 2.79 (m, 1H), 1.42 – 1.36 (m, 2H), 1.19 – 1.13 (m, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 200.4, 153.0, 152.8, 134.3, 132.5, 132.1, 131.5, 124.1, 113.9, 29.0, 20.0, 13.1. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{17}N_2O_2^+$, 229.0972; Found: 229.0972.

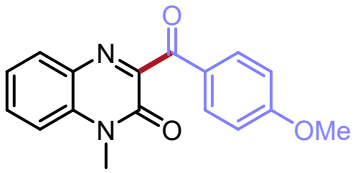
3-(cyclohexanecarbonyl)-1-methylquinoxalin-2(1H)-one (5l)



Purification by flash column chromatography (PE:EA, 8:1 v/v). Yellow oil (29.7 mg, 55% yield). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.92 (dd, J = 8.0, 1.5 Hz, 1H), 7.65 (ddd, J = 8.6, 7.3, 1.5 Hz, 1H), 7.40 (ddd, J = 8.3, 7.3, 1.2 Hz, 1H), 7.36 (dd, J = 8.5, 1.2 Hz, 1H), 3.72 (s,

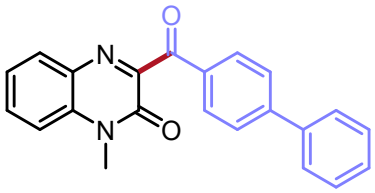
3H), 3.31 (tt, *J* = 11.2, 3.5 Hz, 1H), 1.99 (dt, *J* = 13.4, 3.2 Hz, 2H), 1.81 (dt, *J* = 13.1, 3.7 Hz, 2H), 1.71 – 1.65 (m, 2H), 1.57 – 1.48 (m, 2H), 1.40 – 1.31 (m, 2H), 1.30 – 1.23 (m, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 204.0, 154.3, 153.1, 134.0, 132.13, 132.11, 131.2, 124.1, 113.9, 47.9, 29.0, 27.8, 25.9, 25.5. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{16}H_{19}N_2O_2^+$, 271.1441; Found: 271.1443.

3-(4-methoxybenzoyl)-1-methylquinoxalin-2(1H)-one (5m)



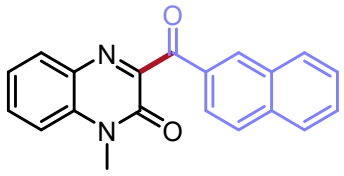
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (32.9 mg, 56% yield), mp 201 – 203 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.9 Hz, 2H), 7.92 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.43 – 7.39 (m, 2H), 6.97 – 6.93 (m, 2H), 3.87 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 190.3, 164.5, 155.0, 153.4, 133.9, 132.5, 132.2, 131.9, 130.9, 128.0, 124.1, 114.0, 114.0, 55.6, 29.1. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{17}H_{15}N_2O_3^+$, 295.1077; Found: 295.1079.

3-([1,1'-biphenyl]-4-carbonyl)-1-methylquinoxalin-2(1H)-one (5n)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (36.7 mg, 54% yield), mp 199 – 201 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.08 – 8.04 (m, 2H), 7.95 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.72 – 7.66 (m, 3H), 7.64 – 7.60 (m, 2H), 7.49 – 7.38 (m, 5H), 3.76 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.4, 154.8, 153.4, 146.9, 139.8, 134.0, 133.6, 132.3, 132.1, 131.1, 130.6, 129.0, 128.4, 127.4, 127.4, 124.2, 114.0, 29.1. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{22}H_{17}N_2O_2^+$, 341.1285; Found:341.1269.

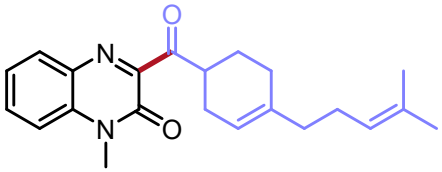
3-(2-naphthoyl)-1-methylquinoxalin-2(1H)-one (5o)



Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow solid (30.2 mg, 48% yield), mp 197 – 199 °C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 1.7 Hz, 1H), 8.13

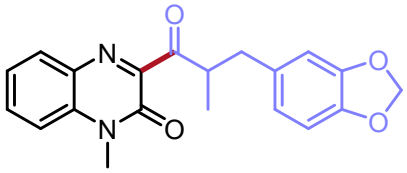
(dd, *J* = 8.7, 1.7 Hz, 1H), 7.98 – 7.92 (m, 2H), 7.88 (d, *J* = 8.3 Hz, 2H), 7.73 – 7.67 (m, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.46 – 7.40 (m, 2H), 3.77 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.8, 154.9, 153.4, 136.2, 134.0, 133.0, 132.41, 132.35, 132.3, 132.1, 131.1, 129.9, 129.1, 128.8, 127.9, 126.8, 124.5, 124.2, 114.0, 29.1. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{15}N_2O_2^+$, 315.1128; Found: 315.1128.

1-methyl-3-(4-(4-methylpent-3-en-1-yl)cyclohex-3-ene-1-carbonyl)quinoxalin-2(1H)-one (5p)



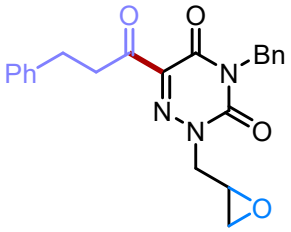
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow oil (23.1 mg, 33% yield). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 – 7.91 (m, 1H), 7.68 – 7.64 (m, 1H), 7.41 – 7.35 (m, 2H), 5.46 – 5.41 (m, 1H), 5.13 – 5.06 (m, 1H), 3.72 (s, 3H), 3.62 – 3.51 (m, 1H), 2.40 – 2.29 (m, 2H), 2.14 – 2.05 (m, 5H), 2.02 – 1.94 (m, 2H), 1.70 – 1.67 (m, 3H), 1.66 – 1.63 (m, 1H), 1.61 – 1.58 (m, 3H).^{13}C NMR (151 MHz, Chloroform-*d*) δ 203.6, 153.8, 153.0, 137.5, 136.2, 134.1, 132.2, 132.1, 131.5, 131.2, 124.25, 124.23, 124.1, 120.3, 118.9, 113.9, 44.6, 44.2, 37.8, 37.6, 29.4, 29.0, 27.9, 26.6, 26.4, 25.7, 24.8, 24.5, 24.3, 17.7. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{22}H_{27}N_2O_2^+$, 351.2067; Found: 351.2068.

3-(3-(benzo[d][1,3]dioxol-5-yl)-2-methylpropanoyl)-1-methylquinoxalin-2(1H)-one (5q)



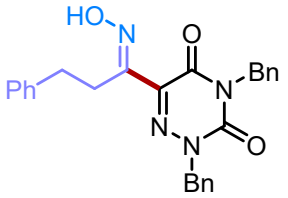
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow oil (30.2 mg, 43% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.68 – 7.62 (m, 1H), 7.41 – 7.32 (m, 2H), 6.72 (s, 1H), 6.65 (d, *J* = 1.5 Hz, 2H), 5.84 (d, *J* = 1.5 Hz, 1H), 5.81 (d, *J* = 1.5 Hz, 1H), 3.92 – 3.80 (m, 1H), 3.69 (s, 3H), 3.09 (dd, *J* = 13.8, 6.2 Hz, 1H), 2.64 (dd, *J* = 13.8, 8.4 Hz, 1H), 1.20 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.3, 152.93, 152.85, 147.5, 145.8, 134.2, 133.2, 132.4, 132.0, 131.3, 124.1, 122.2, 113.8, 109.6, 107.9, 100.7, 45.3, 38.3, 29.0, 15.2. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{19}N_2O_4^+$, 351.1339; Found: 351.1342.

4-benzyl-2-(oxiran-2-ylmethyl)-6-(3-phenylpropanoyl)-1,2,4-triazine-3,5(2H,4H)-dione (6)



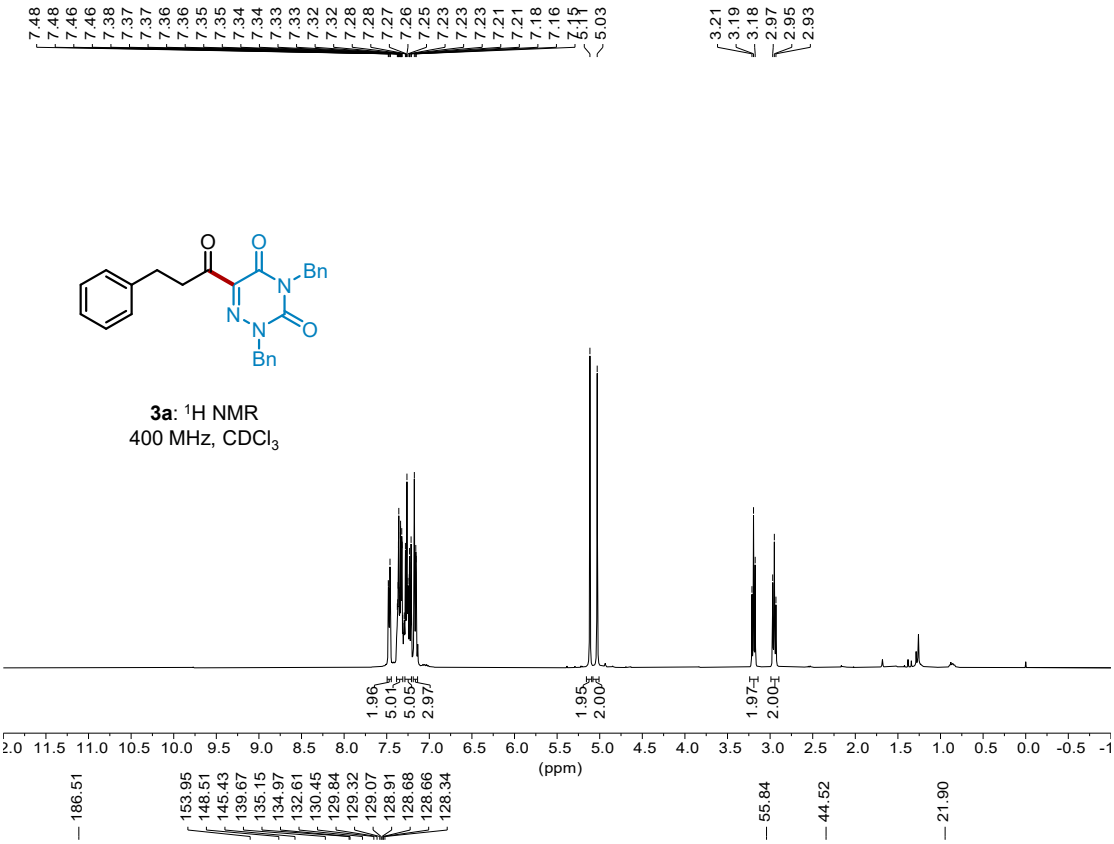
Purification by flash column chromatography (PE:EA, 5:1 v/v). Yellow oil (58.6 mg, 75% yield). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.31 – 7.21 (m, 5H), 7.21 – 7.12 (m, 3H), 5.06 (s, 2H), 4.26 (dd, *J* = 14.2, 4.0 Hz, 1H), 4.01 (dd, *J* = 14.2, 6.2 Hz, 1H), 3.33 – 3.27 (m, 1H), 3.21 (d, *J* = 7.3 Hz, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.86 – 2.81 (m, 1H), 2.63 (dd, *J* = 4.8, 2.5 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.1, 152.9, 148.6, 140.7, 135.0, 129.8, 128.7, 128.5, 128.4, 126.2, 54.6, 48.8, 45.7, 44.5, 41.4, 29.8. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{22}N_3O_4^+$, 392.1605; Found: 392.1609.

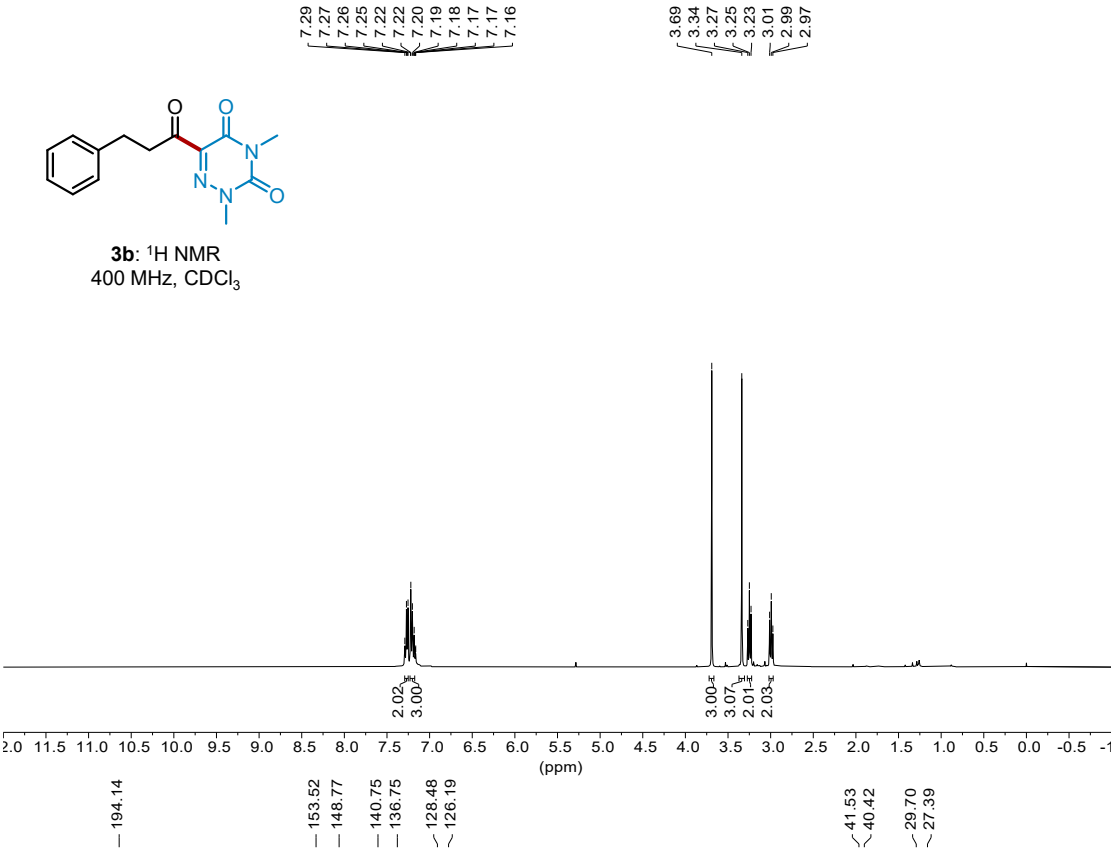
2,4-dibenzyl-6-(1-(hydroxyimino)-3-phenylpropyl)-1,2,4-triazine-3,5(2H,4H)-dione (7)



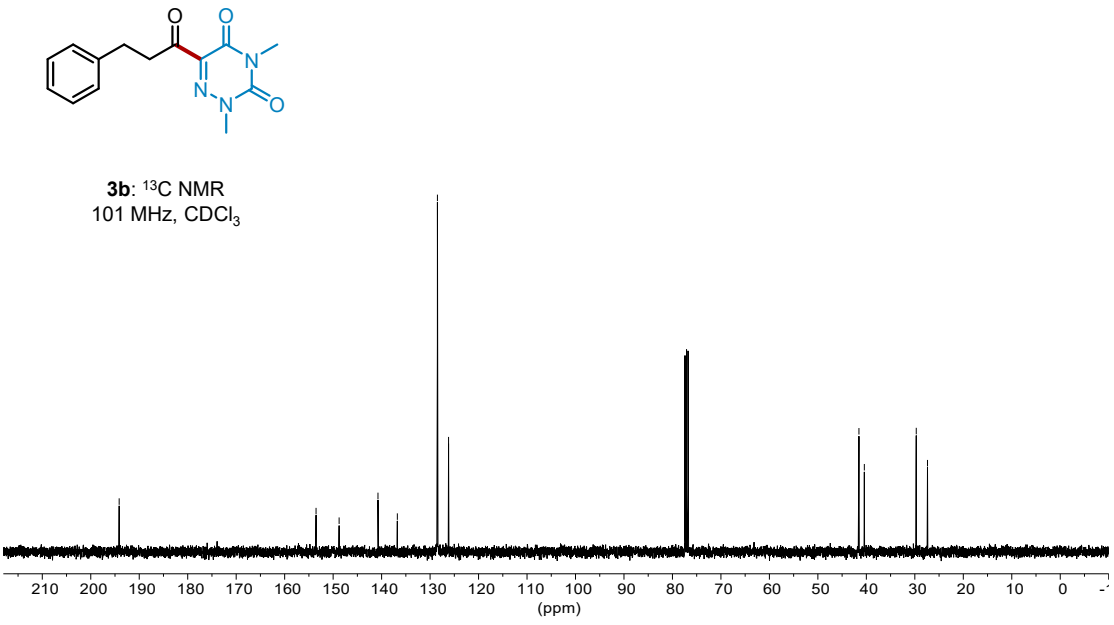
Purification by flash column chromatography (PE:EA, 5:1 v/v). White solid (45.4 mg, 72% yield), mp 130 – 132 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 11.82 (s, 1H), 7.38 – 7.28 (m, 10H), 7.18 – 7.11 (m, 3H), 7.08 – 7.05 (m, 2H), 5.10 (s, 2H), 4.97 (s, 2H), 2.87 (t, *J* = 8.7, 2H), 2.71 (t, *J* = 8.5 Hz, 2H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 154.5, 152.7, 148.8, 141.5, 139.1, 136.6, 136.3, 129.0, 128.9, 128.6, 128.44, 128.40, 128.3, 128.0, 126.3, 55.1, 44.2, 31.6, 28.1. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{25}N_4O_3^+$, 441.1921; Found: 441.1907.

4. NMR Copies of Products

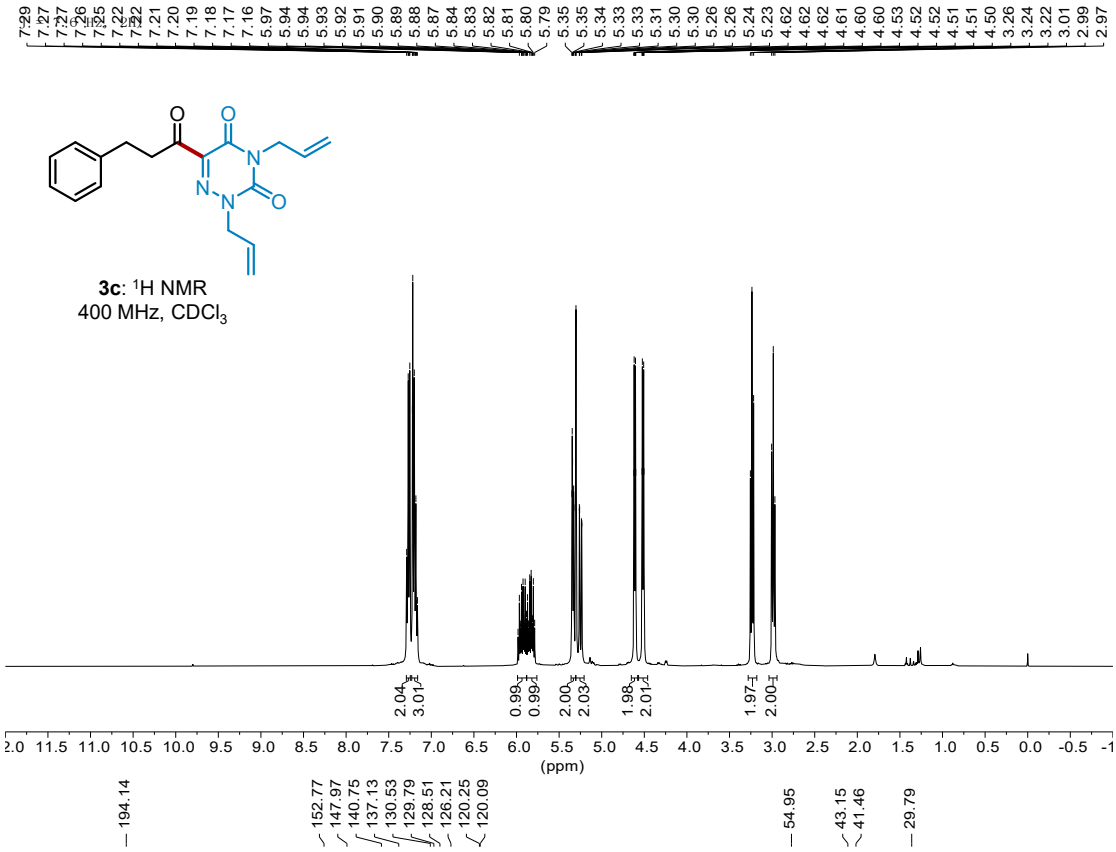




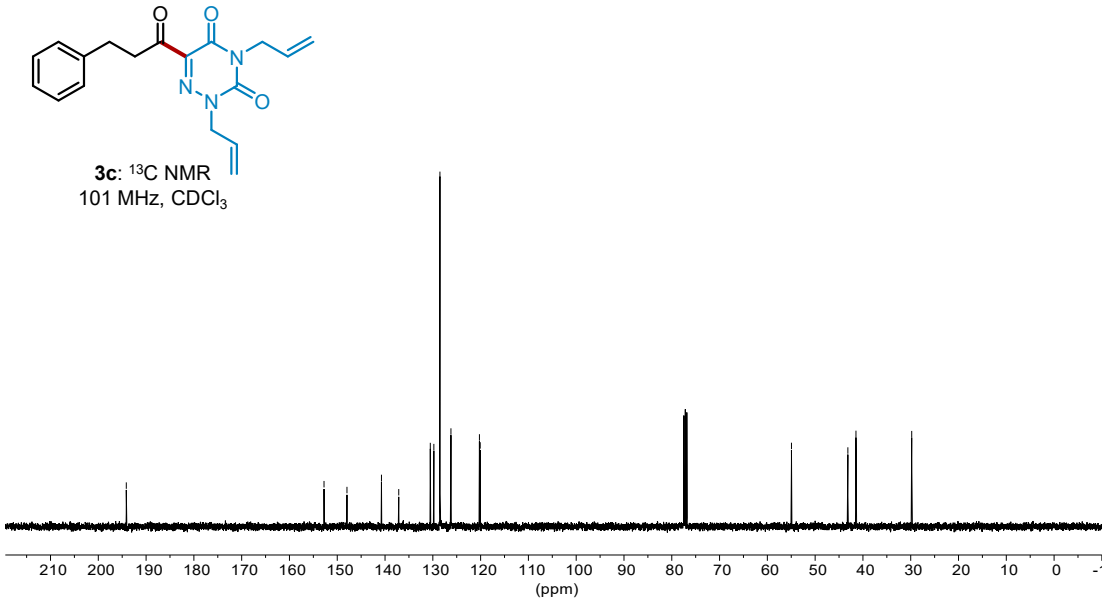
3b: ^{1}H NMR
400 MHz, $CDCl_3$

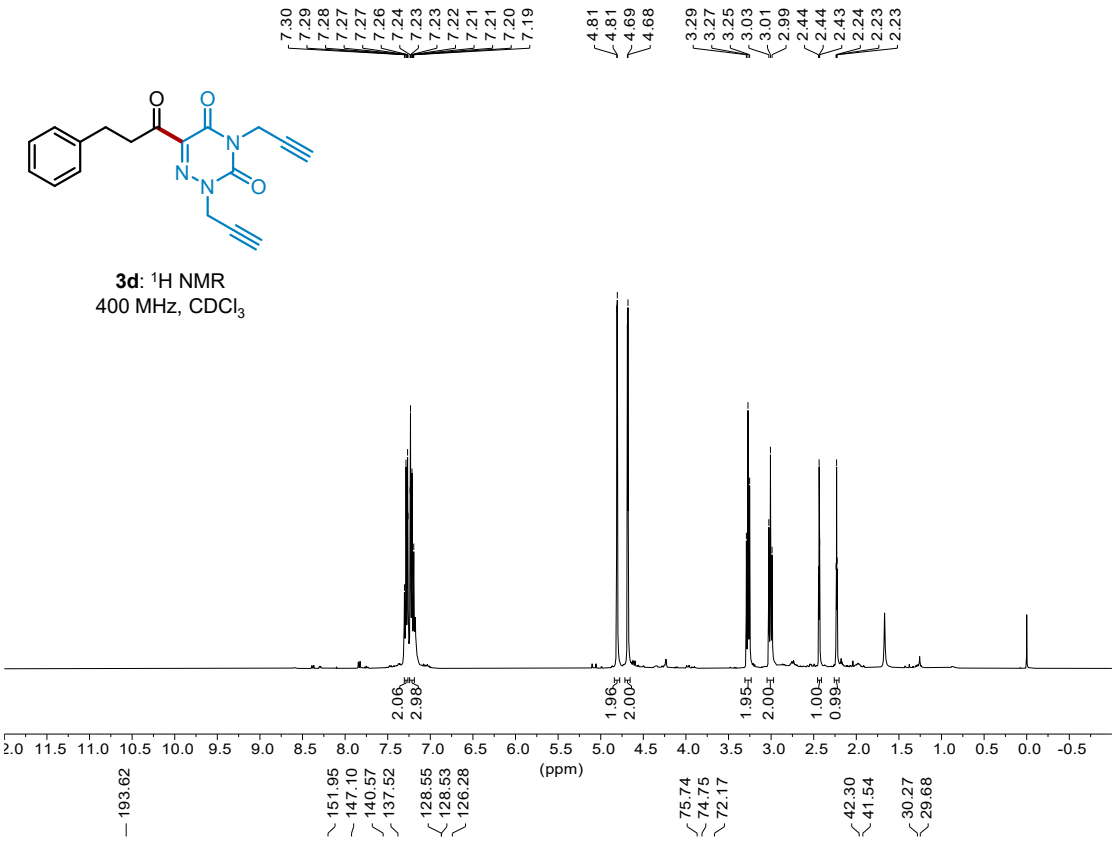


3b: ^{13}C NMR
101 MHz, $CDCl_3$

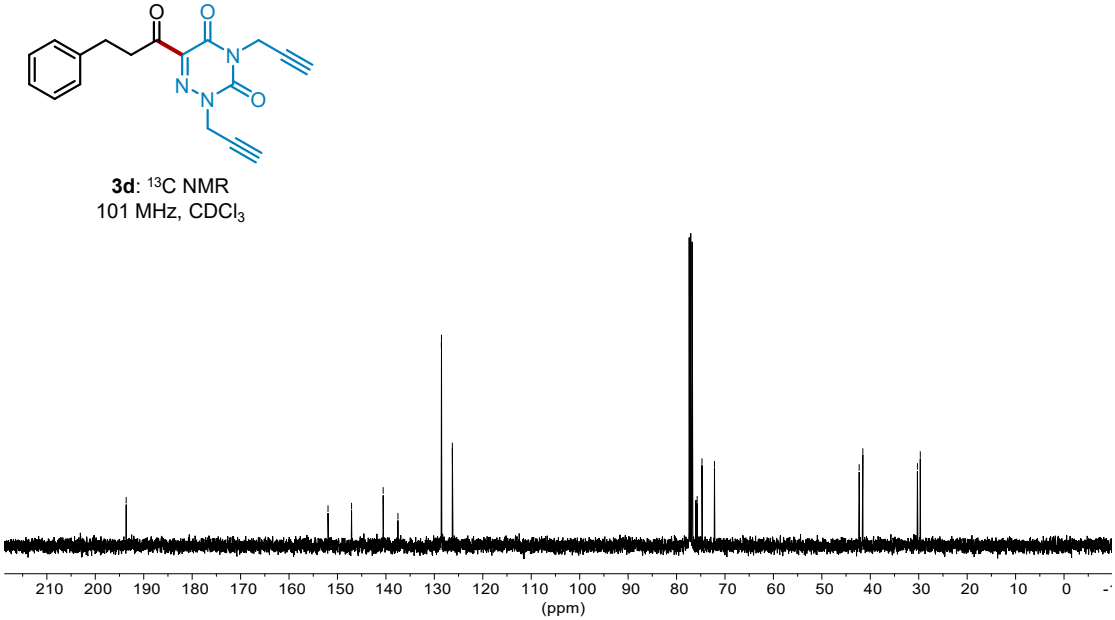

7.29 7.27 7.27 7.26 7.25 7.22 7.22 7.21 7.20 7.19 7.18 7.17 7.16 5.97 5.94 5.94 5.93 5.92 5.91 5.90 5.89 5.88 5.87 5.84 5.83 5.82 5.81 5.80 5.79 5.35 5.35 5.34 5.33 5.33 5.31 5.30 5.30 5.26 5.26 5.24 5.23 4.62 4.62 4.62 4.61 4.60 4.60 4.53 4.52 4.52 4.51 4.51 4.50 3.26 3.24 3.22 3.01 2.99 2.97
3c: 1H NMR
400 MHz, CDCl3
2.04 3.01 0.99 0.99 2.00 2.03 1.98 2.01 1.97 2.00
(ppm)

194.14
152.77 147.97 140.75 137.13 130.53 129.79 128.51 126.21 120.25 120.09
54.95
43.15 41.46
29.79

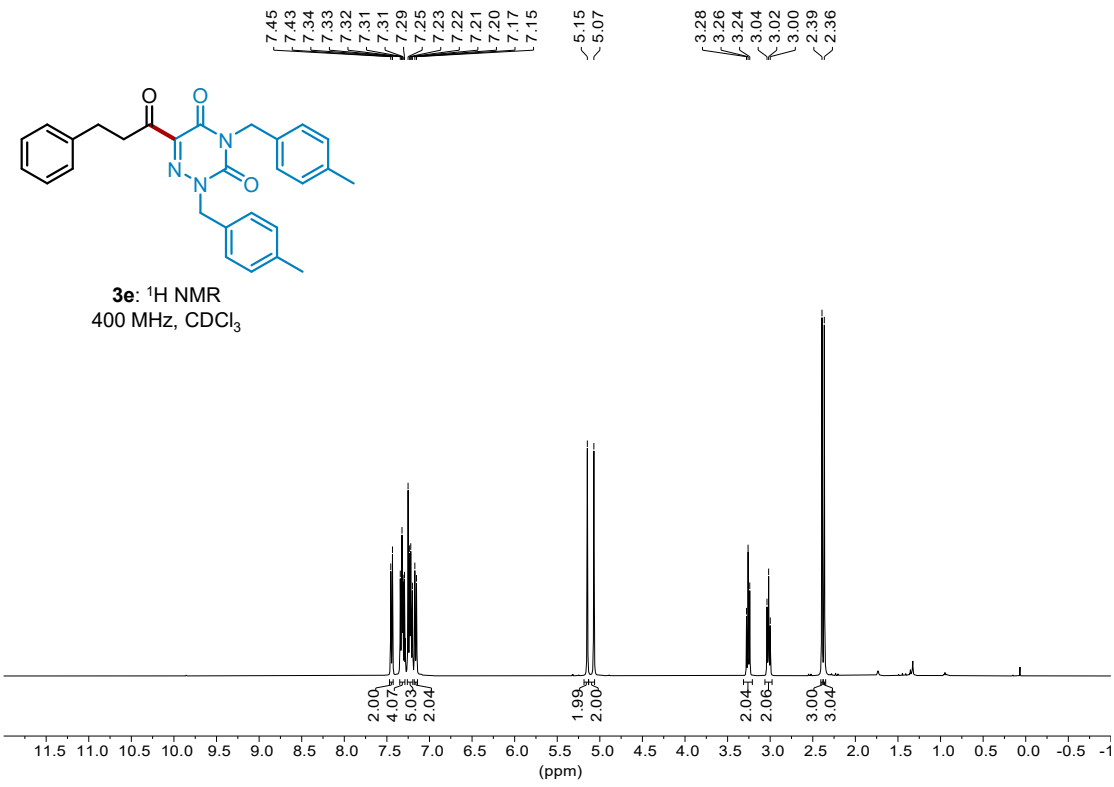

3c: 13C NMR
101 MHz, CDCl3
(ppm)



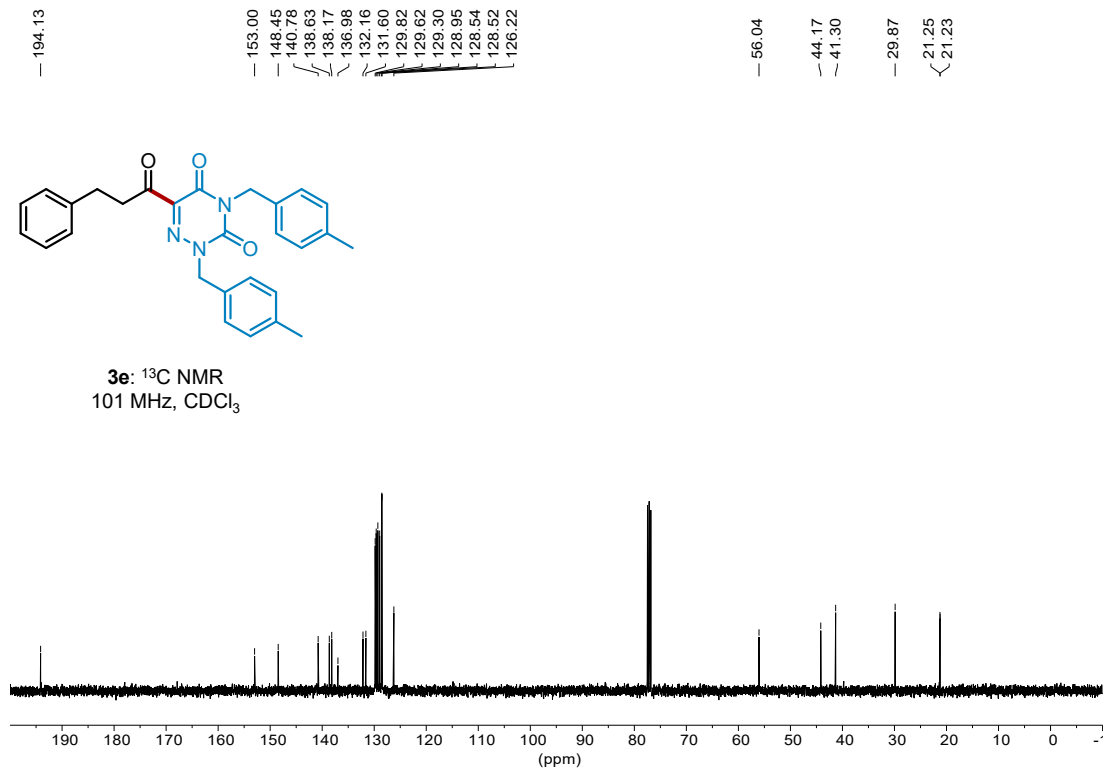
3d: ^{1}H NMR
400 MHz, $CDCl_3$



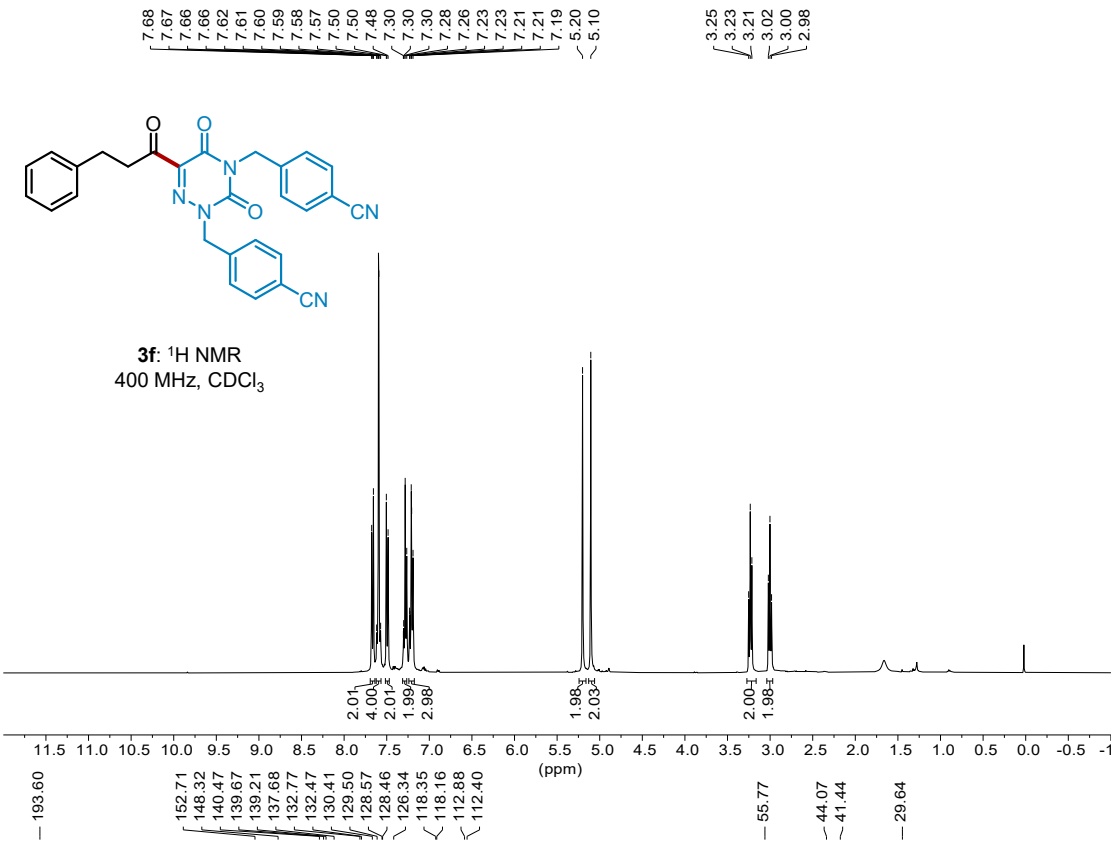
3d: ^{13}C NMR
101 MHz, $CDCl_3$



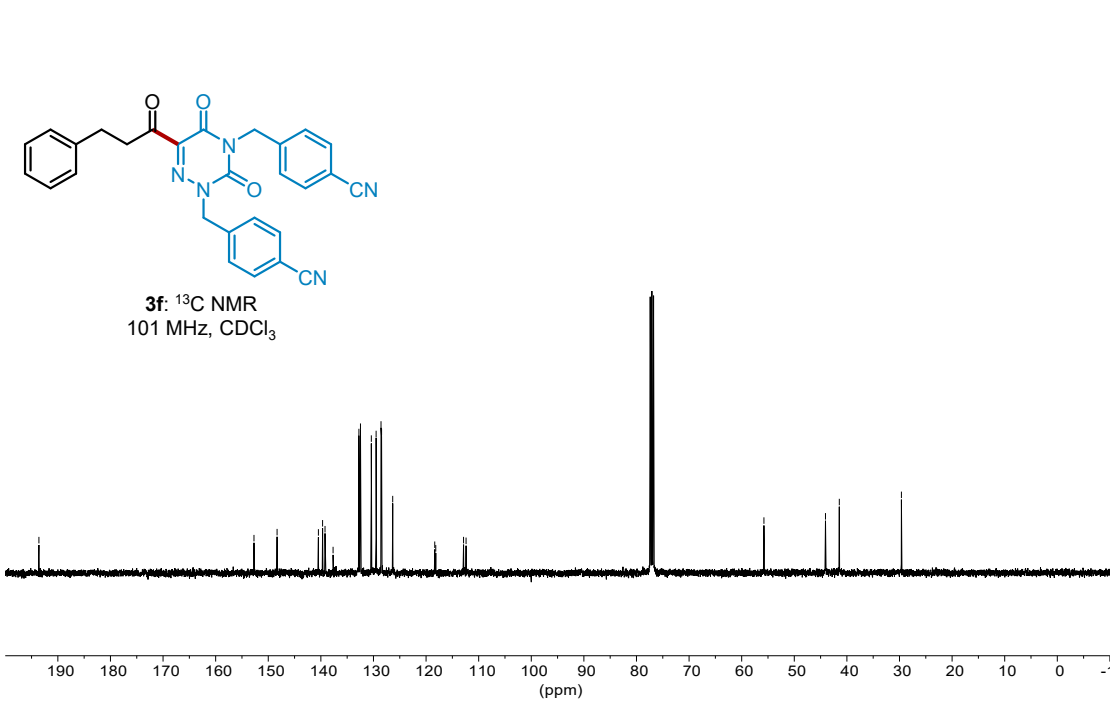
3e: ^{1}H NMR
400 MHz, $CDCl_3$



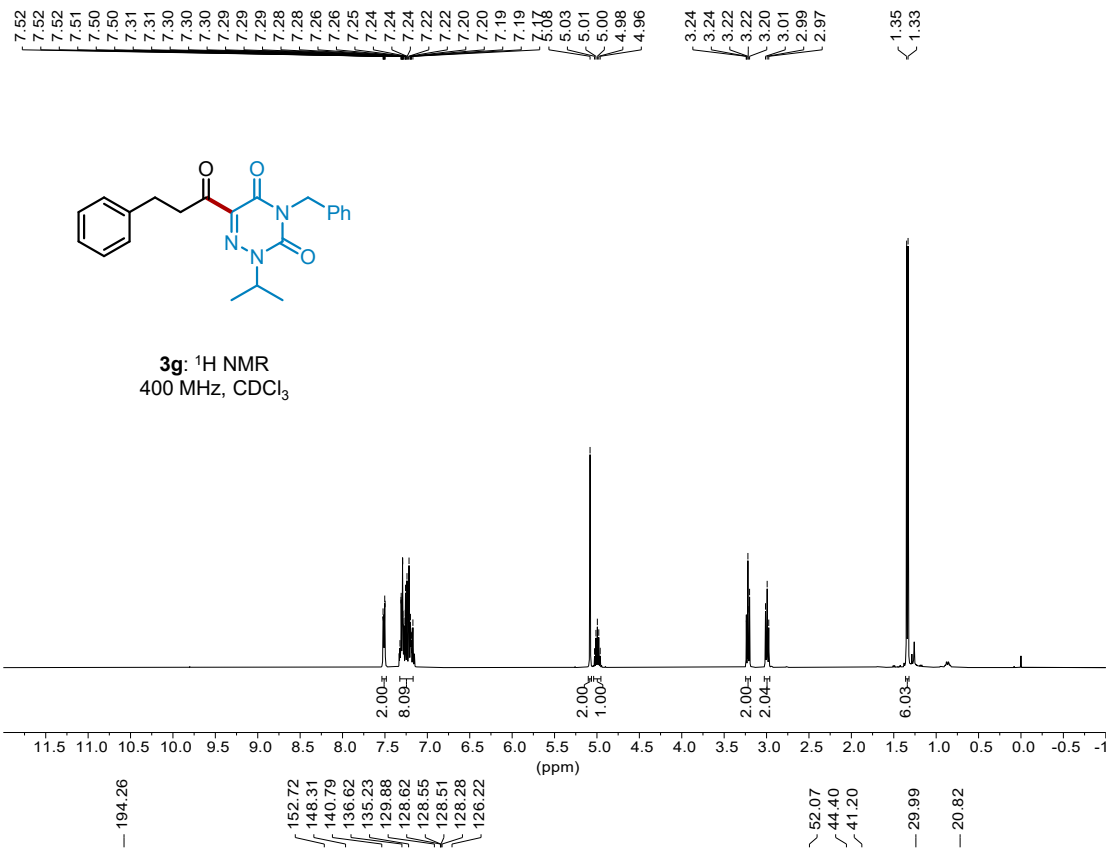
3e: ^{13}C NMR
101 MHz, $CDCl_3$



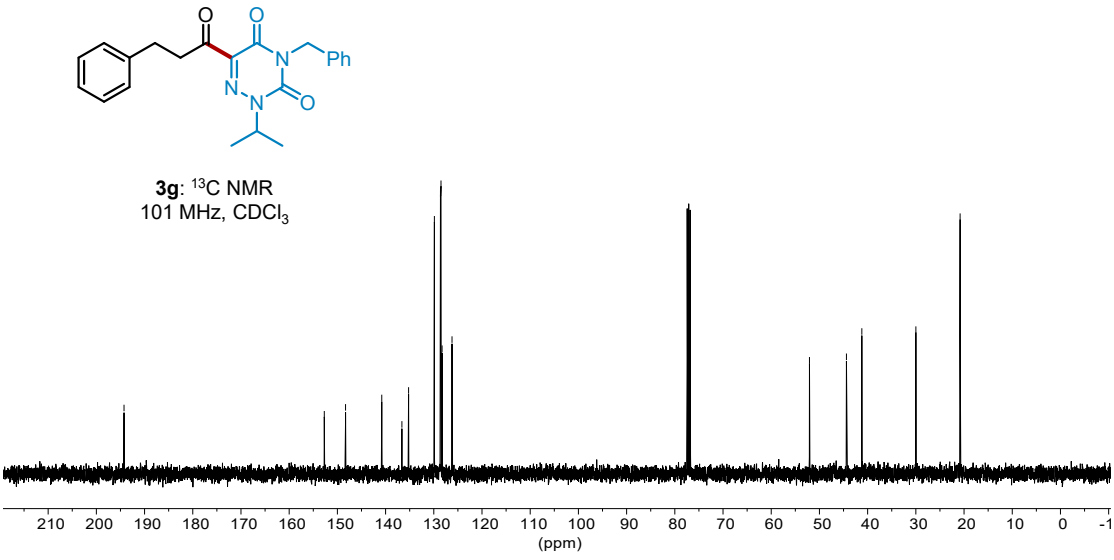
3f: ^{1}H NMR
400 MHz, $CDCl_3$



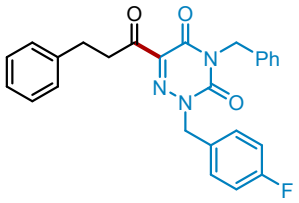
3f: ^{13}C NMR
101 MHz, $CDCl_3$



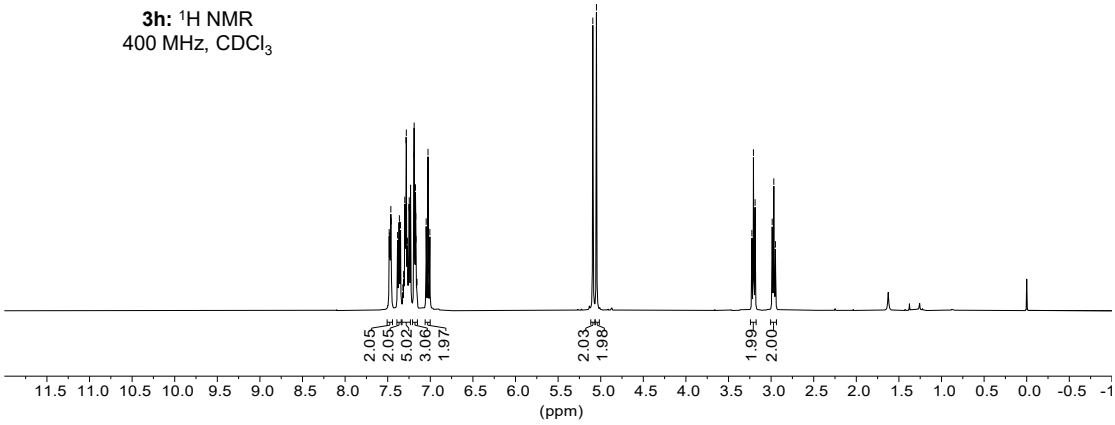
3g: ^{1}H NMR
400 MHz, $CDCl_3$

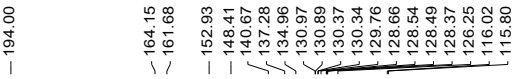


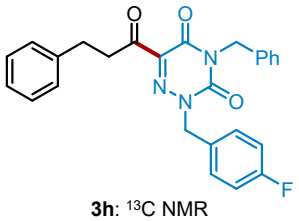
3g: ^{13}C NMR
101 MHz, $CDCl_3$



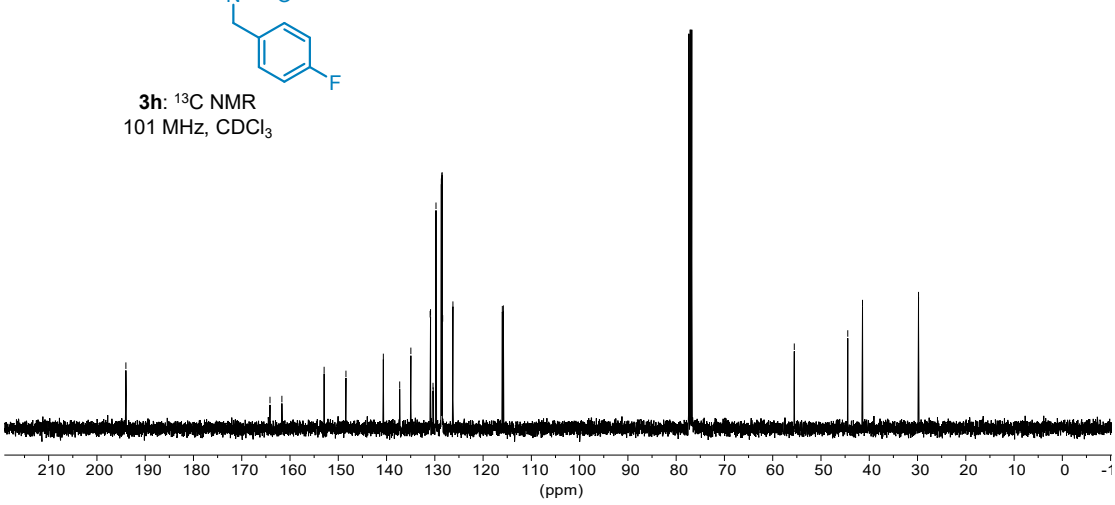
3h: ^{1}H NMR
400 MHz, $CDCl_3$

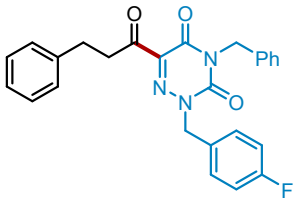




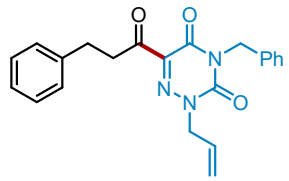


3h: ^{13}C NMR
101 MHz, $CDCl_3$

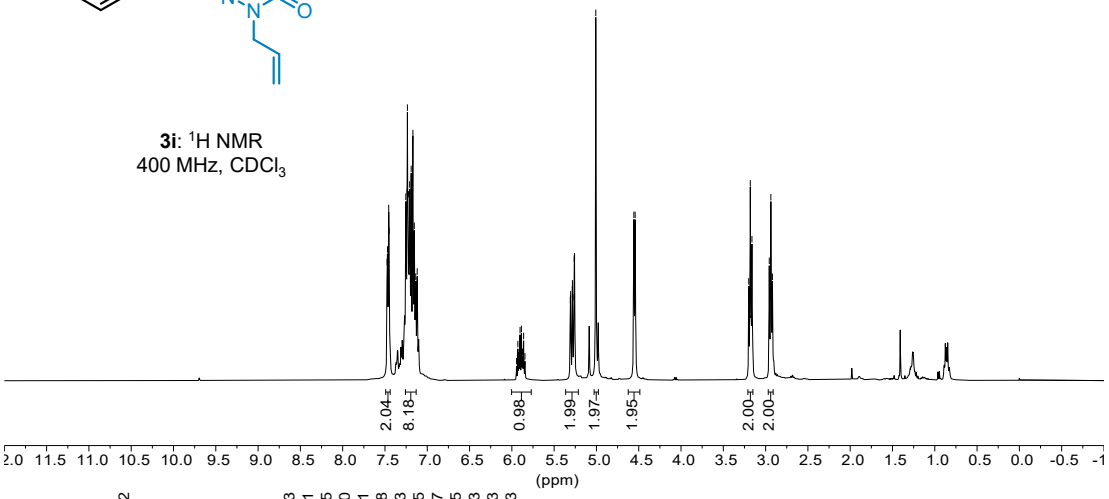


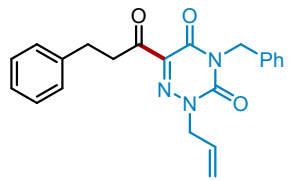


3h: ^{19}F NMR
376 MHz, $CDCl_3$

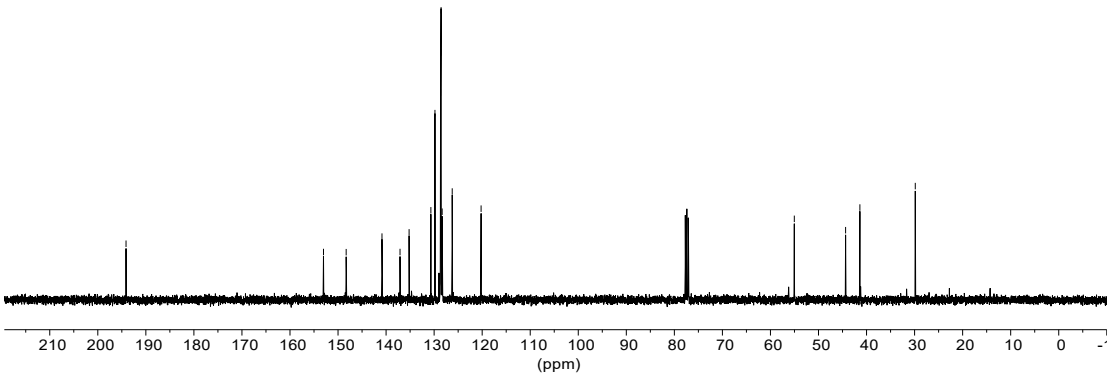


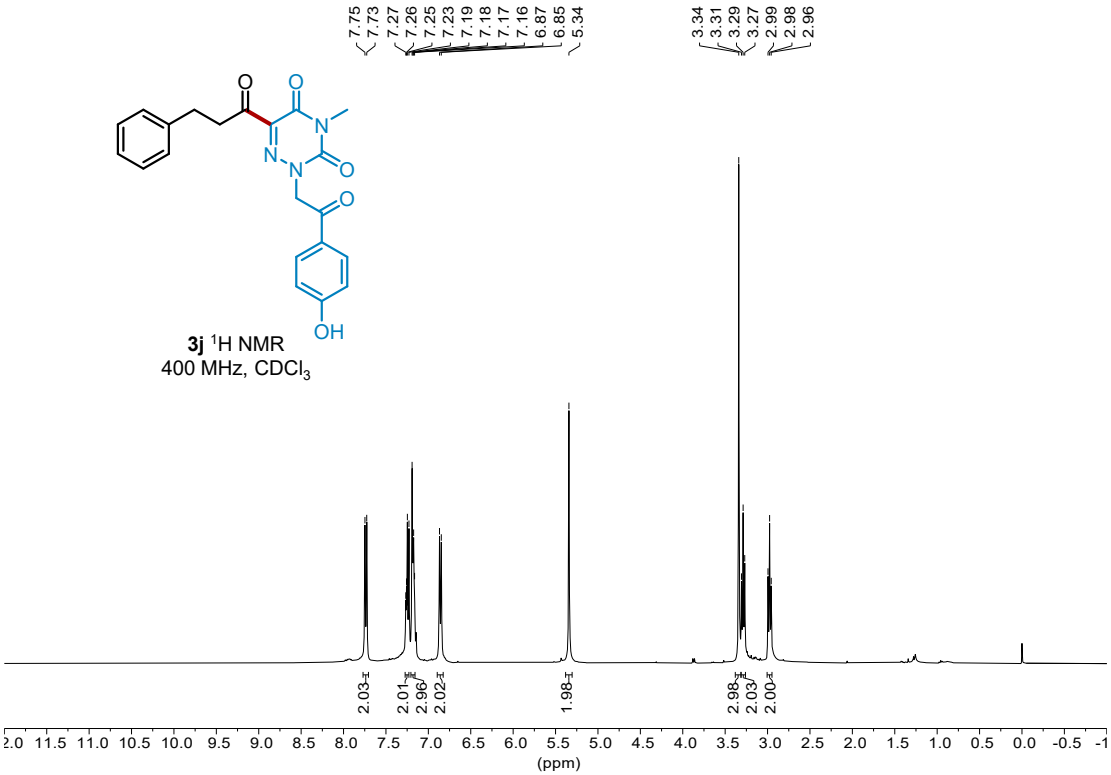
3i: ^{1}H NMR
400 MHz, $CDCl_3$



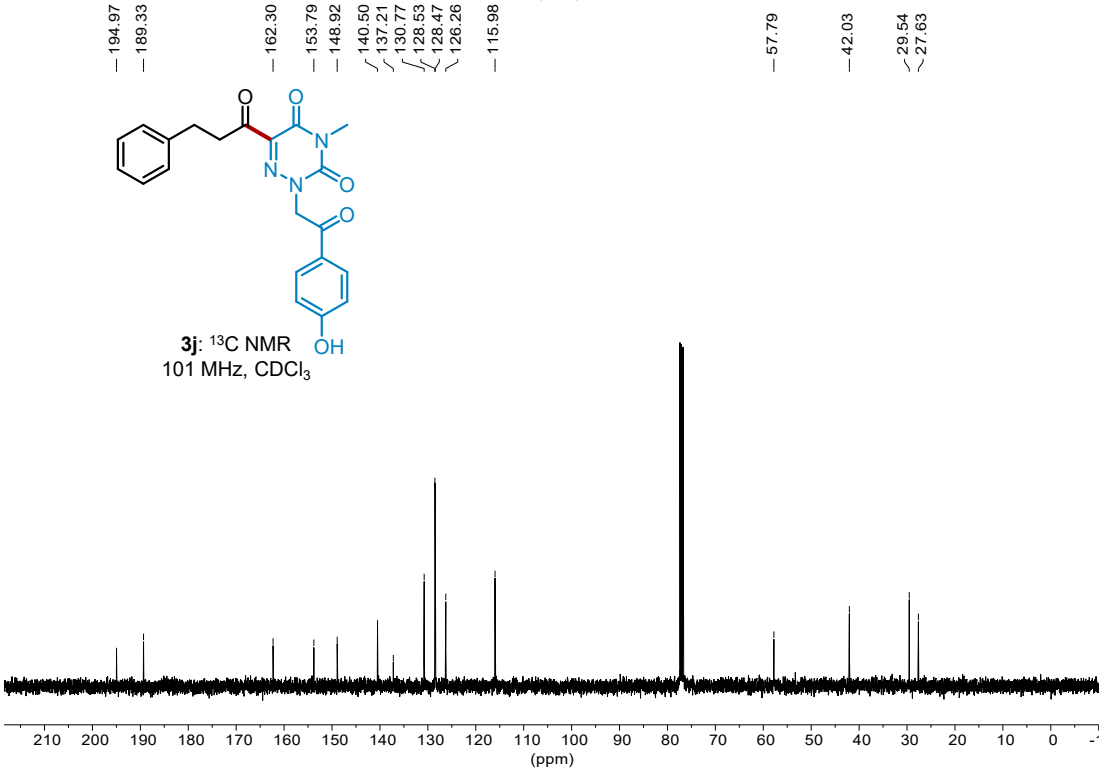


3i: ^{13}C NMR
101 MHz, $CDCl_3$

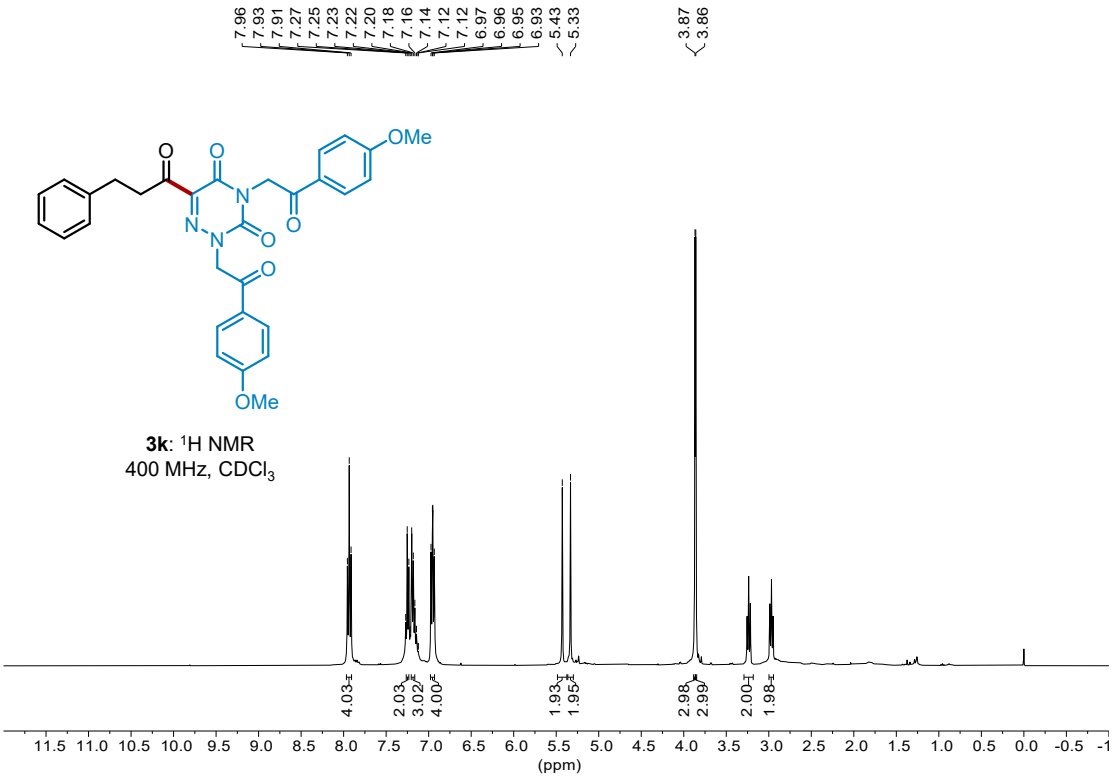




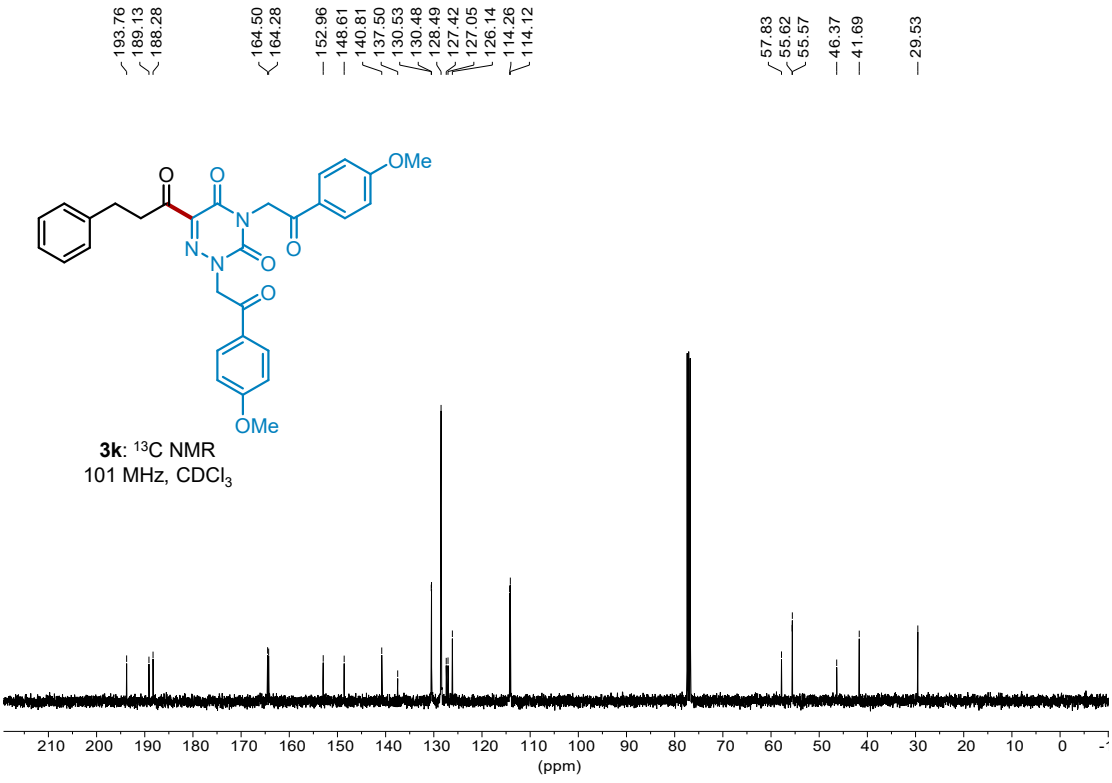
3j ^{1}H NMR
400 MHz, $CDCl_3$



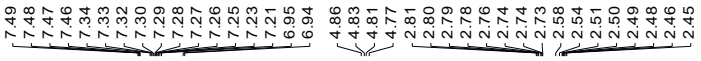
3j: ^{13}C NMR
101 MHz, $CDCl_3$

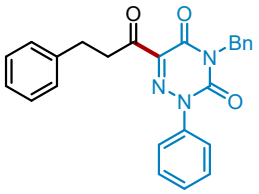


3k: ^{1}H NMR
400 MHz, $CDCl_3$

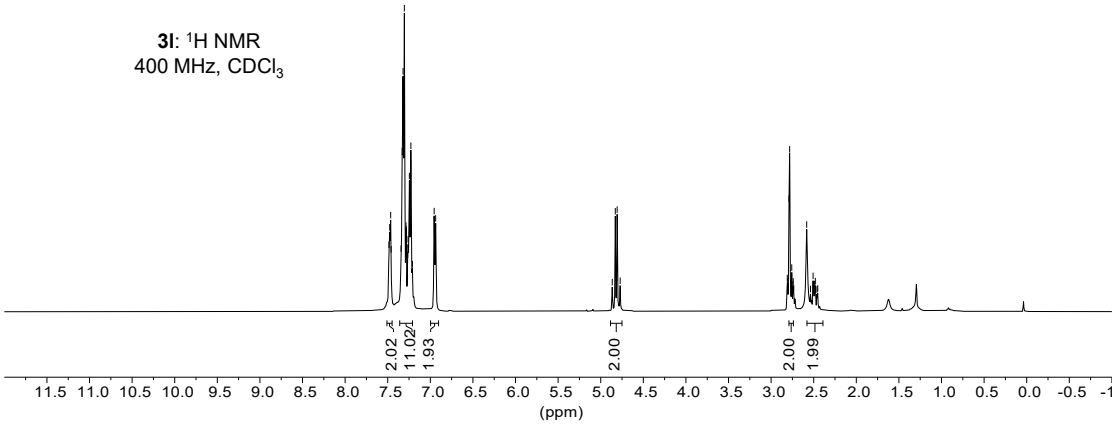


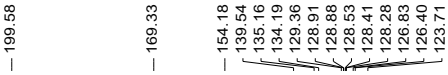
3k: ^{13}C NMR
101 MHz, $CDCl_3$

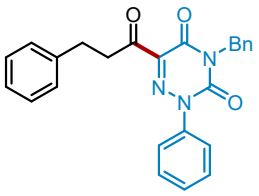




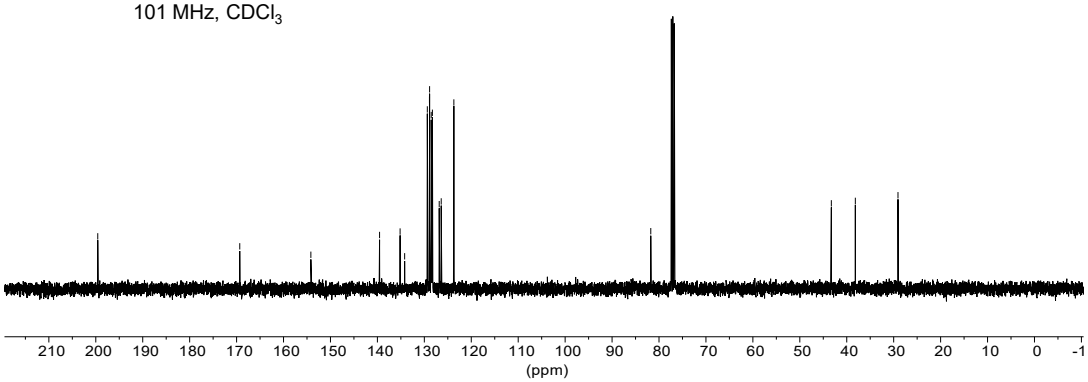
3l: ^{1}H NMR
400 MHz, $CDCl_3$

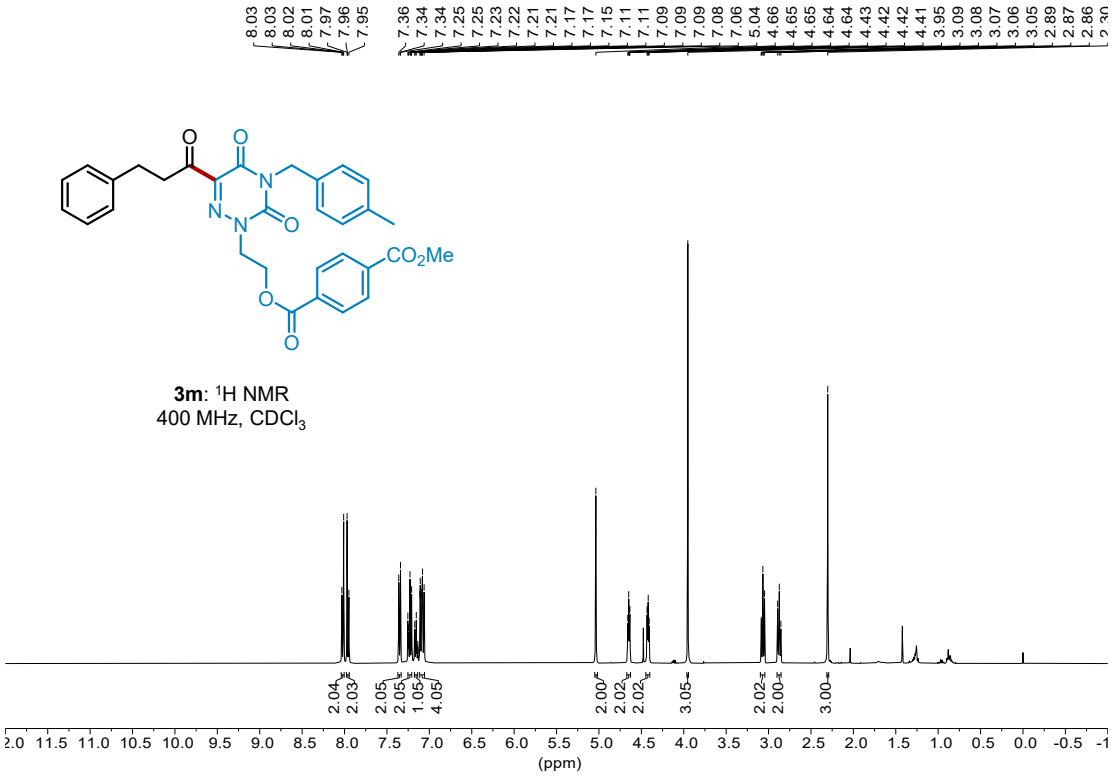




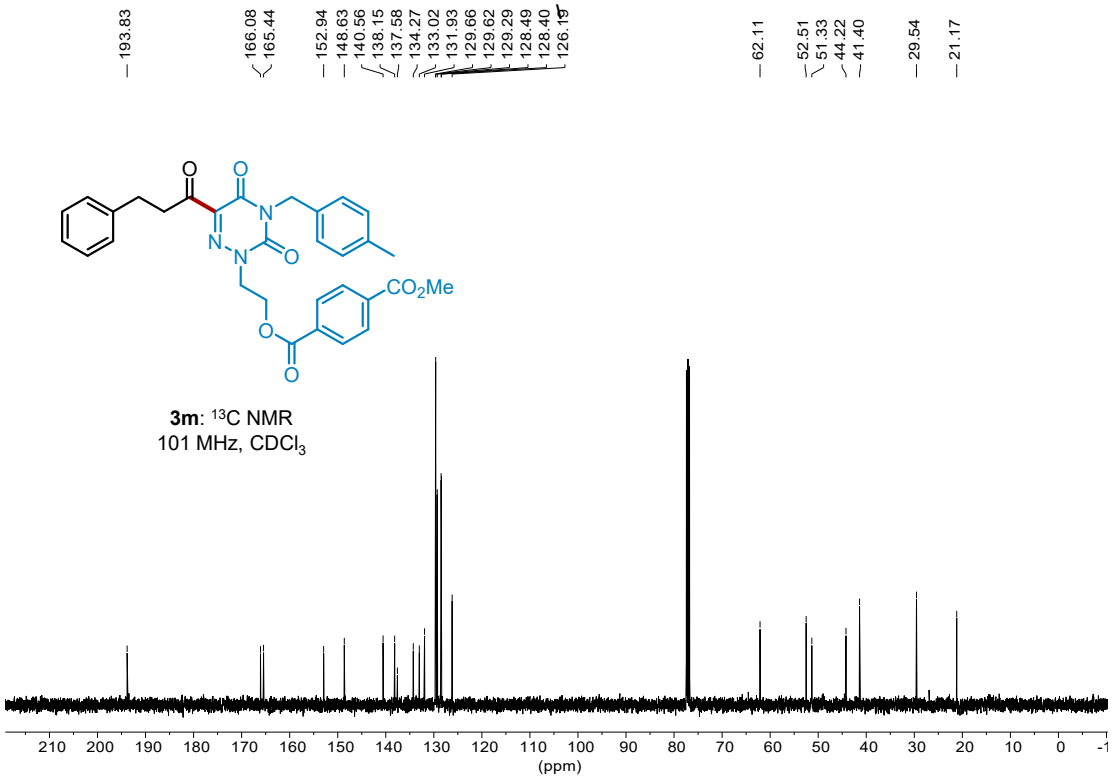


3l: ^{13}C NMR
101 MHz, $CDCl_3$

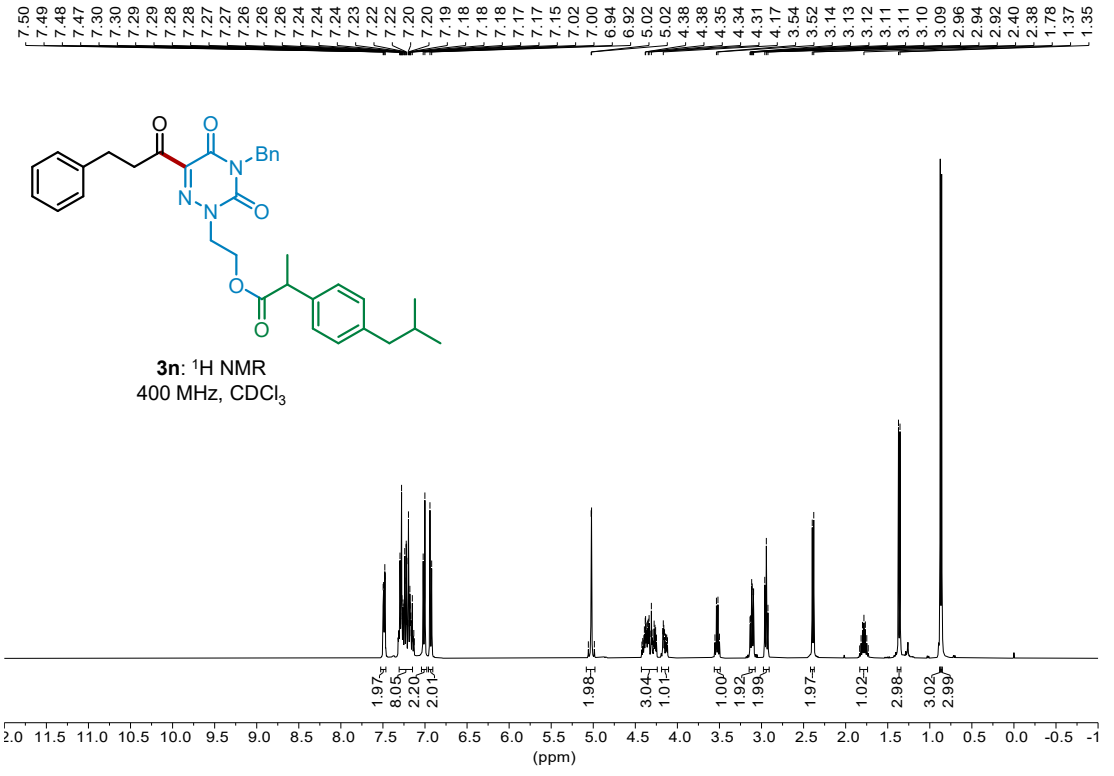


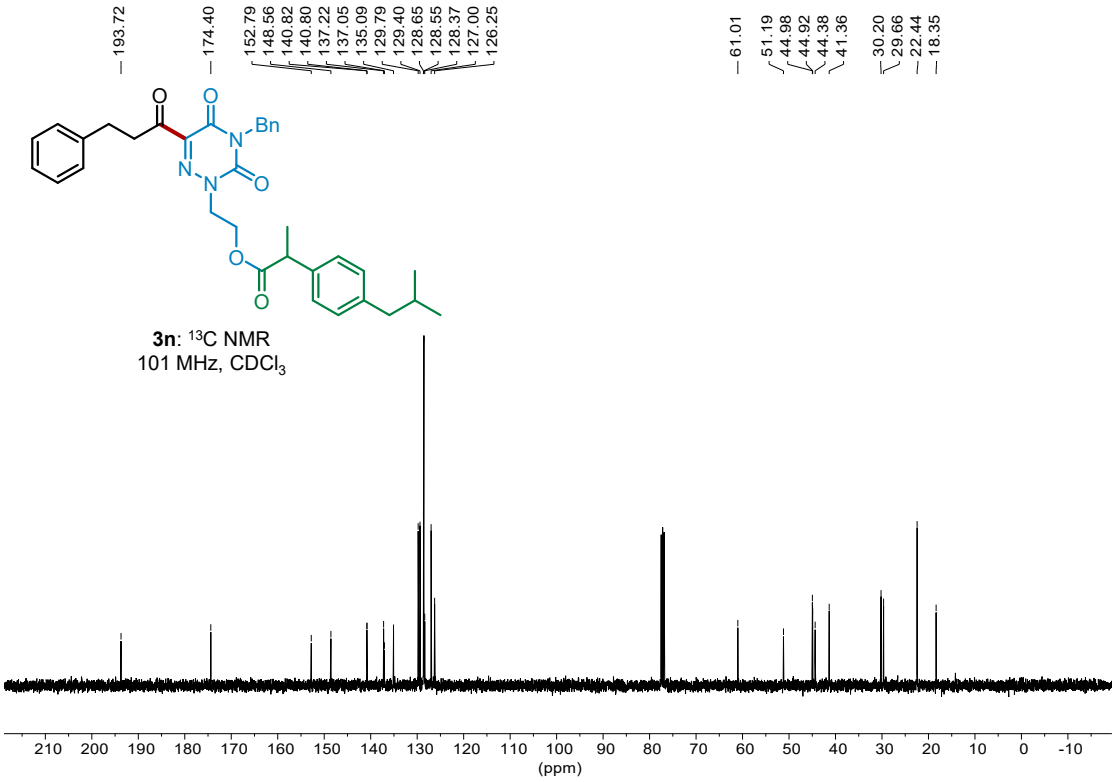


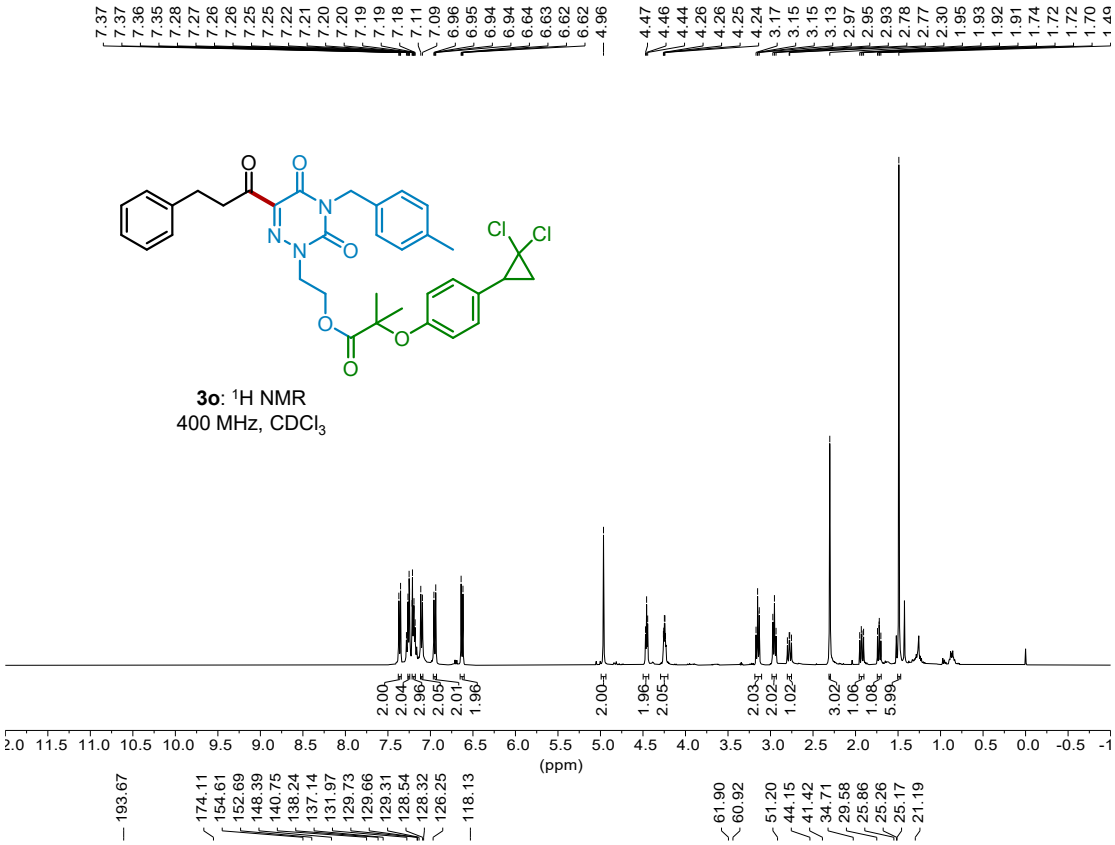
3m: ^{1}H NMR
400 MHz, $CDCl_3$



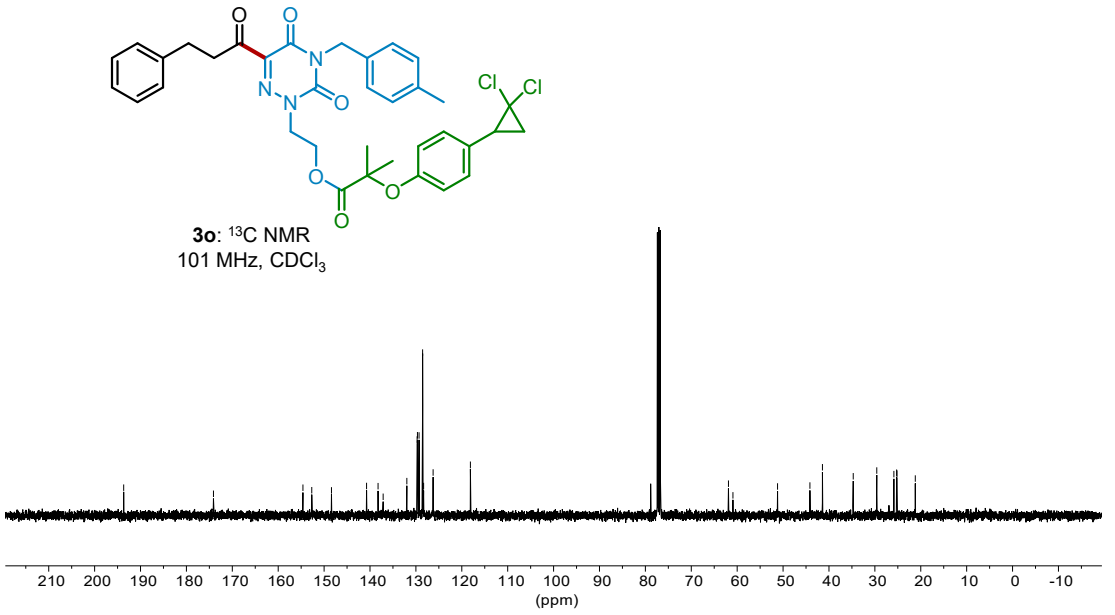
3m: ^{13}C NMR
101 MHz, $CDCl_3$


7.50 7.49 7.48 7.47 7.30 7.30 7.29 7.29 7.28 7.28 7.27 7.27 7.26 7.26 7.26 7.24 7.24 7.24 7.23 7.22 7.22 7.20 7.20 7.19 7.18 7.18 7.18 7.17 7.17 7.15 7.02 7.00 6.94 6.92 5.02 5.02 4.38 4.38 4.35 4.34 4.31 4.17 3.54 3.52 3.14 3.13 3.12 3.11 3.11 3.10 3.09 2.96 2.94 2.92 2.40 2.38 1.78 1.37 1.35
Bn
3n: 1H NMR
400 MHz, CDCl3
1.97 8.05 2.20 2.01 1.98 3.04 1.01 1.00 1.92 1.99 1.97 1.02 2.98 3.02 2.99
(ppm)

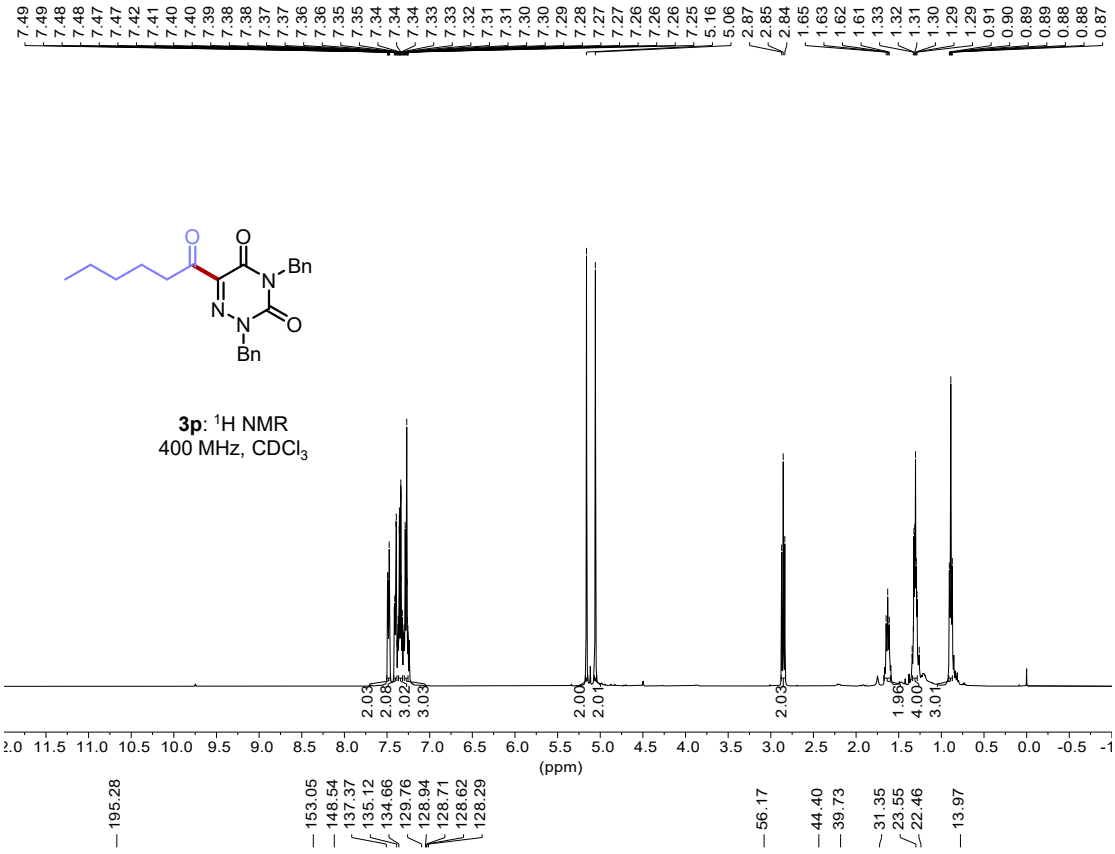

193.72 174.40 152.79 148.56 140.82 140.80 137.22 137.05 135.09 129.79 129.40 128.65 128.55 128.37 127.00 126.25 61.01 51.19 44.98 44.92 44.38 41.36 30.20 29.66 22.44 18.35
Bn
3n: 13C NMR
101 MHz, CDCl3
(ppm)

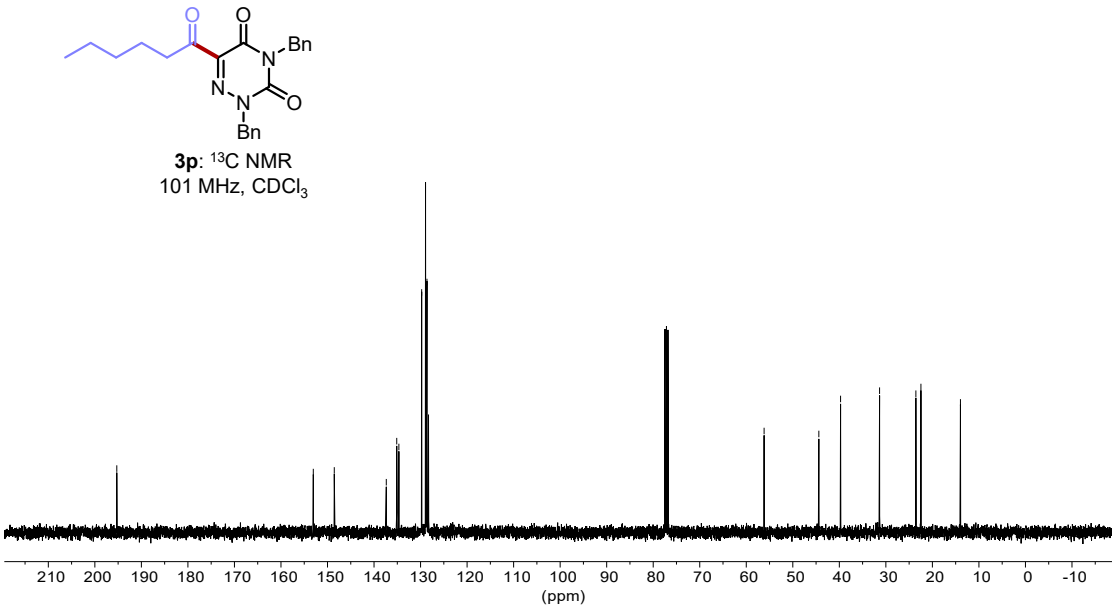


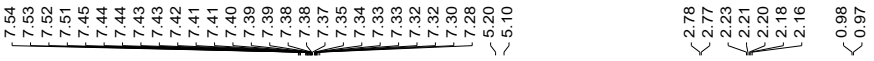
3o: ^{1}H NMR
400 MHz, $CDCl_3$

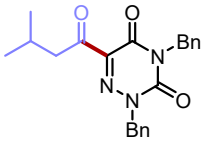


3o: ^{13}C NMR
101 MHz, $CDCl_3$

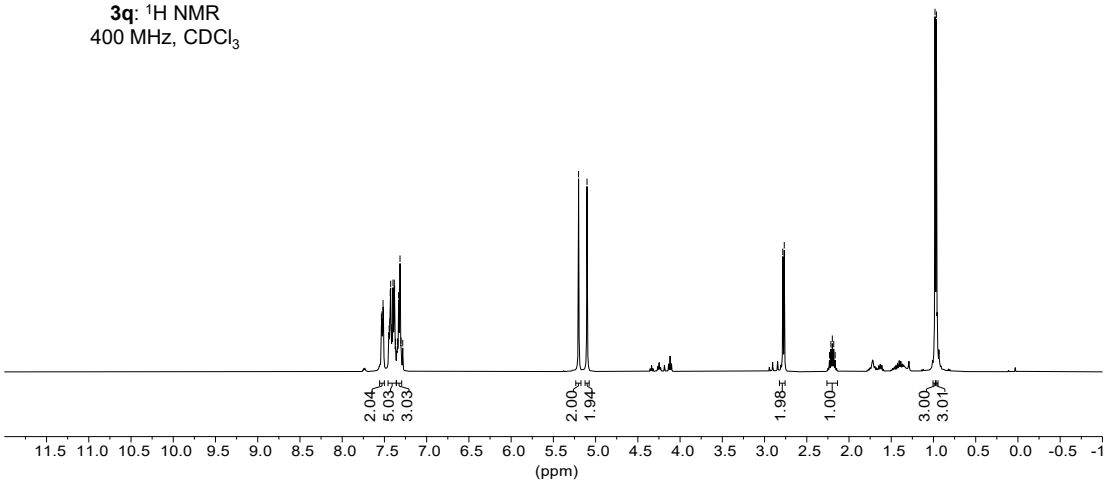

7.49 7.49 7.48 7.48 7.47 7.47 7.42 7.41 7.40 7.40 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.27 7.27 7.26 7.26 7.26 7.25 5.16 5.06 2.87 2.85 2.84 1.65 1.63 1.62 1.61 1.33 1.32 1.31 1.30 1.29 1.29 0.91 0.90 0.89 0.89 0.88 0.88 0.87
O
O
N
Bn
N
N
O
Bn
3p: 1H NMR
400 MHz, CDCl3
2.03 2.08 3.02 3.03 2.00 2.01 2.03 1.96 4.00 3.01
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
(ppm)
195.28 153.05 148.54 137.37 135.12 134.66 129.76 128.94 128.71 128.62 128.29 56.17 44.40 39.73 31.35 23.55 22.46 13.97

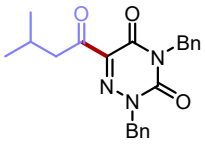

O
O
N
Bn
N
N
O
Bn
3p: 13C NMR
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)



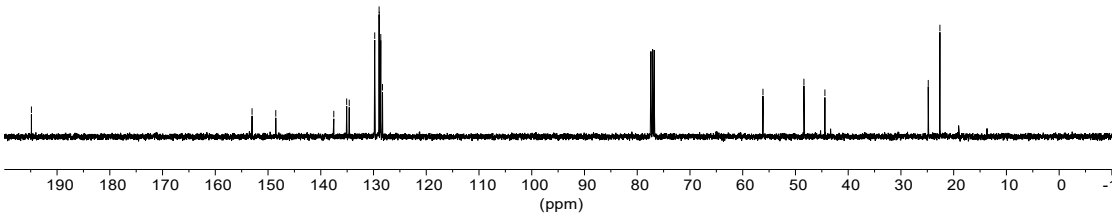


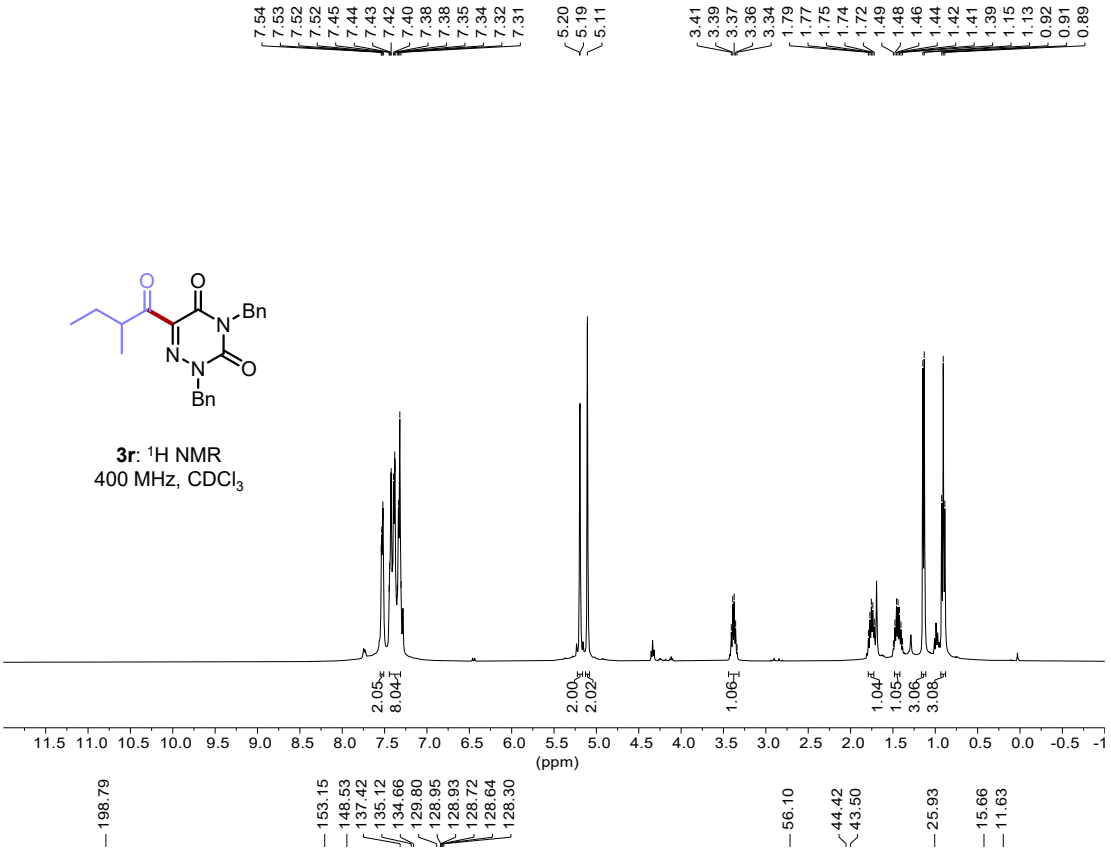
3q: ^{1}H NMR
400 MHz, $CDCl_3$



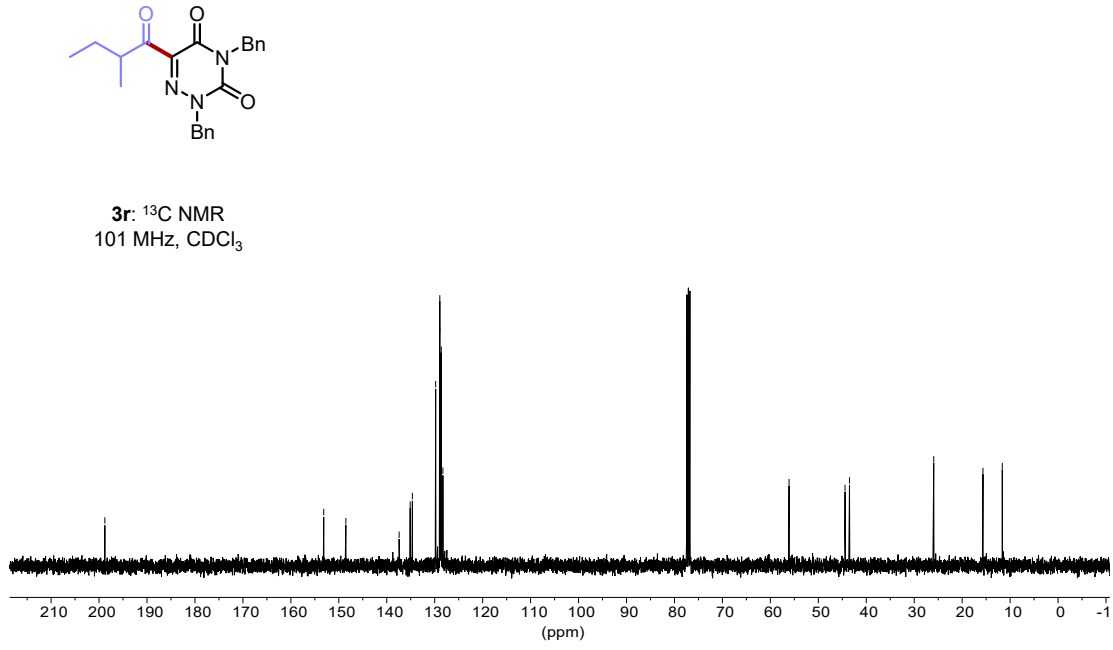


3q: ^{13}C NMR
101 MHz, $CDCl_3$

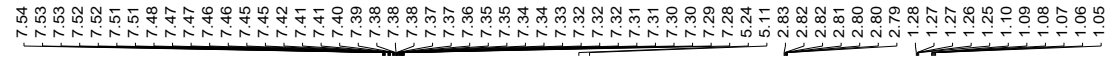


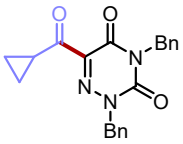


3r: ^{1}H NMR
400 MHz, $CDCl_3$

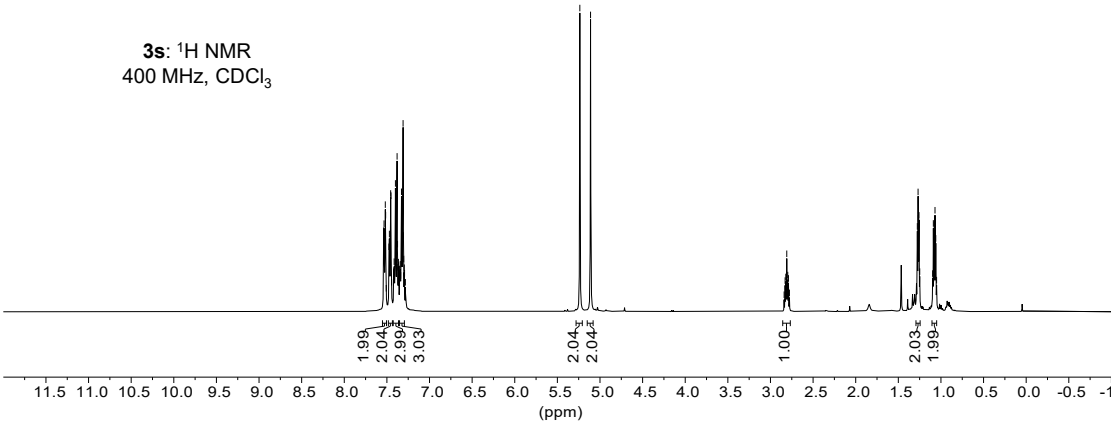


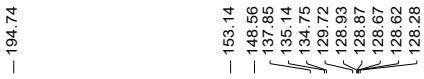
3r: ^{13}C NMR
101 MHz, $CDCl_3$

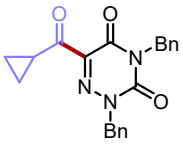




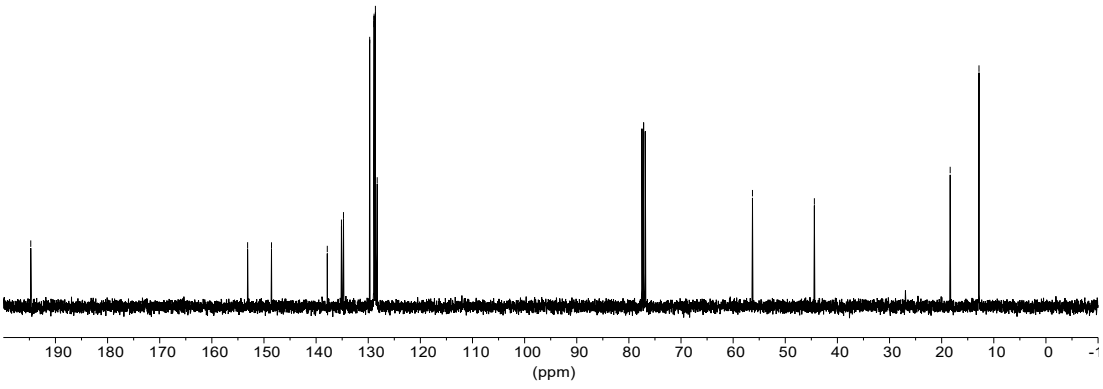
3s: ^{1}H NMR
400 MHz, $CDCl_3$

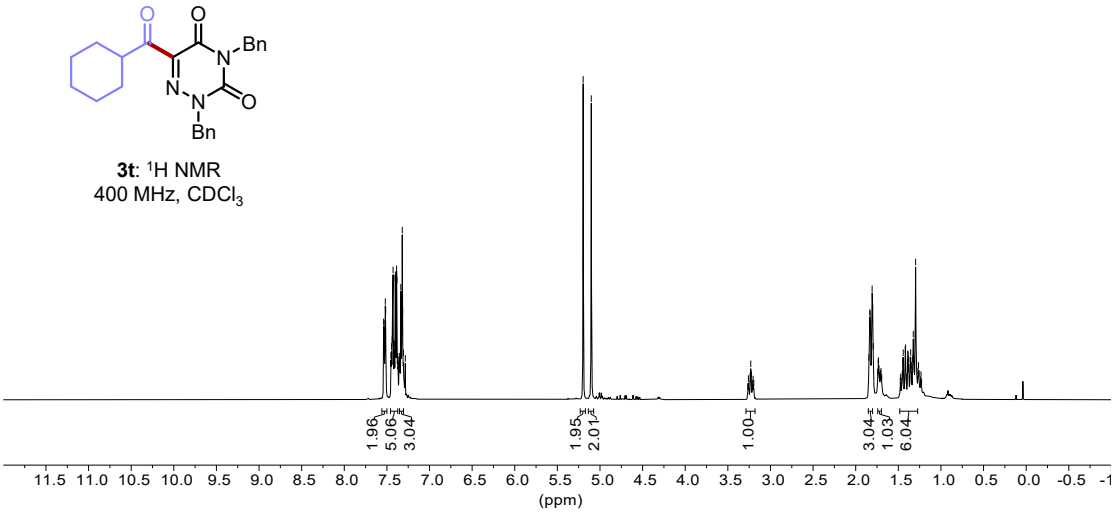




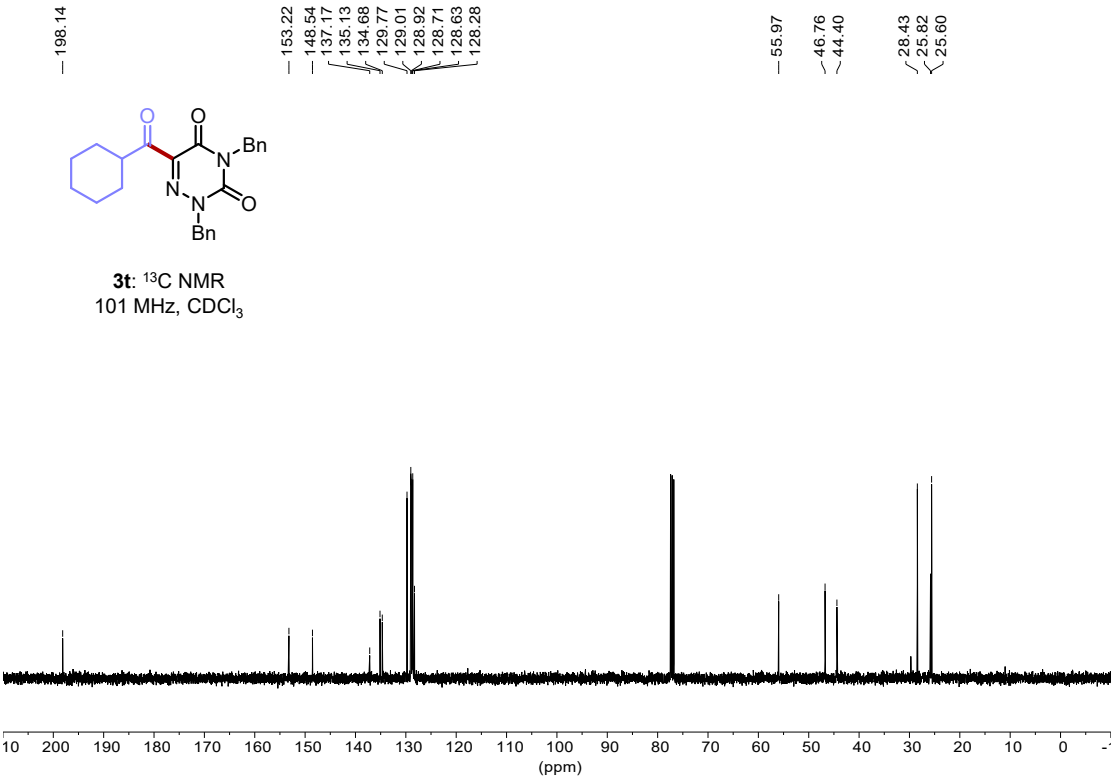


3s: ^{13}C NMR
101 MHz, $CDCl_3$

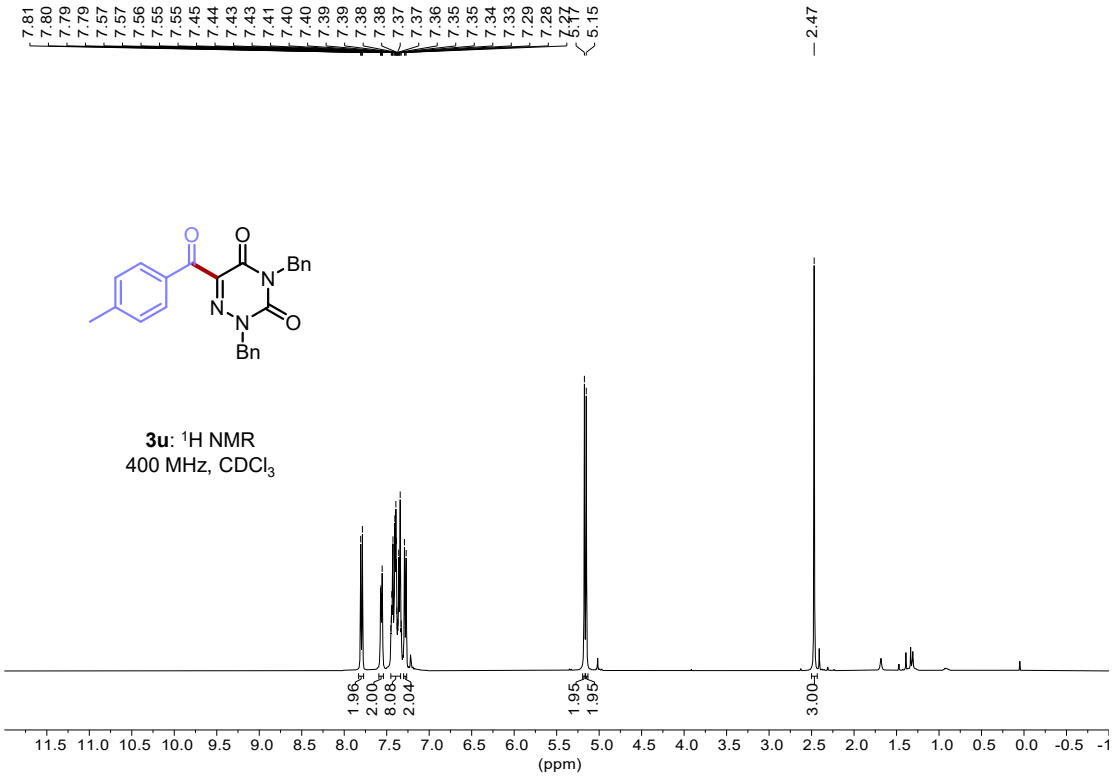




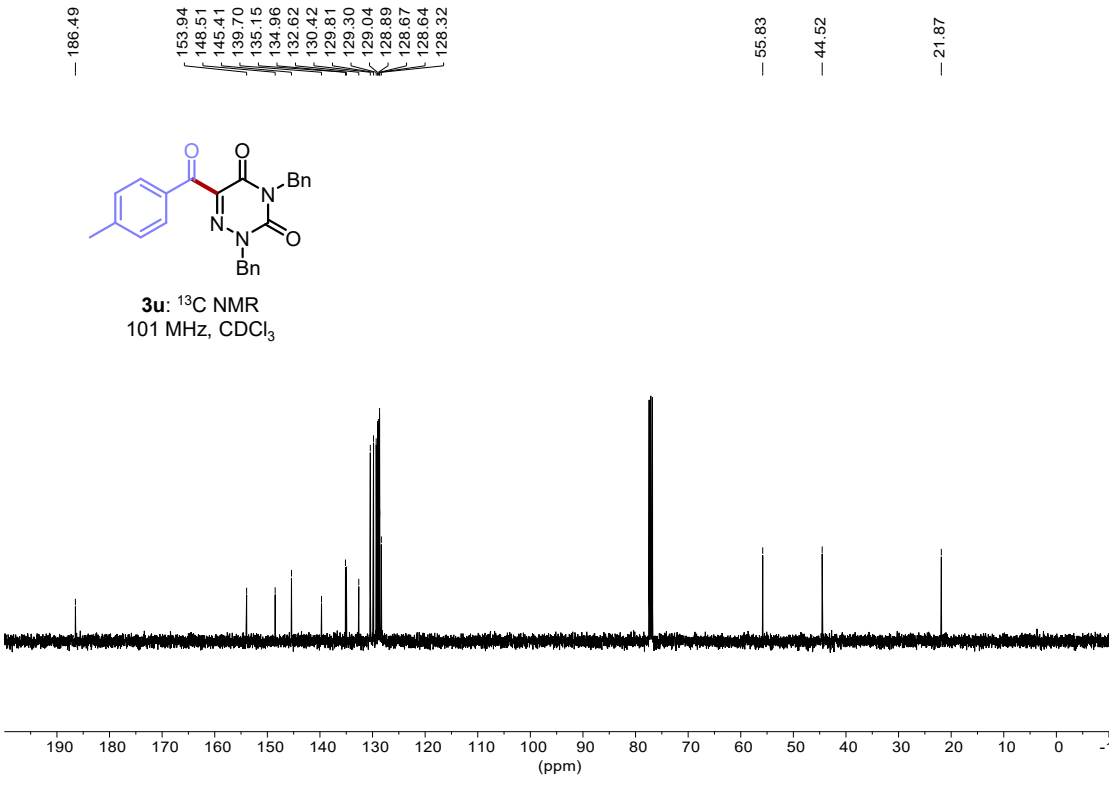
3t: ^{1}H NMR
400 MHz, $CDCl_3$



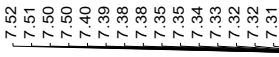
3t: ^{13}C NMR
101 MHz, $CDCl_3$

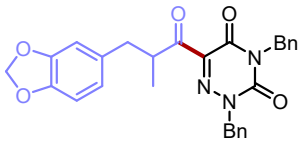


3u: ^{1}H NMR
400 MHz, $CDCl_3$

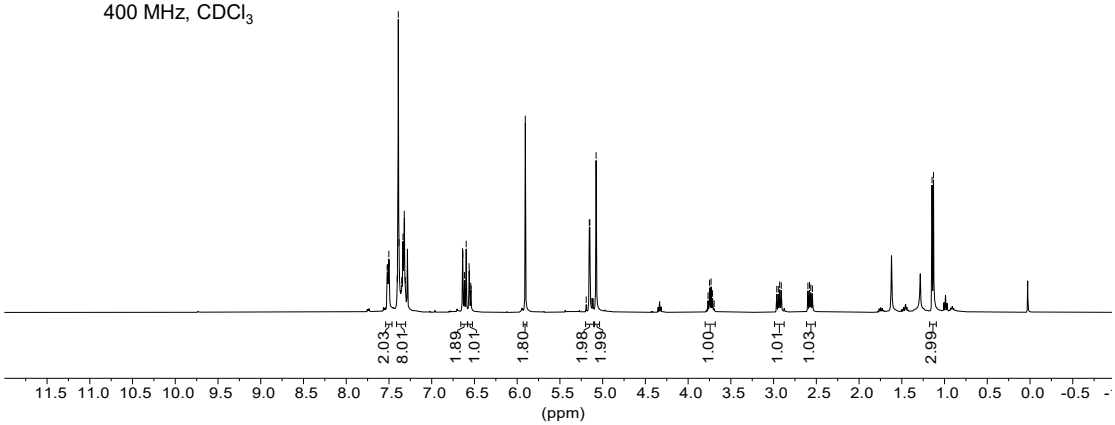


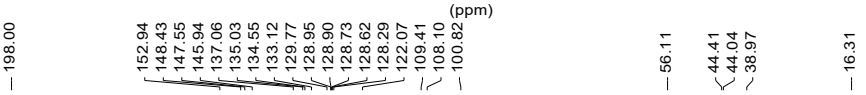
3u: ^{13}C NMR
101 MHz, $CDCl_3$

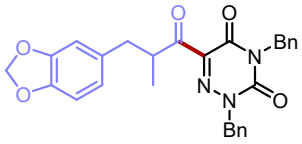




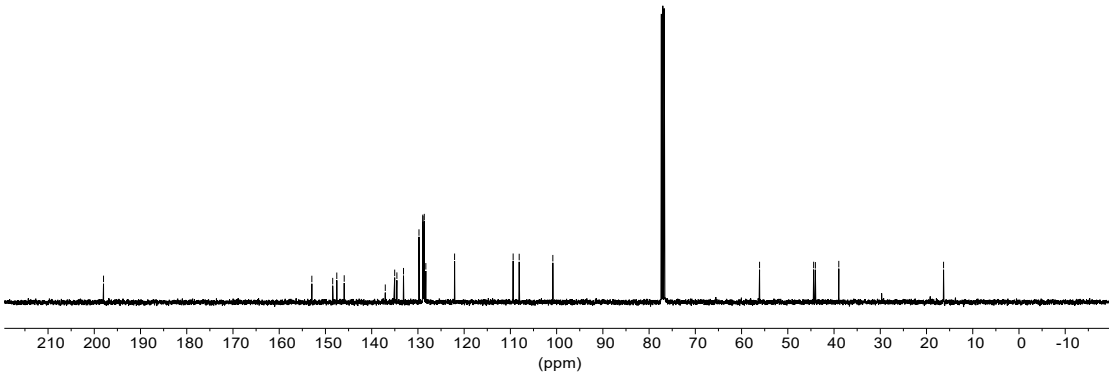
3v: ^{1}H NMR
400 MHz, $CDCl_3$

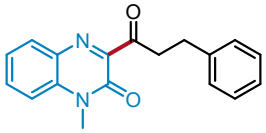




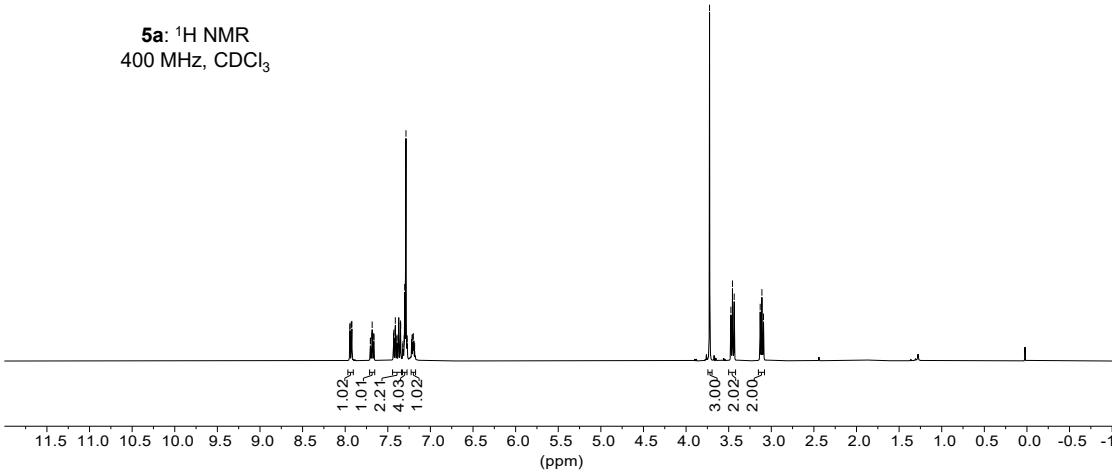


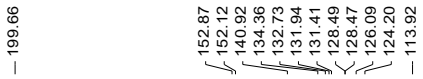
3v: ^{13}C NMR
101 MHz, $CDCl_3$

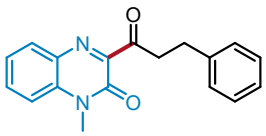




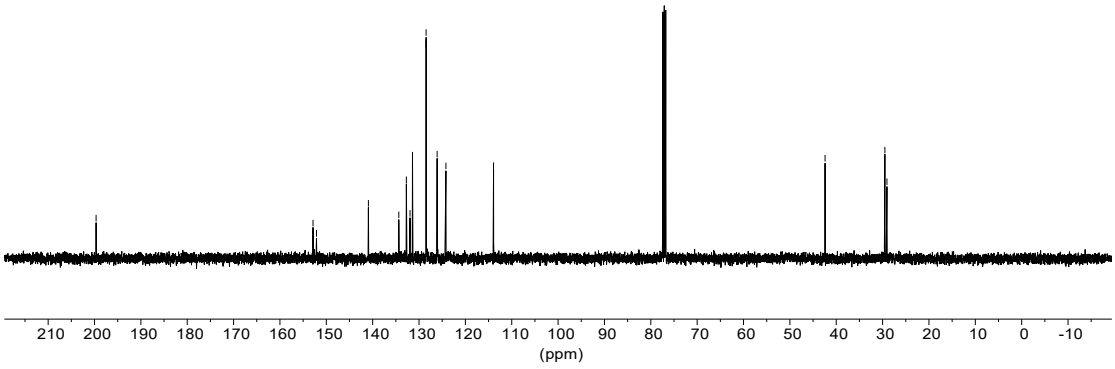
5a: ^{1}H NMR
400 MHz, $CDCl_3$

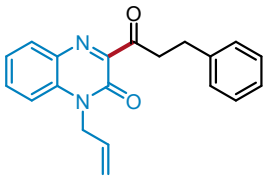




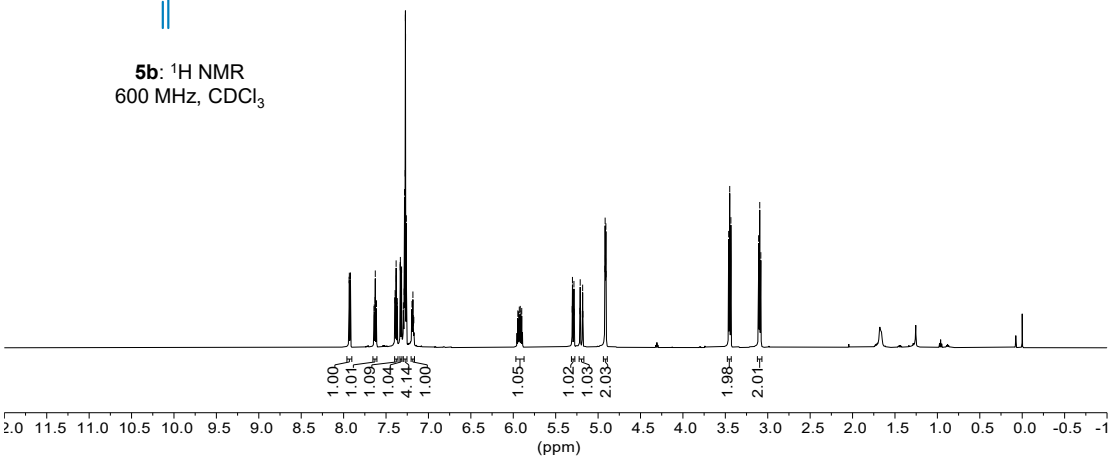


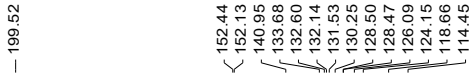
5a: ^{13}C NMR
101 MHz, $CDCl_3$

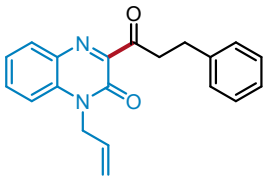




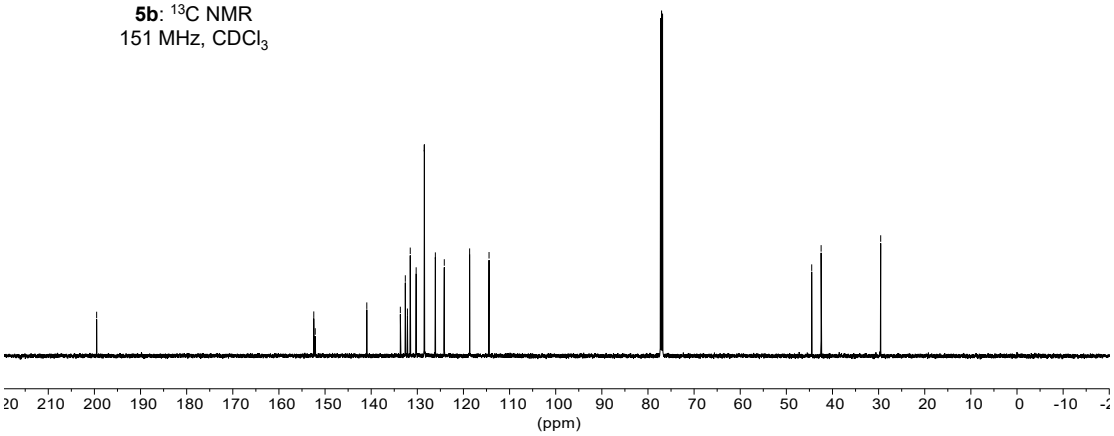
5b: ^{1}H NMR
600 MHz, $CDCl_3$

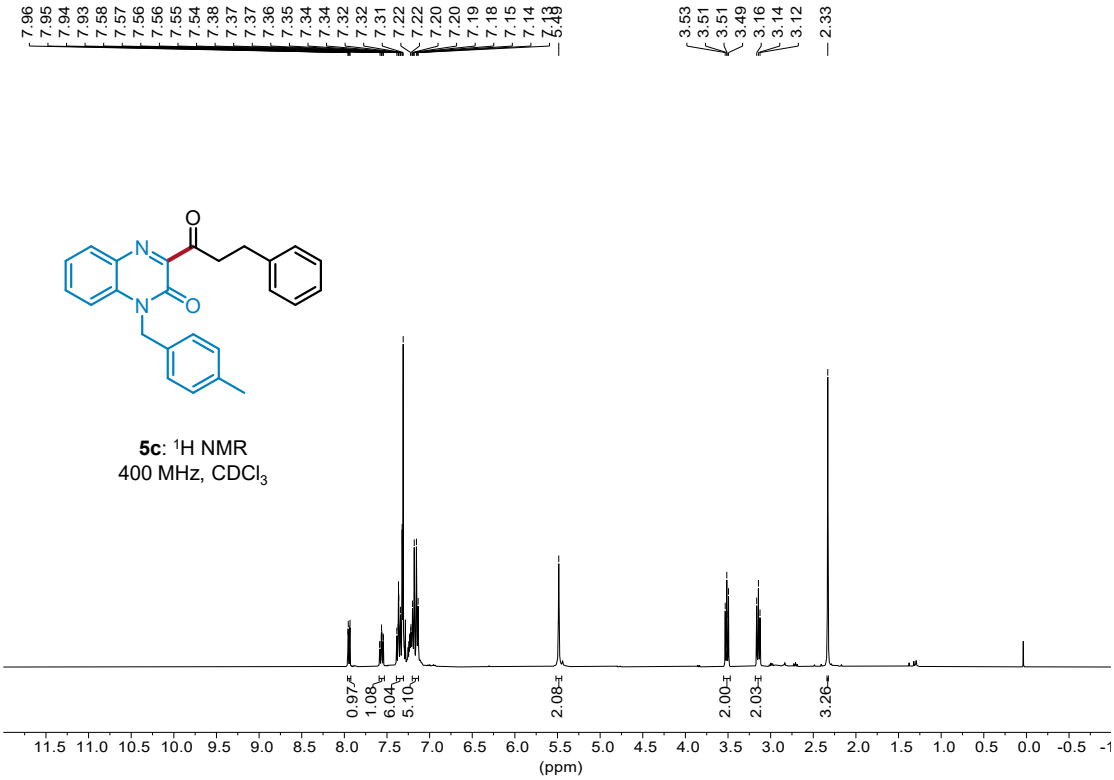




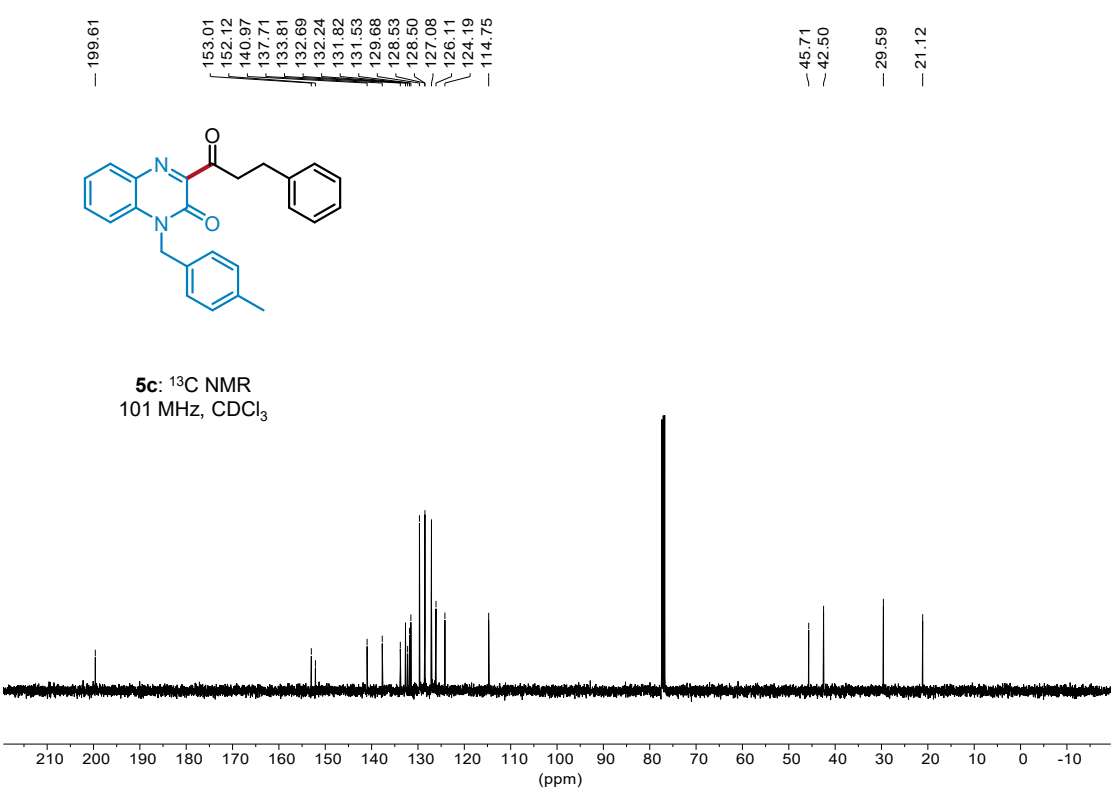


5b: ^{13}C NMR
151 MHz, $CDCl_3$

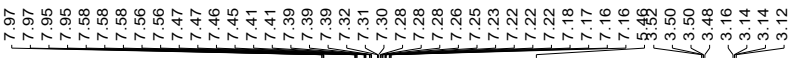


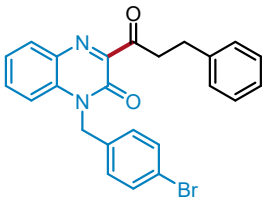


5c: ^{1}H NMR
400 MHz, $CDCl_3$

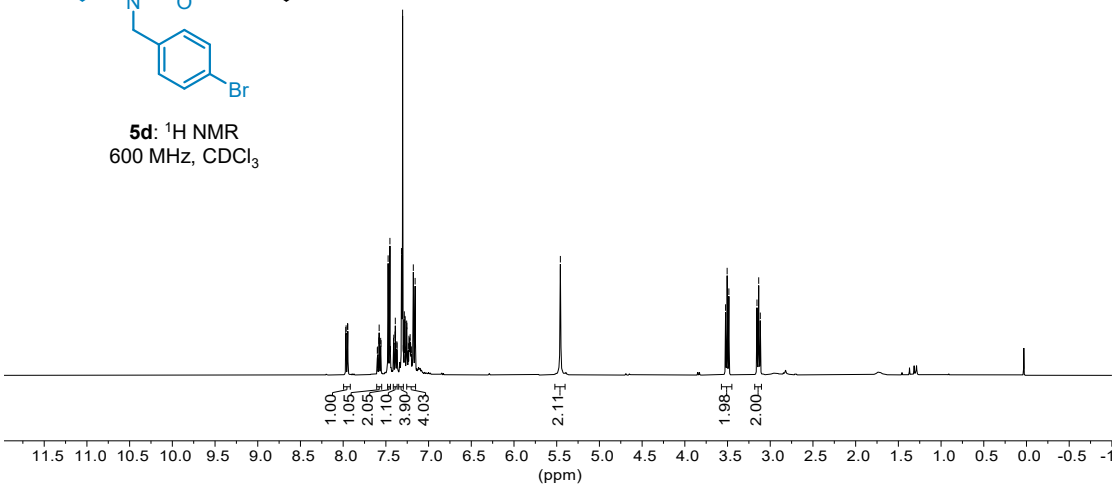


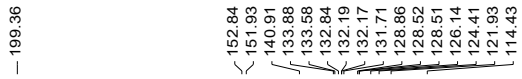
5c: ^{13}C NMR
101 MHz, $CDCl_3$

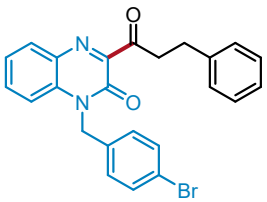




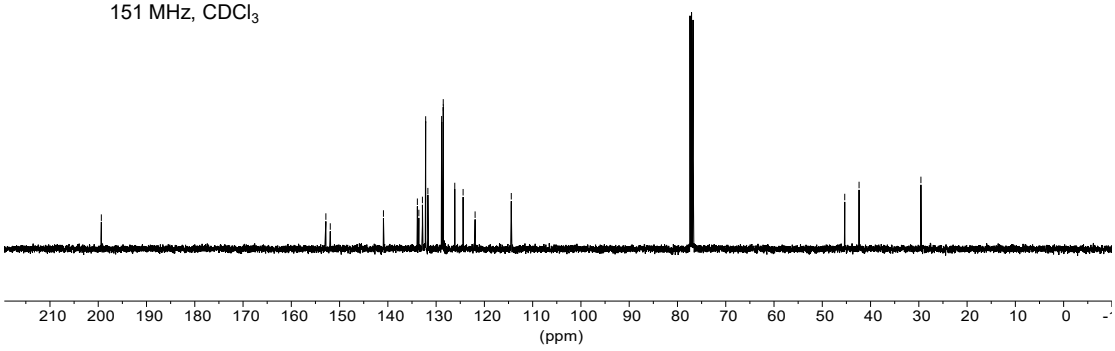
5d: ^{1}H NMR
600 MHz, $CDCl_3$

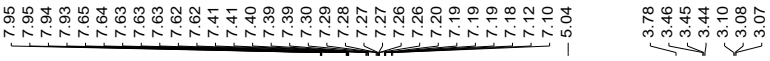


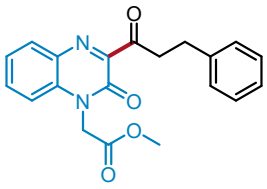




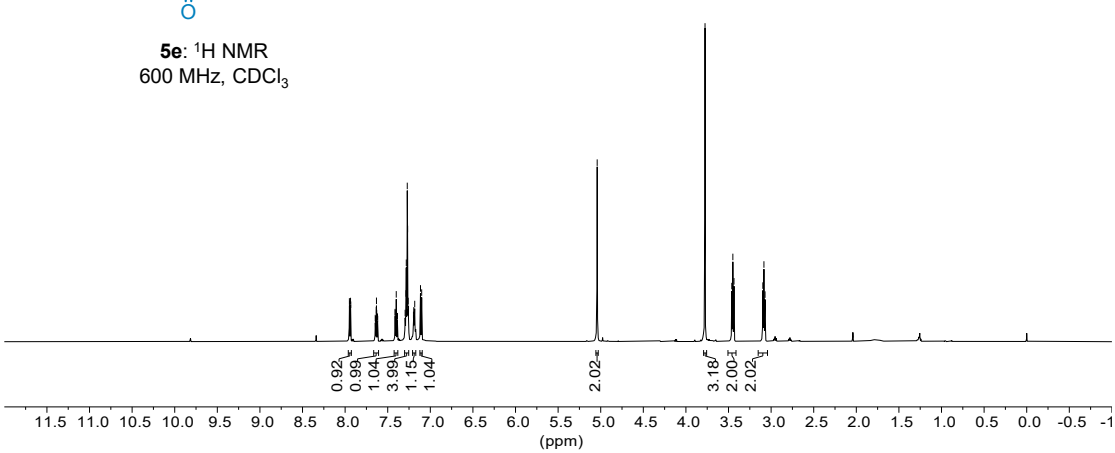
5d: ^{13}C NMR
151 MHz, $CDCl_3$

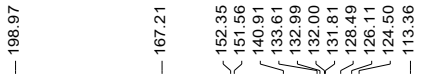


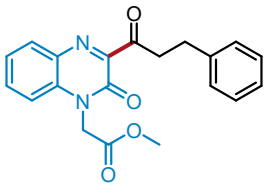




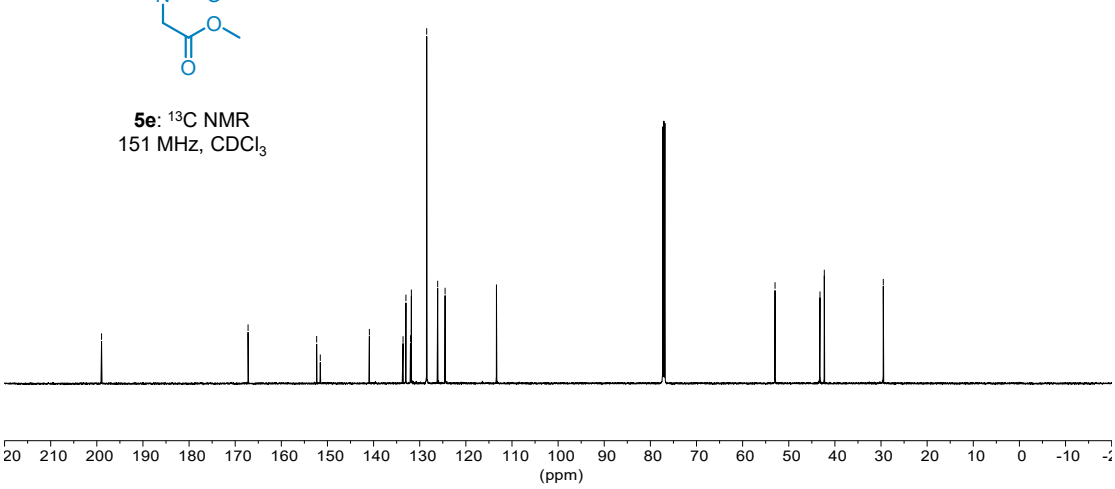
5e: ^{1}H NMR
600 MHz, $CDCl_3$

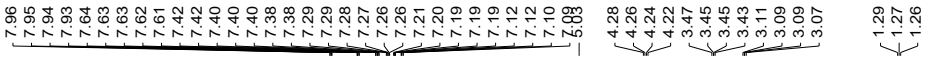


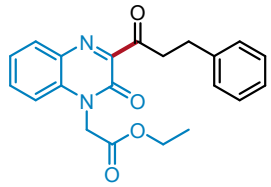




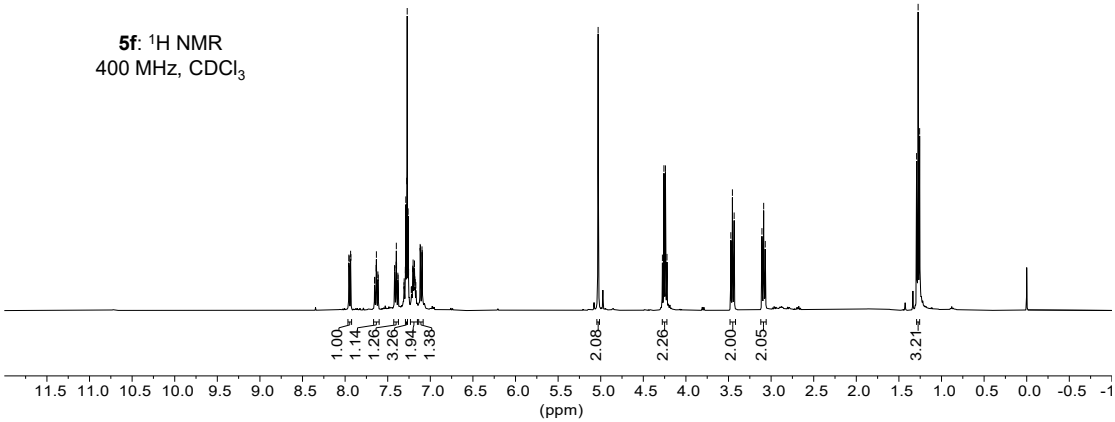
5e: ^{13}C NMR
151 MHz, $CDCl_3$

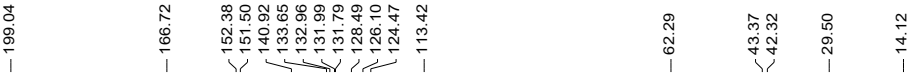


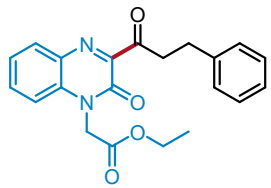




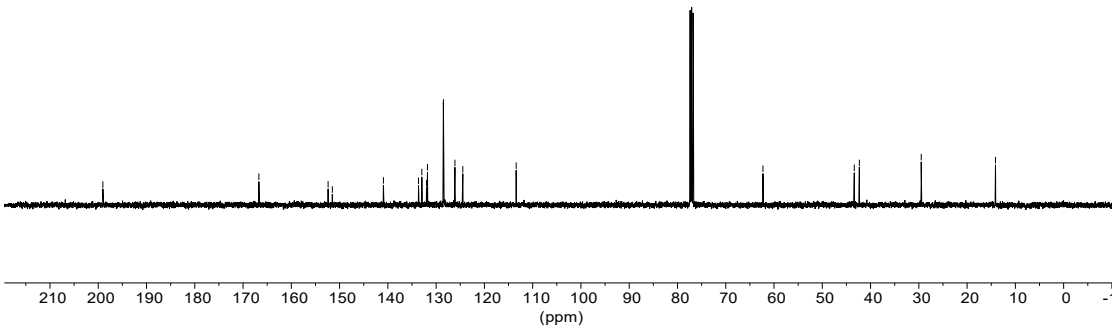
5f: ^{1}H NMR
400 MHz, $CDCl_3$

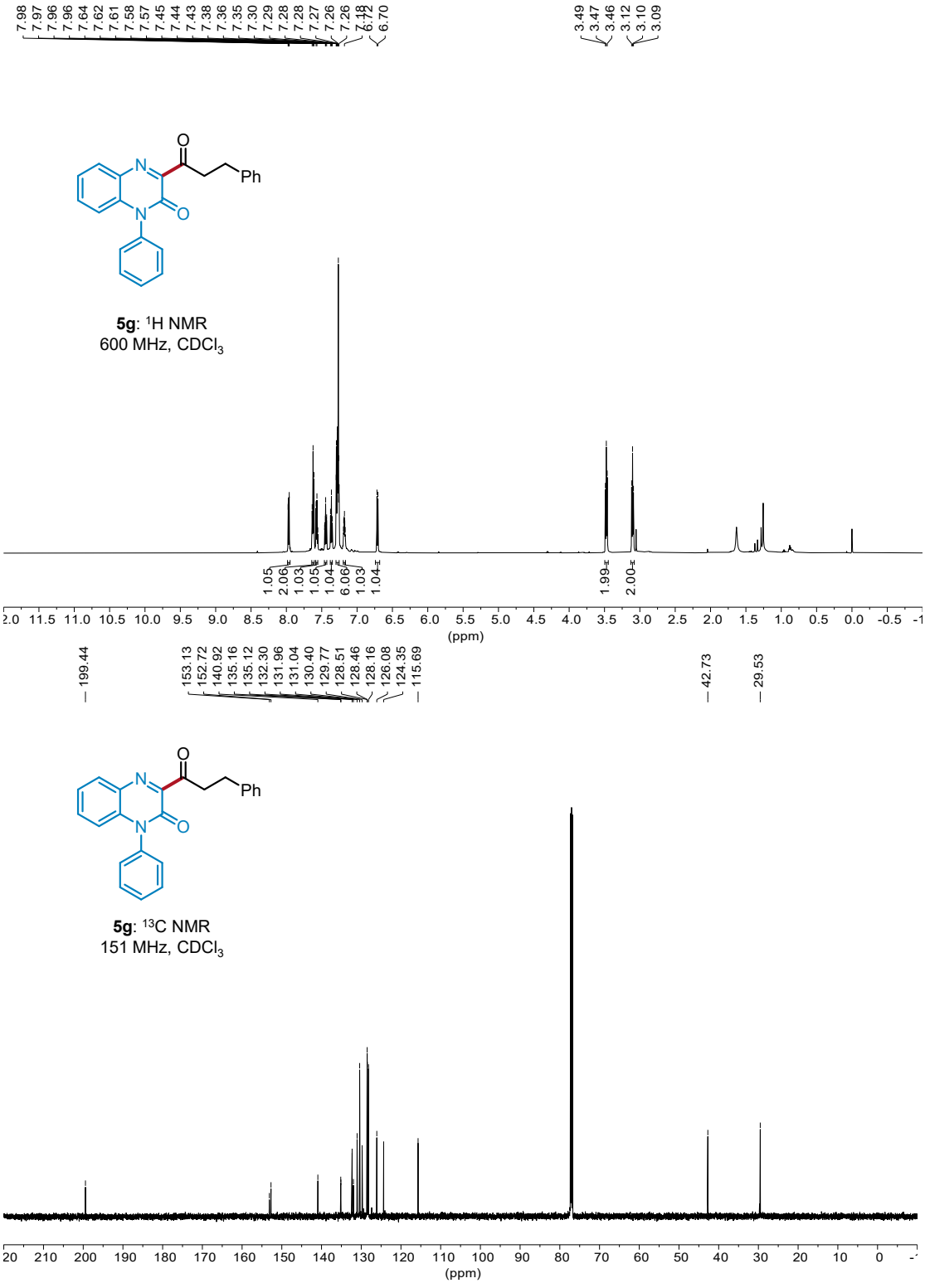






5f: ^{13}C NMR
101 MHz, $CDCl_3$

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7.28
7.28
7.27
7.26
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7.18
7.12
6.70
3.49
3.47
3.46
3.12
3.10
3.09
O
N
Ph
N
O
5g: 1H NMR
600 MHz, CDCl3
1.05
2.06
1.03
1.05
1.04
6.06
1.03
1.04
1.99
2.00
(ppm)
199.44
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152.72
140.92
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128.16
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124.35
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42.73
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O
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N
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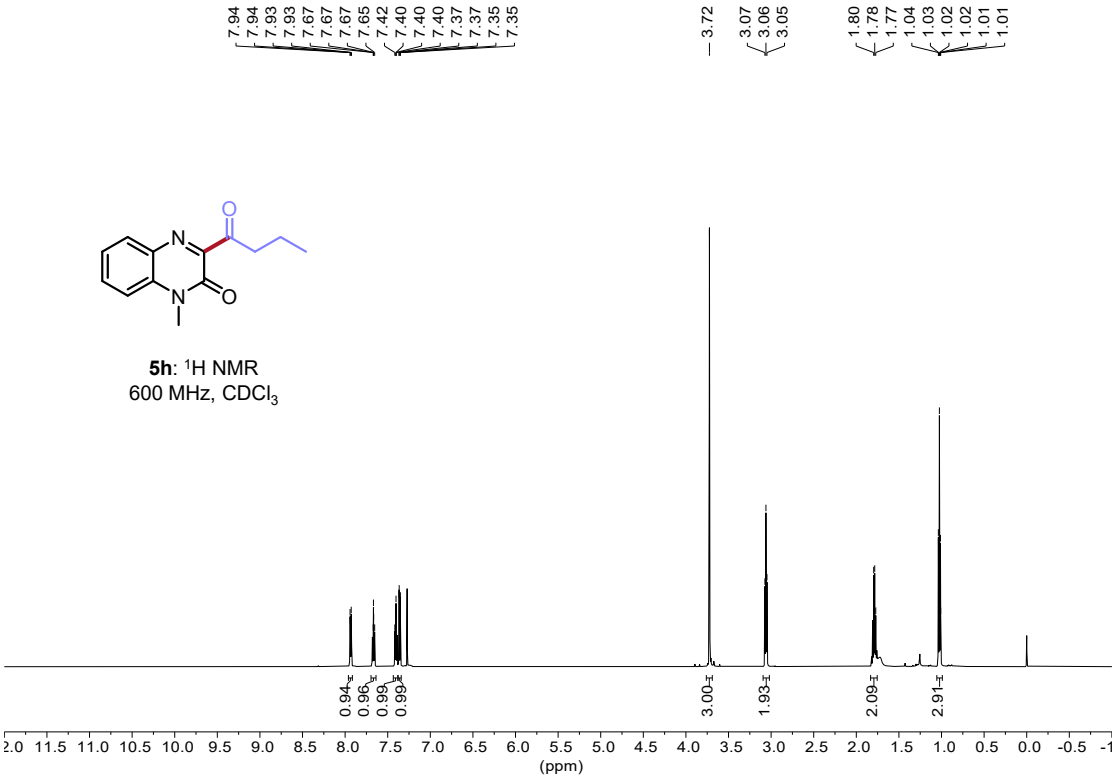
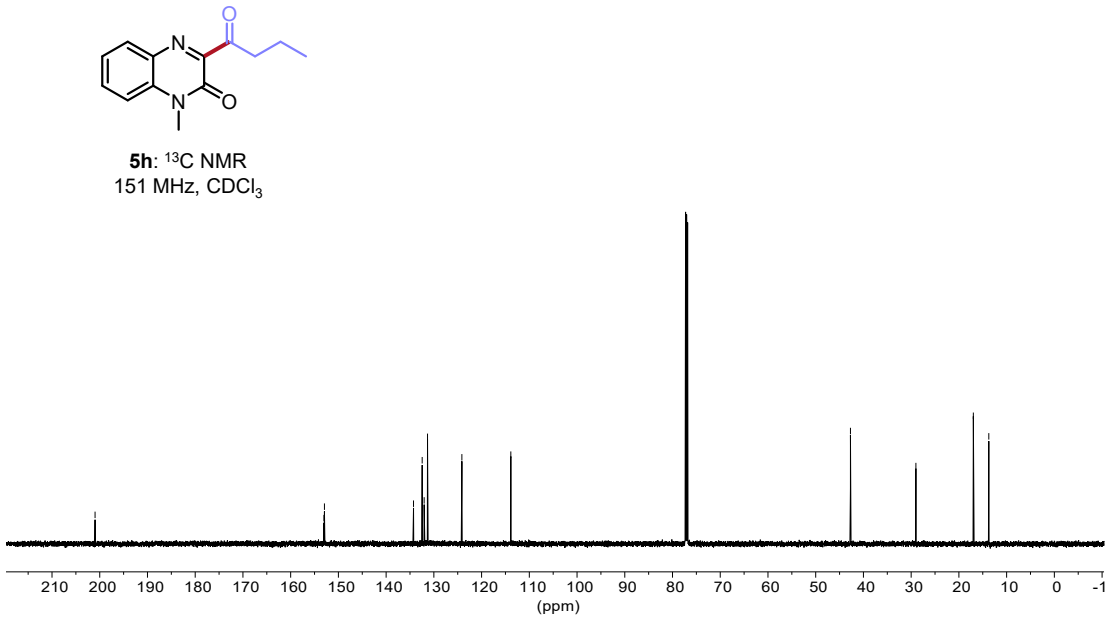
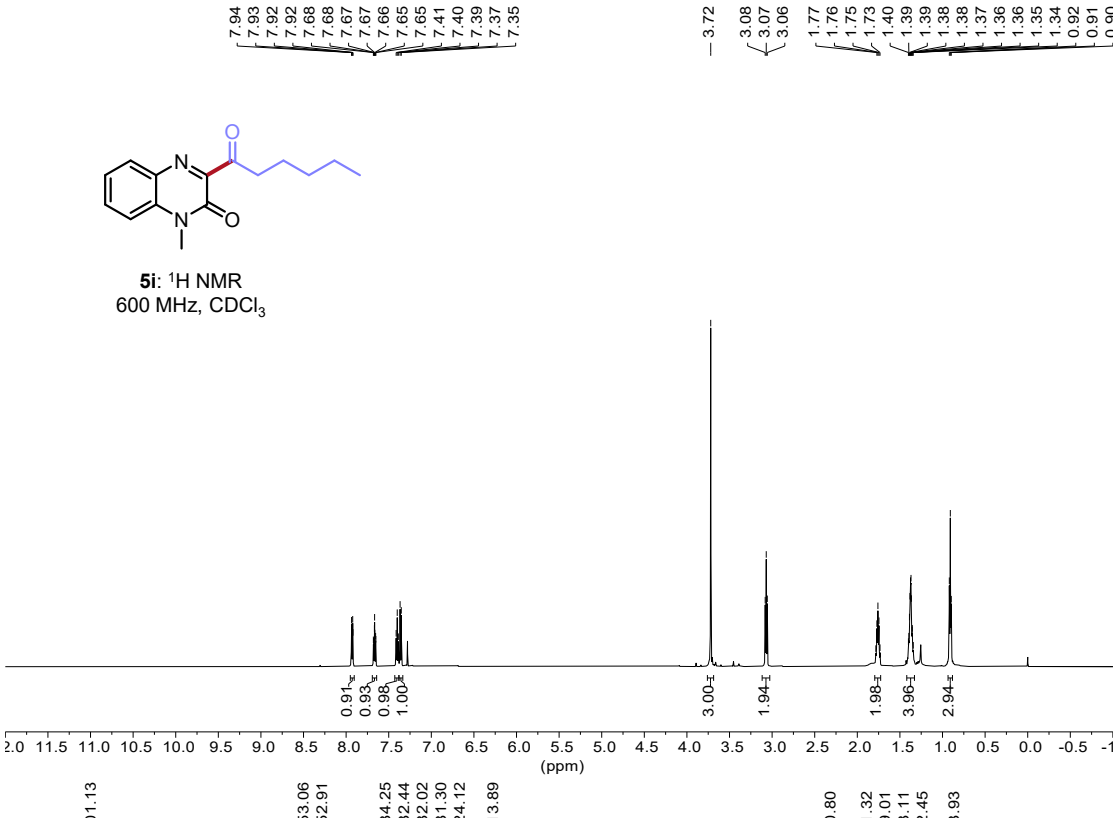
5g: 13C NMR
151 MHz, CDCl3
(ppm)



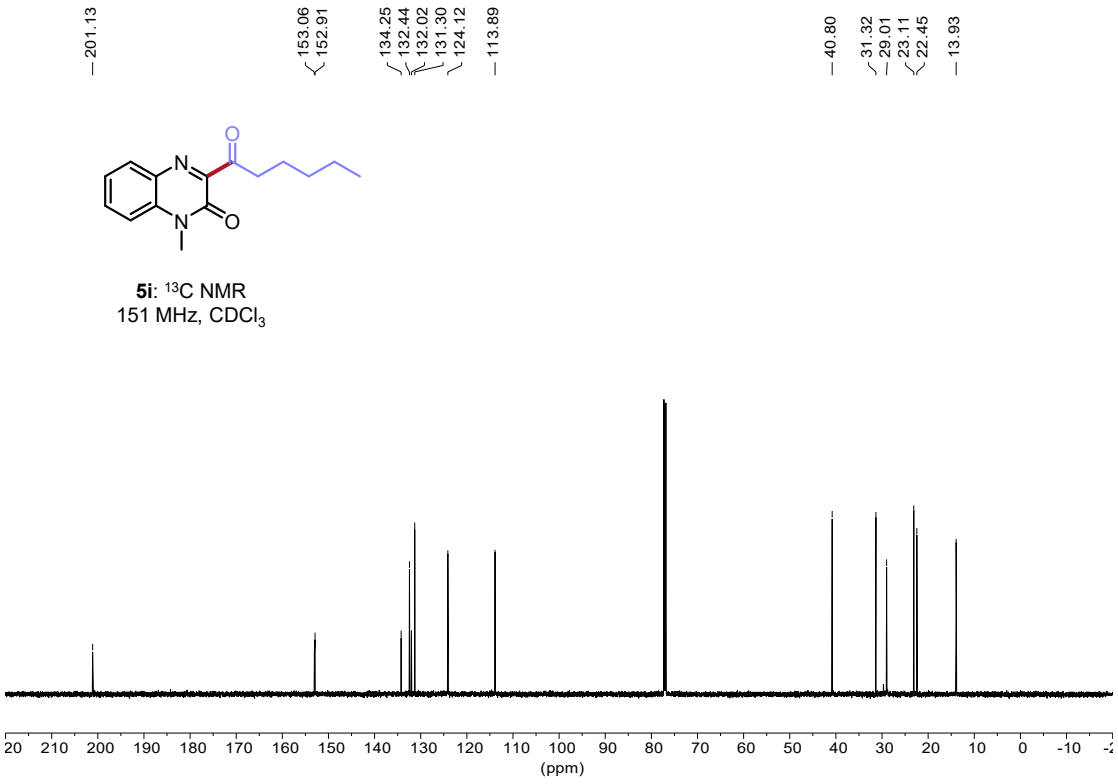
5h: ^{1}H NMR
600 MHz, $CDCl_3$



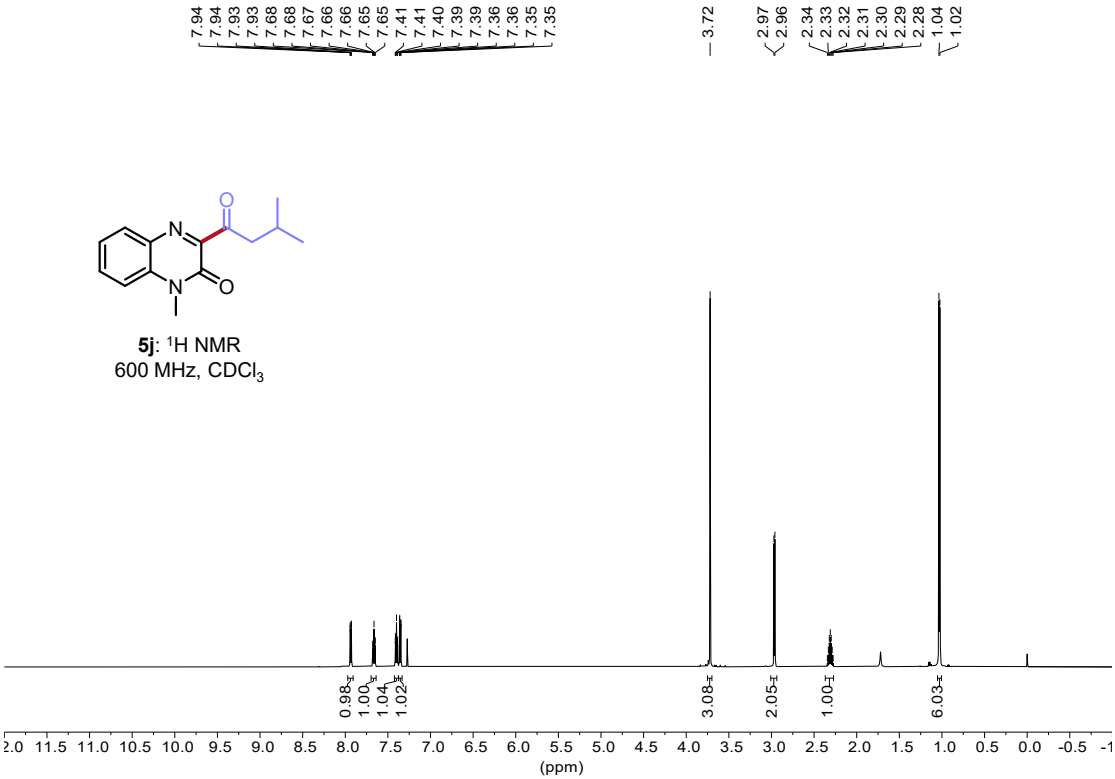
5h: ^{13}C NMR
151 MHz, $CDCl_3$



5i: ^{1}H NMR
600 MHz, $CDCl_3$

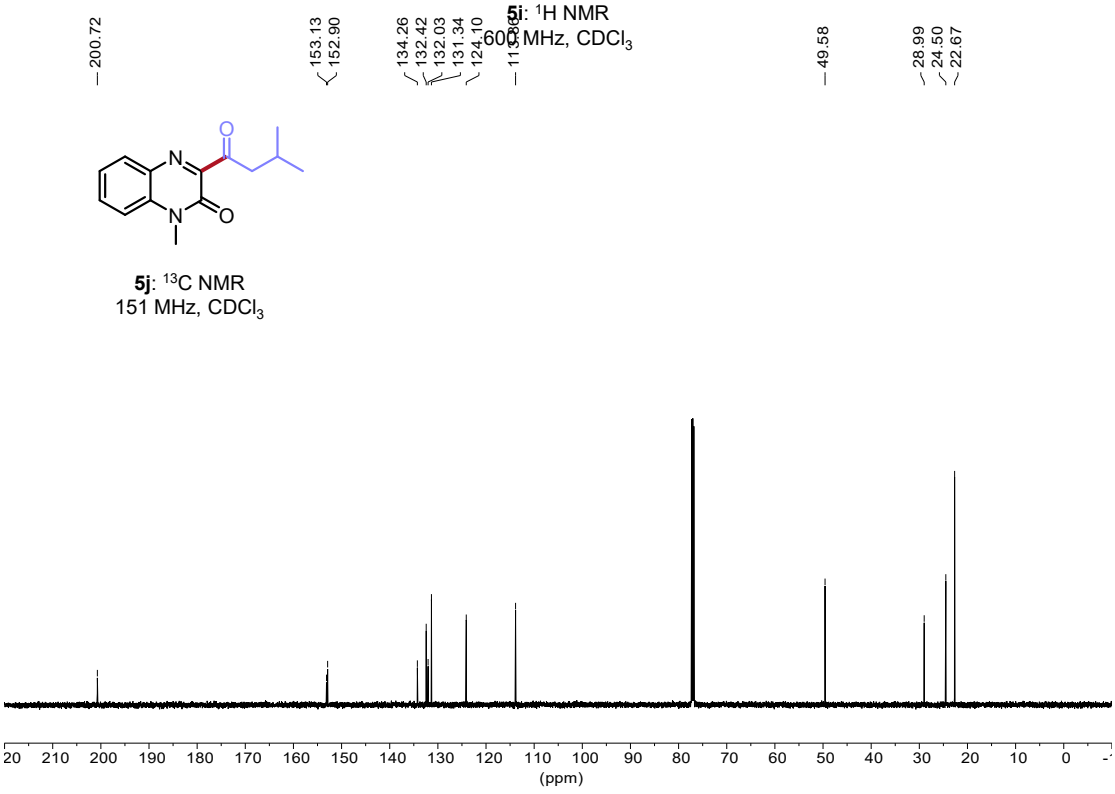


5i: ^{13}C NMR
151 MHz, $CDCl_3$

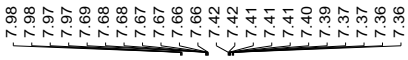


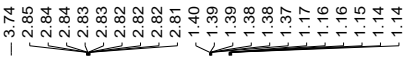
5j: ^{1}H NMR
600 MHz, $CDCl_3$

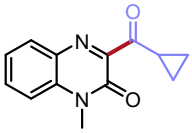
5j: ^{1}H NMR
600 MHz, $CDCl_3$



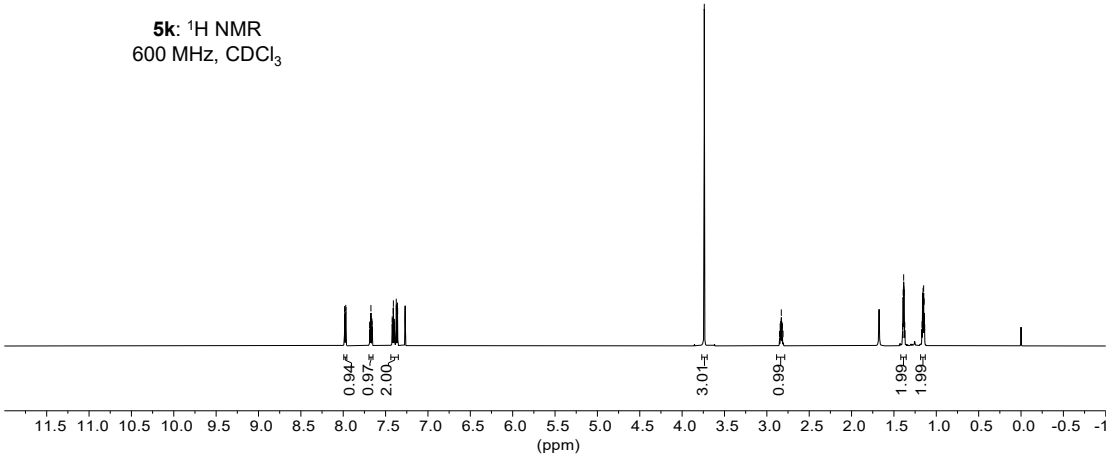
5j: ^{13}C NMR
151 MHz, $CDCl_3$

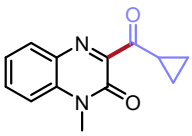




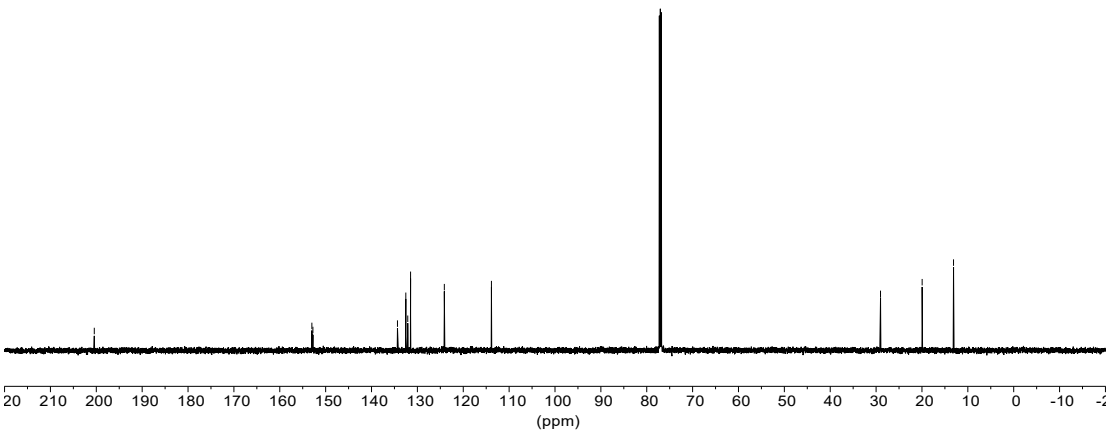


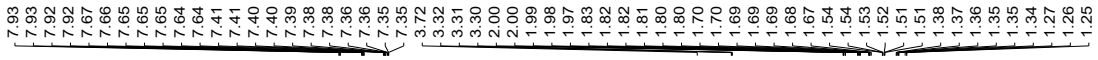
5k: ^{1}H NMR
600 MHz, $CDCl_3$

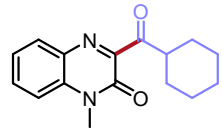




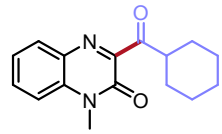
5k: ^{13}C NMR
151 MHz, $CDCl_3$



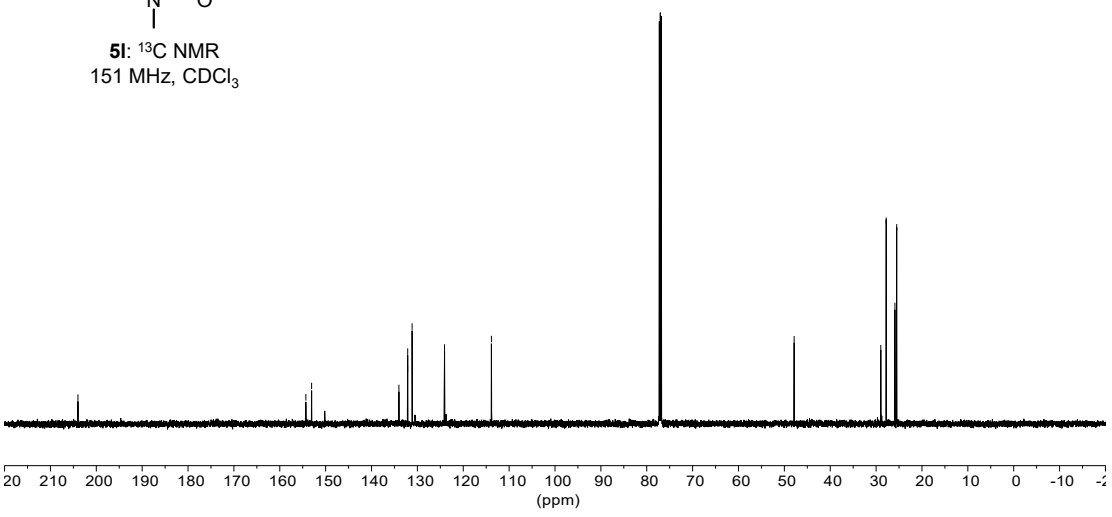


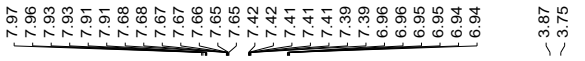


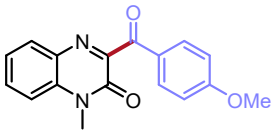
5l: ^{1}H NMR
600 MHz, $CDCl_3$



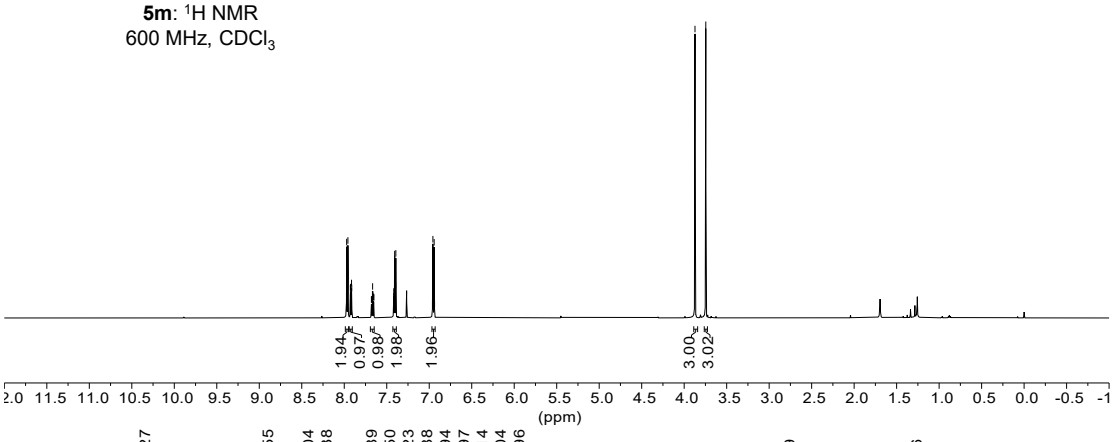
5l: ^{13}C NMR
151 MHz, $CDCl_3$

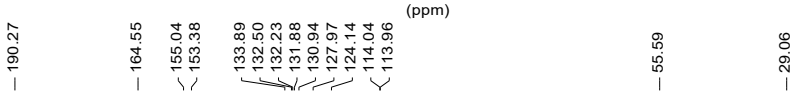


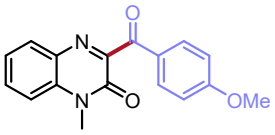




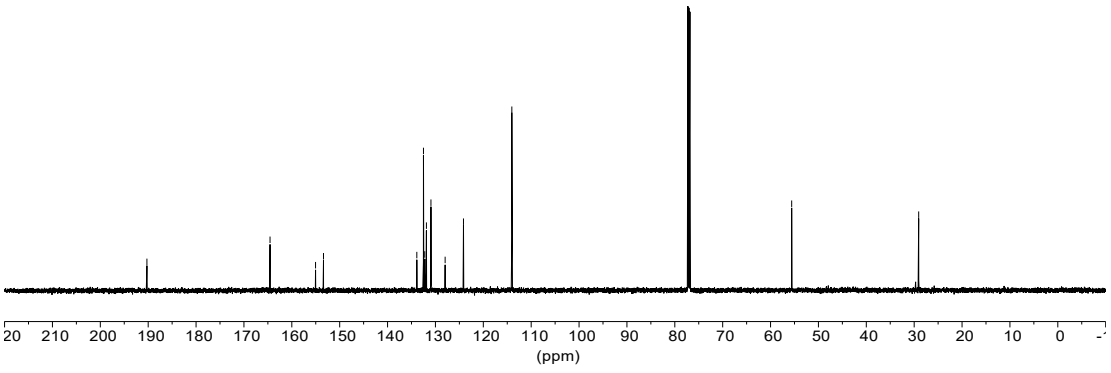
5m: ^{1}H NMR
600 MHz, $CDCl_3$

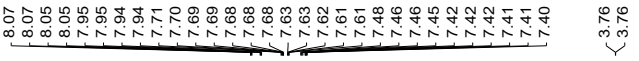


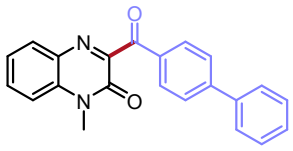




5m: ^{13}C NMR
151 MHz, $CDCl_3$







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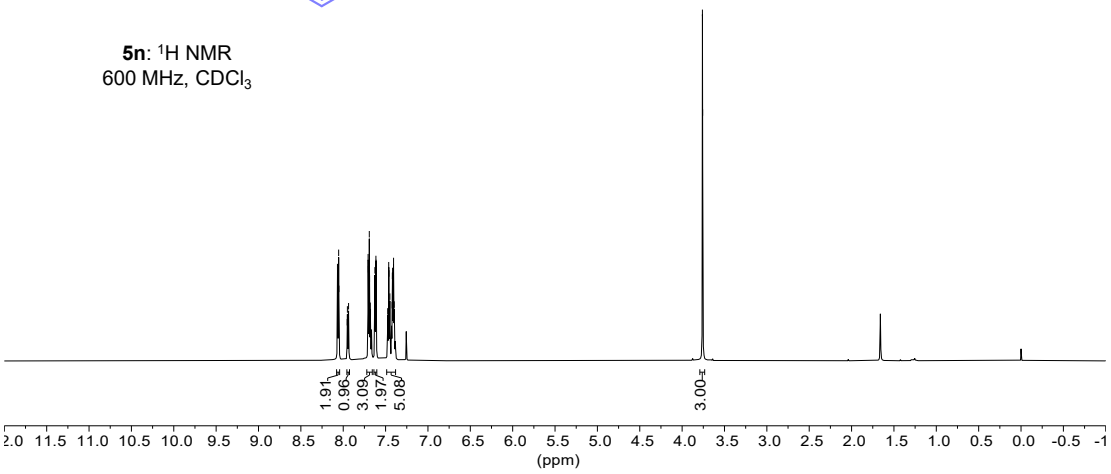
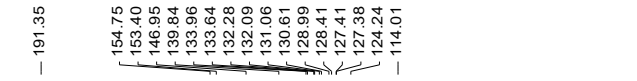
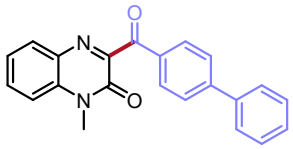
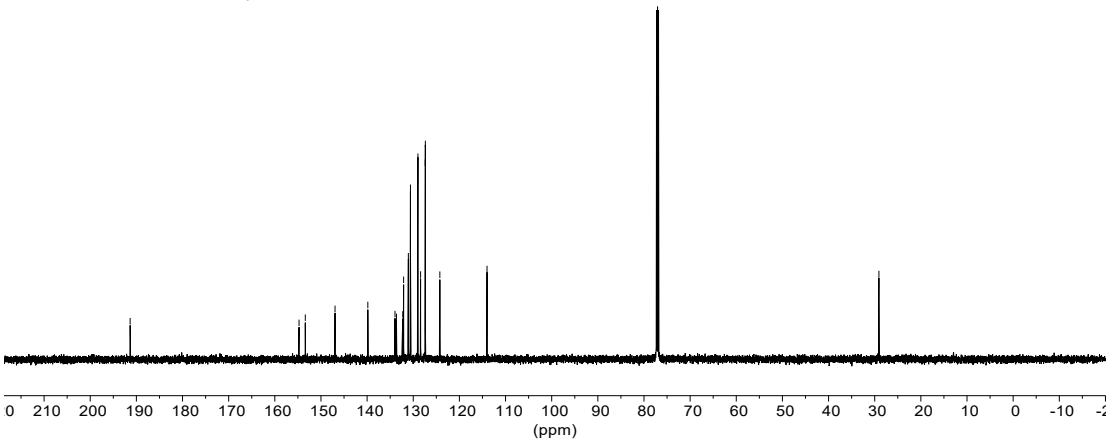
600 MHz, $CDCl_3$

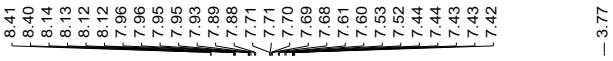


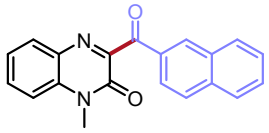




5n: ^{13}C NMR
151 MHz, $CDCl_3$







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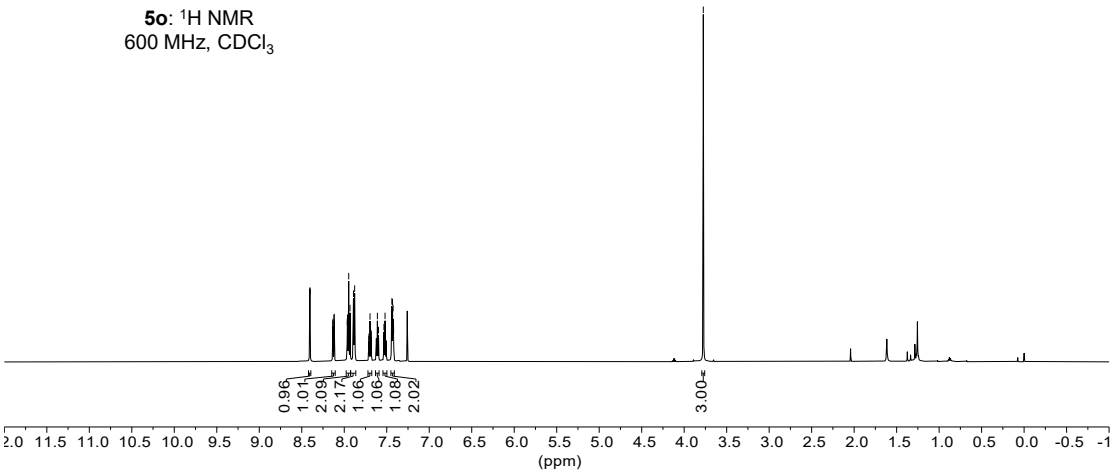
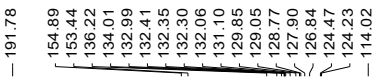
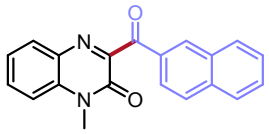
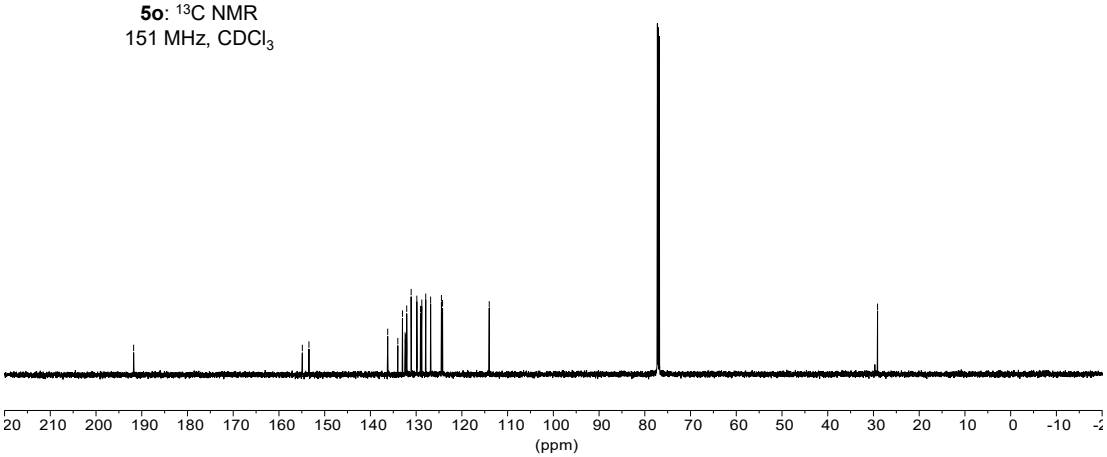
600 MHz, $CDCl_3$

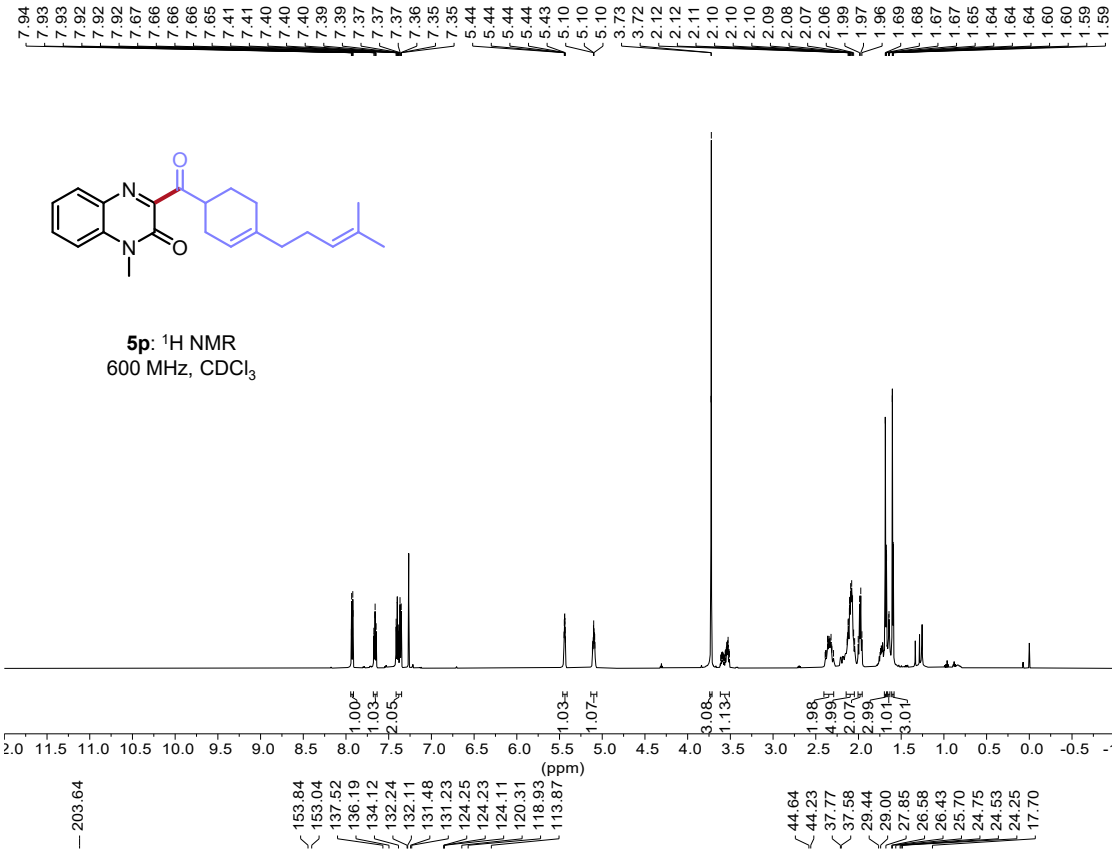




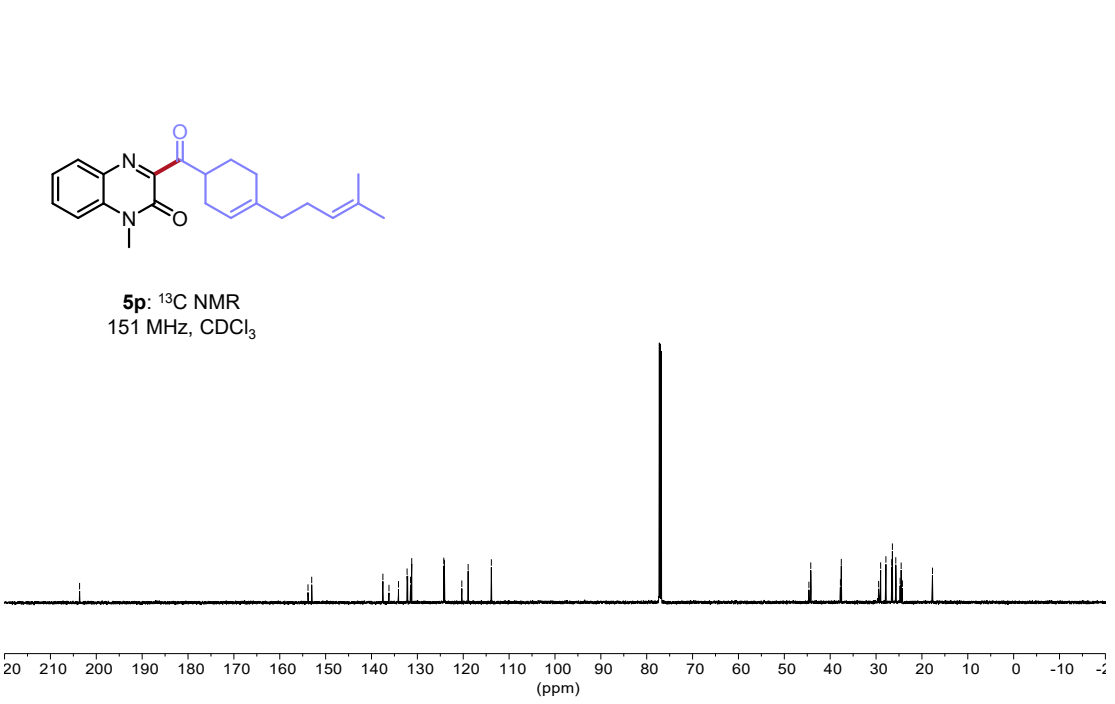


5o: ^{13}C NMR
151 MHz, $CDCl_3$

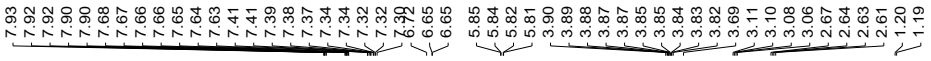


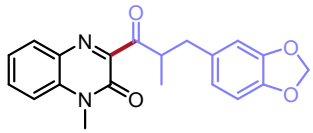


5p: ^{1}H NMR
600 MHz, $CDCl_3$

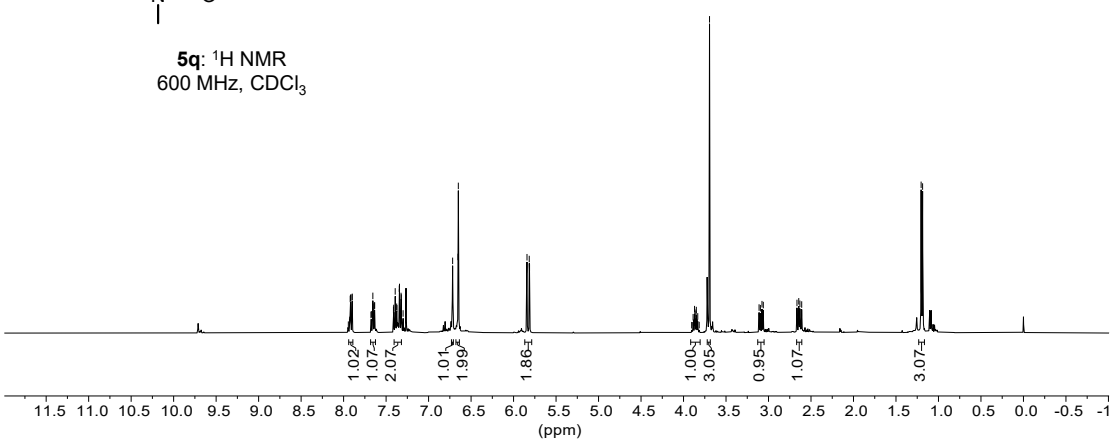


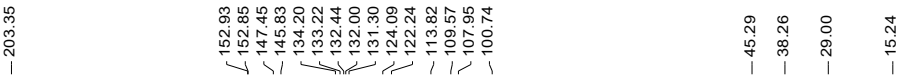
5p: ^{13}C NMR
151 MHz, $CDCl_3$

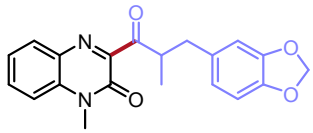




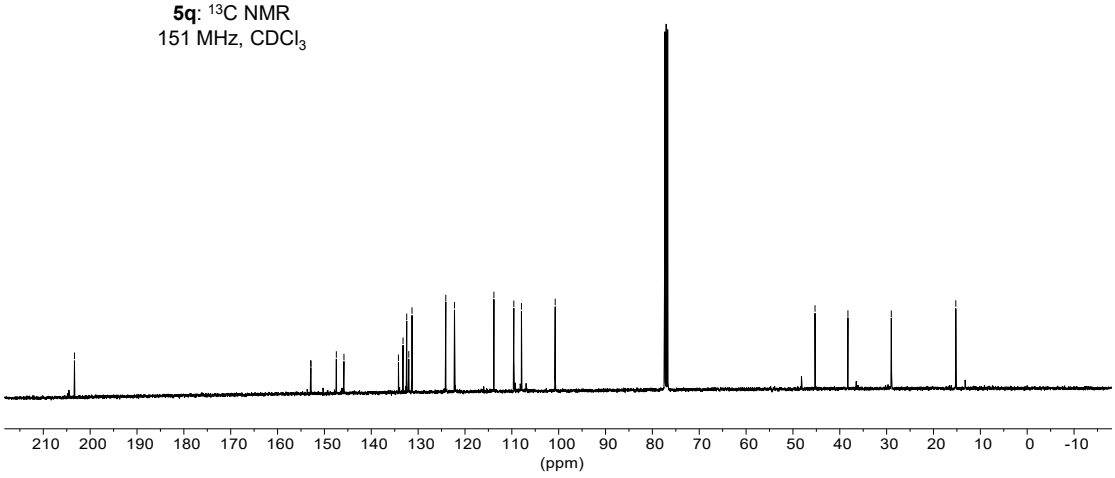
5q: ^{1}H NMR
600 MHz, $CDCl_3$

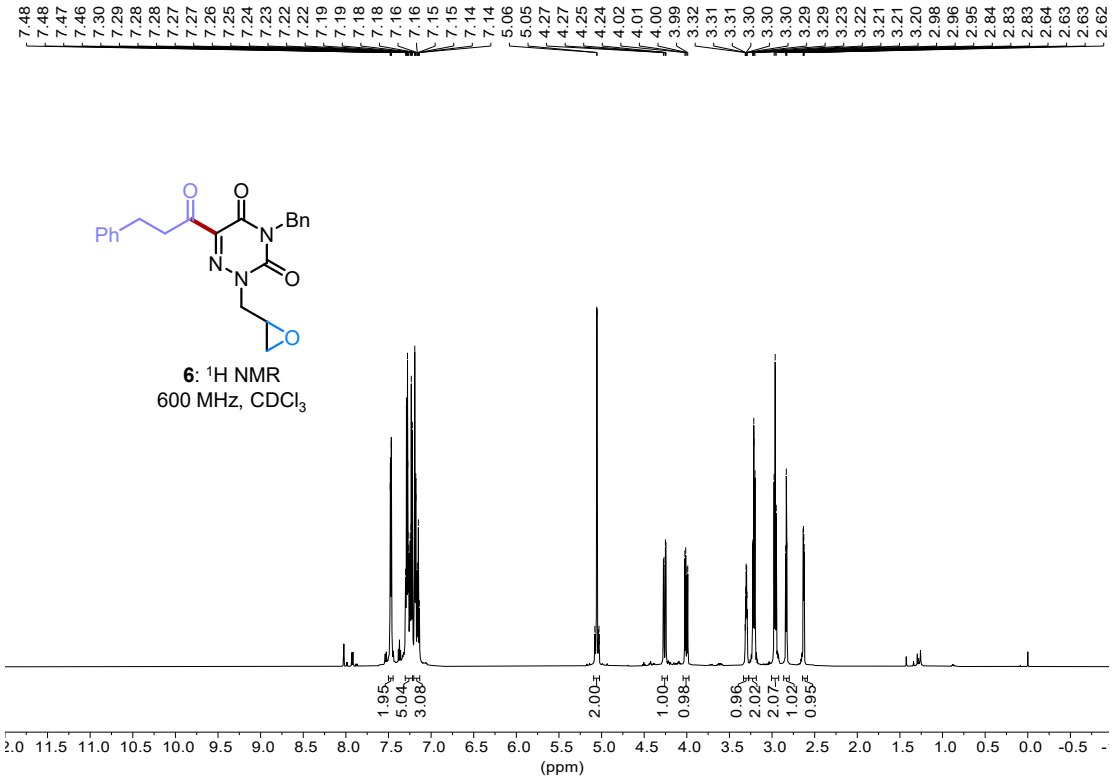




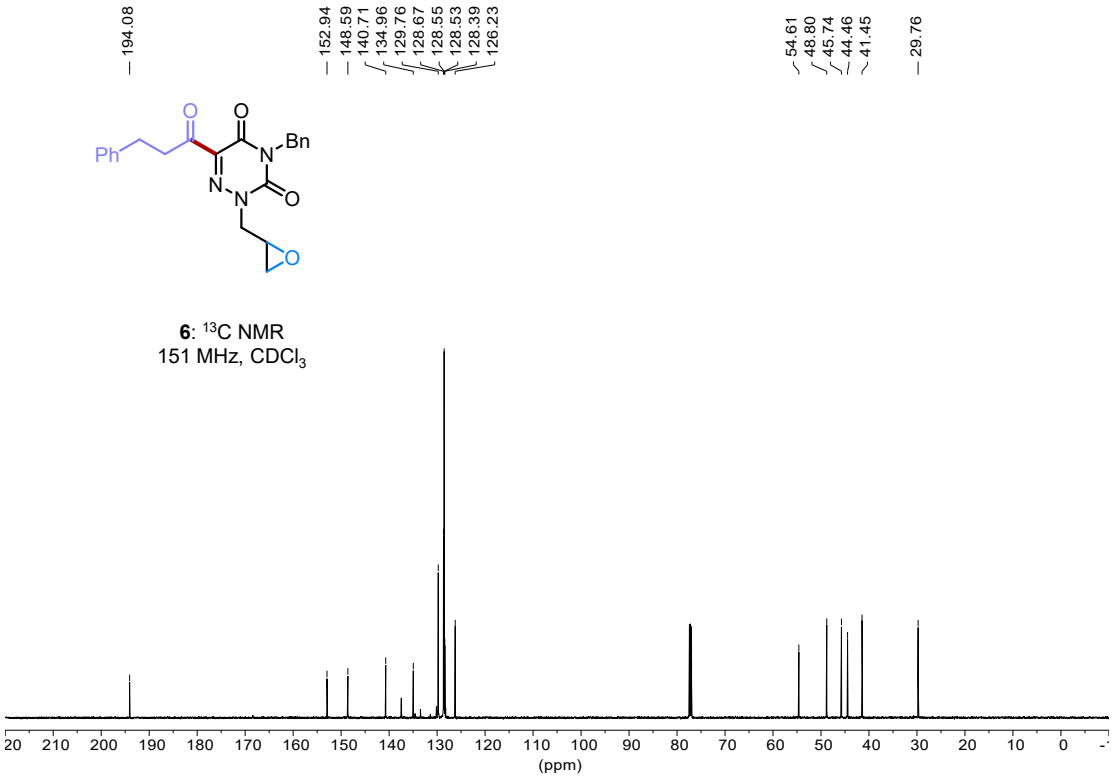


5q: ^{13}C NMR
151 MHz, $CDCl_3$

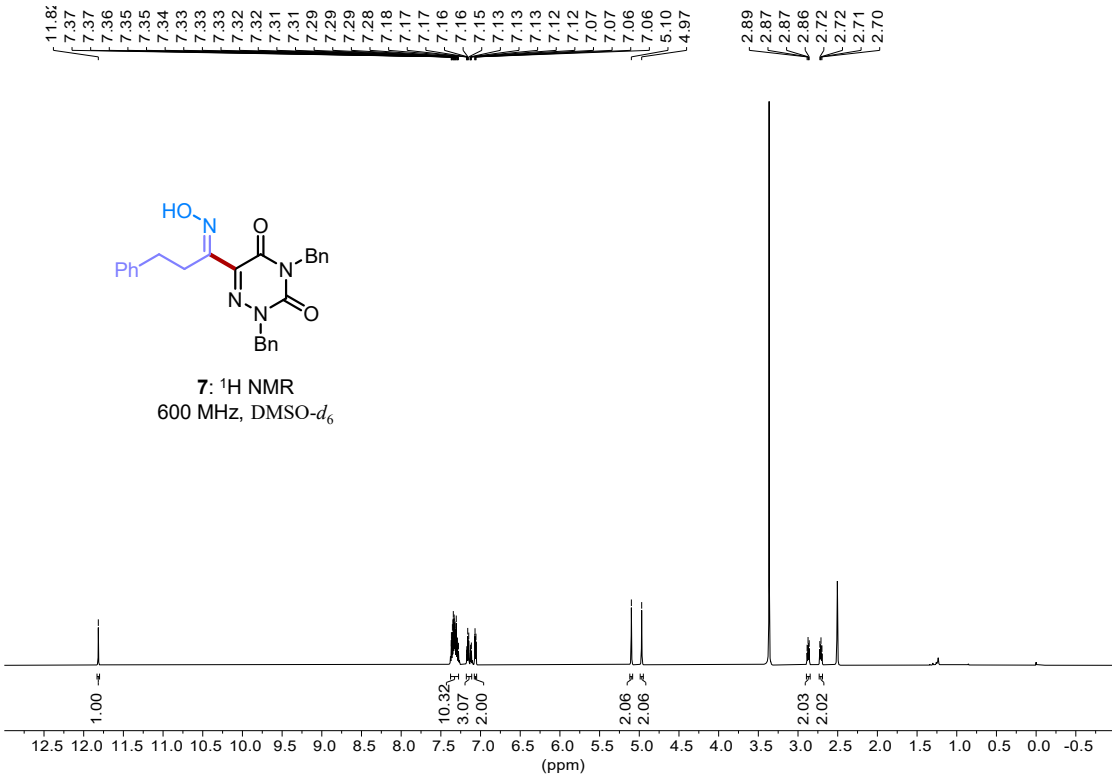




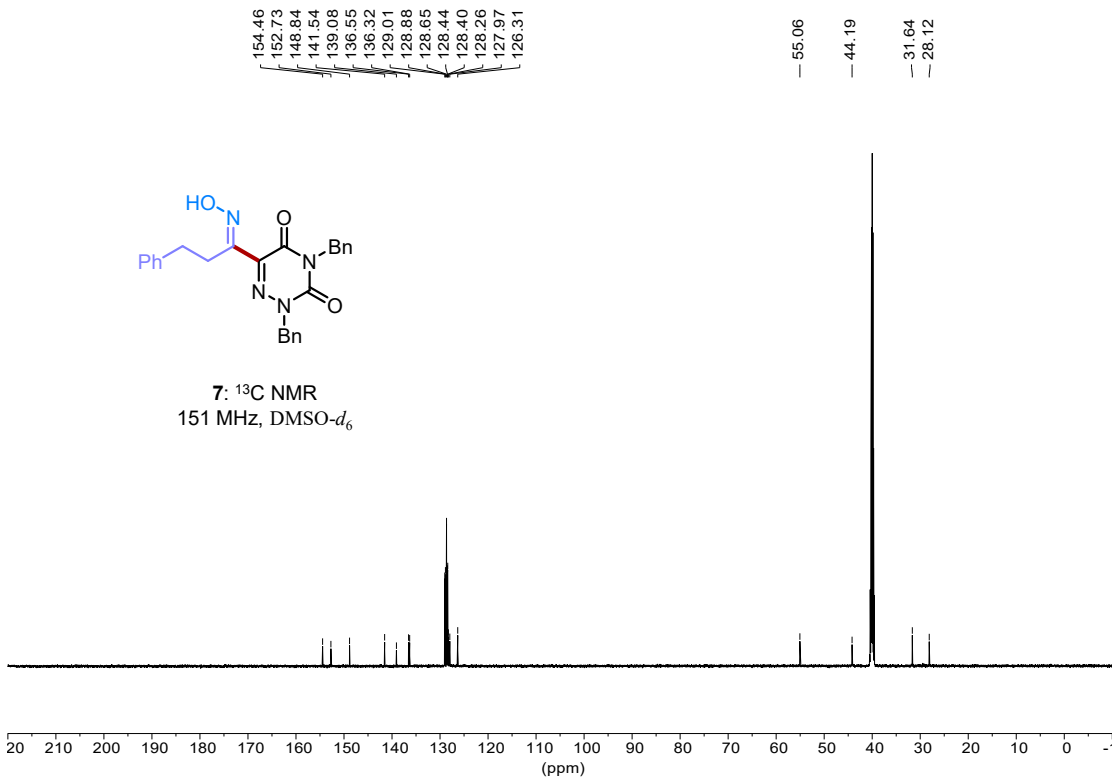
6: ^{1}H NMR
600 MHz, $CDCl_3$



6: ^{13}C NMR
151 MHz, $CDCl_3$



7: ^{1}H NMR
600 MHz, DMSO-d_6



7: ^{13}C NMR
151 MHz, DMSO-d_6

5. Reference

1. L.-C. Hwang, S.-Y. Yang, C.-L. Chuang and G.-H. Lee, *Molecules*, 2017, **22**.
2. X.-K. He, J. Lu, A.-J. Zhang, Q.-Q. Zhang, G.-Y. Xu and J. Xuan, *Org. Lett.*, 2020, **22**, 5984-5989.
3. (a) I. B. Perry, T. F. Brewer, P. J. Sarver, D. M. Schultz, D. A. DiRocco and D. W. C. MacMillan, *Nature*, 2018, **560**, 70-75; (b) C. Liu, J. Xie, W. Wu, M. Wang, W. Chen, S. B. Idres, J. Rong, L.-W.

Deng, S. A. Khan and J. Wu, *Nat. Chem.*, 2021, **13**, 451-457.

4. L. Wang, K. Zhang, Y. Wang, W. Li, M. Chen and J. Zhang, *Angew. Chem. Int. Ed.*, 2020, **59**, 4421-4427.