Supplementary Information

Photoredox β-C(sp^3)-H Heteroarylation of o-Iodoaryl-alkan-1-ones with Heteroarenes via HAT and Dual C-H Functionalizations

Guang-Chuan Xu,[a] Liang Zeng,*[a] Ming Hu,[a] Fu-Jin Sun,*[a] and Jin-Heng Li*[abc]

[a.] *State Key Laboratory Base of Eco-Chemical Engineering, College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266042, China. E-mail: loey_zengliang@hnu.edu.cn, sunfujin@qust.edu.cn and jhli@hnu.edu.cn*

[b.] *State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, China.*

[c.] *School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan 475004, China.*

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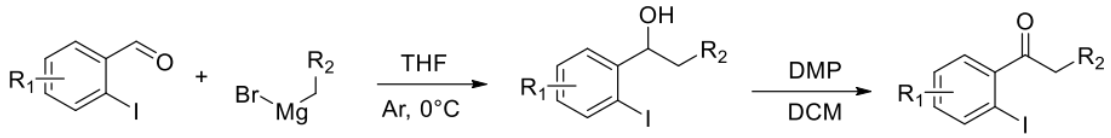
(A) General Experimental Procedures

(a) General Information:

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a JEOL internal standard. High-resolution mass spectra (HRMS) were recorded on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry. All products were identified by ^{1}H and ^{13}C NMR, HRMS; High-resolution mass spectra (HR-MS) were recorded on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry; Cyclic voltammograms were obtained on a CHI 605E potentiostat.

Unless otherwise noted, all reactions were carried out using standard Schlenk techniques. Column chromatography was performed on silica gel (300-400 mesh) using petroleum ether/ethyl acetate. The light source was used 18W Blue LEDs (manufacturer: liang yuan lighting, model: LY-PD001, wavelength range: 450-460 nm, λ max = 455 nm), with wrap in foil, less than 5 cm from the light source to the irradiation vessel. Unless otherwise noted, all reactions were carried out using standard Schlenk techniques, and the starting materials and solvents were commercially available and were used without further purification.

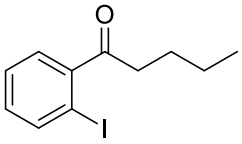
(b) General Procedure for Synthesis of 1-(o-Iodoaryl)alkan-1-ones (1):[1-6]



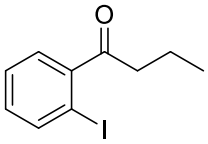
A

Following a modified literature procedure, to aflame-dried three-neck flask were added 2-Iodobenzaldehyde (50 mmol) and THF (50 mL), cool to 0 ℃ under a nitrogen atmosphere, then corresponding Grignard reagent (1.5 equiv) added in dropwise, the resulting mixture was stirred at this temperature for 1.5-3 h, and quenched with a saturated aqueous solution of NH_4Cl. After extraction with ethyl acetate, the organic layer was washed with brine (50 mL) and dried over anhydrous Na_2SO_4, purified by column chromatography on silica gel to give desired secondary benzylic alcohol **A**. To a solution of **A** (1.0 equiv) in DCM (0.1 M) was added DMP (1.5 equiv) under 0 ℃, then the resulted reaction mixture was stirred at room temperature. Upon completion,

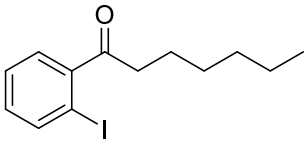
the reaction mixture was filtered and washed with EtOAc. The resulting mixture was concentrated, and the residue was purified by flash column chromatography on silica gel (eluted with petroleumether/ethyl acetate) to afford 1-(*o*-iodoaryl)alkan-1-one.



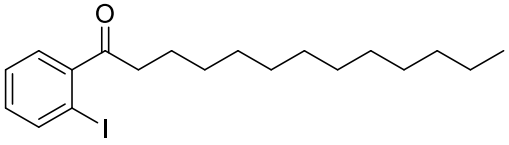
1-(2-iodophenyl)pentan-1-one (1aa): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.89 (d, *J* = 4.0 Hz, 1H), 7.40-7.33 (m, 2H), 7.12-7.08 (m, 1H), 2.88 (t, *J* = 7.6 Hz, 2H), 1.73-1.66 (m, 2H), 1.45-1.35 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.3, 145.0, 140.5, 131.4, 128.0, 127.6, 90.9, 41.9, 26.2, 22.4, 13.9.



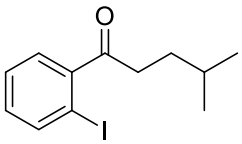
1-(2-iodophenyl)butan-1-one (1ba): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.92-7.89 (m, 1H), 7.42-7.34 (m, 2H), 7.13-7.09 (m, 1H), 2.87 (t, *J* = 7.2 Hz, 2H), 1.80-1.71 (m, 2H), 1.01 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.1, 145.0, 140.5, 131.4, 128.0, 127.6, 90.9, 44.0, 17.6, 13.8.



1-(2-iodophenyl)heptan-1-one (1ca): yellow viscous oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91-7.89 (m, 1H), 7.41-7.33 (m, 2H), 7.13-7.08 (m, 1H), 2.88 (t, *J* = 7.6 Hz, 2H), 1.75-1.67 (m, 2H), 1.36-1.26 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.3, 144.9, 140.4, 131.3, 128.0, 127.6, 90.9, 42.1, 31.6, 28.8, 24.0, 22.5, 14.0.

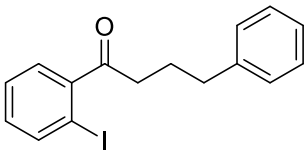


1-(2-iodophenyl)tridecan-1-one (1da): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91-7.89 (m, 1H), 7.41-7.33 (m, 2H), 7.12-7.08 (m, 1H), 2.87 (t, *J* = 7.2 Hz, 2H), 1.65-1.45 (m, 2H), 1.37-1.26 (m, 18H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.3, 145.0, 140.5, 131.4, 128.0, 127.6, 91.0, 42.2, 31.9, 29.7, 29.7, 29.6, 29.5, 29.4, 29.4, 29.2, 24.1, 22.7, 14.2.

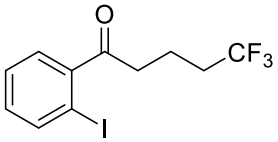


1-(2-iodophenyl)-4-methylpentan-1-one (1ea): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91-7.89 (m, 1H), 7.41-7.33 (m, 2H), 7.12-7.08 (m, 1H), 2.86 (t, *J* = 7.2 Hz, 2H), 1.74-1.68 (m,

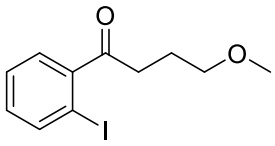
2H), 1.61-1.52 (m, 1H), 1.26-1.24 (m, 2H), 0.90 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.3, 144.9, 140.4, 131.3, 128.0, 127.6, 90.9, 42.3, 38.3, 27.8, 22.5, 21.9.



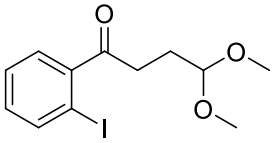
1-(2-iodophenyl)-4-phenylbutan-1-one (1fa): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.89-7.87 (m, 1H), 7.39-7.35 (m, 1H), 7.32-7.23 (m, 3H), 7.10-7.14 (m, 3H), 7.11-7.06 (m, 1H), 2.89 (t, *J* = 7.2 Hz, 2H), 2.65 (t, *J* = 7.2 Hz, 2H), 1.81-1.68 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.9, 144.9, 142.2, 140.5, 131.5, 128.5, 128.4, 128.1, 127.7, 125.8, 91.0, 41.9, 35.8, 31.0, 23.7.



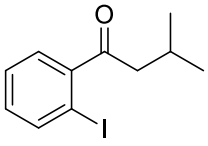
5,5,5-trifluoro-1-(2-iodophenyl)pentan-1-one (1ga): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.92-7.89 (m, 1H), 7.43-7.34 (m, 2H), 7.15-7.11 (m, 1H), 2.98 (t, *J* = 7.2 Hz, 2H), 2.26-2.20 (m, 2H), 2.05-1.99 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 203.3, 144.1, 140.5, 131.7, 128.1, 127.5, 90.77, 40.2, 32.6 (q, *J* = 29.0 Hz), 16.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) 66.02;



1-(2-iodophenyl)-4-methoxybutan-1-one (1ha): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.89-7.87 (m, 1H), 7.38-7.36 (m, 2H), 7.12-7.06 (m, 1H), 3.44 (t, *J* = 6.4 Hz, 2H), 3.31 (s, 3H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.04-1.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.2, 144.5, 140.4, 131.4, 127.9, 127.7, 90.9, 71.4, 58.5, 38.5, 23.9.

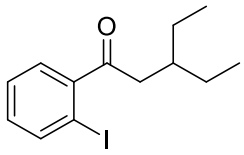


1-(2-iodophenyl)-4,4-dimethoxybutan-1-one (1ia): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-7.99 (m, 2H), 7.70-7.67 (m, 1H), 7.55-7.51 (m, 1H), 4.94-4.92 (m, 1H), 4.04-3.97 (m, 2H), 3.55-3.49 (m, 2H), 3.42 (s, 3H), 3.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 202.1, 161.2, 135.3, 129.9, 126.7, 124.0, 113.5, 92.8, 55.6, 50.0, 25.4, 22.6.

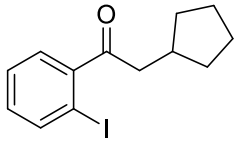


1-(2-iodophenyl)-3-methylbutan-1-one (1ja): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.92-7.90 (m, 1H), 7.41-7.34 (m, 2H), 7.13-7.08 (m, 1H), 2.78 (d, *J* = 6.8 Hz, 2H), 2.33-2.19 (m, 1H), 1.02 (s, 3H), 1.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.7, 144.9, 140.7, 131.5,

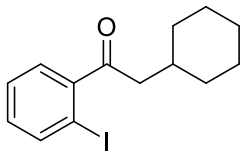
128.0, 127.8, 91.1, 50.9, 24.9, 22.7.



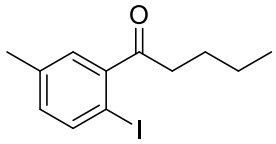
3-ethyl-1-(2-iodophenyl)pentan-1-one (1ka): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.92-7.90 (m, 1H), 7.41-7.35 (m, 2H), 7.12-7.06 (m, 1H), 2.82 (d, *J* = 6.8 Hz, 2H), 1.96-1.90 (m, 1H), 1.45-1.35 (m, 4H), 0.88 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.1, 144.9, 140.6, 131.4, 127.9, 127.7, 91.1, 46.1, 36.8, 25.7, 10.9.



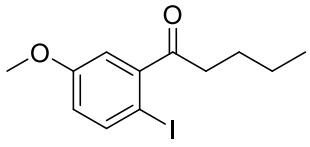
2-cyclopentyl-1-(2-iodophenyl)ethan-1-one (1la): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90-7.88 (m, 1H), 7.40-7.33 (m, 2H), 7.11-7.07 (m, 1H), 2.91 (d, *J* = 6.4 Hz, 2H), 2.37-2.29 (m, 1H), 1.93-1.84 (m, 2H) ,1.65-1.51 (m, 4H), 1.22-1.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.9, 144.8, 140.5, 131.3, 127.9, 127.6, 91.0, 48.2, 35.7, 32.6, 24.9.



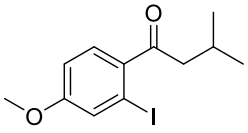
2-cyclohexyl-1-(2-iodophenyl)ethan-1-one (1ma): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90-7.88 (m, 1H), 7.40-7.33 (m, 2H), 7.11-7.07 (m, 1H), 2.76 (d, *J* = 6.8 Hz, 2H), 2.00-1.89 (m, 1H), 1.80-1.75 (m, 2H) ,1.72-1.61 (m, 3H), 1.34-1.23 (m, 3H), 1.04-0.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.6, 144.9, 140.6, 131.4, 127.9, 127.7, 91.0, 49.7, 34.0, 33.2, 26.2, 26.0.



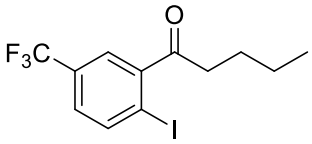
1-(2-iodo-5-methylphenyl)pentan-1-one (1na): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.75-7.74 (m, 1H), 7.30-7.28 (m, 1H), 7.19-7.16 (m, 1H), 2.90-2.84 (m, 2H), 2.31 (s, 3H), 1.71-1.62 (m, 2H) ,1.42-1.32 (m, 2H), 0.94-0.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.1, 159.5, 140.9, 134.2, 117.2, 113.7, 79.0, 55.4, 41.8, 26.0, 22.2, 13.8.



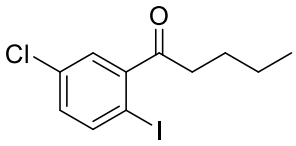
1-(2-iodo-5-methoxyphenyl)pentan-1-one (1oa): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.70 (d, *J* = 8.8 Hz, 1H), 6.85-6.84 (m, 1H), 6.69-6.66 (m, 1H), 3.78 (s, 3H), 2.88-2.83 (m, 2H) ,1.70-1.63 (m, 2H), 1.44-1.34 (m, 2H), 0.94-0.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 205.3, 159.7, 146.1, 141.1, 134.4, 117.4, 113.9, 79.2, 55.6, 42.5, 41.9, 26.2, 22.4, 14.0.



1-(2-iodo-4-methoxyphenyl)-3-methylbutan-1-one (1pa): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.46-7.43 (m, 2H), 6.90-6.87 (m, 1H), 3.80 (s, 3H), 2.74 (d, *J* = 6.8 Hz, 2H), 2.26-2.16 (m, 1H) ,0.97 (s, 3H), 0.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 202.3, 161.3, 135.5, 130.1, 126.9, 113.6, 93.0, 55.7, 50.2, 25.5, 22.8.

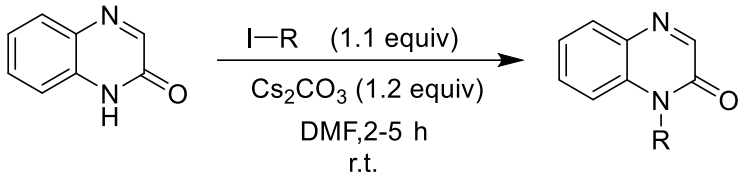


1-(2-iodo-5-(trifluoromethyl)phenyl)pentan-1-one (1qa): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.03 (d, *J* = 8.4 Hz, 1H), 7.53-7.52 (m, 1H), 7.35-7.32 (m, 1H), 2.89 (t, *J* = 7.6 Hz, 2H), 1.74-1.67 (m, 2H) ,1.46-1.36 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.1, 145.9, 141.2, 127.7, 124.1 (q, *J* = 4.0 Hz), 95.39, 41.94, 26.01, 22.36, 13.96. ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) 62.92;



1-(5-chloro-2-iodophenyl)pentan-1-one (1ra): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.78 (d, *J* = 8.4 Hz, 1H), 7.27 (d, *J* = 2.4 Hz, 1H), 7.09-7.06 (m, 1H), 2.84 (t, *J* = 7.2 Hz, 2H), 1.71-1.62 (m, 2H), 1.43-1.34 (m, 2H), 0.92 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 204.0, 146.5, 141.6, 134.8, 131.6, 127.8, 88.1, 41.9, 26.1, 22.4, 14.0.

(c) General Procedure for Synthesis of *N*-Substituted Quinoxalin-2(1*H*)-ones (2):[7-9]

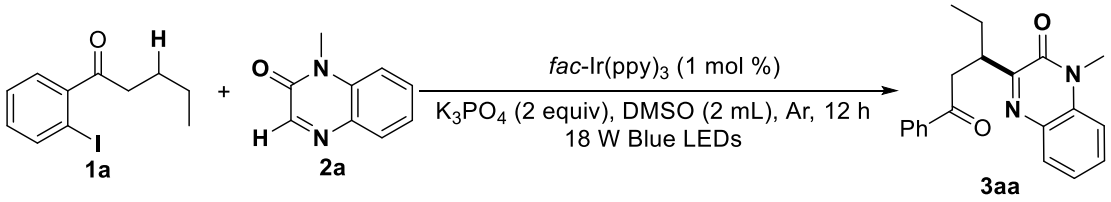


A solution of quinoxalin-2(1*H*)-one (2.92 g, 20 mmol) in DMF (75 mL), added Cesium carbonate (7.8 g, 24mmol, 1.2 equiv) then stirred mixture for 15 min at 25-30 ^{o}C then slowly added alkyl halides (1.1 equiv) further stirred the suspension for 2-5 h, the progress of the reaction was monitored by TLC, after consumption of quinoxalin-2(1*H*)-one, the suspension was quenched with water (50 mL × 3) and the product was extracted twice with ethyl acetate then washed combine ethyl acetate layer with

saturated brine and dried over anhydrous magnesium sulphate then concentrated under vacuum below 45°C to get the crude product, which was further triturated with a mixture of ethyl acetate : n-hexane to obtained pure compound with 50-90% yield. All the *N*-Substituted Quinoxalin-2(1*H*)-ones in the manuscript are known compounds, which the NMR and other data matched the literatures.[7-9]

(d) General Procedure for Photoredox β-C(sp^3)-H Heteroarylation of o-Iodoaryl-alkan-1-ones 1 with Heteroarenes 2

To a Schlenk tube were added **1a** (28.8 mg, 0.20 mmol), **2a** (32.0 mg, 0.20 mmol, 1.0 equiv),*fac*-Ir(ppy)$_3$ (1.3 mg, 1 mol %), K_3PO_4 (84.8 mg, 0.4mmol, 2 equiv), DMSO (2 mL, 0.1 M), Then the tube was charged with argon three times, and was stirred irradiated with a 18 W blue LED lamp (at approximately 5.0 cm away from the light source) with cooled by a fan at room temperature for 12 h until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the reaction mixture was concentrated in vacuum, diluted in diethyl ether, and washed with saturated brine. The combined organic extracts were dried over Na2SO4 and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (PE/EA = 10:1) to provide **3aa** in 87% isolated yield.

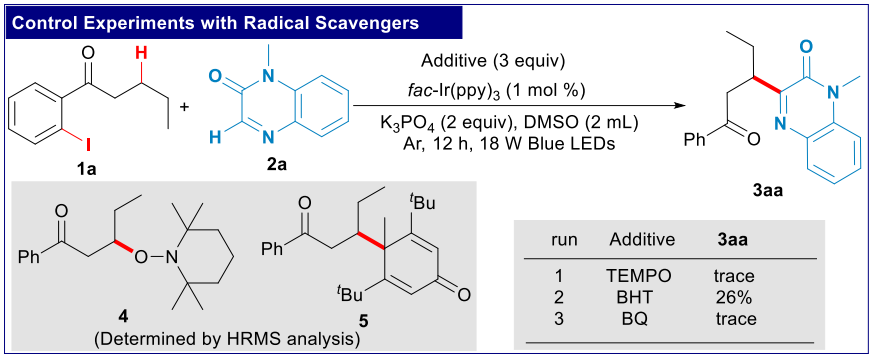


(e) Typical Experimental Procedure for A Scale Up To 1 mmol 1-(2 iodophenyl)pentan-1-one (1a):

To a Schlenk tube were added 1-(2-iodophenyl)pentan-1-one **1a** (288 mg, 1 mmol; 1 equiv), **2a** (160 mg, 1 mmol; 1 equiv), *fac*-Ir(ppy)$_3$ (6.5 mg, 1 mol%), K_3PO_4 (424 mg, 2 mmol; 2 equiv), and DMSO (4 mL). Then the tube was charged with argon and was placed in a photobox and stirred under irradiation of blue LEDs (λmax = 455 nm) and room temperature for the indicated time (about 24 h) until complete consumption of starting material as monitored by TLC. After the reaction was finished, the reaction

mixture was filtered by a crude column with ethyl acetate as eluent, and concentrated in vacuum. The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate = 10:1) to afford product **3aa** in 74% yield (236.8 mg).

(f) Control Experiments



Scheme S1. Control experiments.

To a Schlenk tube were added **1a** (28.8 mg, 0.20 mmol), **2a** (32.0 mg, 0.20 mmol, 1.0 equiv), *fac*-Ir(ppy)$_3$ (1.3 mg, 1 mol %), K_3PO_4 (84.8 mg, 0.4mmol, 2.0 equiv), additive (TEMPO, BHT or BQ; 3.0 equiv), DMSO (2 mL, 0.1 M). Then the tube was charged with argon three times, and was stirred irradiated with a 18 W blue LED lamp (at approximately 5.0 cm away from the light source) with cooled by a fan at room temperature for 12 h. The reaction mixture was concentrated in vacuum, diluted in diethyl ether, and washed with saturated brine. The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. No desired product **3aa** was observed and the product **4** or **5** were detected by HRMS analysis of the crude products.

The product **4**: HRMS m/z (ESI) calcd for $C_{20}H_{31}NO_2$ $[M+Na]^+$ 340.2247, found 340.2246)

The product **5**: HRMS m/z (ESI) calcd for $C_{20}H_{18}N_2O$ $[M+Na]^+$ 403.2608, found 403.2602.)

(g) Stern-Volmer Fluorescence Quenching Experiments

Fluorescence spectra samples for the quenching experiments were prepared in a glass cuvette with a septum screw cap. The *fac*-Ir(ppy)$_3$ was irradiated at 500 nm and the emission intensity at 530 nm was observed. In a typical experiment, the emission spectrum of a 1.0×10^{-5} M solution of the *fac*-Ir(ppy)$_3$ in DMSO was collected. In Figure S1, a stock solution of 1-(2-iodophenyl) pentan-1-one **1a** (28.8 mg, 0.1 mmol) in 1 mL of DMSO was prepared. Then, different amounts of this stock solution were added to a solution of the photocatalyst in DMSO (1.0×10^{-5} M). The results show that the luminescence intensity of the *fac*-Ir(ppy)$_3$ is basically unchanged.

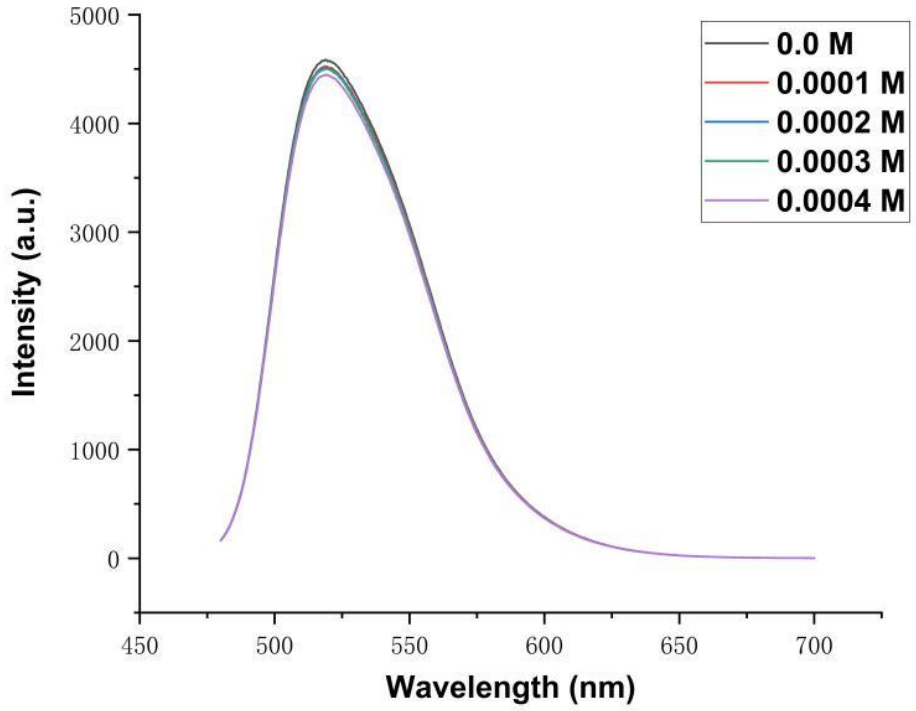


Figure S1. Stern–Volmer fluorescence quenching experiments of *fac*-Ir(ppy)$_3$ with **1a**.

In Figure S2, a stock solution of 1-methylquinoxalin-2(1H)-one **2a** (16.0 mg, 0.1 mmol) in 1 mL of DMSO was prepared. Then, different amounts of this stock solution were added to a solution of the photocatalyst in DMSO (1.0×10^{-5} M). The results show that slight decrease of *fac*-Ir(ppy)$_3$ luminescence was observed.

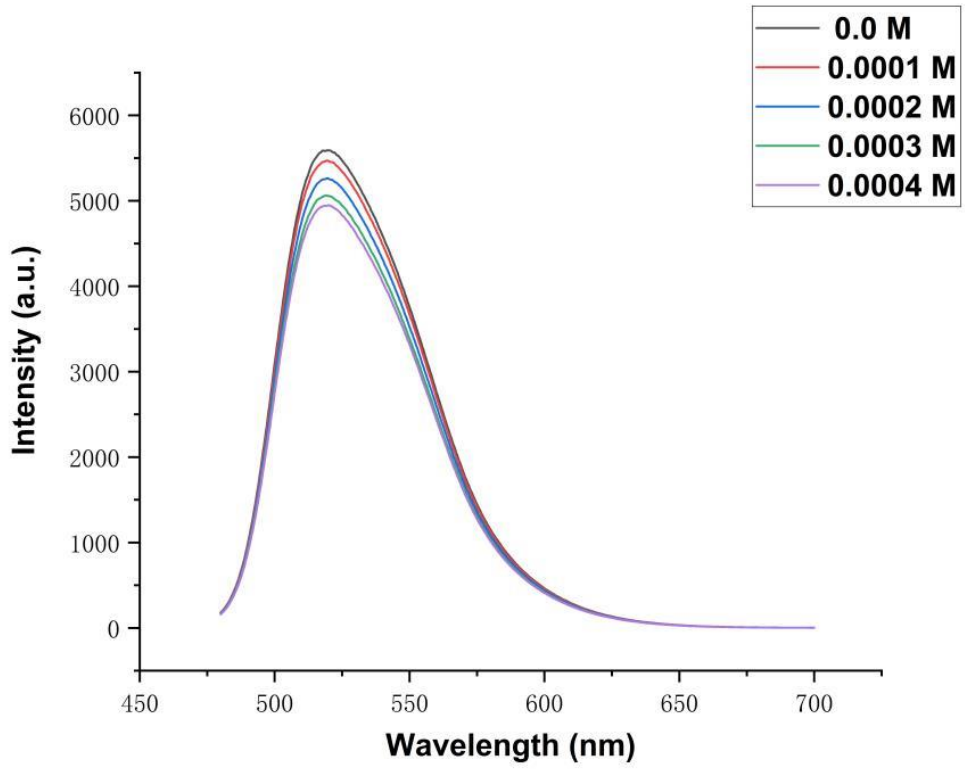


Figure S2. Stern–Volmer fluorescence quenching experiments of *fac*-Ir(ppy)$_3$ with **2a**

In Figure S3, a stock solution of K_3PO_4 (21.2 mg, 0.1 mmol) in 1 mL of DMSO was prepared (use ultrasound to help dissolve). Then, different amounts of this stock solution were added to a solution of the photocatalyst in DMSO (1.0×10^{-5} M). The results show that slight decrease of *fac*-Ir(ppy)$_3$ luminescence was observed.

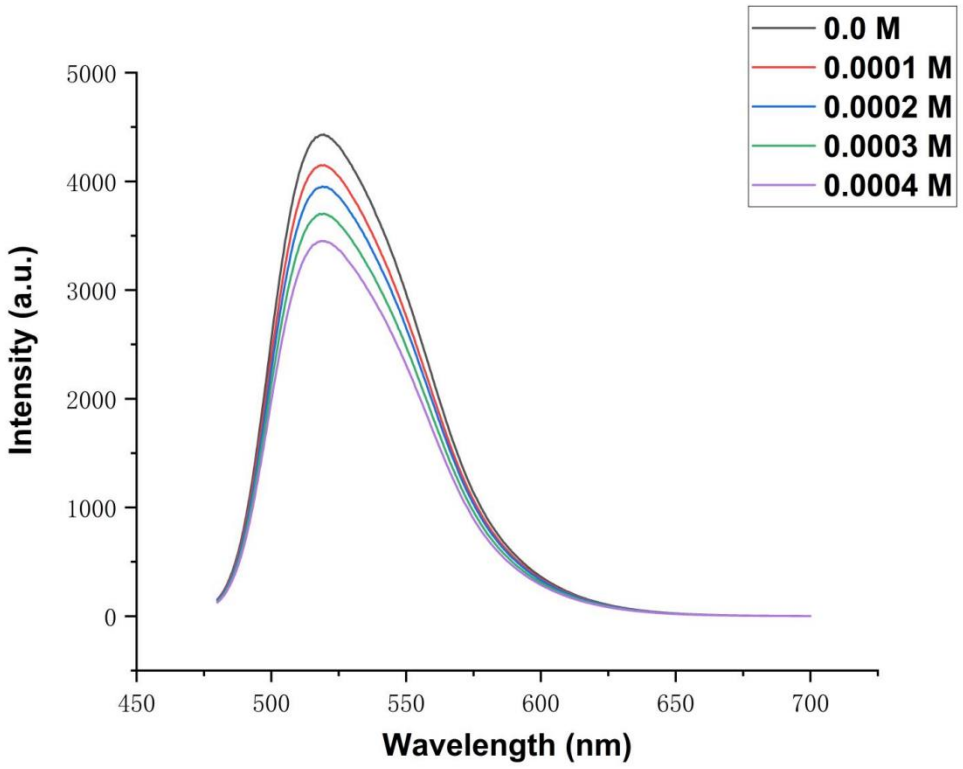


Figure S3. Stern–Volmer fluorescence quenching experiments of *fac*-Ir(ppy)$_3$ with K_3PO_4

In Figure S4, a stock solution of K_3PO_4 (21.2 mg, 0.1 mmol) (use ultrasound to help dissolve) and a stock solution of 1-methylquinoxalin-2(1H)-one **2a** (16.0 mg, 0.1 mmol) in 1 mL of DMSO was prepared. Then, different amounts of this stock solution were added to a solution of the photocatalyst in DMSO (1.0×10^{-5} M). The results show that slight decrease of *fac*-Ir(ppy)$_3$ luminescence was observed.

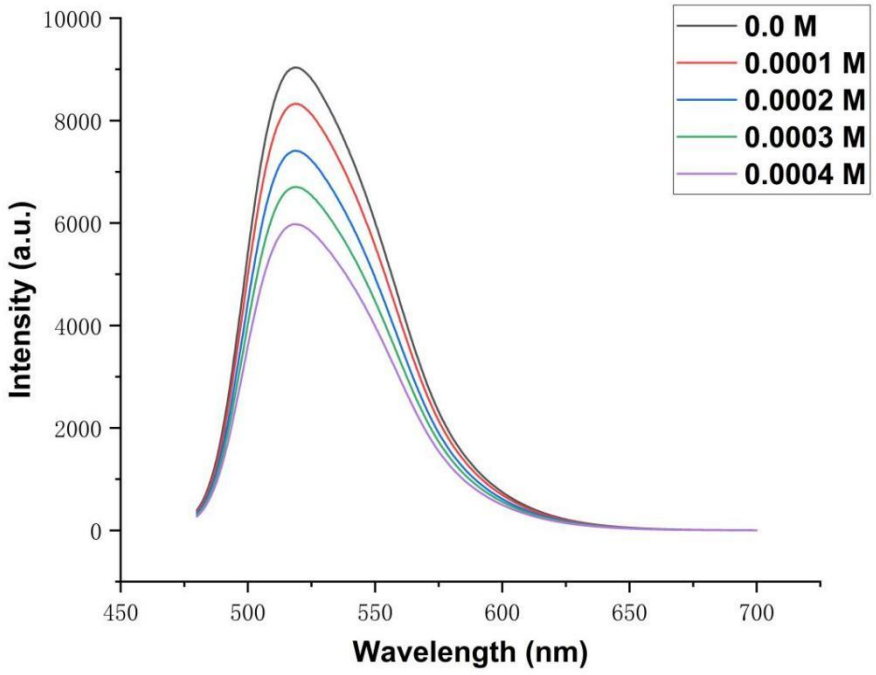


Figure S4. Stern–Volmer fluorescence quenching experiments of *fac*-Ir(ppy)$_3$ with **2a** and K_3PO_4

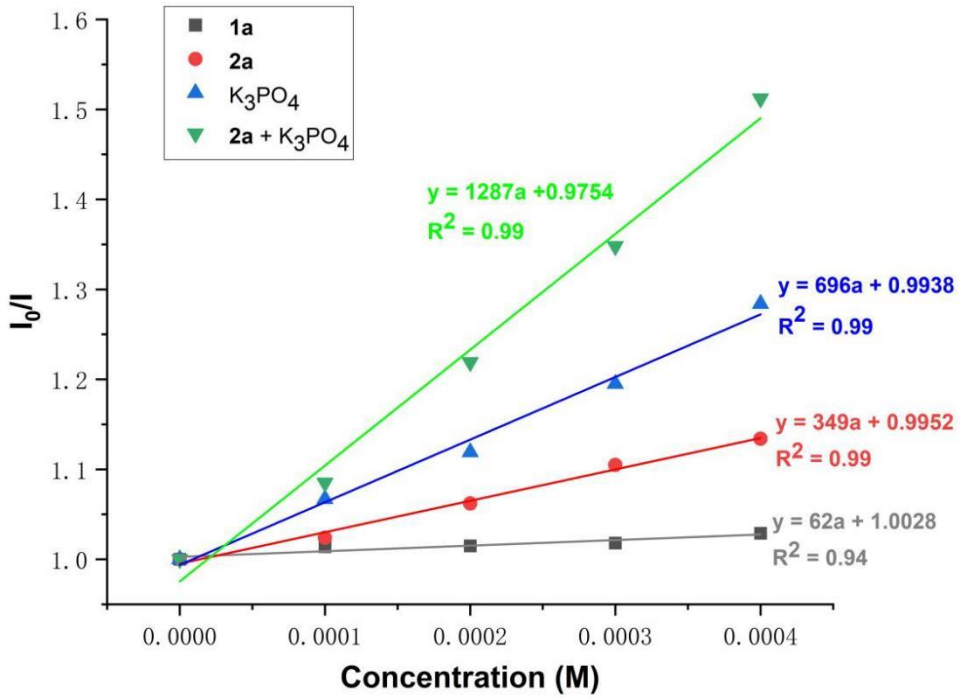


Figure S5. *fac*-Ir(ppy)$_3$ emission quenching with **1a**, **2a**, K_3PO_4 and **2a** with K_3PO_4, respectively.

(h) Light on-off Experiments

Three parallel reactions were performed between **1a** (28.8mg, 0.20 mmol), **2a** (32.0 mg,0.20 mmol) according to the General Procedure (Figure S6). The resulting residue was purfied by silica gel column chromatography (PE/EA = 10:1) to afford the **3aa**. The white area indicates the light irradiation, while the grey area indicates time in the dark. The results demonstrate that the visible light is crucial.

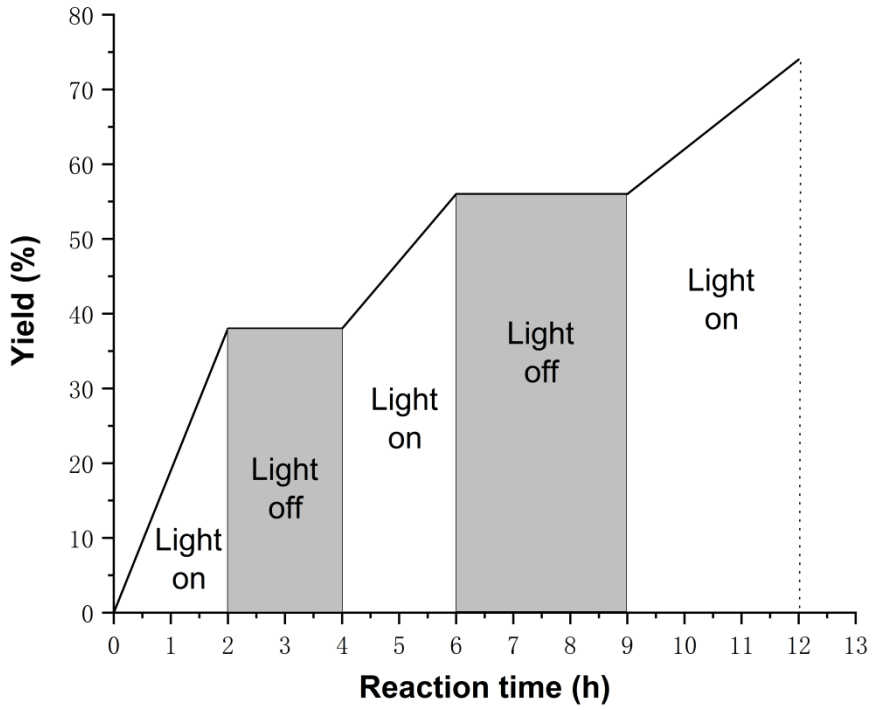
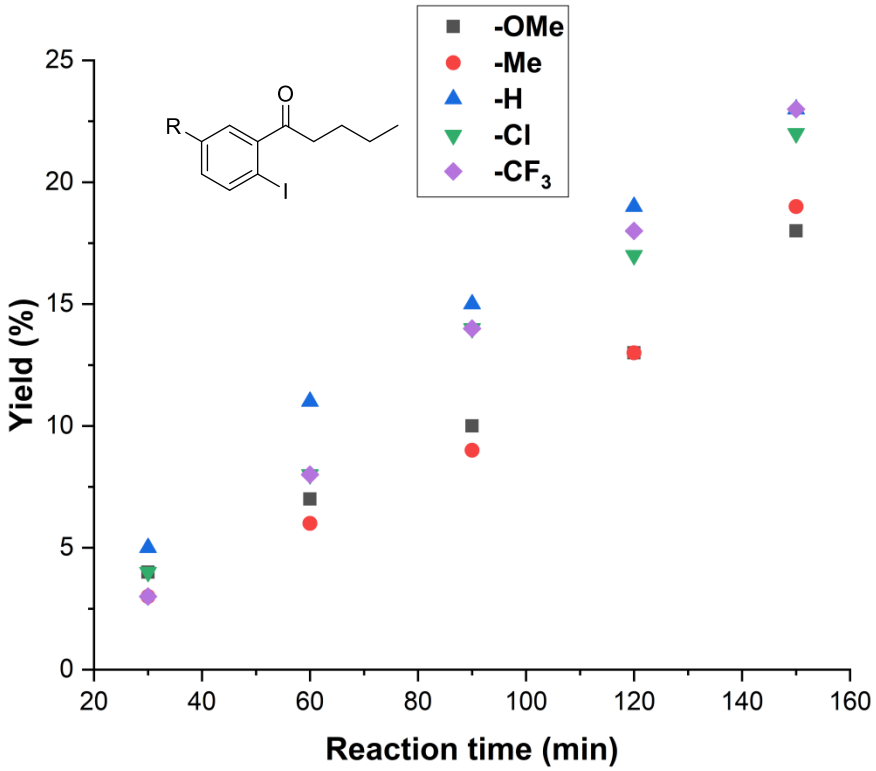


Figure S6: Light on-off experiments plot.

(i) Hammett Studies of the Reaction (Substitution Effect of Iodobenzenes)

To a Schlenk tube were added **1a** (28.8mg, 0.20 mmol), **2a** (32.0 mg, 0.20 mmol, 1.0 equiv), *fac*-Ir(ppy)$_3$ (1.3 mg, 1 mol %), K_3PO_4 (84.8 mg, 0.4mmol, 2 equiv), DMSO (2 mL, 0.1 M), Then the tube was charged with argon three times, and was stirred irradiated with a 18 W blue LED lamp (at approximately 5.0 cm away from the light source) with cooled by a fan at room temperature, five groups were carried out in parallel and stop the one ofreaction every thirty minutes stared fromthirty minutes. After that, the reaction system through simple filtration, wash with ethyl acetate (10 mL) and concentrated in vacuum, followed by addition of diphenylacetonitrile as an internal standard determine the yields.

As the results shown in Figure S7, substituents on iodobenzenes have a significant impact on the reaction rate, and the a positive ρ value (0.19) in Hammett plot was given. These results suggest that there is a buildup of negative charge on the iodobenzene bone in the transition state.



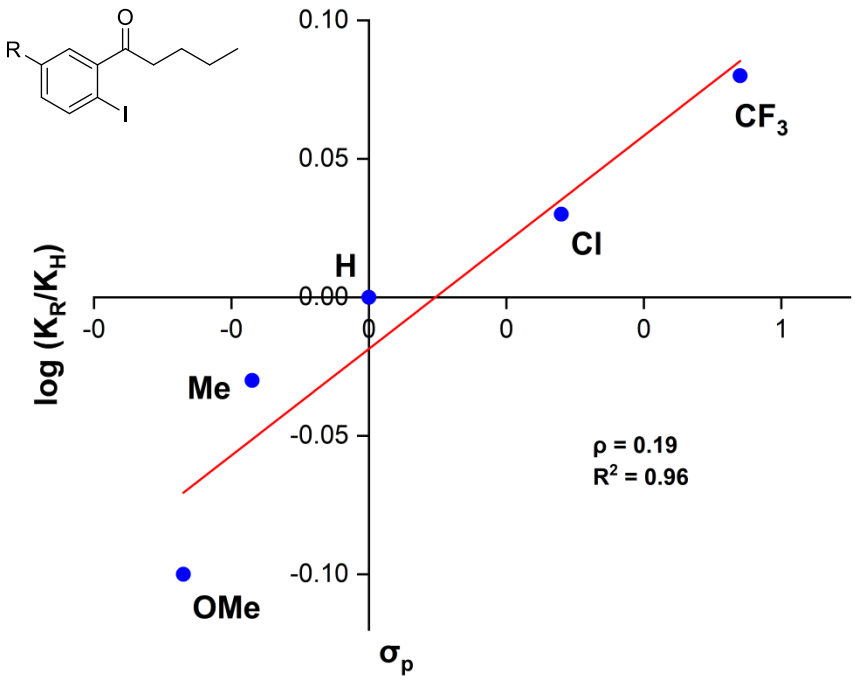


Figure S7. The electronic effect of **1** for the reaction. a) Time course of reaction; b) Hammett plot, $\log(k_R/k_H)$ vs σ.

(j) Cyclic Voltammograms

(I) material

Supporting Electrolyte: *n*-Bu_4NBr was dried under vacuum at 60 °C overnight.

Solvents: MeCN is newly opened ultra-dry reagent.

Working electrode with polishing material and method: The working electrode is a 3 mm diameter glassy carbon working electrode. Polished with 50 nm aluminum oxide and then sonicated in distilled water before drying.

Reference electrode: Ag/AgCl electrode in a saturated solution of KCl.

Counter electrode: The counter electrode is a platinum sheet that was previous burnt for 30 seconds with a butane torch.

(II) The solvent deoxygenation method

An argon filled balloon was attached to the syringe at one end and the other end was placed in the reaction system to be tested and blown up continuously for 2 minutes and keep for use in room temperature.

The cyclic voltammetry was carried out with a Shanghai Chenhua CHI 605E workstation. All CV measurements were conducted in MeCN against saturated calomel electrode (SCE) reference cell and 1 mM *n*-Bu_4NBr supporting electrolyte. All samples should be bubbled with argon for 2 min before test. The scan rate was 100 mV/s.

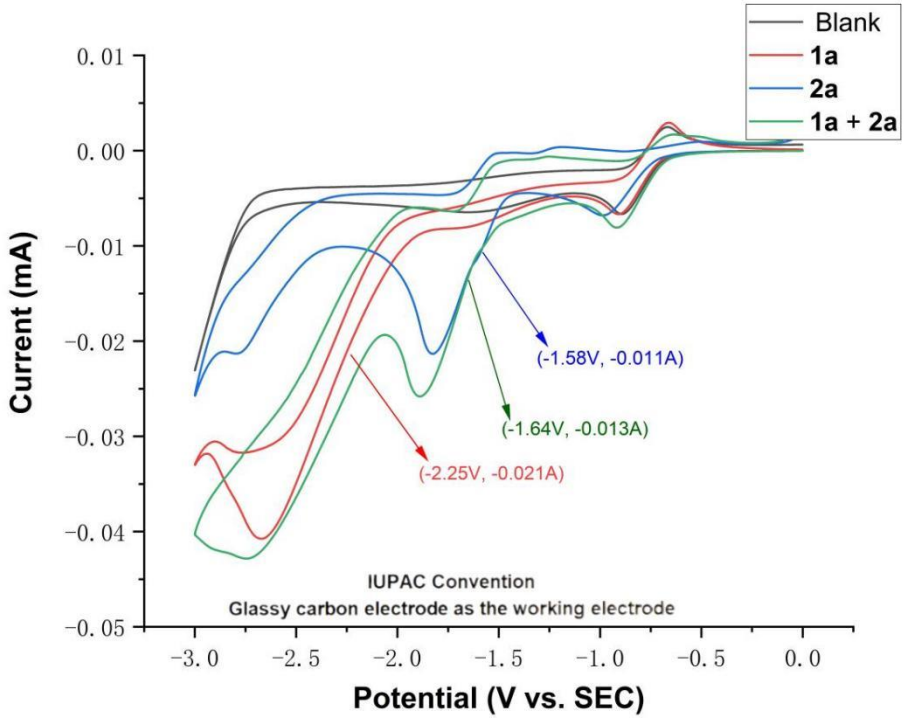


Figure S8. Cyclic Voltammogram Curves. Using GC disk as working electrode, Pt slice, and Ag/AgCl as counter and reference electrode at 100 mV/s scan rate. Cyclic Voltammogram of **1a** (2 mM), $Ep_{1/2red}$ = -2.25 V; **2a** (2 mM), $Ep_{1/2red}$ = -1.58 V;**1a** + **2a** (2 mM), $Ep_{1/2red}$ = -1.64 V;

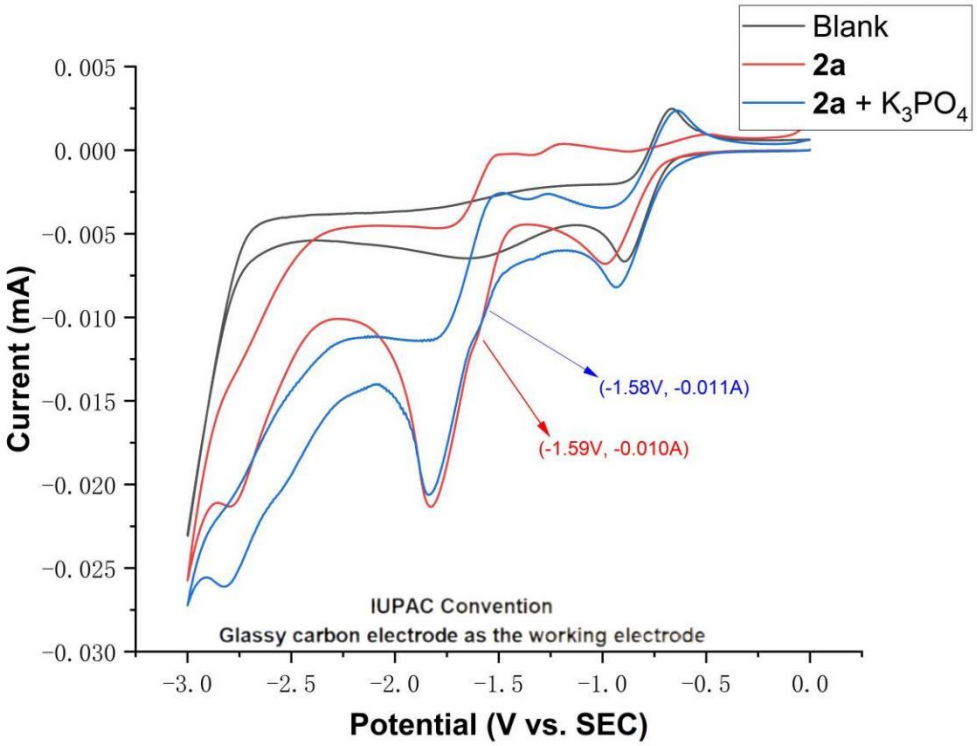


Figure S9. Cyclic Voltammogram Curves. Using GC disk as working electrode, Pt slice, and Ag/AgCl as counter and reference electrode at 100 mV/s scan rate. Cyclic Voltammogram of **2a** (2 mM), $Ep_{1/2red}$ = -1.59 V; **2a** (2 mM), $Ep_{1/2red}$ = -1.58 V.

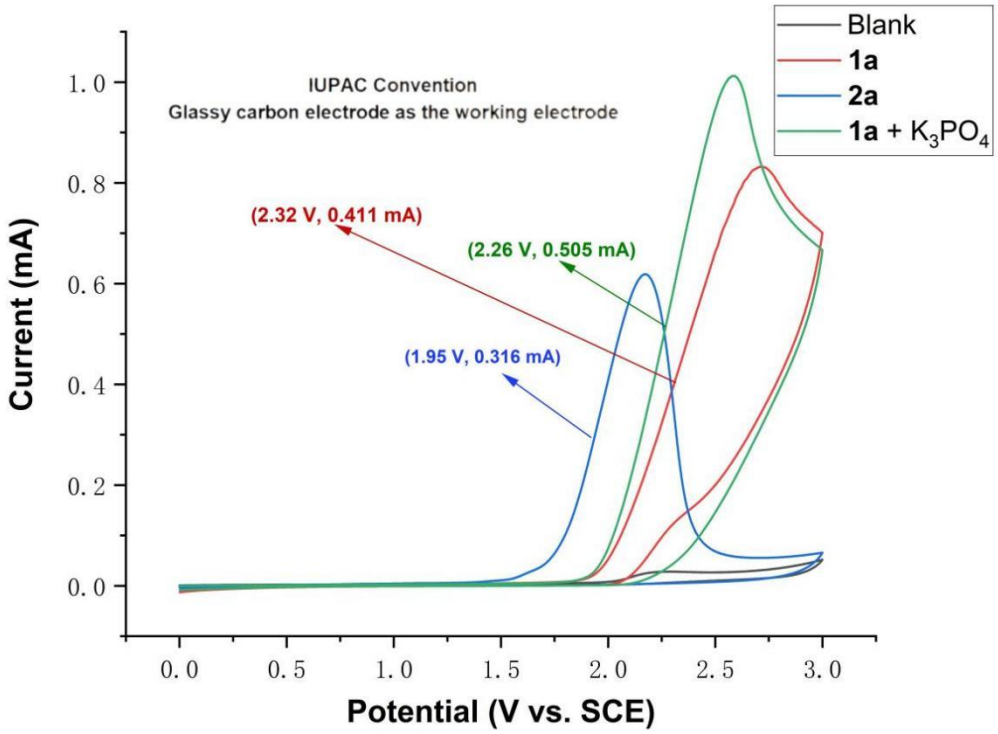


Figure S10. Cyclic Voltammogram Curves. Using GC disk as working electrode, Pt slice, and Ag/AgCl as counter and reference electrode at 100 mV/s scan rate.Cyclic Voltammogram of **1a** (2 mM, 1 equiv) $Ep_{1/2ox}$ = 2.32 V; **2a** (2 mM, 1 equiv) $Ep_{1/2ox}$ = 1.95 V; **1a** (2 mM) + Base (K_3PO_4) (4 Mm, 2 equiv) $Ep_{1/2ox}$ = 2.26 V.

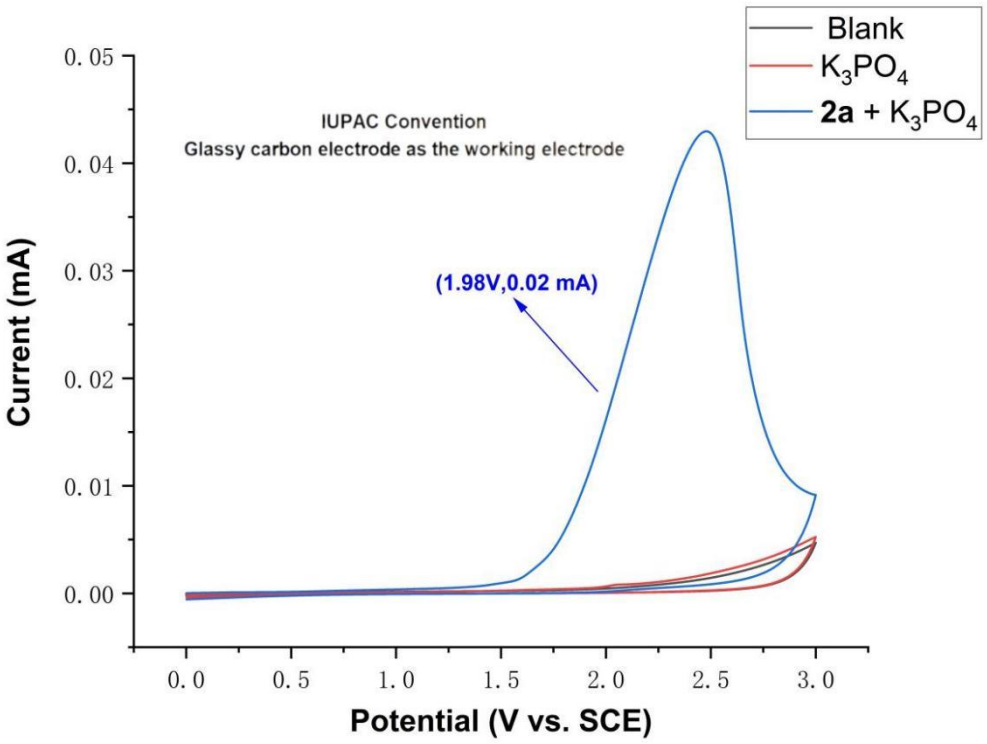


Figure S11. Cyclic Voltammogram Curves. Using GC disk as working electrode, Pt slice, and Ag/AgCl as counter and reference electrode at 100 mV/s scan rate.Cyclic Voltammogram of **2a** (2 mM) + Base (K_3PO_4) (4 Mm, 2 equiv) $Ep_{1/2ox}$ = 1.98 V.

(B) Analytical data

1-Methyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3aa): Following the typical experimental procedure on 0.2 mmol scale, compound **3aa** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 55.7 mg; 87% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-7.99 (m, 2H), 7.68-7.66 (m, 1H), 7.55-7.51 (m, 1H), 7.48-7.42 (m, 3H), 7.27-7.22 (m, 2H), 4.14-4.08 (m, 1H), 3.94-3.87 (m, 1H), 3.70 (s, 3H), 3.28-3.23 (m, 1H), 1.99-1.89 (m, 1H), 1.77-1.67 (m, 1H), 0.99 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 162.7, 154.7, 137.1, 132.9, 132.8, 132.4, 129.5, 129.4, 128.4, 128.0, 123.1, 113.4, 41.3, 38.4, 29.1, 26.2, 11.7; HRMS *m/z* (ESI) calcd for $C_{20}H_{20}N_2O_2$ $[M+H]^+$ 321.1598, found 321.1591.

1-methyl-3-(4-*oxo*-4-phenylbutan-2-yl)quinoxalin-2(1*H*)-one (3ba): Following the typical experimental procedure on 0.2 mmol scale, compound **3ba** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 50.8 mg; 83% yield; Yellow solid; mp 168.4-169.0 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.04-8.02 (m, 2H), 7.69-7.66 (m, 1H), 7.57-7.53 (m, 1H), 7.50-7.44 (m, 3H), 7.27-7.24 (m, 2H), 4.25-4.16 (m, 1H), 3.96-3.90 (m, 1H), 3.71 (s, 3H), 3.17-3.12 (m, 1H), 1.38 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.9, 163.1, 154.4, 137.1, 133.0, 132.8, 132.4, 129.6, 129.5, 128.4, 128.1, 123.2, 113.4, 43.2, 32.5, 29.0, 18.5; HRMS *m/z* (ESI) calcd for $C_{19}H_{18}N_2O_2$ $[M+Na]^+$ 329.1260, found 329.1265.

1-methyl-3-(1-*oxo*-1-phenylheptan-3-yl)quinoxalin-2(1*H*)-one (3ca): Following the typical experimental procedure on 0.2 mmol scale, compound **3ca** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 5:1, v/v). 54.3 mg; 78% yield; Yellow solid; mp 164.4-165.1 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00-7.98 (m, 2H), 7.68-7.65 (m, 1H), 7.54-7.50 (m, 1H), 7.45-7.39 (m, 3H), 7.25-7.21 (m, 2H), 4.19-4.12 (m, 1H), 3.94-3.87 (m, 1H), 3.70 (s, 3H), 3.29-3.23 (m, 1H), 1.93-1.84 (m, 1H), 1.69-1.60 (m, 1H), 1.39-1.29 (m, 4H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.2, 163.1, 154.7, 137.2,

133.0, 132.9, 132.6, 129.6, 129.4, 128.5, 128.1, 123.3, 113.5, 41.8, 37.1, 33.3, 29.6, 29.2, 22.9, 14.1.; HRMS *m/z* (ESI) calcd for $C_{22}H_{24}N_2O_2$ $[M+Na]^+$ 371.1730, found 371.1731.

1-methyl-3-(1-*oxo*-1-phenylpentadecan-3-yl)quinoxalin-2(1*H*)-one (3da): Following the typical experimental procedure on 0.2 mmol scale, compound **3da** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 63.5 mg; 69% yield; Yellow solid; mp 173.4-173.9 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01-7.98 (m, 2H), 7.68-7.65 (m, 1H), 7.54-7.50 (m, 1H), 7.46-7.41 (m, 3H), 7.26-7.21 (m, 2H), 4.20-4.13 (m, 1H), 3.94-3.87 (m, 1H), 3.69 (s, 1H), 3.29-3.23 (m, 1H), 1.94-1.85 (m, 1H), 1.69-1.60 (m, 1H), 1.31-1.23 (m, 20H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 163.0, 154.6, 137.1, 132.9, 132.7, 132.4, 129.5, 129.3, 128.4, 128.4, 128.3, 128.0, 123.1, 113.4, 41.7, 37.1, 33.4, 31.8, 29.7, 29.5, 29.5, 29.4, 29.2, 29.0, 27.3, 22.6, 14.0; HRMS *m/z* (ESI) calcd for $C_{30}H_{40}N_2O_2$ $[M+Na]^+$ 483.2982, found 483.2987.

1-methyl-3-(5-methyl-1-*oxo*-1-phenylhexan-3-yl)quinoxalin-2(1*H*)-one(3ea): Following the typical experimental procedure on 0.2 mmol scale, compound **3ea** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 61.2 mg; 88% yield; Yellow solid; mp 171.4-171.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00-7.97 (m, 2H), 7.68-7.66 (m, 1H), 7.53-7.51 (m, 1H), 7.47-7.42 (m, 3H), 7.27-7.25 (m, 2H), 4.27-4.20 (m, 1H), 3.90-3.84 (m, 1H), 3.71 (t, *J* = 4.0 Hz, 3H), 3.29-3.23 (m, 1H), 1.82-1.75 (m, 1H), 1.69-1.63 (m, 1H), 1.50-1.44 (m, 1H), 0.92 (s, 3H), 0.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.2, 163.3, 154.5, 132.9, 132.7, 132.7, 132.5, 129.4, 129.3, 128.3, 128.0, 123.1, 113.4, 42.7, 42.0, 35.1, 29.0, 26.0, 23.0, 22.3; HRMS *m/z* (ESI) calcd for $C_{22}H_{24}N_2O_2$ $[M+Na]^+$ 371.1730, found 371.1734.

1-methyl-3-(1-*oxo*-1,5-diphenylpentan-3-yl)quinoxalin-2(1*H*)-one (3fa): Following the typical experimental procedure on 0.2 mmol scale, compound **3fa** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 57.0 mg; 72% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00-

7.97 (m, 2H), 7.69-7.66 (m, 1H), 7.53-7.48 (m, 1H), 7.45-7.39 (m, 3H), 7.24-7.22 (m, 1H), 7.21-7.15 (m, 5H), 7.11-7.07 (m, 1H), 4.30-4.23 (m, 1H), 3.96-3.89 (m, 1H), 3.64 (s, 3H), 3.31-3.25 (m, 1H), 2.80-2.64 (m, 2H), 2.32-2.22 (m, 1H), 2.06-1.97 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.7, 162.3, 154.5, 141.8, 136.9, 132.8, 132.8, 132.3, 129.4, 128.3, 128.2, 128.0, 127.9, 125.5, 123.1, 113.45, 41.8, 37.2, 34.8, 33.6, 29.0; HRMS *m/z* (ESI) calcd for $C_{26}H_{24}N_2O_2$ $[M+Na]^+$ 419.1730, found 419.1729.

1-methyl-3-(1,1,1-trifluoro-5-*oxo*-5-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ga): Following the typical experimental procedure on 0.2 mmol scale, compound **3ga** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 59.1 mg; 79% yield; Yellow solid; mp 169.6-170.1 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.0-7.98 (m, 2H), 7.72-7.70 (m, 1H), 7.58-7.50 (m, 2H), 7.48-7.44 (m, 2H), 7.31-7.26 (m, 2H), 4.51-4.44 (m, 1H), 3.93-3.87 (m, 1H), 3.73 (s, 3H), 3.42-3.36 (m, 1H), 2.98-2.84 (m, 1H), 2.68-2.54 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.7, 159.6, 154.2, 136.6, 133.2, 133.1, 132.3, 130.1, 129.8, 128.6, 128.1, 123.5, 113.6, 41.0, 35.8, 35.5, 32.3(q, *J* = 30 Hz), 29.2; HRMS *m/z* (ESI) calcd for $C_{20}H_{17}F_3N_2O_2$ $[M+Na]^+$ 397.1134, found 397.1142.

3-(1-methoxy-4-*oxo*-4-phenylbutan-2-yl)-1-methylquinoxalin-2(1*H*)-one (3ha): Following the typical experimental procedure on 0.2 mmol scale, compound **3ha** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 53.8 mg; 80% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.03-8.00 (m, 2H), 7.69-7.66 (m, 1H), 7.55-7.51 (m, 1H), 7.46-7.42 (m, 3H), 7.24-7.20 (m, 2H), 4.51-4.44 (m, 1H), 4.02-3.95 (m, 1H), 3.83-3.74 (m, 2H), 3.69-3.66 (m, 2H), 3.44-3.39 (m, 2H), 3.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.7, 159.5, 154.5, 137.0, 132.9, 132.8, 132.7, 132.3, 129.6, 128.3, 127.9, 123.1, 113.4, 73.6, 58.7, 38.8, 37.9, 29.0; HRMS *m/z* (ESI) calcd for $C_{20}H_{20}N_2O_3$ $[M+Na]^+$ 359.1366, found 359.1374.

2-(1,1-dimethoxy-4-*oxo*-4-phenylbutan-2-yl)-1-methylquinoxalin-2(1*H*)-one (3ia): Following the typical experimental procedure on 0.2 mmol scale, compound **3ia** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl

acetate = 10:1, v/v). 60.7 mg; 83% yield; Yellow solid; mp 154.4-155.1 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01-7.99 (m, 2H), 7.70-7.67 (m, 1H), 7.55-7.51 (m, 1H), 7.48-7.41 (m, 3H), 7.27-7.21 (m, 2H), 4.92 (d, *J* = 6.0 Hz, 1H), 4.62-4.57 (m, 1H), 4.04-3.97 (m, 1H), 3.71 (t, *J* = 1.6 Hz, 3H), 3.55-3.49 (m, 1H), 3.42 (s, 3H), 3.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.7, 158.9, 154.8, 137.0, 133.0, 132.8, 132.5, 129.7, 129.6, 128.4, 128.1, 123.2, 113.4, 105.4, 54.5, 53.9, 40.5, 37.0, 29.1; HRMS *m/z* (ESI) calcd for $C_{21}H_{22}N_2O_4$ $[M+Na]^+$ 389.1472, found 389.1477.

1-methyl-3-(2-methyl-4-*oxo*-4-phenylbutan-2-yl)quinoxalin-2(1*H*)-one (3ja): Following the typical experimental procedure on 0.2 mmol scale, compound **3ja** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 58.3 mg; 91% yield; Yellow solid; mp 172.4-172.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.94-7.92 (m, 2H), 7.77-7.45 (m, 1H), 7.54-7.45 (m, 2H), 7.44-7.40 (m, 2H), 7.30-7.26 (m, 1H), 7.26-7.24 (m, 1H), 3.90 (s, 2H), 3.62 (s, 3H), 1.58 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.7, 163.9, 154.1, 137.7, 133.2, 132.7, 132.4, 130.0, 129.3, 128.4, 128.0, 123.2, 113.3, 48.8, 41.5, 28.7, 27.1; HRMS *m/z* (ESI) calcd for $C_{20}H_{20}N_2O_2$ $[M+Na]^+$ 343.1417, found 343.1422.

3-(3-ethyl-1-*oxo*-1-phenylpentan-3-yl)-1-methylquinoxalin-2(1*H*)-one (3ka): Following the typical experimental procedure on 0.2 mmol scale, compound **3ka** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 59.9 mg; 86% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.95-7.92 (m, 2H), 7.77-7.75 (m, 1H), 7.53-7.45 (m, 2H), 7.43-7.39 (m, 2H), 7.30-7.28 (m, 1H), 7.26-7.24 (m, 1H), 3.89 (s, 2H), 3.61 (s, 3H), 2.29-2.19 (m, 2H), 2.11-2.02 (m, 2H), 0.80 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.7, 162.8, 154.2, 137.8, 133.0, 132.5, 132.2, 130.0, 129.2, 128.3, 127.9, 123.1, 113.3, 47.9, 43.3, 28.8, 27.1, 8.6; HRMS *m/z* (ESI) calcd for $C_{22}H_{24}N_2O_2$ $[M+Na]^+$ 371.1730, found 371.1731.

1-methyl-3-(1-(2-*oxo*-2-phenylethyl)cyclopentyl)quinoxalin-2(1*H*)-one (3la): Following the typical experimental procedure on 0.2 mmol scale, compound **3la** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 60.2 mg; 87% yield; Yellow solid; mp 160.1-160.3 °C (uncorrected); ^{1}H

NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91-7.89 (m, 2H), 7.74-7.71 (m, 1H), 7.50-7.42 (m, 2H), 7.40-7.36 (m, 2H), 7.27-7.20 (m, 2H), 3.92 (s, 2H), 3.60 (s, 3H), 2.62-2.56 (m, 2H), 1.90-1.76 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.0, 162.7, 154.1, 137.8, 133.1, 132.5, 132.1, 129.9, 129.2, 128.3, 127.9, 123.1, 113.2, 52.3, 47.1, 36.8, 28.7, 25.0; HRMS *m/z* (ESI) calcd for $C_{22}H_{22}N_2O_2$ $[M+Na]^+$ 369.1573, found 369.1578.

1-methyl-3-(1-(2-*oxo*-2-phenylethyl)cyclohexyl)quinoxalin-2(1*H*)-one (3ma): Following the typical experimental procedure on 0.2 mmol scale, compound **3ma** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 62.6 mg; 87% yield; Yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90-7.87 (m, 2H), 7.80-7.78 (m, 1H), 7.48-7.43 (m, 2H), 7.38-7.34 (m, 2H), 7.30-7.25 (m, 1H), 7.22-7.20 (m, 1H), 3.95 (s, 2H), 3.58 (t, *J* = 1.2 Hz, 3H), 2.44-2.37 (m, 2H), 1.93-1.87 (m, 2H), 1.72-1.52 (m, 5H), 1.49-1.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.0, 163.4, 154.0, 138.0, 132.9, 132.5, 132.1, 123.0, 129.2, 128.2, 127.9, 123.0, 113.2, 44.9, 44.5, 34.1, 28.7, 26.1, 22.4; HRMS *m/z* (ESI) calcd for $C_{23}H_{24}N_2O_2$ $[M+Na]^+$ 383.1730, found 383.1734.

1-methyl-3-(1-*oxo*-1-(m-tolyl)pentan-3-yl)quinoxalin-2(1*H*)-one (3na): Following the typical experimental procedure on 0.2 mmol scale, compound **3na** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 51.4 mg; 77% yield; Yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.69-7.61 (m, 2H), 7.49-7.43 (m, 2H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.26-7.22 (m, 2H), 7.09-7.06 (m, 1H), 4.14-4.07 (m, 1H), 3.92-3.85 (m, 1H), 3.81 (t, *J* = 2.4 Hz, 3H), 3.70 (t, *J* = 1.6 Hz, 3H), 3.27-3.22 (m, 1H), 1.99-1.88 (m, 1H), 1.77-1.66 (m, 1H), 0.99 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.9, 162.7, 159.6, 154.6, 138.4, 132.9, 132.4, 129.5, 129.4, 123.1, 120.7, 119.3, 113.4, 112.1, 55.3, 41.4, 38.4, 29.0, 26.2, 11.7; HRMS *m/z* (ESI) calcd for $C_{21}H_{22}N_2O_2$ $[M+Na]^+$ 357.1573, found 357.1574.

2-(1-(3-methoxyphenyl)-1-*oxo*pentan-3-yl)-1-methylquinoxalin-2(1*H*)-one (3oa): Following the typical experimental procedure on 0.2 mmol scale, compound **3oa** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 50.4 mg; 72% yield; Yellow solid; mp 145.6-145.9 °C

(uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.27 (d, *J* = 8.0 Hz, 2H), 7.65-7.62 (m, 1H), 7.41-7.37 (m, 1H), 7.20-7.15 (m, 4H), 4.12-4.05 (m, 1H), 3.8-3.82 (m, 1H), 3.63 (t, *J* = 2.8 Hz, 3H), 3.22-3.17 (m, 1H), 2.34 (s, 3H), 1.96-1.86 (m, 1H), 1.74-1.64 (m, 1H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.6, 162.6, 154.5, 143.3, 134.5, 132.8, 132.3, 129.3, 129.2, 128.9, 128.0, 123.0, 113.3,41.1, 38.3, 28.9, 26.1, 21.4, 11.7; HRMS *m/z* (ESI) calcd for $C_{21}H_{22}N_2O_3$ $[M+Na]^+$ 373.1523, found 373.1526.

1-methyl-3-(1-*oxo*-1-(3-(trifluoromethyl)phenyl)pentan-3-yl)quinoxalin-2(1*H*)-one (3pa) : Following the typical experimental procedure on 0.2 mmol scale, compound **3pa** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 47.3 mg; 61% yield; Yellow solid; mp 172.4-172.6 °C (uncorrected); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21 (s, 1H), 8.19 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 1.2 Hz, 1H), 7.59 (t, *J* = 4.4 Hz, 1H), 7.48-7.44 (m, 1H), 7.29-7.21 (m, 2H), 4.17-4.11 (m, 1H), 4.00-3.93 (m, 1H), 3.69 (t, *J* = 2.8 Hz, 3H), 3.30-3.22 (m, 1H), 2.03-1.93 (m, 1H), 1.79-1.69 (m, 1H), 1.01 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.9, 162.1, 154.5, 137.6, 132.8, 132.2, 131.2, 129.5, 129.4, 129.1, 124.8 (q, *J* = 4 Hz), 123.2, 113.4, 41.0, 38.5, 28.9, 26.1, 11.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) 62.58; HRMS *m/z* (ESI) calcd for $C_{21}H_{19}F_3N_2O_2$ $[M+Na]^+$ 411.1291, found 411.1291.

3-(1-(3-chlorophenyl)-1-oxopentan-3-yl)-1-methylquinoxalin-2(1*H*)-one (3qa): Following the typical experimental procedure on 0.2 mmol scale, compound **3qa** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 39.0 mg; 55% yield; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.27 (s, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.49-7.45 (m, 1H), 7.28-7.22 (m, 2H), 4.17-4.10 (m, 1H), 3.99-3.92 (m, 1H), 3.70 (s, 3H), 3.27-3.21 (m, 1H), 2.03-1.92 (m, 1H), 1.79-1.68 (m, 1H), 1.01 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 163.0, 154.4, 137.0, 135.2, 133.9, 132.9, 131.0, 130.6, 128.5, 128.0, 123.5, 113.5, 41.3, 38.4, 29.3, 26.3, 11.7; HRMS *m/z* (ESI) calcd for $C_{20}H_{19}ClN_2O_2$ $[M+Na]^+$ 377.1027, found

377.1029.

3-(4-(4-methoxyphenyl)-2-methyl-4-oxobutan-2-yl)-1-methylquinoxalin-2(1H)-one (3ra): Following the typical experimental procedure on 0.2 mmol scale, compound **3ra** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 52.5 mg; 75% yield; Yellow solid; mp 166.4-166.7 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84-7.80 (m, 2H), 7.69-7.67 (m, 1H), 7.38-7.34 (m, 1H), 7.20-7.12 (m, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 3.77 (s, 2H), 3.74 (s, 3H), 3.52 (s, 3H), 1.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.2, 164.1, 163.1, 154.0, 133.1, 132.4, 130.7, 130.2, 129.9, 129.1, 123.0, 113.4, 113.2, 55.3, 48.3, 41.5, 28.7, 27.1; HRMS *m/z* (ESI) calcd for $C_{21}H_{22}N_2O_3$ $[M+Na]^+$ 373.1523, found 373.1526.

1-ethyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ab): Following the typical experimental procedure on 0.2 mmol scale, compound **3ab** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 58.7 mg; 88% yield; Yellow solid; mp 182.4-182.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-7.99 (m, 2H), 7.70-7.67 (m, 1H), 7.54-7.52 (m, 1H), 7.49-7.42 (m, 3H), 7.30-7.22 (m, 2H), 4.40-4.27 (m, 2H), 4.13-4.06 (m, 1H), 3.92-3.86 (m, 1H), 3.27-3.21 (m, 1H), 2.00-1.89 (m, 1H), 1.76-1.67 (m, 1H), 1.41-1.37 (m, 3H), 0.99 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 162.4, 154.0, 137.0, 132.6, 131.7, 129.7, 129.2, 128.3, 127.9, 122.8, 113.2, 41.0, 38.4, 37.1, 26.1, 12.3, 11.7; HRMS *m/z* (ESI) calcd for $C_{21}H_{22}N_2O_2$ $[M+Na]^+$ 357.1573, found 357.1573.

1-heptyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ac): Following the typical experimental procedure on 0.2 mmol scale, compound **3ac** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 43.5 mg; 52% yield; Yellow solid; mp 179.3-179.7 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01-7.99 (m, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.53-7.49 (m, 1H), 7.46-7.40 (m, 3H), 7.26-7.19 (m, 2H), 4.32-4.18 (m, 2H), 4.16-4.08 (m, 1H), 3.93-3.86 (m, 1H), 3.27-3.22 (m, 1H), 2.00-1.90 (m, 1H), 1.80-1.67 (m, 3H), 1.49-1.42 (m, 2H), 1.38-1.28 (m, 8H), 0.99 (t, *J* = 7.6 Hz, 3H), 0.88 (t, *J* = 6.4 Hz, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 162.5, 154.2, 137.1, 132.6, 132.6, 132.0, 129.7, 129.2, 128.3, 127.9, 122.8, 113.3, 42.2, 41.1, 38.4, 31.6, 29.1, 29.1, 27.2, 26.9, 26.2, 22.5, 14.0, 11.7; HRMS *m/z* (ESI) calcd for $C_{27}H_{34}N_2O_2$ $[M+Na]^+$ 441.2512, found 441.2512.

1-isopropyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ad): Following the typical experimental procedure on 0.2 mmol scale, compound **3ad** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 54.3 mg; 78% yield; Yellow solid; mp 180.4-180.7 °C (uncorrected); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-8.00 (m, 2H), 7.68-7.66 (m, 1H), 7.54-7.47 (m, 2H), 7.45-7.39 (m, 3H), 7.22-7.18 (m, 1H), 4.13-4.06 (m, 1H), 3.91-3.84 (m, 1H), 3.26-3.20 (m, 1H), 2.00-1.89 (m, 1H), 1.74-1.69 (m, 1H), 1.68-1.64 (m, 7H), 0.99 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 154.8, 137.2, 133.1, 132.6, 130.0, 128.7, 128.3, 128.0, 122.7, 41.1, 38.3, 26.2, 19.3, 11.8; HRMS *m/z* (ESI) calcd for $C_{22}H_{24}N_2O_2$ $[M+Na]^+$ 371.1730, found 371.1733.

1-(cyclopropylmethyl)-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ae): Following the typical experimental procedure on 0.2 mmol scale, compound **3ae** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 56.9 mg; 79% yield; Yellow solid; mp 177.9-178.2 °C (uncorrected); ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-8.00 (m, 2H), 7.69-7.67 (m, 1H), 7.52-7.50 (m, 1H), 7.47-7.41 (m, 3H), 7.36 (d, J = 8.4 Hz, 1H), 7.23-7.20 (m, 1H), 4.19 (t, J = 2.8 Hz, 1H), 3.93-3.86 (m, 1H), 3.27-3.21 (m, 1H), 2.00-1.90 (m, 1H), 1.77-1.66 (m, 1H), 1.32-1.24 (m, 1H), 1.00 (t, J = 7.6 Hz, 3H), 0.61-0.49 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 162.7, 154.5, 137.1, 132.6, 132.3, 129.6, 129.2, 128.3, 127.9, 122.9, 113.6, 45.9, 41.0, 38.5, 26.1, 11.7, 9.5, 4.1, 3.9; HRMS *m/z* (ESI) calcd for $C_{23}H_{24}N_2O_2$ $[M+Na]^+$ 383.1730, found 383.1732.

1-(cyclopentylmethyl)-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3af): Following the typical experimental procedure on 0.2 mmol scale, compound **3af** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 50.4 mg; 79% yield; Yellow solid; mp 176.8-177.0 °C

(uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01-7.99 (m, 2H), 7.69-7.66 (m, 1H), 7.54-7.50 (m, 1H), 7.45-7.41 (m, 3H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.23-7.19 (m, 1H), 4.32-4.22 (m, 2H), 4.14-4.08 (m, 1H), 3.92-3.86 (m, 1H), 3.28-3.23 (m, 1H), 2.47-2.40 (m, 1H), 1.97-1.89 (m, 1H), 1.78-1.68 (m, 5H), 1.57-1.41 (m, 4H), 0.99 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 162.7, 154.8, 137.1, 132.7, 132.6, 132.2, 129.7, 129.1, 128.3, 128.0, 122.8, 113.7, 46.1, 41.2, 38.6, 38.5, 30.3, 30.2, 26.2, 24.7, 24.7, 11.7; HRMS *m/z* (ESI) calcd for $C_{25}H_{28}N_2O_2$ $[M+Na]^+$ 411.2043, found 411.2043.

1-(cyclohexylmethyl)-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ag): Following the typical experimental procedure on 0.2 mmol scale, compound **3ag** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 61.9 mg; 77% yield; Yellow solid; mp 181.4-181.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-7.99 (m, 2H), 7.69-7.66 (m, 1H), 7.53-7.50 (m, 2H), 7.43-7.41 (m, 2H), 7.32-7.28 (m, 1H), 7.24-7.20 (m, 1H), 4.19-4.13 (m, 2H), 3.92-3.85 (m, 1H), 3.28-3.22 (m, 1H), 1.92-1.89 (m, 2H), 1.45-1.64 (m, 6H), 1.22-1.27 (m, 6H), 0.99 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.2, 162.7, 154.9, 137.2, 132.7, 132.5, 129.8, 129.1, 128.4, 128.1, 122.9, 113.9, 48.0, 41.3, 38.6, 36.5, 30.9, 30.8, 26.3, 26.2, 25.8, 25.8, 11.8; HRMS *m/z* (ESI) calcd for $C_{26}H_{30}N_2O_2$ $[M+Na]^+$ 425.2199, found 425.2220.

1-benzyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ah): Following the typical experimental procedure on 0.2 mmol scale, compound **3ah** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 42.8 mg; 54% yield; Yellow solid; mp 168.4-168.7 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-7.99 (m, 2H), 7.68-7.66 (m, 1H), 7.53-7.49 (m, 1H), 7.44-7.40 (t, *J* = 8.0 Hz, 2H), 7.32-7.22 (m, 6H), 7.17-7.14 (m, 2H), 5.58-5.41 (m, 2H), 4.21-4.15 (m, 1H), 3.96-3.89 (m, 1H), 3.32-3.27 (m, 1H), 2.04-1.94 (m, 1H), 1.82-1.72 (m, 1H), 1.03 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 162.8, 154.7, 137.0, 135.3, 132.7, 132.6, 132.1, 129.5, 129.3, 128.7, 128.3, 128.0, 127.4, 126.7, 123.1, 114.2, 45.7, 41.4, 38.5, 26.4, 11.8; HRMS *m/z* (ESI) calcd for $C_{26}H_{24}N_2O_2$

$[M+Na]^+$ 419.1730, found 419.1725.

Ethyl 2-(2-*oxo*-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-1(2*H*)-yl)acetate (3ai): Following the typical experimental procedure on 0.2 mmol scale, compound **3ai** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 47.8 mg; 61% yield; Yellow solid; mp 188.4-188.5 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02-7.99 (m, 2H), 7.85-7.83 (m, 1H), 7.75-7.23 (m, 1H), 7.55-7.49 (m, 2H), 7.48-7.40 (m, 3H), 5.28-5.24 (m, 1H), 5.00-4.96 (m, 1H), 4.26-4.20 (m, 2H), 4.12-3.99 (m, 2H), 3.34-3.29 (m, 1H), 2.08-1.98 (m, 1H), 1.87-1.77 (m, 1H), 1.24 (t, *J* = 6.4 Hz, 3H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.1, 168.5, 154.5, 152.7, 138.9, 137.1, 132.7, 128.8, 128.3, 128.2, 128.0, 126.7, 126.4, 62.6, 60.5, 41.2, 37.8, 26.8, 14.0, 11.7; HRMS *m/z* (ESI) calcd for $C_{23}H_{24}N_2O_4$ $[M+H]^+$ 393.1809, found 393.1810.

2-(1-*oxo*-1-phenylpentan-3-yl)-1-(3,3,3-trifluoropropyl)quinoxalin-2(1*H*)-one (3aj): Following the typical experimental procedure on 0.2 mmol scale, compound **3aj** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 41.8 mg; 52% yield; Yellow solid; mp 177.2-177.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00-7.97 (m, 2H), 7.71-7.69 (m, 1H), 7.54-7.46 (m, 2H), 7.44-7.41 (m, 2H), 7.27-7.22 (m, 2H), 4.56-4.43 (m, 2H), 4.13-4.06 (m, 1H), 3.94-3.87 (m, 1H), 3.29-3.23 (m, 1H), 2.63-2.57 (m, 2H), 1.99-1.88 (m, 1H), 1.77-1.67 (m, 1H), 0.98 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.9, 162.5, 154.0, 136.9, 132.7, 132.6, 131.3, 130.1, 129.7, 128.3, 127.9, 123.5, 112.3, 41.1, 38.2, 35.6, 35.5, 31.1 (q, *J* = 30 Hz), 26.2, 11.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) 65.33. HRMS *m/z* (ESI) calcd for $C_{22}H_{21}F_3N_2O_2$ $[M+Na]^+$ 425.1447, found 425.1454.

7-chloro-1-methyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ak): Following the typical experimental procedure on 0.2 mmol scale, compound **3ak** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 46.7 mg; 66% yield; Yellow solid; mp 188.2-188.4 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99-7.97 (m, 2H), 7.59-7.52 (m, 2H), 7.44 (t, *J* =

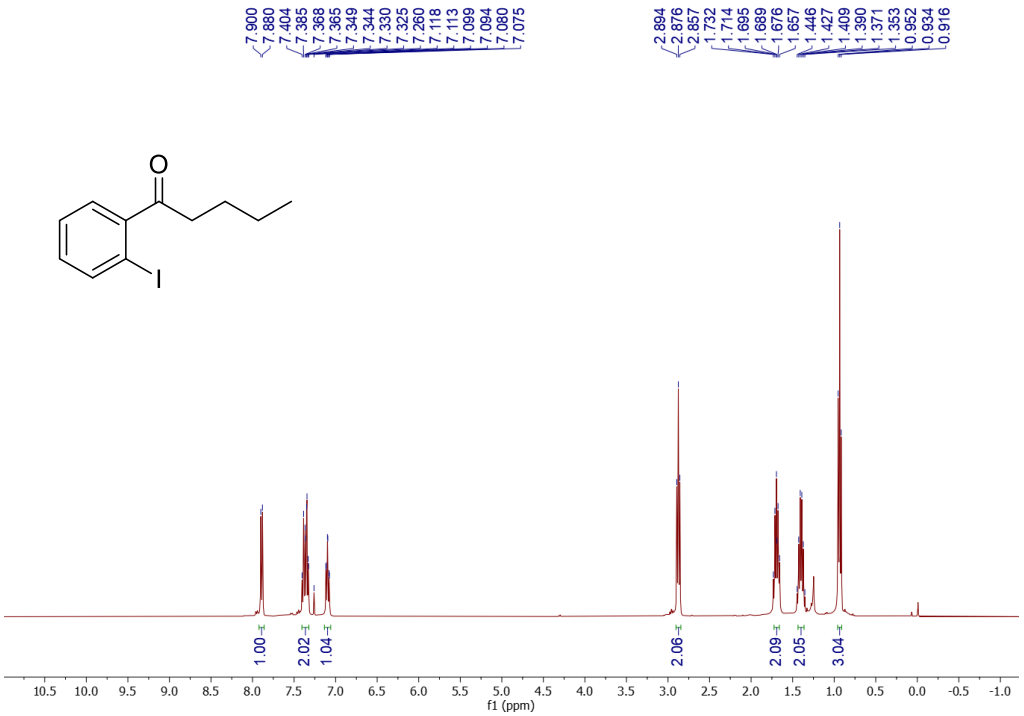
7.6 Hz, 2H), 7.25-7.18 (m, 2H), 4.10-4.04 (m, 1H), 3.91-3.84 (m, 1H), 3.68 (s, 3H), 3.29-3.24 (m, 1H), 1.96-1.86 (m, 1H), 1.75-1.65 (m, 1H), 0.98 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 199.0, 163.0, 154.4, 137.0, 135.2, 133.8, 132.9, 131.0, 130.6, 128.4, 128.0, 123.5, 113.5, 41.3, 38.4, 29.2, 26.3, 11.7; HRMS *m/z* (ESI) calcd for $C_{20}H_{19}ClN_2O_2$ $[M+H]^+$ 355.1208, found 355.1208.

1,6,7-trimethyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3al): Following the typical experimental procedure on 0.2 mmol scale, compound **3al** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 41.8 mg; 90% yield; Yellow solid; mp 173.8-174.0 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01-7.98 (m, 2H), 7.53-7.46 (m, 1H), 7.43-7.40 (m, 3H), 7.00 (s, 1H), 4.13-4.07 (m, 1H), 3.91-3.84 (m, 1H), 3.65 (s, 3H), 3.25-3.20 (m, 1H), 2.33 (s, 3H), 2.24 (s, 3H), 1.99-1.88 (m, 1H), 1.77-1.67 (m, 1H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 198.9, 161.1, 154.6, 138.9, 137.0, 132.6, 131.8, 130.8, 130.7, 129.5, 128.2, 127.9, 113.9, 41.2, 38.2, 28.8, 26.1, 20.2, 18.8, 11.6; HRMS *m/z* (ESI) calcd for $C_{22}H_{24}N_2O_2$ $[M+Na]^+$ 371.1730, found 371.1733.

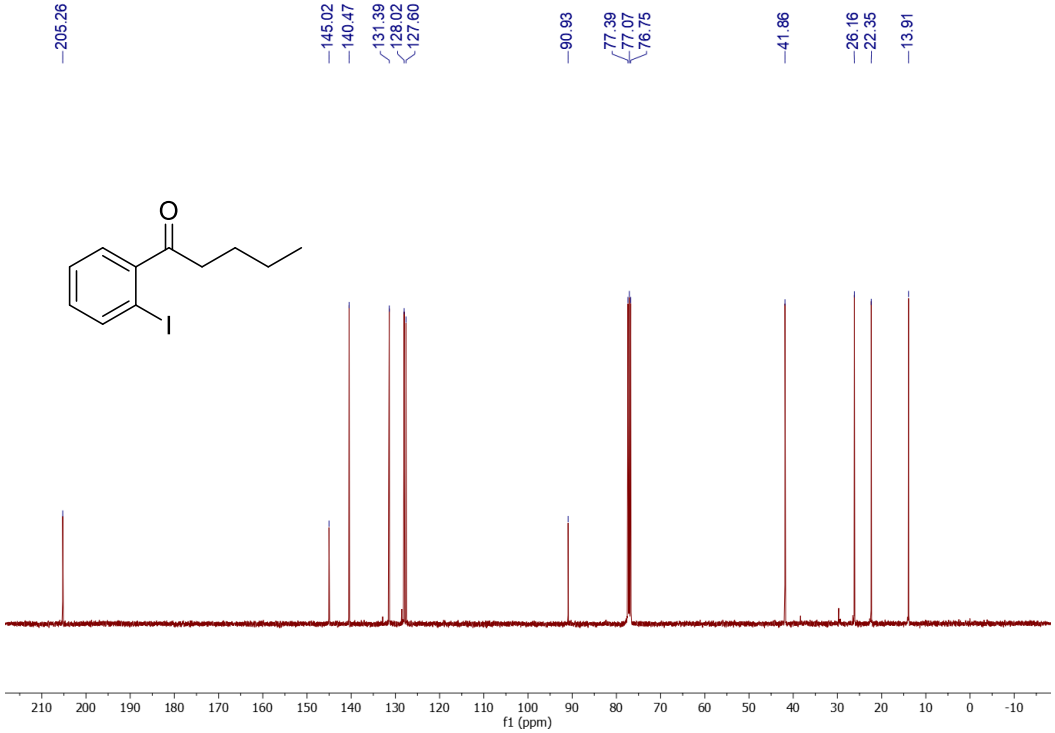
2-(benzo[d]thiazol-2-yl)-3-methyl-1-phenylbutan-1-one (3am): Following the typical experimental procedure on 0.2 mmol scale, compound **3am** was obtained by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1, v/v). 31.9 mg; 54% yield; Yellow solid; mp 160.4-160.8 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.94-7.91 (m, 2H), 7.90-7.88 (m, 1H), 7.85-7.82 (m, 1H), 7.53-7.49 (m, 1H), 7.43-7.38 (m, 3H), 7.33-7.29 (m, 1H), 3.67 (s, 2H), 1.67 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.6, 180.4, 153.2, 137.5, 134.9, 128.0, 122.5, 122.5, 121.5, 121.5, 49.9, 40.0, 29.1, 28.9; HRMS *m/z* (ESI) calcd for $C_{18}H_{17}NOS$ $[M+Na]^+$ 318.0923, found 318.0921.

(C) Spectra

1-(2-iodophenyl)pentan-1-one (1aa)

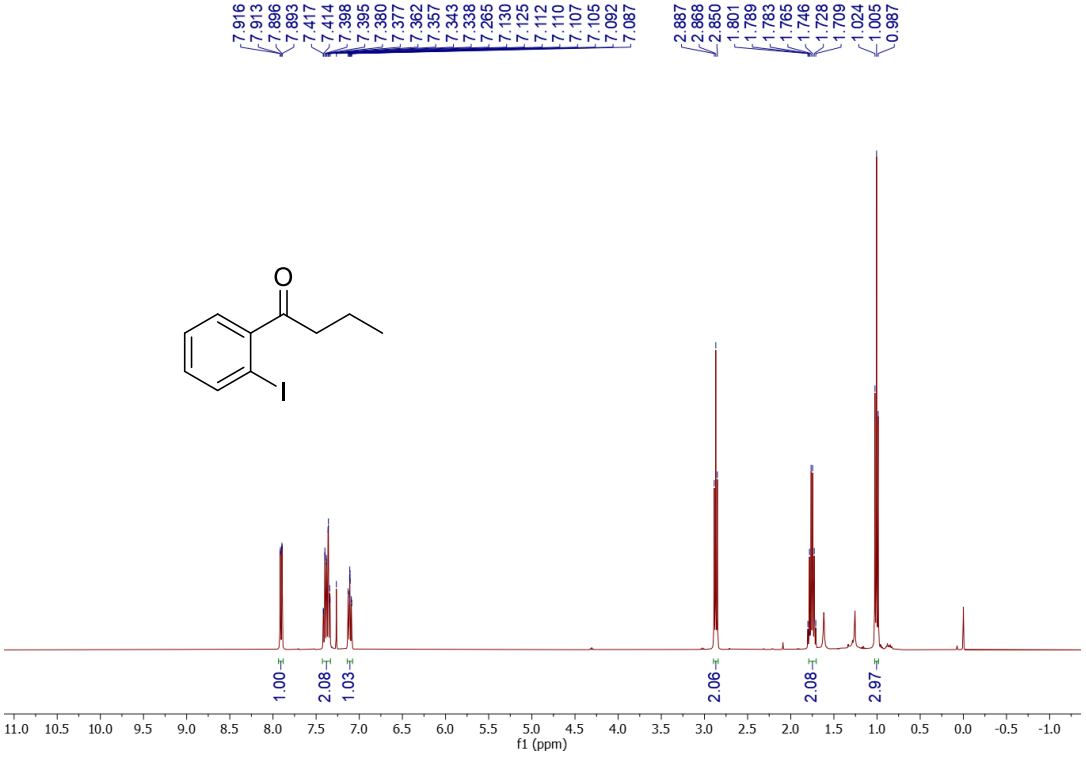


^{1}H NMR (400 MHz, $CDCl_3$)

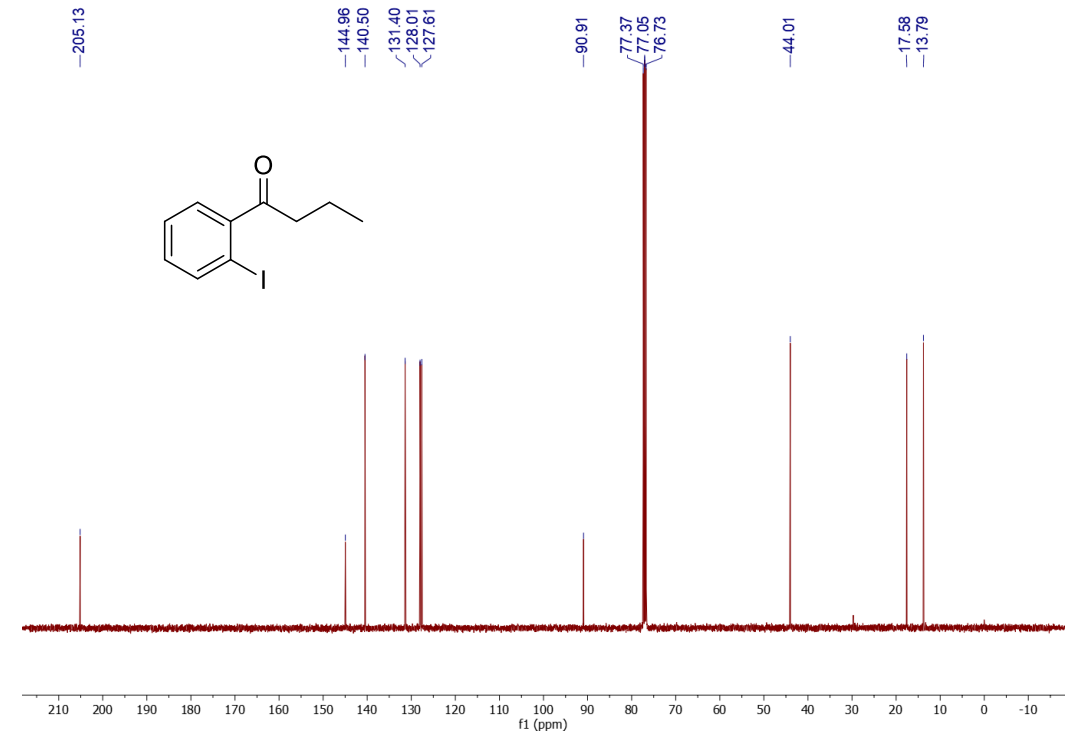


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)butan-1-one (1ba)

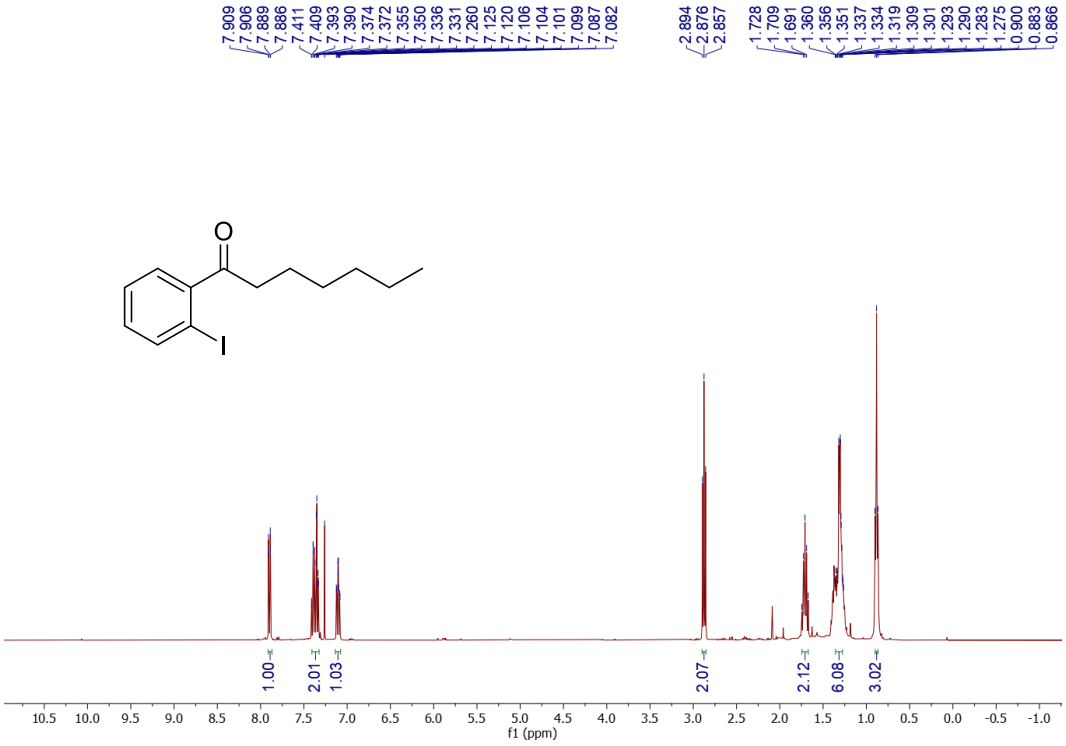


^{1}H NMR (400 MHz, $CDCl_3$)

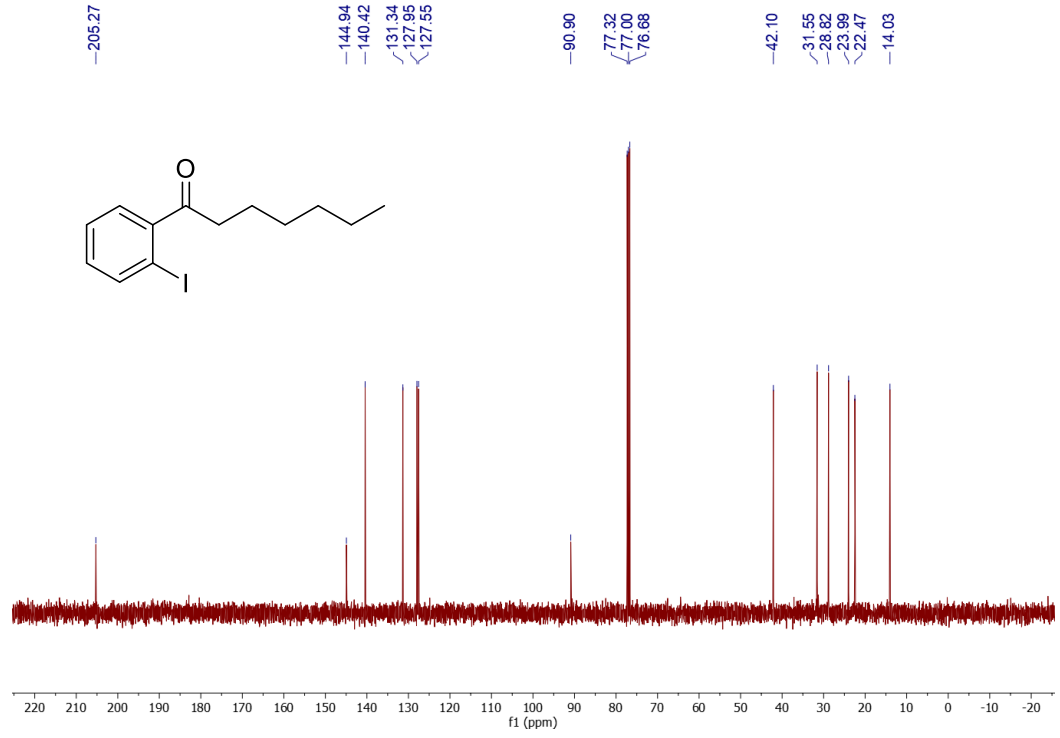


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)heptan-1-one (1ca)

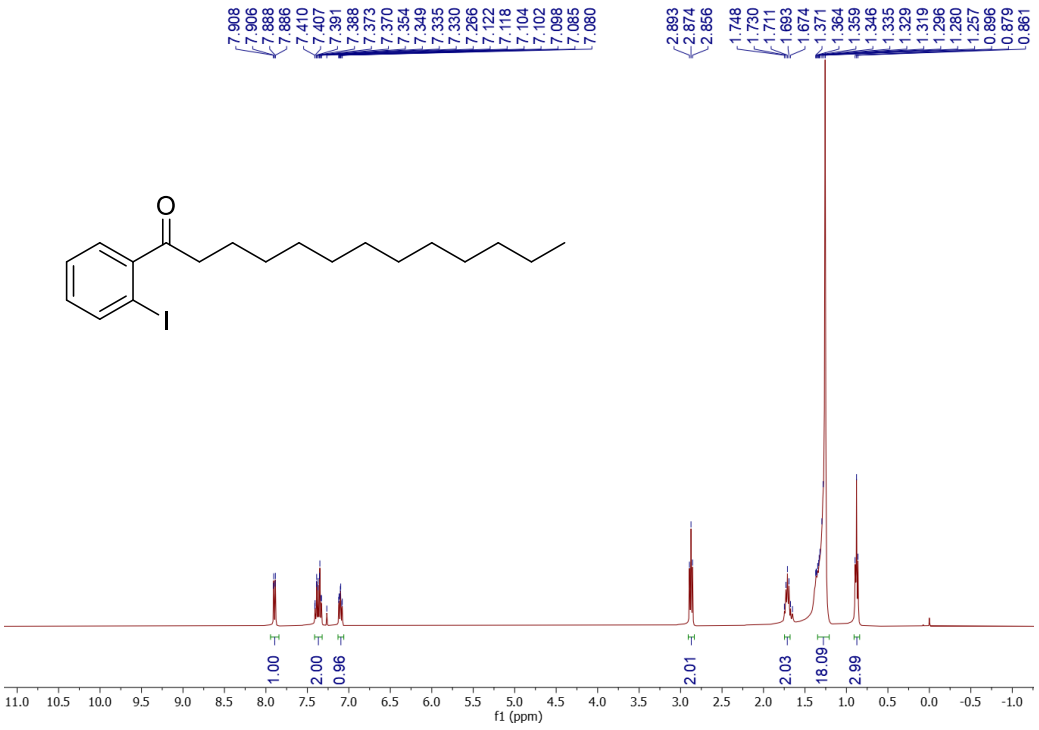


^{1}H NMR (400 MHz, $CDCl_3$)

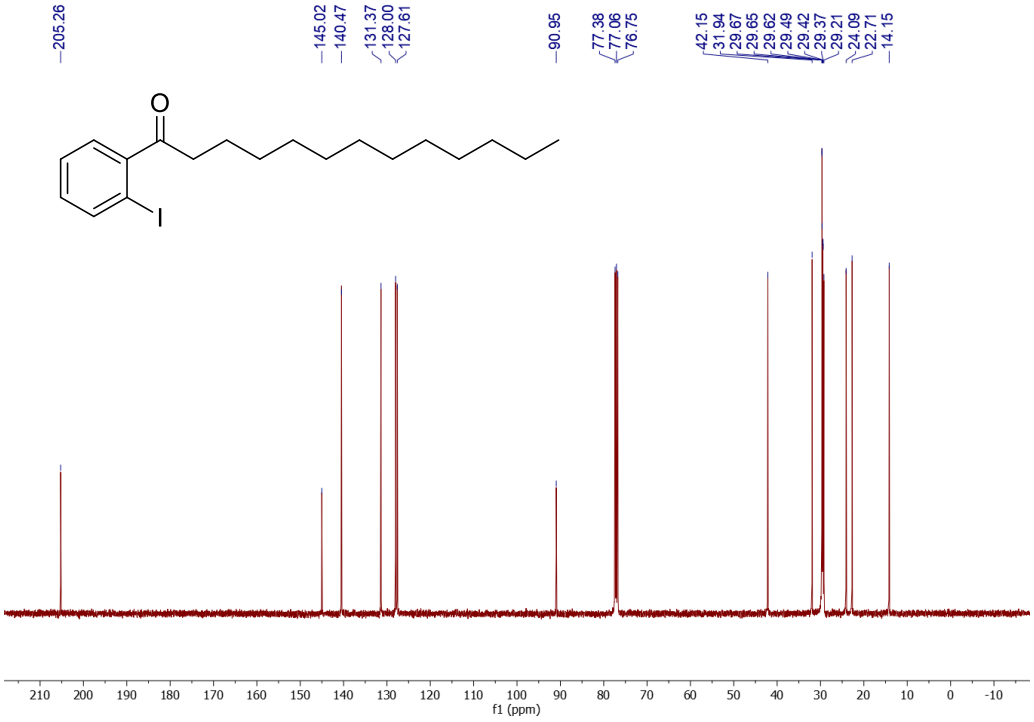


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)tridecan-1-one (1da)

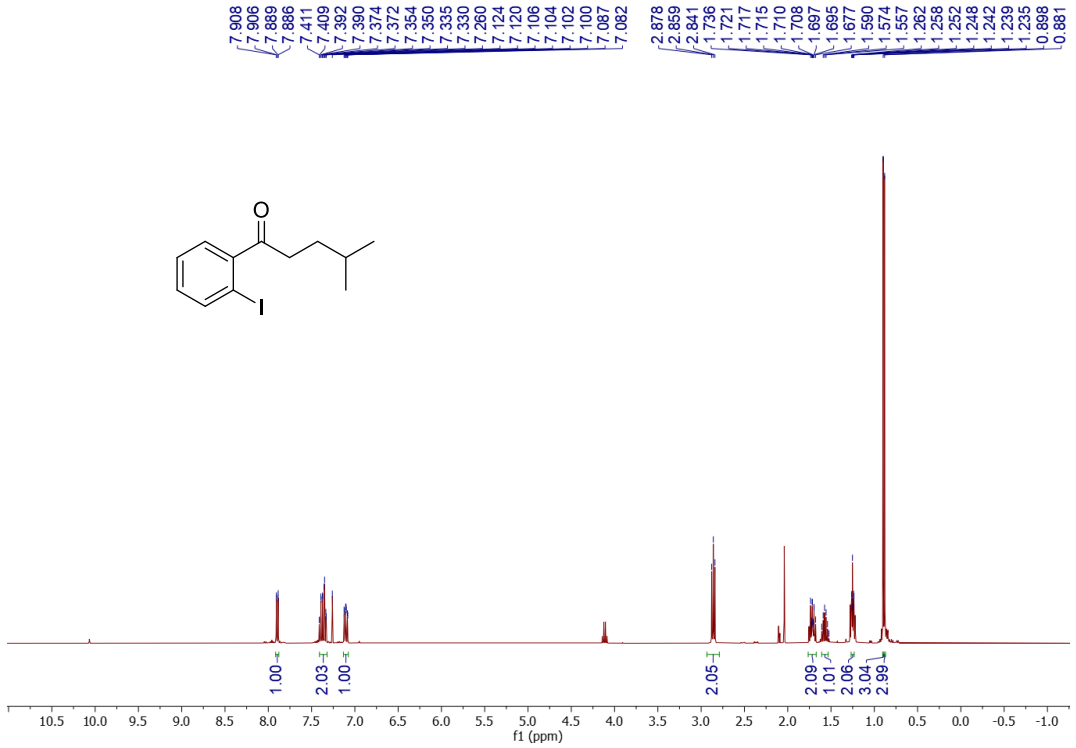


^{1}H NMR (400 MHz, $CDCl_3$)

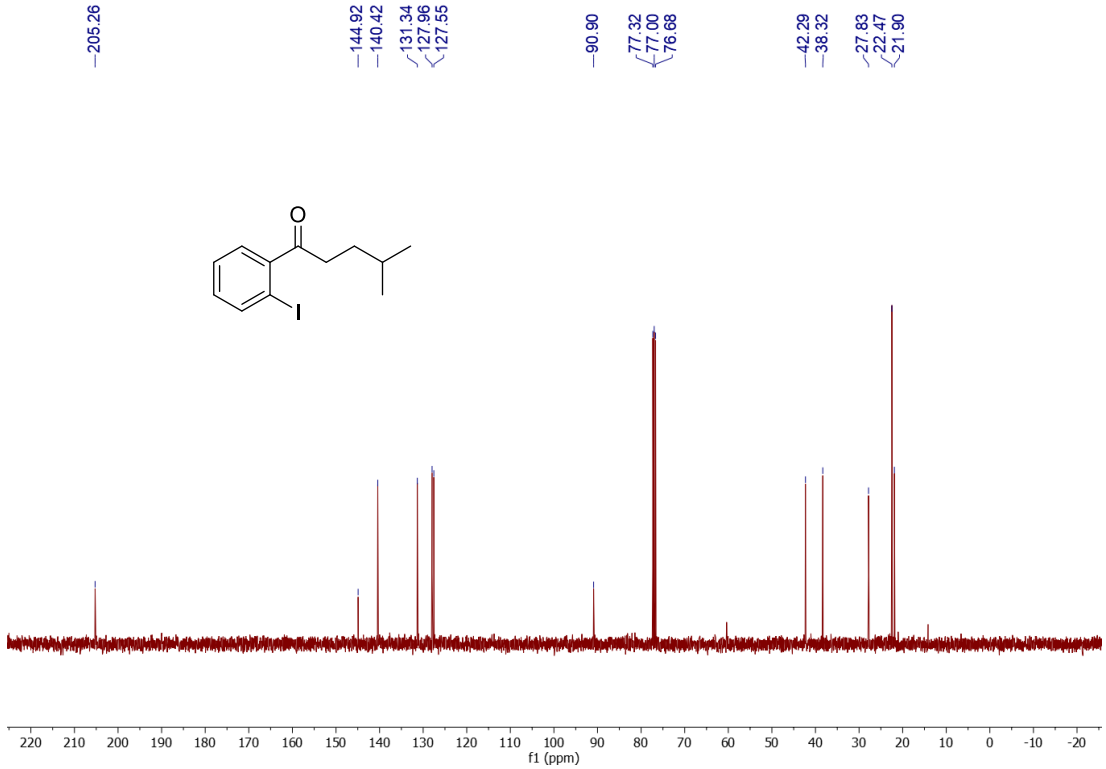


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)-4-methylpentan-1-one (1ea)

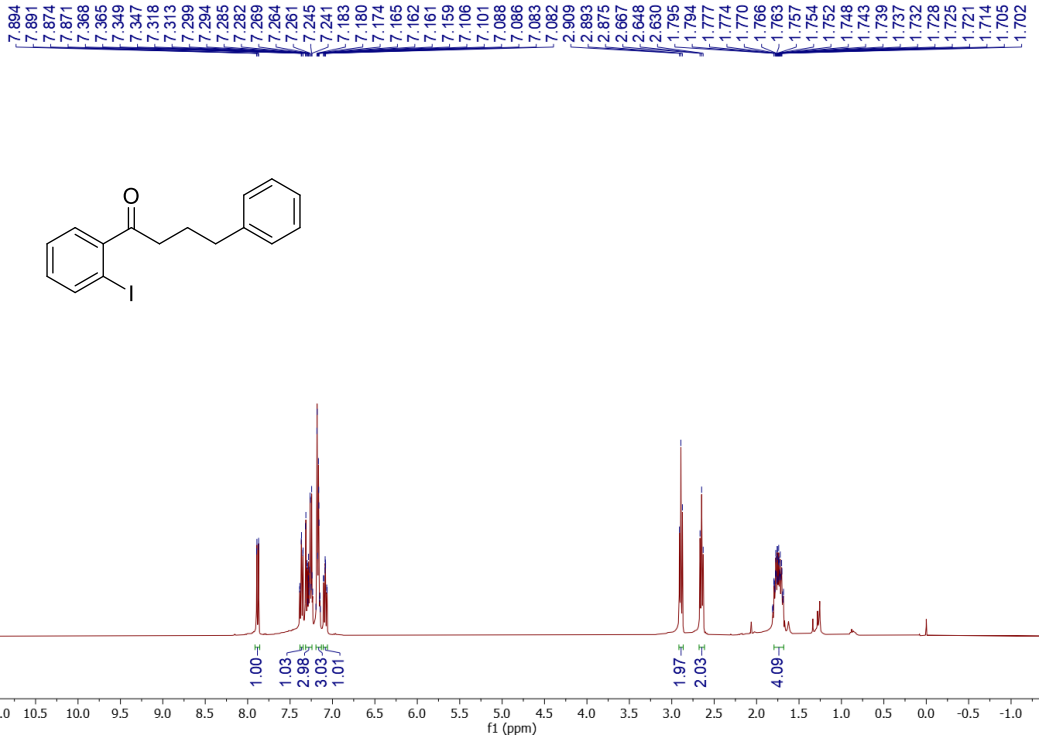


^{1}H NMR (400 MHz, $CDCl_3$)

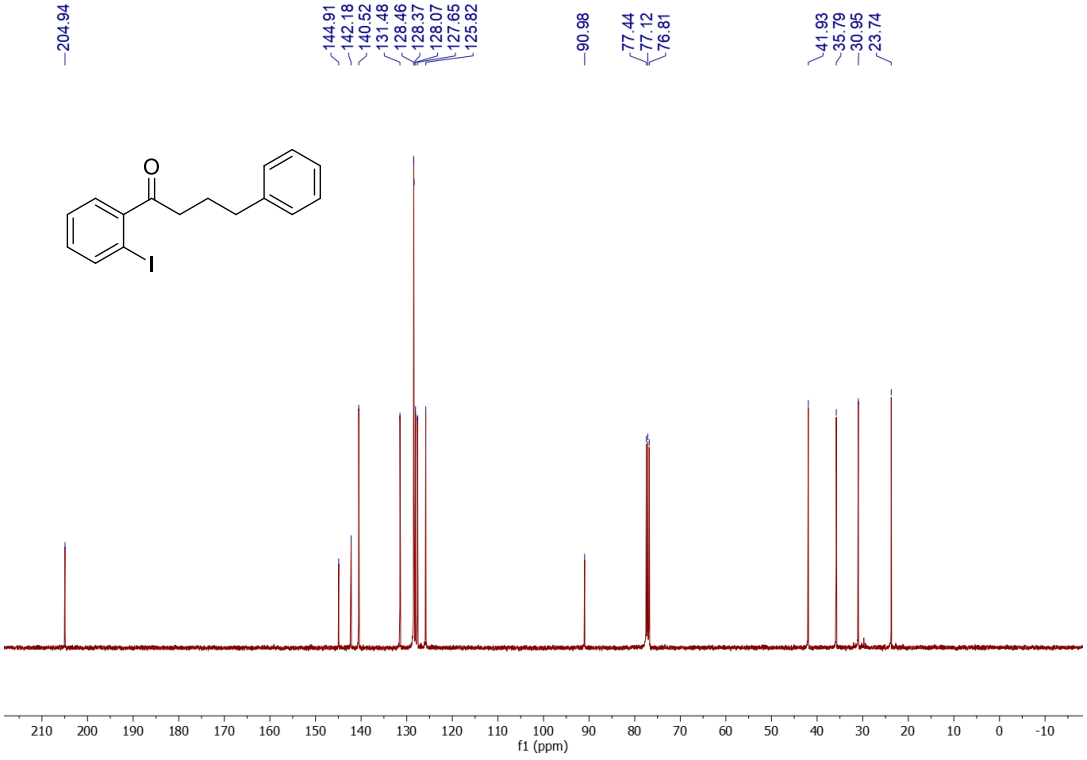


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)-4-phenylbutan-1-one (1fa)

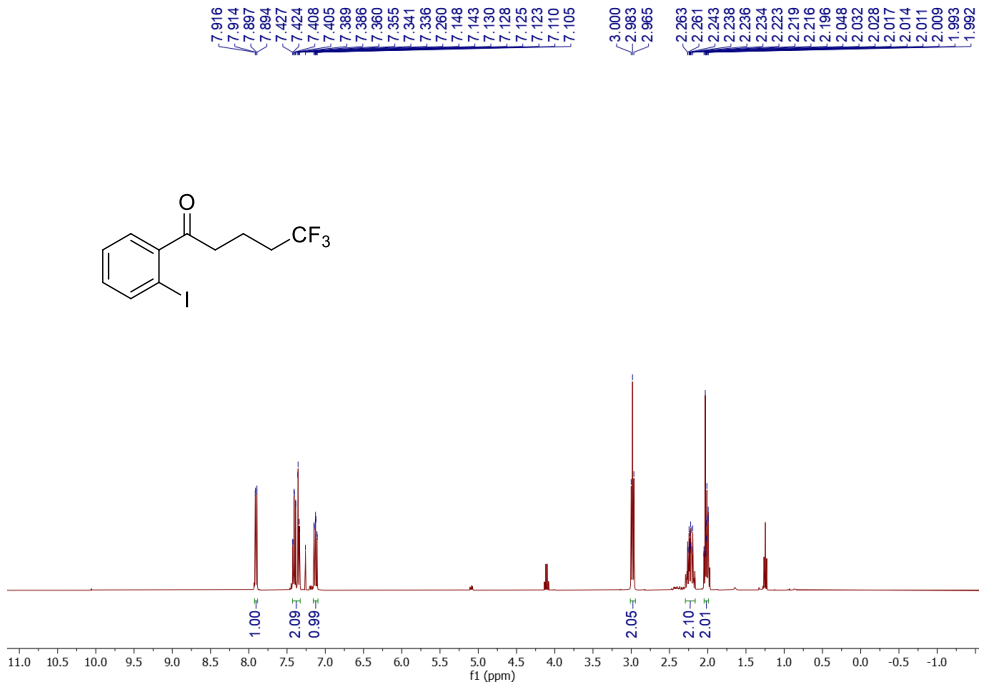


^{1}H NMR (400 MHz, $CDCl_3$)

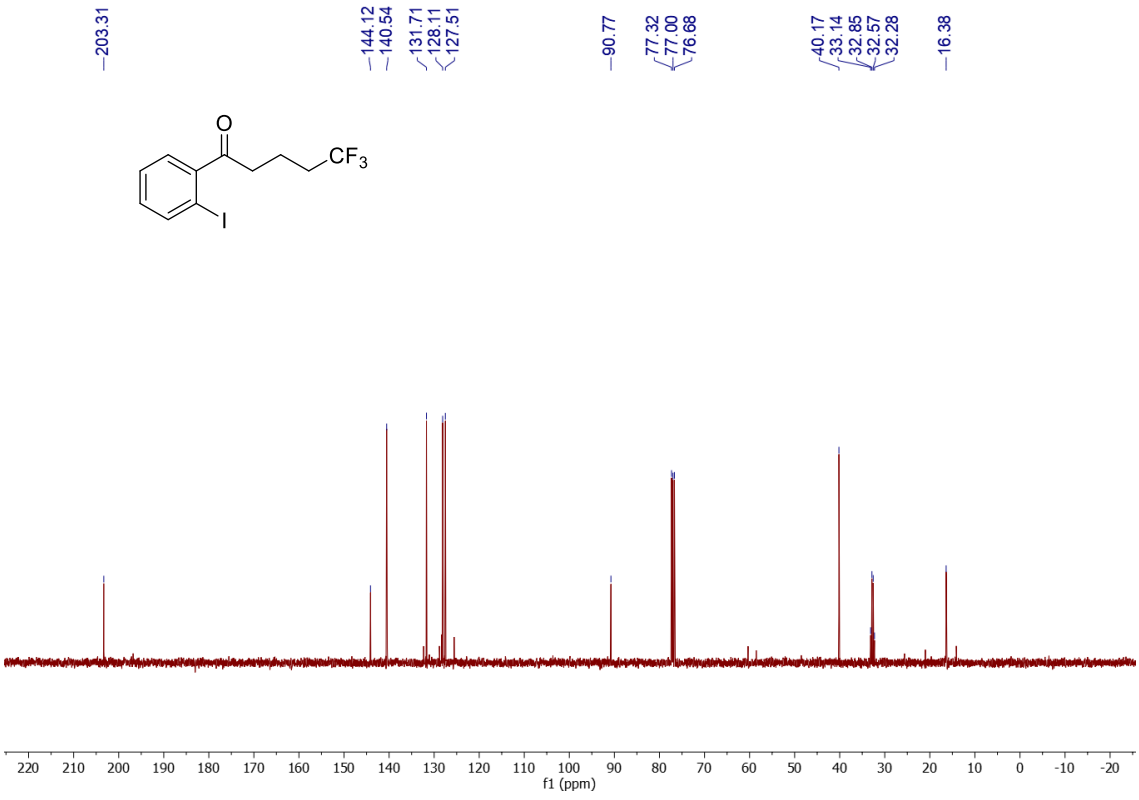


^{13}C NMR (100 MHz, $CDCl_3$)

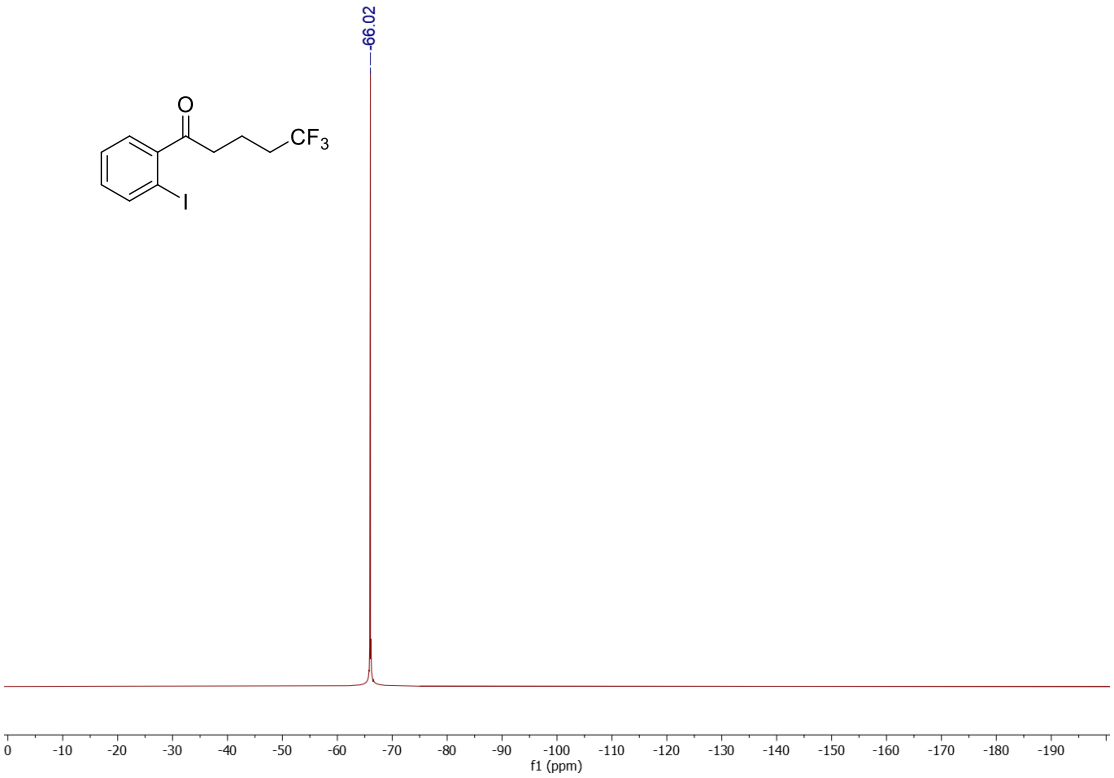
5,5,5-trifluoro-1-(2-iodophenyl)pentan-1-one (1ga)



^{1}H NMR (400 MHz, $CDCl_3$)

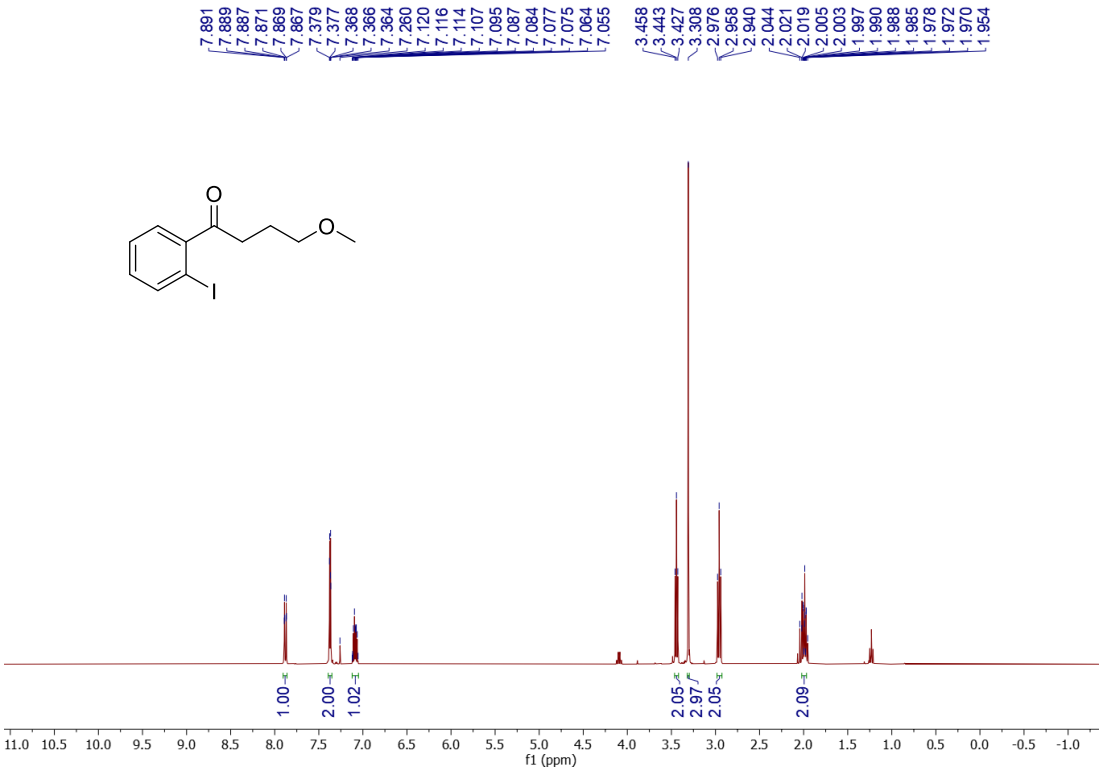


^{13}C NMR (100 MHz, $CDCl_3$)

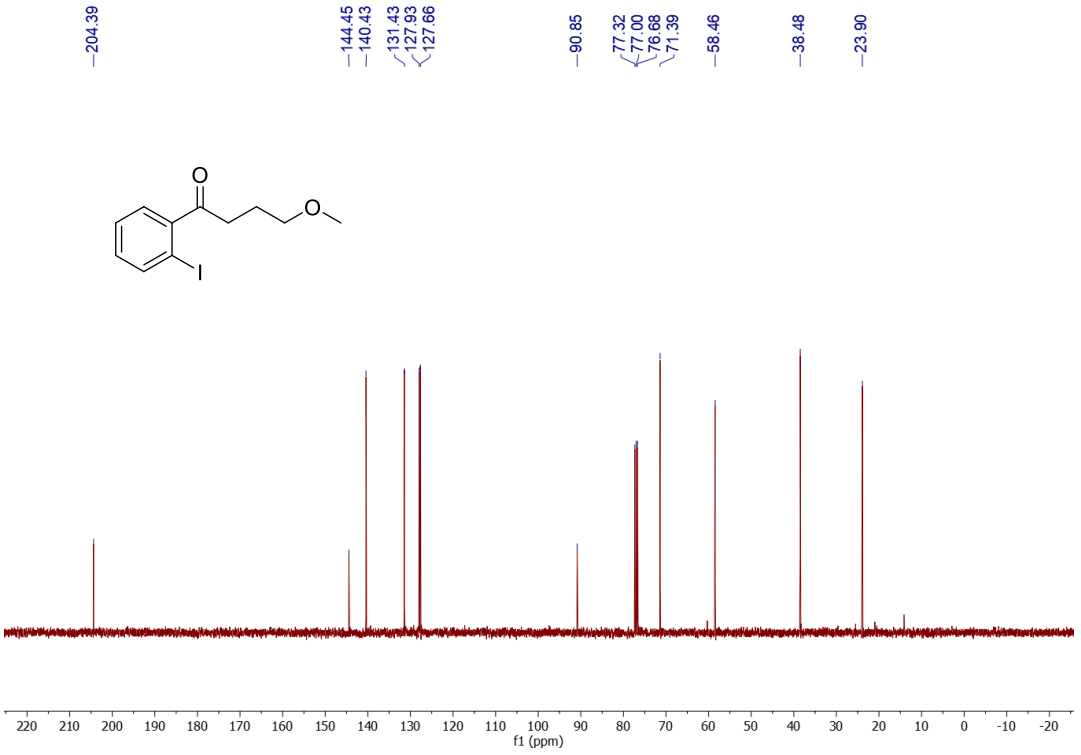


^{19}F NMR (376 MHz, $CDCl_3$)

1-(2-iodophenyl)-4-methoxybutan-1-one (1ha)

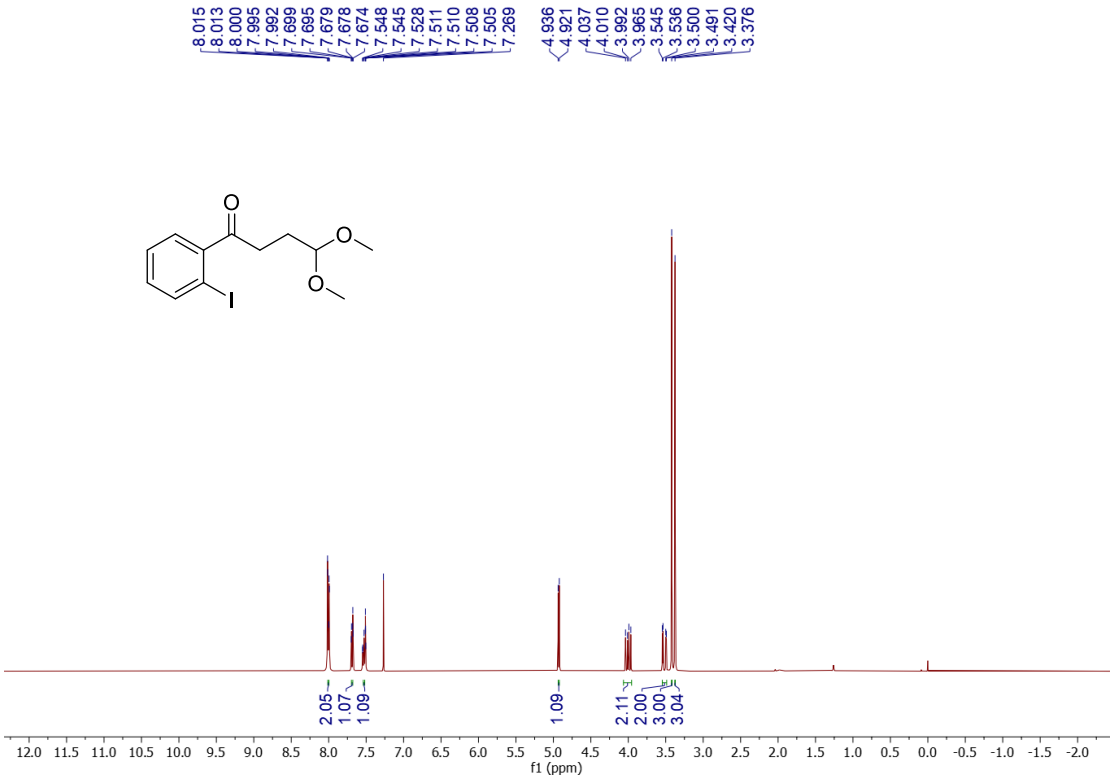


^{1}H NMR (400 MHz, $CDCl_3$)

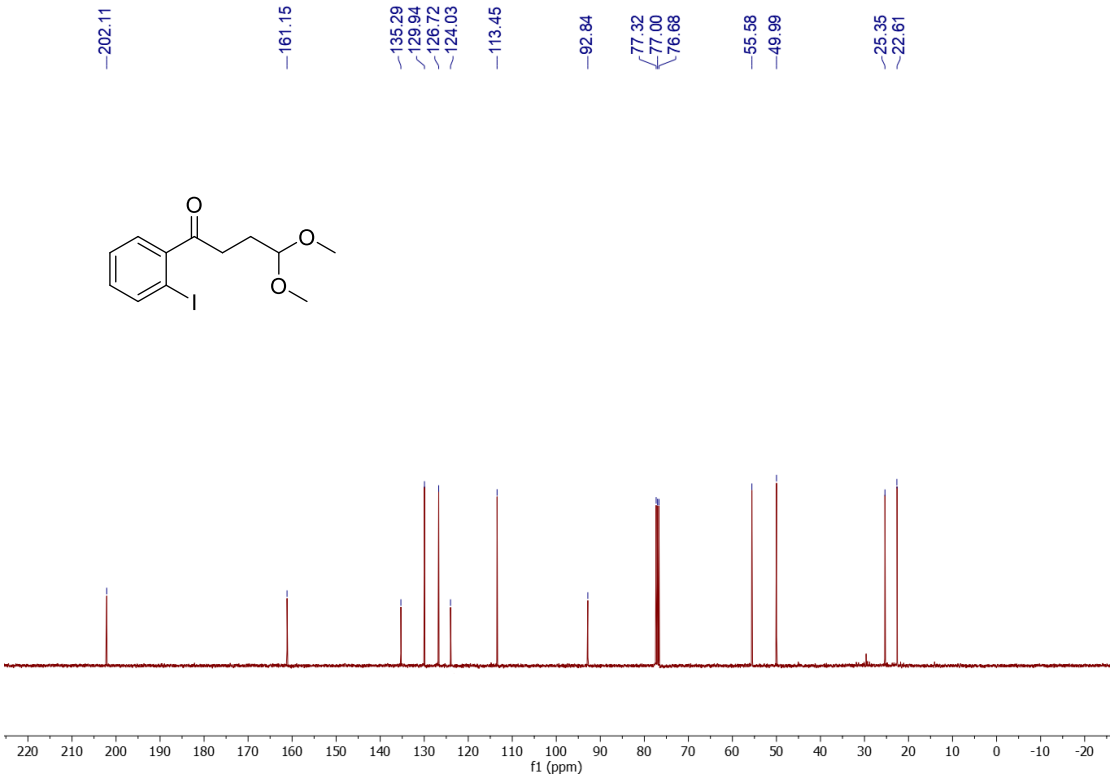


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)-4,4-dimethoxybutan-1-one (1ia)

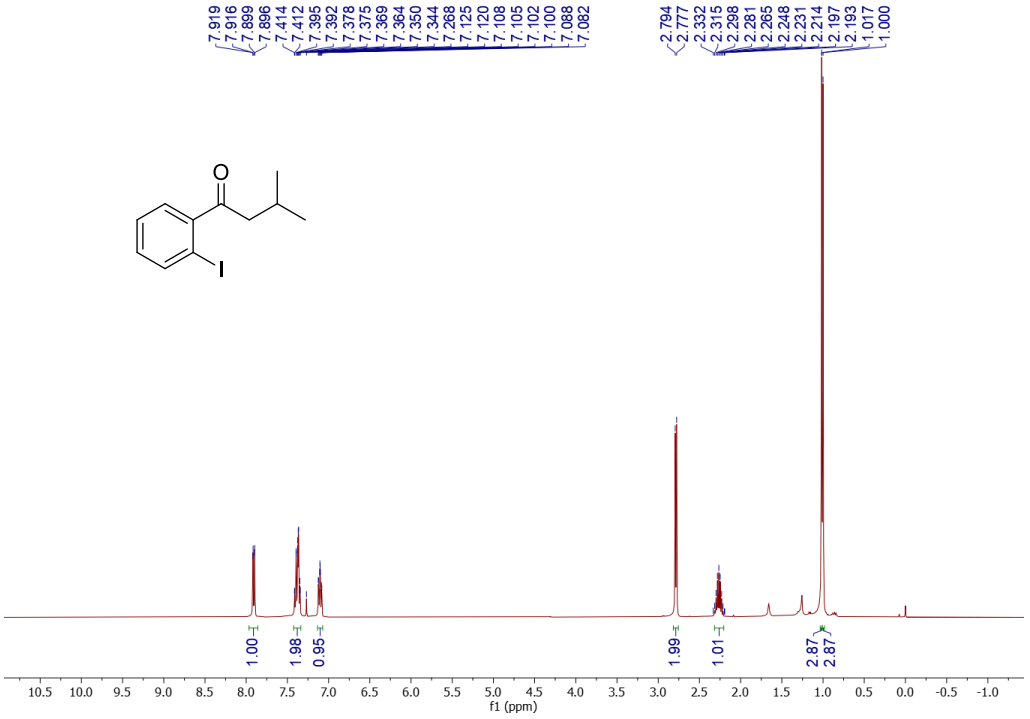


^{1}H NMR (400 MHz, $CDCl_3$)

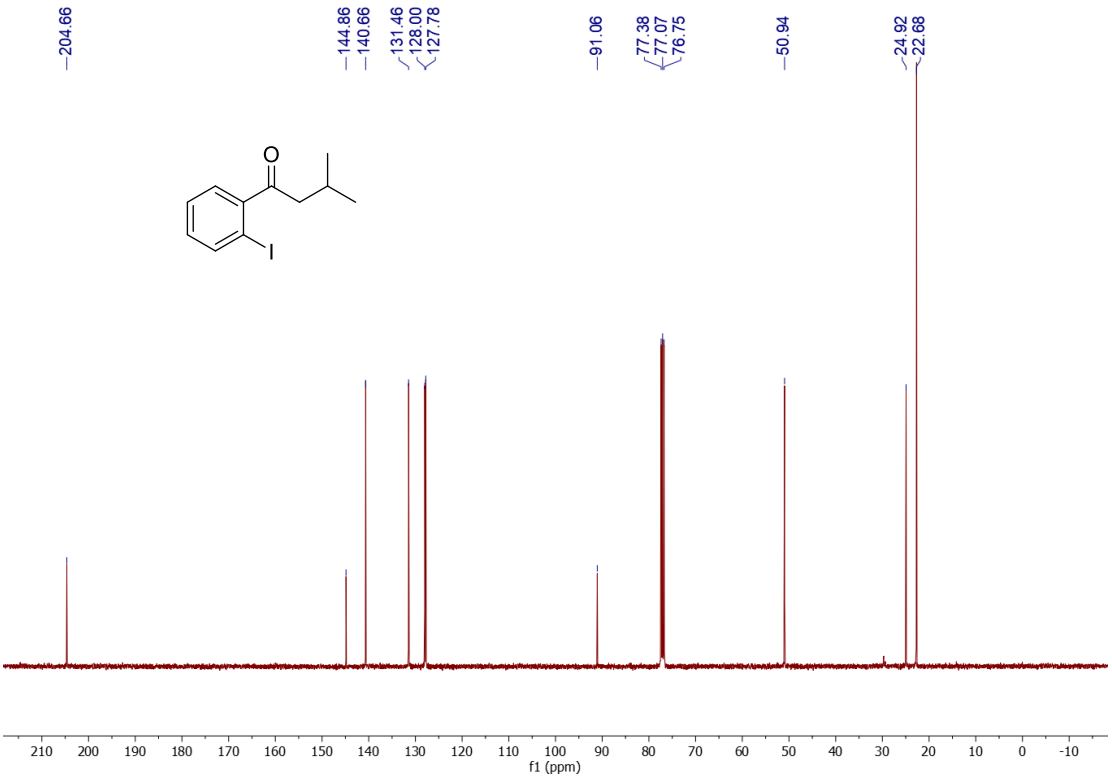


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodophenyl)-3-methylbutan-1-one (1ja)

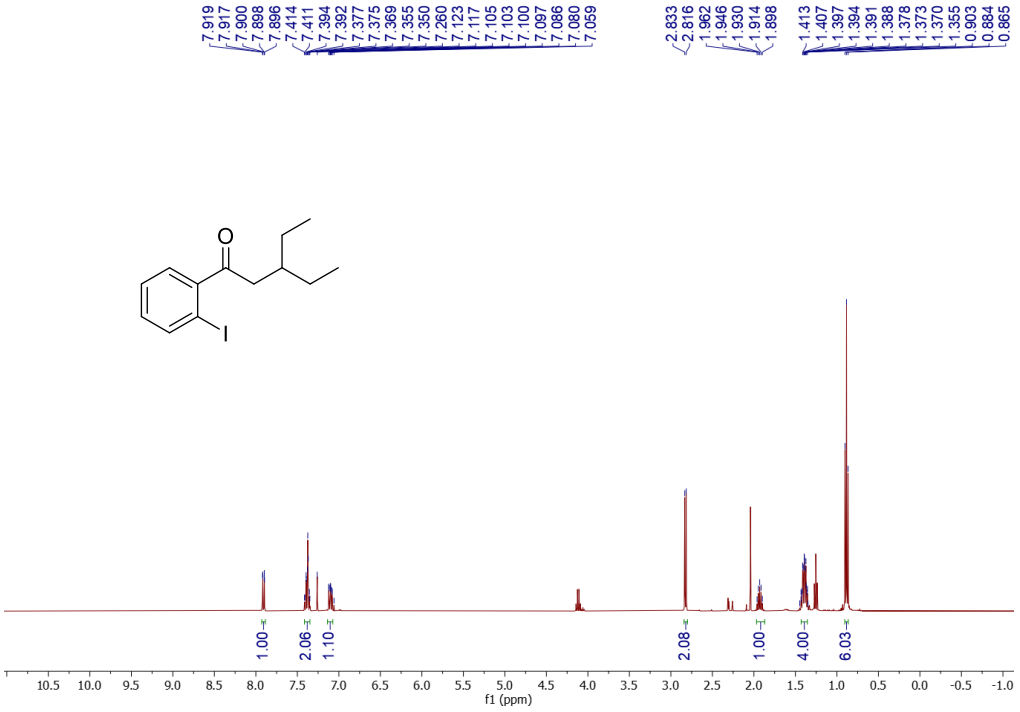


^{1}H NMR (400 MHz, $CDCl_3$)

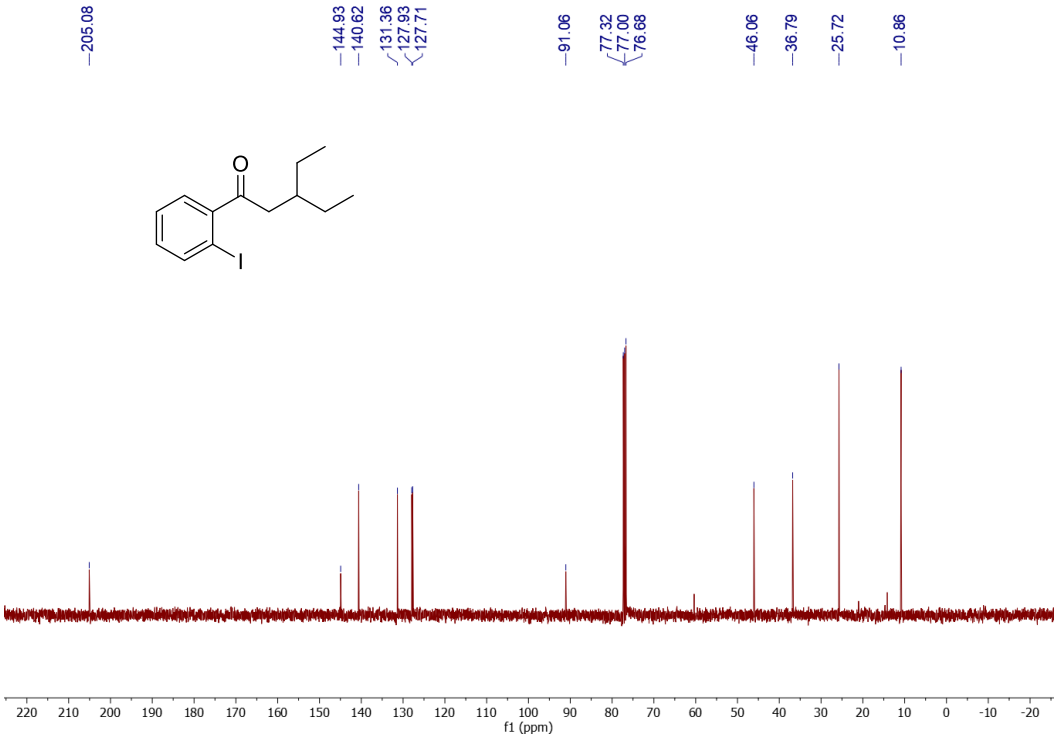


^{13}C NMR (100 MHz, $CDCl_3$)

3-ethyl-1-(2-iodophenyl)pentan-1-one (1ka)

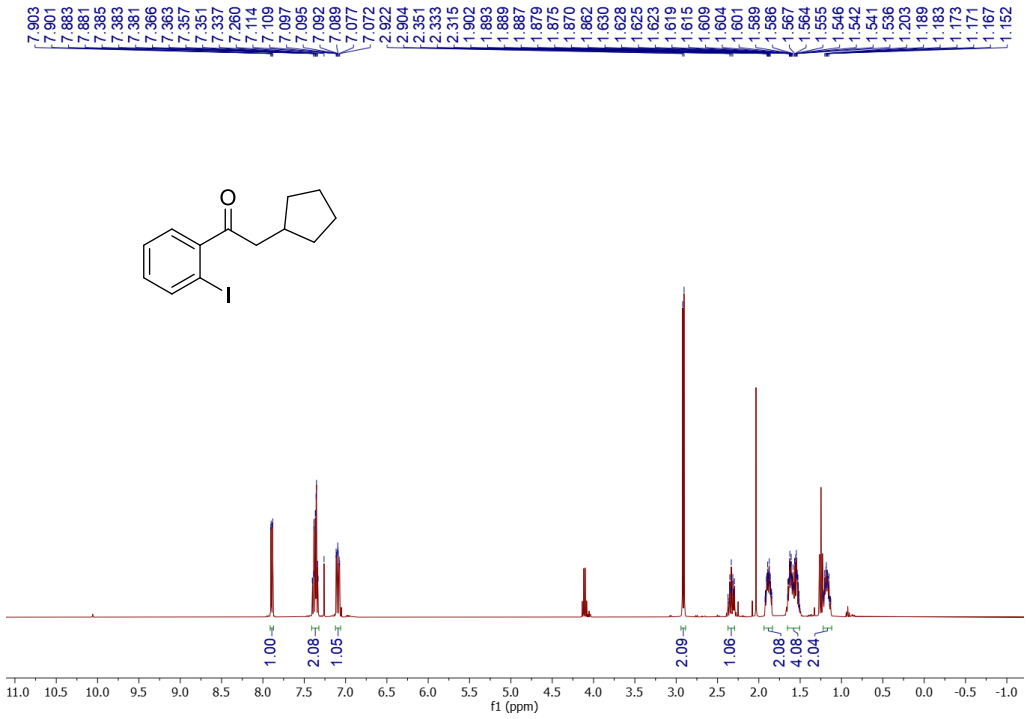


^{1}H NMR (400 MHz, $CDCl_3$)

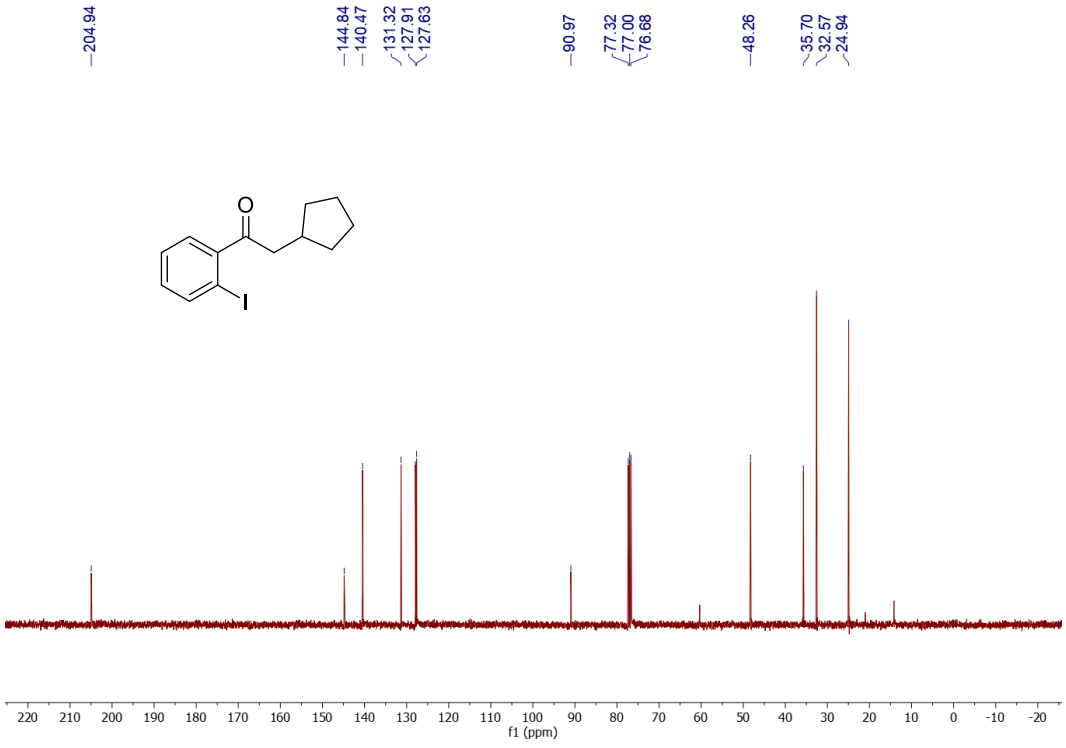


^{13}C NMR (100 MHz, $CDCl_3$)

2-cyclopentyl-1-(2-iodophenyl)ethan-1-one (1la)

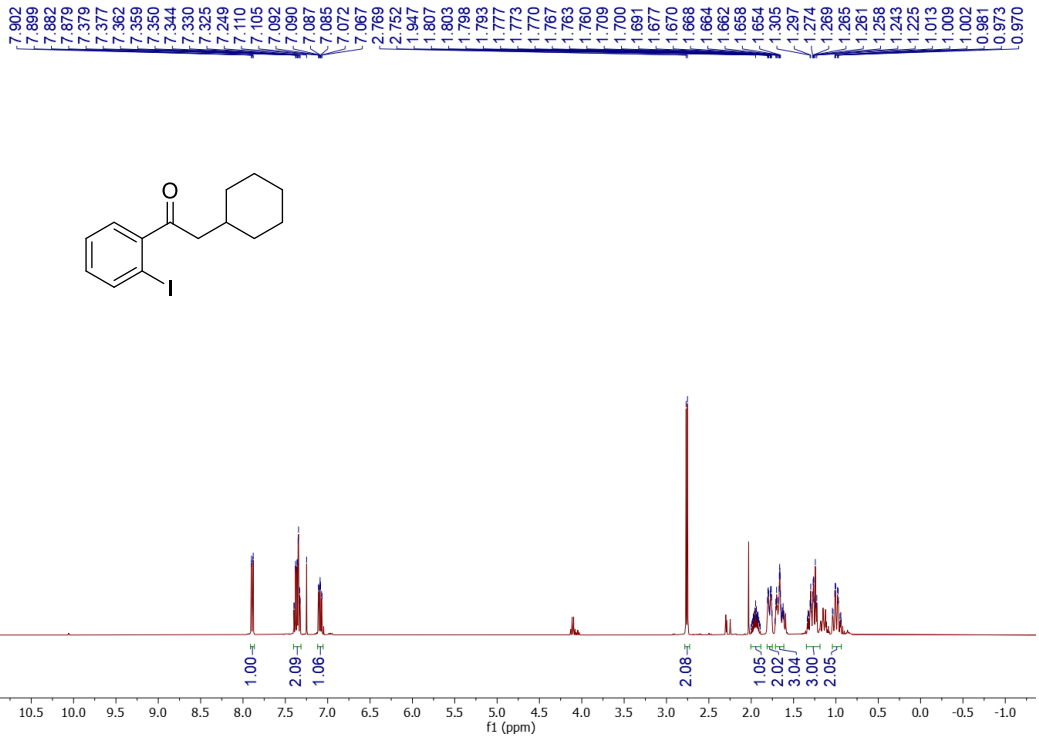


^{1}H NMR (400 MHz, $CDCl_3$)

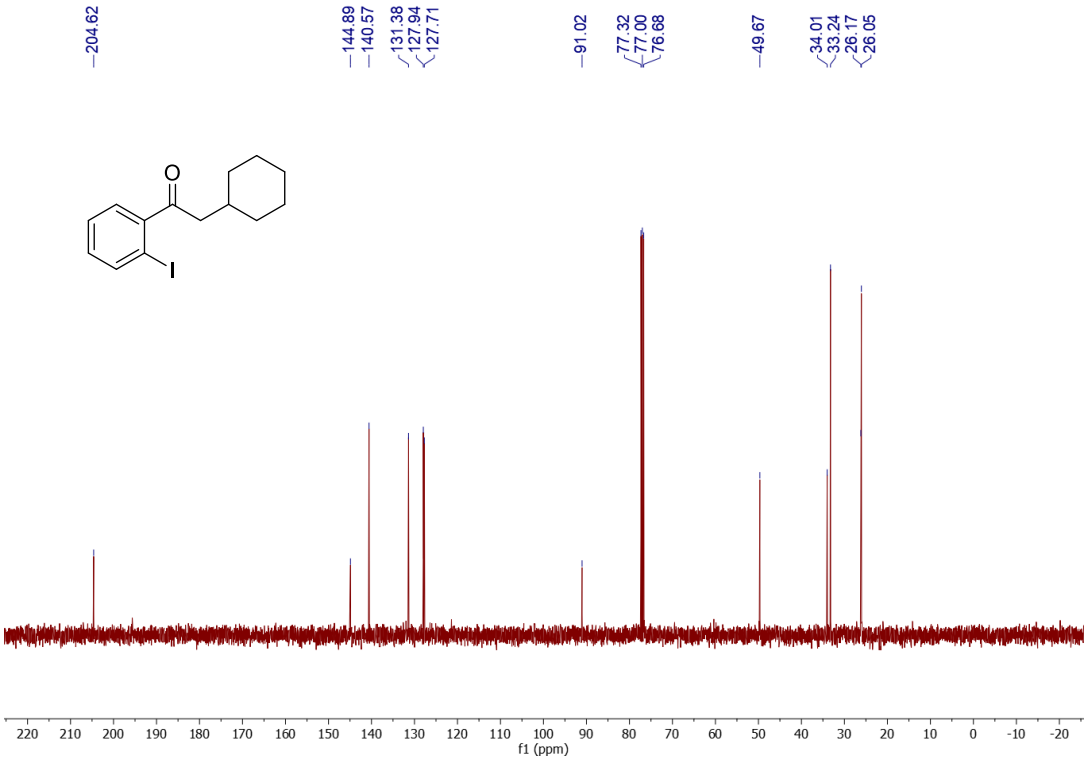


^{13}C NMR (100 MHz, $CDCl_3$)

2-cyclohexyl-1-(2-iodophenyl)ethan-1-one (1ma)

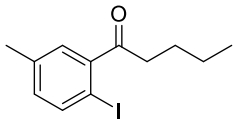


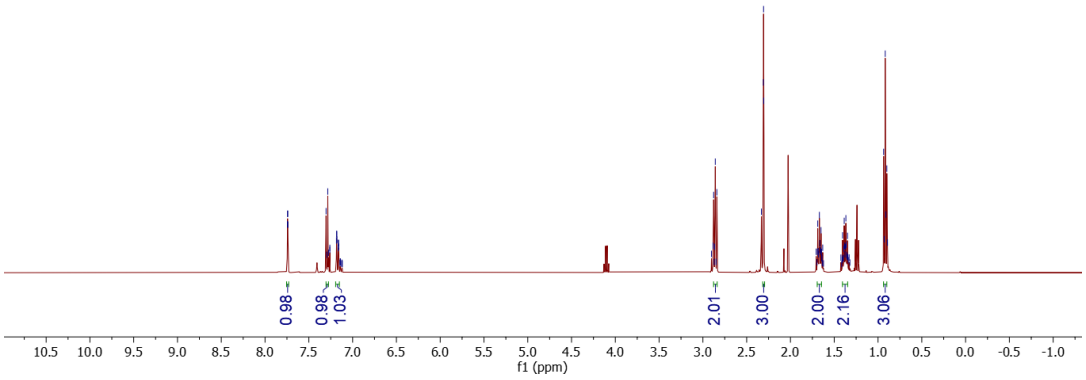
^{1}H NMR (400 MHz, $CDCl_3$)



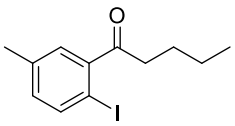
^{13}C NMR (100 MHz, $CDCl_3$)

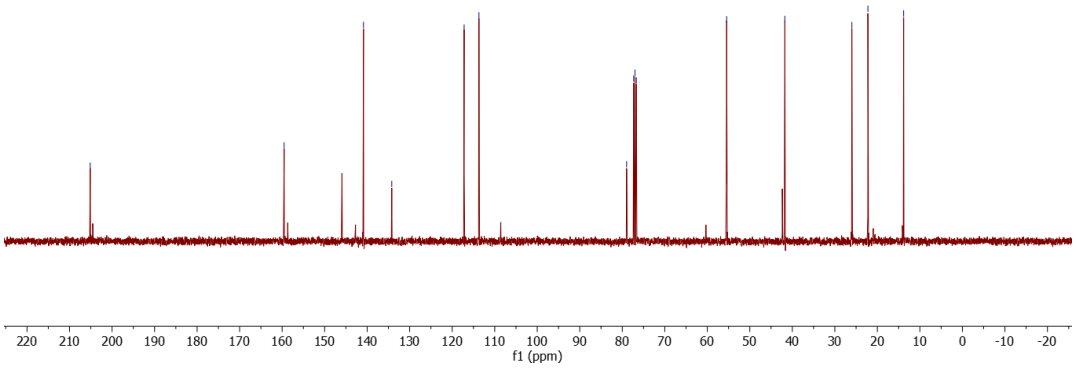
1-(2-iodo-5-methylphenyl)pentan-1-one (1na)





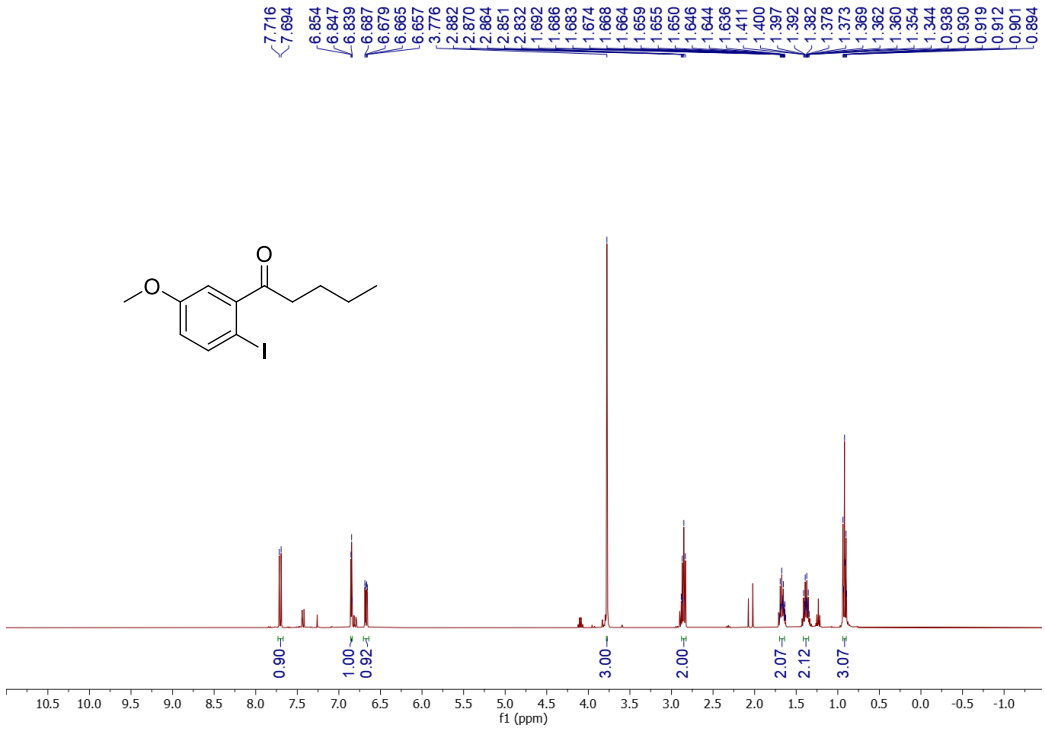
^{1}H NMR (400 MHz, $CDCl_3$)



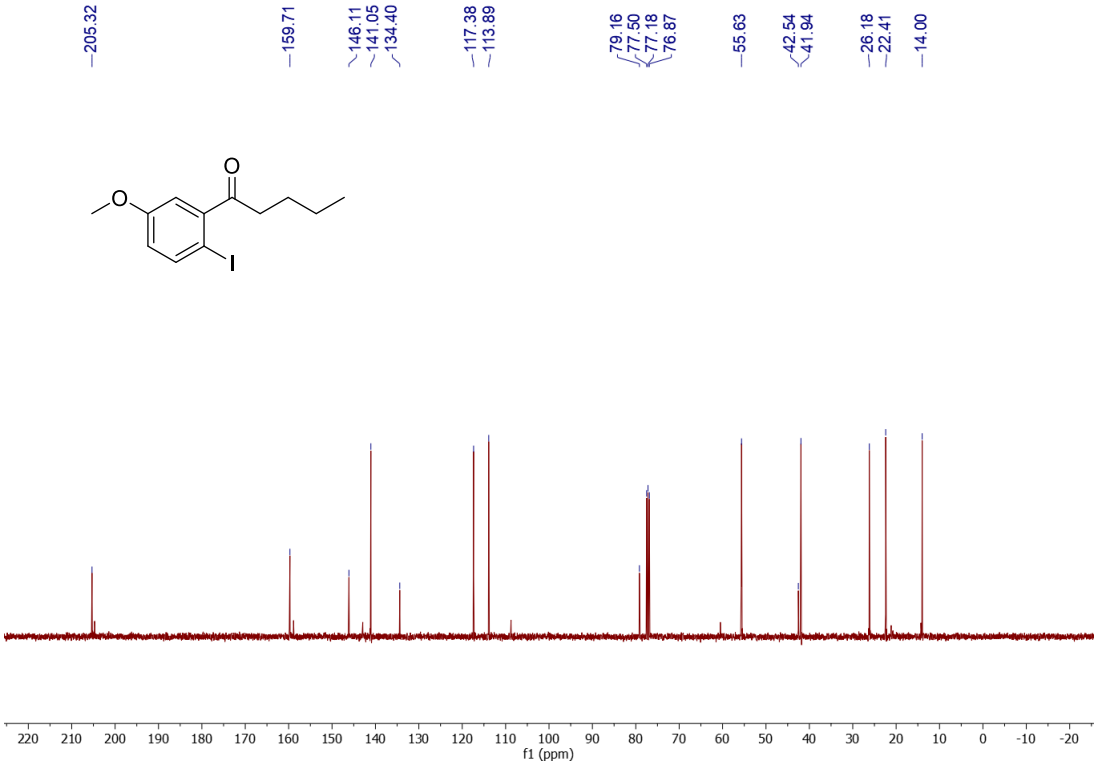


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodo-5-methoxyphenyl)pentan-1-one (1oa)

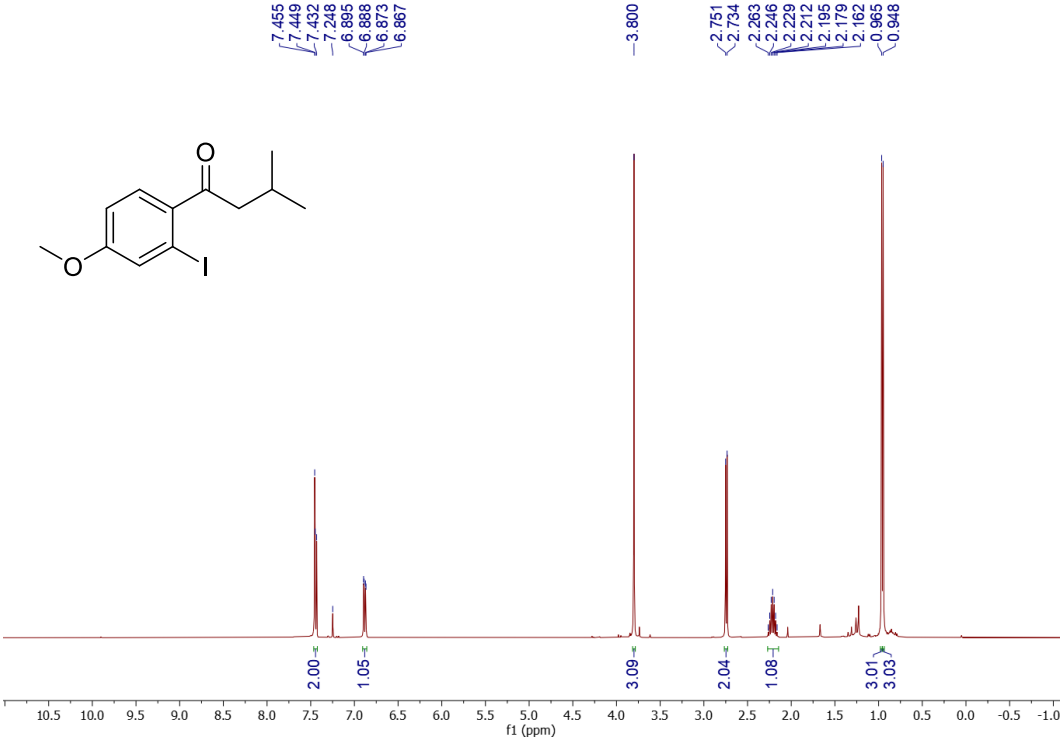


^{1}H NMR (400 MHz, $CDCl_3$)

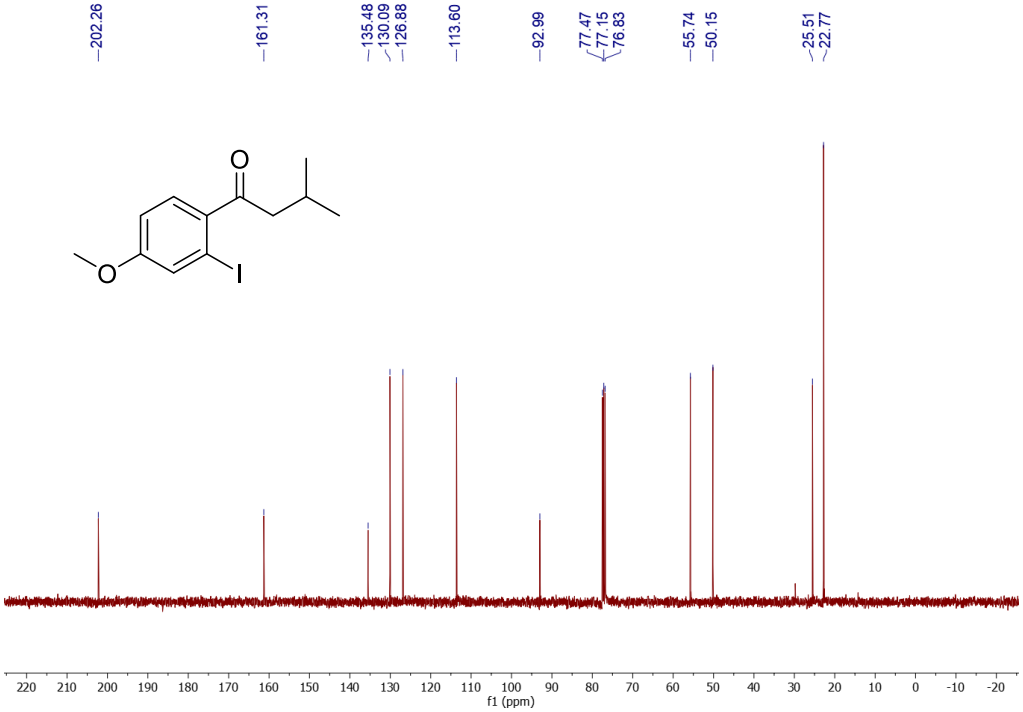


^{13}C NMR (100 MHz, $CDCl_3$)

1-(2-iodo-4-methoxyphenyl)-3-methylbutan-1-one (1pa)

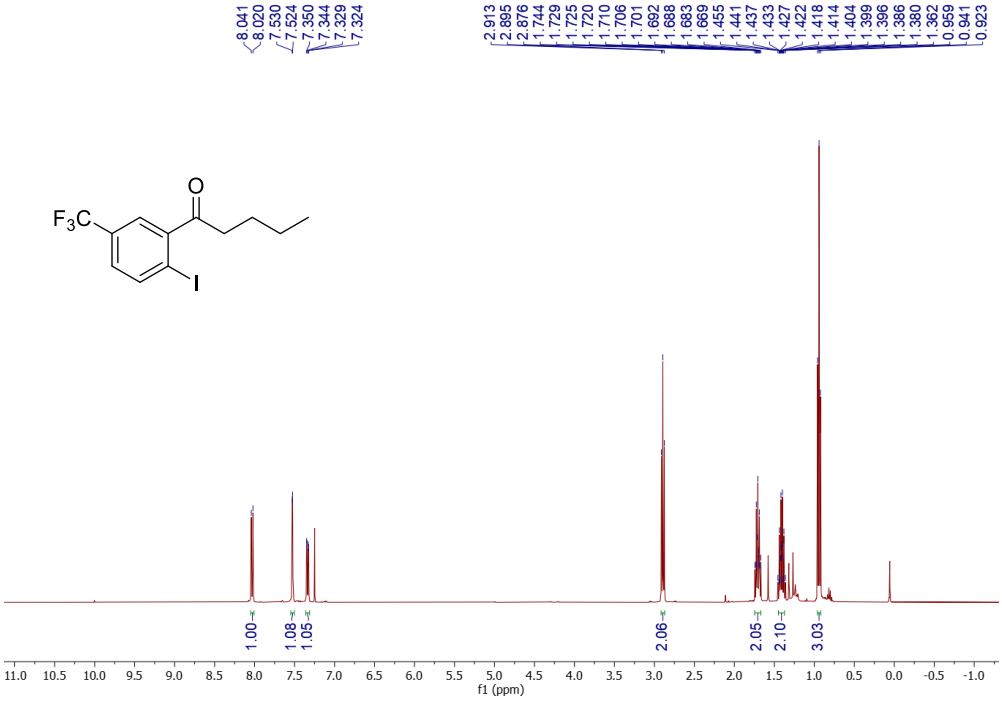


^{1}H NMR (400 MHz, $CDCl_3$)

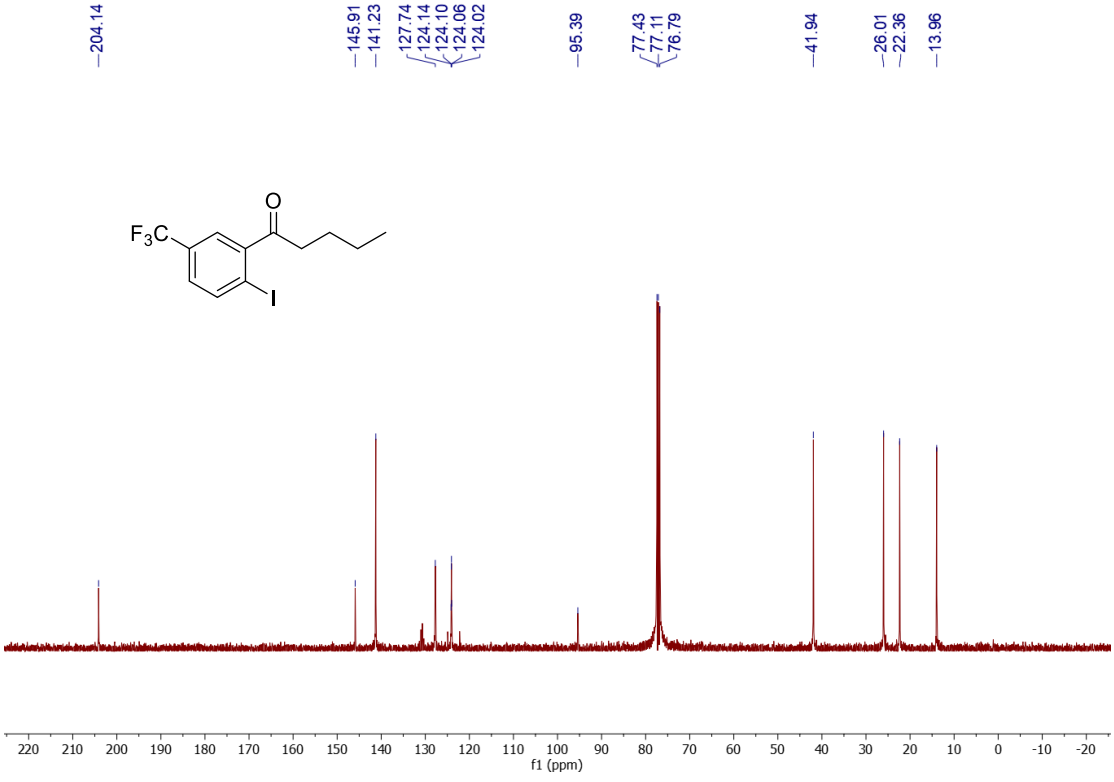


^{13}C NMR (100 MHz, $CDCl_3$)

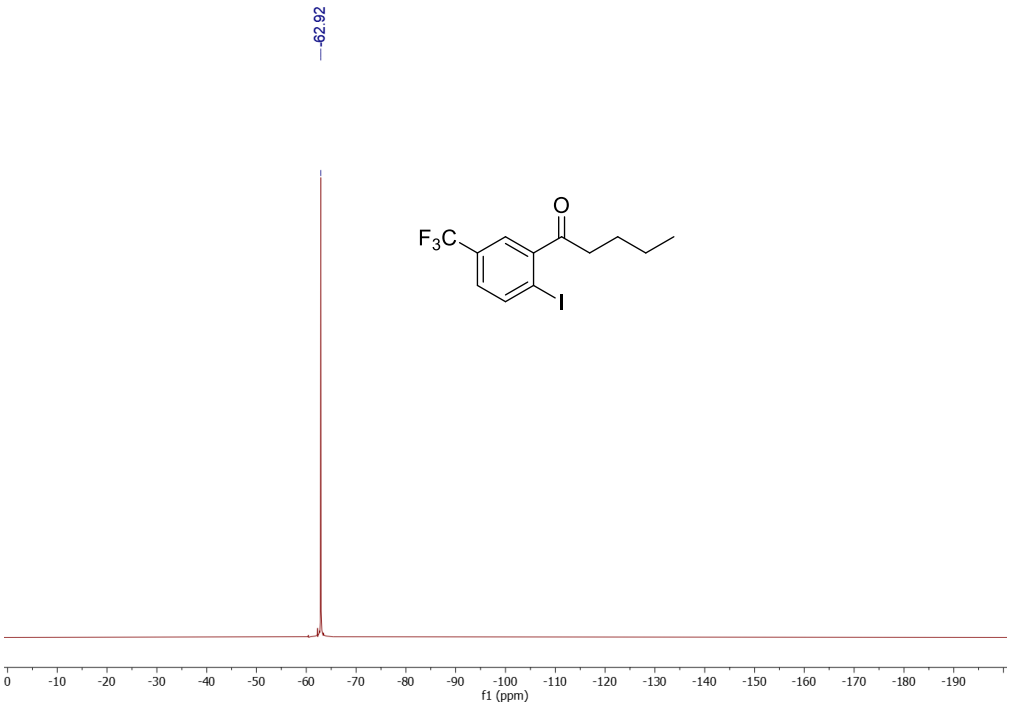
1-(2-iodo-5-(trifluoromethyl)phenyl)pentan-1-one (1qa)



^{1}H NMR (400 MHz, $CDCl_3$)

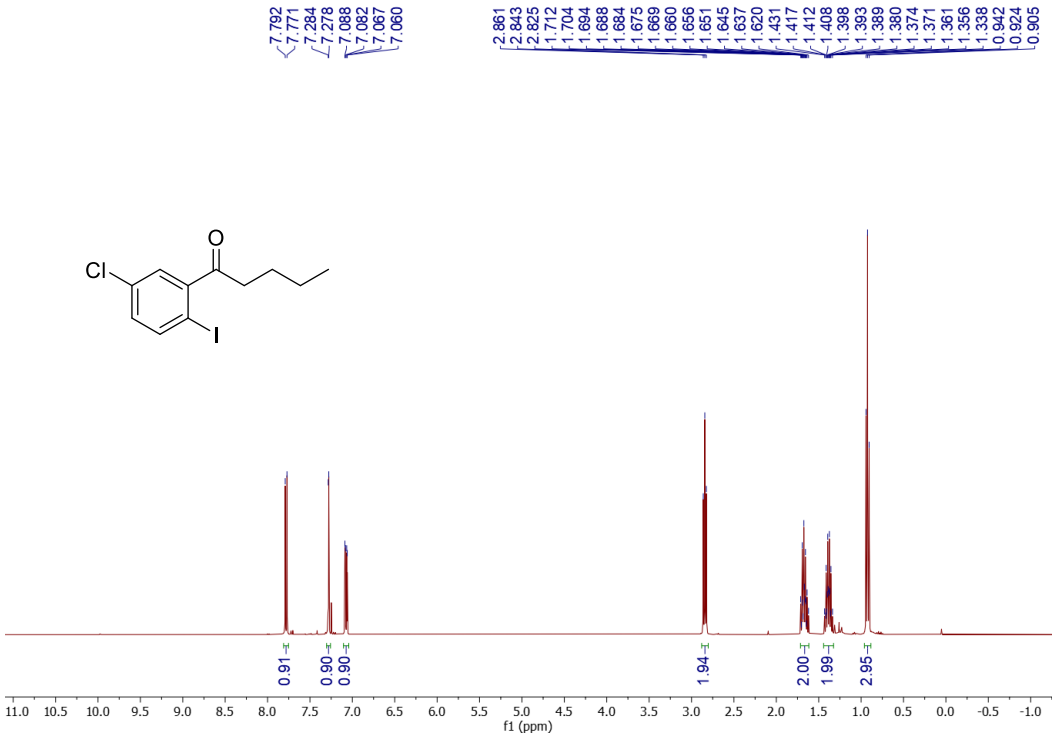


^{13}C NMR (100 MHz, $CDCl_3$)

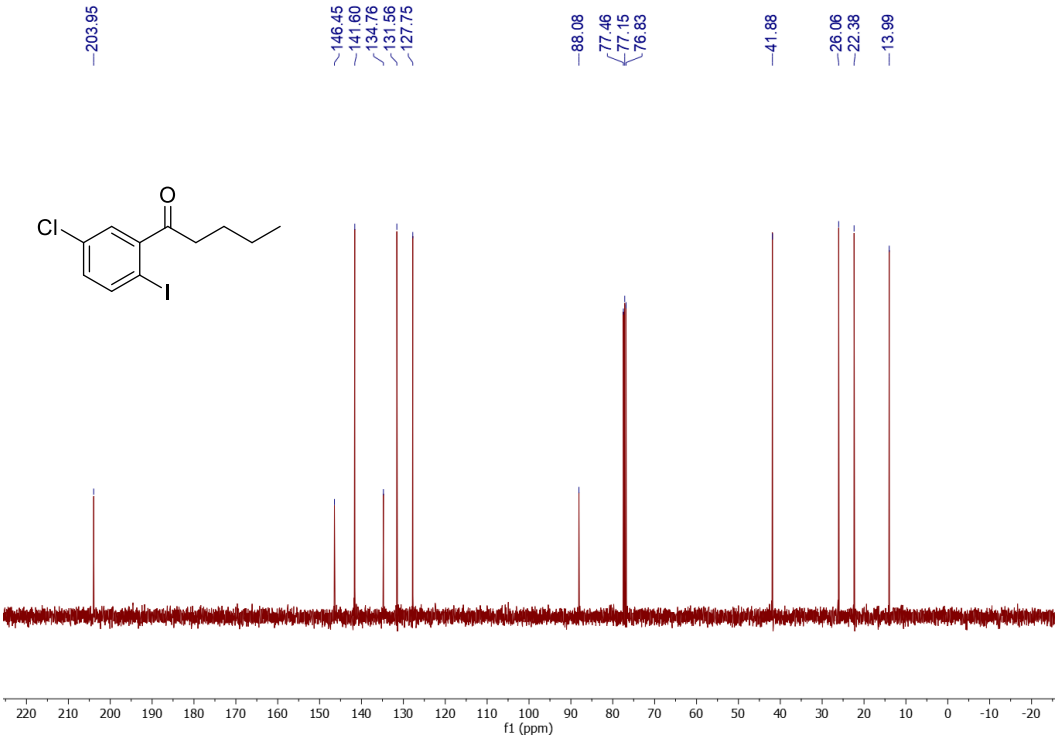


^{19}F NMR (376 MHz, $CDCl_3$)

1-(5-chloro-2-iodophenyl)pentan-1-one (1ra)

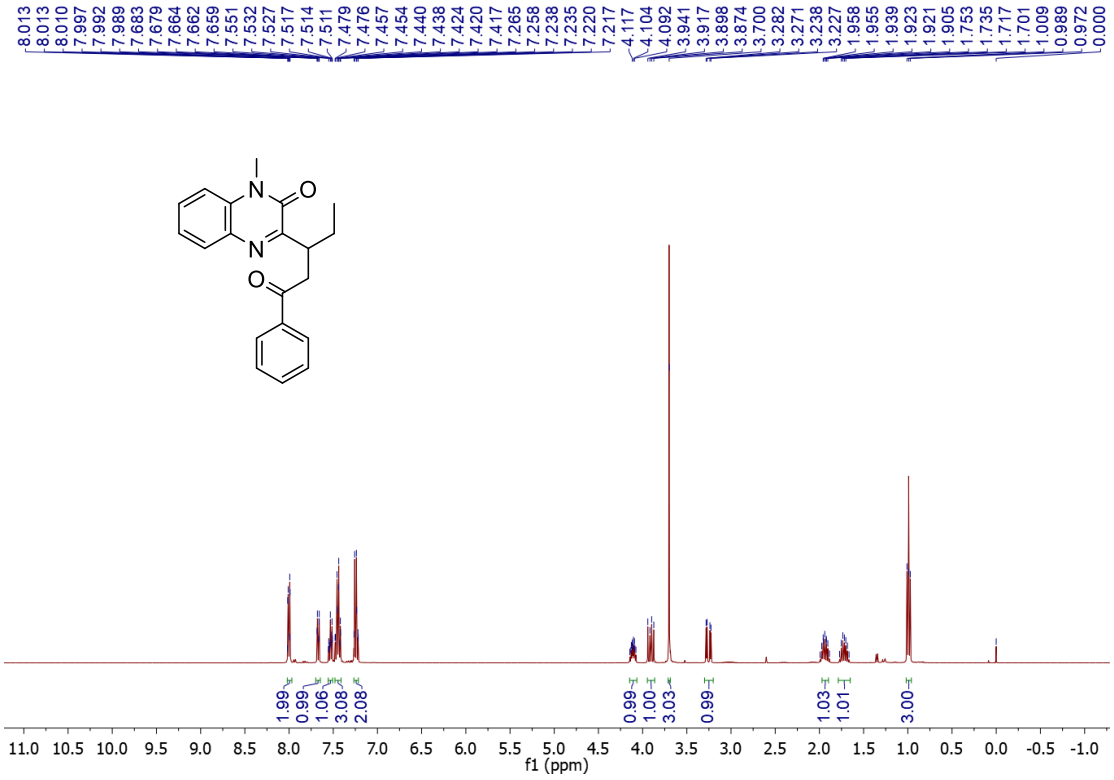


^{1}H NMR (400 MHz, $CDCl_3$)

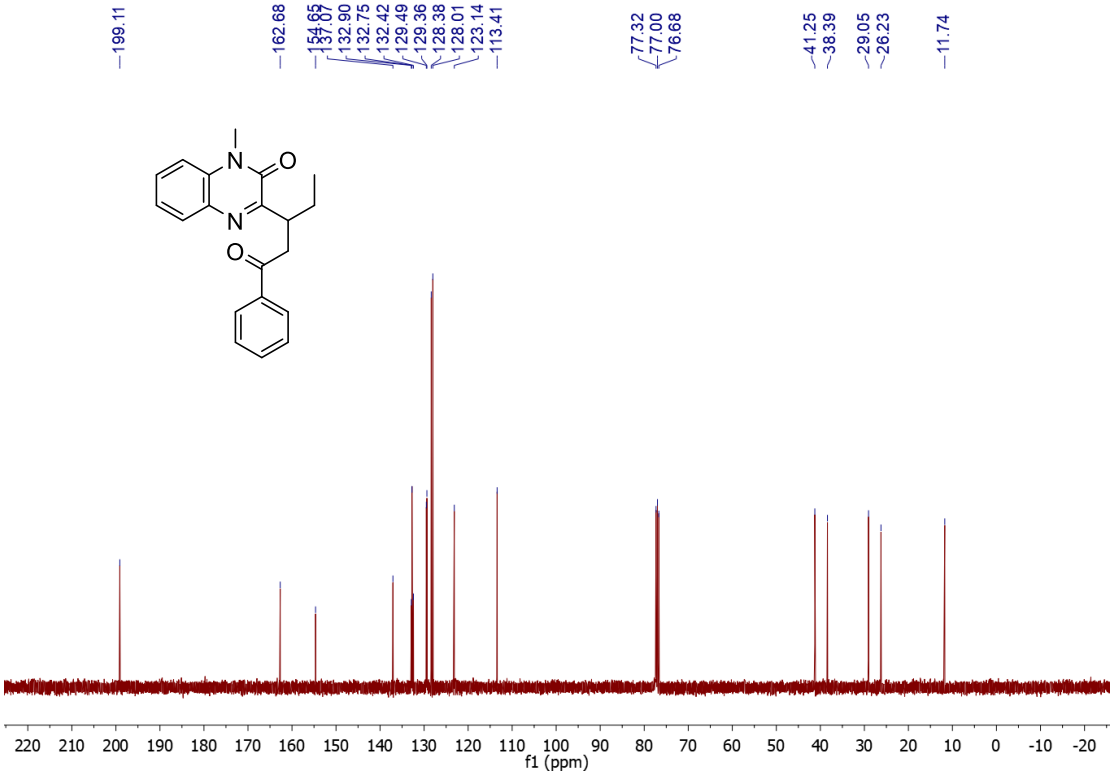


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3aa)

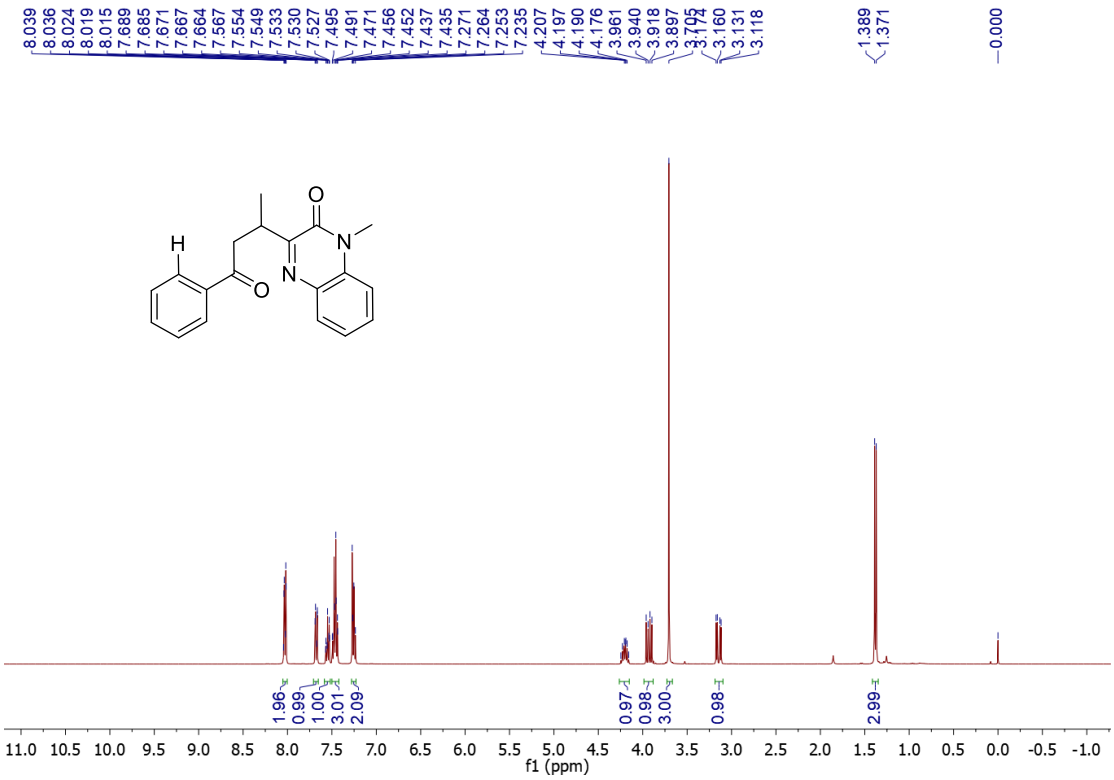


^{1}H NMR (400 MHz, CDCl$_3$)

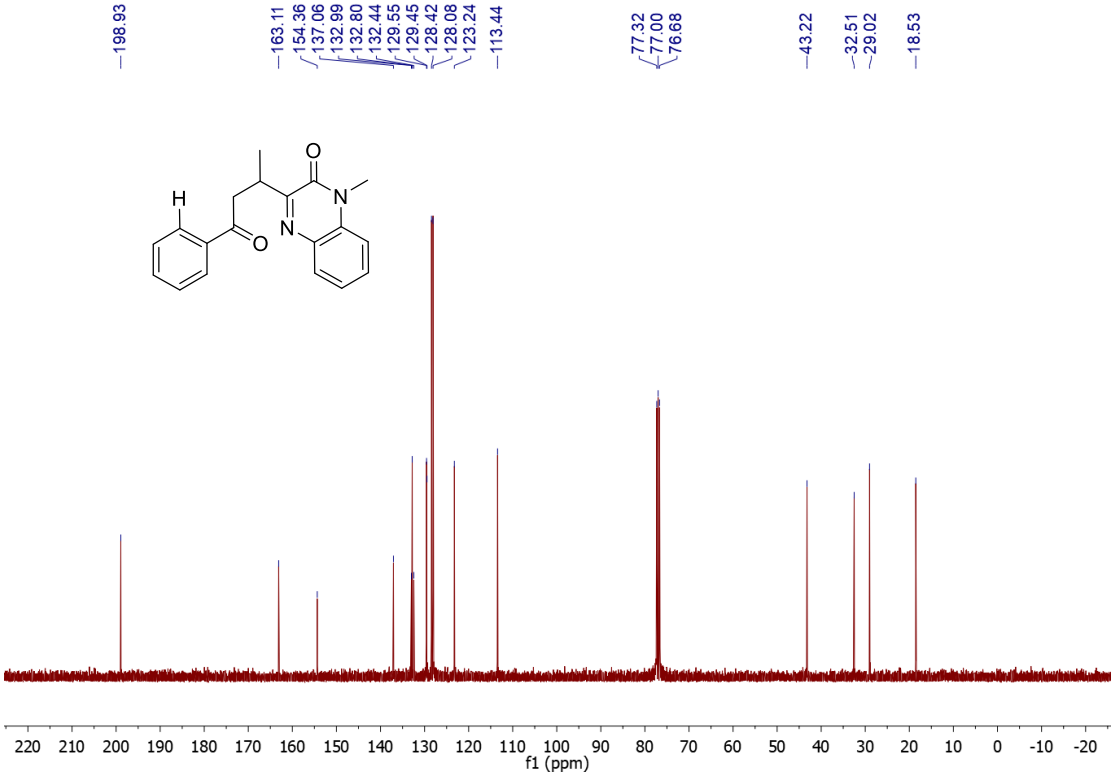


^{13}C NMR (100 MHz, CDCl$_3$)

1-methyl-3-(4-*oxo*-4-phenylbutan-2-yl)quinoxalin-2(1*H*)-one (3ba)

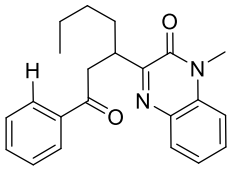


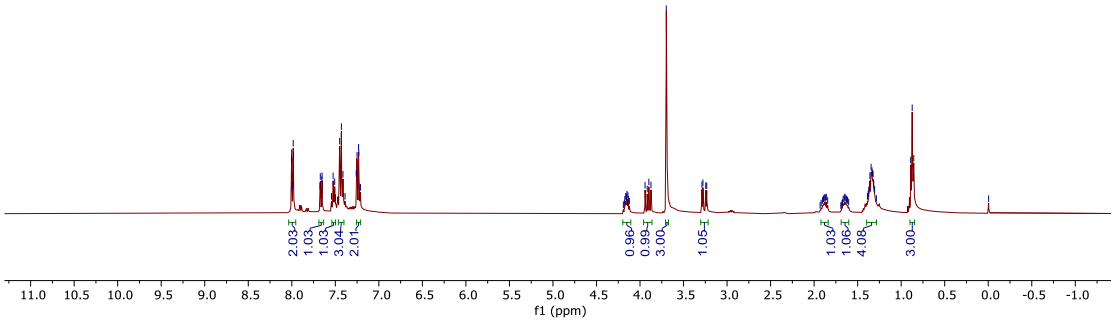
^{1}H NMR (400 MHz, CDCl$_3$)



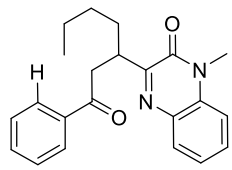
^{13}C NMR (100 MHz, CDCl$_3$)

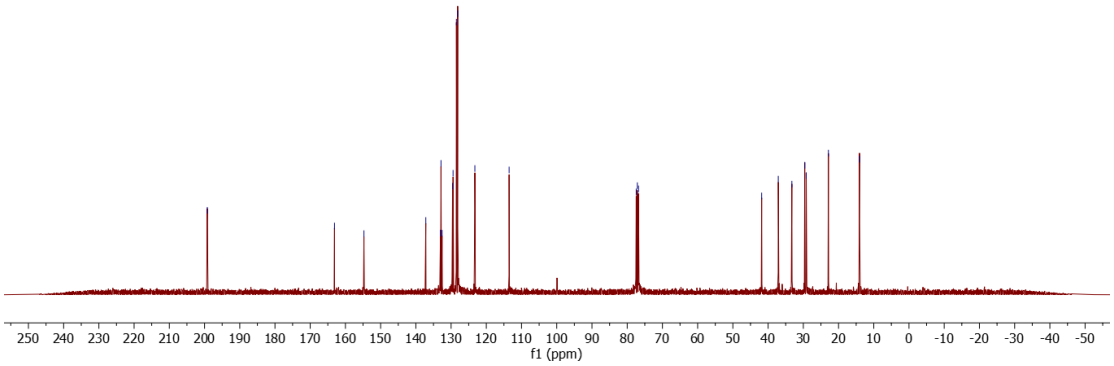
1-methyl-3-(1-*oxo*-1-phenylheptan-3-yl)quinoxalin-2(1*H*)-one (3ca)





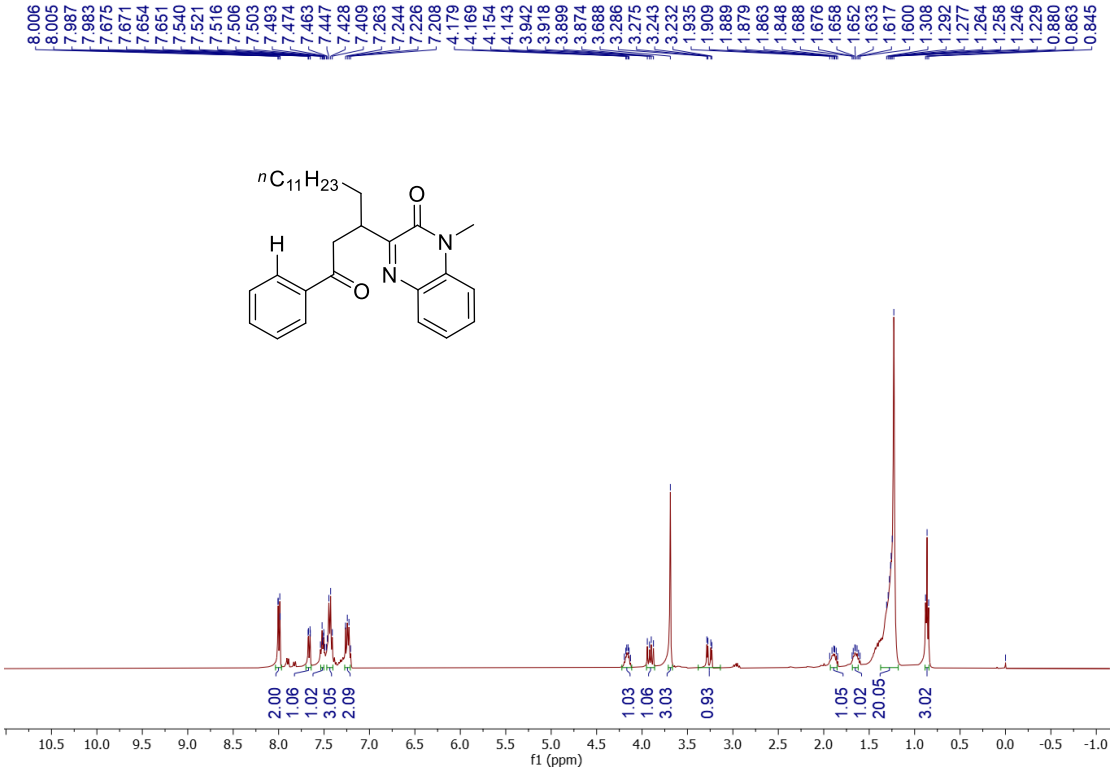
^{1}H NMR (400 MHz, $CDCl_3$)



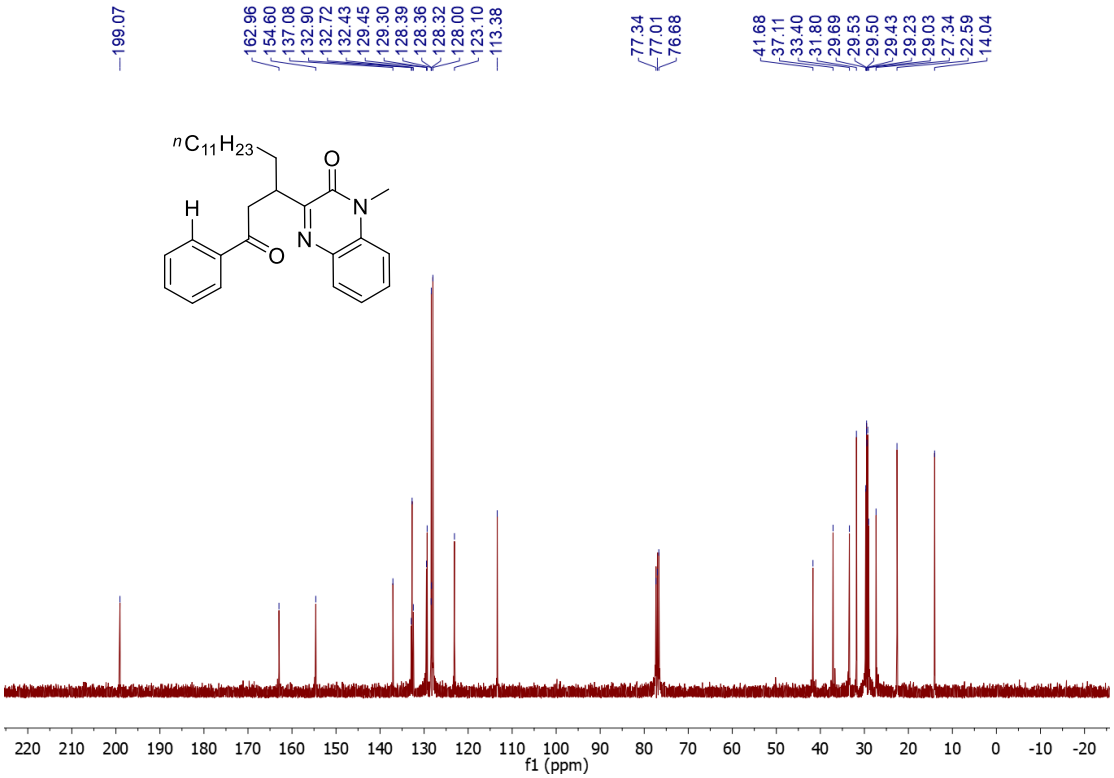


^{13}C NMR (100 MHz, $CDCl_3$)

1- methyl-3-(1-*oxo*-1-phenylpentadecan-3-yl)quinoxalin-2(1*H*)-one (3da)

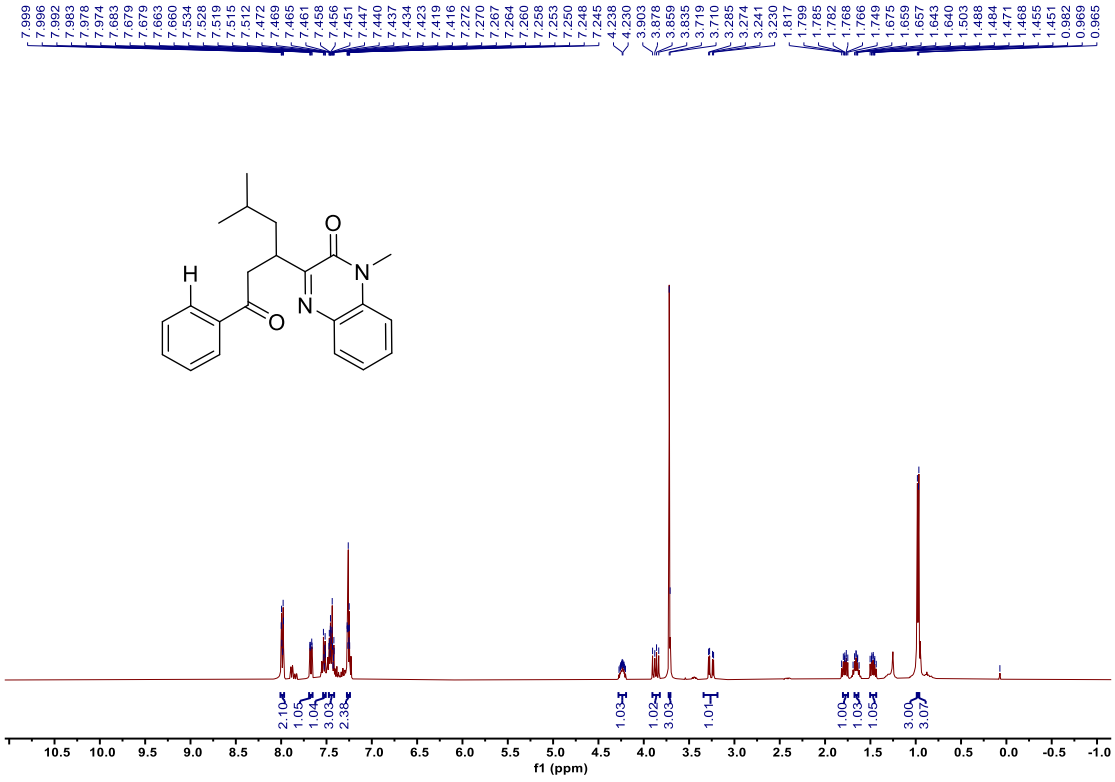


^{1}H NMR (400 MHz, $CDCl_3$)

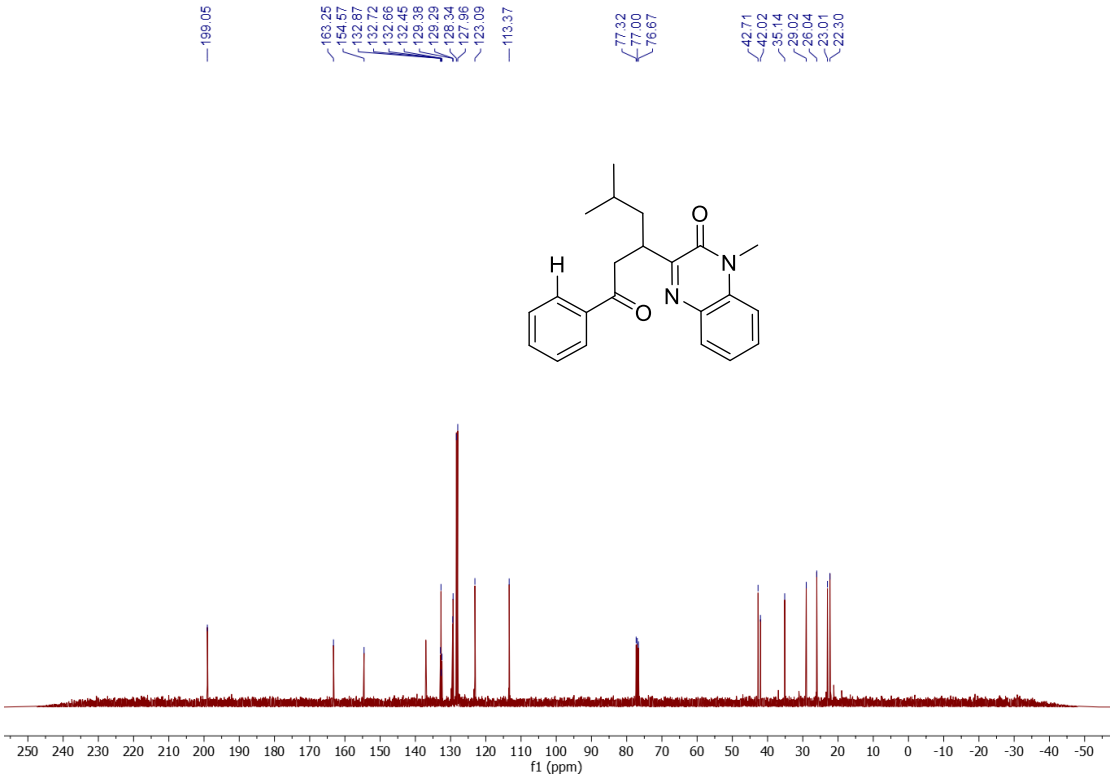


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(5-methyl-1-*oxo*-1-phenylhexan-3-yl)quinoxalin-2(1*H*)-one (3ea)

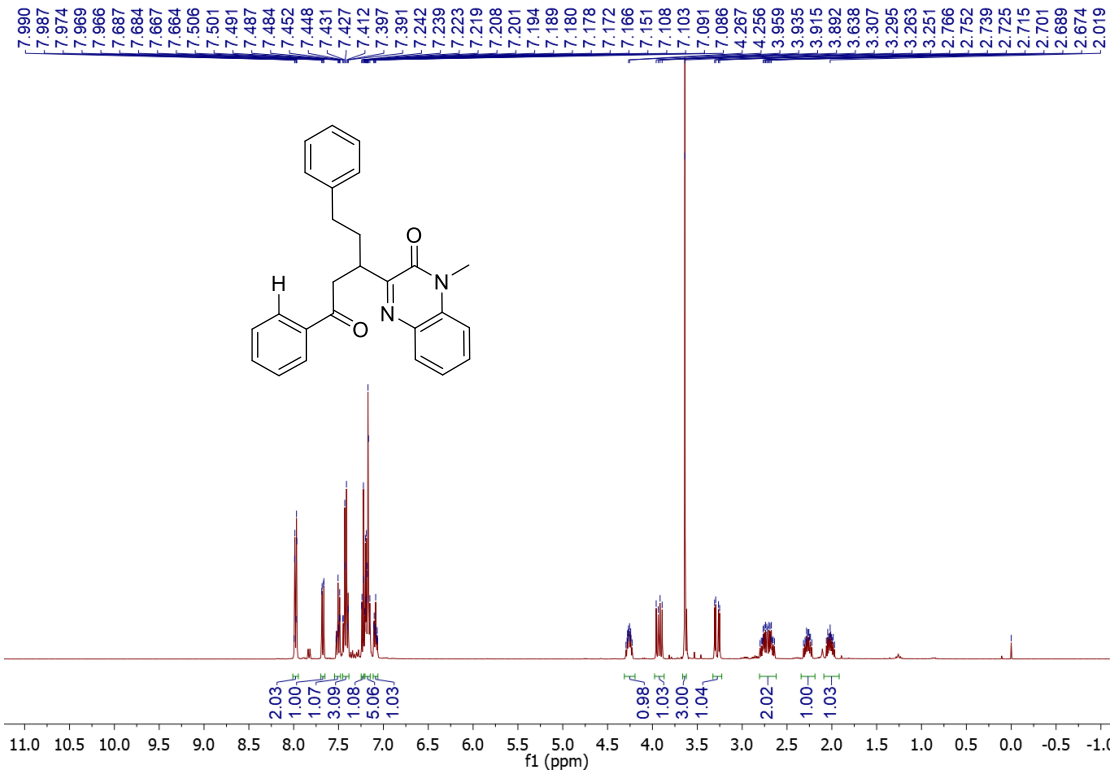


^{1}H NMR (400 MHz, $CDCl_3$)

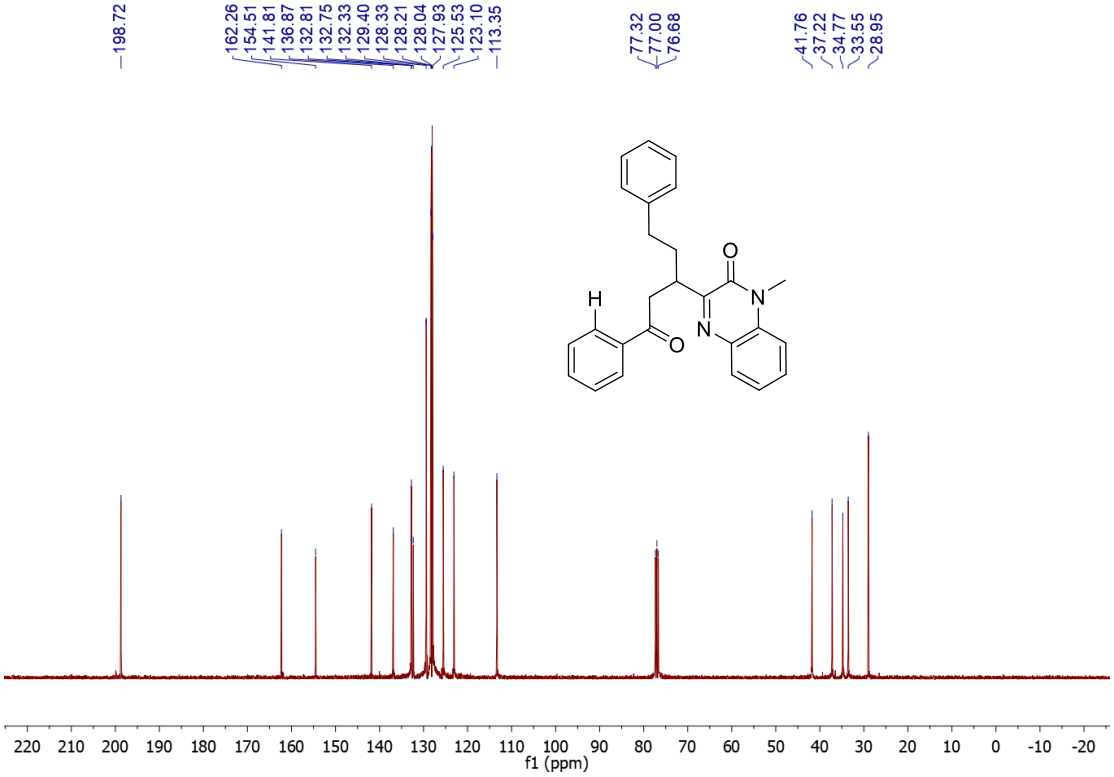


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(1-*oxo*-1,5-diphenylpentan-3-yl)quinoxalin-2(1*H*)-one (3fa)



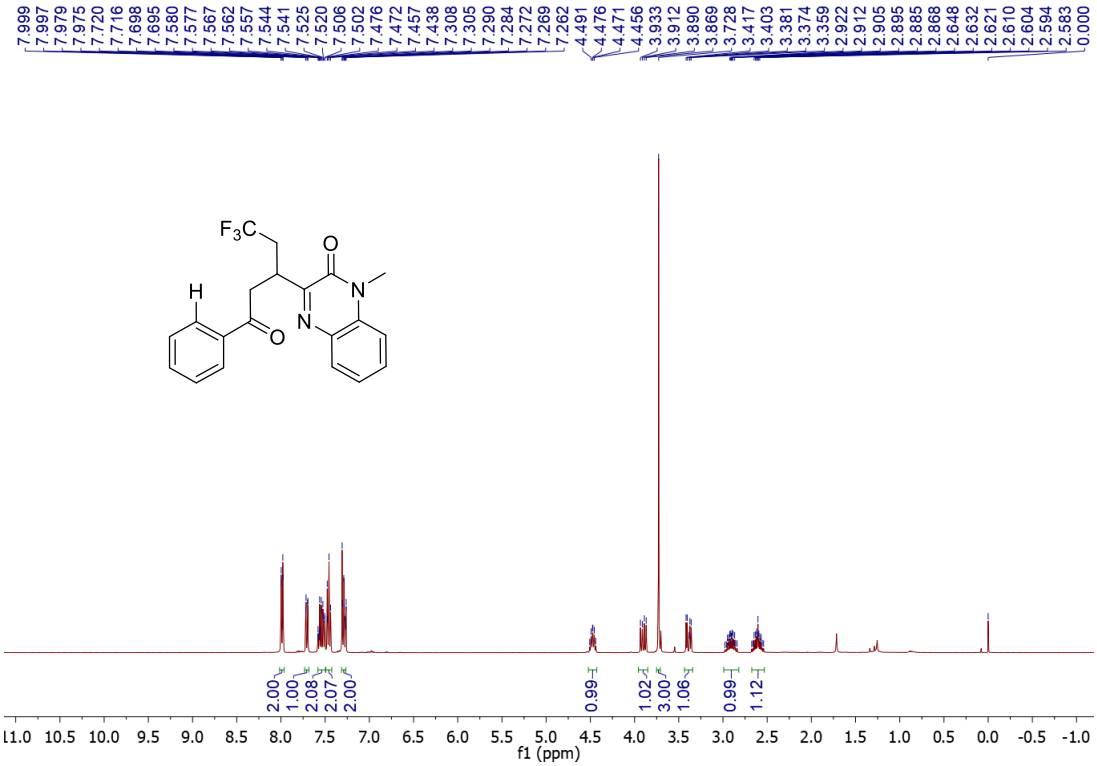
^{1}H NMR (400 MHz, $CDCl_3$)



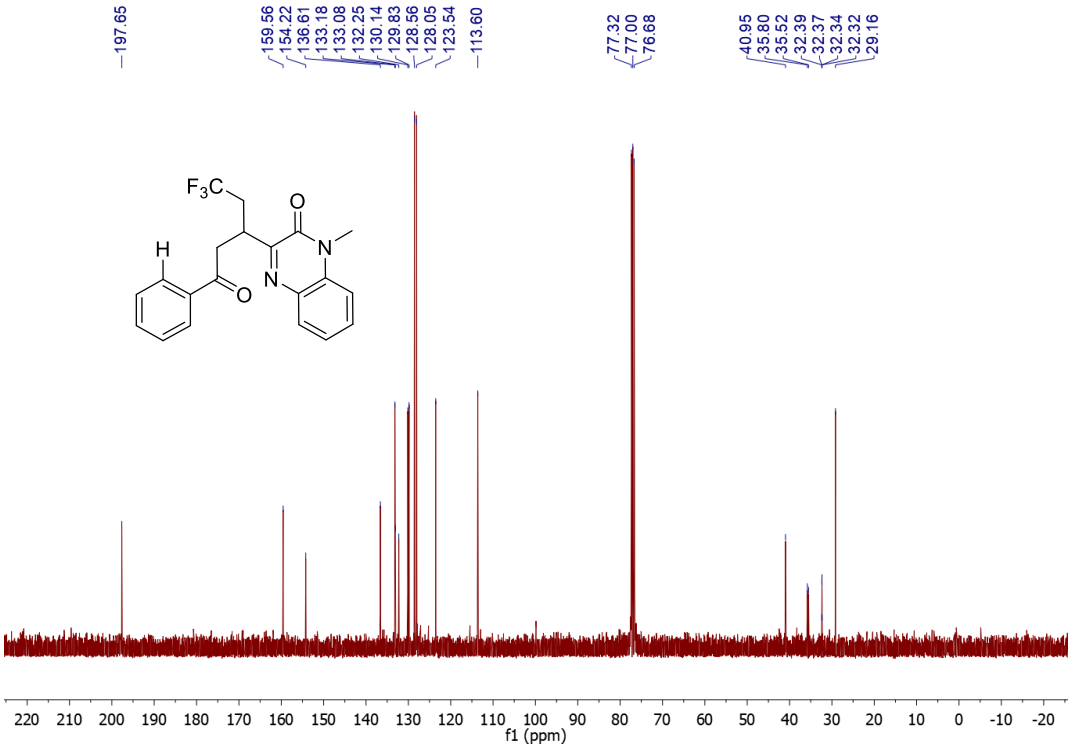
^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(1,1,1-trifluoro-5-*oxo*-5-phenylpentan-3-yl)quinoxalin-2(1*H*)-one

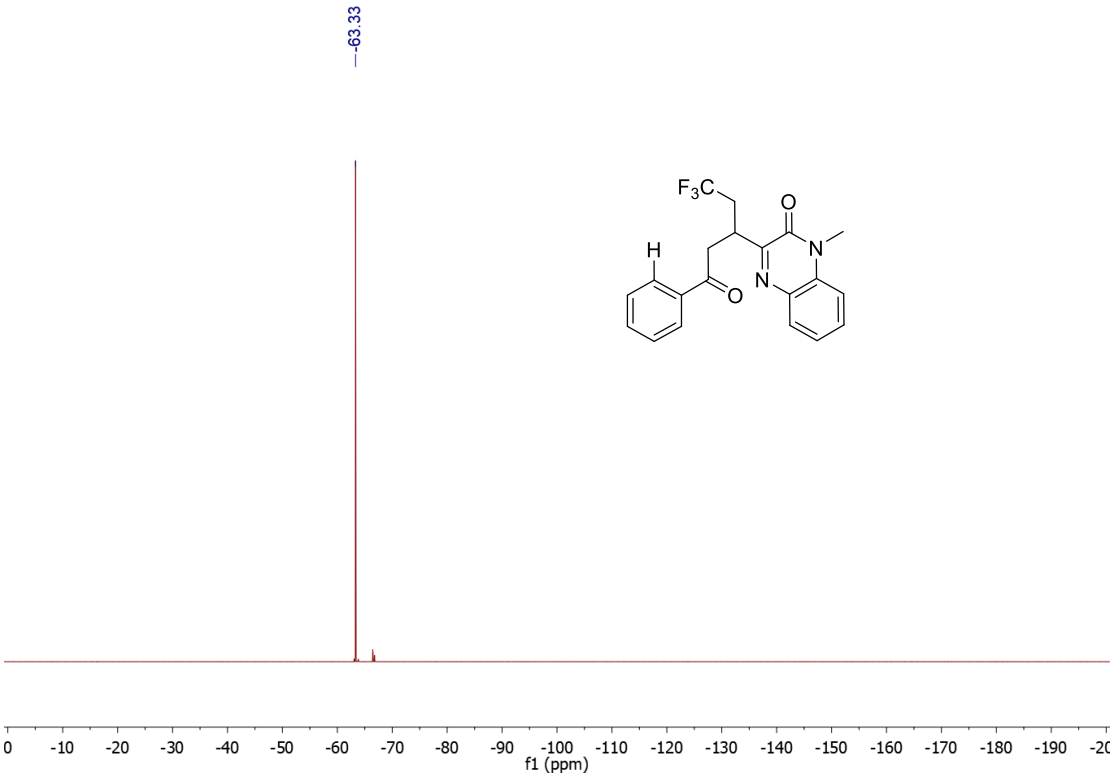
(3ga)



^{1}H NMR (400 MHz, CDCl$_3$)

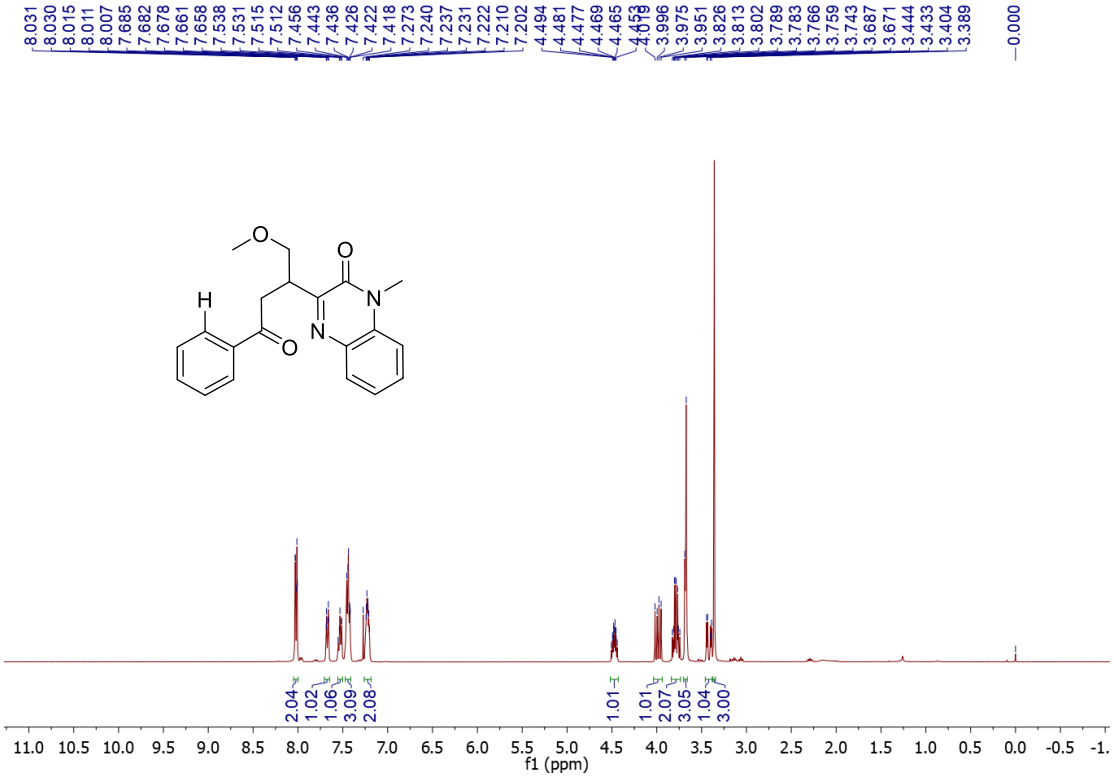


^{13}C NMR (100 MHz, CDCl$_3$)

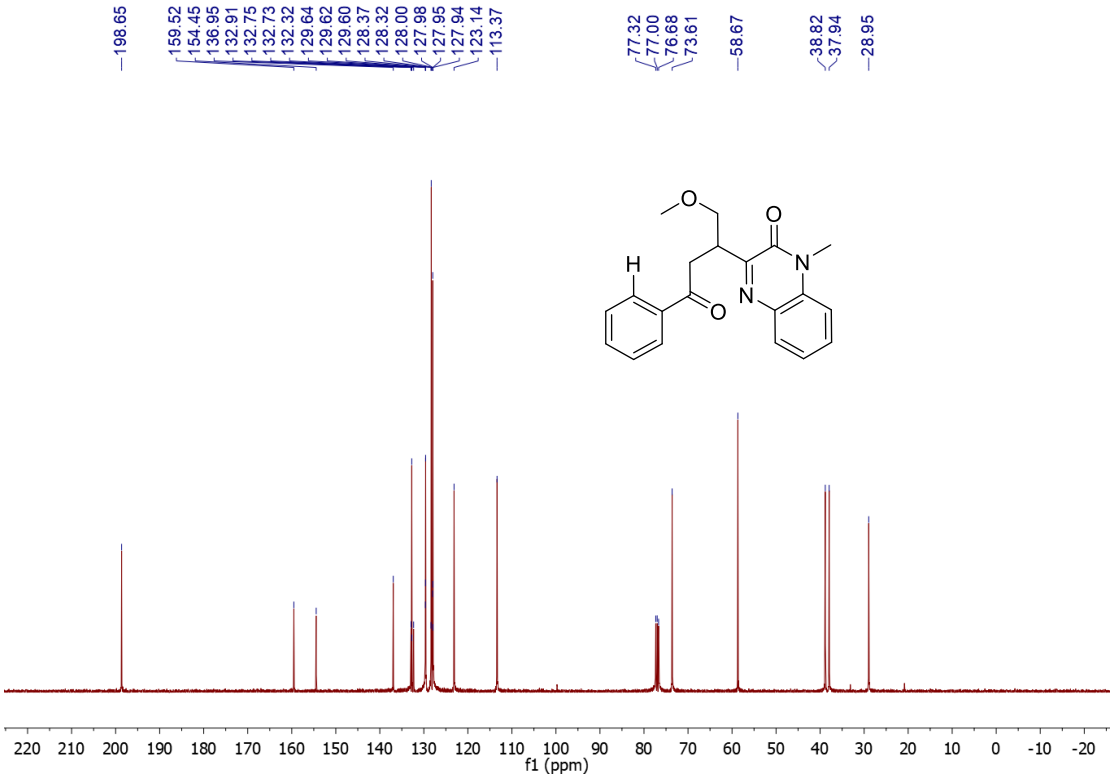


^{19}F NMR (376 MHz, $CDCl_3$)

2-(1-methoxy-4-*oxo*-4-phenylbutan-2-yl)-1-methylquinoxalin-2(1*H*)-one (3ha)

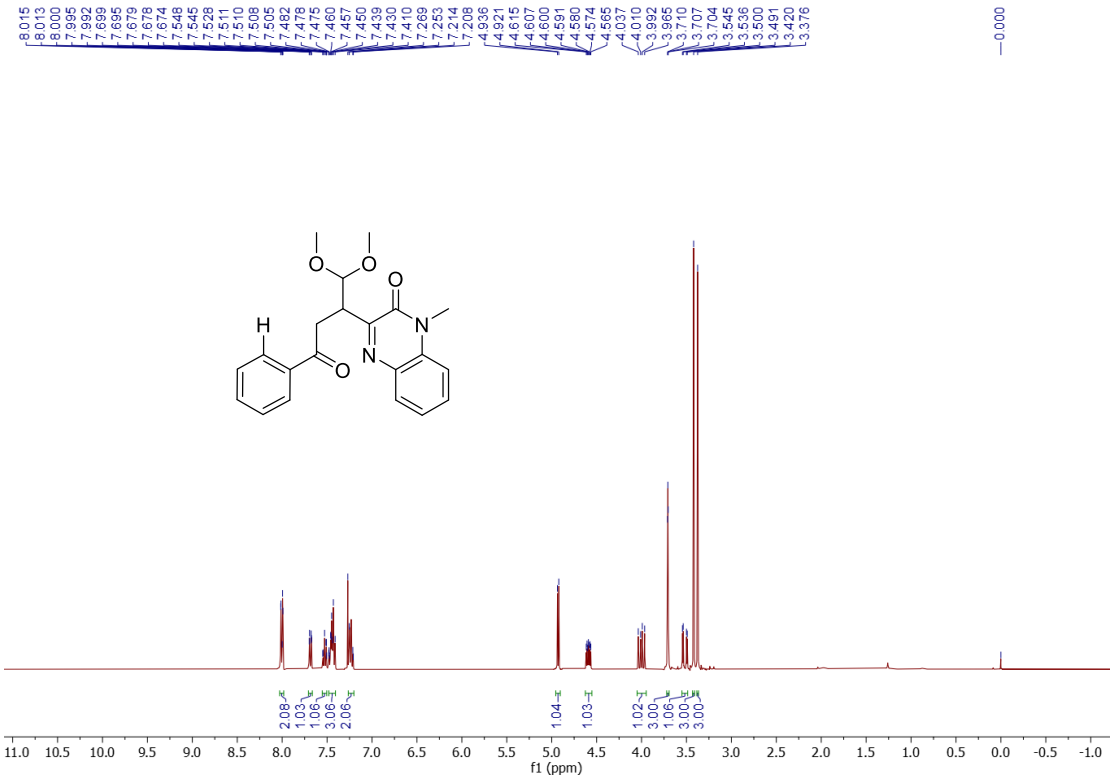


^{1}H NMR (400 MHz, CDCl$_3$)

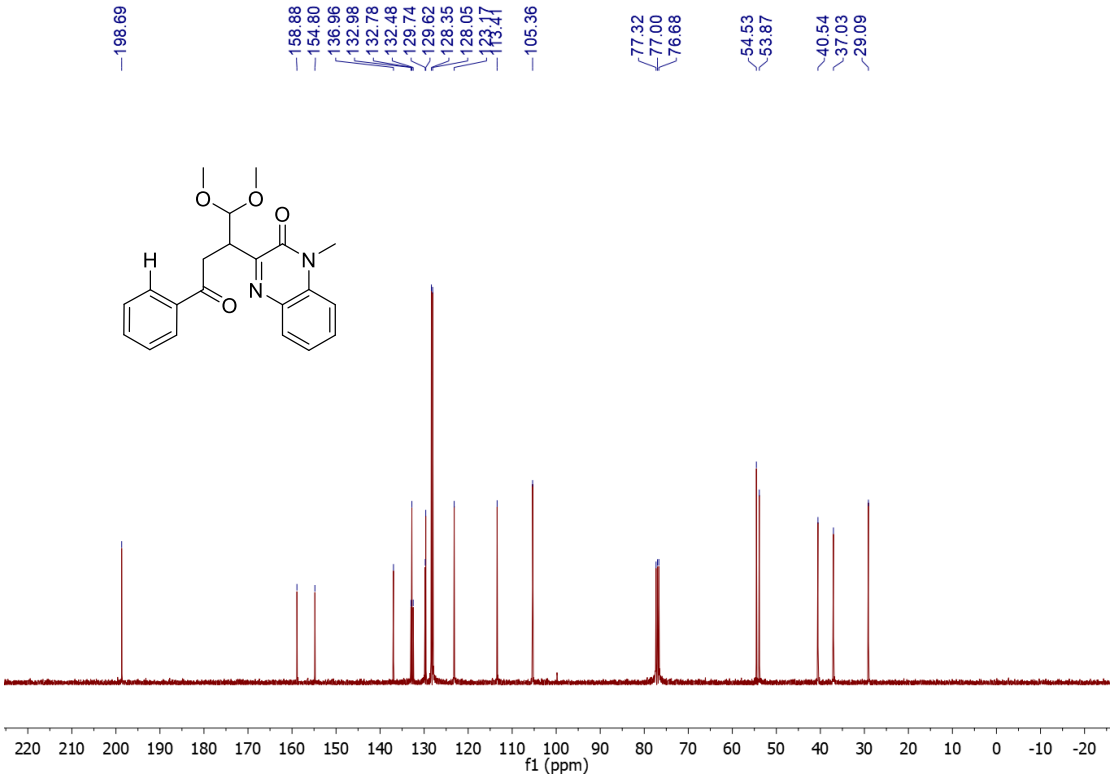


^{13}C NMR (100 MHz, CDCl$_3$)

2-(1,1-dimethoxy-4-*oxo*-4-phenylbutan-2-yl)-1-methylquinoxalin-2(1*H*)-one (3ia)

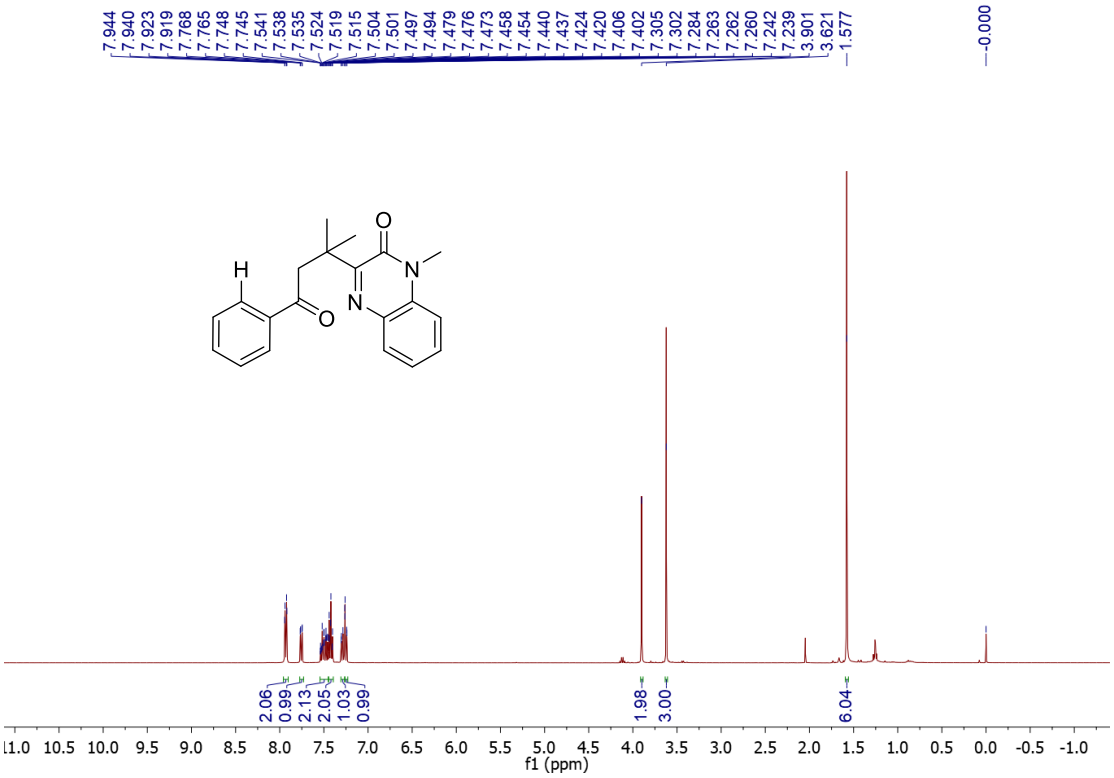


^{1}H NMR (400 MHz, $CDCl_3$)

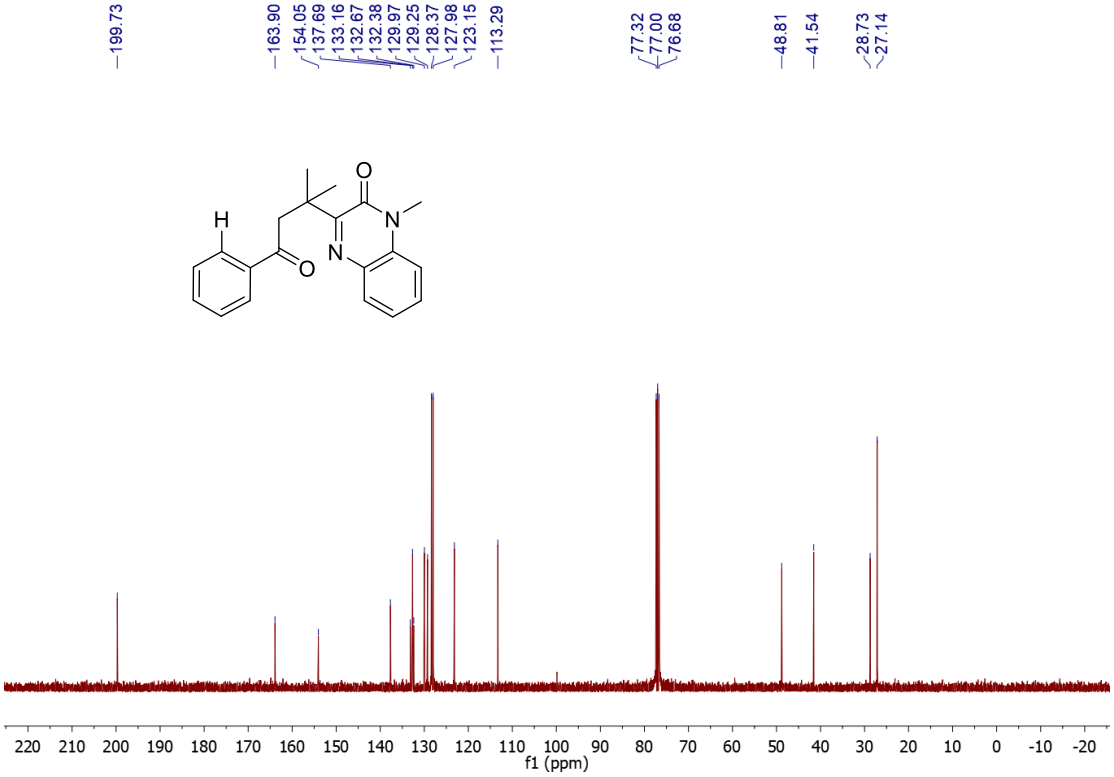


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(2-methyl-4-*oxo*-4-phenylbutan-2-yl)quinoxalin-2(1*H*)-one (3ja)

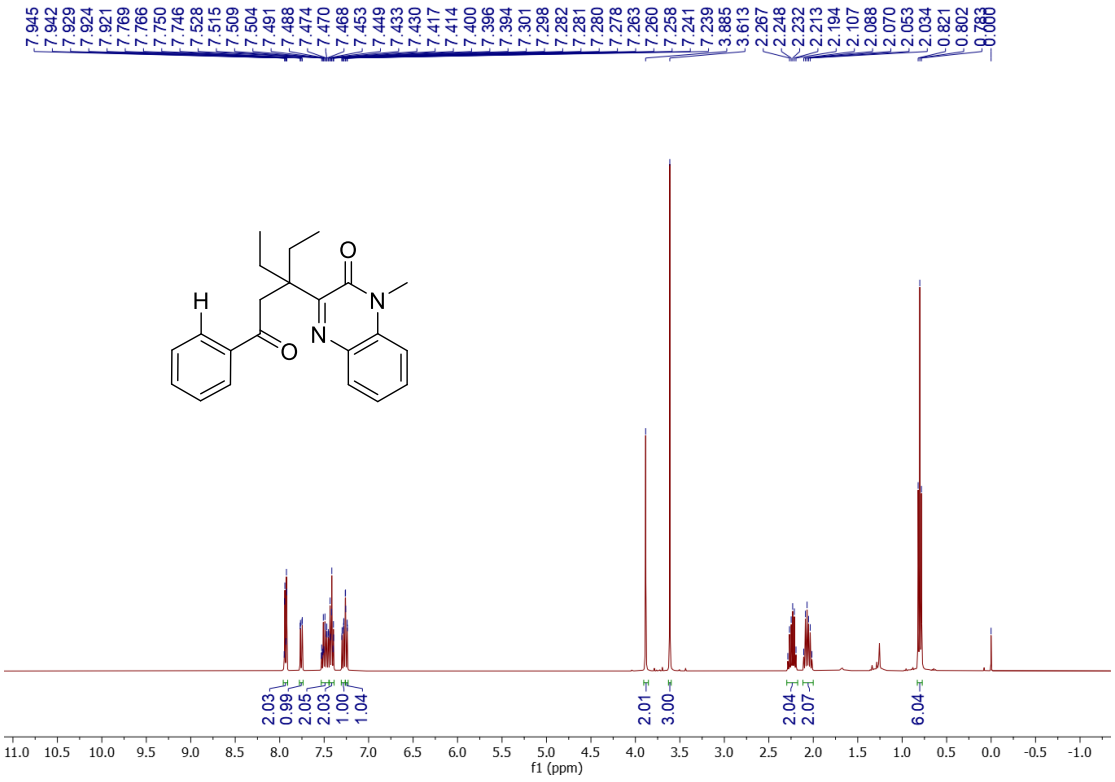


^{1}H NMR (400 MHz, $CDCl_3$)

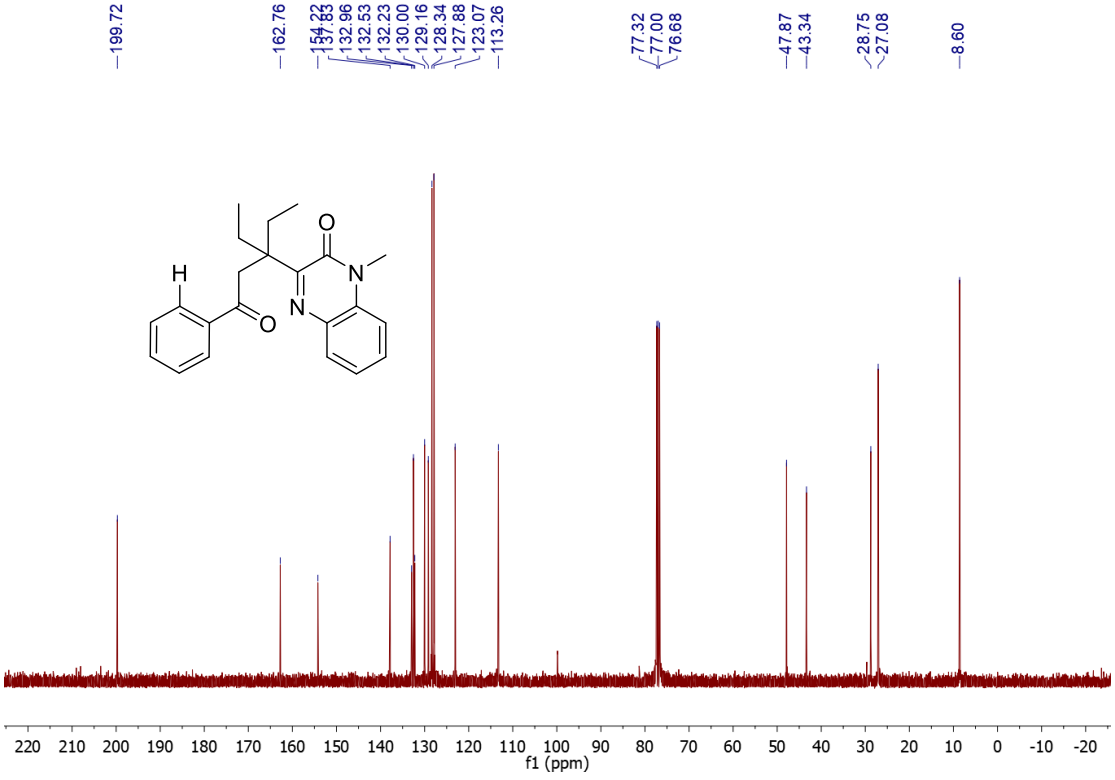


^{13}C NMR (100 MHz, $CDCl_3$)

3-(3-ethyl-1-*oxo*-1-phenylpentan-3-yl)-1-methylquinoxalin-2(1*H*)-one (3ka)

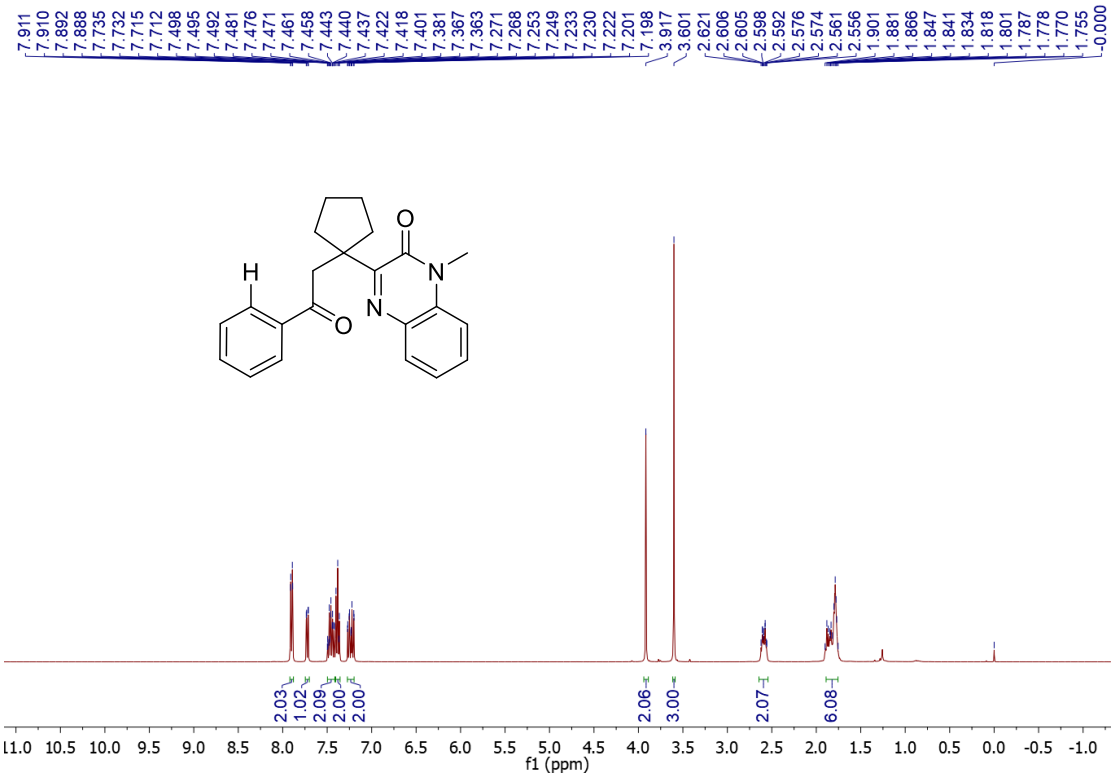


^{1}H NMR (400 MHz, $CDCl_3$)

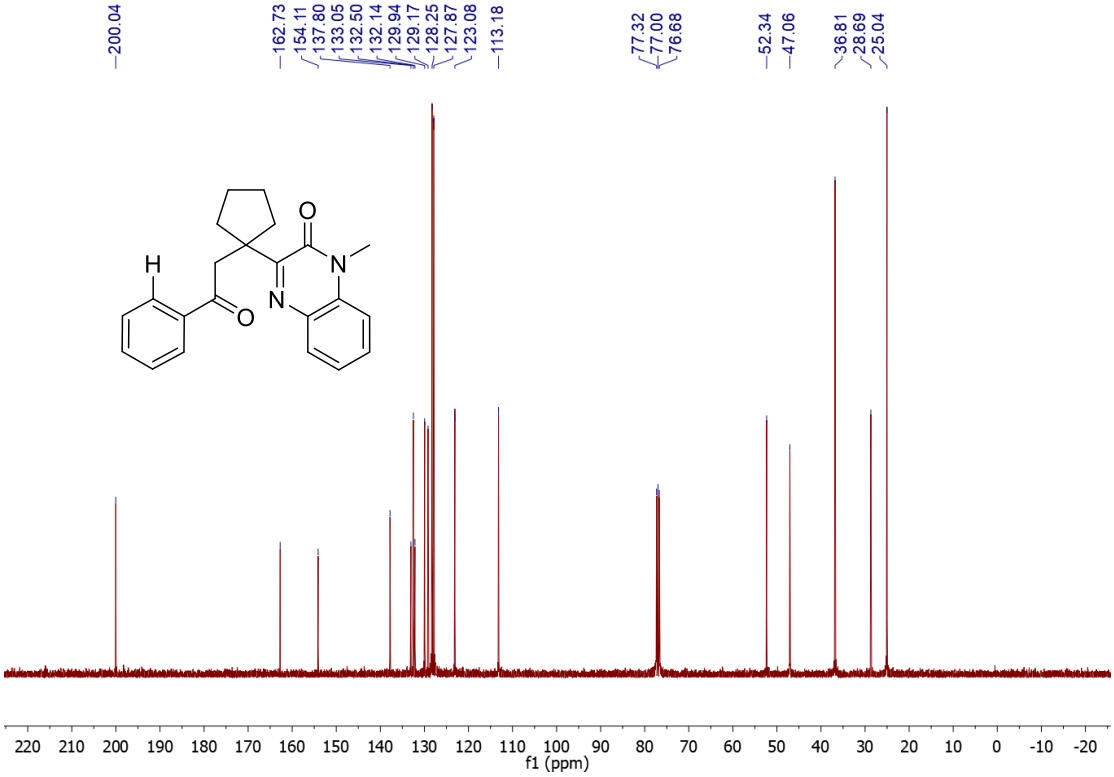


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(1-(2-*oxo*-2-phenylethyl)cyclopentyl)quinoxalin-2(1*H*)-one (3la)

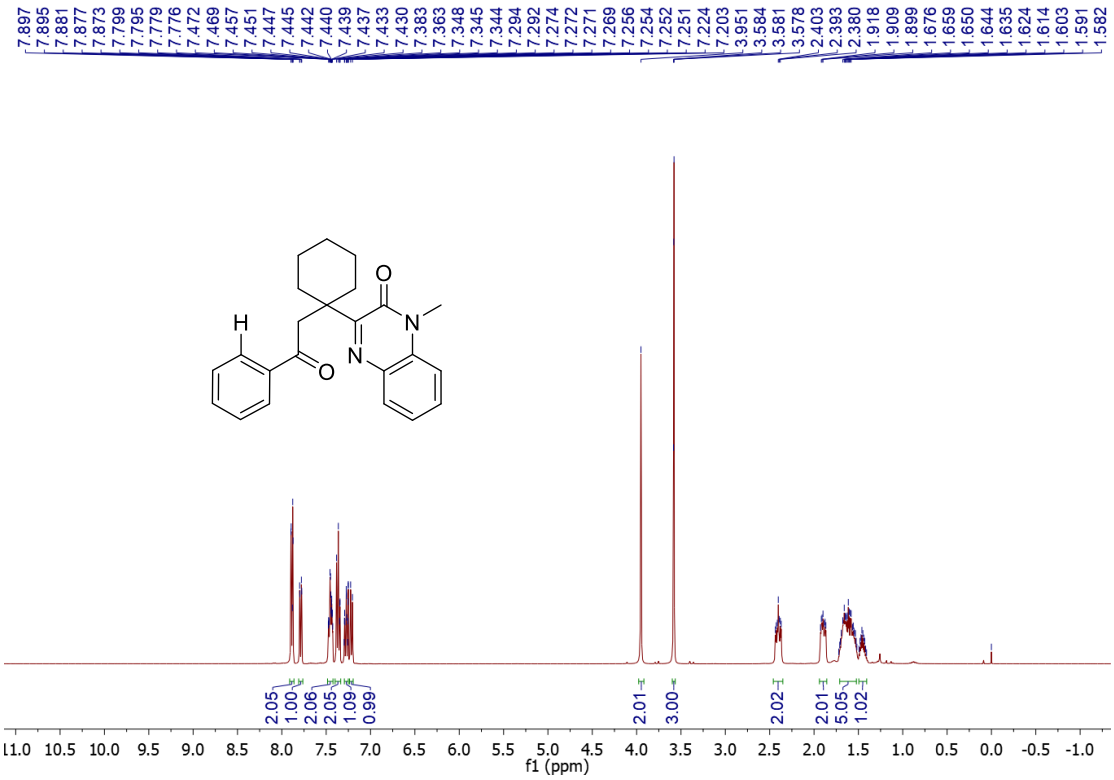


^{1}H NMR (400 MHz, $CDCl_3$)

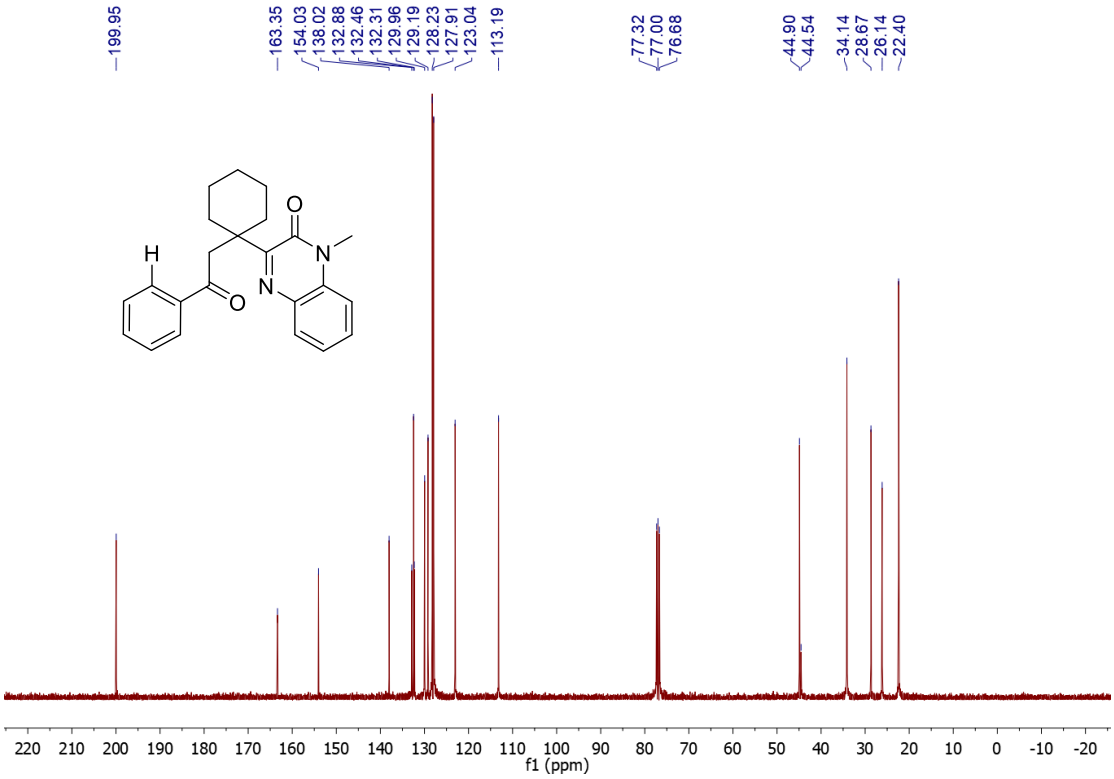


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(1-(2-*oxo*-2-phenylethyl)cyclohexyl)quinoxalin-2(1*H*)-one (3ma)

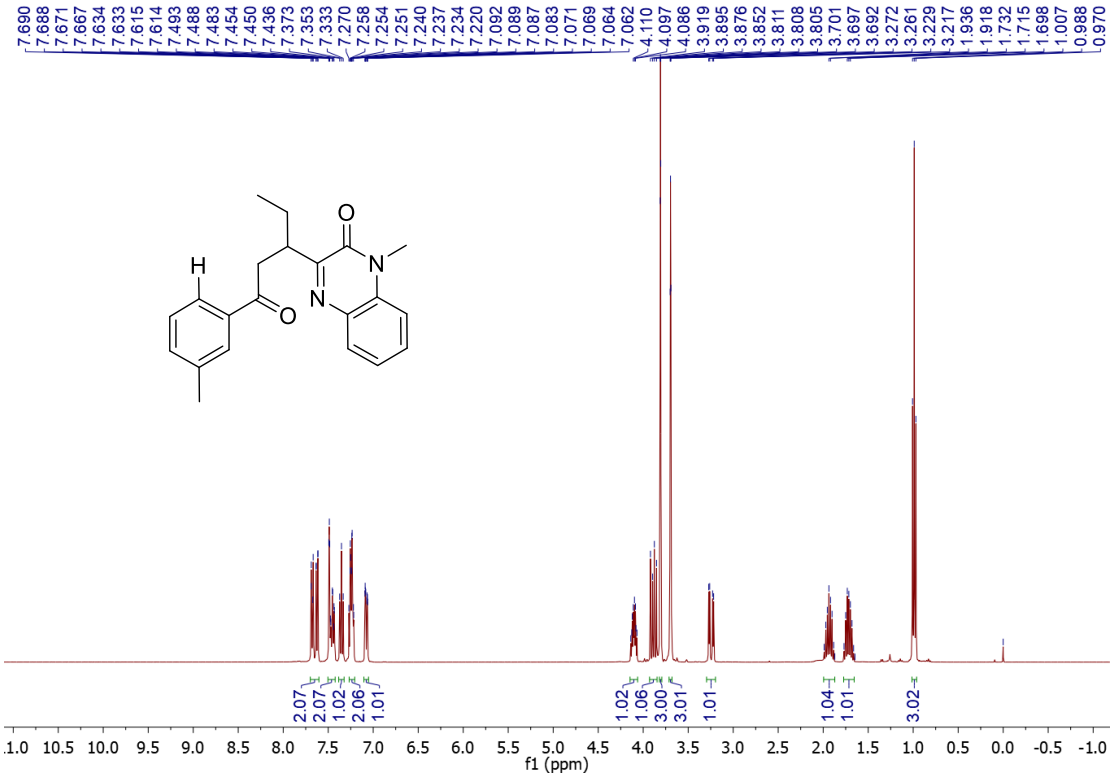


^{1}H NMR (400 MHz, $CDCl_3$)

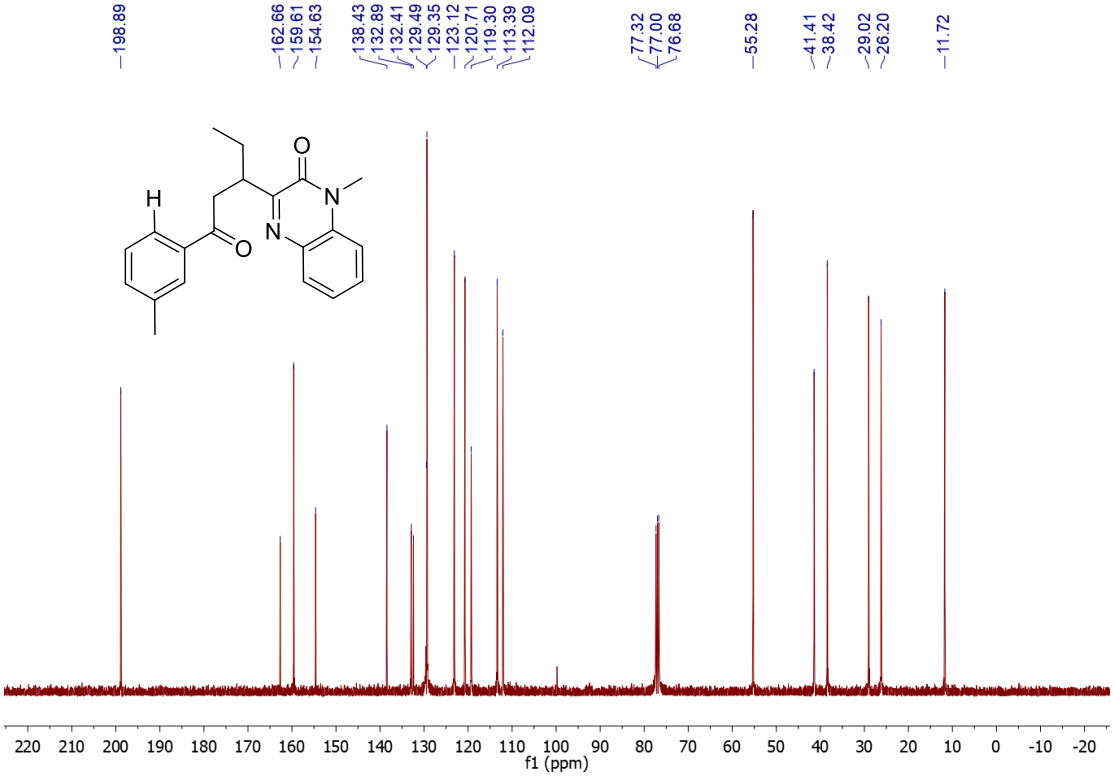


^{13}C NMR (100 MHz, $CDCl_3$)

1-methyl-3-(1-*oxo*-1-(m-tolyl)pentan-3-yl)quinoxalin-2(1*H*)-one (3na)

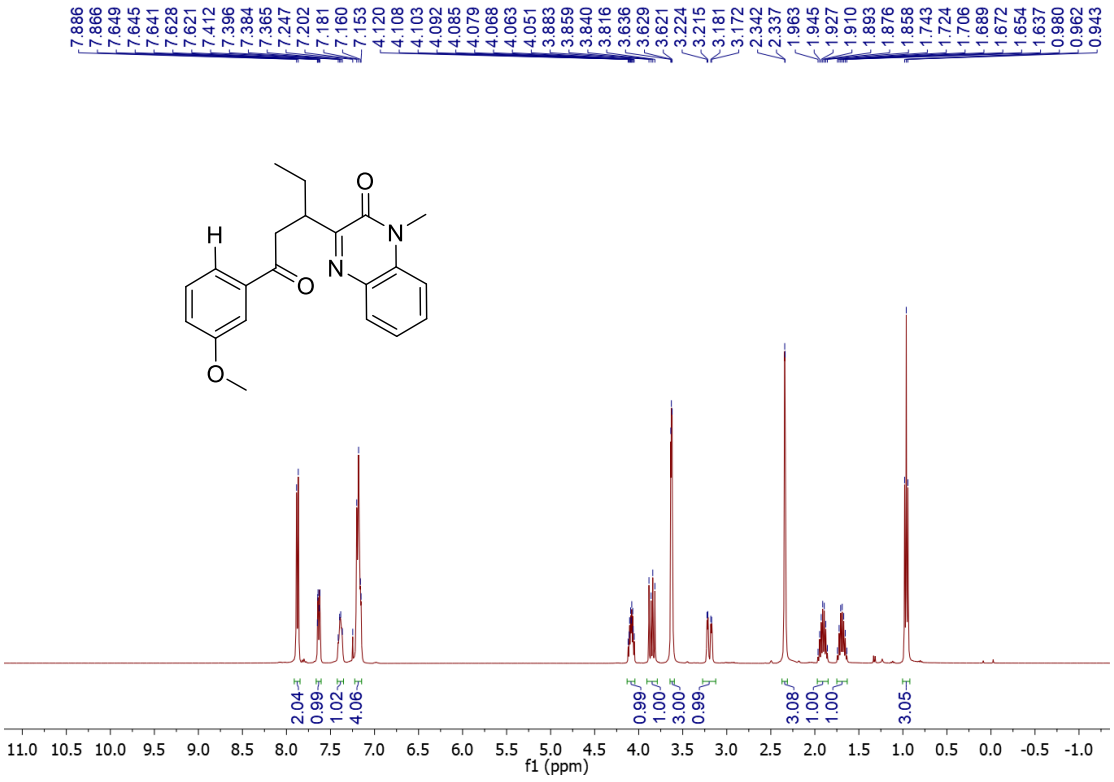


^{1}H NMR (400 MHz, CDCl$_3$)

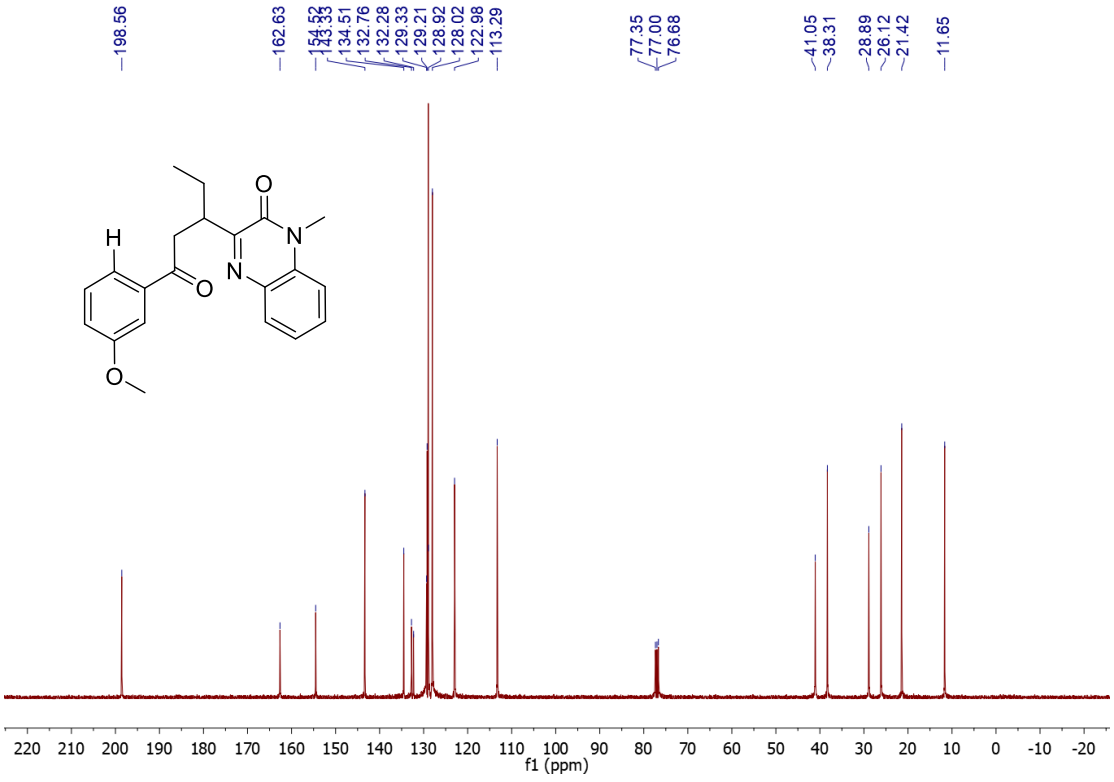


^{13}C NMR (100 MHz, CDCl$_3$)

2-(1-(3-methoxyphenyl)-1-*oxo*pentan-3-yl)-1-methylquinoxalin-2(1*H*)-one (3oa)

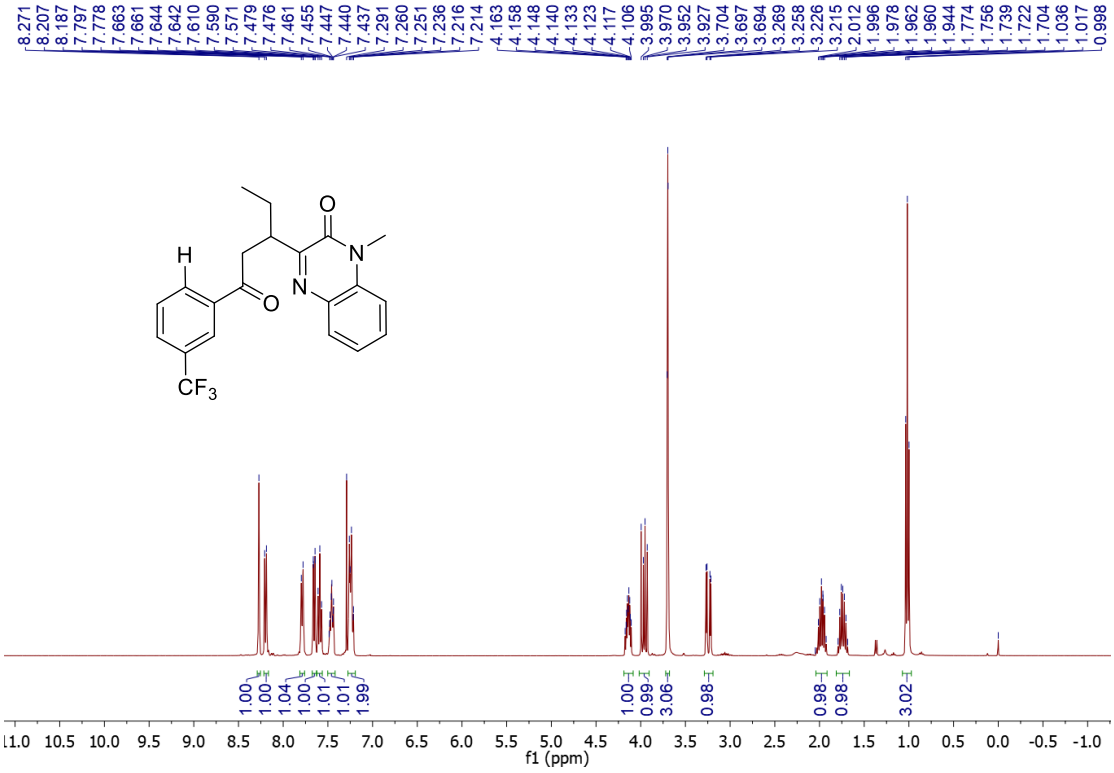


^{1}H NMR (400 MHz, $CDCl_3$)

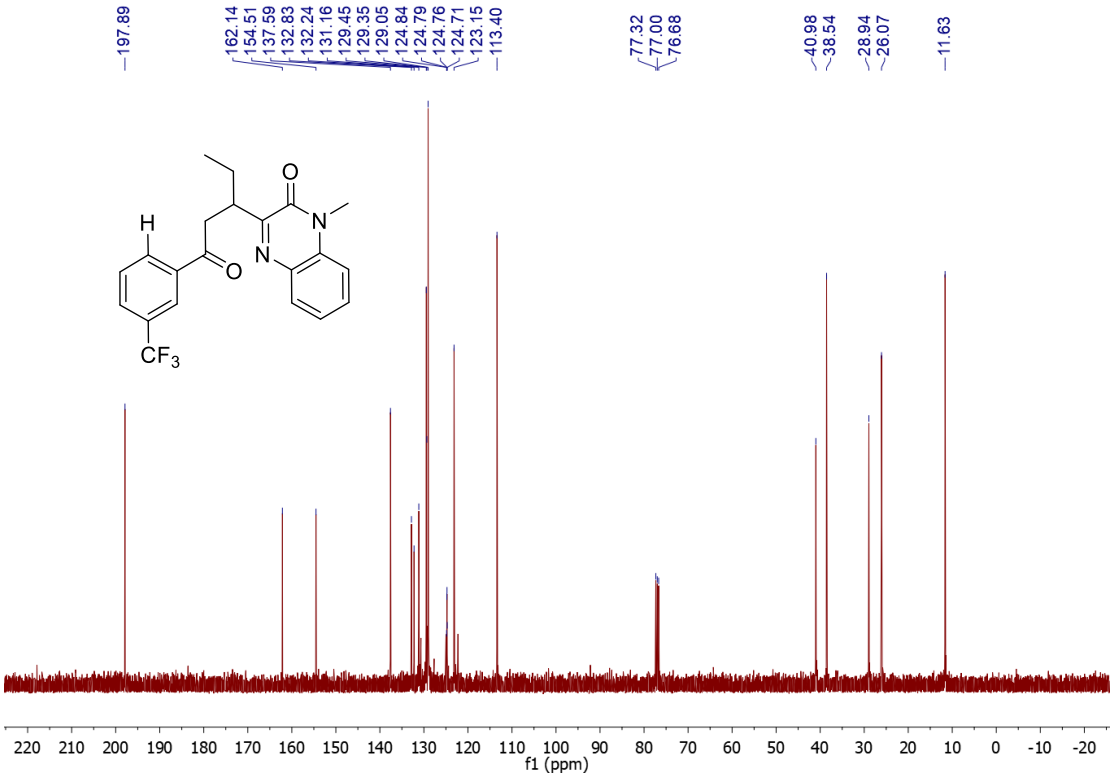


^{13}C NMR (100 MHz, $CDCl_3$)

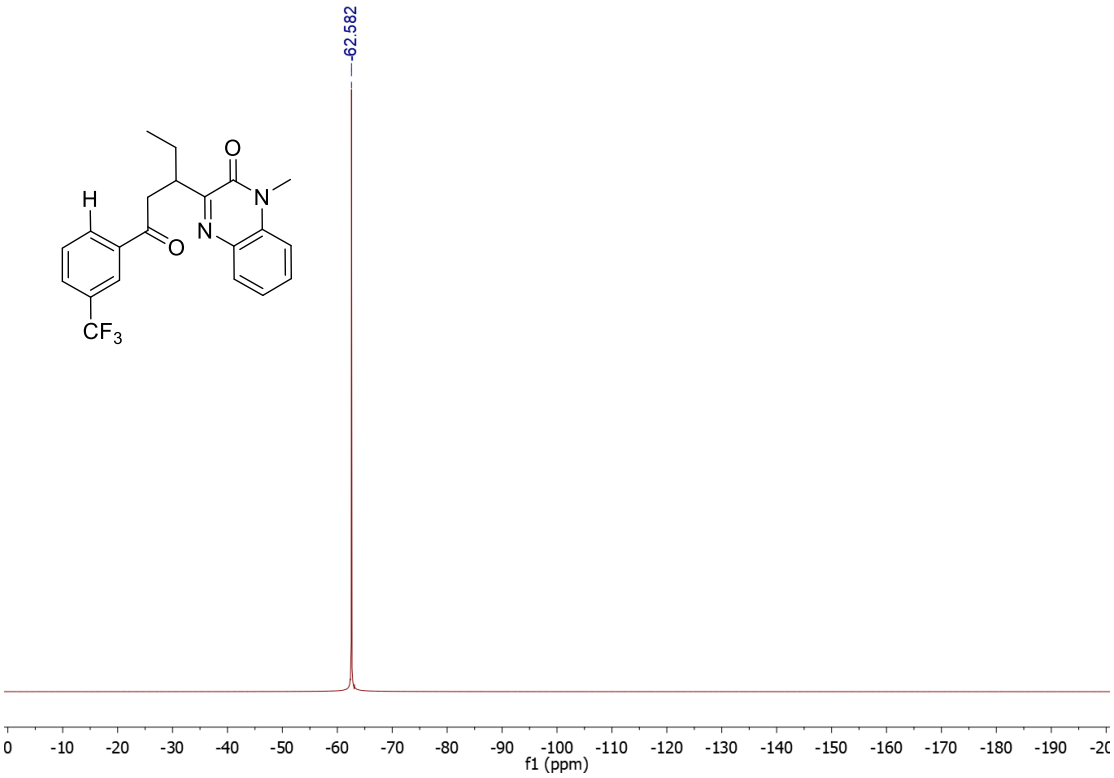
1-methyl-3-(1-*oxo*-1-(3-(trifluoromethyl)phenyl)pentan-3-yl)quinoxalin-2(1*H*)-one (3pa)



^{1}H NMR (400 MHz, CDCl$_3$)

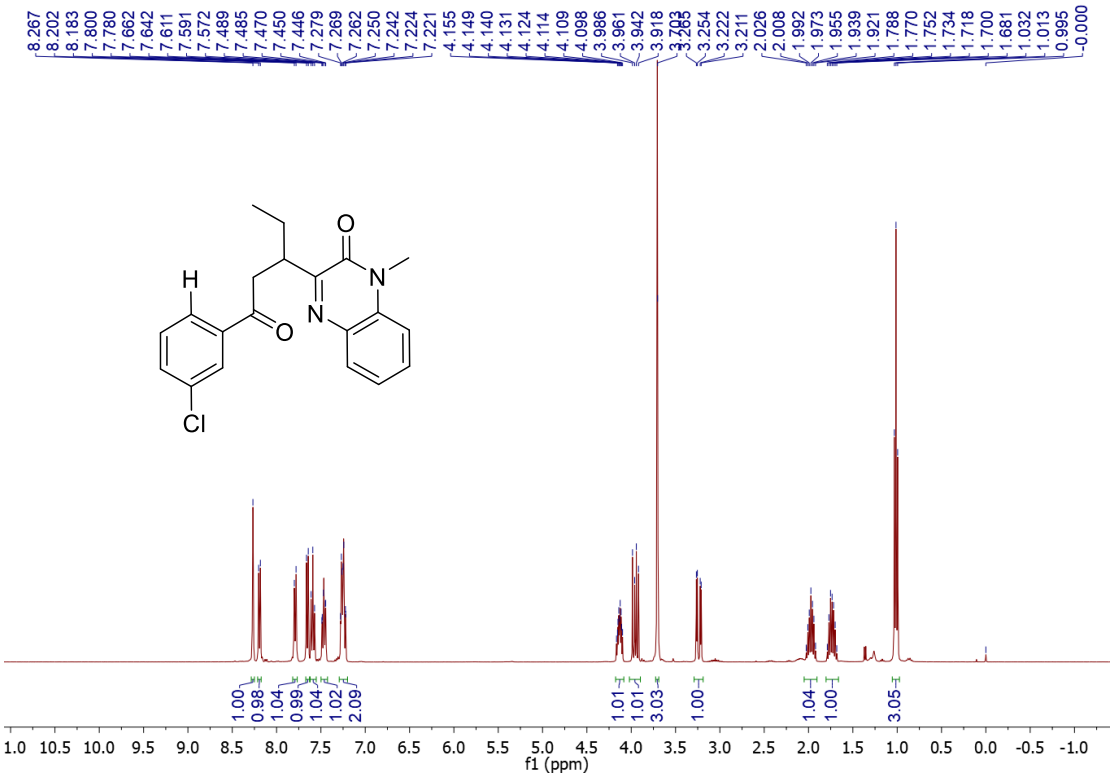


^{13}C NMR (100 MHz, CDCl$_3$)

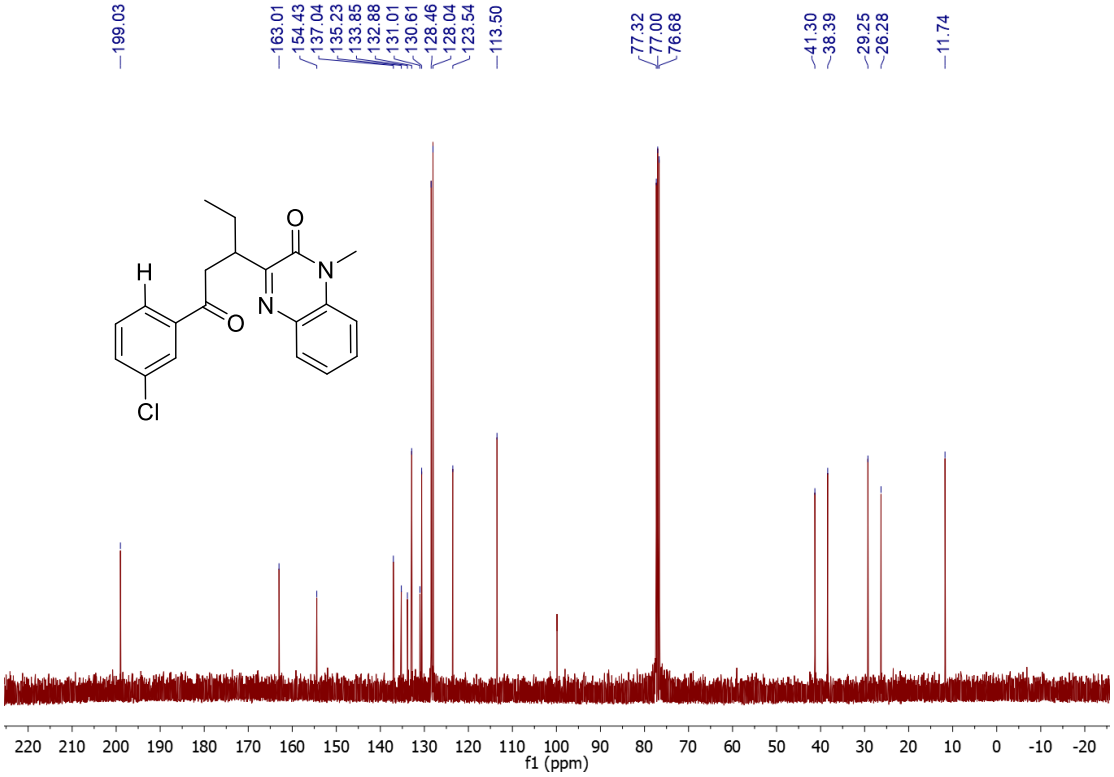


^{19}F NMR (376 MHz, $CDCl_3$)

3-(1-(3-chlorophenyl)-1-oxopentan-3-yl)-1-methylquinoxalin-2(1*H*)-one (3qa)

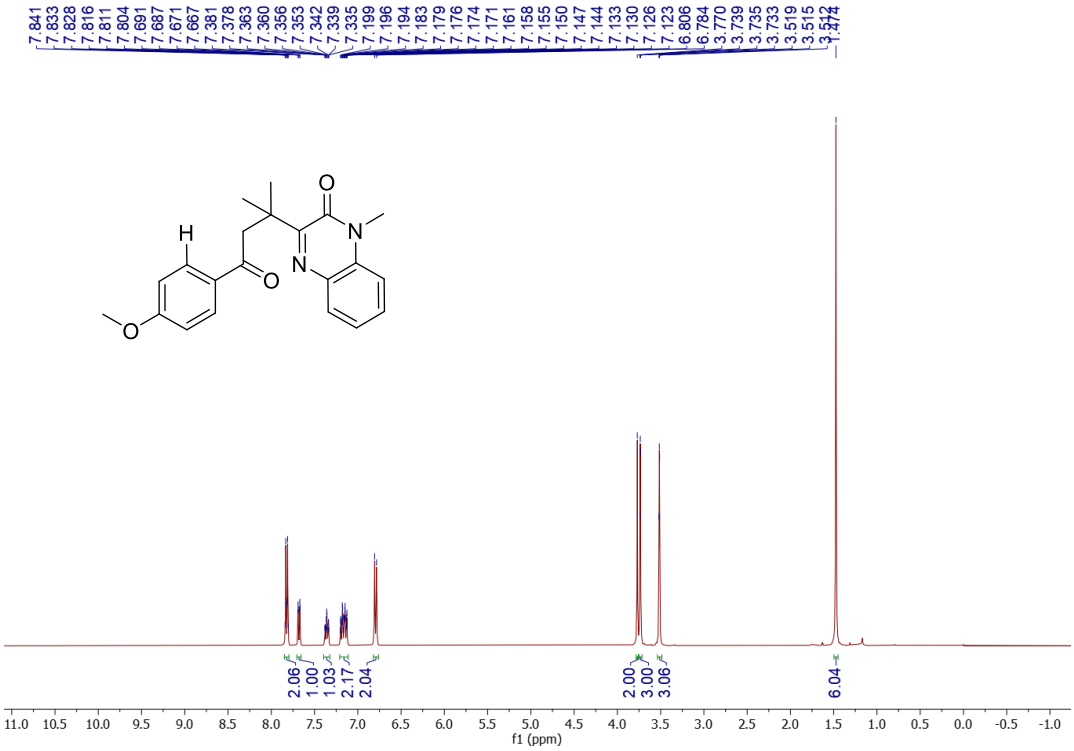


^{1}H NMR (400 MHz, CDCl$_3$)

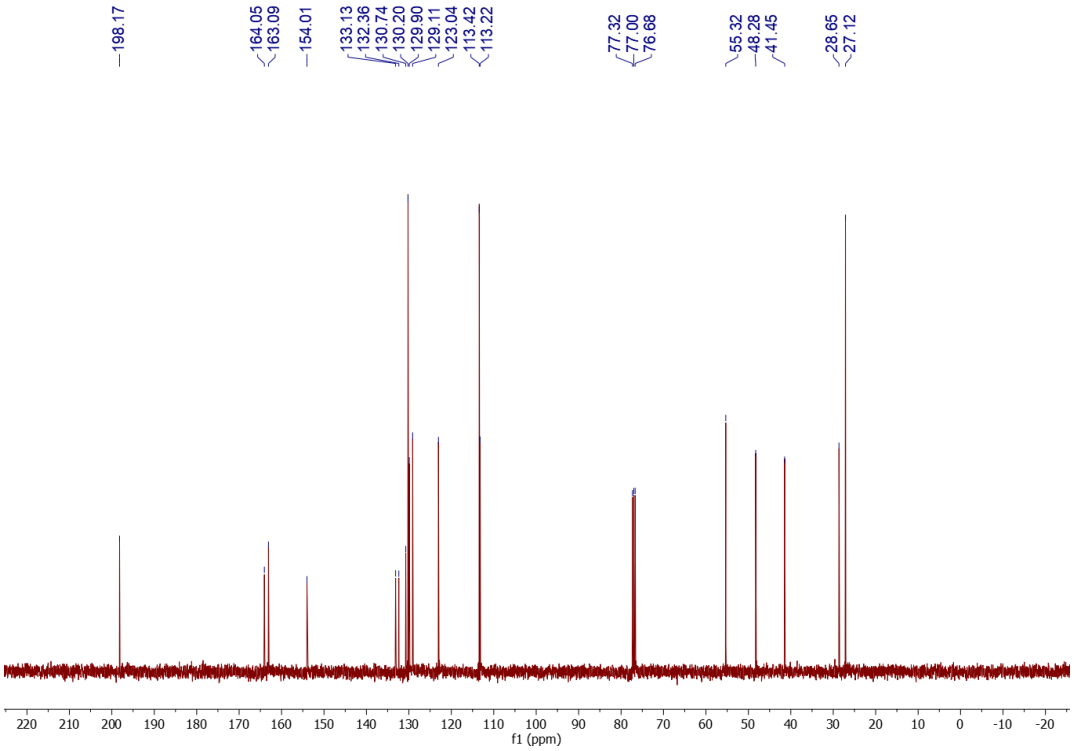


^{13}C NMR (100 MHz, CDCl$_3$)

3-(4-(4-methoxyphenyl)-2-methyl-4-oxobutan-2-yl)-1-methylquinoxalin-2(1*H*)-one(3ra)

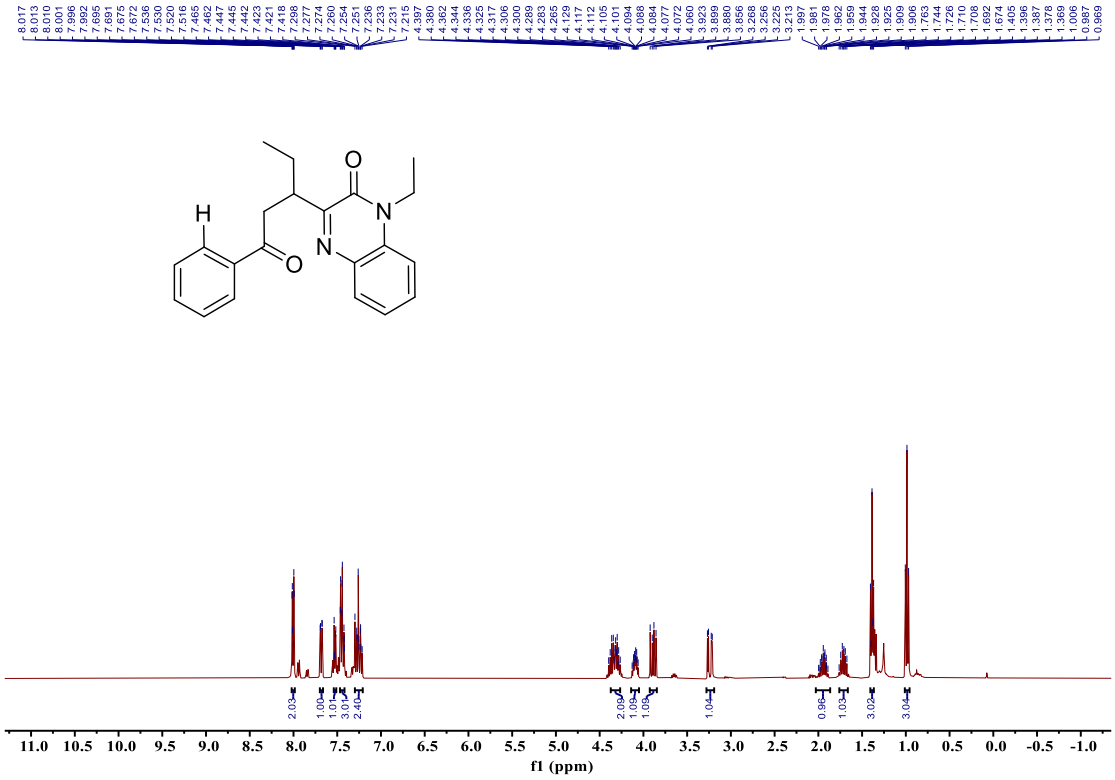


^{1}H NMR (400 MHz, CDCl$_3$)

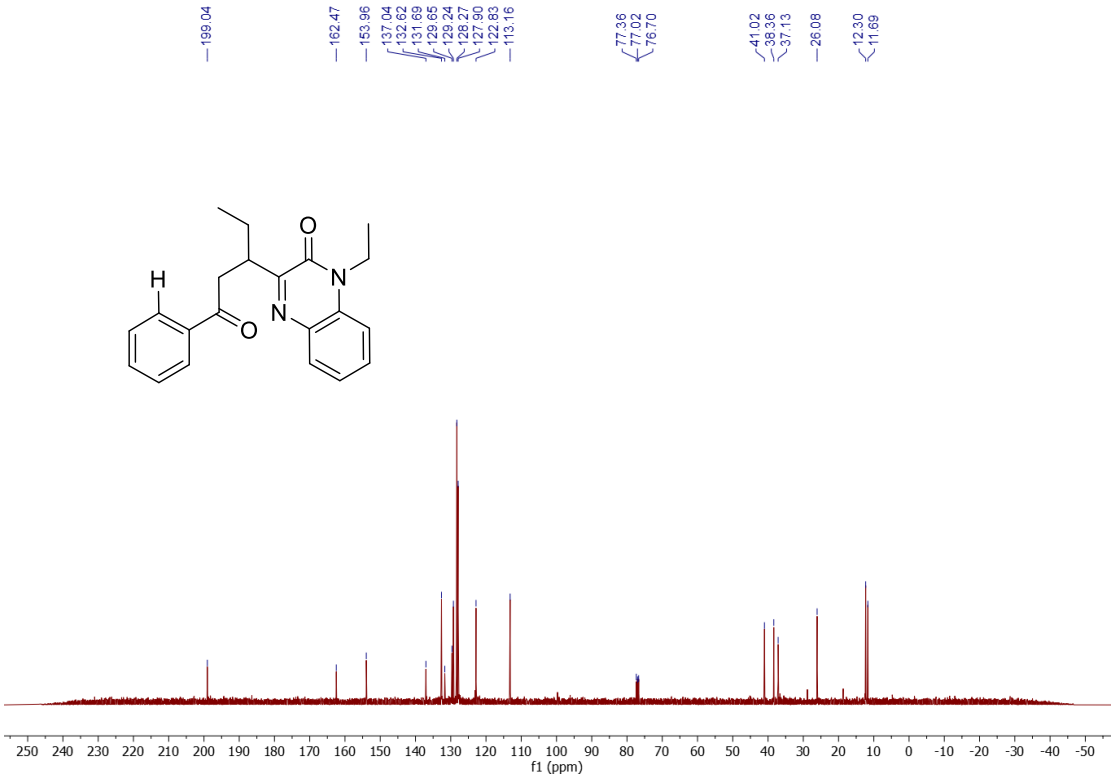


^{13}C NMR (100 MHz, CDCl$_3$)

1-ethyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ab)

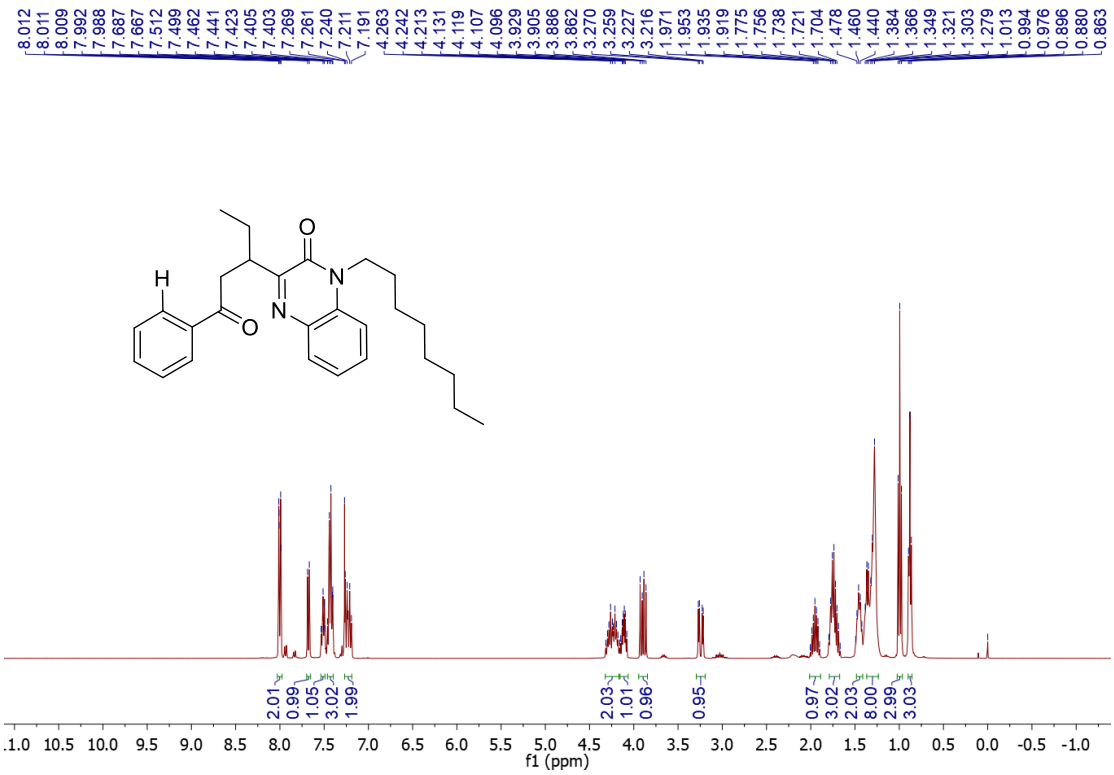


^{1}H NMR (400 MHz, $CDCl_3$)

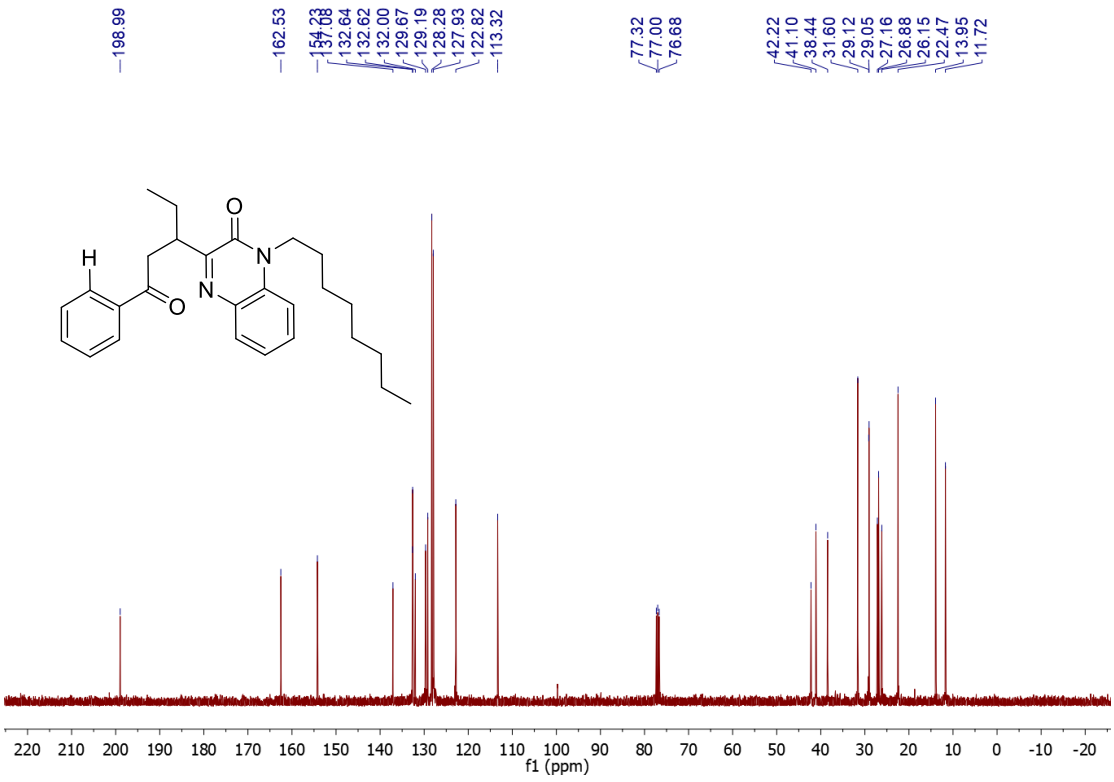


^{13}C NMR (100 MHz, $CDCl_3$)

1-heptyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ac)

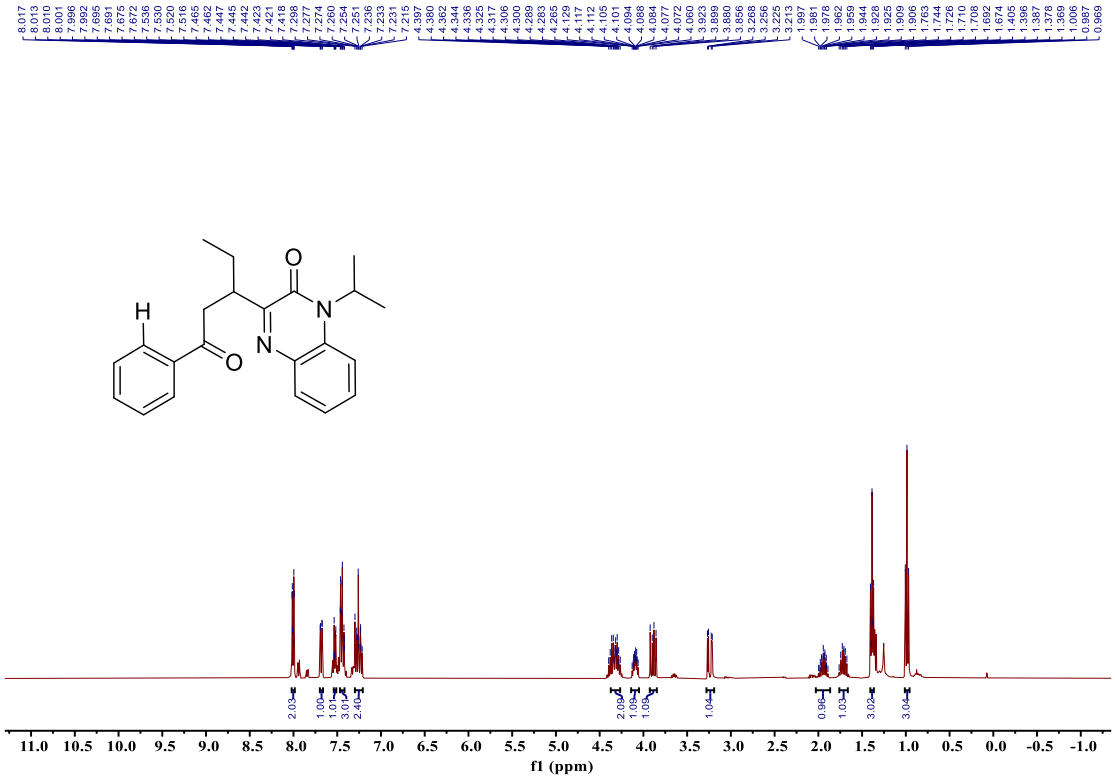


^{1}H NMR (400 MHz, CDCl$_3$)

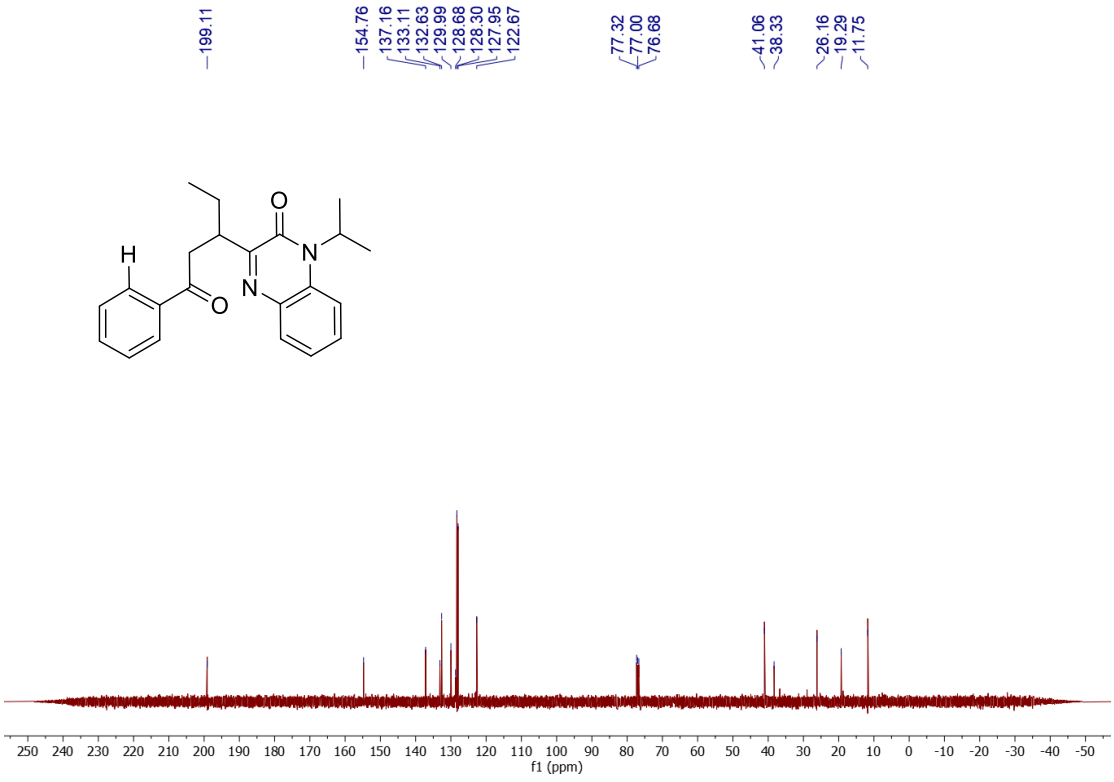


^{13}C NMR (100 MHz, CDCl$_3$)

1-isopropyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ad)

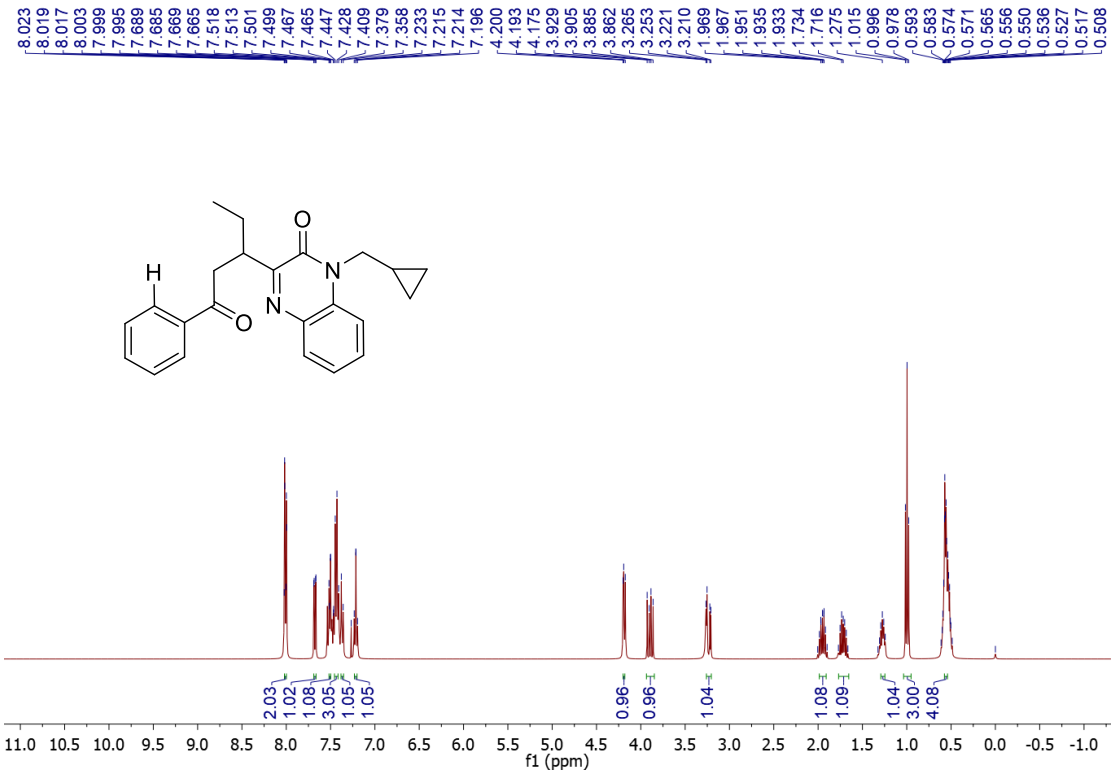


^{1}H NMR (400 MHz, $CDCl_3$)

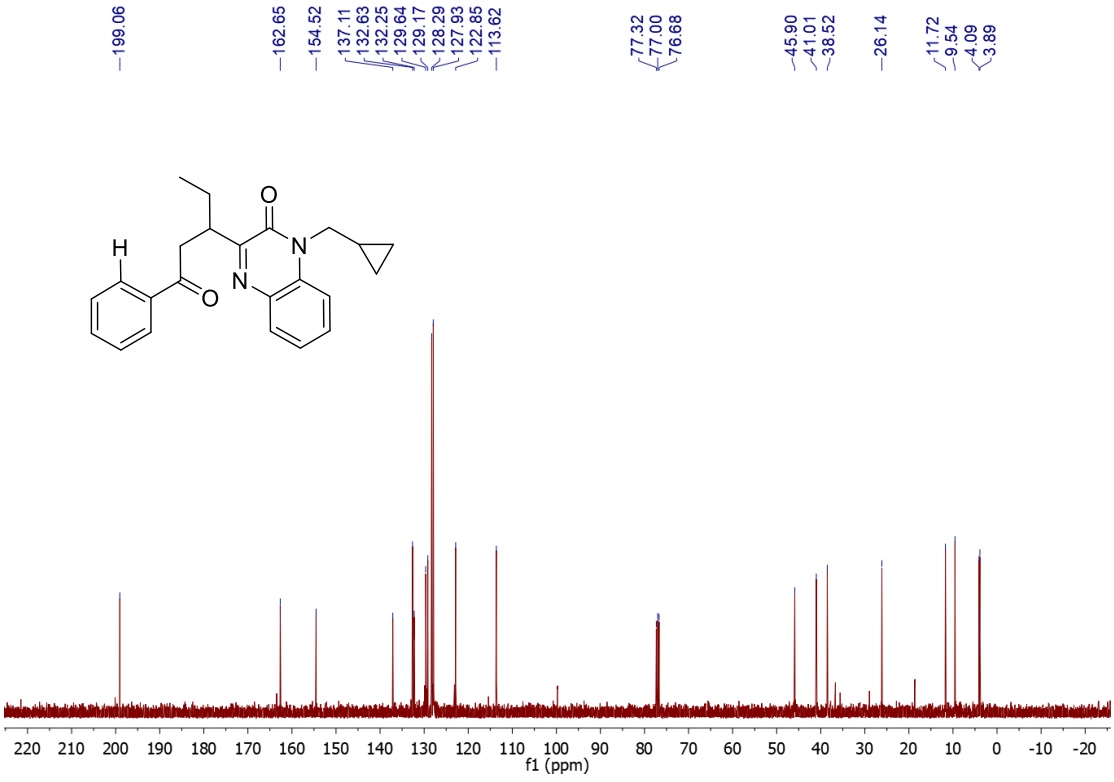


^{13}C NMR (100 MHz, $CDCl_3$)

1-(cyclopropylmethyl)-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ae)

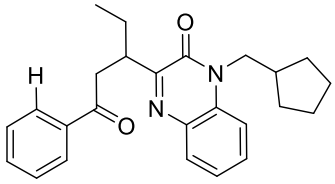


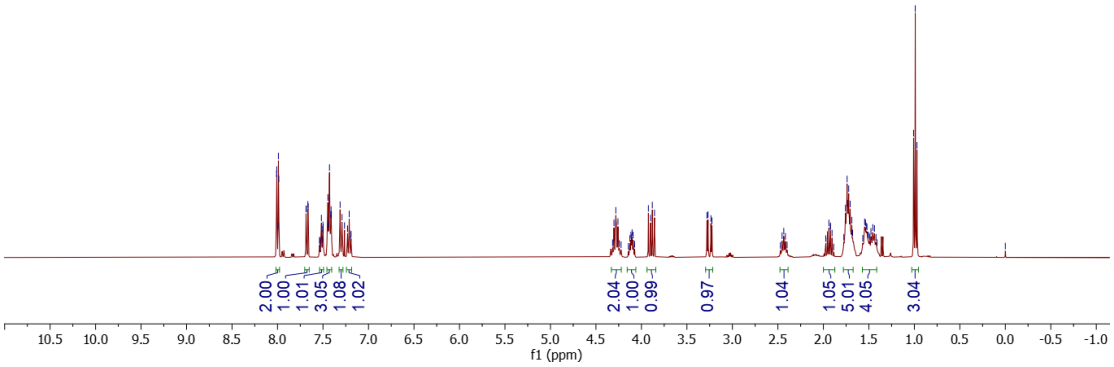
^{1}H NMR (400 MHz, CDCl$_3$)



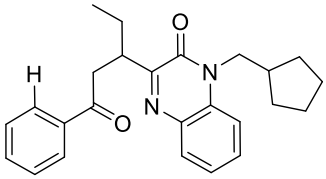
^{13}C NMR (100 MHz, CDCl$_3$)

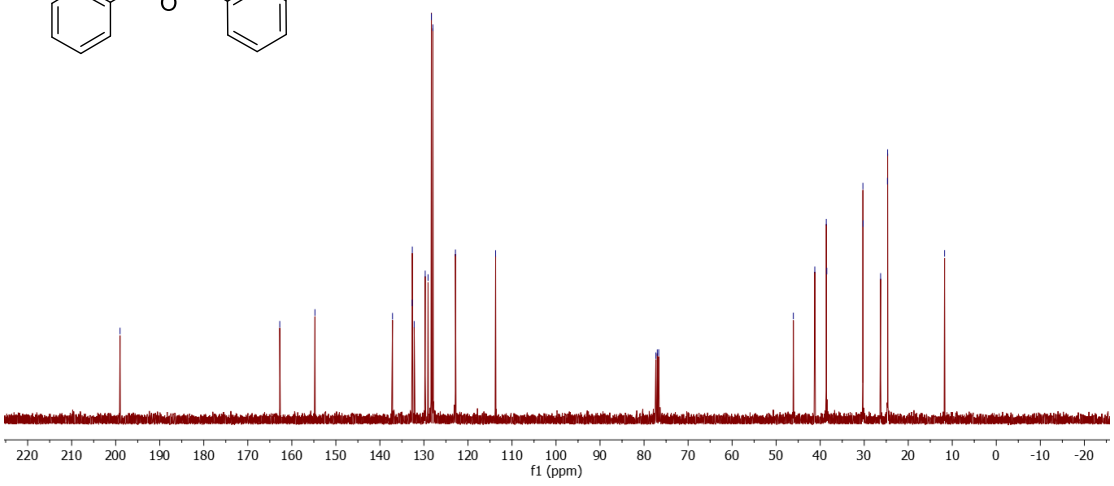
1-(cyclopentylmethyl)-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3af)





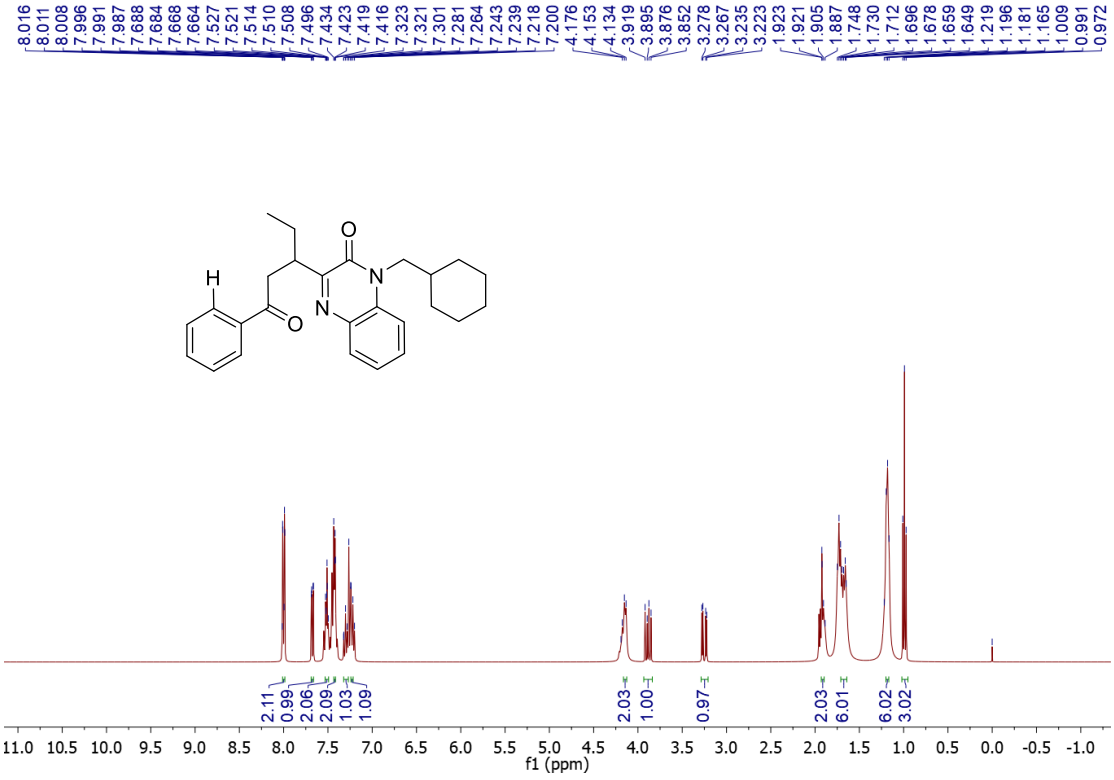
^{1}H NMR (400 MHz, $CDCl_3$)



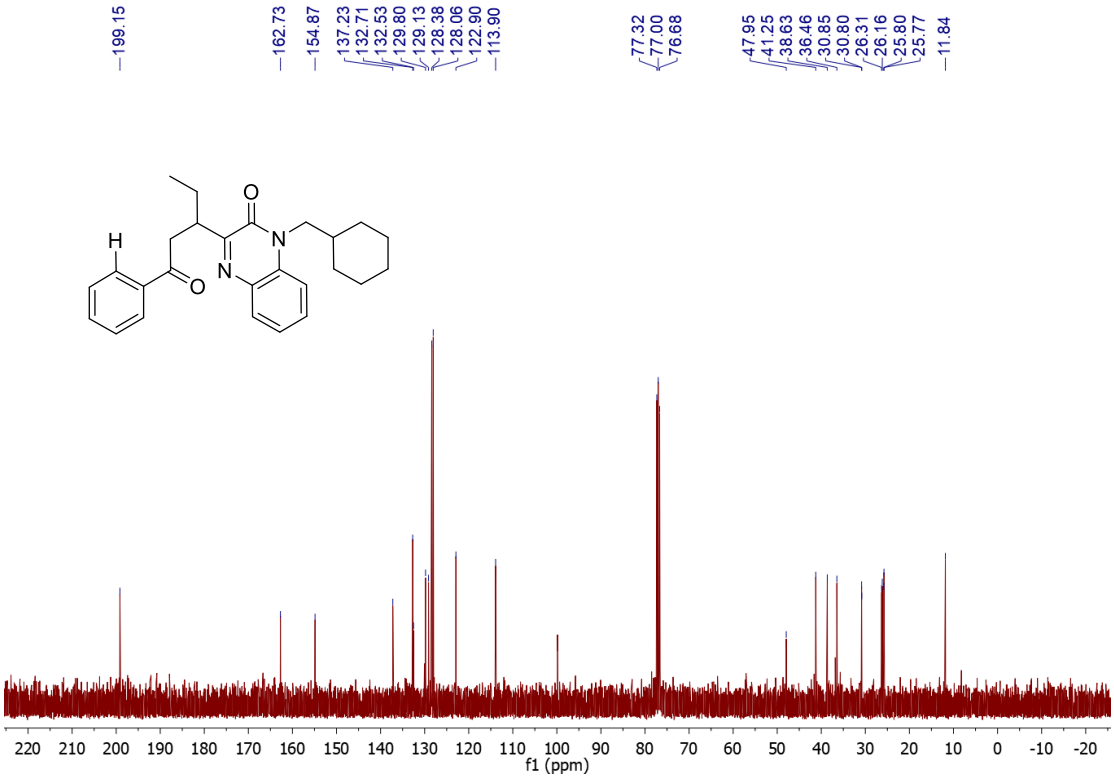


^{13}C NMR (100 MHz, $CDCl_3$)

1-(cyclohexylmethyl)-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ag)

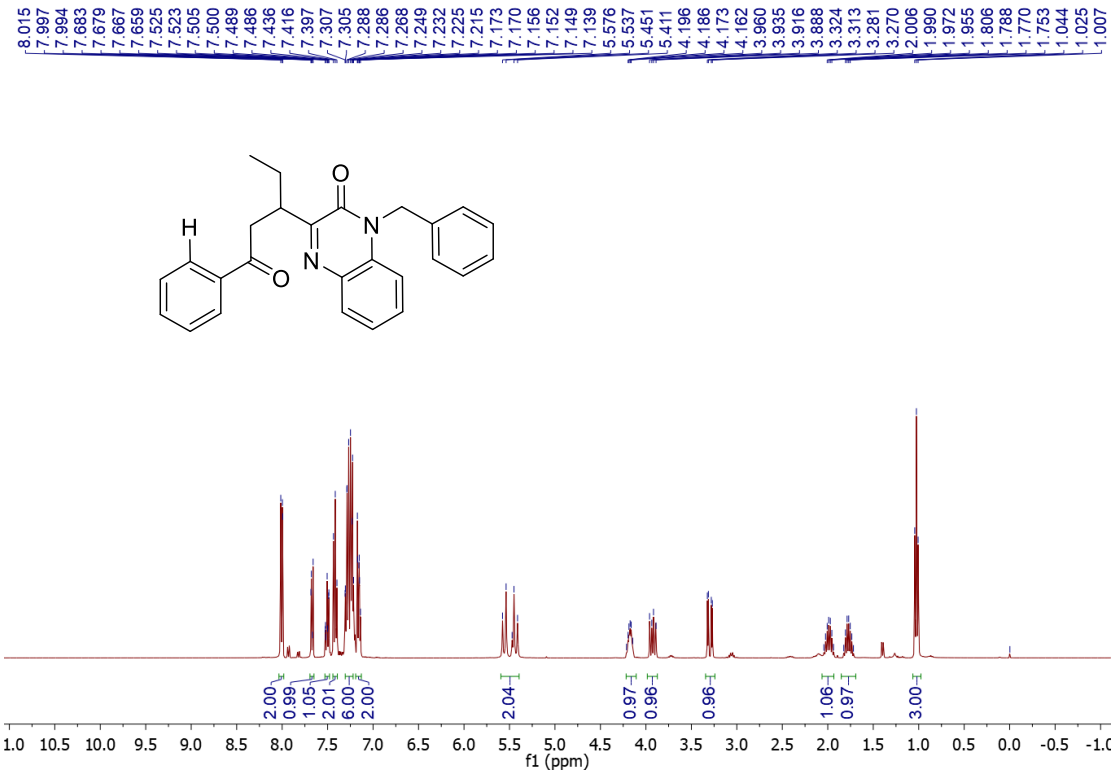


^{1}H NMR (400 MHz, CDCl$_3$)

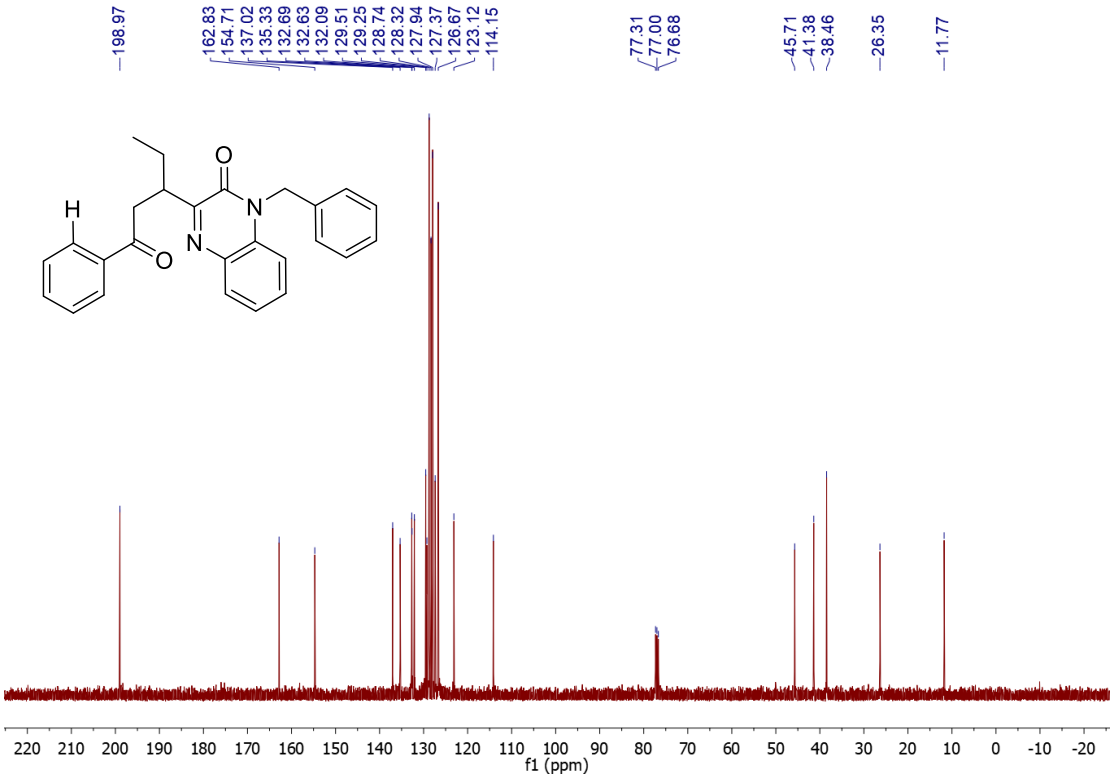


^{13}C NMR (100 MHz, CDCl$_3$)

1-benzyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ah)

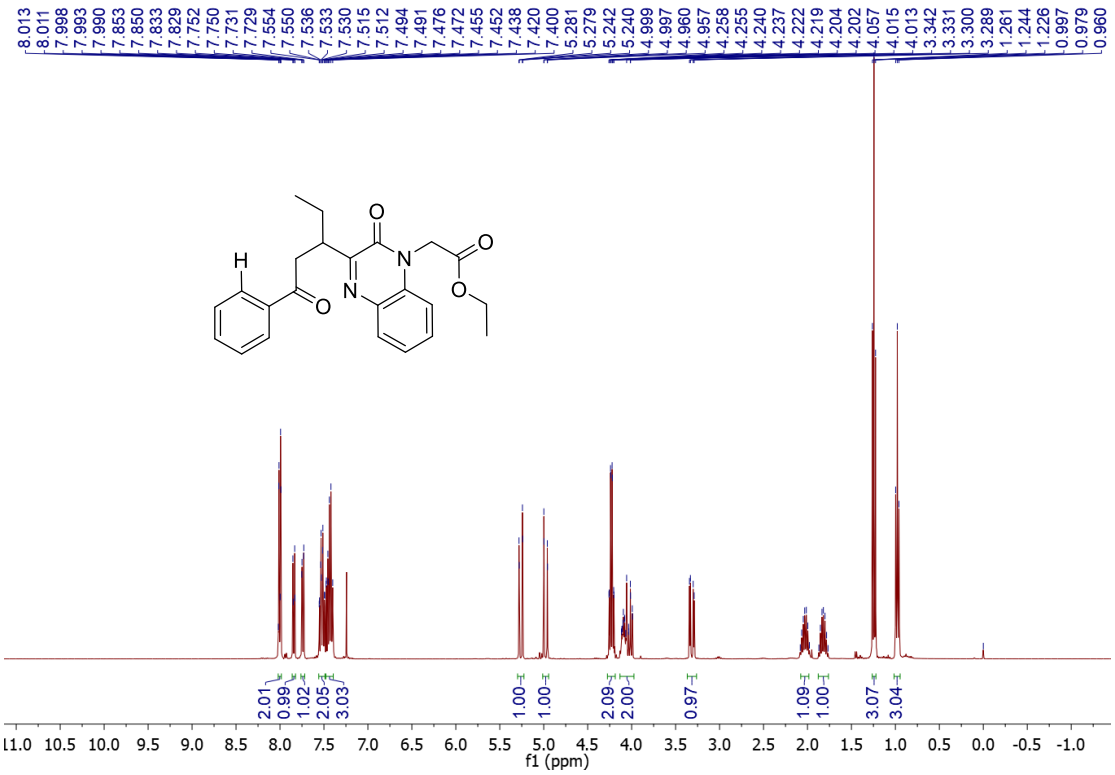


^{1}H NMR (400 MHz, CDCl$_3$)

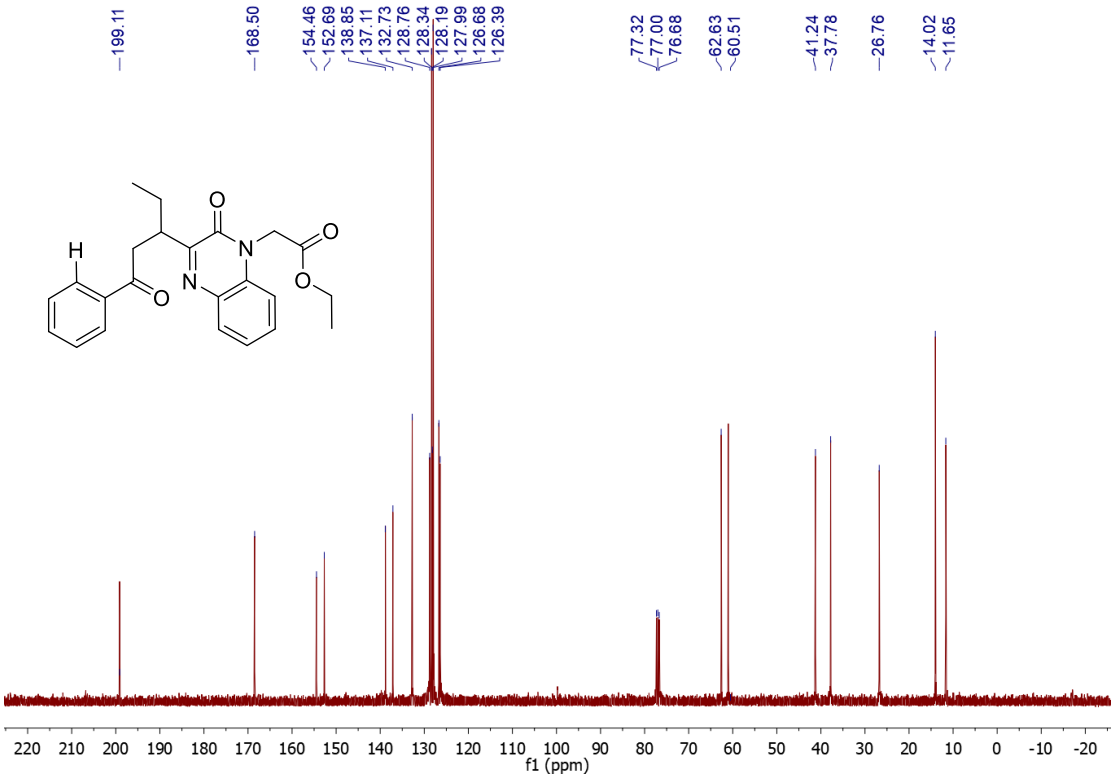


^{13}C NMR (100 MHz, CDCl$_3$)

Ethyl-2-(2-*oxo*-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-1(2*H*)-yl)acetate (3ai)



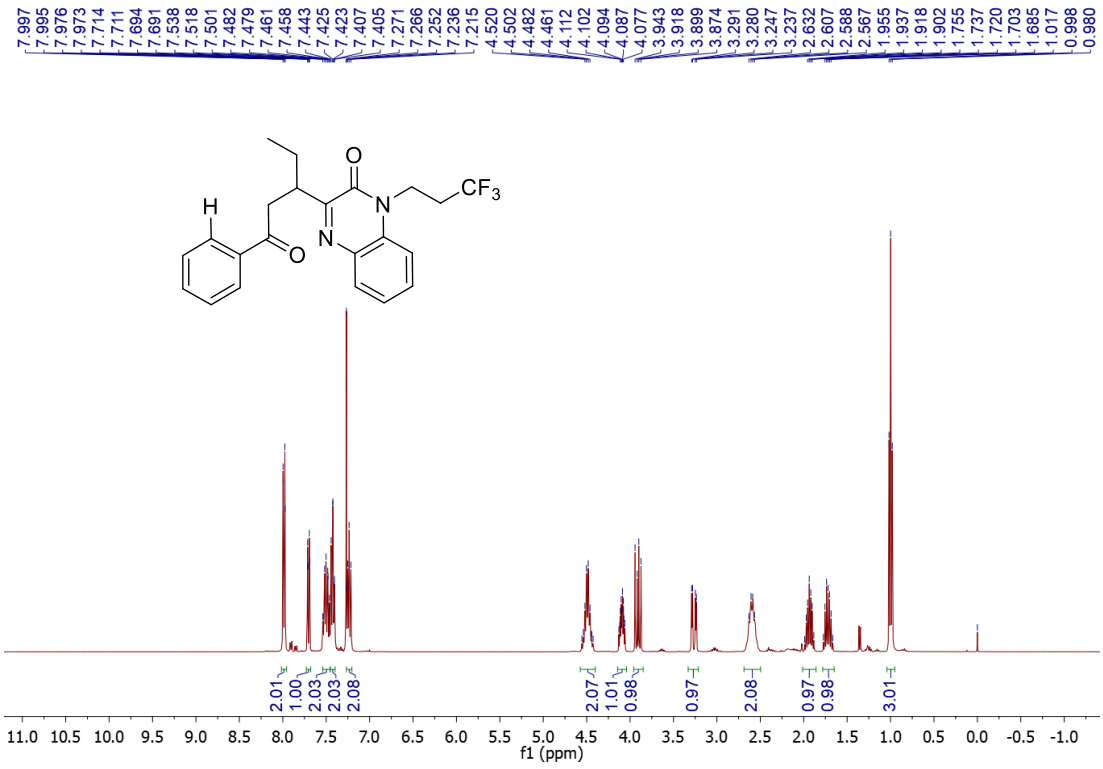
^{1}H NMR (400 MHz, $CDCl_3$)



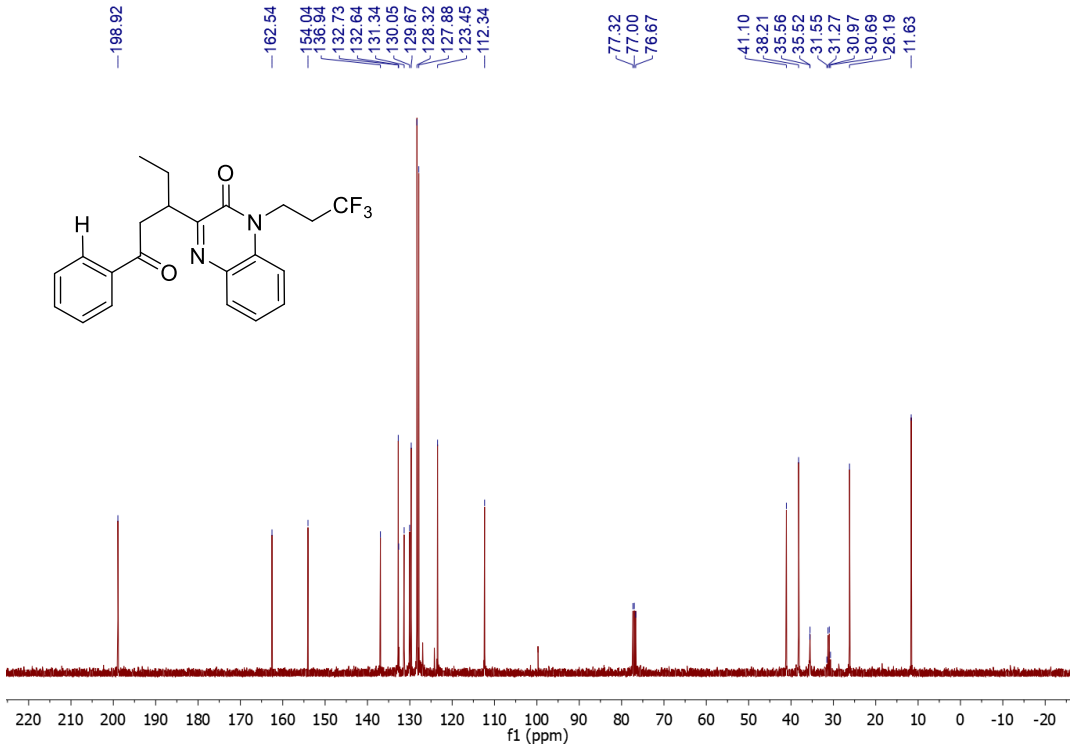
^{13}C NMR (100 MHz, $CDCl_3$)

2-(1-*oxo*-1-phenylpentan-3-yl)-1-(3,3,3-trifluoropropyl)quinoxalin-2(1*H*)-one

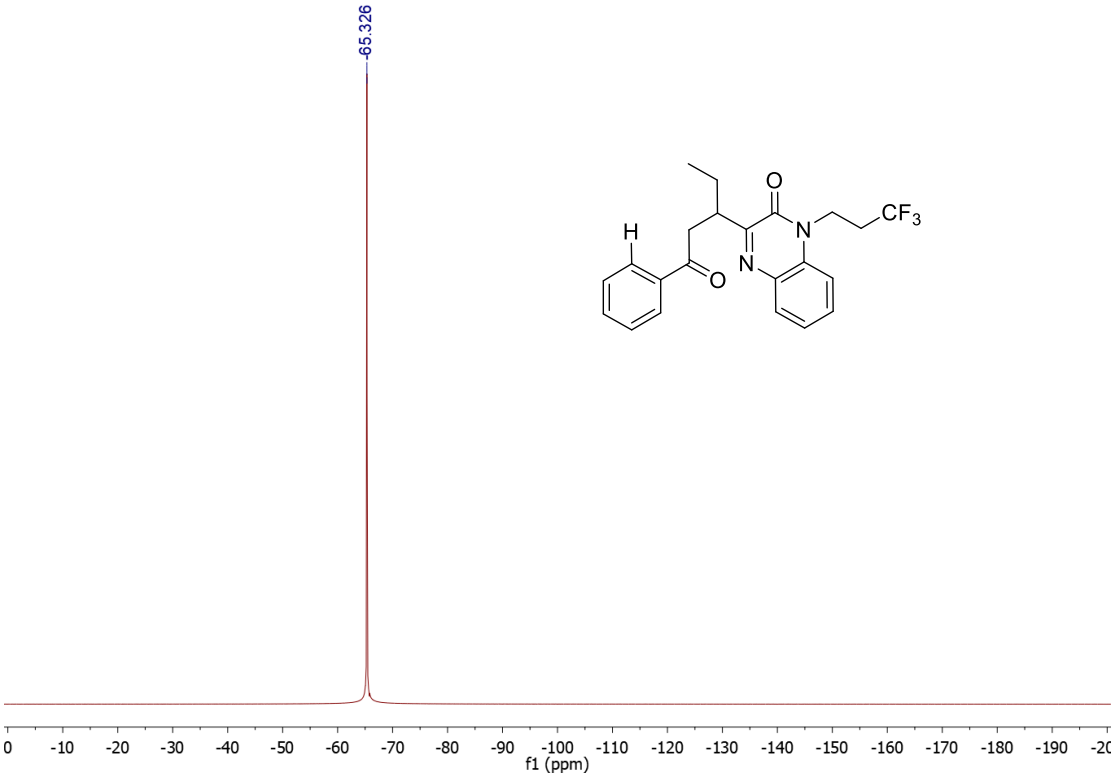
(3aj)



^{1}H NMR (400 MHz, CDCl$_3$)

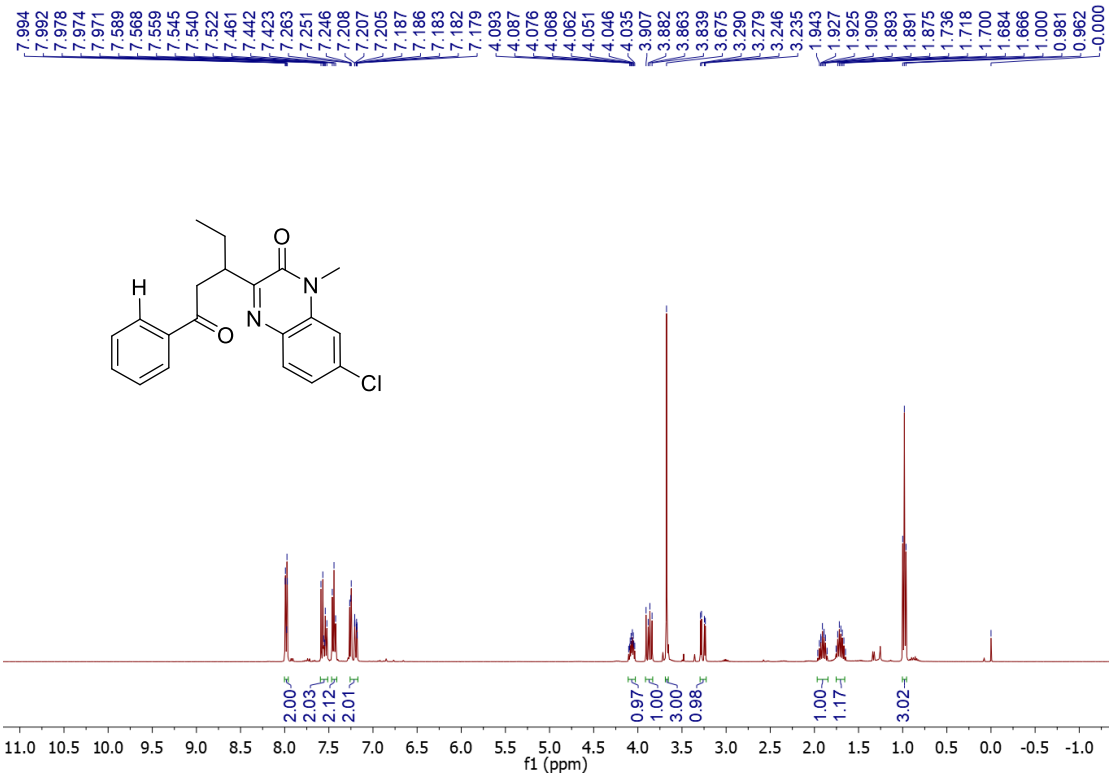


^{13}C NMR (100 MHz, CDCl$_3$)

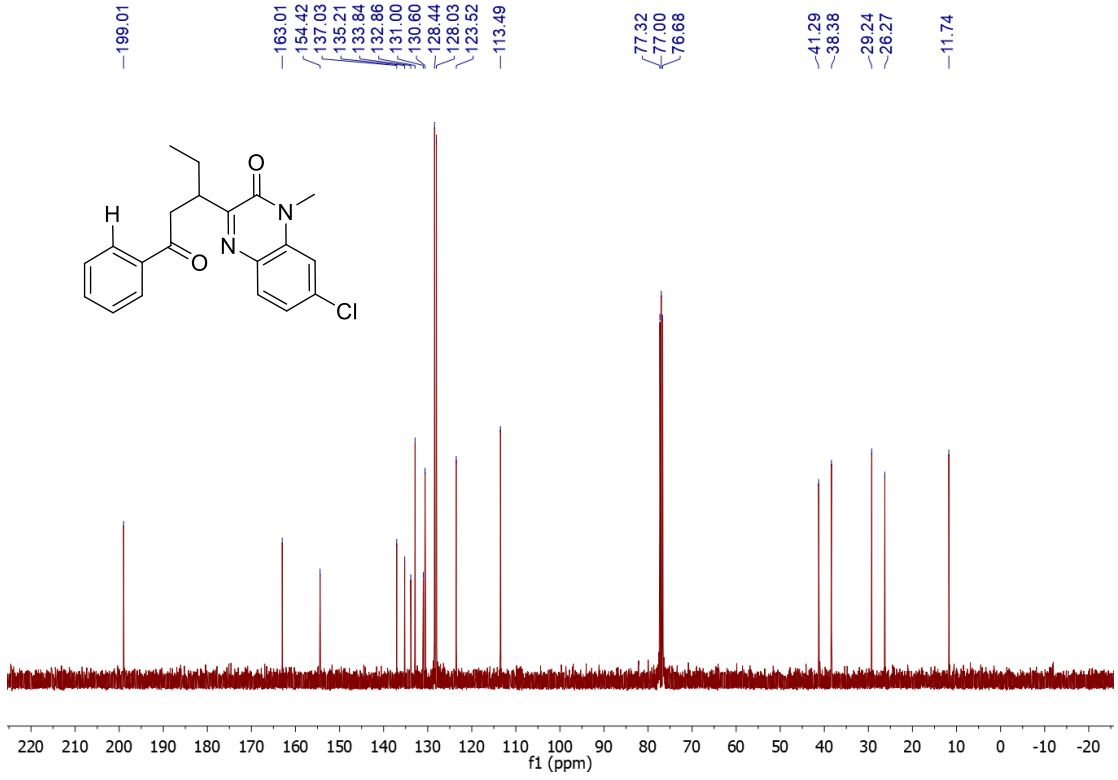


^{19}F NMR (376 MHz, $CDCl_3$)

7-chloro-1-methyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3ak)

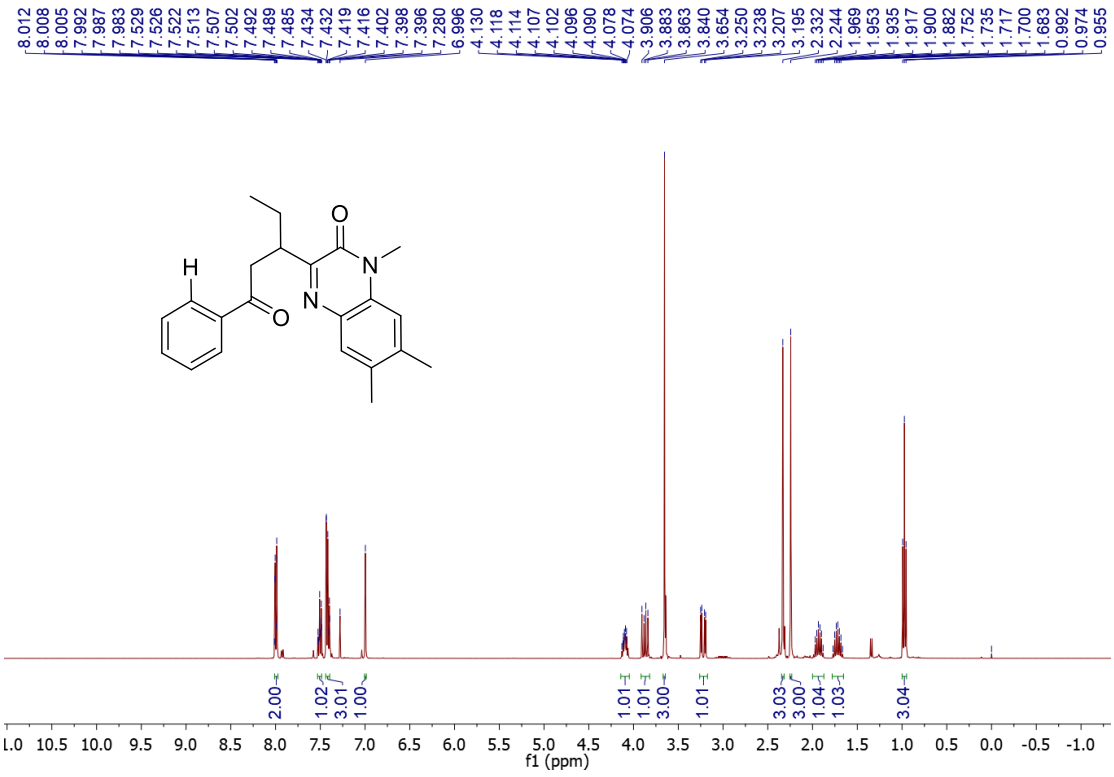


^{1}H NMR (400 MHz, CDCl$_3$)

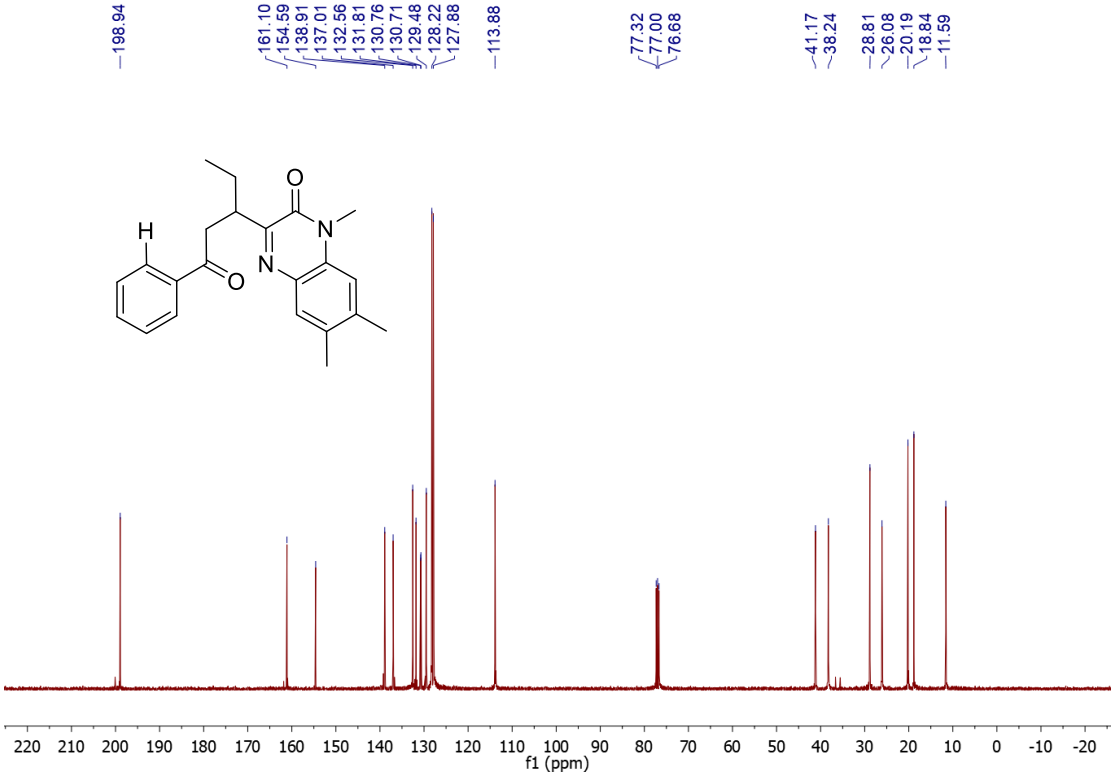


^{13}C NMR (100 MHz, CDCl$_3$)

1,6,7-trimethyl-3-(1-*oxo*-1-phenylpentan-3-yl)quinoxalin-2(1*H*)-one (3al)

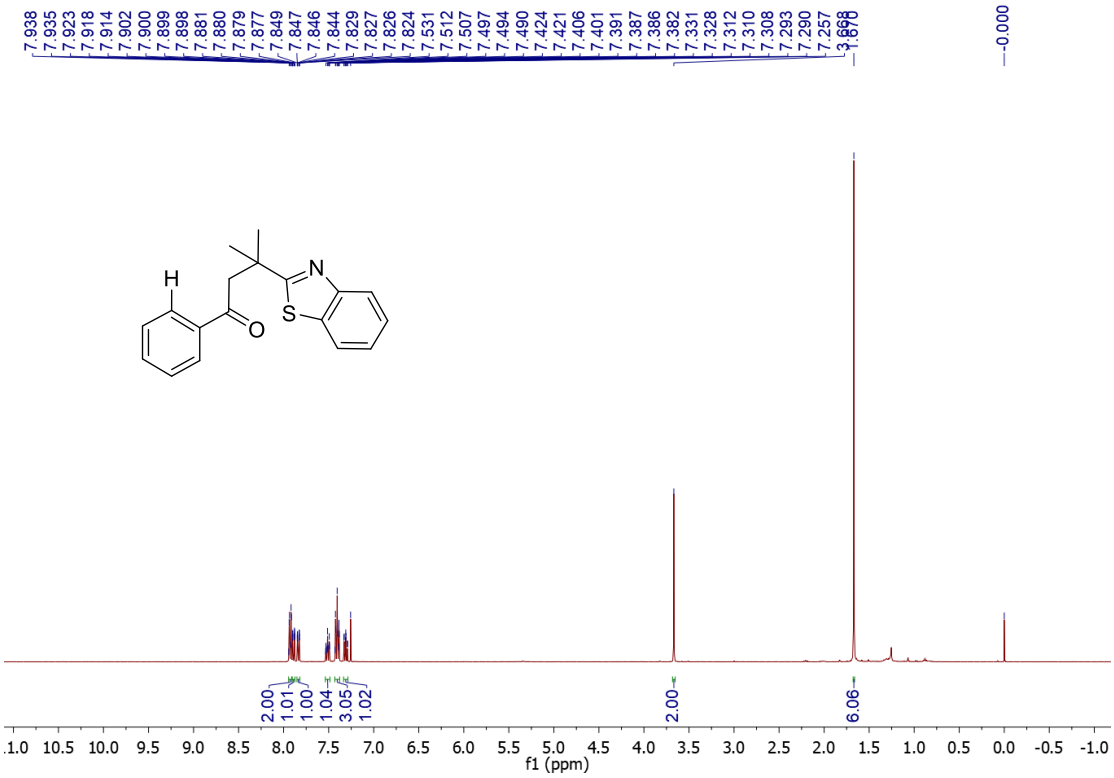


^{1}H NMR (400 MHz, $CDCl_3$)

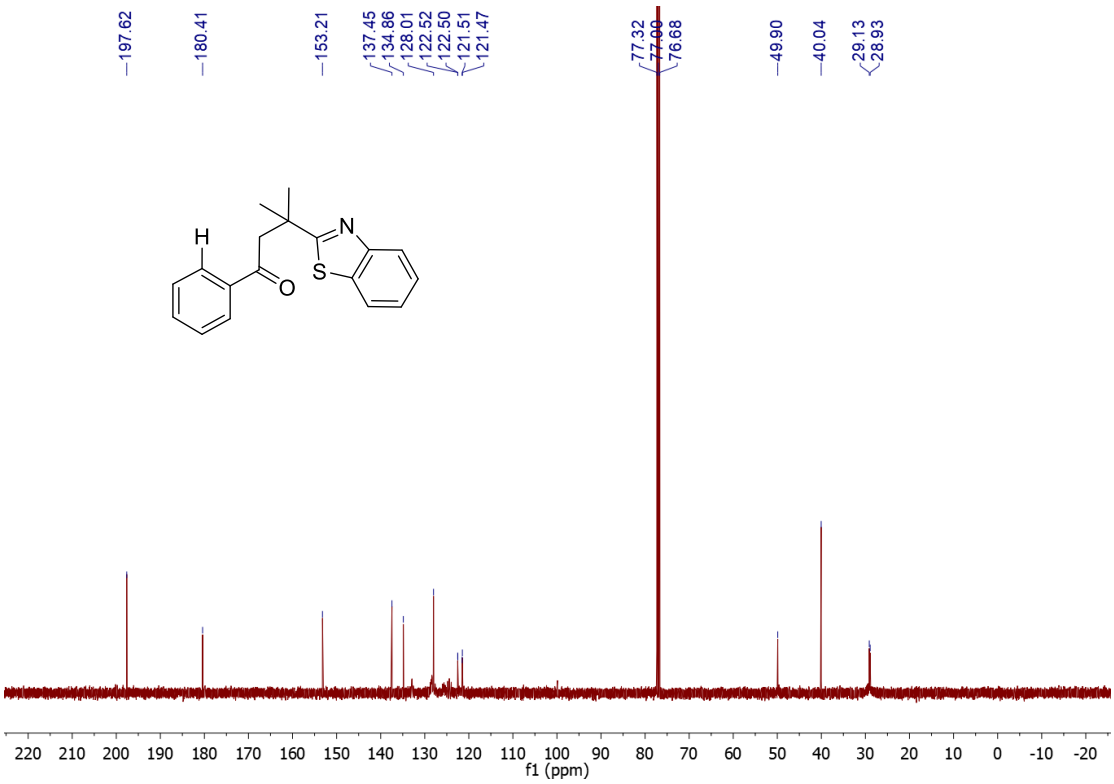


^{13}C NMR (100 MHz, $CDCl_3$)

2-(benzo[d]thiazol-2-yl)-3-methyl-1-phenylbutan-1-one (3am)



^{1}H NMR (400 MHz, CDCl$_3$)



^{13}C NMR (100 MHz, CDCl$_3$)

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