Supporting information

Visible-light-promoted Acridine Red catalyzed aerobic oxidative decarboxylative acylation of α-oxo-carboxylic acids with quinoxalin-2(1H)-ones

Pengli Bao,[a] Fei Liu,[a] Yufen Lv,[a] Huilan Yue,[b*] Jiang-Sheng Li,[c] and Wei Wei[*a,b]

[a]*School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, Shandong, China*

[b]*Qinghai Provincial Key Laboratory of Tibetan Medicine Research and Key Laboratory of Tibetan Medicine Research, Northwest Institute of Plateau Biology, Chinese Academy of Sciences, Qinghai 810008, China*

[c]*School of Chemistry and Food Engineering, Changsha University of Science and Technology, Changsha, 410114, P. R. China*

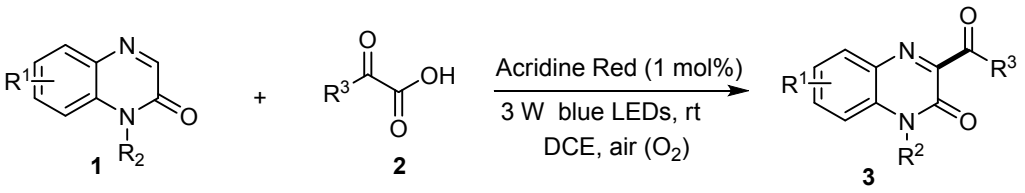
**E-mail: weiweiqfnu@163.com; hlyue@nwipb.cas.cn*

Table of Content

1. General information

All commercially available reagent grade chemicals were purchased from Aldrich, Acros, Alfa Aesar and Energy Chemical Company and used as received without further purification unless otherwise stated. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a Bruker Avance III spectrometer with TMS as internal standard (500 MHz ^{1}H, 125 MHz ^{13}C) at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Mass analyses and HRMS were obtained on a Finnigan-LCQDECA mass spectrometer and a Bruker Daltonics Bio-TOF-Q mass spectrometer by the ESI method, respectively. Column chromatography was performed on silica gel (200-300 mesh).

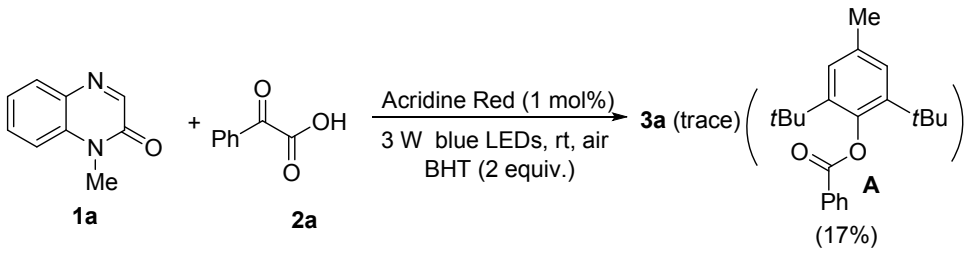
2. General procedure for visible-light-mediated oxidative decarboxylative acylation of α-oxo-carboxylic acids with quinoxalin-2(1H)-ones leading to 3-acyl quinoxalin-2(1H)-ones.



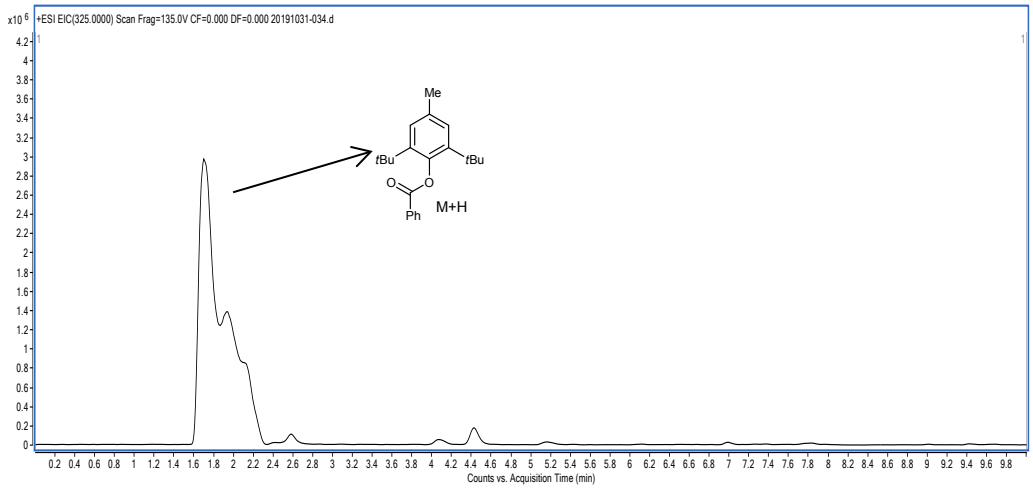
To a solution of quinoxalin-2(H)-one **1** (0.2 mmol), Acridine Red (0.002 mmol, 1 mol %), and DCE (2 mL) was added keto acid **2** (0.4 mmol). The reaction mixture was opened to the air and stirred under the irradiation of 3 W blue LEDs at room temperature for 8 h. After completion of the reaction, the solvent was concentrated under reduced pressure and the crude mixtures were purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate (5:1) as eluent to give the desired products **3**.

3. Preliminary mechanistic studies

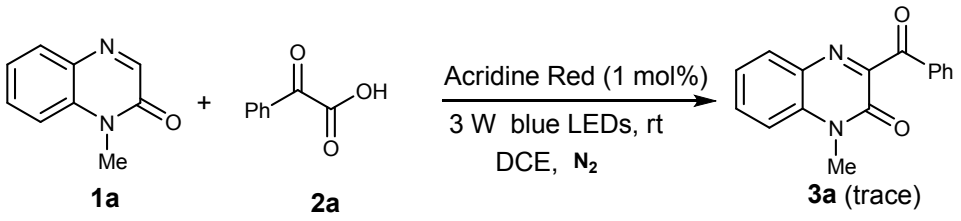
3.1 The addition of BHT in the model reaction system.



To a solution of 1-methylquinoxalin-2(1H)-one **1a** (0.1 mmol), BHT (0.2 mmol), Acridine Red (0.001 mmol, 1 mol %), and DCE (2 mL) was added 2-oxo-2-phenylacetic acid **2a** (0.2 mmol). The reaction mixture was opened to the air and stirred under the irradiation of 3 W white LEDs at room temperature for 8 h. Only a trace amount of desired product **3a** was detected and BHT-trapped complex (A) was detected.

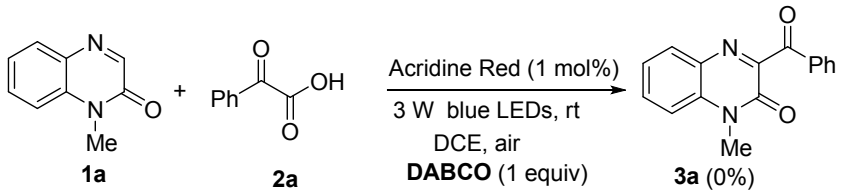


3.3 The model reaction was carried under N_2.



Under N_2 atmosphere, to a mixture of 1-methylquinoxalin-2(1*H*)-one **1a** (0.1 mmol), 2-oxo-2-phenylacetic acid **2a** (0.2 mmol) and Acridine Red (0.001 mmol, 1 mol %) was added DCE (2 mL). Then, the reaction mixture was stirred under the irradiation of 3W blue LEDs at room temperature for 8 h. After completion of the reaction, the solution was concentrated in vacuum. Only a trace amount of the desired product **3a** was detected.

3.4 The $^1O_2$ inhibition experiment.



To a solution of 1-methylquinoxalin-2(1H)-one **1a** (0.2 mmol), DABCO (0.2 mmol), Acridine Red (0.002 mmol, 1 mol %), and DCE (2 mL) was added 2-oxo-2-phenylacetic acid **2a** (0.4 mmol). The reaction mixture was opened to the air and stirred under the irradiation of 3 W blue LEDs at room temperature for 8 h. None of the desired product **3a** was detected.

3.5 The UV-visible spectroscopy and Fluorescence quenching studies (Stern–Volmer Studies)

UV-visible spectroscopy of reaction solution was recorded on a SHIMADZU UV-3600 UV-visible spectrophotometer. The sample was prepared by mixing Acridine Red, 2-oxo-2-phenylacetic acid and 1-methylquinoxalin-2(1H)-one with solvent V[DCE] = 2 mL, (M[Acridine Red] = 1.0×10^{-5} mol/L, M[1-methylquinoxalin-2(1H)-

one] = 1×10^{-3} mol/L, M[2-oxo-2-phenylacetic acid] = 2×10^{-3} mol/L in a light path quartz UV cuvette. The UV-visible spectroscopy indicated that the maximum absorption wavelength of reaction solution was found to be 521 nm. The absorption was collected and the result was listed in Figure S1.

The fluorescence emission intensity of reaction solution was recorded on a Fluoromax-4600 spectrofluorimeter. The excitation wavelength was fixed at 521 nm, and the emission wavelength was measured at 557 nm. The sample was prepared by mixing Acridine Red, 1-methylquinoxalin-2(1H)-one, 2-oxo-2-phenylacetic acid with solvent (V[DCE] = 2 mL) (M[Acridine Red] = 1.0×10^{-5} mol/L, M[1-methylquinoxalin-2(1H)-one] = 1×10^{-5} mol/L, M[2-oxo-2-phenylacetic acid] = 2.0×10^{-5} mol) in a light path quartz fluoresence cuvette. The emission intensity was collected and the result was listed in Figure S2.

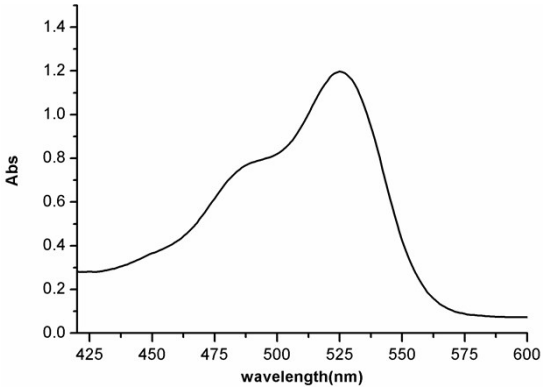


Figure S1. UV–vis spectrum of the reaction mixture.

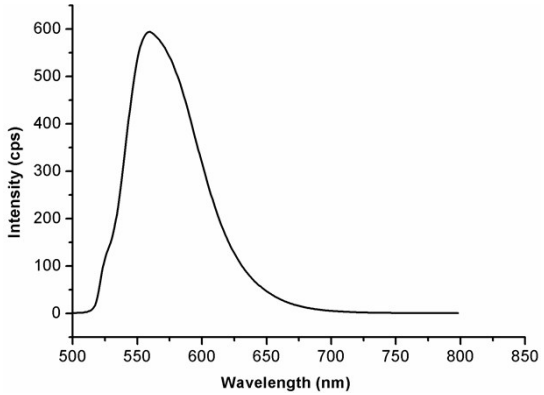


Figure S2. Fluorescence spectrum of the reaction mixture.

The fluorescence emission intensities were recorded on a Fluormax-4600 spespectrofluorimeter. The excitation wavelength was fixed at 521nm, and the emission

wavelength was measured at 556 nm (emission maximum). The samples were prepared by mixing by Acridine Red (1.0×10^{-5} mol/L) and different amount of 2-oxo-2-phenylacetic acid **2a** in DCE (total volume = 0.2 mL) in a light path quartz fluorescence cuvette. The concentration of 2-oxo-2-phenylacetic acid **2a** stock solution is 2.0×10^{-6} mol/L in DCE. For each quenching experiment, 0.1 mL of 2-oxo-2-phenylacetic acid stock solution was titrated to a mixed solution of 0.1 mL Rose Bengal (in a total volume = 0.2 mL). Then the emission intensity was collected and the results were presented in Figure S3. An fluorescence quenching phenomenon of Acridine Red under various concentrations of 2-oxo-2-phenylacetic acid was shown in Figure S4 (Stern-Volmer plots).

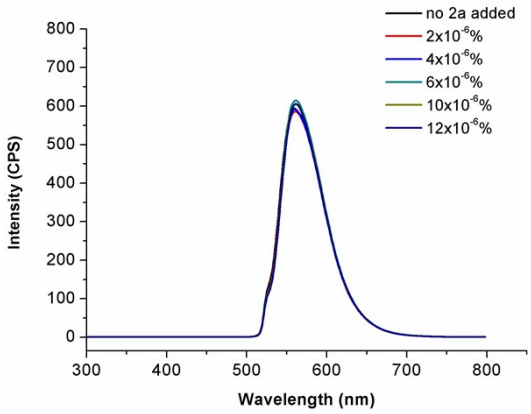


Figure S3. Quenching of Acridine Red fluorescence emission in the presence of 2-oxo-2-phenylacetic acid.

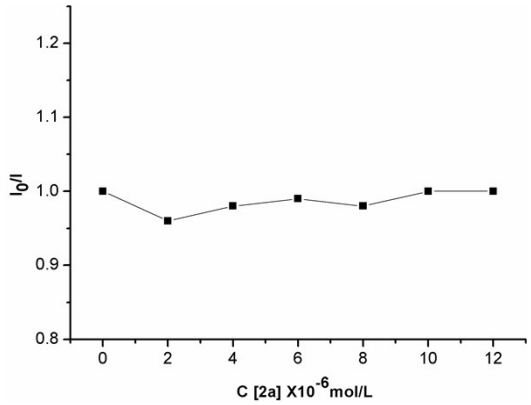
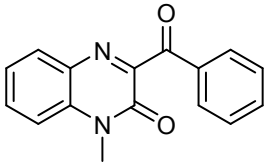
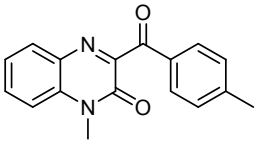


Figure S4. Stern-volmer plots.

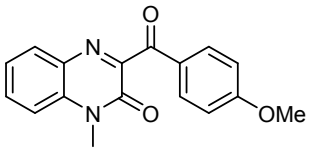
4. Characterization data of products 3a- 3zb



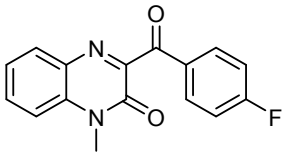
3-benzoyl-1-methylquinoxalin-2(1H)-one[1], Compound **3a** was obtained in 84 % yield according to the general procedure. Yellow solid, mp = 189.9°C – 190.2 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.99 (d, J = 7.7 Hz, 2H), 7.94 (d, J = 8.1 Hz, 1H), 7.69 (t, J = 7.8 Hz, 1H), 7.63 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.6 Hz, 2H), 7.42 (t, J = 7.6 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 191.8, 154.7, 153.4, 134.9, 134.3, 133.9, 132.2, 132.1, 131.1, 130.0, 128.7, 124.3, 114.0, 29.1; MS (EI); $[M+H]^+$: 265.1.



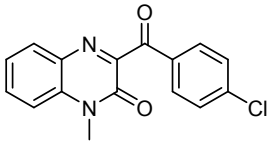
1-methyl-3-(4-methylbenzoyl)quinoxalin-2(1H)-one[1], Compound **3b** was obtained in 81 % yield according to the general procedure. Yellow solid, mp = 213.0°C – 213.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, J = 7.5 Hz, 1H), 7.88 (d, J = 8.1 Hz, 2H), 7.67 (t, J = 7.5 Hz, 1H), 7.41 (t, J = 7.4 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 3.75 (s, 3H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 191.4, 155.0, 153.4, 145.4, 133.9, 132.5, 132.3, 132.0, 130.2, 129.4, 129.2, 124.2, 114.0, 29.1, 21.9; MS (EI); $[M+H]^+$: 279.1.



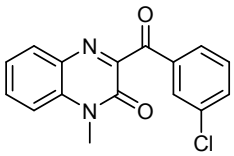
3-(4-methoxybenzoyl)-1-methylquinoxalin-2(1H)-one[1], Compound **3c** was obtained in 63 % yield according to the general procedure. White solid, mp = 180.1°C – 180.9 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.97 (d, J = 8.8 Hz, 2H), 7.93 (d, J = 8.0 Hz, 1H), 7.67 (t, J = 7.8 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H), 3.75 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.3, 164.6, 155.1, 153.4, 133.9, 132.5, 132.2, 131.9, 131.0, 128.0, 124.2, 114.0, 113.9, 55.6, 29.1; MS (EI); $[M+H]^+$: 295.1.



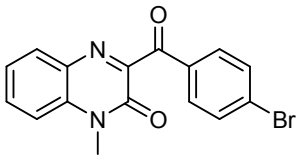
3-(4-fluorobenzoyl)-1-methylquinoxalin-2(1H)-one[2], Compound **3d** was obtained in 72 % yield according to the general procedure. Yellow solid, mp = 158.6°C – 159.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.03 (q, J = 7.7 Hz, 2H), 7.92 (d, J = 8.2 Hz, 1H), 7.69 (t, J = 7.8 Hz, 1H), 7.42 (t, J = 7.6 Hz, 2H), 7.16 (t, J = 8.3 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.11, 154.22, 153.29, 133.93, 132.85, 132.77, 132.25, 132.15, 131.37(d, J = 1.25 Hz) 131.04, 124.30, 115.99 (d, J = 21.25Hz), 114.04, 29.02; MS (EI); $[M+H]^+$: 283.1.



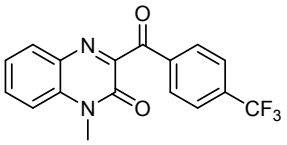
3-(4-chlorobenzoyl)-1-methylquinoxalin-2(1H)-one[1], Compound **3e** was obtained in 82 % yield according to the general procedure. Yellow solid, mp = 155.6°C – 155.9 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.93 – 7.78 (m, 3H), 7.65 – 7.60 (m, 1H), 7.41 – 7.37 (m, 2H), 7.36 – 7.26 (m, 2H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.5, 154.0, 153.3, 140.8, 134.0, 133.3, 132.3, 132.2, 131.4, 131.1, 129.1, 124.3, 114.0, 29.1; MS (EI); $[M+H]^+$: 299.1.



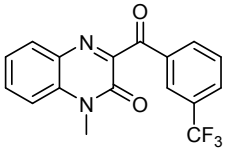
3-(3-chlorobenzoyl)-1-methylquinoxalin-2(1H)-one, Compound **3f** was obtained in 81 % yield according to the general procedure. Yellow solid, mp = 135.7°C – 136.2 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.94 (d, J = 11.7 Hz, 2H), 7.87 (d, J = 7.7 Hz, 1H), 7.70 (t, J = 7.8 Hz, 1H), 7.60 (d, J = 7.9 Hz, 1H), 7.43 (t, J = 8.1 Hz, 3H), 3.76 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.4, 153.8, 153.3, 136.5, 135.0, 134.1, 134.0, 132.4, 132.2, 131.2, 130.1, 129.9, 128.1, 124.4, 114.1, 29.1; MS (EI); $[M+H]^+$: 299.1.



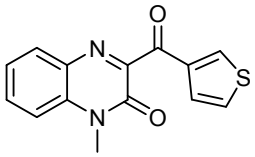
3-(4-bromobenzoyl)-1-methylquinoxalin-2(1H)-one[1], Compound **3g** was obtained in 63 % yield according to the general procedure. Yellow solid, mp = 145.6°C – 145.9 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.93 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.5 Hz, 2H), 7.72 – 7.66 (m, 1H), 7.63 (d, J = 8.5 Hz, 2H), 7.42 (t, J = 8.7 Hz, 2H), 3.76 (s, 3H).; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.7, 154.0, 153.3, 134.0, 133.7, 132.3, 132.2, 132.1, 131.4, 131.1, 129.7, 124.3, 114.0, 29.1; MS (EI); $[M+H]^+$: 343.0.



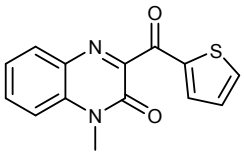
1-methyl-3-(4-(trifluoromethyl)benzoyl)quinoxalin-2(1H)-one, Compound **3h** was obtained in 71% yield according to the general procedure. Yellow solid, mp = 158.6°C – 159.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.11 (d, J = 8.1 Hz, 2H), 7.94 (d, J = 7.9 Hz, 1H), 7.80 – 7.67 (m, 3H), 7.44 (t, J = 8.3 Hz, 2H), 3.77 (s, 3H).; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.62, 153.54, 153.27, 137.68, 135.30, 135.04, 134.04 132.57, 132.17, 131.23, 130.27, 125.73 (q, J = 3.75 Hz), 124.43, 114.09, 29.15; MS (EI); $[M+H]^+$: 333.1.



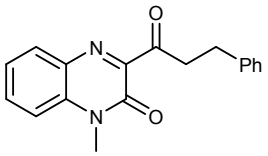
1-methyl-3-(3-(trifluoromethyl)benzoyl)quinoxalin-2(1H)-one, Compound **3i** was obtained in 71 % yield according to the general procedure. Yellow solid, mp = 191.2°C – 191.8 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.19 (s, 1H), 8.10 (d, J = 7.8 Hz, 1H), 7.86 (q, J = 8.4 Hz, 1H), 7.81 (d, J = 7.8 Hz, 1H), 7.67 – 7.61 (m, 1H), 7.56 (t, J = 7.8 Hz, H), 7.38 – 7.35 (m, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.26, 153.39, 153.26, 135.53, 134.06, 133.19, 132.57, 132.13, 131.49, 131.21, 130.47 (q, J = 2.5 Hz), 129.36, 126.73 (q, J = 3.75 Hz), 124.42, 123.58 (d, J = 270 Hz), 114.10, 29.16. MS (EI); $[M+H]^+$: 333.1.



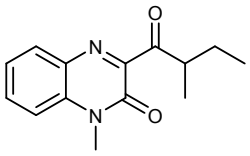
1-methyl-3-(thiophene-3-carbonyl)quinoxalin-2(1H)-one, Compound **3j** was obtained in 55 % yield according to the general procedure. Yellow solid, mp = 133.4°C – 134.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.18 (q, J = 2.8 Hz, 1H), 7.94 (q, J = 8.0 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.45 – 7.36 (m, 3H), 3.76 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 184.7, 153.9, 153.1, 140.0, 136.3, 134.1, 132.3, 132.0, 131.1, 127.8, 126.6, 124.2, 114.0, 29.2; MS (EI); $[M+H]^+$: 271.0.



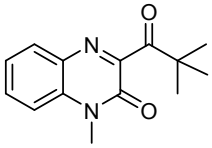
1-methyl-3-(thiophene-2-carbonyl)quinoxalin-2(1H)-one[1], Compound **3k** was obtained in 52 % yield according to the general procedure. Yellow solid, mp = 131.4°C – 131.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.88-7.86 (m, 1H), 7.73 (t, J = 5.2 Hz, 2H), 7.65 – 7.61 (m, 1H), 7.39 – 7.31 (m, 2H), 7.10 – 7.08 (m, 1H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 183.1, 153.0, 152.8, 141.6, 136.2, 136.1, 134.2, 132.5, 131.9, 131.1, 128.4, 124.3, 114.0, 29.2; MS (EI); $[M+H]^+$: 271.0.



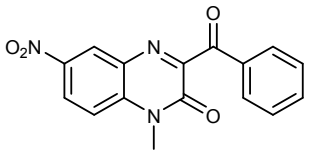
1-methyl-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one, Compound **3l** was obtained in 51 % yield according to the general procedure. Yellow solid, mp = 131.3°C – 132.0 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.92 (dd, J_1= 1.2 Hz, J_2= 8.0 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.39 (t, J = 7.7 Hz, 1H), 7.34 (d, J = 8.5 Hz, 1H), 7.31 – 7.28 (m, 2H), 7.27-7.25 (m, 1H), 7.22 – 7.17 (m, 2H), 3.71 (s, 3H), 3.43 (t, J = 7.5 Hz, 2H), 3.09 (t, J = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 199.7, 152.9, 152.1, 140.9, 134.4, 132.7, 131.4, 128.5, 128.5, 128.3, 126.1, 124.2, 113.9, 42.4, 29.5, 29.1; MS (EI); $[M+H]^+$: 293.1.



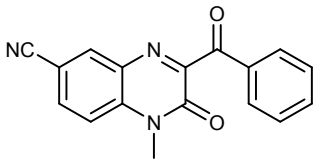
1-methyl-3-(2-methylbutanoyl)quinoxalin-2(1H)-one, Compound **3m** was obtained in 53 % yield according to the general procedure. Yellow solid, mp = 145.7 ^{o}C – 146.9 ^{o}C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.93-7.92 (dd, J_1 = 1.4 Hz, J_2 = 8 Hz, 1H), 7.70 – 7.62 (m, 1H), 7.41 – 7.35 (m, 2H), 3.72 (s, 3H), 3.48-3.43 (m, 1H), 1.90 – 1.83 (m, 1H), 1.57 – 1.50 (m, 1H), 1.24 (d, J = 6.3 Hz, 3H), 0.98 (t, J = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 204.4, 154.0, 153.0, 134.1, 132.2, 132.1, 131.2, 124.1, 113.9, 44.9, 29.0, 25.3, 14.8, 11.5; MS (EI); $[M+H]^+$: 245.1.



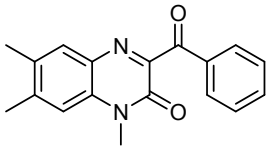
1-methyl-3-pivaloylquinoxalin-2(1H)-one, Compound **3n** was obtained in 72 % yield according to the general procedure. Yellow solid, mp = 199.6^{o}C – 201.7 ^{o}C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.88 (d, J = 8.0, 1H), 7.66 – 7.59 (m, 1H), 7.41 – 7.33 (m, 2H), 3.71 (s, 3H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 208.1, 156.4, 153.0, 133.5, 132.0, 131.4, 130.7, 124.0, 113.9, 44.4, 28.9, 26.4; MS (EI); $[M+H]^+$: 245.1.



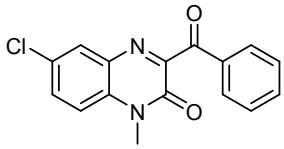
3-benzoyl-1-methyl-6-nitroquinoxalin-2(1H)-one, Compound **3o** was obtained in 62 % yield according to the general procedure. Yellow solid. mp = 199.6^{o}C – 201.7 ^{o}C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.74 (d, J = 2.6 Hz, 1H), 8.46-8.43 (m, 1H), 7.93 – 7.89 (m, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.46-7.43 (m, 3H), 3.74 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.5, 156.9, 152.9, 143.7, 138.3, 134.8, 134.2, 131.2, 130.0, 128.9, 126.7, 126.3, 114.8, 29.7; MS (EI); $[M+H]^+$: 310.1.



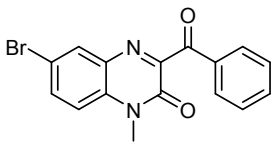
3-benzoyl-1-methyl-2-oxo-1,2-dihydroquinoxaline-6-carbonitrile, Compound **3p** was obtained in 44 % yield according to the general procedure. Yellow solid, mp = 142.9°C – 143.7 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.16 (d, J = 1.7 Hz, 1H), 7.89 (d, J = 7.4 Hz, 2H), 7.83 – 7.81 (m, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.46 – 7.40 (m, 3H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.6, 156.6, 152.9, 137.0, 135.2, 134.7, 134.3, 131.7, 130.0, 128.9, 117.5, 115.2, 108.0, 29.4; MS (EI); $[M+H]^+$: 290.1.



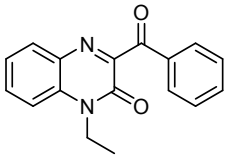
3-benzoyl-1,6,7-trimethylquinoxalin-2(1H)-one[1], Compound **3q** was obtained in 81 % yield according to the general procedure. Yellow solid, mp = 161.0°C – 162.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.97 (d, J = 7.7 Hz, 2H), 7.65 (s, 1H), 7.60 (t, J = 6.9 Hz, 1H), 7.46 (t, J = 7.3 Hz, 2H), 7.16 (s, 1H), 3.71 (s, 3H), 2.45 (s, 3H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 192.1, 153.5, 153.2, 142.6, 135.1, 134.1, 133.4, 132.0, 130.9, 130.6, 130.0, 128.6, 114.5, 29.0, 20.8, 19.2; MS (EI); $[M+H]^+$: 293.1.



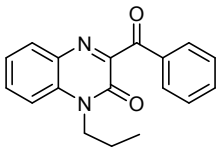
3-benzoyl-6-chloro-1-methylquinoxalin-2(1H)-one[2], Compound **3r** was obtained in 83 % yield according to the general procedure. Yellow solid, mp = 142.0°C – 143.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.90 (d, J = 7.9 Hz, 2H), 7.78 (d, J = 8.5 Hz, 1H), 7.56 (t, J = 7.2 Hz, 1H), 7.42 (t, J = 7.6 Hz, 2H), 7.35 – 7.27 (m, 2H), 3.65 (s, 3H).; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 191.4, 154.6, 153.1, 138.3, 134.8, 134.7, 134.4, 132.1, 130.7, 130.0, 128.8, 124.7, 114.1, 29.2; MS (EI); $[M+H]^+$: 299.0.



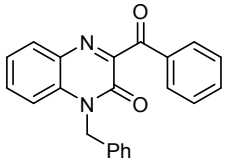
3-benzoyl-6-bromo-1-methylquinoxalin-2(1H)-one[2], Compound **3s** was obtained in 67 % yield according to the general procedure. Yellow solid, mp = 211.7°C – 212.2 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.07 (d, J = 2.2 Hz, 1H), 7.99 – 7.94 (m, 2H), 7.77 – 7.74 (m, 1H), 7.65 – 7.62 (m, 1H), 7.49 (t, J = 7.9 Hz, 2H), 7.29 (d, J = 9.0 Hz, 1H), 3.73 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 191.2, 155.8, 153.0, 134.8, 134.4, 133.3, 133.0, 130.2, 130.0, 128.8, 128.5, 116.8, 115.5, 29.3; MS (EI); $[M+H]^+$: 343.0.



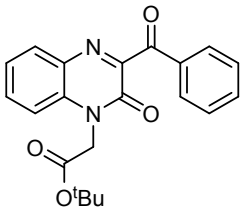
3-benzoyl-1-ethylquinoxalin-2(1H)-one, Compound **3t** was obtained in 62 % yield according to the general procedure. Yellow oil, mp = 102.5°C – 103.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.92 (d, J = 7.6 Hz, 2H), 7.87 (d, J = 7.9 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.55 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.7 Hz, 2H), 7.38 – 7.30 (m, 2H), 4.30 (q, J = 7.2 Hz, 2H), 1.36 (t, J = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.9, 153.7, 151.8, 133.9, 133.2, 131.9, 131.5, 131.0, 130.3, 129.0, 127.7, 123.0, 112.8, 36.4, 11.4; MS (EI); $[M+H]^+$: 279.1.



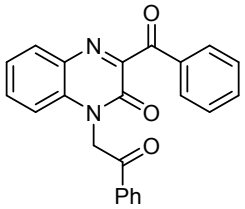
3-benzoyl-1-propylquinoxalin-2(1H)-one, Compound **3u** was obtained in 73 % yield according to the general procedure. Yellow solid, mp = 158.5°C – 159.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.93 – 7.89 (m, 2H), 7.88 – 7.85 (m, 1H), 7.61 – 7.54 (m, 2H), 7.41 (t, J = 7.8 Hz, 2H), 7.33 (t, J = 7.6 Hz, 2H), 4.22 – 4.17 (m, 2H), 1.80 – 1.76 (m, 2H), 1.00 (t, J = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.9, 153.8, 152.1, 133.9, 133.2, 132.1, 131.5, 130.9, 130.2, 128.9, 127.7, 123.0, 113.0, 42.8, 19.7, 10.4; MS (EI); $[M+H]^+$: 293.1.



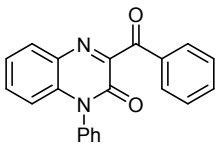
3-benzoyl-1-benzylquinoxalin-2(1H)-one[2], Compound **3v** was obtained in 60 % yield according to the general procedure. Yellow solid, mp = 178.9°C – 179.9 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.95 (d, *J* = 8.2 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.42 (m, 3H), 7.33 – 7.20 (m, 7H), 5.46 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): *δ* 191.7, 154.8, 153.5, 134.9, 134.9, 134.3, 133.3, 132.5, 132.0, 131.2, 130.0, 129.1, 128.8, 128.0, 127.2, 124.3, 114.8, 45.9; MS (EI); $[M+H]^+$: 341.1.



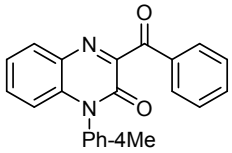
tert-butyl 2-(3-benzoyl-2-oxoquinoxalin-1(2H)-yl)acetate, Compound **3w** was obtained in 77 % yield according to the general procedure. Yellow solid, mp = 222.0°C – 222.8 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): *δ* 7.91 (d, *J* = 7.4 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.58 – 7.53 (m, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 4.90 (s, 2H), 1.39 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): *δ* 191.4, 165.7, 154.5, 152.9, 134.8, 134.3, 133.2, 132.3, 132.2, 131.3, 130.0, 128.7, 124.4, 113.5, 83.5, 44.0, 28.0; MS (EI); $[M+H]^+$: 365.1.



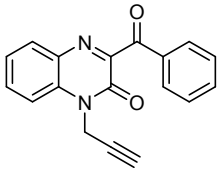
3-benzoyl-1-(2-oxo-2-phenylethyl)quinoxalin-2(1H)-one[2], Compound **3x** was obtained in 79 % yield according to the general procedure. Yellow solid, mp = 139.6°C – 140.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): *δ* 8.00 – 7.96 (m, 2H), 7.95 – 7.90 (m, 2H), 7.88 – 7.86 (m, 1H), 7.61 – 7.50 (m, 2H), 7.49 – 7.43 (m, 3H), 7.42 – 7.37 (m, 2H), 7.31 – 7.28 (m, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 5.69 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): *δ* 190.5, 189.7, 153.3, 152.1, 133.8, 133.4, 133.2, 132.3, 131.3, 131.1, 130.2, 129.0, 128.1, 127.7, 127.2, 123.3, 112.9, 47.3, 28.7; MS (EI); $[M+H]^+$: 369.1.



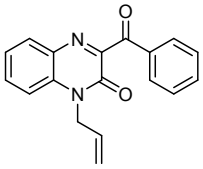
3-benzoyl-1-phenylquinoxalin-2(1H)-one, Compound **3y** was obtained in 81 % yield according to the general procedure. Yellow solid, mp = 157.6°C – 159.1 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.03 (d, J = 8.0 Hz, 2H), 7.95 (d, J = 8.0 Hz, 1H), 7.63 – 7.59 (m, 3H), 7.54 (t, J = 7.0 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.38 – 7.33 (m, 3H), 6.78 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 191.6, 155.4, 153.0, 134.9, 134.9, 134.8, 134.3, 132.1, 131.7, 130.6, 130.4, 130.1, 129.8, 128.7, 128.3, 124.4, 115.8; MS (EI); $[M+H]^+$: 327.1



A name could not be generated for this structure, Compound **3z** was obtained in 80 % yield according to the general procedure. Yellow solid, mp = 128.5°C – 129.5 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.96 (d, J = 7.3 Hz, 2H), 7.88 – 7.87 (m, 1H), 7.55 (t, J = 7.4 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.39 – 7.35 (m, 1H), 7.33 (d, J = 8.0 Hz, 2H), 7.31 – 7.27 (m, 1H), 7.15 (d, J = 8.2 Hz, 2H), 6.75 (d, J = 8.4 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 191.6, 155.4, 153.1, 139.8, 135.0, 139.4, 134.2, 132.2, 132.1, 131.6, 131.0, 130.6, 130.1, 128.7, 127.9, 124.2, 115.9, 21.3; MS (EI); $[M+H]^+$: 250.0.



3-benzoyl-1-(prop-2-ynyl)quinoxalin-2(1H)-one, Compound **3za** was obtained in 66 % yield according to the general procedure. Yellow solid, mp = 228.9°C – 230.2 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.95 – 7.91 (m, 2H), 7.89 – 7.87 (m, 1H), 7.67 – 7.62 (m, 1H), 7.56 (t, J = 7.4 Hz, 1H), 7.51 (d, J = 8.1 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.40 – 7.34 (m, 1H), 5.03 (d, J = 2.5 Hz, 2H), 2.26 (t, J = 2.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.3, 153.4, 151.3, 133.7, 133.3, 131.4, 131.3, 131.1, 130.2, 129.1, 127.7, 123.6, 113.6, 75.3, 72.8, 30.4; MS (EI); $[M+H]^+$: 289.1.



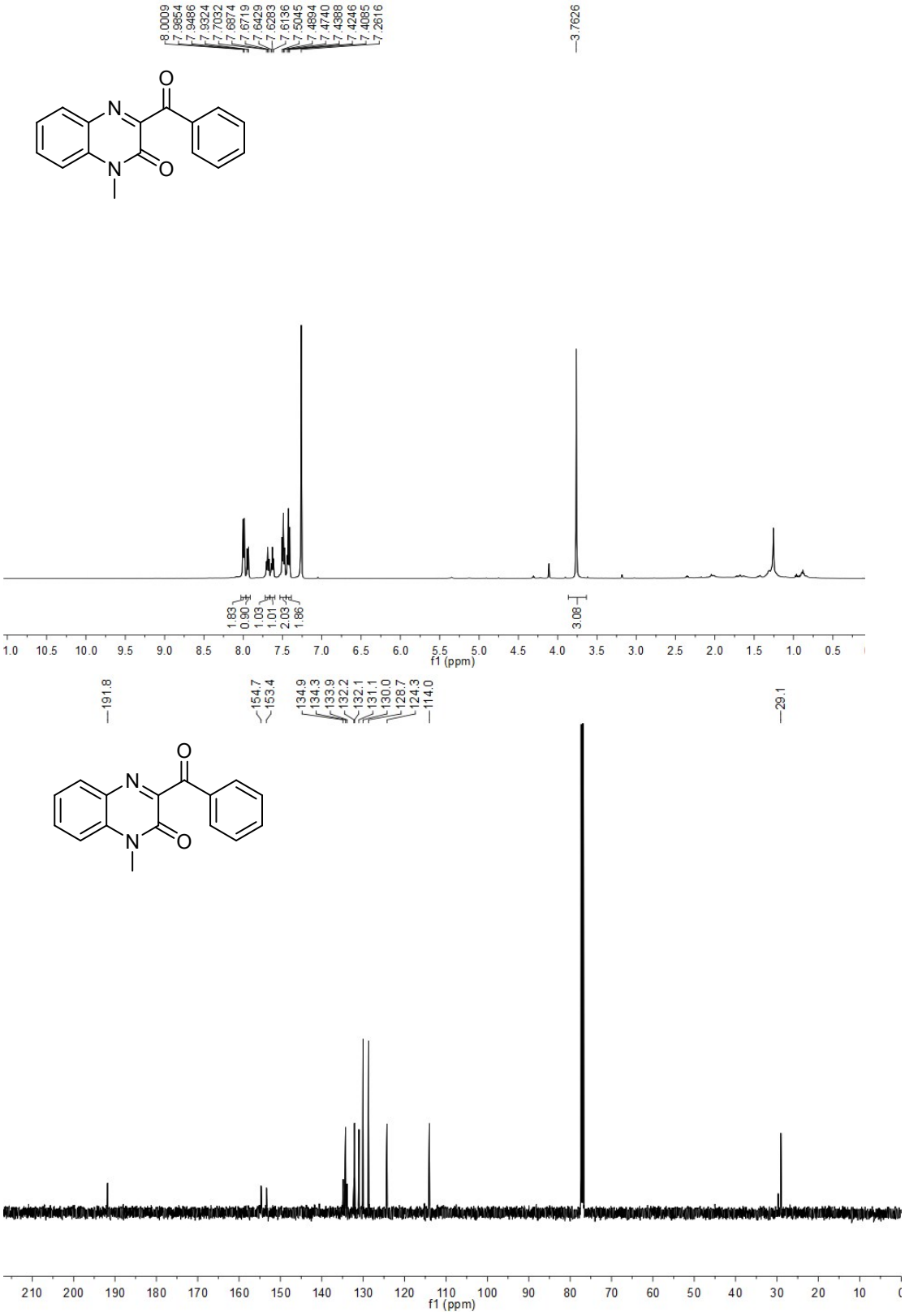
1-allyl-3-benzoylquinoxalin-2(1H)-one, Compound **3zb** was obtained in 80 % yield according to the general procedure. Yellow solid, mp = 118.7°C – 119.9 °C. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.96 – 7.89 (m, 2H), 7.88 – 7.85 (m, 1H), 7.60 – 7.52 (m, 2H), 7.41 (t, J = 7.8 Hz, 2H), 7.34 – 7.31 (m, 2H), 5.92 – 5.84 (m, 1H), 5.26 – 5.17 (m, 2H), 4.93 – 4.83 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 190.7, 153.7, 151.9, 133.8, 133.2, 132.2, 131.4, 130.9, 130.1, 129.3, 129.0, 127.7, 123.2, 117.8, 113.5, 43.5; MS (EI); $[M+H]^+$: 291.1.

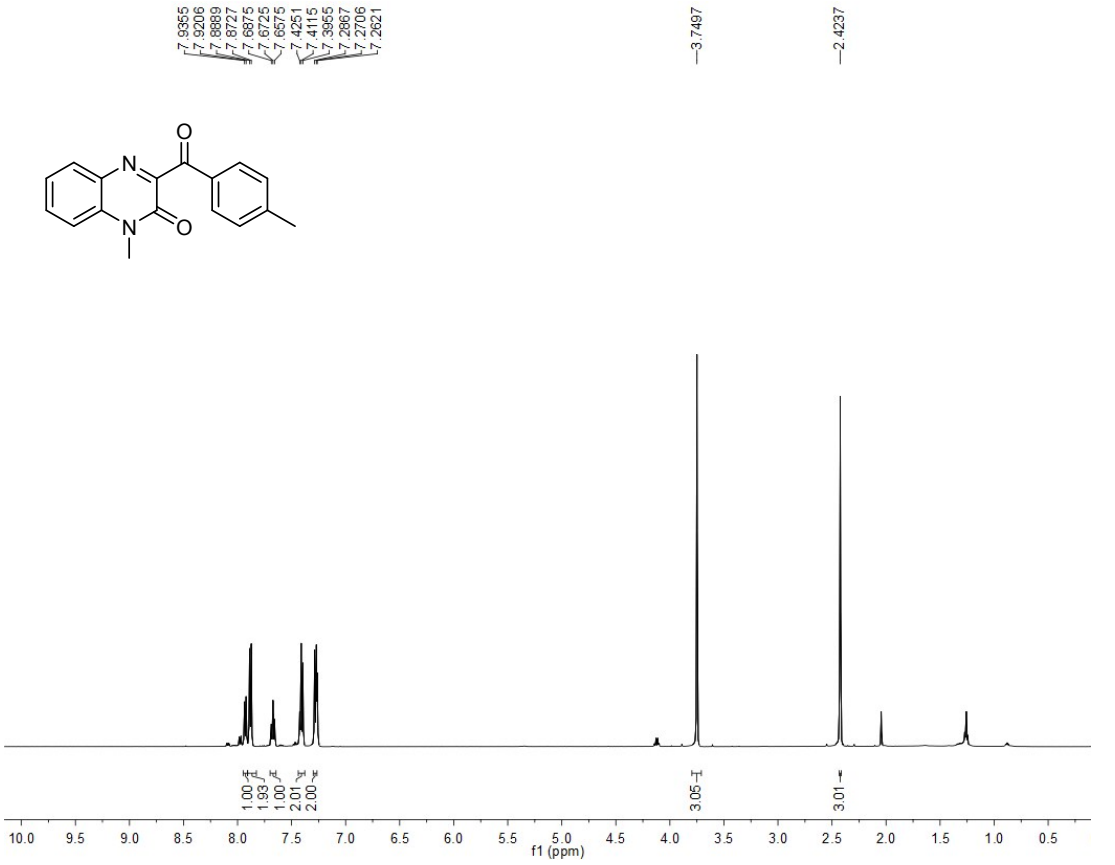
References：

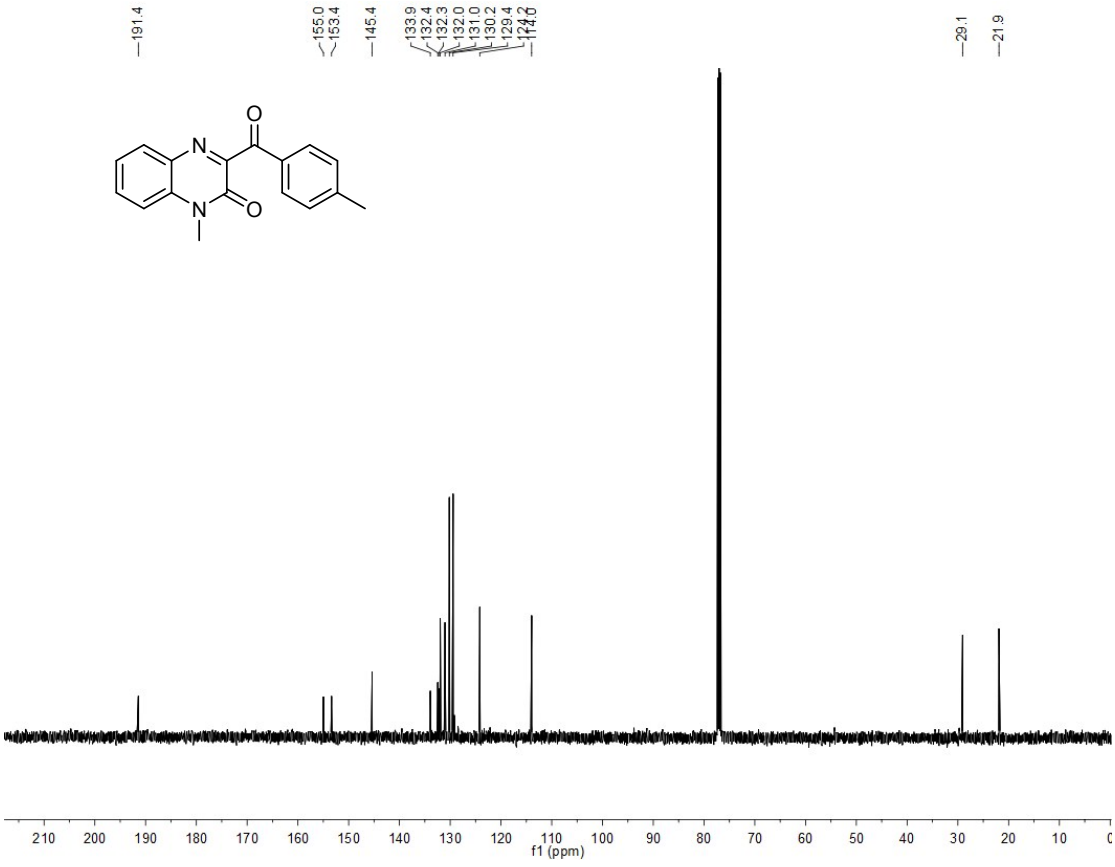
[1] X. Zeng, C. Liu, X. Wang, J. Zhang, X. Wang , Y. Hu. *Org. Biomol. Chem.* 2017, **15**, 8929–8935.

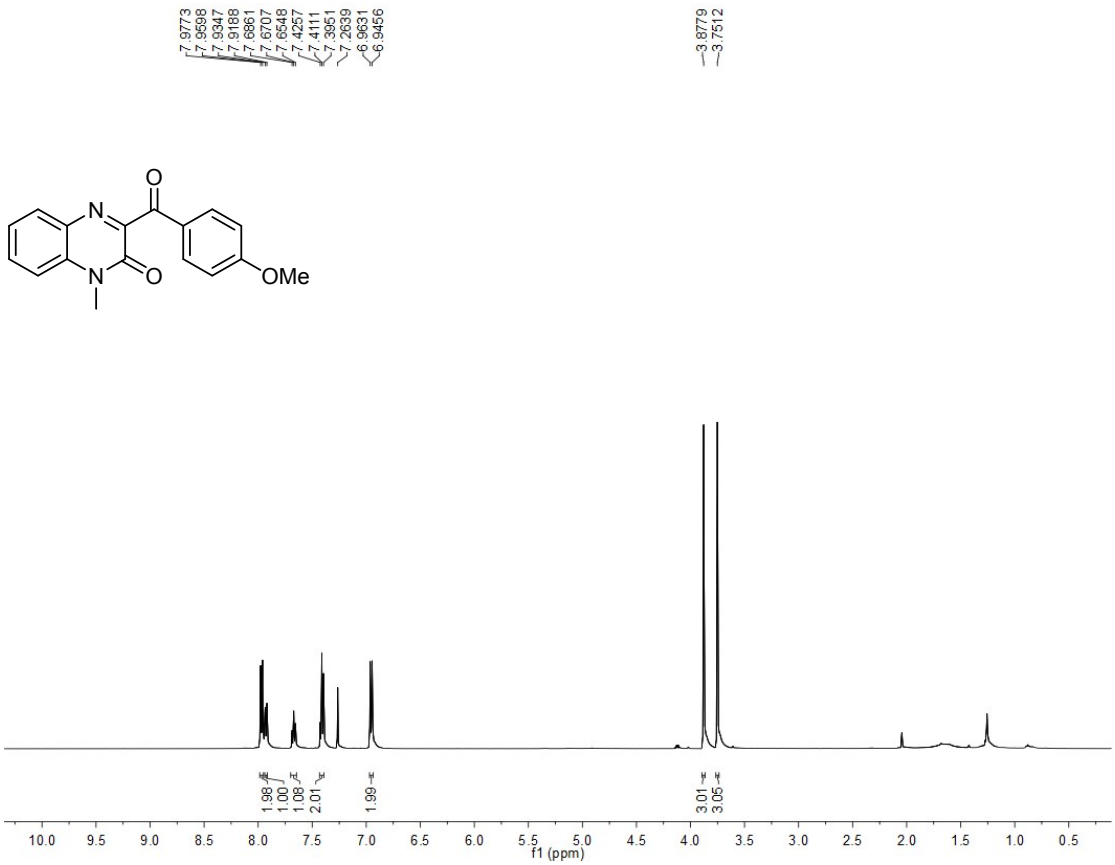
[2] J. Yuan, J. Fu, S. Liu, Y. Xiao, P. Mao, L. Qu. *Org. Biomol. Chem.* 2018, **16**, 3203–3212.

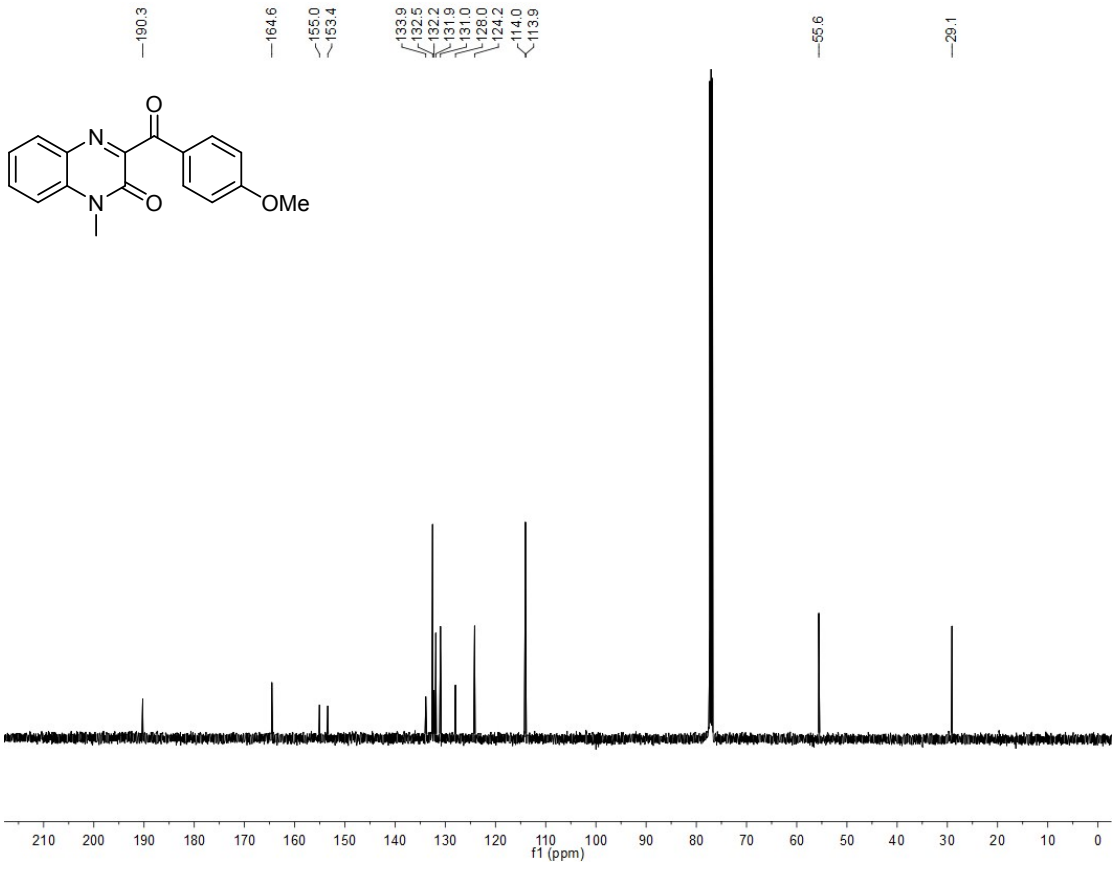
6. Copies of NMR Spectra for 3a−3zb.




7.9355
7.9206
7.8889
7.8727
7.6875
7.6725
7.6575
7.4251
7.4115
7.3955
7.2867
7.2706
7.2621
3.7497
2.4237
O
N
N
O
1.00
1.93
1.00
2.01
2.00
3.05
3.01
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
f1 (ppm)

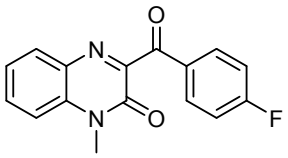

191.4
155.0
153.4
145.4
133.9
132.4
132.3
132.0
131.0
130.2
129.4
29.1
21.9
O
N
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

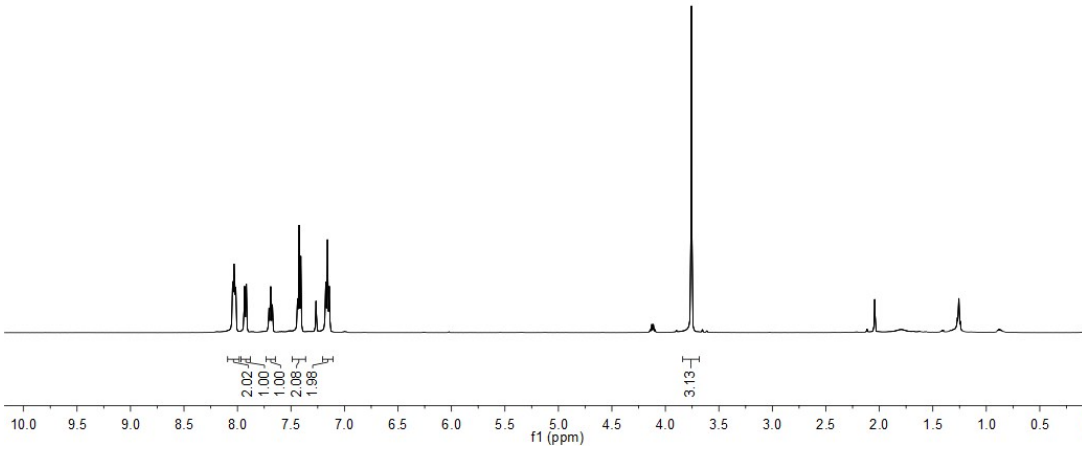

7.9773
7.9698
7.9347
7.9188
7.6861
7.6707
7.6548
7.4257
7.4111
7.3951
7.2639
6.9631
6.9456
3.8779
3.7512
O
N
O
N
OMe
1.98
1.00
1.08
2.01
1.99
3.01
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

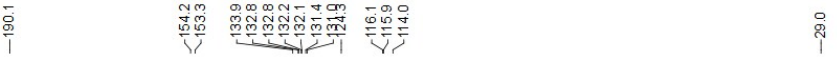

190.3
164.6
155.0
153.4
133.9
132.5
132.2
131.9
131.0
128.0
124.2
114.0
113.9
55.6
29.1
O
N
O
N
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

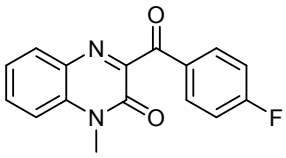

8.0440
8.0326
8.0284
8.0173
7.9331
7.9168
7.7050
7.6895
7.6737
7.4380
7.4237
7.4078
7.2657
7.1749
7.1584
7.1418

3.7560

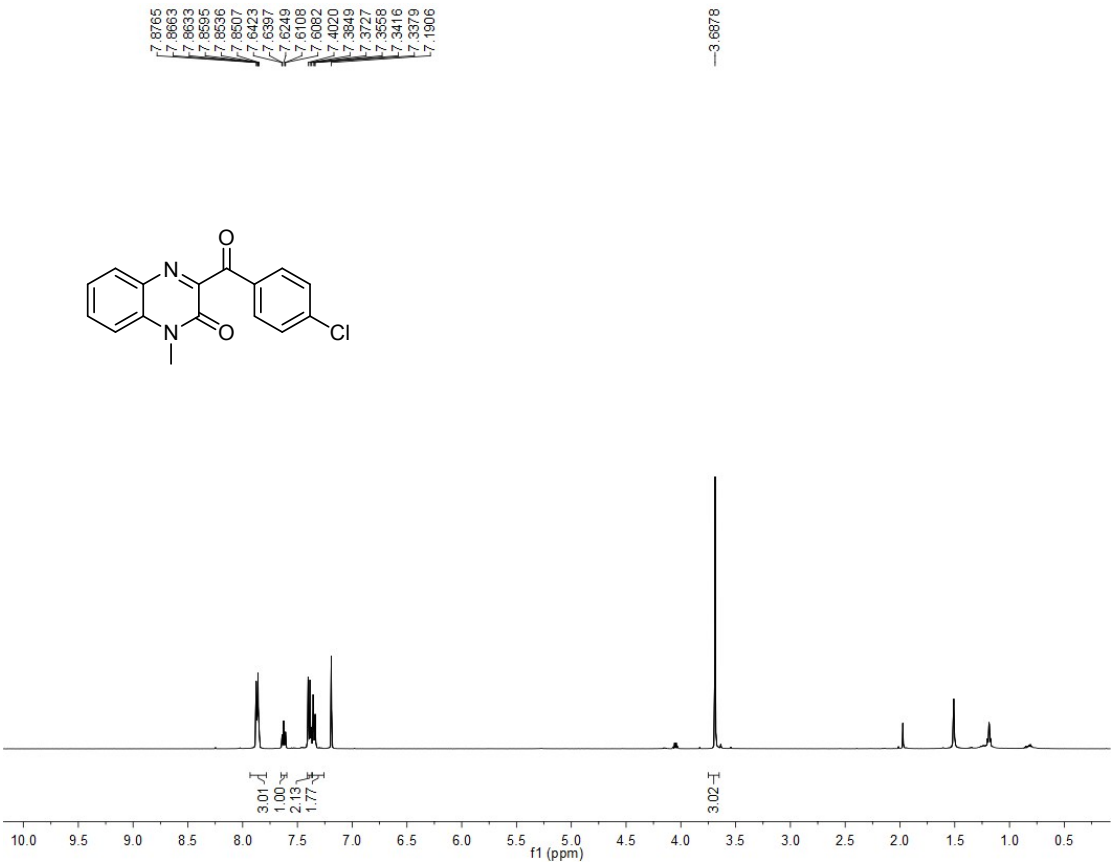

O
N
N
O
F

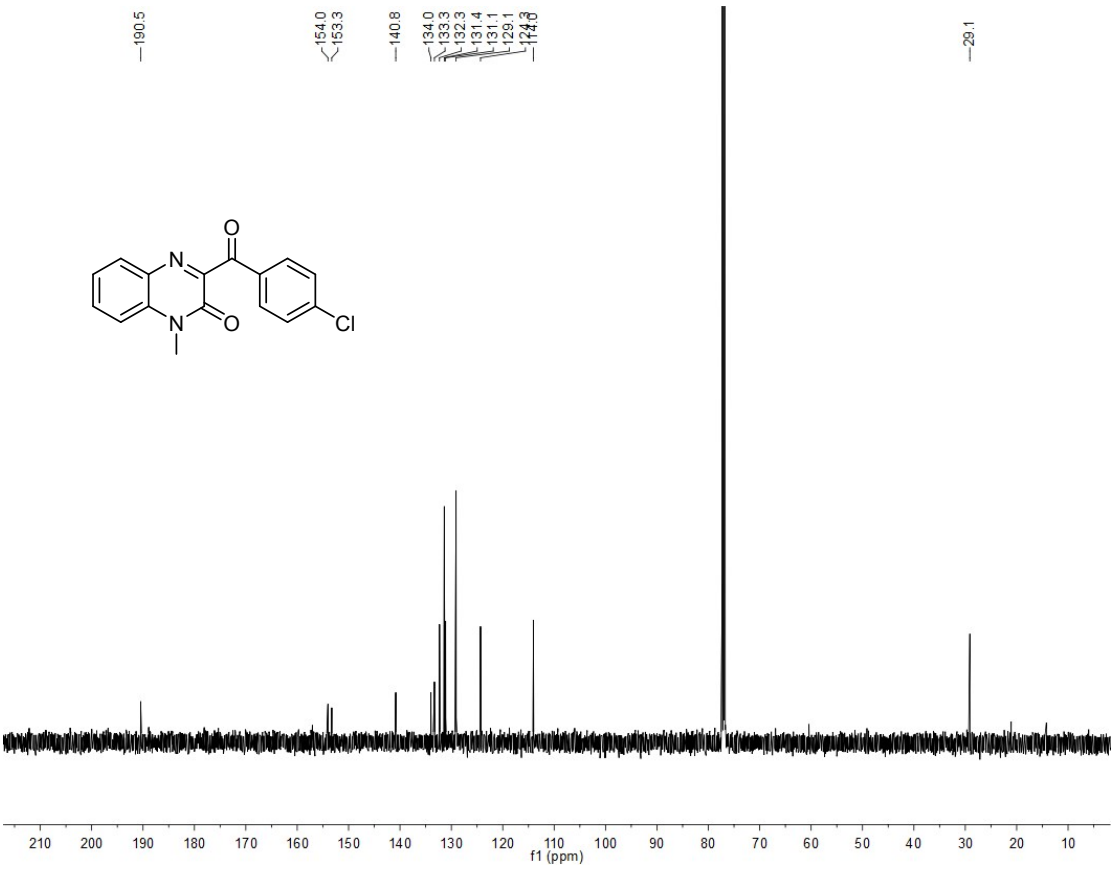

2.02
1.00
1.00
2.08
1.98
3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

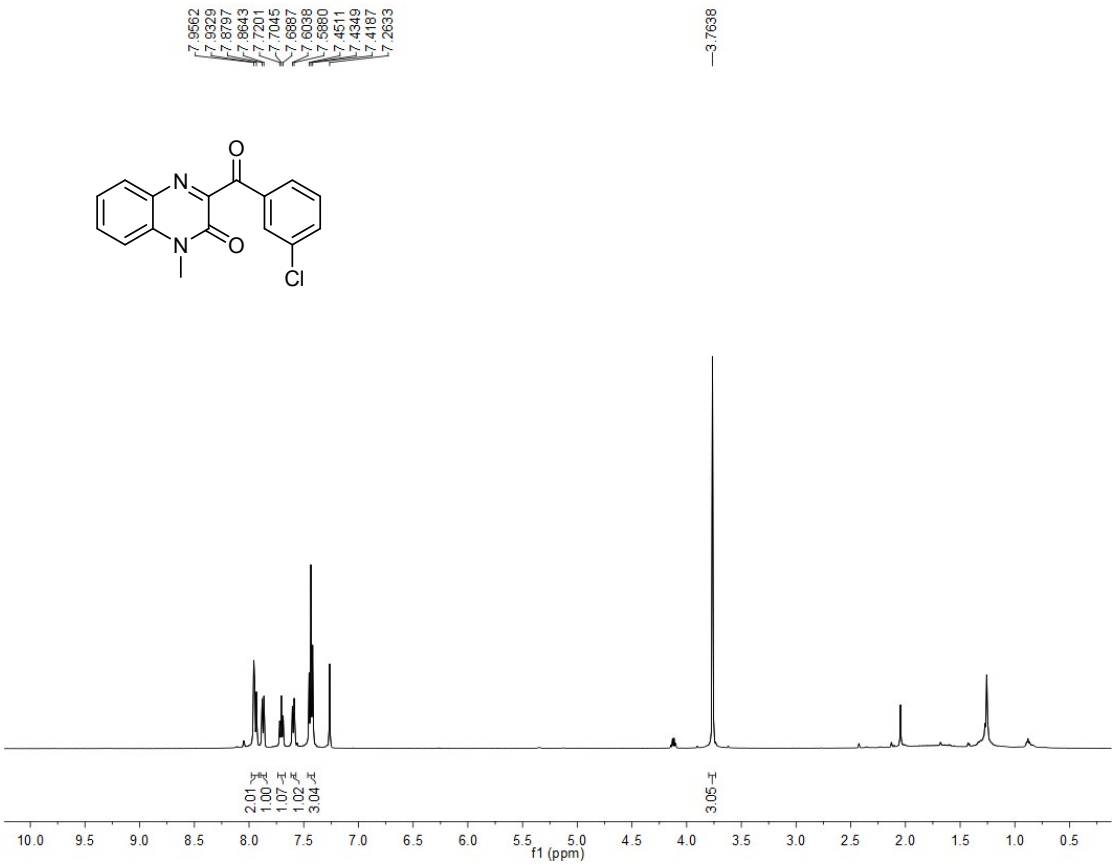

190.1
154.2
153.3
133.9
132.8
132.8
132.2
132.1
131.4
116.1
115.9
114.0
29.0

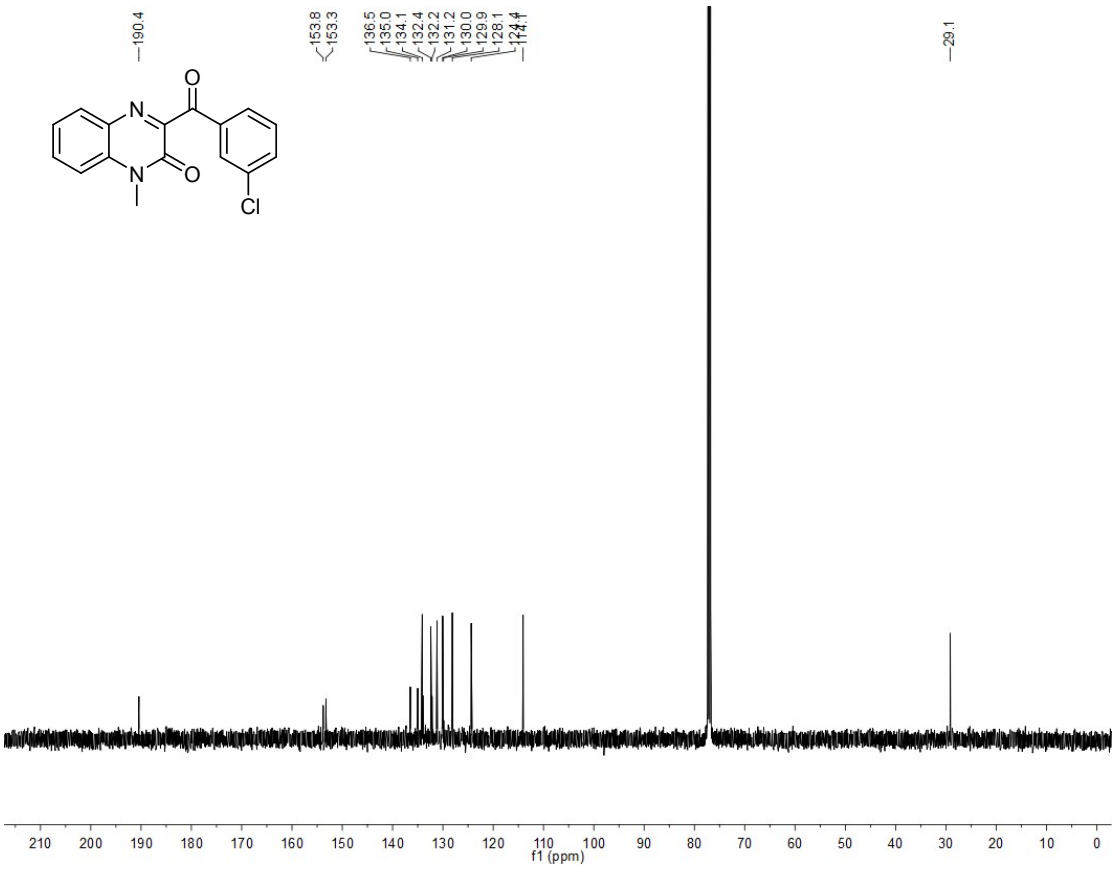

O
N
N
O
F

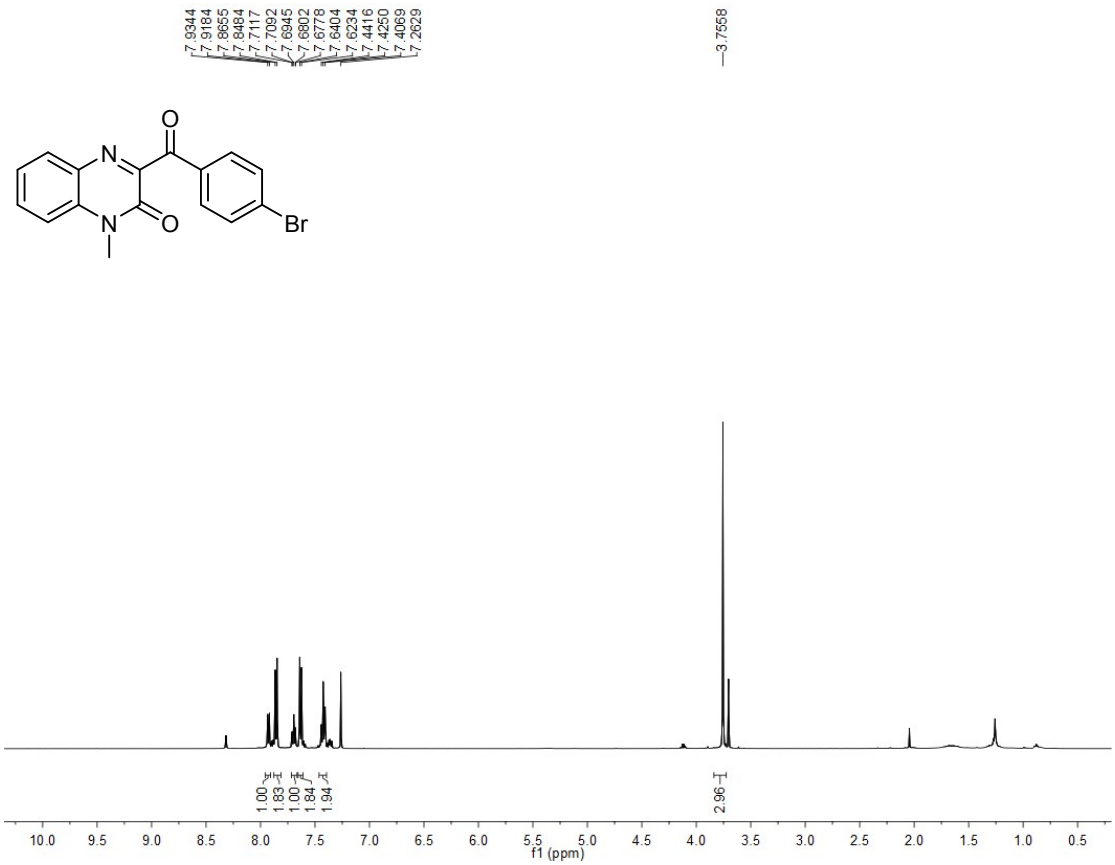
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

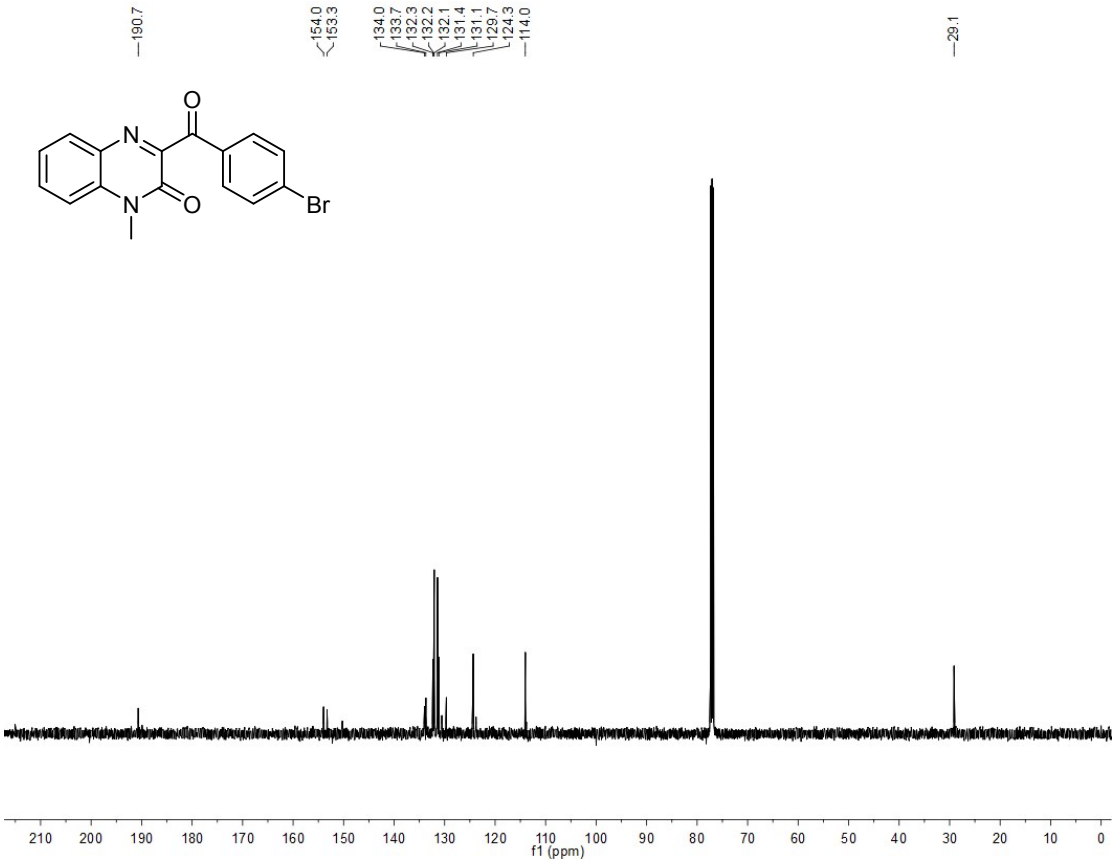

7.8765
7.8663
7.8633
7.8595
7.8536
7.8507
7.6423
7.6397
7.6249
7.6108
7.6082
7.4020
7.3849
7.3727
7.3558
7.3416
7.3379
7.1906
3.6878
O
N
O
N
Cl
3.01
1.00
2.13
1.77
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

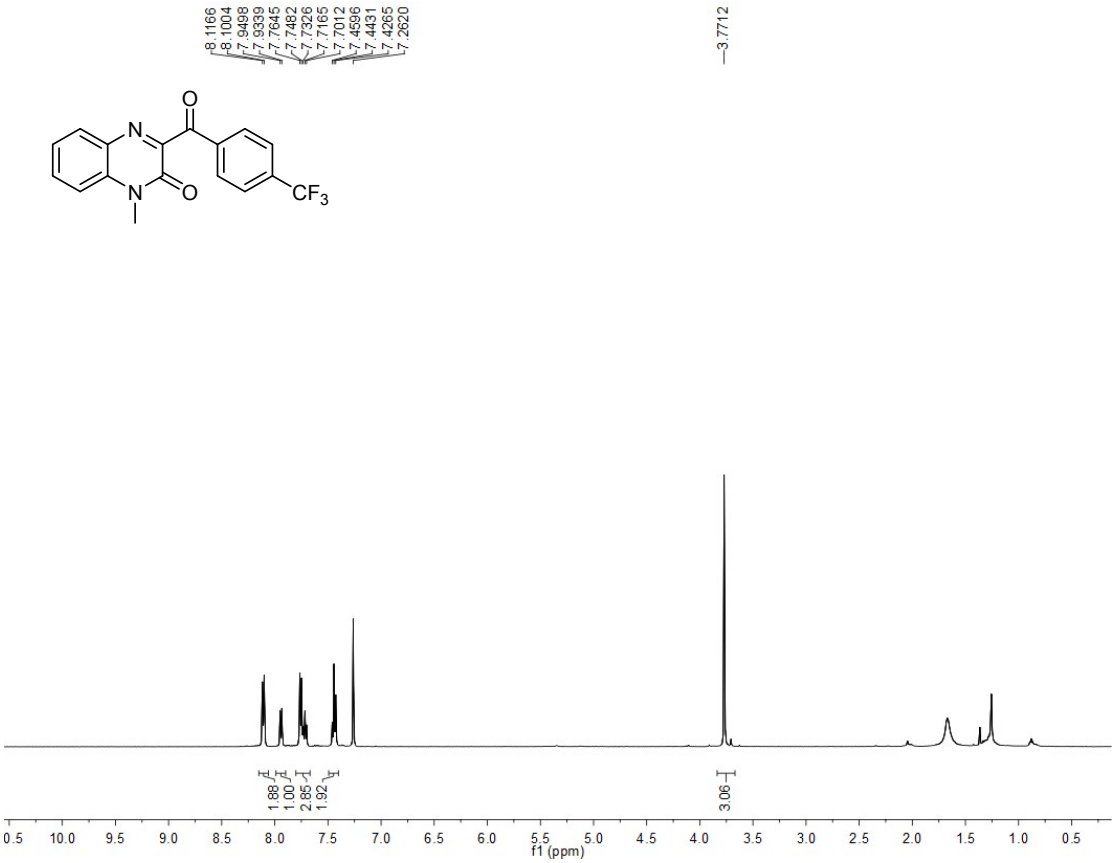

190.5
154.0
153.3
140.8
134.0
133.3
132.3
131.4
131.1
129.1
29.1
O
N
O
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

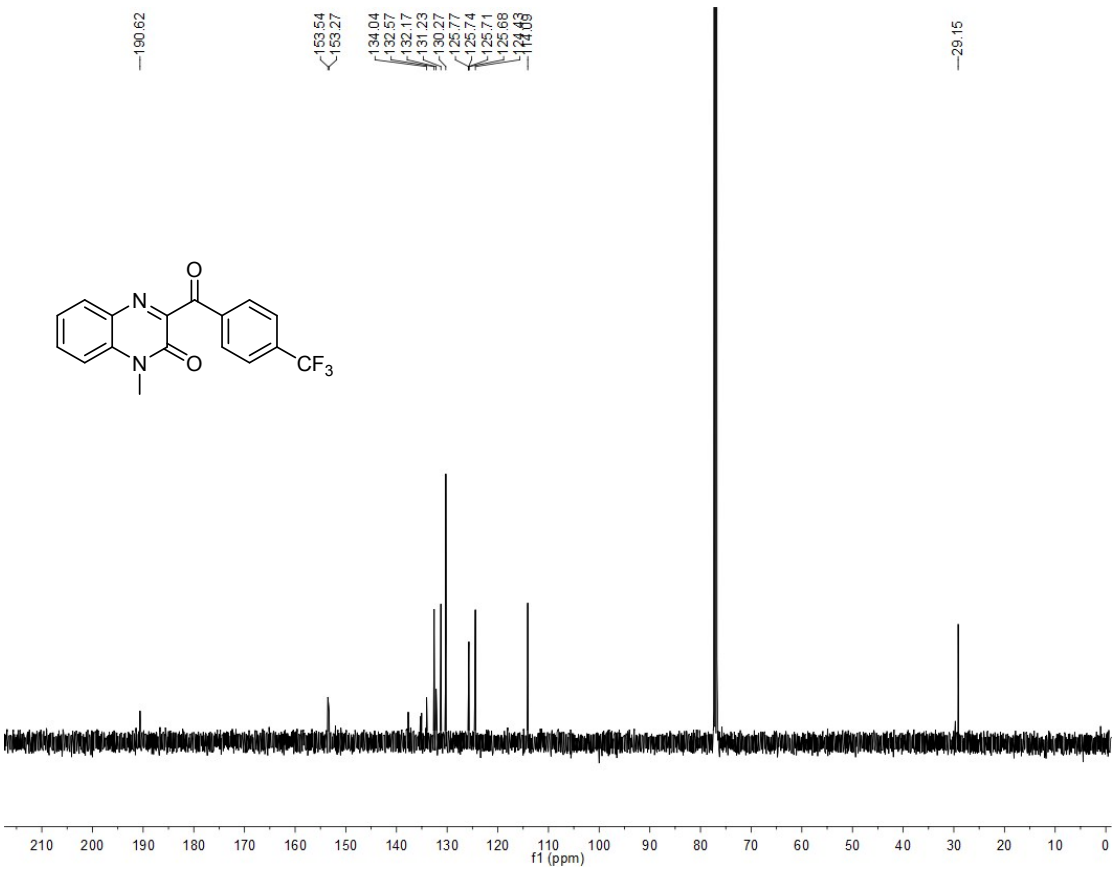

7.9562
7.9329
7.8797
7.8643
7.7201
7.7045
7.6887
7.6038
7.5980
7.4511
7.4349
7.4187
7.2633
3.7638
O
N
O
N
Cl
2.01
1.00
1.07
1.02
3.04
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

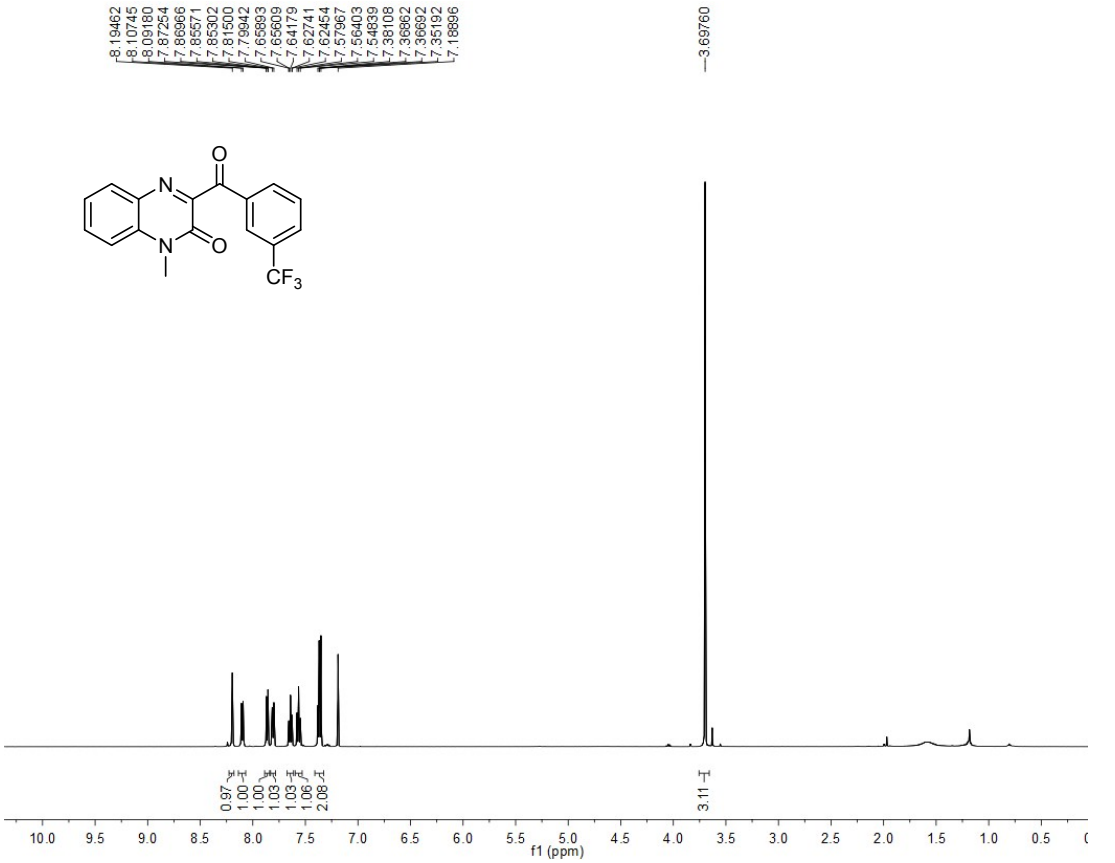

190.4
153.8
153.3
136.5
135.0
134.1
132.4
132.2
131.2
130.0
129.9
128.1
29.1
O
N
O
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

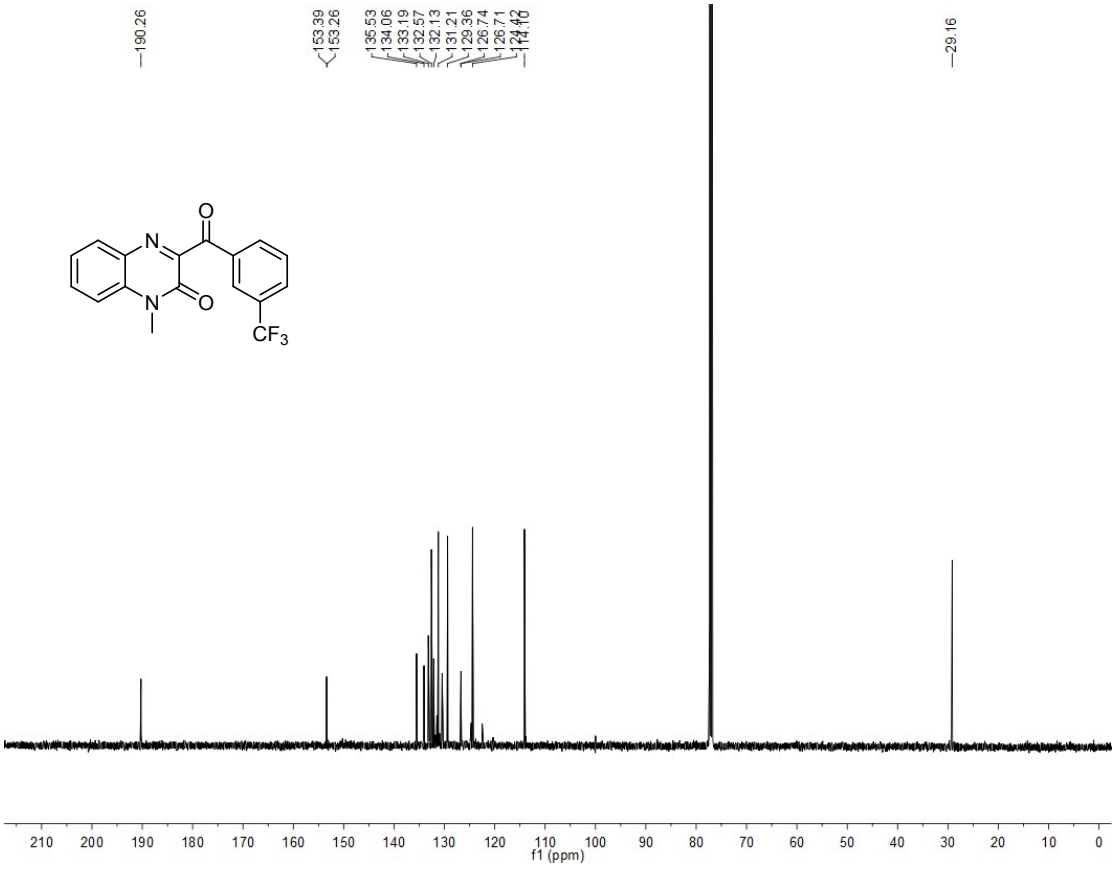

7.9344
7.9184
7.8655
7.8484
7.7117
7.7092
7.6945
7.6802
7.6778
7.6404
7.6234
7.4416
7.4250
7.4069
7.2629
3.7558
O
N
O
N
Br
1.00
1.83
1.00
1.84
1.94
2.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

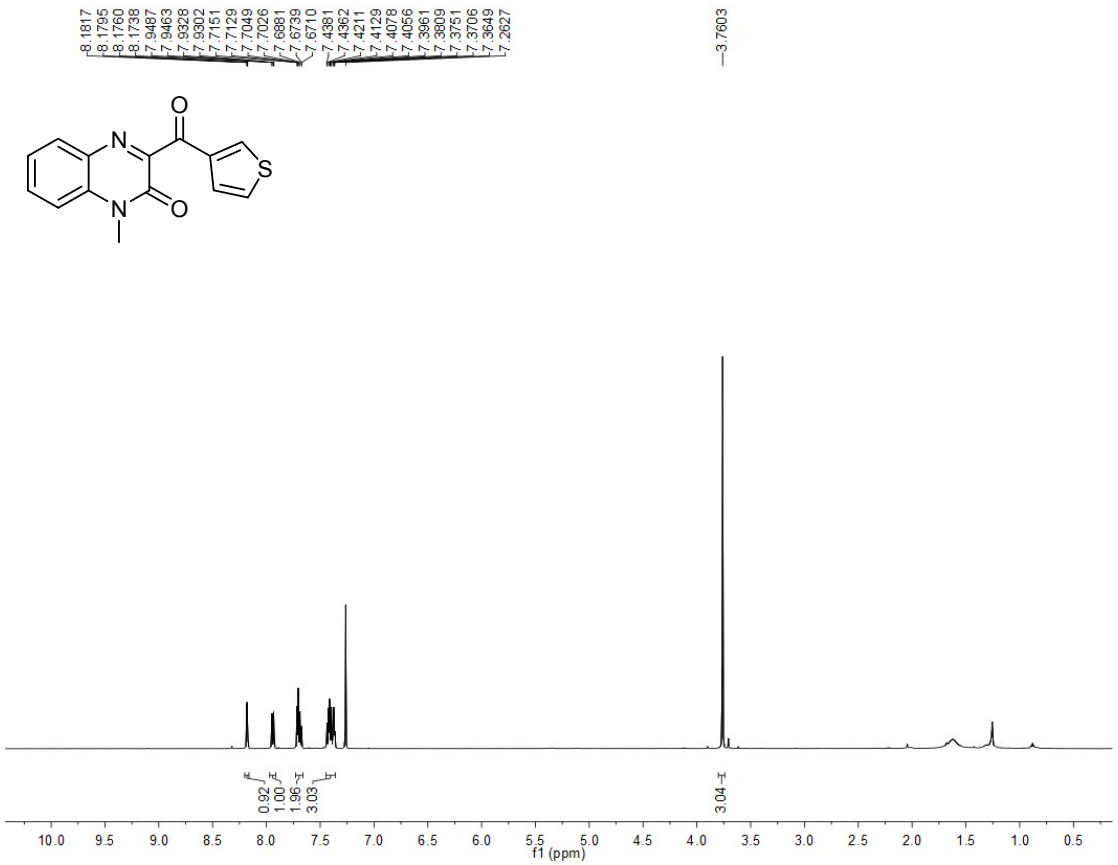

190.7
154.0
153.3
134.0
133.7
132.3
132.2
132.1
131.4
131.1
129.7
124.3
114.0
29.1
O
N
O
N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

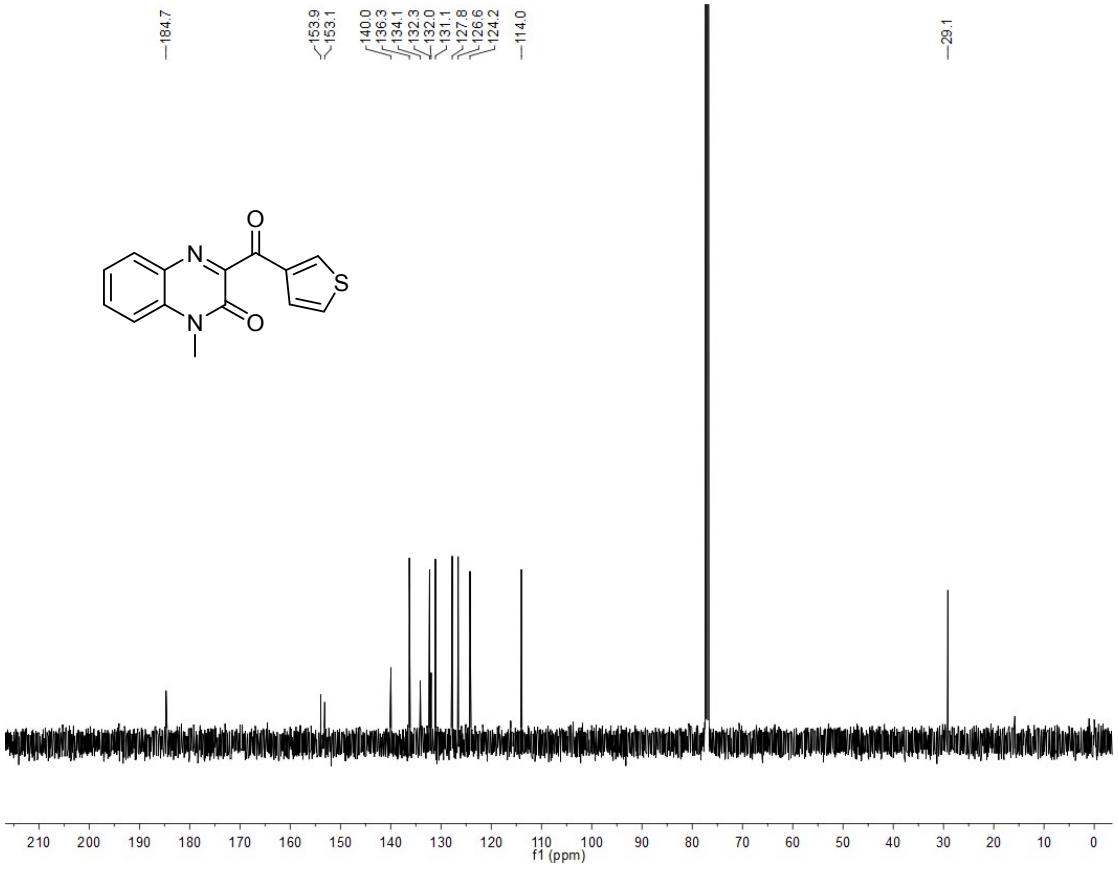

8.1166
8.1004
7.9498
7.9339
7.7645
7.7482
7.7326
7.7165
7.7012
7.4596
7.4431
7.4265
7.2620
3.7712
O
N
O
N
CF3
1.88
1.00
2.85
1.92
3.06
f1 (ppm)

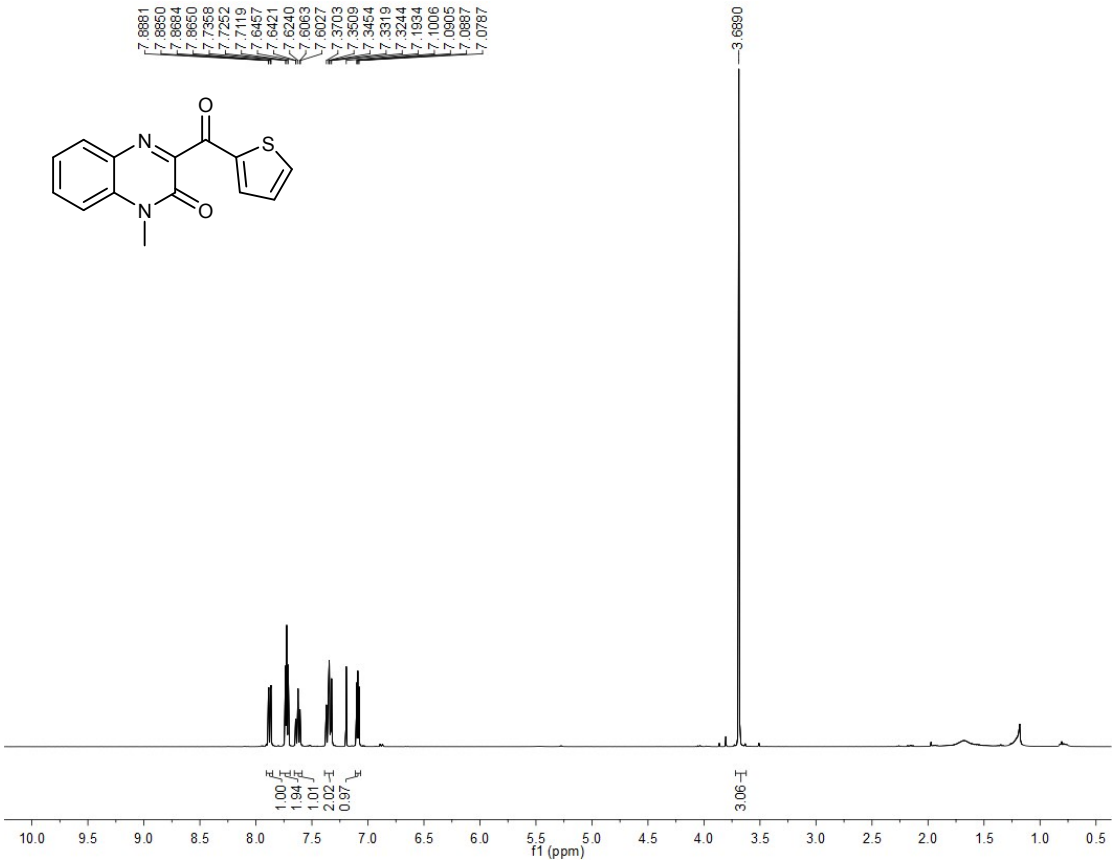

190.62
153.54
153.27
134.04
132.57
132.17
131.23
130.27
125.77
125.74
125.71
125.68
29.15
O
N
O
N
CF3
f1 (ppm)

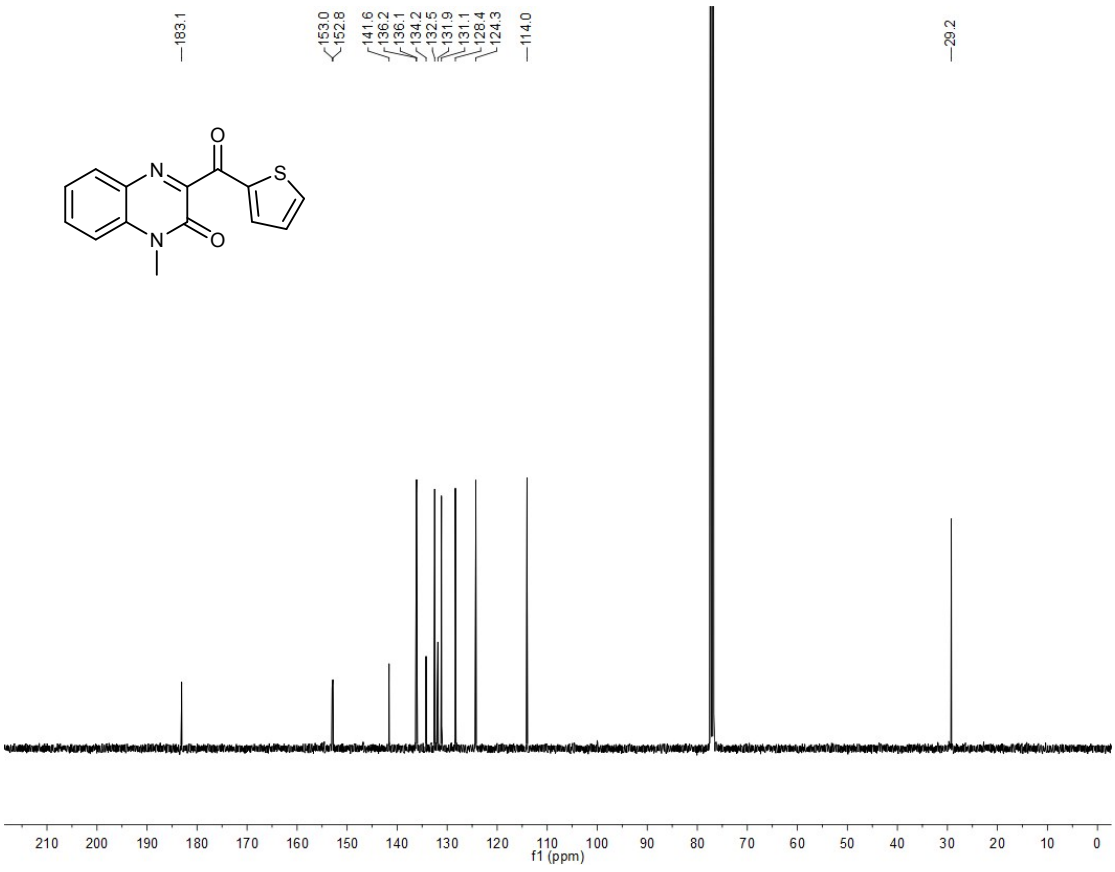

8.19462
8.10745
8.09180
7.87254
7.86966
7.85571
7.85302
7.81500
7.79942
7.65893
7.65609
7.64179
7.62741
7.62454
7.57967
7.56403
7.54839
7.38108
7.36862
7.36692
7.35192
7.18896
3.69760
O
N
N
O
CF3
0.97
1.00
1.00
1.03
1.06
2.08
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

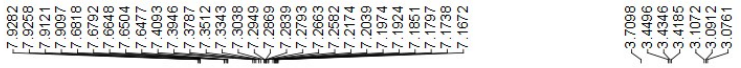

190.26
153.39
153.26
135.53
134.06
133.19
132.57
132.13
131.21
129.36
126.74
126.71
124.42
124.16
29.16
O
N
N
O
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

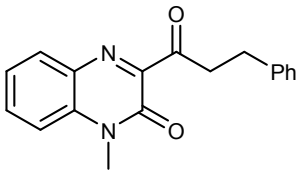

8.1817
8.1795
8.1760
8.1738
7.9487
7.9463
7.9328
7.9302
7.7151
7.7129
7.7049
7.7026
7.6881
7.6739
7.6710
7.4381
7.4362
7.4211
7.4129
7.4078
7.4056
7.3961
7.3809
7.3751
7.3706
7.3649
7.2627
3.7603
O
N
S
N
O
0.92
1.00
1.96
3.03
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

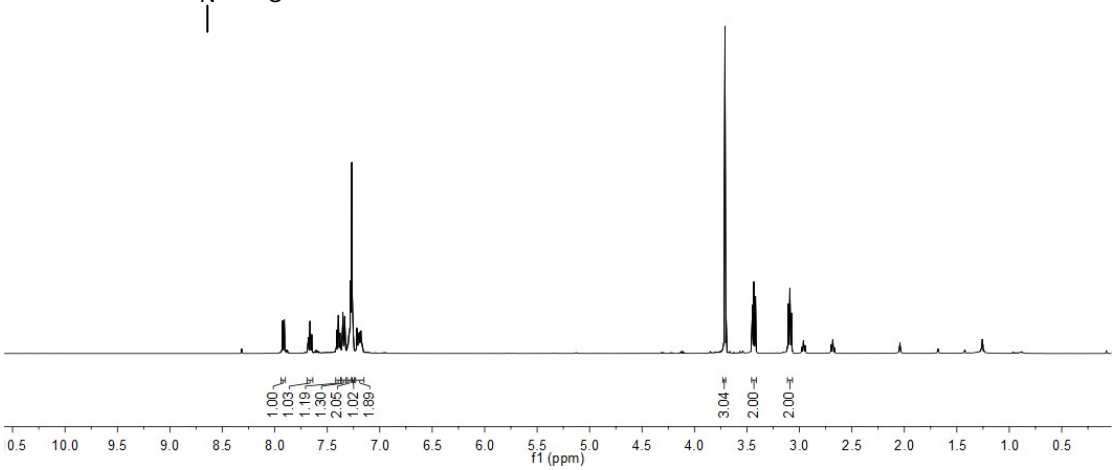

184.7
153.9
153.1
140.0
136.3
134.1
132.3
132.0
131.1
127.8
126.6
124.2
114.0
29.1
O
N
S
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

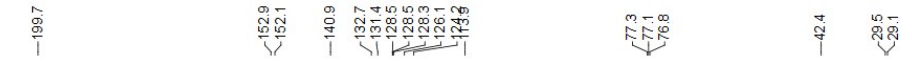

7.8881
7.8850
7.8684
7.8650
7.7358
7.7252
7.7119
7.6457
7.6421
7.6240
7.6063
7.6027
7.3703
7.3509
7.3454
7.3319
7.3244
7.1934
7.1006
7.0905
7.0887
7.0787
3.6890
1.00
1.94
1.01
2.02
0.97
3.06
f1 (ppm)

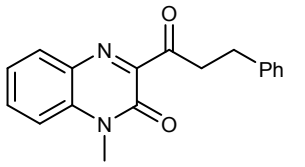

183.1
153.0
152.8
141.6
136.2
136.1
134.2
132.5
131.9
131.1
128.4
124.3
114.0
29.2
f1 (ppm)

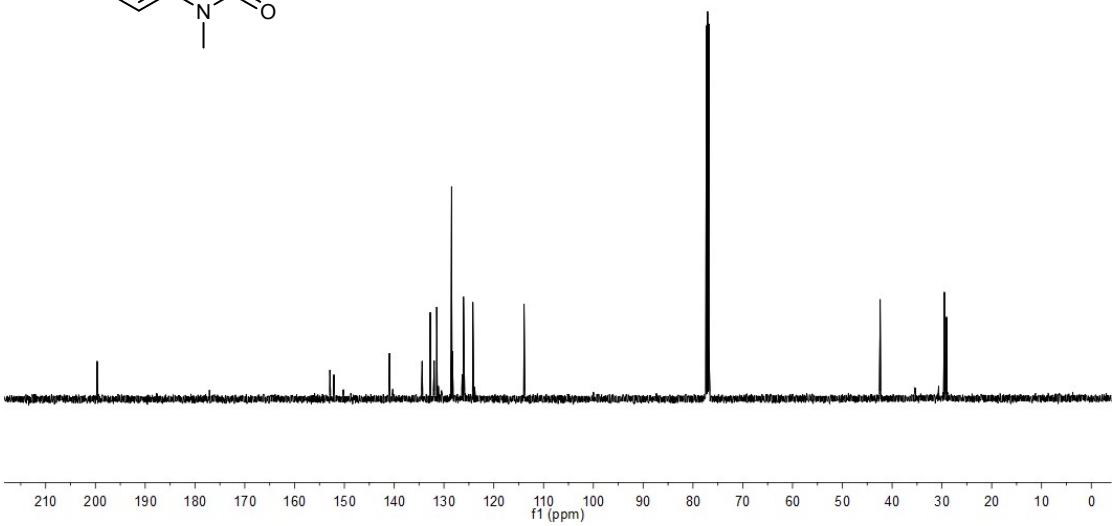

7.9282
7.9258
7.9121
7.9097
7.6818
7.6792
7.6648
7.6504
7.6477
7.4093
7.3946
7.3787
7.3512
7.3343
7.3038
7.2949
7.2869
7.2839
7.2793
7.2663
7.2582
7.2174
7.2039
7.1974
7.1924
7.1851
7.1797
7.1738
7.1672
3.7098
3.4496
3.4346
3.4185
3.1072
3.0912
3.0761

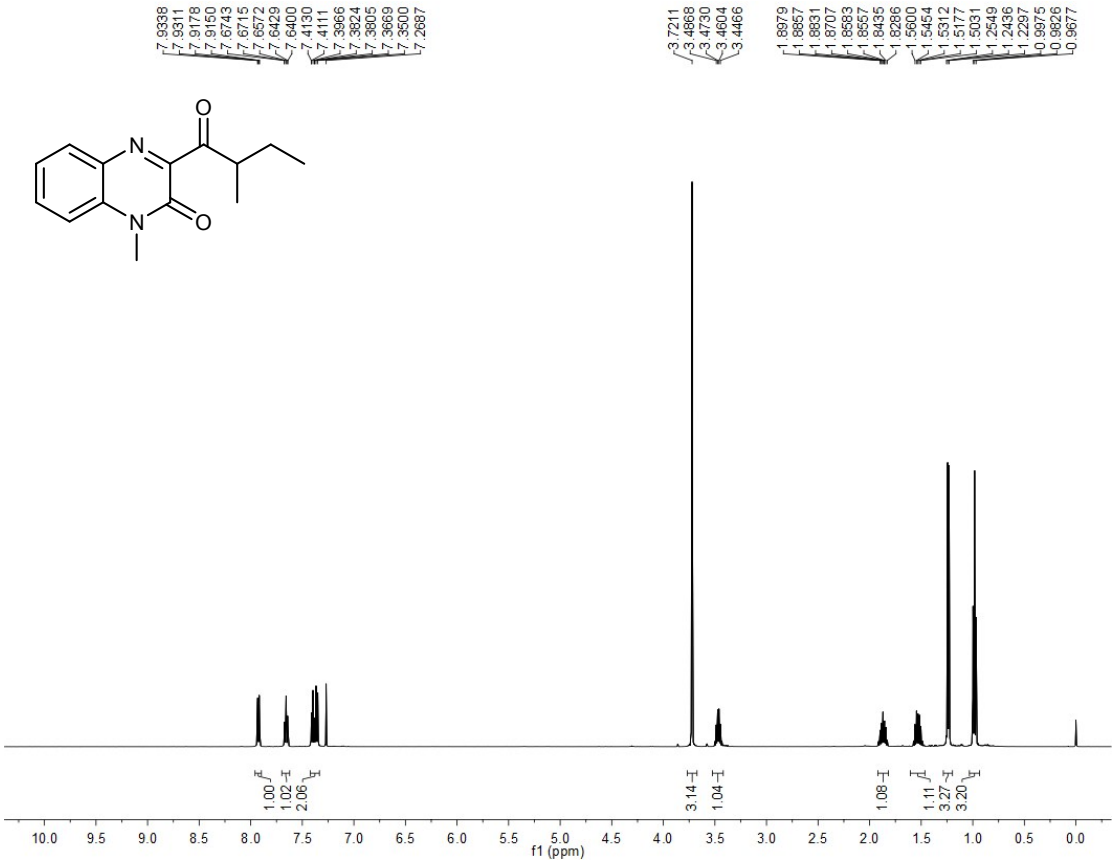

O
N
Ph
N
O

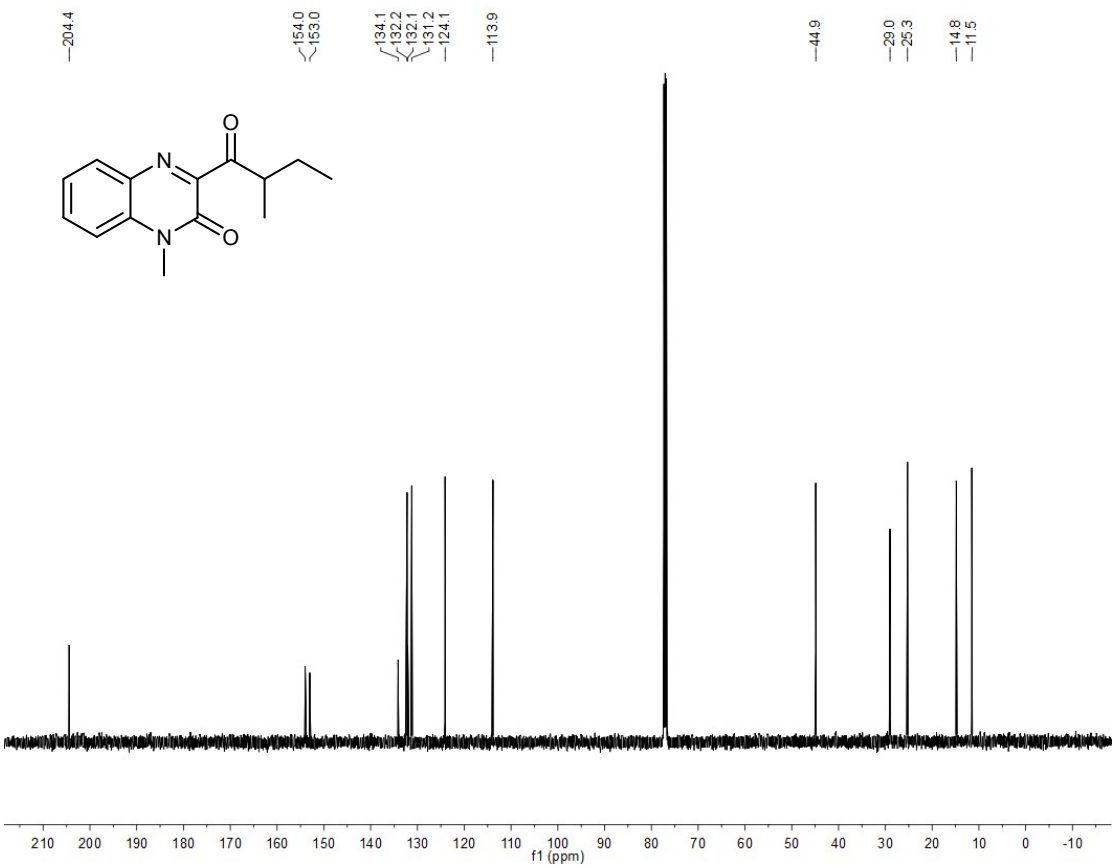

1.00
1.03
1.19
1.30
2.05
1.02
1.89
3.04
2.00
2.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

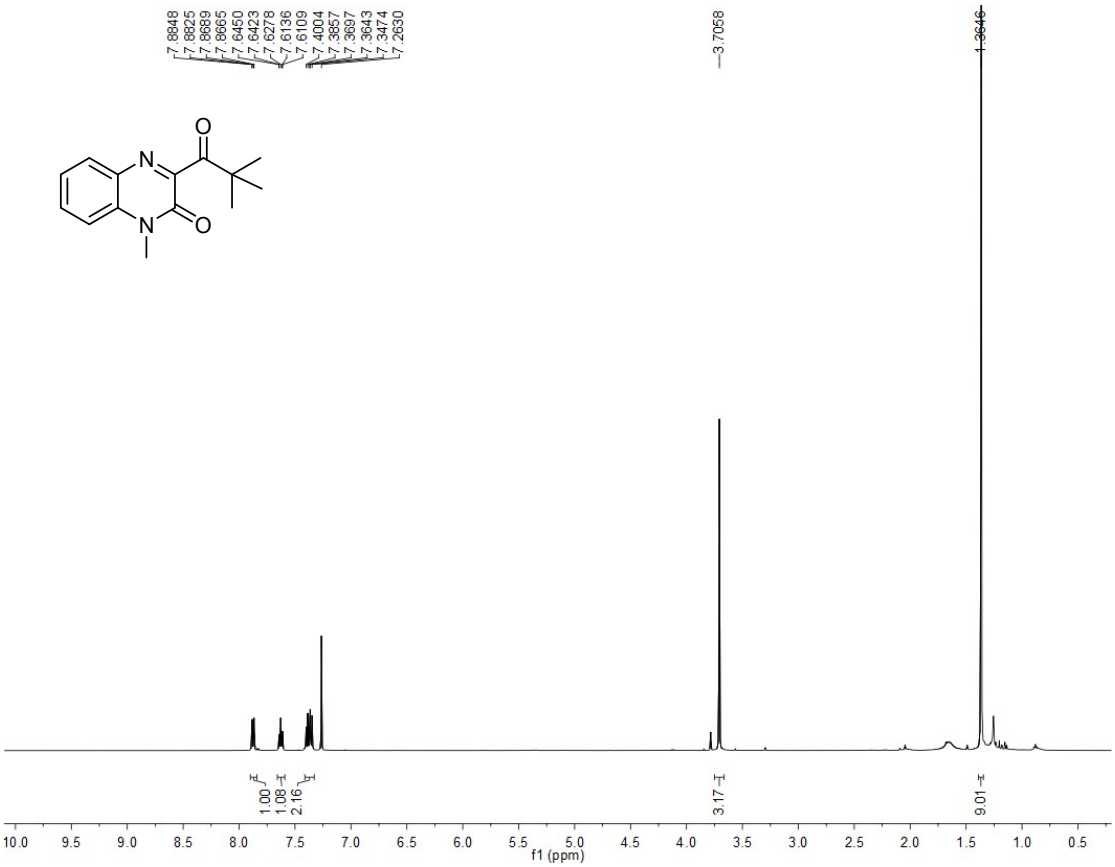

199.7
152.9
152.1
140.9
132.7
131.4
128.5
128.5
128.3
126.1
124.2
113.9
77.3
77.1
76.8
42.4
29.5
29.1

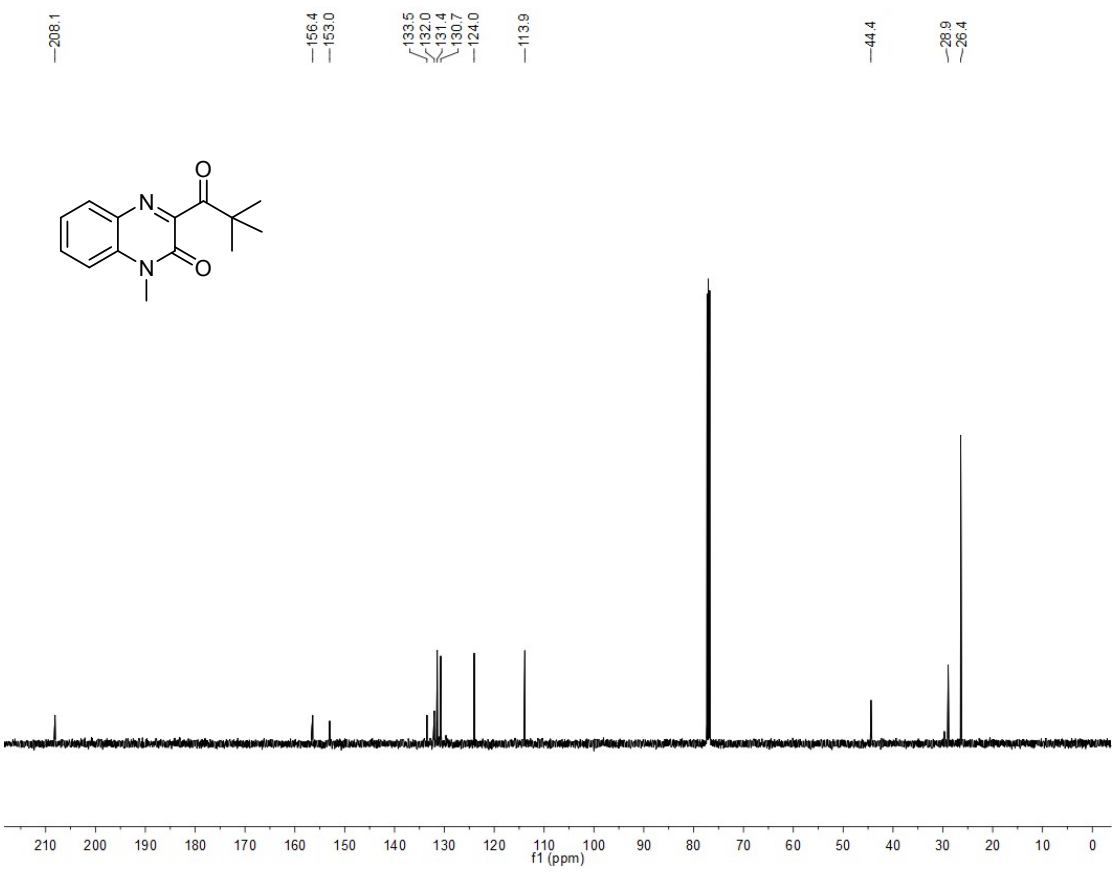

O
N
Ph
N
O

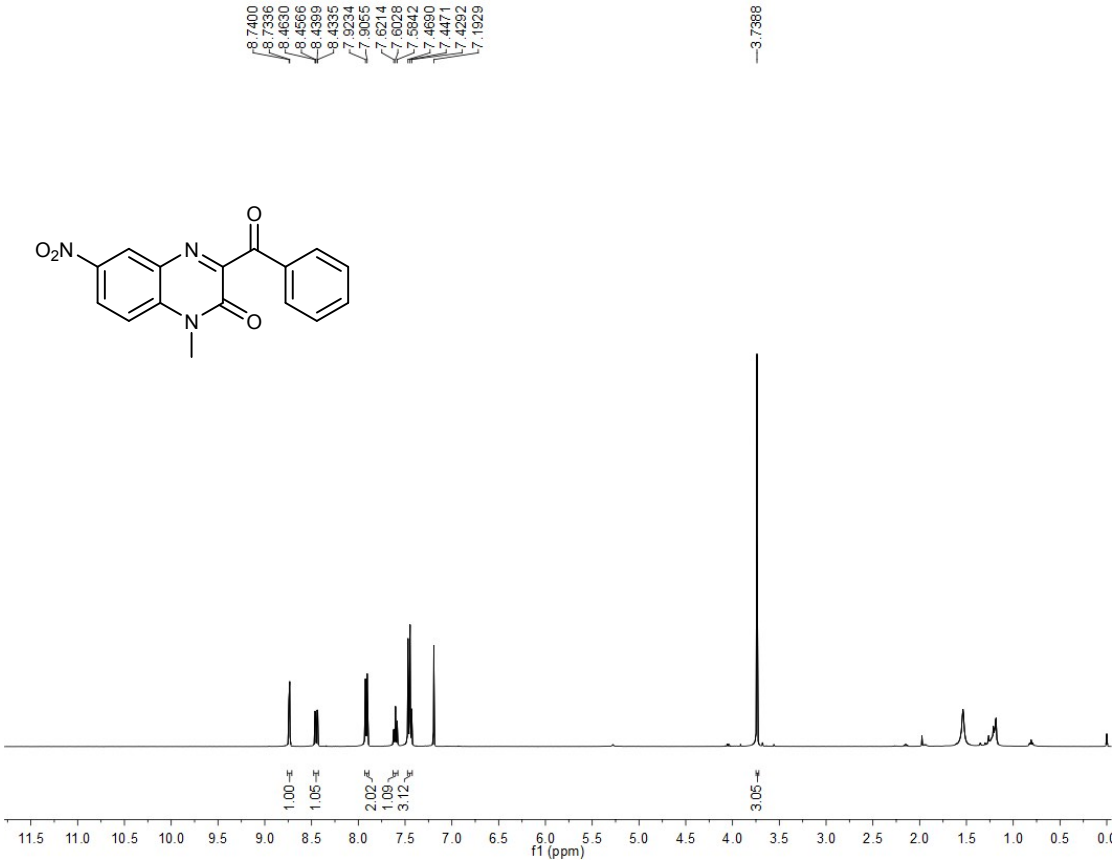

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

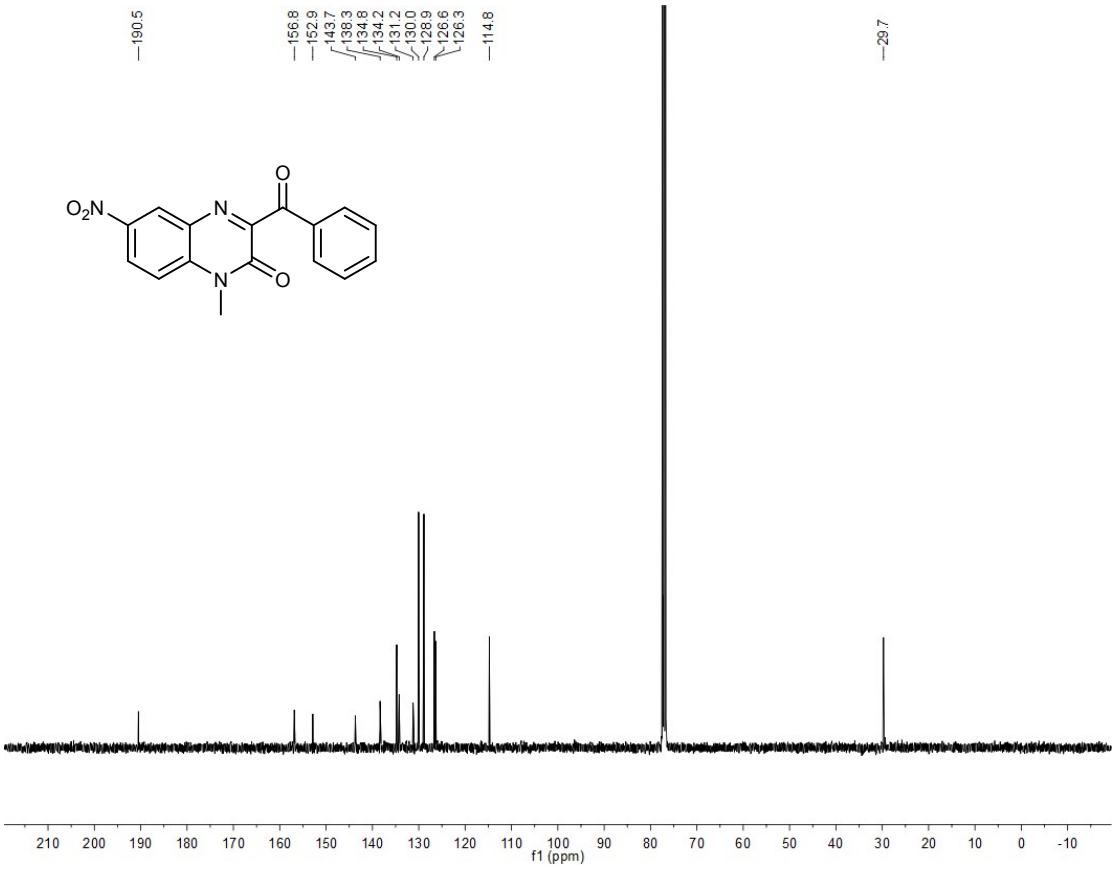

7.9338
7.9311
7.9178
7.9150
7.6743
7.6715
7.6572
7.6429
7.6400
7.4130
7.4111
7.3966
7.3824
7.3805
7.3669
7.3500
7.2687
3.7211
3.4868
3.4730
3.4604
3.4466
1.8979
1.8857
1.8831
1.8707
1.8583
1.8557
1.8435
1.8286
1.5600
1.5454
1.5312
1.5177
1.5031
1.2549
1.2436
1.2297
0.9975
0.9826
0.9677
1.00
1.02
2.06
3.14
1.04
1.08
1.11
3.27
3.20
f1 (ppm)

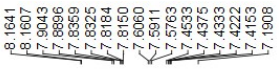

204.4
154.0
153.0
134.1
132.2
132.1
131.2
124.1
113.9
44.9
29.0
25.3
14.8
11.5
f1 (ppm)


7.8848
7.8825
7.8689
7.8665
7.6450
7.6423
7.6278
7.6136
7.6109
7.4004
7.3857
7.3697
7.3643
7.3474
7.2630
3.7058
1.3646
1.00
1.08
2.16
3.17
9.01
f1 (ppm)

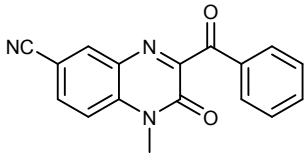

208.1
156.4
153.0
133.5
132.0
131.4
130.7
124.0
113.9
44.4
28.9
26.4
f1 (ppm)

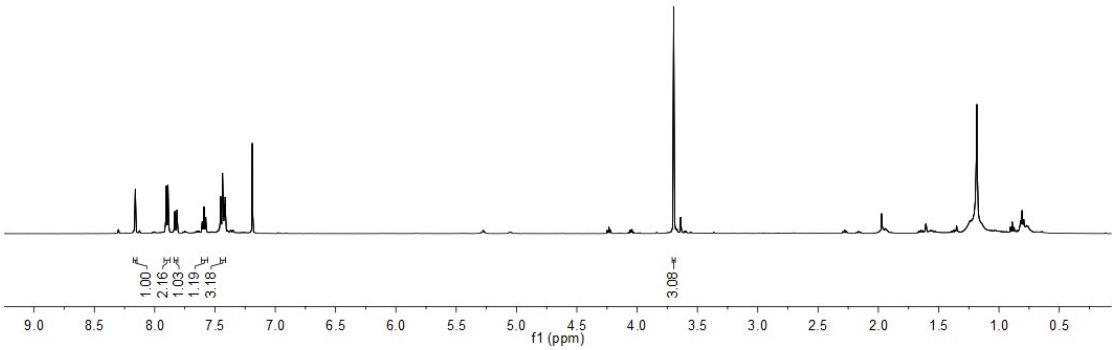

8.7400
8.7336
8.4630
8.4566
8.4399
8.4335
7.9234
7.9055
7.6214
7.6028
7.5842
7.4690
7.4471
7.4292
7.1929
3.7388
O2N
N
O
N
O
1.00
1.05
2.02
1.09
3.12
3.05
f1 (ppm)

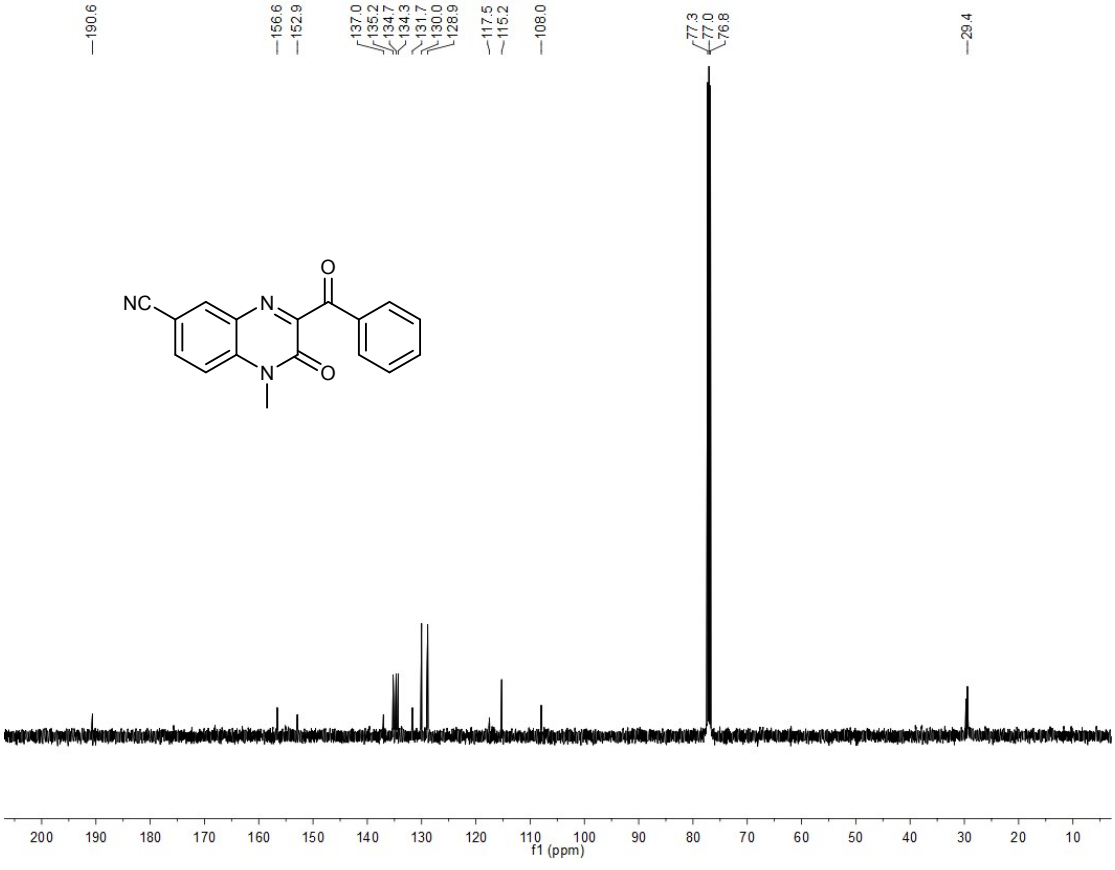

190.5
156.8
152.9
143.7
138.3
134.8
134.2
131.2
130.0
128.9
126.6
126.3
114.8
29.7
O2N
N
O
N
O
f1 (ppm)


8.1641
8.1607
7.9043
7.8896
7.8359
7.8325
7.8184
7.8150
7.6060
7.5911
7.5763
7.4533
7.4375
7.4333
7.4222
7.4153
7.1908

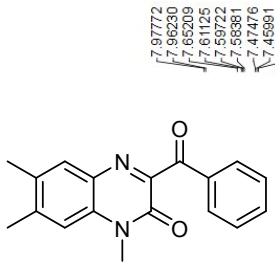

3.6969


NC
N
O
N
O

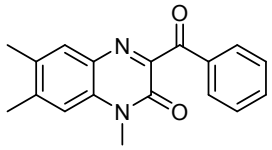

1.00
2.16
1.03
1.19
3.18
3.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


190.6
156.6
152.9
137.0
135.2
134.7
134.3
131.7
130.0
128.9
117.5
115.2
108.0
77.3
77.0
76.8
29.4
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

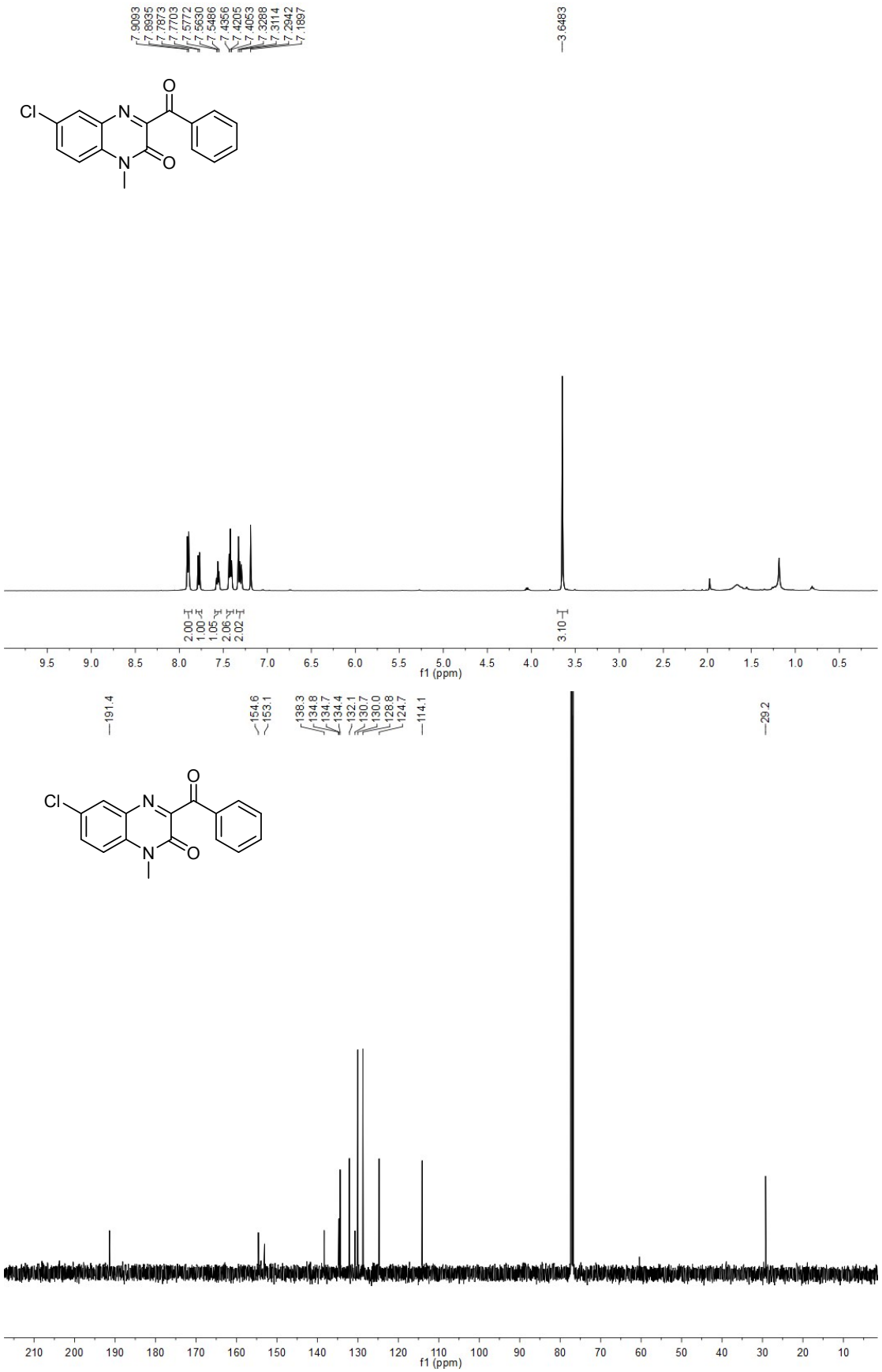
NC
N
O
N
O

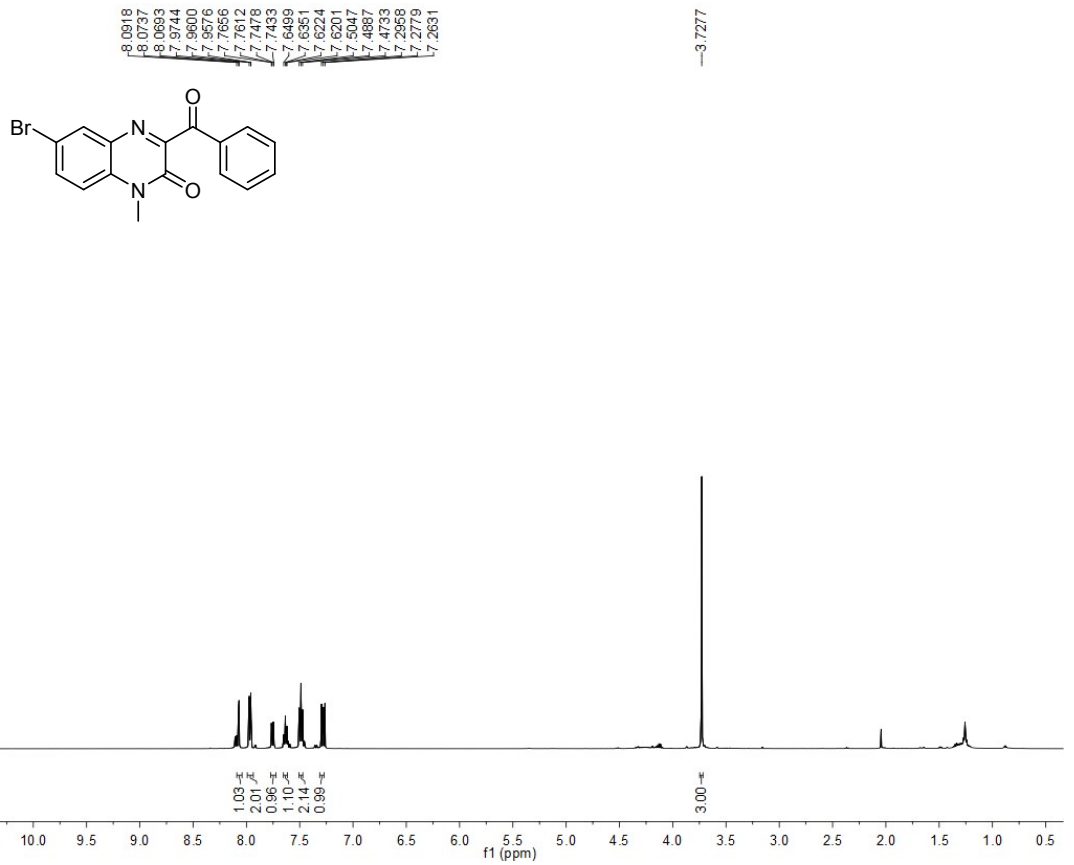


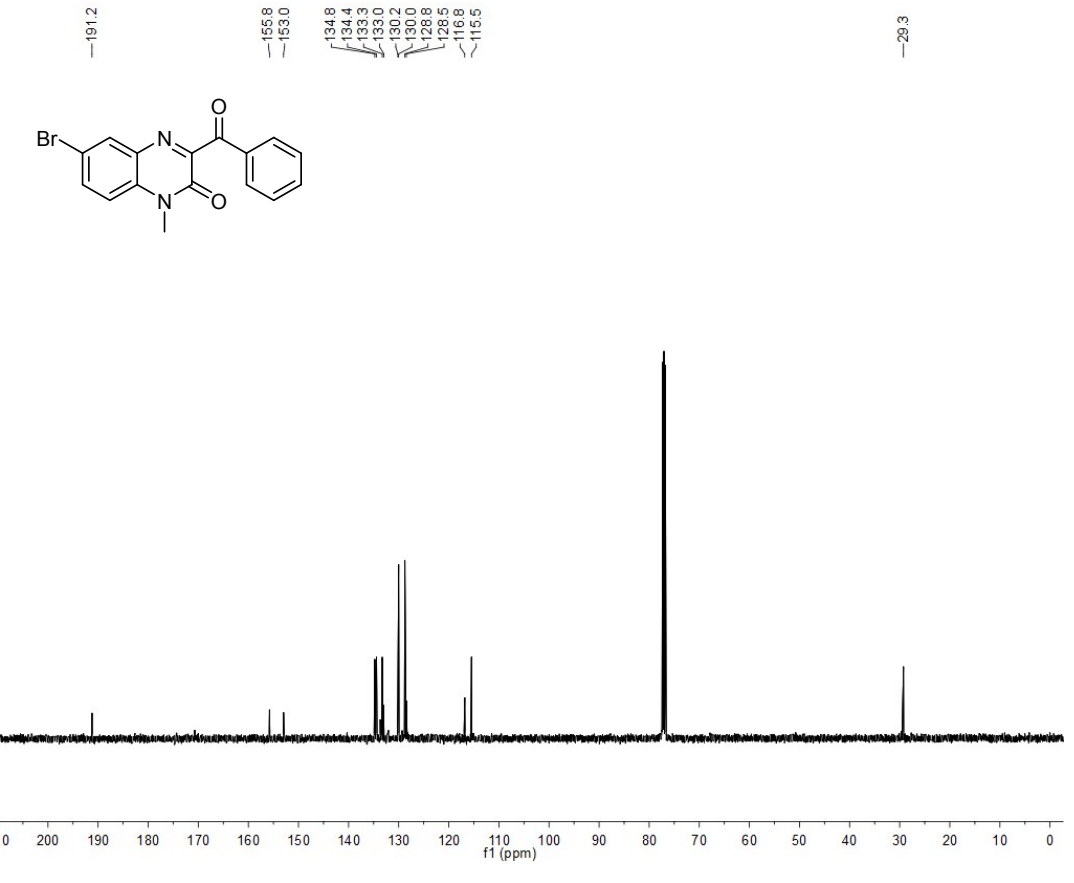
7.97772
7.96230
7.65209
7.61125
7.59722
7.58381
7.47476
7.45991
7.44538
7.27126
7.26905
7.16460
3.70878
2.45162
2.34928
1.94
1.05
1.12
2.16
0.97
3.20
3.29
3.00
f1 (ppm)



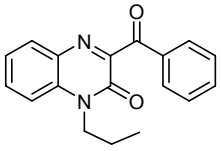
192.1
153.4
153.2
142.6
135.1
134.1
133.4
132.0
130.9
130.6
130.0
128.6
29.0
20.8
19.2
f1 (ppm)

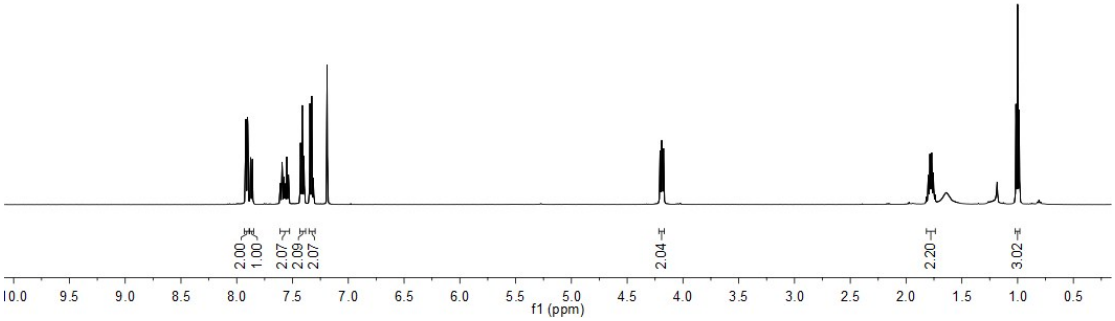

7.9093
7.8935
7.7873
7.7703
7.5772
7.5630
7.5486
7.4356
7.4205
7.4053
7.3288
7.3114
7.2942
7.1897
3.6483
Cl
O
N
O
N
2.00
1.00
1.05
2.06
2.02
3.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
191.4
154.6
153.1
138.3
134.8
134.7
134.4
132.1
130.7
130.0
128.8
124.7
114.1
29.2
Cl
O
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

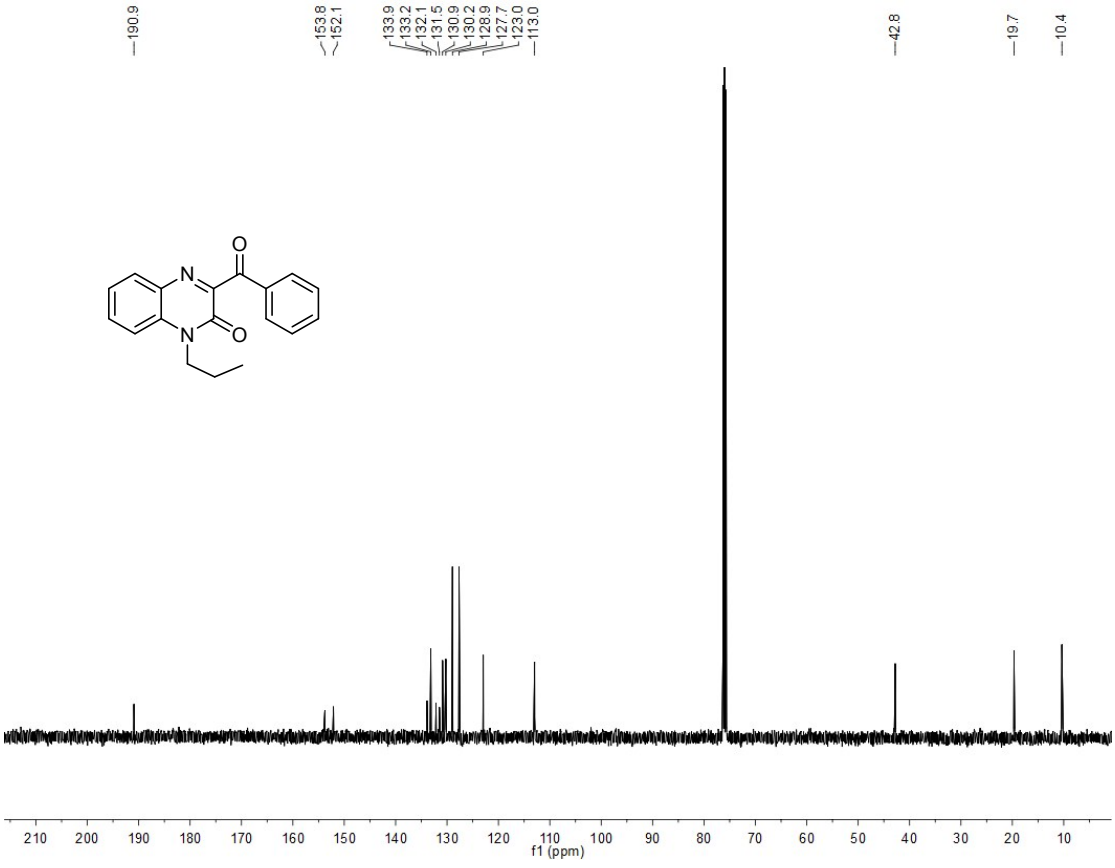

8.0918
8.0737
8.0693
7.9744
7.9600
7.9576
7.7656
7.7612
7.7478
7.7433
7.6499
7.6351
7.6224
7.6201
7.5047
7.4887
7.4733
7.2958
7.2779
7.2631
3.7277
Br
N
O
O
N
1.03
2.01
0.96
1.10
2.14
0.99
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


191.2
155.8
153.0
134.8
134.4
133.3
133.0
130.2
130.0
128.8
128.5
116.8
115.5
29.3
Br
N
O
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.9179
7.9033
7.9012
7.8762
7.8616
7.8596
7.6101
7.6078
7.5936
7.5786
7.5762
7.5657
7.5508
7.5360
7.4282
7.4124
7.3970
7.3436
7.3278
7.3134
7.1898
4.2056
4.1900
4.1743
1.8011
1.7859
1.7704
1.7552
1.0153
1.0005
0.9856

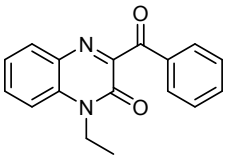

O
N
O
N

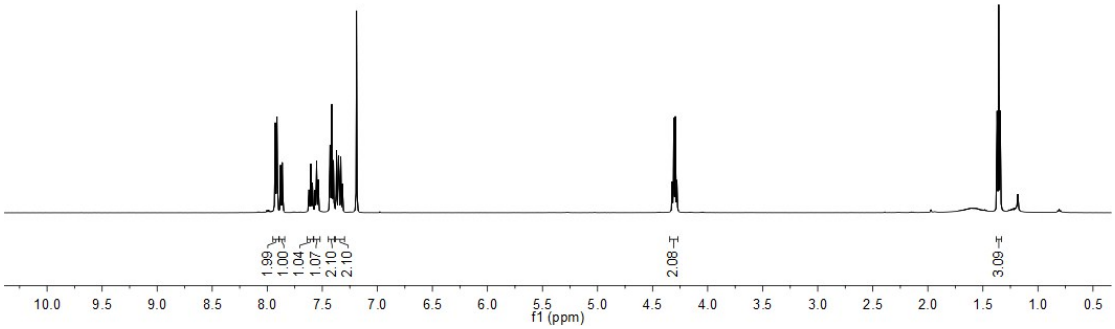

2.00
1.00
2.07
2.09
2.07
2.04
2.20
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

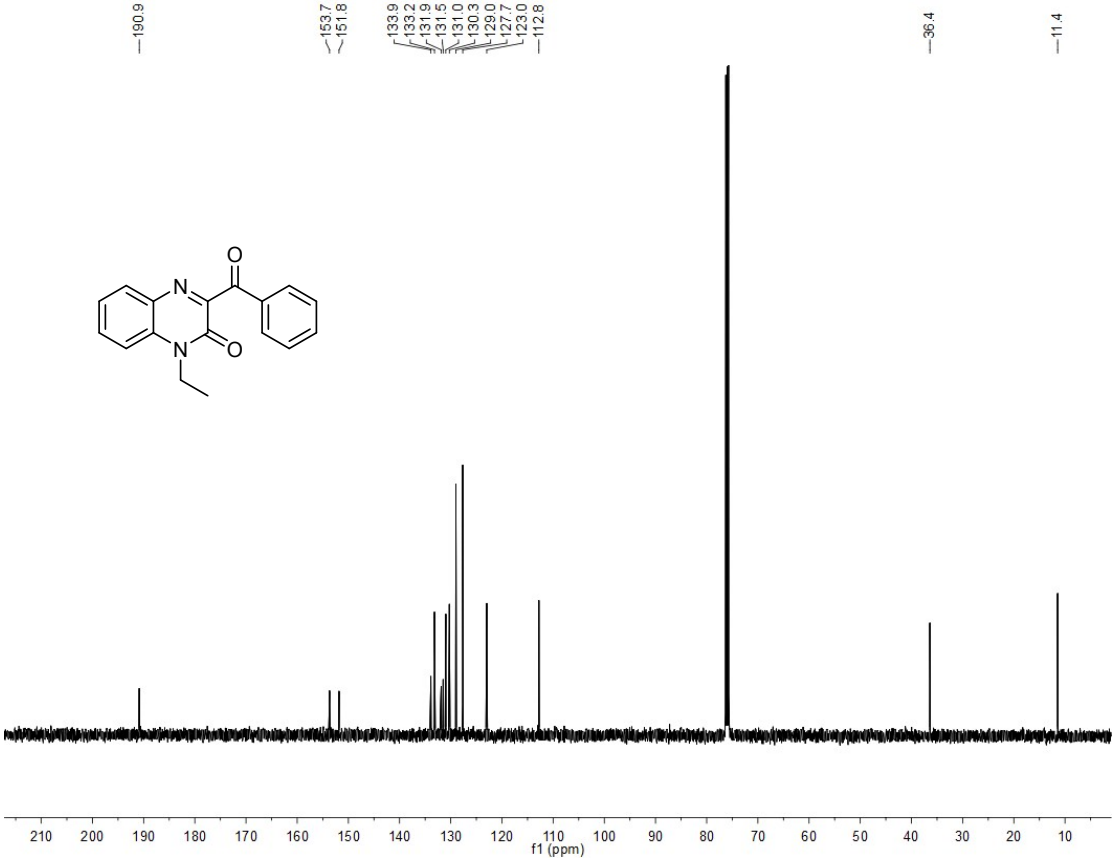

190.9
153.8
152.1
133.9
133.2
132.1
131.5
130.9
130.2
128.9
127.7
123.0
113.0
42.8
19.7
10.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

O
N
O
N

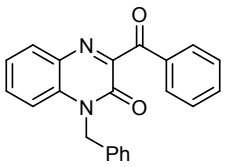

7.9271
7.9120
7.8796
7.8637
7.6209
7.6188
7.6040
7.5894
7.5874
7.5666
7.5520
7.5370
7.4296
7.4142
7.3987
7.3702
7.3530
7.3487
7.3324
7.3177
7.1893
4.3223
4.3079
4.2935
4.2792
1.3709
1.3565
1.3421

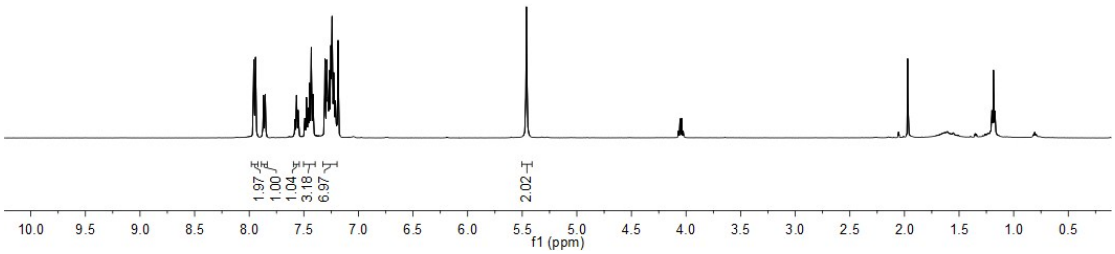

O
N
N
O

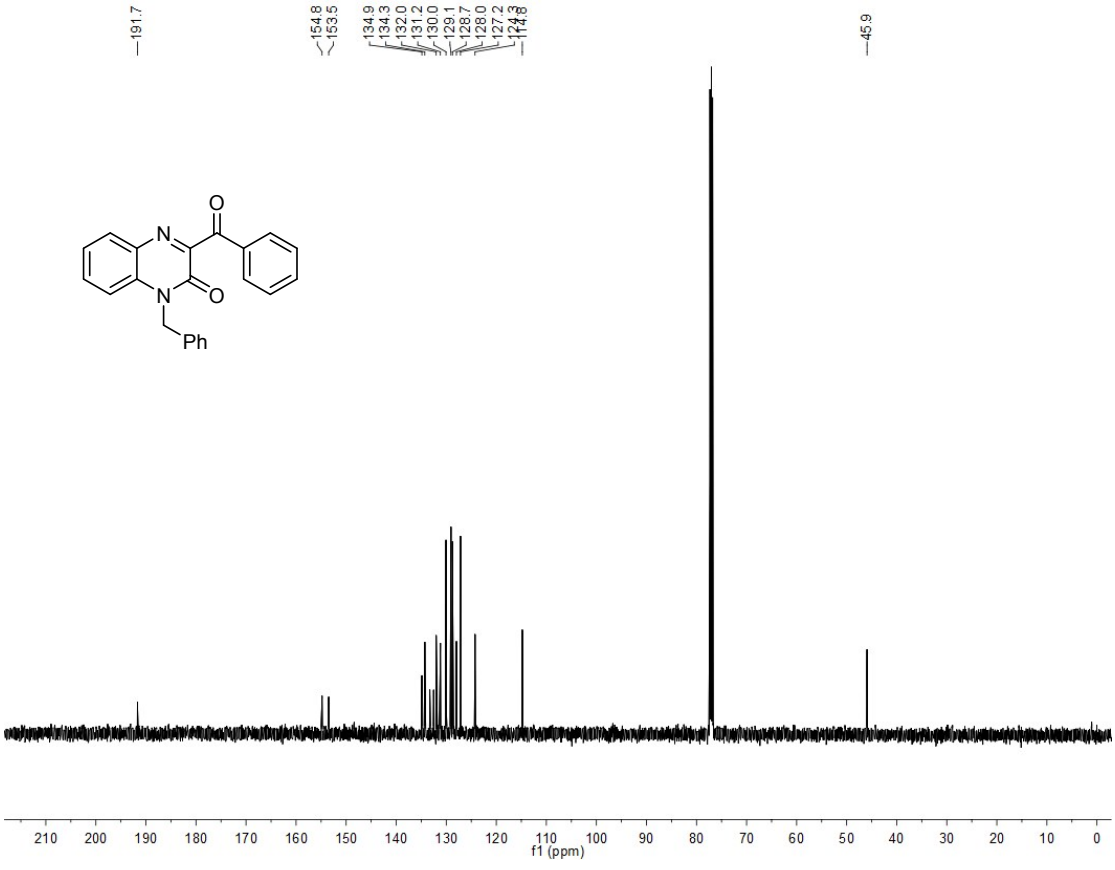

1.99
1.00
1.04
1.07
2.10
2.10
2.08
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

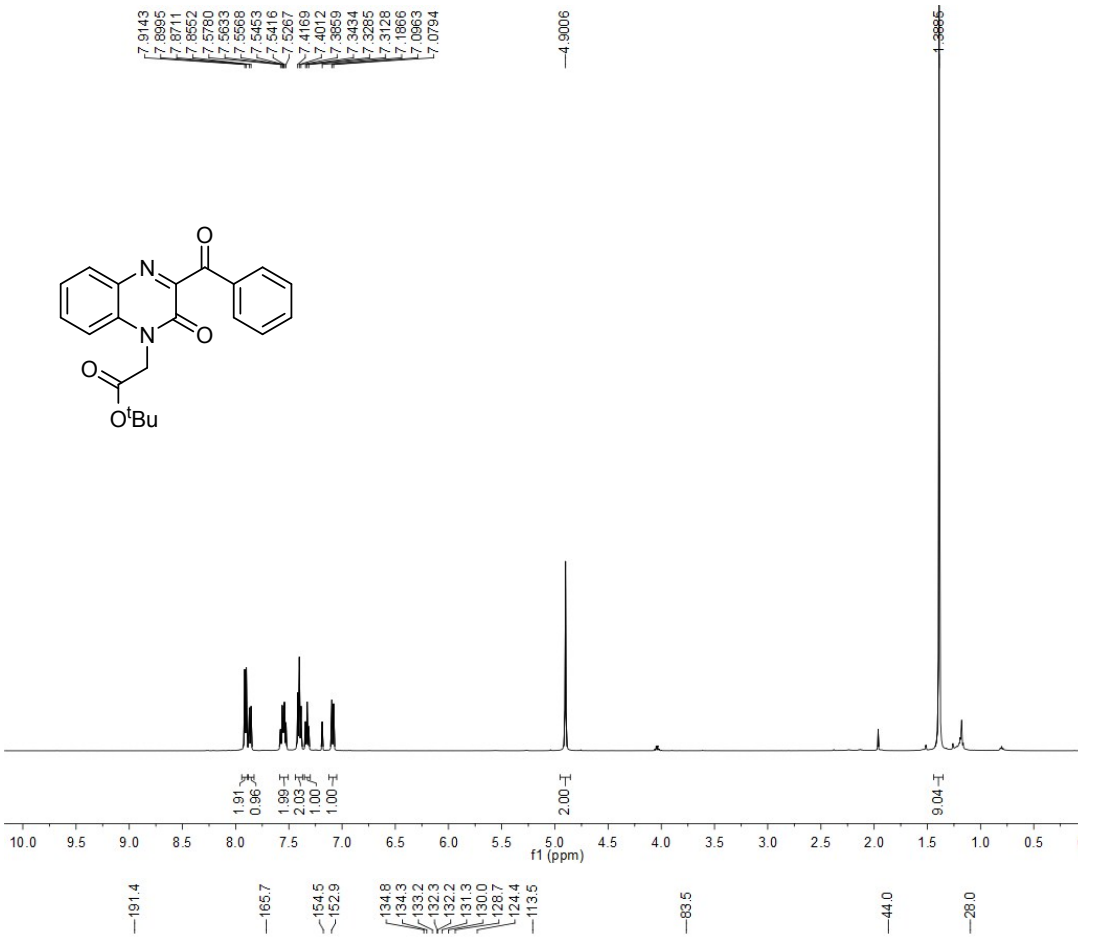

190.9
153.7
151.8
133.9
133.2
131.9
131.5
131.0
130.3
129.0
127.7
123.0
112.8
36.4
11.4
O
N
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

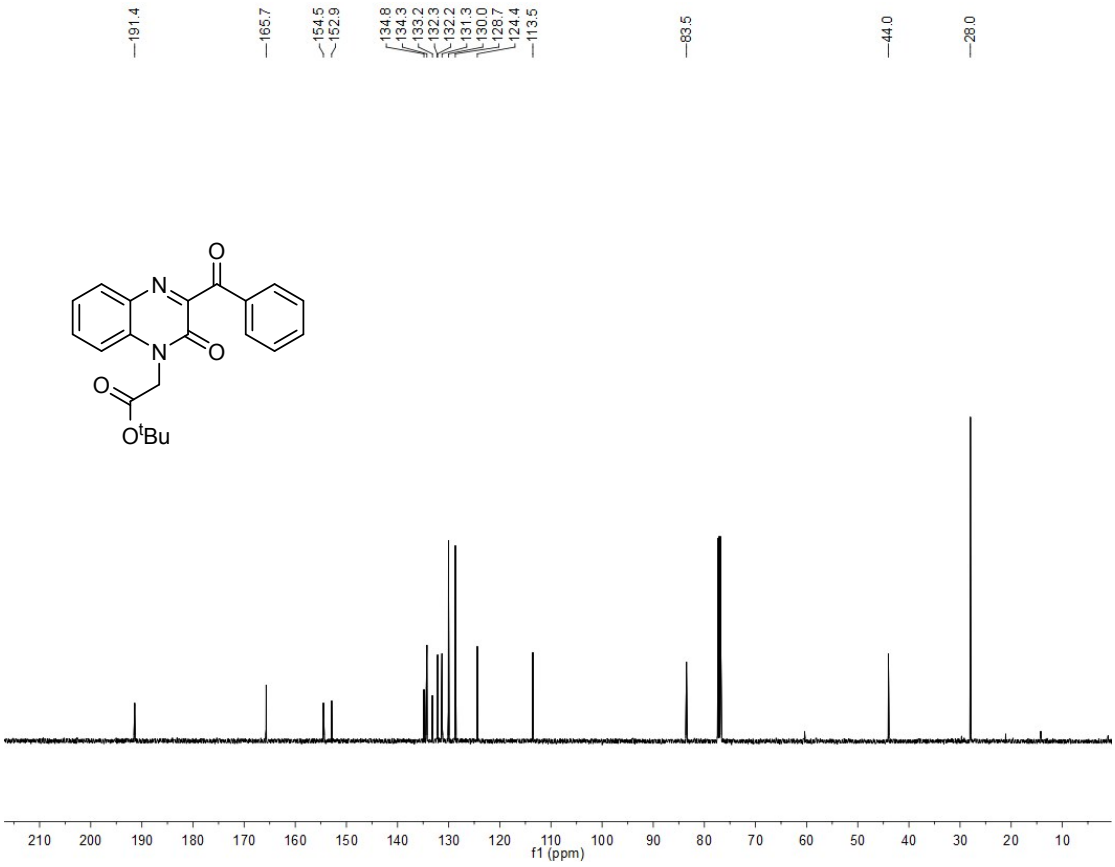

7.9584
7.9421
7.8691
7.8531
7.5820
7.5672
7.5525
7.4906
7.4761
7.4591
7.4475
7.4320
7.4168
7.3068
7.2908
7.2788
7.2660
7.2522
7.2411
7.2262
7.2097
7.1959
7.1865
5.4622


O
N
N
O
Ph

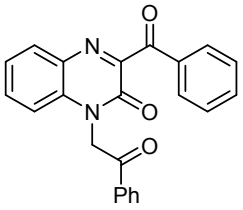

1.97
1.00
1.04
3.18
6.97
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

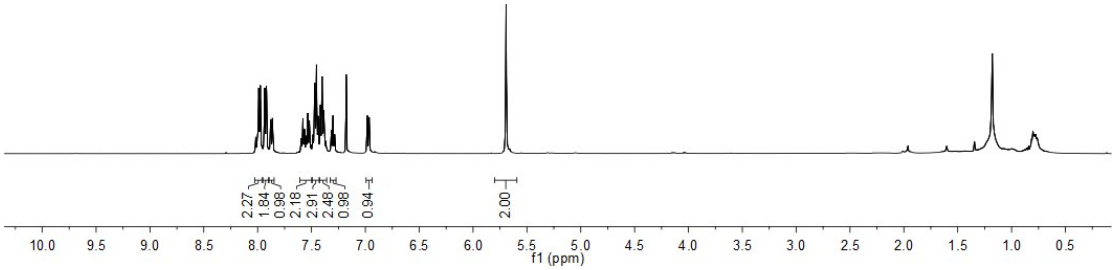

191.7
154.8
153.5
134.9
134.3
132.0
131.2
130.0
129.1
128.7
128.0
127.2
114.8
45.9
O
N
N
O
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

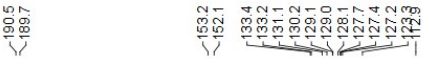

7.9143
7.8995
7.8711
7.8552
7.5780
7.5633
7.5568
7.5453
7.5416
7.5267
7.4169
7.4012
7.3859
7.3434
7.3285
7.3128
7.1866
7.0963
7.0794
4.9006
1.3885
O
N
O
N
O
O
O
O
tBu
1.91
0.96
1.99
2.03
1.00
1.00
2.00
9.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

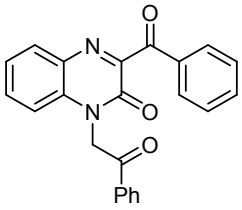

191.4
165.7
154.5
152.9
134.8
134.3
133.2
132.3
132.2
131.3
130.0
128.7
124.4
113.5
83.5
44.0
28.0
O
N
O
N
O
O
O
O
tBu
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

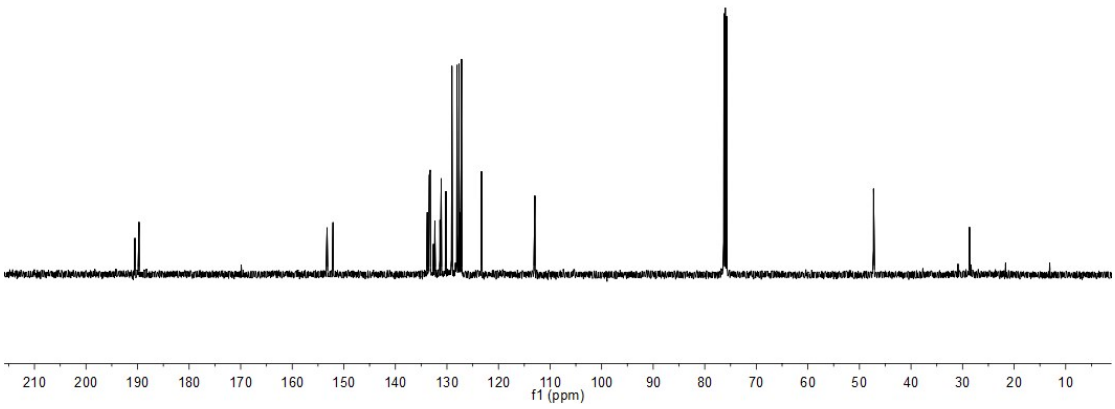

8.0026
8.0002
7.9899
7.9753
7.9732
7.9337
7.9192
7.9169
7.8793
7.8770
7.8632
7.8610
7.5797
7.5649
7.5344
7.5196
7.4855
7.4692
7.4537
7.4381
7.4175
7.4014
7.3861
7.3149
7.3004
7.2860
7.2843
7.1777
6.9814
6.9645
6.9533

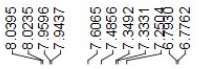

O
N
O
N
O
O
Ph

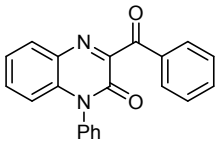

2.27
1.84
0.98
2.18
2.91
2.48
0.98
0.94
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

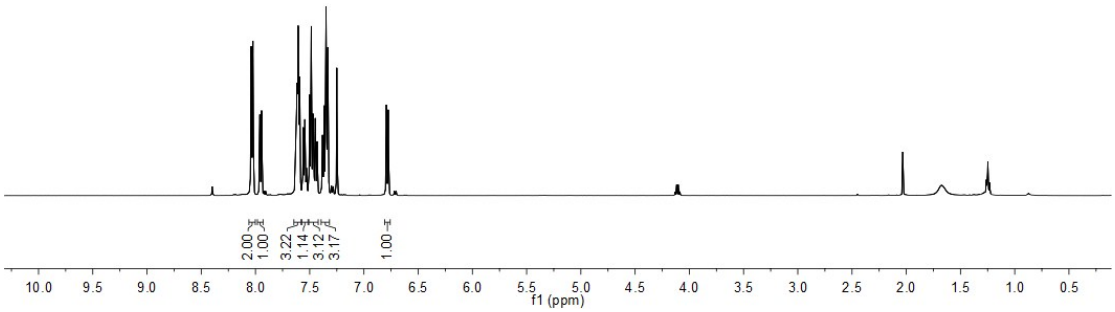

190.5
189.7
153.2
152.1
133.4
133.2
131.1
130.2
129.1
129.0
128.1
127.7
127.4
127.2
123.3
112.9
47.3
28.7

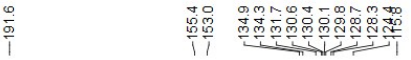

O
N
O
N
O
O
Ph

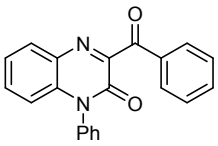

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

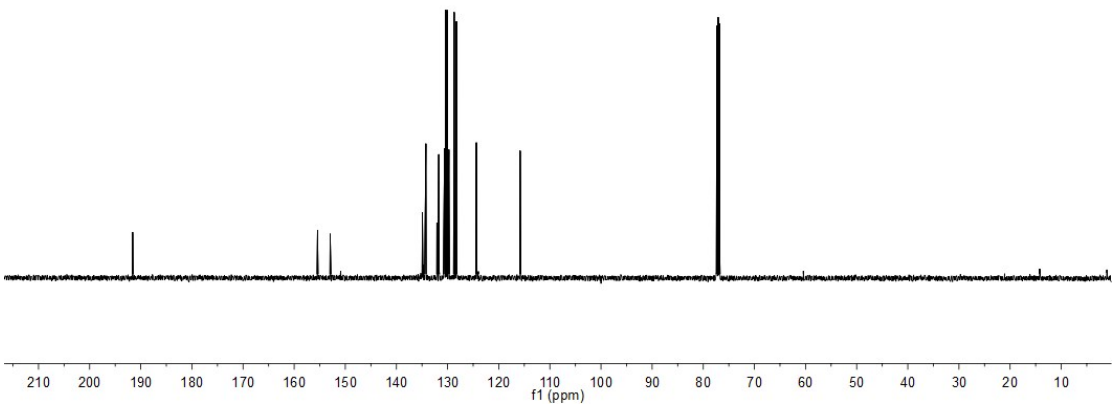

8.0395
8.0235
7.9596
7.9437
7.6065
7.4856
7.3492
7.3331
6.7762

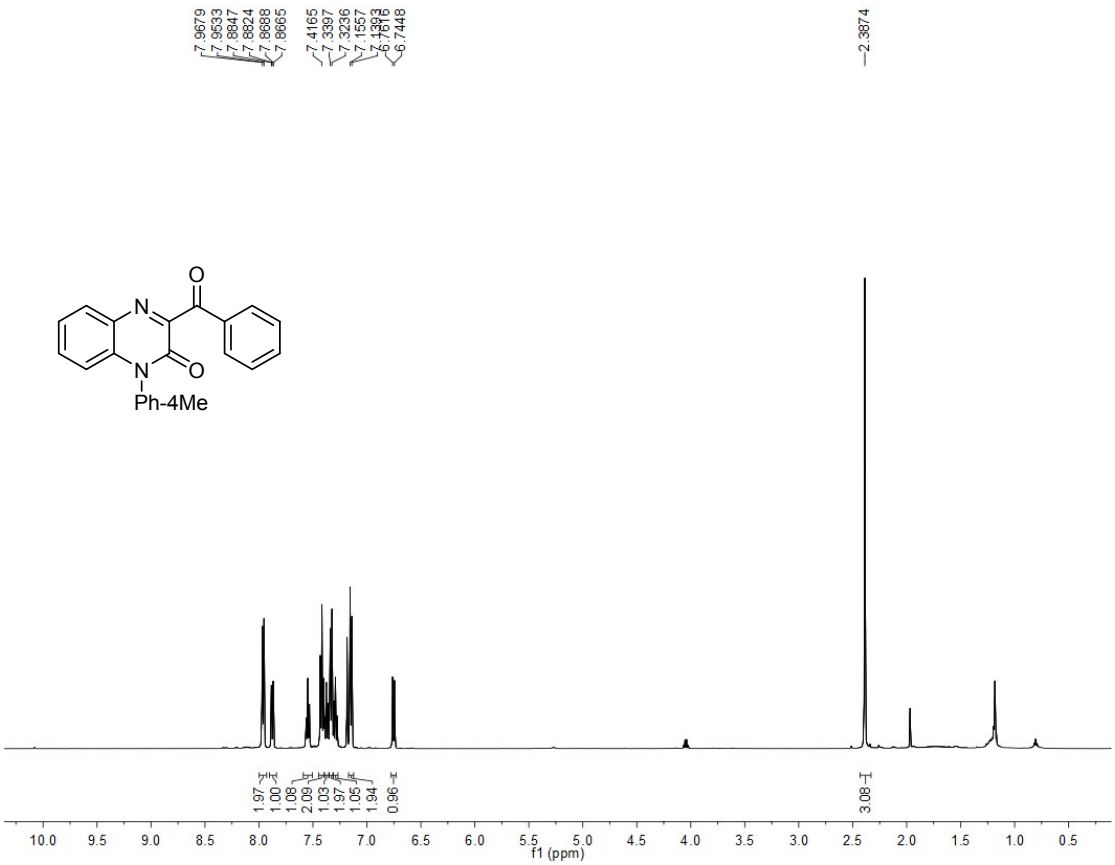

O
N
O
N
Ph

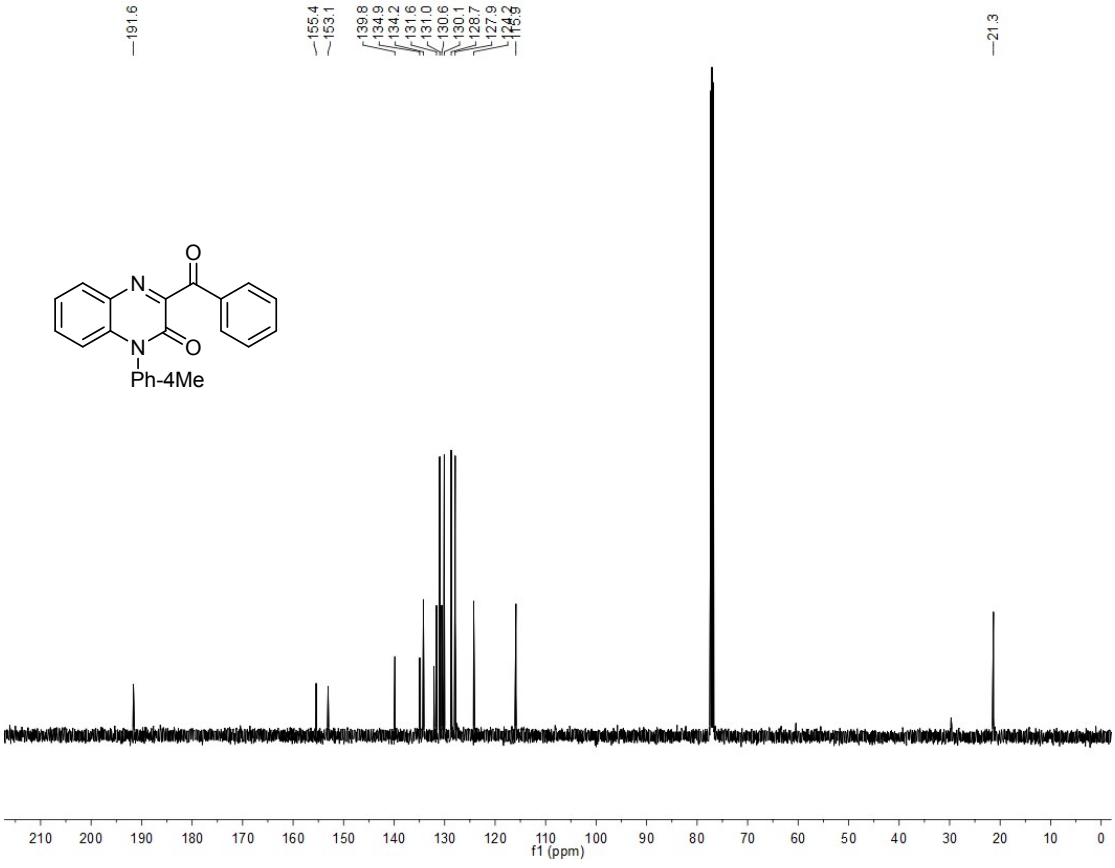

2.00
1.00
3.22
1.14
3.12
3.17
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

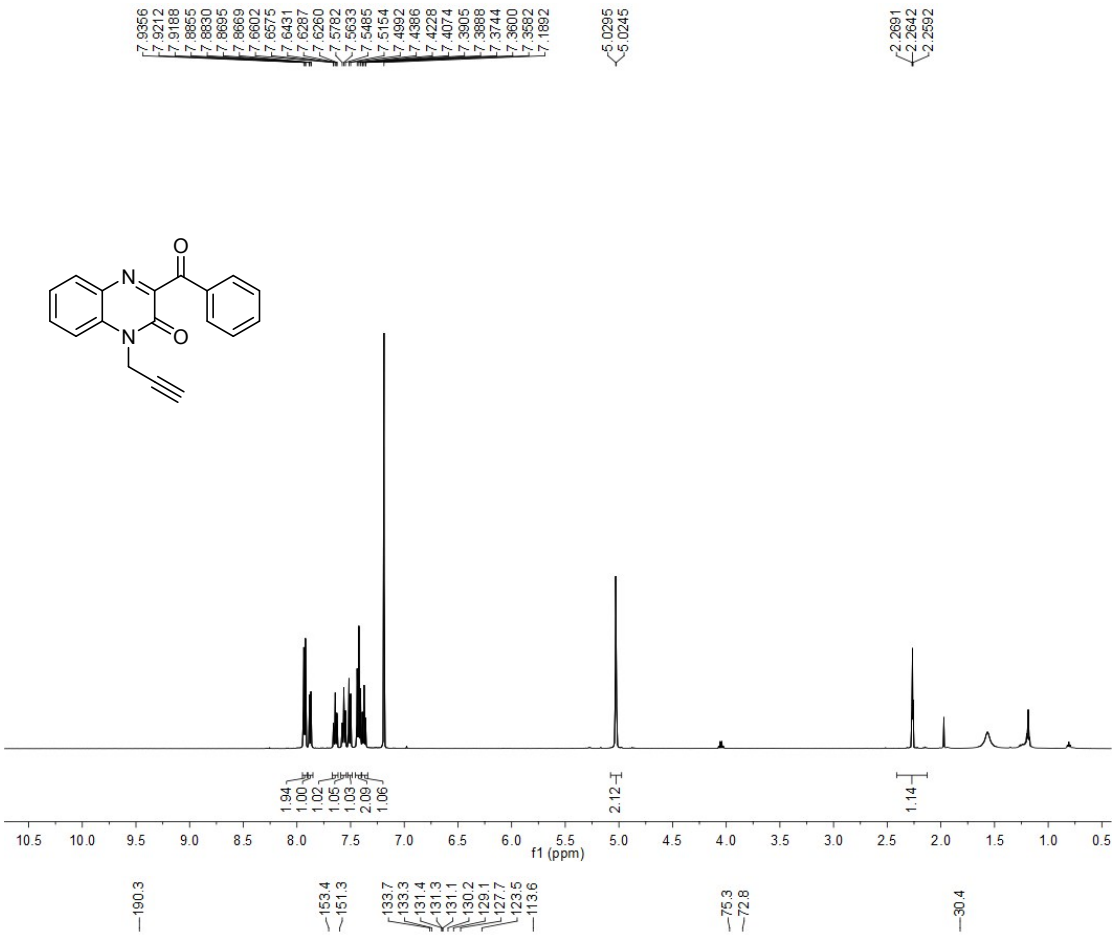

191.6
155.4
153.0
134.9
134.3
131.7
130.6
130.4
130.1
129.8
128.7
128.3
124.4
115.8


O
N
O
N
Ph

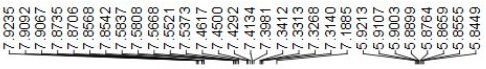

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

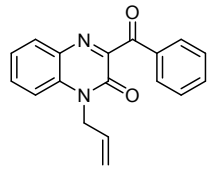

7.9679
7.9533
7.8847
7.8824
7.8688
7.8665
7.4165
7.3397
7.3236
7.1557
7.1393
6.7616
6.7448
2.3874
O
N
O
N
Ph-4Me
1.97
1.00
1.08
2.09
1.03
1.97
1.05
1.94
0.96
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

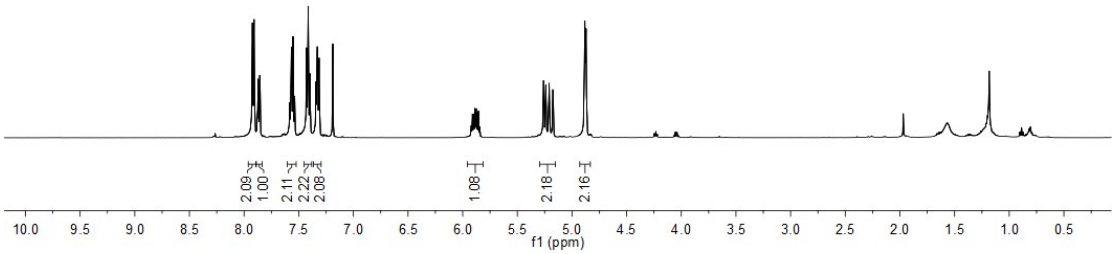

191.6
155.4
153.1
139.8
134.9
134.2
131.6
131.0
130.6
130.1
128.7
127.9
21.3
O
N
O
N
Ph-4Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

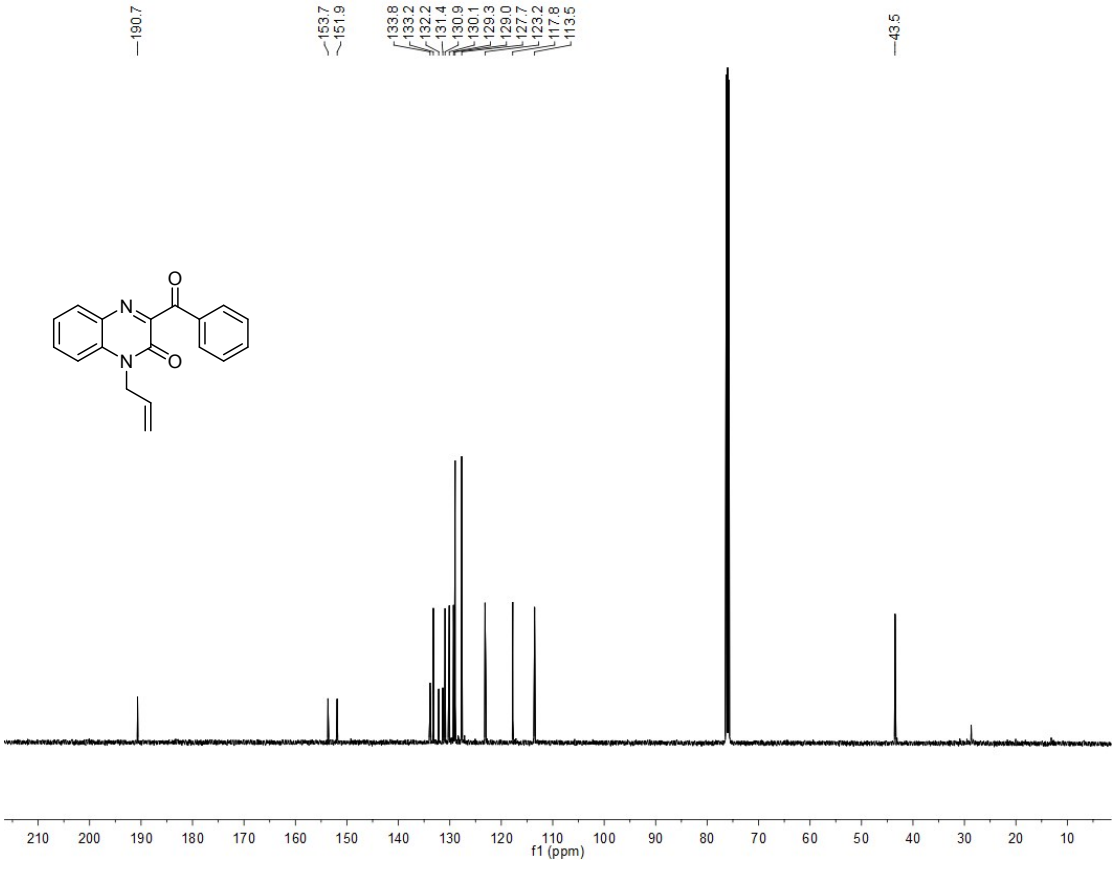

7.9356
7.9212
7.9188
7.8855
7.8830
7.8695
7.8669
7.6602
7.6575
7.6431
7.6287
7.6260
7.5782
7.5633
7.5485
7.5154
7.4992
7.4386
7.4228
7.4074
7.3905
7.3888
7.3744
7.3600
7.3582
7.1892
5.0295
5.0245
2.2691
2.2642
2.2592
O
N
O
N
1.94
1.00
1.02
1.05
1.03
2.09
1.06
2.12
1.14
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 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
f1 (ppm)

190.3
153.4
151.3
133.7
133.3
131.4
131.3
131.1
130.2
129.1
127.7
123.5
113.6
75.3
72.8
30.4
O
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.9235
7.9092
7.9067
7.8735
7.8706
7.8568
7.8542
7.5837
7.5808
7.5668
7.5521
7.5373
7.4617
7.4500
7.4292
7.4134
7.3981
7.3412
7.3313
7.3268
7.3140
7.1885
5.9213
5.9107
5.9003
5.8899
5.8764
5.8659
5.8555
5.8449


O
N
N
O


2.09
1.00
2.11
2.22
2.08
1.08
2.18
2.16
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
f1 (ppm)


190.7
153.7
151.9
133.8
133.2
132.2
131.4
130.9
130.1
129.3
129.0
127.7
123.2
117.8
113.5
43.5
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

O
N
N
O