Supporting Information

Phenanthrenequinone (PQ) catalyzed cross-dehydrogenative coupling of alkanes with quinoxalin-2(1*H*)-ones and simple *N*-heteroarenes under visible light irradiation

Min Wang,[a,b] Yicheng Zhang,[b] Xinyu Yang[b] and Peipei Sun[*a]

[a.] School of Chemistry and Materials Science, Jiangsu Provincial Key Laboratory of Material Cycle Processes and Pollution Control, Jiangsu Collaborative Innovation Center of Biomedical Functional Materials, Nanjing Normal University, Nanjing 210023, China; E-mail: sunpeipei@njnu.edu.cn

[b.] Key Laboratory of Green and Precise Synthetic Chemistry and Applications, Ministry of Education; Department of Chemistry, Huaibei Normal University, Huaibei, Anhui 235000, China; E-mail: wangmin204@chnu.edu.cn

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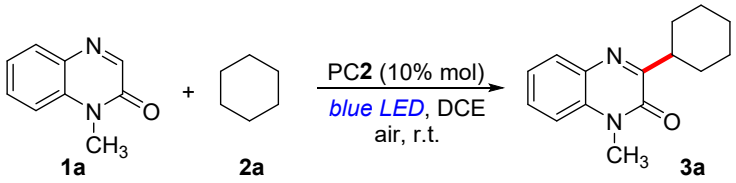
1. General considerations

The ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker FT-NMR spectrometer (600 MHz or 150 MHz, respectively). All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, *J*, are reported in Hertz (Hz). High resolution mass spectroscopy data of the product were collected on an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS (ESI). Electron paramagnetic resonance (EPR) spectra were recorded at room temperature on a Bruker A300 EPR spectrometer. The chemicals and solvents were purchased from commercial suppliers and used without further purification. Products were purified by flash chromatography on 200–300 mesh silica gels, SiO_2.

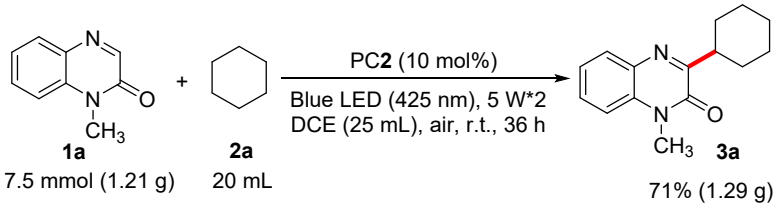
2. Typical experimental procedure

2.1 Typical experimental procedure for the synthesis of 3a



A 15 mL oven-dried quartz tube equipped with a magnetic stirrer was charged with quinoxalin-2(1*H*)-one (**1a**, 0.25 mmol), cyclohexane (**2a**, 1.0 mL), phenanthrenequinone (PC**2**, 0.025 mmol) and 1,2-dichloroethane (DCE, 1.0 mL). The reaction vessel was exposed to blue LED (425 nm, 5 W) irradiation at room temperature in air with stirring for 16 h. After completion of the reaction, the mixture was concentrated to yield the crude product, which was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 10:1, V/V) to give the desired product **3a** in 86% yield as white power.

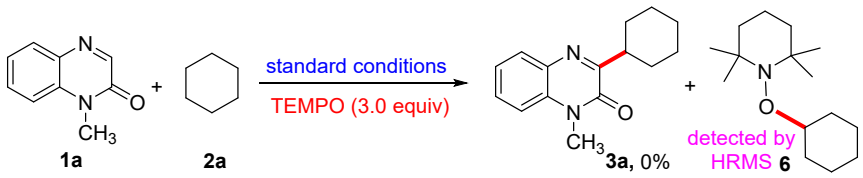
2.2 Gram-scale synthesis of 3a



A 100 mL oven-dried quartz tube equipped with a magnetic stirrer was charged with quinoxalin-2(1*H*)-one (**1a**, 7.5 mmol), cyclohexane (**2a**, 20.0 mL), phenanthrenequinone (PC**2**, 0.75 mmol) and 1,2-dichloroethane (DCE, 25.0 mL). The reaction vessel was exposed to blue LED (425 nm, 5 W, two lamps) irradiation at room temperature in air with stirring for 36 h. After completion of the reaction, the mixture was concentrated to yield the crude product, which was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 10:1, V/V) to give the desired product **3a** in 71% yield.

3. Mechanism investigation

3.1 Free radical-trapping experiment



A 15 mL oven-dried quartz tube equipped with a magnetic stirrer was charged with quinoxalin-2(1*H*)-one (**1a**, 0.25 mmol), cyclohexane (**2a**, 1.0 mL), phenanthrenequinone (PC**2**, 0.025 mmol), TEMPO (2,2,6,6-tetramethyl-1-piperidinyloxy, 0.75 mmol, 3.0 equiv.) and 1,2-dichloroethane (DCE, 1.0 mL). The reaction vessel was exposed to blue LED (425 nm, 5 W) irradiation at room temperature in air with stirring for 16 h. After the reaction was stopped, no desired product **3a** was detected in the mixture, while an adduct (**6**) of TEMPO with a cyclohexyl radical was formed, which was detected by HPLC/HRMS. The model reaction was completely inhibited, indicating that a radical pathway was involved in the reaction.

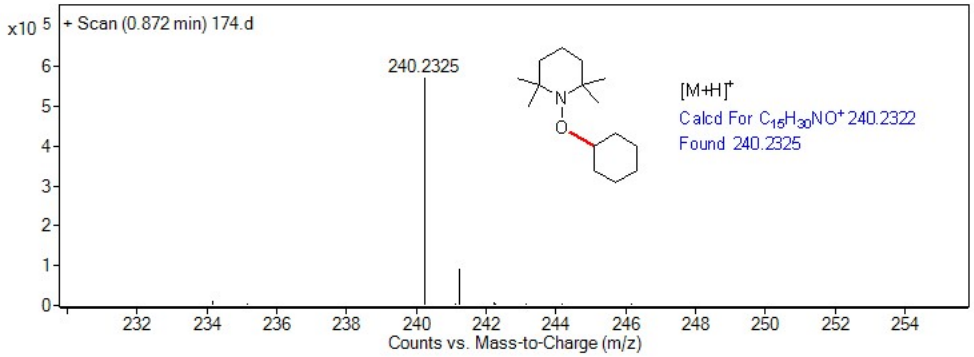


Figure S1. HRMS analysis of **6**

3.2 Determination of electron paramagnetic resonance (EPR)

3.2.1 Determination of singlet oxygen species

In order to determine the active species of oxygen involved in the present reaction, 2,2,6,6-tetramethylpiperidine (TEMP) was used to trap $^1O_2$. Irradiation of the air-saturated solution of TEMP and phenanthrenequinone (PQ) in DCE with blue LED (425 nm, 5 W) resulted in the formation of a strong characteristic signal of $^1O_2$ adduct with TEMP (Figure S2b, c, d and e), implying that $^1O_2$ is present during the reaction.

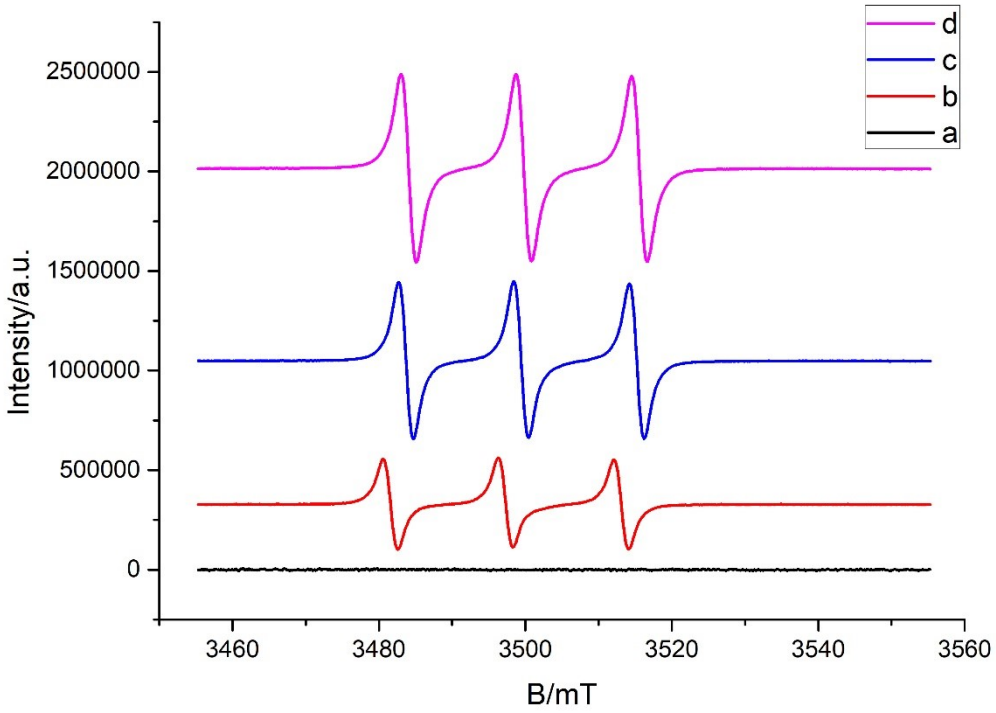


Figure S2. Electron paramagnetic resonance (EPR) spectra of $^1O_2$ adduct with DMPO

(a) A solution of PQ (0.025 mol/L) with TEMP (0.05 mol/L) in air-saturated DCE without light irradiation.

(b) A solution of PQ (0.025 mol/L) with TEMP (0.05 mol/L) in air-saturated DCE under blue LED (425 nm, 5 W) irradiation for 30 s.

(c) A solution of PQ (0.025 mol/L) with TEMP (0.05 mol/L) in air-saturated DCE under blue LED (425 nm, 5 W) irradiation for 60 s.

(d) A solution of PQ (0.025 mol/L) with TEMP (0.05 mol/L) in air-saturated DCE under blue LED (425 nm, 5 W) irradiation for 90 s.

3.2.2 Determination of alkyl radical species

For further explore the active species of $O_2^{\bullet-}$ involved during the reaction, 5,5-dimethyl-pyrroline-*N*-oxide (DMPO) was used to trap $O_2^{\bullet-}$. In the standard reaction mixture, DMPO (0.1 mmol) was added. Irradiation of the reaction solution in air with blue LED (425 nm, 5 W) resulted in the formation of a strong characteristic signal of alkyl radical adduct with DMPO (Figure S3b, c and d), while the characteristic signal of $O_2^{\bullet-}$ adduct with DMPO was not observed, which implying that alkyl radical is present during the reaction.

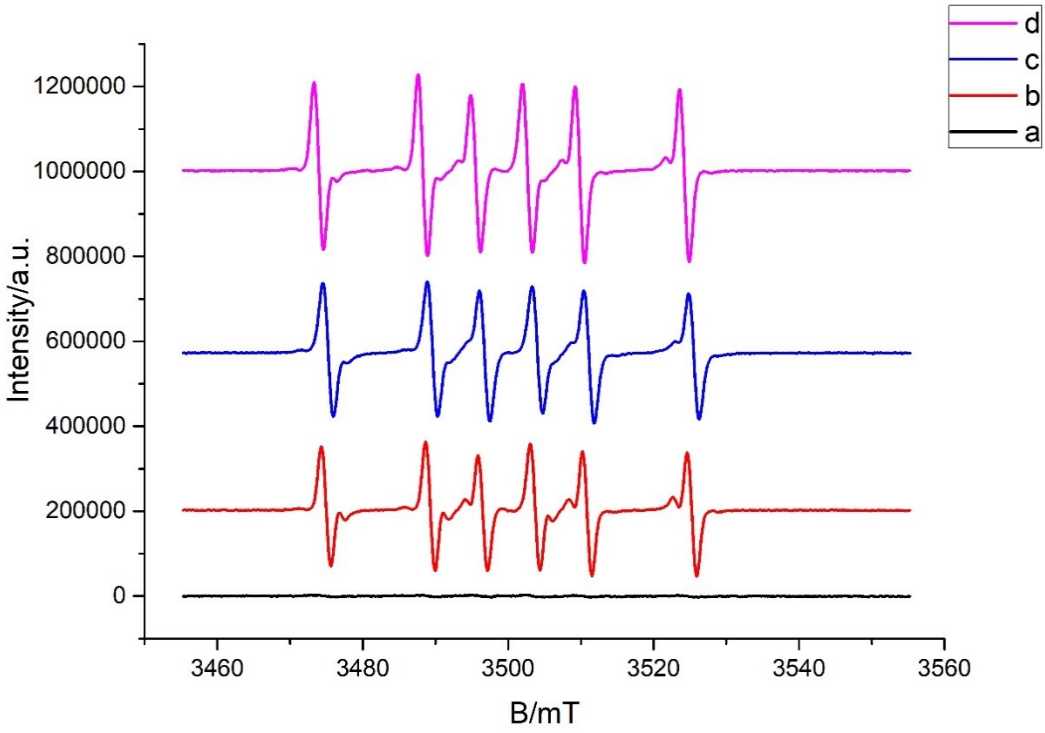


Figure S3. Electron paramagnetic resonance (EPR) spectra of alkyl radical adduct with DMPO

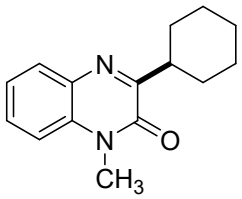
(a) An air-saturated solution of standard reaction with DMPO (0.20 mol/L) without light irradiation.

(b) An air-saturated solution of standard reaction with DMPO (0.20 mol/L) under blue LED (425 nm, 5 W) irradiation for 30 s.

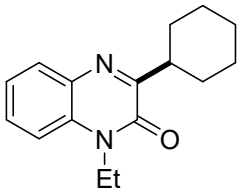
(c) An air-saturated solution of standard reaction with DMPO (0.20 mol/L) under blue LED (425 nm, 5 W) irradiation for 60 s.

(d) An air-saturated solution of standard reaction with DMPO (0.20 mol/L) under blue LED (425 nm, 5 W) irradiation for 90 s.

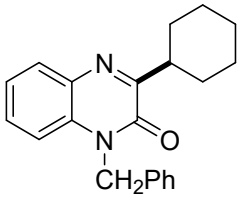
4. Characterization data for the products



3-cyclohexyl-1-methylquinoxalin-2(1H)-one (3a).[1] White solid; 86% yield (52.1 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.84 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.52–7.49 (m, 1H), 7.34–7.31 (m, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 3.69 (s, 3H), 3.34 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.96 (d, *J* =12.0, 2H), 1.88–1.85 (m, 2H), 1.78–1.75 (m, 1H), 1.58 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.47 (qt, *J* = 12.6, 3.0 Hz, 2H), 1.31 (qt, *J* = 12.0, 3.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 164.2, 154.4, 132.8, 132.8, 129.7, 129.3, 123.3, 113.4, 40.7, 30.5, 29.0, 26.3, 26.1.

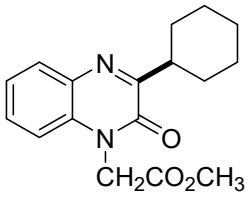


3-cyclohexyl-1-ethylquinoxalin-2(1H)-one (3b).[2] White solid; 87% yield (55.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.84 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.32–7.29 (m, 2H), 4.31 (q, *J* = 7.2 Hz, 2H), 3.35 (tt, *J* = 11.4, 3.6 Hz, 1H), 1.97–1.95 (m, 2H), 1.88–1.86 (m, 2H), 1.78–1.75 (m, 1H), 1.57 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.47 (qt, *J* = 13.2, 3.6 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 1.33–1.27 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.3, 154.0, 133.2, 131.8, 130.0, 129.3, 123.1, 113.2, 40.6, 37.2, 30.5, 26.3, 26.1, 12.4.

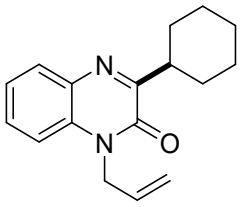


1-benzyl-3-cyclohexylquinoxalin-2(1H)-one (3c).[1] White solid; 82% yield (65.3 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.83 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.38–7.35 (m, 1H), 7.31–

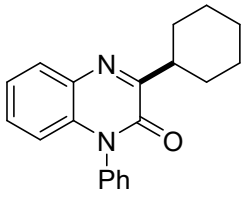
7.28 (m, 2H), 7.26–7.25 (m, 1H), 7.24–7.21 (m, 4H), 5.48 (s, 2H), 3.40 (tt, *J* = 11.4, 3.2 Hz, 1H), 2.03–2.00 (m, 2H), 1.88 (dt, *J* = 13.2, 3.4 Hz, 2H), 1.79–1.76 (m, 1H), 1.61 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.48 (qt, *J* = 13.2, 3.6 Hz, 2H), 1.32 (qt, *J* = 12.6, 3.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ = 164.3, 154.5, 135.4, 133.1, 132.1, 129.8, 129.3, 128.8, 127.6, 126.9, 123.4, 114.2, 45.9, 40.8, 30.5, 26.3, 26.1.



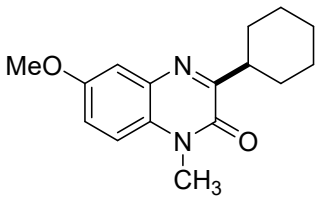
ethyl 2-(3-cyclohexyl-2-oxoquinoxalin-1(2H)-yl)acetate (3d).[3] White solid; 84% yield (63.1 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 7.8, 1H), 7.46 (t, *J* = 7.8, 1H), 7.32 (t, *J* = 7.8, 1H), 7.04 (d, *J* = 8.4, 1H), 5.01 (s, 2H), 4.24 (q, *J* = 7.2 Hz, 2H), 3.32 (tt, *J* = 11.4, 3.6 Hz, 1H), 1.99–1.95 (m, 2H), 1.87 (dt, *J* = 13.2, 3.6 Hz, 2H), 1.78–1.75 (m, 1H), 1.58 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.45 (qt, *J* = 13.2, 3.6 Hz, 2H), 1.35–1.29 (m, 1H), 1.27 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (151 MHz,$CDCl_3$): δ = 167.2, 164.0, 154.1, 132.9, 132.0, 130.1, 129.5, 123.6, 112.8, 61.9, 43.5, 40.8, 30.4, 26.3, 26.1, 14.1.



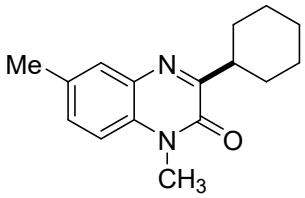
1-allyl-3-cyclohexylquinoxalin-2(1H)-one (3e).[1] White solid; 81% yield (54.3 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.84 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.48–7.45 (m, 1H), 7.32–7.29 (m, 1H), 7.27–7.25 (m, 1H), 5.97–5.91 (m, 1H), 5.26 (dd, *J* = 10.2, 0.6 Hz, 1H), 5.17 (dd, *J* = 17.4, 0.6 Hz, 1H), 4.90 (dt, *J* = 5.4, 1.8 Hz, 2H), 3.35 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.98–1.95 (m, 2H), 1.86 (dt, *J* = 12.6, 3.6 Hz, 2H), 1.79–1.74 (m, 1H), 1.58 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.46 (qt, *J* = 12.6, 3.6 Hz, 2H), 1.31 (qt, *J* = 12.6, 3.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 164.3, 154.0, 133.0, 132.0, 130.8, 129.8, 129.2, 123.3, 117.9, 113.9, 44.5, 40.7, 30.5, 26.3, 26.1.



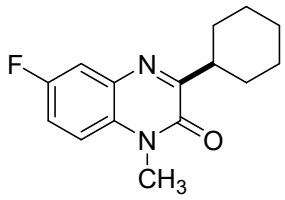
3-cyclohexyl-1-phenylquinoxalin-2(1H)-one (3f). White solid; 83% yield (63.2 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.88–7.87 (m, 1H), 7.60 (t, *J* =7.2 Hz, 2H), 7.55–7.53 (m, 1H), 7.30–7.27 (m, 4H), 6.66–6.64 (m, 1H), 3.35 (tt, *J* = 12.0, 3.6 Hz, 1H), 2.02–2.00 (m, 2H), 1.87 (d, *J* = 13.2 Hz, 2H), 1.76 (d, *J* = 12.6 Hz, 1H), 1.67–1.60 (m, 2H), 1.49–1.42 (m, 2H), 1.36–1.28 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.0, 154.2, 136.1, 133.6, 132.7, 130.2, 129.3, 129.3, 129.2, 129.0, 128.3, 123.5, 115.3, 40.8, 30.5, 26.3, 26.1; HRMS (ESI): $[M+H]^+$ calculated for $C_{20}H_{21}N_2O^+$: 305.1648, found: 305.1647.



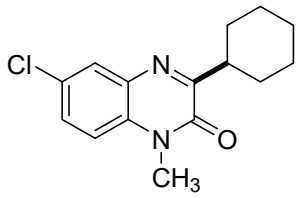
3-cyclohexyl-6-methoxy-1-methylquinoxalin-2(1H)-one (3g).[1] White solid; 79% yield (53.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.33 (d, *J* = 3.0 Hz, 1H), 7.20 (d, *J* = 9.0 Hz, 1H), 7.14–7.12 (m, 1H), 3.89 (s, 3H), 3.68 (s, 3H), 3.36 (tt, *J* = 11.4, 3.6 Hz, 1H), 1.97–1.95 (m, 2H), 1.88–1.85 (m, 2H), 1.78–1.76 (m, 1H), 1.57 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.47 (qt, *J* = 12.6, 3.0 Hz, 2H), 1.31 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.9, 155.8, 154.2, 133.5, 127.1, 118.6, 114.3, 111.2, 55.8, 40.8, 30.5, 29.2, 26.3, 26.1.



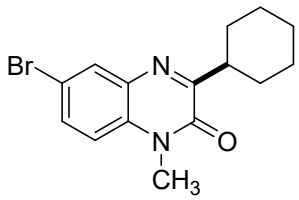
3-cyclohexyl-1,6-dimethylquinoxalin-2(1H)-one (3h).[2] White solid; 88% yield (56.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.65 (s, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 1H), 3.67 (s, 2H), 3.33 (tt, *J* = 12.0, 3.6 Hz, 1H), 2.44 (s, 3H), 1.96–1.93 (m, 2H), 1.86 (dt, *J* = 13.2, 3.6 Hz, 2H), 1.78–1.75 (m, 1H), 1.56 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.50–1.43 (m, 2H), 1.34–1.25 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.2, 154.4, 133.1, 132.7, 130.6, 130.4, 129.6, 113.2, 40.7, 30.5, 29.0, 26.3, 26.1, 20.5.



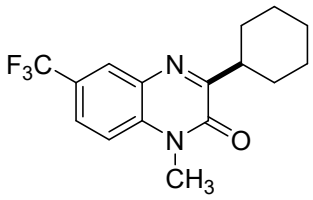
3-cyclohexyl-6-fluoro-1-methylquinoxalin-2(1H)-one (3i).[1] White solid; 85% yield (55.3 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.54–7.52 (m, 1H), 7.27–7.23 (m, 2H), 3.69 (s, 3H), 3.33 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.95–1.93 (m, 2H), 1.86 (dt, *J* = 12.6, 3.0 Hz, 2H), 1.78–1.75 (m, 1H), 1.54 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.46 (qt, *J* = 12.0, 3.0 Hz, 2H), 1.30 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ = 165.8, 158.6 (d, *J* = 241.6 Hz), 154.1, 133.4 (d, *J* = 11.1), 129.5, 116.9 (*J* = 23.7 Hz), 115.2 (d, *J* = 22.5 Hz), 114.4 (d, *J* = 8.7 Hz), 40.8, 30.4, 29.3, 26.2, 26.1.



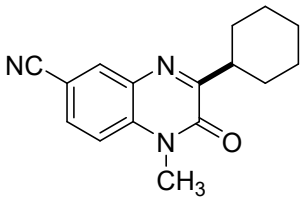
6-chloro-3-cyclohexyl-1-methylquinoxalin-2(1H)-one (3j).[1] White solid; 83% yield (57.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 2.4 Hz, 1H), 7.45 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.21–7.20 (m, 1H), 3.68 (s, 3H), 3.33 (tt, *J* = 11.4, 3.6 Hz, 1H), 1.95–1.93 (m, 2H), 1.86 (dt, *J* = 13.2, 3.6 Hz, 2H), 1.78–1.75 (m, 1H), 1.53 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.46 (qt, *J* = 12.6, 3.0 Hz, 2H), 1.30 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.7, 154.2, 133.4, 131.5, 129.3, 129.1, 128.6, 114.6, 40.8, 30.4, 29.0, 26.2, 26.1.



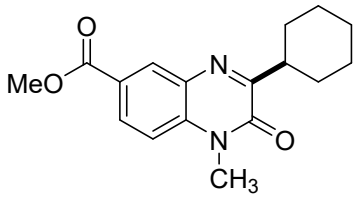
6-bromo-3-cyclohexyl-1-methylquinoxalin-2(1H)-one (3k).[2] White solid; 84% yield (67.5 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.98 (s, 1H), 7.58–7.50 (m, 1H), 7.14 (dd, *J* = 9.0, 1.8 Hz, 1H), 3.66 (s, 3H), 3.34–3.30 (m, 1H), 1.95–1.92 (m, 2H), 1.88–1.85 (m, 2H), 1.78–1.74 (m, 1H), 1.56–1.50 (m, 2H), 1.49–1.42 (m, 2H), 1.33–1.26 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.6, 154.1, 133.6, 132.1, 132.0, 131.9, 115.8, 114.8, 40.7, 30.4, 29.1, 26.2, 26.0.



3-cyclohexyl-1-methyl-6-(trifluoromethyl)quinoxalin-2(1H)-one (3l).[1] White solid; 81% yield (62.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.13 (d, *J* = 1.2 Hz, 1H), 7.72 (dd, *J* = 13.2, 2.4 Hz, 1H), 7.38 (d, *J* = 13.2 Hz, 1H), 3.72 (s, 3H), 3.34 (tt, *J* = 13.2, 3.6 Hz, 1H), 1.98–1.94 (m, 2H), 1.89–1.86 (m, 2H), 1.79–1.76 (m, 1H), 1.60–1.41 (m, 4H), 1.36–1.26 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ = 166.0, 154.3, 135.2, 132.2, 127.2 (q, *J* = 5.7 Hz), 125.8, 125.6 (q, *J* = 5.4 Hz), 123.8 (q, *J* = 272.5 Hz), 114.0, 40.8, 30.4, 29.2, 26.2, 26.1.

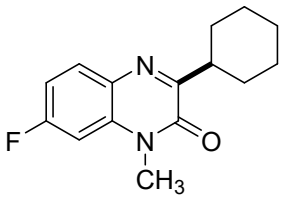


3-cyclohexyl-1-methyl-2-oxo-1,2-dihydroquinoxaline-6-carbonitrile (3m).[2] White solid; 80% yield (53.5 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.14 (s, 1H), 7.73 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 3.71 (s, 3H), 3.32 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.95–1.93 (m, 2H), 1.89–1.86 (m, 2H), 1.79–1.76 (m, 1H), 1.53 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.49–1.42 (m, 2H), 1.34–1.29 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.5, 154.1, 136.2, 134.0, 132.4, 132.0, 118.1, 114.5, 106.8, 40.9, 30.4, 29.3, 26.1, 26.0.

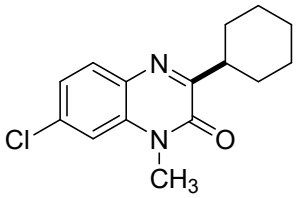


Methyl 3-cyclohexyl-1-methyl-2-oxo-1,2-dihydroquinoxaline-6-carboxylate (3n). White solid; 85% yield (63.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.52 (d, *J* = 1.8 Hz, 1H), 8.15 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.31 (d, *J* = 9.0 Hz, 1H), 3.96 (s, 3H), 3.71 (s, 3H), 3.33 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.98–1.94 (m, 2H), 1.90–1.85 (m, 2H), 1.79–1.76 (m, 1H), 1.60–1.53 (m, 2H), 1.50–1.44 (m, 2H), 1.31 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 166.2, 165.2, 154.4, 136.2, 132.2, 131.6, 130.2, 125.3, 113.5,

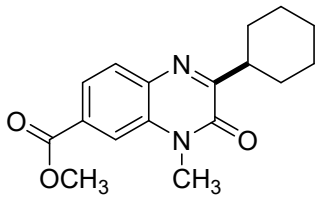
52.2, 40.8, 30.5, 29.3, 26.2, 26.1; HRMS (ESI): $[M+H]^+$ calculated for $C_{17}H_{21}N_2O_3^+$: 301.1547, found: 301.1546.



3-cyclohexyl-7-fluoro-1-methylquinoxalin-2(1H)-one (3o). White solid; 84% yield (54.7 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.80 (t, *J* = 7.8 Hz, 1H), 7.02 (t, *J* = 8.4 Hz, 1H), 6.96 (d, *J* = 9.6 Hz, 1H), 3.65 (s, 3H), 3.32–3.28 (m, 1H), 1.94 (d, *J* = 13.9 Hz, 2H), 1.86 (d, *J* = 13.0 Hz, 2H), 1.76 (d, *J* = 13.0 Hz, 1H), 1.58–1.51 (m, 2H), 1.49–1.43 (m, 2H), 1.34–1.27 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 163.0 (d, *J* = 3.4 Hz), 162.9 (d, *J* = 249.5 Hz), 154.3, 134.2 (d, *J* = 11.5 Hz), 131.5 (d, *J* = 10.3 Hz), 129.5 (d, *J* = 2.2 Hz), 111.0 (d, *J* = 23.3 Hz), 100.3 (d, *J* = 27.8 Hz), 40.6, 30.4, 29.2, 26.2, 26.1; HRMS (ESI): $[M+H]^+$ calculated for $C_{15}H_{17}{}^{19}FN_2O^+$: 261.1398, found: 261.1397.

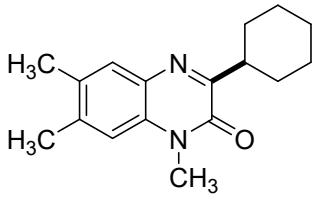


7-chloro-3-cyclohexyl-1-methylquinoxalin-2(1H)-one (3p). White solid; 87% yield (60.2 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.75 (d, *J* = 8.4 Hz, 1H), 7.28–7.27 (m, 2H), 3.66 (s, 3H), 3.33–3.29 (m, 1H), 1.95–1.93 (m, 2H), 1.87–1.85 (m, 2H), 1.77–1.75 (m, 1H), 1.57–1.51 (m, 2H), 1.49–1.43 (m, 2H), 1.33–1.27 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.4, 154.2, 135.2, 133.7, 131.3, 130.8, 123.7, 113.5, 40.8, 30.4, 29.2, 26.2, 26.1; HRMS (ESI): $[M+H]^+$ calculated for $C_{15}H_{17}{}^{35}ClN_2O^+$: 277.1102, found: 277.1101.

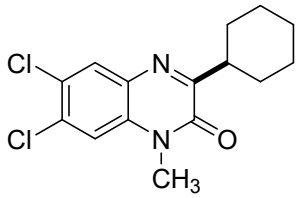


Methyl 2-cyclohexyl-4-methyl-3-oxo-3,4-dihydroquinoxaline-6-carboxylate (3q). White solid; 84% yield (63.1 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.98 (s, 1H), 7.97–7.95 (m, 1H), 7.87 (dd, *J* = 8.4, 3.0 Hz, 1H), 3.98 (s, 3H), 3.74 (s, 3H), 3.38–3.34 (m,

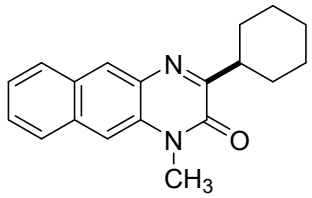
1H), 1.97–1.95 (m, 2H), 1.88–1.86 (m, 2H), 1.78–1.76 (m, 1H), 1.60–1.53 (m, 2H), 1.47 (qt, J = 12.6, 3.0 Hz, 2H), 1.31 (qt, J = 12.6, 3.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.9, 166.2, 154.3, 135.5, 132.7, 130.3, 129.7, 124.1, 115.2, 52.5, 41.0, 30.4, 29.2, 26.2, 26.1; HRMS (ESI): $[M+H]^+$ calculated for $C_{17}H_{21}N_2O_3^+$: 301.1547, found: 301.1545.



3-cyclohexyl-1,6,7-trimethylquinoxalin-2(1H)-one (3r).[1] White solid; 85% yield (57.5 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.60 (s, 1H), 7.03 (s, 1H), 3.66 (s, 3H), 3.31(br, 1H), 2.40 (s, 3H), 2.33 (s, 3H), 1.95–1.87 (m, 5H), 1.56–1.45 (m, 5H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 162.9, 154.6, 138.9, 132.1, 131.2, 130.7, 129.8, 114.0, 40.6, 30.5, 28.9, 26.3, 26.1, 20.4, 19.0.

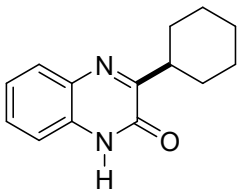


6,7-dichloro-3-cyclohexyl-1-methylquinoxalin-2(1H)-one (3s).[1] White solid; 84% yield (65.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.92 (s, 1H), 7.36 (s, 1H), 3.64 (s, 3H), 3.30 (tt, J = 11.4, 3.0 Hz, 1H), 1.94–1.92 (m, 2H), 1.85 (dt, J = 10.2, 3.0 Hz, 2H), 1.78–1.75 (m, 1H), 1.55–1.48 (m, 2H), 1.47–1.41 (m, 2H), 1.34–1.25 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.8, 153.9, 133.3, 132.3, 132.0, 130.6, 127.1, 114.9, 40.8, 30.4, 29.3, 26.2, 26.1.

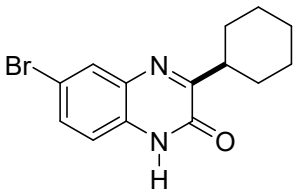


3-cyclohexyl-1-methylbenzo[g]quinoxalin-2(1H)-one (3t).[1] White solid; 81% yield (59.2 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.32 (s, 1H), 7.93 (d, J = 12.0 Hz, 1H), 7.87 (d, J = 12.6 Hz, 1H), 7.55–7.51 (m, 2H), 7.47–7.43 (m, 1H), 3.73 (s, 3H), 3.38 (tt, J = 16.8, 4.8 Hz, 1H), 2.02–1.99 (m, 2H), 1.91–1.87 (m, 2H), 1.80–1.77 (m, 1H), 1.61 (qd,

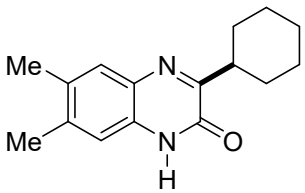
J = 18.6, 4.2 Hz, 2H), 1.49 (qt, *J* = 18.0, 3.6 Hz, 2H), 1.33 (qt, *J* = 18.6, 4.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.8, 154.4, 133.2, 132.2, 131.6, 129.7, 128.6, 128.3, 127.4, 127.0, 125.0, 109.7, 40.8, 30.6, 29.0, 26.3, 26.1.



3-cyclohexylquinoxalin-2(1H)-one (3u).[3] White solid; 64% yield (36.5 mg). ^{1}H NMR (600 MHz, DMSO-d_6): δ = 12.30 (s, 1H), 7.70 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.48–7.45 (m, 1H), 7.28–7.25 (m, 2H), 3.17 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.88–1.86 (m, 2H), 1.82–1.80 (m, 2H), 1.73–1.71 (m, 1H), 1.45 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.37 (qt, *J* = 12.6, 3.0 Hz, 2H), 1.24 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ = 164.8, 154.2, 131.7, 131.5, 129.4, 128.2, 123.0, 115.1, 30.1, 25.8, 25.7.

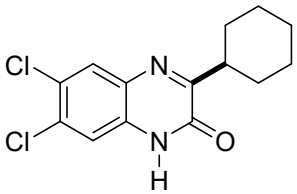


6-bromo-3-cyclohexylquinoxalin-2(1H)-one (3v).[3] White solid; 70% yield (53.8 mg). ^{1}H NMR (600 MHz, DMSO-d_6): δ = 12.43 (s, 1H), 7.87 (d, *J* = 2.4 Hz, 1H), 7.62 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 3.17 (tt, *J* = 11.4, 3.0 Hz, 1H), 1.87–1.85 (m, 2H), 1.82–1.80 (m, 2H), 1.73–1.70 (m, 1H), 1.47–1.40 (m, 2H), 1.38–1.33 (m, 2H), 1.27–1.22 (m, 1H); ^{13}C NMR (151 MHz, DMSO-d_6): δ = 166.3, 153.9, 132.6, 131.9, 130.8, 130.2, 117.1, 114.3, 29.9, 25.7, 25.6.

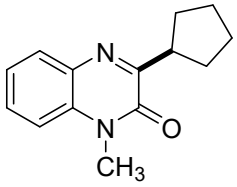


3-cyclohexyl-6,7-dimethylquinoxalin-2(1H)-one (3w).[3] White solid; 61% yield (39.1 mg). ^{1}H NMR (600 MHz, DMSO-d_6): δ: 12.16 (s, 1H), 7.49 (s, 1H), 7.02 (s, 1H), 3.14 (tt, *J* = 11.4, 3.6 Hz, 1H), 2.29 (s, 3H), 2.27 (s, 3H), 1.86–1.84 (m, 2H), 1.81–1.79 (m, 2H), 1.72–1.70 (m, 1H), 1.46–1.40 (m, 2H), 1.37–1.33 (m, 2H), 1.26–1.22 (m, 1H); ^{13}C

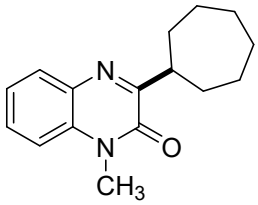
NMR (151 MHz, DMSO-d_6): δ = 163.5, 154.2, 138.6, 131.6, 130.1, 129.4, 128.2, 115.2, 30.1, 25.8, 25.7, 19.7, 18.9.



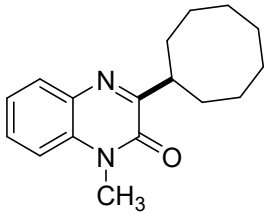
6,7-dichloro-3-cyclohexylquinoxalin-2(1H)-one(3x).[3] White solid; 73% yield (54.2 mg). ^{1}H NMR (600 MHz, DMSO-d_6): δ = 12.45 (s, 1H), 7.93 (s, 1H), 7.40 (s, 1H), 3.14 (tt, *J* = 11.4, 3.6 Hz, 1H), 1.87–1.85 (m, 2H), 1.82–1.80 (m, 2H), 1.73–1.70 (m, 1H), 1.45–1.33 (m, 4H), 1.26–1.20 (m, 1H); ^{13}C NMR (151 MHz, DMSO-d_6): δ = 166.8, 153.7, 131.4, 131.3, 131.1, 129.1, 124.7, 116.2, 29.9, 25.7, 25.6.



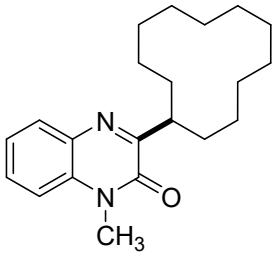
3-cyclopentyl-1-methylquinoxalin-2(1H)-one (3y).[2] White solid; 89% yield (50.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 3.72–3.71 (m, 1H), 3.69 (s, 3H), 2.09–2.04 (m, 2H), 1.95–1.90 (m, 2H), 1.85–1.80 (m, 2H), 1.74–1.69 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 163.7, 154.9, 132.9, 132.7, 129.7, 129.2, 123.3, 113.3, 42.7, 30.8, 28.9, 25.9.



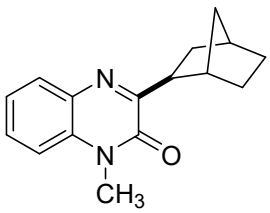
3-cycloheptyl-1-methylquinoxalin-2(1H)-one (3z).[4] White solid; 82% yield (52.6 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 3.69 (s, 3H), 3.51–3.46 (m, 1H), 1.98–1.96 (m, 2H), 1.84–1.77 (m, 4H), 1.71–1.70 (m, 2H), 1.63–1.60 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.3, 154.4, 132.9, 132.8, 129.7, 129.2, 123.3, 113.4, 42.4, 32.2, 29.0, 28.2, 27.1.



3-cyclooctyl-1-methylquinoxalin-2(1H)-one (3aa).[4] White solid; 81% yield (54.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 8.4 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 3.70 (s, 3H), 3.58–3.54 (m, 1H), 1.88 (q, *J* = 5.4 Hz, 4H), 1.84–1.77 (m, 2H), 1.71–1.68 (m, 3H), 1.66–1.62 (m, 5H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.7, 154.4, 132.8, 132.7, 129.7, 129.2, 123.3, 113.4, 40.4, 30.6, 29.0, 26.7, 26.6, 25.9.

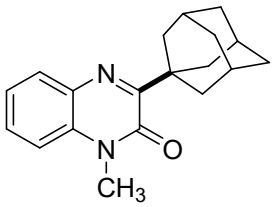


3-cyclododecyl-1-methylquinoxalin-2(1H)-one (3ab). White solid; 83% yield (67.7 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.85 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.51–7.49 (m, 1H), 7.33–7.31 (m, 1H), 7.28 (d, *J* = 8.4, 1H), 3.72–3.67 (m, 4H), 1.81–1.74 (m, 4H), 1.64–1.59 (m, 2H), 1.55–1.51 (m, 1H), 1.48–1.42 (m, 6H), 1.39–1.29 (m, 9H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.4, 154.9, 132.8, 129.7, 129.3, 123.3, 113.4, 36.2, 29.1, 28.1, 23.9, 23.8, 23.6, 23.2, 23.0; HRMS (ESI): $[M+H]^+$ calculated for $C_{21}H_{30}N_2O^+$: 327.2431, found: 327.2433.

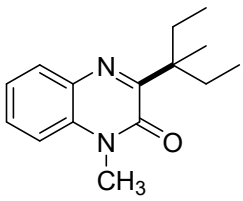


3-bicyclo[2.2.1]heptan-2-yl)-1-methylquinoxalin-2(1H)-one (3ac). White solid; 78% yield (49.6 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.84 (dd, J =7.8, 1.8 Hz, 1H), 7.49 (m, 1H), 7.31 (m, 1H), 7.27 (dd, J = 8.4, 1.2 Hz, 1H), 3.69 (s, 3H), 3.32–3.30 (m, 1H), 2.49–2.48 (m, 1H), 2.38–2.37 (m, 1H), 2.23–2.19 (m, 1H), 1.66–1.50 (m, 5H), 1.36–1.33 (m, 1H), 1.12–1.10 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 162.8, 155.0, 132.8,

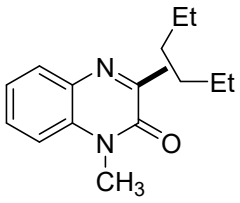
132.5, 129.8, 129.2, 123.3, 113.3, 44.5, 41.5, 36.6, 35.5, 33.9, 30.1, 29.2, 29.0; HRMS (ESI): $[M+H]^+$ calculated for $C_{16}H_{18}N_2O^+$: 255.1492, found: 255.1490.



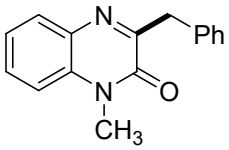
3-adamantan-1-yl)-1-methylquinoxalin-2(1H)-one (3ad).[2] White solid; 76% yield (55.9 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 7.8, 1H), 7.47 (t, *J* = 8.4, 1H), 7.29 (*J* = 7.8, 1H), 7.23 (d, *J* = 8.4, 1H), 3.64 (s, 3H), 2.25 (d, *J* = 2.4 Hz, 6H), 2.14–2.05 (m, 3H), 1.83–1.78 (m, 6H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.6, 153.5, 132.9, 132.3, 130.0, 129.3, 123.0, 113.1, 41.8, 38.7, 36.9, 28.5, 28.5; HRMS (ESI): $[M+H]^+$ calculated for $C_{19}H_{22}N_2O^+$: 295.1805, found: 295.1806.



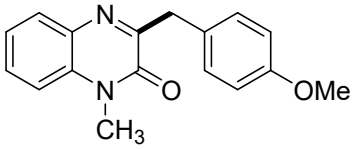
1-methyl-3-(3-methylpentan-3-yl)quinoxalin-2(1H)-one (3ae). White solid; 77% yield (47.0 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 3.67 (s, 3H), 2.34–2.28 (m, 2H), 1.79–1.73 (m, 2H), 1.38 (s, 3H), 0.73 (t, *J* = 7.2, 6H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.1, 153.8, 133.1, 132.2, 130.2, 129.4, 123.1, 113.2, 46.7, 30.9, 28.8, 22.1, 9.2; HRMS (ESI): $[M+H]^+$ calculated for $C_{15}H_{20}N_2O^+$: 245.1648, found: 245.1646.



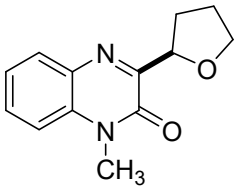
(3af, mixture).[5] Colorless oil; 70% yield (42.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.87–7.86 (m, 1H), 7.53–50 (m, 1H), 7.34–7.31 (m, 1H), 7.30–7.28 (m, 1H), 3.71 (s, 3H), 3.55–3.42 (m, 1H), 1.92–1.70 (m, 2H), 1.65–1.55 (m, 1H), 1.36–1.26 (m, 5H), 0.90–0.87 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.8, 164.1, 155.0, 154.7, 132.9, 132.8, 132.7, 129.7, 129.4, 129.4, 123.4, 113.4, 42.9, 36.1, 35.3, 34.4, 29.8, 29.1, 29.1, 26.2, 22.8, 20.7, 18.2, 14.3, 14.0, 12.0.



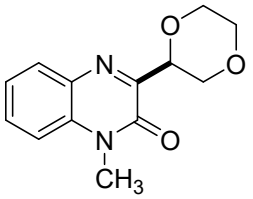
3-benzyl-1-methylquinoxalin-2(1H)-one (3ag).[4] White solid; 58% yield (36.3 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.85 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.51–7.48 (m, 1H), 7.47–7.46 (m, 2H), 7.33–7.27 (m, 3H), 7.24–7.23 (m, 1H), 7.21–7.18 (m, 1H), 4.26 (s, 2H), 3.64 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 159.2, 154.6, 137.0, 133.3, 132.6, 129.8, 129.8, 129.5, 128.3, 126.5, 123.5, 113.5, 40.7, 29.1.



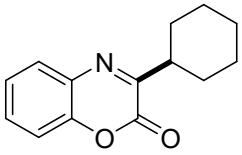
3-(4-methoxybenzyl)-1-methylquinoxalin-2(1H)-one (3ah).[4] White solid; 52% yield (36.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.86 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 9.0 Hz, 2H), 7.33 (t, *J* = 7.2, 1H), 7.25 (d, *J* = 8.4, 1H), 6.83 (t, *J* = 8.4, 2H), 4.20 (s, 2H), 3.76 (s, 3H), 3.65 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 159.5, 158.3, 154.7, 133.3, 132.7, 130.5, 129.8, 128.9, 123.5, 113.8, 113.5, 55.2, 39.9, 29.1.



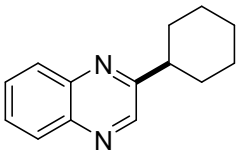
1-methyl-3-(tetrahydrofuran-2-yl)quinoxalin-2(1*H*)-one (3ai).[7] Colorless oil; 89% yield (51.2 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.86 (d, *J* = 7.8, 1H), 7.56–7.54 (m, 1H), 7.36–7.34 (m, 1H),7.32 (d, *J* = 8.4 Hz, 1H), 5.41–5.38 (m, 1H), 4.26–4.22 (m, 1H), 4.04–4.00 (m, 1H), 3.70 (s, 3H), 2.53–2.49 (m, 1H), 2.05 (br, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 159.4, 154.0, 133.1, 132.4, 130.4, 130.1, 123.6, 113.5, 77.5, 69.1, 30.4, 28.7, 25.6.



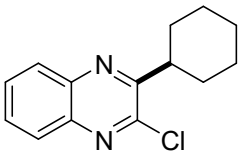
3-(1,4-dioxan-2-yl)-1-methylquinoxalin-2(1*H*)-one (3aj).[7] White solid; 91% yield (56.1 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.03 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.60–7.57 (m, 1H), 7.38–7.36 (m, 1H), 7.33 (d, *J* = 8.4, 1H), 5.30 (dd, *J* = 9.6, 2.4 Hz, 1H), 4.28 (dd, *J* = 11.4, 2.4 Hz, 1H), 4.12 (d, *J* = 11.4 Hz, 1H), 4.01–3.97 (m, 1H), 3.85–3.83 (m, 2H), 3.71 (s, 3H), 3.67–3.64 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.0, 153.6, 133.0, 132.5, 130.7, 130.6, 123.8, 113.5, 74.5, 69.3, 67.4, 66.2, 28.9.



3-cyclohexyl-2H-benzo[b][1,4]oxazin-2-one (5a). White solid; 84% yield (48.1 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.74 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.45 (td, *J* = 8.4, 1.6 Hz, 1H), 7.34 (td, *J* = 8.0, 1.2 Hz, 1H), 7.27 (dd, *J* = 8.4, 1.2 Hz, 1H), 3.16 (tt, *J* = 11.2, 3.2 Hz, 1H), 1.99 (m, 2H), 1.88 (dt, *J* = 12.8, 2.8 Hz, 2H), 1.79–1.75 (m, 1H), 1.61–1.53 (m, 2H), 1.42 (qt, *J* = 12.4, 3.2 Hz, 2H), 1.29 (qt, *J* = 12.4, 3.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 161.3, 152.6, 146.2, 131.3, 130.3, 128.9, 125.2, 116.2, 41.4, 30.2, 26.1, 25.9. HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{14}H_{16}NO_2$: 230.1176, Found: 230.1175.

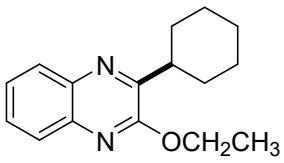


2-cyclohexylquinoxaline (5b).[6] White solid; 76% yield (40.3 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.77 (s, 1H), 8.07–8.04 (m, 2H), 7.75–7.72 (m, 1H), 7.71–7.68 (m, 1H), 2.97 (tt, *J* = 12.0, 3.6 Hz, 1H), 2.05–2.03 (m, 2H), 1.93 (dt, *J* = 12.6, 3.0 Hz, 2H), 1.82–1.80 (m, 1H), 1.71 (qd, J = 12.6, 3.0 Hz, 2H), 1.48 (qt, *J* = 12.6, 3.6 Hz, 2H), 1.36 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 161.1, 145.0, 142.2, 141.4, 129.8, 129.1, 129.0, 128.8, 45.0, 32.3, 26.3, 25.8.

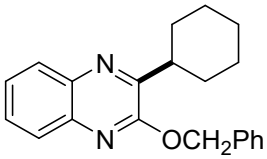


2-chloro-3-cyclohexylquinoxaline (5c).[6] White solid; 78% yield (48.1 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.06–8.05 (m, 1H), 7.98–7.96 (m, 1H), 7.74–7.69 (m, 2H), 3.35 (tt, *J* = 12.0, 3.0 Hz, 1H), 2.03–2.02 (m, 2H), 1.93 (dt, *J* = 13.2, 3.0 Hz, 2H), 1.82–1.80

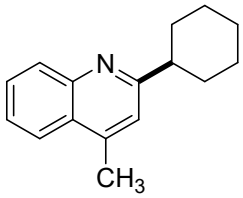
(m, 1H), 1.71 (qd, *J* = 12.2, 3.6 Hz, 2H), 1.49 (qt, *J* = 13.2, 3.0 Hz, 2H), 1.36 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 159.1, 147.4, 141.1, 140.6, 129.8, 128.8, 128.0, 42.5, 31.2, 26.4, 25.9.



2-cyclohexyl-3-ethoxyquinoxaline (5d). Colorless oil; 81% yield (51.9 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.95 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.76 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.56 (ddd, *J* =8.4, 7.2, 1.8 Hz, 1H), 7.49 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 4.55 (q, *J* = 6.6 Hz, 2H), 3.19 (tt, *J* = 12.0, 3.0 Hz, 1H), 1.98–1.95 (m, 2H), 1.89 (dt, *J* = 13.2, 3.0 Hz, 2H), 1.79–1.77 (m, 1H), 1.70 (qd, *J* = 12.6, 3.0 Hz, 2H), 1.49–1.42 (m, 5H), 1.34 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.5, 154.8, 139.5, 138.6, 128.6, 128.3, 126.5, 125.9, 62.1, 40.5, 30.6, 26.5, 26.1, 14.4; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{16}H_{21}N_2O$: 257.1648, Found: 257.1646.

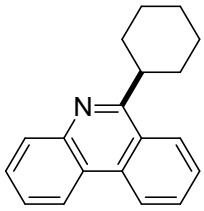


2-(benzyloxy)-3-cyclohexylquinoxaline (5e). Colorless oil; 82% yield (52.6 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.97 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.81 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.58 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.53–7.50 (m, 3H), 7.40 (t, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 5.57 (s, 2H), 3.25 (tt, *J* = 11.4, 3.0 Hz, 1H), 2.00–1.98 (m, 2H), 1.89 (dt, *J* = 13.2, 3.0 Hz, 2H), 1.78–1.68 (m, 3H), 1.44 (qt, *J* = 12.6, 3.6 Hz, 2H), 1.33 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.2, 154.7, 139.3, 138.8, 136.9, 128.7, 128.5, 128.4, 127.9, 127.8, 126.6, 126.2, 67.8, 40.6, 30.7, 26.4, 26.1; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{21}H_{23}N_2O$: 319.1805, Found: 319.1804.

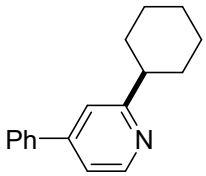


2-cyclohexyl-4-methylquinoline (6f).[6] White solid; 81% yield (45.6 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.07 (d, *J* = 8.4 Hz, 1H), 7.94 (dd, *J* = 7.8, 0.6 Hz, 1H), 7.67 (ddd, *J*

= 7.8, 6.6, 1.2 Hz, 1H), 7.49 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.17 (s, 1H), 2.89 (tt, *J* = 12.0, 3.6 Hz, 1H), 2.68 (s, 3H), 2.01 (m, 2H), 1.89 (dt, *J* = 13.8, 3.6 Hz, 2H), 1.79 (m, 1H), 1.62 (qd, *J* = 12.6, 3.6 Hz, 2H), 1.47 (qt, *J* = 12.6, 3.0 Hz, 2H), 1.34 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 166.4, 147.4, 144.5, 129.3, 129.0, 127.0, 125.4, 123.5, 120.2, 47.5, 32.8, 26.5, 26.1, 18.8.



6-cyclohexylphenanthridine (5g).[6] White solid; 88% yield (57.5 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.65 (d, *J* = 8.4 Hz, 1H), 8.53 (d, *J* = 8.4 Hz, 1H), 8.32 (d, *J* = 7.8 Hz, 1H), 8.14(b, 1H), 7.81 (t, *J* = 7.2 Hz, 1H), 7.69 (q, *J* = 7.8 Hz, 2H), 7.60 (t, *J* = 7.8 Hz, 1H), 3.62 (b, 1H), 2.08–2.06 (m, 2H), 1.98–1.96 (m, 4H), 1.85–1.83 (m, 1H), 1.57 (qt, *J* = 12.6, 3.0 Hz, 2H), 1.45 (t, *J* = 12.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 165.3, 133.0, 129.9, 128.4, 127.1, 126.2, 125.7, 124.7, 123.3, 122.6, 121.8, 42.0, 32.2, 26.9, 26.3.



2-cyclohexyl-4-phenylpyridine (5h).[6] White solid; 83% yield (49.3 mg). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.57 (d, *J* = 4.8 Hz, 1H), 7.64–7.62 (m, 2H), 7.48–7.46 (m, 2H), 7.44–7.41 (m, 1H), 7.37 (s, 1H), 7.32 (dd, *J* = 4.8, 1.8 Hz, 1H), 2.78 (tt, *J* = 12.0, 3.0 Hz, 1H), 2.02–2.00 (m, 2H), 1.88 (dt, *J* = 13.2, 3.0 Hz, 2H), 1.78–1.76 (m, 1H), 1.60 (qd, *J* = 12.6, 3.6 Hz, 2H), 1.44 (qt, *J* = 13.2, 3.5 Hz, 2H), 1.31 (qt, *J* = 12.6, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 166.9, 149.3, 149.0, 138.7, 129.0, 128.8, 127.0, 119.2, 119.1, 46.6, 33.0, 26.6, 26.1.

References :

1. K. Niu, Y. Hao, L. Song, Y. Liu and Q. Wang, *Green Chem.*, 2021, **23**, 302.

2. K. Niu, L. Song, Y. Hao, Y. Liu and Q. Wang, *Chem. Commun.*, 2020, **56**, 11673.

3.F. Lian, K. Xu, W. Meng, H. Zhang, Z. Tan and C. Zeng, *Chem. Commun.*, **2019**, *55*, 14685.

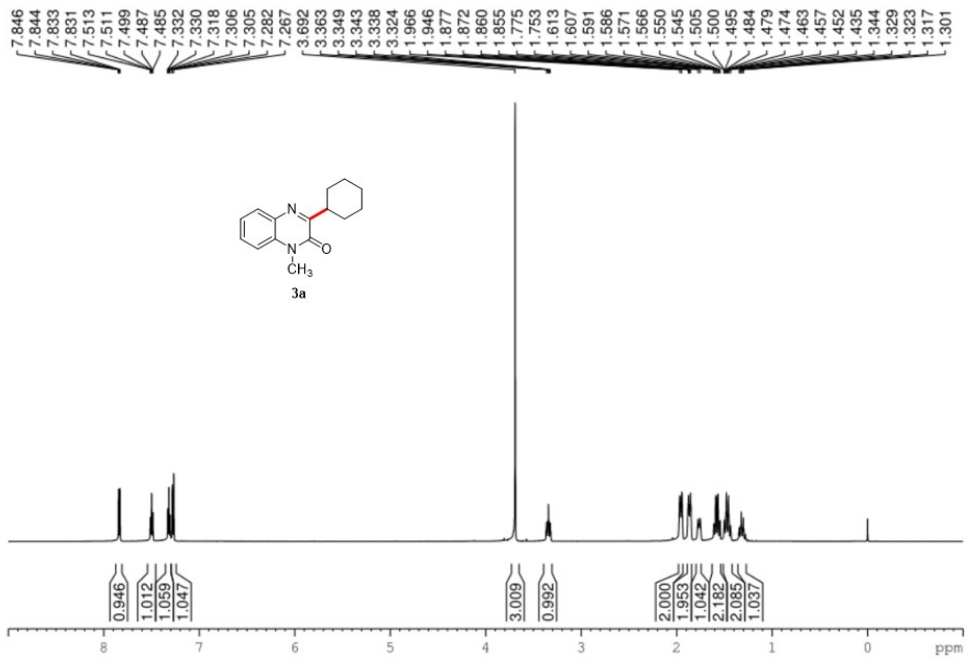
4. S. Singh, N. Dagar and S. R. Roy, *Org. Biomol. Chem.*, 2021, **19**, 5383.

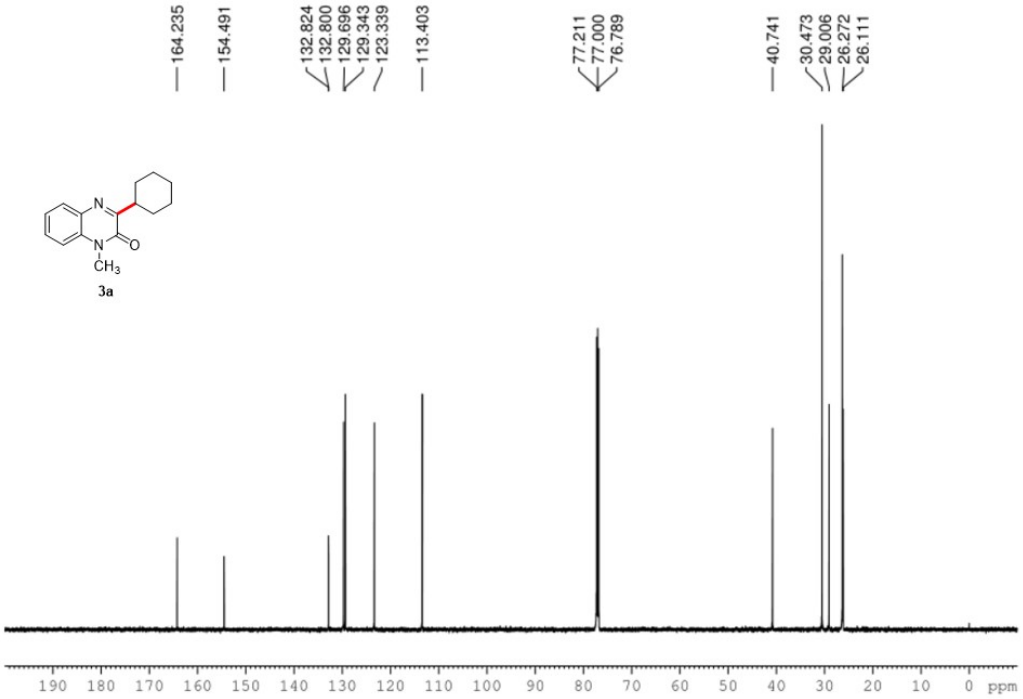
5. X.-K. He, J. Lu, A.-J. Zhang, Q.-Q. Zhang, G.-Y. Xu and J. Xuan, *Org. Lett.*, 2020, **22**, 5984.

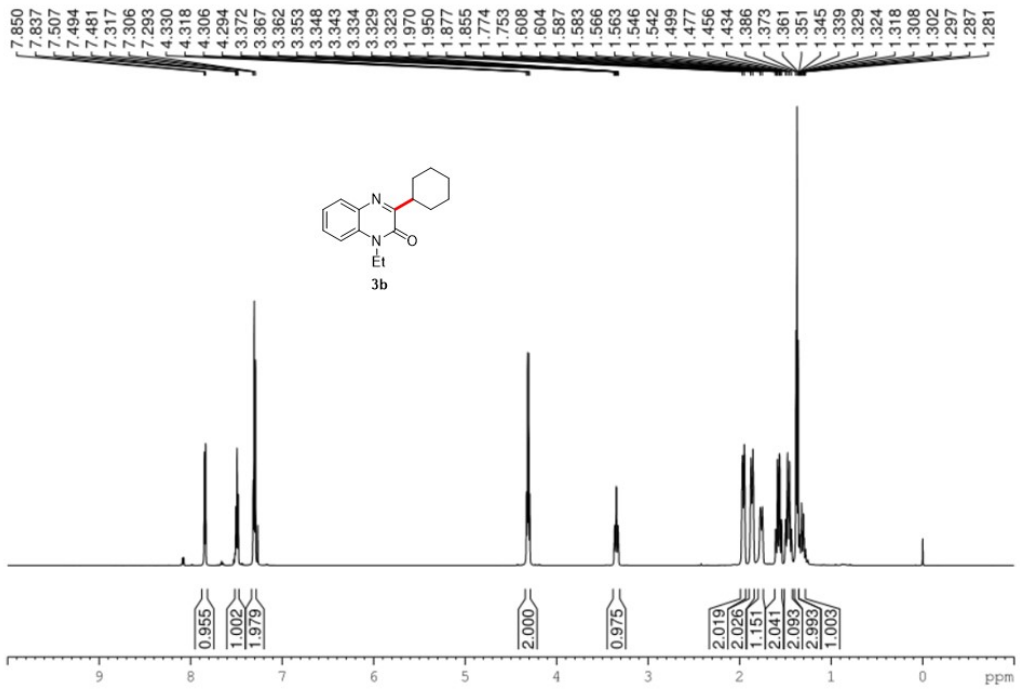
6. X. Shao, X. Wu, S. Wu and C. Zhu, *Org. Lett.*, 2020, **22**, 7450.

7. J. Yuan, J. Fu, J. Yin, Z. Dong, Y. Xiao, P. Mao and L. Qu, *Org. Chem. Front.*, **2018**, *5*, 2820.

5. ^{1}H and ^{13}C NMR spectra of the products



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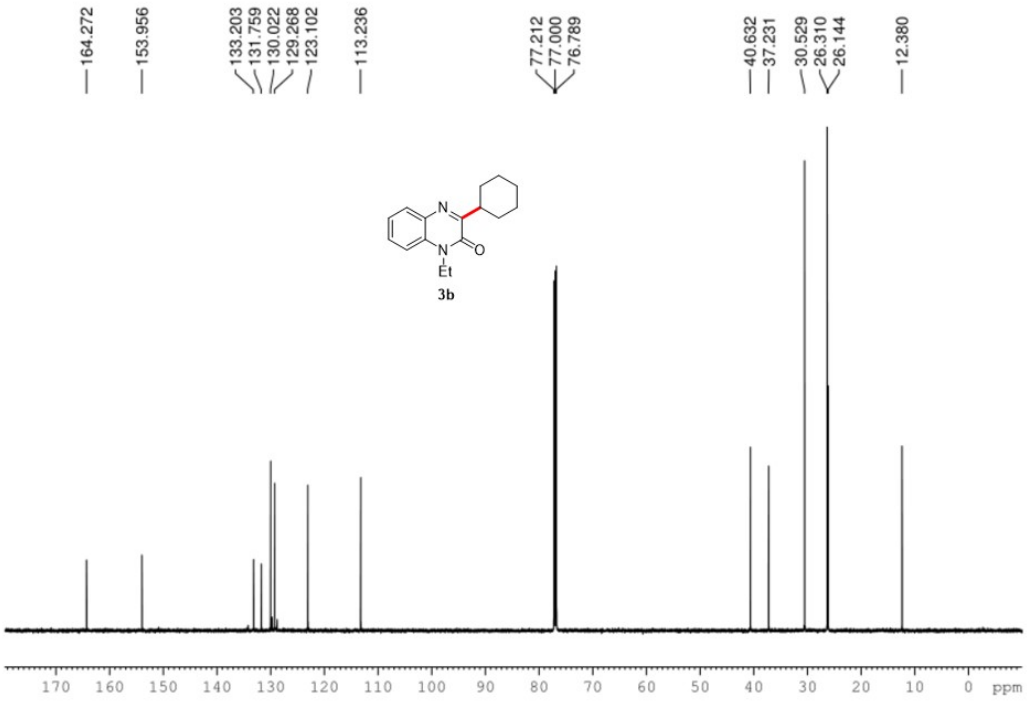
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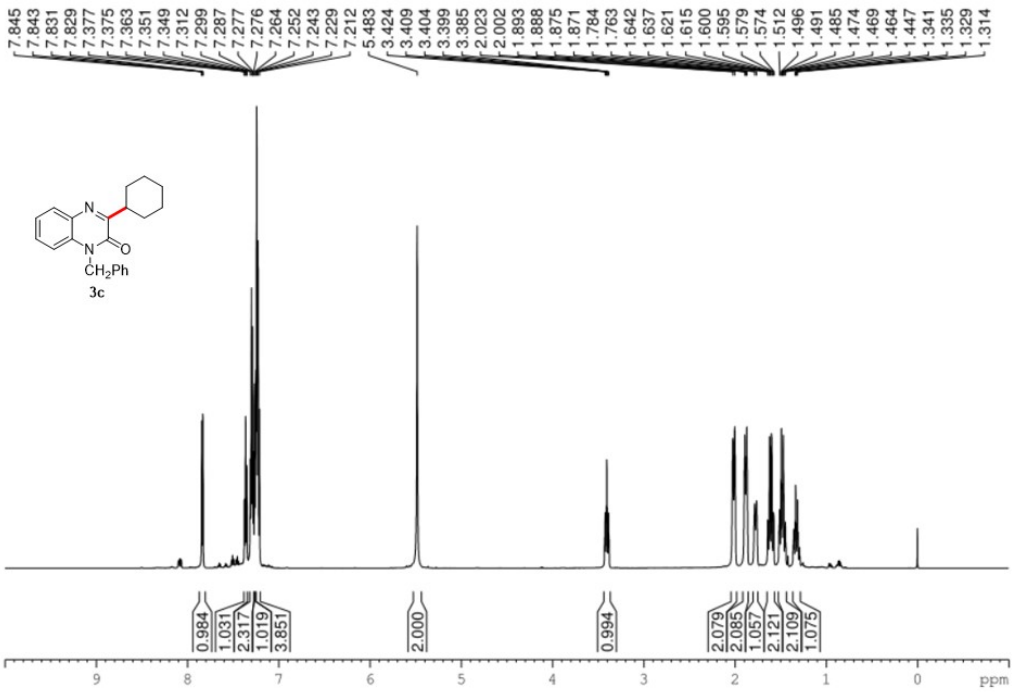
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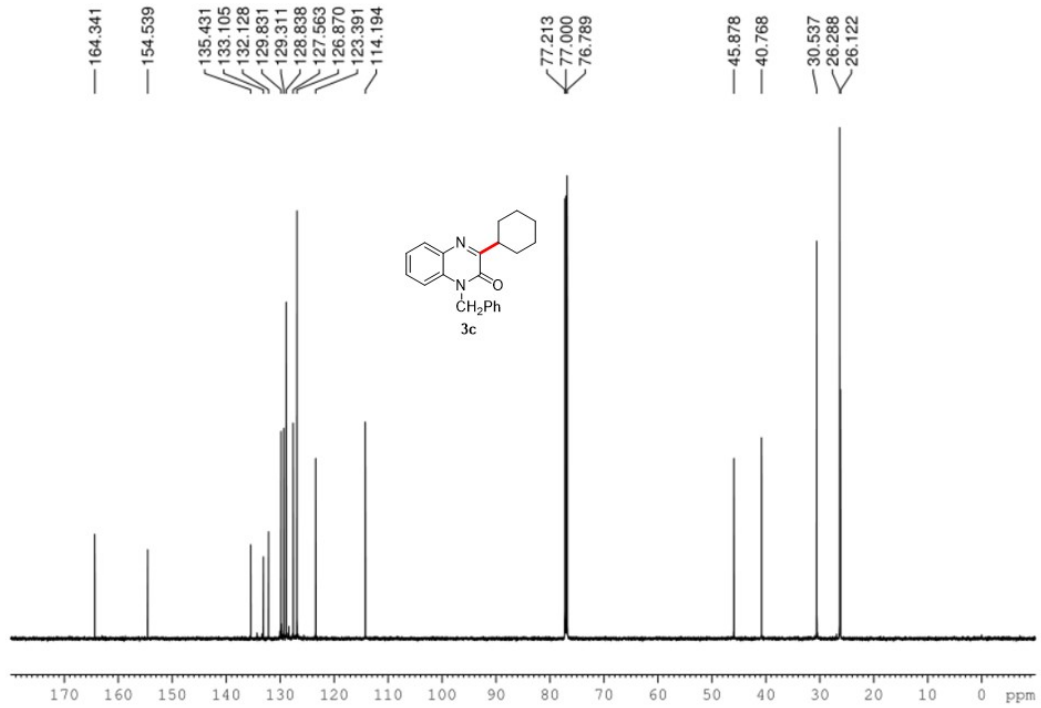
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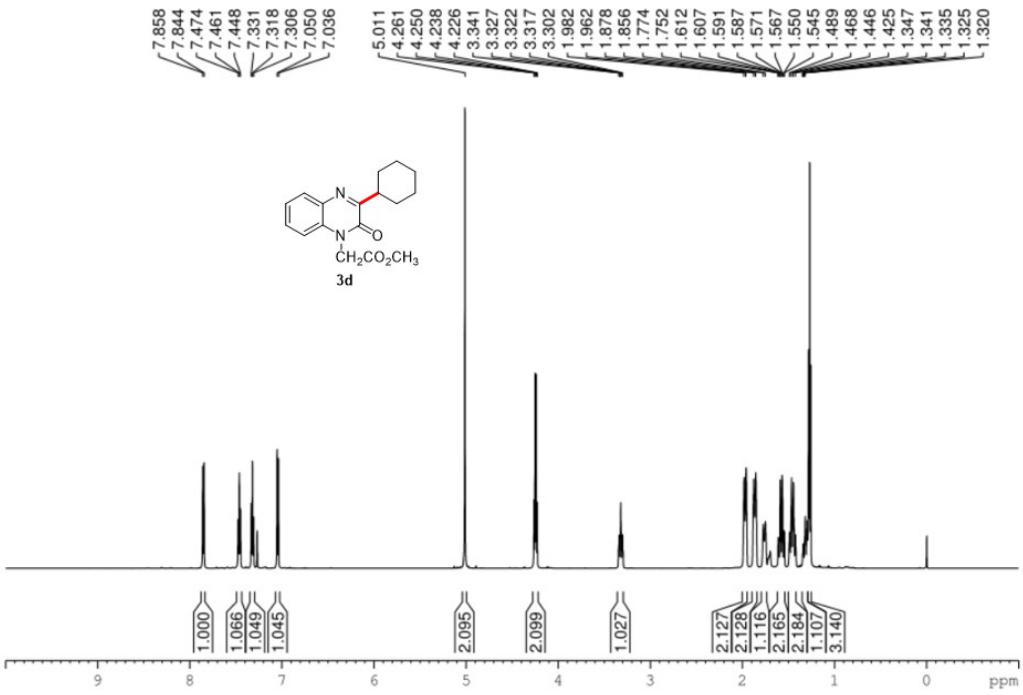
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O
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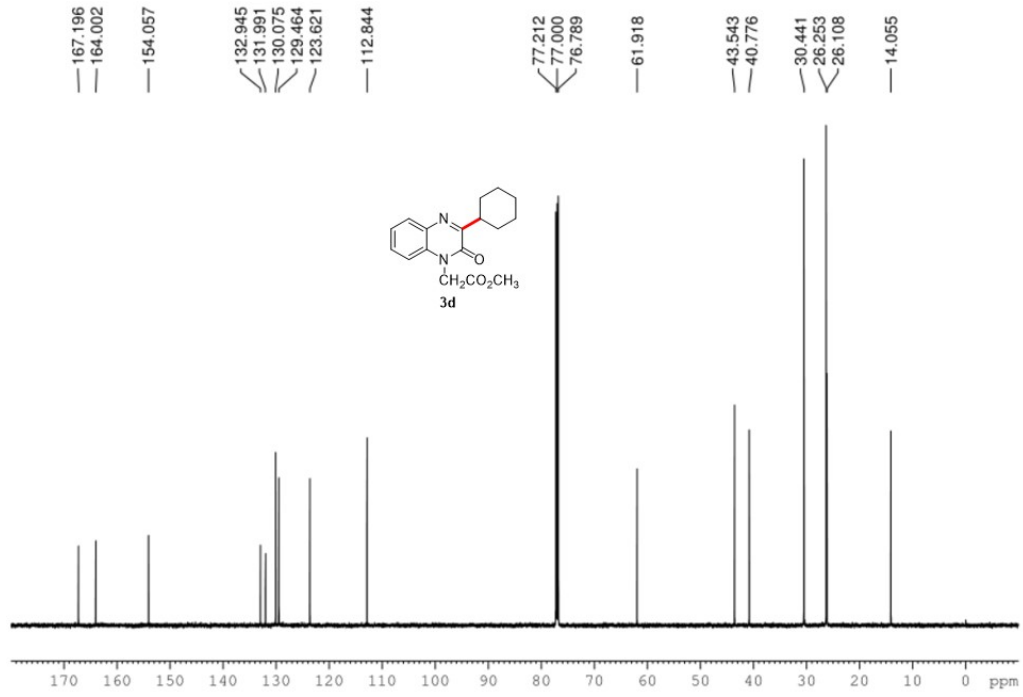
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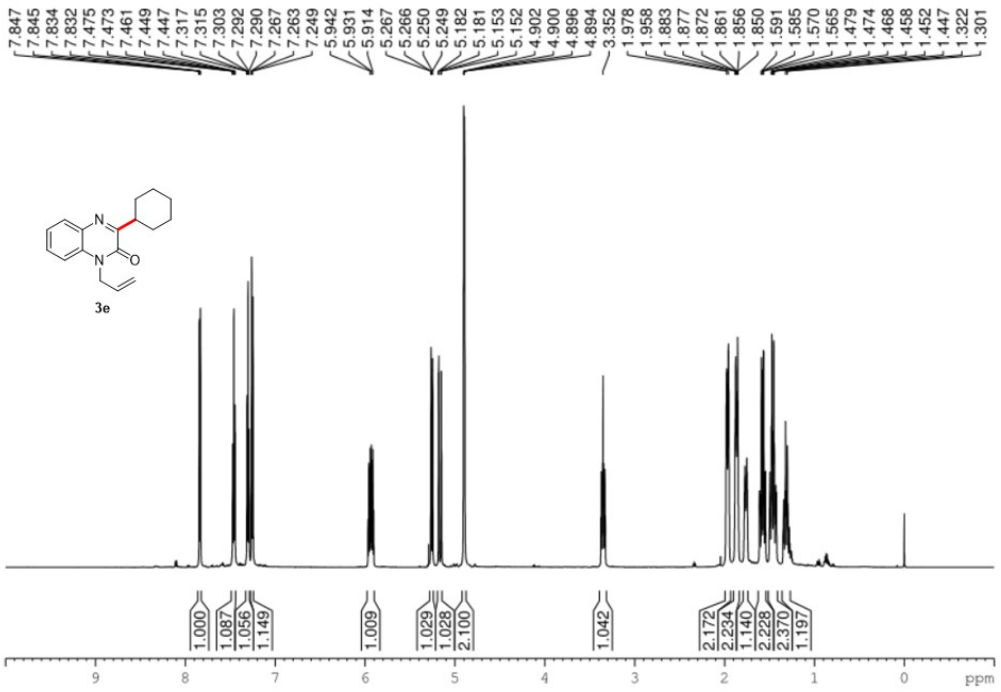
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5.152
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1.301
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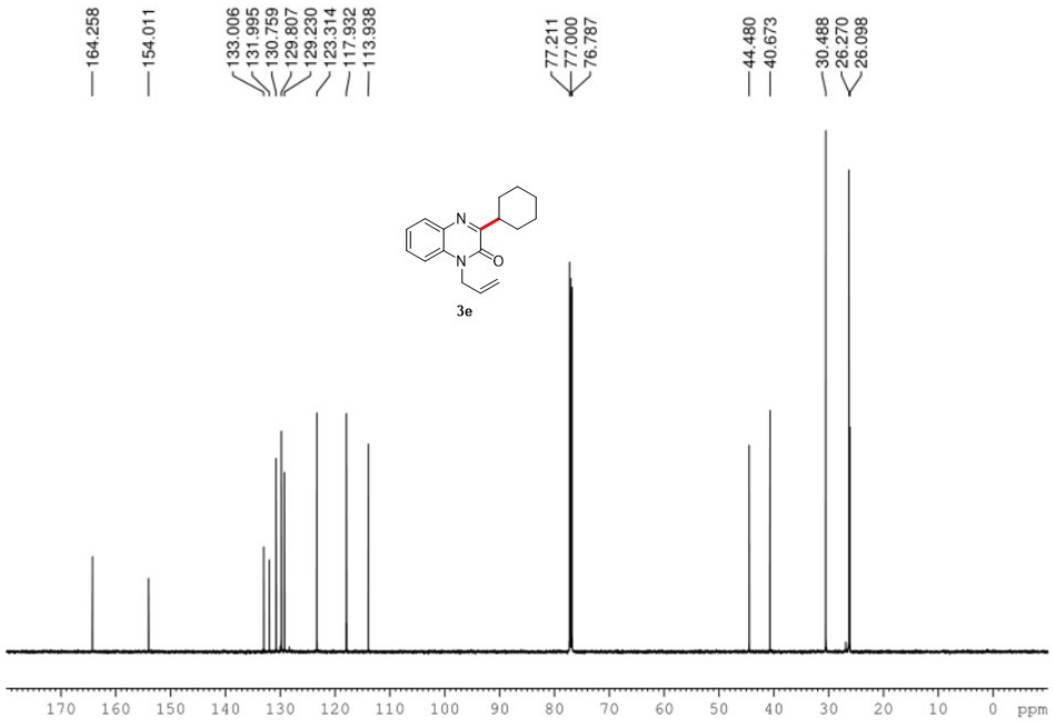
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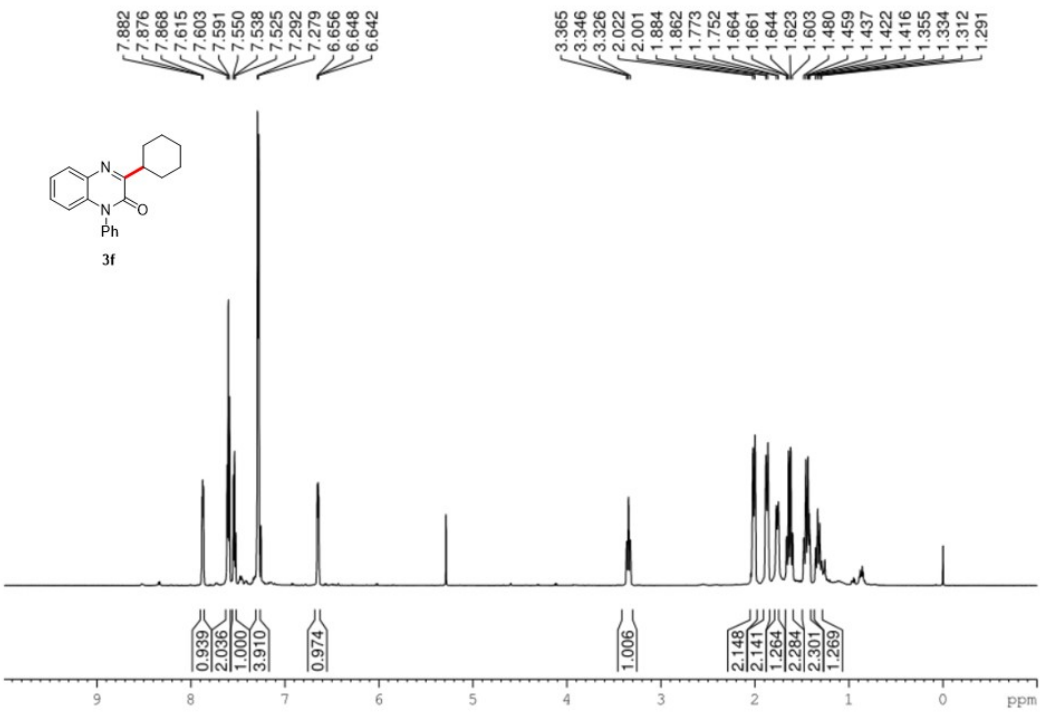
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Ph
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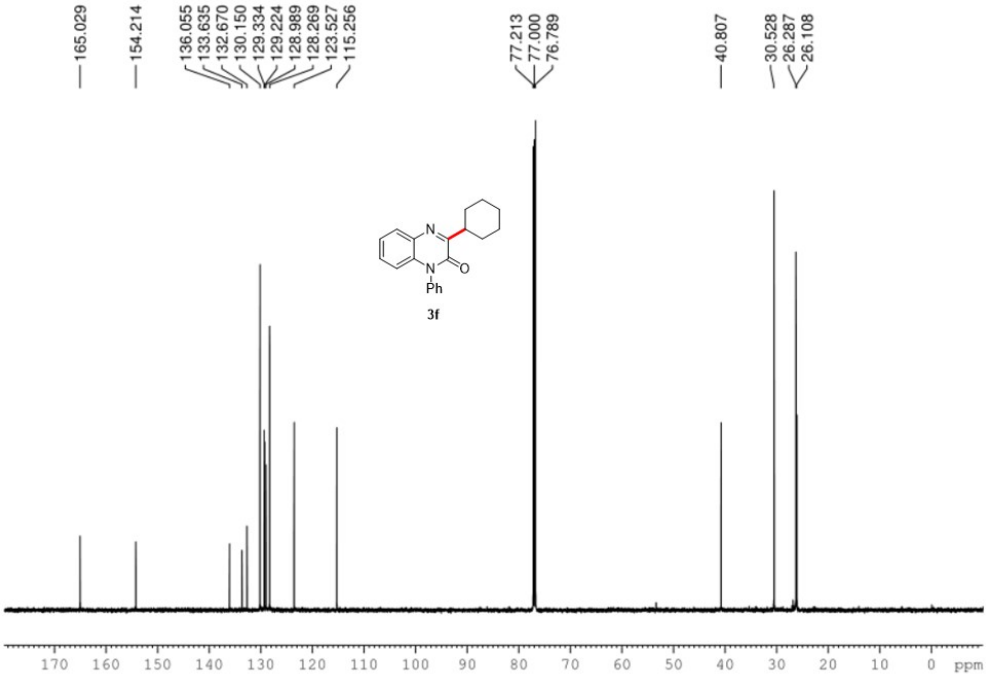
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N
Ph
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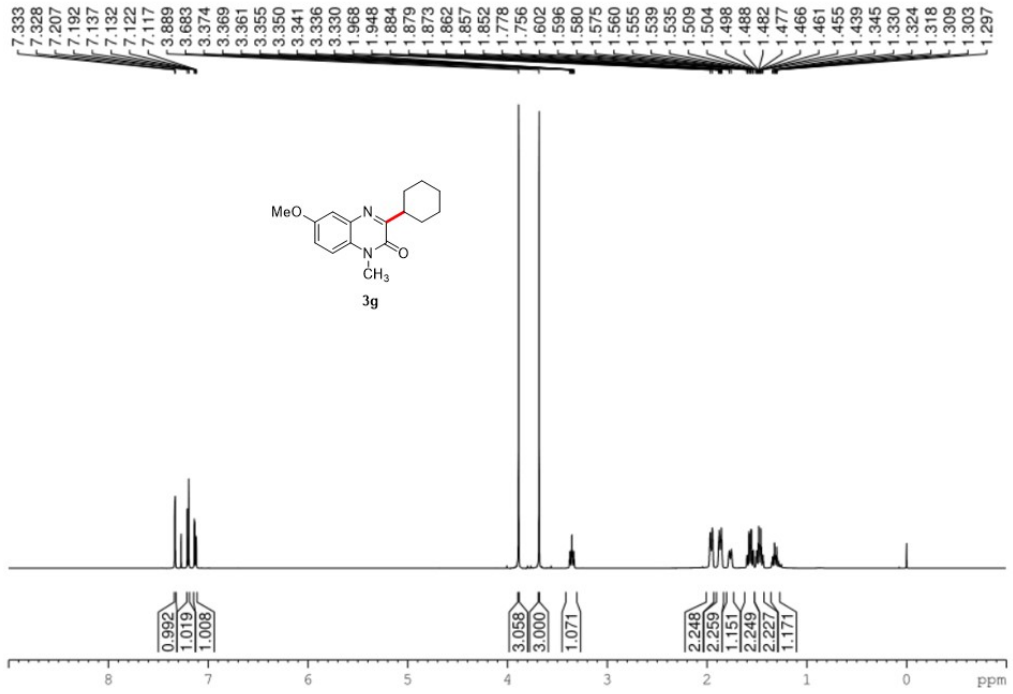
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1.560
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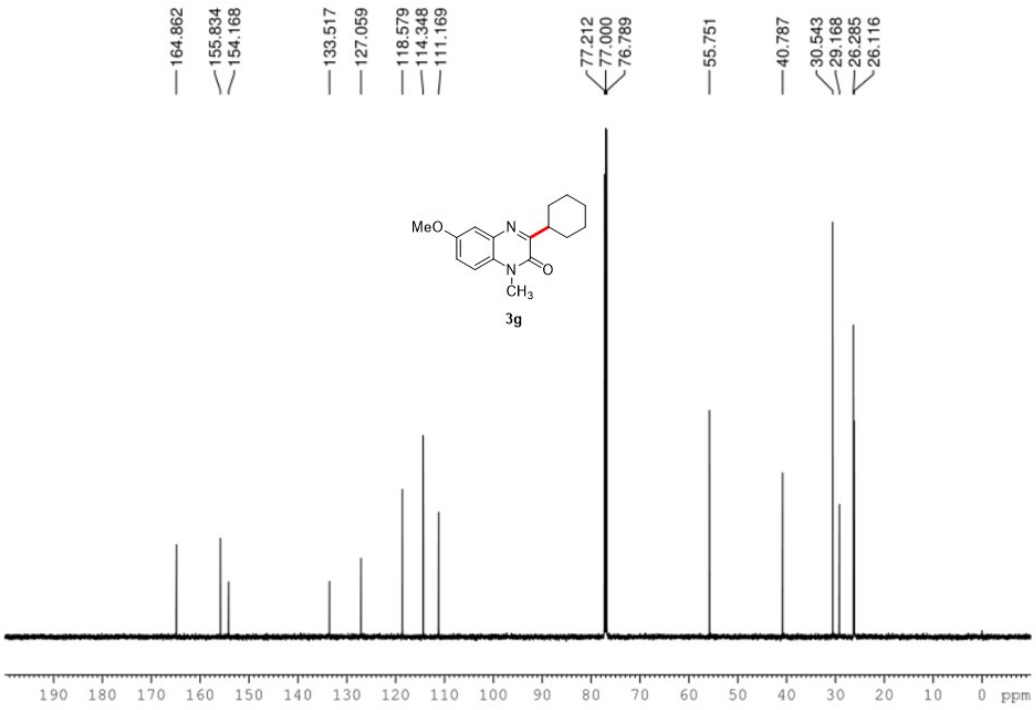
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N
O
CH3
3g
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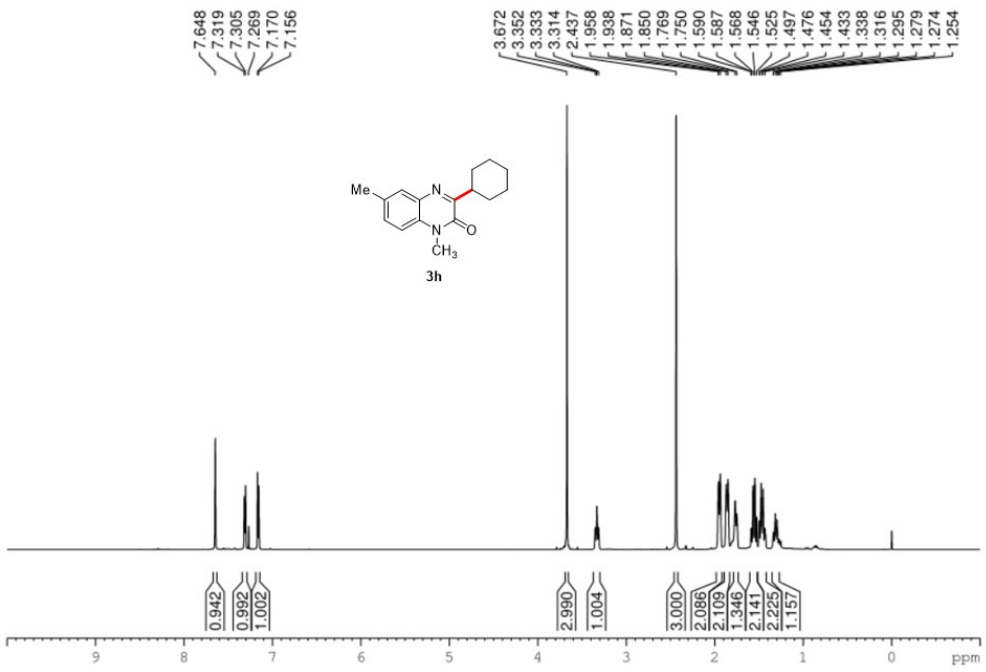
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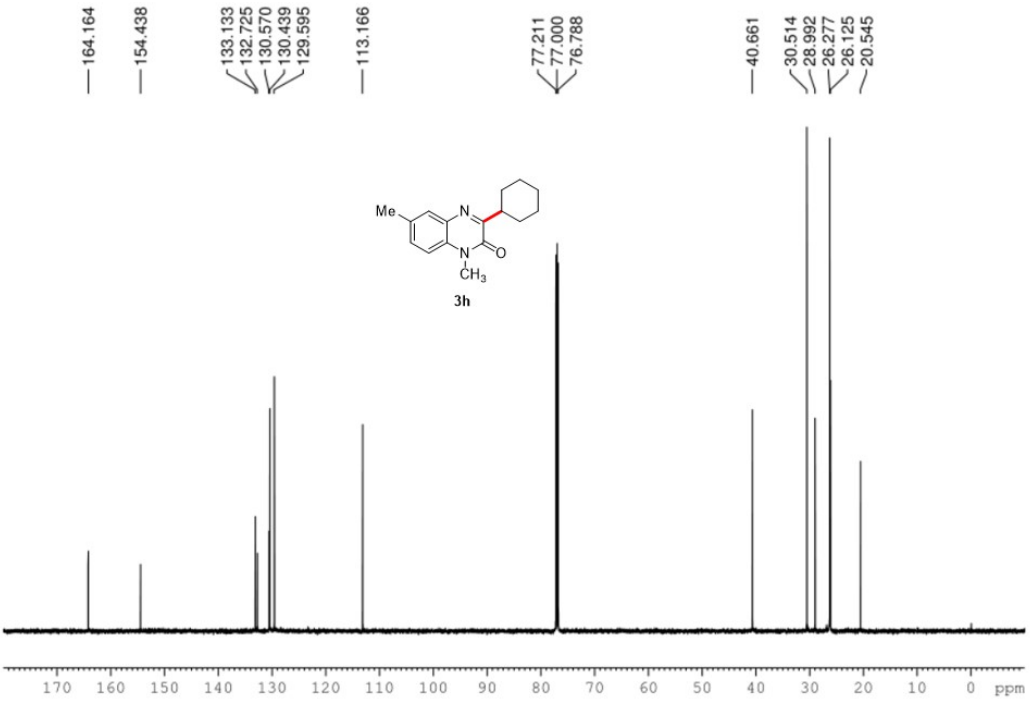
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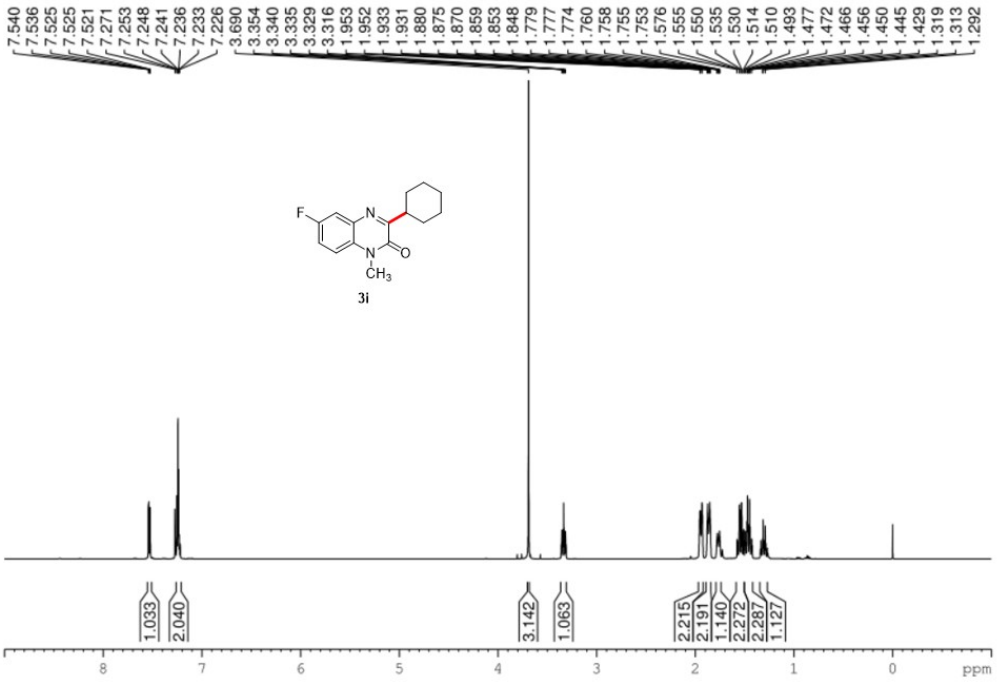
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O
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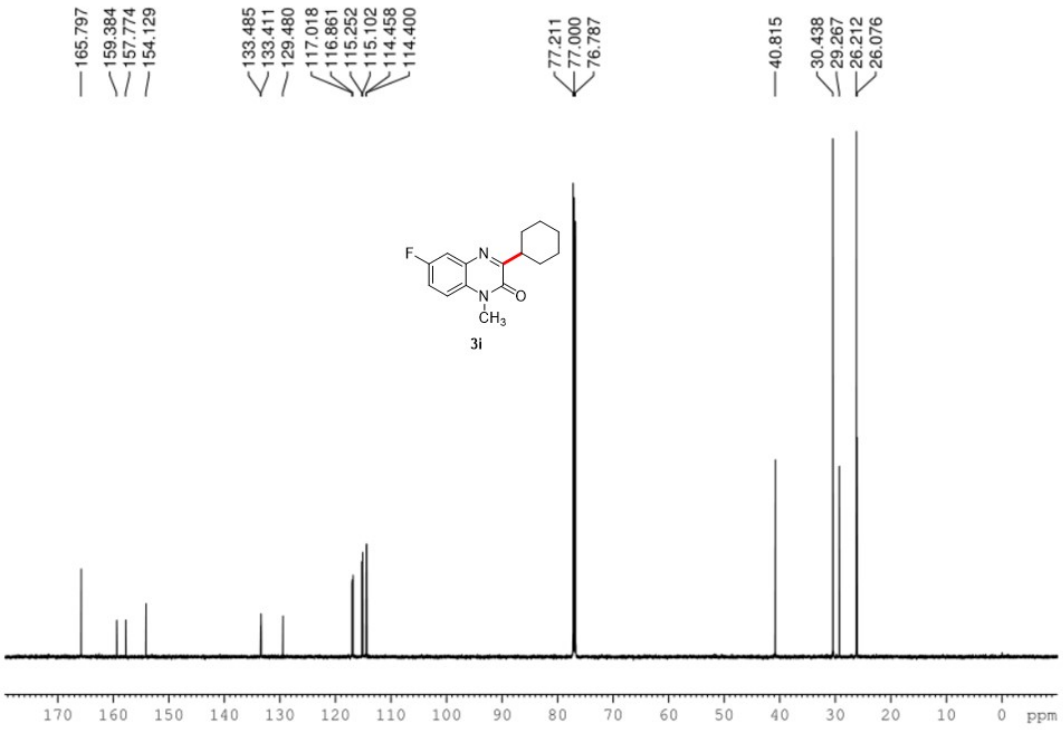
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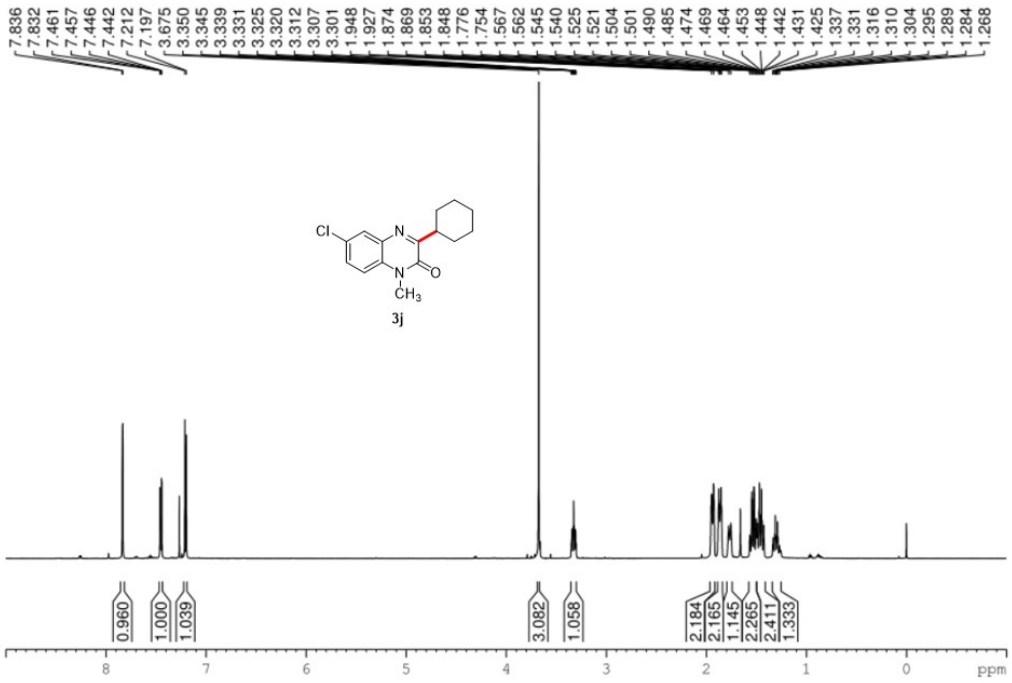
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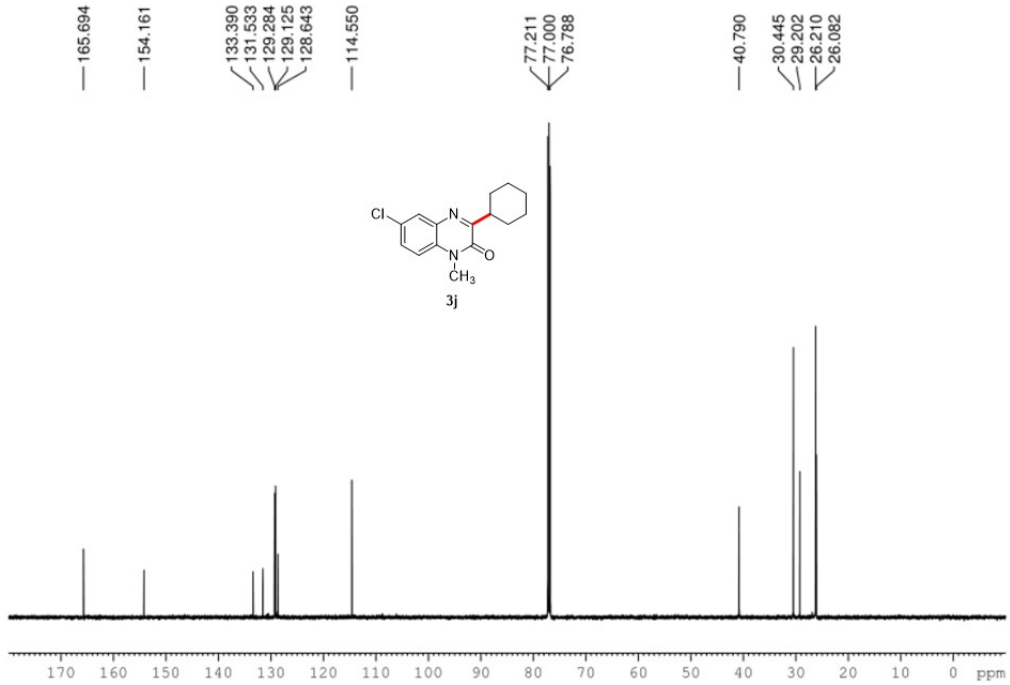
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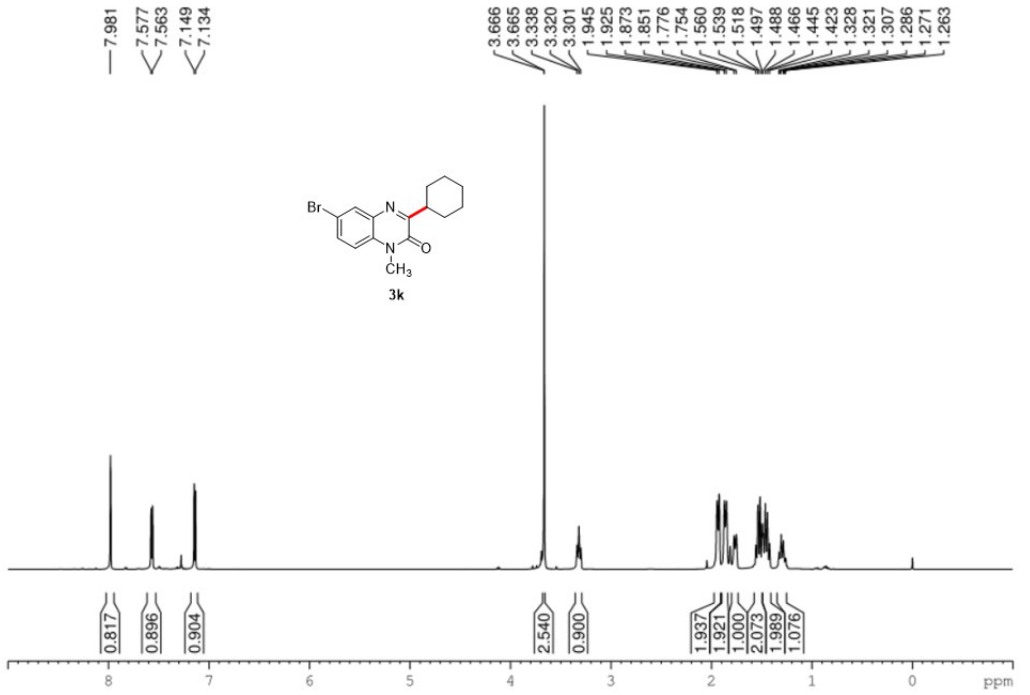
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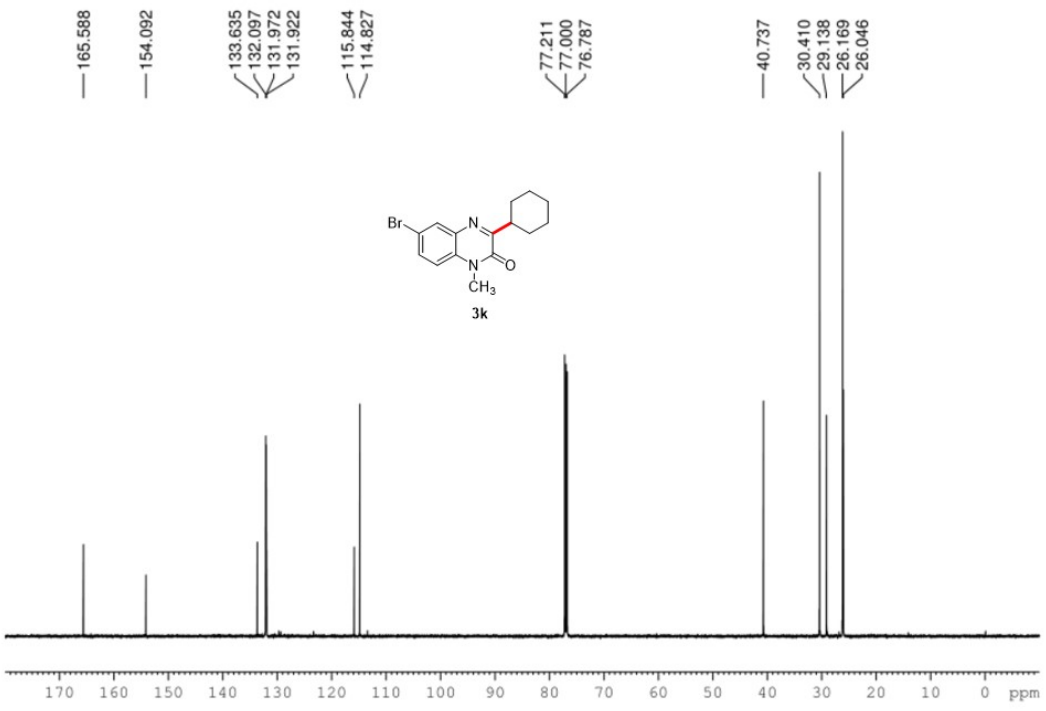
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O
N
CH3
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60
50
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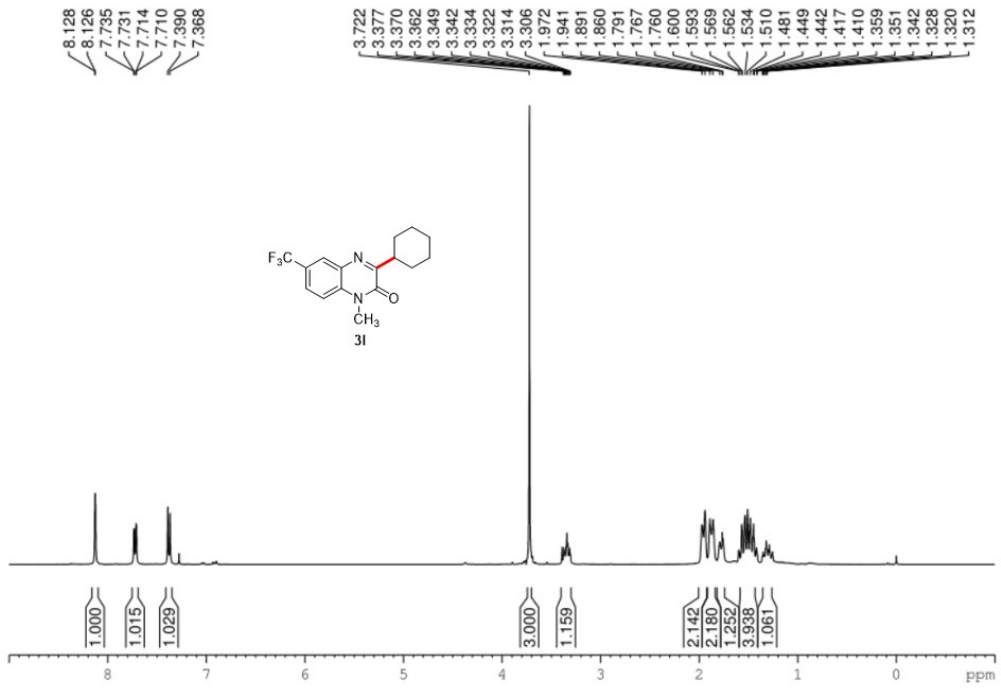
0
ppm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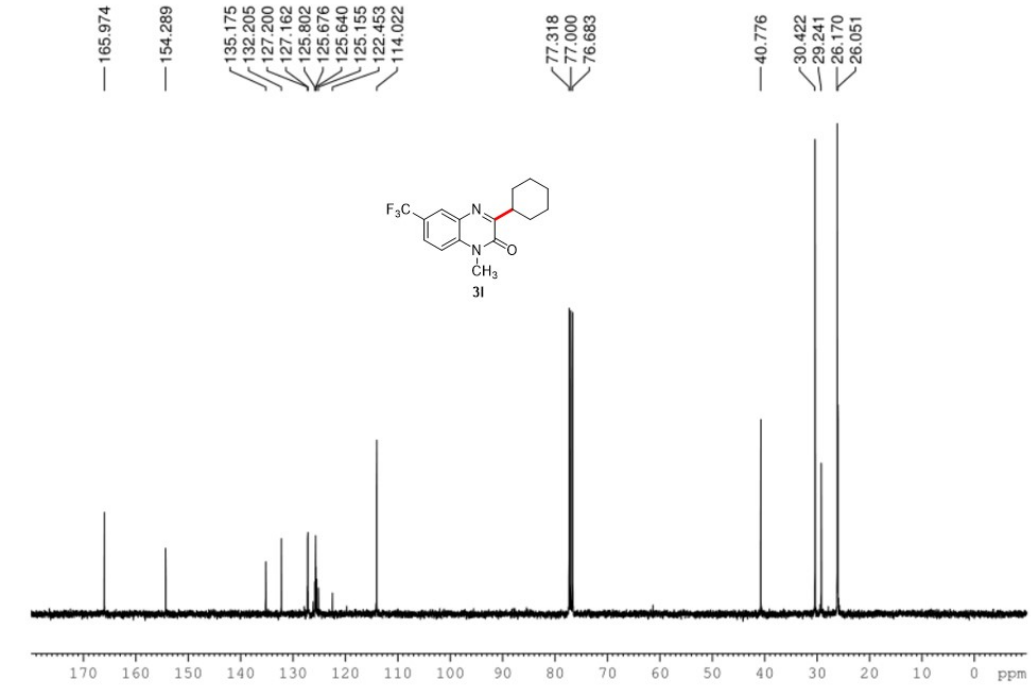
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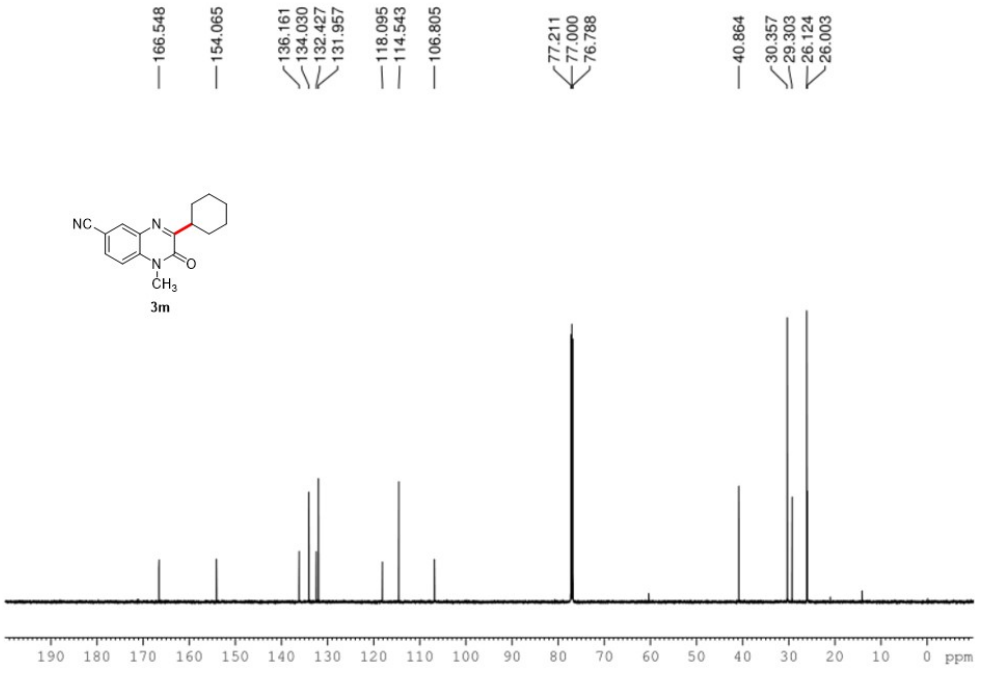
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O
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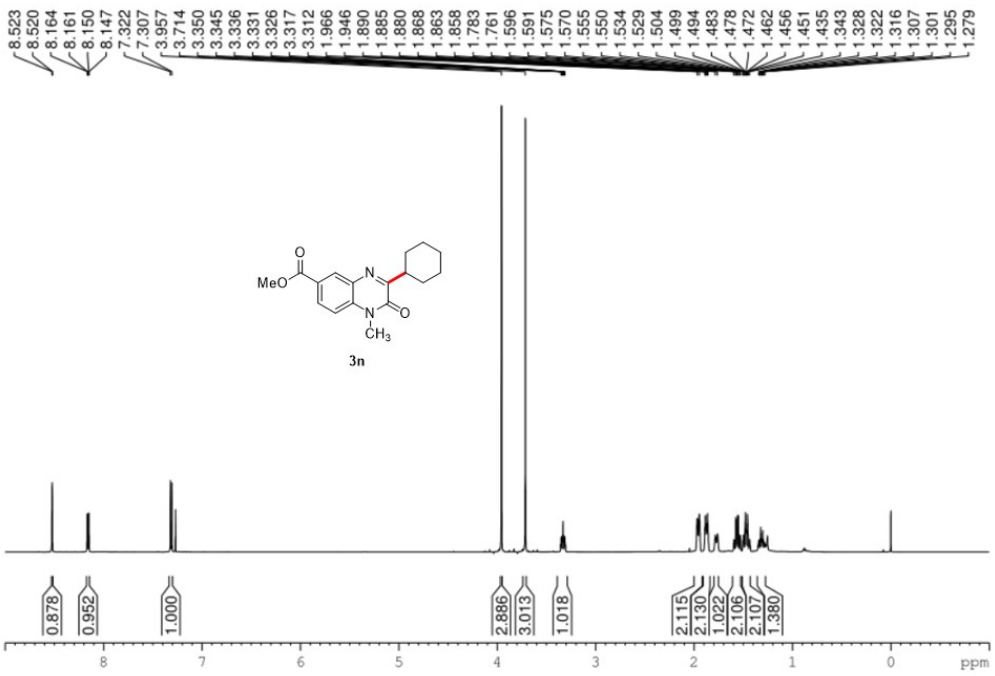
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1.783
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1.550
1.534
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1.504
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CH3
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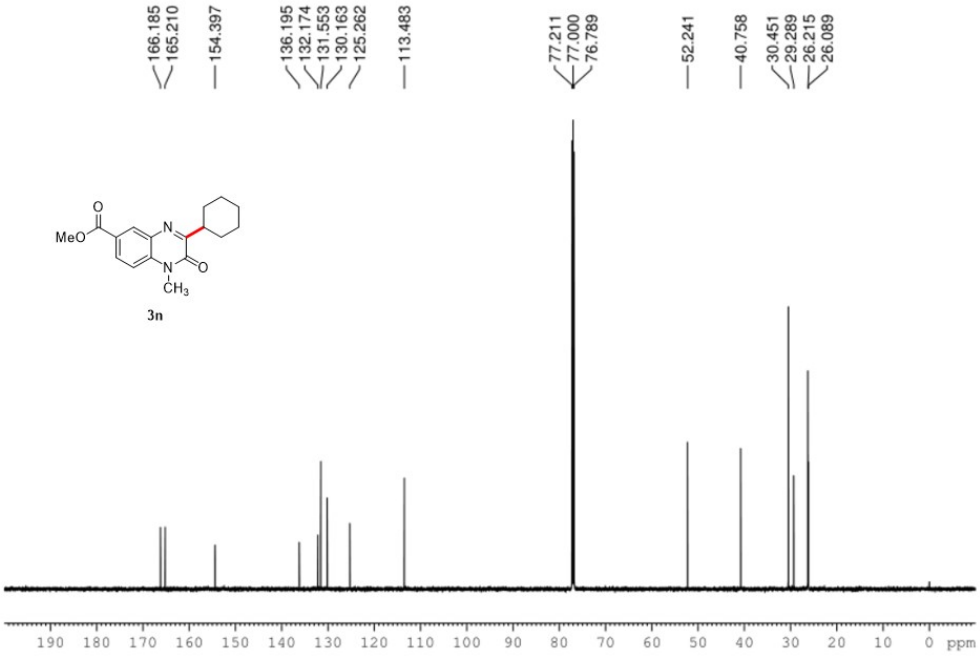
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26.215
26.089
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O
N
N
O
CH3
3n
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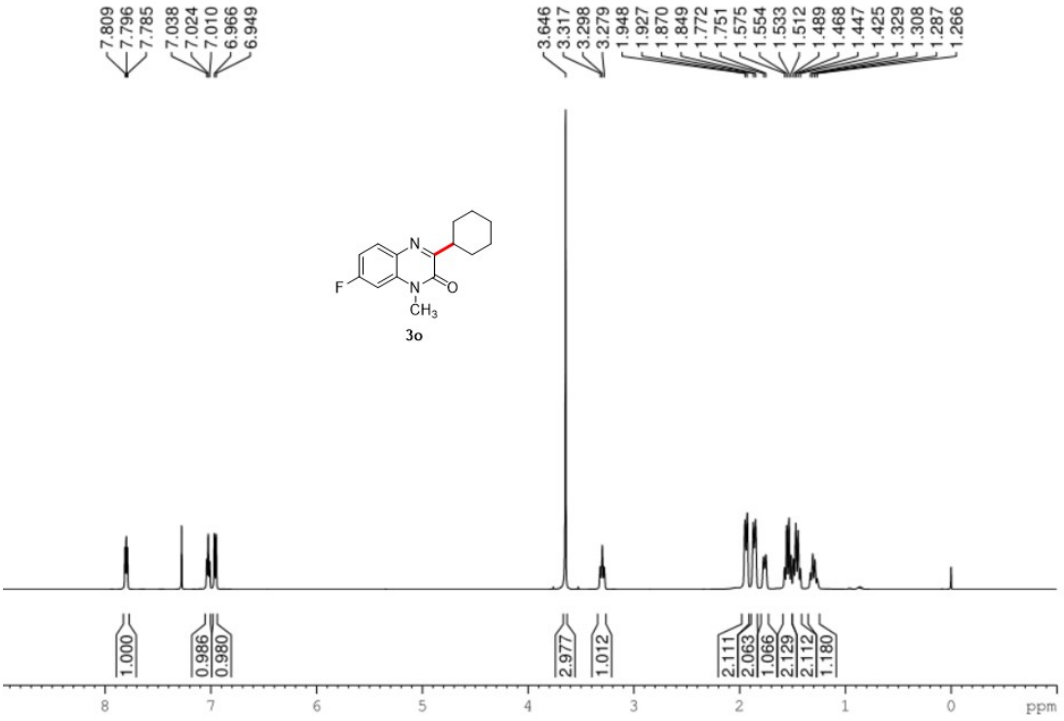
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1.468
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1.287
1.266
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N
O
CH3
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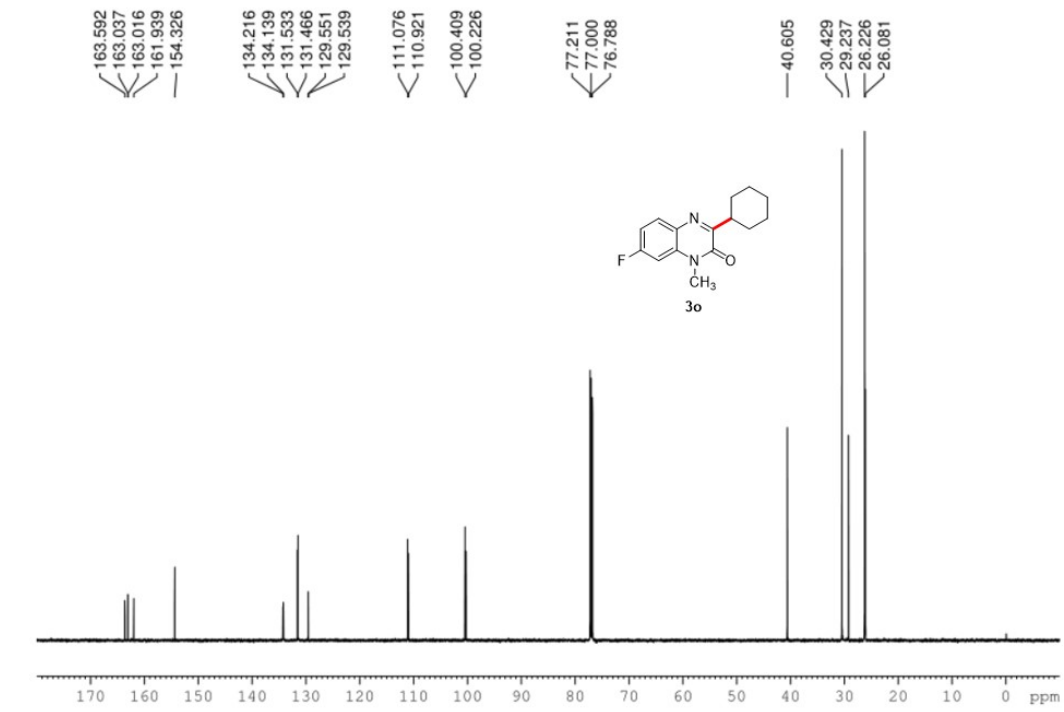
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77.000
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40.605
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29.237
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26.081
F
N
O
CH3
3o
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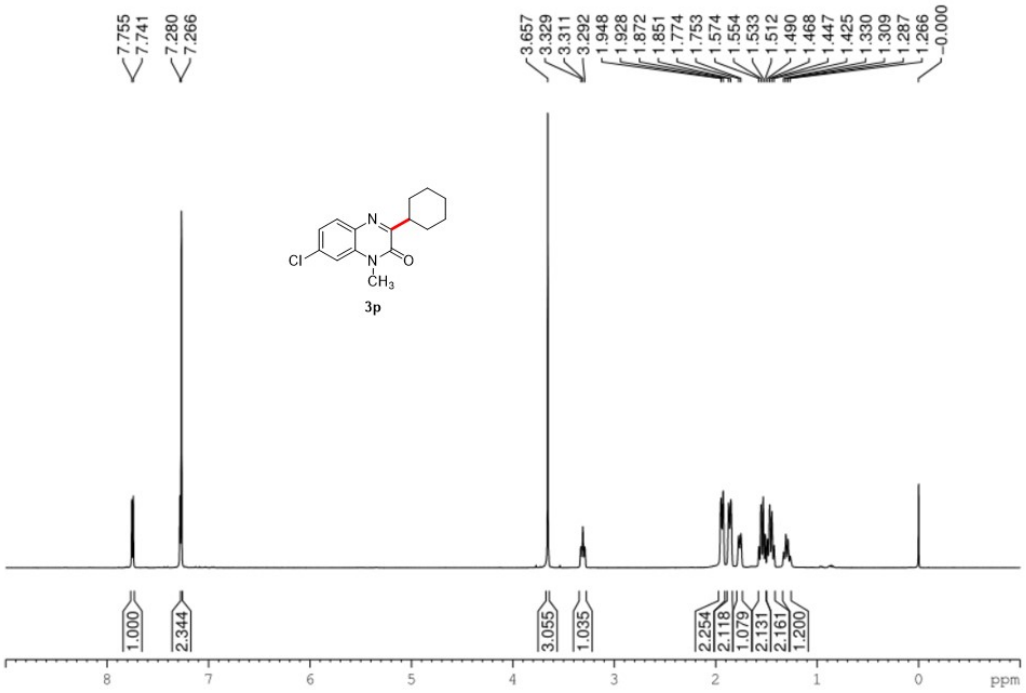
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1.468
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1.425
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1.309
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N
O
CH3
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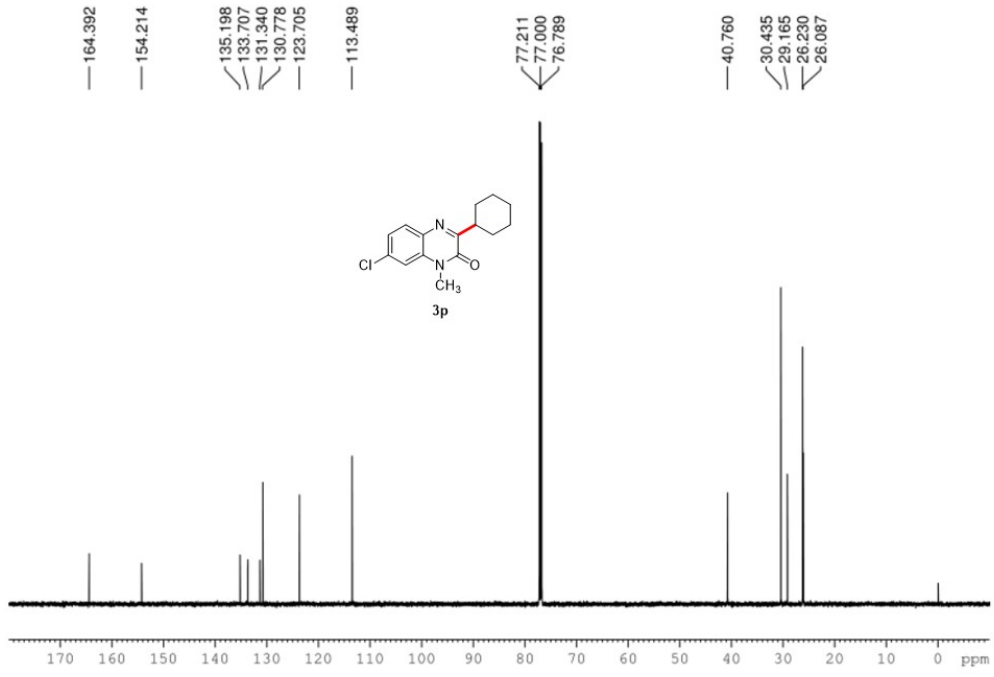
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26.230
26.087
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O
CH3
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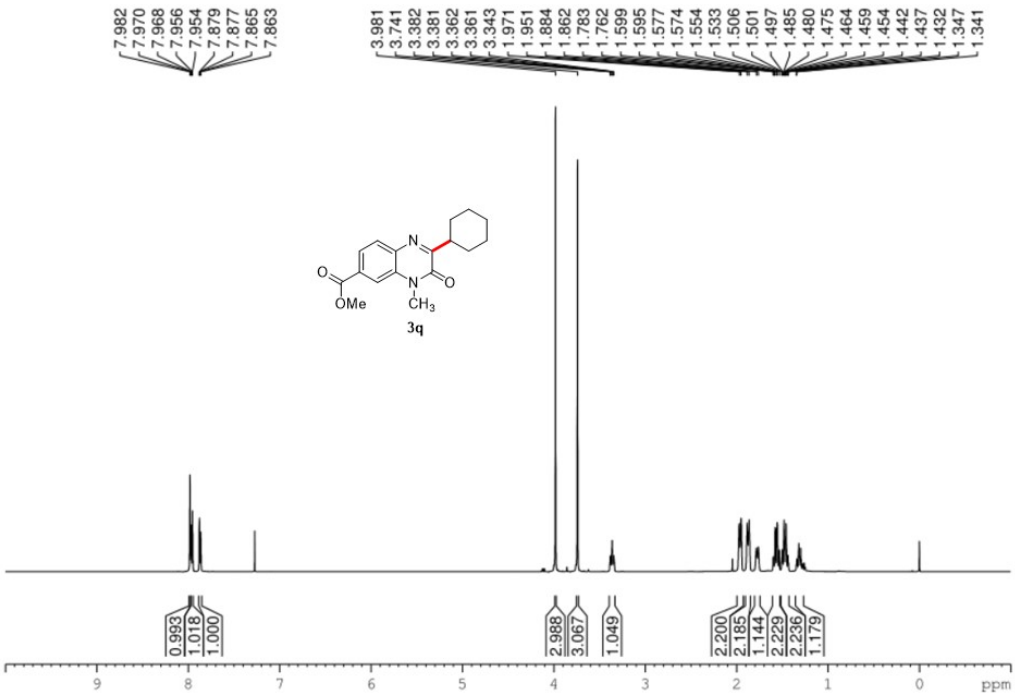
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1.506
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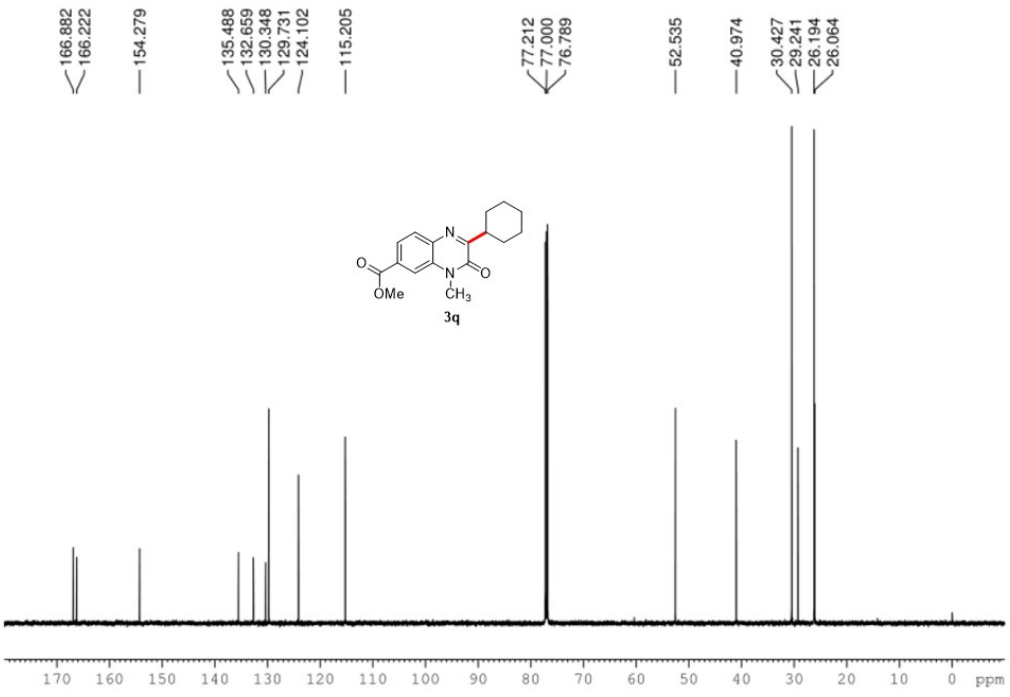
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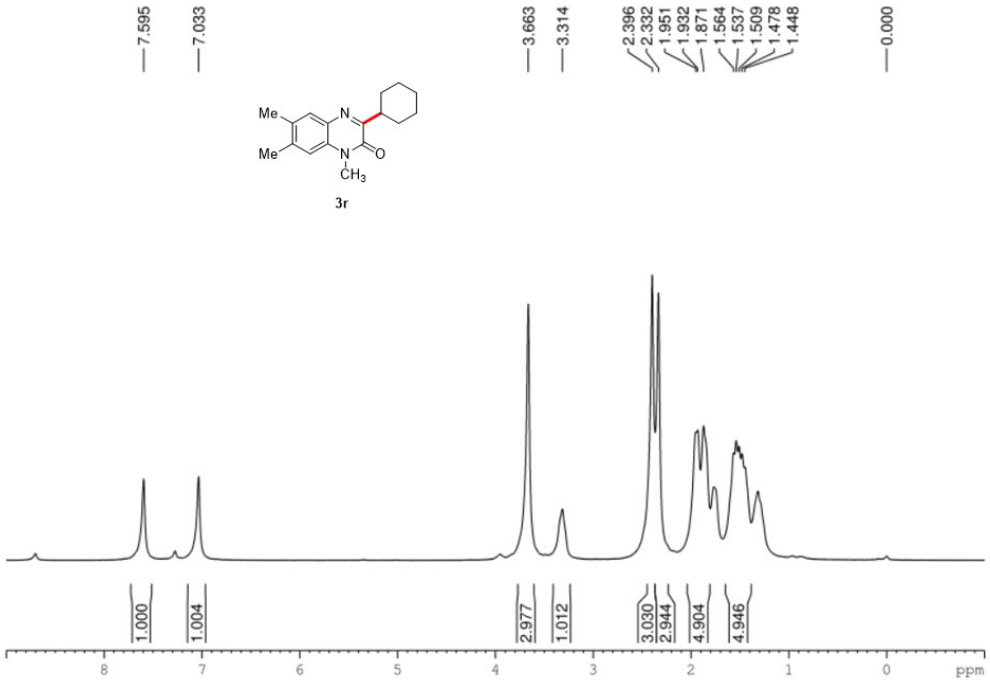
OMe
CH3
3q
ppm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N
N
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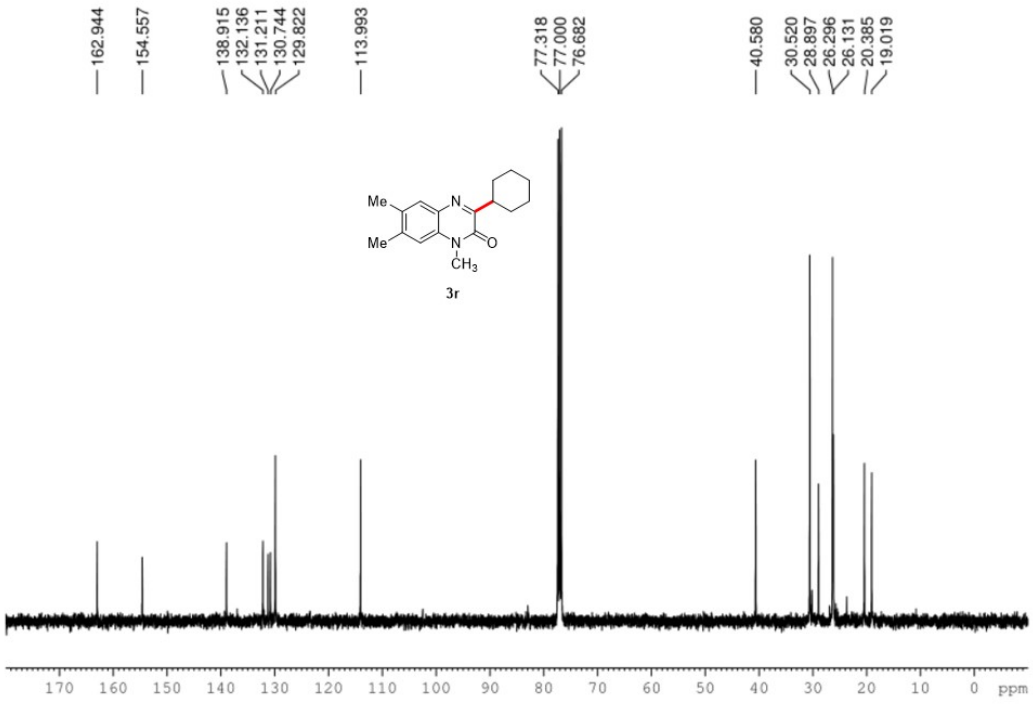
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Me
Me
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N
O
CH3
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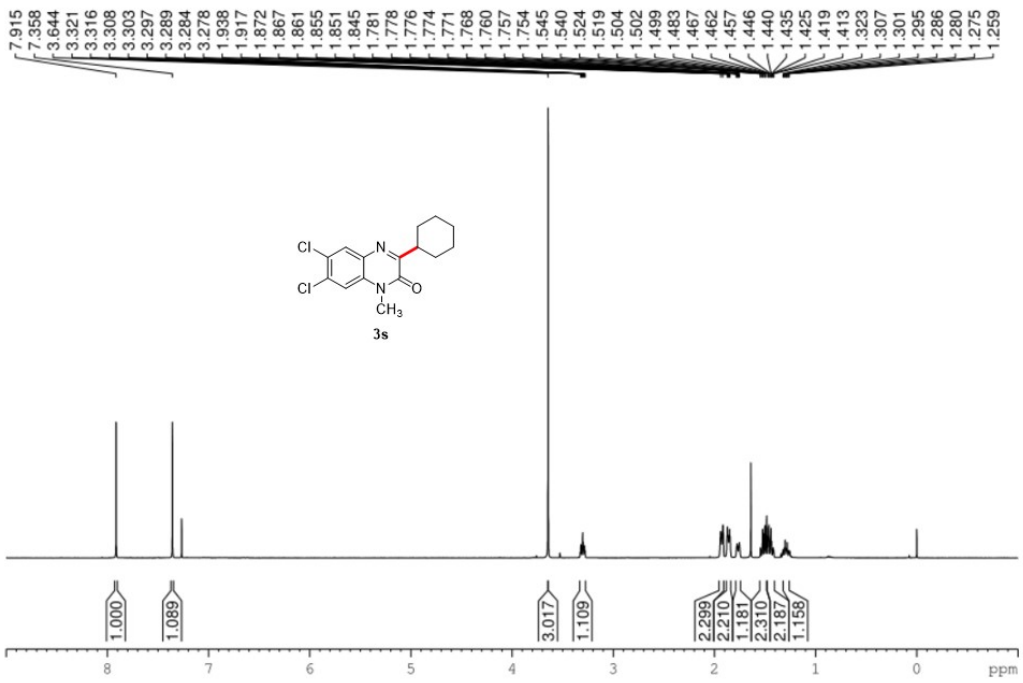
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1.757
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1.524
1.519
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1.502
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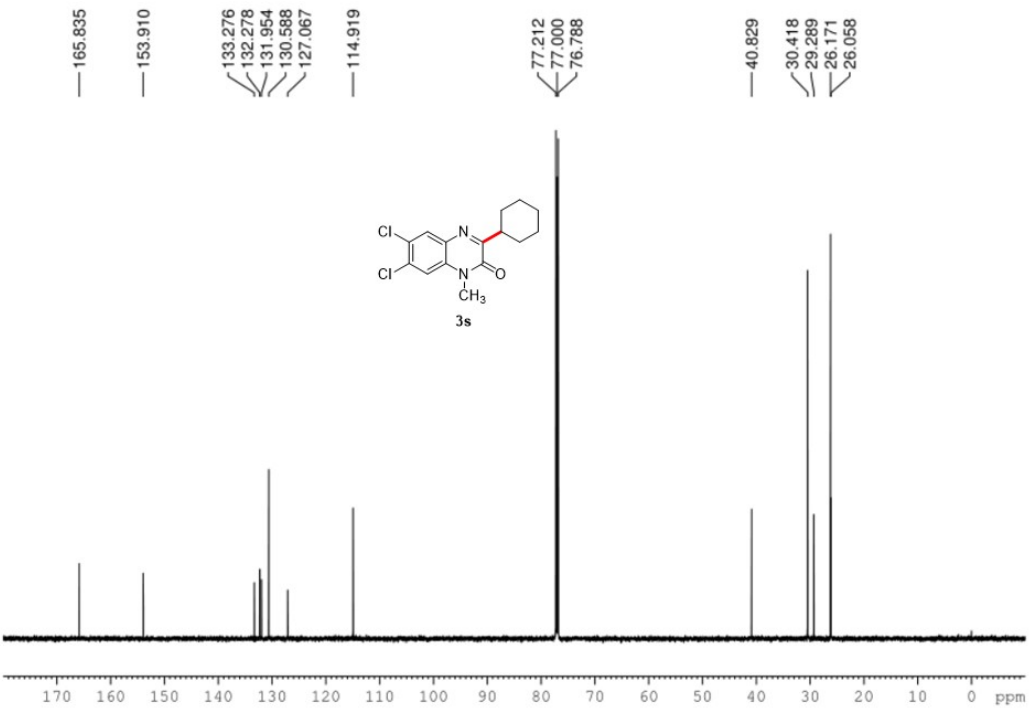
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26.171
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O
CH3
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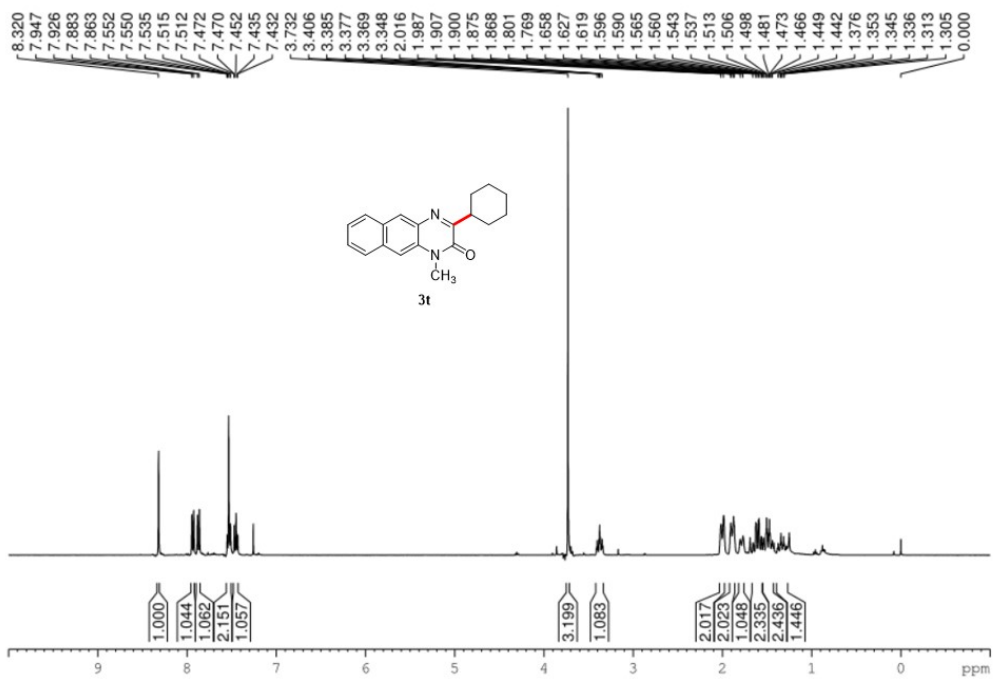
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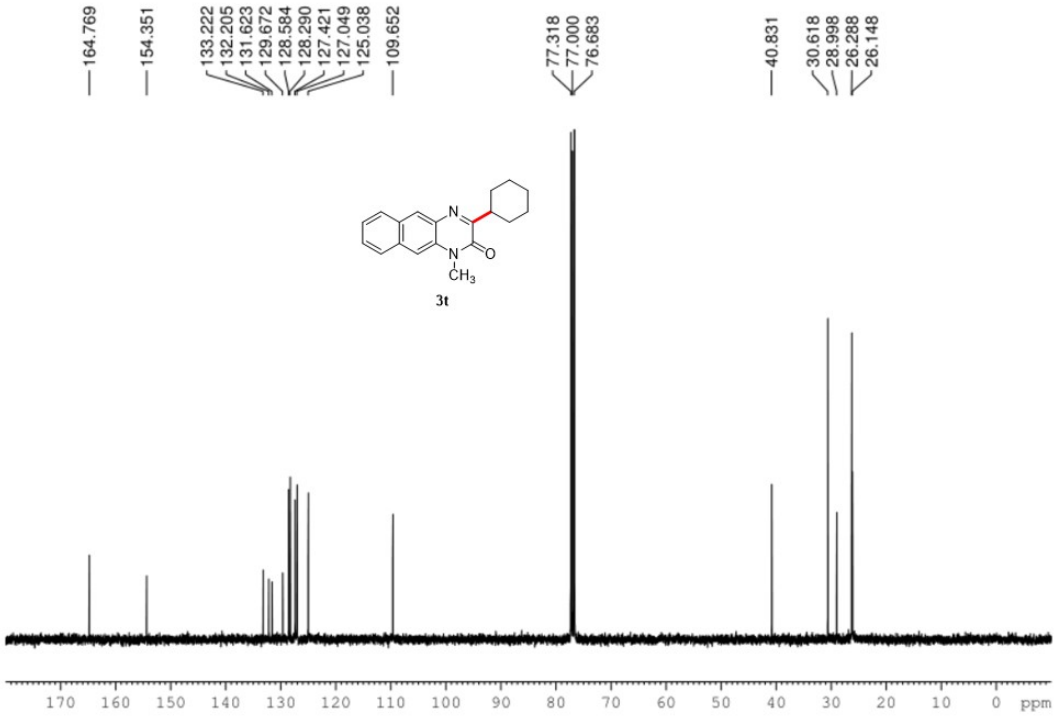
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O
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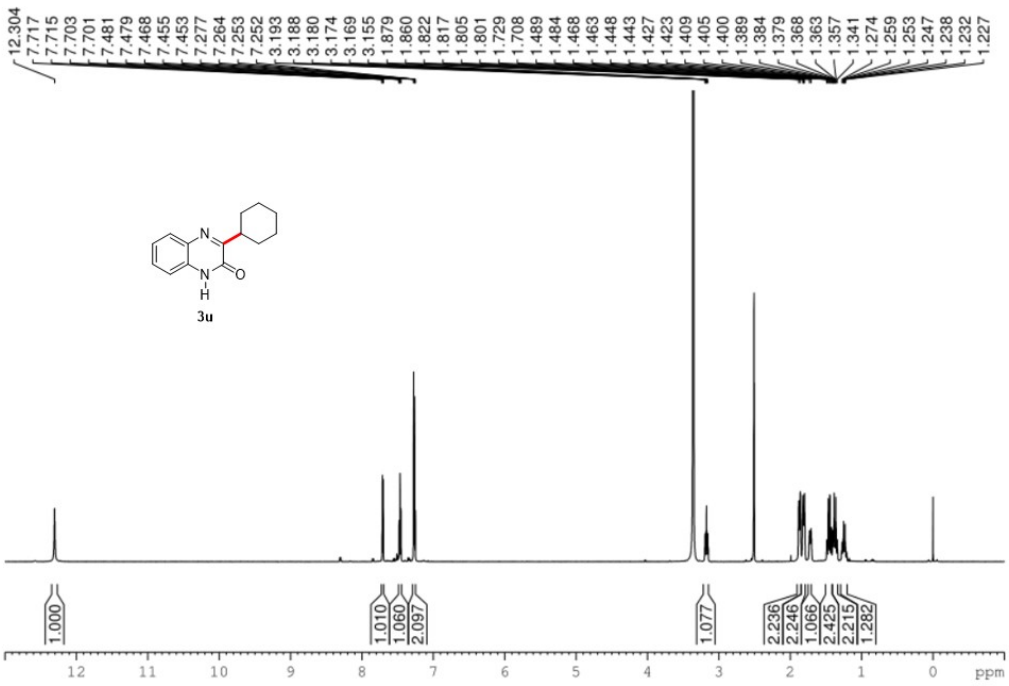
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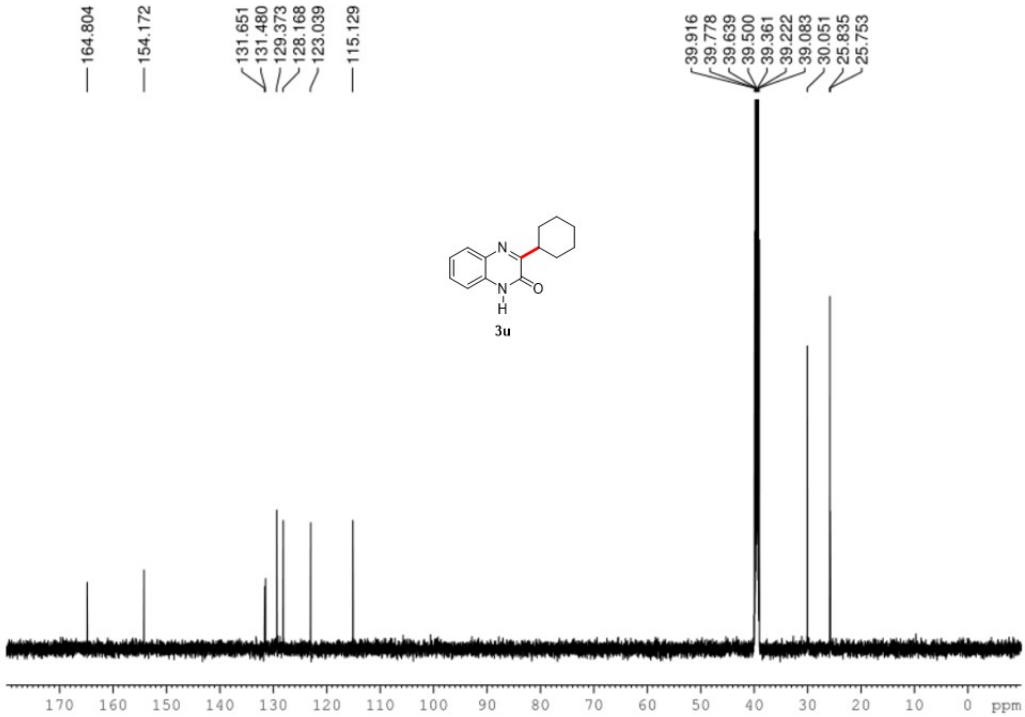
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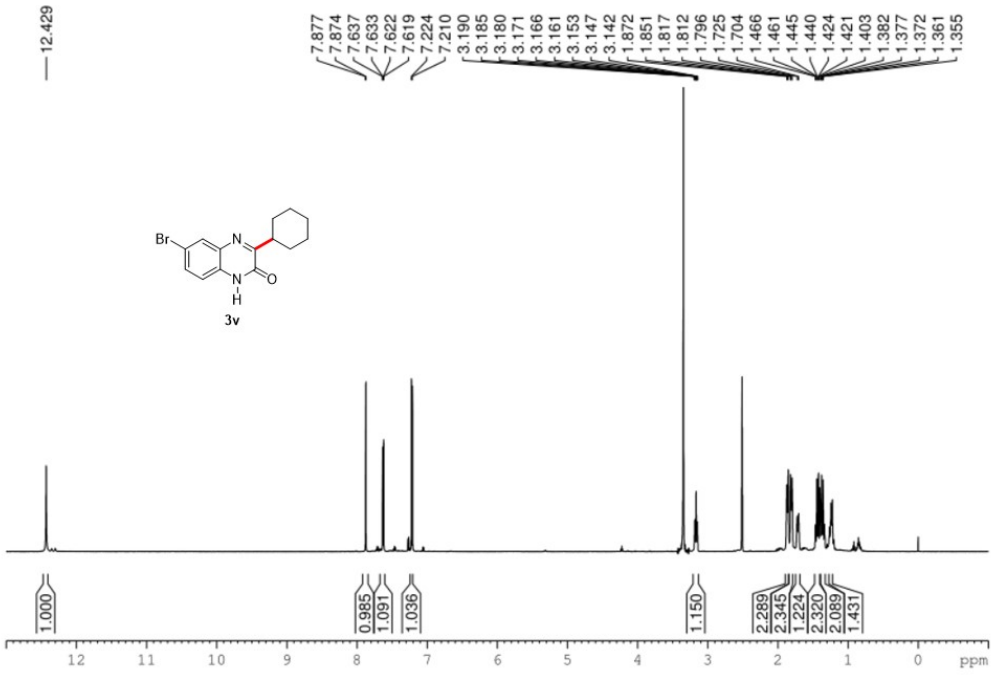
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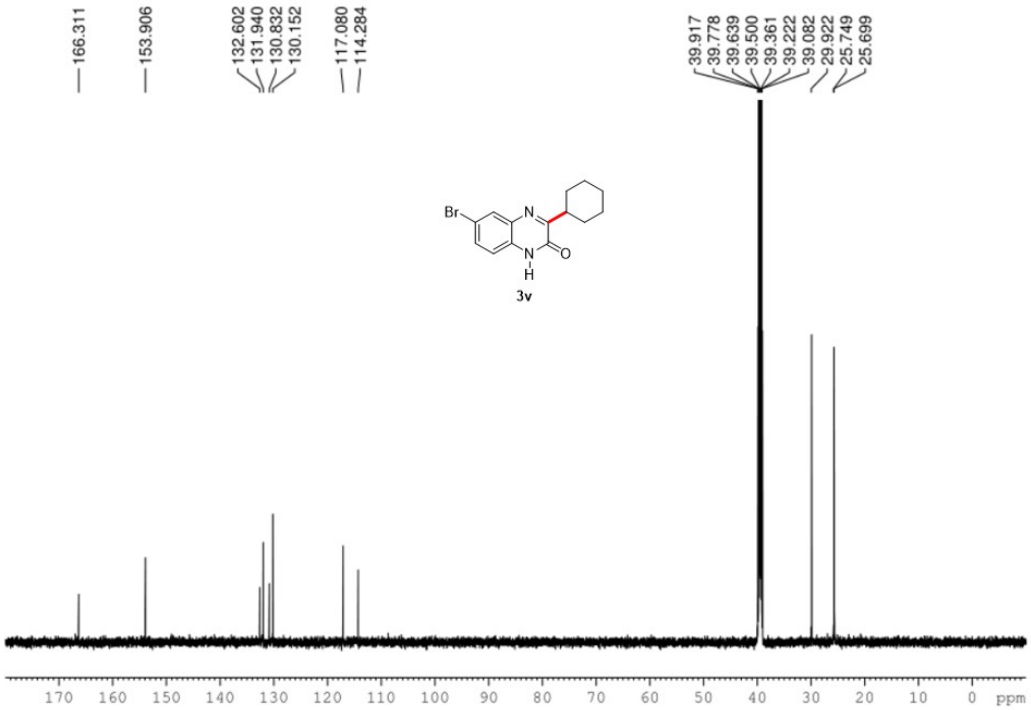
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N
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O
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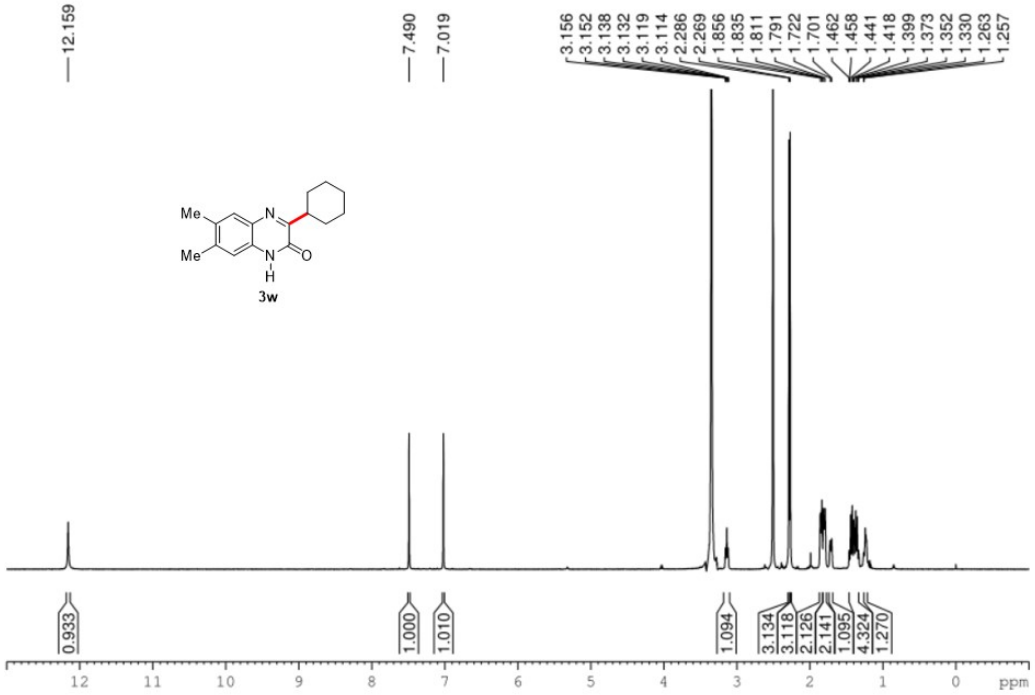
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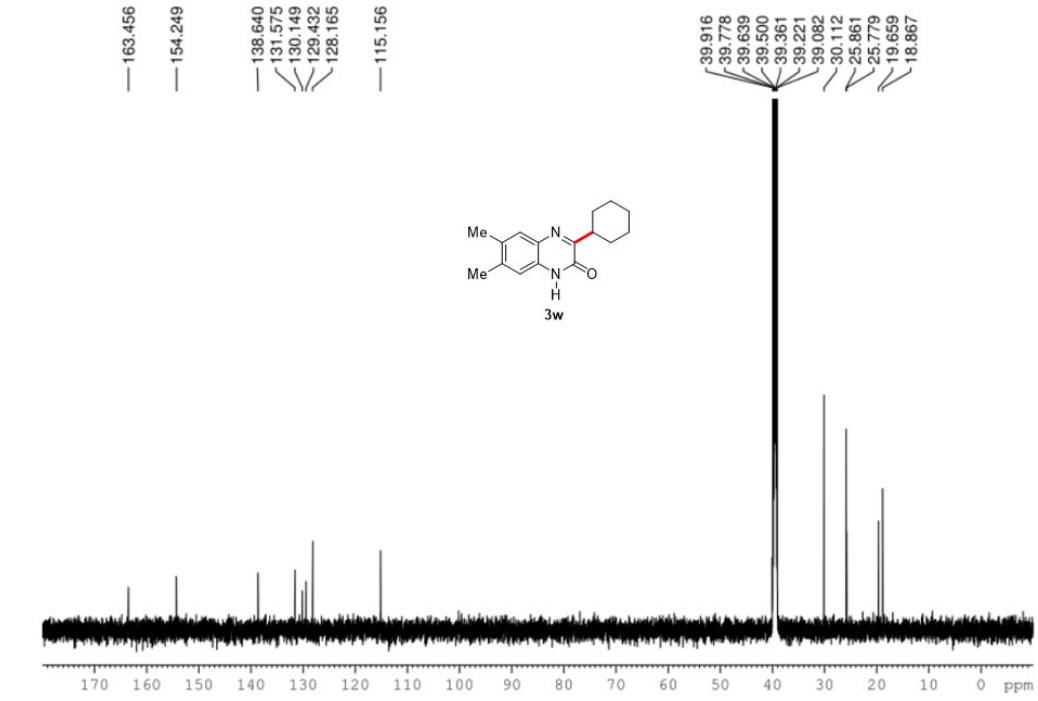
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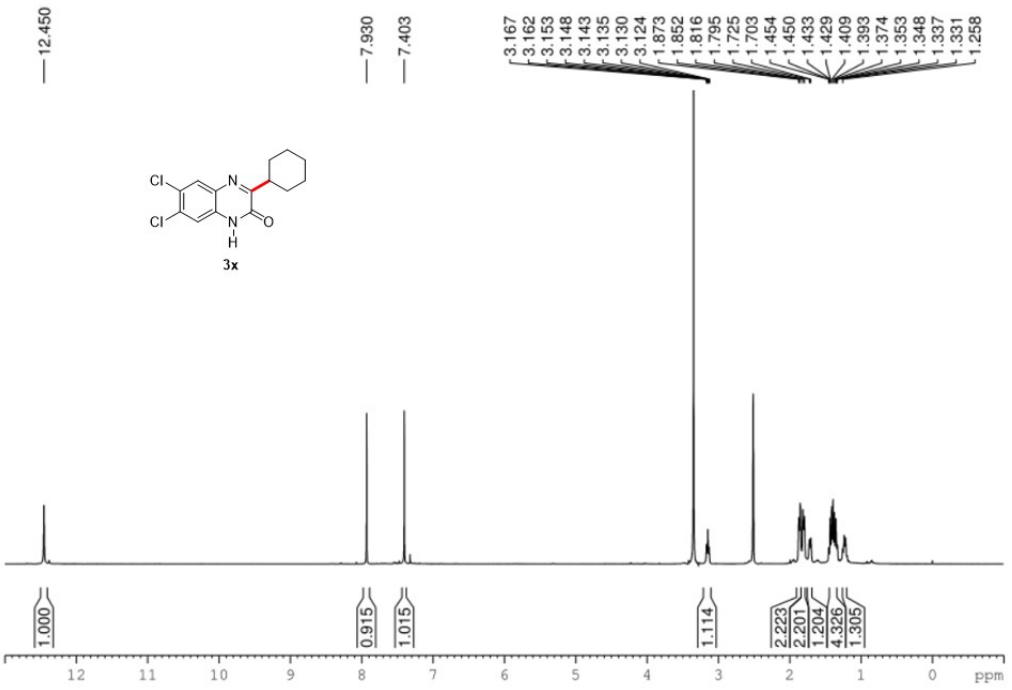
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1.795
1.725
1.703
1.454
1.450
1.433
1.429
1.409
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1.374
1.353
1.348
1.337
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1.258
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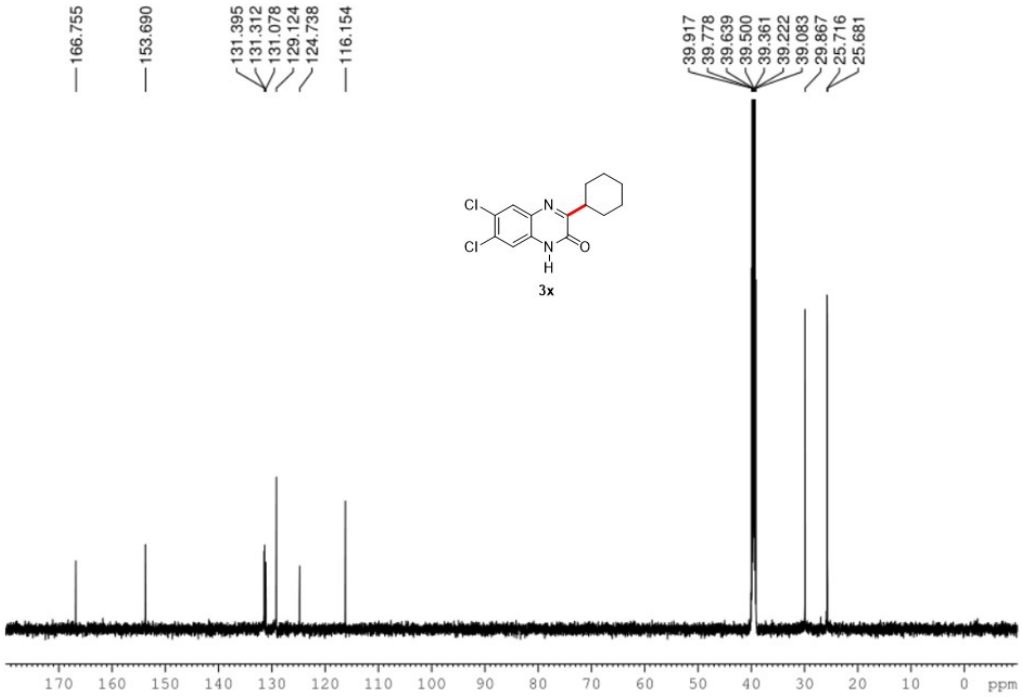
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39.222
39.083
29.867
25.716
25.681
Cl
Cl
N
N
H
O
3x
170
160
150
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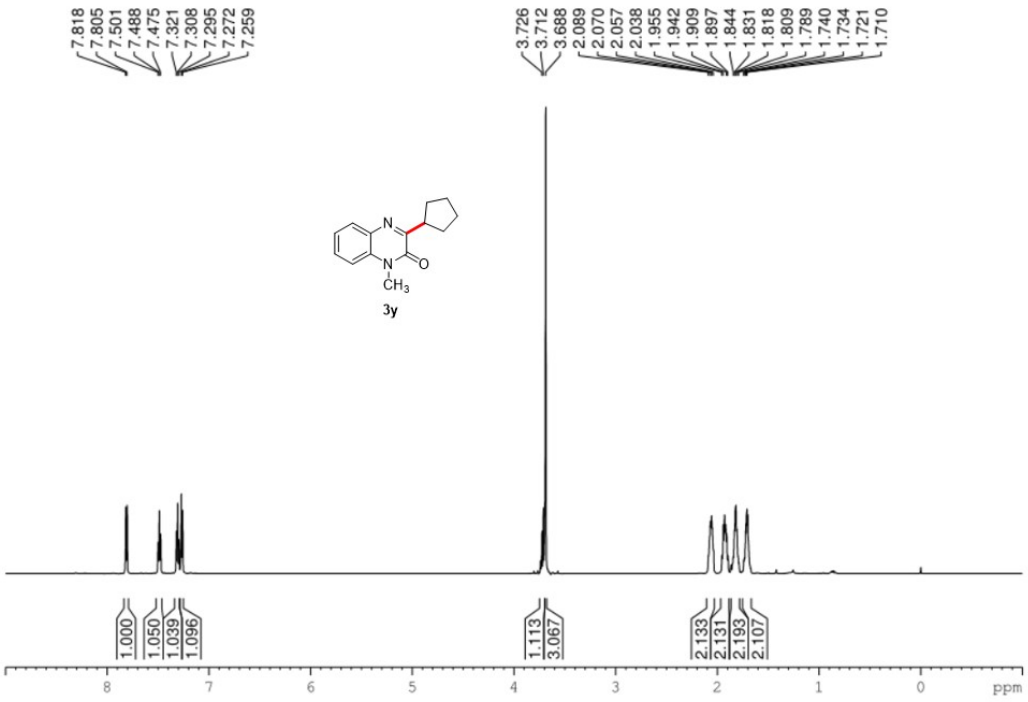
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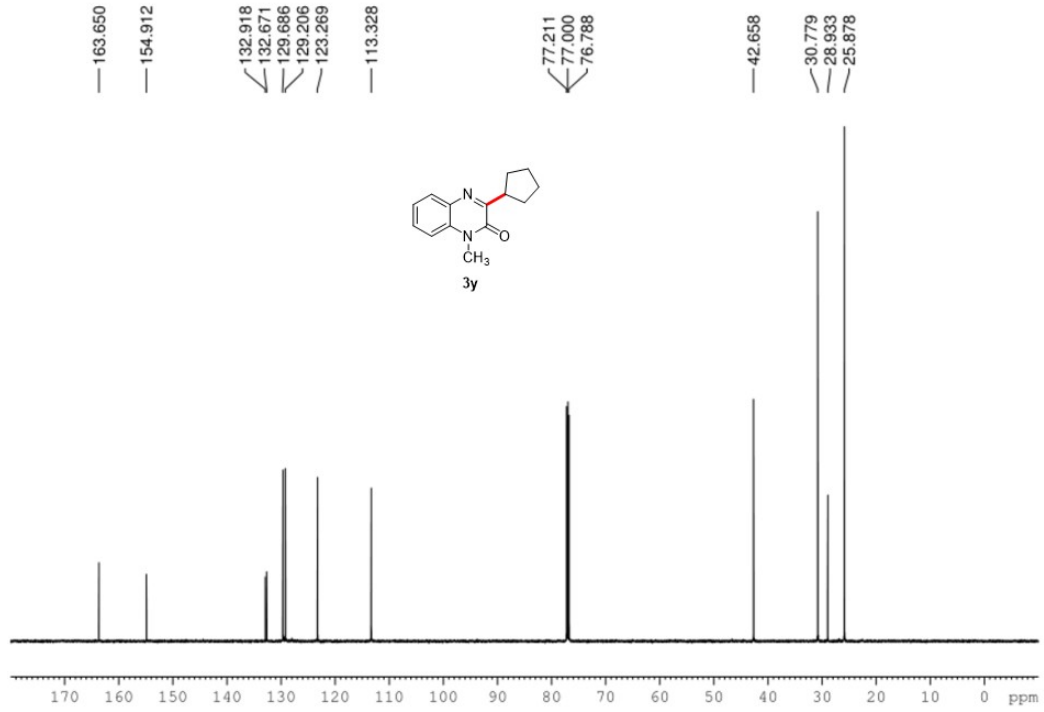
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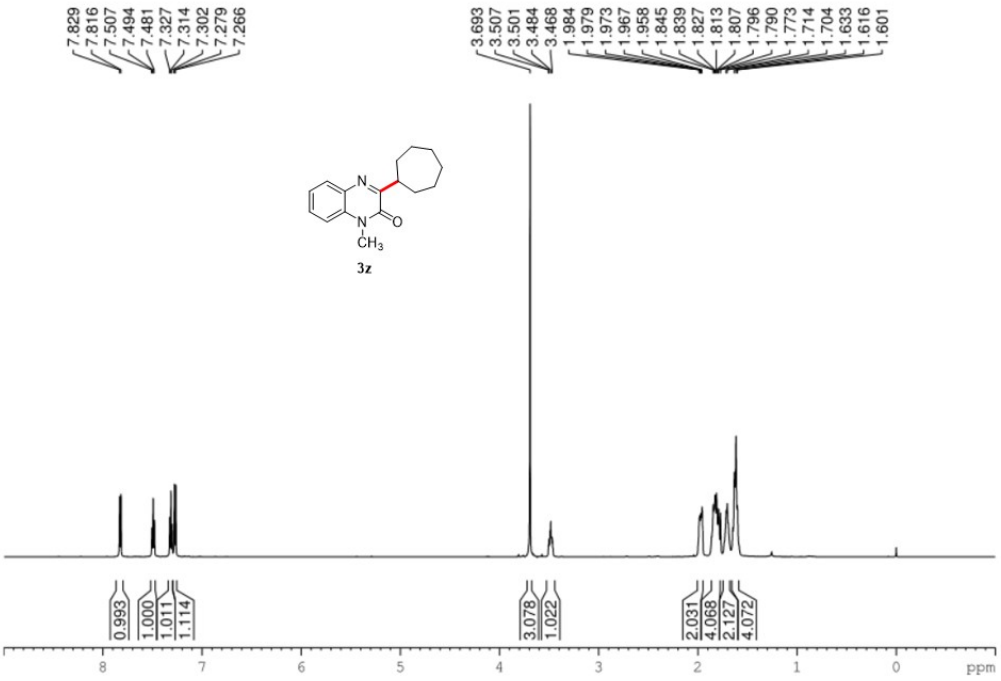
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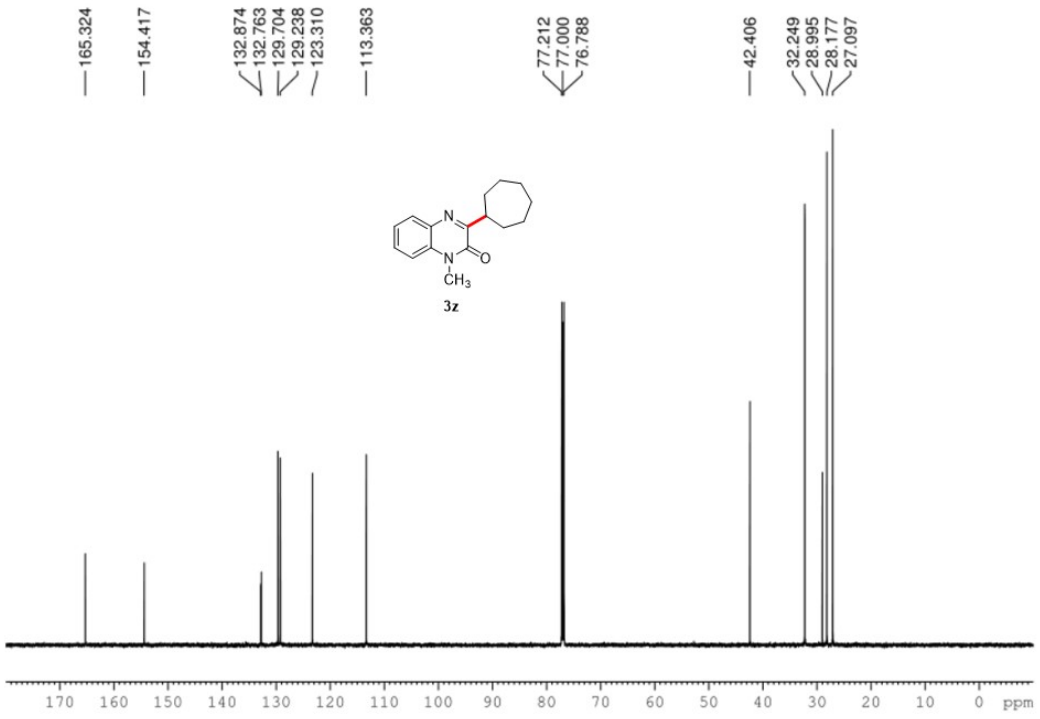
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CH3
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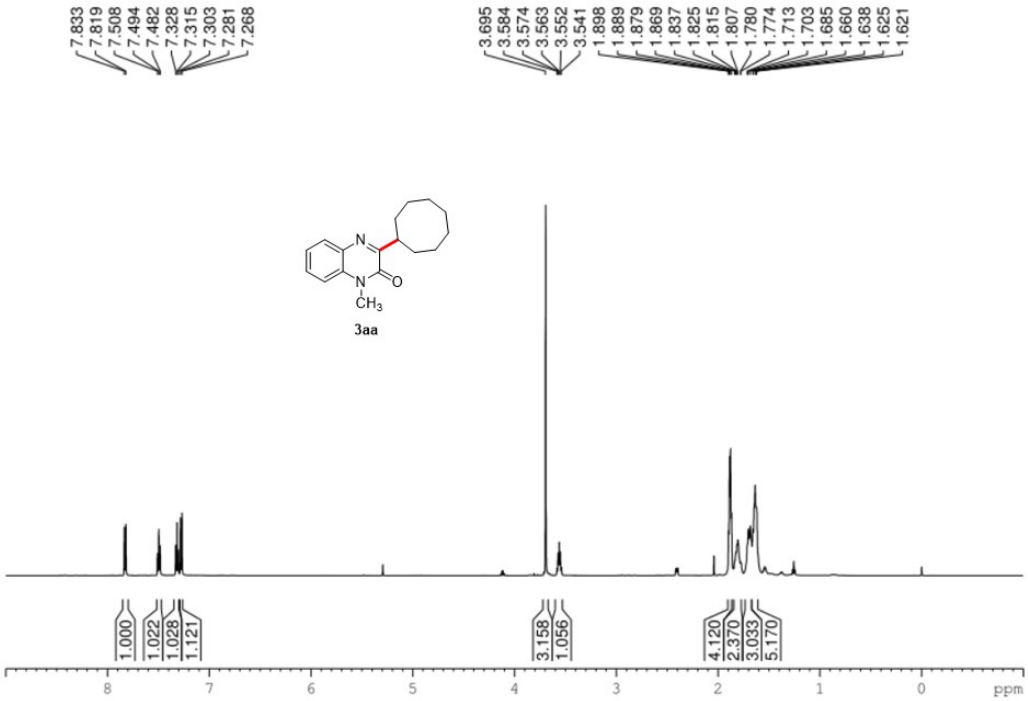
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1.889
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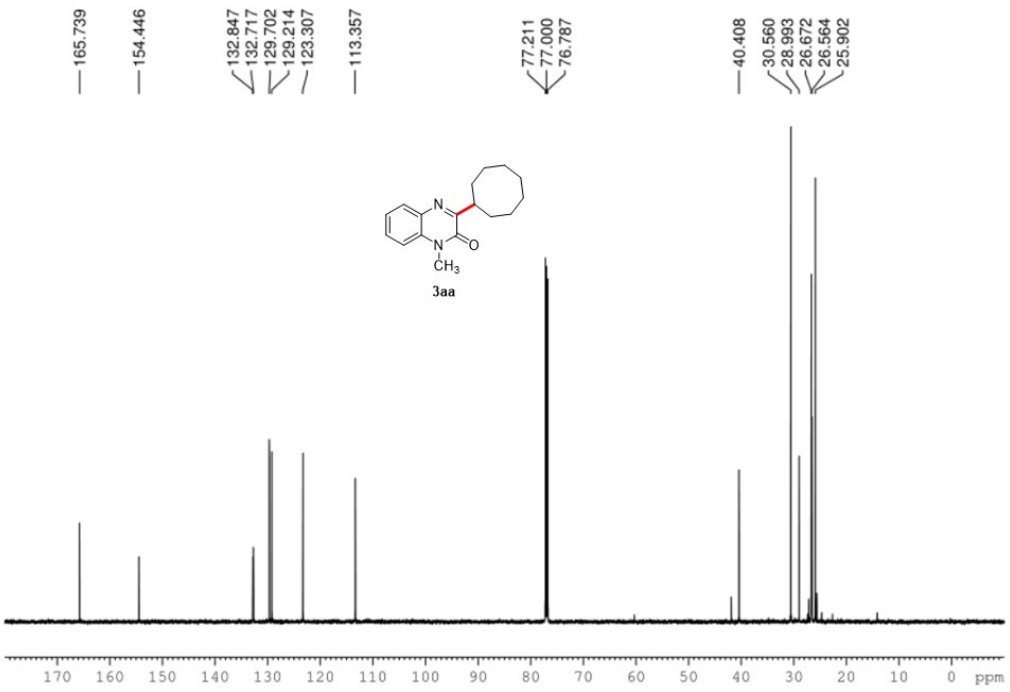
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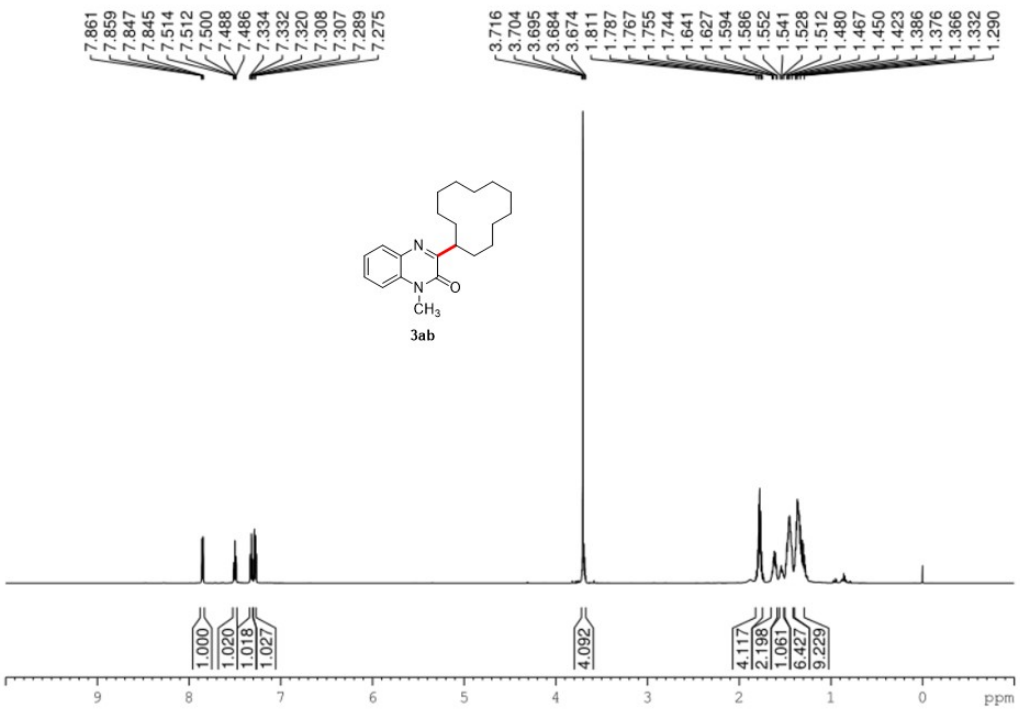
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1.541
1.528
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1.467
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1.423
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1.376
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1.332
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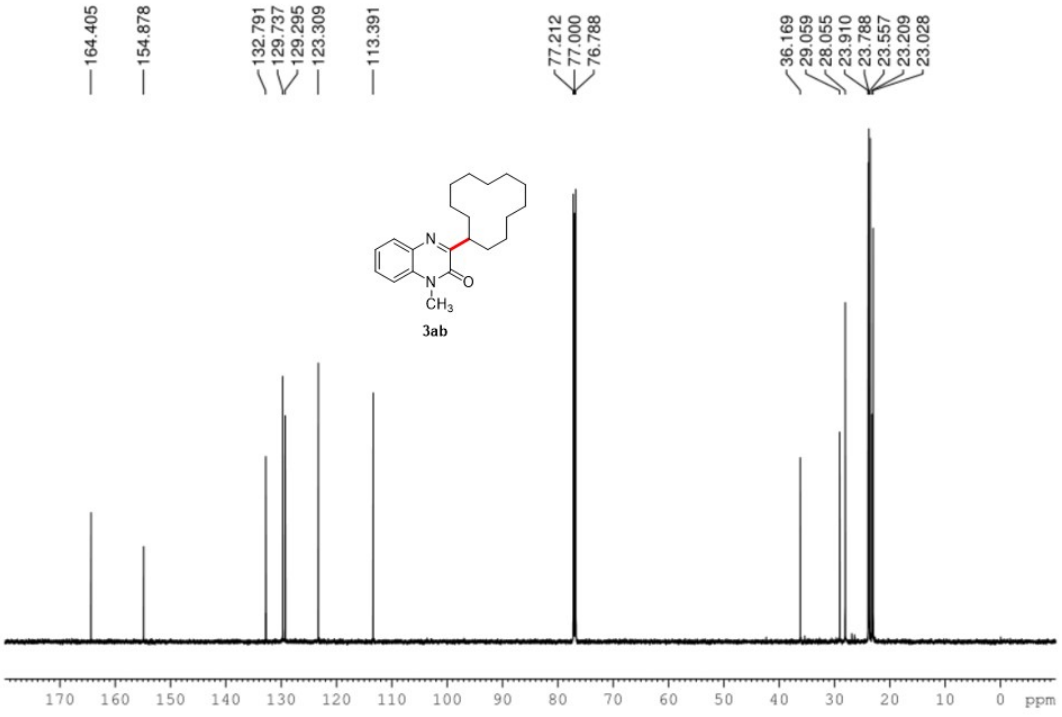
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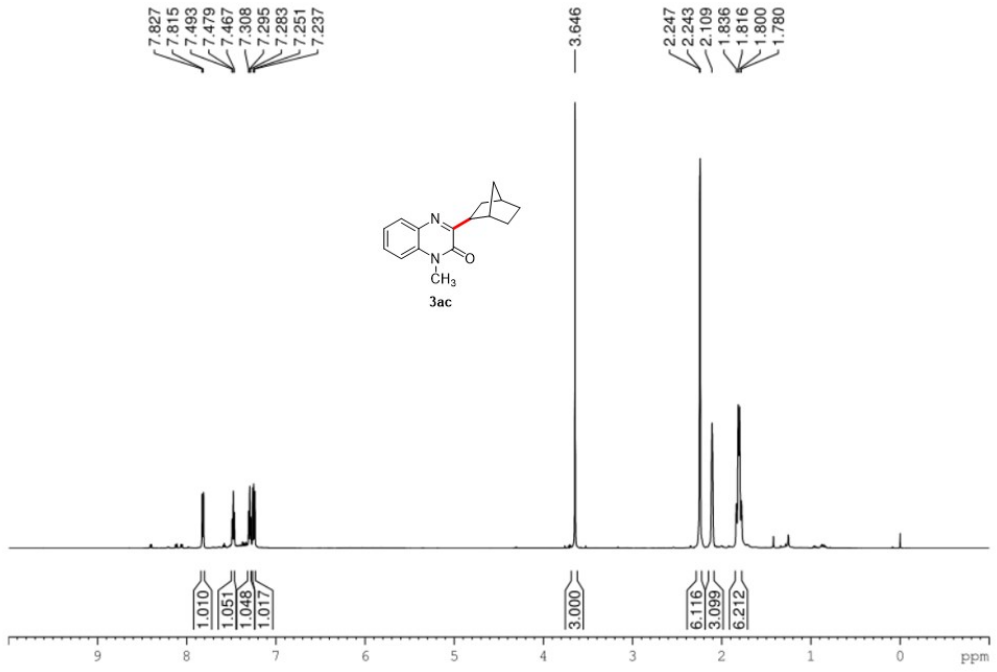
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7.237
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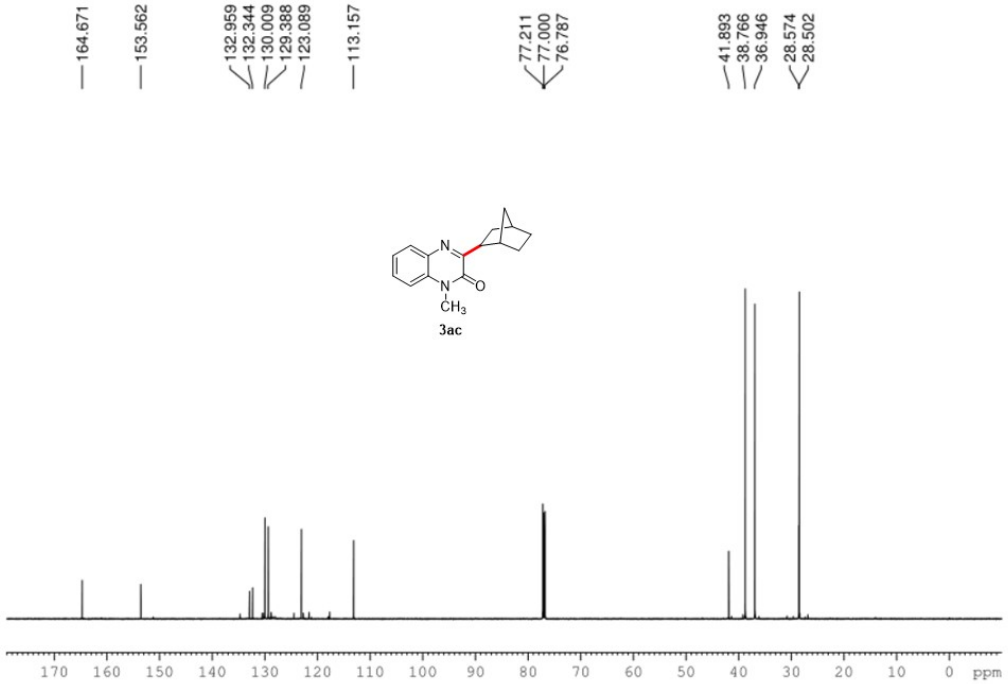
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38.766
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28.574
28.502
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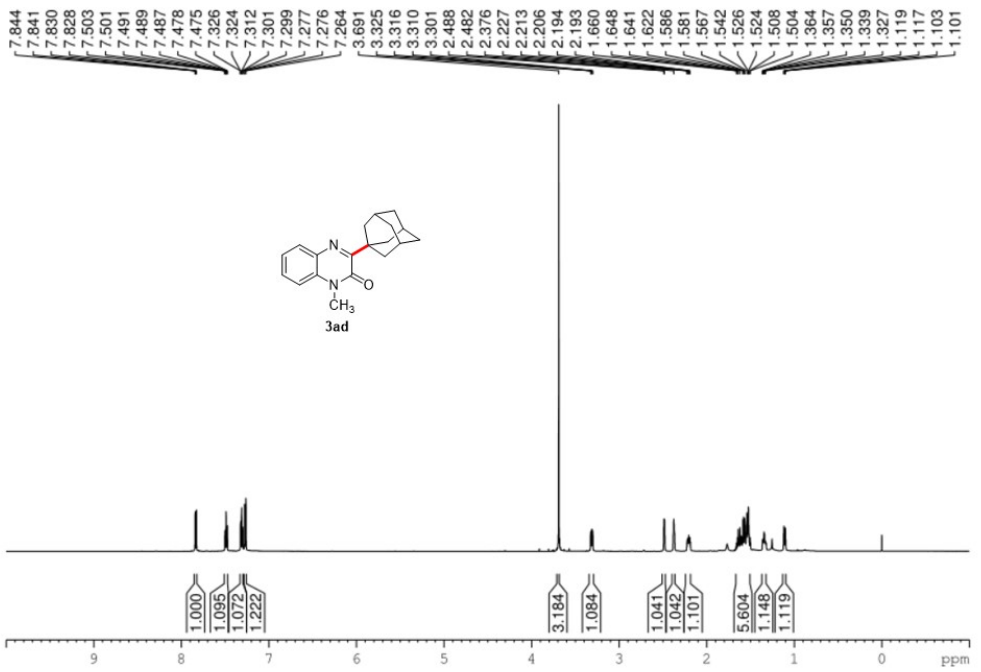
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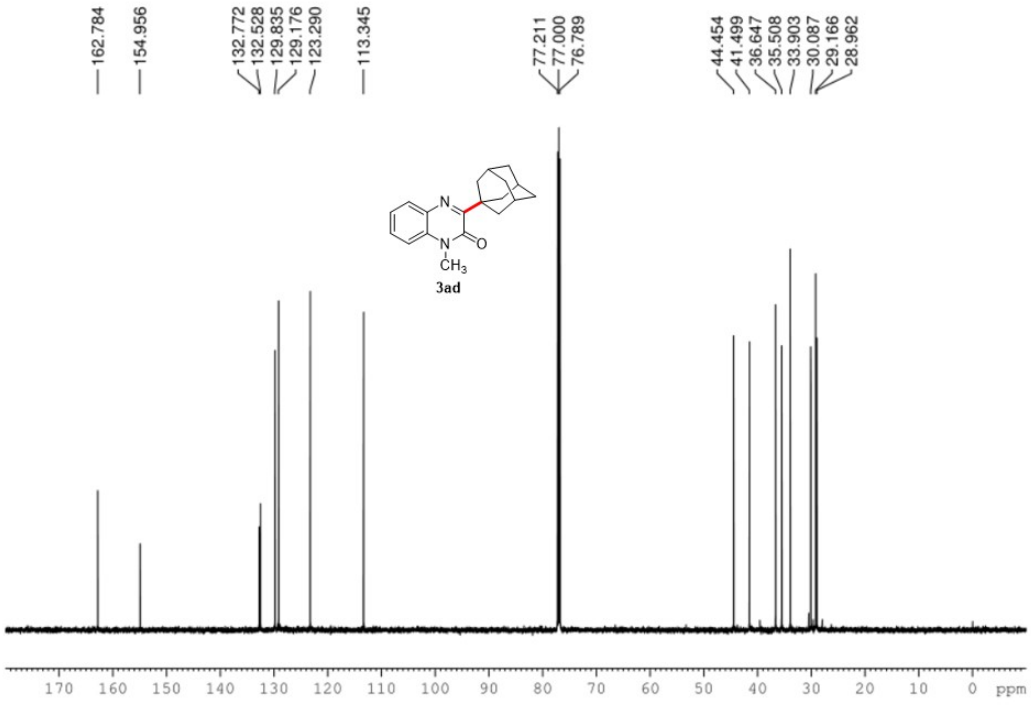
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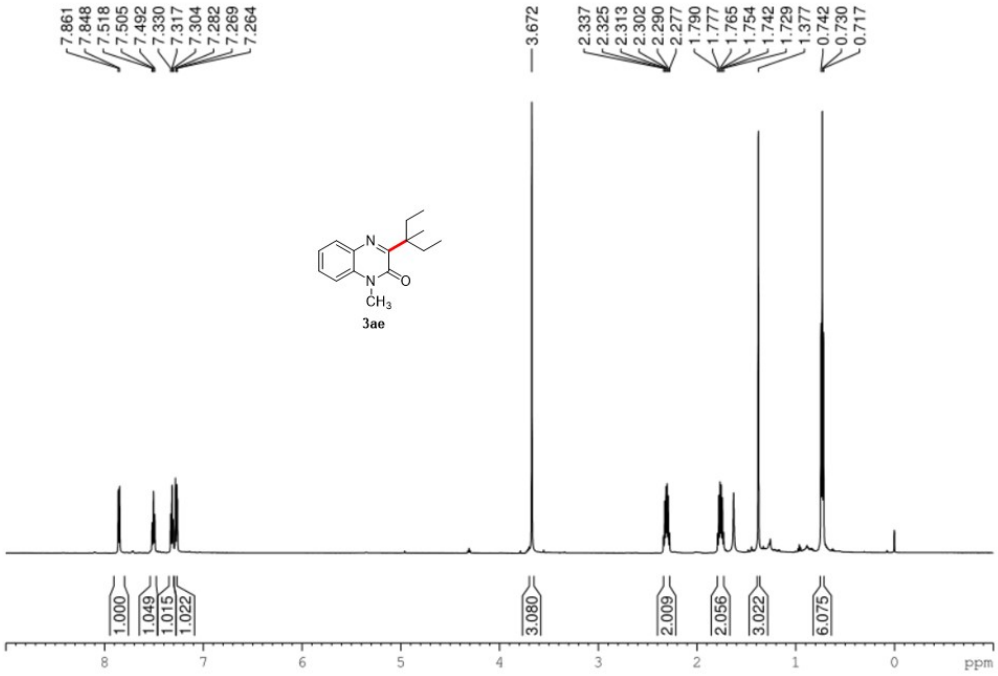
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2.337
2.325
2.313
2.302
2.290
2.277
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1.742
1.729
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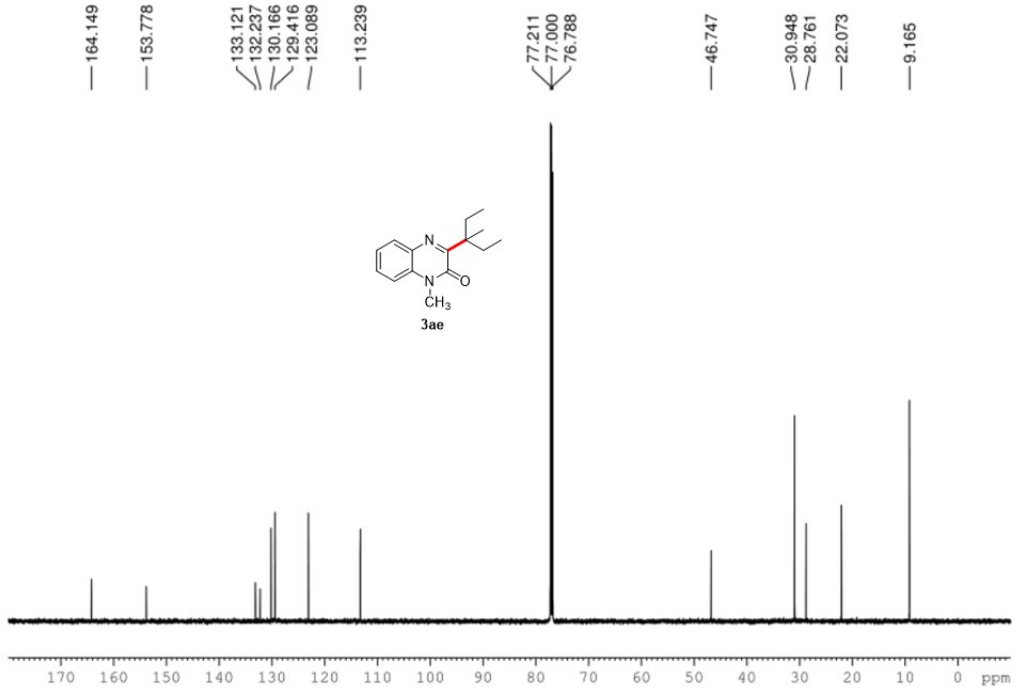
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O
CH3
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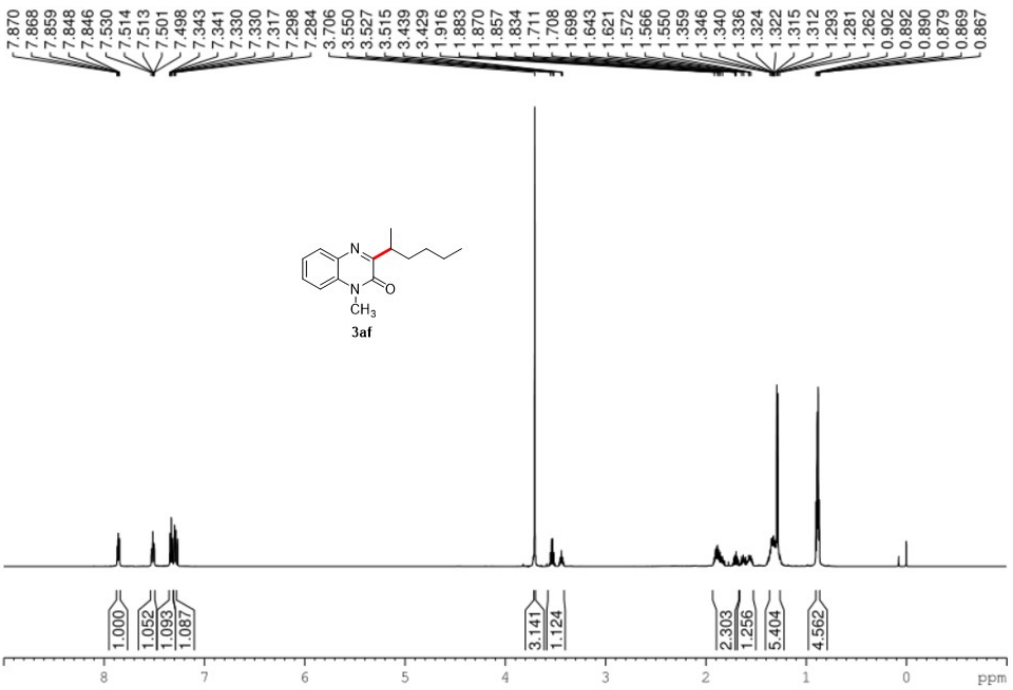
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7.330
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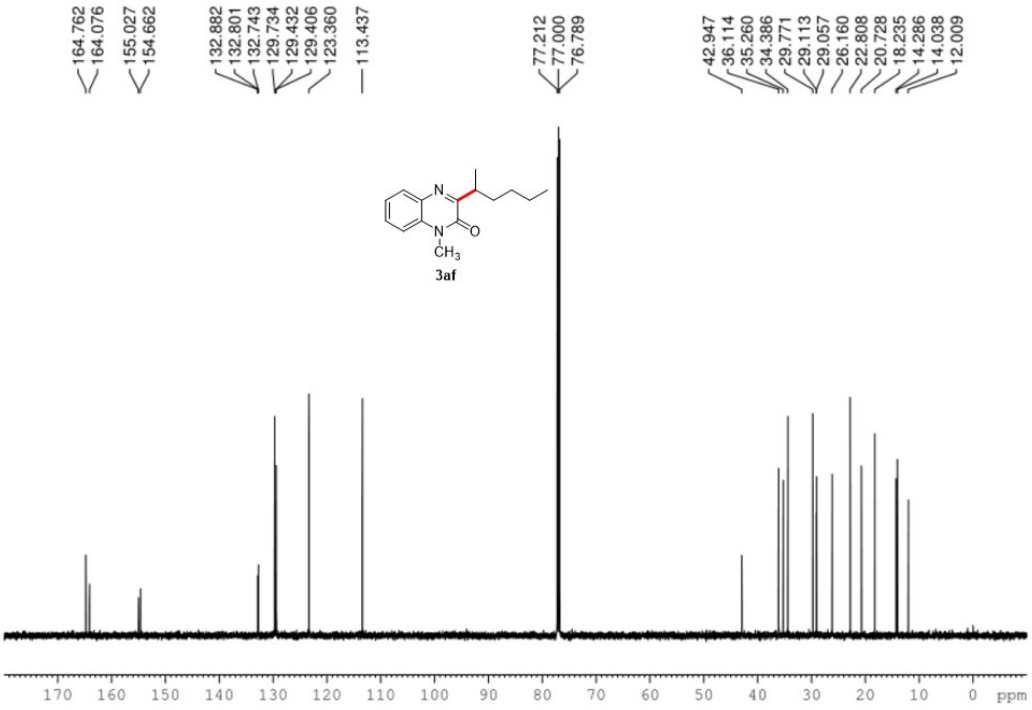
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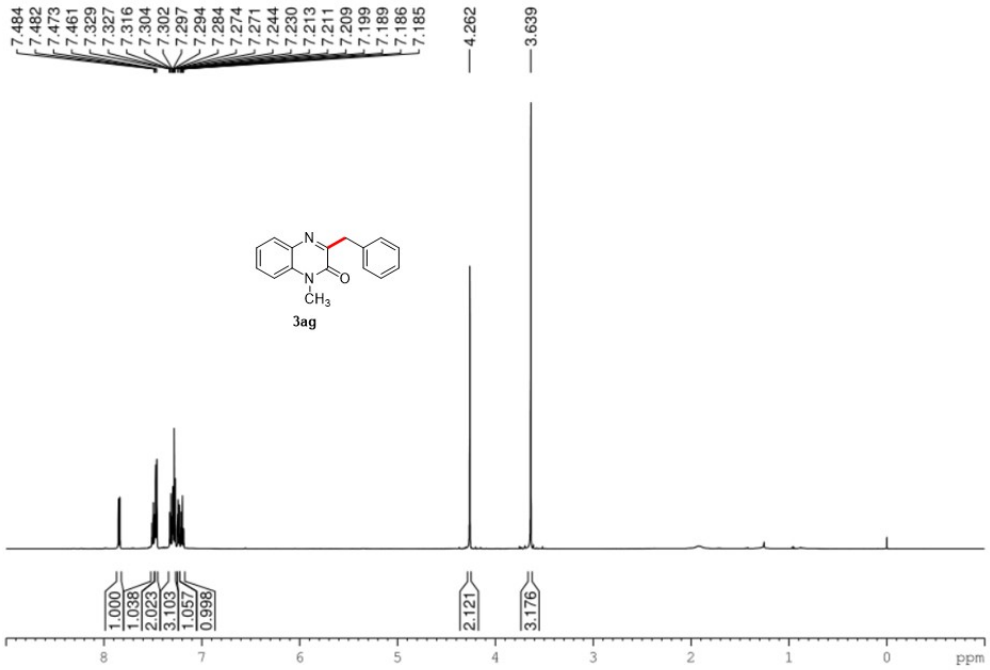
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7.244
7.230
7.213
7.211
7.209
7.199
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7.186
7.185
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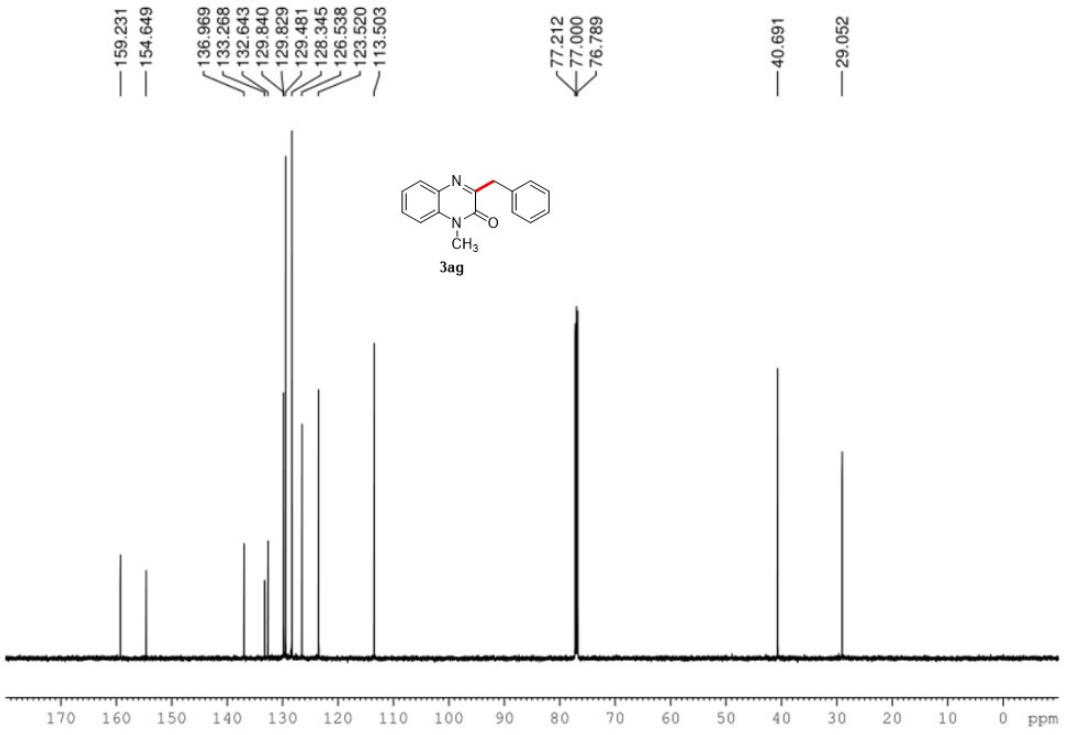
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29.052
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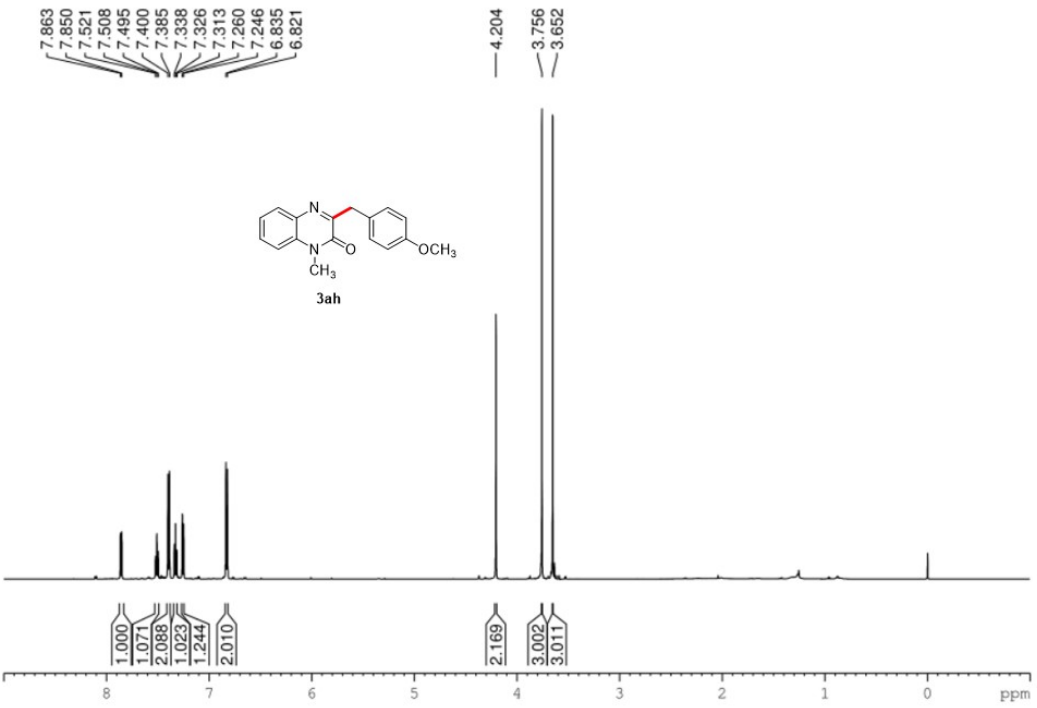
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6.821
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N
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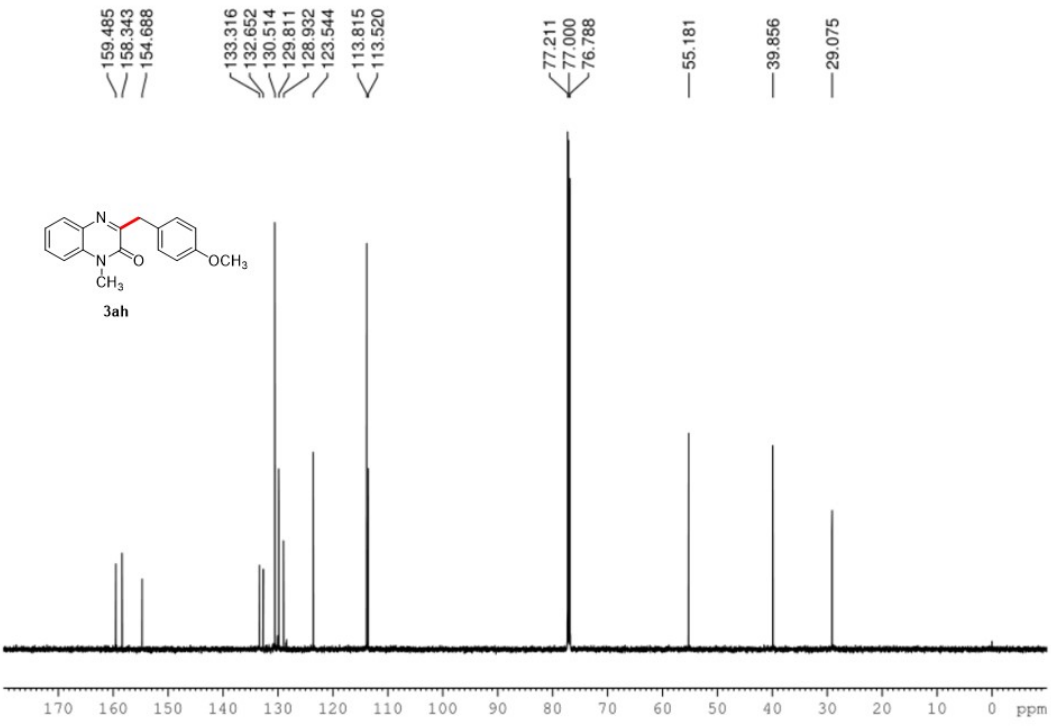
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OCH3
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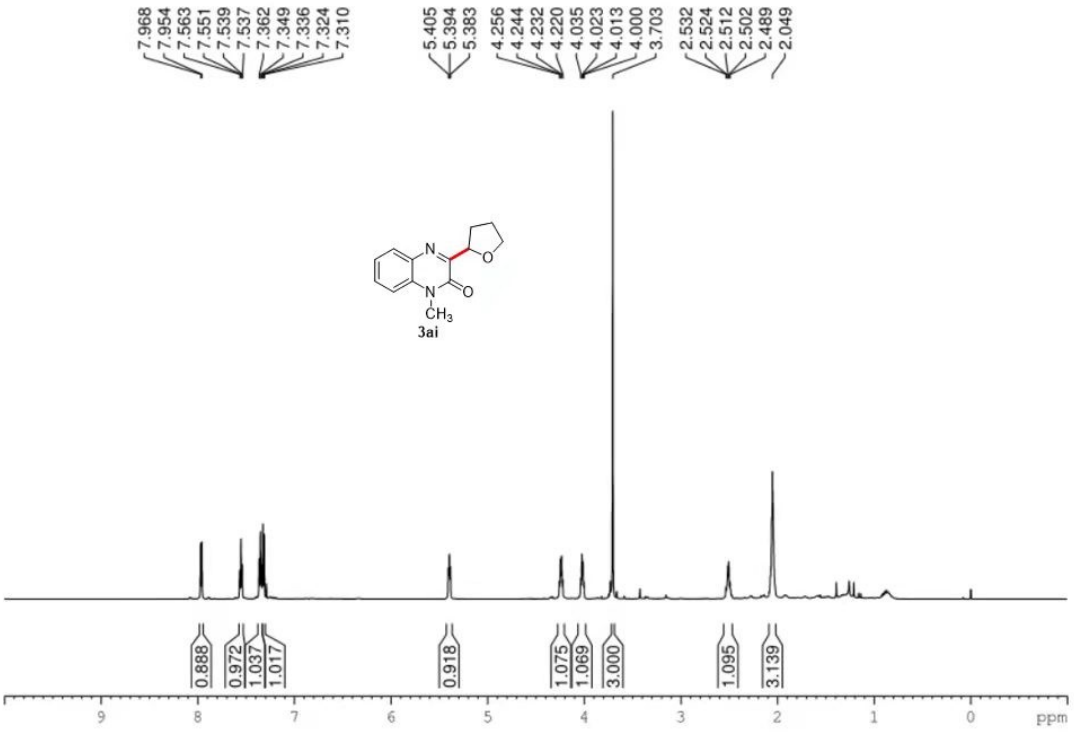
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4.220
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2.524
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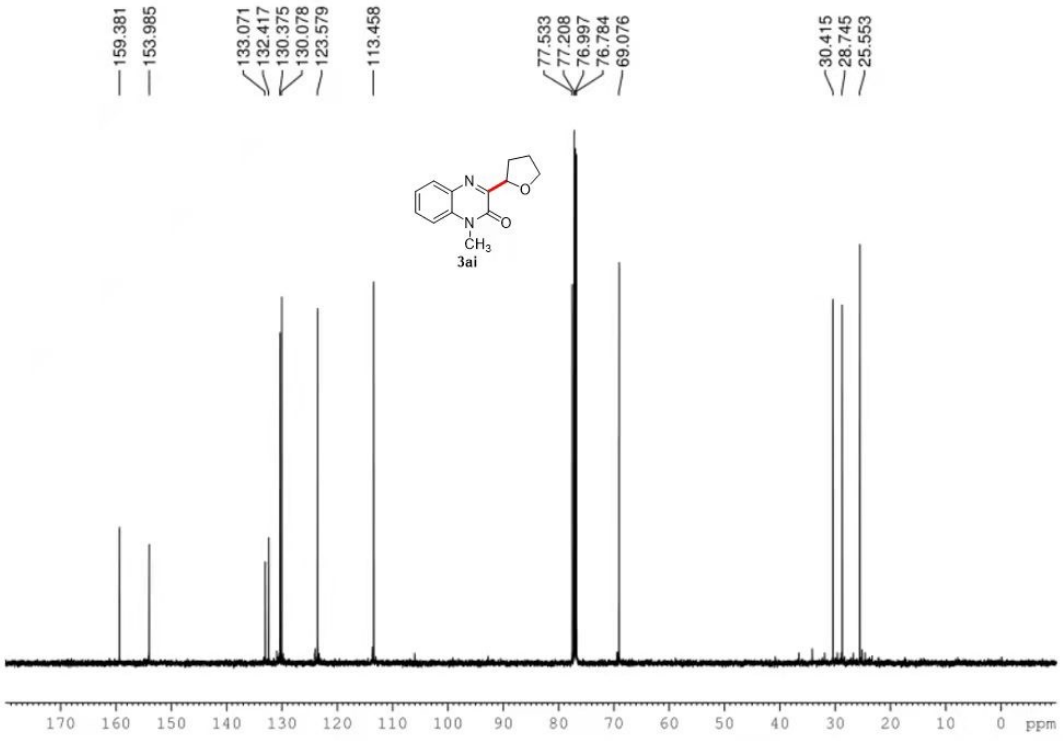
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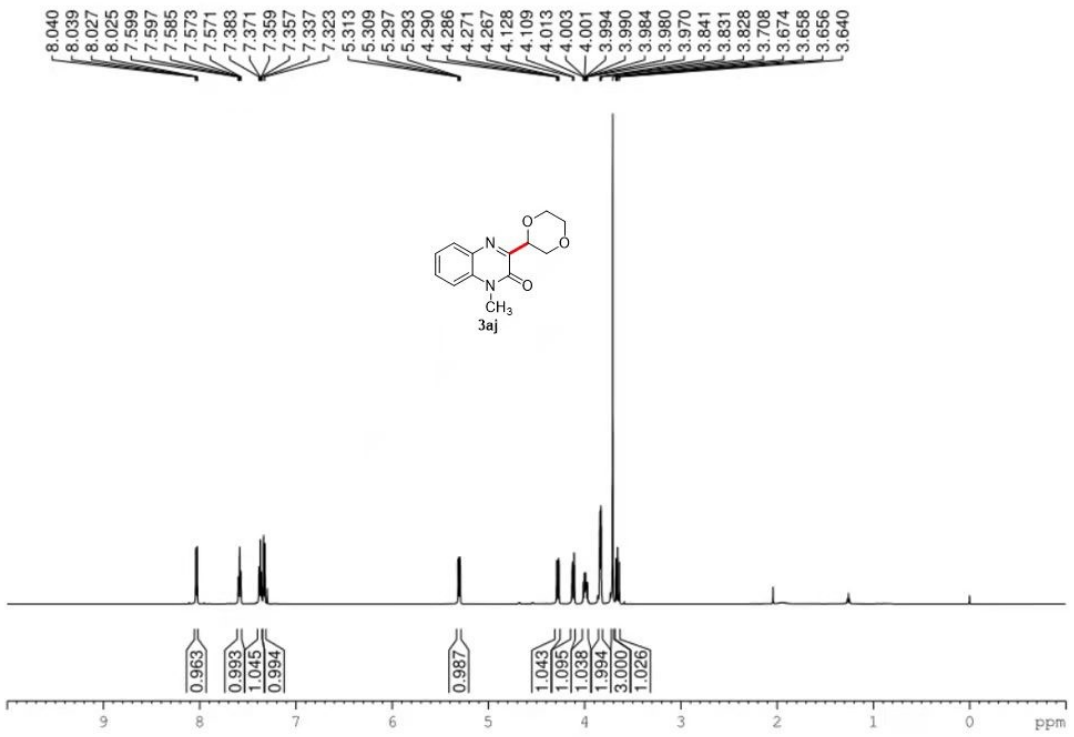
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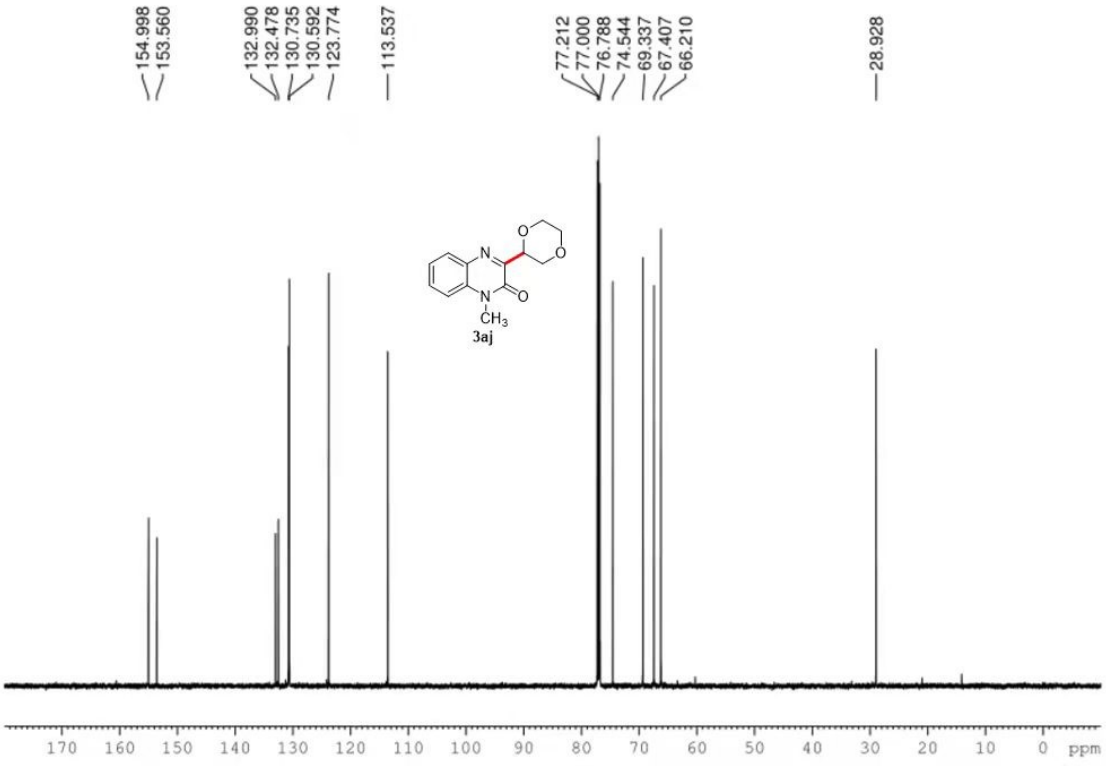
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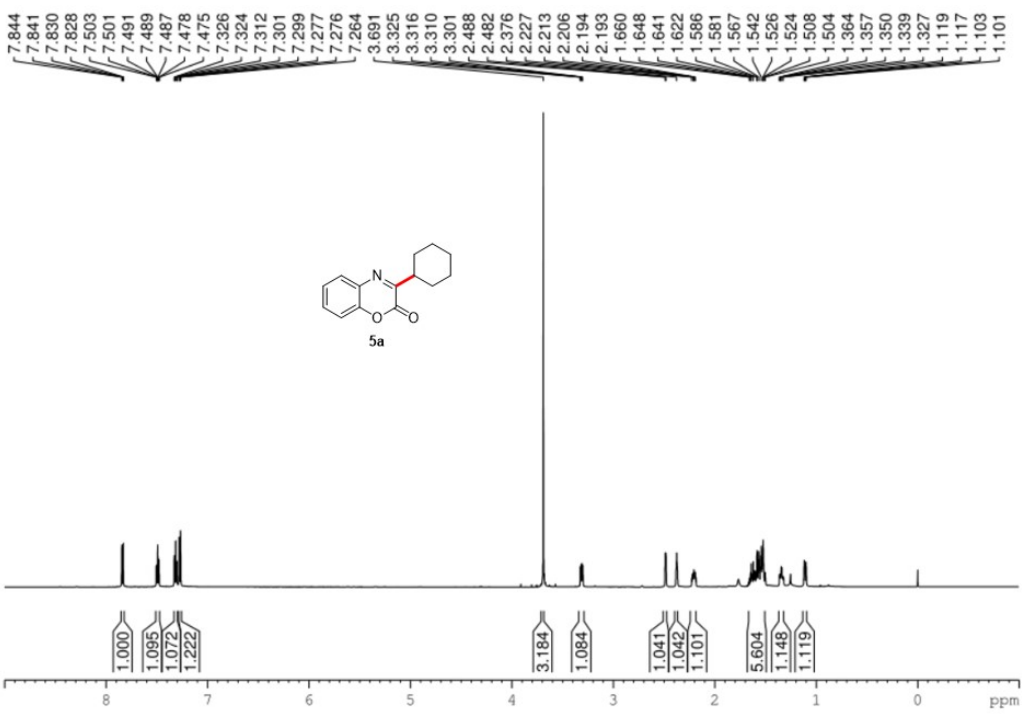
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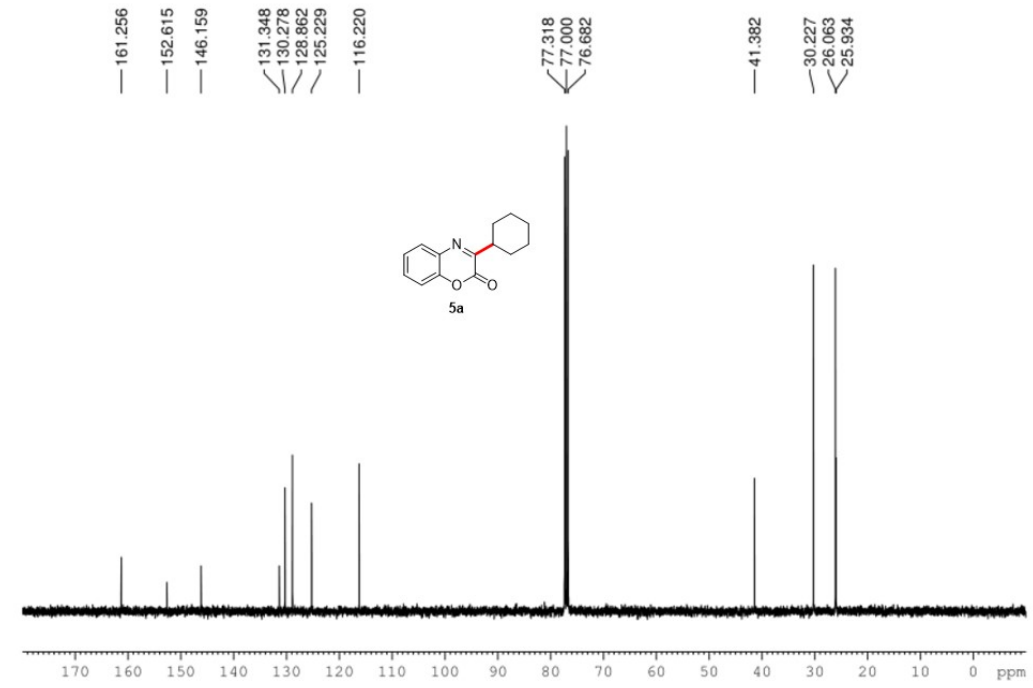
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77.000
76.682
41.382
30.227
26.063
25.934
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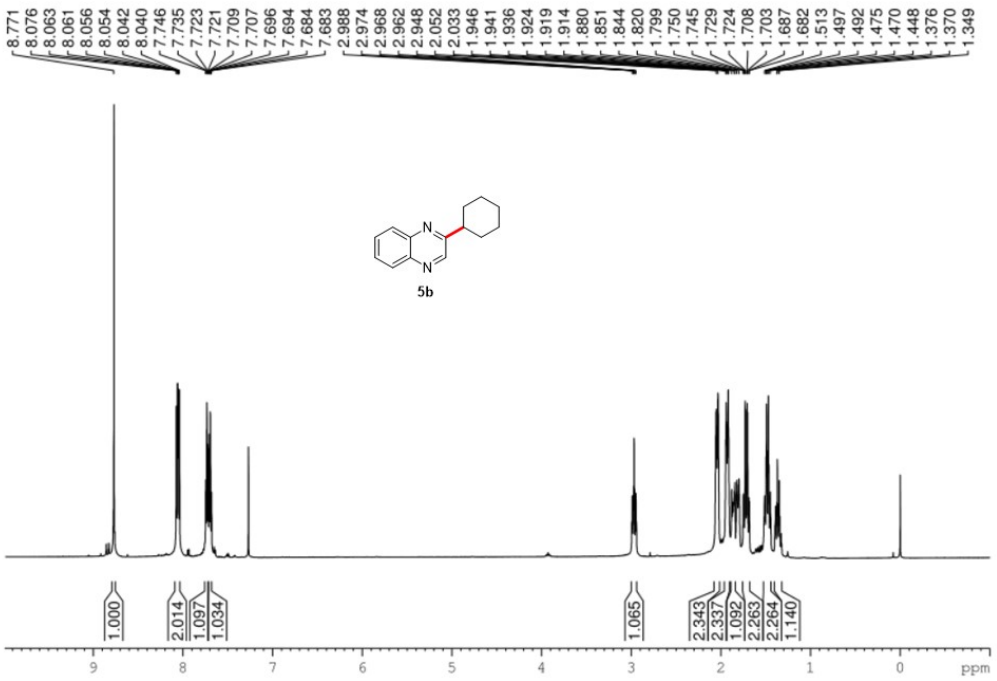
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7.707
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7.694
7.684
7.683
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2.962
2.948
2.052
2.033
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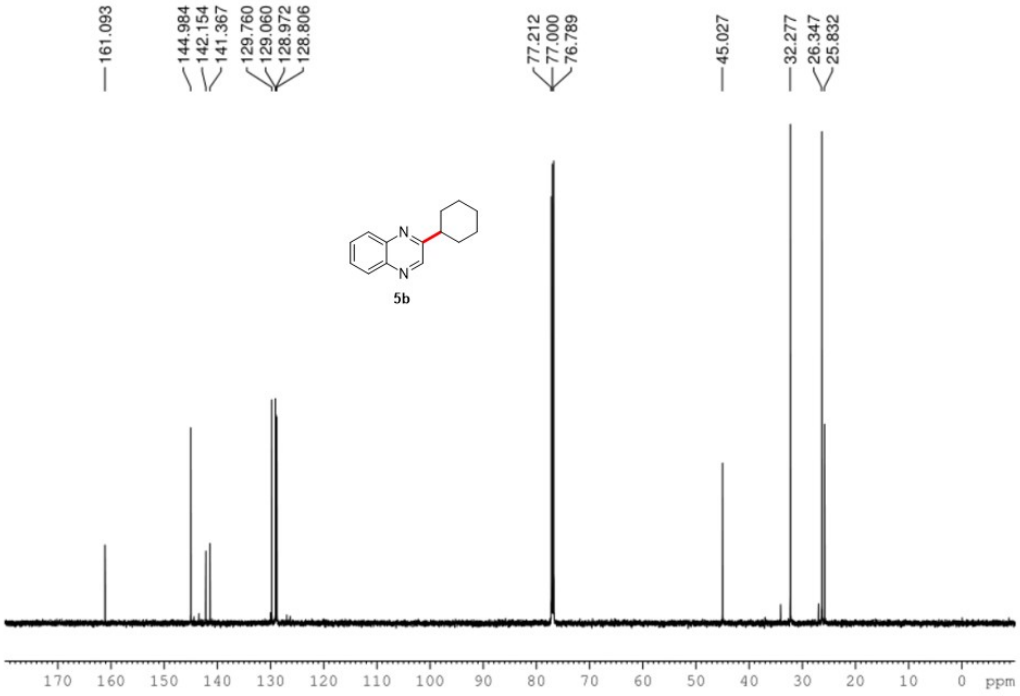
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26.347
25.832
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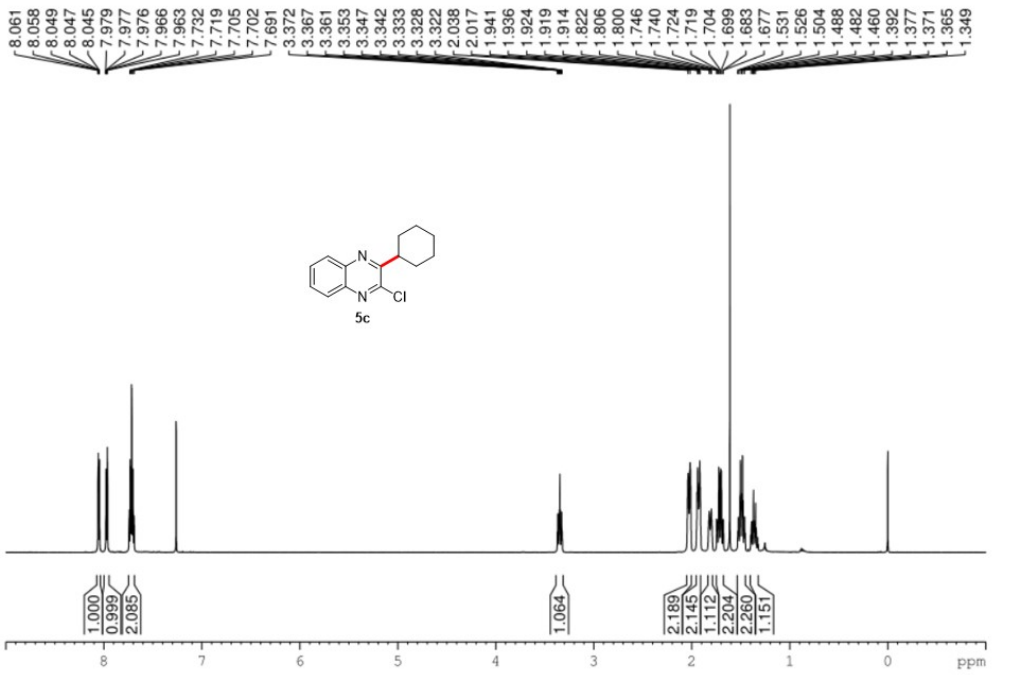
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7.976
7.966
7.963
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7.719
7.705
7.702
7.691
3.372
3.367
3.361
3.353
3.347
3.342
3.333
3.328
3.322
2.038
2.017
1.941
1.936
1.924
1.919
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1.822
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1.746
1.740
1.724
1.719
1.704
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1.683
1.677
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1.504
1.488
1.482
1.460
1.392
1.377
1.371
1.365
1.349
N
N
Cl
5c
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0.999
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6
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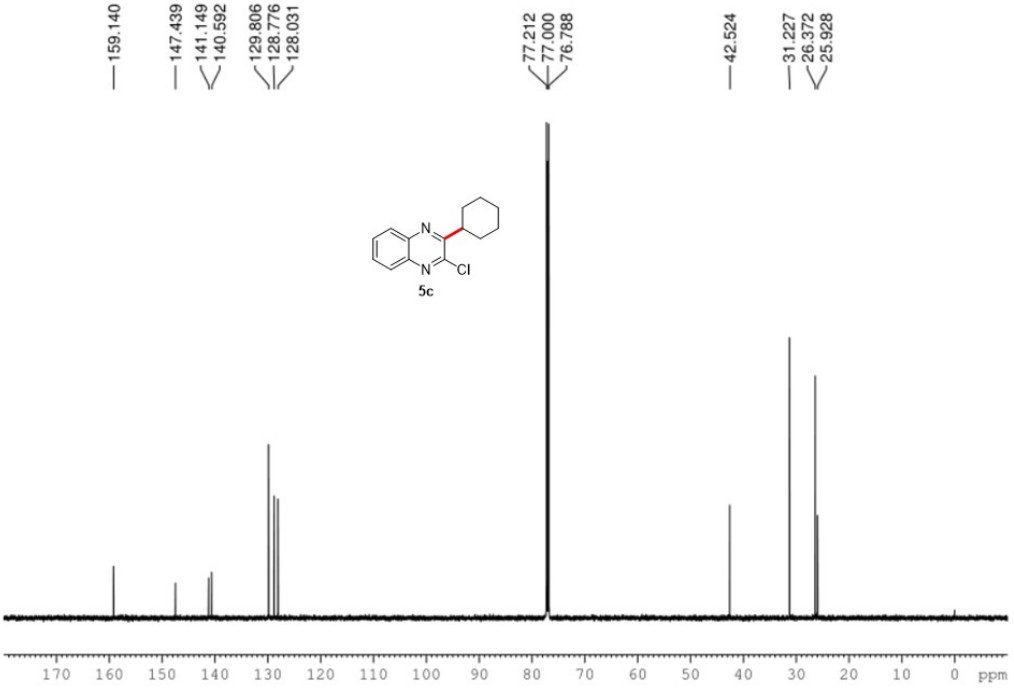
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Cl
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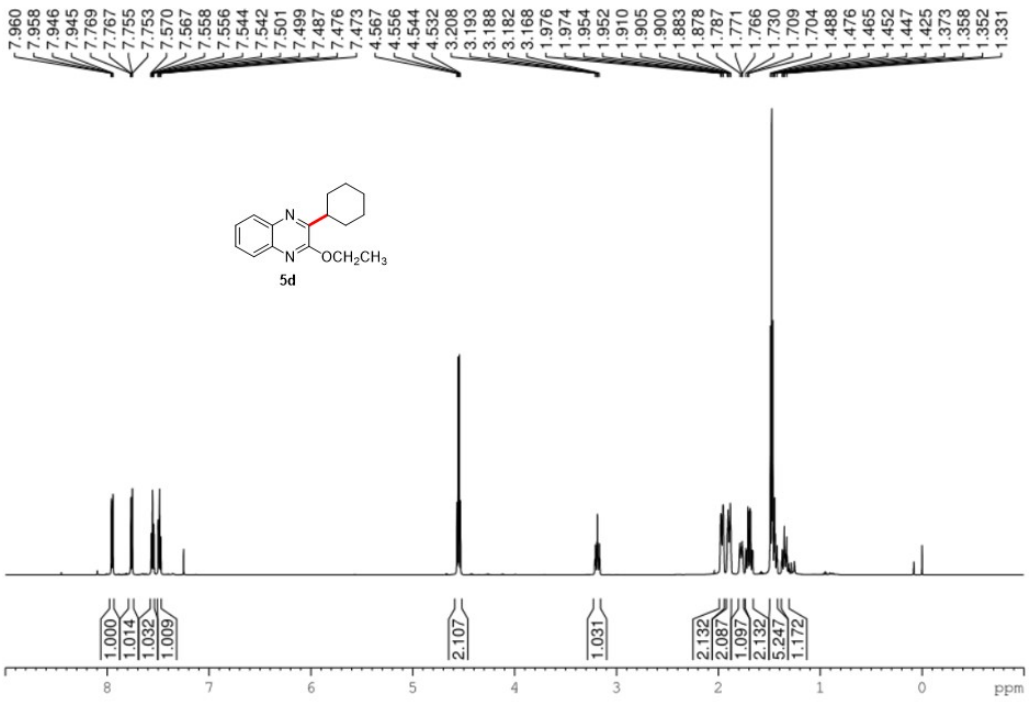
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7.556
7.544
7.542
7.501
7.499
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7.476
7.473
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4.556
4.544
4.532
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3.193
3.188
3.182
3.168
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1.905
1.900
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1.878
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1.331
N
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2.107
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6
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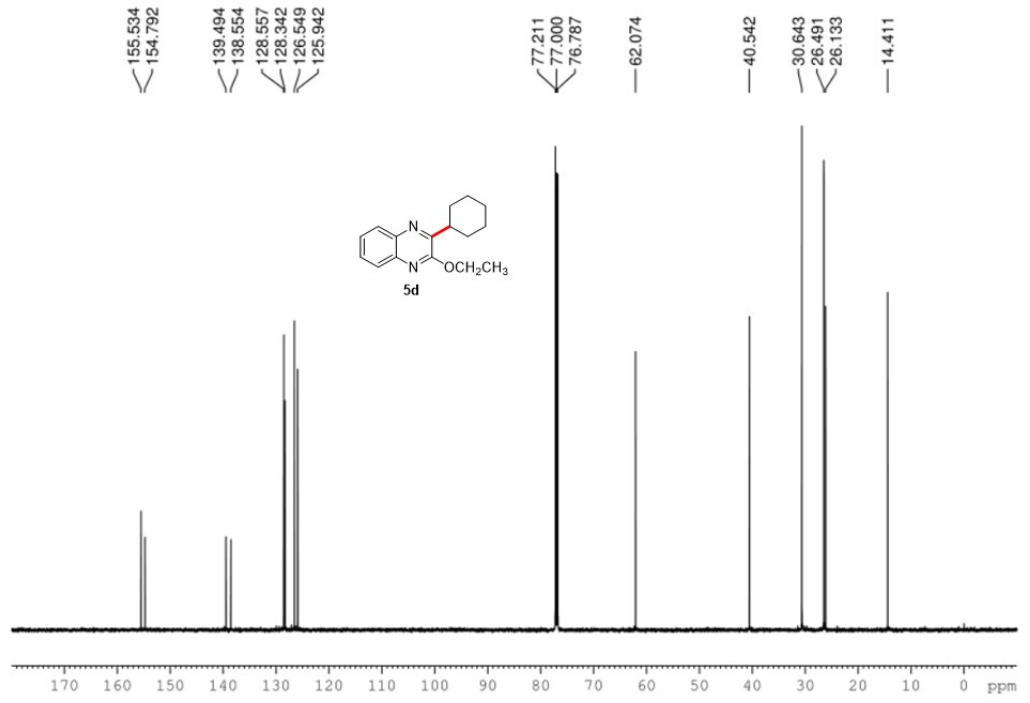
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30.643
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26.133
14.411
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OCH2CH3
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140
130
120
110
100
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80
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60
50
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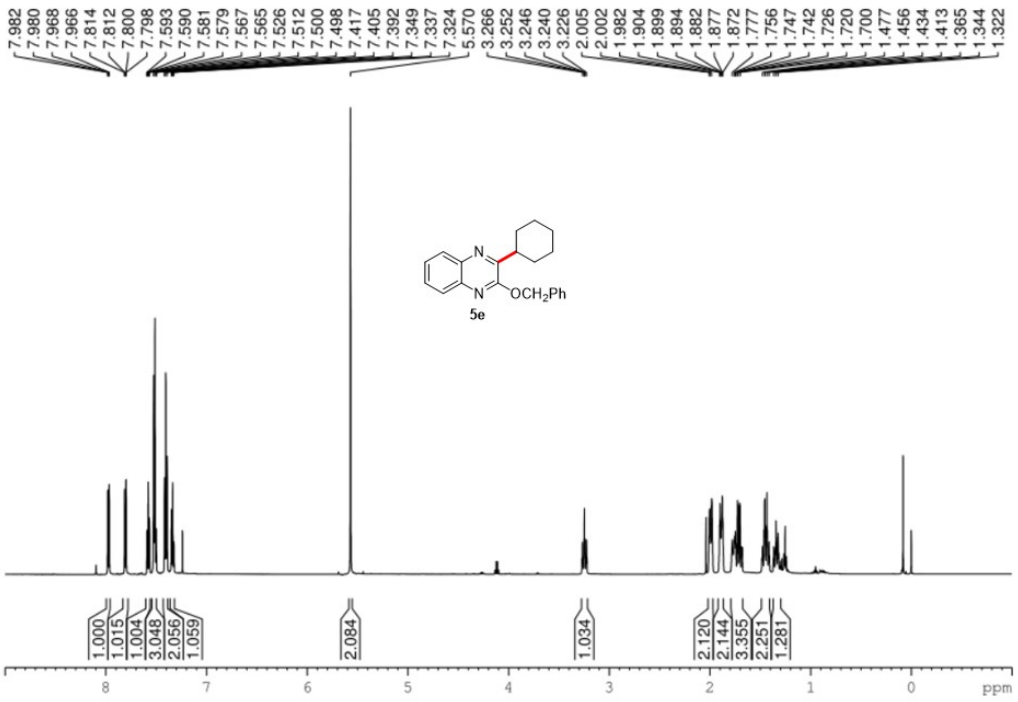
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7.567
7.565
7.526
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7.500
7.498
7.417
7.405
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7.324
5.570
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3.252
3.246
3.240
3.226
2.005
2.002
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1.904
1.899
1.894
1.882
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1.477
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1.344
1.322
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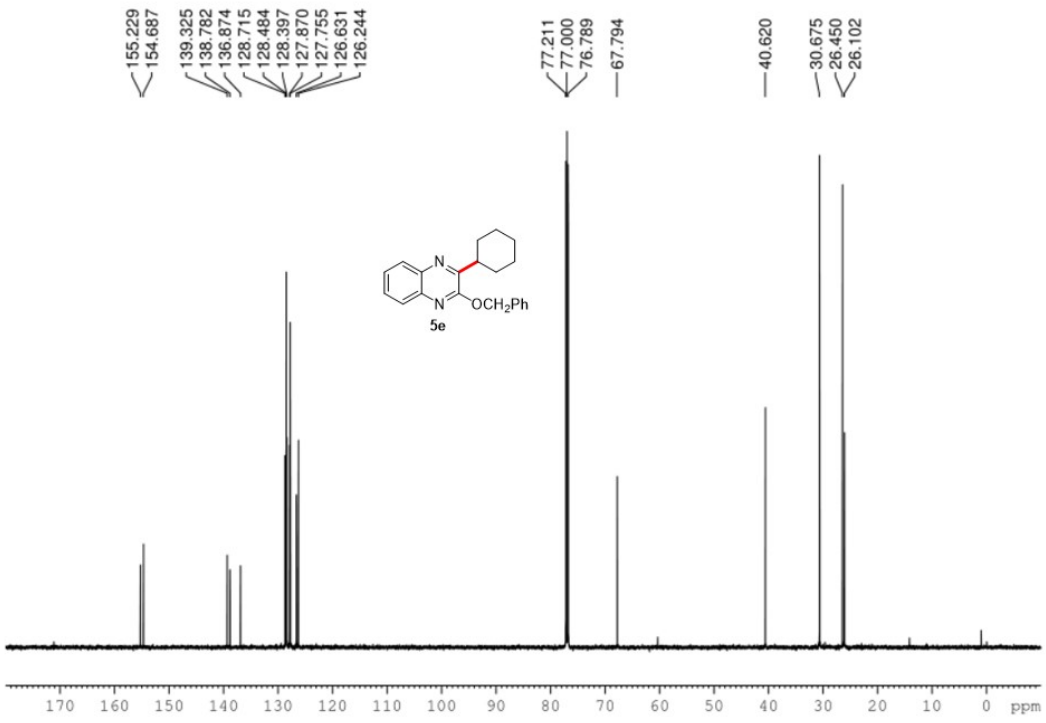
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126.244
77.211
77.000
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67.794
40.620
30.675
26.450
26.102
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N
OCH2Ph
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110
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50
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20
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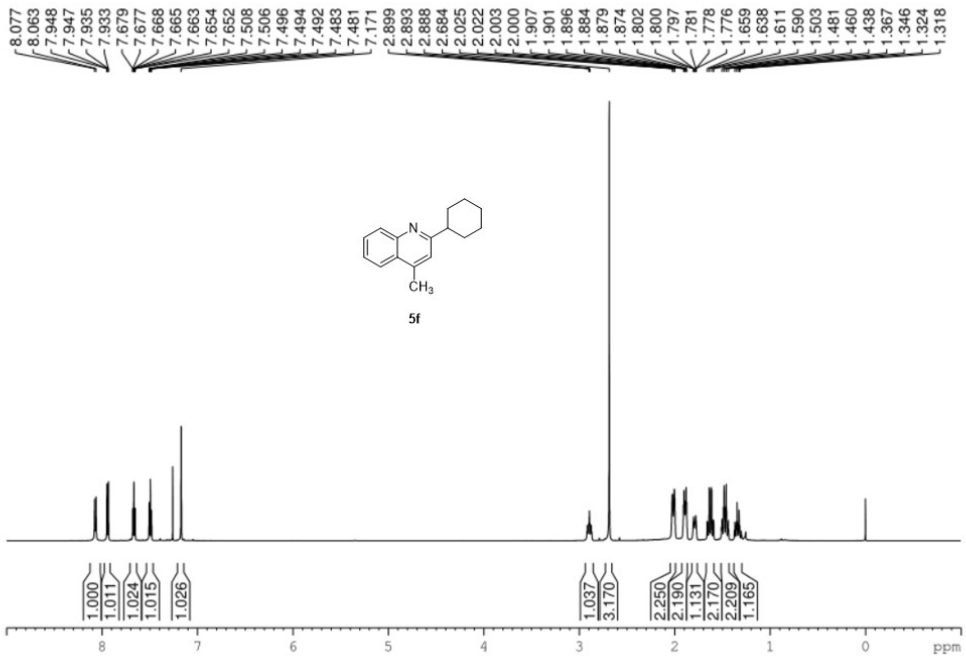
ppm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CH3
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1.024
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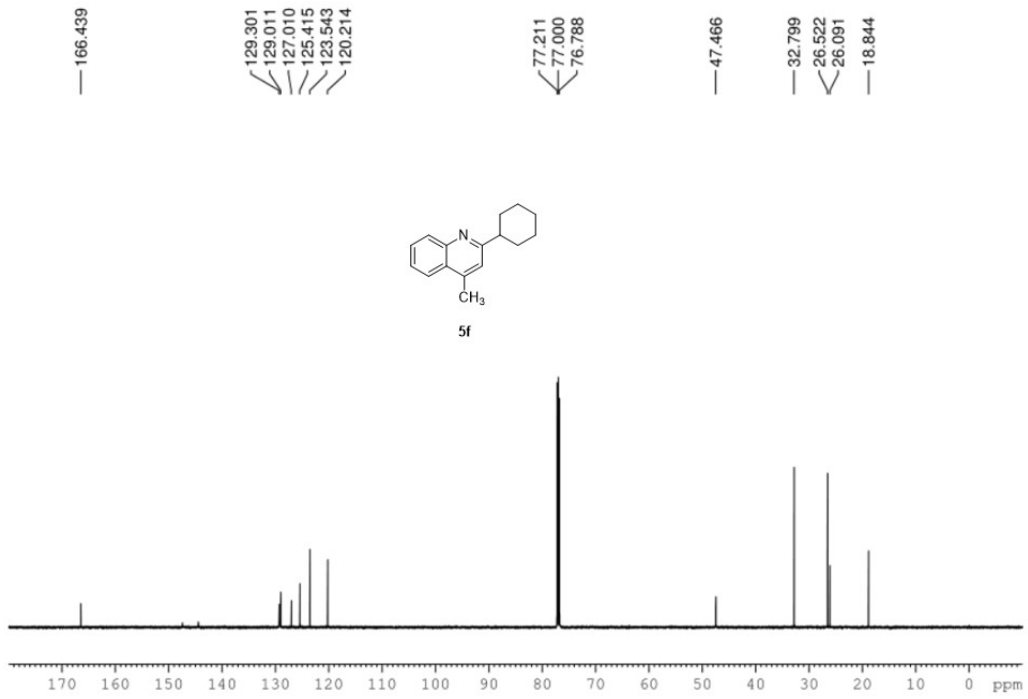
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26.091
18.844
N
CH3
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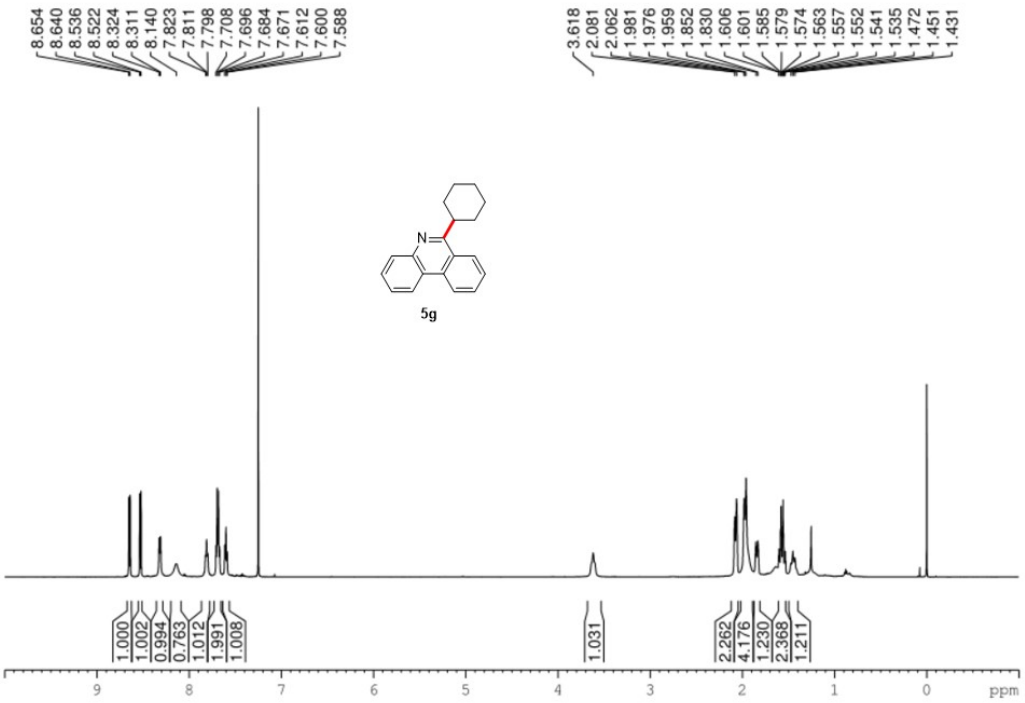
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7.823
7.811
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7.696
7.684
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7.612
7.600
7.588
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2.081
2.062
1.981
1.976
1.959
1.852
1.830
1.606
1.601
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1.579
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1.563
1.557
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1.541
1.535
1.472
1.451
1.431
N
5g
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1.002
0.994
0.763
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1.008
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6
5
4
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2
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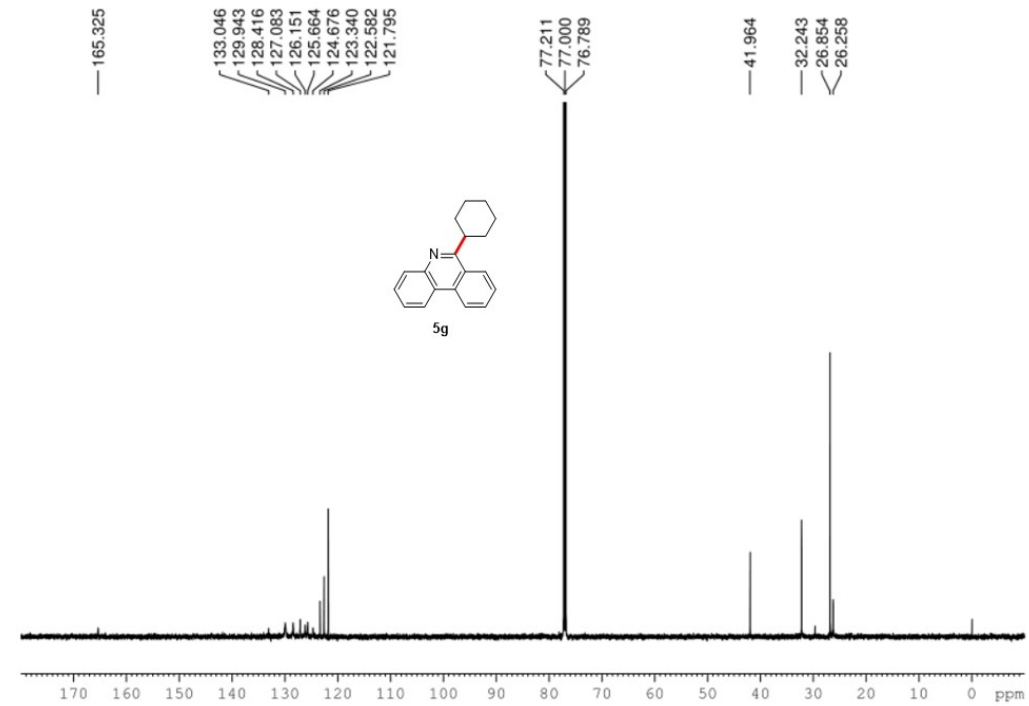
ppm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124.676
123.340
122.582
121.795
77.211
77.000
76.789
41.964
32.243
26.854
26.258
N
5g
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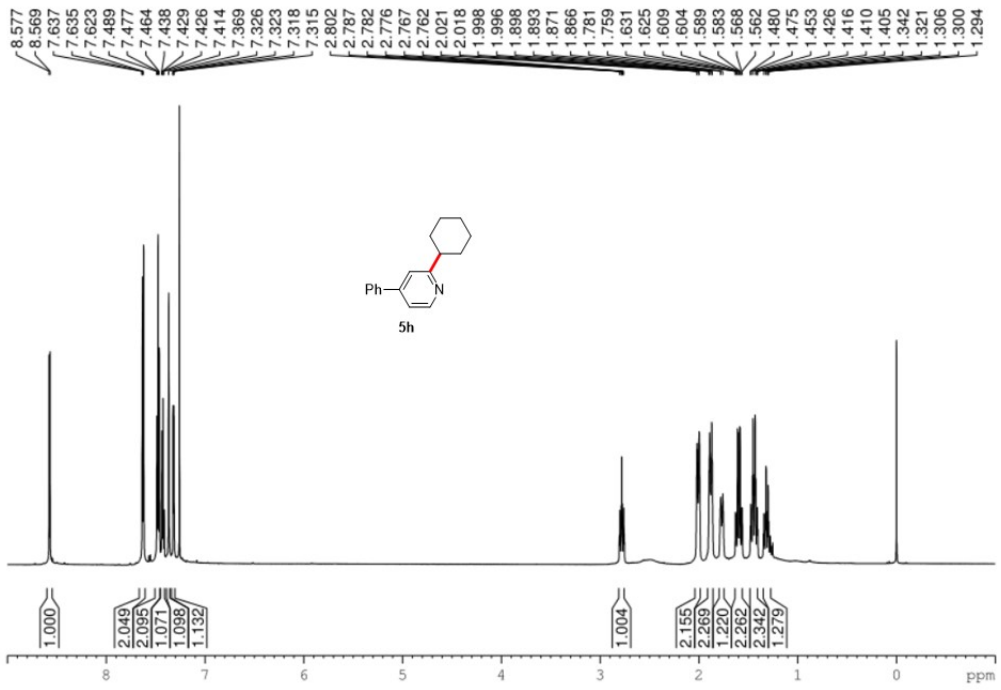
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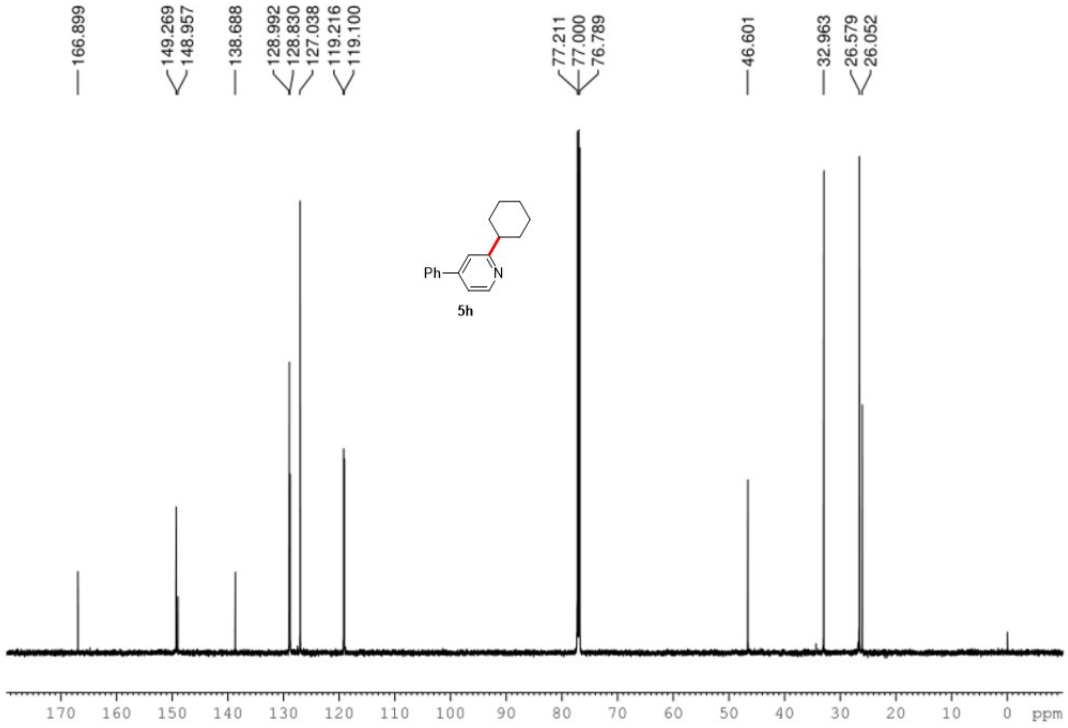
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5h
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80
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50
40
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10
0
ppm