Supporting Information

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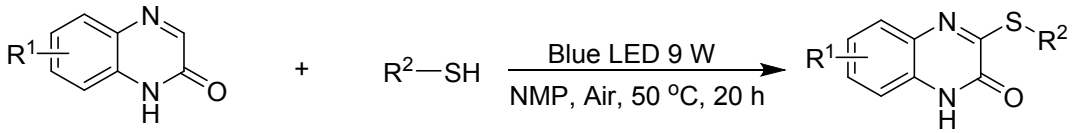
General information.

All manipulations were performed under an air atmosphere unless otherwise statement. Column chromatography was performed on silica gel (300−400 mesh). NMR spectra were obtained using a Bruker Avance 400 or 600 spectrometer (^{1}H at 400 or 600 MHz and ^{13}C at 100 or 150 MHz). Chemical shifts were reported in ppm. ^{1}H NMR spectra were referenced to DMSO (2.50 ppm), and ^{13}C-NMR spectra were referenced to DMSO (40.00 ppm). Peak multiplicities were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; m, multiplet; brs, broad singlet and J, coupling constant in Hz. High resolution mass spectra (HRMS) were recorded on the Exactive Mass Spectrometer (Agilent Technologies 6545Q-TOF LC/MS, USA) equipped with ESI ionization source. Unless stated otherwise, commercial reagents were used without further purification.

1 were prepared by reported methods.[1]

Experimental Procedures

Typical experimental procedure for the synthesis of 3 and **5.**



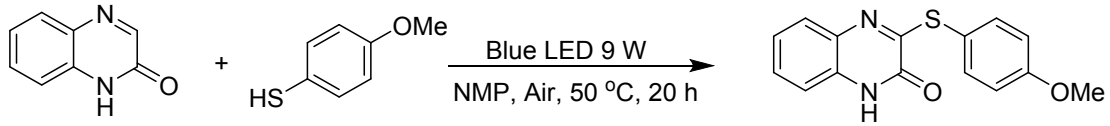
1 **2** **3** or **5**

To a solution of **1** (0.5 mmol) and **2** (1 mmol) in NMP (1.5 mL) was stirred under the irradiation of blue LEDs at 50 °C for 20 h. The mixture was diluted with EA (10 mL) and extracted with NaCl aqueous solution (10 mL). Then the organic layer was concentrated under reduced pressure, and the residue was purified by flash column chromatography to give **3** or **5**.

Photoreactor configuration

Reactions were irradiated by using a simple photoreactor consisting of a 9 W LED lamp with a magnetic stirrer, meanwhile the inside of reaction box was equipped with tin foil to reflect light. The distance between blue lamp and the reaction tube was 5 cm. And the temperature of reaction box was about 35-80 °C by measured with a standard alcohol thermometer.

Synthesis of 3a on a Gram Scale



1a
7 mmol, 1.02 g

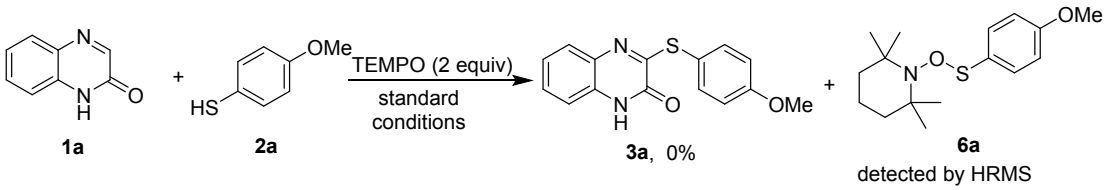
2a
14 mmol, 1.96 g

3a
56%, 1.11 g

To a solution of **1a** (7 mmol) and **2a** (14 mmol) in NMP (8 mL) was stirred under the irradiation of blue LEDs at 50 °C for 20 h. The mixture was diluted with EA (30 mL) and extracted with NaCl aqueous solution (30 mL). Then the organic layer was

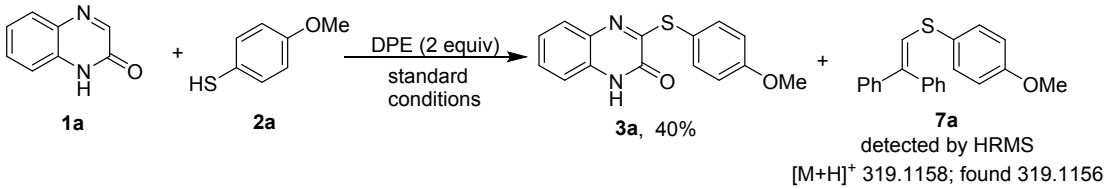
concentrated under reduced pressure, and the residue was purified by flash column chromatography to give **3a** in yield of 56%.

Controlled Experiments for Mechanism Study



To a solution of **1a** (0.5 mmol), **2a** (1 mmol) and TEMPO (1 mmol, 2 equiv) in NMP (1.5 mL) was stirred under the irradiation of blue LEDs at 50 °C for 20 h. The mixture was diluted with EA (10 mL) and extracted with NaCl aqueous solution (10 mL). Then the organic layer was concentrated under reduced pressure, and the residue was purified by flash column chromatography to give **3a** in 0% yield.

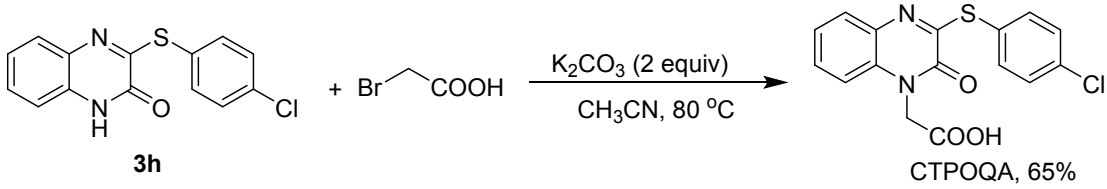
The molecular weight of **6a** is $[M+H]^+$ 296.1677, and it was detected by LC-MS.



To a solution of **1a** (0.5 mmol), **2a** (1 mmol) and 1,1-diphenylethylene (1 mmol, 2 equiv) in NMP (1.5 mL) was stirred under the irradiation of blue LEDs at 50 °C for 20 h. The mixture was diluted with EA (10 mL) and extracted with NaCl aqueous solution (10 mL). Then the organic layer was concentrated under reduced pressure, and the residue was purified by flash column chromatography to give **3a** in 40% yield.

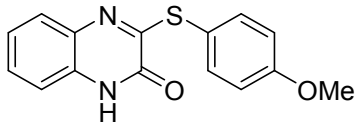
The molecular weight of **7a** is $[M+H]^+$ 319.1156, and it was detected by LC-MS.

Synthesis of bioactive quinoxalinone derivative CTPOQA

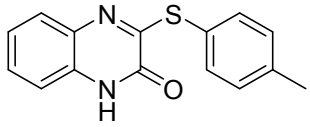


To a solution of **3h** (0.5 mmol), 2-bromoacetic acid (1 mmol) and K_2CO_3 (1 mmol, 2 equiv) in CH_3CN (2 mL) was stirred at 80 °C for 2 h. The mixture was diluted with EA (10 mL) and extracted with NaCl aqueous solution (10 mL). Then the organic layer was concentrated under reduced pressure, and the residue was purified by flash column chromatography to give **CTPOQA** in 65% yield.

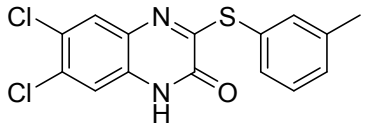
Characterization of the Compounds.



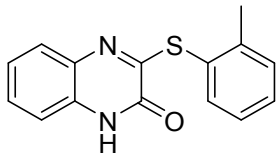
3-((4-Methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**3a**, 76%), white solid, M. P. 238-240 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.58 (s, 1H), 7.52 – 7.47 (m, 2H), 7.43 – 7.33 (m, 2H), 7.28 (dd, J = 8.1, 1.0 Hz, 1H), 7.20 – 7.15 (m, 1H), 7.08 – 7.04 (m, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 160.7, 153.2, 137.3, 132.5, 130.9, 129.0, 127.5, 123.9, 118.7, 116.0, 115.4, 55.8 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_2S$ $[M + H]^+$ 285.0692, found 285.0693.



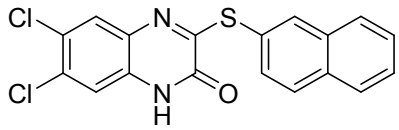
3-(*p*-Tolylthio)quinoxalin-2(1*H*)-one (**3b**, 68%), white solid, M. P. 265.5-275.5 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.75 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.36 – 7.32 (m, 1H), 7.29 (t, *J* = 7.9 Hz, 3H), 7.21 – 7.16 (m, 1H), 2.37 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.6, 153.3, 139.7, 135.7, 132.7, 131.0, 130.6, 129.3, 127.6, 125.0, 124.1, 116.2, 21.5 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2OS$ $[M + H]^+$ 269.0743, found 269.0748.



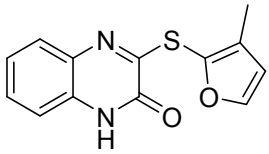
6,7-Dichloro-3-(m-tolylthio)quinoxalin-2(1*H*)-one (**3c**, 80%), white solid, M. P. 276.2-278.8 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.80 (s, 1H), 7.56 (s, 1H), 7.45 (s, 1H), 7.42 – 7.37 (m, 3H), 7.32 (d, *J* = 3.7 Hz, 1H), 2.36 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 152.9, 139.2, 135.7, 132.5, 131.9, 131.0, 130.8, 130.7, 129.7, 128.3, 127.8, 125.6, 117.2, 21.3 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{11}Cl_2N_2OS$ $[M + H]^+$ 336.9964, found 336.9965.



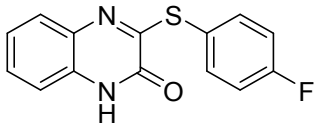
3-(*o*-Tolylthio)quinoxalin-2(1*H*)-one (**3d**, 43%), white solid, M. P. 210-211 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.76 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 4.1 Hz, 2H), 7.42 – 7.35 (m, 2H), 7.30 (t, *J* = 6.2 Hz, 2H), 7.20 – 7.15 (m, 1H), 2.33 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.6, 153.3, 151.9, 143.2, 136.8, 132.6, 131.1, 130.6, 129.1, 127.7, 127.4, 127.2, 123.9, 116.1, 20.8 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2OS$ $[M + H]^+$ 269.0743, found 269.0748.



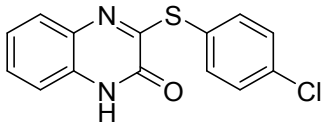
6,7-Dichloro-3-(naphthalen-2-ylthio)quinoxalin-2(1*H*)-one (**3e**, 82%), yellow solid, M. P. 301-303 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 8.24 (s, 1H), 8.01 (t, *J* = 9.3 Hz, 3H), 7.62 (dd, *J* = 13.3, 7.6 Hz, 3H), 7.48 (d, *J* = 22.9 Hz, 2H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 152.9, 136.2, 134.7, 133.7, 133.4, 132.1, 130.8, 130.1, 129.1, 128.3, 128.2, 127.8, 127.2, 125.7, 125.7, 125.4, 117.2 ppm; HRMS (ESI) m/z calcd for $C_{18}H_{11}Cl_2N_2OS$ $[M + H]^+$ 372.9964, found 372.9963.



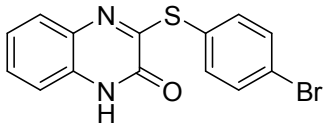
3-((3-Methylfuran-2-yl)thio)quinoxalin-2(1*H*)-one (**3f**, 20%), yellow solid, M. P. 270-272 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 7.72 (d, *J* = 1.9 Hz, 1H), 7.48 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.29 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.24 – 7.19 (m, 1H), 6.56 (d, *J* = 1.9 Hz, 1H), 2.28 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.4, 156.5, 153.3, 142.2, 132.6, 130.9, 129.2, 127.6, 124.0, 116.1, 116.0, 104.3, 12.4 ppm; HRMS (ESI) m/z calcd for C13H11N2O2S $[M + H]^+$ 259.0536, found 259.0535.



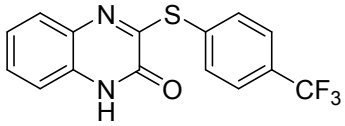
3-((4-Fluorophenyl)thio)quinoxalin-2(1*H*)-one (**3g**, 72%), white solid, M. P. 284-286 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.64 (s, 1H), 7.64 (dd, *J* = 8.4, 5.6 Hz, 2H), 7.44 – 7.38 (m, 1H), 7.38 – 7.31 (m, 3H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.21 – 7.16 (m, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ163.3 (d, *J* = 247.0 Hz), 160.3, 153.2, 138.1 (d, *J* = 8.7 Hz), 132.5, 131.0, 129.3, 127.6, 124.3 (d, *J* = 3.3 Hz), 124.0, 116.9 (d, *J* = 22.0 Hz), 116.1 ppm; HRMS (ESI) m/z calcd for $C_{14}H_{10}FN_2OS$ $[M + H]^+$ 273.0492, found 273.0496.



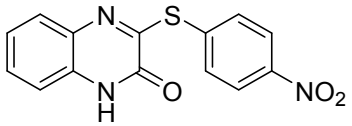
3-((4-Chlorophenyl)thio)quinoxalin-2(1*H*)-one (**3h**, 73%), white solid, M. P. 254-255.6 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 (s, 1H), 7.60 (dd, *J* = 22.8, 8.5 Hz, 4H), 7.42 (dd, *J* = 16.8, 8.1 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.8, 153.1, 137.3, 134.8, 132.4, 131.0, 129.8, 129.3, 127.7, 127.6, 124.0, 116.1 ppm; HRMS (ESI) m/z calcd for $C_{14}H_{10}ClN_2OS$ $[M + H]^+$ 289.0197, found 289.0196.



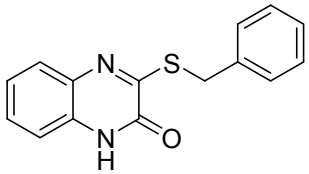
3-((4-Bromophenyl)thio)quinoxalin-2(1*H*)-one (**3i**, 75%), white solid, M. P. >300 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.74 (s, 1H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 7.7 Hz, 2H), 7.46 – 7.30 (m, 3H), 7.20 (t, *J* = 7.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.7, 153.1, 137.5, 132.7, 132.4, 131.0, 129.3, 128.2, 127.6, 124.0, 123.5, 116.1 ppm; HRMS (ESI) m/z calcd for $C_{14}H_{10}BrN_2OS$ $[M + H]^+$ 332.9692, found 332.9691.



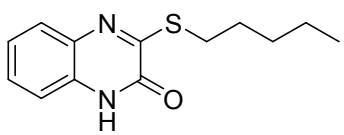
3-((4-(Trifluoromethyl)phenyl)thio)quinoxalin-2(1*H*)-one (**3j**, 10%), white solid, M. P. 254-256 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.76 (s, 1H), 7.87 (s, 4H), 7.47 – 7.39 (m, 2H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.22 (dd, *J* = 11.2, 4.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.2, 153.1, 135.9, 134.5 (q, *J* = 1.0 Hz), 132.4, 131.2, 130.0 (q, *J* = 32.0 Hz), 129.5, 127.7, 126.3 (q, *J* = 3.7 Hz), 123.20 (q, *J* = 274.0 Hz), 123.19, 116.2 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{10}F_3N_2OS$ $[M + H]^+$ 323.0460, found 323.0458.



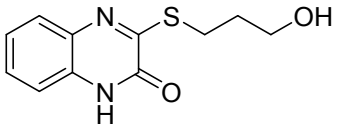
3-((4-Nitrophenyl)thio)quinoxalin-2(1*H*)-one (**3k**, 8%,), yellow solid, M. P. 295-297 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.74 (s, 1H), 8.35 – 8.30 (m, 2H), 7.98 – 7.92 (m, 2H), 7.46 (ddd, *J* = 10.2, 6.4, 2.2 Hz, 2H), 7.32 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.26 – 7.21 (m, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.7, 153.1, 148.1, 138.1, 135.9, 132.3, 131.2, 129.7, 127.7, 124.3, 124.1, 116.2 ppm; HRMS (ESI) m/z calcd for $C_{14}H_{10}N_3O_3S$ $[M + H]^+$ 300.0437, found 300.0439.



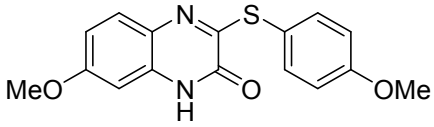
3-(Benzylthio)quinoxalin-2(1*H*)-one (**3l**, 75%), white solid, M. P. 245-247 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.53 (s, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.3 Hz, 2H), 7.45 – 7.38 (m, 1H), 7.34 – 7.19 (m, 5H), 4.38 (s, 2H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.1, 153.3, 138.0, 132.6, 130.6, 129.7, 128.9, 127.6, 127.3, 124.0, 116.1, 33.2 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2OS$ $[M + H]^+$ 269.0743, found 269.0740.



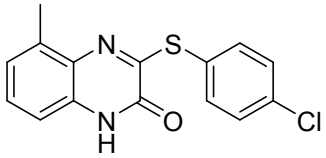
3-(Pentylthio)quinoxalin-2(1*H*)-one (**3m**, 66%), yellow solid, M. P. 165.7-167.5 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.47 (s, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.27 (dd, *J* = 12.1, 4.4 Hz, 2H), 3.14 – 3.07 (m, 2H), 1.73 – 1.61 (m, 2H), 1.39 (ddd, *J* = 20.7, 11.4, 7.3 Hz, 4H), 0.89 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.9, 153.4, 132.7, 130.4, 128.7, 127.2, 124.0, 116.1, 31.1, 28.9, 28.3, 22.1, 14.3 ppm; HRMS (ESI) m/z calcd for $C_{13}H_{17}N_2OS$ $[M + H]^+$ 249.1056, found 249.1060.



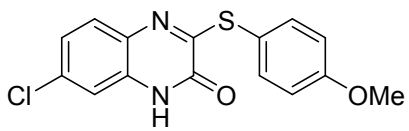
3-((3-Hydroxypropyl)thio)quinoxalin-2(1*H*)-one (**3n**, 57%), white solid, M. P. 195.5-196.6 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.47 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.27 (t, *J* = 8.6 Hz, 2H), 4.61 (s, 1H), 3.53 (t, *J* = 5.7 Hz, 2H), 3.15 (t, *J* = 7.2 Hz, 2H), 1.88 – 1.77 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.0, 153.4, 132.7, 130.4, 128.7, 127.3, 124.0, 116.1, 60.1, 31.8, 26.1 ppm; HRMS (ESI) m/z calcd for $C_{11}H_{13}N_2O_2S$ $[M + H]^+$ 237.0692, found 237.0696.



7-Methoxy-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5a**, 53%), white solid, M. P. 238.6-240 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.51 (s, 1H), 7.51 – 7.48 (m, 2H), 7.21 (d, *J* = 8.9 Hz, 1H), 7.08 (d, *J* = 2.1 Hz, 1H), 7.05 (dd, *J* = 9.3, 2.4 Hz, 2H), 6.82 (d, *J* = 2.7 Hz, 1H), 3.83 (s, 3H), 3.73 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 160.7, 156.0, 152.7, 137.3, 133.2, 124.9, 118.7, 118.3, 116.9, 115.5, 109.2, 56.0, 55.8 ppm; HRMS (ESI) m/z calcd for $C_{16}H_{15}N_2O_3S$ $[M + H]^+$ 315.0798, found 315.0802.

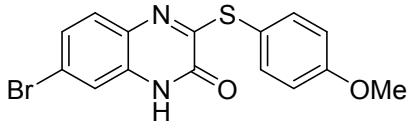


3-((4-Chlorophenyl)thio)-5-methylquinoxalin-2(1*H*)-one (**5b**, 47%), white solid, M. P. >300 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 7.1 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 1H), 7.11 (t, *J* = 7.7 Hz, 1H), 2.42 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.25, 153.70, 137.31, 134.79, 132.57, 130.61, 129.77, 129.47, 127.73, 125.72, 124.86, 123.66, 17.43 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{11}ClN_2OS$ $[M + H]^+$ 303.0353, found 303.0357.

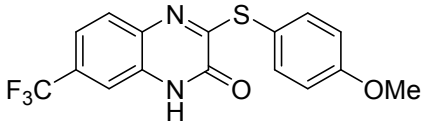


7-Chloro-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5c**, 62%), white solid, M. P. 206.5-208.7 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.75 (s, 1H), 7.51 – 7.42 (m,

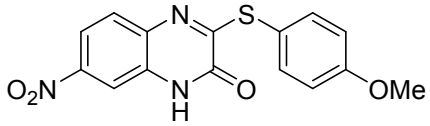
3H), 7.36 (d, *J* = 2.3 Hz, 1H), 7.31 (d, *J* = 8.7 Hz, 1H), 7.10 – 7.04 (m, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 160.8, 153.0, 137.2, 133.1, 130.0, 128.8, 127.6, 126.4, 118.4, 117.7, 115.5, 55.8 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{12}ClN_2O_2S$ $[M + H]^+$ 319.0303, found 319.0307.



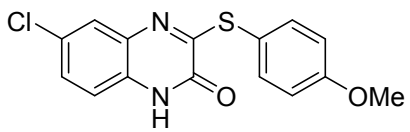
7-Bromo-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5d**, 65%), white solid, M. P. 260-262 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.53 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.49 (s, 1H), 7.48 – 7.45 (m, 2H), 7.21 (d, *J* = 8.7 Hz, 1H), 7.06 (t, *J* = 5.8 Hz, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 160.8, 153.3, 137.2, 133.5, 131.4, 130.7, 129.3, 118.5, 118.2, 115.4, 115.1, 55.8, ppm; HRMS (ESI) m/z calcd for $C_{15}H_{12}BrN_2O_2S$ $[M + H]^+$ 362.9797, found 362.9800.



3-((4-Methoxyphenyl)thio)-7-(trifluoromethyl)quinoxalin-2(1*H*)-one (**5e**, 67%), white solid, M. P. 248.3-250 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.89 (s, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.59 (s, 1H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.3 Hz, 1H), 7.09 (d, *J* = 8.2 Hz, 2H), 3.84 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.6, 160.9, 153.1, 137.3, 134.5, 131.2, 128.6, 128.3 (q, *J* = 32.5 Hz), 124.3 (q, *J* = 272.7 Hz), 120.1 (q, *J* =3.3 Hz), 118.2, 115.5, 113.2 (q, *J* = 4.4 Hz), 55.8 ppm; HRMS (ESI) m/z calcd for $C_{16}H_{12}F_3N_2O_2S$ $[M + H]^+$ 353.0566, found 353.0572.

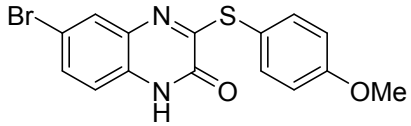


3-((4-Methoxyphenyl)thio)-7-nitroquinoxalin-2(1*H*)-one (**5f**, 49%), yellow solid, M. P. 266-267.8 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.89 (s, 1H), 8.08 (d, *J* = 2.4 Hz, 1H), 7.95 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.52 (dd, *J* = 8.8, 7.3 Hz, 3H), 7.09 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 166.0, 161.0, 153.1, 146.1, 137.2, 136.1, 131.3, 128.5, 118.4, 117.9, 115.6, 111.7, 55.8 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{12}N_3O_4S$ $[M + H]^+$ 330.0543, found 330.0547.

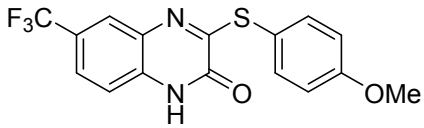


6-Chloro-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5g**, 65%), yellow solid, M. P. 262-264 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 (s, 1H), 7.52 – 7.46 (m, 2H), 7.36 (d, *J* = 8.6 Hz, 1H), 7.27 (d, *J* = 2.2 Hz, 1H), 7.20 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.09 – 7.05 (m, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 160.8, 153.0, 137.3, 132.8, 132.0, 131.3, 129.1, 123.9, 118.4, 115.5, 115.3, 55.8 ppm; HRMS

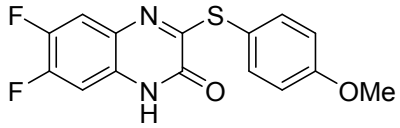
(ESI) m/z calcd for $C_{15}H_{12}ClN_2O_2S$ $[M + H]^+$ 319.0303, found 319.0307.



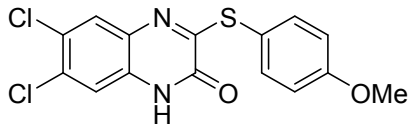
6-Bromo-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5h**, 68%), yellow solid, M. P. 263.4-264.4 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (s, 1H), 7.48 (d, *J* = 7.8 Hz, 2H), 7.40 (s, 1H), 7.27 (t, *J* = 7.2 Hz, 2H), 7.05 (d, *J* = 7.9 Hz, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.7, 160.8, 153.0, 137.2, 132.3, 131.6, 129.2, 126.7, 121.2, 118.4, 118.3, 115.4, 55.8 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{12}BrN_2O_2S$ $[M + H]^+$ 362.9797, found 362.9800.



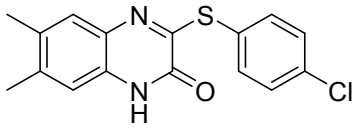
3-((4-Methoxyphenyl)thio)-6-(trifluoromethyl)quinoxalin-2(1*H*)-one (**5i**, 66%), white solid, M. P. 222.8-225 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.79 (s, 1H), 7.60 – 7.42 (m, 5H), 7.08 (d, *J* = 8.6 Hz, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.3, 160.8, 153.3, 137.2, 133.9, 131.9, 125.1 (q, *J* = 3.7 Hz), 124.5 (q, *J* = 271.7 Hz), 124.3 (q, *J* =3.9 Hz), 124.2 (q, *J* = 33.2 Hz), 118.2, 117.3, 115.5, 55.8 ppm; HRMS (ESI) m/z calcd for $C_{16}H_{12}F_3N_2O_2S$ $[M + H]^+$ 353.0566, found 353.0573.



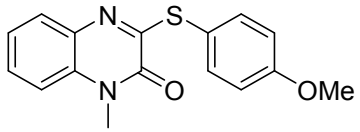
6,7-Difluoro-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5j**, 67%), white solid, M. P. 258.6-260 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.67 (s, 1H), 7.50 – 7.40 (m, 3H), 7.20 (dd, *J* = 11.0, 7.7 Hz, 1H), 7.09 – 7.02 (m, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.0, 160.8, 152.9, 149.4 (dd, *J* = 13.9, 83.1 Hz), 144.4 (dd, *J* = 14.5, 87 Hz), 137.2, 128.6 (dd, *J* =2.4, 10.1 Hz), 125.4 (d, *J* = 9 Hz), 118.3, 115.5, 115.3 (d, *J* = 18.8 Hz), 103.9 (d, *J* = 21.8 Hz), 55.8 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{11}F_2N_2O_2S$ $[M + H]^+$ 321.0504, found 321.0509.



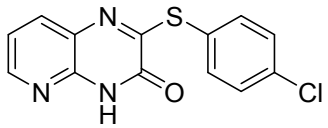
6,7-Dichloro-3-((4-methoxyphenyl)thio)quinoxalin-2(1*H*)-one (**5k**, 80%), yellow solid, M. P. 278-280 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.62 (s, 1H), 7.53 (s, 1H), 7.48 (d, *J* = 8.7 Hz, 2H), 7.06 (d, *J* = 8.7 Hz, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.3, 160.9, 153.0, 137.2, 132.0, 130.9, 130.8, 128.3, 125.7, 118.2, 117.1, 115.6, 55.9 ppm; HRMS (ESI) m/z calcd for $C_{15}H_{11}Cl_2N_2O_2S$ $[M + H]^+$ 352.9913, found 352.9914.



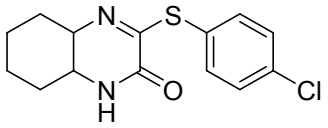
3-((4-Chlorophenyl)thio)-6,7-dimethylquinoxalin-2(1*H*)-one (**5l**, 81%), white solid, M. P. >300 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.54 (s, 1H), 7.63 – 7.55 (m, 4H), 7.20 (s, 1H), 7.05 (s, 1H), 2.27 (s, 3H), 2.21 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.2, 153.1, 138.7, 137.3, 134.7, 132.7, 131.0, 129.7, 128.9, 127.9, 127.6, 116.1, 20.1, 19.2 ppm; HRMS (ESI) m/z calcd for $C_{16}H_{14}ClN_2OS$ $[M + H]^+$ 317.0510, found 317.0513.



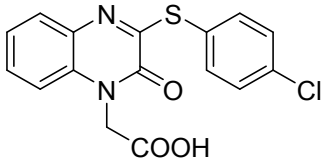
3-((4-Methoxyphenyl)thio)-1-methylquinoxalin-2(1*H*)-one (**5m**, 47%), white solid, M. P. 187-188 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.56 – 7.47 (m, 4H), 7.39 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.27 (ddd, *J* = 8.2, 6.7, 1.8 Hz, 1H), 7.10 – 7.05 (m, 2H), 3.83 (s, 3H), 3.66 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.7, 159.8, 152.8, 137.3, 132.9, 132.6, 132.2, 129.3, 128.2, 124.2, 118.9, 115.4, 55.8, 29.8 ppm; HRMS (ESI) m/z calcd for $C_{16}H_{15}N_2O_2S$ $[M + H]^+$ 299.0849, found 299.0853.



2-((4-Chlorophenyl)thio)pyrido[2,3-b]pyrazin-3(4*H*)-one (**5n**, 53%), yellow solid, M. P. 270.6-272 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.11 (s, 1H), 8.42 (dd, *J* = 4.7, 1.5 Hz, 1H), 7.82 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.58 (d, *J* = 8.6 Hz, 2H), 7.26 (dd, *J* = 8.0, 4.7 Hz, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 154.6, 149.0, 143.4, 137.3, 135.3, 135.0, 129.8, 127.7, 127.3, 120.4 ppm; HRMS (ESI) m/z calcd for $C_{13}H_9ClN_3OS$ $[M + H]^+$ 290.0149, found 290.0151.



3-((4-Chlorophenyl)thio)-4a,5,6,7,8,8a-hexahydroquinoxalin-2(1*H*)-one (**5o**, 33%), white solid, M. P. 209-211 °C, ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (s, 1H), 7.47 (s, 4H), 3.12 – 3.00 (m, 2H), 1.90 (dd, *J* = 24.3, 11.6 Hz, 2H), 1.65 (d, *J* = 8.2 Hz, 2H), 1.27 – 1.15 (m, 4H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 156.3, 136.9, 134.2, 129.4, 128.4, 63.6, 54.2, 32.0, 30.4, 25.0, 23.6 ppm; HRMS (ESI) m/z calcd for $C_{14}H_{16}ClN_2OS$ $[M + H]^+$ 295.0666, found 295.0668.



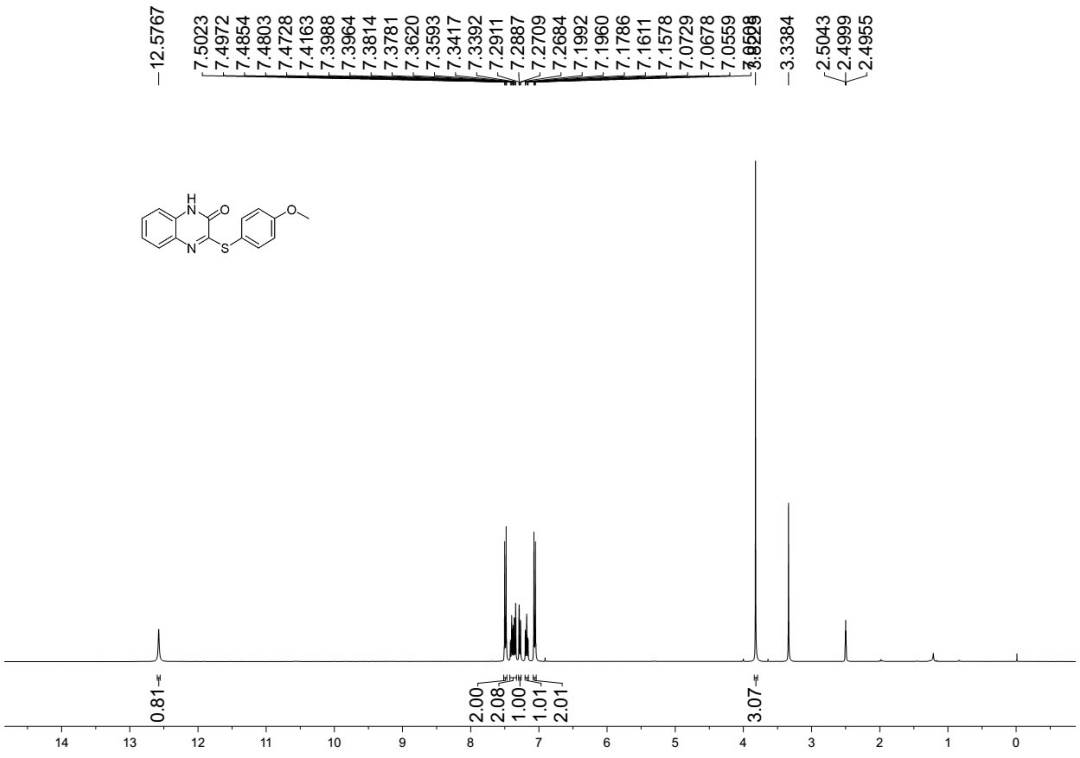
2-(3-((4-Chlorophenyl)thio)-2-oxoquinoxalin-1(2*H*)-yl)acetic acid[2] (65%), white solid, M. P. 279-281 ^{o}C, ^{1}H NMR (400 MHz, DMSO) δ 7.66 – 7.62 (m, 2H), 7.61 – 7.57 (m, 2H), 7.45 (dd, *J* = 11.3, 4.2 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 4.52 (s, 2H) ppm; ^{13}C NMR (100 MHz, DMSO) δ 167.6, 158.8, 152.3, 137.4, 134.8, 1328, 132.5, 129.8, 129.2, 128.1, 128.0, 123.6, 116.1, 47.5 ppm; HRMS (ESI) m/z calcd for $C_{16}H_{12}ClN_2O_3S$ $[M + H]^+$ 347.0252, found 347.0257.

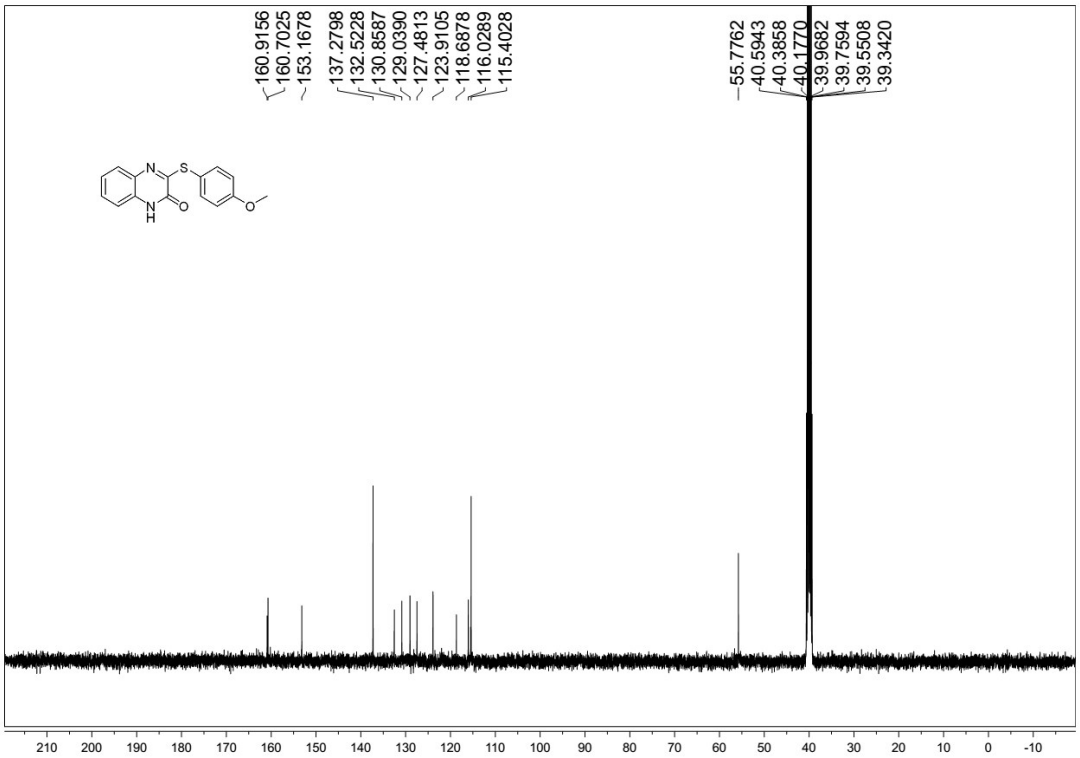
References

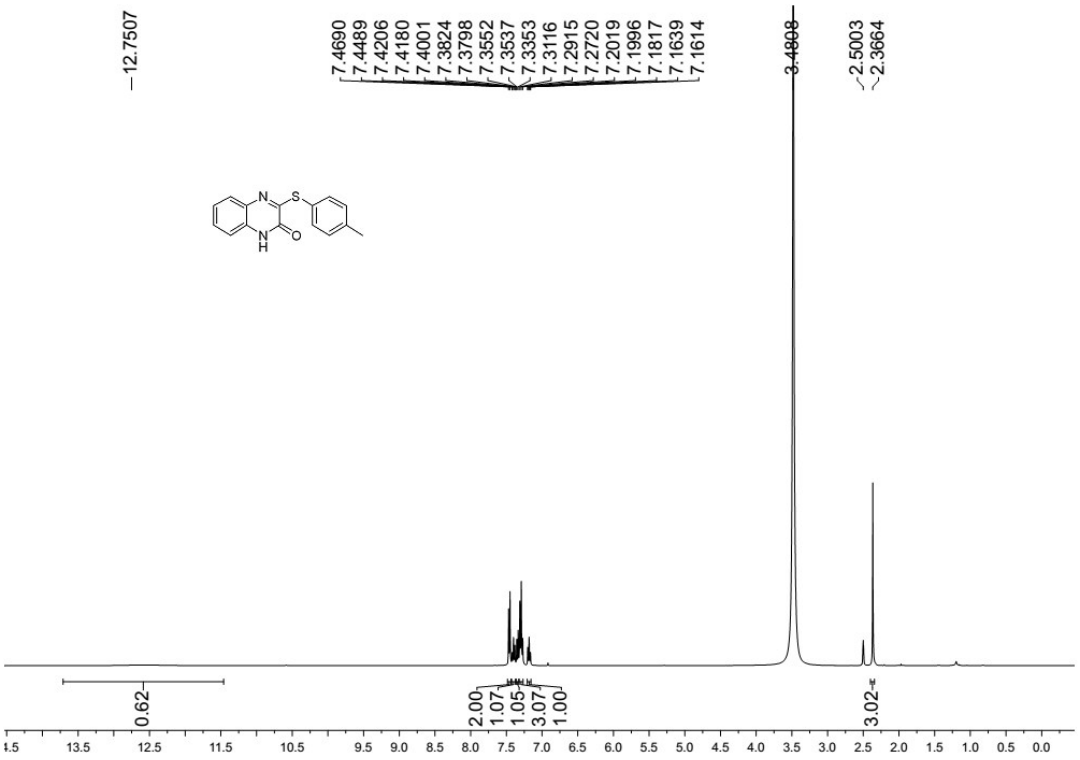
[1] A. Carrer, J.-D. Brion, S.Messaoudi, and M. Alami, *Org. Lett.*, 2013, **15**, 5606–5609.

[2] X. Y. Qin, X. Hao, H. Han, S. J. Zhu, Y. C. Yang, B. B. Wu, S. Hussain, S. Parveen, C. J. Jing, B. Ma, and C. J. Zhu, *J. Med. Chem*., 2015, **58**, 1254−1267.

Copies of ^{1}H NMR and ^{13}C NMR Spectra of Products



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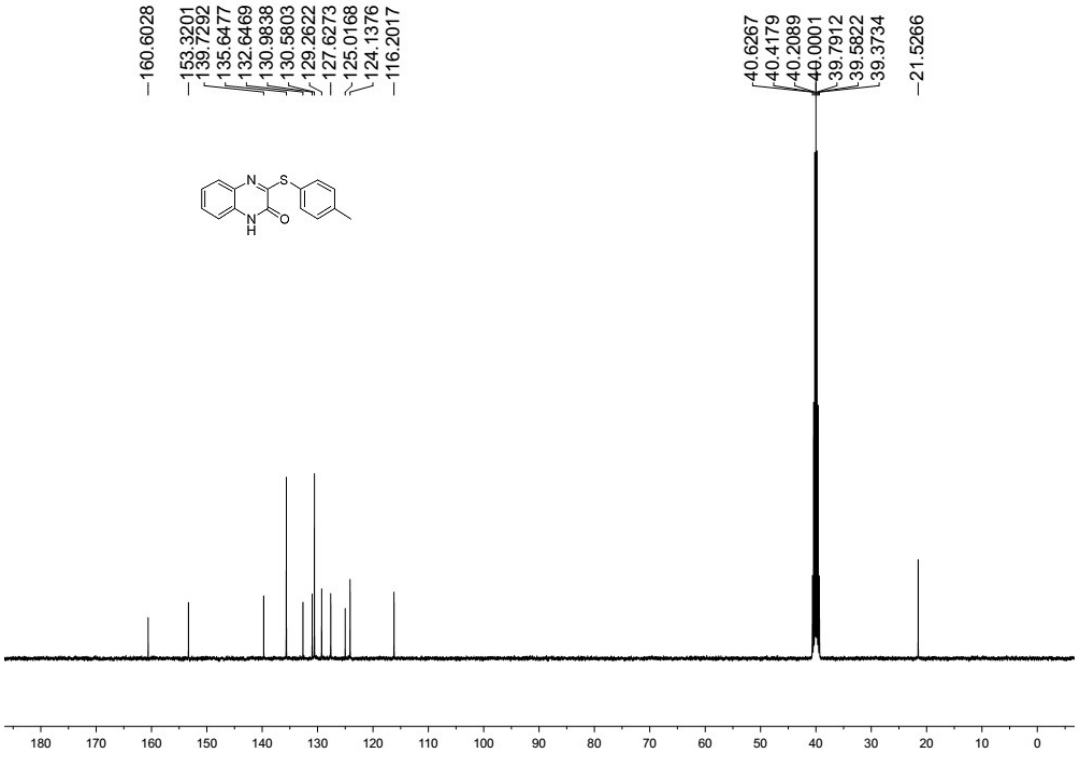
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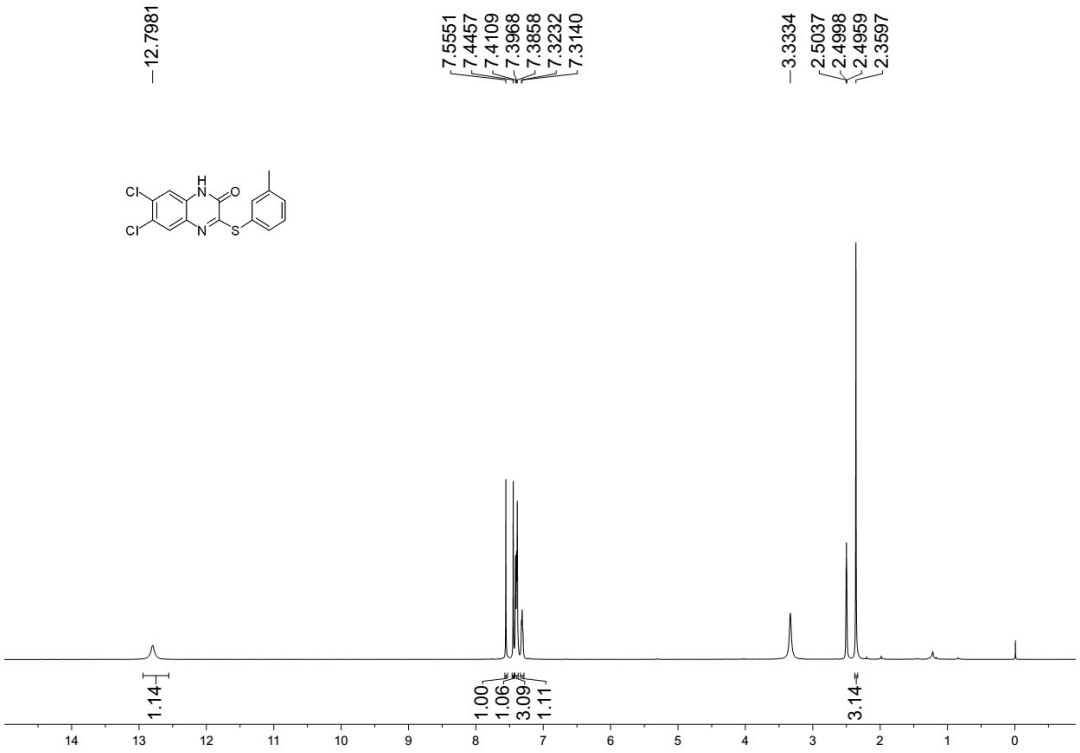
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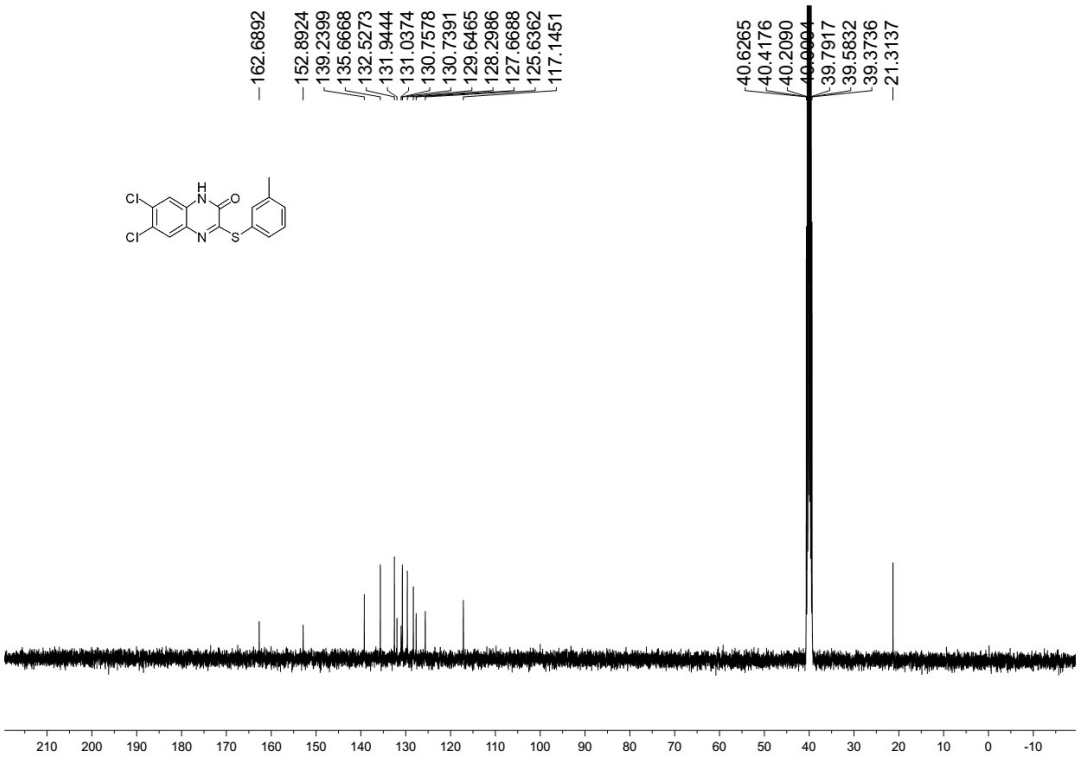
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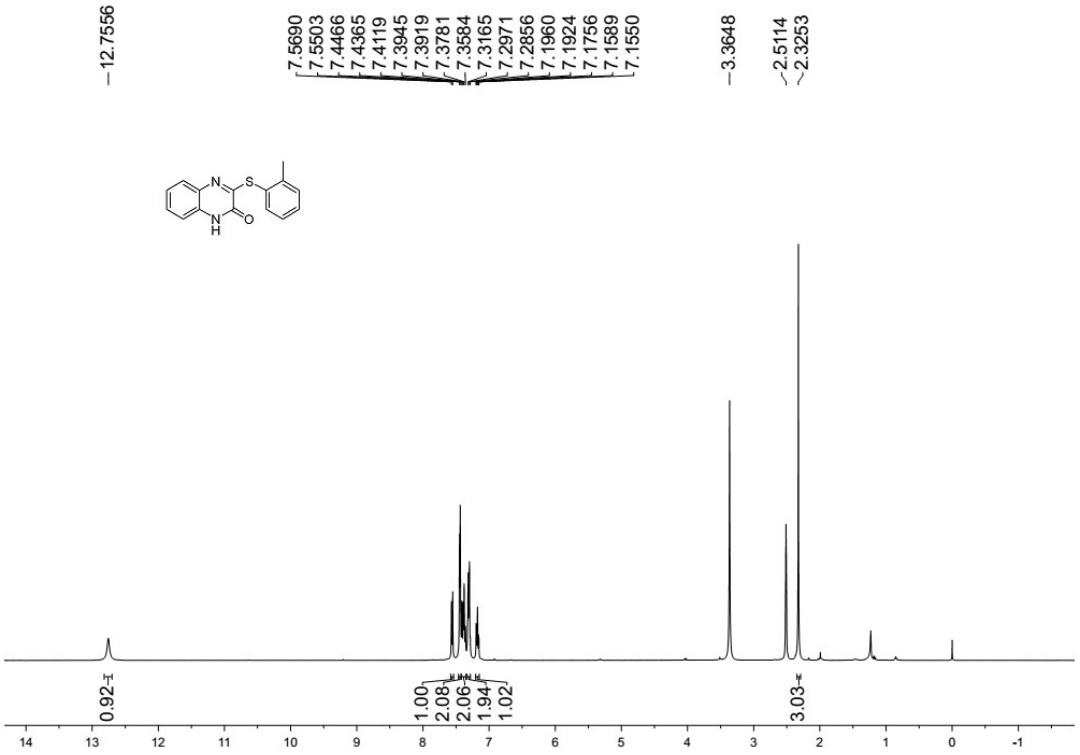
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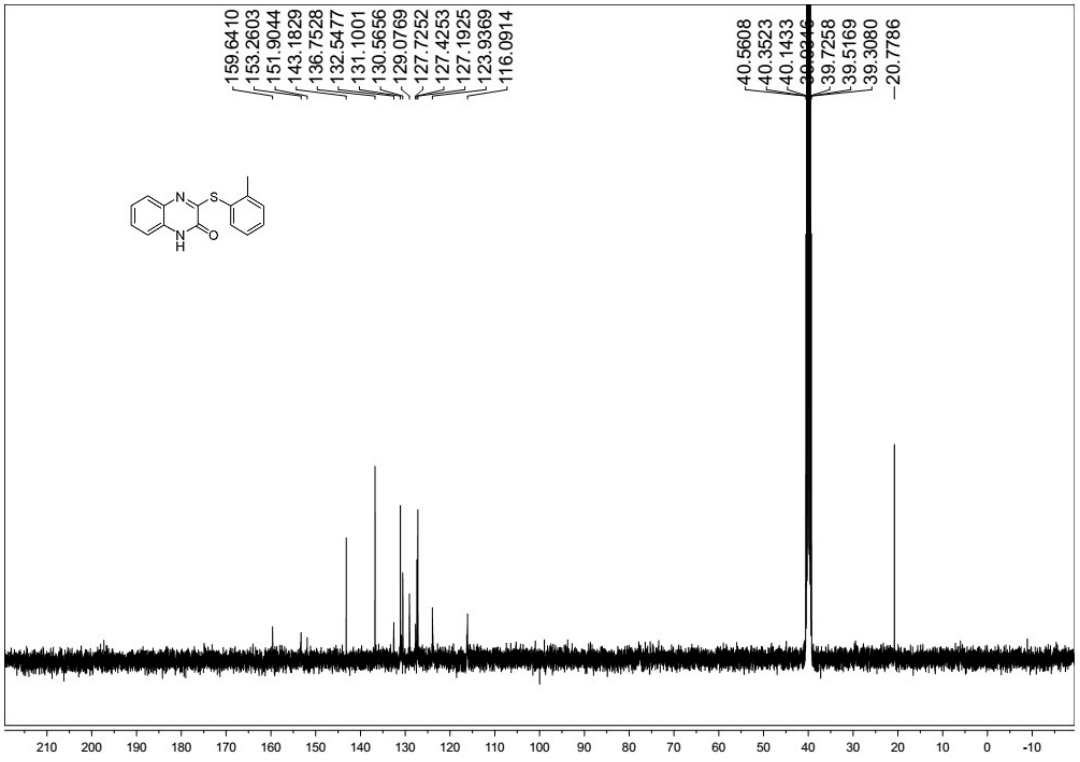
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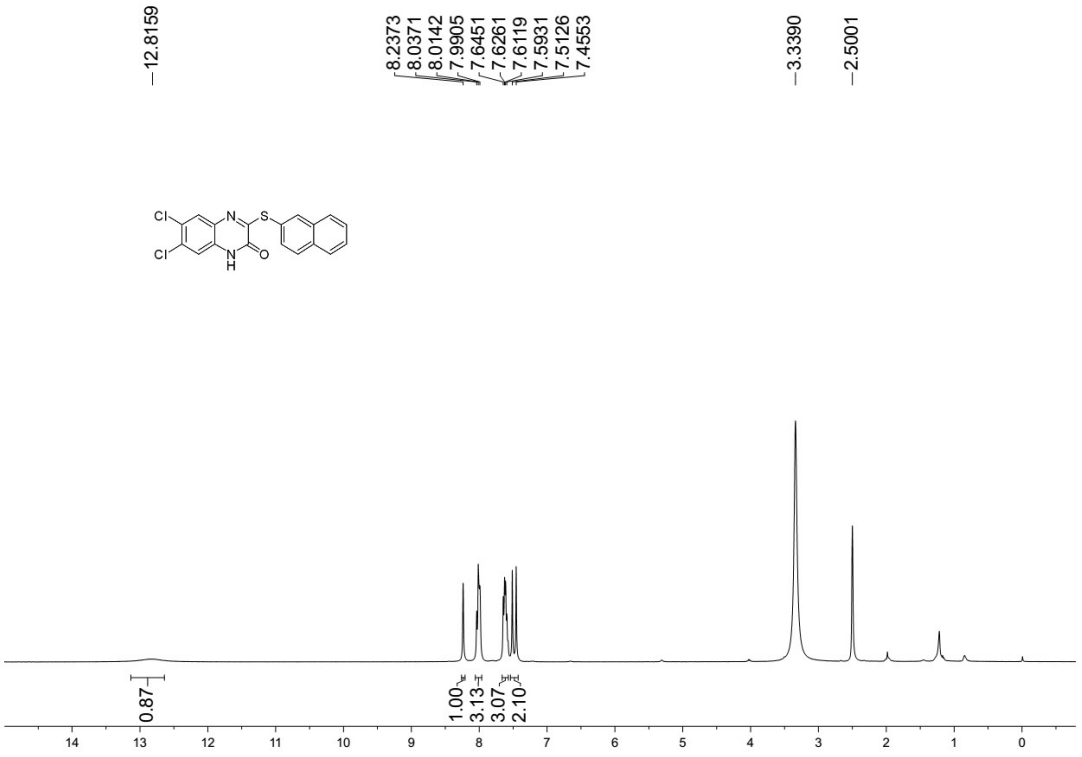
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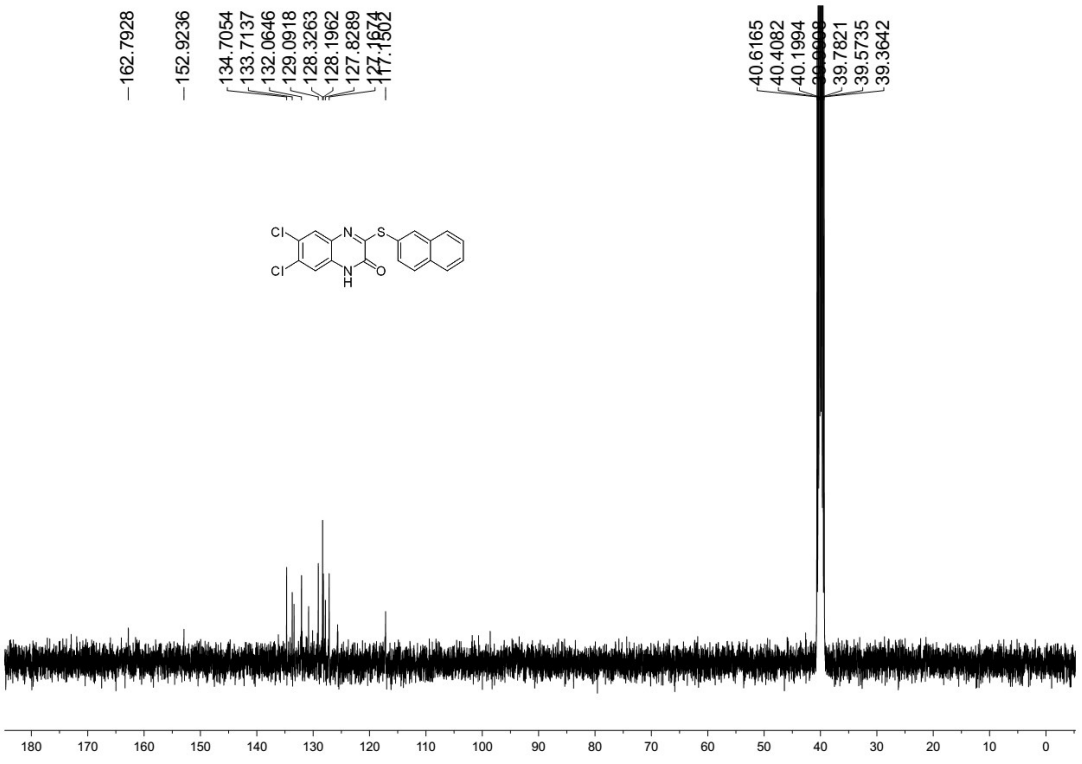
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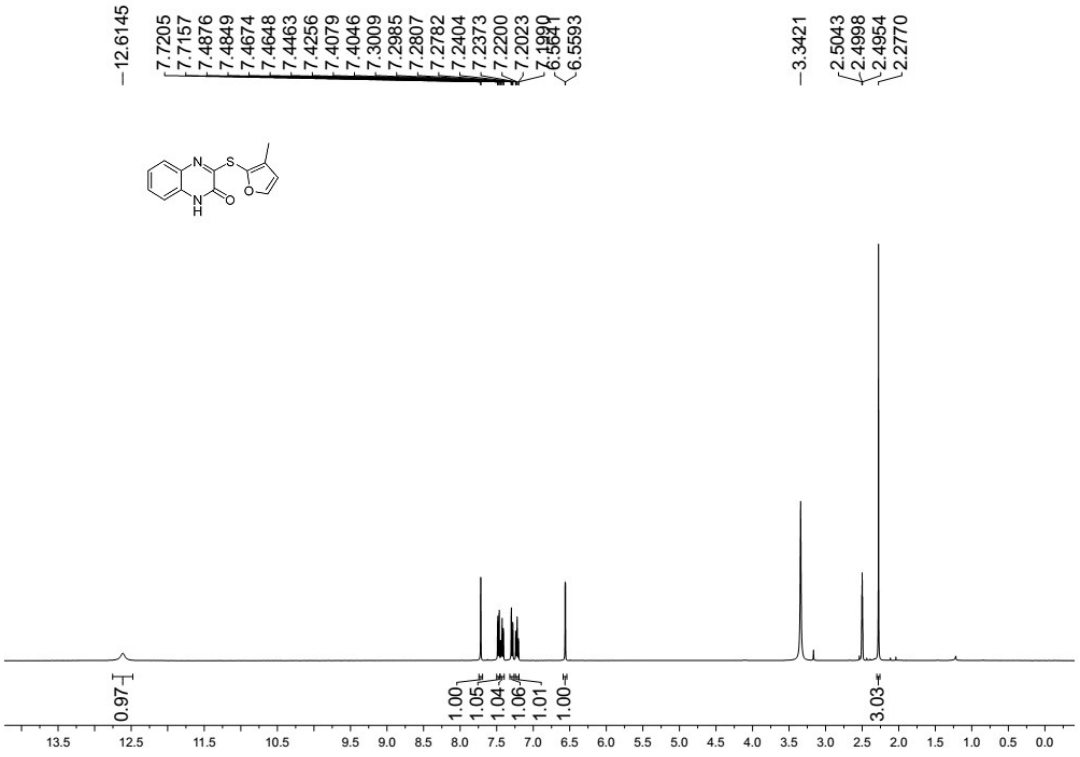
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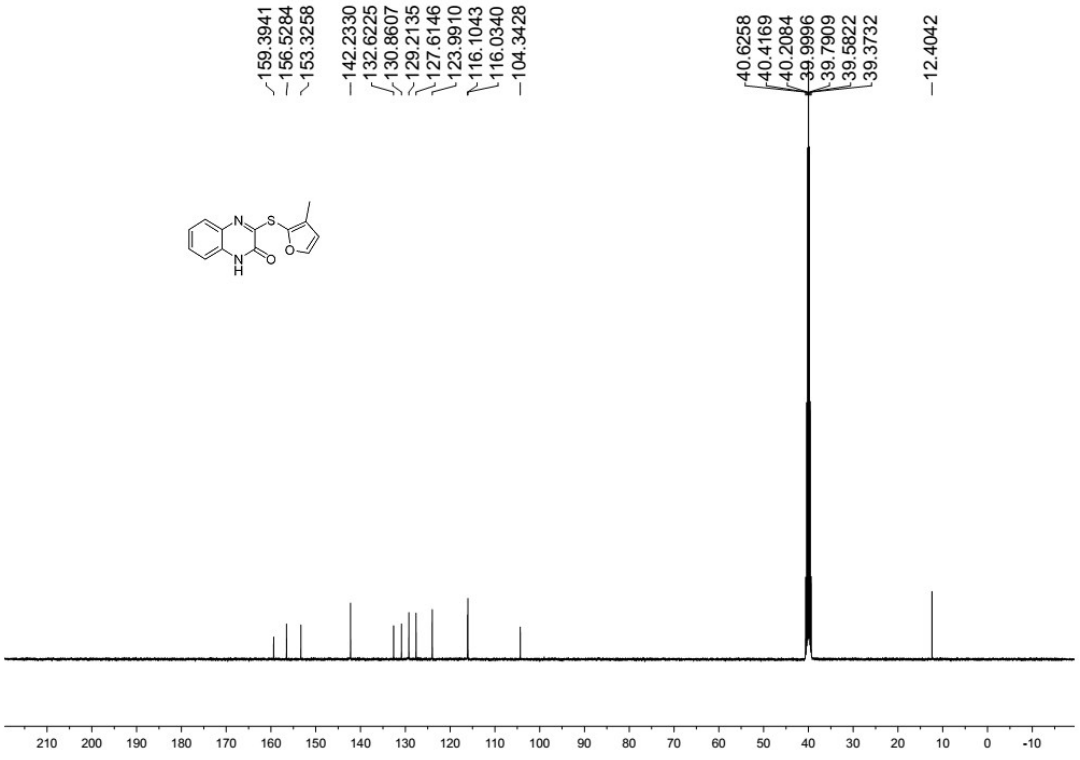
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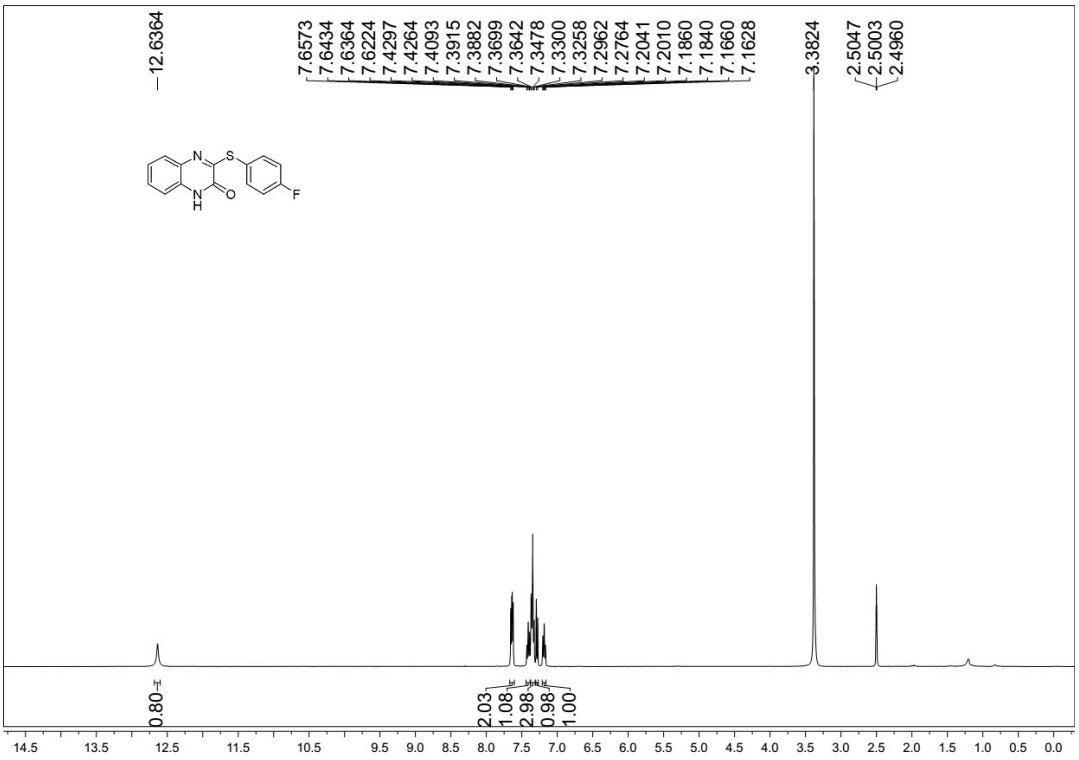
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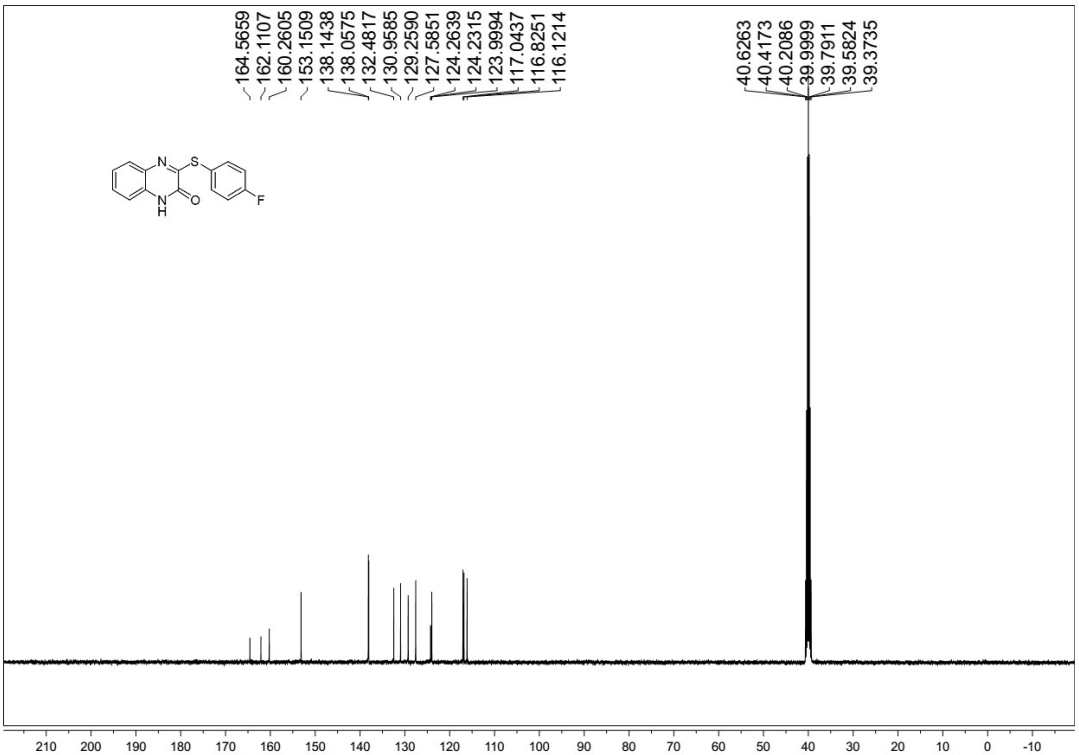
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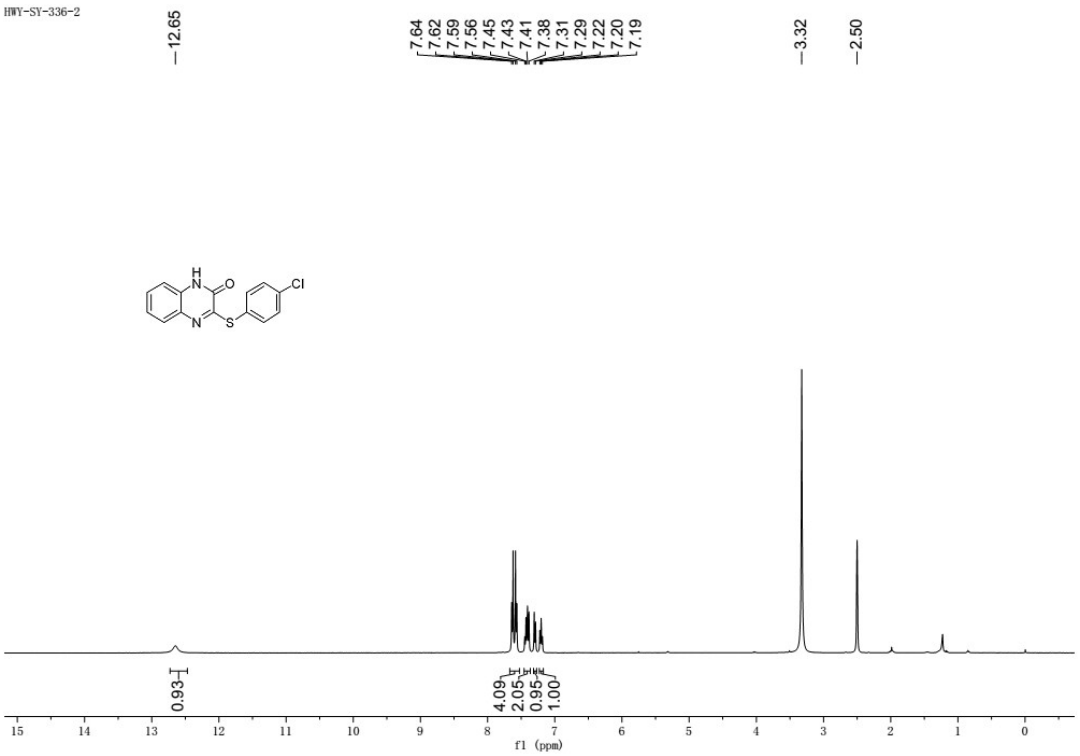
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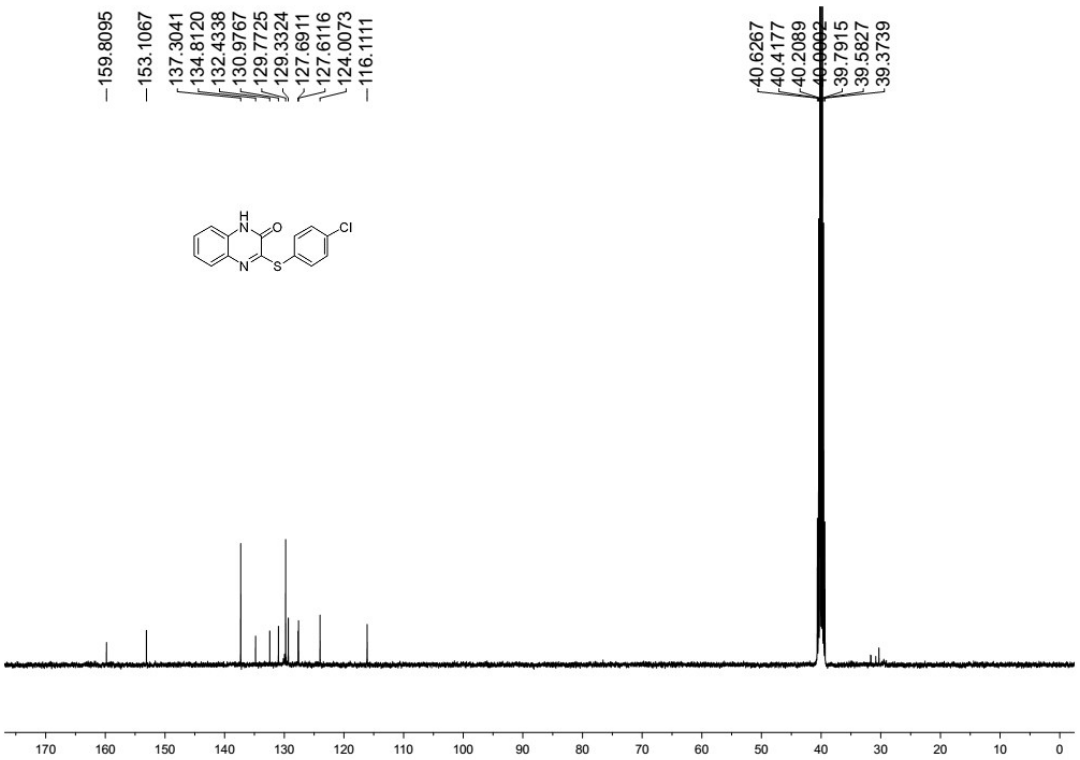
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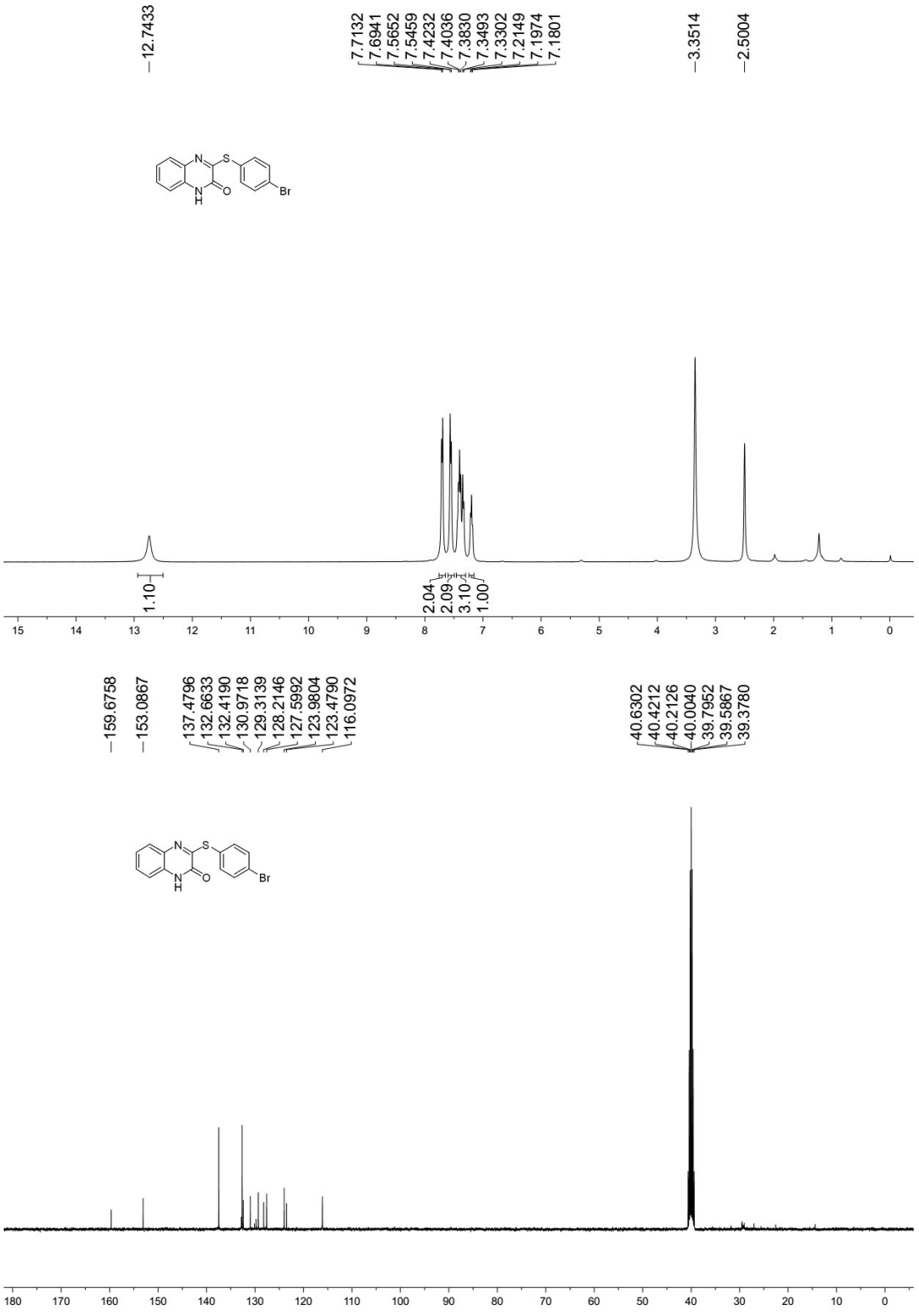
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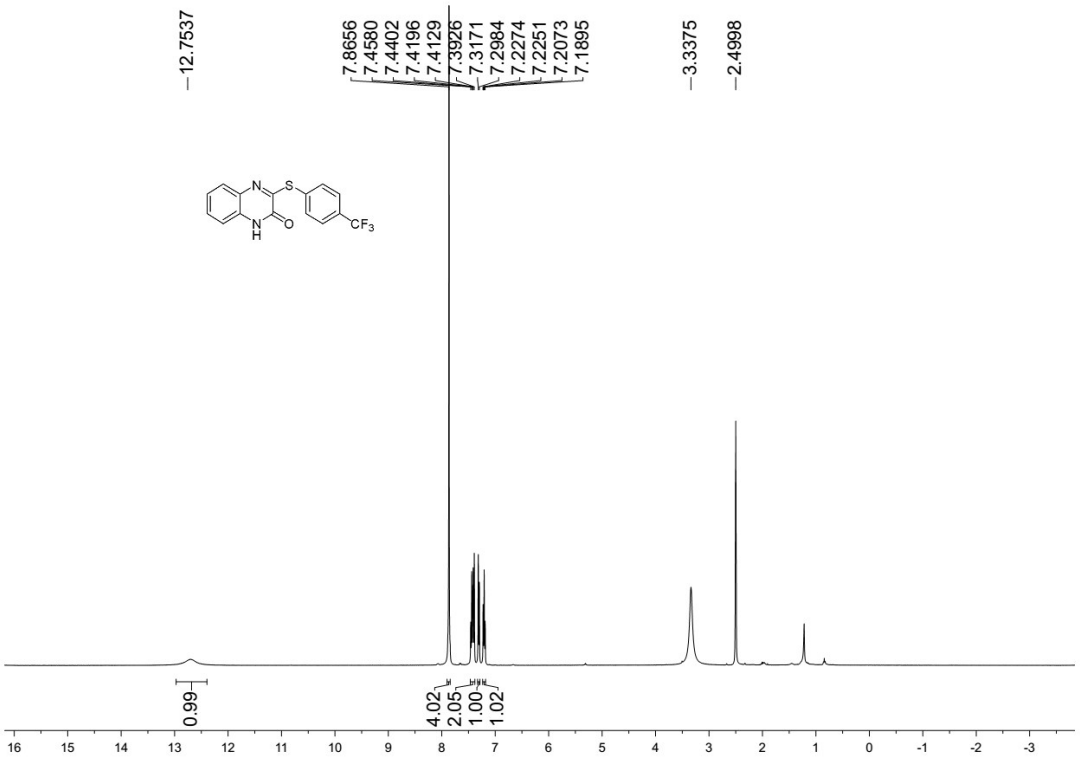
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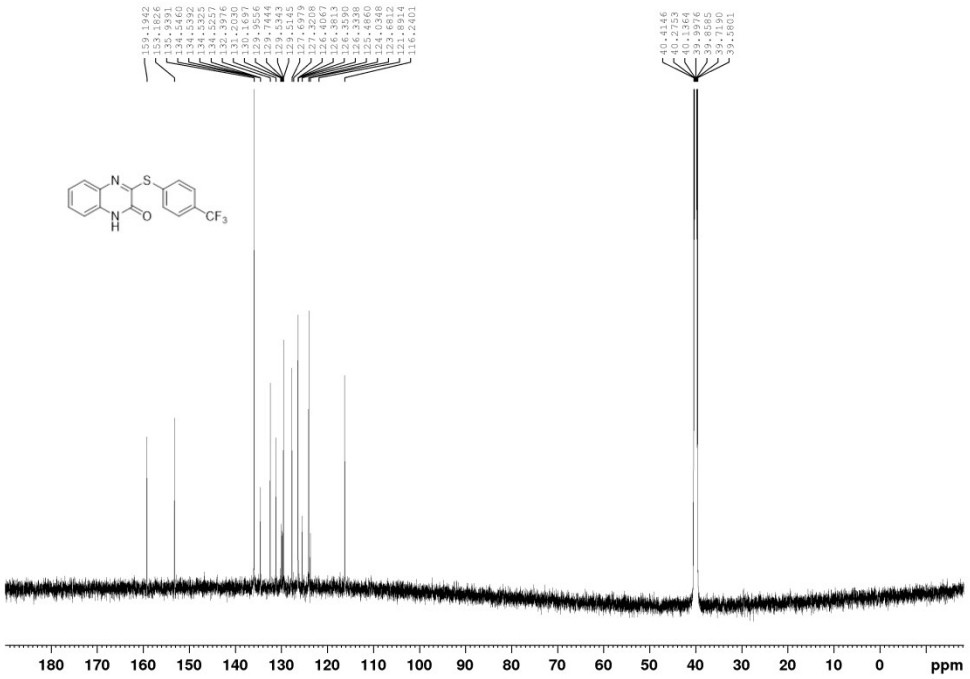
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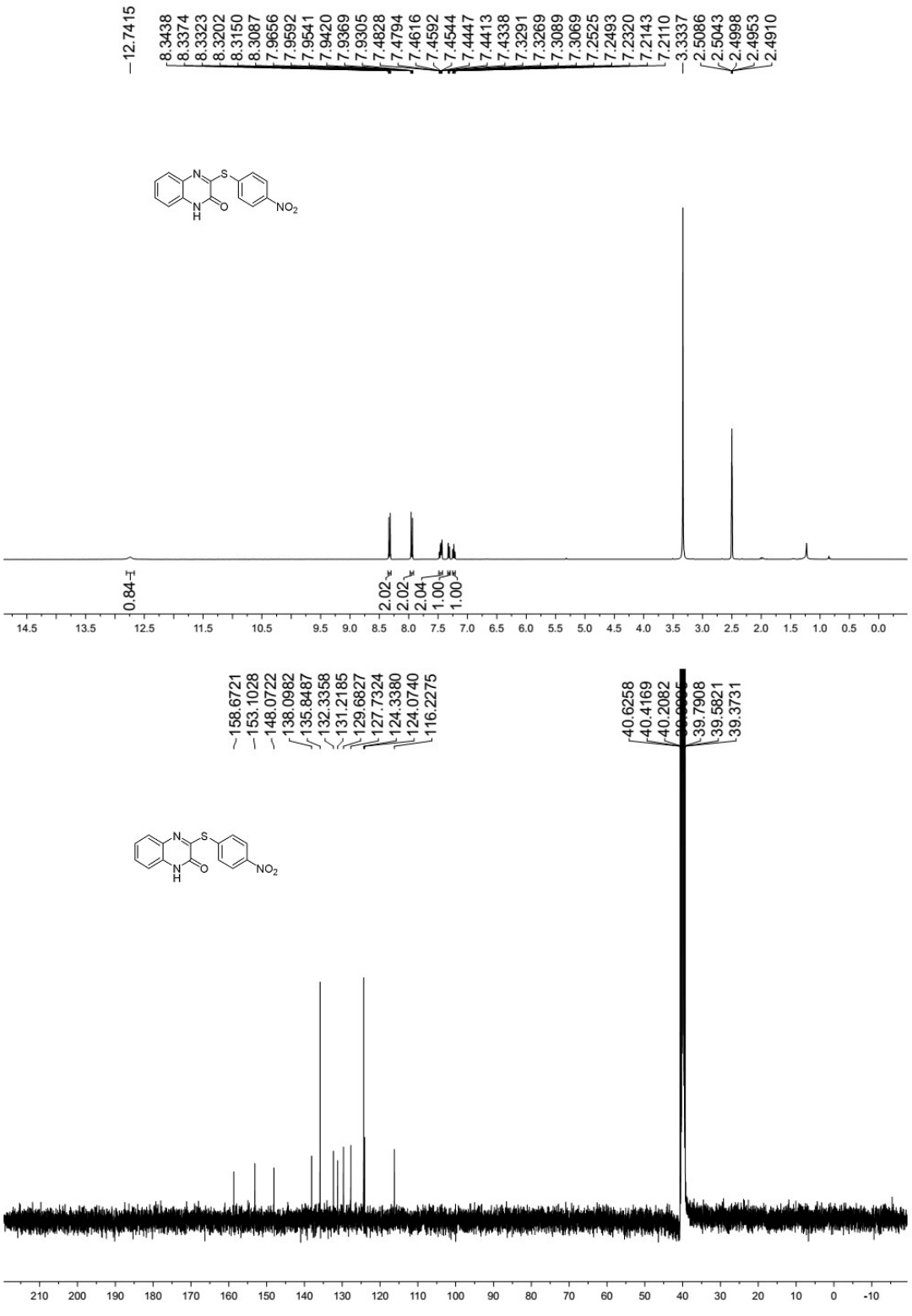
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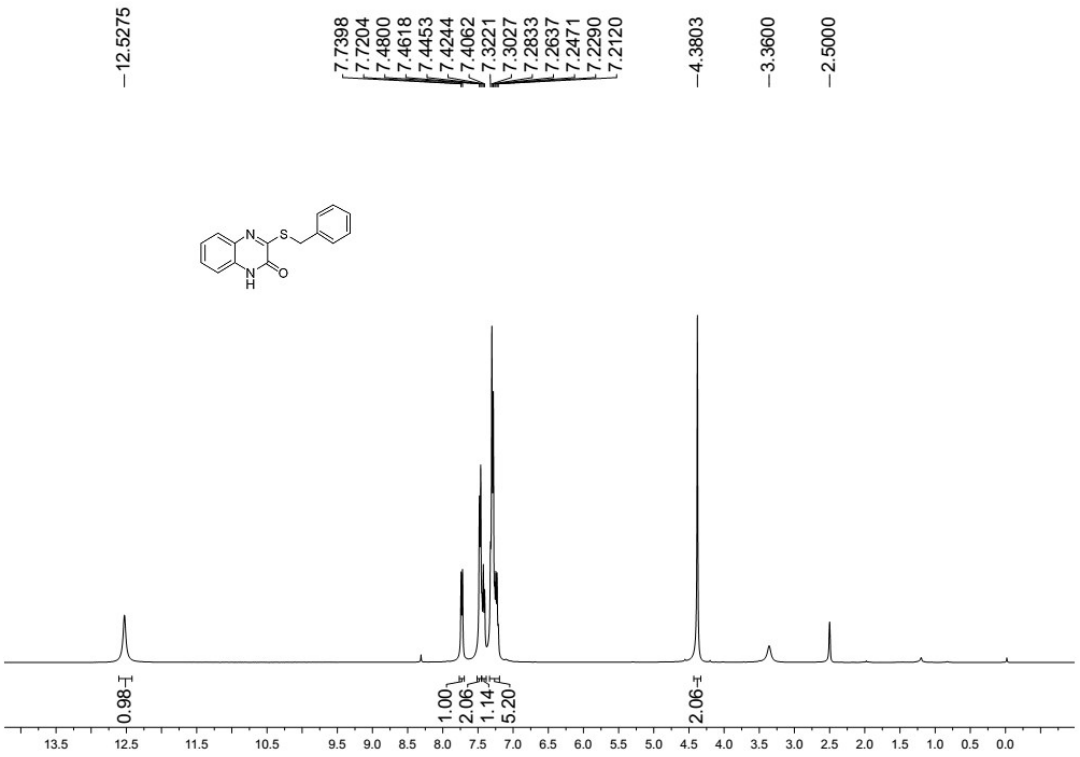
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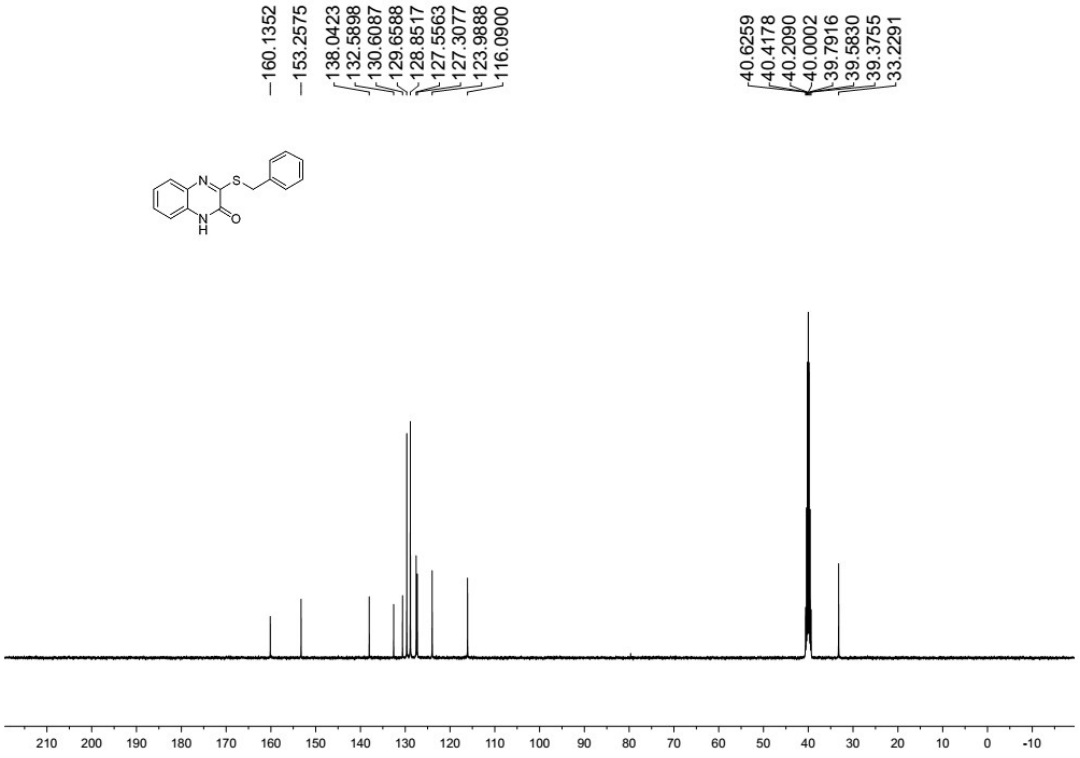
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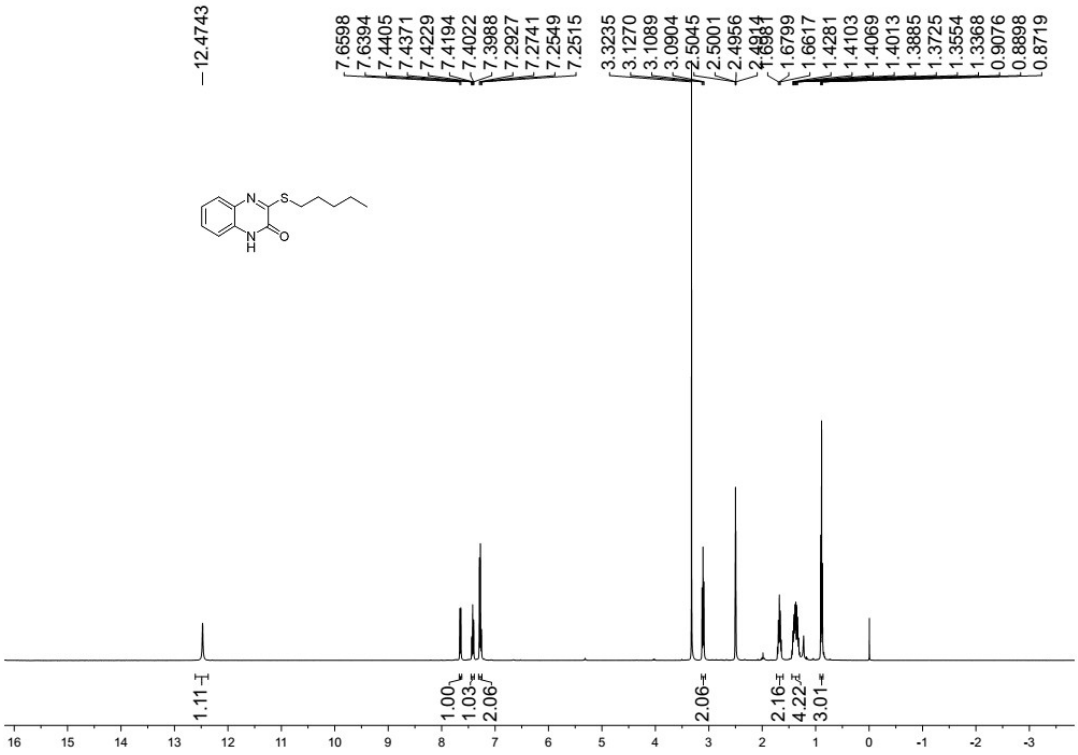
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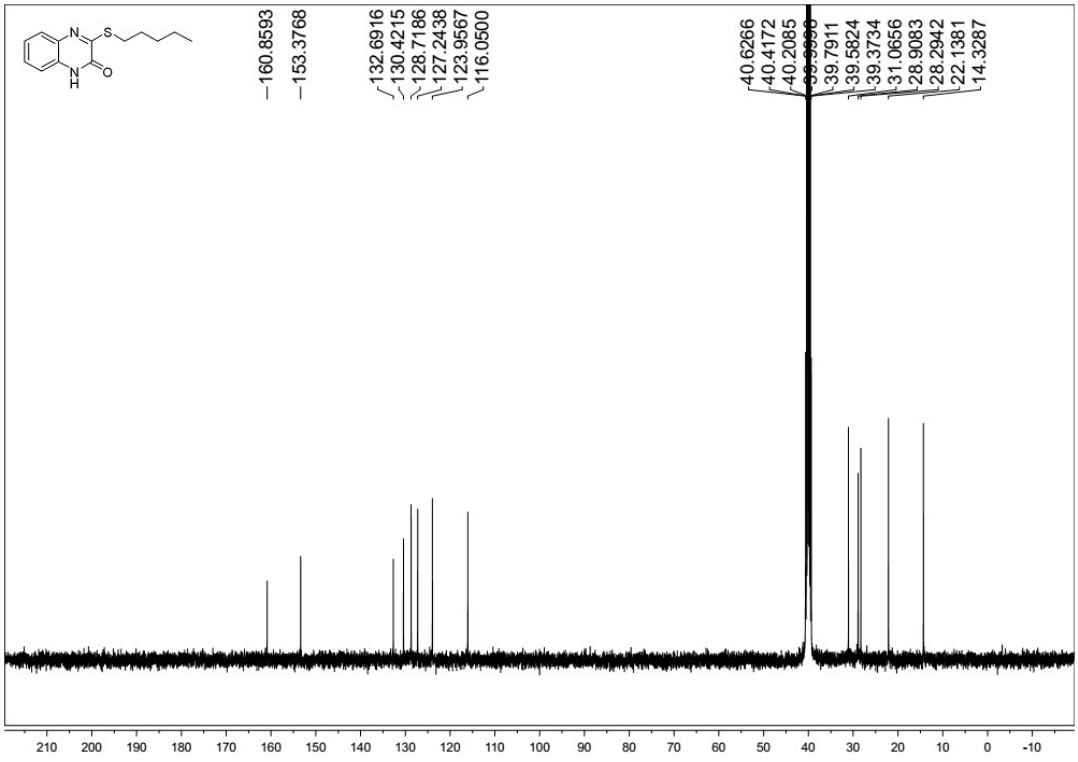
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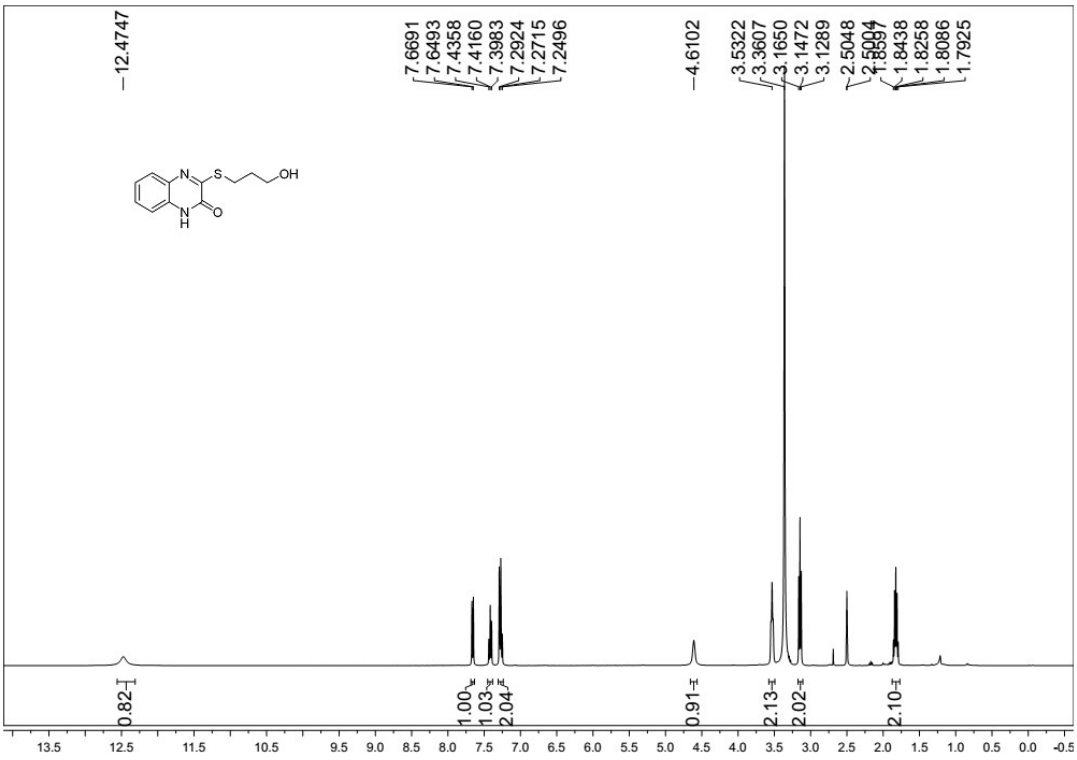
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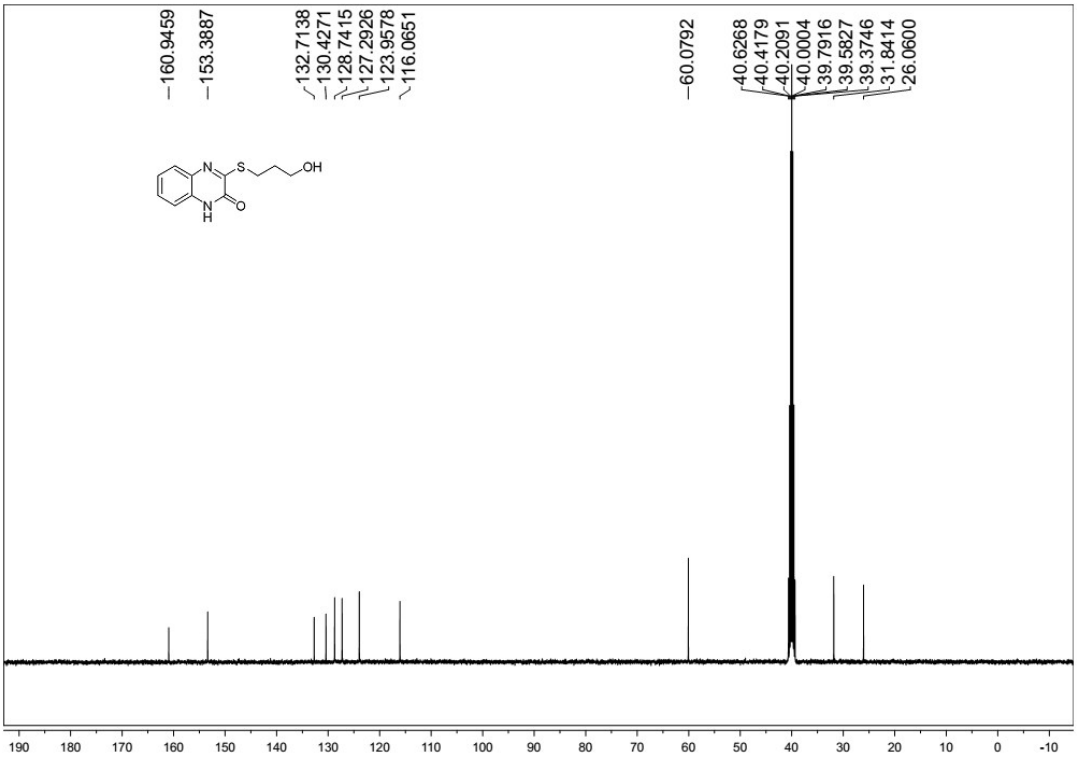
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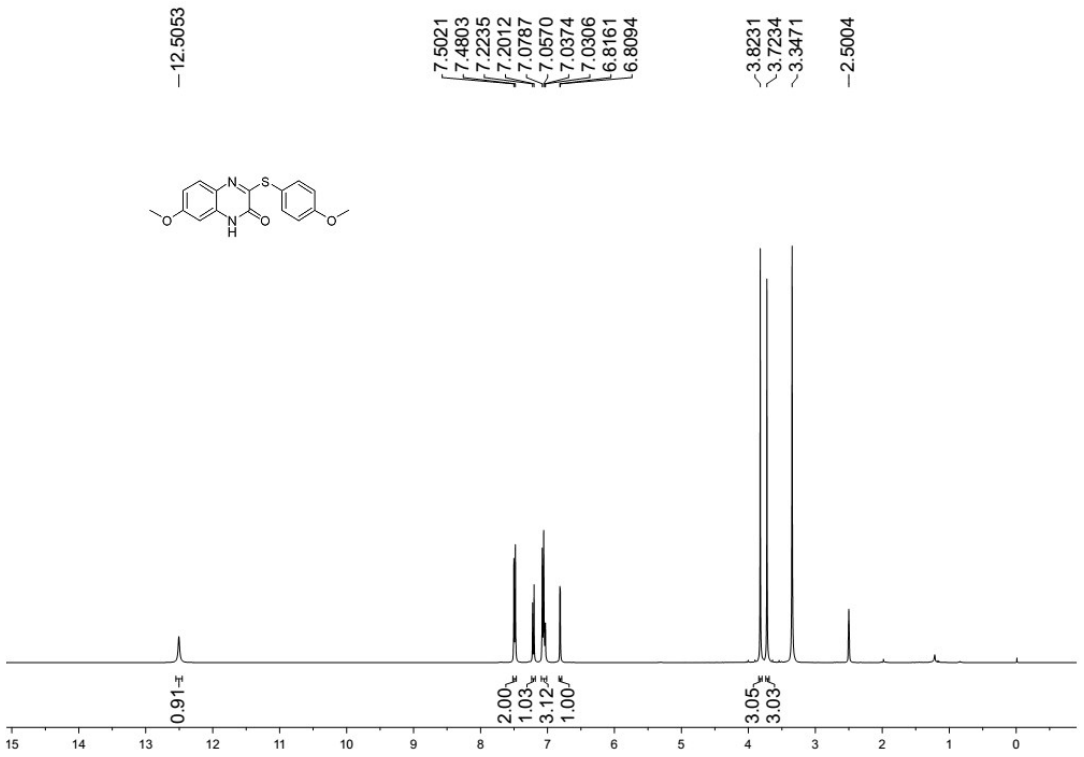
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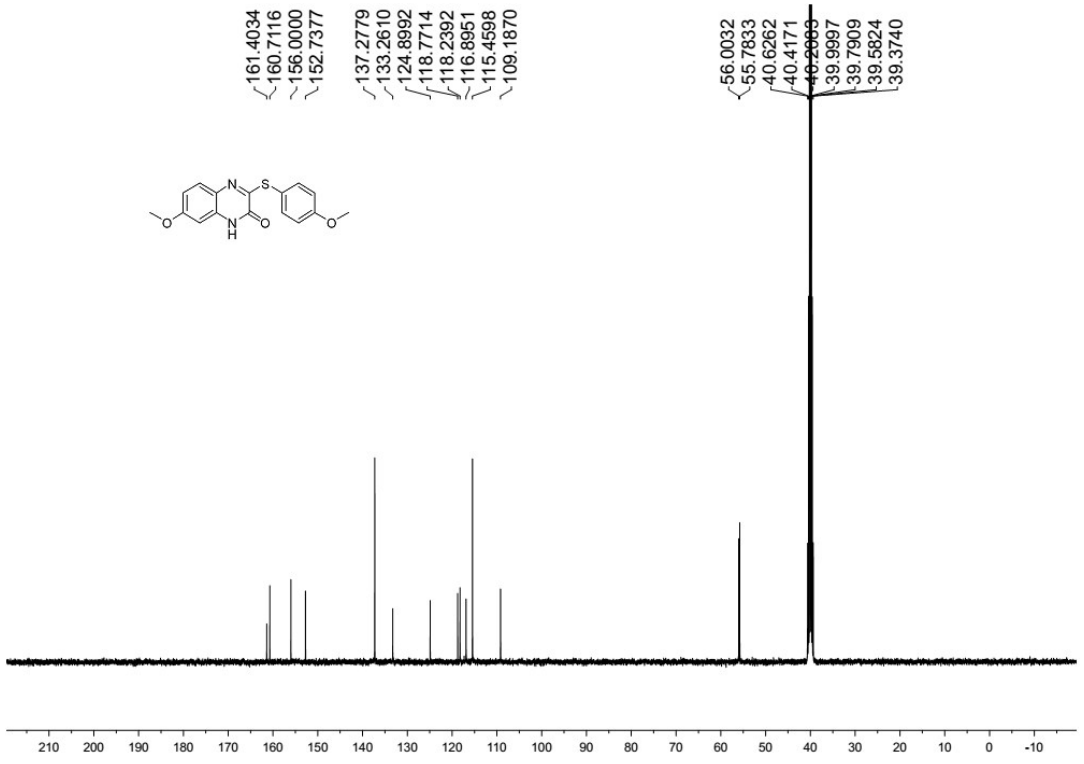
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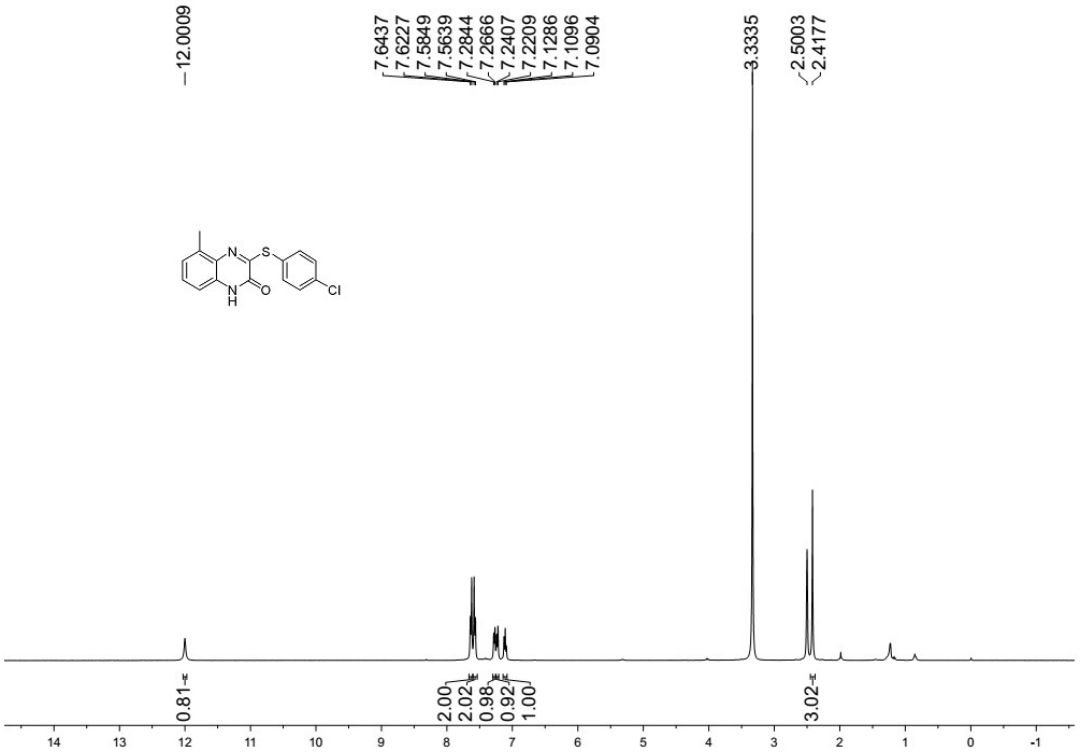
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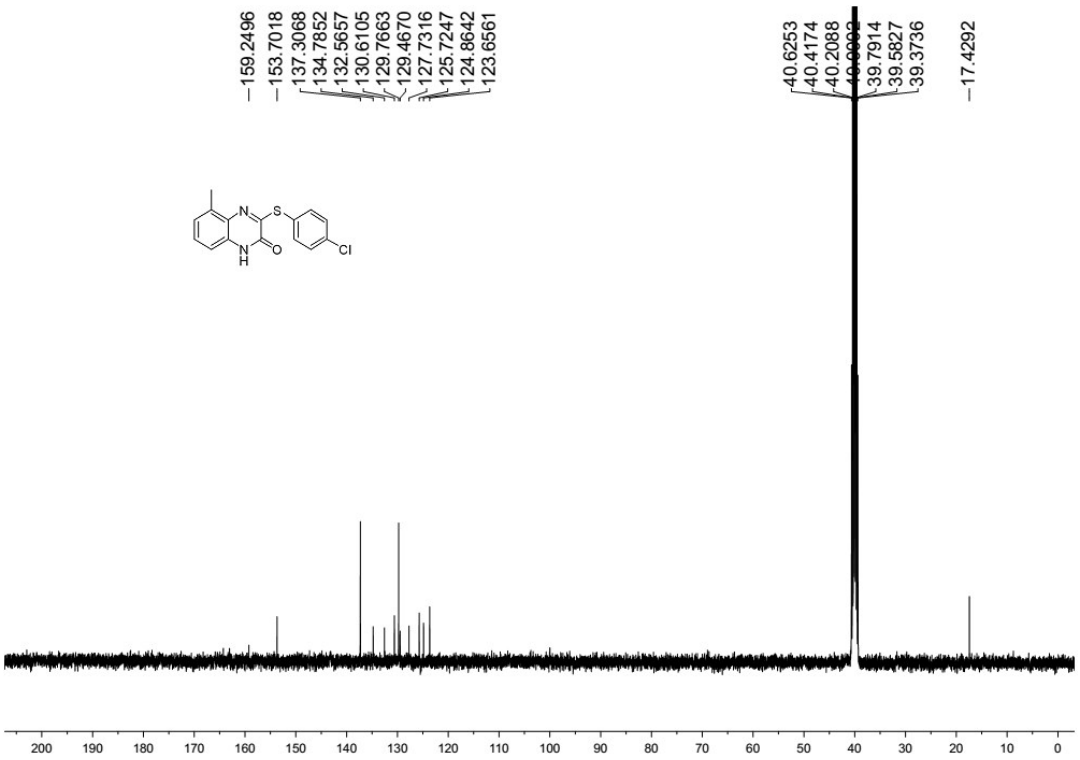
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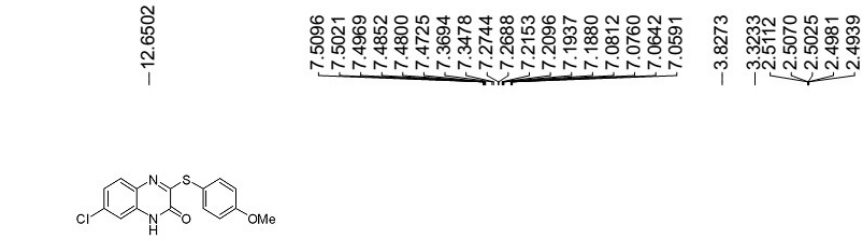
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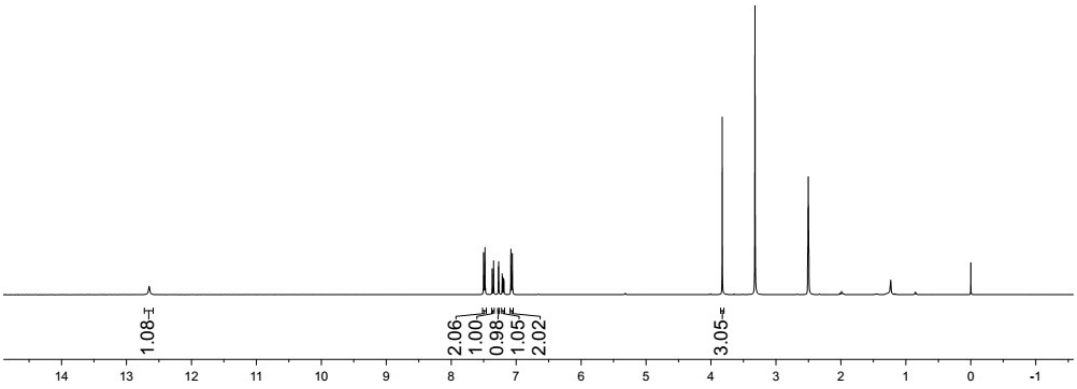
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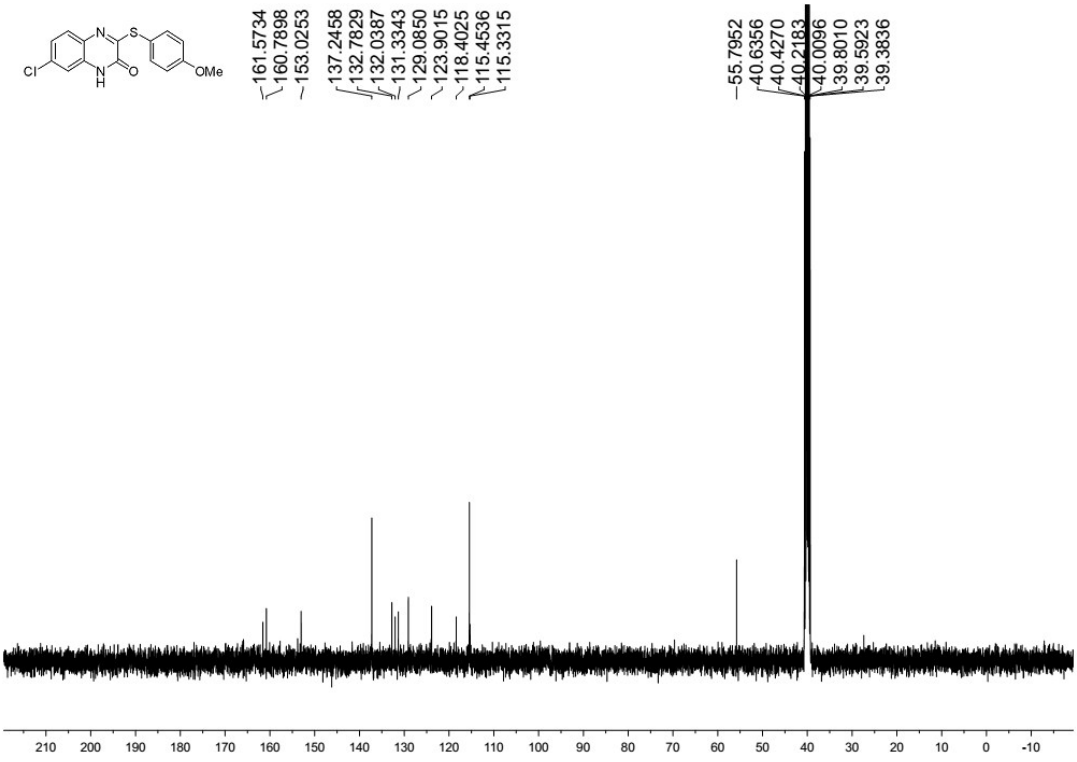
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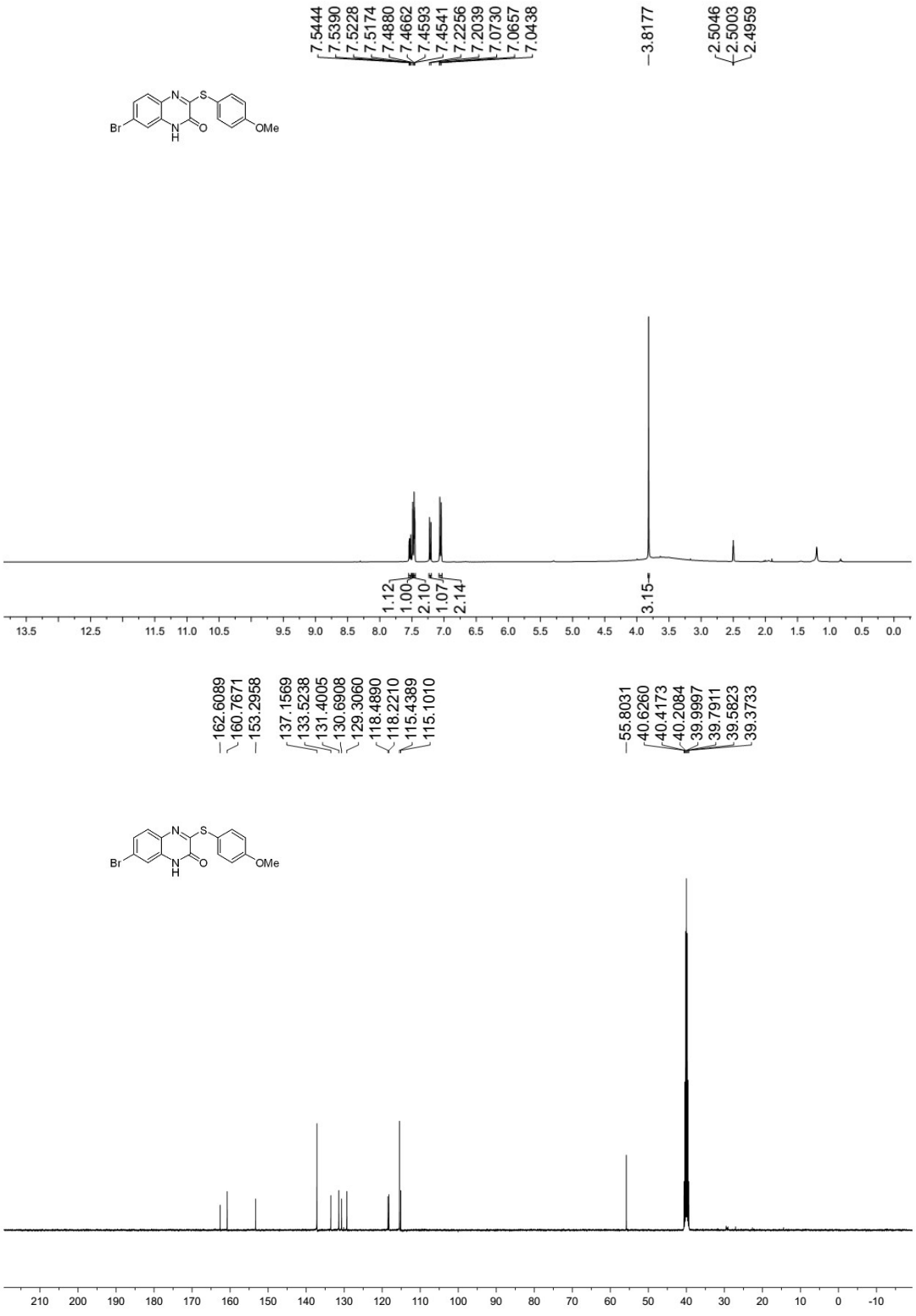
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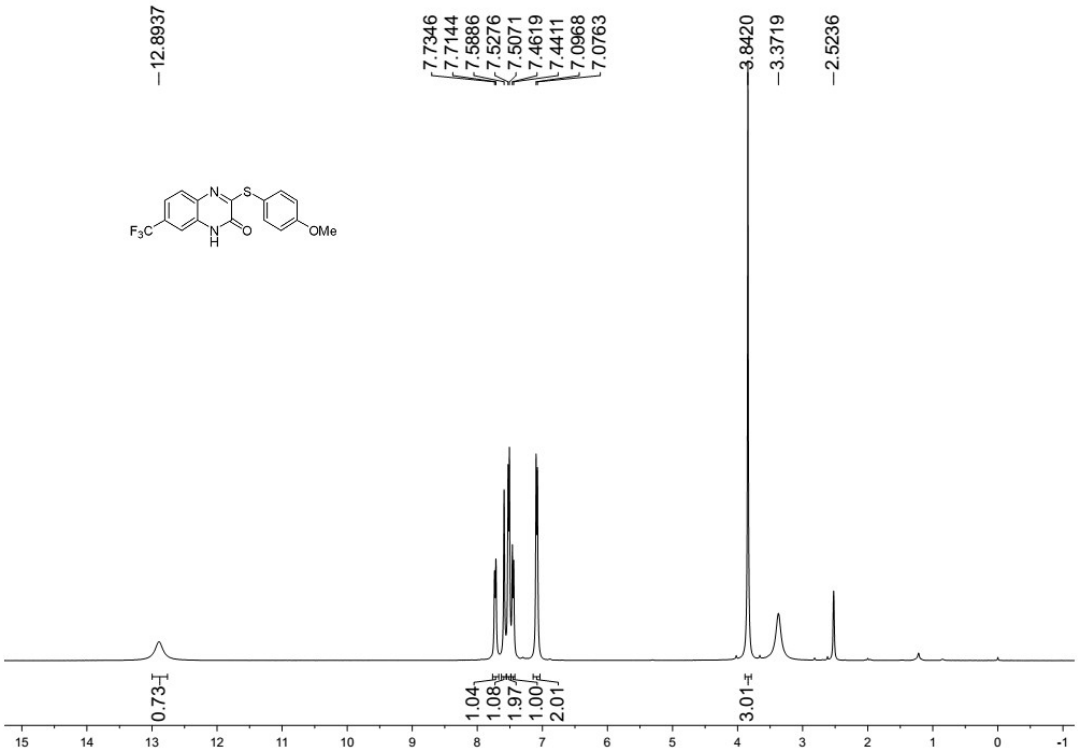
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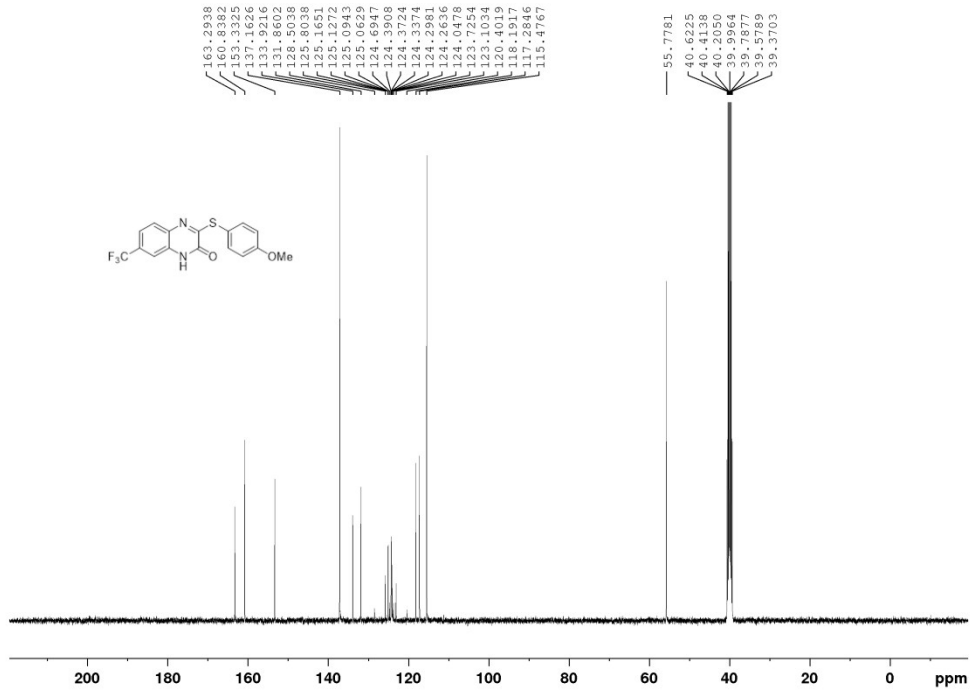
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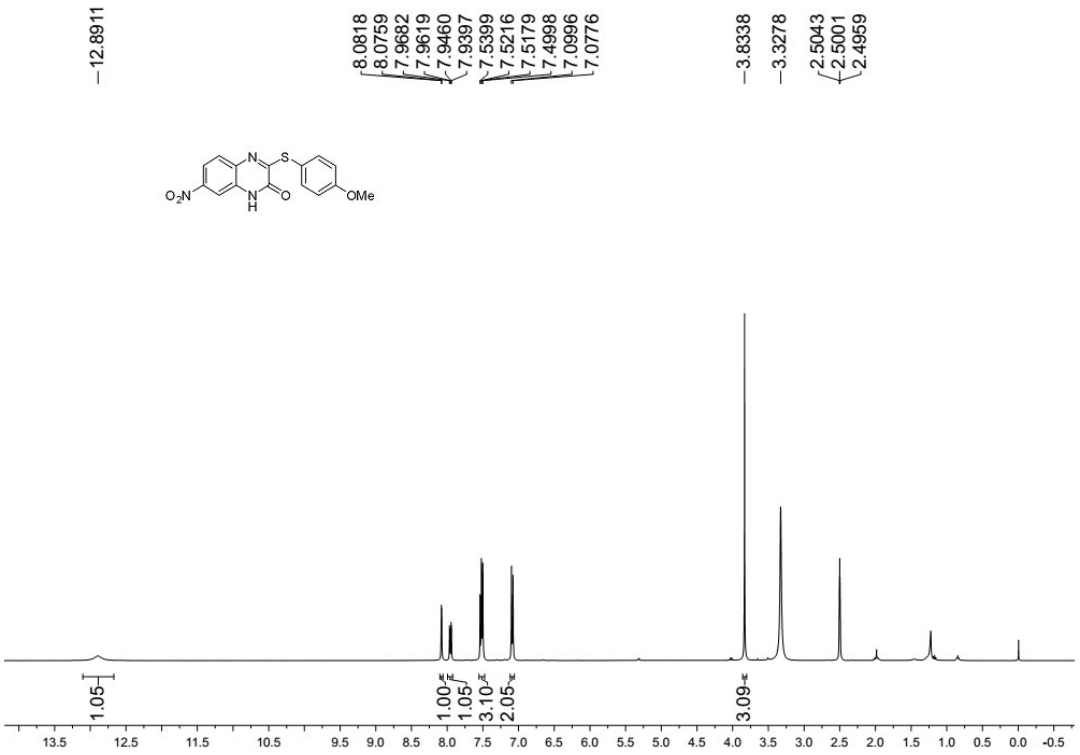
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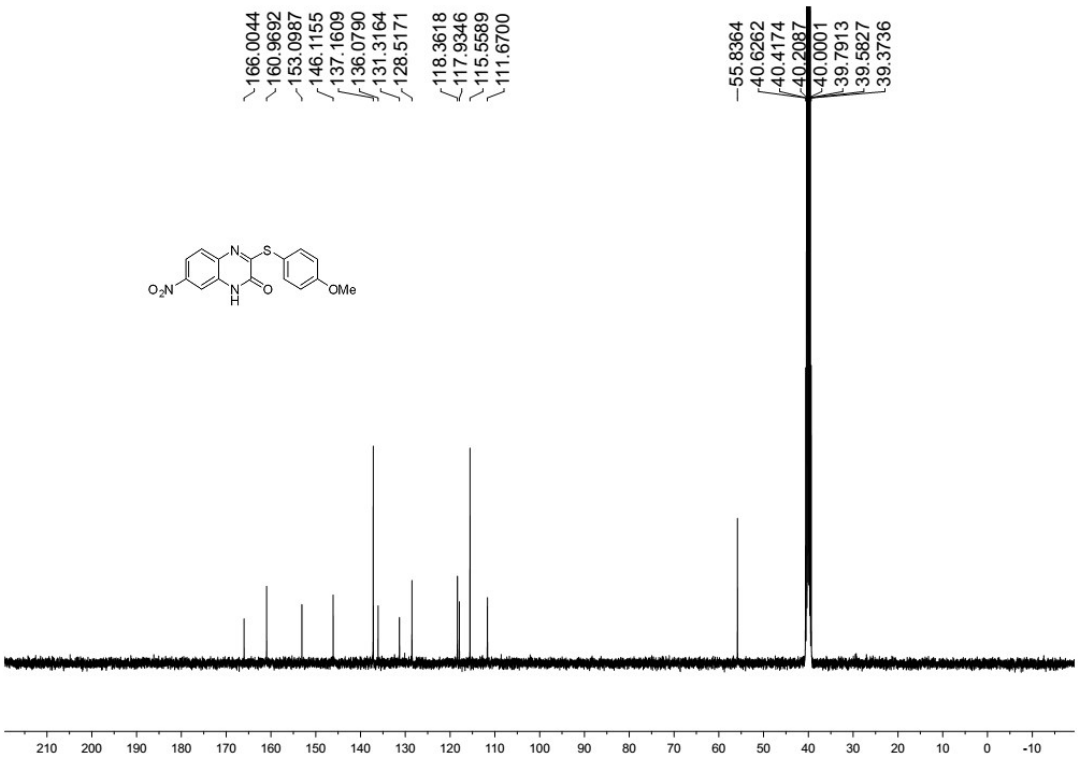
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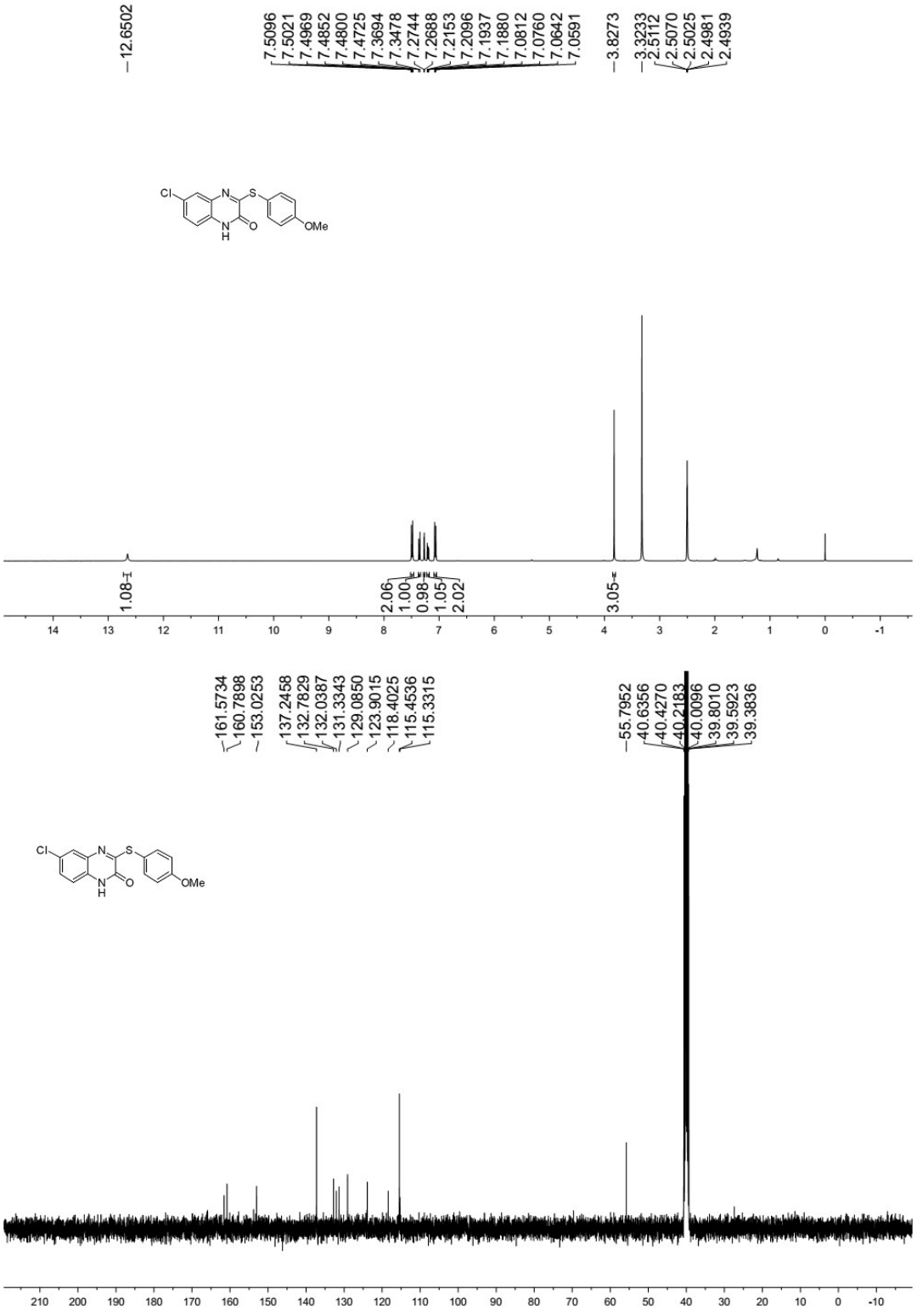
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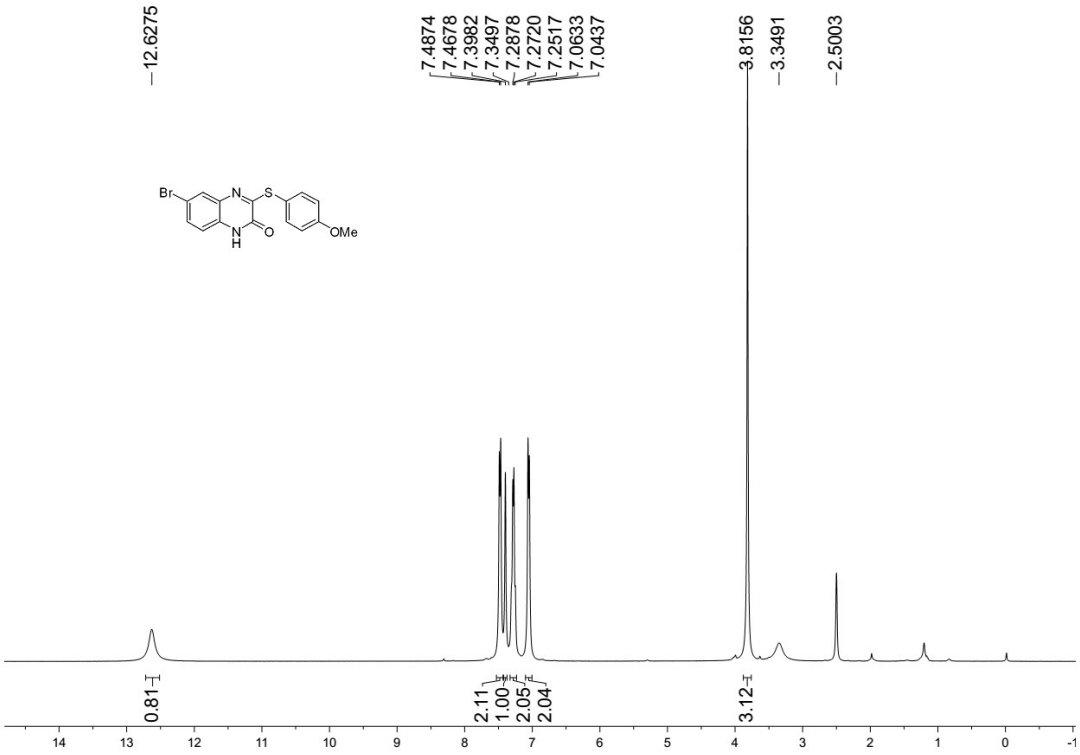
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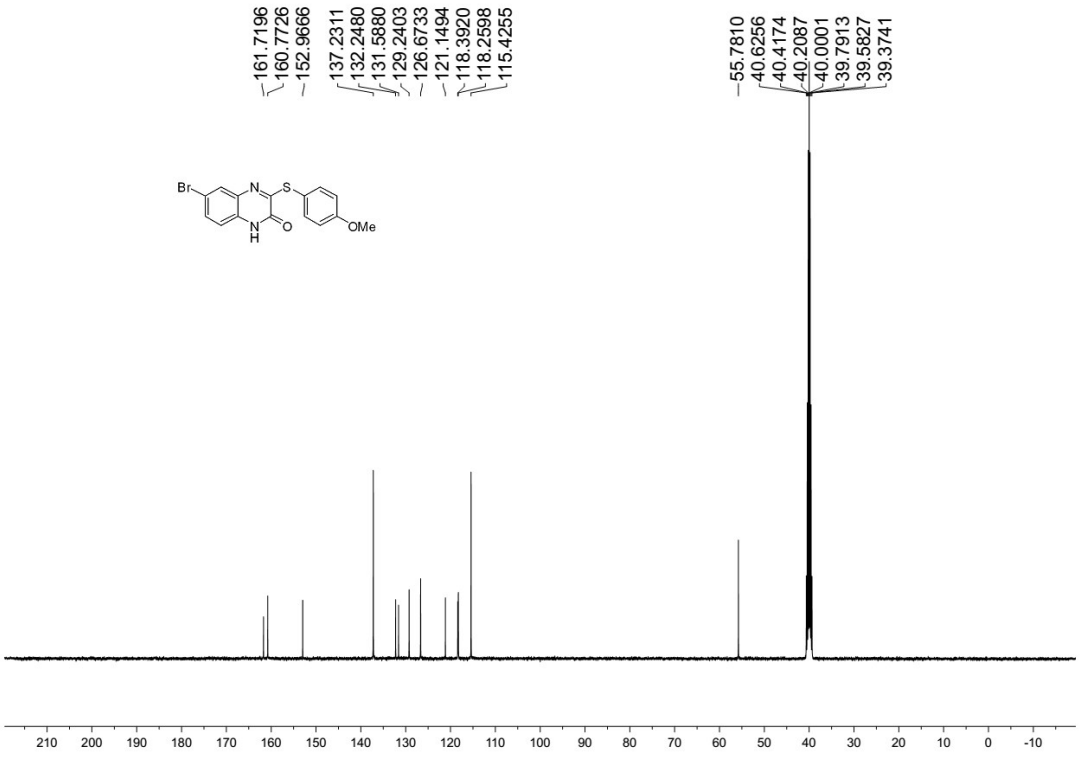
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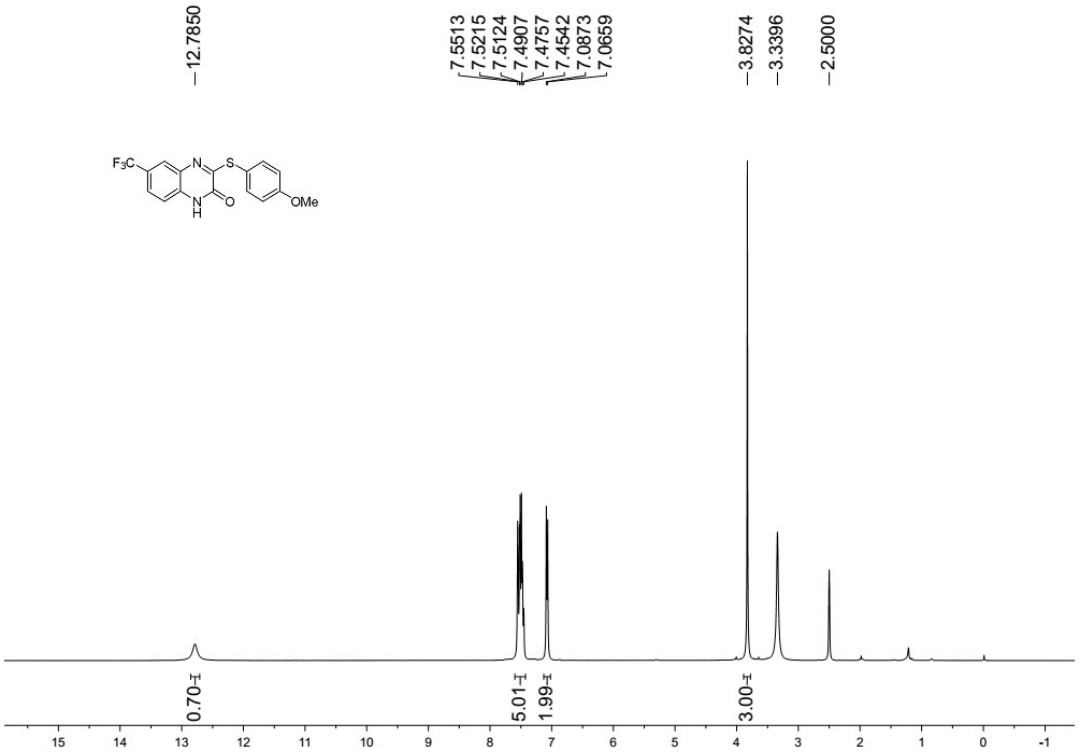
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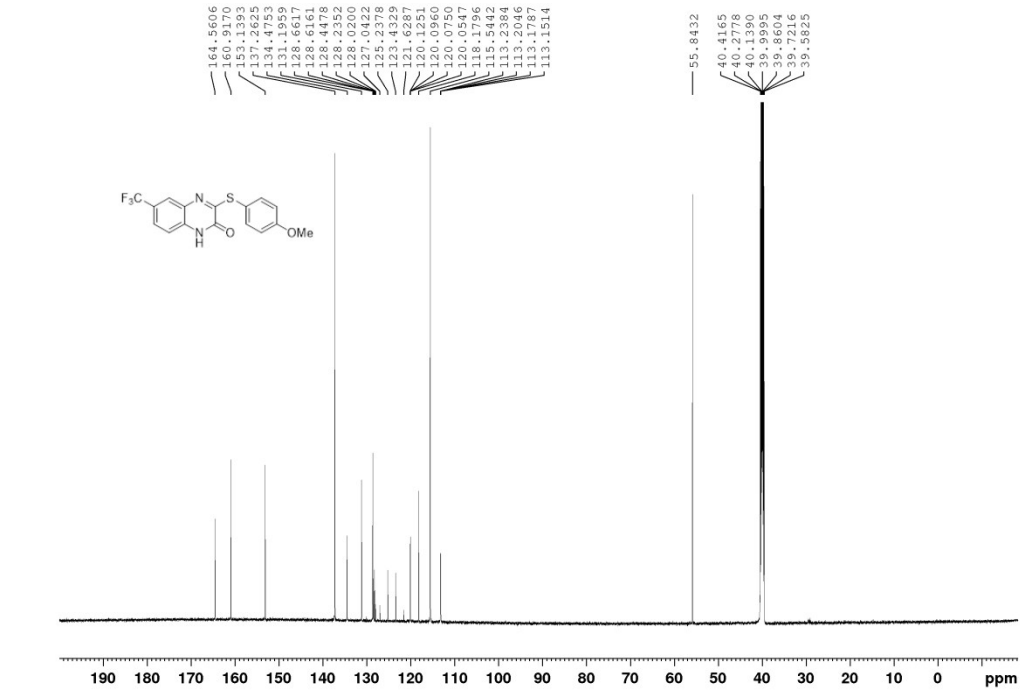
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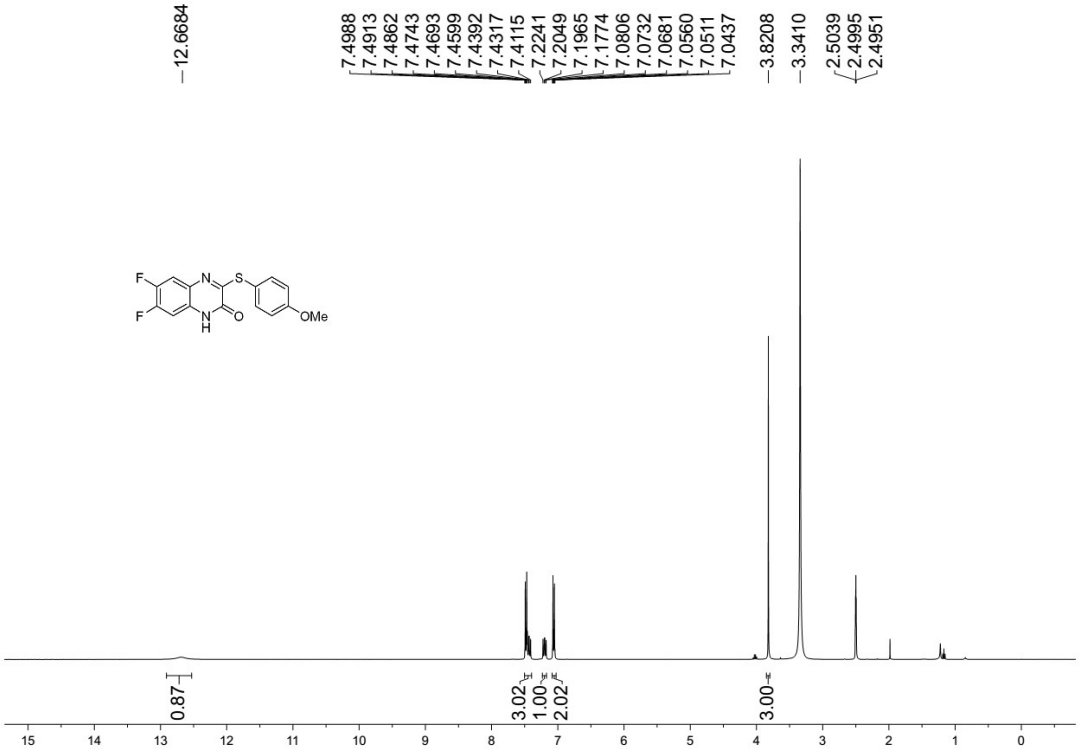
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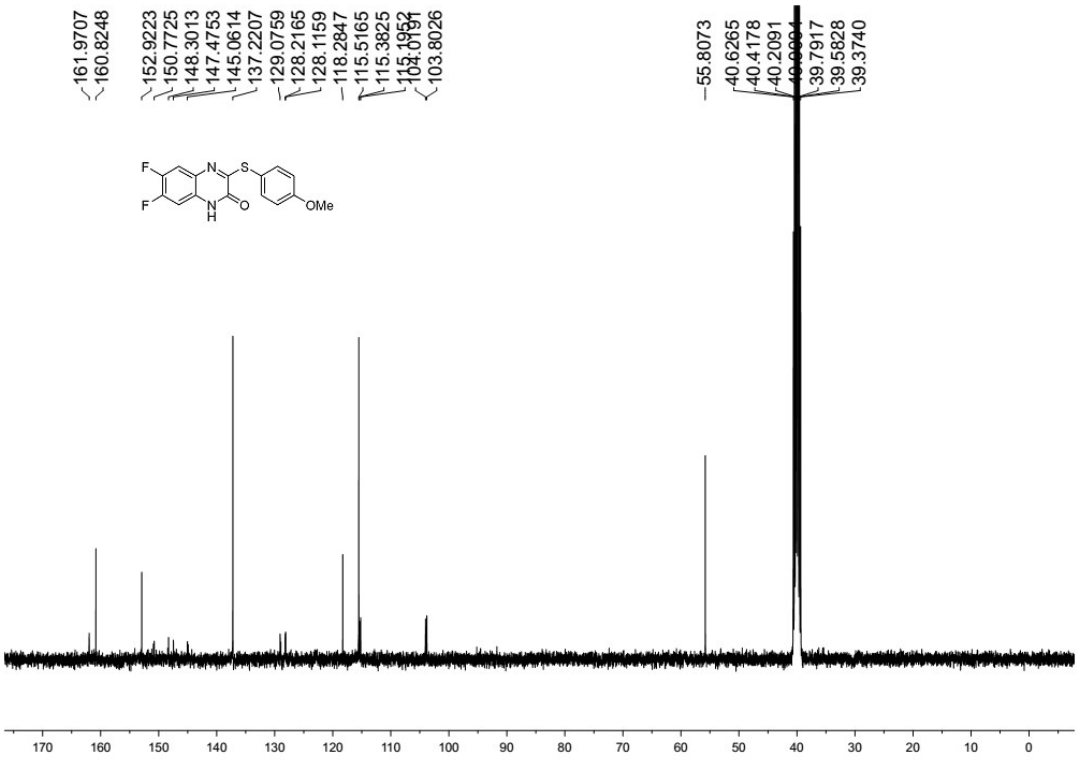
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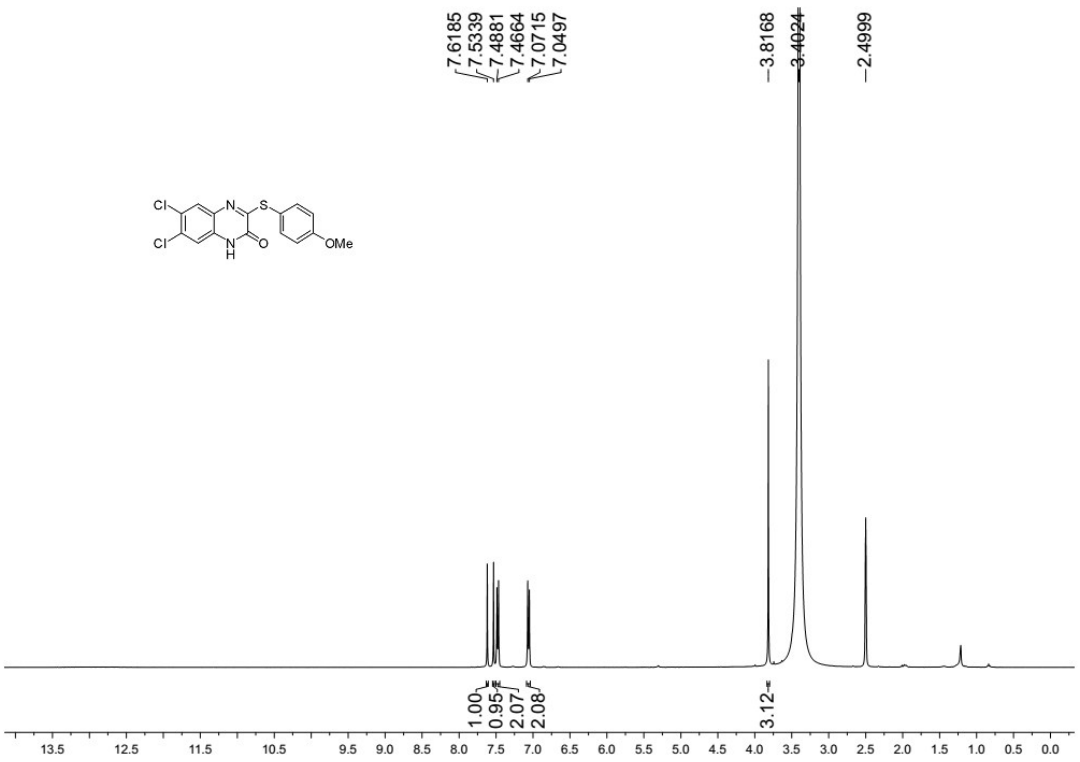
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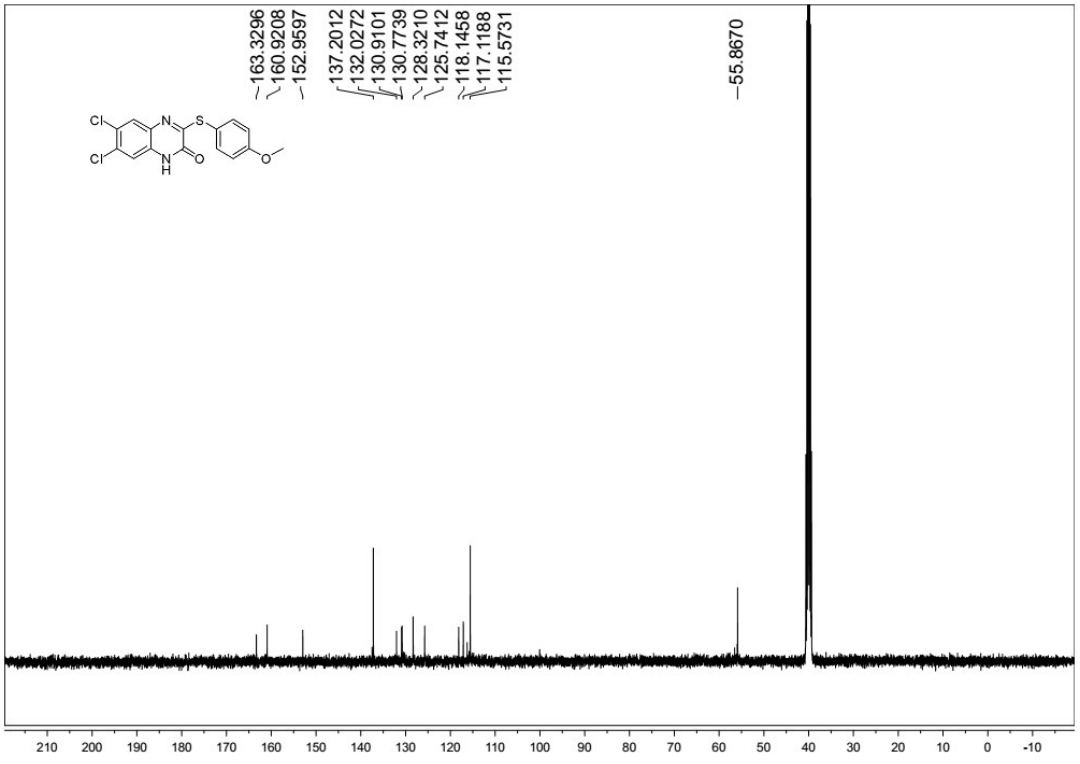
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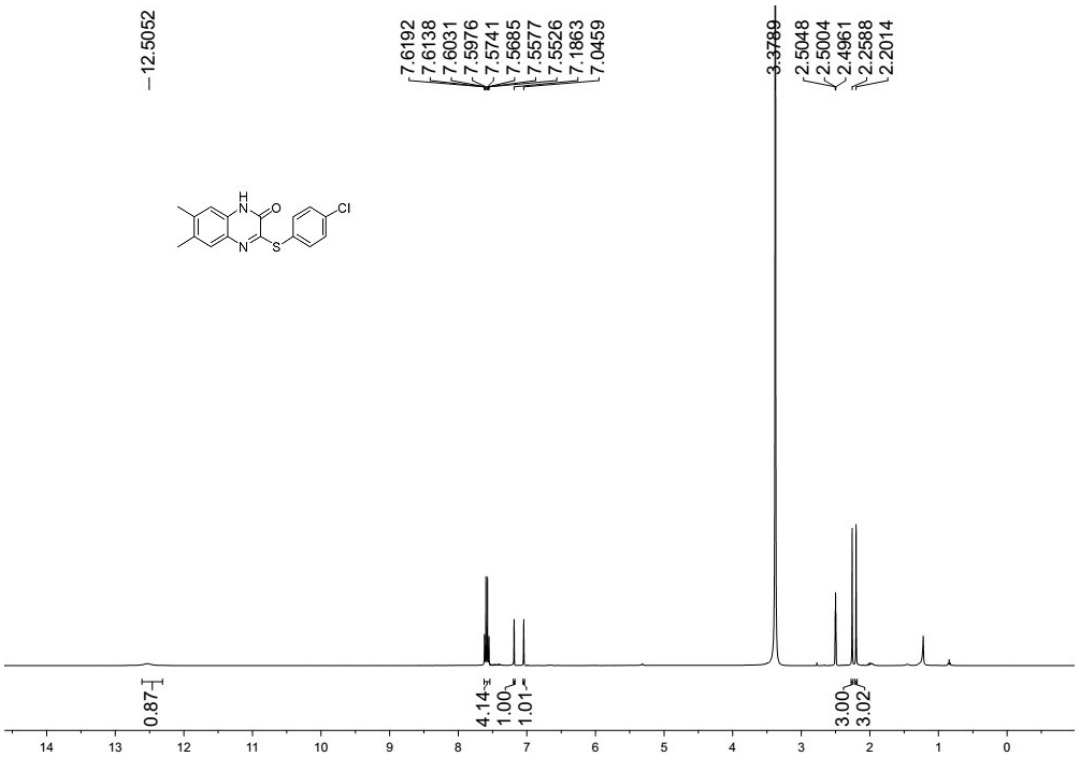
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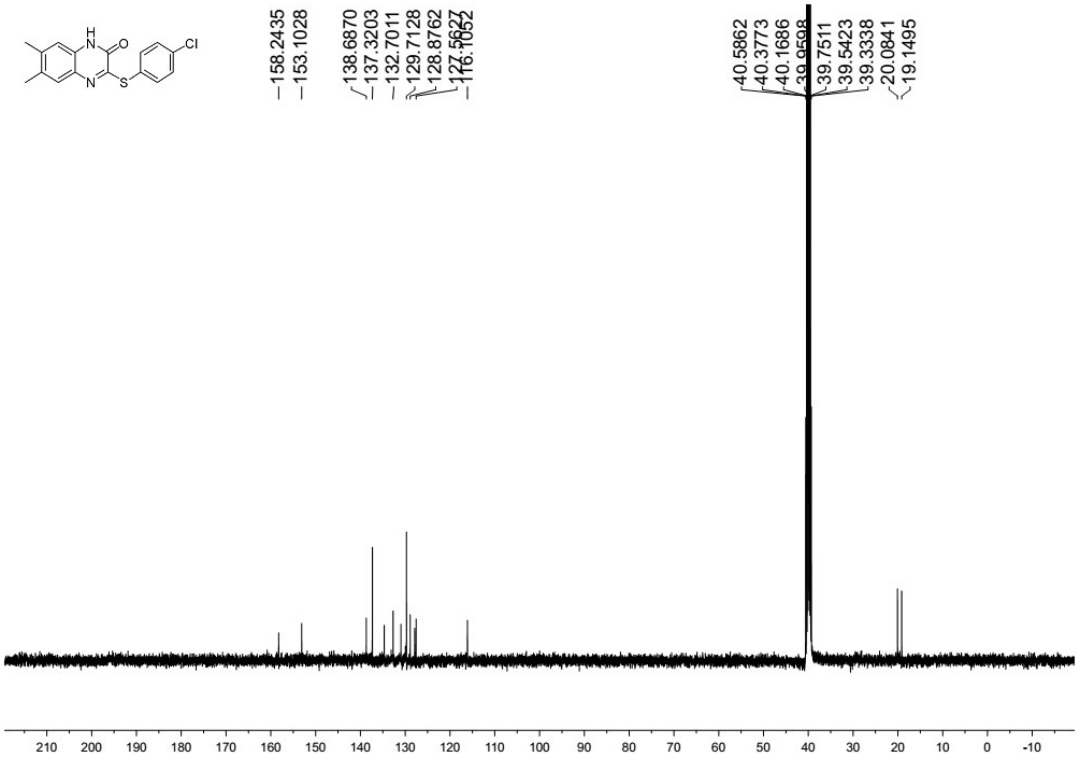
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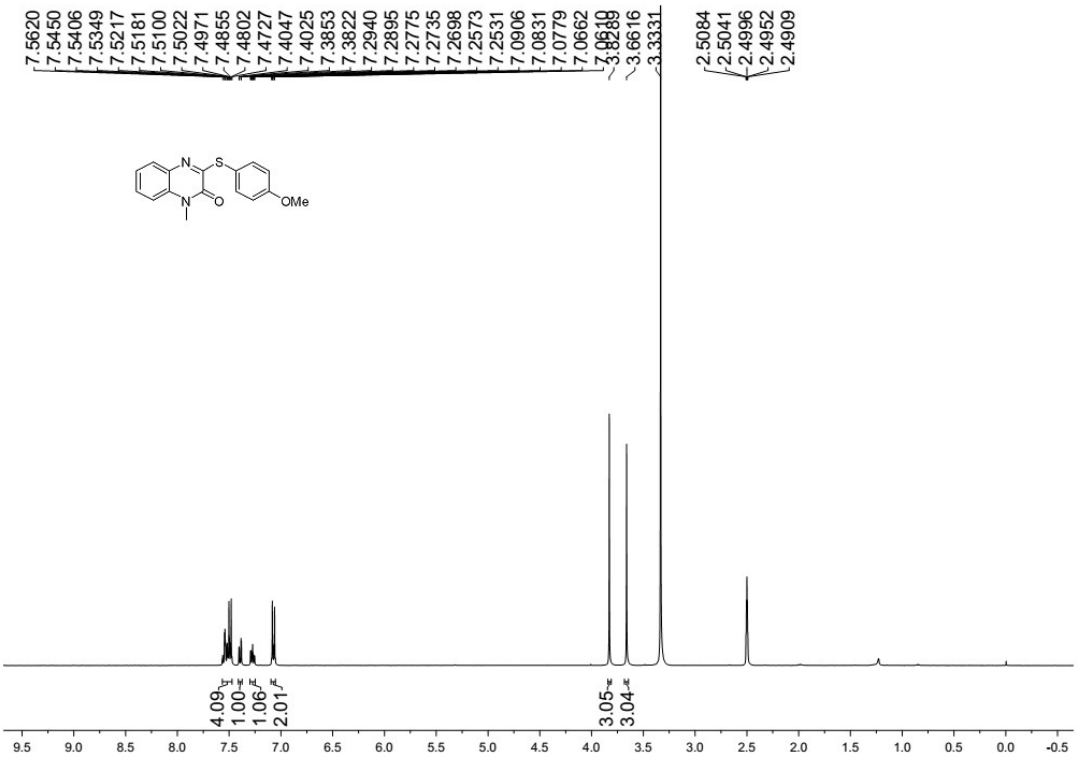
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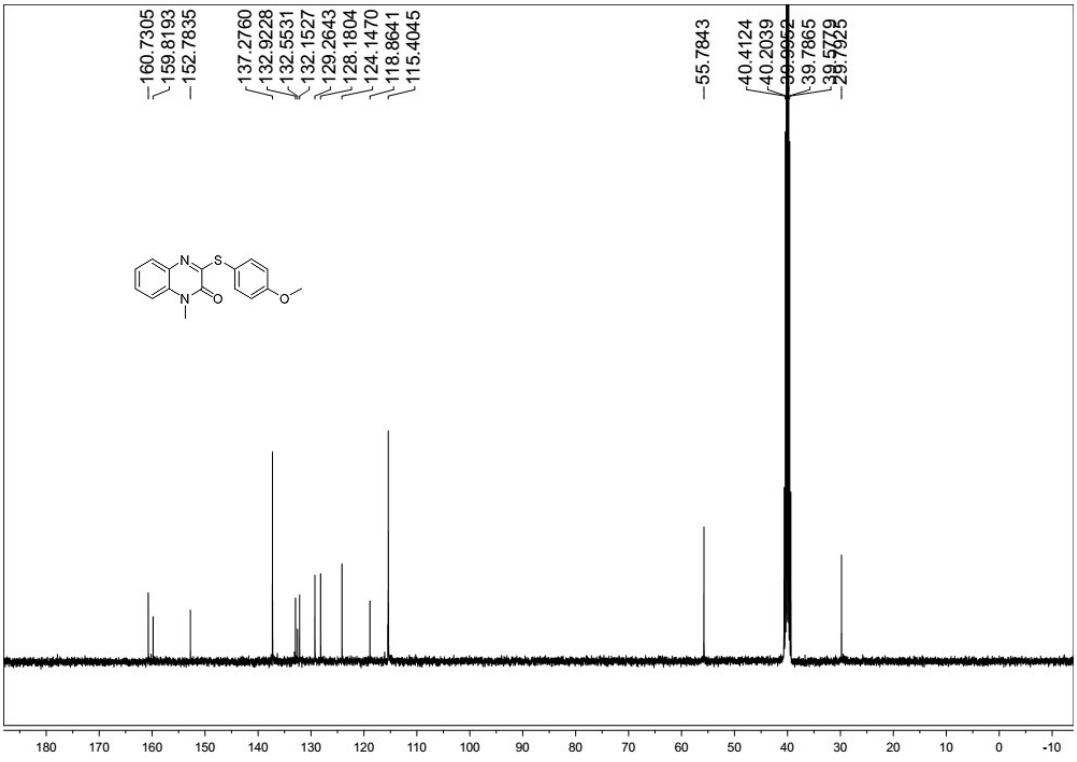
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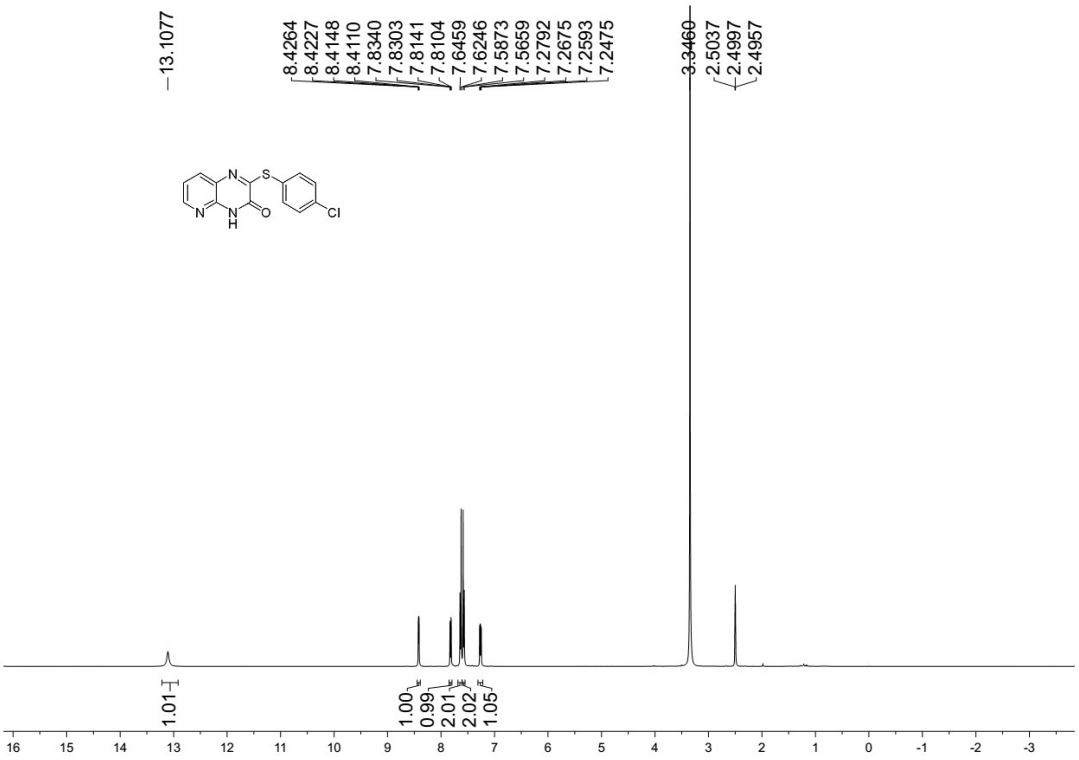
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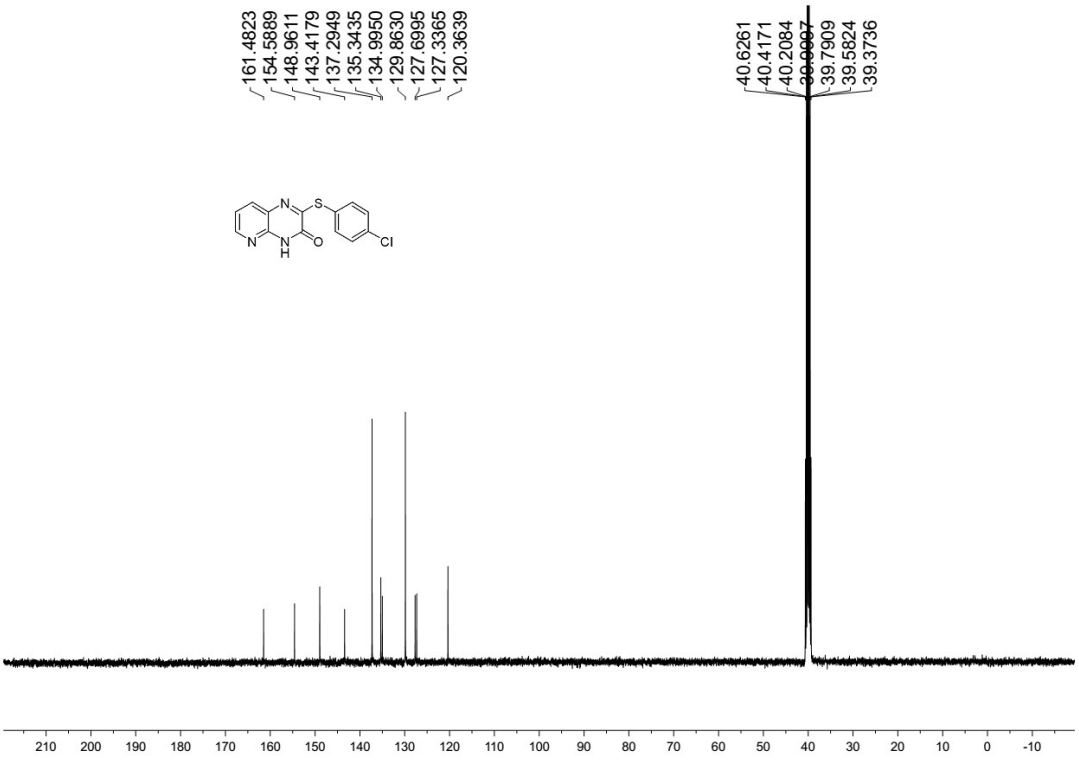
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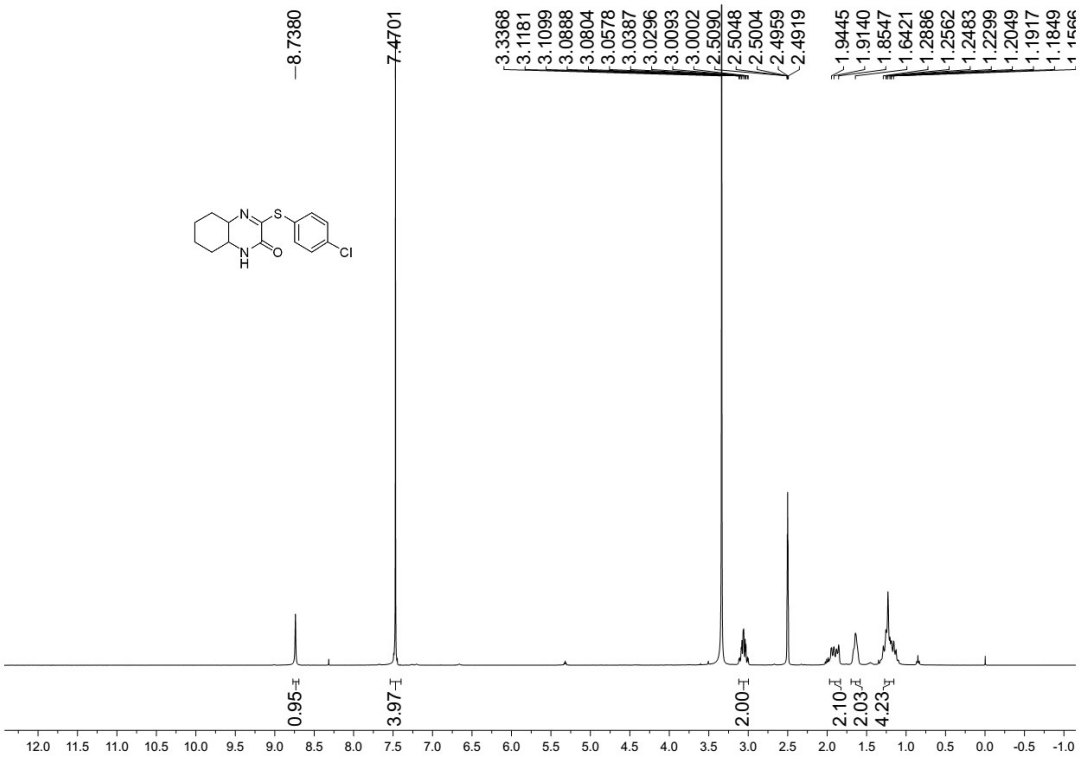
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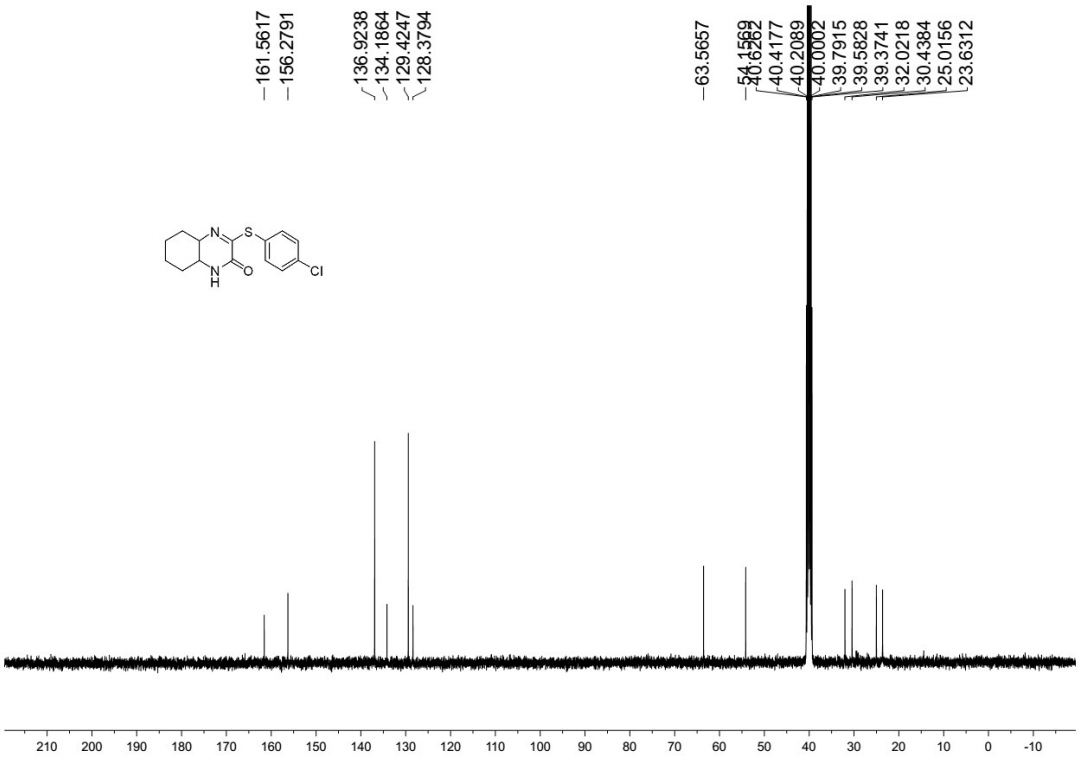
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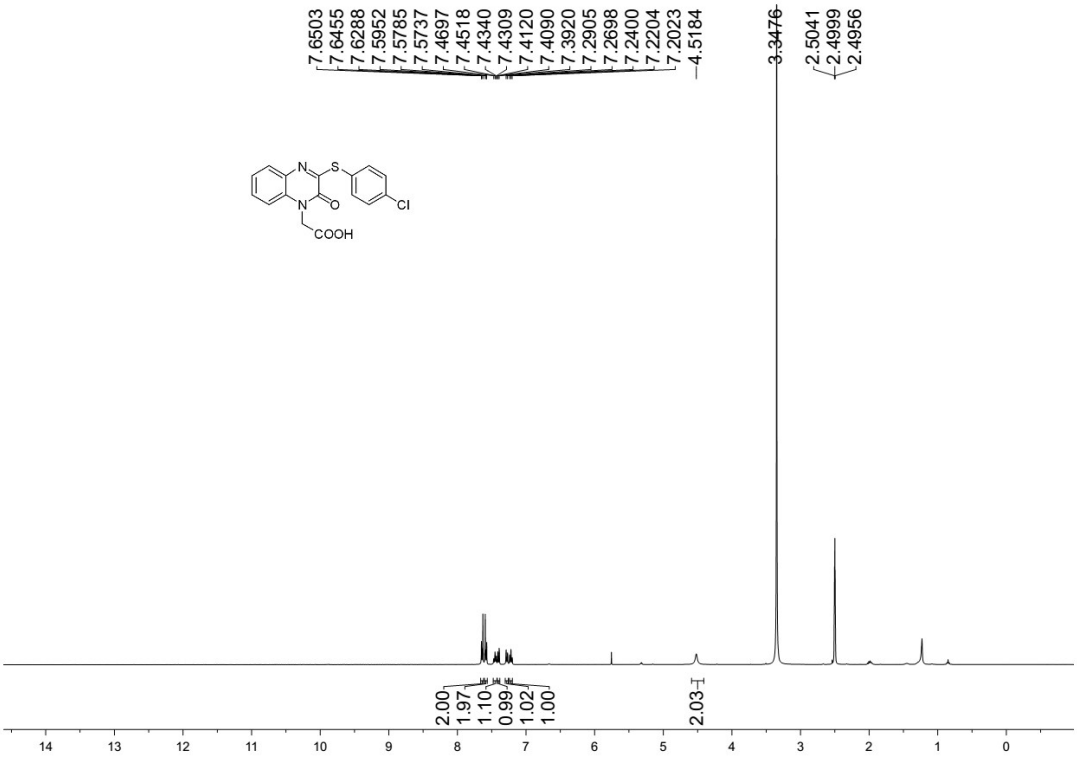
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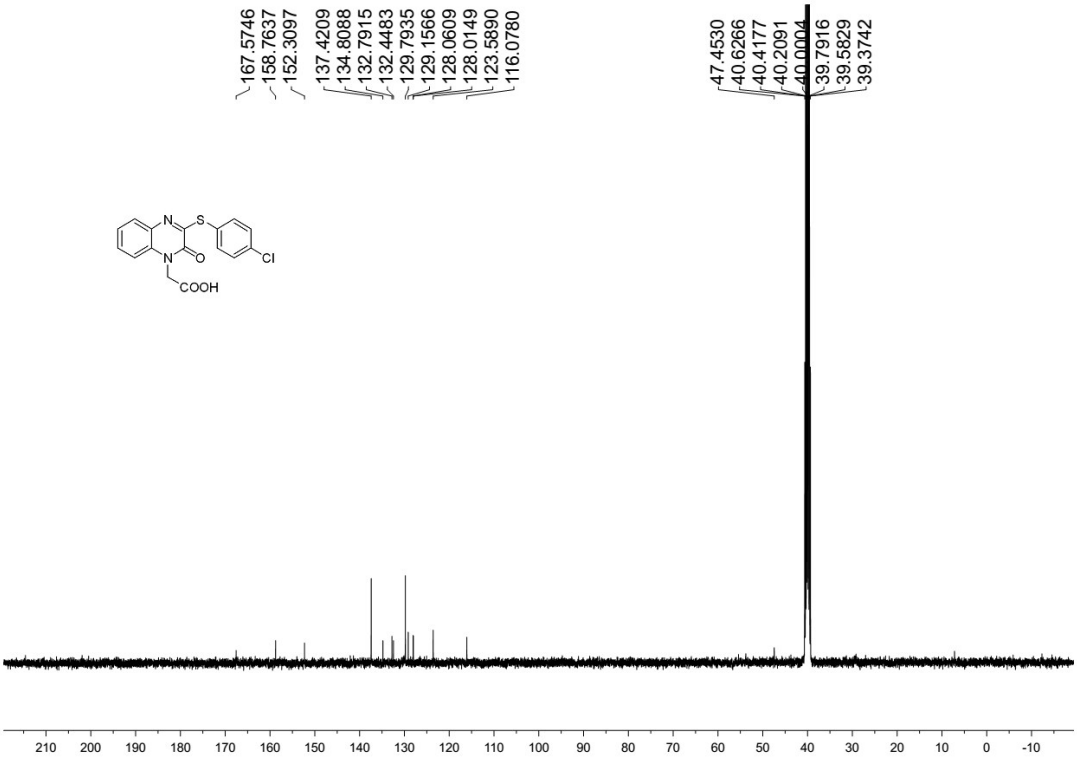
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