

Supporting Information

HBr as a dual functional catalyst enabling aerobic CDC coupling of quinoxalin-2(1H)-ones with electron-rich heteroarenes

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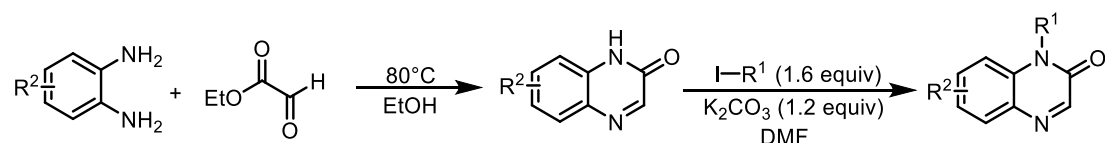
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1. General information

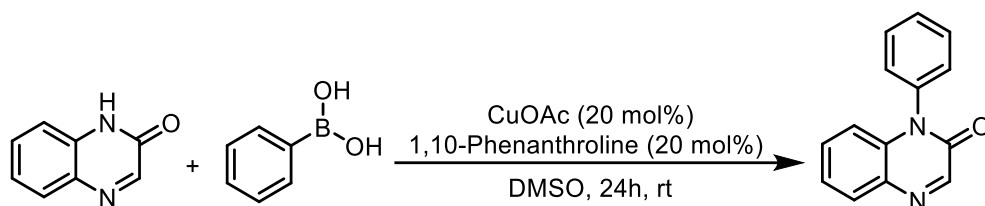
All reactions were carried out with magnetic stirring and in dried glassware. Standard syringe techniques were applied for transfer of dry solvents. The reactions via general procedure were carried out under an atmosphere of oxygen unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh) and thin layer chromatography was performed using silica gel (GF254). ^1H NMR and ^{13}C NMR spectra were recorded on Bruker-AVANCE-III-HD (400 and 100 MHz, respectively) and processed using MestReNova. Spectra were calibrated relative to resonances of the deuterated solvents for proton and carbon chemical shifts: DMSO ($\delta = 2.50$ for ^1H NMR and $\delta = 39.50$ for ^{13}C NMR), CDCl_3 ($\delta = 0$ for ^1H NMR and $\delta = 77.00$ for ^{13}C NMR). Mass spectra were measured on Agilent 5977 GC-MS instrument (EI). High-resolution mass spectra (ESI) were obtained with the Thermo Scientific LTQ Orbitrap XL mass spectrometer. The structures of known compounds were further corroborated by comparing their ^1H NMR, ^{13}C NMR data and MS data with those in literature. Melting points were measured with a YUHUA X-5 melting point instrument and were uncorrected. Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification.

2. Preparation of substrates and characterization data

Preparation of substrates and characterization data.^{1,2}



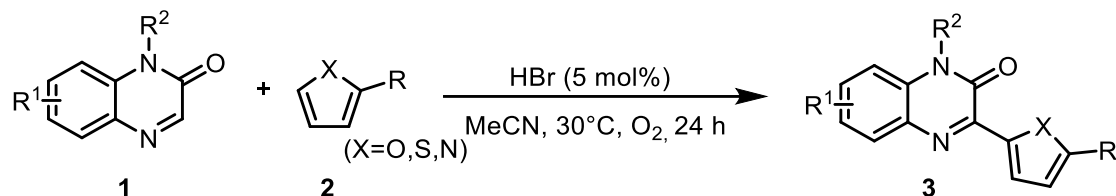
Quinoxalin-2(1H)-ones were prepared by two-step reactions based on the literature procedure. To an oven-dried 50 mL round-bottom flask charged with a magnetic stirring bar, *o*-aryl diamine (5.0 mmol, 1.0 equiv), ethyl glyoxylate (6.0 mmol, 1.2 equiv), and 20 mL of EtOH were added. The reaction mixture was stirred at 80 °C in an oil bath until the starting material was fully consumed as monitored by TLC (12–18 h). The resulting precipitate was filtered, washed with EtOH (3 × 10 mL), and dried to provide quinoxalin-2(1H)-ones, which was directly used in the next step without further purification. In the next step, the corresponding quinoxalin-2(1H)-ones (4.5 mmol, 1.0 equiv) was dissolved in DMF (20 mL), followed by addition of K₂CO₃ (5.4 mmol, 1.2 equiv) and the corresponding alkyl halide (7.2 mmol, 1.6 equiv). The reaction mixture was stirred at room temperature for 12 h. After completion of the reaction (confirmed by TLC), saturated aqueous NH₄Cl (5 mL) was added, and the mixture was extracted with ethyl acetate (3 × 25 mL). The combined organic layers were washed with water (90 mL), dried over anhydrous MgSO₄, concentrated, and subjected to silica gel flash column chromatography using 20% ethyl acetate in hexanes as eluent to afford the N1-protected quinoxalin-2(1H)-ones.



1-phenylquinoxalin-2(1H)-one was prepared by one step reactions based on the literature procedure. To an oven-dried 50 mL round-bottom flask charged with a magnetic stirring bar, quinoxalin-2(1H)-one (5.0 mmol, 1.0 equiv), phenylboronic acid (7.5 mmol, 1.5 equiv), CuOAc (1.0 mmol, 0.2 equiv), 1,10-phenanthroline (1.0 mmol, 0.2 equiv), and 12 mL of DMSO were added. The resulting reaction mixture was stirred at room temperature for 24 h. The reaction was monitored by TLC. After completion of the reaction, the mixture was worked up with ethyl acetate. The product and other organic residues were carefully removed from the supernatant. The combined organic layers were dried under reduced pressure and concentrated. The crude product was adsorbed onto silica gel and purified by column chromatography (eluent: hexane/ethyl acetate) to afford analytically pure 1-phenylquinoxalin-2(1H)-one as a white solid.

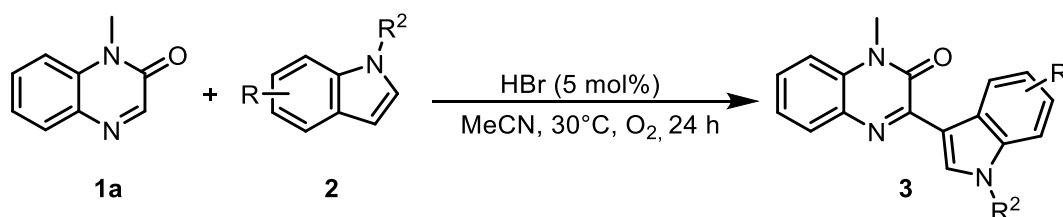
4. General experimental procedure

General reaction procedure for the synthesis of 3a-3u:



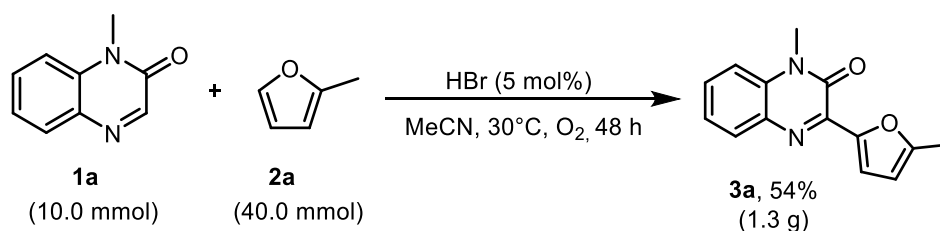
To a 10 mL reactor were added **1** (0.2 mmol, 1.0 equiv), **2** (0.8 mmol, 4.0 equiv), HBr (0.01 mmol, 5 mol%), and MeCN (0.1 M, 2 mL). The atmosphere was exchanged by applying vacuum and backfilling with O_2 (this process was repeated three times). The resulting mixture was stirred at 30 °C for 24 h. Upon completion of the reaction as confirmed by TLC, the residue was purified by flash column chromatography using a mixed solvent of petroleum ether and ethyl acetate to afford the target product **3**.

General reaction procedure for the synthesis of 3v-3al:



To a 10 mL reactor were added **1a** (0.2 mmol, 1.0 equiv), **2** (0.3 mmol, 1.5 equiv), HBr (0.01 mmol, 5 mol%), and MeCN (0.1 M, 2 mL). The atmosphere was exchanged by applying vacuum and backfilling with O_2 (this process was repeated three times). The resulting mixture was stirred at 30 °C for 24 h. Upon completion of the reaction as confirmed by TLC, the residue was purified by flash column chromatography using a mixed solvent of petroleum ether and ethyl acetate to afford the target product **3**.

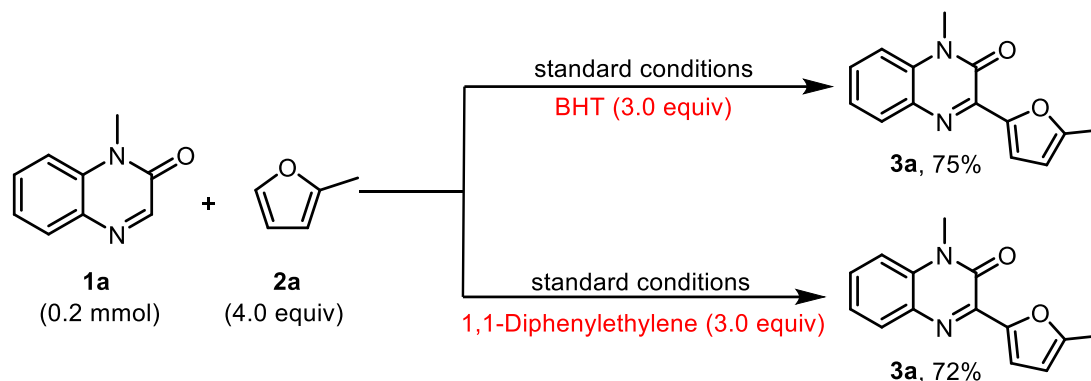
5. Scale-up experiments



In a 100 mL Schlenk tube, quinoxalin-2(1H)-ones (**1a**, 1.6 g, 10.0 mmol), 2-methylfuran (**2a**, 3.6 mL, 40.0 mmol, 4.0 equiv), HBr (60.0 μ L, 0.5 mmol, 5 mol%) and MeCN (40 mL) were added. The atmosphere was exchanged by applying vacuum and backfilling with O_2 (this process was repeated three times). The resulting mixture was stirred at 30 °C for 48 h. After completion of the reaction (monitored by TLC), the residue was purified by column chromatography using a mixture of petroleum ether and ethyl acetate as the eluent to afford the desired product **3a** in 54% yield (1.3 g).

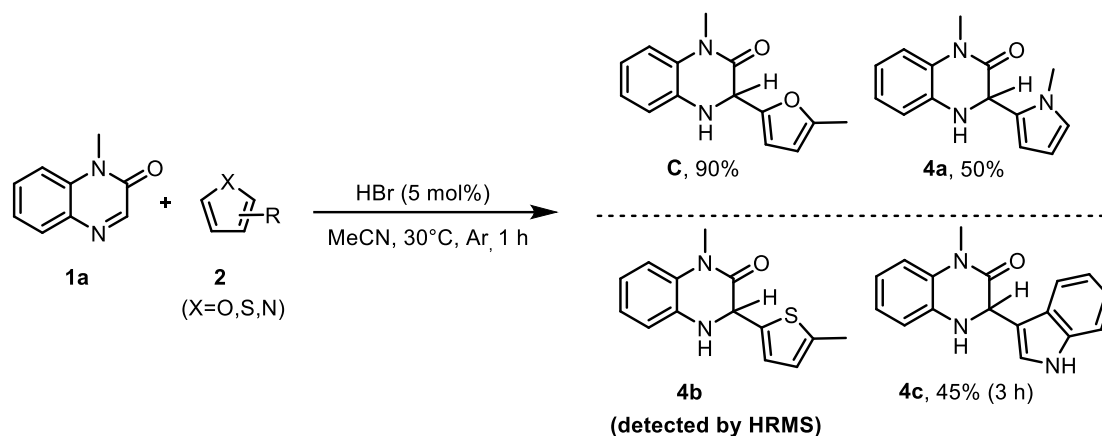
6. Mechanistic studies

6.1 Radical trapping experiments



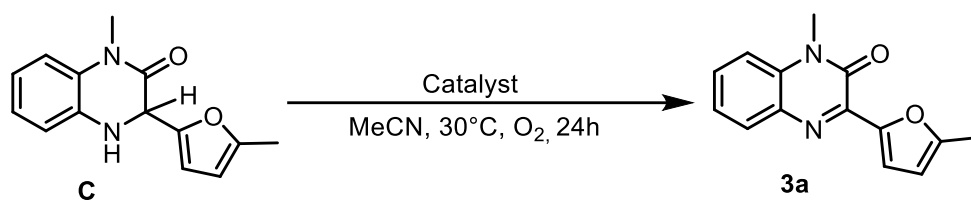
A 10 mL reaction vessel was charged with quinoxalin-2(1H)-ones (0.2 mmol), 2-methylfuran (0.8 mmol, 4.0 equiv), HBr (0.01 mmol, 5 mol%), and MeCN (0.1 M, 2 mL). Subsequently, a radical scavenger was added: either BHT (0.6 mmol, 3.0 equiv) or 1,1-diphenylethylene (0.6 mmol, 3.0 equiv). The atmosphere was exchanged by applying vacuum and backfilling with O₂ (this process was repeated three times). The resulting mixture was stirred at 30 °C for 24 h. Upon completion of the reaction, the yields of **3a** were 75% and 72%, respectively.

6.2 Intermediate trapping



Four separate 10 mL reaction vessels were each charged with quinoxalin-2(1H)-ones (0.2 mmol), HBr (0.01 mmol, 5 mol%), and MeCN (0.1 M, 2 mL). To these mixtures were then added the following substrates respectively: 2-methylfuran (0.8 mmol, 4.0 equiv), N-methylpyrrole (0.8 mmol, 4.0 equiv), 2-methylthiophene (0.8 mmol, 4.0 equiv), and indole (0.3 mmol, 1.5 equiv). The atmosphere was exchanged by applying vacuum and backfilling with O₂ (this process was repeated three times). The resulting mixtures were stirred at 30 °C for 1-3 h. After the reaction, intermediates **C**, **4a**, and **4d** were isolated in 90%, 50%, and 45% yields, respectively. The structure of product **4b** was confirmed by HRMS analysis.

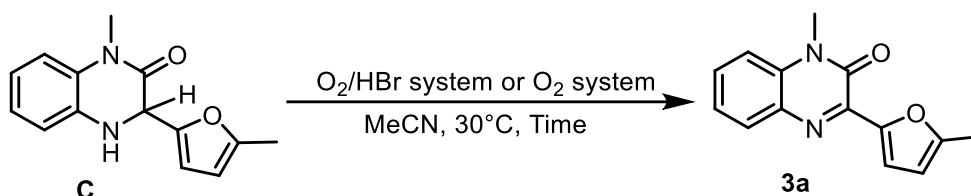
6.3 Role of HBr in the conversion of **C** to **3a**



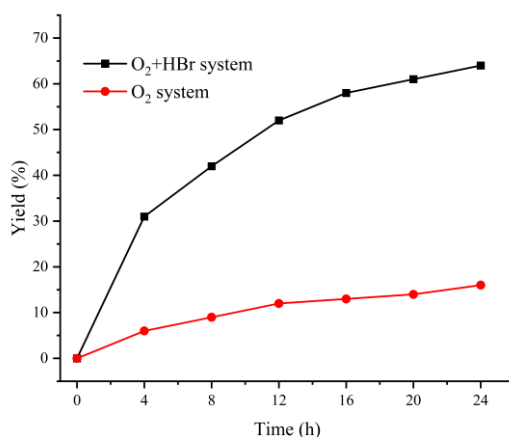
| Entry | Catalyst | Yield (%) ^b |
|----------------|--------------------------------|------------------------|
| 1 | – | 15 |
| 2 | HBr (5 mol%) | 64 |
| 3 | LiBr (25 mol%) | 16 |
| 4 | TFA (25 mol%) + LiBr (25 mol%) | 51 |
| 5 ^c | Br ₂ (25 mol%) | 39 |

^aReaction conditions: **C** (0.2 mmol), and additive in MeCN (2.0 mL) at 30 °C under O₂ atmosphere for 24 h. ^bIsolated yield. ^cUnder Ar atmosphere.

6.4 Comparison between the O₂/HBr system and the O₂ system



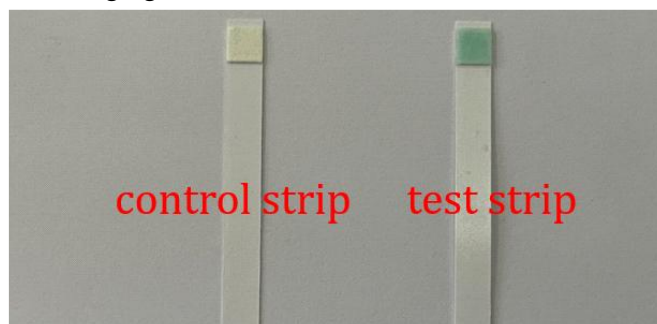
Two separate 10 mL reaction vessels were each charged with **C** (0.2 mmol) and MeCN (0.1 M, 2 mL). To one of the systems was added HBr (0.01 mmol, 5 mol%). The atmosphere was exchanged by applying vacuum and backfilling with O₂ (this process was repeated three times). The resulting mixtures were stirred at 30 °C. Subsequently, the yield of **3a** was recorded at 4-hour intervals, and a total of six sets of data were collected. The results are shown in the following figure.



6.5 Hydrogen peroxide test strips

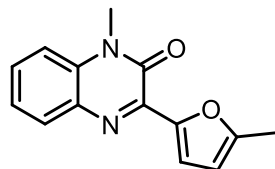
In a 10 mL reaction vessel, quinoxalin-2(1H)-ones (**1a**, 0.2 mmol, 1.0 equiv) and 2-methylfuran (**2a**, 0.8 mmol, 4.0 equiv) were added, followed by MeCN (2 mL) and hydrobromic acid (5 mol%). The atmosphere was exchanged by applying vacuum and backfilling with O₂ (this process was repeated

three times). The resulting mixture was stirred at 30 °C for 24 h. The reaction mixture was extracted with 20 mL of deionized water. A 10 mL aliquot of the aqueous extract was taken, into which a hydrogen peroxide test strip was immersed for 10 seconds. The strip was then promptly removed, excess liquid was shaken off, and it was left to stand for 60 seconds to allow for full color development. By comparing the developed color with a standard color chart, the formation of hydrogen peroxide in the reaction system was confirmed. The corresponding experimental results are presented in the following figure.



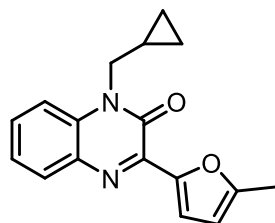
7. Characterization data of products

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



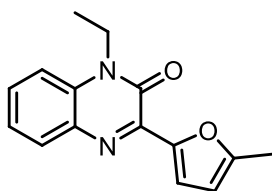
3a (78%, 37.4 mg) as a yellow solid (mp 174-176 °C); ^1H NMR (400 MHz, CDCl_3) δ 7.98 (dd, $J = 8.1, 1.6$ Hz, 1H), 7.88 (d, $J = 3.4$ Hz, 1H), 7.55 – 7.46 (m, 1H), 7.38 – 7.29 (m, 2H), 6.27 – 6.22 (m, 1H), 3.76 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.7, 152.9, 148.0, 143.9, 133.0, 132.2, 129.9, 129.4, 123.8, 121.2, 113.5, 109.4, 29.1, 14.2; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}_2^+$ 241.0972, found 241.0971.

1-(cyclopropylmethyl)-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3b)



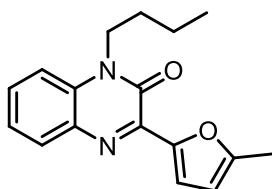
3b (73%, 40.9 mg) as a brown solid (mp 122-124 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, $J = 7.8$ Hz, 1H), 7.86 (d, $J = 3.5$ Hz, 1H), 7.50 (t, $J = 7.7$ Hz, 1H), 7.44 (s, 1H), 7.40 – 7.26 (m, 1H), 6.23 (d, $J = 3.8$ Hz, 1H), 4.27 (d, $J = 7.0$ Hz, 2H), 2.50 (s, 3H), 1.32 (dd, $J = 10.0, 5.0$ Hz, 1H), 0.57 (t, $J = 8.1$ Hz, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.5, 152.9, 148.1, 144.1, 133.2, 131.6, 130.1, 129.3, 123.6, 121.1, 113.7, 109.3, 46.0, 14.2, 9.6, 4.1; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_2^+$ 281.1285, found 281.1286.

1-ethyl-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3c)



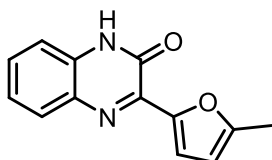
3c (71%, 36.1 mg) as a brown solid (mp 139-141 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, $J = 7.9$ Hz, 1H), 7.88 (d, $J = 3.4$ Hz, 1H), 7.54 – 7.47 (m, 1H), 7.35 (t, $J = 7.6$ Hz, 2H), 6.24 (d, $J = 3.5$ Hz, 1H), 4.40 (q, $J = 7.2$ Hz, 2H), 2.51 (s, 3H), 1.42 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.6, 152.5, 148.0, 143.9, 133.3, 131.1, 130.2, 129.4, 123.6, 121.1, 113.3, 109.4, 37.4, 14.2, 12.3; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_2^+$ 255.1128, found 255.1128.

1-butyl-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3d)



3d (70%, 39.5 mg) as a brown liquid; ^1H NMR (400 MHz, CDCl_3) δ 8.00 (dd, $J = 8.1$, 1.6 Hz, 1H), 7.88 (d, $J = 3.4$ Hz, 1H), 7.54 – 7.45 (m, 1H), 7.38 – 7.29 (m, 2H), 6.24 (d, $J = 3.5$ Hz, 1H), 4.38 – 4.25 (m, 2H), 2.50 (s, 3H), 1.77 (q, $J = 8.0$ Hz, 2H), 1.52 (q, $J = 7.5$ Hz, 2H), 1.01 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.6, 152.6, 148.1, 143.9, 133.3, 131.3, 130.2, 129.3, 123.6, 121.1, 113.5, 109.4, 42.2, 29.2, 20.3, 14.2, 13.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{19}\text{N}_2\text{O}_2^+$ 283.1441, found 283.1444.

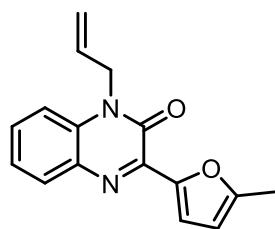
3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3e)



3e (61%, 27.6 mg) as a yellow solid (mp 229-231 °C); ^1H NMR (400 MHz, DMSO) δ 12.57 (s, 1H), 7.80 (d, $J = 8.3$ Hz, 1H), 7.72 (d, $J = 3.4$ Hz, 1H), 7.47 (t, $J = 7.7$ Hz,

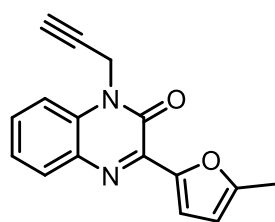
1H), 7.31 (d, $J = 7.6$ Hz, 2H), 6.35 (d, $J = 3.7$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 155.9, 152.9, 147.8, 144.5, 132.1, 131.0, 129.5, 128.2, 123.6, 120.1, 115.2, 109.3, 13.7; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{11}\text{N}_2\text{O}_2^+$ 227.0815, found 227.0812.

1-allyl-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3f)



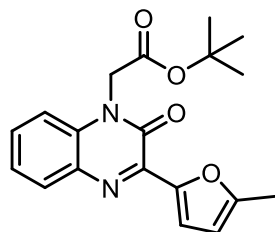
3f (80%, 42.6 mg) as a brown solid (mp 149-151 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.00 (dd, $J = 8.0, 1.7$ Hz, 1H), 7.88 (d, $J = 3.4$ Hz, 1H), 7.51 – 7.42 (m, 1H), 7.39 – 7.32 (m, 1H), 7.30 – 7.27 (m, 1H), 6.27 – 6.22 (m, 1H), 6.04 – 5.92 (m, 1H), 5.28 (d, $J = 10.4$ Hz, 1H), 5.17 (d, $J = 17.2$ Hz, 1H), 5.01 – 4.94 (m, 2H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.7, 152.5, 148.0, 143.9, 133.2, 131.4, 130.4, 130.0, 129.3, 123.8, 121.3, 117.9, 114.0, 109.5, 44.5, 14.2; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}_2^+$ 267.1128, found 267.1129.

3-(5-methylfuran-2-yl)-1-(prop-2-yn-1-yl)quinoxalin-2(1H)-one (3g)



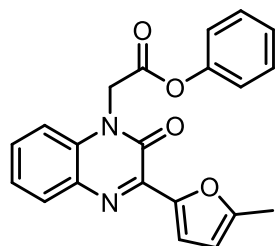
3g (61%, 32.2 mg) as a yellow solid (mp 195-197 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.00 (dd, $J = 8.1, 1.6$ Hz, 1H), 7.88 (d, $J = 3.4$ Hz, 1H), 7.58 – 7.51 (m, 1H), 7.46 (d, $J = 7.1$ Hz, 1H), 7.39 (t, $J = 7.6$ Hz, 1H), 6.24 (d, $J = 3.7$ Hz, 1H), 5.12 (d, $J = 2.6$ Hz, 2H), 2.50 (s, 3H), 2.31 (t, $J = 2.6$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.9, 152.1, 147.8, 143.7, 133.2, 130.7, 130.1, 129.5, 124.2, 121.5, 113.9, 109.6, 76.7, 73.1, 31.5, 14.2; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{13}\text{N}_2\text{O}_2^+$ 265.0972, found 265.0962.

tert-butyl 2-(3-(5-methylfuran-2-yl)-2-oxoquinoxalin-1(2H)-yl)acetate (3h)



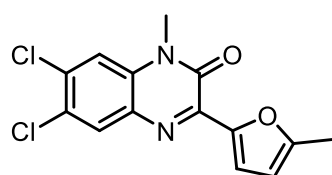
3h (55%, 37.4 mg) as a brown solid (mp 109-111 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.00 (d, *J* = 7.9 Hz, 1H), 7.85 (d, *J* = 3.5 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.07 (d, *J* = 8.3 Hz, 1H), 6.24 (d, *J* = 3.5 Hz, 1H), 5.01 (s, 2H), 2.50 (s, 3H), 1.46 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 166.0, 156.8, 152.6, 147.9, 143.8, 133.0, 131.4, 130.2, 129.5, 124.0, 121.4, 113.0, 109.5, 83.1, 44.2, 27.9, 14.2; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₉H₂₁N₂O₄⁺ 341.1496, found 341.1497.

phenyl 2-(3-(5-methylfuran-2-yl)-2-oxoquinoxalin-1(2H)-yl)acetate (3i)



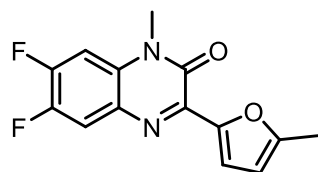
3i (56%, 40.3 mg) as a yellow solid (mp 187-189 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 3.4 Hz, 1H), 7.55 – 7.47 (m, 1H), 7.40 – 7.33 (m, 3H), 7.25 – 7.18 (m, 2H), 7.09 (d, *J* = 8.6 Hz, 2H), 6.25 (d, *J* = 3.5 Hz, 1H), 5.33 (s, 2H), 2.50 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 165.8, 157.0, 152.6, 150.0, 147.8, 143.7, 133.2, 131.3, 130.4, 129.6, 129.5, 126.3, 124.3, 121.5, 121.1, 112.8, 109.6, 43.6, 14.2; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₁H₁₇N₂O₄⁺ 361.1183, found 361.1180.

6,7-dichloro-1-methyl-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3j)



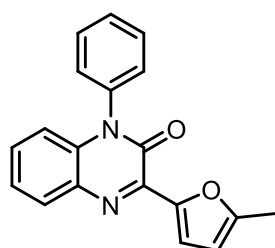
3j (66%, 40.7 mg) as a yellow solid (mp 175-177 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.02 (s, 1H), 7.87 (d, *J* = 3.7 Hz, 1H), 7.35 (s, 1H), 6.24 (d, *J* = 3.7 Hz, 1H), 3.69 (s, 3H), 2.49 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.6, 152.3, 147.7, 144.5, 133.0, 132.2, 131.5, 130.4, 127.6, 122.5, 114.9, 109.8, 29.3, 14.2; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₁Cl₂N₂O₂⁺ 309.0192, found 309.0190.

6,7-difluoro-1-methyl-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3k)



3k (55%, 30.7 mg) as a yellow solid (mp 201-203 °C); ¹H NMR (400 MHz, CDCl₃) δ 7.85 (d, *J* = 3.4 Hz, 1H), 7.77 (dd, *J* = 10.5, 8.2 Hz, 1H), 7.09 (dd, *J* = 11.3, 7.2 Hz, 1H), 6.27 – 6.22 (m, 1H), 3.70 (s, 3H), 2.50 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.2, 152.5, 150.7 (dd, *J* = 251.6, 14.6 Hz), 147.7, 146.8 (dd, *J* = 245.2, 13.9 Hz), 144.0 (d, *J* = 3.6 Hz), 129.4 (d, *J* = 17.3 Hz), 129.4 (d, *J* = 2.3 Hz), 121.9, 117.2 (dd, *J* = 18.2, 2.0 Hz), 109.7, 102.1 (d, *J* = 23.3 Hz), 29.6, 14.2; ¹⁹F NMR (376 MHz, CDCl₃) δ -131.67, -131.73, -141.71, -141.77; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₁F₂N₂O₂⁺ 277.0783, found 277.0795.

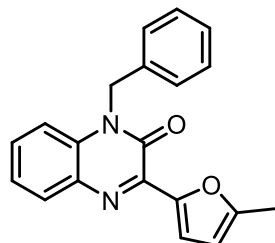
3-(5-methylfuran-2-yl)-1-phenylquinoxalin-2(1H)-one (3l)



3l (54%, 32.6 mg) as a yellow solid (mp 182-184 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.03 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.84 (d, *J* = 3.4 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 2H), 7.61 – 7.55 (m, 1H), 7.36 – 7.27 (m, 4H), 6.66 (dd, *J* = 7.9, 1.8 Hz, 1H), 6.22 (dd, *J* = 3.5, 1.1 Hz, 1H), 2.52 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 156.9, 152.9, 147.9, 144.4, 135.8, 133.0, 132.9, 130.3, 129.5, 129.5, 129.0, 128.2, 124.0, 121.5, 115.3, 109.6, 14.2;

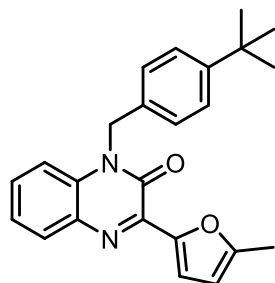
HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{19}H_{15}N_2O_2^+$ 303.1128, found 303.1129.

1-benzyl-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3m)



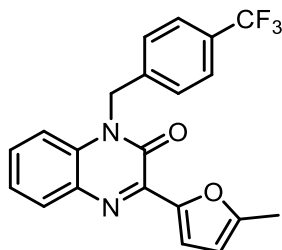
3m (60%, 37.9 mg) as a yellow solid (mp 156-158 °C); 1H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, $J = 7.9, 1.7$ Hz, 1H), 7.91 (d, $J = 3.4$ Hz, 1H), 7.39 – 7.28 (m, 4H), 7.25 (t, $J = 6.7$ Hz, 4H), 6.25 (d, $J = 3.7$ Hz, 1H), 5.57 (s, 2H), 2.51 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 153.1, 148.0, 144.0, 135.1, 133.3, 131.5, 130.0, 129.4, 128.9, 127.6, 126.6, 123.9, 121.4, 114.3, 109.5, 45.9, 14.2; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{20}H_{17}N_2O_2^+$ 317.1285, found 317.1294.

1-(4-(tert-butyl)benzyl)-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3n)



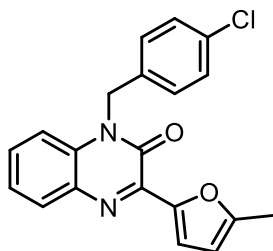
3n (63%, 46.9 mg) as a brown solid (mp 184-186 °C); 1H NMR (400 MHz, $CDCl_3$) δ 7.99 (dd, $J = 7.9, 1.7$ Hz, 1H), 7.91 (d, $J = 3.4$ Hz, 1H), 7.41 – 7.35 (m, 1H), 7.34 – 7.26 (m, 4H), 7.18 (d, $J = 8.4$ Hz, 2H), 6.28 – 6.17 (m, 1H), 5.53 (s, 2H), 2.51 (s, 3H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 153.0, 150.5, 148.0, 144.0, 133.2, 132.0, 131.6, 130.0, 129.4, 126.4, 125.8, 123.8, 121.4, 114.3, 109.5, 45.5, 34.4, 31.2, 14.2; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{24}H_{25}N_2O_2^+$ 373.1911, found 373.1912.

3-(5-methylfuran-2-yl)-1-(4-(trifluoromethyl)benzyl)quinoxalin-2(1H)-one (3o)



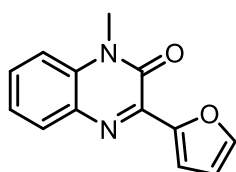
3o (65%, 49.9 mg) as a yellow solid (mp 156-158 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, $J = 7.9, 1.8$ Hz, 1H), 7.89 (d, $J = 3.4$ Hz, 1H), 7.58 (d, $J = 8.3$ Hz, 2H), 7.42 – 7.32 (m, 4H), 7.16 (dd, $J = 8.2, 1.3$ Hz, 1H), 6.26 (d, $J = 3.5$ Hz, 1H), 5.61 (s, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.0, 153.0, 147.9, 143.9, 139.2, 133.3, 131.3, 130.2, 130.0 (q, $J = 32.0$ Hz), 129.5, 127.0, 125.9 (q, $J = 3.5$ Hz), 124.2, 123.8 (q, $J = 270.1$ Hz), 121.6, 113.9, 109.6, 45.5, 14.2; ^{19}F NMR (376 MHz, CDCl_3) δ -62.60; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{21}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_2^+$ 385.1158, found 385.1159.

1-(4-chlorobenzyl)-3-(5-methylfuran-2-yl)quinoxalin-2(1H)-one (3p)



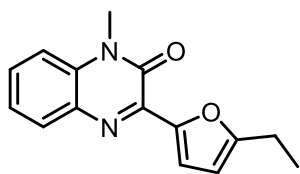
3p (65%, 45.5 mg) as a yellow solid (mp 187-189 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.00 (dd, $J = 7.9, 1.8$ Hz, 1H), 7.89 (d, $J = 3.5$ Hz, 1H), 7.41 – 7.36 (m, 1H), 7.35 – 7.26 (m, 3H), 7.19 (d, $J = 8.6$ Hz, 3H), 6.25 (d, $J = 3.5$ Hz, 1H), 5.52 (s, 2H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.9, 153.0, 147.9, 143.9, 133.6, 133.5, 133.3, 131.3, 130.1, 129.4, 129.1, 128.1, 124.0, 121.5, 114.0, 109.5, 45.3, 14.2; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{16}\text{ClN}_2\text{O}_2^+$ 351.0895, found 351.0893.

3-(furan-2-yl)-1-methylquinoxalin-2(1H)-one (3q)³



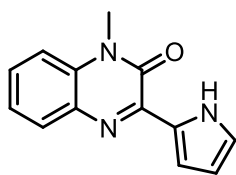
3q (62%, 28.0 mg) as a yellow solid (mp 151-153 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.02 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.94 (d, *J* = 3.5 Hz, 1H), 7.73 (s, 1H), 7.59 – 7.51 (m, 1H), 7.43 – 7.31 (m, 2H), 6.63 (dd, *J* = 3.5, 1.8 Hz, 1H), 3.79 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 152.9, 149.2, 145.7, 144.1, 132.9, 132.4, 130.2, 130.0, 124.0, 119.2, 113.6, 112.5, 29.1.

3-(5-ethylfuran-2-yl)-1-methylquinoxalin-2(1H)-one (3r)



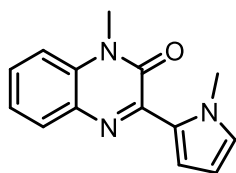
3r (74%, 37.6 mg) as a yellow solid (mp 144-146 °C); ¹H NMR (400 MHz, CDCl₃) δ 7.97 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.89 (d, *J* = 3.4 Hz, 1H), 7.52 – 7.45 (m, 1H), 7.36 – 7.28 (m, 2H), 6.26 (d, *J* = 3.5 Hz, 1H), 3.75 (s, 3H), 2.87 (q, *J* = 7.6 Hz, 2H), 1.33 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 162.3, 152.9, 147.8, 143.9, 133.0, 132.1, 129.9, 129.3, 123.7, 121.0, 113.4, 107.7, 29.0, 21.7, 11.7; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₅N₂O₂⁺ 255.1128, found 255.1128.

1-methyl-3-(1H-pyrrol-2-yl)quinoxalin-2(1H)-one (3s)⁴



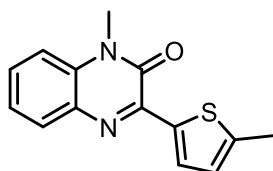
3s (58%, 26.1 mg) as a yellow solid (mp 174-176 °C); ¹H NMR (400 MHz, CDCl₃) δ 10.75 (s, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.37 – 7.26 (m, 2H), 7.04 (d, *J* = 1.6 Hz, 1H), 6.38 (q, *J* = 2.7 Hz, 1H), 3.75 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.4, 144.9, 133.5, 131.9, 129.4, 129.1, 128.5, 123.9, 122.2, 114.7, 113.5, 110.8, 29.0.

1-methyl-3-(1-methyl-1H-pyrrol-2-yl)quinoxalin-2(1H)-one (3t)⁵



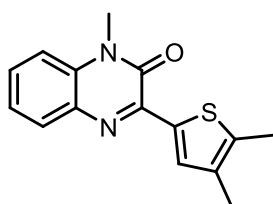
3t (61%, 29.2 mg) as a yellow solid (mp 150-152 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.08 (t, $J = 2.0$ Hz, 1H), 7.83 (dd, $J = 7.9, 1.6$ Hz, 1H), 7.46 – 7.38 (m, 1H), 7.32 – 7.25 (m, 2H), 7.06 (dd, $J = 2.9, 1.7$ Hz, 1H), 6.65 (t, $J = 2.5$ Hz, 1H), 3.73 (s, 3H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 154.3, 150.1, 133.5, 132.0, 129.1, 128.1, 128.0, 123.4, 122.6, 120.9, 113.3, 109.2, 36.4, 29.0.

1-methyl-3-(5-methylthiophen-2-yl)quinoxalin-2(1H)-one (3u)⁶



3u (53%, 27.1 mg) as a yellow solid (mp 183-185 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.28 (d, $J = 3.8$ Hz, 1H), 7.83 (d, $J = 7.9$ Hz, 1H), 7.48 (t, $J = 7.8$ Hz, 1H), 7.35 – 7.26 (m, 2H), 6.85 (d, $J = 3.9$ Hz, 1H), 3.75 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.6, 148.1, 146.9, 137.0, 133.1, 132.3, 132.3, 129.5, 129.2, 126.5, 123.8, 113.5, 29.2, 15.6.

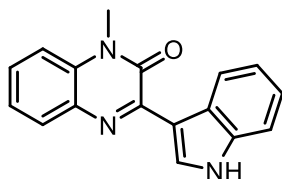
3-(4,5-dimethylthiophen-2-yl)-1-methylquinoxalin-2(1H)-one (3v)



3v (63%, 34.0 mg) as a yellow solid (mp 189-191 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.16 (s, 1H), 7.81 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.49 – 7.41 (m, 1H), 7.31 (t, $J = 7.6$ Hz, 1H), 7.26 (d, $J = 8.5$ Hz, 1H), 3.73 (s, 3H), 2.41 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.7, 148.1, 140.9, 134.8, 134.5, 134.2, 133.2, 132.3, 129.5, 129.0, 123.7, 113.4, 29.1, 13.6, 13.5; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{OS}^+$

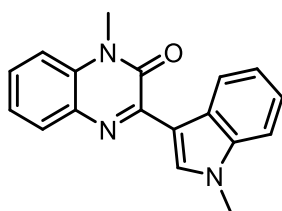
271.0900, found 271.0897.

3-(1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3w)⁷



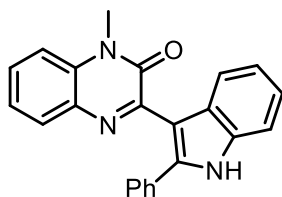
3w (91%, 50.1 mg) as a yellow solid (mp 217-219 °C); ¹H NMR (400 MHz, DMSO) δ 11.80 (s, 1H), 8.98 – 8.85 (m, 2H), 7.89 (d, *J* = 7.3 Hz, 1H), 7.58 – 7.45 (m, 3H), 7.42 – 7.31 (m, 1H), 7.30 – 7.20 (m, 2H), 3.69 (s, 3H); ¹³C NMR (100 MHz, DMSO) δ 153.7, 150.7, 136.3, 133.2, 133.0, 131.5, 128.4, 128.3, 126.4, 123.5, 123.1, 122.6, 121.1, 114.5, 112.0, 111.5, 29.1.

1-methyl-3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3x)⁸



3x (90%, 52.0 mg) as a orange solid (mp 232-234 °C); ¹H NMR (400 MHz, CDCl₃) δ 9.06 – 8.97 (m, 1H), 8.82 (d, *J* = 2.9 Hz, 1H), 8.01 – 7.94 (m, 1H), 7.48 – 7.40 (m, 1H), 7.38 – 7.30 (m, 4H), 7.28 – 7.25 (m, 1H), 3.85 (s, 3H), 3.75 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.5, 150.7, 137.1, 136.6, 133.8, 131.5, 129.2, 128.0, 127.4, 123.6, 123.5, 122.8, 121.5, 113.3, 111.3, 109.3, 33.3, 29.1.

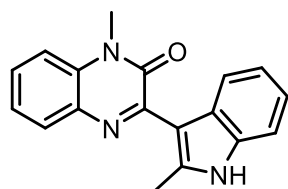
1-methyl-3-(2-phenyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3y)⁸



3y (77%, 54.1 mg) as a yellow solid (mp 210-212 °C); ¹H NMR (400 MHz, DMSO) δ 11.86 (s, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 7.7 Hz,

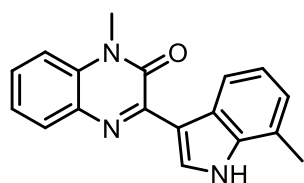
1H), 7.52 (dd, $J = 15.0, 8.0$ Hz, 4H), 7.40 – 7.30 (m, 4H), 7.19 (t, $J = 7.6$ Hz, 1H), 7.08 (t, $J = 7.5$ Hz, 1H), 3.58 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 153.7, 153.6, 139.2, 136.0, 133.2, 133.0, 132.7, 129.7, 129.0, 128.6, 128.4, 127.9, 127.8, 123.4, 122.1, 120.4, 120.0, 114.6, 111.5, 109.1, 29.3.

1-methyl-3-(2-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3z)⁷



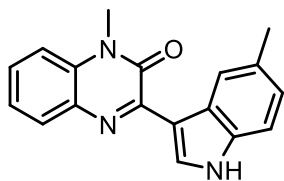
3z (50%, 28.9 mg) as a yellow solid (mp 249-251 °C); ^1H NMR (400 MHz, DMSO) δ 11.51 (s, 1H), 7.83 – 7.73 (m, 2H), 7.56 (d, $J = 2.3$ Hz, 2H), 7.40 – 7.31 (m, 2H), 7.11 – 6.99 (m, 2H), 3.70 (s, 3H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 154.0, 153.2, 139.3, 135.1, 132.8, 132.5, 129.1, 128.7, 128.0, 123.3, 120.9, 120.8, 119.5, 114.5, 110.6, 109.5, 29.3, 14.3.

1-methyl-3-(7-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3aa)⁹



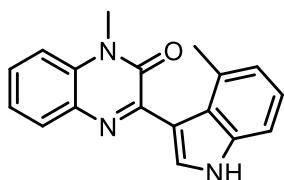
3aa (82%, 47.4 mg) as a yellow solid (mp 289-291 °C); ^1H NMR (400 MHz, DMSO) δ 11.79 (s, 1H), 8.92 (d, $J = 3.1$ Hz, 1H), 8.74 (d, $J = 7.9$ Hz, 1H), 7.89 (d, $J = 7.7$ Hz, 1H), 7.50 (d, $J = 4.3$ Hz, 2H), 7.40 – 7.33 (m, 1H), 7.15 (t, $J = 7.5$ Hz, 1H), 7.04 (d, $J = 7.1$ Hz, 1H), 3.70 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 153.7, 150.6, 135.7, 133.0, 132.9, 131.5, 128.4, 128.2, 126.1, 123.4, 123.2, 121.2, 121.0, 120.7, 114.4, 111.8, 29.1, 16.8.

1-methyl-3-(5-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3ab)⁹



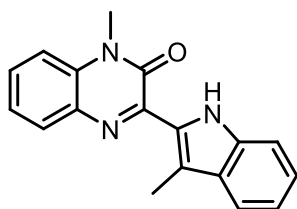
3ab (78%, 45.1 mg) as a yellow solid (mp >300 °C); ¹H NMR (400 MHz, DMSO) δ 11.69 (s, 1H), 8.89 (d, *J* = 2.9 Hz, 1H), 8.71 (s, 1H), 7.94 (d, *J* = 7.7 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.40 (dd, *J* = 8.3, 3.7 Hz, 2H), 7.07 (dd, *J* = 8.3, 1.8 Hz, 1H), 3.73 (s, 3H), 2.50 (s, 3H); ¹³C NMR (100 MHz, DMSO) δ 153.7, 150.7, 134.6, 133.2, 133.0, 131.4, 129.7, 128.4, 128.2, 126.6, 124.0, 123.4, 122.8, 114.4, 111.5, 111.0, 29.1, 21.7.

1-methyl-3-(4-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3ac)



3ac (66%, 38.2 mg) as a brown solid (mp 209-211 °C); ¹H NMR (400 MHz, DMSO) δ 11.70 (s, 1H), 8.23 (d, *J* = 3.1 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 7.0 Hz, 2H), 7.42 – 7.30 (m, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 7.2 Hz, 1H), 3.71 (s, 3H), 2.59 (s, 3H); ¹³C NMR (100 MHz, DMSO) δ 154.4, 151.2, 136.6, 132.4, 132.3, 131.3, 131.2, 128.9, 128.4, 125.1, 123.5, 122.6, 122.1, 114.6, 112.8, 109.7, 29.3, 22.9. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₈H₁₆N₃O⁺ 290.1288, found 290.1287.

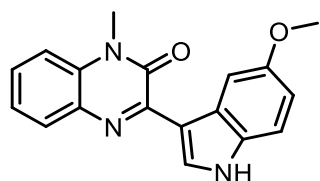
1-methyl-3-(3-methyl-1H-indol-2-yl)quinoxalin-2(1H)-one (3ad)⁸



3ad (65%, 37.6 mg) as a yellow solid (mp 280-282 °C); ¹H NMR (400 MHz, CDCl₃) δ 11.17 (s, 1H), 7.79 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.42 – 7.31 (m, 2H), 7.31 – 7.25 (m, 1H), 7.24 – 7.19 (m, 1H), 7.13 – 7.03 (m, 2H), 3.54 (s, 3H), 2.74 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 155.2, 146.5, 135.5, 133.5, 131.3, 129.6, 129.5,

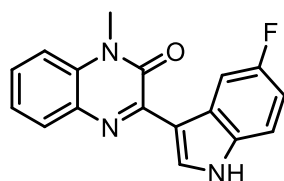
129.1, 128.4, 124.1, 123.9, 119.7, 119.2, 118.3, 113.4, 111.6, 28.9, 11.9.

3-(5-methoxy-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3ae)⁷



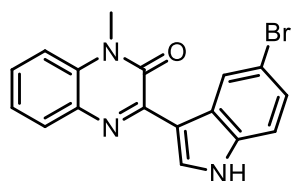
3ae (71%, 43.3 mg) as a brown solid (mp 230-232 °C); ¹H NMR (400 MHz, DMSO) δ 11.67 (s, 1H), 8.88 (d, *J* = 3.1 Hz, 1H), 8.47 (d, *J* = 2.6 Hz, 1H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.51 (d, *J* = 4.6 Hz, 2H), 7.45 – 7.34 (m, 2H), 6.92 – 6.86 (m, 1H), 3.88 (s, 3H), 3.71 (s, 3H); ¹³C NMR (100 MHz, DMSO) δ 154.9, 153.7, 150.7, 133.5, 132.9, 131.4, 131.2, 128.3, 128.1, 127.0, 123.5, 114.4, 112.5, 112.1, 111.2, 105.1, 55.2, 29.1.

3-(5-fluoro-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3af)



3af (66%, 38.7 mg) as a brown liquid; ¹H NMR (400 MHz, DMSO) δ 11.87 (s, 1H), 8.95 (d, *J* = 2.1 Hz, 1H), 8.56 (dd, *J* = 10.6, 2.7 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.45 (m, 3H), 7.39 – 7.31 (m, 1H), 7.13 – 7.04 (m, 1H), 3.68 (s, 3H); ¹³C NMR (100 MHz, DMSO) δ 158.3 (d, *J* = 231.0 Hz), 153.6, 150.4, 134.7, 132.94, 132.86, 131.5, 128.5, 126.8 (d, *J* = 9.0 Hz), 123.5, 114.5, 113.0 (d, *J* = 9.8 Hz), 111.5 (d, *J* = 4.3 Hz), 110.6 (d, *J* = 25.7 Hz), 107.8 (d, *J* = 24.5 Hz), 29.1; ¹⁹F NMR (376 MHz, DMSO) δ -122.20; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₇H₁₃FN₃O⁺ 294.1037, found 294.1042.

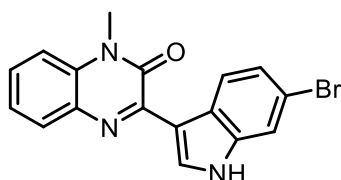
3-(5-bromo-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3ag)⁷



3ag (55%, 38.8 mg) as a yellow solid (mp 291-293 °C); ¹H NMR (400 MHz, DMSO)

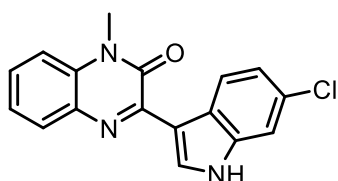
δ 11.95 (s, 1H), 8.98 (d, $J = 2.1$ Hz, 1H), 8.91 (d, $J = 3.1$ Hz, 1H), 7.83 (d, $J = 8.1$ Hz, 1H), 7.49 (q, $J = 8.4$ Hz, 3H), 7.39 – 7.31 (m, 2H), 3.66 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 153.5, 150.2, 135.1, 134.3, 132.8, 131.5, 128.6, 128.4, 128.0, 125.1, 123.5, 114.5, 113.9, 113.8, 110.9, 29.1.

3-(6-bromo-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3ah)⁸



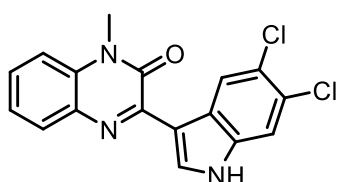
3ah (80%, 56.5 mg) as a yellow solid (mp 286-288 °C); ^1H NMR (400 MHz, DMSO) δ 11.85 (s, 1H), 8.89 (s, 1H), 8.78 (d, $J = 8.6$ Hz, 1H), 7.86 (d, $J = 7.8$ Hz, 1H), 7.69 (d, $J = 1.8$ Hz, 1H), 7.49 (d, $J = 6.0$ Hz, 2H), 7.38 – 7.29 (m, 2H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 153.5, 150.2, 137.2, 133.9, 132.8, 131.5, 128.5, 128.5, 125.3, 124.7, 123.7, 123.4, 115.2, 114.5, 114.4, 111.5, 29.1.

3-(6-chloro-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3ai)⁸



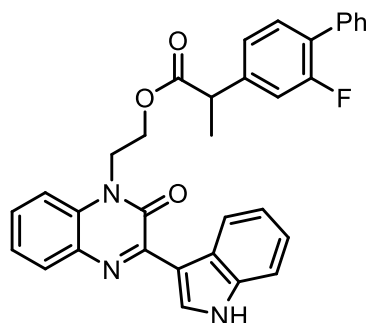
3ai (81%, 50.1 mg) as a yellow solid (mp 271-272 °C); ^1H NMR (400 MHz, DMSO) δ 11.84 (s, 1H), 8.90 (d, $J = 2.9$ Hz, 1H), 8.82 (d, $J = 8.7$ Hz, 1H), 7.84 (d, $J = 7.9$ Hz, 1H), 7.58 – 7.51 (m, 1H), 7.46 (d, $J = 10.8$ Hz, 2H), 7.33 (t, $J = 7.5$ Hz, 1H), 7.25 – 7.16 (m, 1H), 3.66 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 153.5, 150.2, 136.8, 133.9, 132.8, 131.5, 128.4, 127.1, 125.1, 124.3, 123.4, 121.1, 114.3, 111.6, 111.5, 29.0.

3-(5,6-dichloro-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3aj)⁸



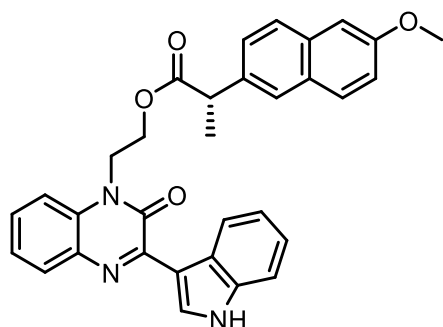
3aj (45%, 30.9 mg) as an orange solid (mp 256-258 °C); ¹H NMR (400 MHz, DMSO) δ 11.93 (s, 1H), 8.89 (d, *J* = 4.9 Hz, 2H), 7.80 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.68 (s, 1H), 7.56 – 7.43 (m, 2H), 7.39 – 7.30 (m, 1H), 3.64 (s, 3H); ¹³C NMR (100 MHz, DMSO) δ 153.8, 150.2, 135.6, 135.5, 133.0, 132.0, 129.1, 128.9, 126.5, 125.1, 124.1, 123.9, 114.8, 113.8, 111.4, 29.5.

2-(3-(1H-indol-3-yl)-2-oxoquinoxalin-1(2H)-yl)ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (3ak)



3ak (84%, 89.2 mg) as a yellow liquid; ¹H NMR (400 MHz, DMSO) δ 11.86 (s, 1H), 9.03 – 8.92 (m, 2H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 2H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.40 – 7.31 (m, 6H), 7.28 (dd, *J* = 6.2, 3.2 Hz, 2H), 7.19 (t, *J* = 8.2 Hz, 1H), 7.03 (d, *J* = 12.0 Hz, 1H), 6.96 – 6.90 (m, 1H), 4.73 – 4.58 (m, 2H), 4.52 (dd, *J* = 11.7, 5.4 Hz, 1H), 4.47 – 4.38 (m, 1H), 3.67 (q, *J* = 7.1 Hz, 1H), 1.26 (d, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, DMSO) δ 173.3, 158.8 (d, *J* = 244.9 Hz), 153.9, 150.5, 141.9 (d, *J* = 7.9 Hz), 136.4, 134.8, 133.3 (d, *J* = 4.7 Hz), 130.8, 130.6 (d, *J* = 3.9 Hz), 128.75, 128.68 (d, *J* = 2.7 Hz), 128.6, 128.2, 127.8, 126.8 (d, *J* = 13.0 Hz), 126.4, 123.8 (d, *J* = 3.2 Hz), 123.5, 123.2, 122.7, 121.2, 115.1 (d, *J* = 23.2 Hz), 114.4, 112.0, 111.4, 61.5, 44.0, 40.7, 17.9; ¹⁹F NMR (376 MHz, DMSO) δ -118.16; HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₃₃H₂₇FN₃O₃⁺ 532.2031, found 532.2026.

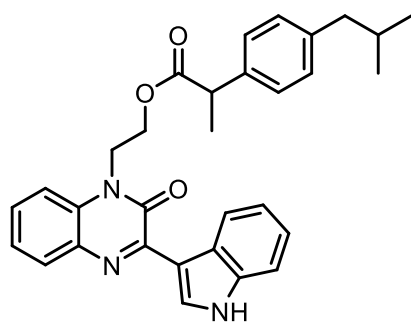
2-(3-(1H-indol-3-yl)-2-oxoquinoxalin-1(2H)-yl)ethyl (S)-2-(6-methoxynaphthalen-2-yl)propanoate (3al)



3al (78%, 80.7 mg) as a yellow solid (mp 117-119 °C); ^1H NMR (400 MHz, CDCl_3) δ 8.98 (d, $J = 7.8$ Hz, 1H), 8.79 (s, 2H), 7.95 – 7.88 (m, 1H), 7.57 (dd, $J = 14.9, 8.8$ Hz, 2H), 7.50 (s, 1H), 7.33 (q, $J = 7.9$ Hz, 2H), 7.27 – 7.20 (m, 5H), 7.08 (dd, $J = 8.9, 2.6$ Hz, 1H), 6.99 (d, $J = 2.7$ Hz, 1H), 4.59 – 4.50 (m, 1H), 4.50 – 4.39 (m, 3H), 3.84 (s, 3H), 3.72 (q, $J = 7.2$ Hz, 1H), 1.47 (d, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 174.8, 157.6, 154.3, 150.7, 136.1, 135.1, 133.9, 133.7, 132.4, 131.0, 129.6, 129.3, 128.9, 128.3, 127.3, 126.6, 126.0, 123.6, 123.5, 123.2, 121.7, 119.0, 113.5, 112.6, 111.3, 105.6, 61.4, 55.3, 45.4, 40.9, 18.4; HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{32}\text{H}_{28}\text{N}_3\text{O}_4^+$ 518.2074, found 518.2071.

2-(3-(1H-indol-3-yl)-2-oxoquinoxalin-1(2H)-yl)ethyl
isobutylphenyl)propanoate (3am)

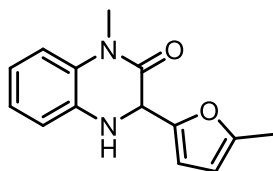
2-(4-



3am (76%, 75.0 mg) as a yellow solid (mp 124-126 °C); ^1H NMR (400 MHz, CDCl_3) δ 9.01 (s, 1H), 8.97 (d, $J = 7.9$ Hz, 1H), 8.82 (d, $J = 3.1$ Hz, 1H), 7.93 (d, $J = 7.9$ Hz, 1H), 7.38 – 7.30 (m, 3H), 7.29 – 7.21 (m, 3H), 7.06 (d, $J = 7.9$ Hz, 2H), 6.98 (d, $J = 7.9$ Hz, 2H), 4.55 – 4.36 (m, 4H), 3.57 (q, $J = 7.1$ Hz, 1H), 2.36 (d, $J = 7.2$ Hz, 2H), 1.83 – 1.70 (m, 1H), 1.38 (d, $J = 7.2$ Hz, 3H), 0.83 (d, $J = 6.6$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 174.8, 154.2, 150.5, 140.6, 137.0, 136.0, 133.8, 132.3, 130.9, 129.4, 129.3, 128.2, 127.0, 126.5, 123.5, 123.3, 123.0, 121.5, 113.4, 112.4, 111.2, 61.1, 44.9, 44.8,

40.6, 30.0, 22.3, 18.1; HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{31}H_{32}N_3O_3^+$ 494.2437, found 494.2438.

1-methyl-3-(5-methylfuran-2-yl)-3,4-dihydroquinoxalin-2(1H)-one (C)



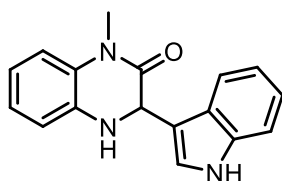
C as a colorless liquid; 1H NMR (400 MHz, $CDCl_3$) δ 6.97 – 6.91 (m, 2H), 6.90 – 6.83 (m, 1H), 6.75 – 6.69 (m, 1H), 6.01 (d, $J = 3.3$ Hz, 1H), 5.83 (d, $J = 3.2$ Hz, 1H), 5.07 (s, 1H), 3.41 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 152.5, 149.2, 134.0, 128.5, 123.6, 119.8, 114.7, 114.4, 108.5, 106.3, 55.3, 29.2, 13.5; HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{14}H_{14}N_2O_2Na^+$ 265.0947, found 265.0949.

1-methyl-3-(1-methyl-1H-pyrrol-2-yl)-3,4-dihydroquinoxalin-2(1H)-one (4a)



4a as a yellow liquid; 1H NMR (400 MHz, $CDCl_3$) δ 6.92 (dd, $J = 7.9, 6.3$ Hz, 2H), 6.87 – 6.82 (m, 1H), 6.70 (dd, $J = 7.8, 1.6$ Hz, 1H), 6.49 (t, $J = 2.1$ Hz, 1H), 6.45 (t, $J = 2.5$ Hz, 1H), 5.98 (t, $J = 2.3$ Hz, 1H), 4.96 (s, 1H), 3.53 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 134.9, 128.7, 123.4, 122.1, 122.0, 119.5, 119.3, 114.5, 114.2, 106.9, 55.2, 36.1, 29.1; HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{14}H_{15}N_3ONa^+$ 264.1107, found 264.1118.

3-(1H-indol-3-yl)-1-methyl-3,4-dihydroquinoxalin-2(1H)-one (4c)



4c as a yellow liquid; 1H NMR (400 MHz, DMSO) δ 10.93 (s, 1H), 7.63 (d, $J = 8.0$ Hz,

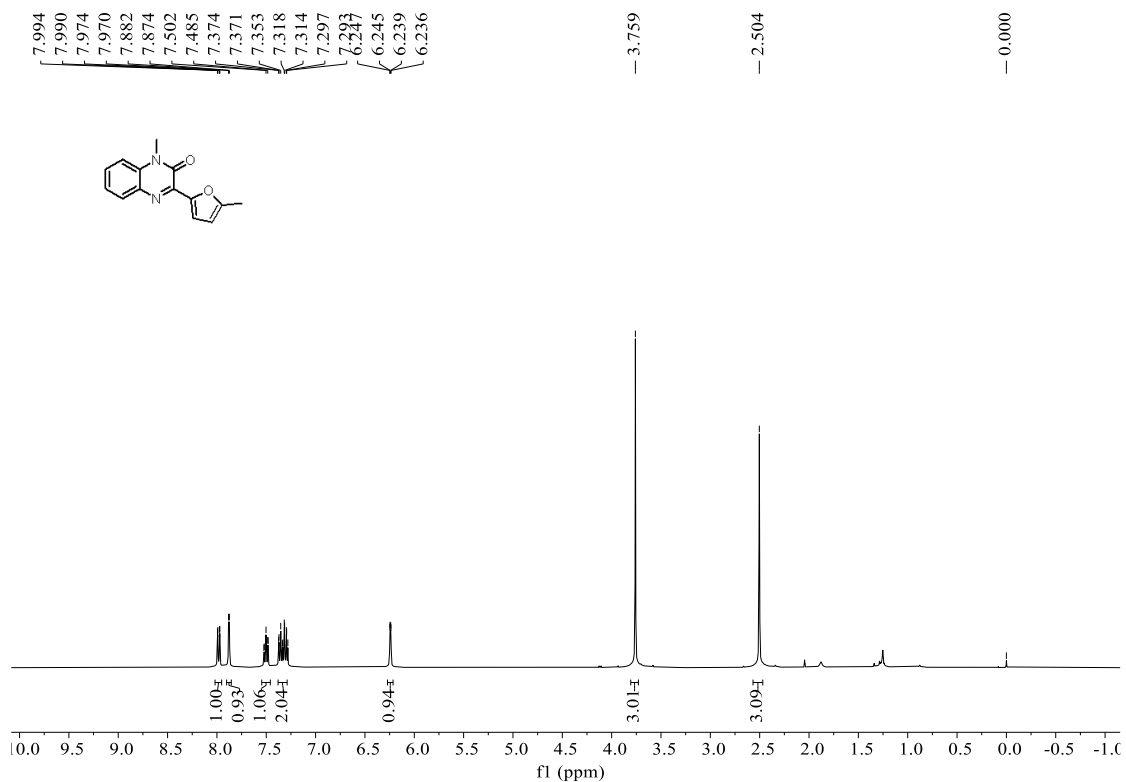
1H), 7.34 (d, $J = 8.1$ Hz, 1H), 7.11 – 7.04 (m, 1H), 7.03 – 6.94 (m, 3H), 6.90 – 6.81 (m, 2H), 6.78 – 6.71 (m, 1H), 6.59 (d, $J = 1.9$ Hz, 1H), 5.21 (d, $J = 1.8$ Hz, 1H), 3.29 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 165.5, 136.2, 136.0, 128.2, 125.7, 123.3, 123.2, 121.3, 119.5, 118.7, 118.0, 114.5, 113.7, 113.3, 111.4, 53.4, 28.6; HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{17}\text{H}_{15}\text{N}_3\text{ONa}^+$ 300.1107, found 300.1108.

8. Reference

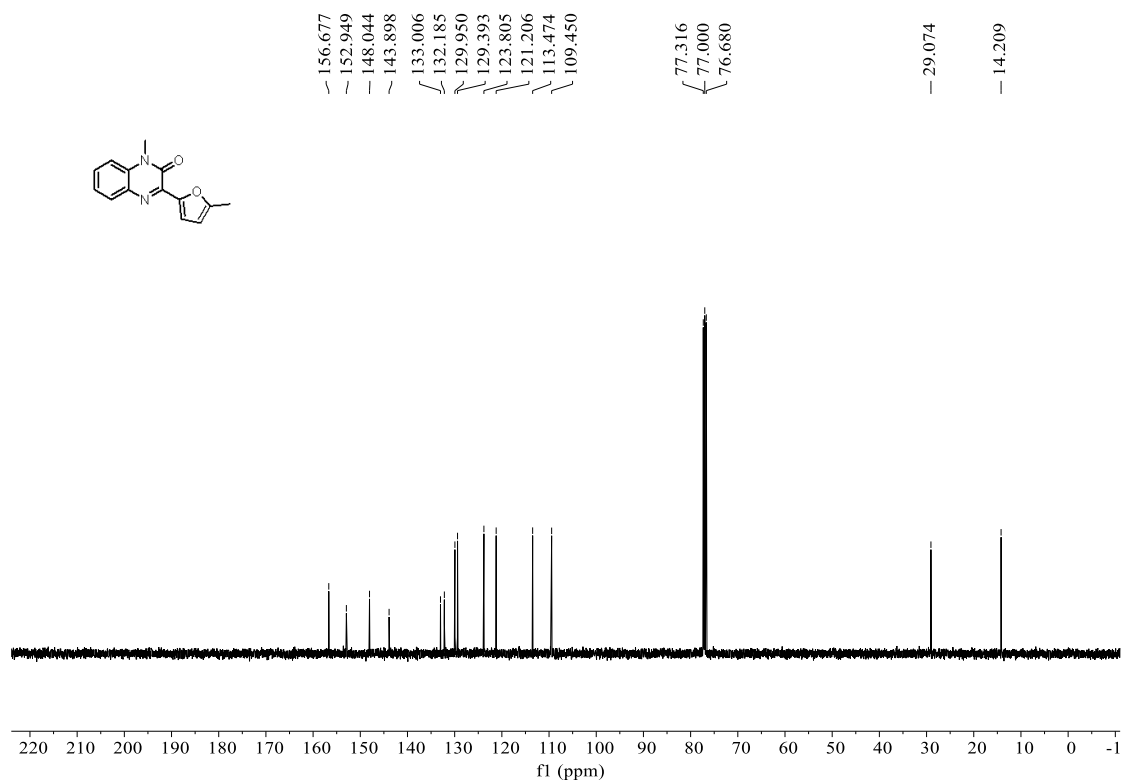
1. K.-J. Li, Y.-Y. Jiang, K. Xu, C.-C. Zeng, B.-G. Sun, *Green Chem.*, **2019**, *21*, 4412-4421.
2. K. A. Kumar, P. Kannaboina, C. K. Jaladanki, P. V. Bharatam, P. Das, *ChemSelect*, **2016**, *3*, 601-607.
3. H Bao, Z. Lin, M. Jin, H. Zhang, J. Xua, B. Chen, W. Lia, *Tetrahedron Lett.*, **2021**, *66*, 152841.
4. X. Lu, Z. Luo, R. Huang, D. C. Lo, W. Huang, *Chem. Eur. J.*, **2022**, *28*, e202201421.
5. W. Huang, T. Wang, S.-Y. Chen, Q. Zhou, L. Wang, *Org. Biomol. Chem.*, **2025**, *23*, 5564–5568.
6. P. Swami, N. Meena, H. Joshi, R. Roy, K. Rangan, A. Kumar, *Organometallics*, **2025**, *44*, 912-921.
7. Y.-Y. Han, Z.-J. Wu, X.-M. Zhang, W.-C. Yuan, *Tetrahedron Lett.*, **2010**, *51*, 2023-2028.
8. J. Huang, L. Wang, X.-Y. Tang, *Org. Biomol. Chem.*, **2023**, *21*, 2709–2714.
9. H. Ni, H. Mao, Y. Huang, Y. Lu, Z. Liu, *Molecules*, **2024**, *29*, 2649.

9. Copies of ^1H , ^{13}C and ^{19}F NMR spectra of all products

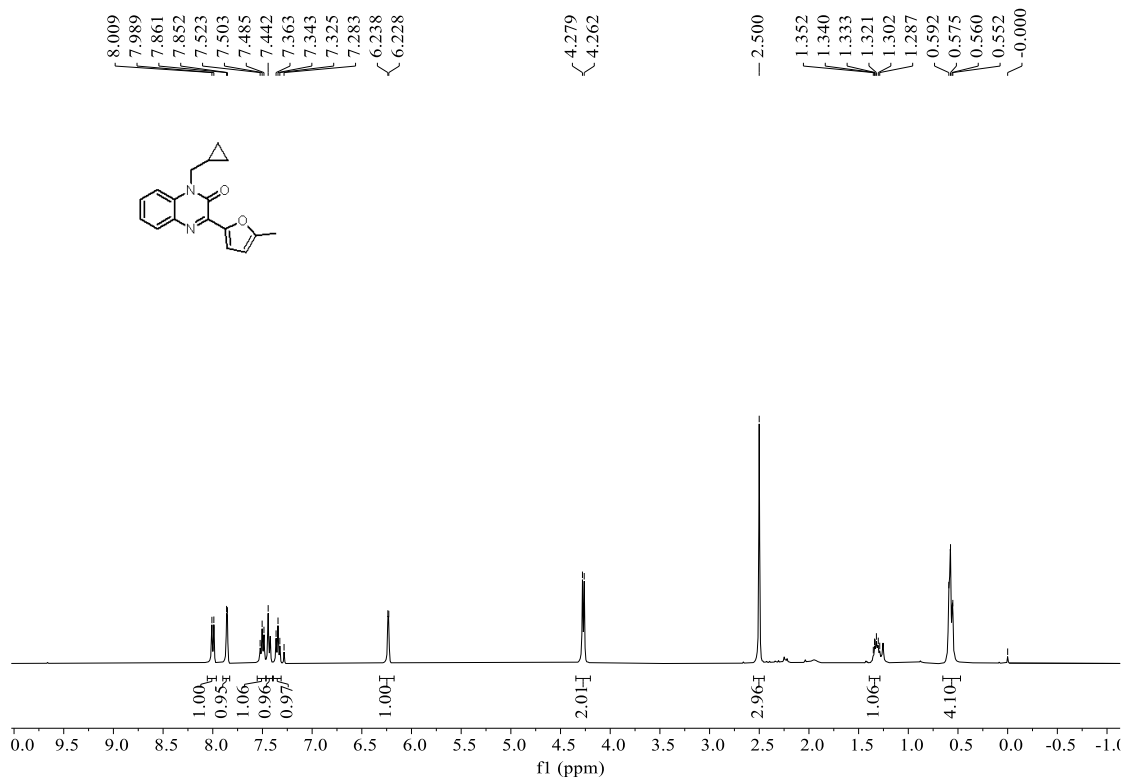
^1H NMR spectra of 3a (400 MHz, CDCl_3)



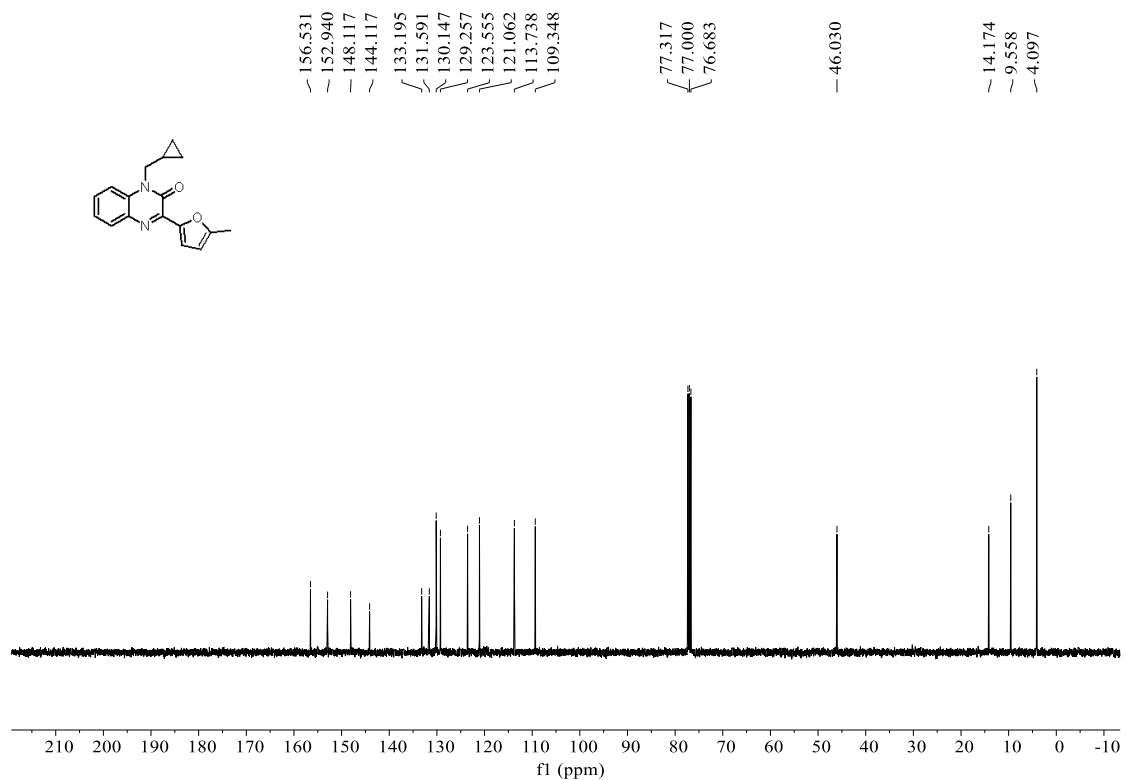
^{13}C NMR spectra of 3a (100 MHz, CDCl_3)



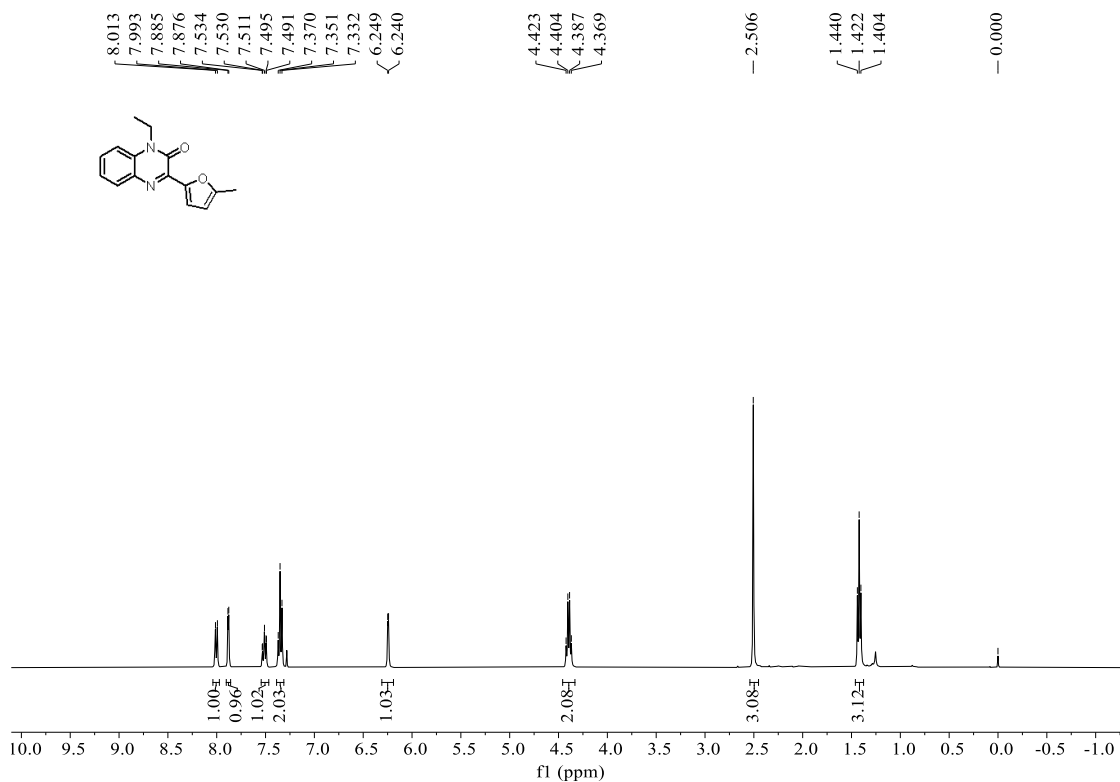
¹H NMR spectra of 3b (400 MHz, CDCl₃)



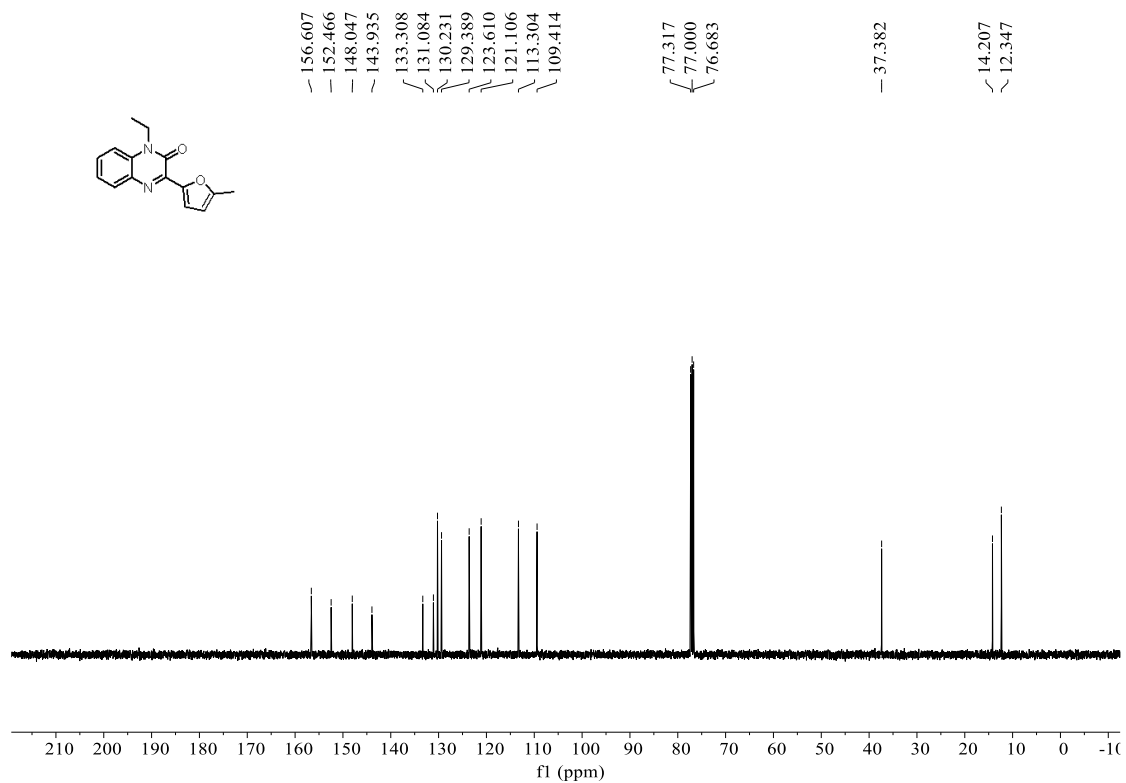
¹³C NMR spectra of 3b (100 MHz, CDCl₃)



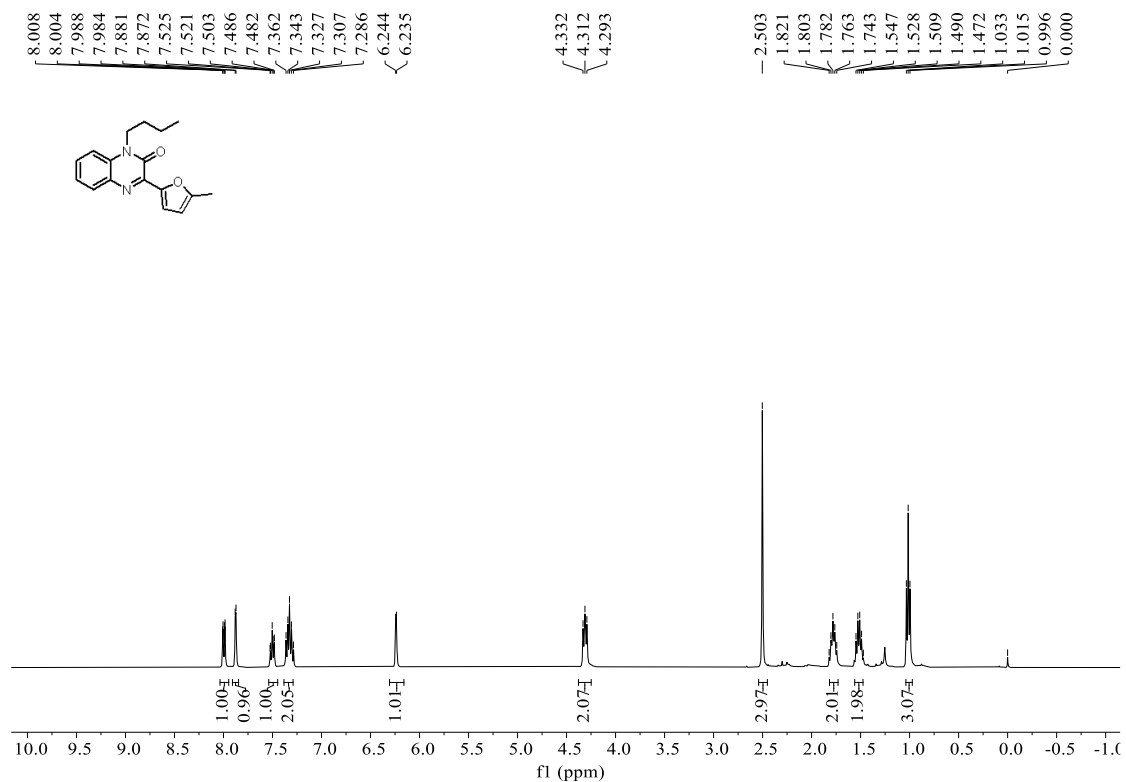
¹H NMR spectra of 3c (400 MHz, CDCl₃)



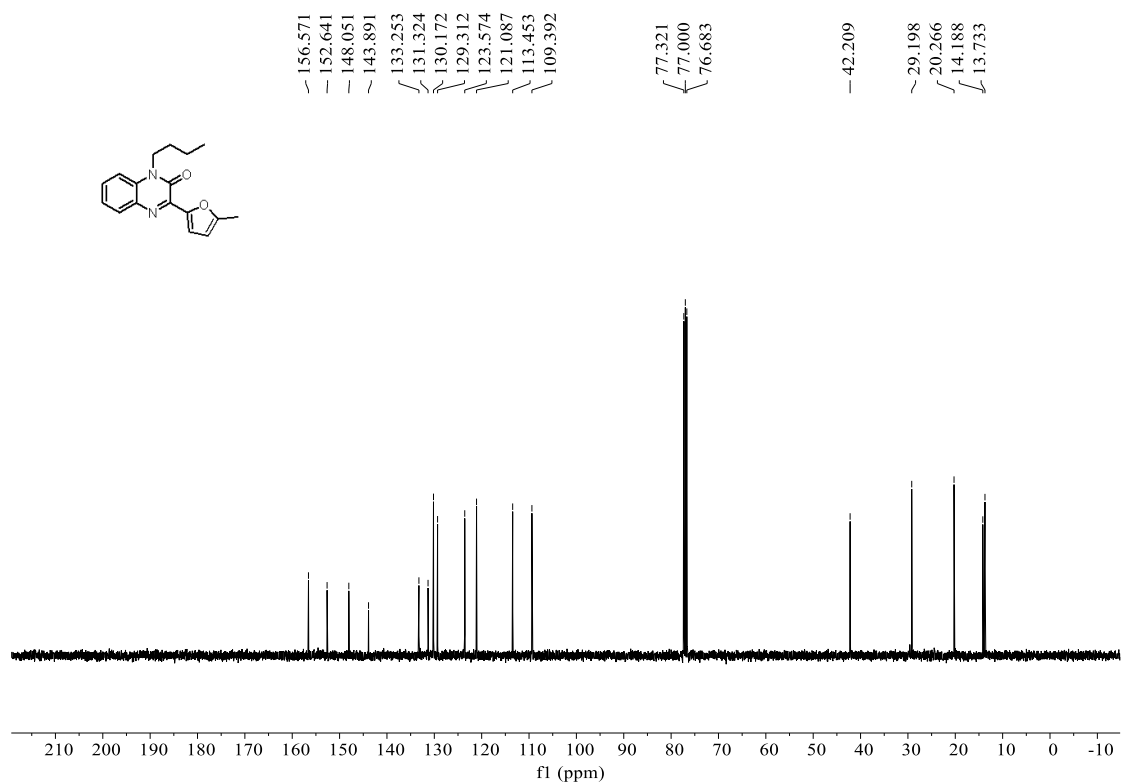
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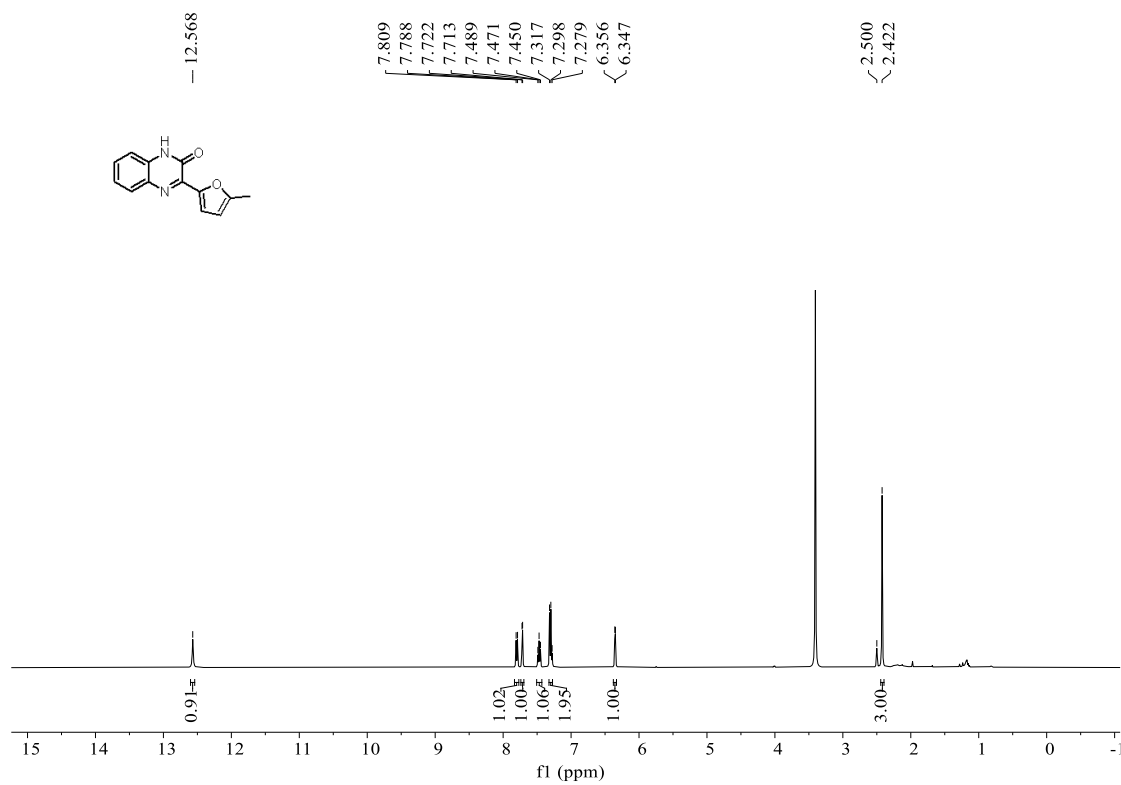
¹H NMR spectra of 3d (400 MHz, CDCl₃)



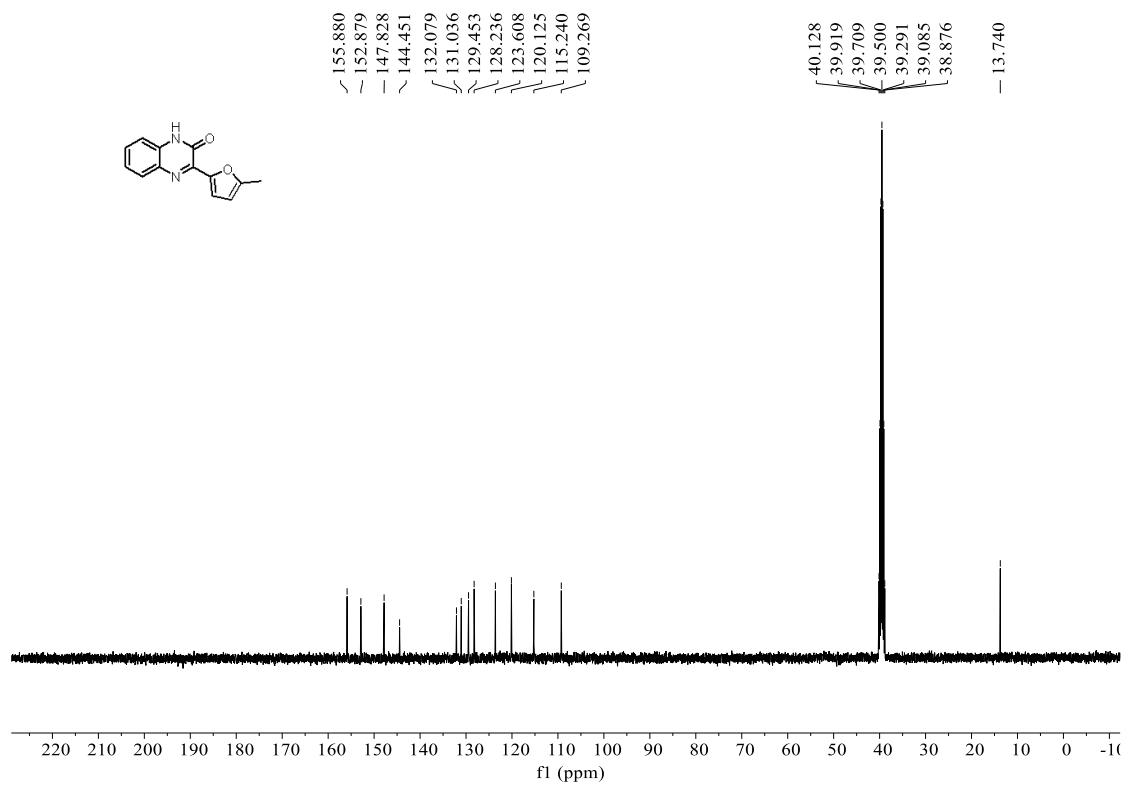
¹³C NMR spectra of 3d (100 MHz, CDCl₃)



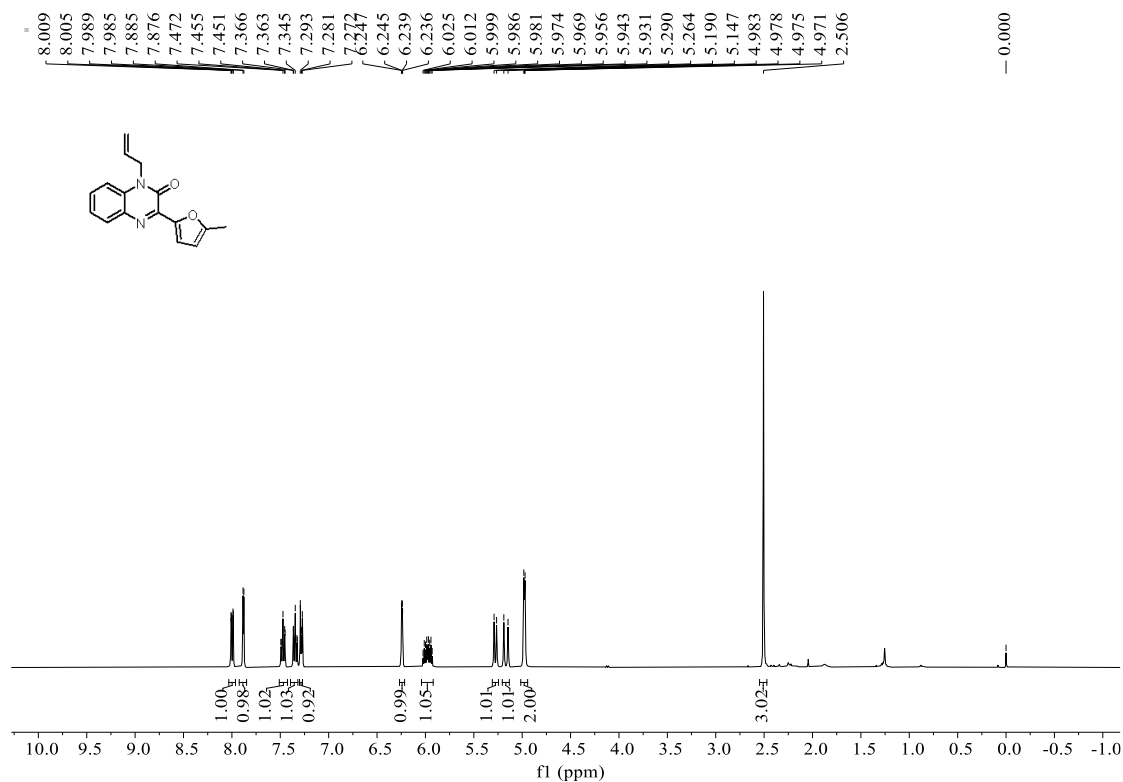
¹H NMR spectra of 3e (400 MHz, DMSO)



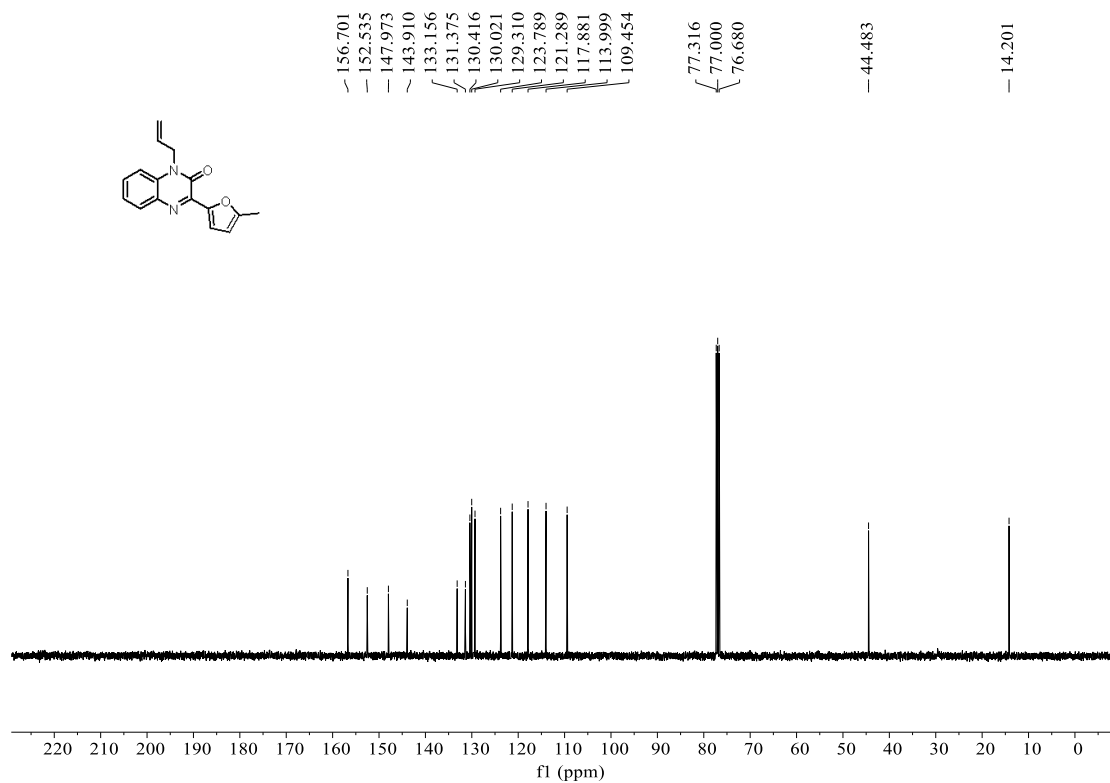
¹³C NMR spectra of 3e (100 MHz, DMSO)



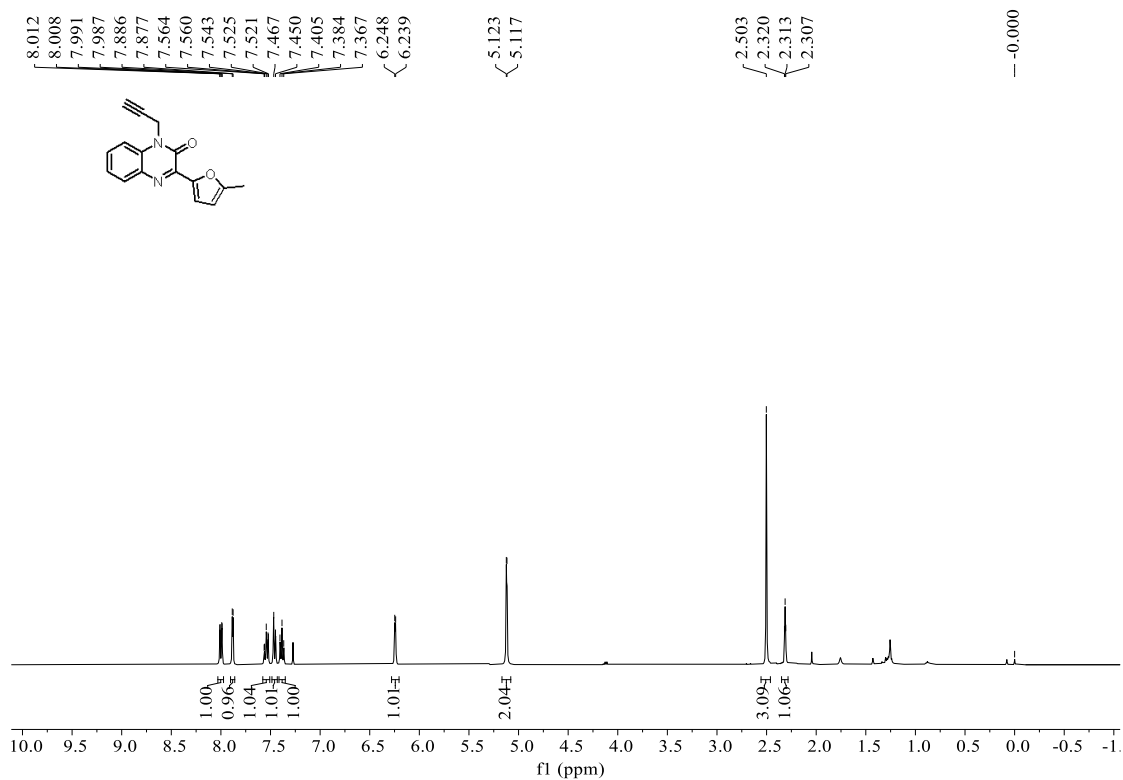
¹H NMR spectra of 3f (400 MHz, CDCl₃)



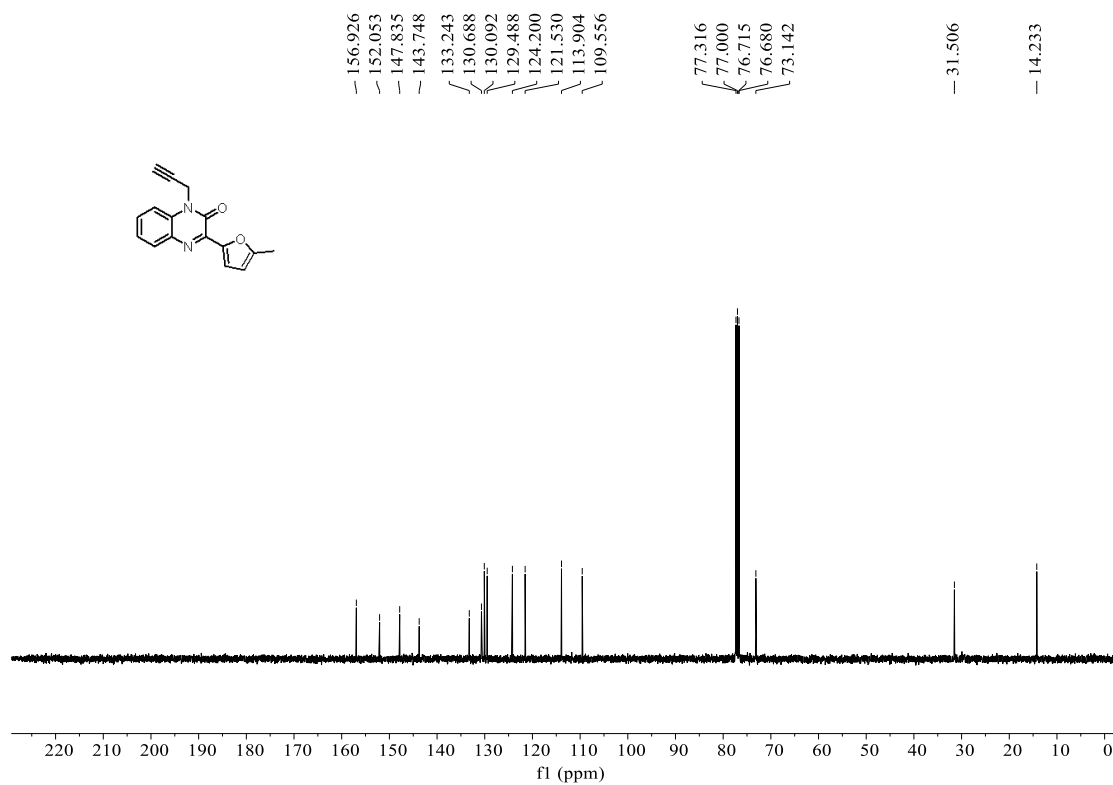
¹³C NMR spectra of 3f (100 MHz, CDCl₃)



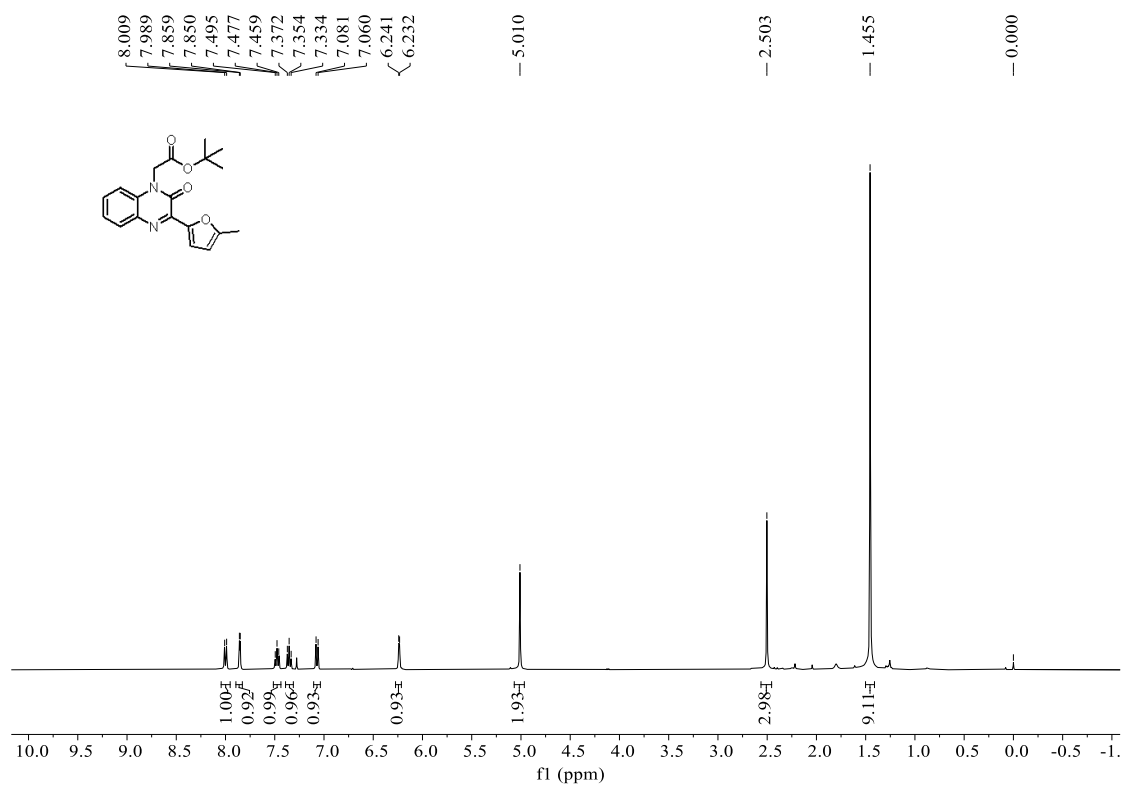
¹H NMR spectra of 3g (400 MHz, CDCl₃)



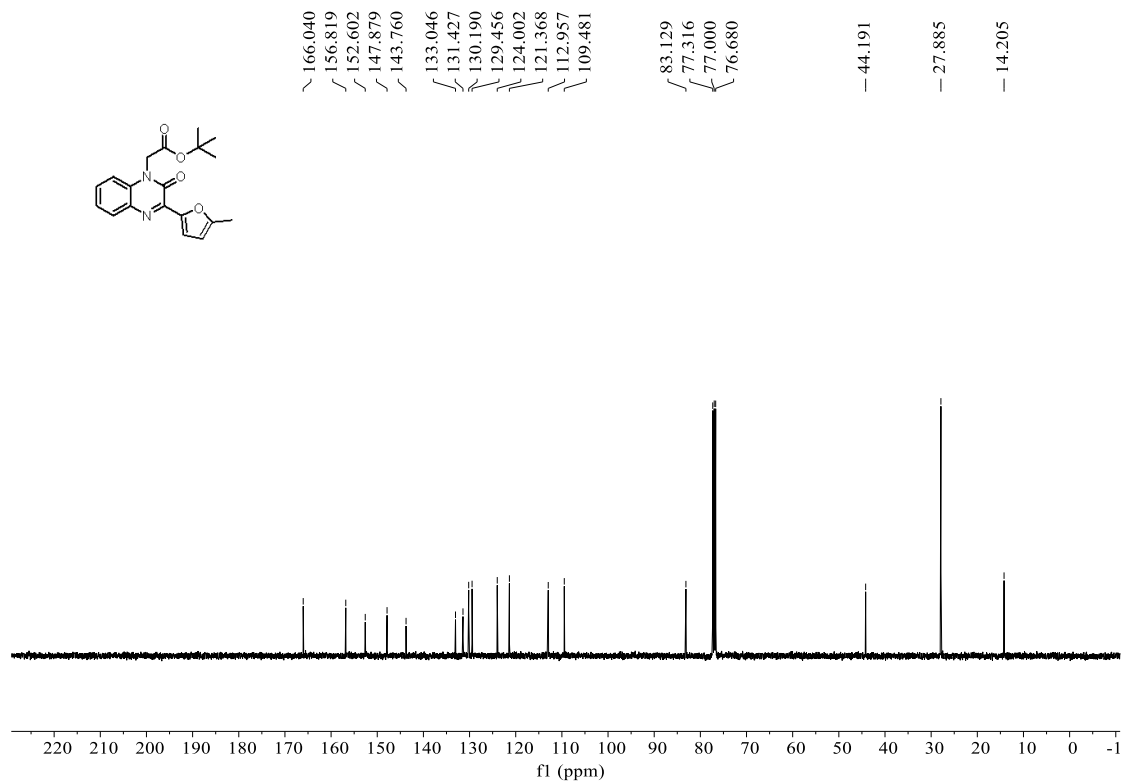
¹³C NMR spectra of 3g (100 MHz, CDCl₃)



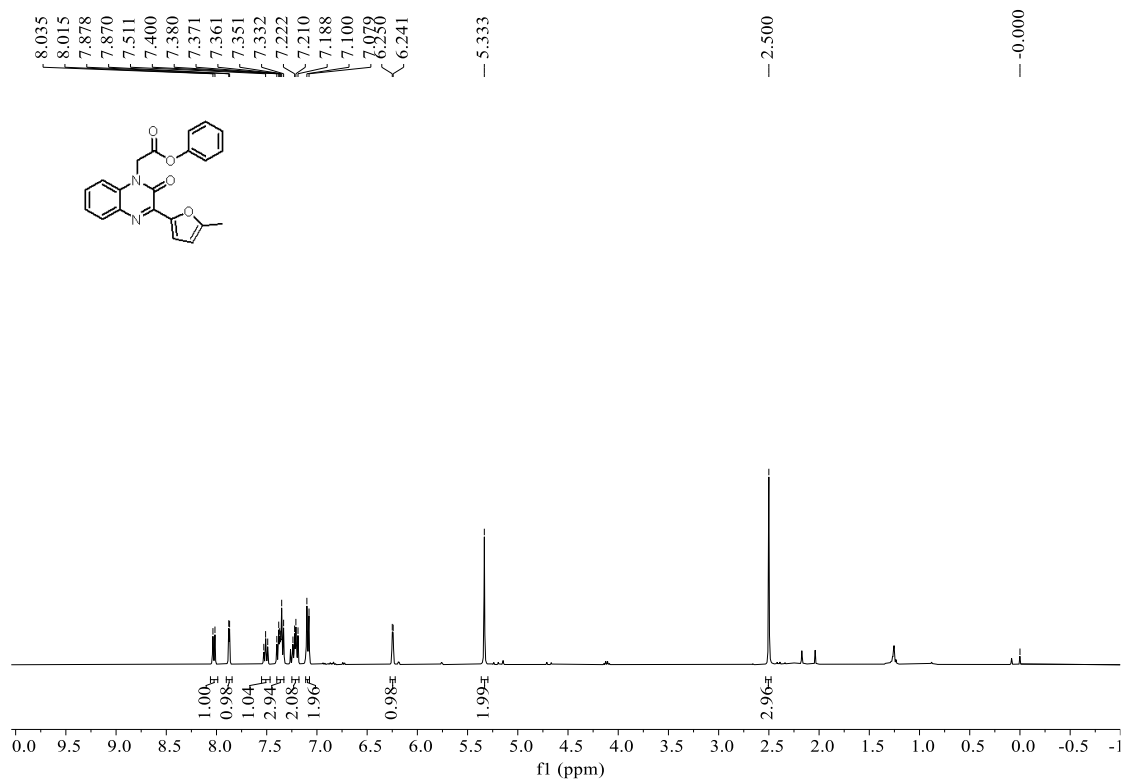
¹H NMR spectra of 3h (400 MHz, CDCl₃)



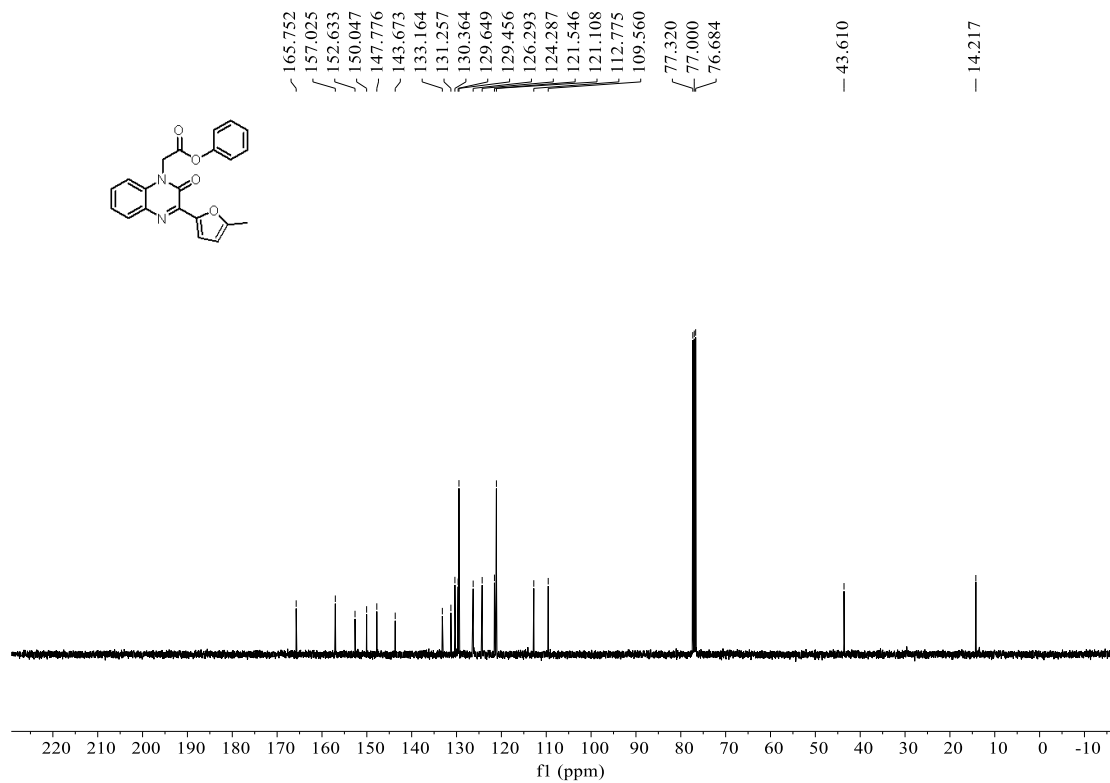
¹³C NMR spectra of 3h (100 MHz, CDCl₃)



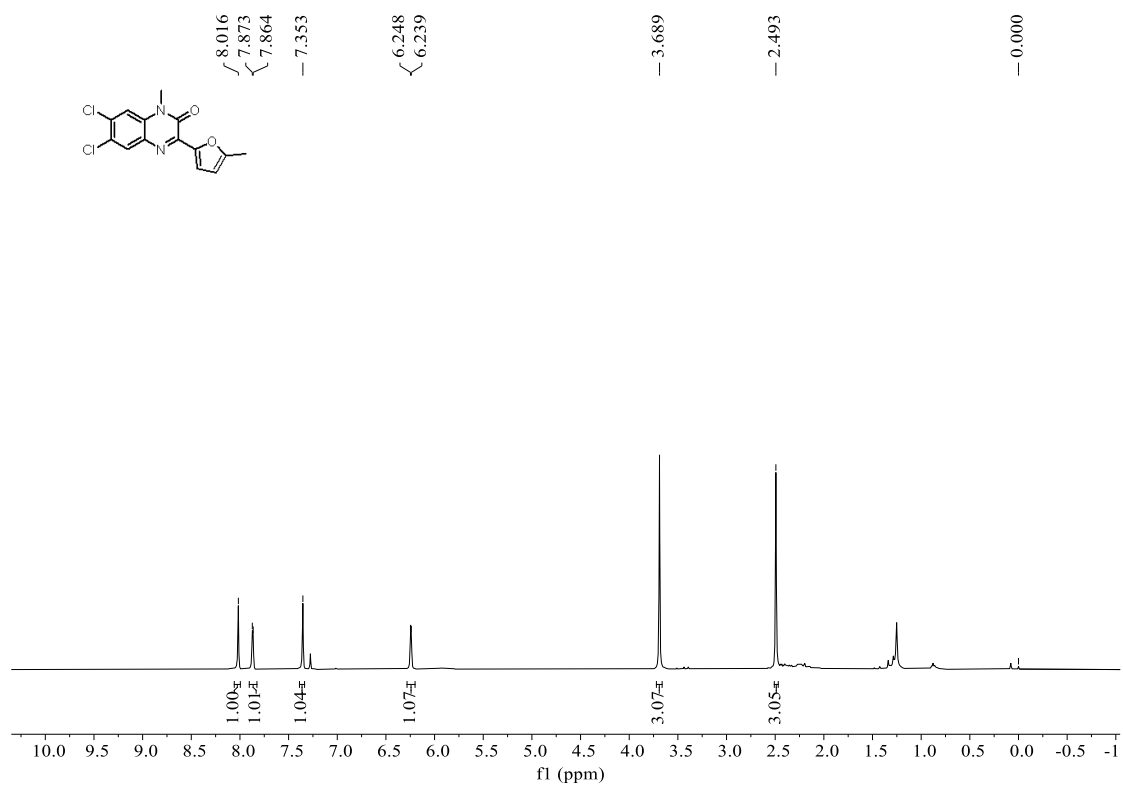
¹H NMR spectra of 3i (400 MHz, CDCl₃)



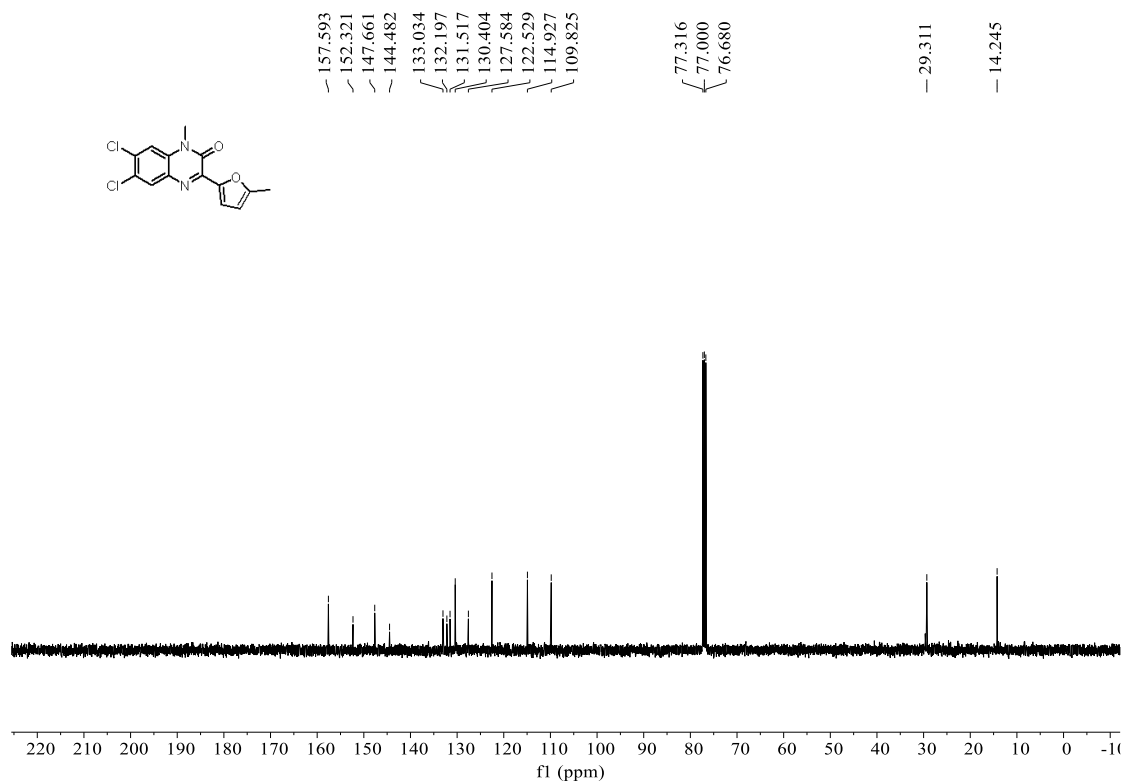
¹³C NMR spectra of 3i (100 MHz, CDCl₃)



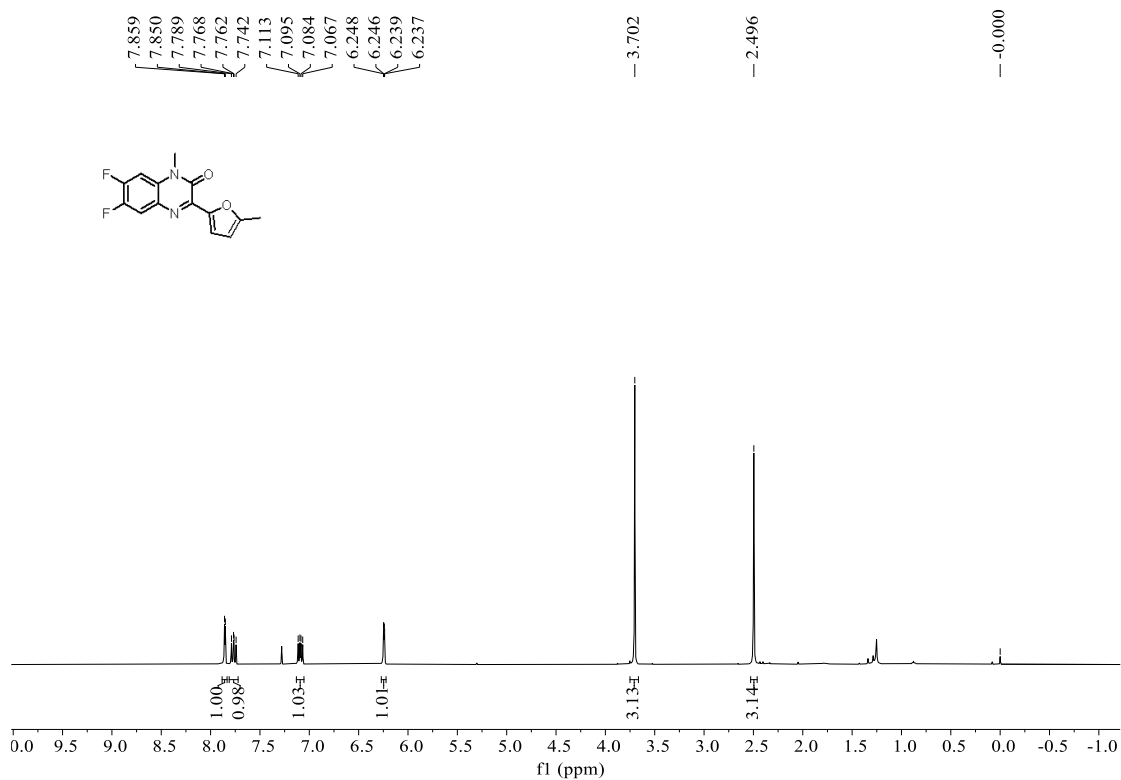
¹H NMR spectra of 3j (400 MHz, CDCl₃)



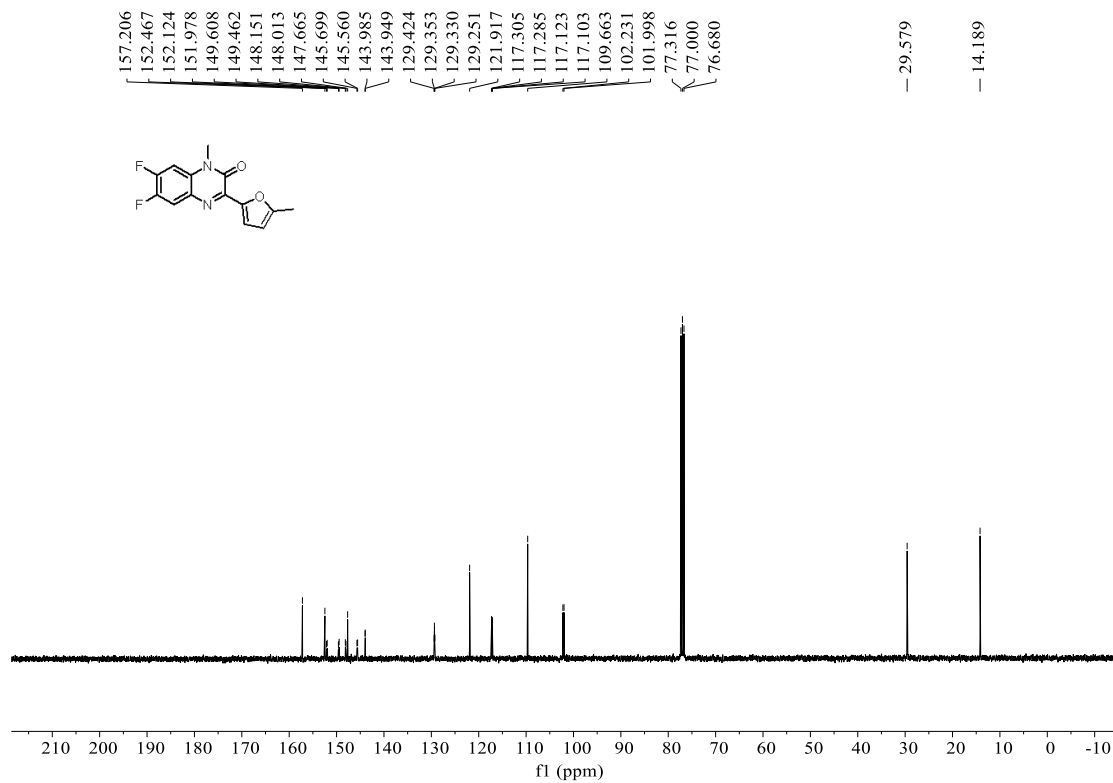
¹³C NMR spectra of 3j (100 MHz, CDCl₃)



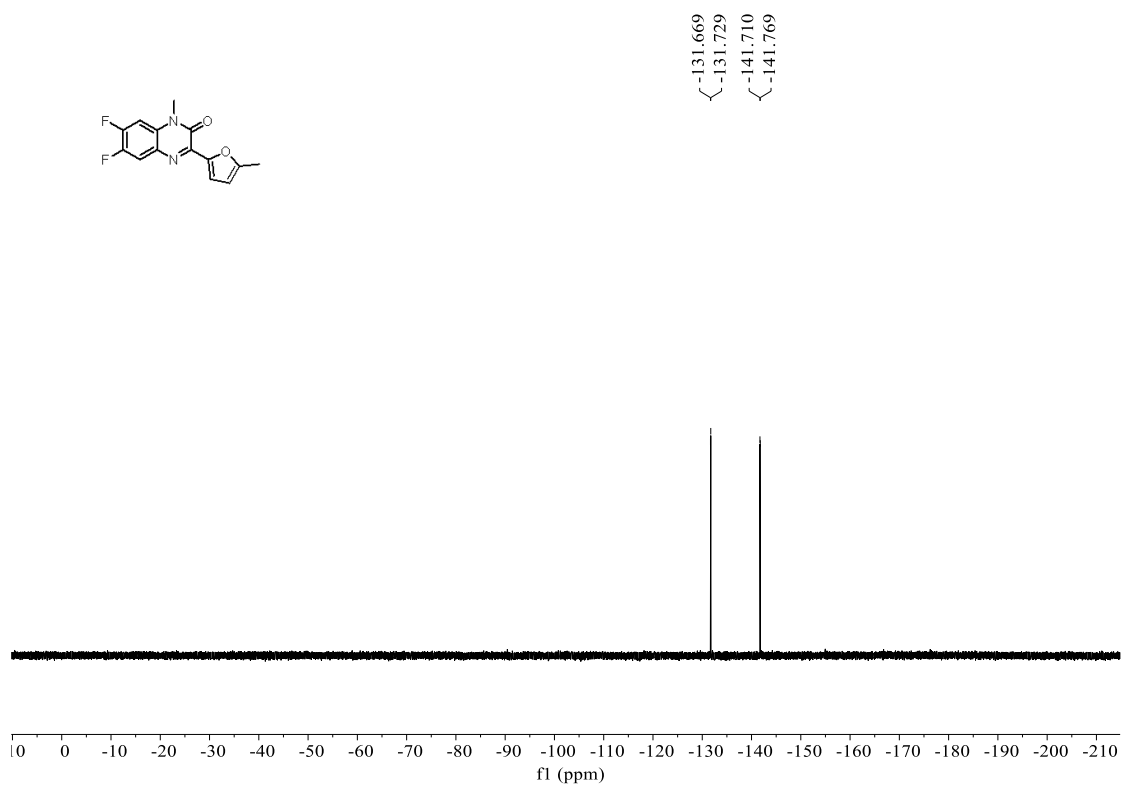
¹H NMR spectra of 3k (400 MHz, CDCl₃)



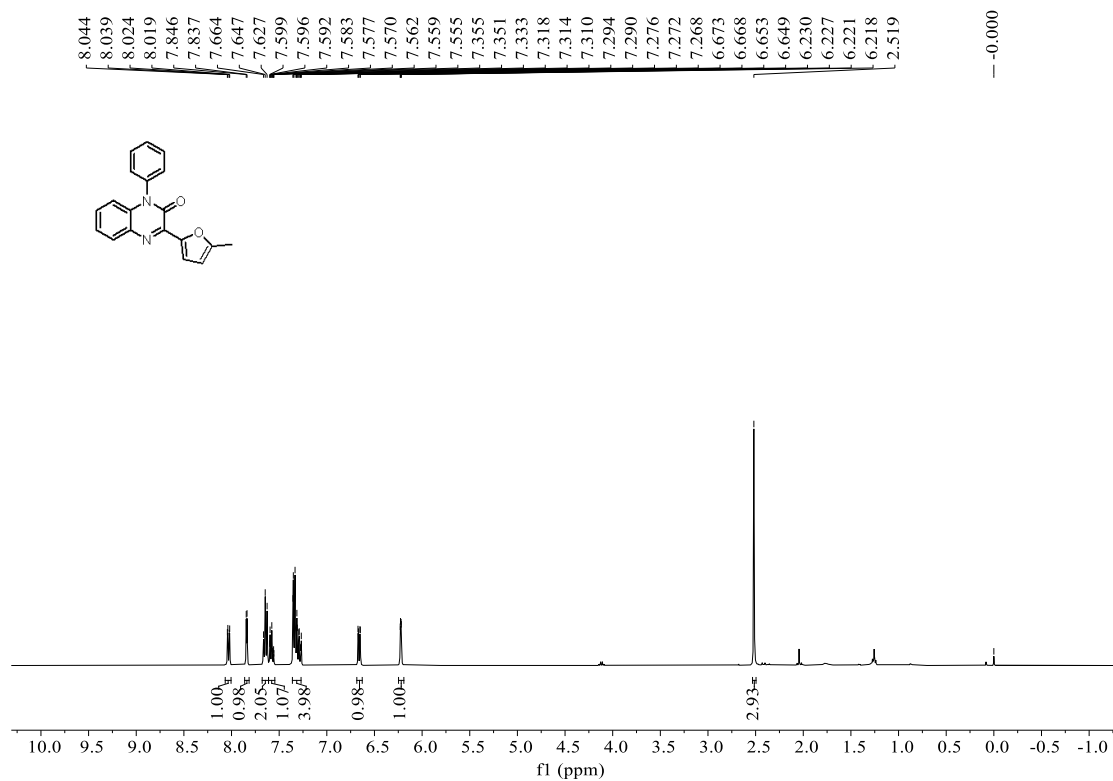
¹³C NMR spectra of 3k (100 MHz, CDCl₃)



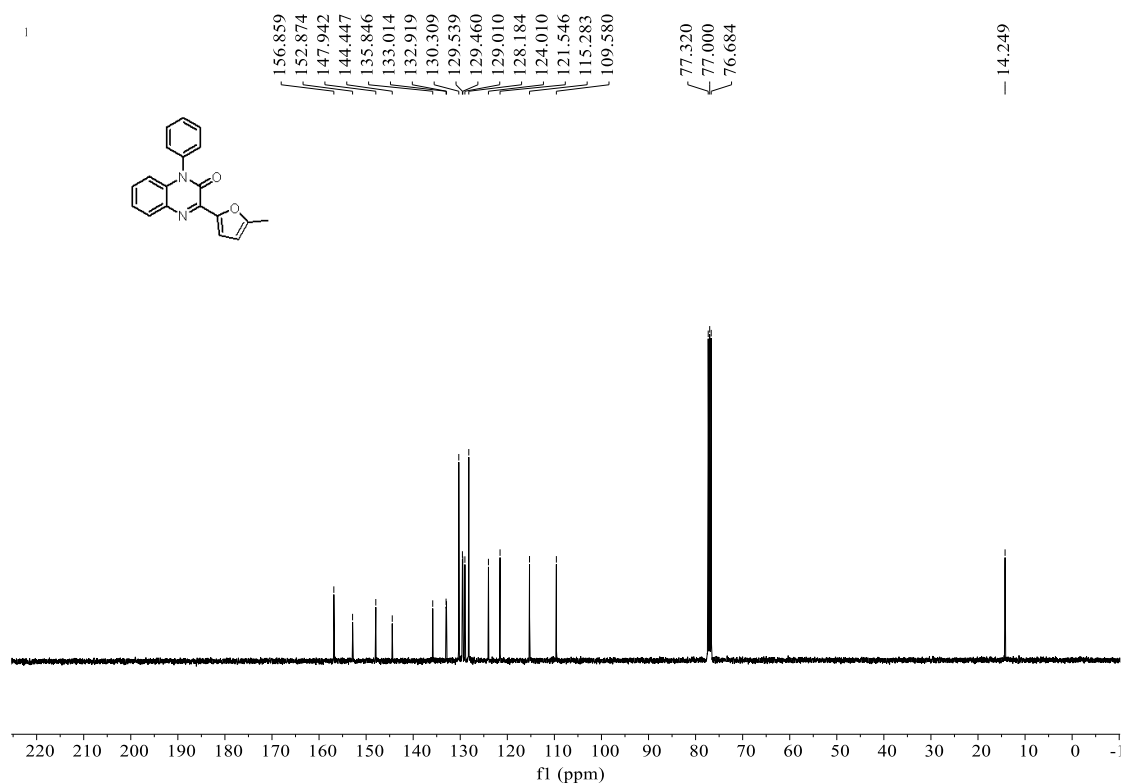
¹⁹F NMR spectra of 3k (376 MHz, CDCl₃)



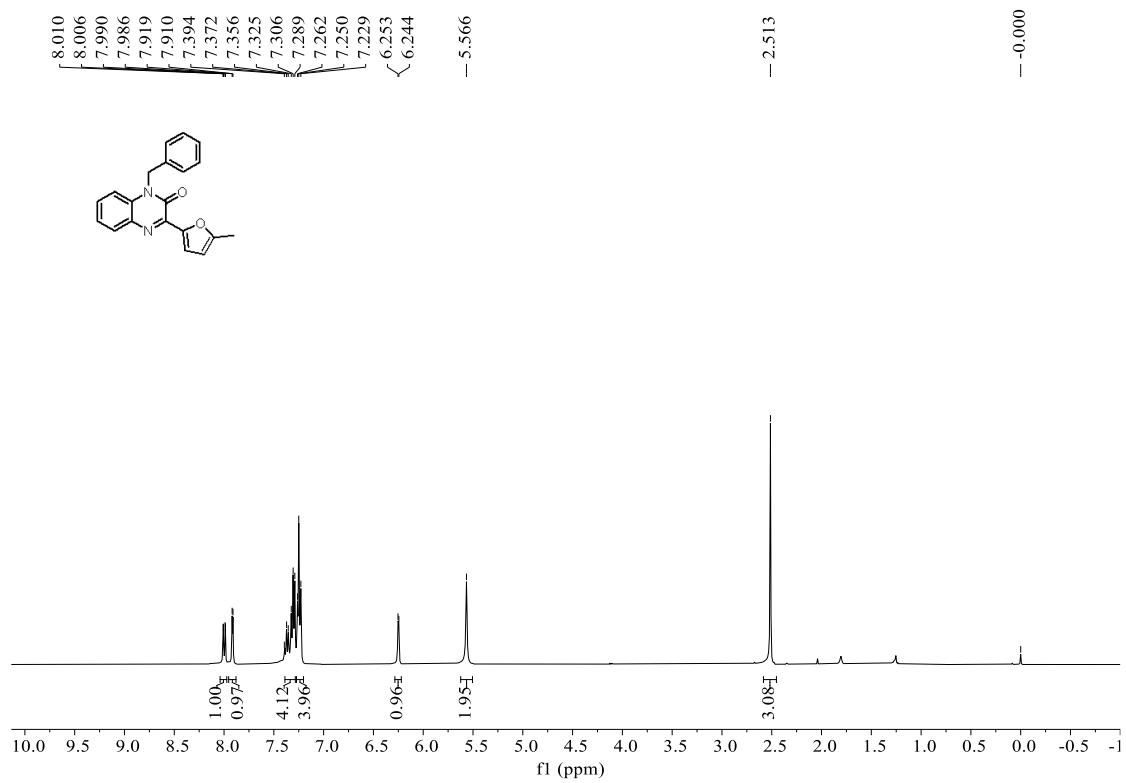
¹H NMR spectra of 3l (400 MHz, CDCl₃)



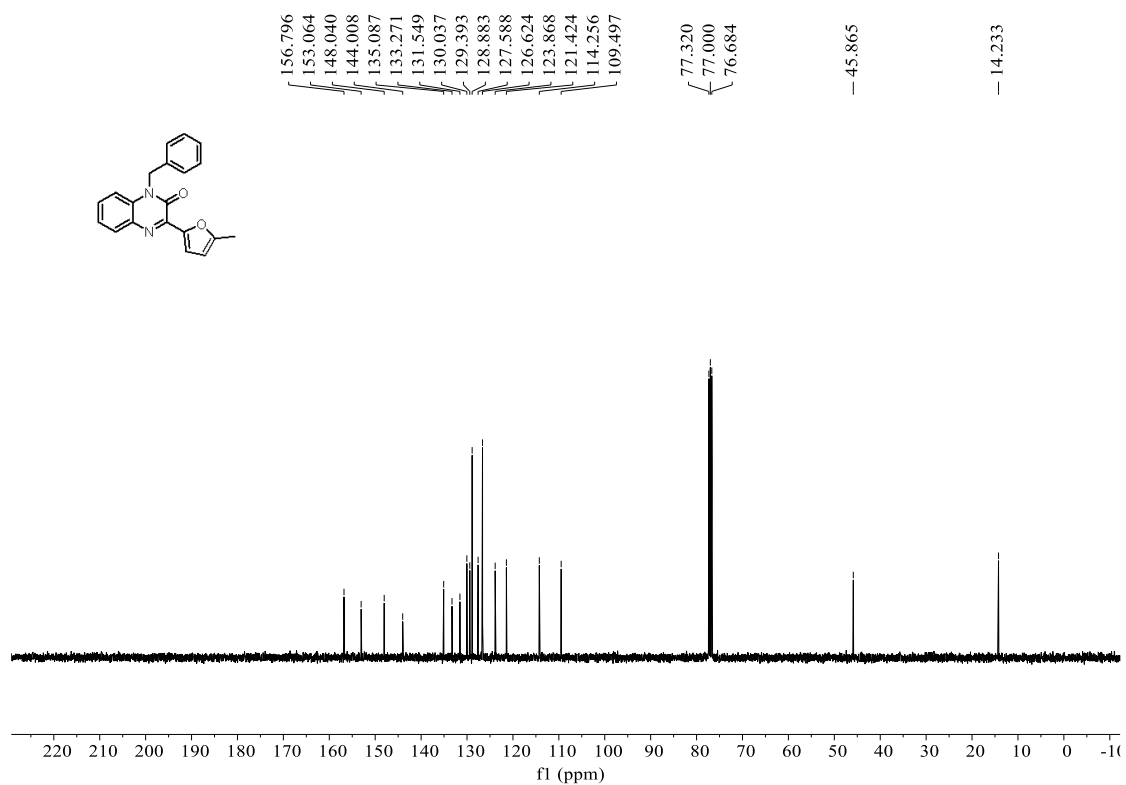
¹³C NMR spectra of 3l (100 MHz, CDCl₃)



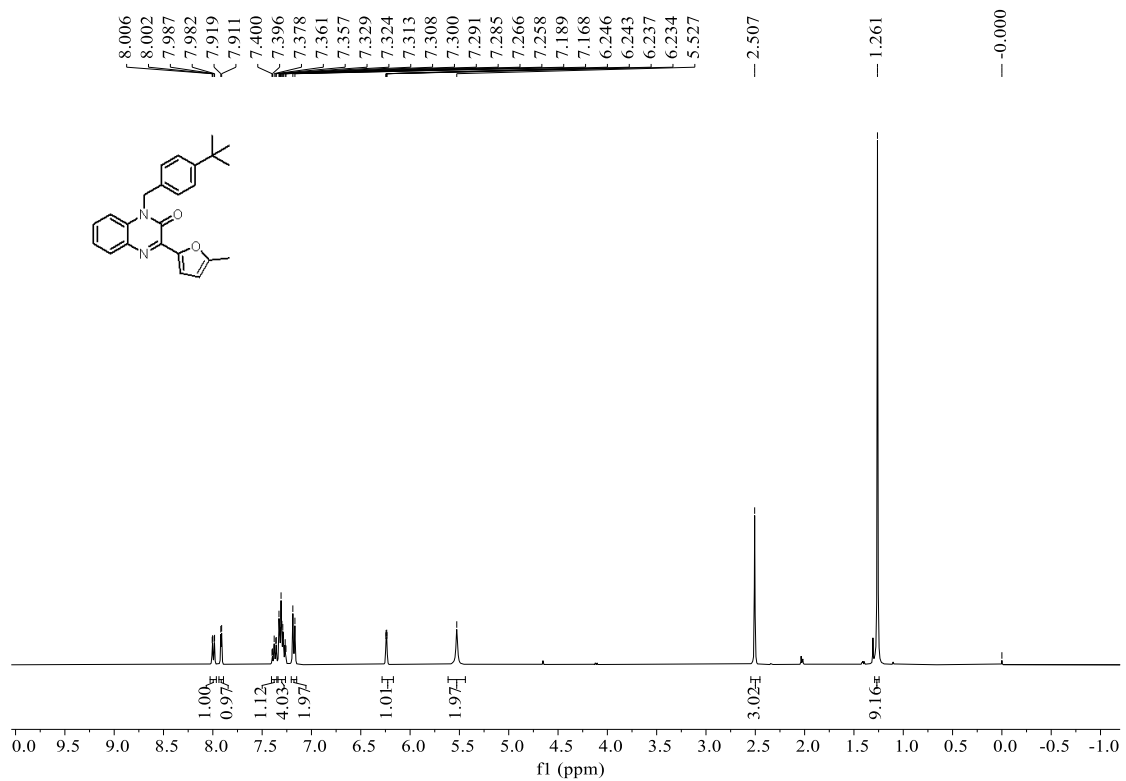
¹H NMR spectra of 3m (400 MHz, CDCl₃)



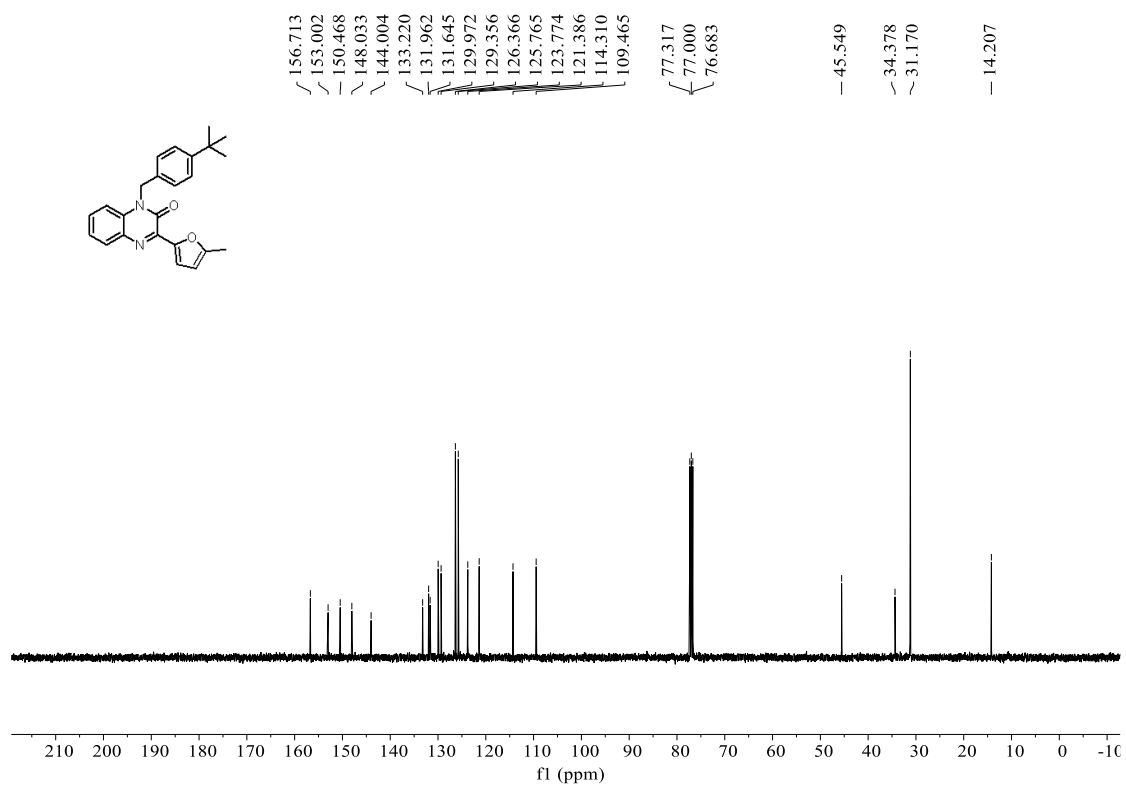
¹³C NMR spectra of 3m (100 MHz, CDCl₃)



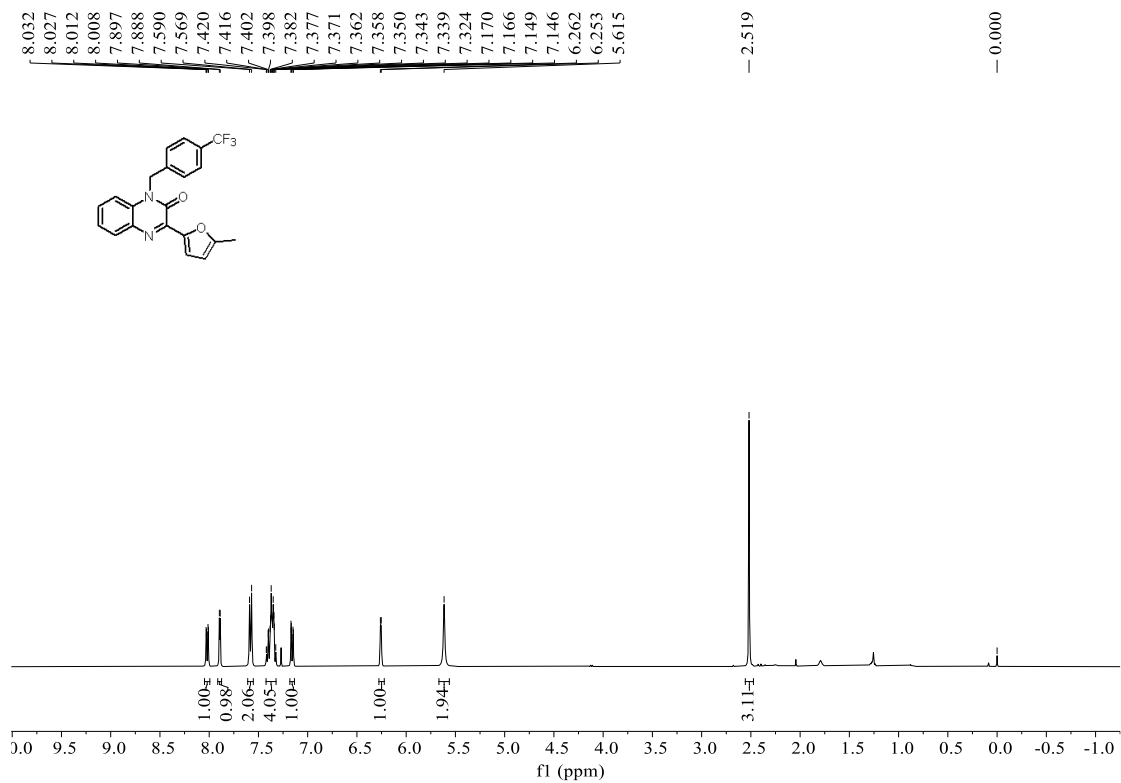
¹H NMR spectra of 3n (400 MHz, CDCl₃)



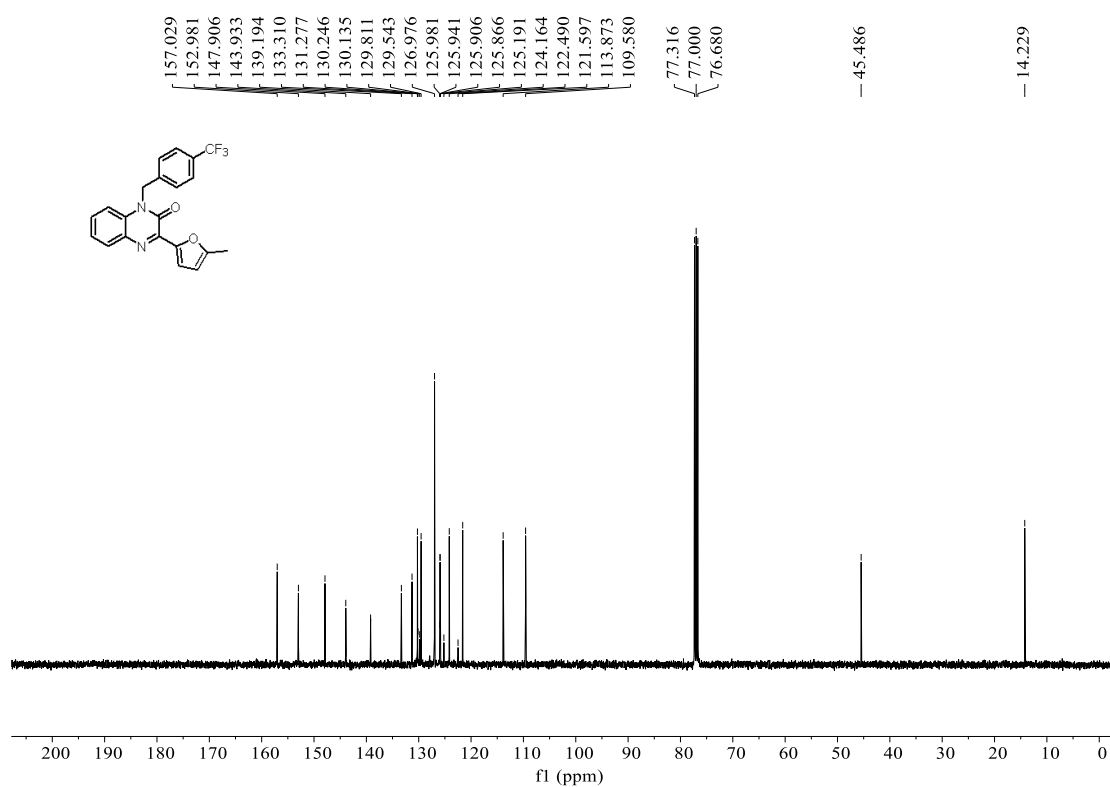
¹³C NMR spectra of 3n (100 MHz, CDCl₃)



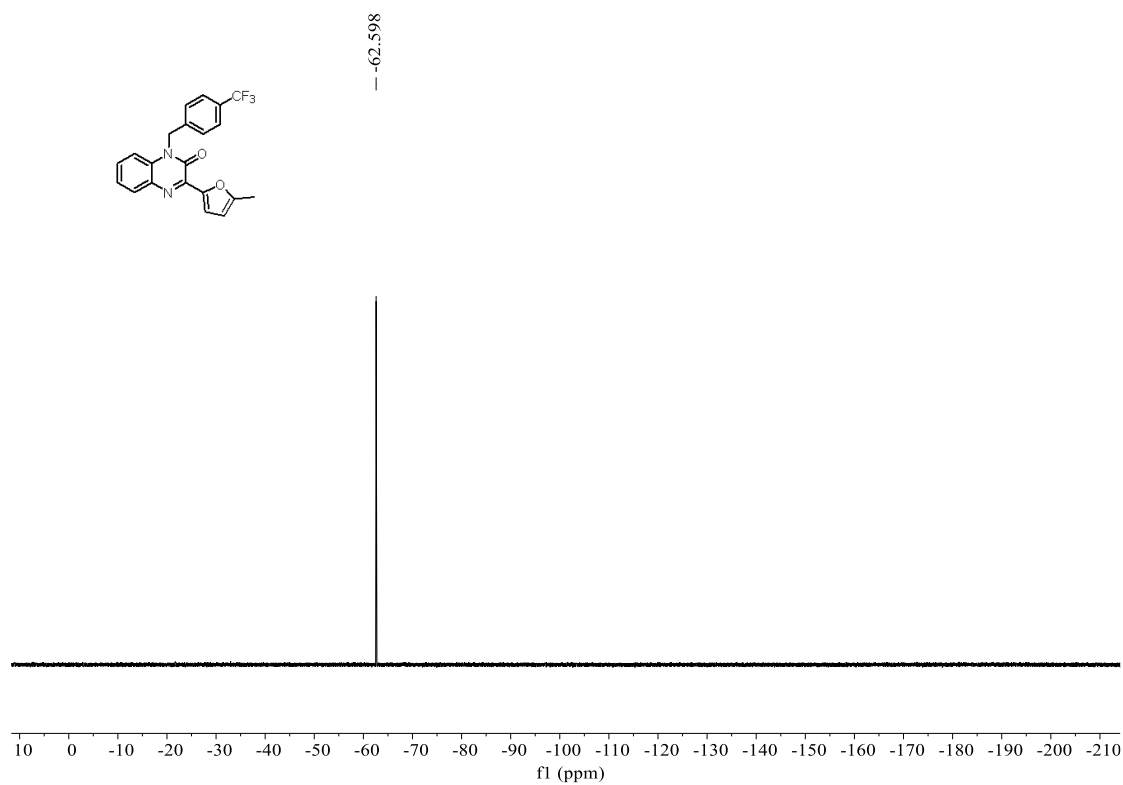
¹H NMR spectra of 3o (400 MHz, CDCl₃)



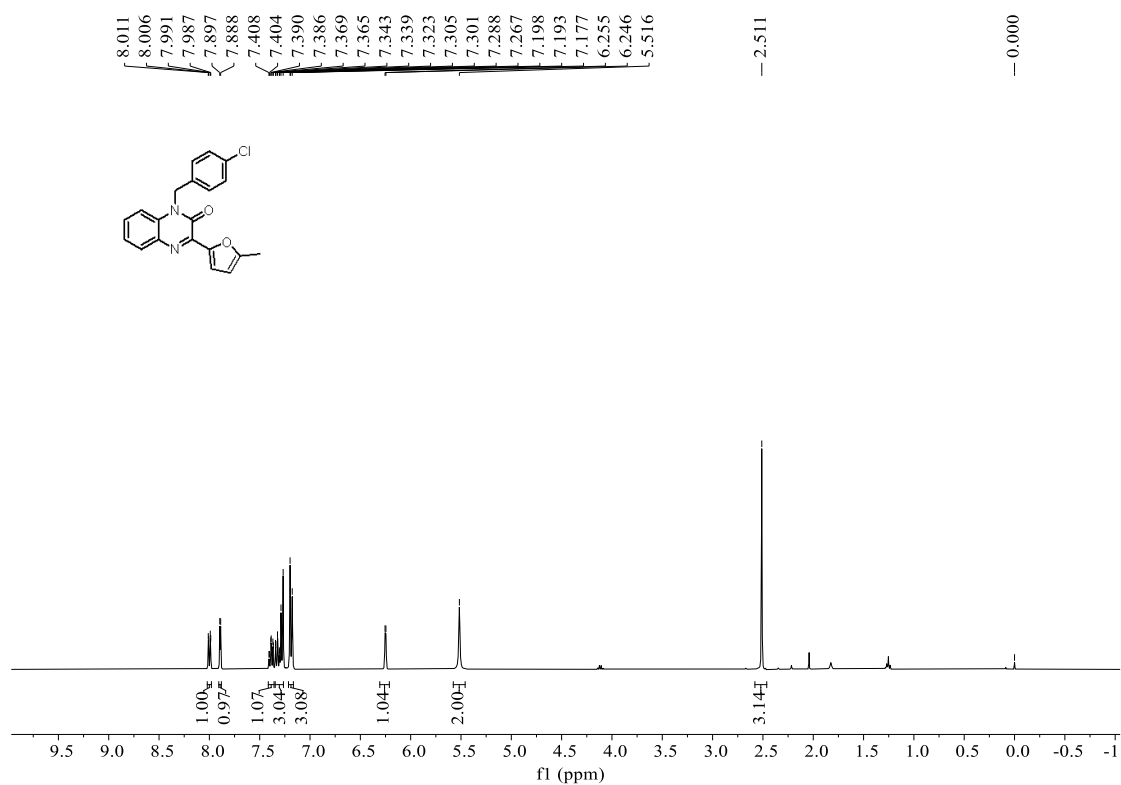
¹³C NMR spectra of 3o (100 MHz, CDCl₃)



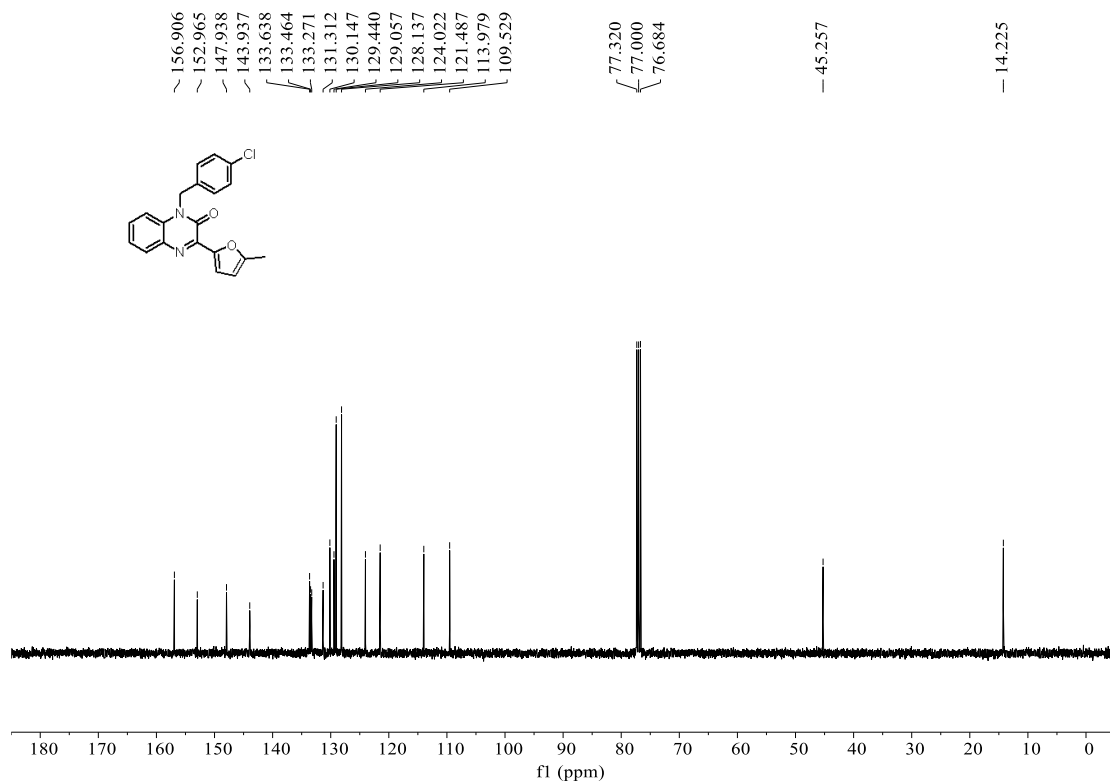
¹⁹F NMR spectra of 3o (376 MHz, CDCl₃)



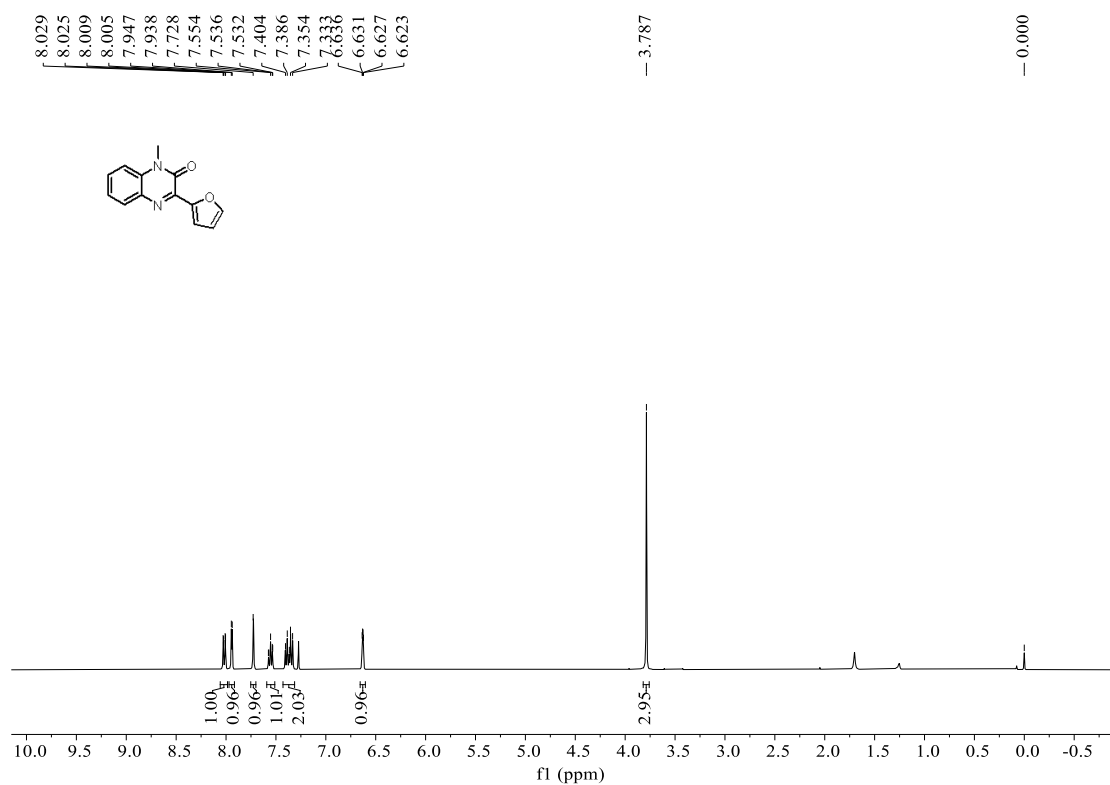
¹H NMR spectra of 3p (400 MHz, CDCl₃)



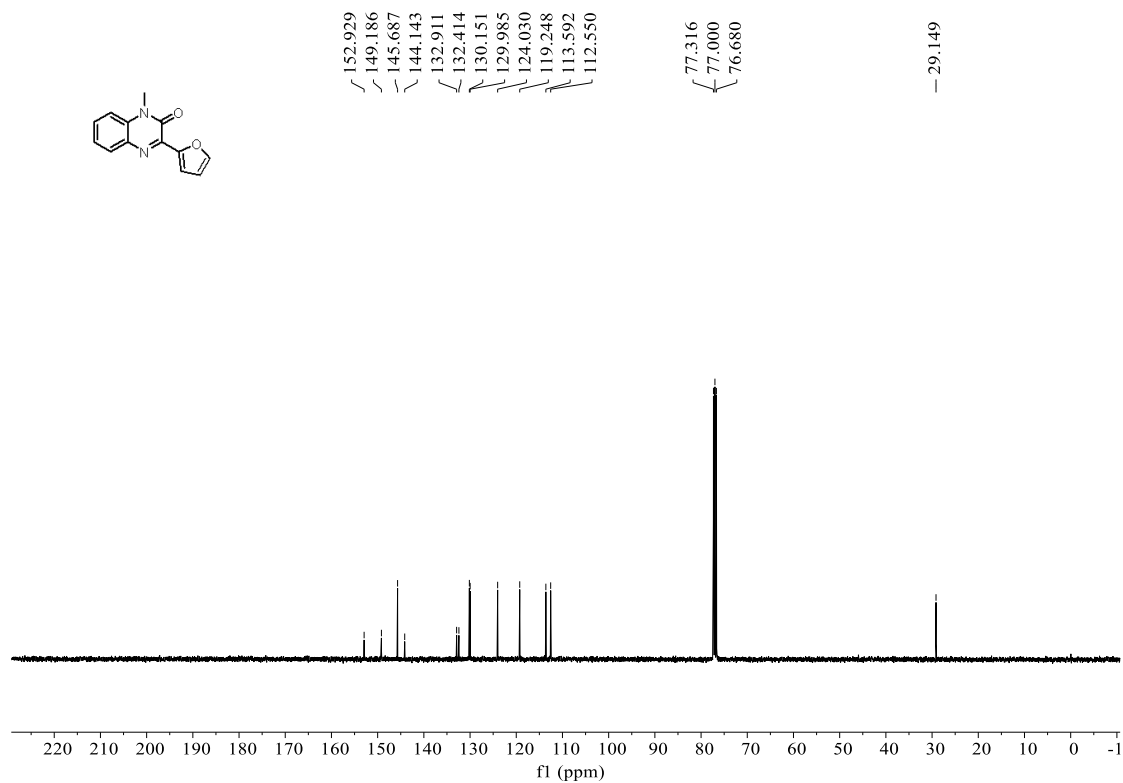
¹³C NMR spectra of 3p (100 MHz, CDCl₃)



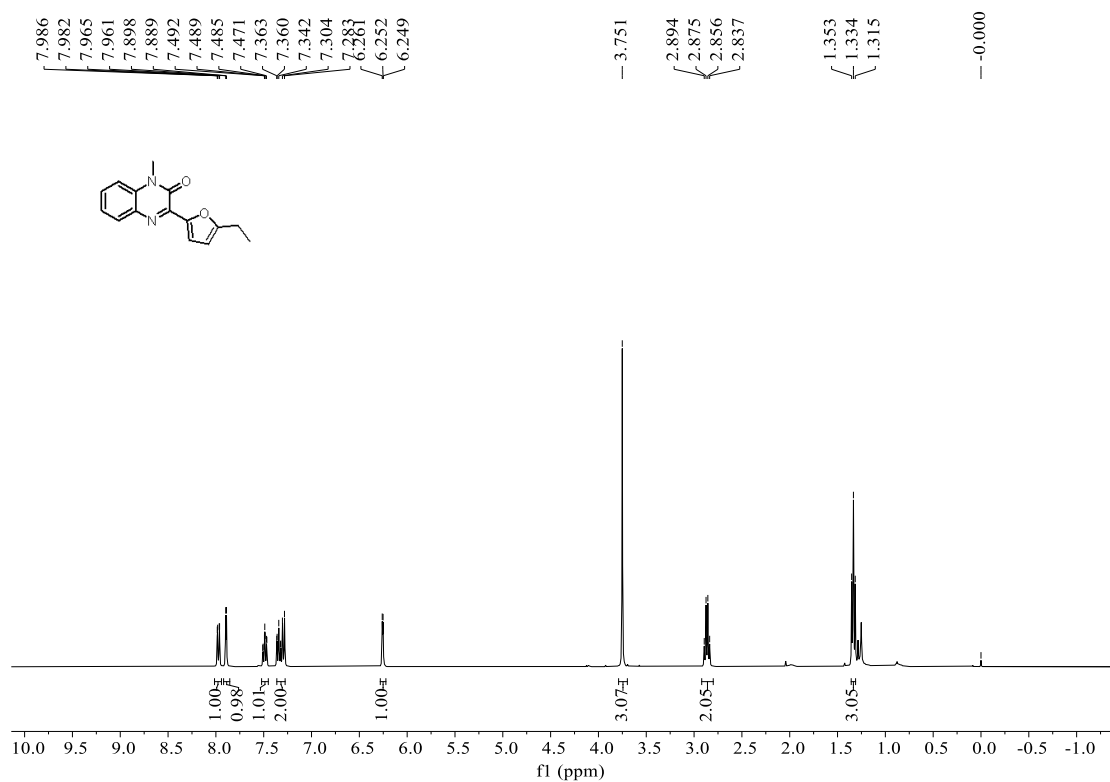
¹H NMR spectra of 3q (400 MHz, CDCl₃)



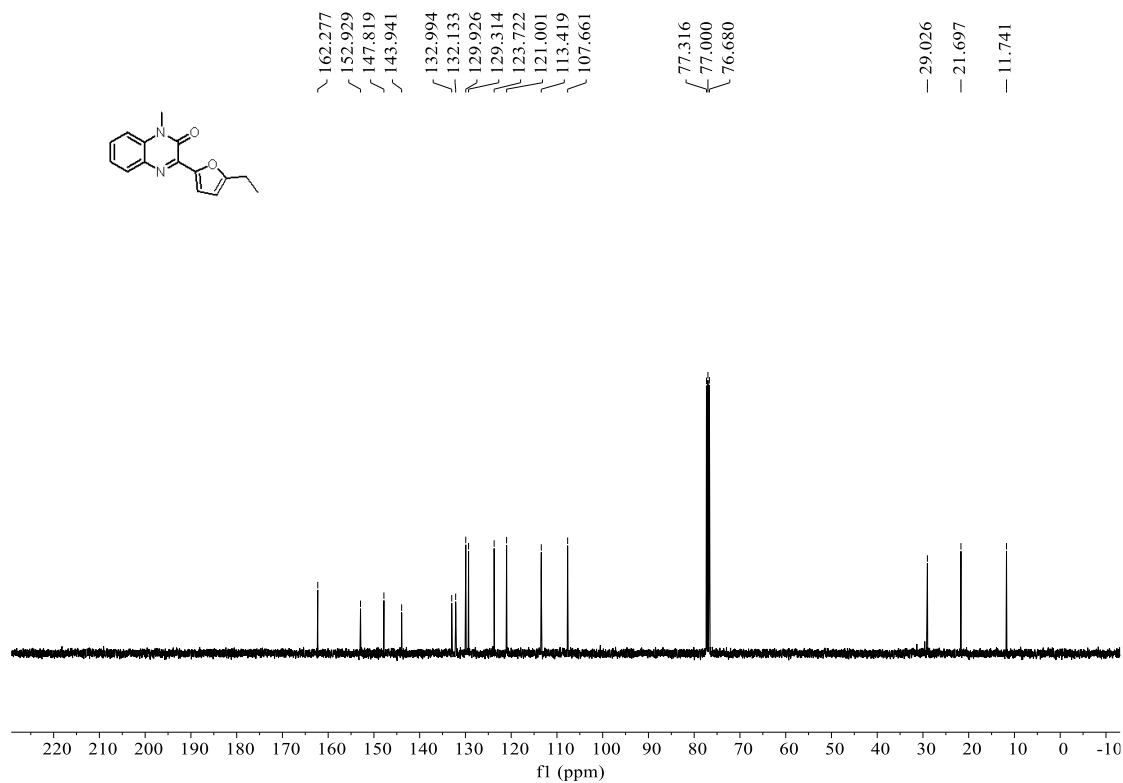
¹³C NMR spectra of 3q (100 MHz, CDCl₃)



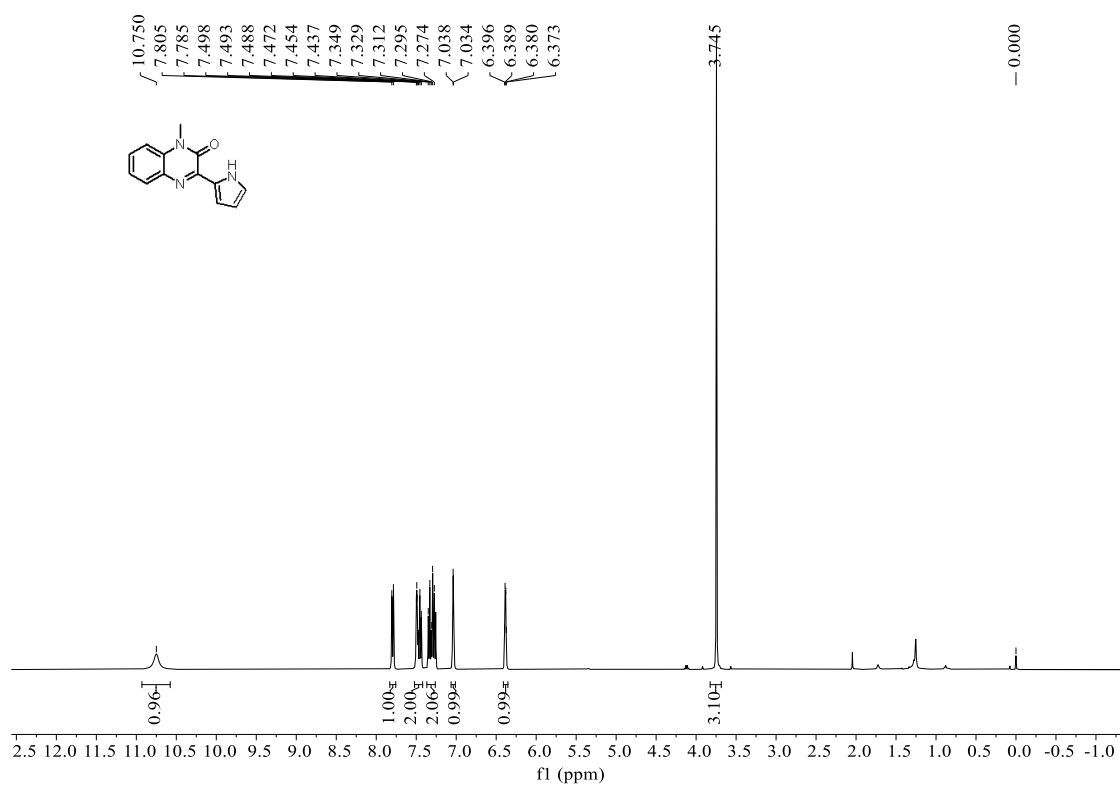
¹H NMR spectra of 3r (400 MHz, CDCl₃)



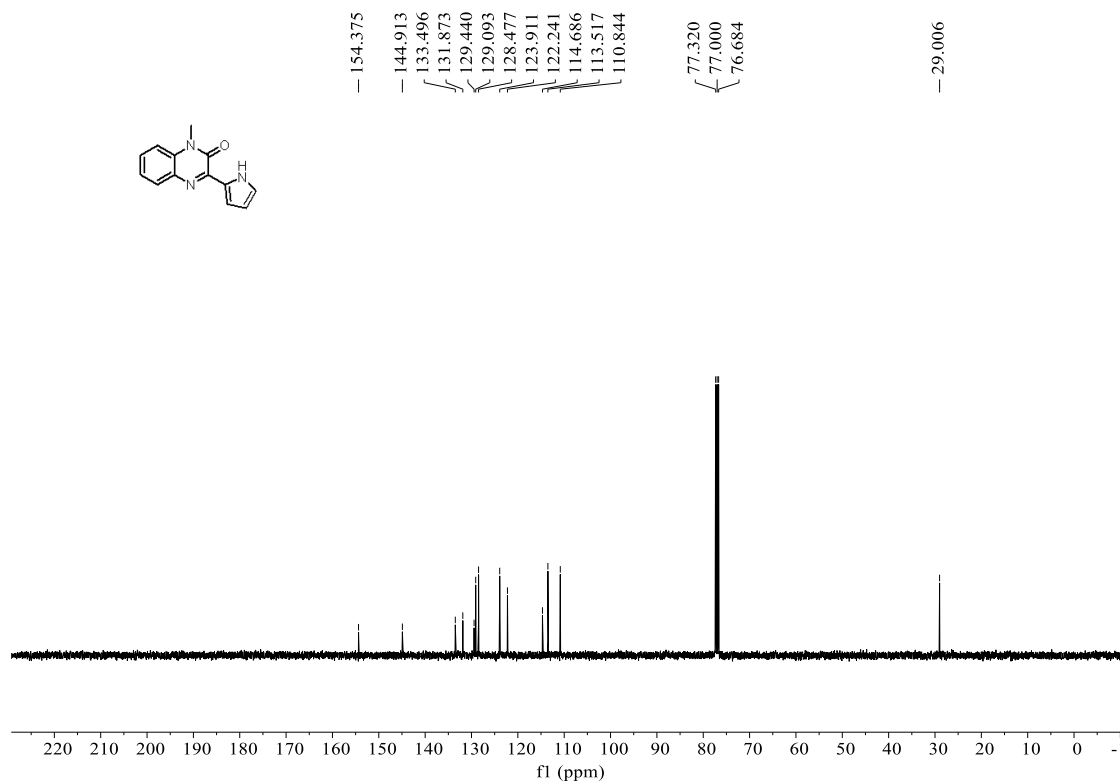
¹³C NMR spectra of 3r (100 MHz, CDCl₃)



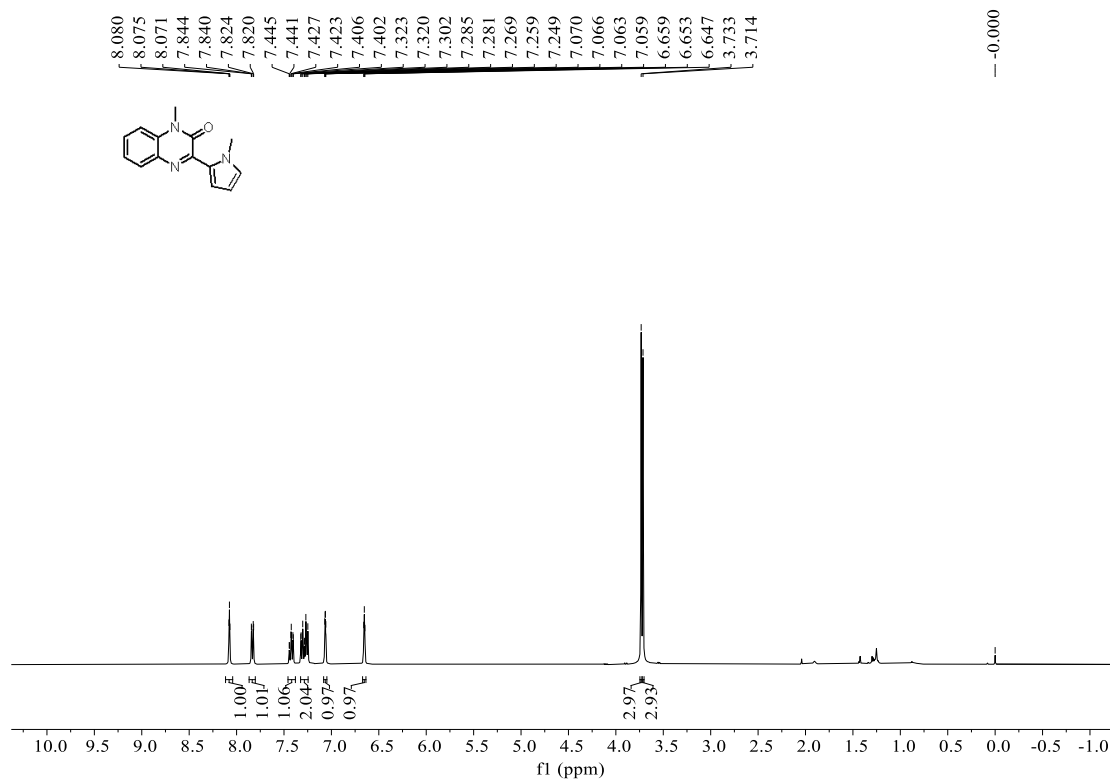
¹H NMR spectra of 3s (400 MHz, CDCl₃)



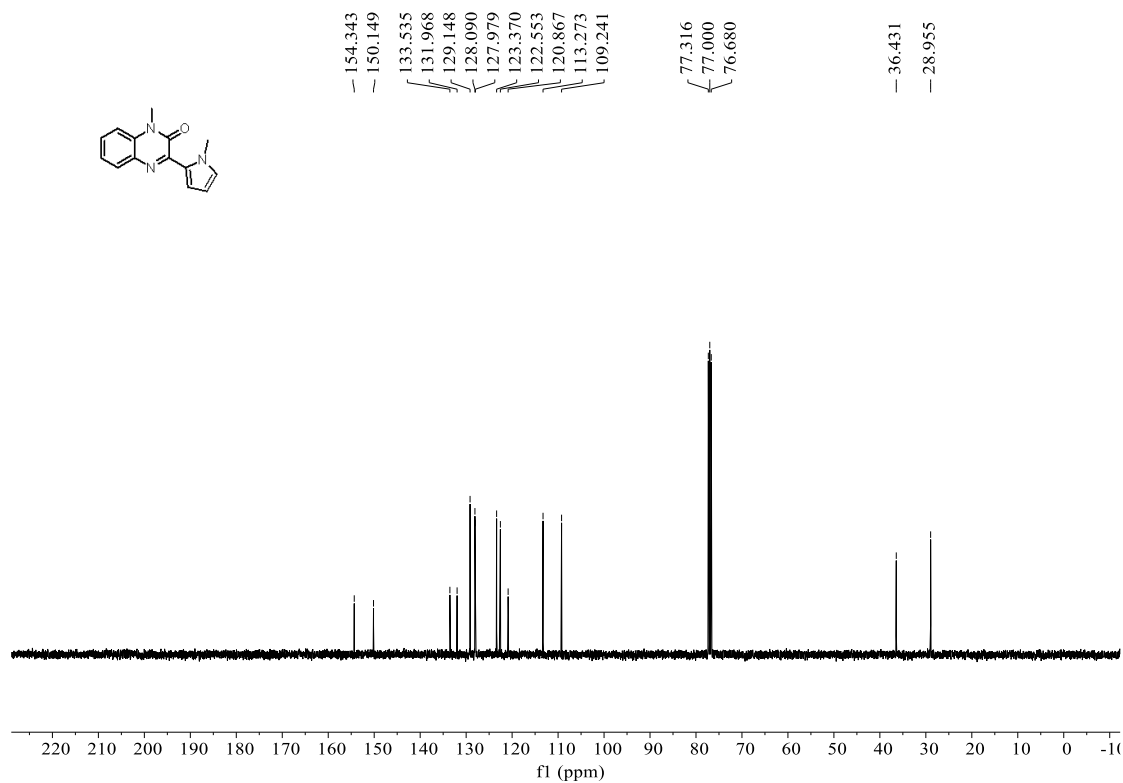
¹³C NMR spectra of 3s (100 MHz, CDCl₃)



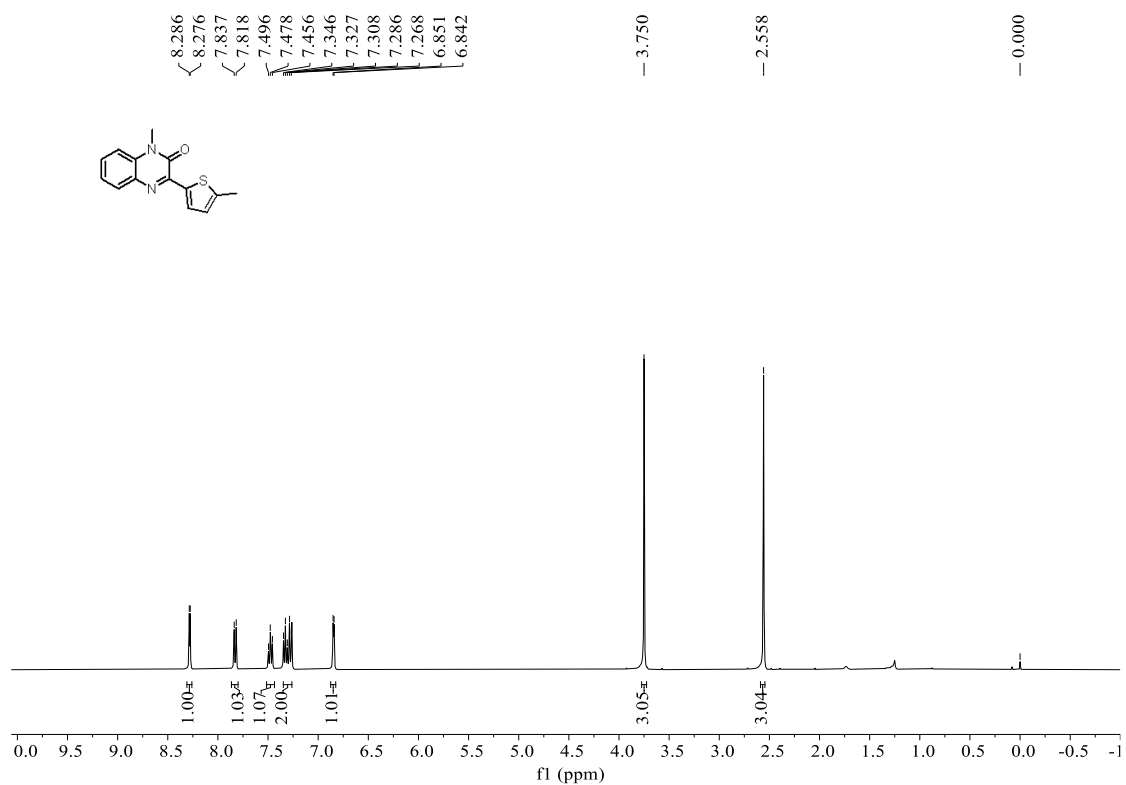
¹H NMR spectra of 3t (400 MHz, CDCl₃)



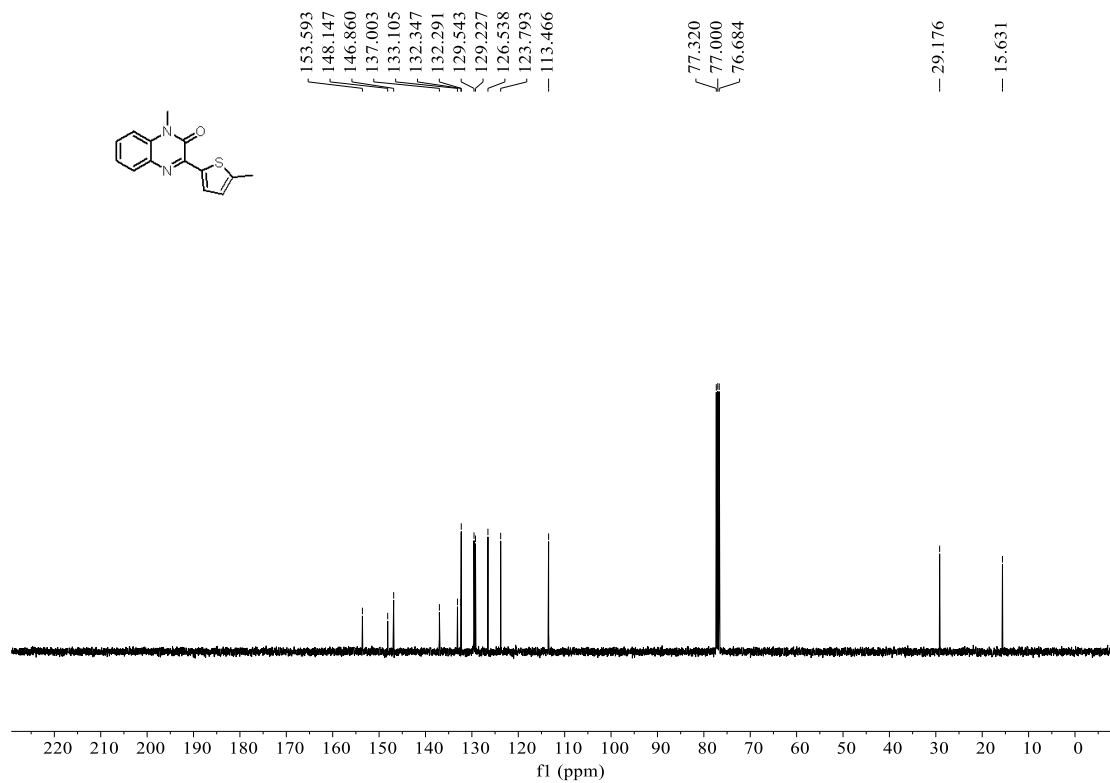
¹³C NMR spectra of 3t (100 MHz, CDCl₃)



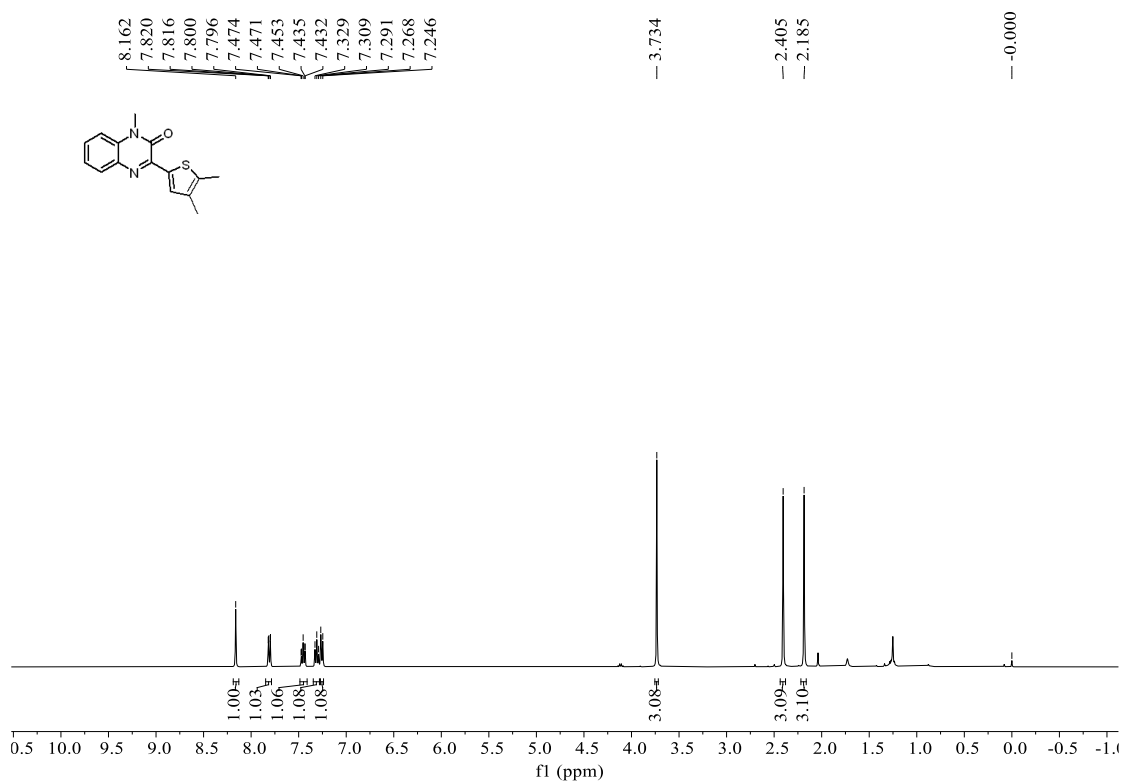
¹H NMR spectra of 3u (400 MHz, CDCl₃)



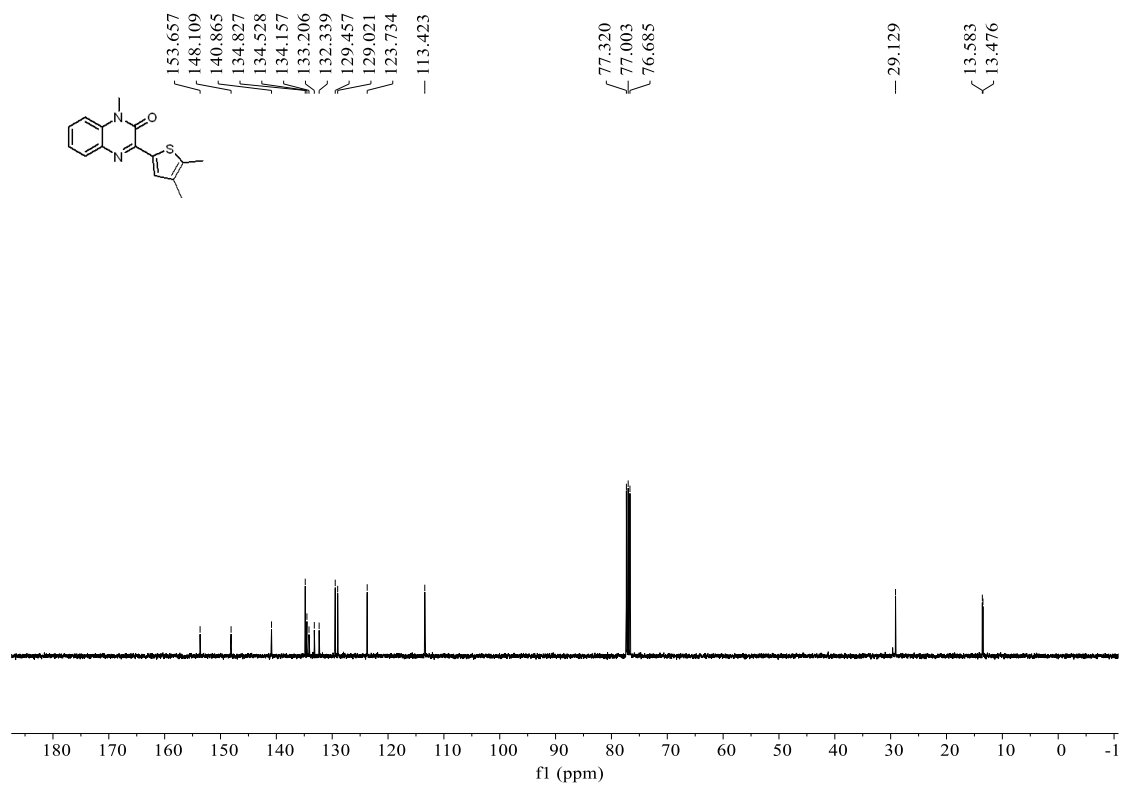
¹³C NMR spectra of 3u (100 MHz, CDCl₃)



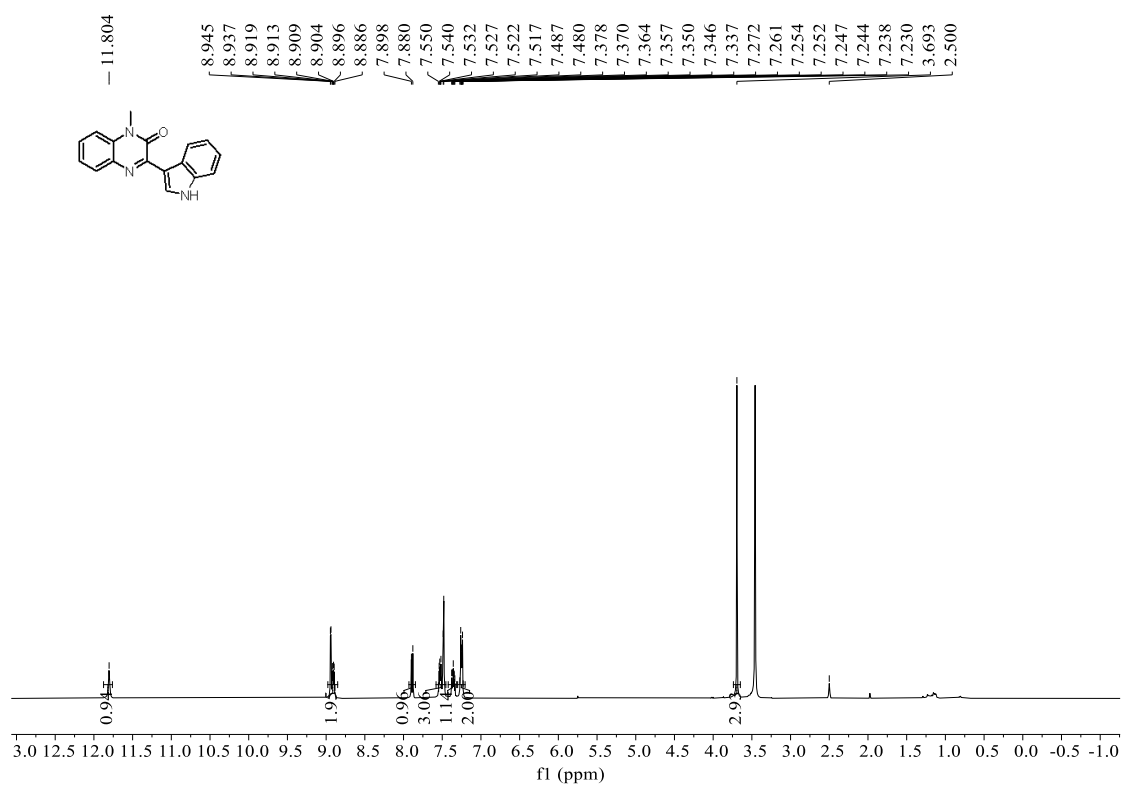
¹H NMR spectra of 3v (400 MHz, CDCl₃)



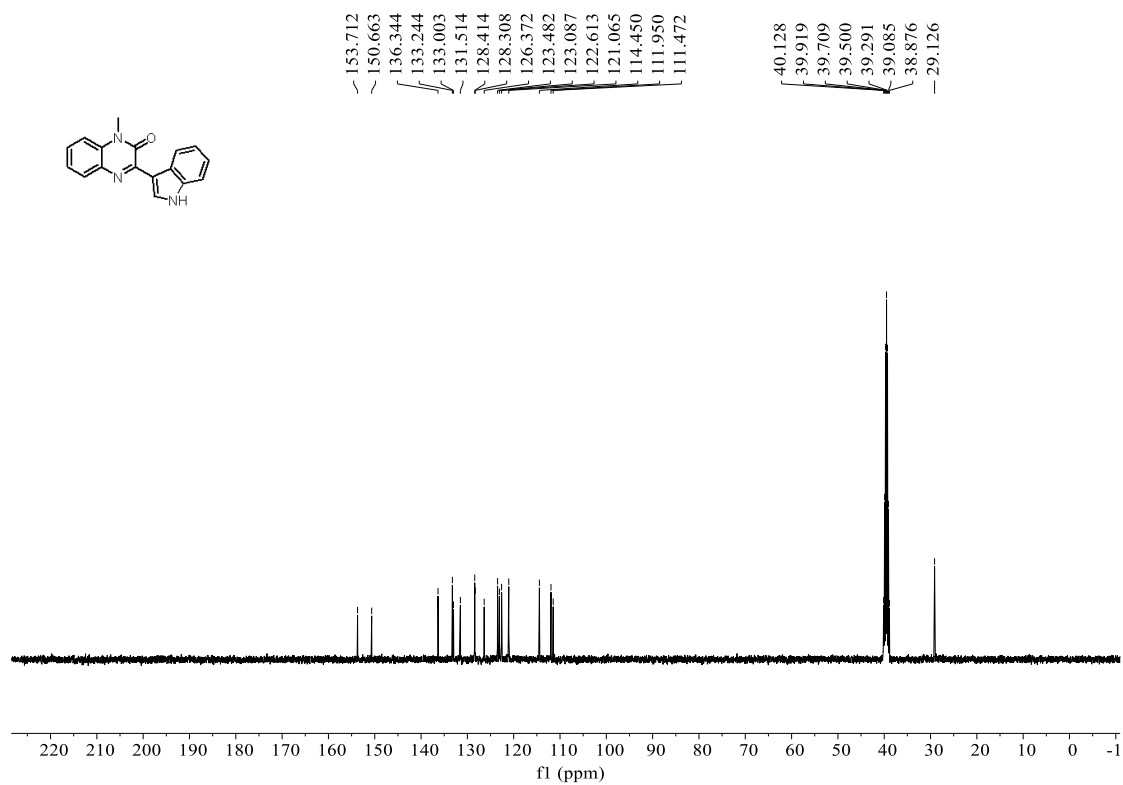
¹³C NMR spectra of 3v (100 MHz, CDCl₃)



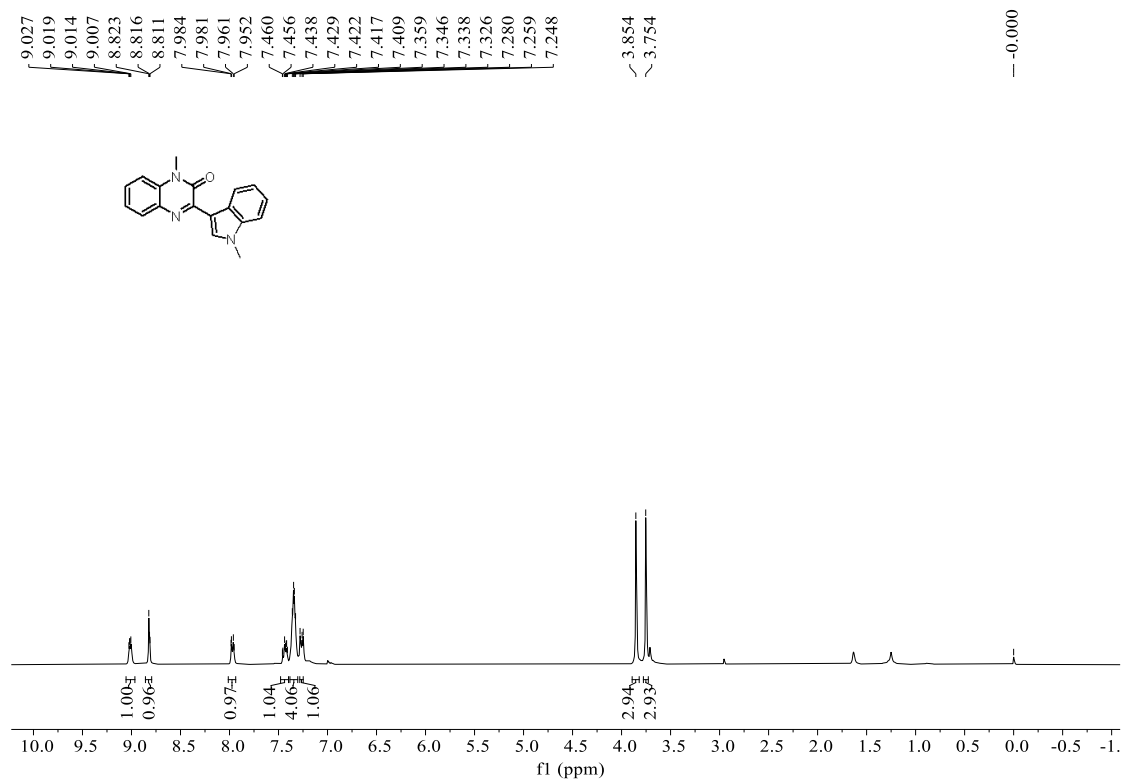
¹H NMR spectra of 3w (400 MHz, DMSO)



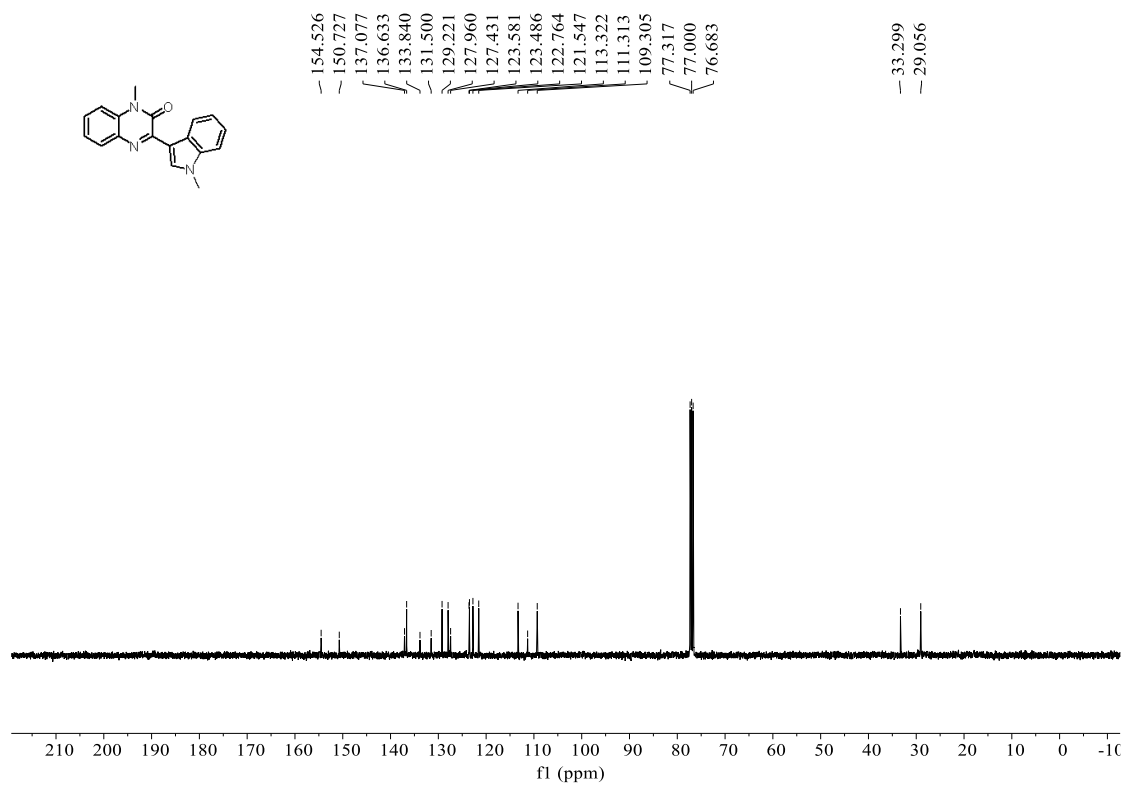
¹³C NMR spectra of 3w (100 MHz, DMSO)



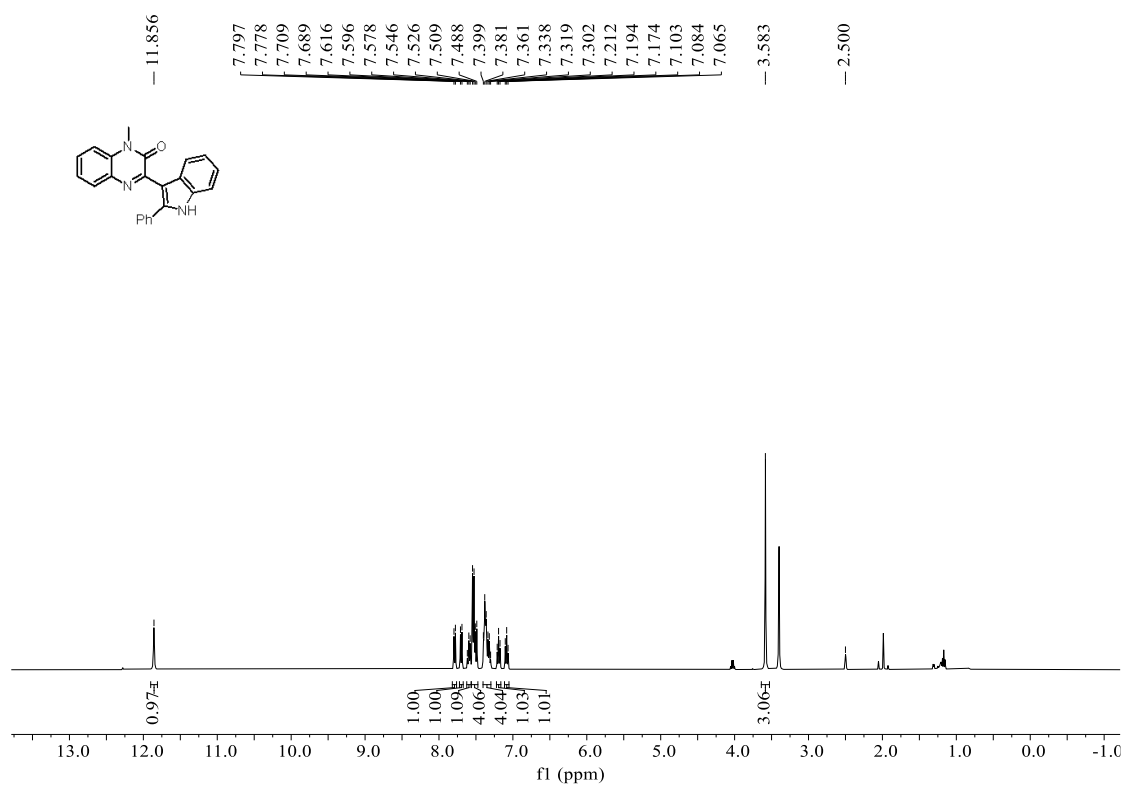
¹H NMR spectra of 3x (400 MHz, CDCl₃)



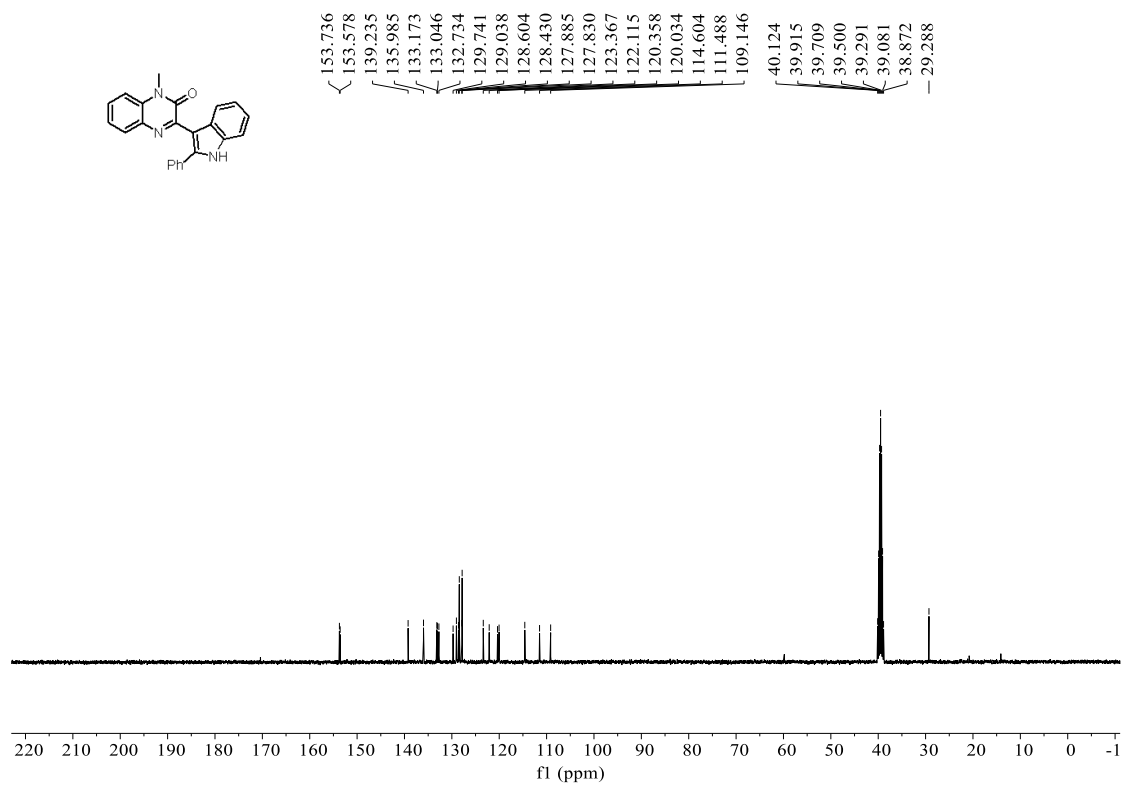
¹³C NMR spectra of 3x (100 MHz, CDCl₃)



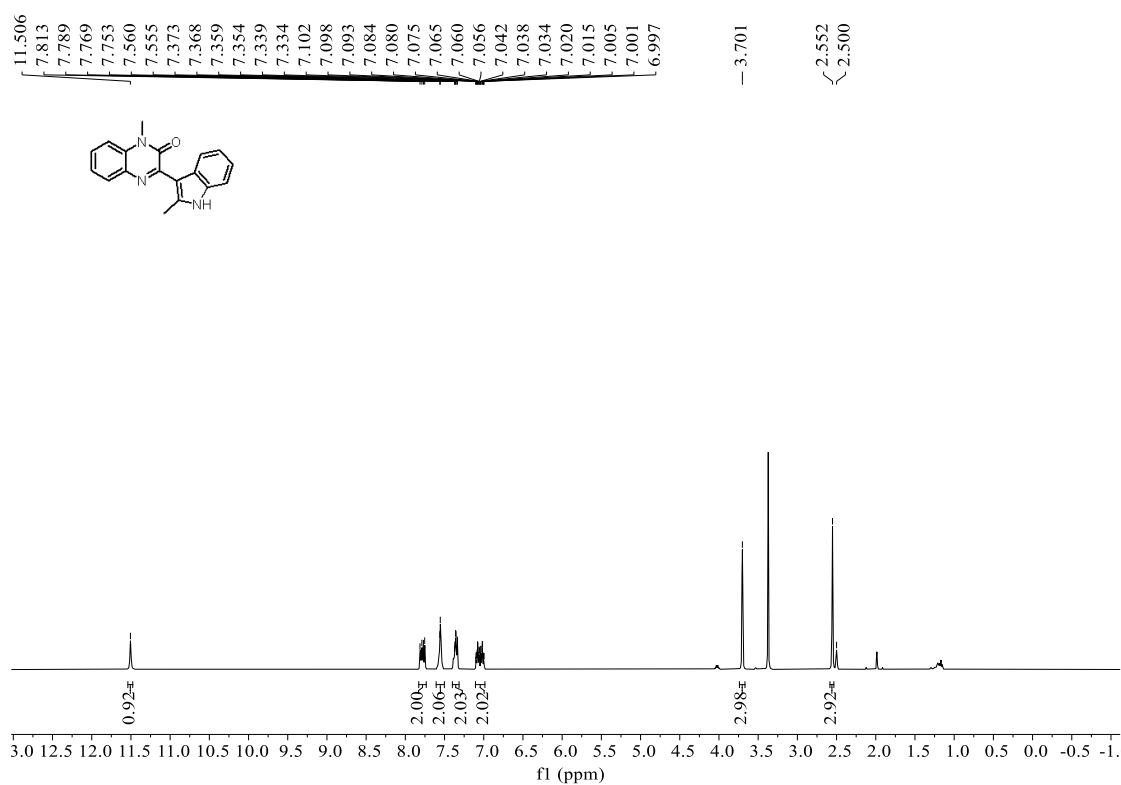
¹H NMR spectra of 3y (400 MHz, DMSO)



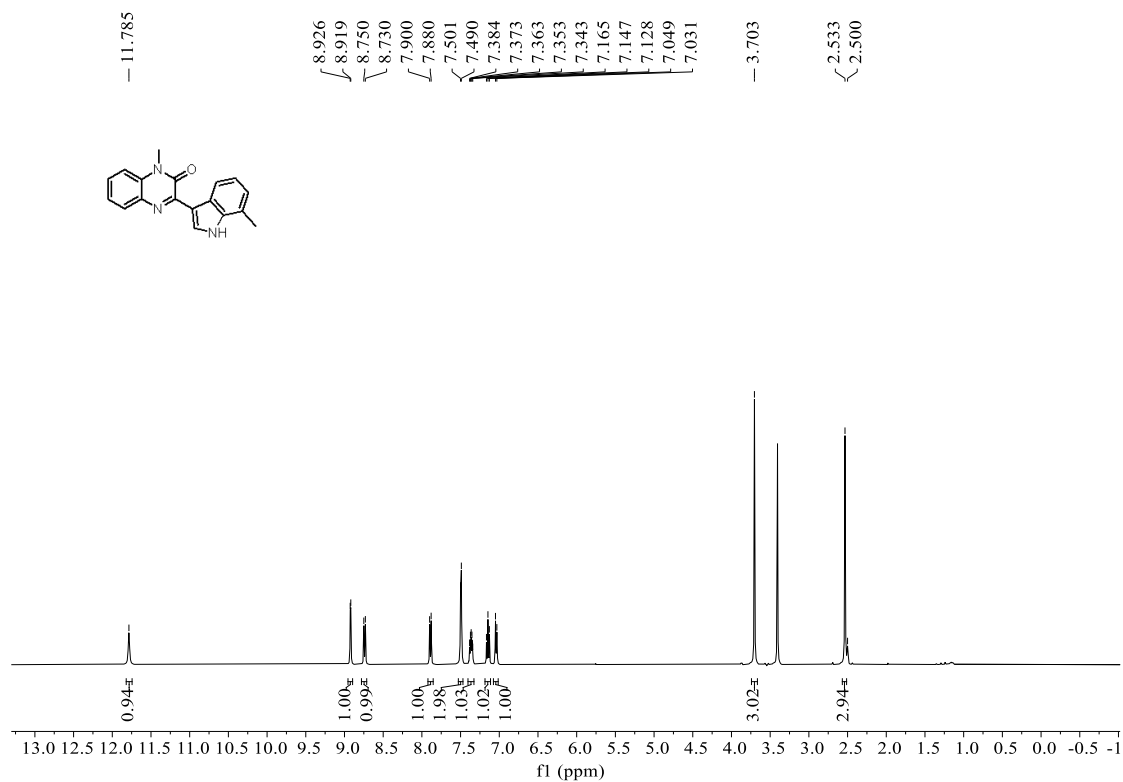
¹³C NMR spectra of 3y (100 MHz, DMSO)



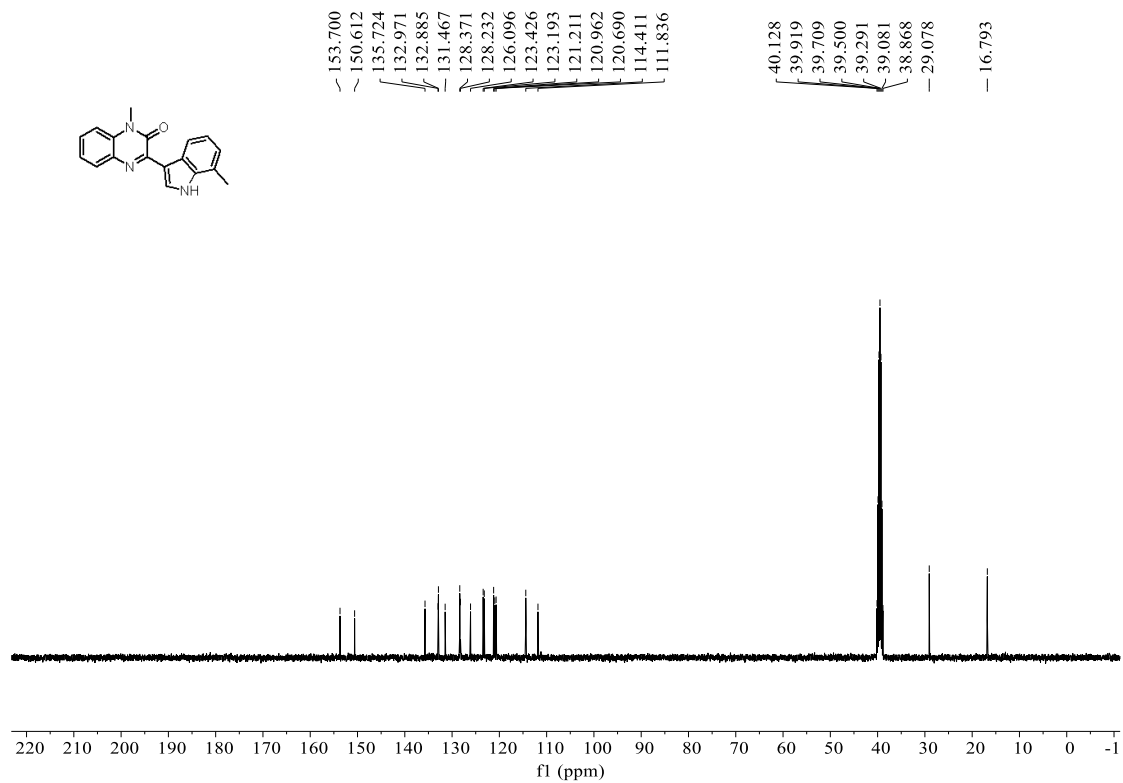
¹H NMR spectra of 3z (400 MHz, DMSO)



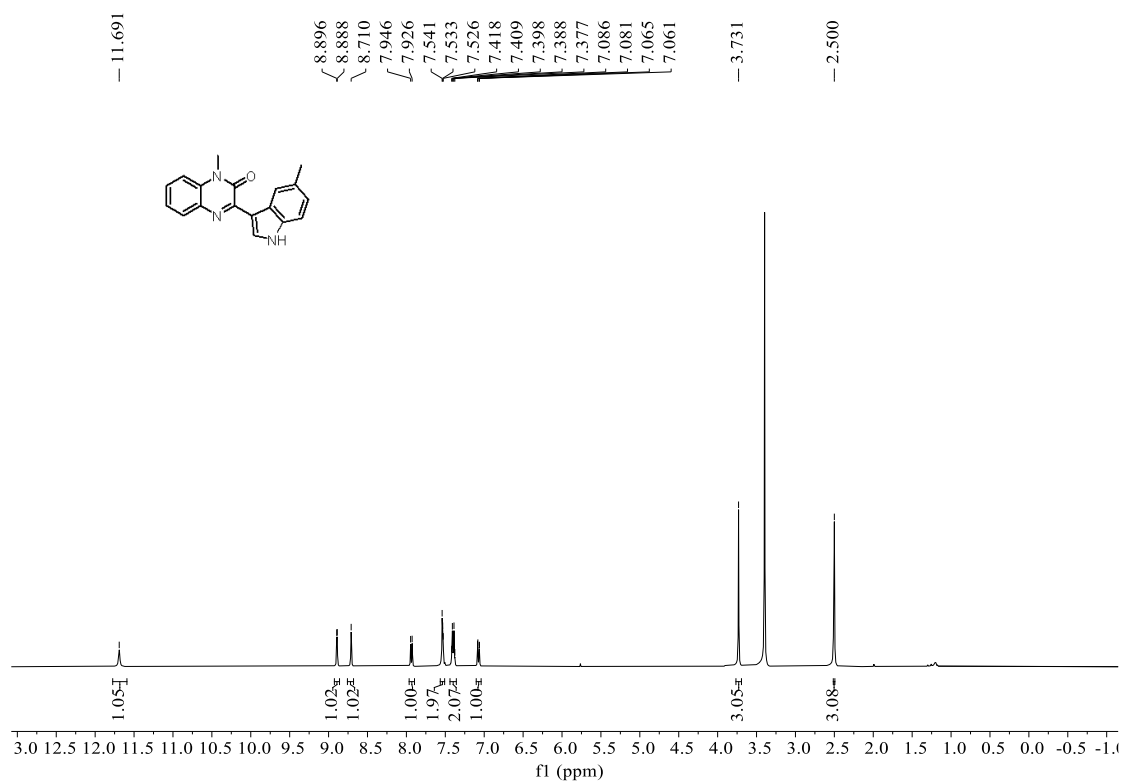
¹H NMR spectra of 3aa (400 MHz, DMSO)



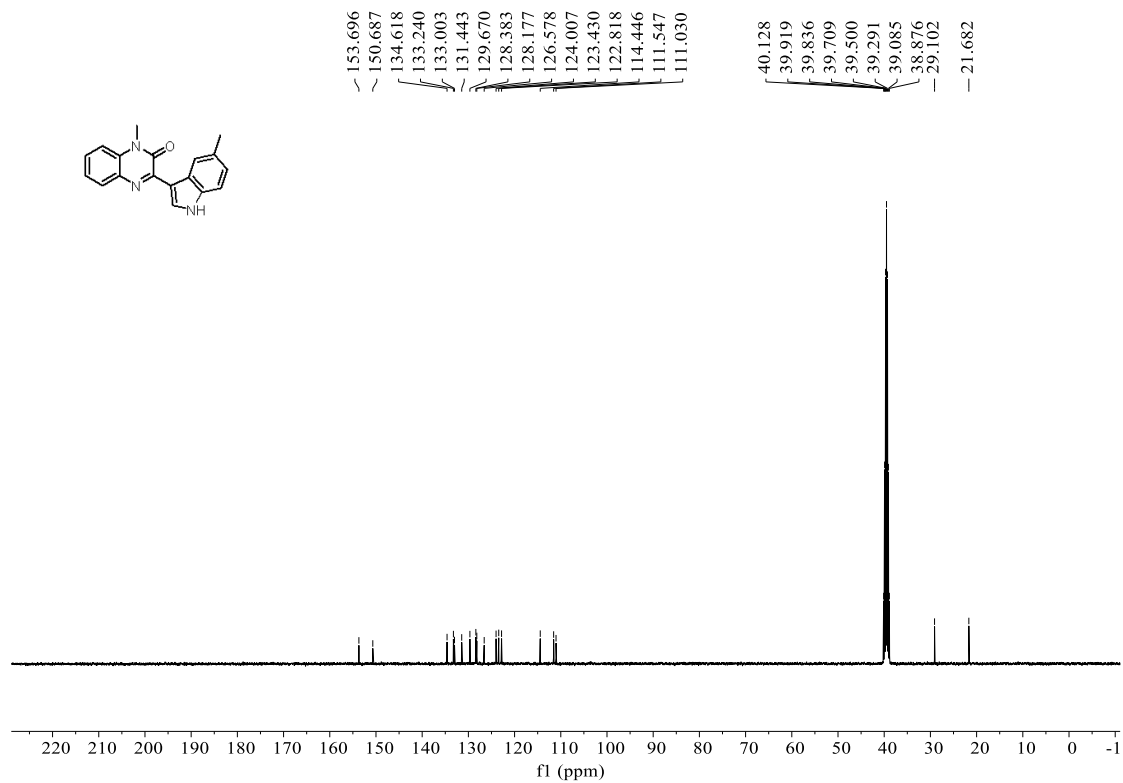
¹³C NMR spectra of 3aa (100 MHz, DMSO)



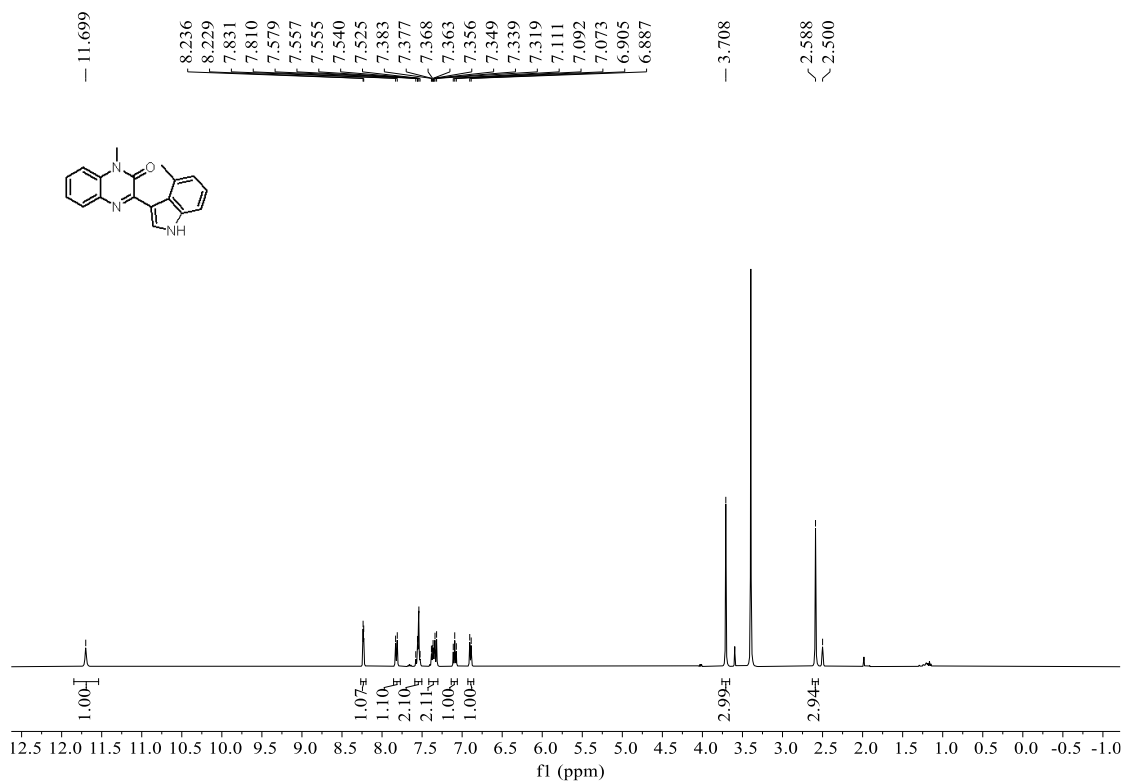
¹H NMR spectra of 3ab (400 MHz, DMSO)



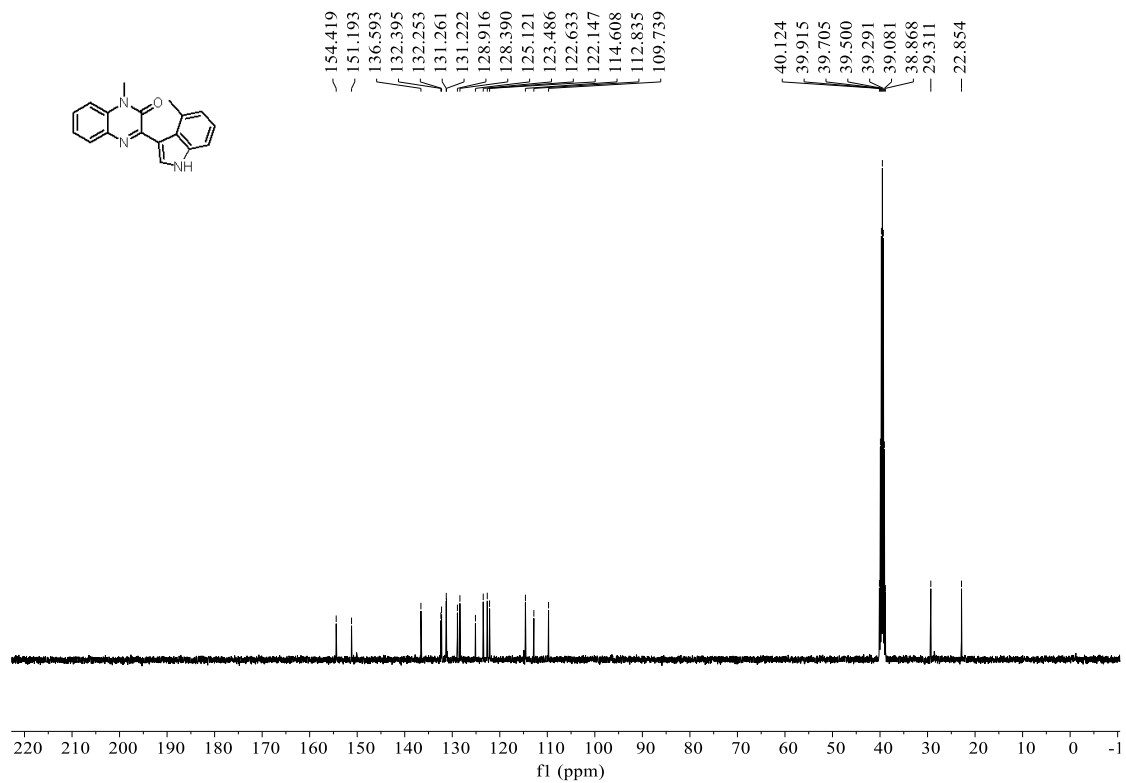
¹³C NMR spectra of 3ab (100 MHz, DMSO)



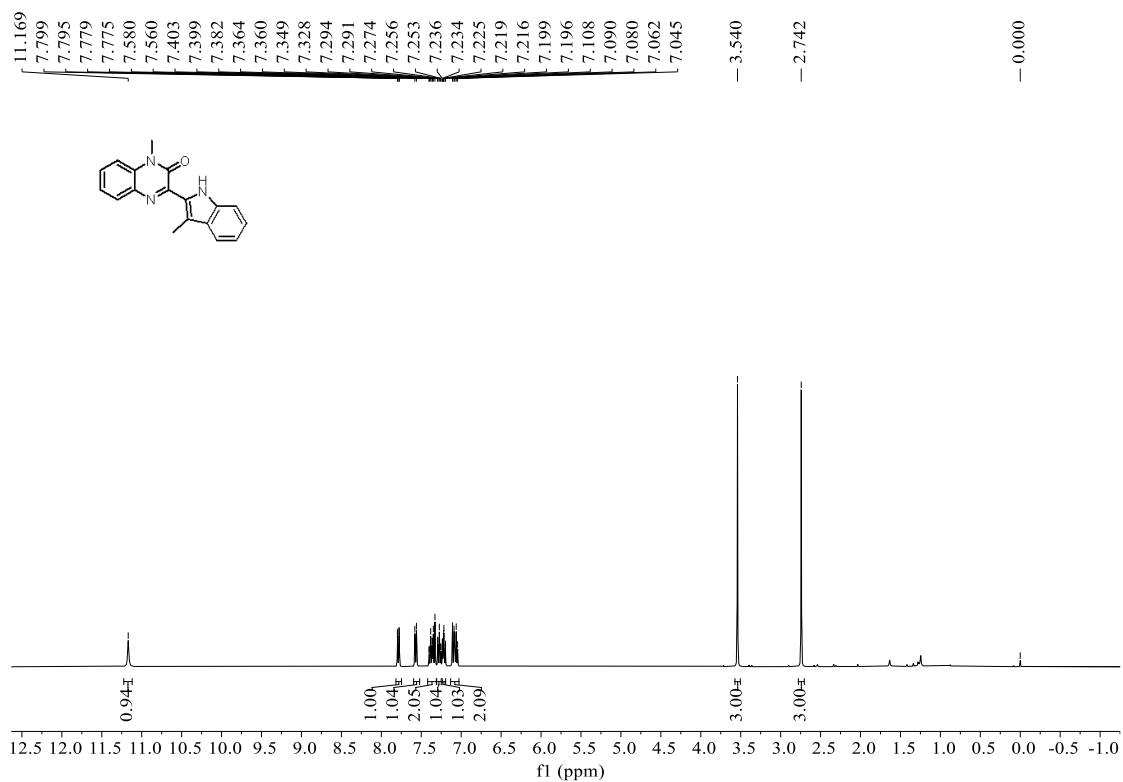
¹H NMR spectra of 3ac (400 MHz, DMSO)



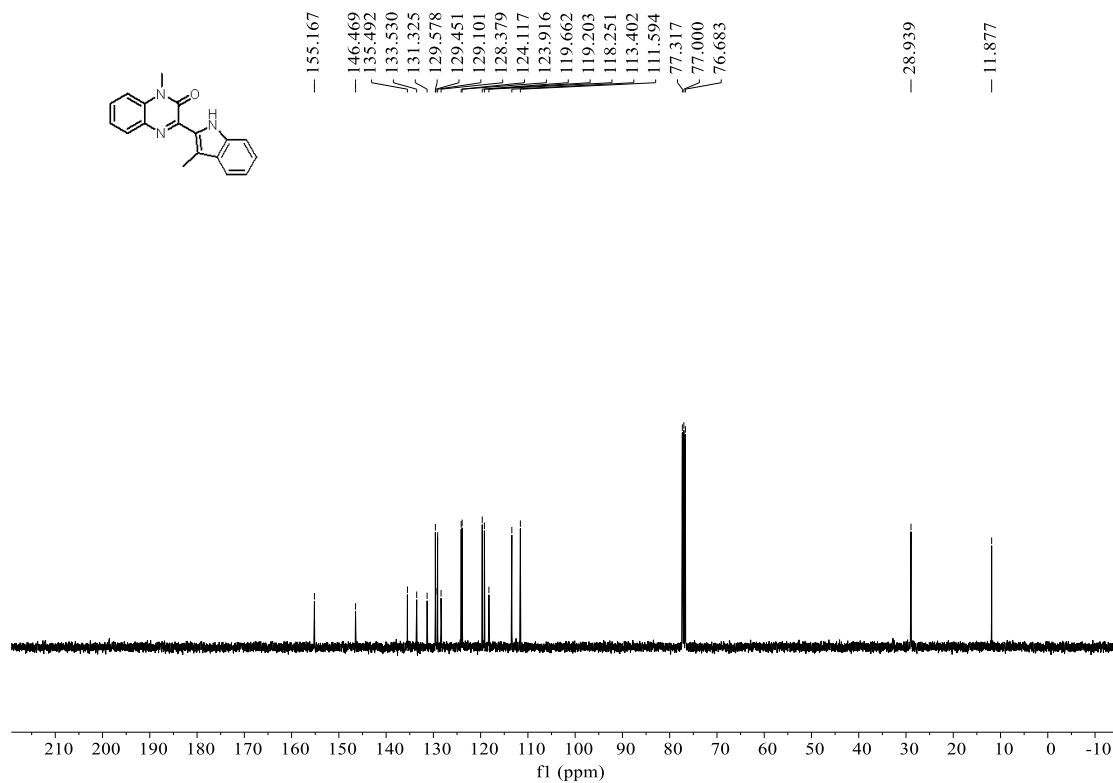
¹³C NMR spectra of 3ac (100 MHz, DMSO)



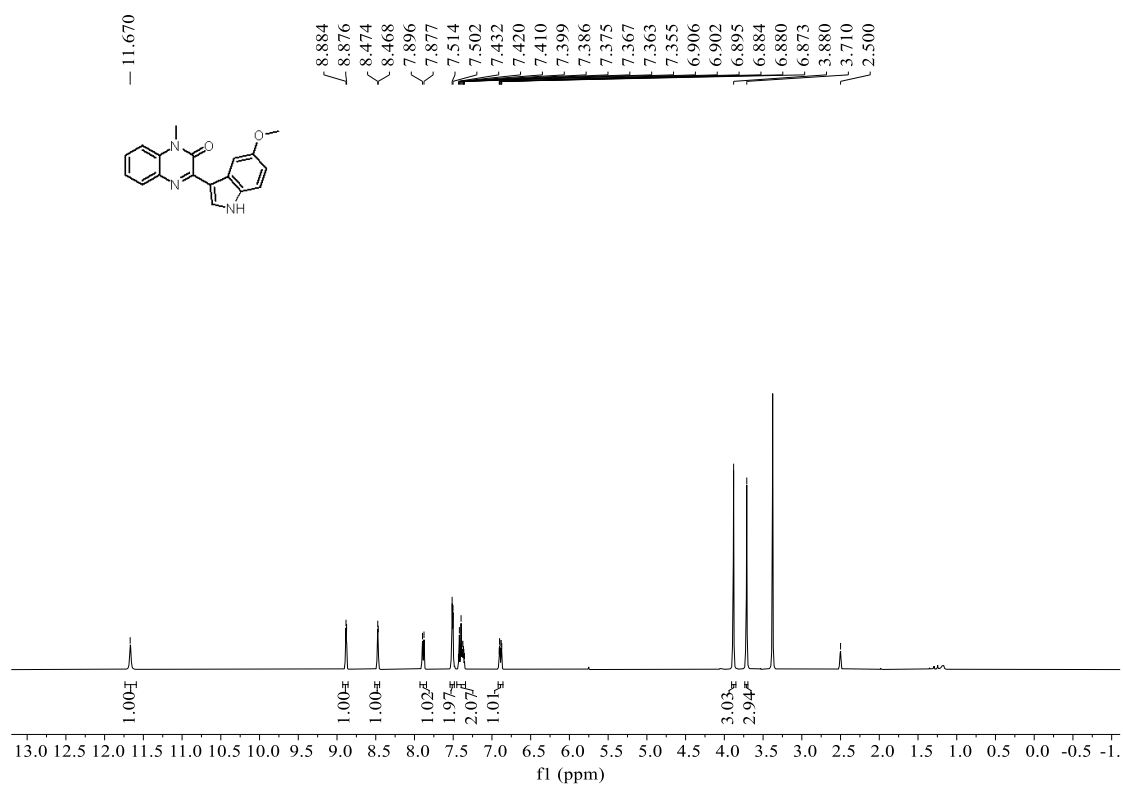
¹H NMR spectra of 3ad (400 MHz, CDCl₃)



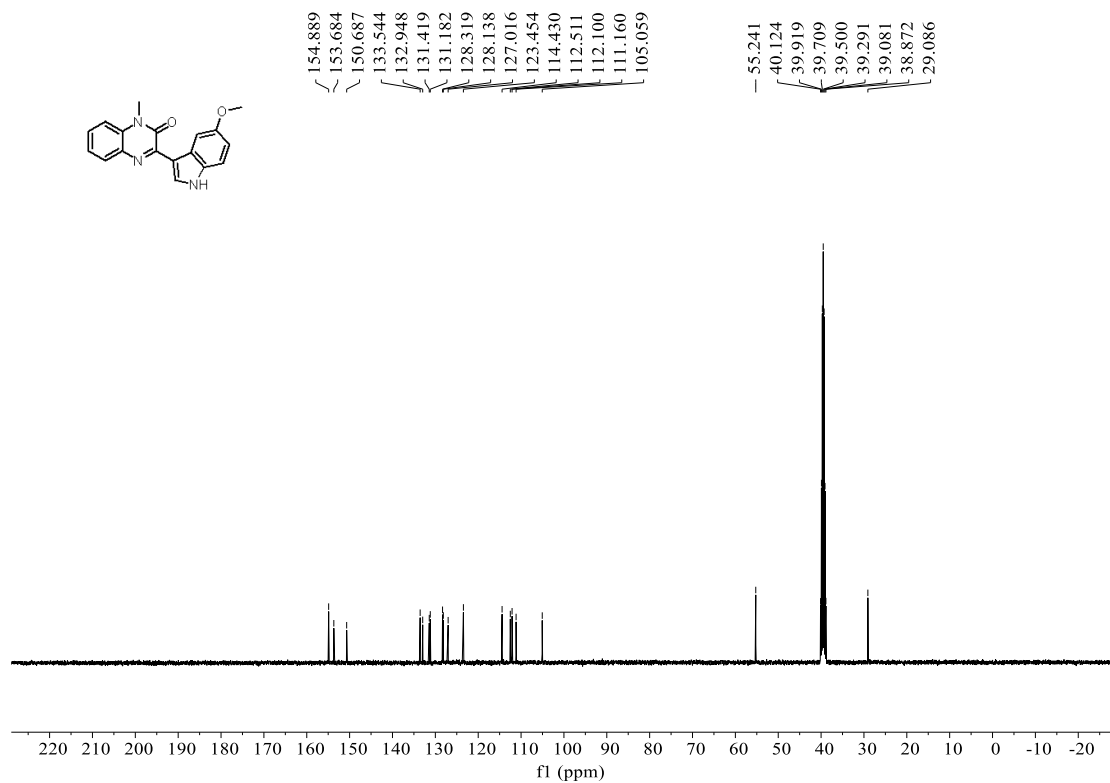
¹³C NMR spectra of 3ad (100 MHz, CDCl₃)



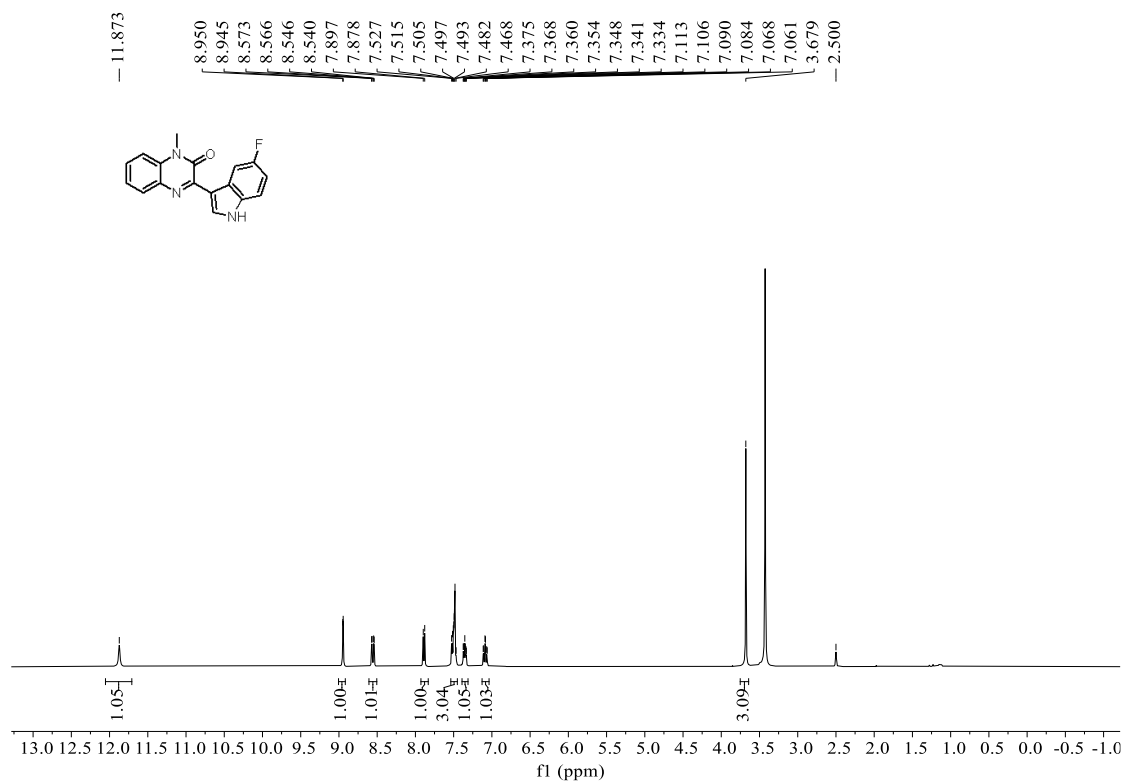
¹H NMR spectra of 3ae (400 MHz, DMSO)



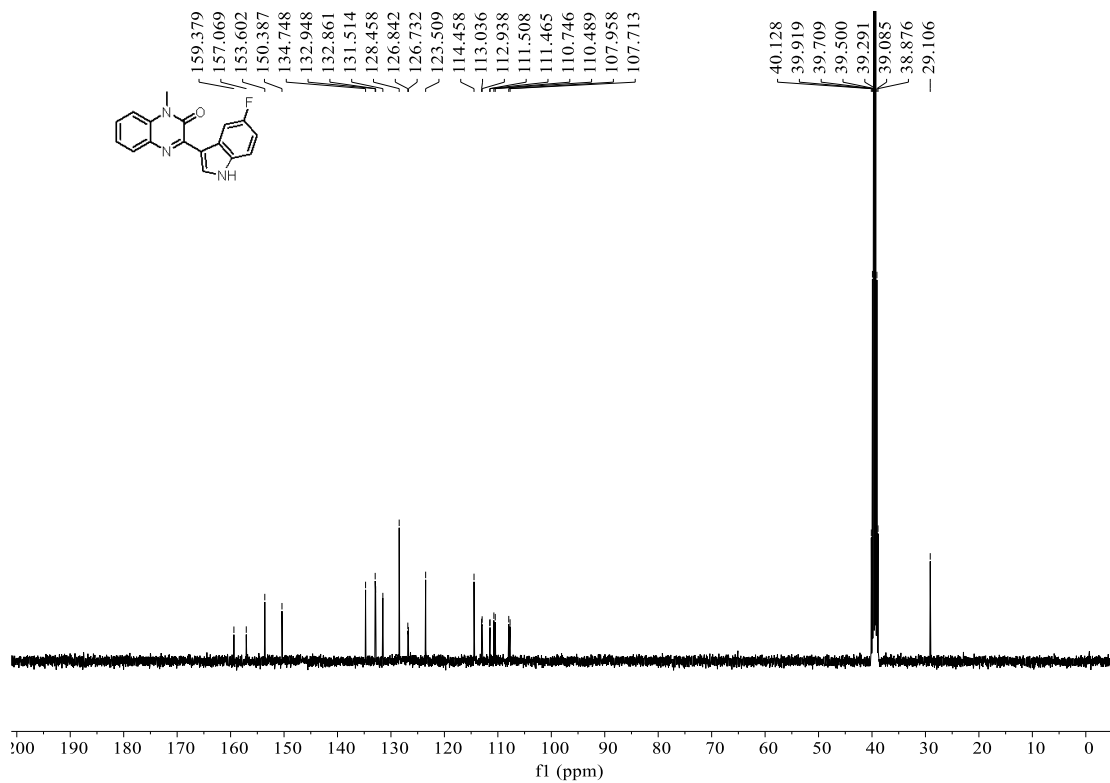
¹³C NMR spectra of 3ae (100 MHz, DMSO)



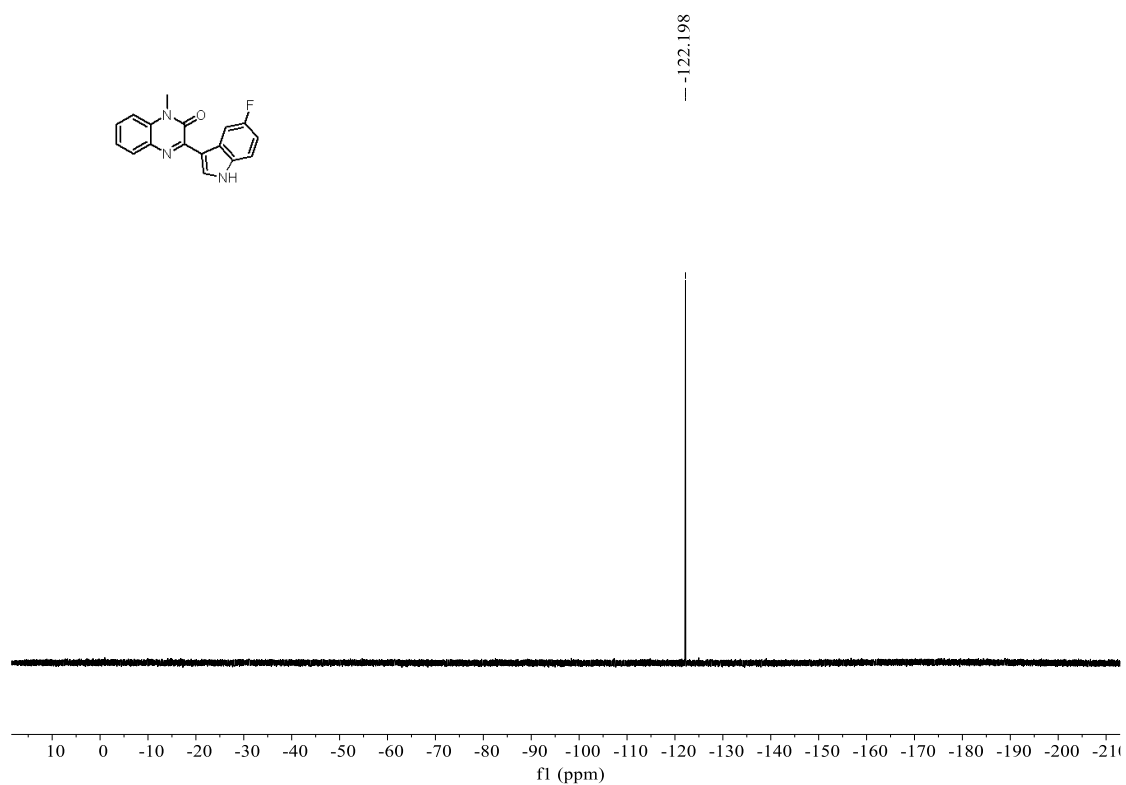
¹H NMR spectra of 3af (400 MHz, DMSO)



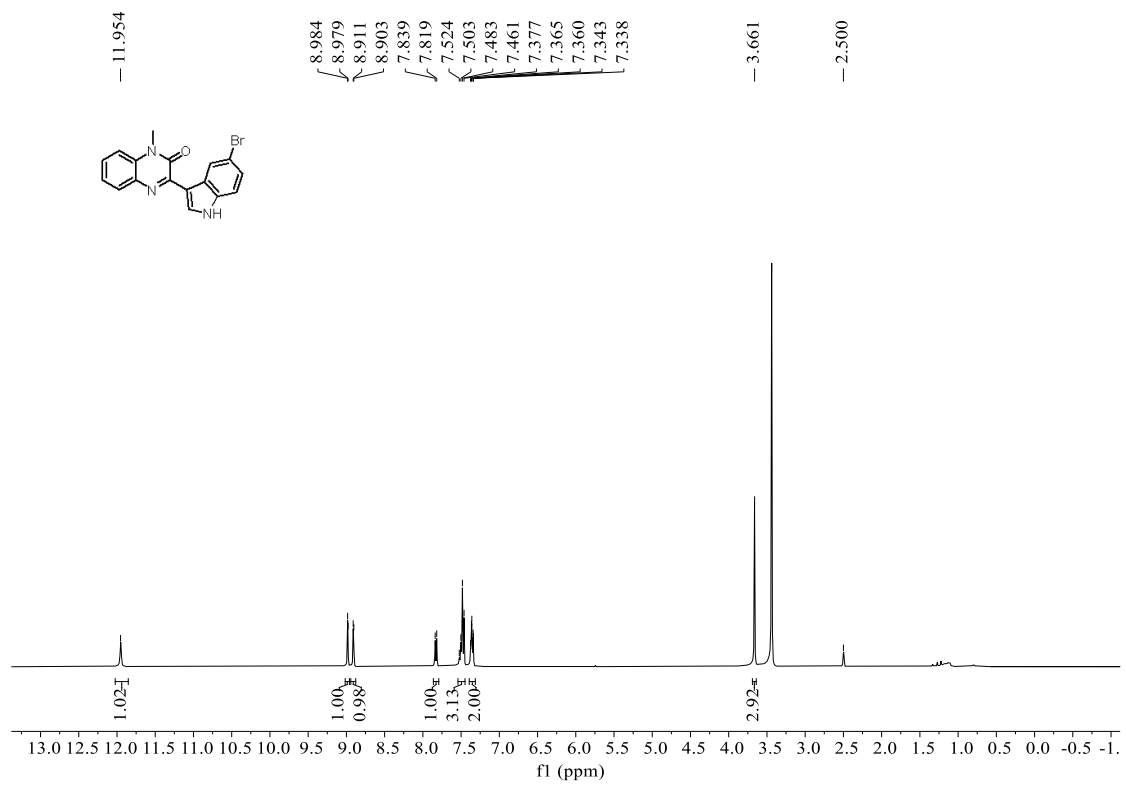
¹³C NMR spectra of 3af (100 MHz, DMSO)



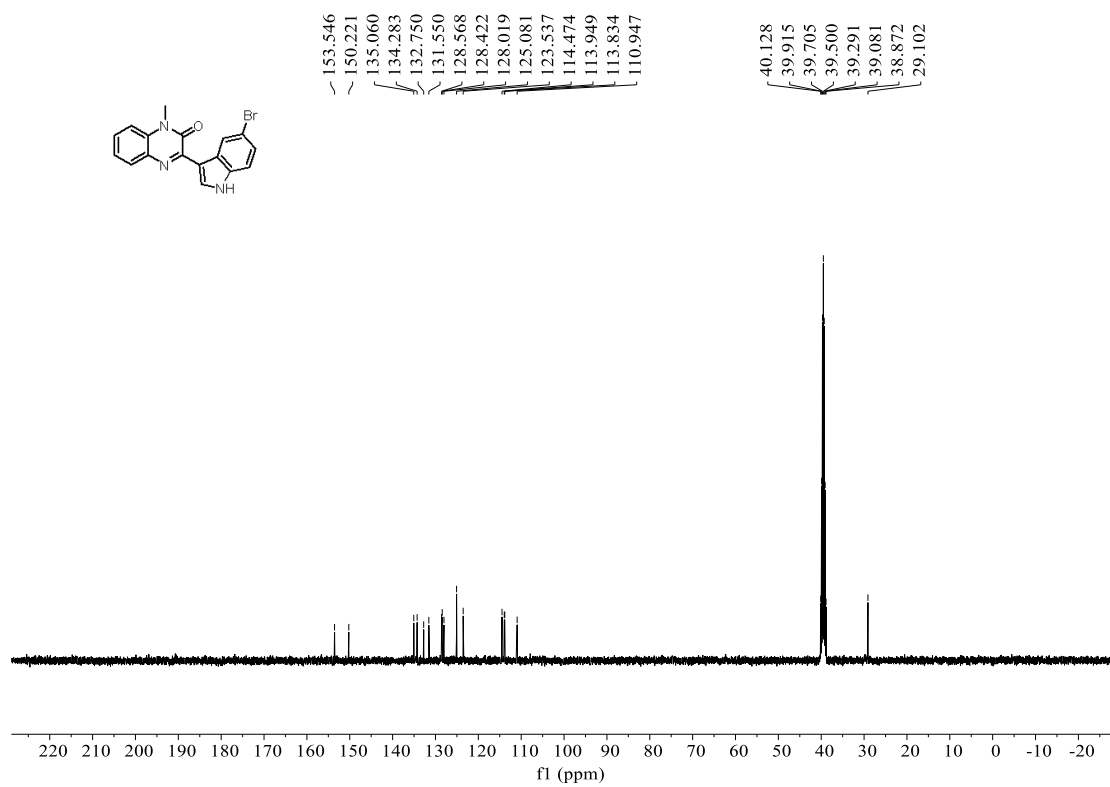
¹⁹F NMR spectra of 3af (376 MHz, DMSO)



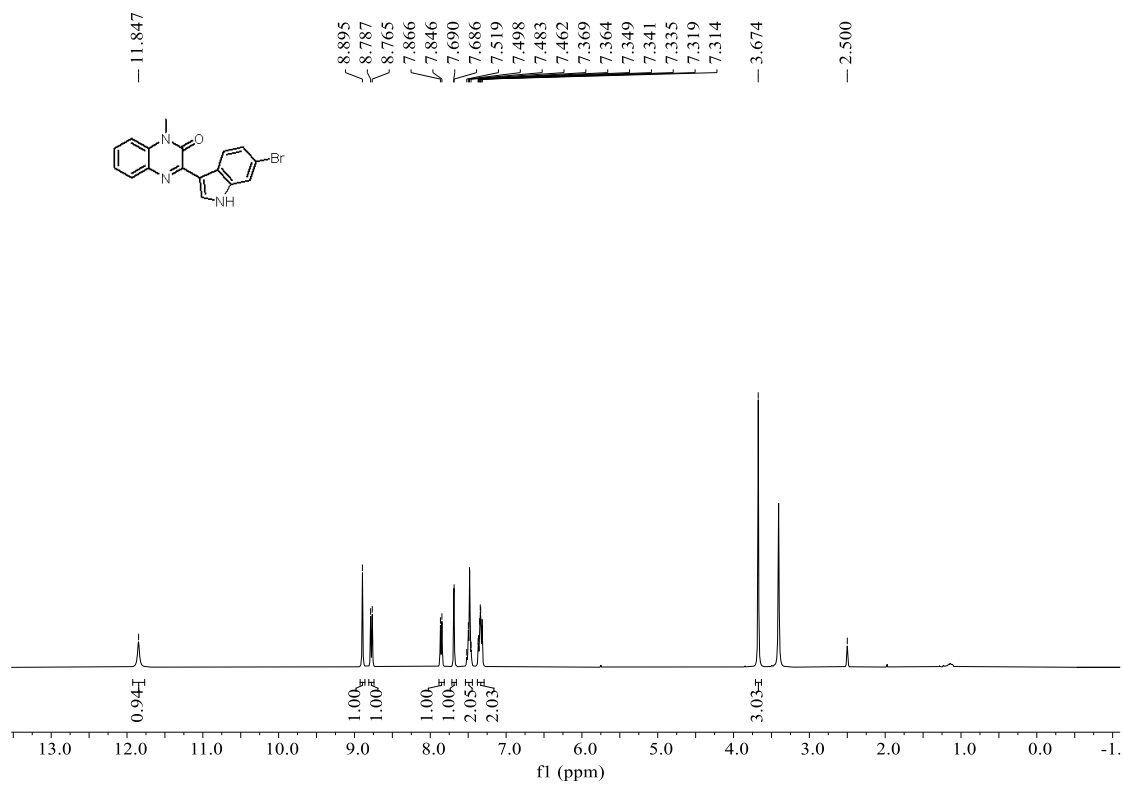
¹H NMR spectra of 3ag (400 MHz, DMSO)



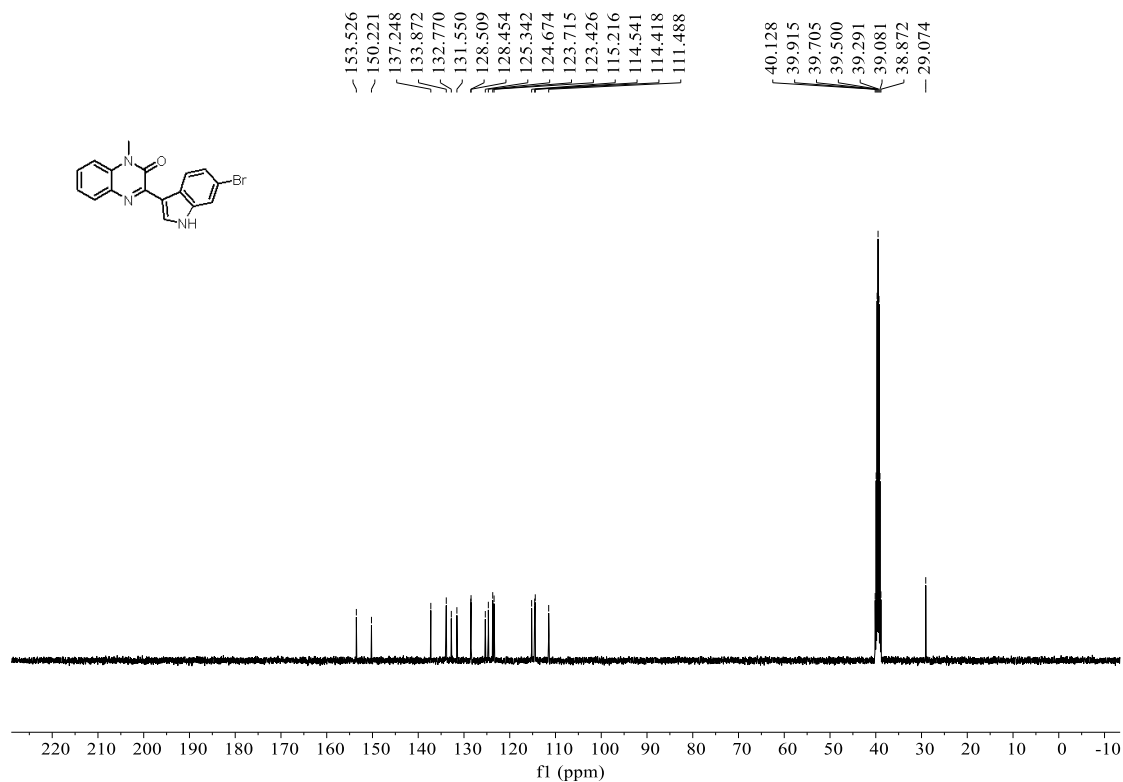
¹³C NMR spectra of 3ag (100 MHz, DMSO)



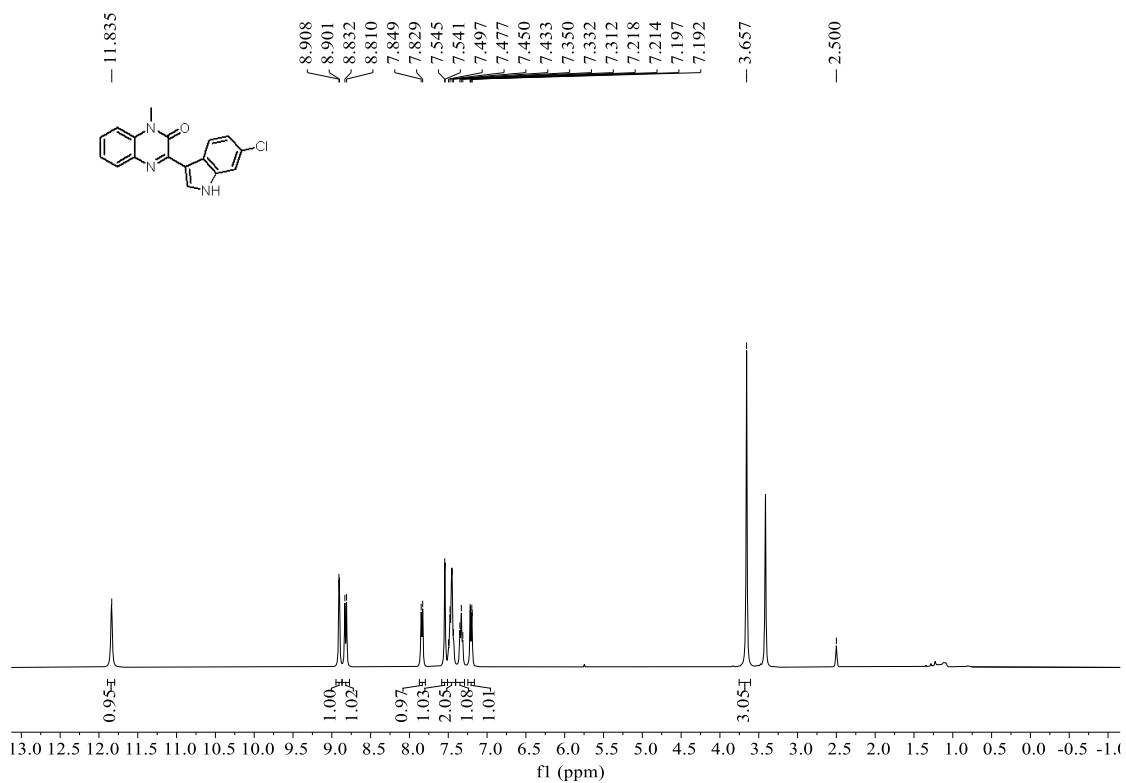
¹H NMR spectra of 3ah (400 MHz, DMSO)



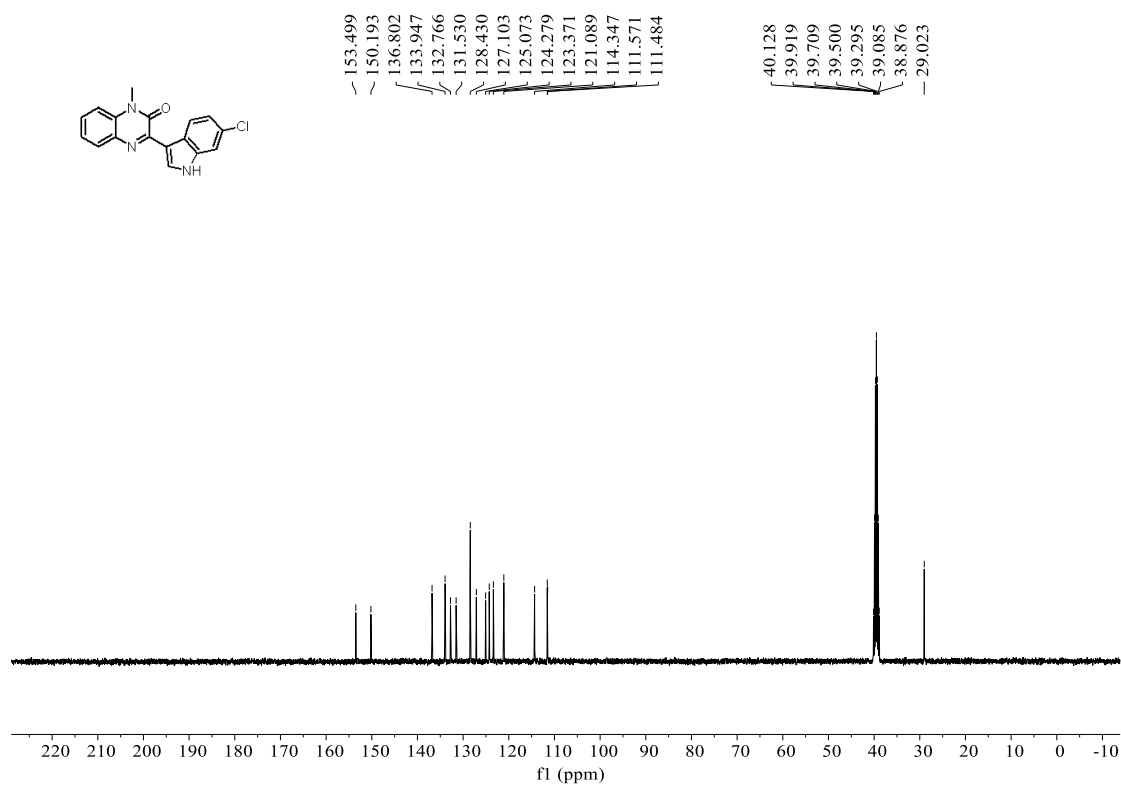
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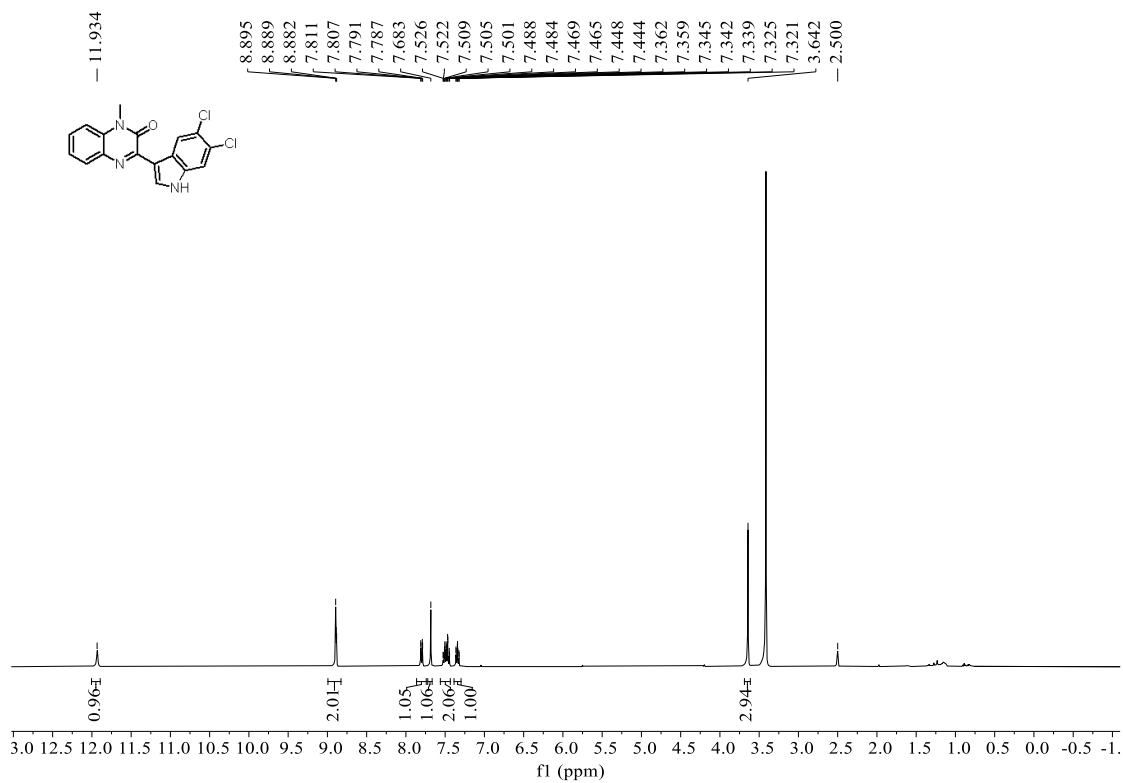
¹H NMR spectra of 3ai (400 MHz, DMSO)



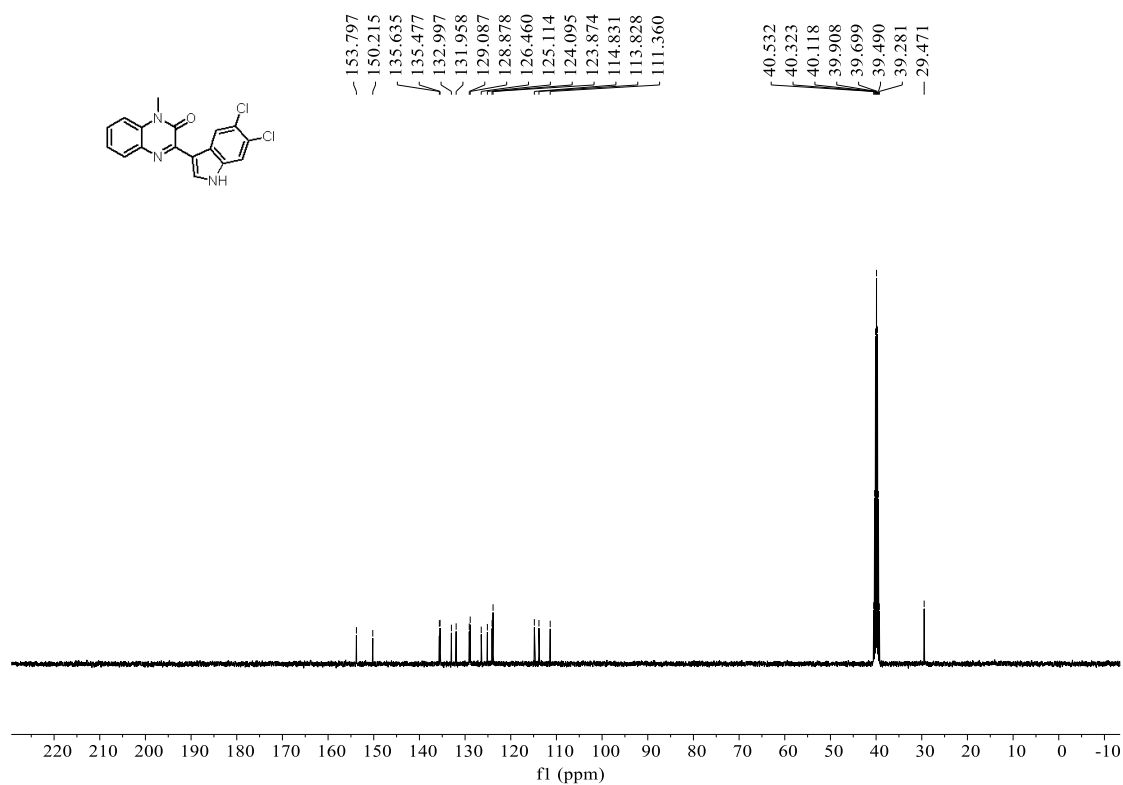
¹³C NMR spectra of 3ai (100 MHz, DMSO)



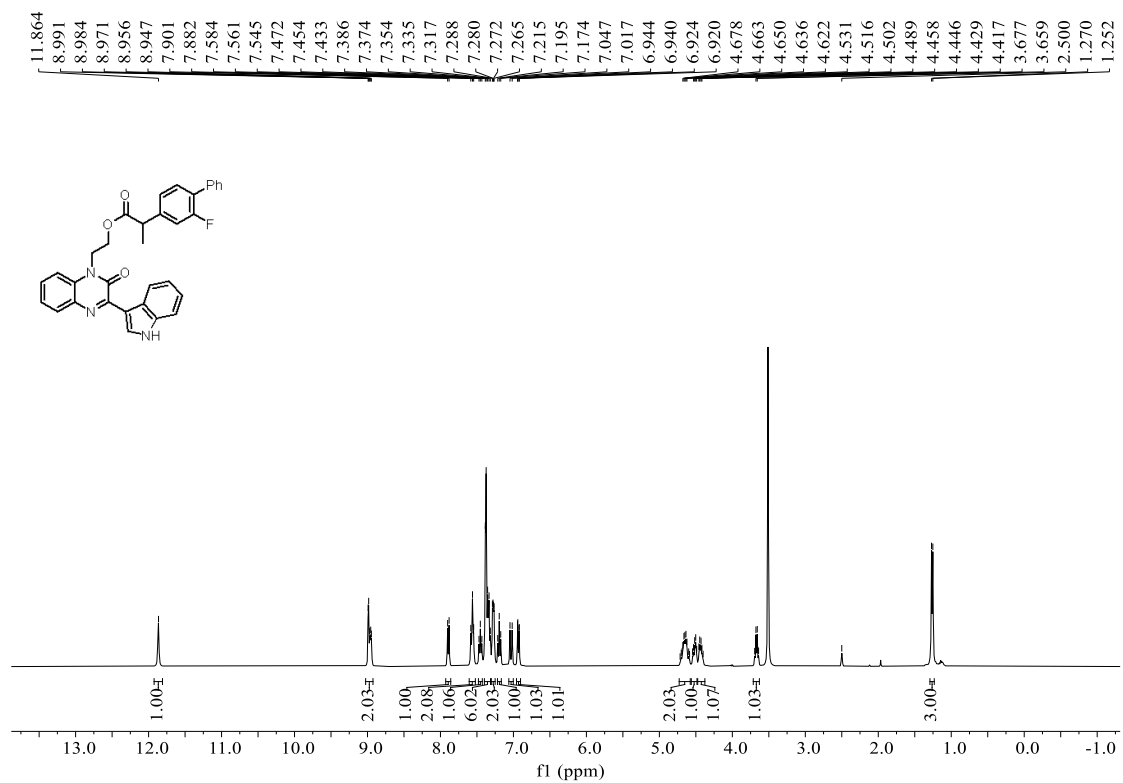
¹H NMR spectra of 3aj (400 MHz, DMSO)



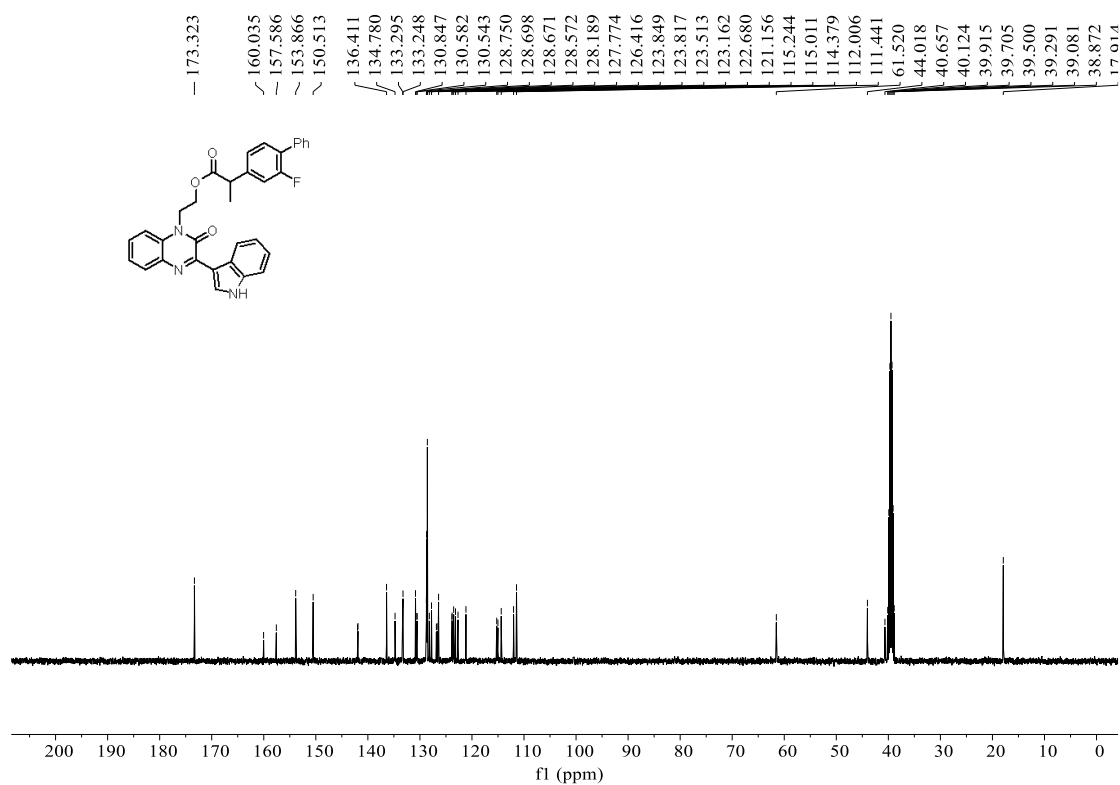
¹³C NMR spectra of 3aj (100 MHz, DMSO)



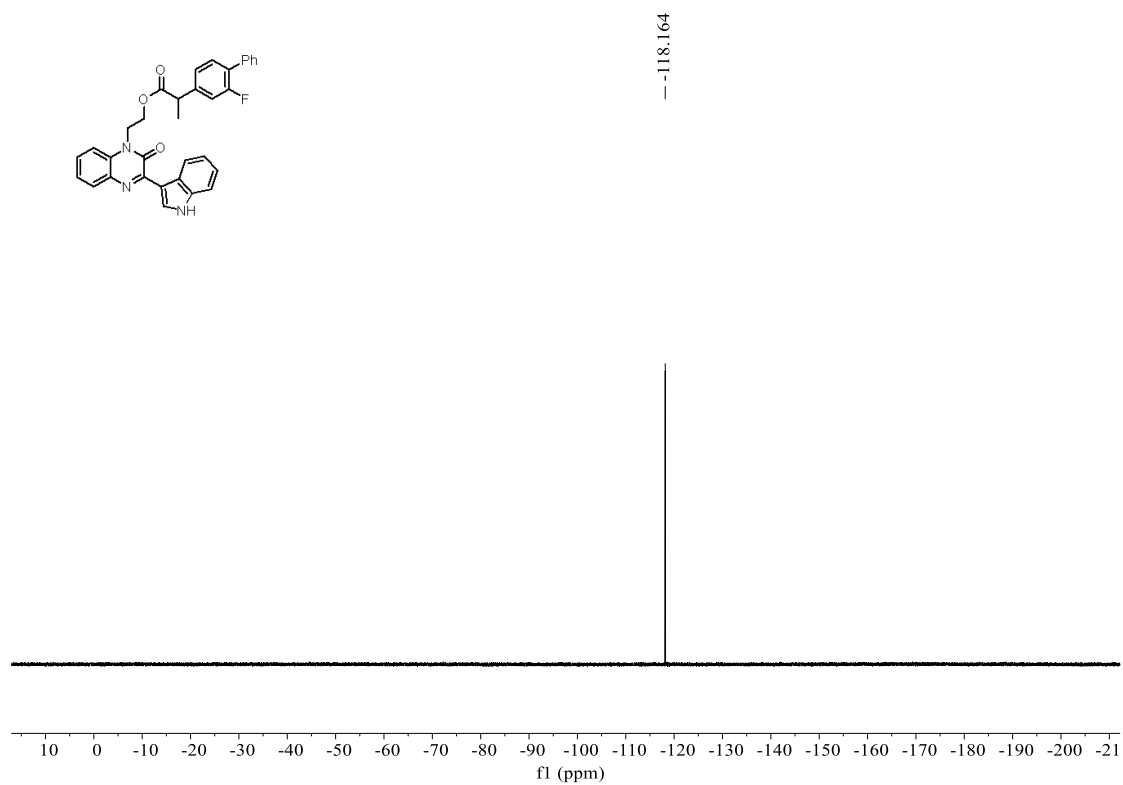
¹H NMR spectra of 3ak (400 MHz, DMSO)



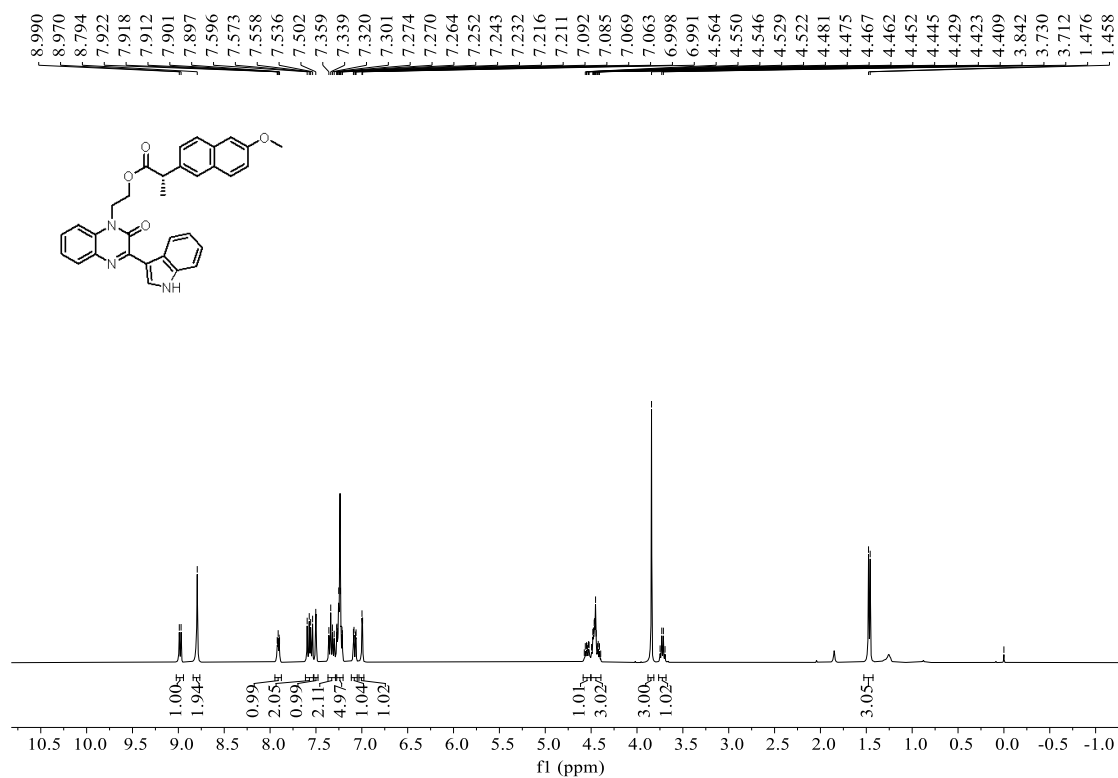
¹³C NMR spectra of 3ak (100 MHz, DMSO)



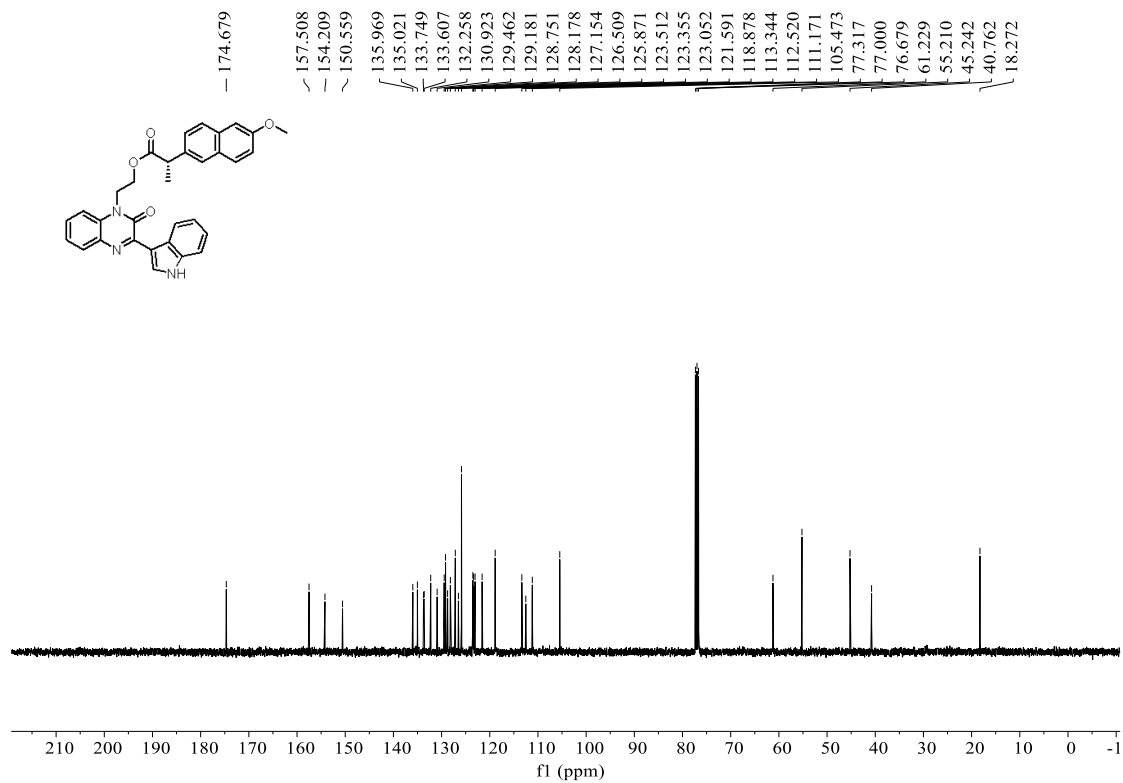
¹⁹F NMR spectra of 3ak (376 MHz, DMSO)



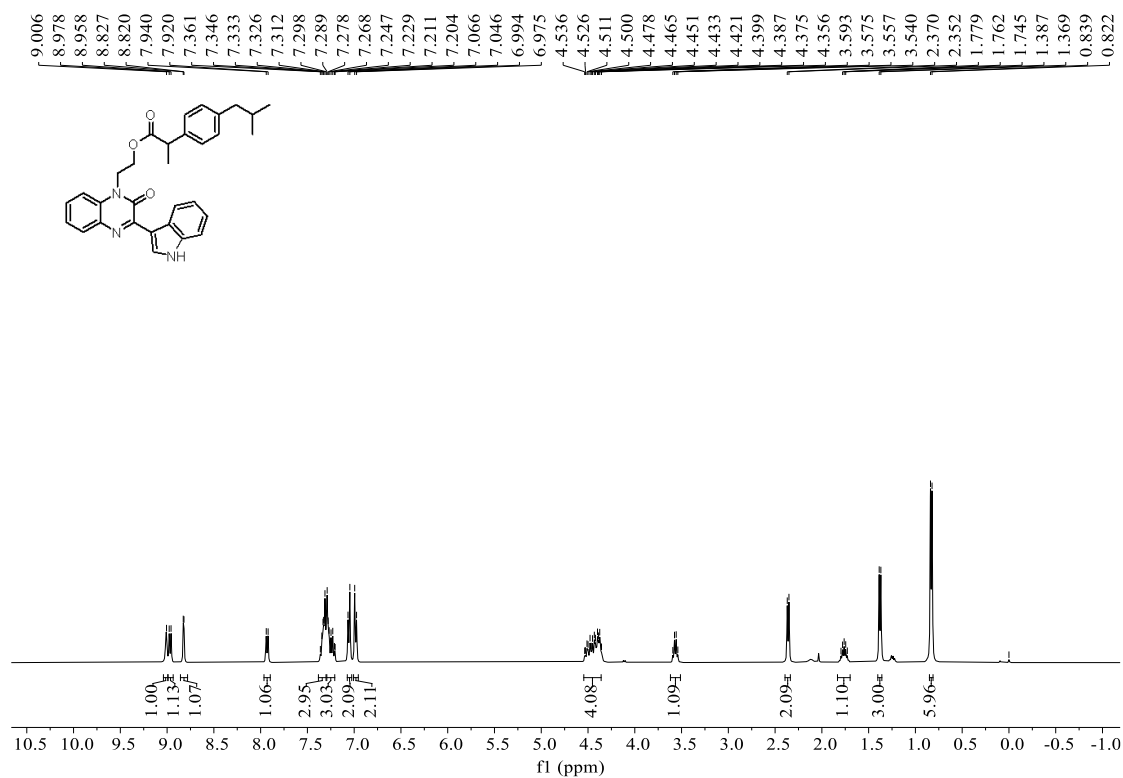
¹H NMR spectra of 3al (400 MHz, CDCl₃)



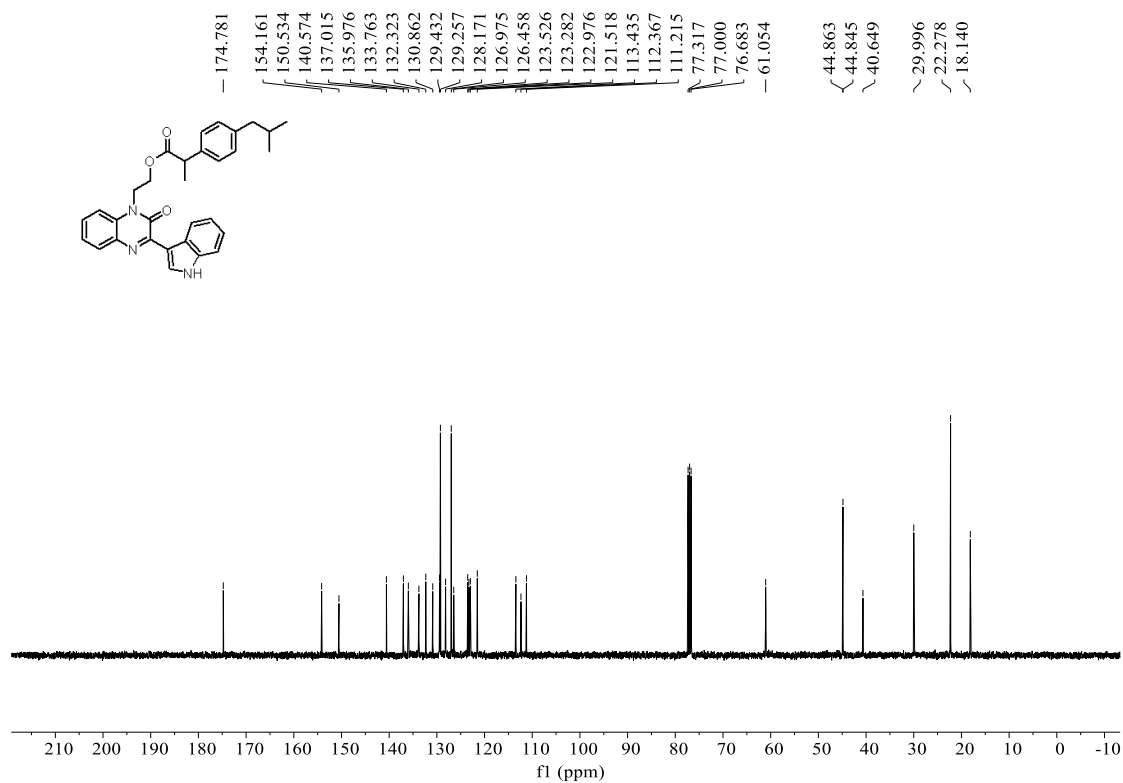
¹³C NMR spectra of 3al (100 MHz, CDCl₃)



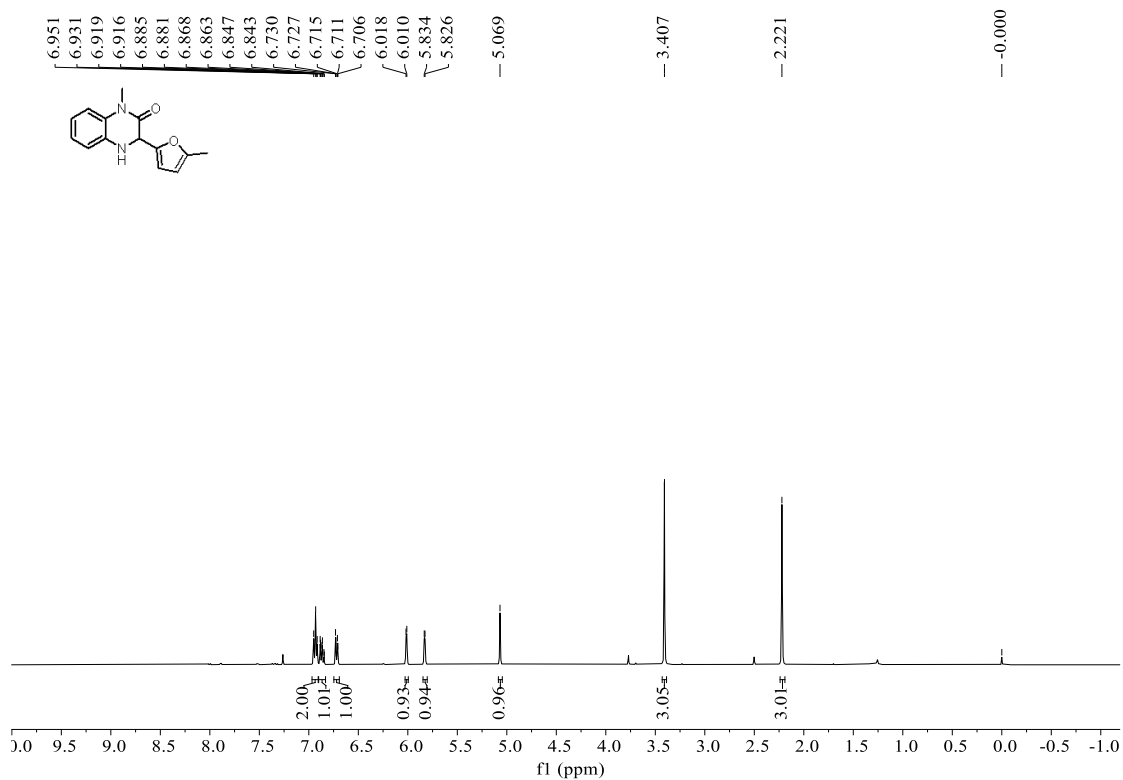
¹H NMR spectra of 3am (400 MHz, CDCl₃)



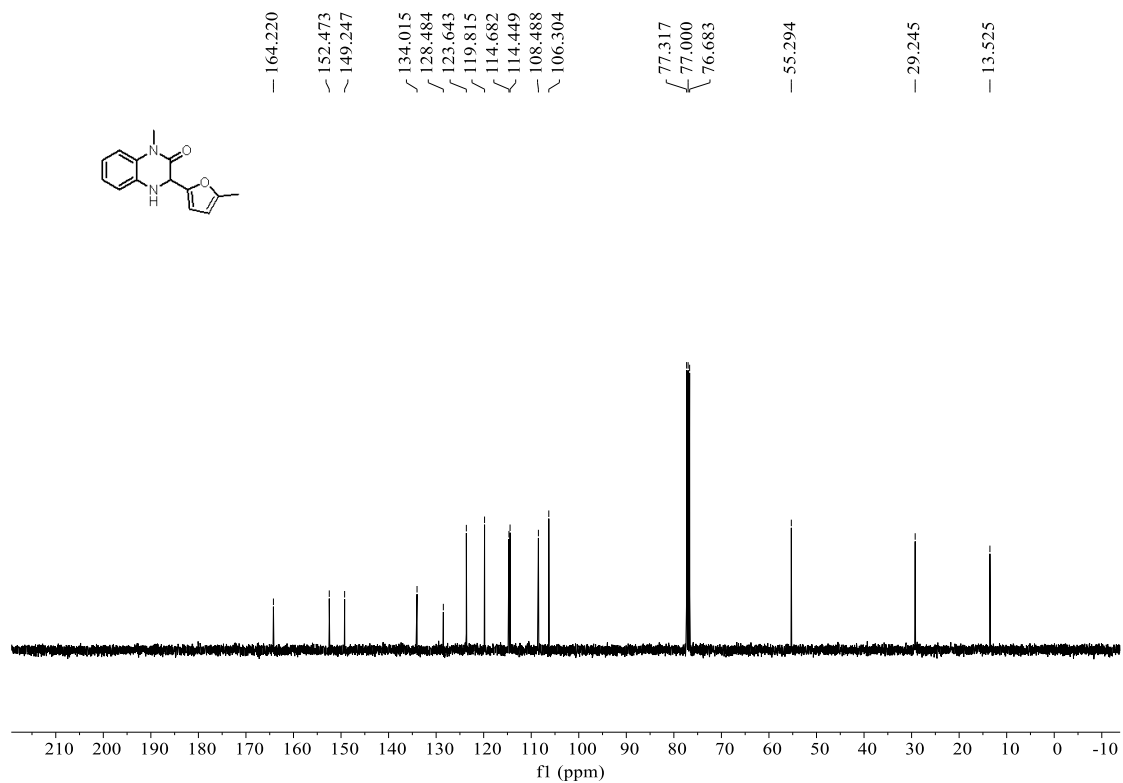
¹³C NMR spectra of 3am (100 MHz, CDCl₃)



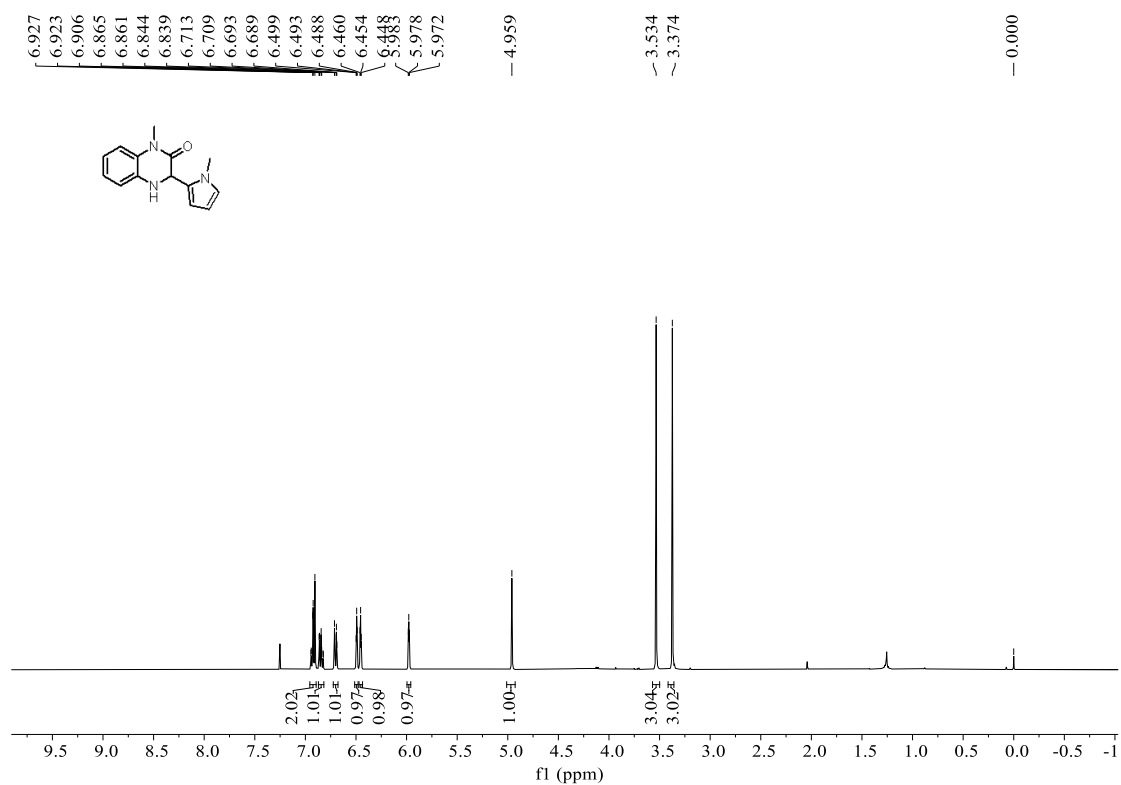
¹H NMR spectra of C (400 MHz, CDCl₃)



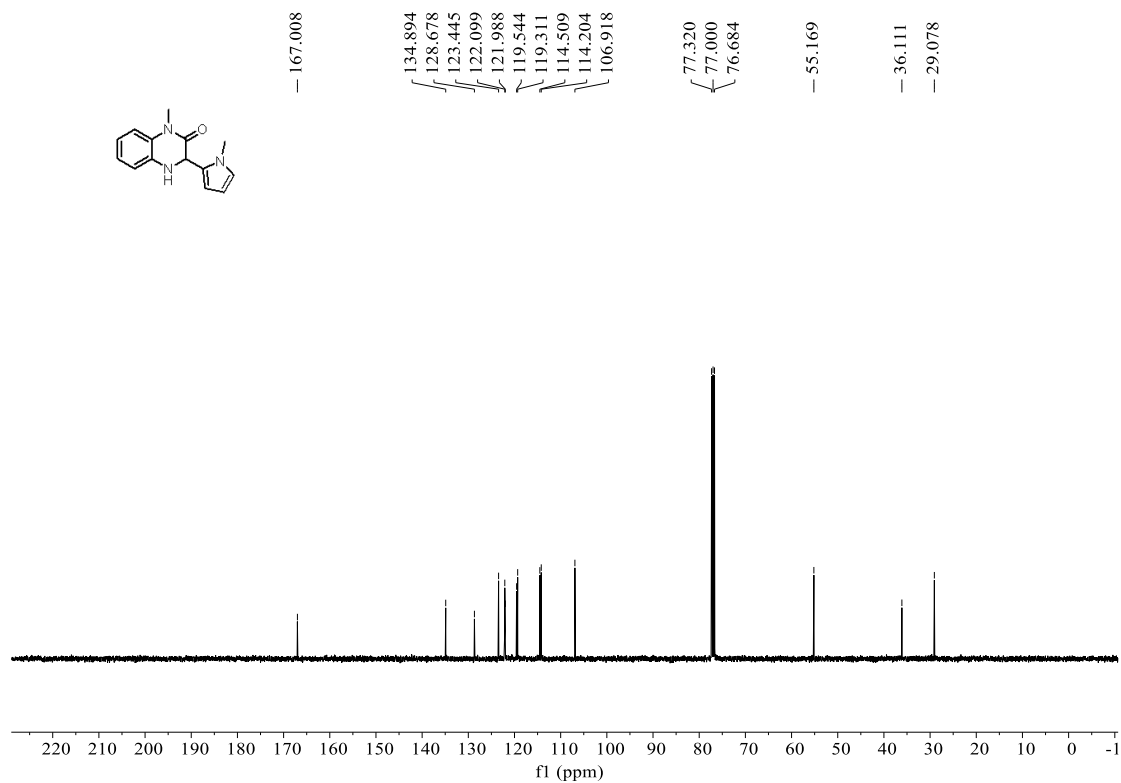
¹³C NMR spectra of C (100 MHz, CDCl₃)



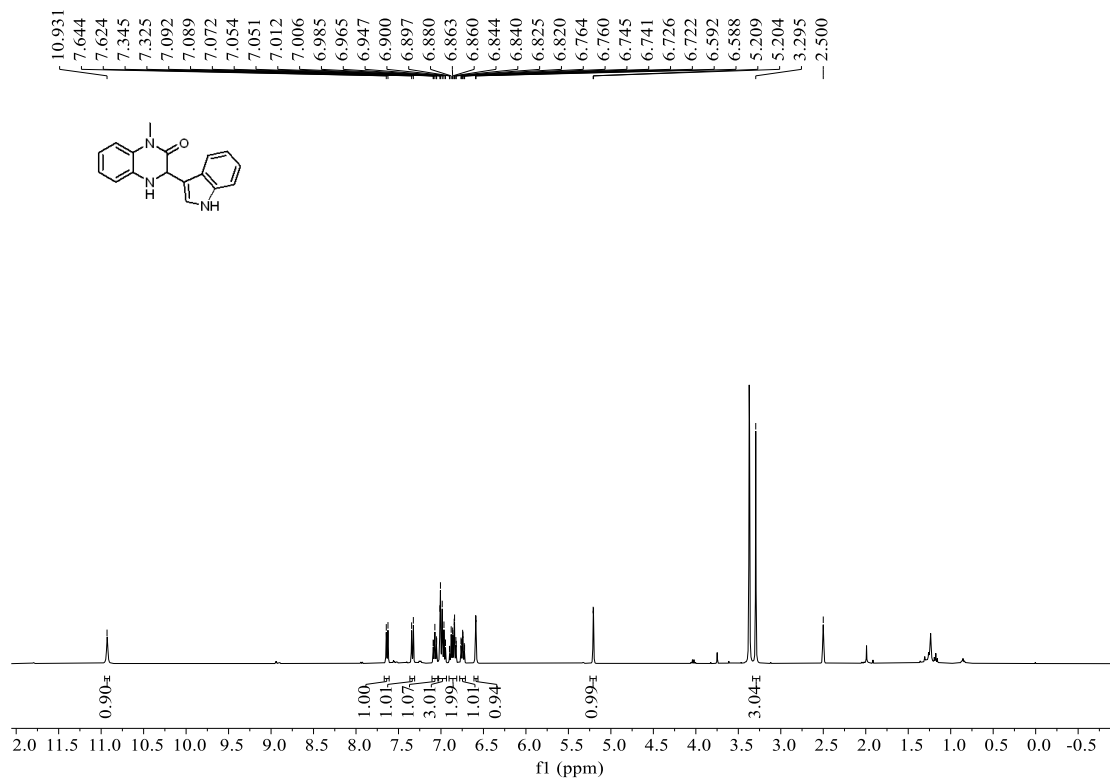
¹H NMR spectra of 4a (400 MHz, CDCl₃)



¹³C NMR spectra of 4a (100 MHz, CDCl₃)



¹H NMR spectra of 4c (400 MHz, DMSO)



¹³C NMR spectra of 4c (100 MHz, DMSO)

