

Supporting Information

Radical relay cyclization/C–C bond formation of allyloxy-tethered aryl iodides with quinoxalin-2(1*H*)-ones via polysulfide anions photocatalysis

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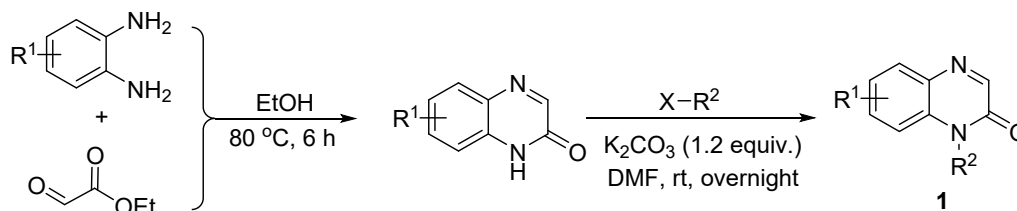
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1. General information

Unless otherwise stated, commercially available reagents were used without further purification. ^1H NMR spectra were recorded at 400 MHz or 600 MHz. The chemical shifts were reported in parts per million (ppm) relative to tetramethylsilane and with the solvent resonance as the interior standard. Data were recorded as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration. ^{13}C NMR data were collected at 100 MHz or 150 MHz with complete proton decoupling. Chemical shifts were reported in parts per million (ppm) from the tetramethylsilane with the solvent resonance as interior standard. ^{19}F NMR data were collected at 376 MHz or 564 MHz with complete proton decoupling. Chemical shifts were reported in parts per million (ppm) from the tetramethylsilane with the solvent resonance as interior standard. High resolution mass spectroscopy (HRMS) was recorded on a Thermofisher Q Exactive Accurate-Mass Q-Orbitrap LC/MS (HESI), and the samples were dissolved by acetonitrile. X-Ray data were collected on a Bruker SMART APEX instrument with an I II μS Mo microsource ($\lambda = 0.7107 \text{ \AA}$). Column chromatography was carried out on silica gel (200–300 mesh). The light source for the photocatalytic reaction is a Kessil PR160L-blue LED lamp (30 W High Luminous DEX 2100 LED, $\lambda = 425 \text{ nm}$) was placed 1.0 inches away from the reaction vials.

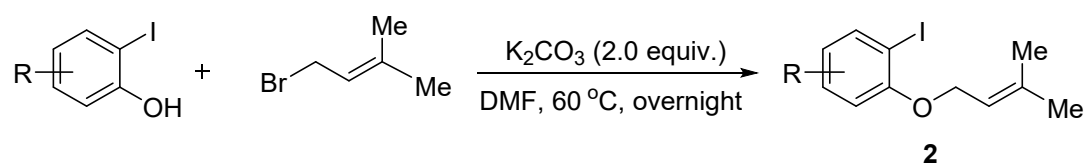
2. Experimental section

2.1 General procedure for the preparation of 1 and 2



Starting materials **1** were prepared according to a literature procedure (Xiang, P.; Sun, K.; Wang, S.; Chen, X.; Qu, L.; Yu, B. *Chin. Chem. Lett.* **2022**, *33*, 5074–5079; Wang M.; Zhang Z.; Xiong C.; Sun P.; Zhou C. *ChemistrySelect* **2022**, e202200816). To a suspension of *o*-arylenediamine (10 mmol, 1.0 equiv.) in ethanol (30 mL) was

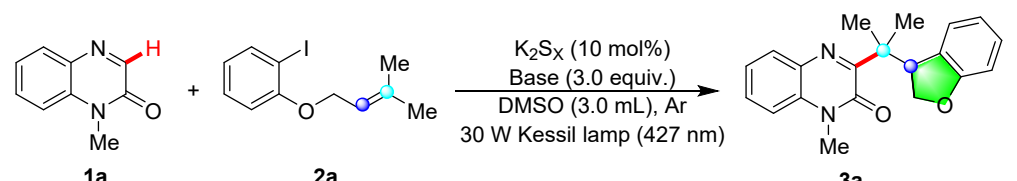
added ethyl 2-oxoacetate (12 mmol, 1.2 equiv.). The mixture was stirred at 80 °C for 6 h. The precipitated solid was filtered, washed with ethanol, and finally dried to afford the corresponding product quinoxalinone. To a suspension of obtained quinoxalinone (5.0 mmol, 1.0 equiv.) in DMF (20 mL) was added potassium carbonate (6.0 mmol, 1.2 equiv.) and the corresponding alkyl halide (R²-X, 9.0 mmol, 1.6 equiv.). The mixture was stirred at room temperature overnight. After that, ethyl acetate (100 mL) and water (20 mL) were added and the aqueous layer was extracted with EtOAc (50 mL×2). The combined organic layers were washed with a saturated solution of NH₄Cl (30 mL), followed by brine (40 mL), then dried over Na₂SO₄, filtered and evaporated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/ethyl acetate = 5/1) over silica gel to afford the desired product **1** as a colorless solid.



Starting materials **2** were prepared according to a reported procedure (Koy, M.; Bellotti, P.; Katzenburg, F.; Daniliuc, C. G.; Glorius, F. *Angew. Chem. Int. Ed.* **2020**, *59*, 2375–2379). Under air, the corresponding phenol (10 mmol, 1.0 equiv.), K₂CO₃ (2.0 equiv.), DMF (0.5 M), and the corresponding bromide (1.1 equiv.) were added to a Schlenk tube. The reaction mixture was stirred at 60 °C overnight. After cooling to room temperature, the reaction mixture was transferred to a separation funnel with EtOAc/water. The aqueous phase was extracted with EtOAc (50 mL×2). After the combined organic phases were washed with water (40 mL×2) and brine (20 mL×1), dried over MgSO₄, filtered and concentrated under reduced pressure, the residue was purified by flash column chromatography (petroleum ether) to give the compound **2** as a colorless oil.

2.2 The optimization of reaction conditions

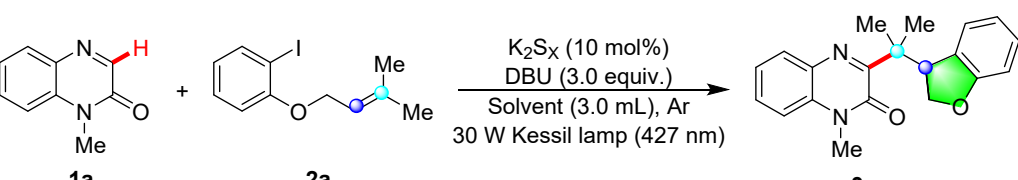
Table S1. Screening base^[a]



Entry	Base	Yield of 3a (%) ^[b]
1	Cs ₂ CO ₃	30
2	LiO ^t Bu	45
3	KOH	34
4	KO ^t Bu	53
5	Pyridine	0
6	Et ₃ N	0
7	DBU	80

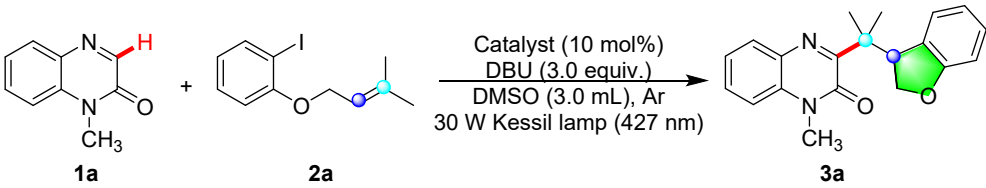
^[a]Reaction conditions: **1a** (0.40 mmol), **2a** (0.20 mmol), base (3.0 equiv.) and K₂S_X (10 mol% per S) in DMSO (3.0 mL) under argon atmosphere with Kessil[®] LED (427 nm, 30 W) at room temperature for 12 h. ^[b]Isolated yield of the product **3a**.

Table S2. Screening solvent^[a]



Entry	Solvent	Yield of 3a (%) ^[b]
1	DMF	61
2	MeCN	23
3	DMSO	80
4	DCM	<10
5	THF	0
6	DCE	<10
7	Et ₃ N	0
8	1,4-Dioxane	0

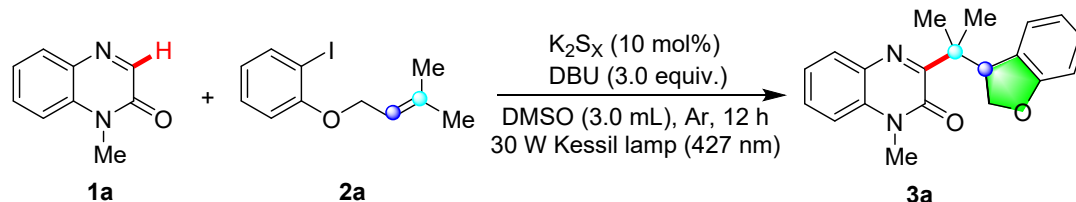
^[a]Reaction conditions: **1a** (0.40 mmol), **2a** (0.20 mmol), DBU (3.0 equiv.) and K₂S_X (10 mol% per S) in solvent (3.0 mL) under argon atmosphere with Kessil[®] LED (427 nm, 30 W) at room temperature for 12 h. ^[b]Isolated yield of the product **3a**.

Table S3. Screening catalyst^[a]

Entry	Catalyst	Yield of 3a (%) ^[b]
1	Phenothiazine	52
2	10-Phenylphenothiazine	63
3	9,10-Dicyanoanthracene	13
4	4CzIPN	39
5	K ₂ S _X	80
6	Ru(bpy) ₃ (PF ₆) ₂	28
7	[Ir(dtbbpy)(ppy) ₂](PF ₆) ₃	43

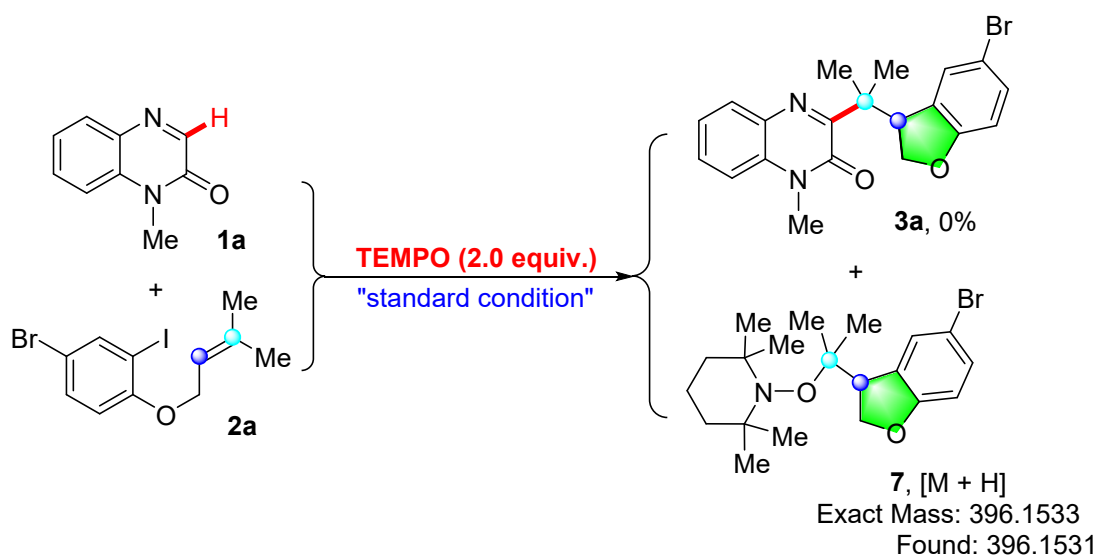
^[a]Reaction conditions: **1a** (0.40 mmol), **2a** (0.20 mmol), DBU (3.0 equiv.) and catalyst in DMSO (3.0 mL) under argon atmosphere with Kessil® LED (427 nm, 30 W) at room temperature for 12 h. ^[b]Isolated yield of the product **3a**.

2.3 General procedure for the model reaction



To a 15 mL reaction tube equipped with a magnetic stirring bar, 1-methylquinoxalin-2(1*H*)-one (**1a**, 0.40 mmol, 2.0 equiv.), 1-iodo-2-((3-methylbut-2-en-1-yl)oxy)benzene (**2a**, 0.20 mmol, 1.0 equiv.), DBU (0.6 mmol, 3.0 equiv.), K₂S_X (10 mol%) and DMSO (3.0 mL) were added. The vessel was evacuated and backfilled with argon atmosphere three times. The tube was screw-capped and stirred at room temperature under irradiation of a Kessil PR160L-blue LED lamp (30 W, High Luminous DEX 2100 LED, $\lambda = 427$ nm) was placed 1.0 inches for 12 h. Thereafter, EtOAc (60 mL) was added to the reaction mixture, and the obtained organic layer was washed with brine (20 mL×3), dried over Na₂SO₄, and concentrated under reduced pressure. The crude product was further purified by flash chromatography using silica gel to afford the desired product **3a** (51.3 mg, 80% yield) as a colorless solid.

2.4 The radical inhibiting experiment



When a radical scavenger (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) in 3.0 equivalents was added to the model reaction, the reactions were inhibited, demonstrating a possible radical pathway in this system. Meanwhile, an adduct (**7**) of the carbon-centered radical intermediate with TEMPO was formed during the reaction, and was detected by HRMS analysis (Figure S1).

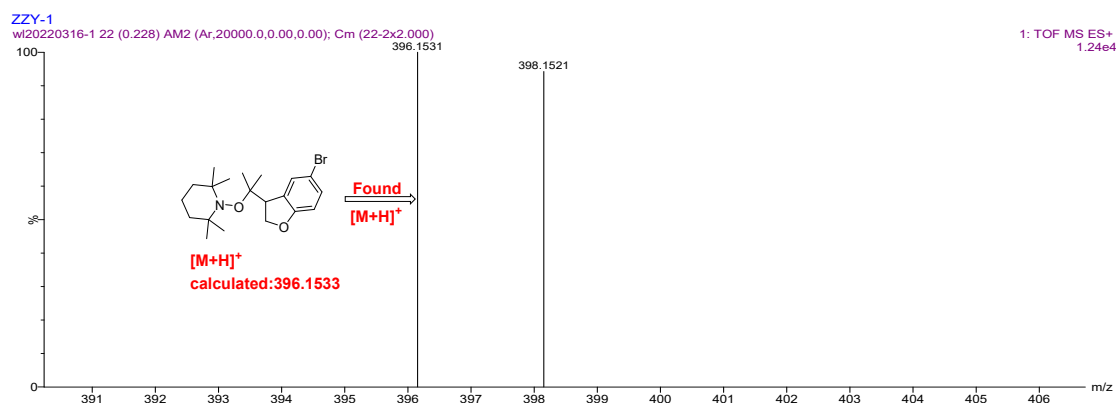


Figure S1. HRMS analysis of an adduct (**7**) of a radical intermediate with TEMPO

2.5 Fluorescence quenching experiment of K_2S_X with **2a**

In order to investigate the possible reaction pathway, a fluorescence quenching experiment was conducted. The fluorescence emission intensity was recorded on the

Cary Eclipse Fluorescence Spectrometer with the excitation wavelength was fixed at 427 nm, and the fluorescence quenching result of K_2S_x (2.2 mg) in 3.0 mL DMSO by the addition of 1-iodo-2-((3-methylbut-2-en-1-yl)oxy)benzene (**2a**, 0.1–0.9 mmol, respectively) was shown in Figure S2. The results were also presented in the SI, as well as in the main text. Please see the revised version for details.

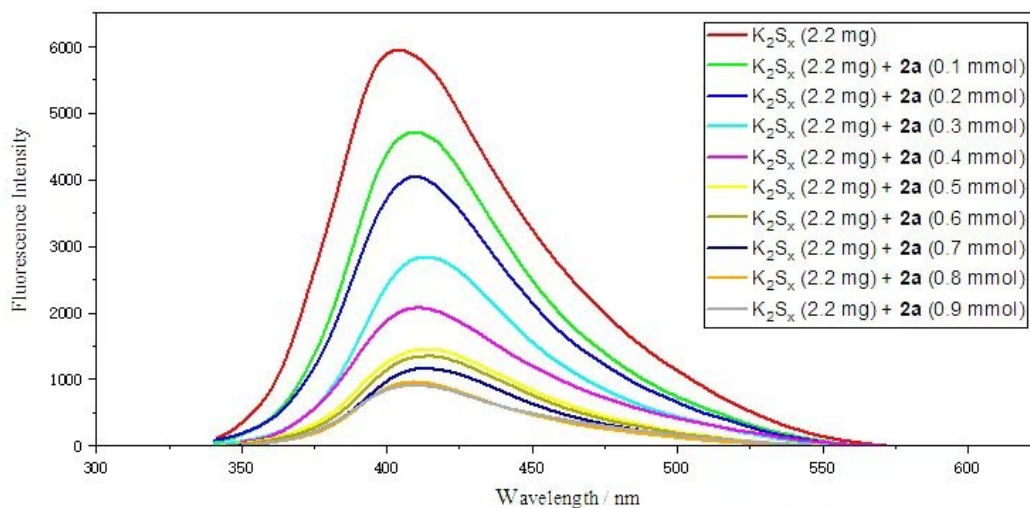
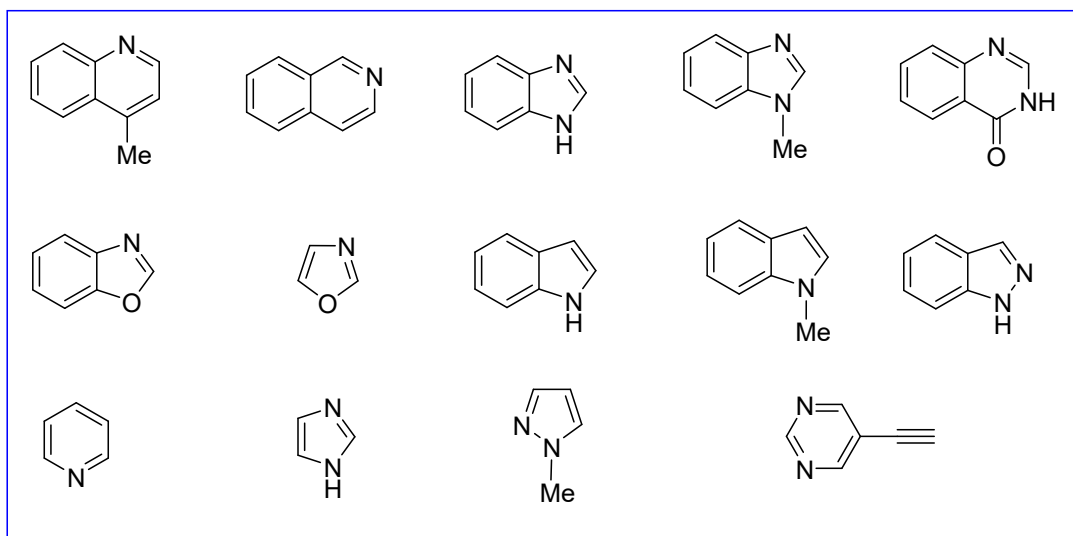


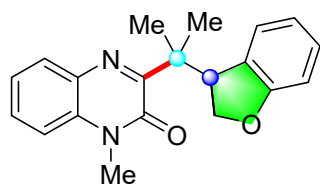
Figure S2. Fluorescence quenching experiment of K_2S_x with **2a** in DMSO

3. Unsuccessful heterocycles for the substrates in the reactions

Unsuccessful heterocycles for the substrates

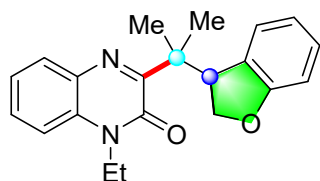


4. Characterization data for the products



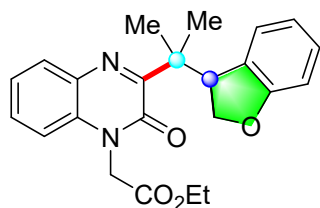
3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-2(1H)-one

(3a): Purification by column chromatography (EtOAc/hexane, V/V = 1:50) afforded **3a** (colorless solid, 51.3 mg, 80% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.83 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.56–7.53 (m, 1H), 7.35–7.31 (m, 2H), 7.11 (td, $J = 7.8, 1.8$ Hz, 1H), 7.01–6.99 (m, 1H), 6.78–6.74 (m, 2H), 4.68 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.53 (t, $J = 9.6$ Hz, 1H), 4.38 (dd, $J = 9.6, 3.6$ Hz, 1H), 3.71 (s, 3H), 1.52 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 162.9, 161.1, 153.8, 133.2, 131.9, 130.4, 130.0, 128.2, 128.1, 126.1, 123.4, 119.7, 113.3, 109.3, 74.1, 47.4, 46.4, 28.9, 22.4, 20.9. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{21}\text{N}_2\text{O}_2]^+$: 321.1598, Found: 321.1598.

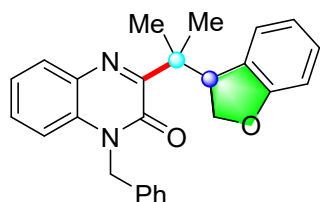


3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-1-ethylquinoxalin-2(1H)-one (3b)

Purification by column chromatography (EtOAc/hexane, V/V = 1:50) afforded **3b** (light yellow oil, 51.5 mg, 77% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.84 (dd, $J = 7.8, 1.8$ Hz, 1H), 7.57–7.54 (m, 1H), 7.35–7.32 (m, 2H), 7.11 (td, $J = 7.8, 1.8$ Hz, 1H), 6.97 (d, $J = 7.8$ Hz, 1H), 6.79–6.73 (m, 2H), 4.69 (dd, $J = 9.6, 4.2$ Hz, 1H), 4.54 (t, $J = 9.6$ Hz, 1H), 4.40 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.38–4.30 (m, 2H), 1.51 (s, 3H), 1.41 (t, $J = 7.2$ Hz, 3H), 1.35 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 163.0, 161.1, 153.3, 132.2, 132.1, 130.7, 130.0, 128.2, 126.1, 123.3, 119.7, 113.2, 109.3, 74.1, 47.5, 46.4, 37.2, 22.4, 21.0, 12.5. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}_2]^+$: 335.1754, Found: 335.1752.

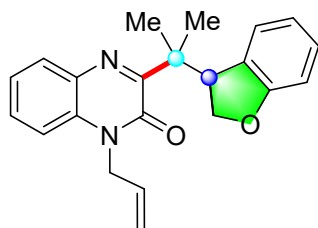


Ethyl-2-(3-(2-(2,3-dihydrobenzofuran-3-yl)propan-2-yl)-2-oxoquinoxalin-1(2H)-yl)acetate (3c): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3c** (colorless solid, 45.5 mg, 58% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.85 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.54–7.51 (m, 1H), 7.36–7.34 (m, 1H), 7.12–7.09 (m, 2H), 6.93 (d, $J = 7.2$ Hz, 1H), 6.78 (dd, $J = 8.4, 1.2$ Hz, 1H), 6.73 (td, $J = 7.2, 0.6$ Hz, 1H), 5.12 (d, $J = 17.4$ Hz, 1H), 4.97 (d, $J = 17.4$ Hz, 1H), 4.67 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.54 (t, $J = 9.6$ Hz, 1H), 4.44 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.26 (q, $J = 7.2$ Hz, 2H), 1.47 (s, 3H), 1.37 (s, 3H), 1.28 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 167.2, 162.8, 161.0, 153.4, 132.3, 132.0, 130.8, 130.2, 128.2, 128.1, 126.0, 123.8, 119.8, 112.8, 109.3, 73.9, 62.1, 47.5, 46.5, 43.4, 22.2, 21.3, 14.1. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{23}\text{H}_{25}\text{N}_2\text{O}_4]^+$: 393.1809, Found: 393.1808.



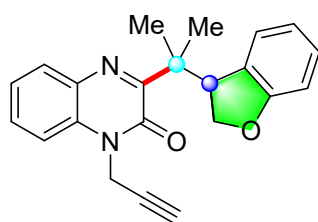
1-Benzyl-3-(2-(2,3-dihydrobenzofuran-3-yl)propan-2-yl)quinoxalin-2(1H)-one (3d): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **3d** (light yellow oil, 68.2 mg, 86% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.84 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.44–7.42 (m, 1H), 7.34–7.29 (m, 3H), 7.28–7.26 (m, 2H), 7.25–7.23 (m, 2H), 7.12 (td, $J = 7.8, 1.2$ Hz, 1H), 6.98–6.96 (m, 1H), 6.79 (d, $J = 8.4$ Hz, 1H), 6.75 (td, $J = 7.8, 1.2$ Hz, 1H), 5.57 (d, $J = 15.6$ Hz, 1H), 5.48 (d, $J = 15.6$ Hz, 1H), 4.73 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.56 (t, $J = 9.0$ Hz, 1H), 4.44 (dd, $J = 9.6, 4.2$ Hz, 1H), 1.54 (s, 3H), 1.39 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 163.1, 161.1, 153.8, 135.4, 132.6, 132.2, 130.5, 130.0, 129.0, 128.2 (2C), 127.7, 126.8, 126.0, 123.5, 119.8,

114.1, 109.3, 74.1, 47.5, 46.5, 45.7, 22.5, 21.2. HRMS (ESI) m/z : ($[M + H]^+$) Calcd for $[C_{20}H_{20}N_2O_2]^+$: 320.1519, Found: 320.1520.



1-Allyl-3-(2-(2,3-dihydrobenzofuran-3-yl)propan-2-yl)quinoxalin-2(1H)-one (3e):

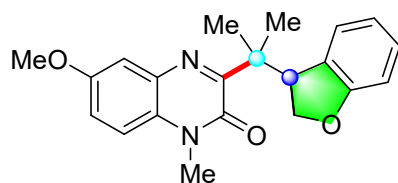
Purification by column chromatography (EtOAc/hexane, V/V = 1:40) afforded **3e** (light yellow oil, 61.7 mg, 89% yield). 1H NMR (600 MHz, $CDCl_3$) δ : 7.84 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.53–7.51 (m, 1H), 7.35–7.32 (m, 1H), 7.30 (dd, $J = 8.4, 1.2$ Hz, 1H), 7.13–7.10 (m, 1H), 6.97 (dt, $J = 7.2, 1.2$ Hz, 1H), 6.78 (d, $J = 7.2$ Hz, 1H), 6.75 (td, $J = 7.2, 1.2$ Hz, 1H), 6.00–5.94 (m, 1H), 5.30–5.27 (m, 1H), 5.19–5.15 (m, 1H), 4.98–4.88 (m, 2H), 4.69 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.53 (t, $J = 9.0$ Hz, 1H), 4.41 (dd, $J = 9.6, 4.2$ Hz, 1H), 1.51 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ : 163.0, 161.1, 153.3, 132.4, 132.1, 130.8, 130.5, 130.0, 128.2 (2C), 126.0, 123.5, 119.8, 117.9, 113.9, 109.3, 74.1, 47.5, 46.4, 44.4, 22.4, 21.1. HRMS (ESI) m/z : ($[M + H]^+$) Calcd for $[C_{22}H_{23}N_2O_2]^+$: 347.1754, Found: 347.1753.



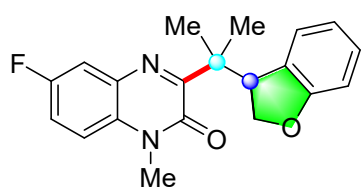
3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-1-(prop-2-yn-1-yl)quinoxalin-

2(1H)-one (3f): Purification by column chromatography (EtOAc/hexane, V/V = 1:15) afforded **3f** (light yellow solid, 42.0 mg, 61% yield). 1H NMR (600 MHz, $CDCl_3$) δ : 7.85 (dd, $J = 8.4, 1.8$ Hz, 1H), 7.60–7.57 (m, 1H), 7.47 (dd, $J = 8.4, 1.2$ Hz, 1H), 7.39–7.36 (m, 1H), 7.13–7.10 (m, 1H), 6.99–6.97 (m, 1H), 6.78 (d, $J = 8.4$ Hz, 1H), 6.75 (td, $J = 7.8, 1.2$ Hz, 1H), 5.12–5.02 (m, 2H), 4.64 (dd, $J = 9.6, 4.2$ Hz, 1H), 4.54 (t, $J = 9.6$ Hz, 1H), 4.40 (dd, $J = 9.6, 4.2$ Hz, 1H), 2.30 (t, $J = 2.4$ Hz, 1H), 1.51 (s, 3H),

1.35 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 162.9, 161.1, 152.7, 132.1, 131.7, 130.5, 130.2, 128.3, 128.0, 126.1, 123.9, 119.8, 113.8, 109.3, 77.0, 74.1, 73.1, 47.5, 46.5, 31.3, 22.4, 21.0. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_2]^+$: 345.1598, Found: 345.1598.

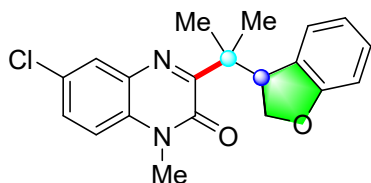


3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-6-methoxy-1-methylquinoxalin-2(1H)-one (3g): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **3g** (light yellow oil, 55.4 mg, 79% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.30 (d, $J = 2.4$ Hz, 1H), 7.25 (d, $J = 9.0$ Hz, 1H), 7.19 (dd, $J = 9.0, 3.0$ Hz, 1H), 7.13–7.10 (m, 1H), 6.97 (d, $J = 7.2$ Hz, 1H), 6.78 (d, $J = 7.8$ Hz, 1H), 6.75 (td, $J = 7.2, 1.2$ Hz, 1H), 4.71 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.52 (t, $J = 9.6$ Hz, 1H), 4.38 (dd, $J = 9.6, 4.2$ Hz, 1H), 3.90 (s, 3H), 3.71 (s, 3H), 1.50 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 163.5, 161.1, 155.9, 153.5, 132.7, 128.2, 127.5, 126.1, 119.8, 119.3, 114.3, 111.7, 109.3, 74.1, 55.8, 47.3, 46.4, 29.1, 22.4, 21.1. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}_3]^+$: 351.1703, Found: 351.1699.



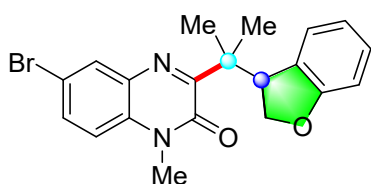
3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-6-fluoro-1-methylquinoxalin-2(1H)-one (3h): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3h** (light yellow oil, 52.8 mg, 78% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.53 (dd, $J = 8.4, 3.0$ Hz, 1H), 7.33–7.27 (m, 2H), 7.12 (td, $J = 7.8, 1.2$ Hz, 1H), 6.97 (d, $J = 7.2$ Hz, 1H), 6.78 (d, $J = 7.8$ Hz, 1H), 6.76 (td, $J = 7.2, 1.2$ Hz, 1H), 4.66 (dd, $J = 9.6, 4.2$ Hz, 1H), 4.52 (t, $J = 9.0$ Hz, 1H), 4.37 (dd, $J = 9.0, 3.6$ Hz, 1H), 3.72 (s, 3H), 1.50 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ : 164.6, 161.1, 158.6 (d,

$J = 243.6$ Hz), 153.5, 132.4 (d, $J = 11.4$ Hz), 129.9 (d, $J = 1.8$ Hz), 128.3, 128.0, 126.0, 119.8, 117.8 (d, $J = 24.0$ Hz), 115.7 (d, $J = 22.3$ Hz), 114.5 (d, $J = 8.8$ Hz), 109.4, 74.0, 47.4, 46.6, 29.2, 22.4, 21.0; ^{19}F NMR (564 MHz, CDCl_3) δ : -119.2. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{20}\text{FN}_2\text{O}_2]^+$: 339.1503, Found: 339.1502.



6-Chloro-3-(2-(2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-

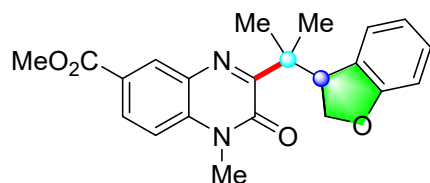
2(1H)-one (3i): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3i** (light yellow oil, 50.4 mg, 71% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.84 (d, $J = 2.4$ Hz, 1H), 7.51 (dd, $J = 8.8, 2.4$ Hz, 1H), 7.26 (d, $J = 8.8$ Hz, 1H), 7.13 (td, $J = 7.6, 1.2$ Hz, 1H), 6.96 (d, $J = 7.2$ Hz, 1H), 6.80–6.74 (m, 2H), 4.64 (dd, $J = 9.2, 3.6$ Hz, 1H), 4.52 (t, $J = 9.2$ Hz, 1H), 4.36 (dd, $J = 9.2, 3.6$ Hz, 1H), 3.71 (s, 3H), 1.49 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 164.5, 161.0, 153.4, 132.4, 131.9, 130.0, 129.7, 128.8, 128.3, 127.9, 126.0, 119.8, 114.6, 109.4, 74.0, 47.3, 46.6, 29.1, 22.3, 20.9. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{20}^{35}\text{ClN}_2\text{O}_2]^+$: 355.1208, Found: 355.1207.



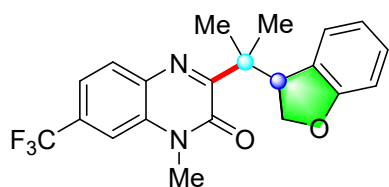
6-Bromo-3-(2-(2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-

2(1H)-one (3j): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **3j** (light yellow oil, 58.3 mg, 73% yield). ^1H NMR (400 MHz, CDCl_3) δ : 8.00 (d, $J = 2.4$ Hz, 1H), 7.64 (dd, $J = 8.8, 2.4$ Hz, 1H), 7.20 (d, $J = 8.8$ Hz, 1H), 7.13 (td, $J = 7.6, 1.2$ Hz, 1H), 6.96 (d, $J = 7.2$ Hz, 1H), 6.80 – 6.74 (m, 2H), 4.64 (dd, $J = 9.2, 3.6$ Hz, 1H), 4.52 (t, $J = 9.6$ Hz, 1H), 4.36 (dd, $J = 9.2, 3.6$ Hz, 1H), 3.70 (s, 3H), 1.49 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 164.4, 161.0, 153.4, 132.8, 132.7 (2C), 132.3, 128.3, 127.9, 126.0, 119.8, 116.0, 114.9, 109.4, 74.0, 47.3, 46.6,

29.1, 22.4, 20.9. HRMS (ESI) m/z : $([M + H]^+)$ Calcd for $[C_{20}H_{20}^{79}BrN_2O_2]^+$: 399.0703, Found: 399.0703.

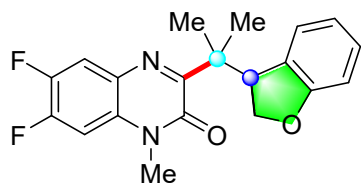


Methyl-3-(2-(2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methyl-2-oxo-1,2-dihydroquinoxaline-6-carboxylate (3k): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3k** (light yellow solid, 46.2 mg, 61% yield). 1H NMR (400 MHz, $CDCl_3$) δ : 8.51 (d, $J = 2.0$ Hz, 1H), 8.22 (dd, $J = 8.8, 2.0$ Hz, 1H), 7.37 (d, $J = 8.4$ Hz, 1H), 7.13 (t, $J = 8.0$ Hz, 1H), 6.98 (d, $J = 7.6$ Hz, 1H), 6.80–6.74 (m, 2H), 4.63 (dd, $J = 9.2, 3.6$ Hz, 1H), 4.54 (t, $J = 9.2$ Hz, 1H), 4.38 (dd, $J = 9.6, 3.6$ Hz, 1H), 3.97 (s, 3H), 3.75 (s, 3H), 1.51 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 166.1, 164.1, 161.1, 153.7, 136.5, 132.2, 131.2, 130.8, 128.4, 127.9, 126.1, 125.4, 119.8, 113.5, 109.4, 74.0, 52.3, 47.4, 46.6, 29.2, 22.4, 20.8. HRMS (ESI) m/z : $([M + H]^+)$ Calcd for $[C_{22}H_{23}N_2O_4]^+$: 379.1652, Found: 379.1651.

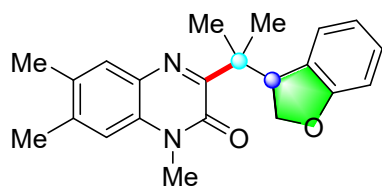


3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-1-methyl-7-(trifluoromethyl)quinoxalin-2(1H)-one (3l): Purification by column chromatography (EtOAc/hexane, V/V = 1:40) afforded **3l** (light yellow oil, 41.9 mg, 54% yield). 1H NMR (400 MHz, $CDCl_3$) δ : 7.95 (d, $J = 8.4$ Hz, 1H), 7.60–7.57 (m, 2H), 7.13 (td, $J = 8.0, 1.6$ Hz, 1H), 6.96 (d, $J = 7.2$ Hz, 1H), 6.80–6.74 (m, 2H), 4.66 (dd, $J = 9.2, 3.6$ Hz, 1H), 4.53 (t, $J = 9.2$ Hz, 1H), 4.38 (dd, $J = 9.6, 3.6$ Hz, 1H), 3.76 (s, 3H), 1.51 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 165.8, 161.0, 153.4, 133.5, 133.2, 131.5 (q, $J = 32.8$ Hz), 131.1, 128.4, 127.8, 126.0, 123.6 (q, $J = 272.5$ Hz), 120.0 (q, $J = 3.6$ Hz), 119.8, 110.9 (q, $J = 4.2$ Hz), 109.4, 73.9, 47.3, 46.8, 29.2,

22.3, 21.0; ^{19}F NMR (376 MHz, CDCl_3) δ : -62.2. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{21}\text{H}_{20}\text{F}_3\text{N}_2\text{O}_2]^+$: 389.1471, Found: 389.1468.

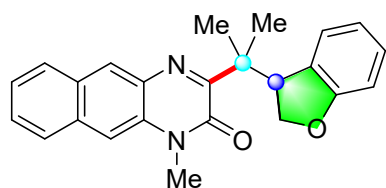


3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-6,7-difluoro-1-methylquinoxalin-2(1H)-one (3m): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3m** (light yellow solid, 52.0 mg, 73% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.64 (dd, $J = 10.2, 8.2$ Hz, 1H), 7.15–7.10 (m, 2H), 6.94 (d, $J = 7.4$ Hz, 1H), 6.80–6.73 (m, 2H), 4.62 (dd, $J = 9.2, 3.7$ Hz, 1H), 4.51 (t, $J = 9.3$ Hz, 1H), 4.36 (dd, $J = 9.4, 3.8$ Hz, 1H), 3.67 (s, 3H), 1.47 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.6 (d, $J = 3.6$ Hz), 161.0, 153.4, 151.4 (dd, $J = 253.4, 14.4$ Hz), 146.6 (dd, $J = 247.2, 13.9$ Hz), 130.4 (dd, $J = 8.8, 1.2$ Hz), 128.4, 128.1 (dd, $J = 9.1, 2.6$ Hz), 127.9, 126.0, 119.8, 117.9 (dd, $J = 18.1, 2.3$ Hz), 109.4, 102.0 (d, $J = 23.3$ Hz), 73.9, 47.3, 46.5, 29.5, 22.3, 21.0; ^{19}F NMR (376 MHz, CDCl_3) δ : -130.9, -142.2. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{19}\text{F}_2\text{N}_2\text{O}_2]^+$: 357.1409, Found: 357.1408.



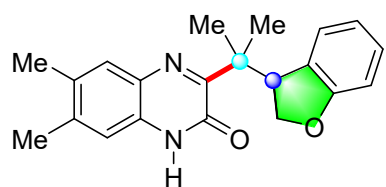
3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-1,6,7-trimethylquinoxalin-2(1H)-one (3n): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3n** (colorless solid, 59.9 mg, 86% yield). ^1H NMR (600 MHz, CDCl_3) δ : 7.59 (s, 1H), 7.12 – 7.09 (m, 2H), 6.97 (d, $J = 7.8$ Hz, 1H), 6.79 – 6.73 (m, 1H), 4.69 (dd, $J = 9.0, 3.6$ Hz, 1H), 4.52 (t, $J = 9.0$ Hz, 1H), 4.37 (dd, $J = 9.0, 3.6$ Hz, 1H), 3.69 (s, 3H), 2.43 (s, 3H), 2.35 (s, 3H), 1.49 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3) δ : 161.6, 161.0, 153.9, 139.8, 132.4, 131.2, 130.4 (2C), 128.3, 128.1, 126.1,

119.7, 113.9, 109.2, 74.1, 47.4, 46.2, 28.8, 22.4, 21.0, 20.5, 19.1. HRMS (ESI) m/z : ([M + H]⁺) Calcd for [C₂₂H₂₅N₂O₂]⁺: 349.1911, Found: 349.1906.



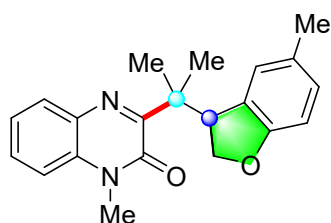
3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-1-methylbenzo[g]quinoxalin-

2(1H)-one (3o): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **3o** (light yellow solid, 38.5 mg, 52% yield). ¹H NMR (400 MHz, CDCl₃) δ : 8.36 (s, 1H), 7.96 (dd, J = 17.2, 8.0 Hz, 2H), 7.63–7.56 (m, 2H), 7.51–7.47 (m, 1H), 7.13 (t, J = 8.0 Hz, 1H), 7.00 (d, J = 7.2 Hz, 1H), 6.80 (d, J = 8.0 Hz, 1H), 6.77–6.73 (m, 1H), 4.71 (dd, J = 9.6, 4.0 Hz, 1H), 4.57 (td, J = 9.2, 1.6 Hz, 1H), 4.46–4.42 (m, 1H), 3.80 (s, 3H), 1.54 (s, 3H), 1.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ : 163.6, 161.1, 153.7, 133.7, 131.8, 131.3, 129.8, 129.6, 128.5, 128.3, 128.2, 127.9, 127.2, 126.2, 125.3, 119.8, 109.7, 109.4, 74.1, 47.7, 46.7, 29.0, 22.6, 21.3. HRMS (ESI) m/z : ([M + H]⁺) Calcd for [C₂₄H₂₃N₂O₂]⁺: 371.1754, Found: 371.1753.

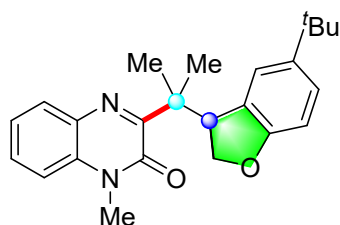


3-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)-6,7-dimethylquinoxalin-2(1H)-

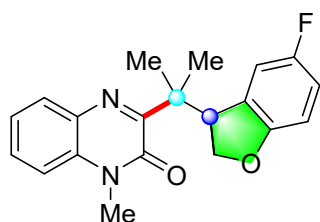
one (3p): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **3p** (light yellow solid, 39.5 mg, 59% yield). ¹H NMR (400 MHz, CDCl₃) δ : 12.16 (d, J = 18.8 Hz, 1H), 7.59 (s, 1H), 7.13 (t, J = 8.0 Hz, 1H), 7.08 (s, 1H), 7.01 (d, J = 7.6 Hz, 1H), 6.81–6.75 (m, 2H), 4.78–4.74 (m, 1H), 4.59 (td, J = 9.2, 1.6 Hz, 1H), 4.45–4.42 (m, 1H), 2.38 (s, 3H), 2.35 (s, 3H), 1.56 (s, 3H), 1.41 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ : 162.1, 161.1, 155.9 (2C), 140.2, 133.2, 130.7, 129.3, 129.2, 128.3, 128.2, 126.1, 119.8, 115.2, 109.4, 74.1, 47.6, 46.0, 22.4, 21.0, 20.3, 19.4. HRMS (ESI) m/z : ([M + H]⁺) Calcd for [C₂₁H₂₃N₂O₂]⁺: 335.1754, Found: 335.1753.



1-Methyl-3-(2-(5-methyl-2,3-dihydrobenzofuran-3-yl)propan-2-yl)quinoxalin-2(1H)-one (4a): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **4a** (light yellow oil, 35.4 mg, 53% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.84 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.57–7.53 (m, 1H), 7.36–7.31 (m, 2H), 6.94–6.91 (m, 1H), 6.87 (s, 1H), 6.67 (d, $J = 8.0$ Hz, 1H), 4.60 (dd, $J = 9.2, 3.6$ Hz, 1H), 4.49 (t, $J = 9.2$ Hz, 1H), 4.33 (dd, $J = 9.2, 3.6$ Hz, 1H), 3.72 (s, 3H), 2.22 (s, 3H), 1.54 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.1, 159.0, 153.8, 133.1, 131.9, 130.3, 130.0, 128.8, 128.6, 128.1, 126.9, 123.4, 113.3, 108.7, 74.3, 47.6, 46.4, 28.9, 22.7, 20.9, 20.6. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}_2]^+$: 335.1754, Found: 335.1753.

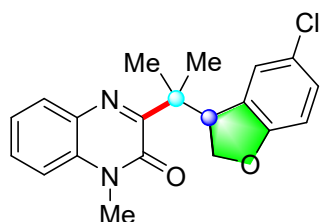


3-(2-(5-(tert-Butyl)-2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-2(1H)-one (4b): Purification by column chromatography (EtOAc/hexane, V/V = 1:30) afforded **4b** (light yellow solid, 37.7 mg, 50% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.81 (dd, $J = 8.4, 1.6$ Hz, 1H), 7.57–7.53 (m, 1H), 7.35–7.31 (m, 2H), 7.11 (dd, $J = 8.4, 2.0$ Hz, 1H), 6.83 (d, $J = 2.0$ Hz, 1H), 6.69 (d, $J = 8.4$ Hz, 1H), 4.63 (dd, $J = 8.8, 3.6$ Hz, 1H), 4.51 (t, $J = 9.2$ Hz, 1H), 4.43 (dd, $J = 9.6, 3.6$ Hz, 1H), 3.74 (s, 3H), 1.45 (s, 3H), 1.39 (s, 3H), 1.11 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.0, 158.7, 153.9, 142.4, 133.1, 132.0, 130.4, 130.0, 127.7, 124.9, 123.5, 123.1, 113.3, 108.2, 74.1, 47.5, 46.4, 34.0, 31.5, 28.9, 22.2, 21.4. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{24}\text{H}_{29}\text{N}_2\text{O}_2]^+$: 377.2224, Found: 377.2223.



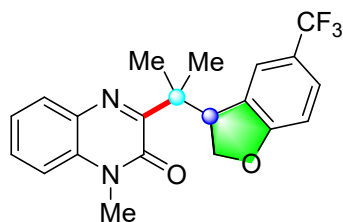
3-(2-(5-Fluoro-2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-

2(1H)-one (4c): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **4c** (colorless solid, 60.2 mg, 89% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.84 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.58–7.54 (m, 1H), 7.37–7.32 (m, 2H), 6.83–6.77 (m, 1H), 6.74–6.71 (m, 1H), 6.67 (dd, $J = 8.8, 4.4$ Hz, 1H), 4.68 (dd, $J = 9.2, 4.0$ Hz, 1H), 4.56 (t, $J = 9.6$ Hz, 1H), 4.39 (dd, $J = 9.2, 4.0$ Hz, 1H), 3.72 (s, 3H), 1.52 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 162.5, 157.1, 156.9 (d, $J = 236.1$ Hz), 153.8, 133.2, 131.8, 130.4, 130.2, 129.6 (d, $J = 8.1$ Hz), 123.5, 114.3 (d, $J = 24.1$ Hz), 113.4, 113.1 (d, $J = 24.6$ Hz), 109.2 (d, $J = 8.7$ Hz), 74.7, 47.8, 46.3, 28.9, 22.3, 20.9; ^{19}F NMR (376 MHz, CDCl_3) δ : –125.1 (td, $J = 15.04, 3.76$ Hz, 1F). HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{20}\text{FN}_2\text{O}_2]^+$: 339.1503, Found: 339.1502.

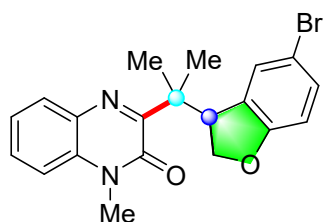


3-(2-(5-Chloro-2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-

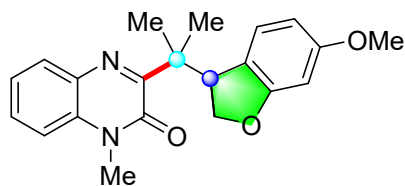
2(1H)-one (4d): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **4d** (light yellow solid, 62.5 mg, 88% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.84 (dd, $J = 7.6, 1.2$ Hz, 1H), 7.57 (t, $J = 7.6$ Hz, 1H), 7.38–7.32 (m, 2H), 7.09–7.03 (m, 2H), 6.69 (d, $J = 8.8$ Hz, 1H), 4.64 (dd, $J = 9.2, 4.0$ Hz, 1H), 4.55 (t, $J = 9.2$ Hz, 1H), 4.37 (dd, $J = 9.2, 4.0$ Hz, 1H), 3.72 (s, 3H), 1.54 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 162.5, 159.9, 153.7, 133.1, 131.8, 130.4, 130.20 (2C), 128.1, 126.2, 124.3, 123.5, 113.4, 110.1, 74.8, 47.7, 46.3, 29.0, 22.5, 20.6. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{20}^{35}\text{ClN}_2\text{O}_2]^+$: 355.1208, Found: 355.1207.



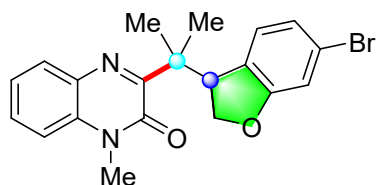
1-Methyl-3-(2-(5-(trifluoromethyl)-2,3-dihydrobenzofuran-3-yl)propan-2-yl)quinoxalin-2(1H)-one (4e): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **4e** (colorless solid, 67.6 mg, 87% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.83 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.59–7.55 (m, $J = 8.6$, 1H), 7.42–7.33 (m, 3H), 7.27–7.26 (m, 1H), 6.83 (d, $J = 8.4$ Hz, 1H), 4.68 (dd, $J = 9.2, 3.6$ Hz, 1H), 4.62 (t, $J = 9.2$ Hz, 1H), 4.46 (dd, $J = 8.8, 3.6$ Hz, 1H), 3.73 (s, 3H), 1.53 (s, 3H), 1.34 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ : 163.8, 162.3, 153.8, 133.2, 131.8, 130.4, 130.3, 129.1, 126.3 (q, $J = 3.9$ Hz), 124.6 (q, $J = 270.0$ Hz), 123.6, 123.4 (q, $J = 3.7$ Hz), 123.4, 122.1 (q, $J = 32.2$ Hz), 113.4, 109.3, 75.1, 47.3, 46.3, 29.0, 22.5, 20.6; ^{19}F NMR (376 MHz, CDCl_3) δ : -61.0 (s, 1F). HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{21}\text{H}_{20}\text{F}_3\text{N}_2\text{O}_2]^+$: 389.1471, Found: 389.1472.



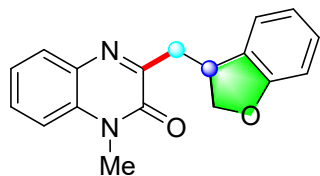
3-(2-(5-Bromo-2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-2(1H)-one (4f): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **4f** (colorless solid, 67.9 mg, 85% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.85–7.83 (m, 1H), 7.60–7.55 (m, 1H), 7.39–7.32 (m, 2H), 7.22 (dd, $J = 8.4, 2.0$ Hz, 1H), 7.17 (s, 1H), 6.66 (dd, $J = 8.4, 2.4$ Hz, 1H), 4.66–4.62 (m, 1H), 4.58–4.53 (m, 1H), 4.38–4.35 (m, 1H), 3.72 (s, 3H), 1.54 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 162.5, 160.4, 153.7, 133.2, 131.8, 131.0, 130.8, 130.4, 130.2, 129.1, 123.6, 113.4, 111.5, 110.9, 74.9, 47.7, 46.3, 29.0, 22.6, 20.5. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{20}^{79}\text{BrN}_2\text{O}_2]^+$: 399.0703, Found: 399.0703.



3-(2-(6-Methoxy-2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-2(1H)-one (4g): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **4g** (colorless solid, 59.6 mg, 85% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.84 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.58–7.53 (m, 1H), 7.37–7.31 (m, 2H), 6.87 (d, $J = 8.4$ Hz, 1H), 6.38 (d, $J = 2.4$ Hz, 1H), 6.32 (dd, $J = 8.0, 2.4$ Hz, 1H), 4.61–4.52 (m, 2H), 4.39 (dd, $J = 8.4, 2.8$ Hz, 1H), 3.75 (s, 3H), 3.72 (s, 3H), 1.50 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.1, 162.4, 160.5, 153.8, 133.2, 131.9, 130.4, 130.0, 126.1, 123.5, 120.2, 113.4, 105.4, 95.8, 75.0, 55.4, 46.9, 46.5, 28.9, 22.4, 20.8. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}_3]^+$: 351.1703, Found: 351.1703.

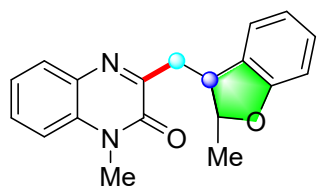


3-(2-(6-Bromo-2,3-dihydrobenzofuran-3-yl)propan-2-yl)-1-methylquinoxalin-2(1H)-one (4h): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **4h** (light yellow solid, 71.1 mg, 89% yield). ^1H NMR (400 MHz, CDCl_3) δ : 7.83 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.59–7.54 (m, 1H), 7.37–7.32 (m, 2H), 6.92 (d, $J = 1.6$ Hz, 1H), 6.88 (dd, $J = 8.0, 1.6$ Hz, 1H), 6.83 (d, $J = 8.0$ Hz, 1H), 4.63 (dd, $J = 9.6, 4.0$ Hz, 1H), 4.56 (t, $J = 9.2$ Hz, 1H), 4.40 (dd, $J = 9.2, 4.0$ Hz, 1H), 3.72 (s, 3H), 1.49 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 162.5, 162.2, 153.8, 133.2, 131.8, 130.4, 130.2, 127.6, 127.0, 123.5, 122.8, 121.3, 113.4, 112.9, 74.9, 47.1, 46.2, 29.0, 22.3, 20.9. HRMS (ESI) m/z : ($[\text{M} + \text{H}]^+$) Calcd for $[\text{C}_{20}\text{H}_{20}^{79}\text{BrN}_2\text{O}_2]^+$: 399.0703, Found: 399.0704.

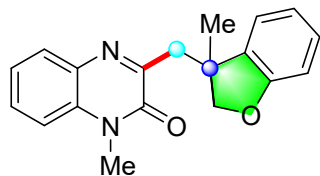


3-((2,3-Dihydrobenzofuran-3-yl)methyl)-1-methylquinoxalin-2(1H)-one (4i):

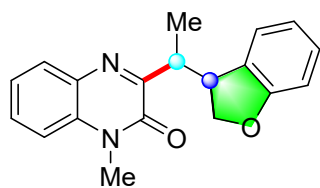
Purification by column chromatography (EtOAc/hexane, V/V = 1:15) afforded **4i** (colorless solid, 38.6 mg, 66% yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.86 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.58–7.54 (m, 1H), 7.39–7.31 (m, 2H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.87–6.80 (m, 2H), 4.86 (t, *J* = 9.2 Hz, 1H), 4.34 (dd, *J* = 9.2, 6.8 Hz, 1H), 4.21–4.14 (m, 1H), 3.72 (s, 3H), 3.53 (dd, *J* = 17.2, 4.8 Hz, 1H), 3.15 (dd, *J* = 17.2, 9.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ: 160.0, 158.3, 154.8, 133.1, 132.5, 130.2, 130.0, 129.9, 128.3, 124.5, 123.7, 120.3, 113.6, 109.5, 77.1, 39.3, 38.9, 29.0. HRMS (ESI) *m/z*: ([M + H]⁺) Calcd for [C₁₈H₁₇N₂O₂]⁺: 293.1285, Found: 293.1282.



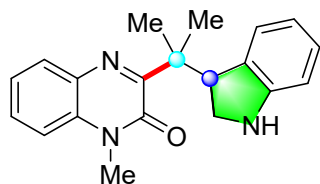
1-Methyl-3-((2-methyl-2,3-dihydrobenzofuran-3-yl)methyl)quinoxalin-2(1H)-one (4j): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **4j** (colorless solid, 41.7 mg, 68% yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.87 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.59–7.55 (m, 1H), 7.40–7.33 (m, 2H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.84–6.77 (m, 2H), 4.74–4.68 (m, 1H), 3.84–3.79 (m, 1H), 3.73 (s, 3H), 3.38 (dd, *J* = 16.4, 5.6 Hz, 1H), 3.20 (dd, *J* = 16.8, 8.4 Hz, 1H), 1.47 (d, *J* = 6.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 159.1, 158.4, 154.8, 133.1, 132.5, 130.3, 130.0, 129.8, 128.3, 124.9, 123.7, 120.2, 113.7, 109.5, 85.3, 45.8, 39.2, 29.1, 21.2. HRMS (ESI) *m/z*: ([M + H]⁺) Calcd for [C₁₉H₁₉N₂O₂]⁺: 307.1441, Found: 307.1440.



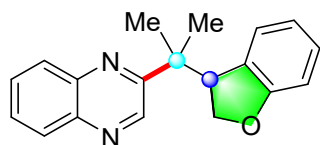
1-Methyl-3-((3-methyl-2,3-dihydrobenzofuran-3-yl)methyl)quinoxalin-2(1H)-one (4k): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **4k** (light yellow solid, 51.5 mg, 84% yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.78 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.56–7.52 (m, 1H), 7.36–7.28 (m, 2H), 7.27–7.25 (m, 1H), 7.13 (td, *J* = 7.6, 1.6 Hz, 1H), 6.90 (td, *J* = 7.2, 0.8 Hz, 1H), 6.76 (dd, *J* = 8.0, 0.8 Hz, 1H), 4.88 (d, *J* = 8.8 Hz, 1H), 4.42 (d, *J* = 8.8 Hz, 1H), 3.69 (s, 3H), 3.58 (d, *J* = 15.6 Hz, 1H), 3.15 (d, *J* = 15.6 Hz, 1H), 1.48 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 159.1, 157.8, 155.2, 135.4, 133.0, 132.4, 129.9 (2C), 128.2, 123.6, 123.1, 120.4, 113.6, 109.6, 82.3, 45.6, 42.2, 29.2, 25.4. HRMS (ESI) *m/z*: ([M + H]⁺) Calcd for [C₁₉H₁₉N₂O₂]⁺: 307.1441, Found:307.1441.



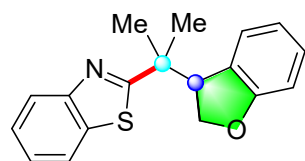
3-(1-(2,3-Dihydrobenzofuran-3-yl)ethyl)-1-methylquinoxalin-2(1H)-one (4l): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **4l** (yellow solid, 46.6 mg, 76% yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.86 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.57–7.53 (m, 1H), 7.38–7.31 (m, 2H), 7.19–7.10 (m, 2H), 6.84–6.77 (m, 2H), 4.73–4.31 (m, 2H), 4.12–4.05 (m, 1H), 3.99–3.74 (m, 1H), 3.72–3.71 (m, 3H), 1.34–1.17 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 162.4, 162.3, 160.7, 160.4, 154.4, 154.3, 133.0, 132.9, 132.5, 132.4, 130.0 (2C), 129.9 (2C), 129.2, 128.4, 128.3, 126.3, 124.5, 123.6, 120.3, 119.8, 113.5, 109.4, 109.3, 76.3, 73.0, 44.5, 44.1, 40.5, 39.7, 29.1, 15.3, 12.9. HRMS (ESI) *m/z*: ([M + H]⁺) Calcd for [C₁₉H₁₉N₂O₂]⁺: 307.1441, Found:307.1441.



3-(2-(Indolin-3-yl)propan-2-yl)-1-methylquinoxalin-2(1H)-one (4m): Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **4m** (yellow solid, 46.6 mg, 73% yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.85 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.57–7.53 (m, 1H), 7.36–7.31 (m, 2H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.63–6.57 (m, 2H), 4.68 (dd, *J* = 10.0, 4.4 Hz, 1H), 3.72 (s, 3H), 3.60 (t, *J* = 10.0 Hz, 1H), 3.34 (dd, *J* = 10.0, 4.8 Hz, 1H), 1.53 (s, 3H), 1.38 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 163.7, 153.9, 152.7, 133.2, 132.0, 130.4, 130.3, 129.8, 127.5, 126.0, 123.4, 117.9, 113.3, 109.4, 49.7, 47.0, 46.7, 28.9, 22.7, 21.8. HRMS (ESI) *m/z*: ([M + H]⁺) Calcd for [C₂₀H₂₂N₃O]⁺: 320.1757 Found: 320.1759.

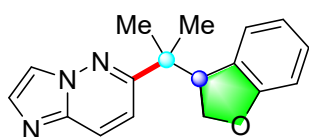


2-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)quinoxaline (6a): Purification by column chromatography (EtOAc/hexane, V/V = 1:20) afforded **6a** (yellow oil, 60.3 mg, 78% yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.83 (s, 1H), 8.12–8.07 (m, 2H), 7.80–7.73 (m, 2H), 7.16–7.10 (m, 1H), 6.77–6.71 (m, 3H), 4.54 (t, *J* = 9.2 Hz, 1H), 4.44 (dd, *J* = 9.6, 3.6 Hz, 1H), 4.27 (dd, *J* = 9.2, 3.6 Hz, 1H), 1.53 (s, 3H), 1.45 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 161.5, 161.0, 143.6, 141.5, 140.9, 130.0, 129.4, 129.0, 128.7, 127.5, 125.8, 120.0, 109.6, 73.9, 50.8, 43.8, 24.6, 23.7. HRMS (ESI) *m/z*: ([M + H]⁺) Calcd for [C₁₉H₁₉N₂O]⁺: 291.1492, Found: 291.1490.



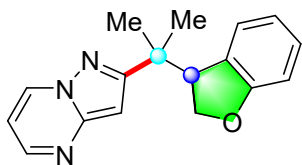
2-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)benzo[d]thiazole (6b): Purification by column chromatography (EtOAc/hexane, V/V = 1:100) afforded **6b** (colorless oil,

39.0 mg, 66% yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.03 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.52–7.47 (m, 1H), 7.41–7.37(m, 1H), 7.14 (td, *J* = 7.6, 1.2 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.80–6.73 (m, 2H), 4.56–4.48 (m, 2H), 4.18 (dd, *J* = 8.4, 4.0 Hz, 1H), 1.51 (s, 3H), 1.41 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 179.9, 161.0, 153.1, 134.7, 128.8, 126.9, 126.0, 124.8, 122.9, 121.6, 120.1, 109.6, 73.8, 51.8, 44.7, 25.6, 24.7. HRMS (ESI) *m/z*: ([*M* + *H*]⁺) Calcd for [C₁₈H₁₈NOS]⁺: 296.1104, Found: 296.1102.



6-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)imidazo[1,2-*b*]pyridazine (6c):

Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **6c** (colorless solid, 48.6 mg, 87% yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.24 (d, *J* = 4.8 Hz, 1H), 8.00 (d, *J* = 1.2 Hz, 1H), 7.78 (d, *J* = 1.2 Hz, 1H), 7.10 (td, *J* = 8.0, 1.6 Hz, 1H), 6.79–6.76 (m, 2H), 6.68 (td, *J* = 7.6, 1.2 Hz, 1H), 6.53 (d, *J* = 7.2 Hz, 1H), 5.10 (dd, *J* = 8.8, 3.6 Hz, 1H), 4.44–4.35 (m, 2H), 1.47 (s, 3H), 1.44 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 160.7, 146.4, 142.9, 138.3, 132.1, 128.4, 127.7, 125.7, 119.8, 116.5, 113.8, 109.3, 73.6, 47.7, 42.2, 23.1, 22.6. HRMS (ESI) *m/z*: ([*M* + *H*]⁺) Calcd for [C₁₇H₁₈N₃O]⁺: 280.1444, Found:280.1443.

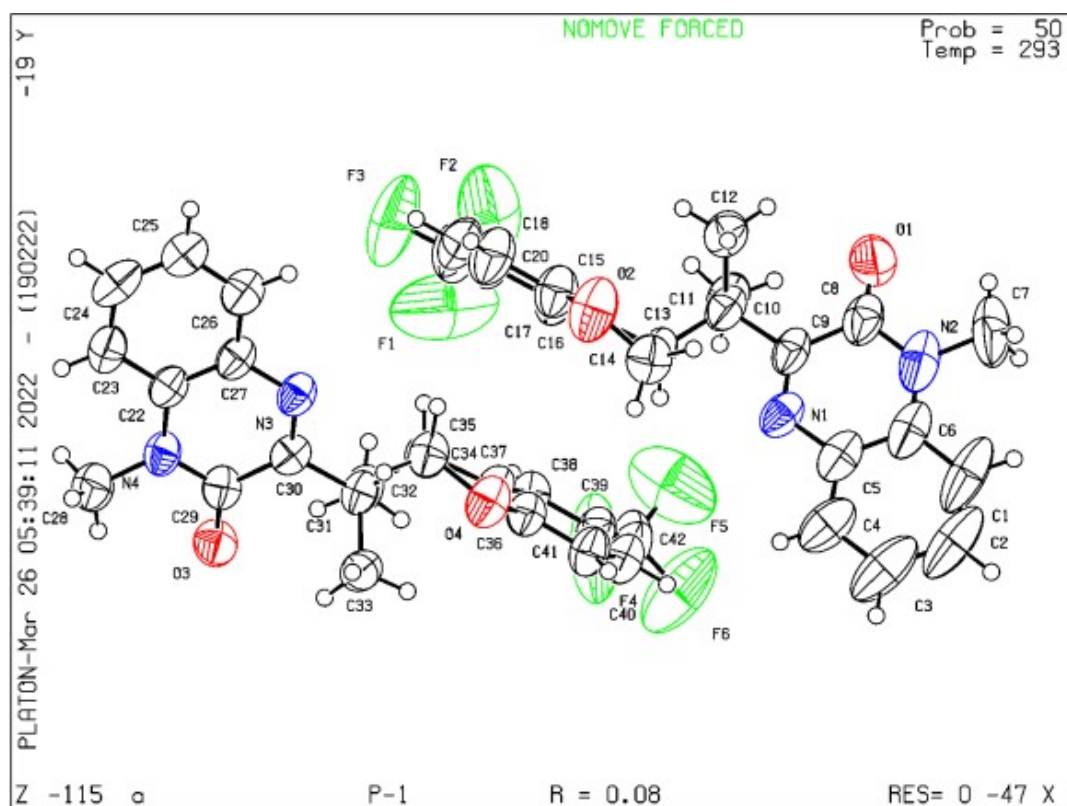


2-(2-(2,3-Dihydrobenzofuran-3-yl)propan-2-yl)pyrazolo[1,5-*a*]pyrimidine (6d):

Purification by column chromatography (EtOAc/hexane, V/V = 1:10) afforded **6d** (colorless solid, 24.0 mg, 43% yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.35 (d, *J* = 4.4 Hz, 1H), 8.10 (d, *J* = 2.4 Hz, 1H), 7.03 (td, *J* = 7.6, 1.2 Hz, 1H), 6.72–6.70 (m, 2H), 6.60–6.56 (m, 2H), 6.20 (d, *J* = 7.2 Hz, 1H), 5.26 (t, *J* = 6.0 Hz, 1H), 4.34 (d, *J* = 6.0 Hz, 2H), 1.47 (s, 3H), 1.42 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 160.7, 153.9,

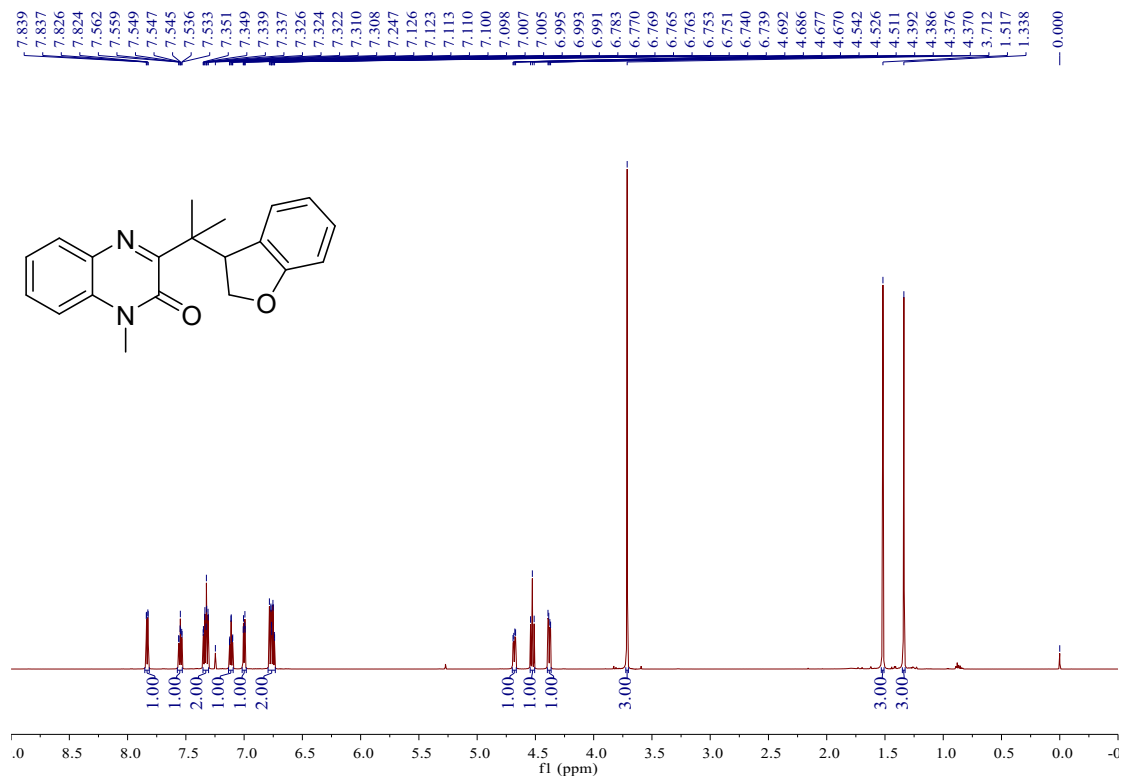
150.0, 148.8, 143.5, 128.6, 127.2, 125.3, 120.0, 109.4, 106.2, 96.7, 73.3, 44.3, 42.8, 21.8, 21.2. HRMS (ESI) m/z : ($[M + H]^+$) Calcd for $[C_{17}H_{18}N_3O]^+$: 280.1444, Found: 280.1444.

5. X-Ray Crystallographic Data for 4e (CCDC: 2211108).

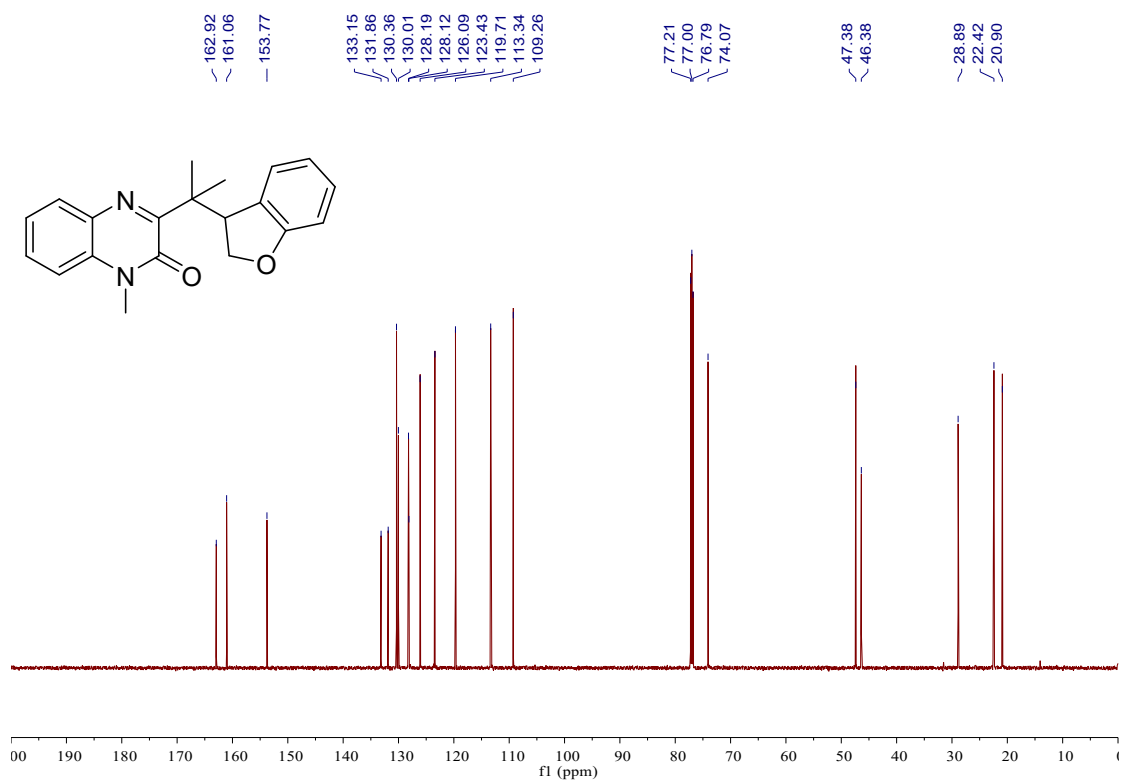


6. Copies of ^1H , ^{13}C NMR and ^{19}F NMR spectra

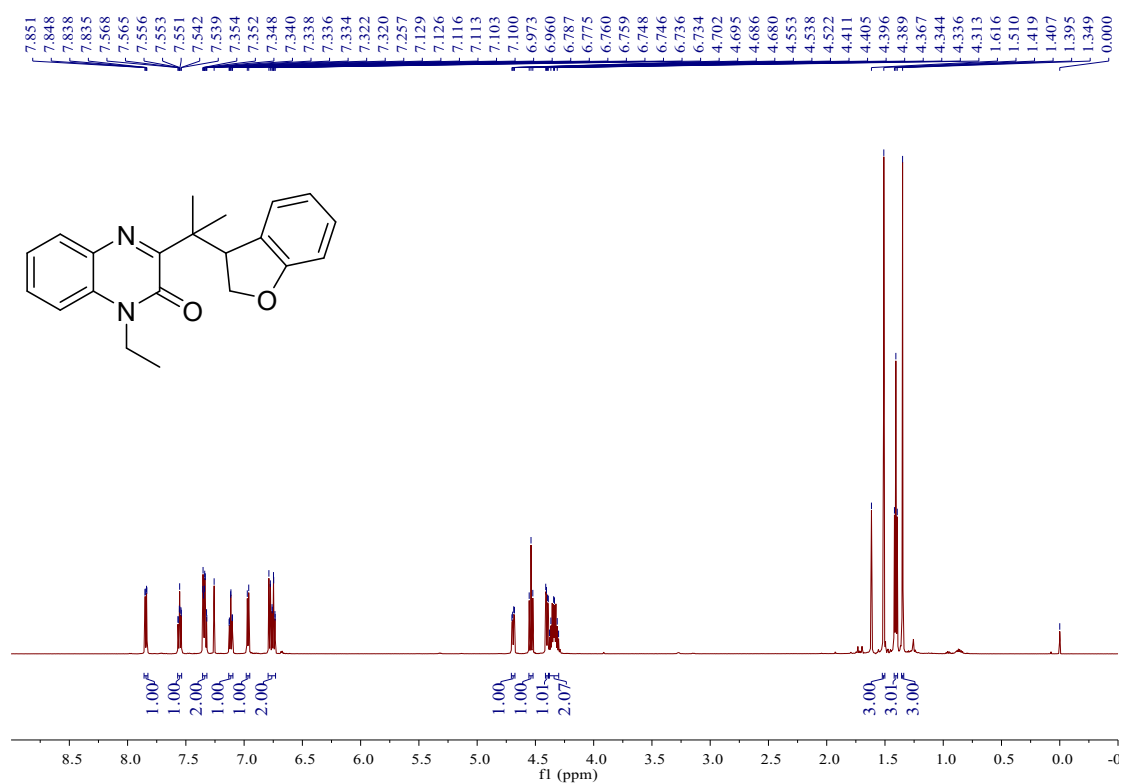
^1H NMR spectrum of **3a** (600 MHz, CDCl_3)



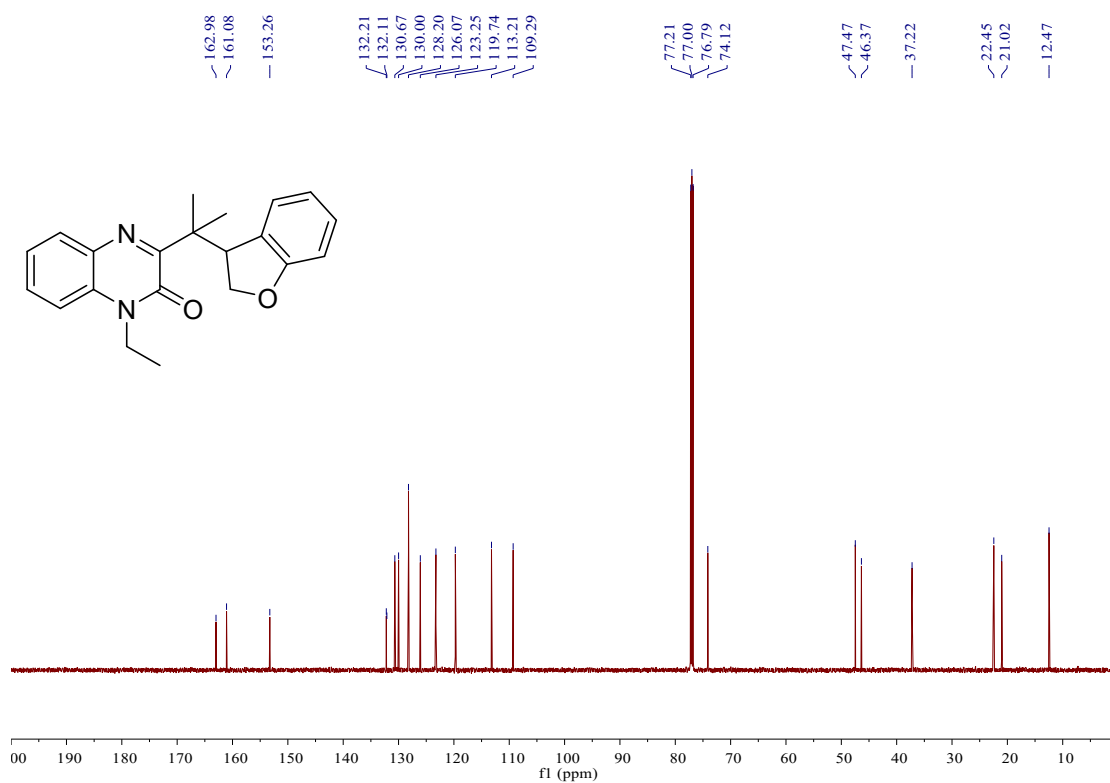
^{13}C NMR spectrum of **3a** (150 MHz, CDCl_3)



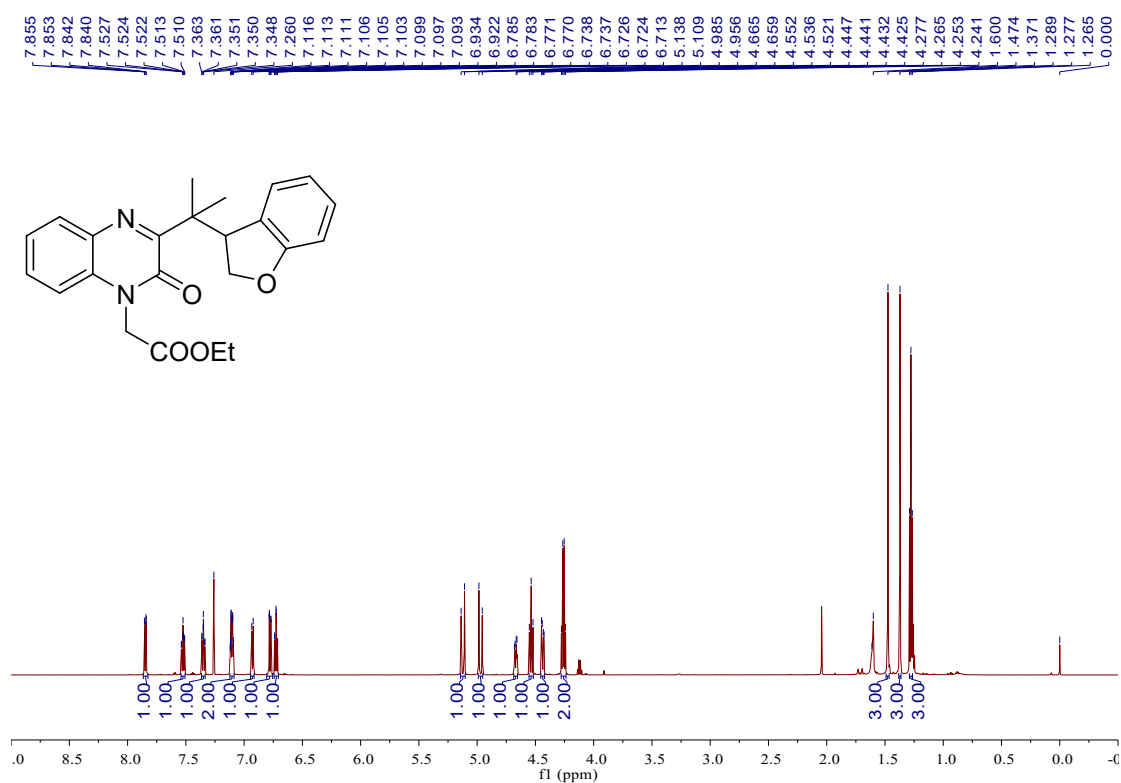
¹H NMR spectrum of **3b** (600 MHz, CDCl₃)



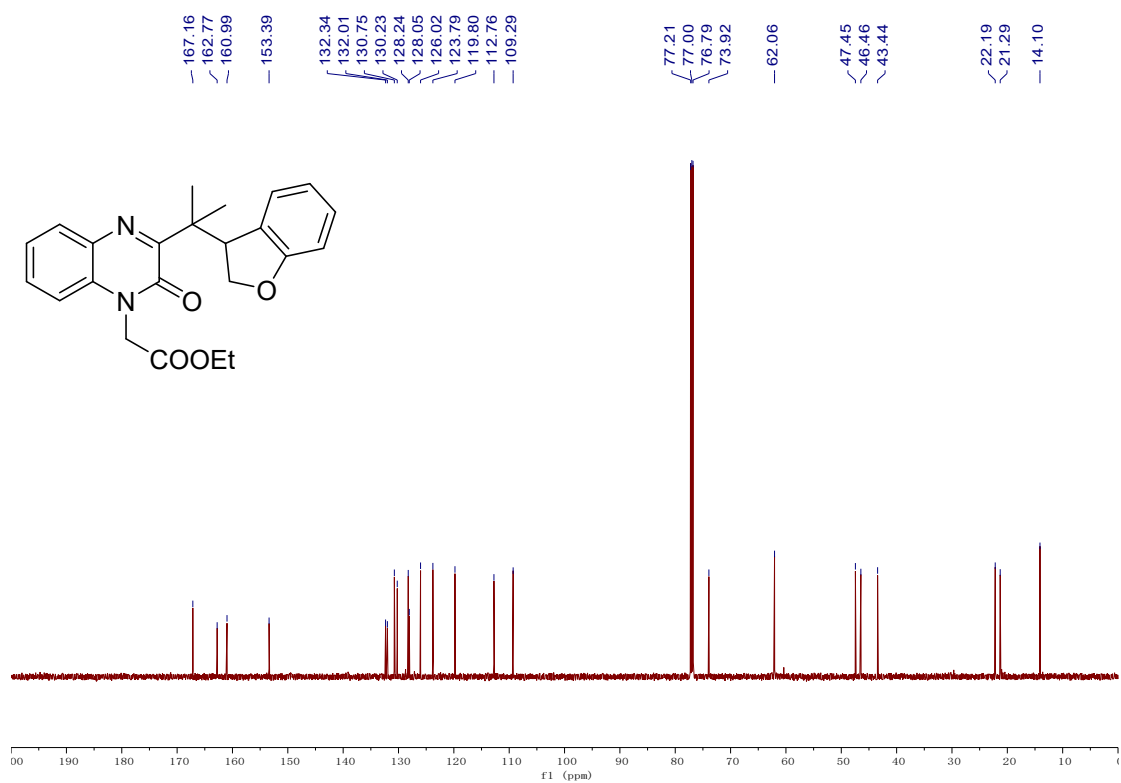
¹³C NMR spectrum of **3b** (150 MHz, CDCl₃)



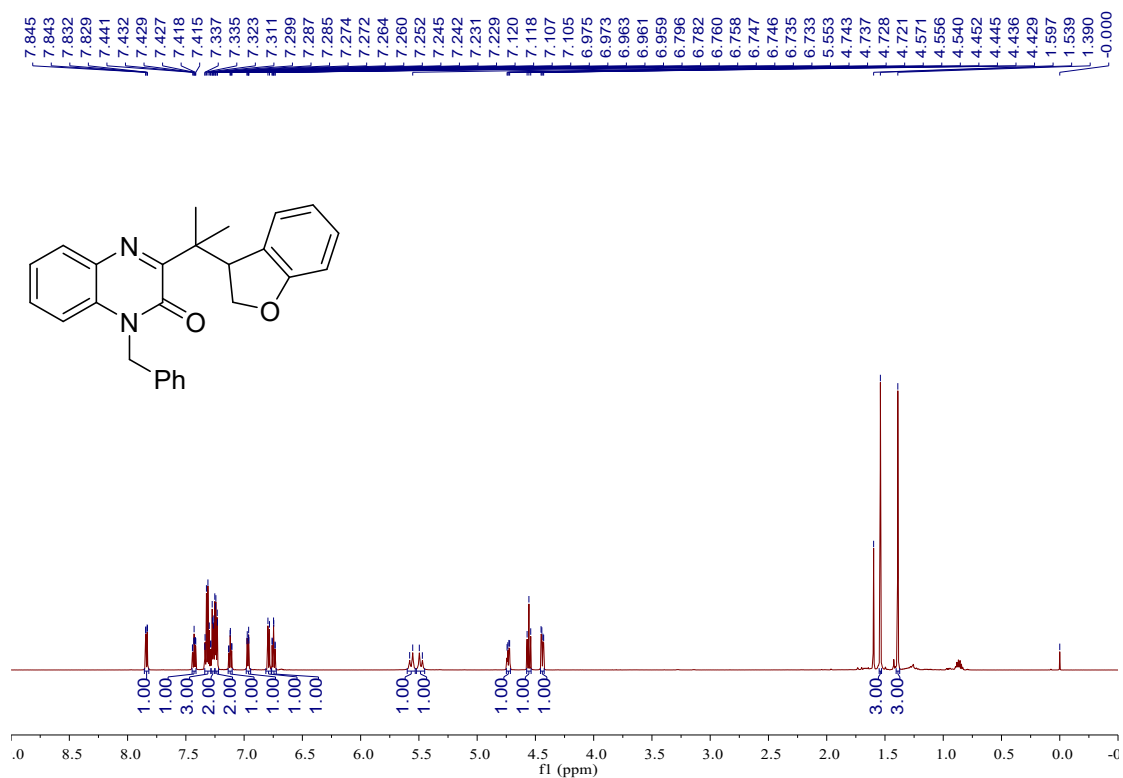
¹H NMR spectrum of **3c** (600 MHz, CDCl₃)



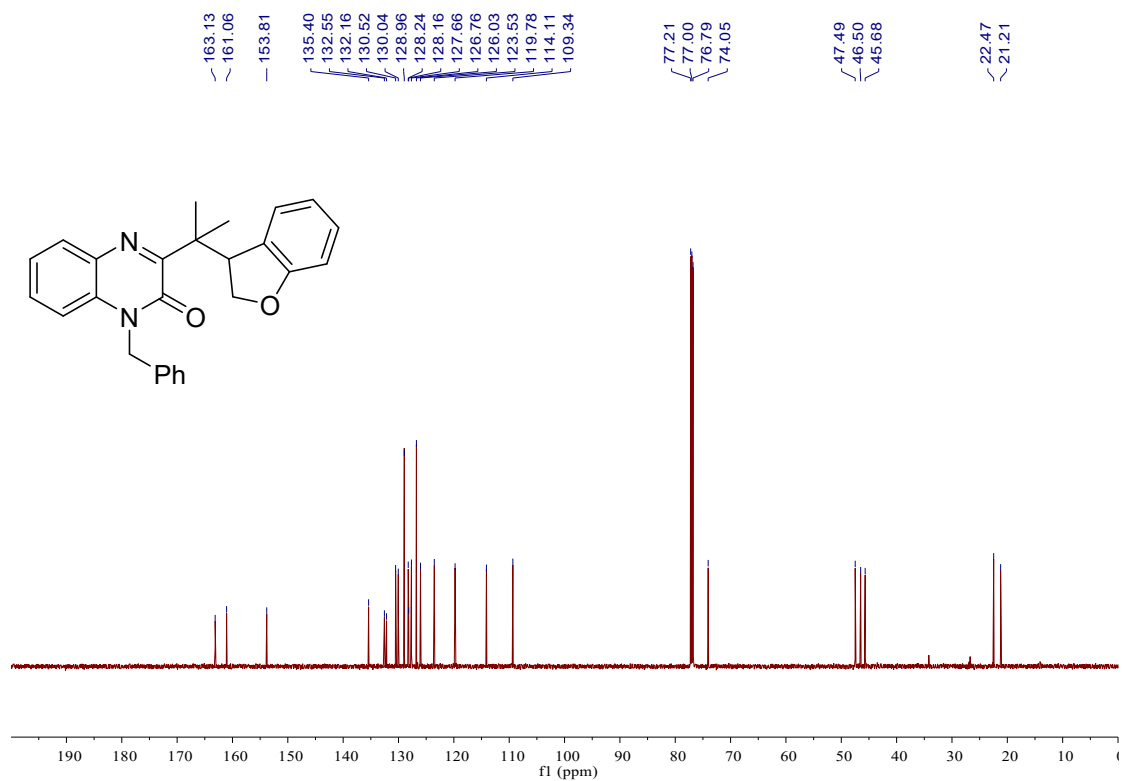
¹³C NMR spectrum of **3c** (150 MHz, CDCl₃)



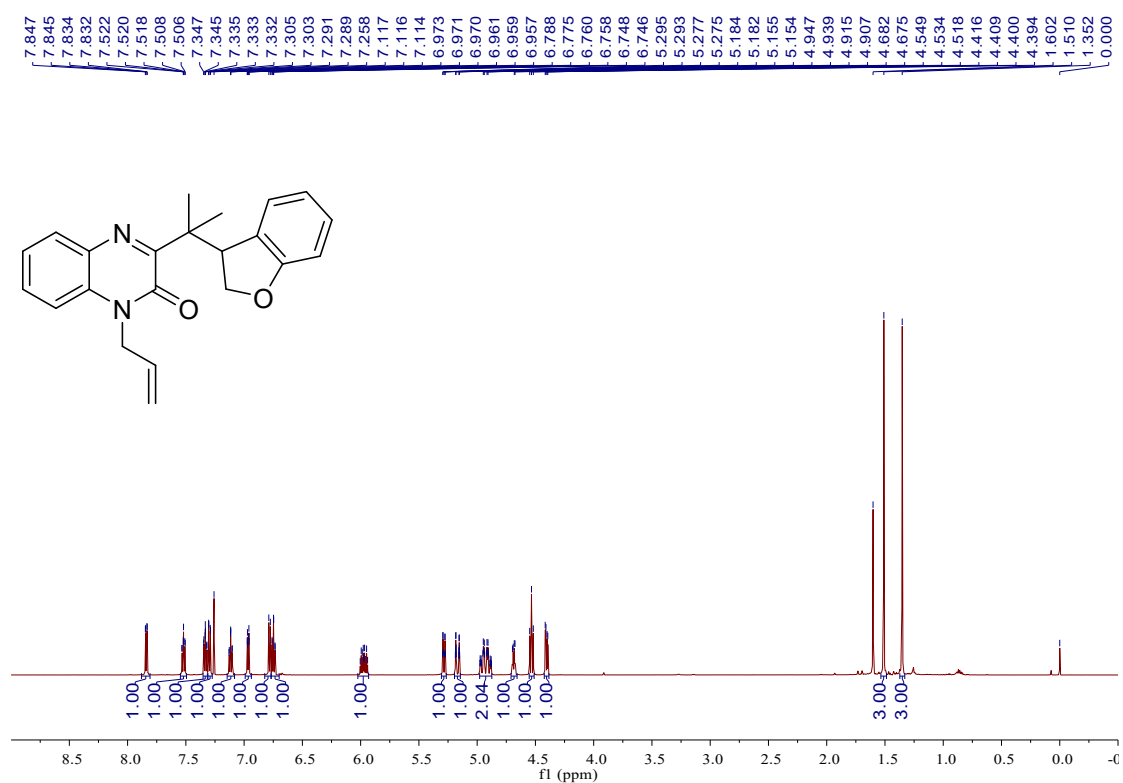
¹H NMR spectrum of **3d** (600 MHz, CDCl₃)



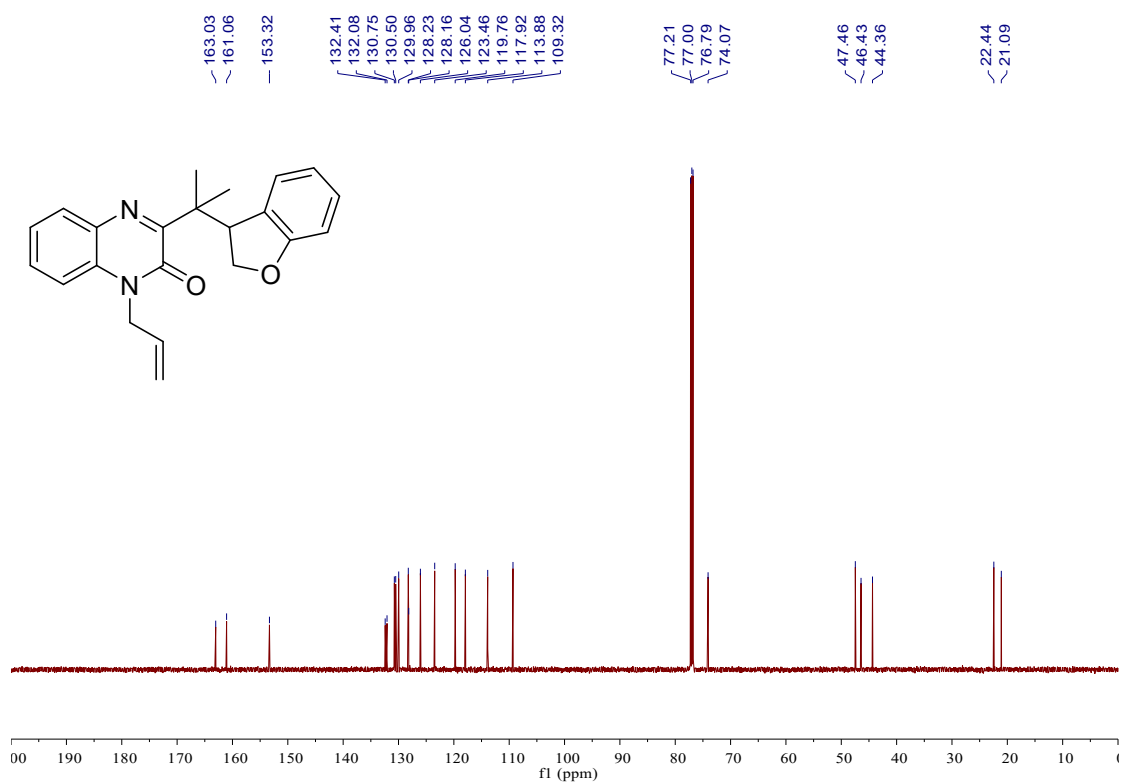
¹³C NMR spectrum of **3d** (150 MHz, CDCl₃)



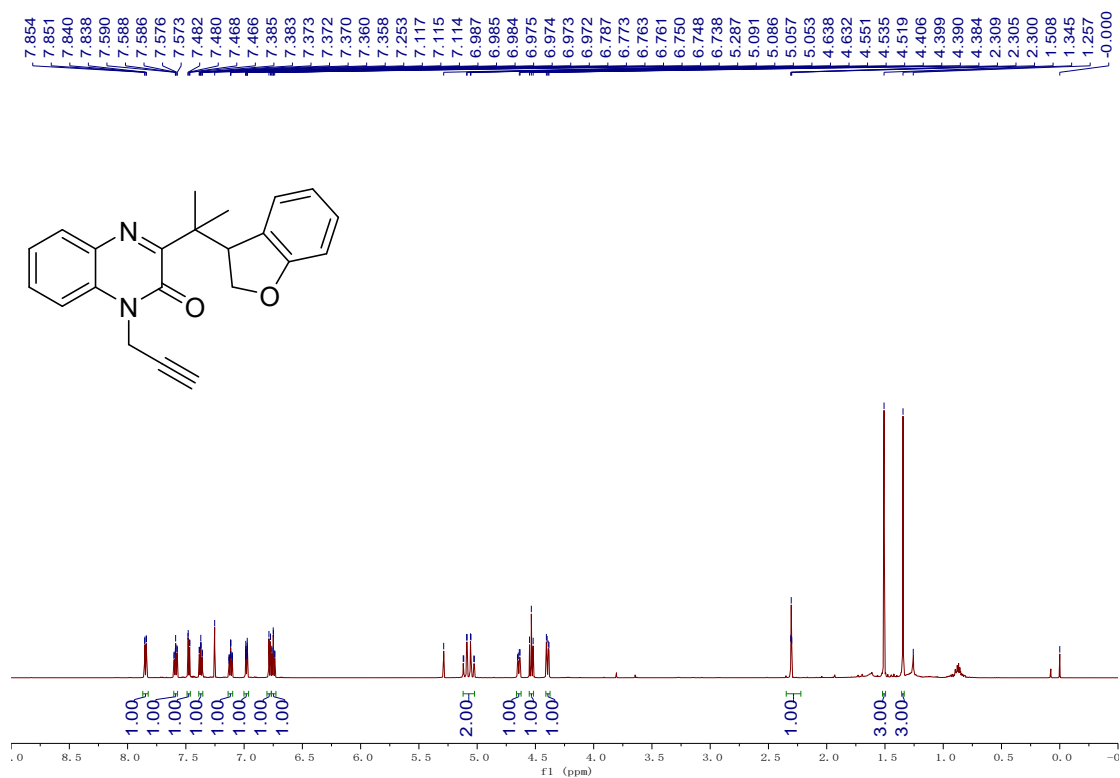
¹H NMR spectrum of **3e** (600 MHz, CDCl₃)



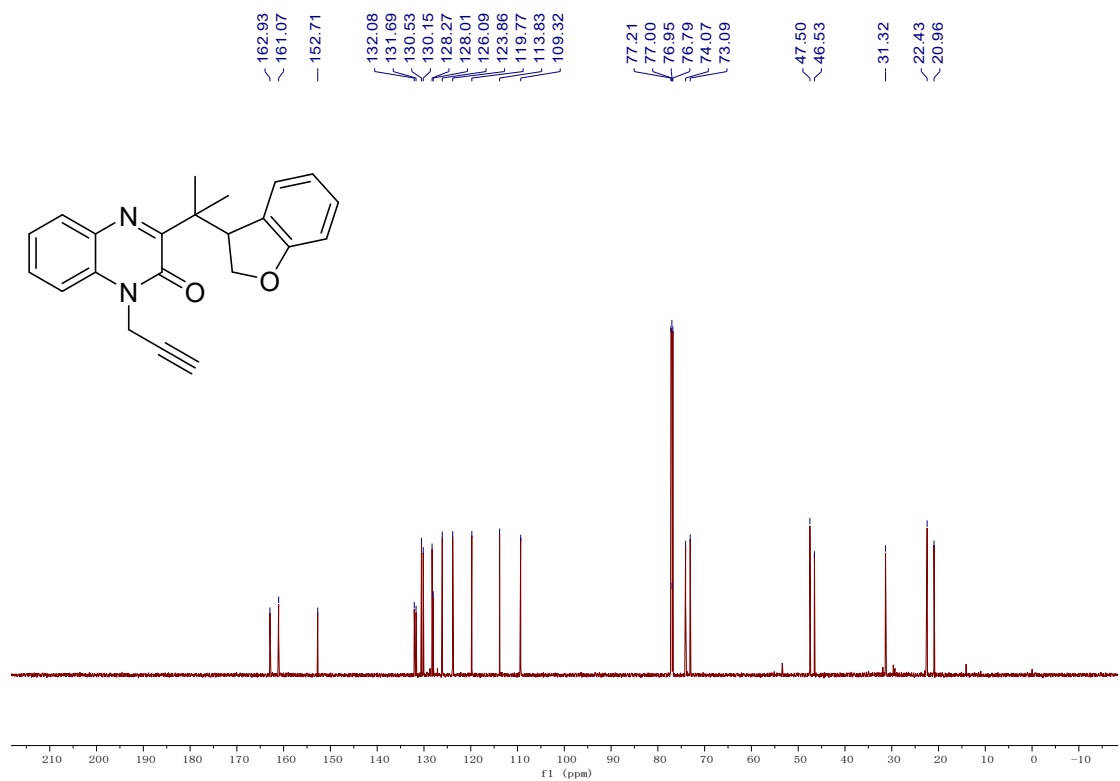
¹³C NMR spectrum of **3e** (150 MHz, CDCl₃)



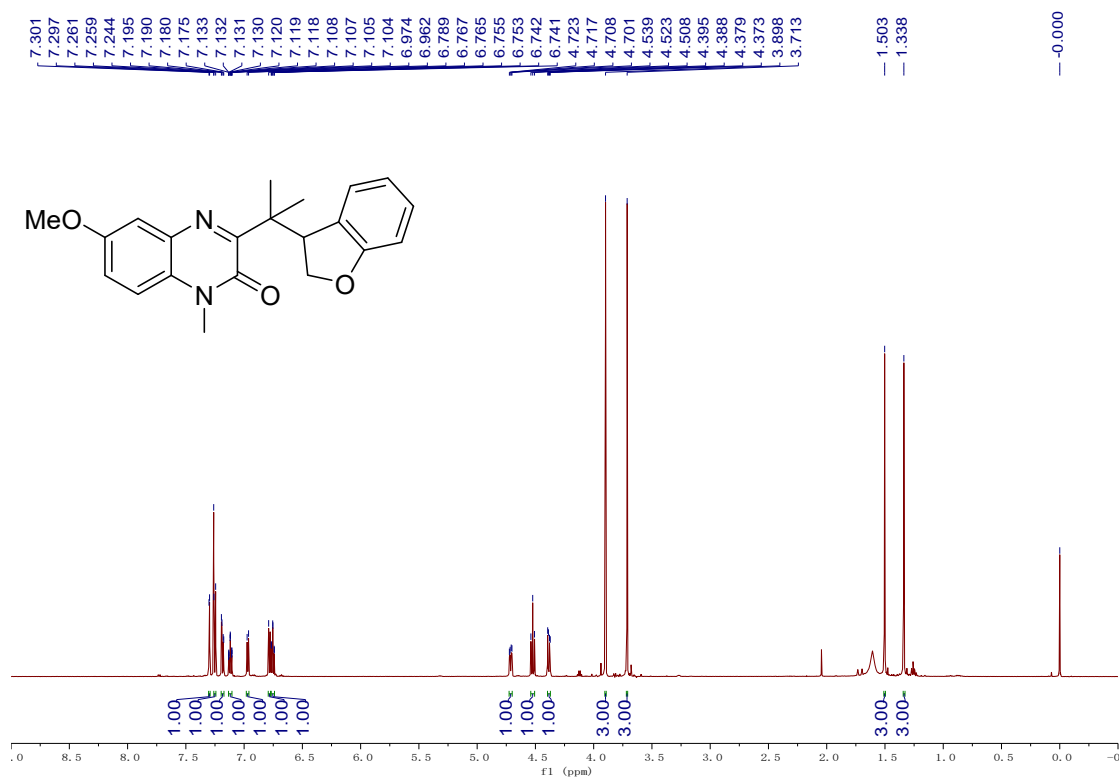
¹H NMR spectrum of **3f** (600 MHz, CDCl₃)



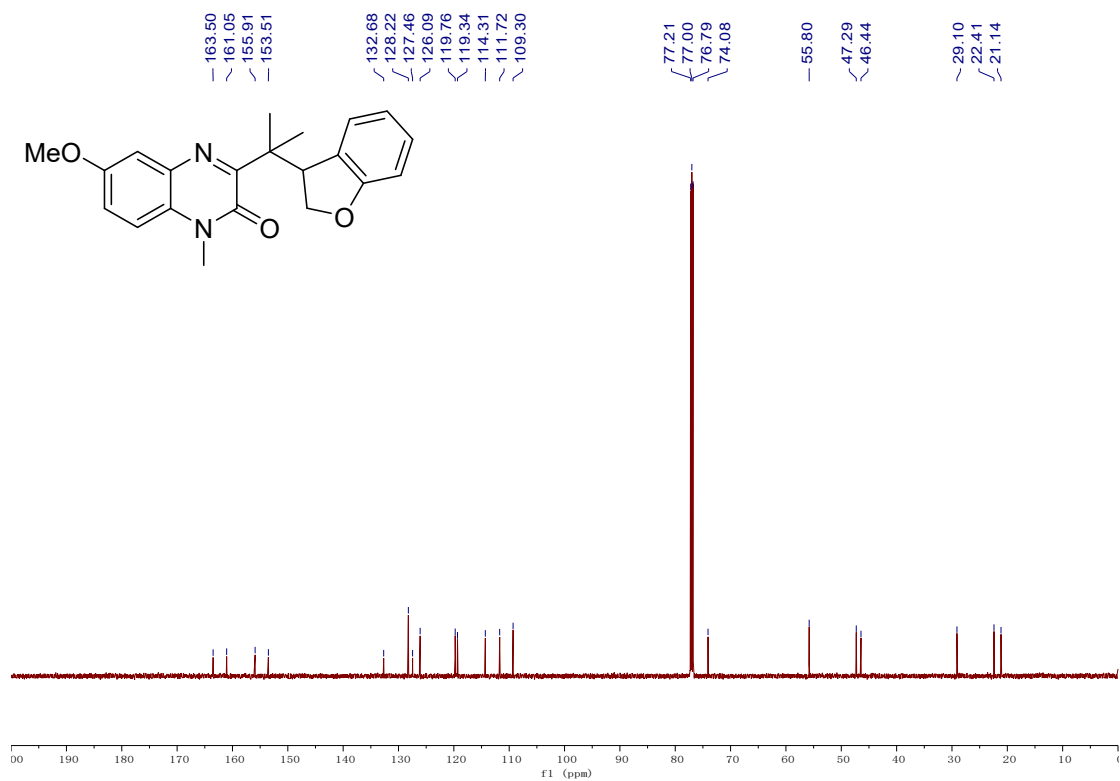
¹³C NMR spectrum of **3f** (150 MHz, CDCl₃)



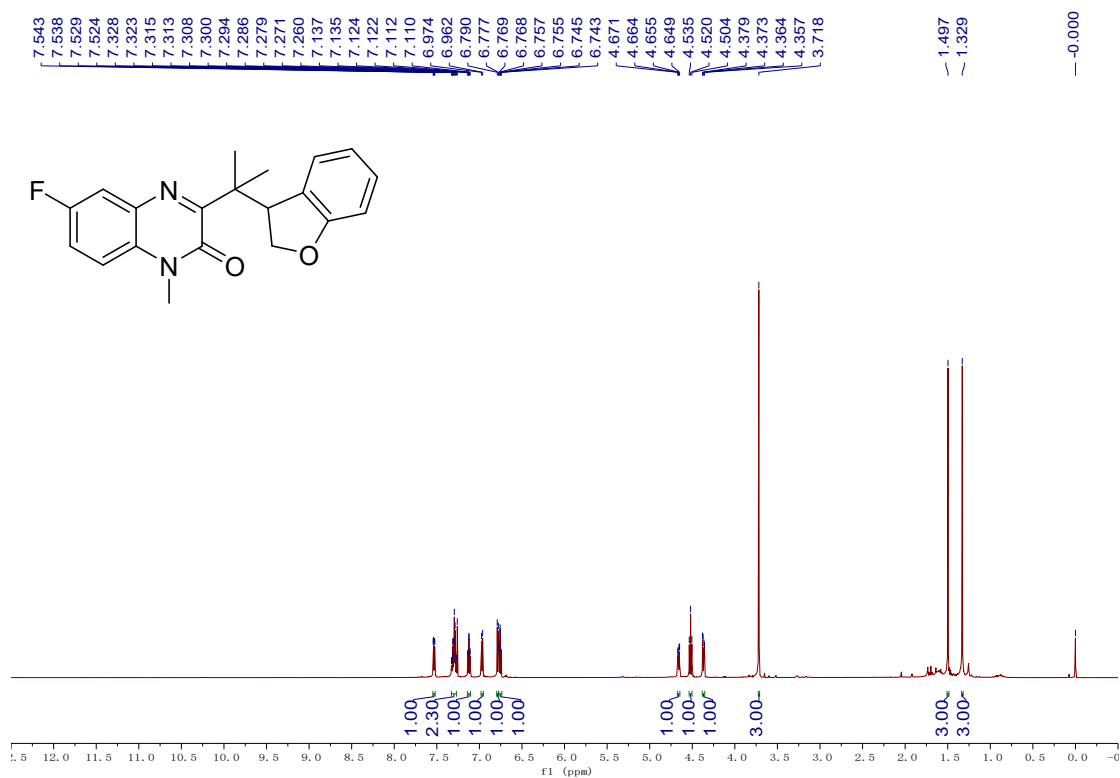
¹H NMR spectrum of **3g** (600 MHz, CDCl₃)



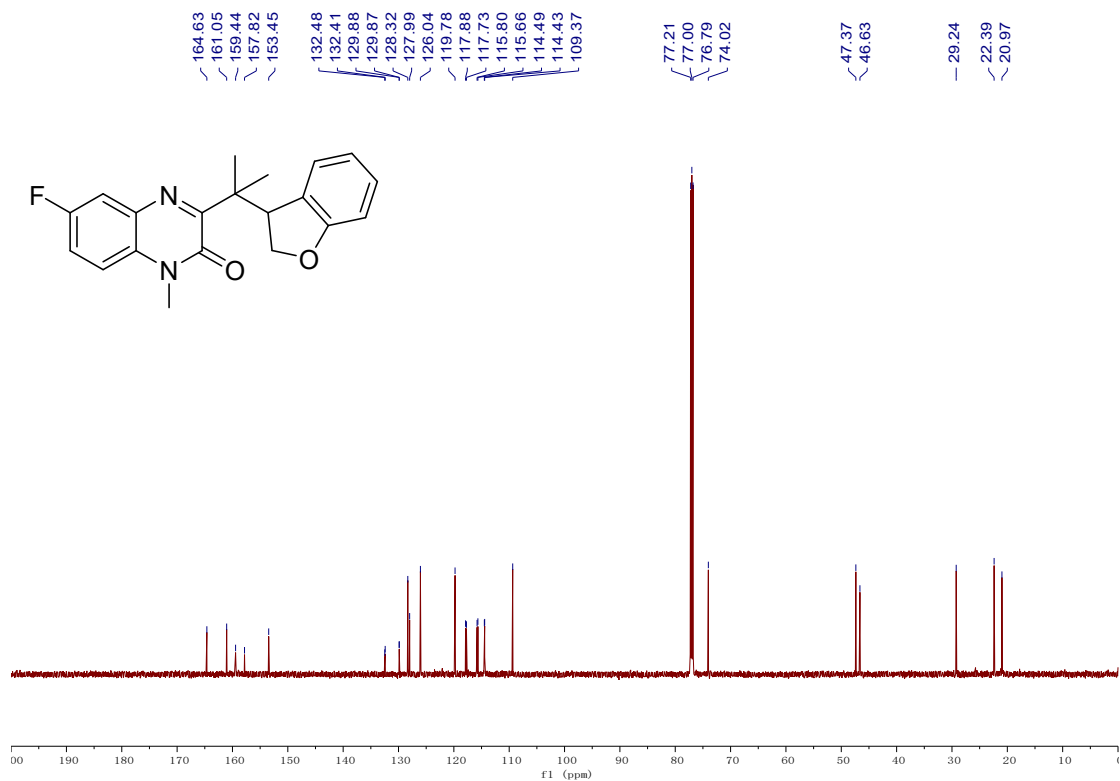
¹³C NMR spectrum of **3g** (150 MHz, CDCl₃)



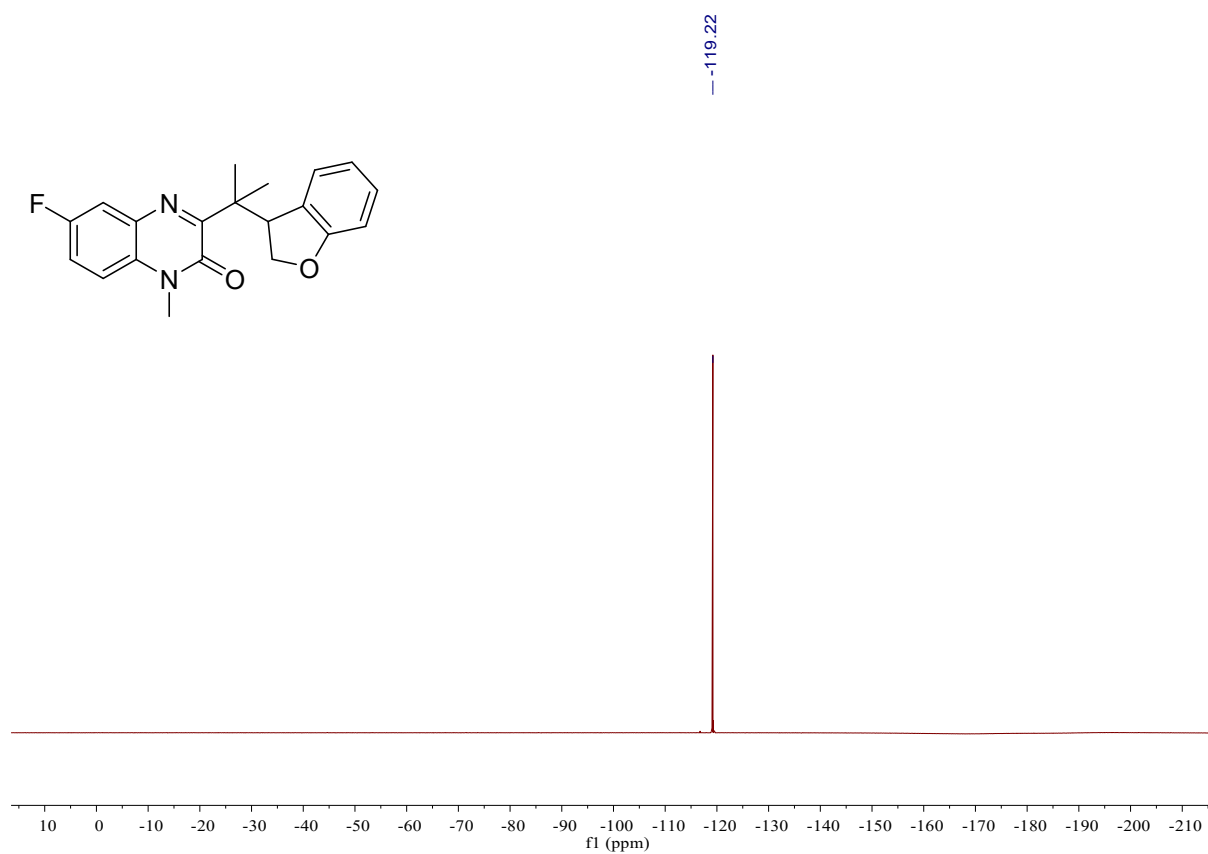
¹H NMR spectrum of **3h** (600 MHz, CDCl₃)



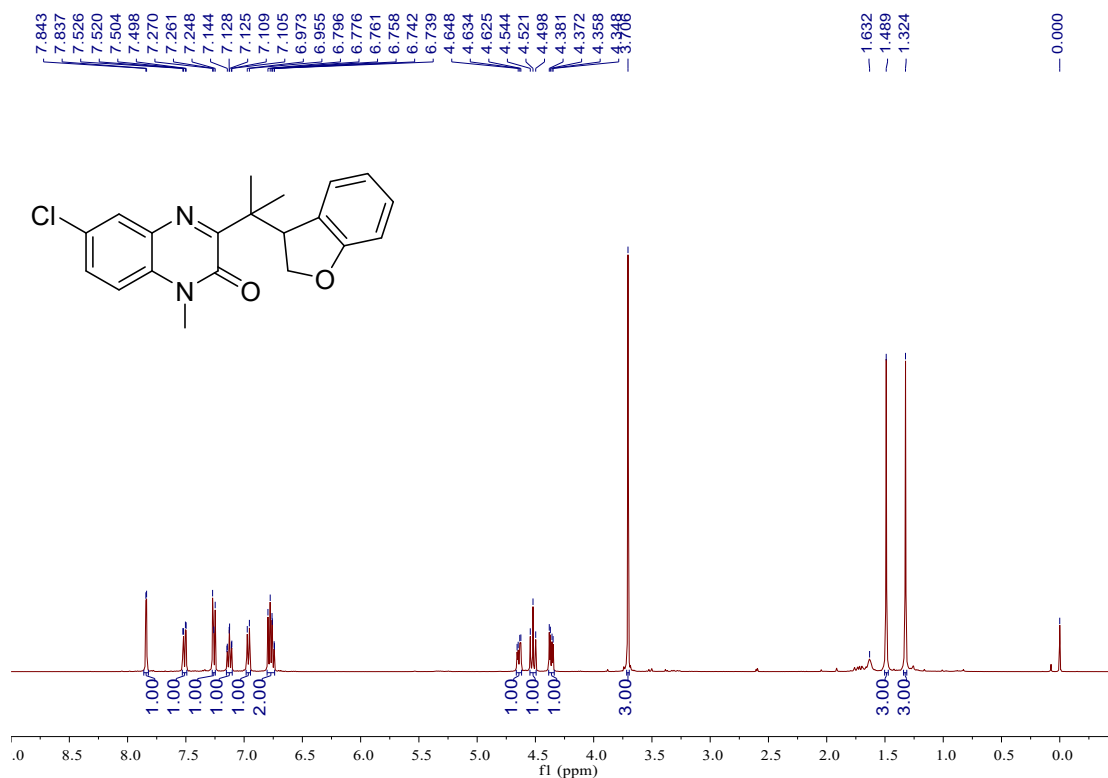
¹³C NMR spectrum of **3h** (150 MHz, CDCl₃)



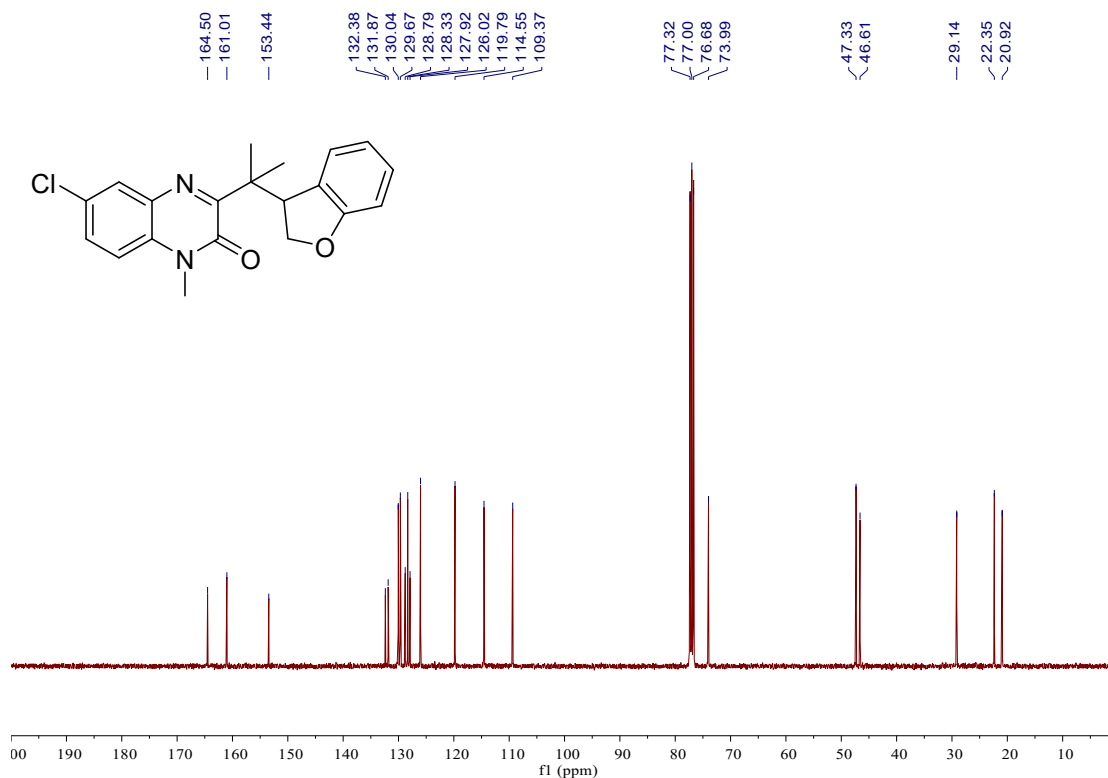
¹⁹F NMR spectrum of **3h** (564 MHz, CDCl₃)



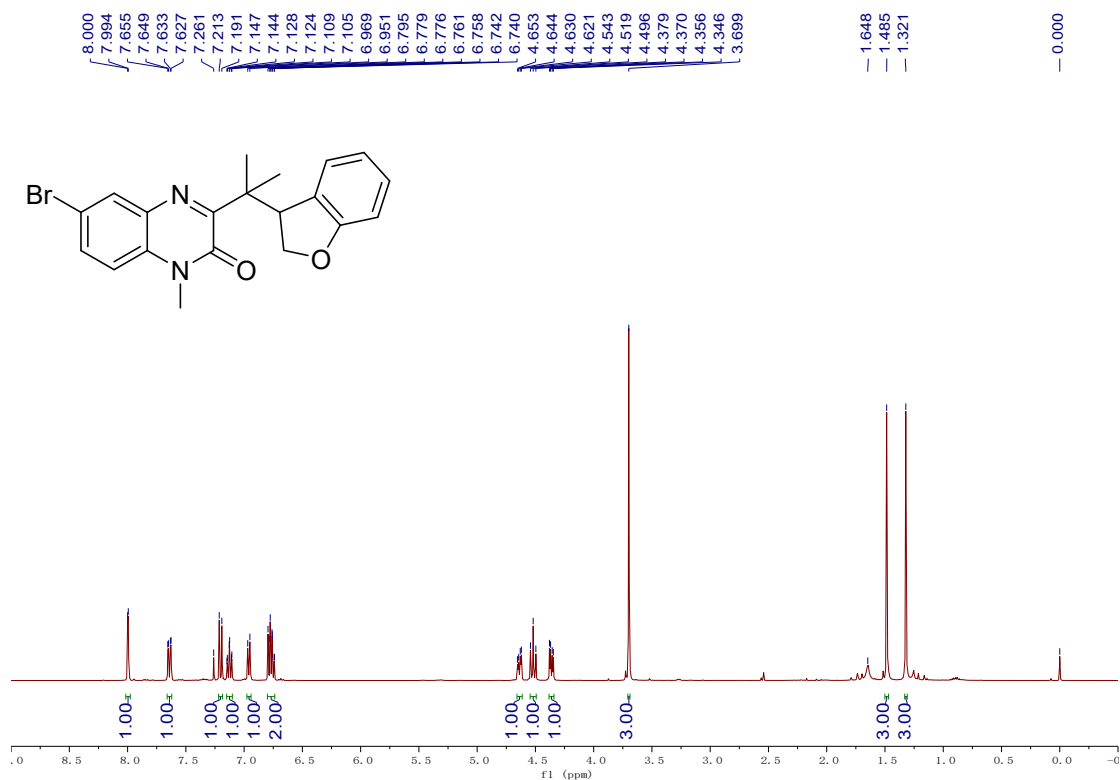
¹H NMR spectrum of **3i** (400 MHz, CDCl₃)



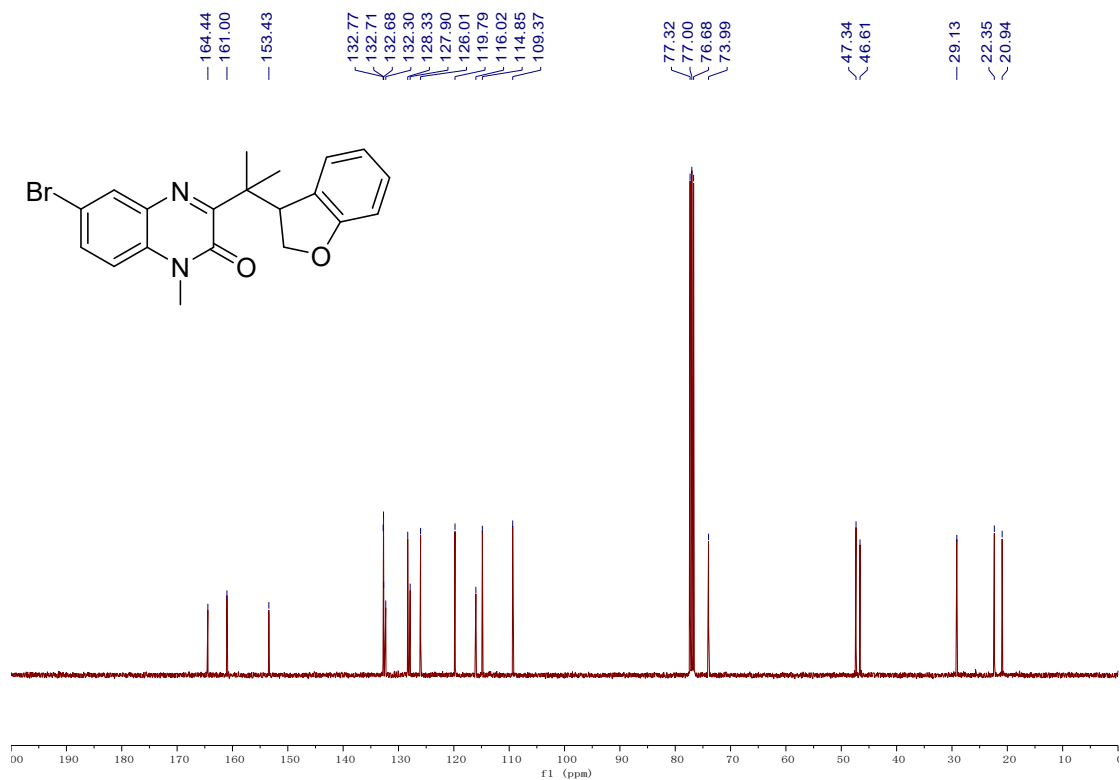
¹³C NMR spectrum of **3i** (100 MHz, CDCl₃)



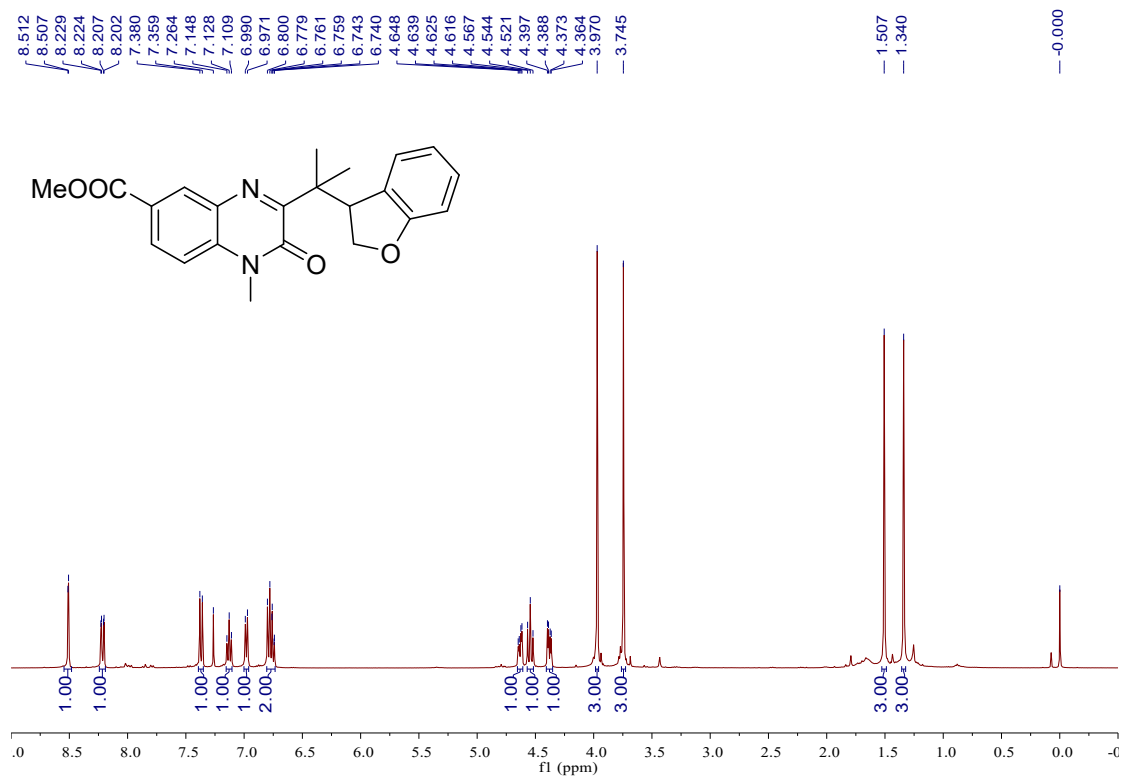
¹H NMR spectrum of **3j** (400 MHz, CDCl₃)



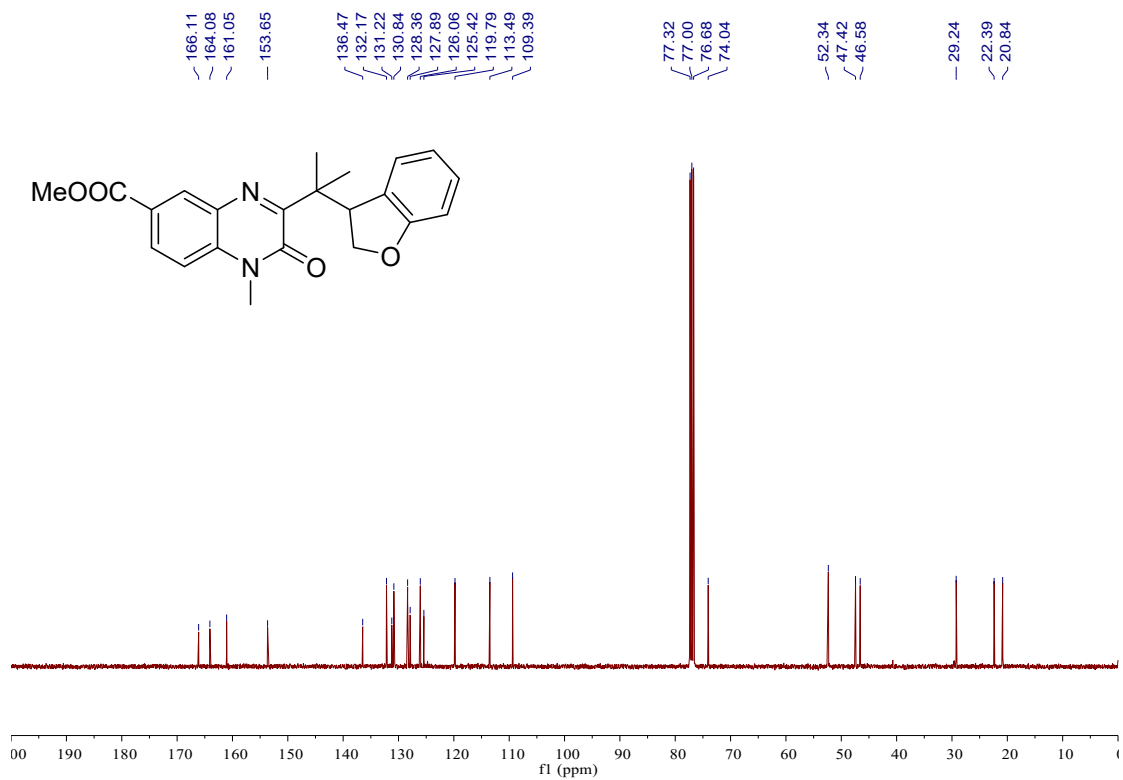
¹³C NMR spectrum of **3j** (100 MHz, CDCl₃)



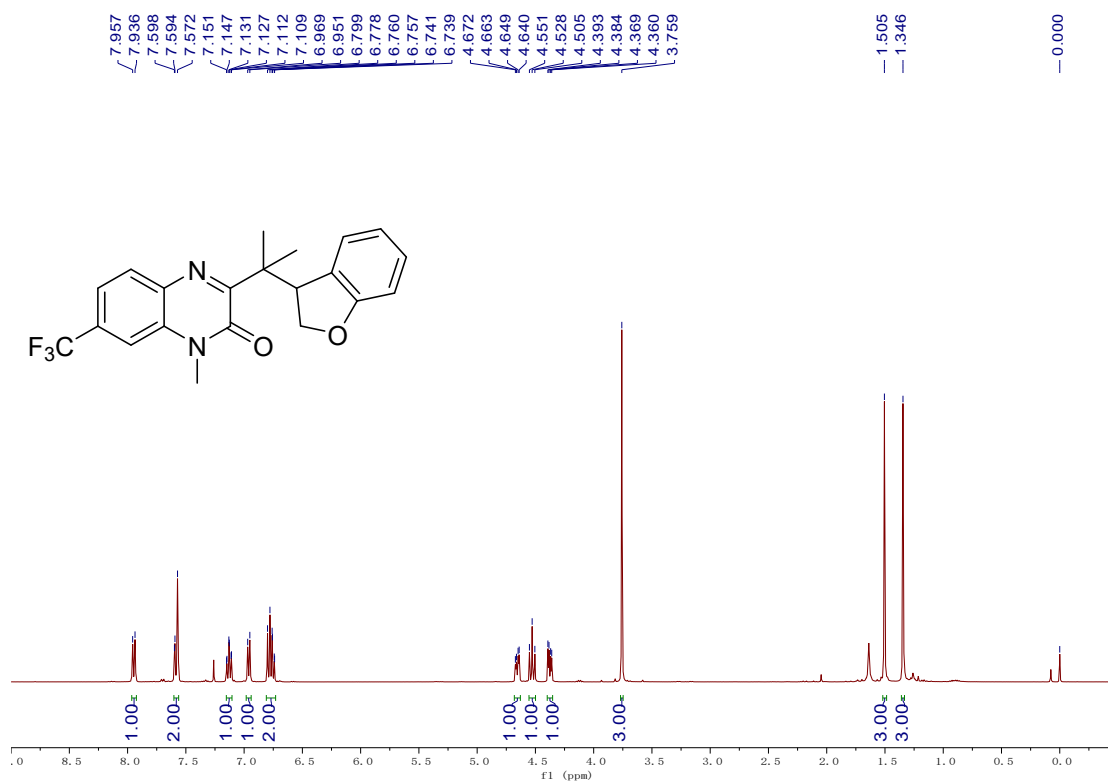
¹H NMR spectrum of **3k** (400 MHz, CDCl₃)



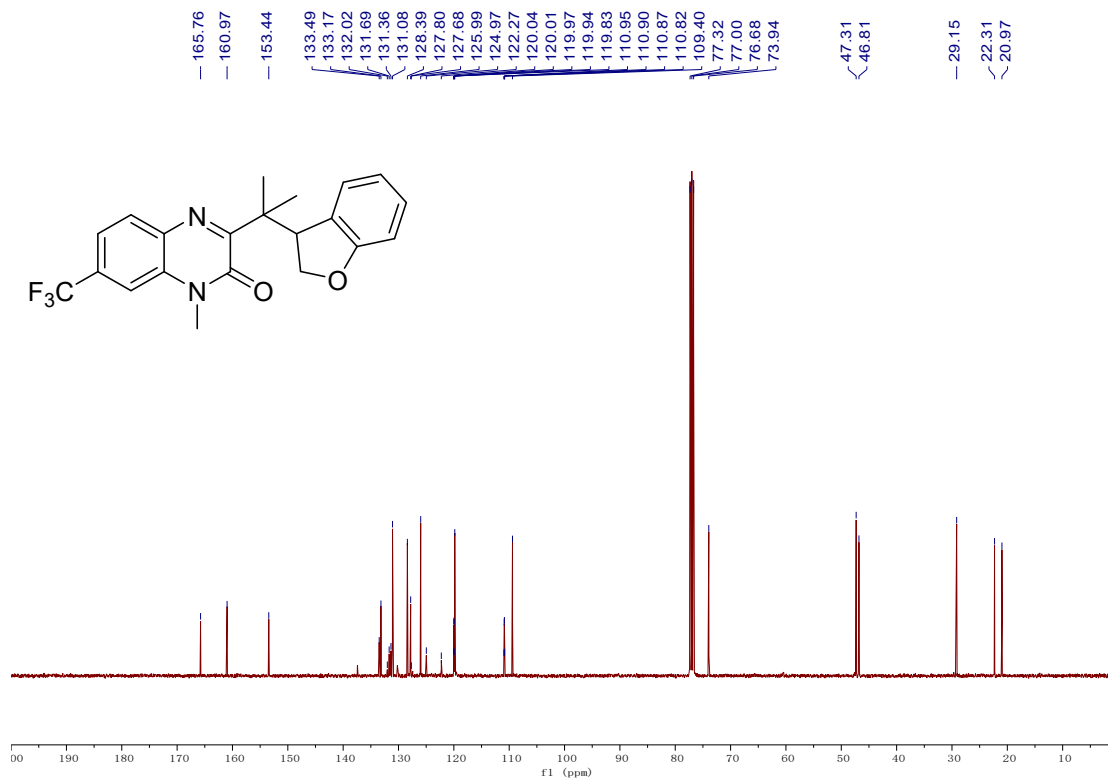
¹³C NMR spectrum of **3k** (100 MHz, CDCl₃)



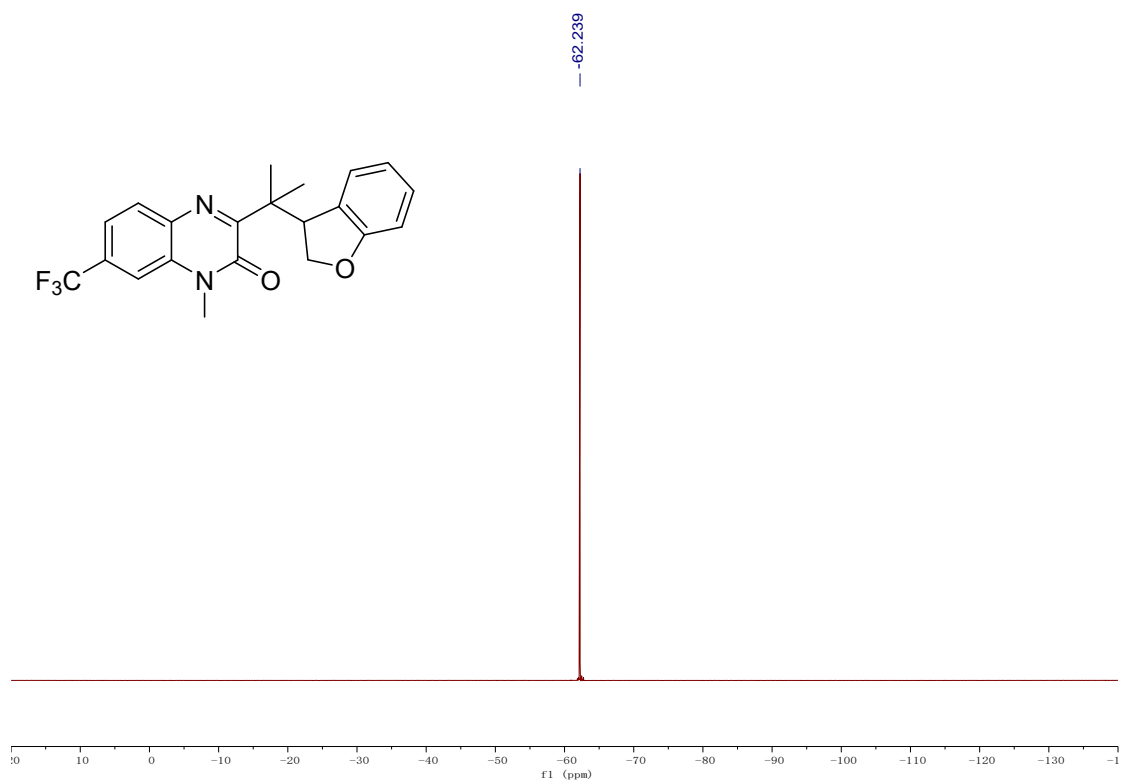
¹H NMR spectrum of **31** (400 MHz, CDCl₃)



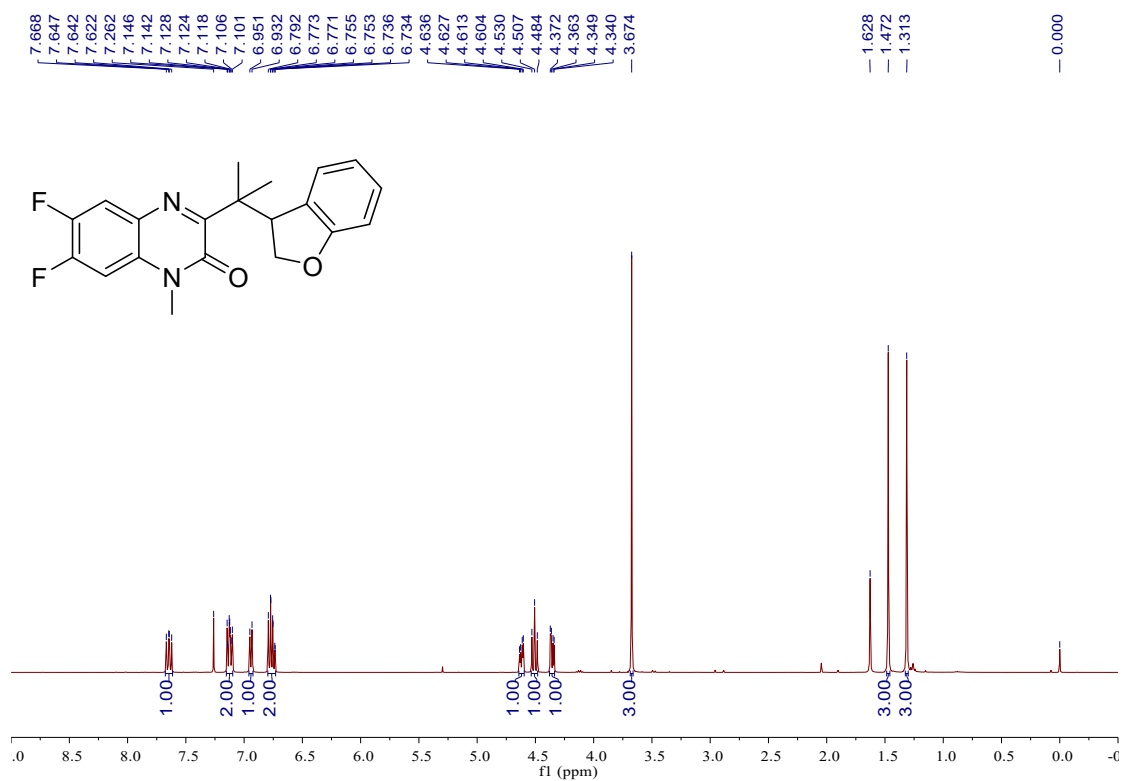
¹³C NMR spectrum of **31** (100 MHz, CDCl₃)



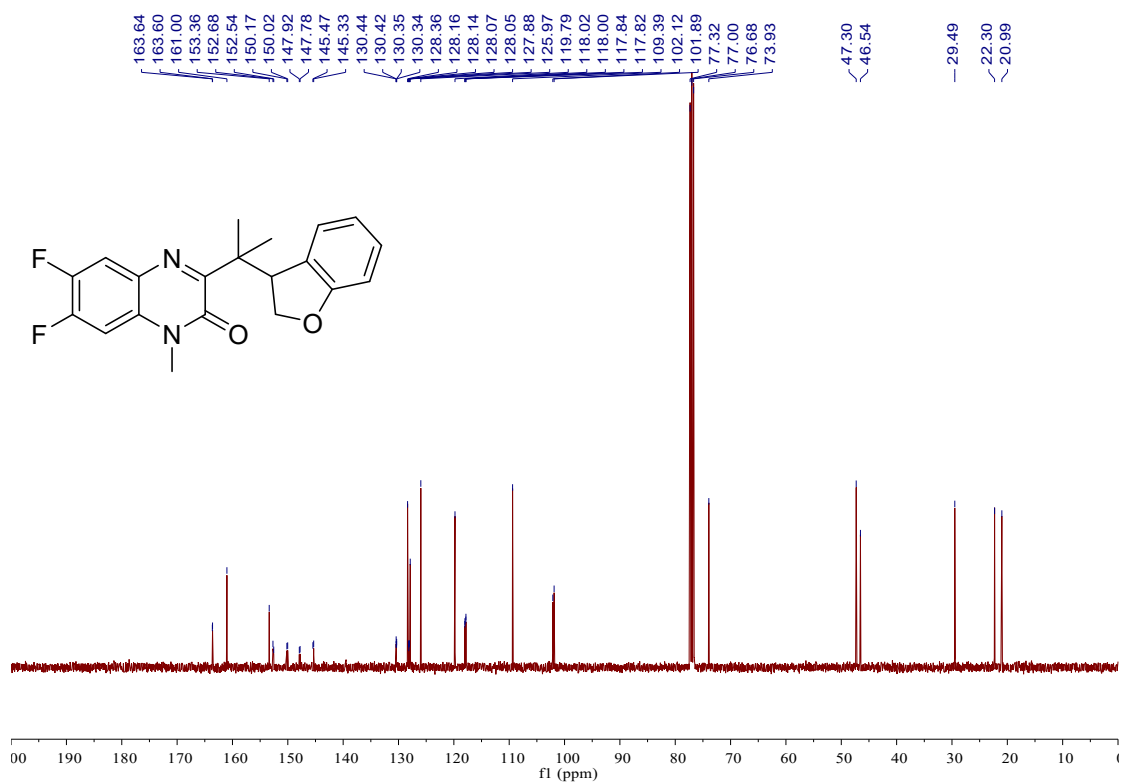
¹⁹F NMR spectrum of **31** (376 MHz, CDCl₃)



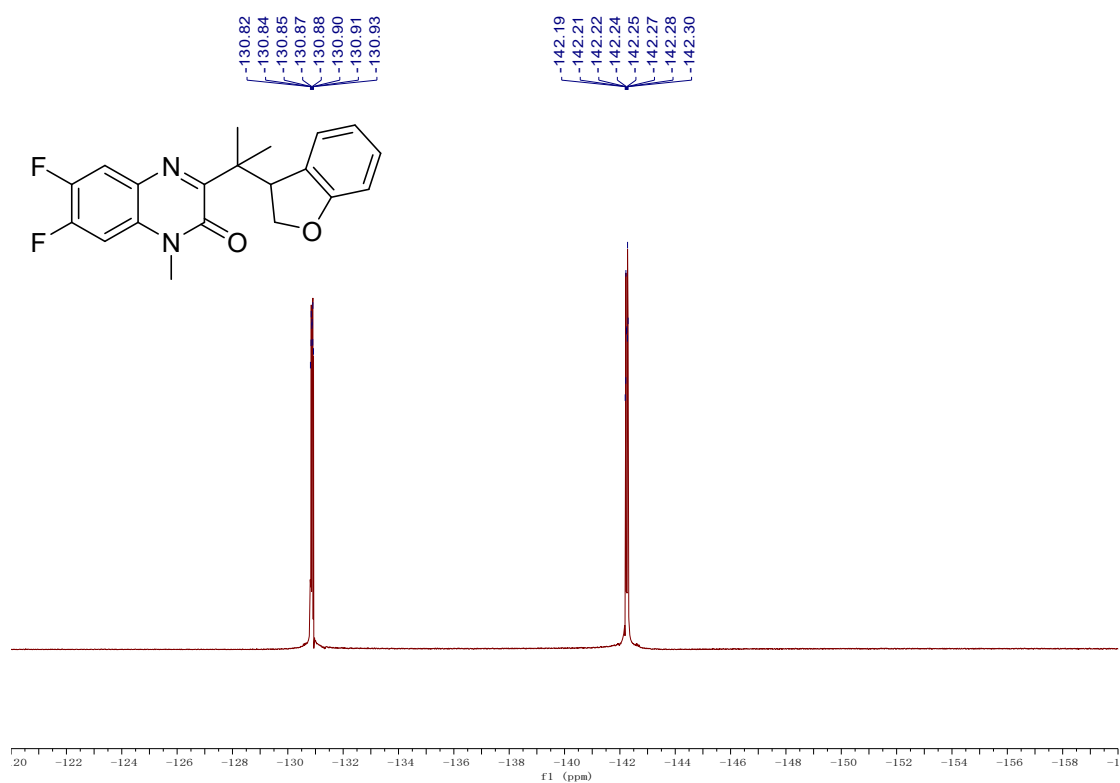
¹H NMR spectrum of **3m** (400 MHz, CDCl₃)



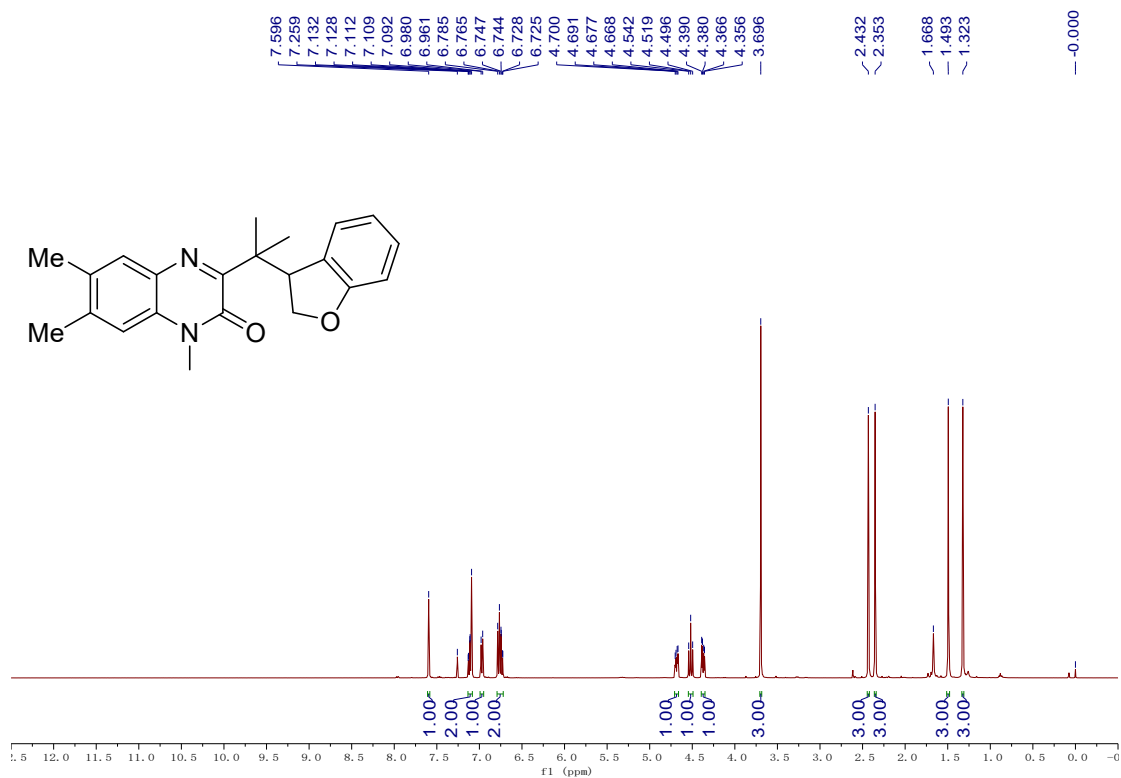
¹³C NMR spectrum of **3m** (100 MHz, CDCl₃)



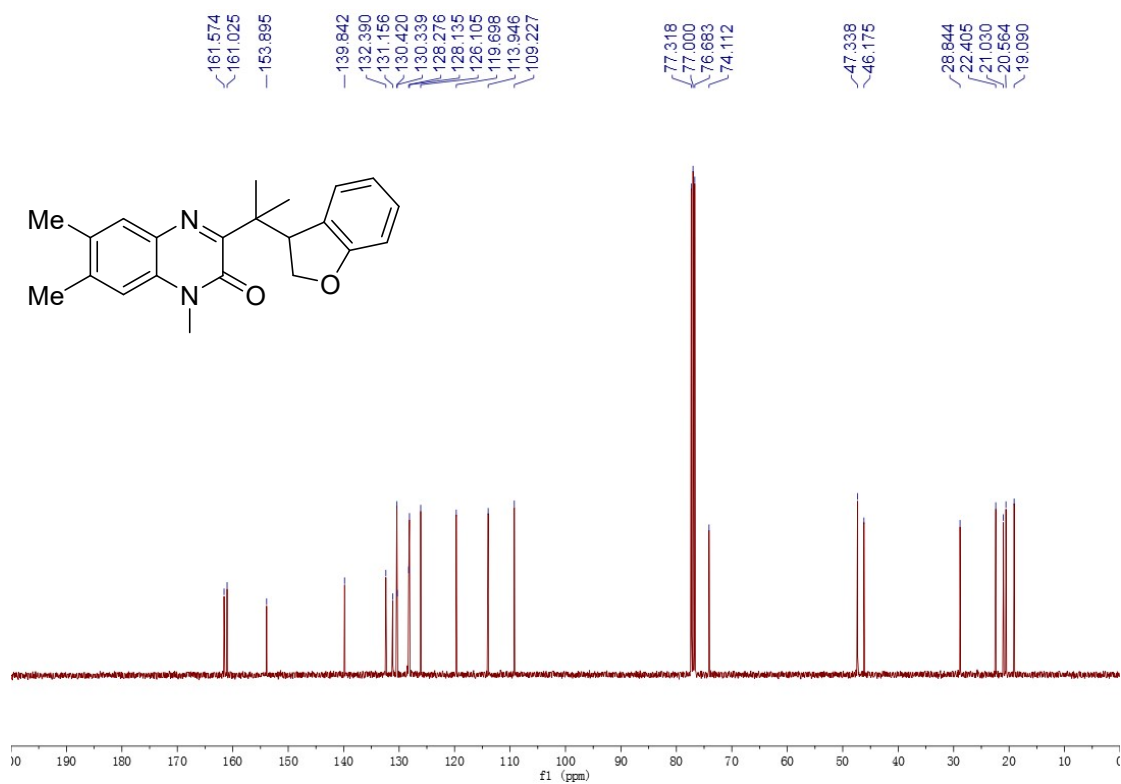
^{19}F NMR spectrum of **3m** (376 MHz, CDCl_3)



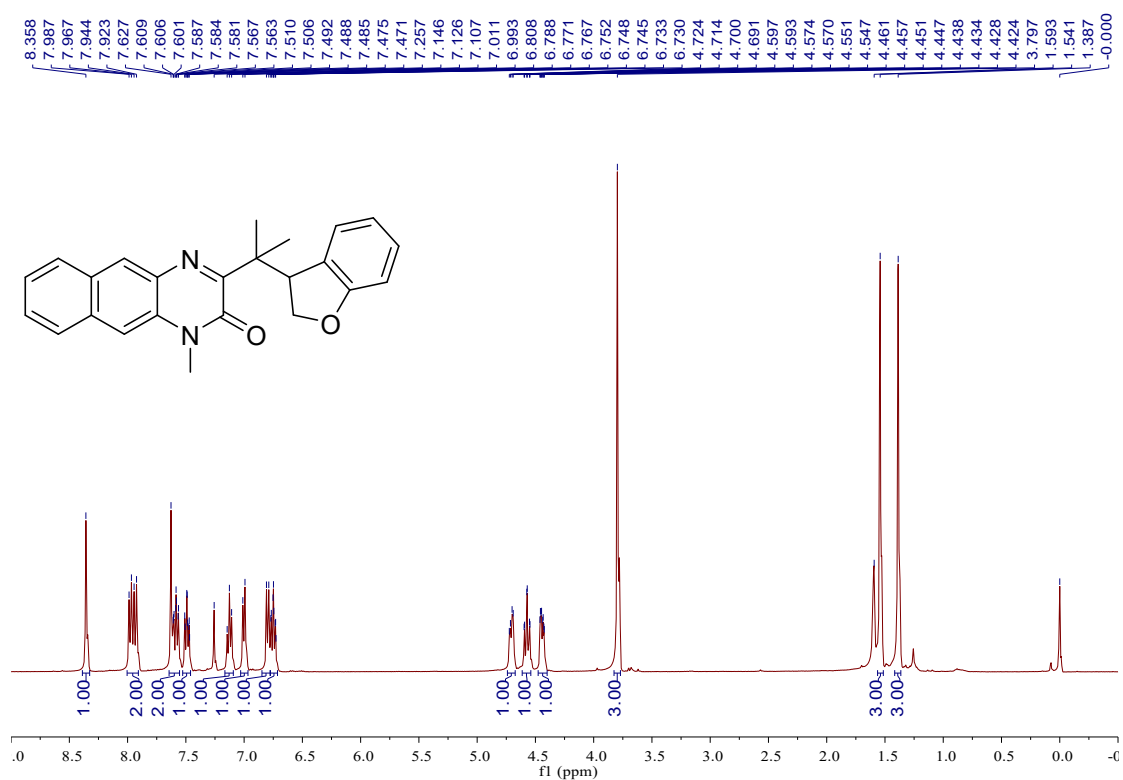
^1H NMR spectrum of **3n** (400 MHz, CDCl_3)



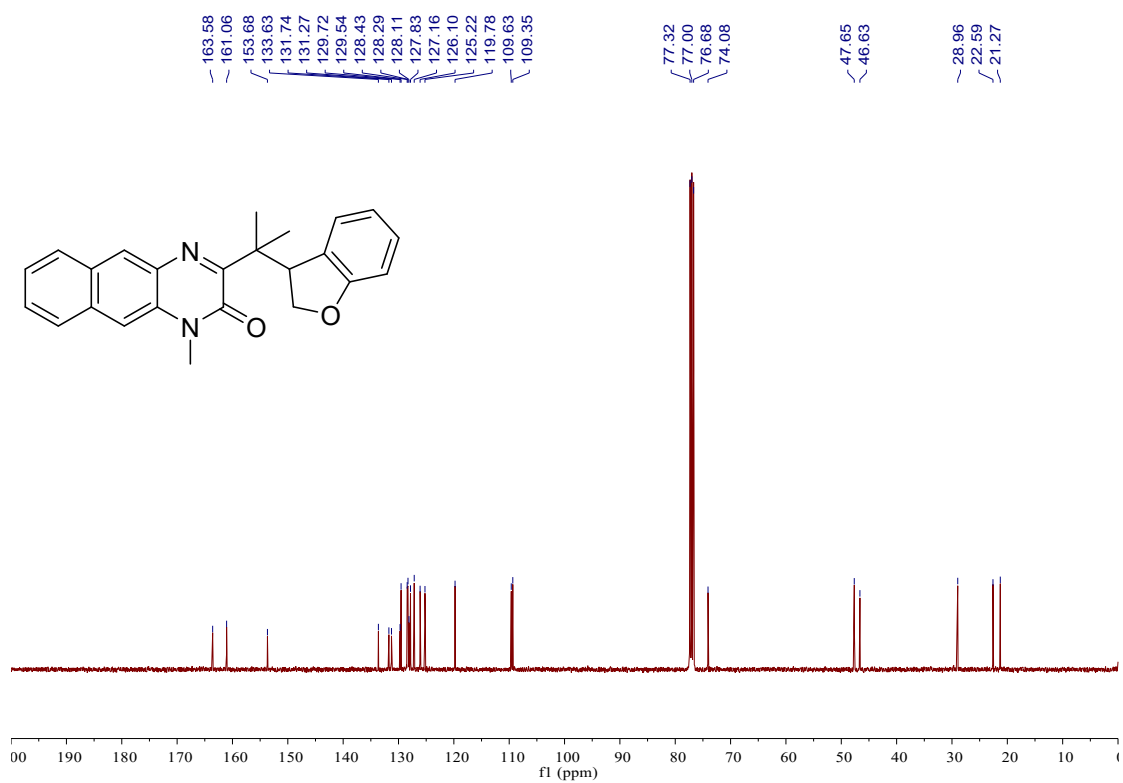
^{13}C NMR spectrum of **3n** (100 MHz, CDCl_3)



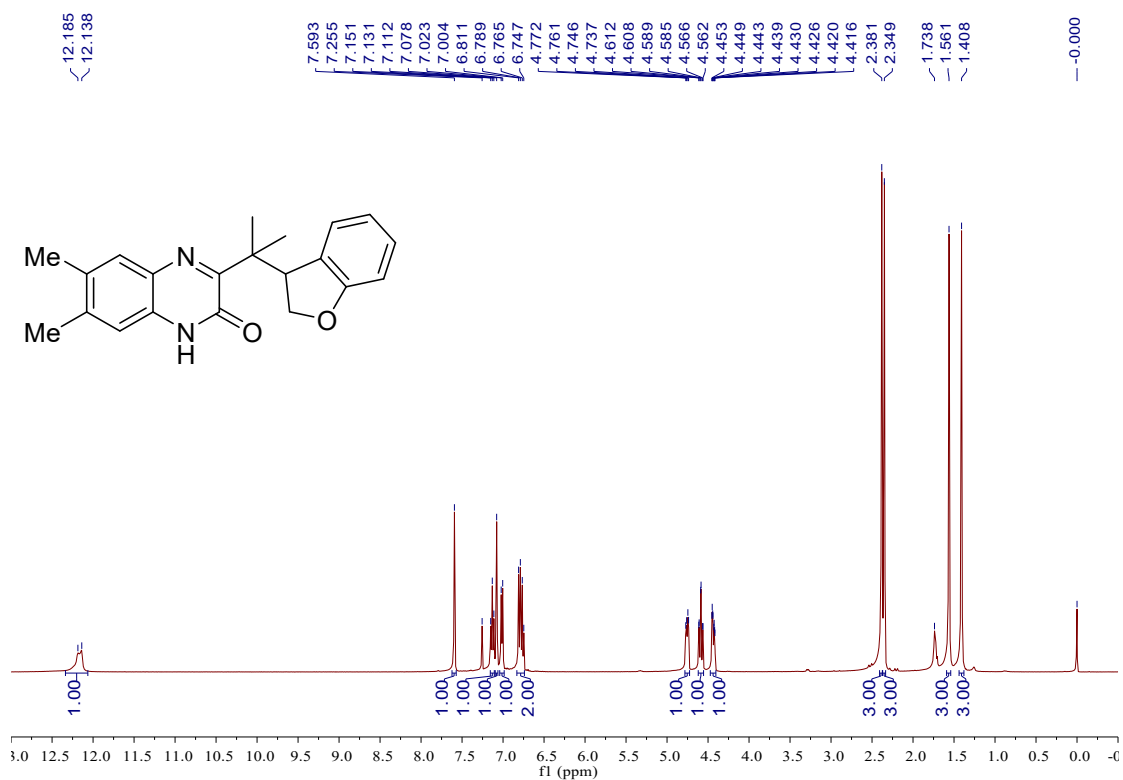
¹H NMR spectrum of **3o** (400 MHz, CDCl₃)



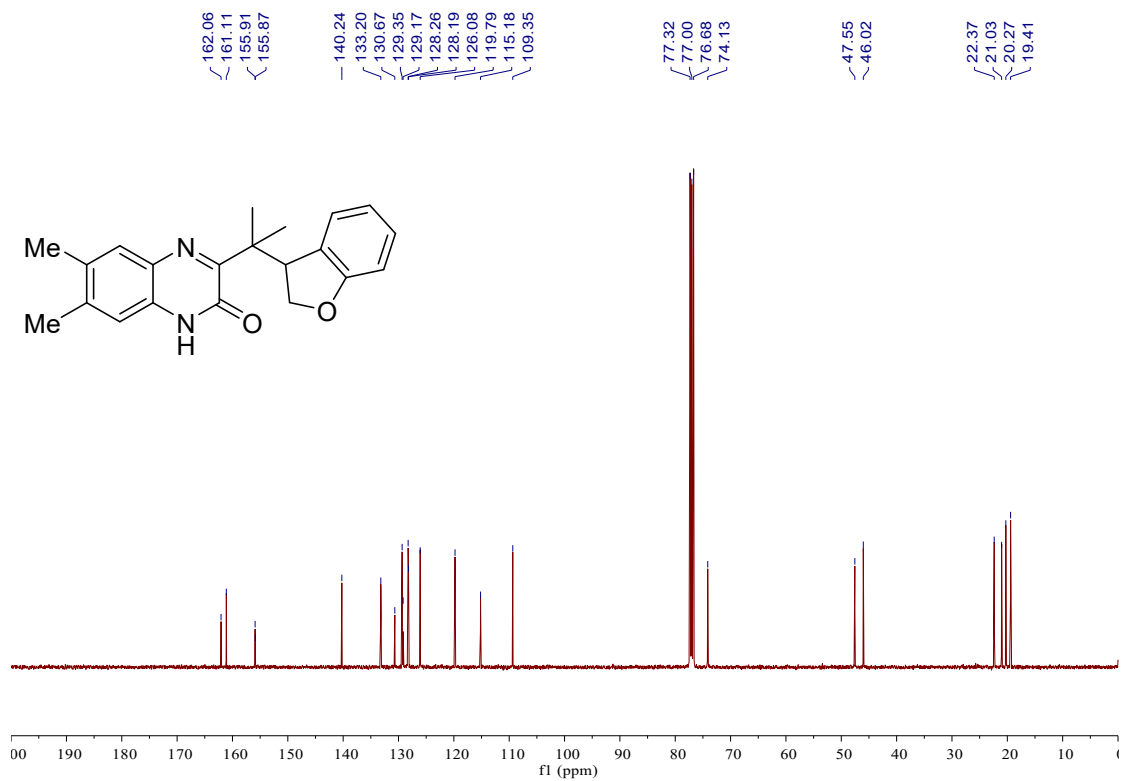
¹³C NMR spectrum of **3o** (100 MHz, CDCl₃)



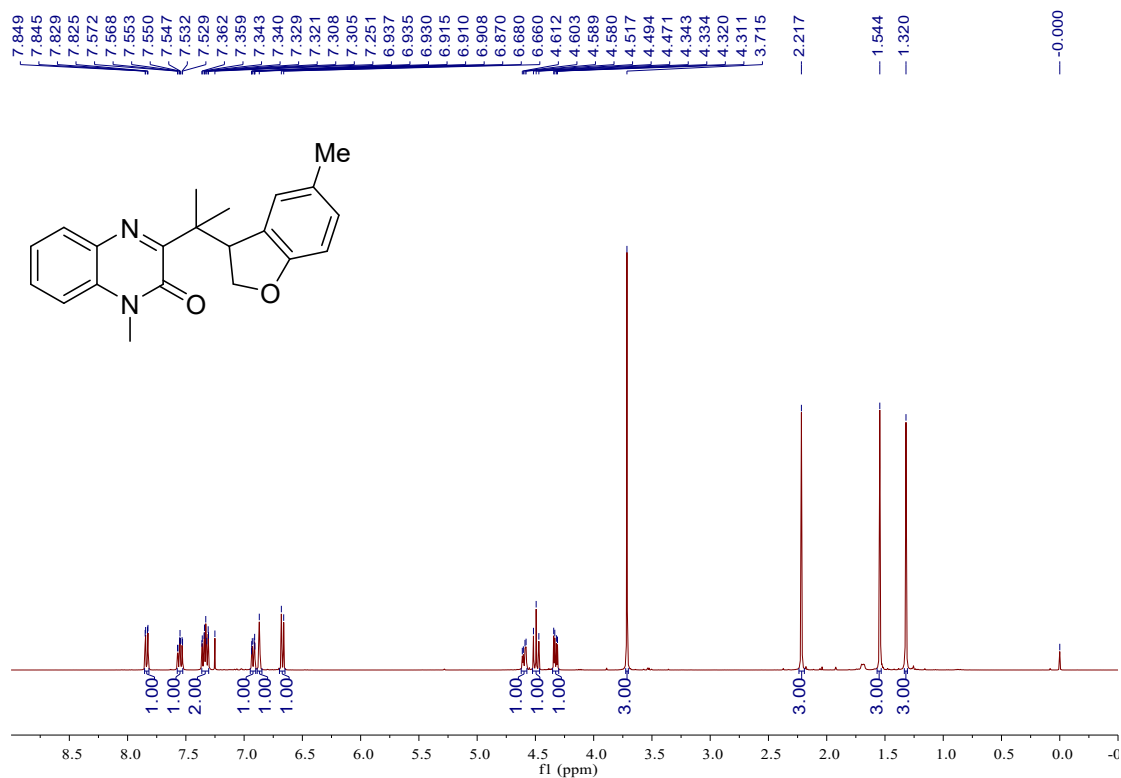
¹H NMR spectrum of **3p** (400 MHz, CDCl₃)



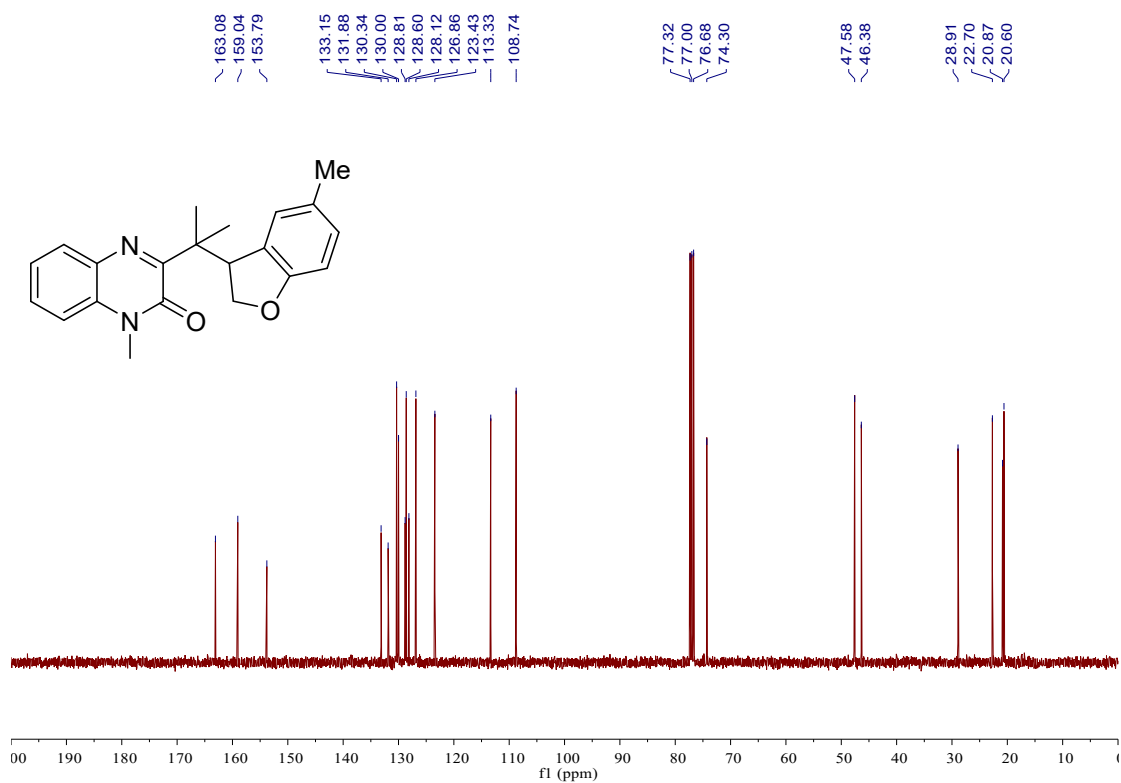
¹³C NMR spectrum of **3p** (100 MHz, CDCl₃)



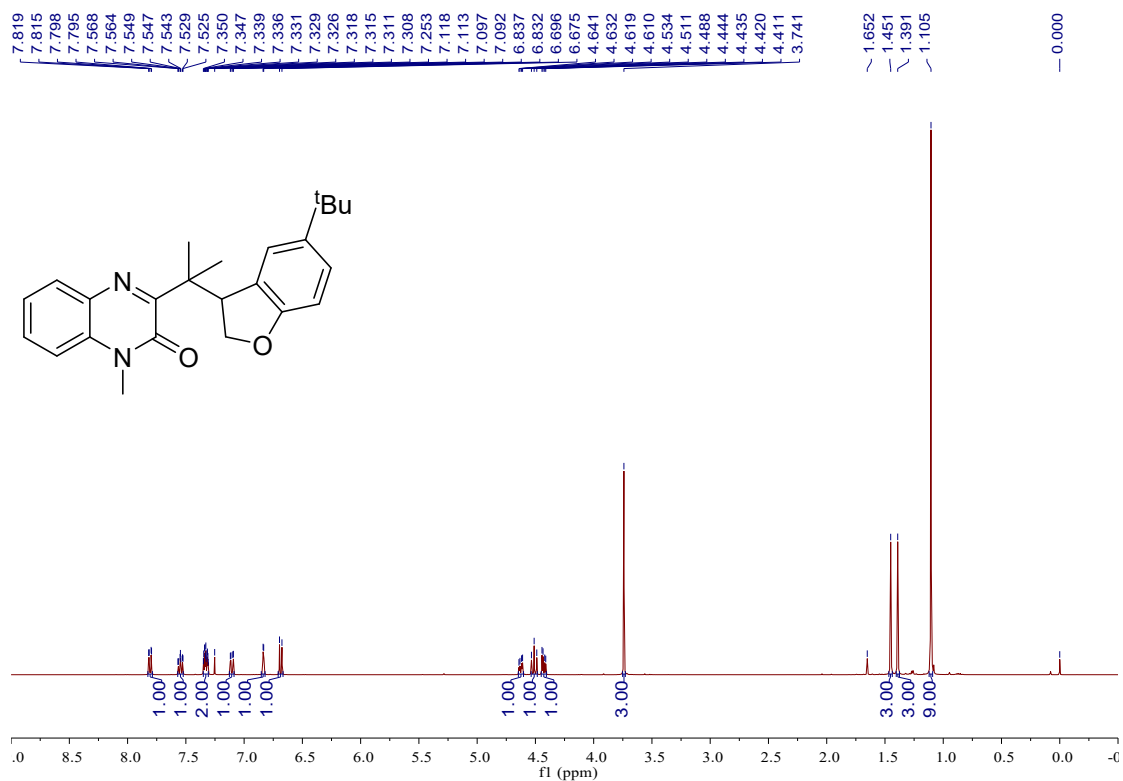
¹H NMR spectrum of **4a** (400 MHz, CDCl₃)



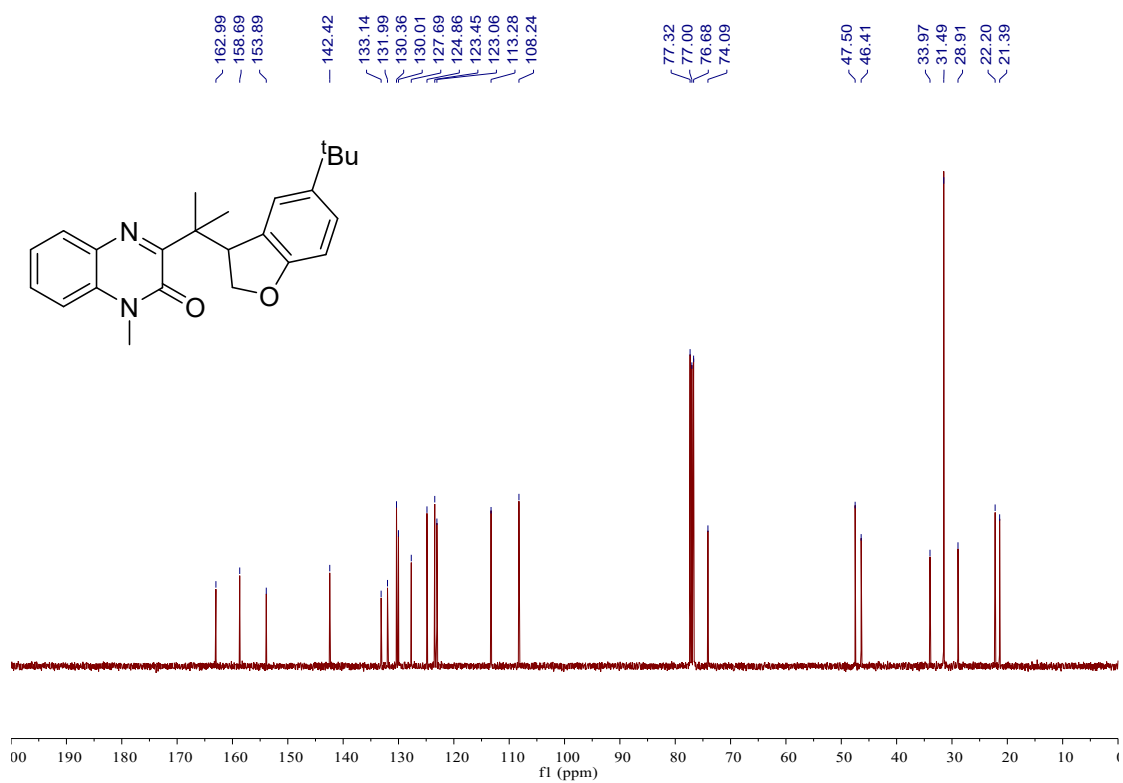
¹³C NMR spectrum of **4a** (100 MHz, CDCl₃)



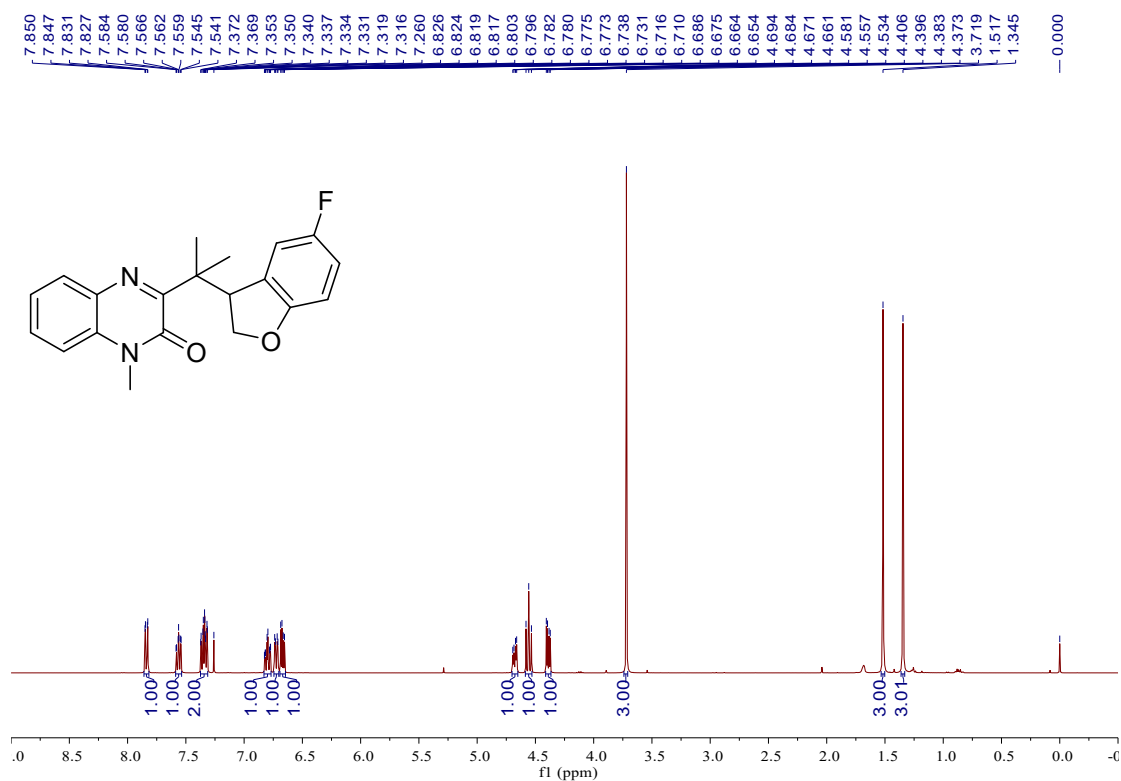
¹H NMR spectrum of **4b** (400 MHz, CDCl₃)



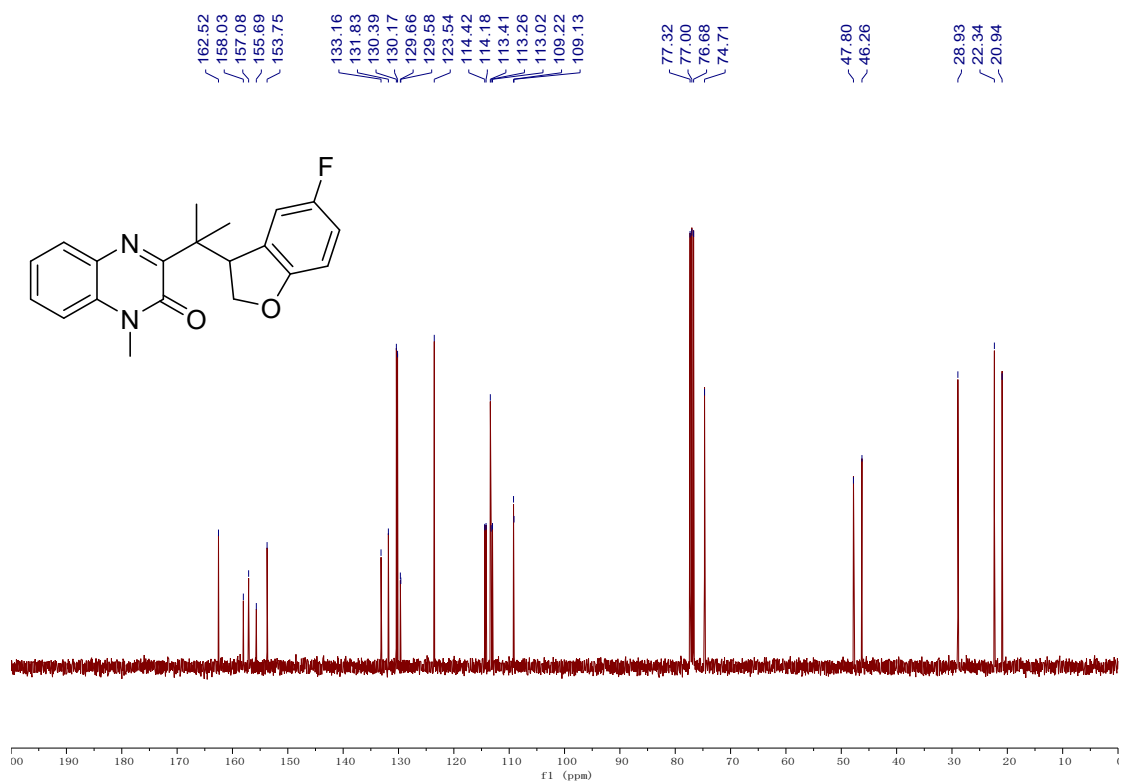
¹³C NMR spectrum of **4b** (100 MHz, CDCl₃)



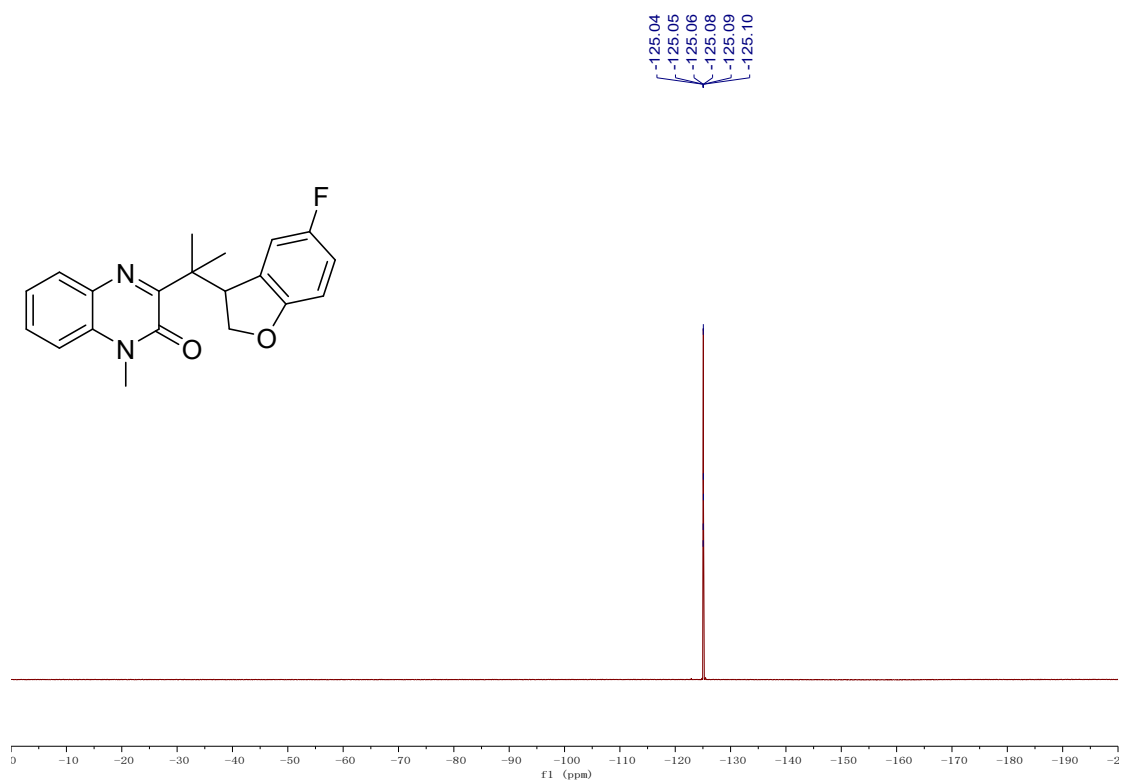
¹H NMR spectrum of **4c** (400 MHz, CDCl₃)



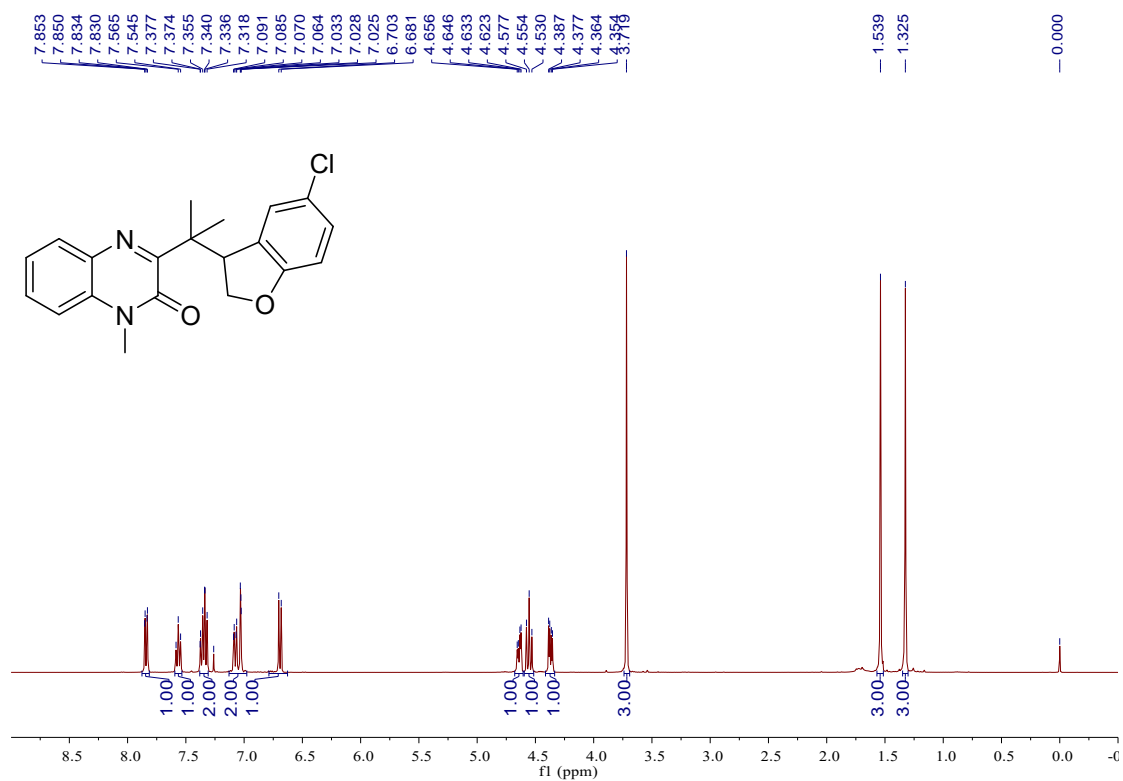
¹³C NMR spectrum of **4c** (100 MHz, CDCl₃)



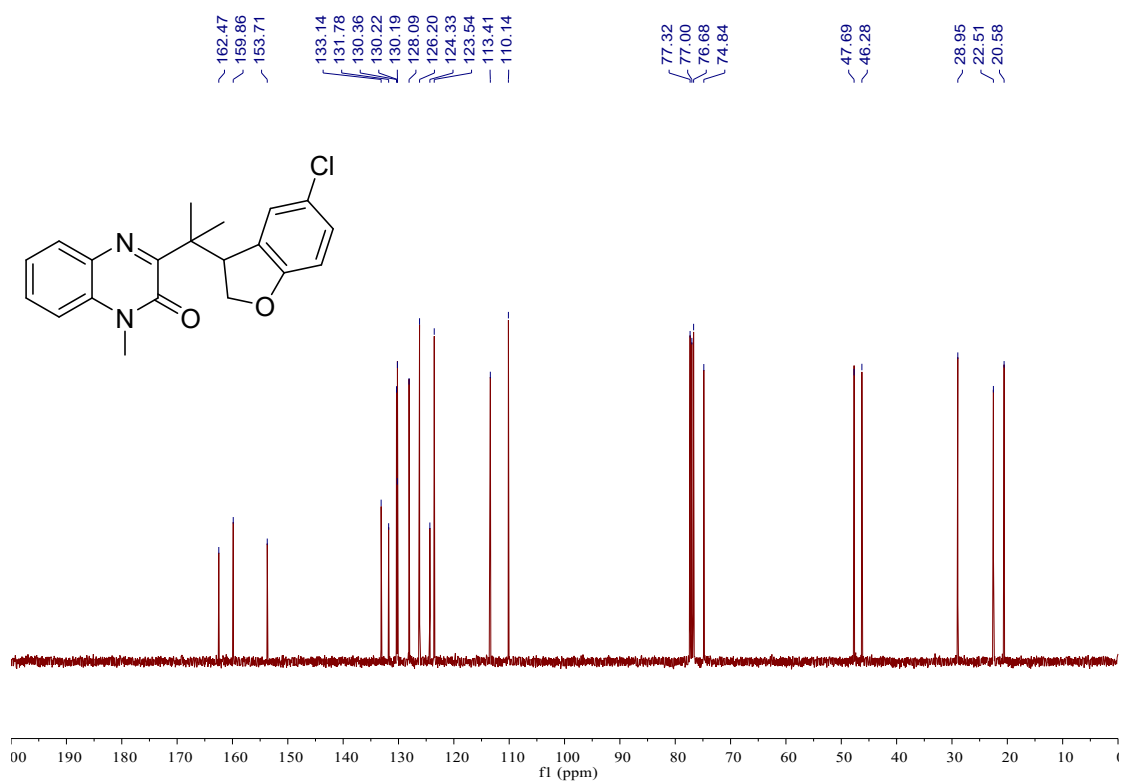
^{19}F NMR spectrum of **4c** (376 MHz, CDCl_3)



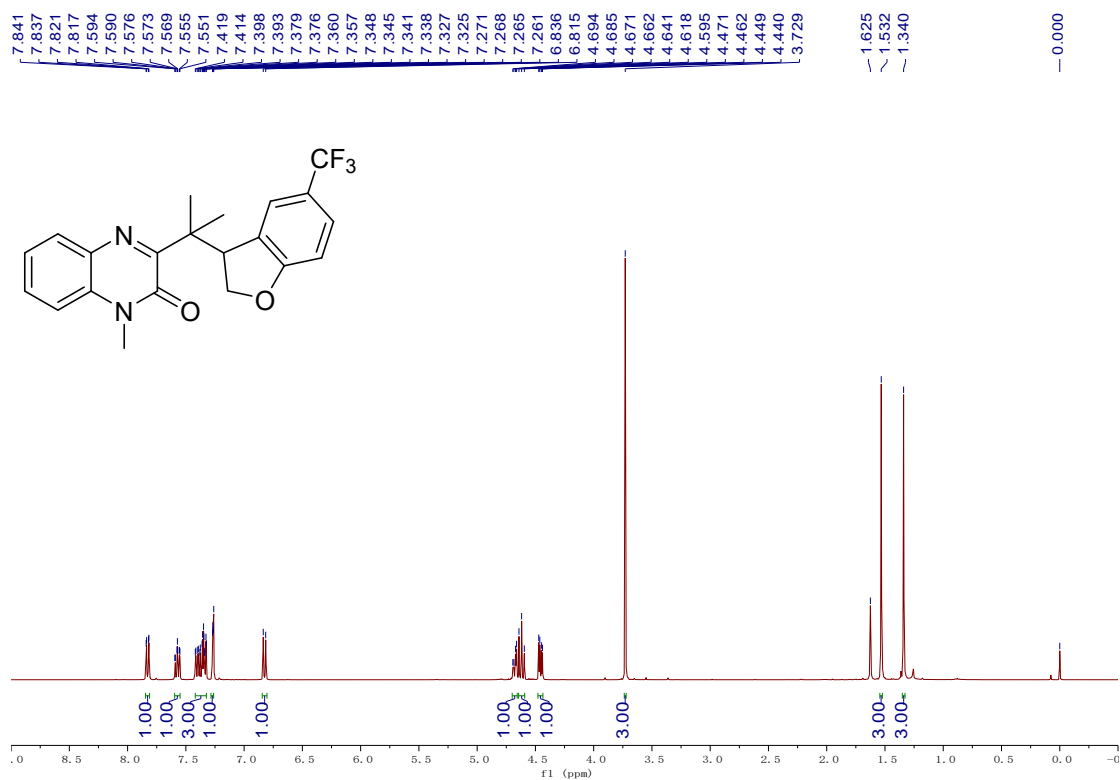
¹H NMR spectrum of **4d** (400 MHz, CDCl₃)



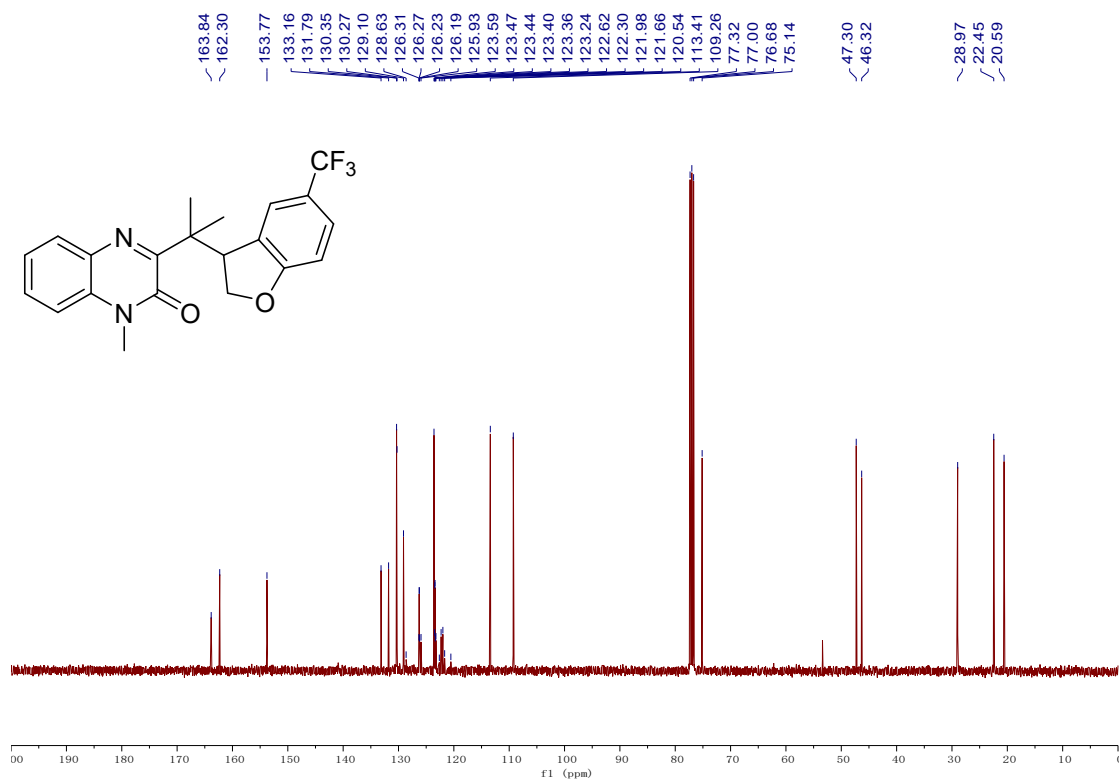
¹³C NMR spectrum of **4d** (100 MHz, CDCl₃)



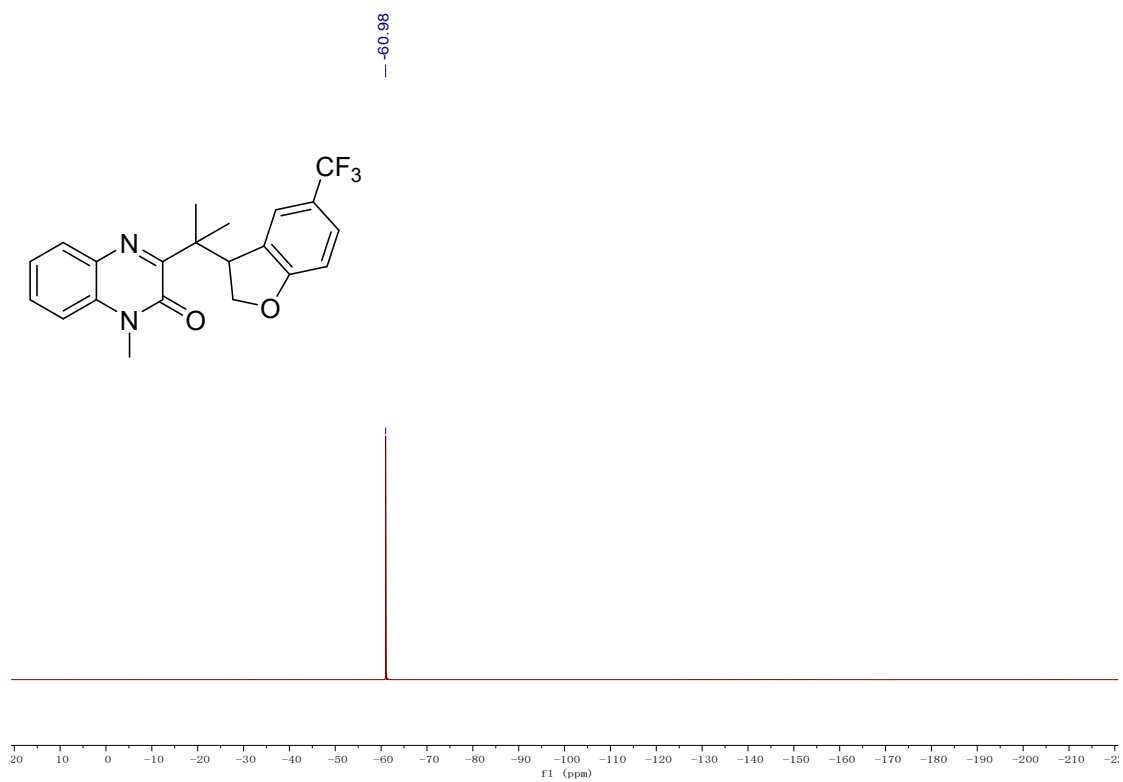
¹H NMR spectrum of **4e** (400 MHz, CDCl₃)



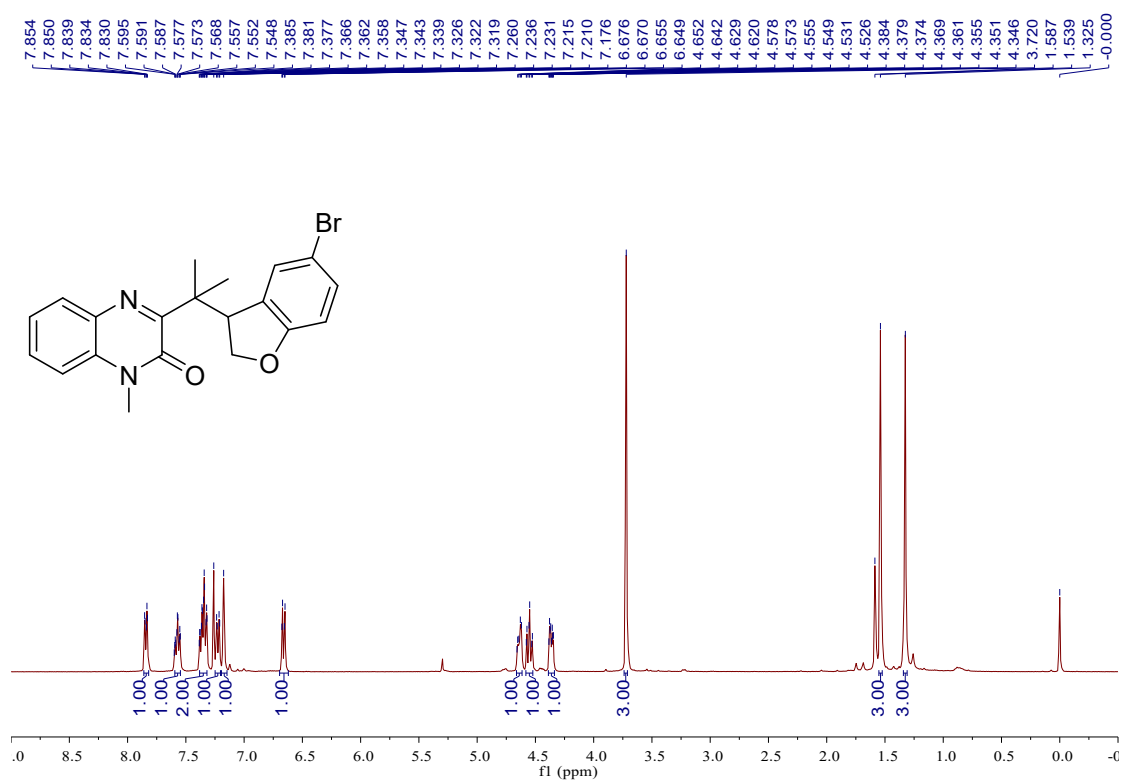
¹³C NMR spectrum of **4e** (100 MHz, CDCl₃)



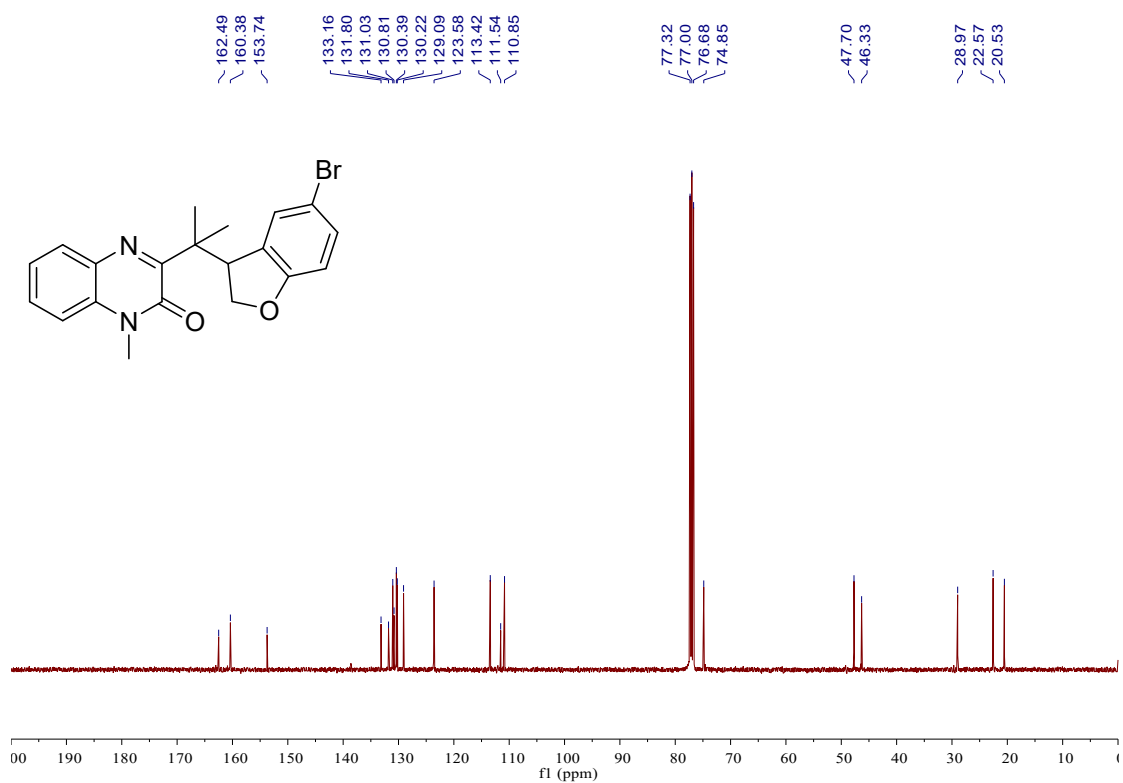
^{19}F NMR spectrum of **4e** (376 MHz, CDCl_3)



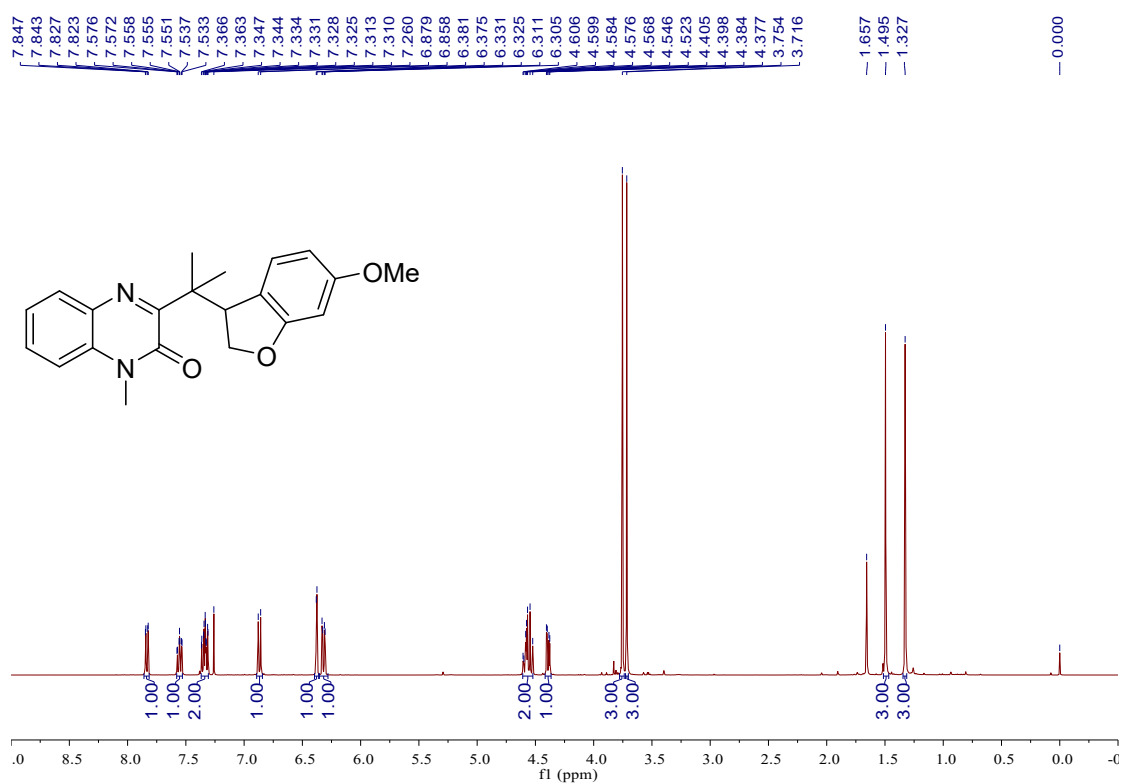
¹H NMR spectrum of **4f** (400 MHz, CDCl₃)



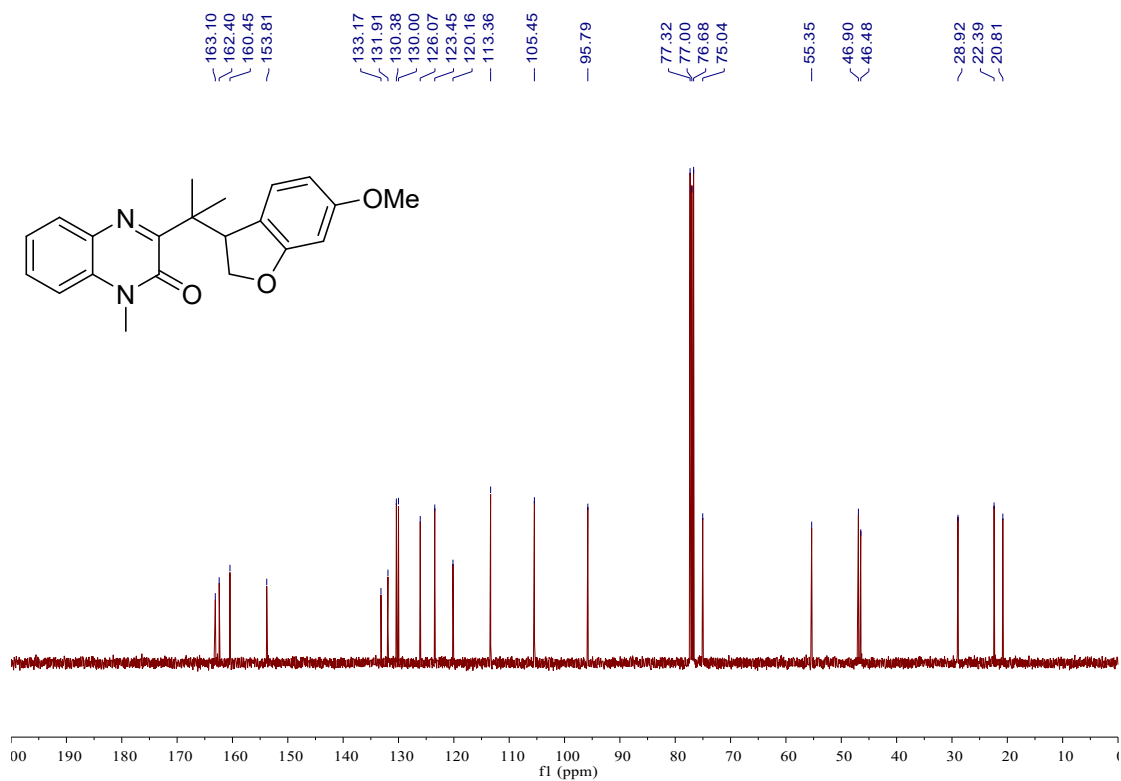
¹³C NMR spectrum of **4f** (100 MHz, CDCl₃)



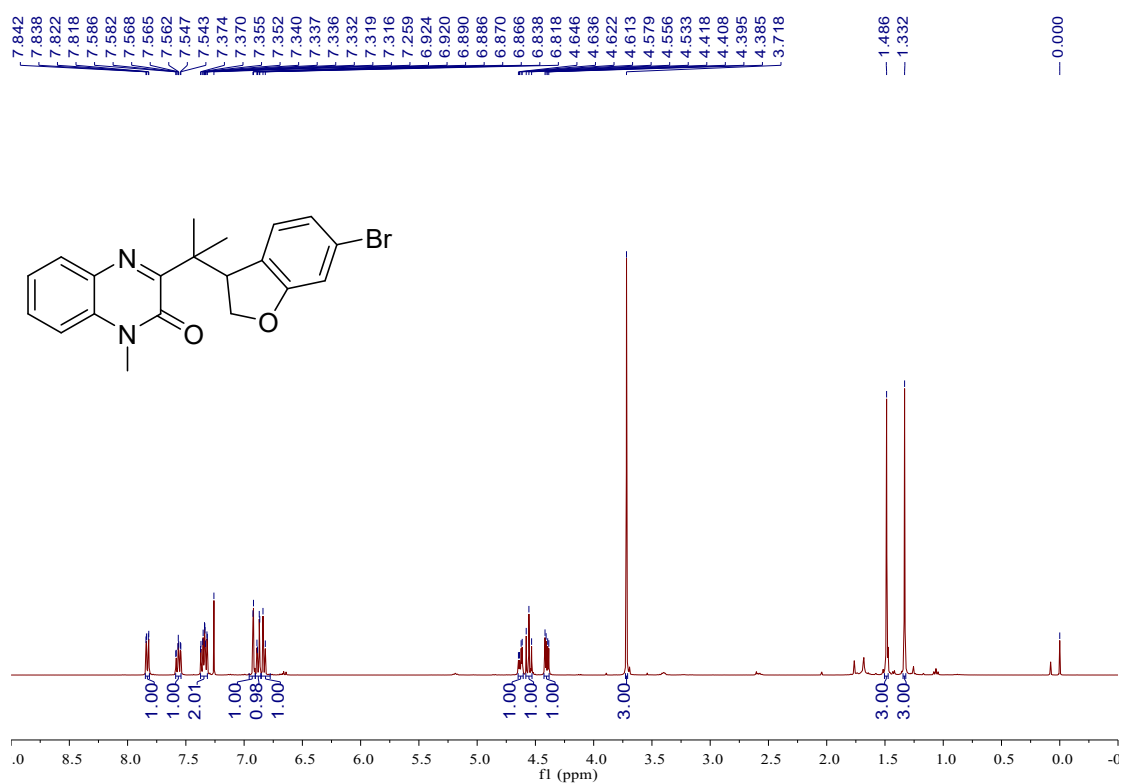
¹H NMR spectrum of **4g** (400 MHz, CDCl₃)



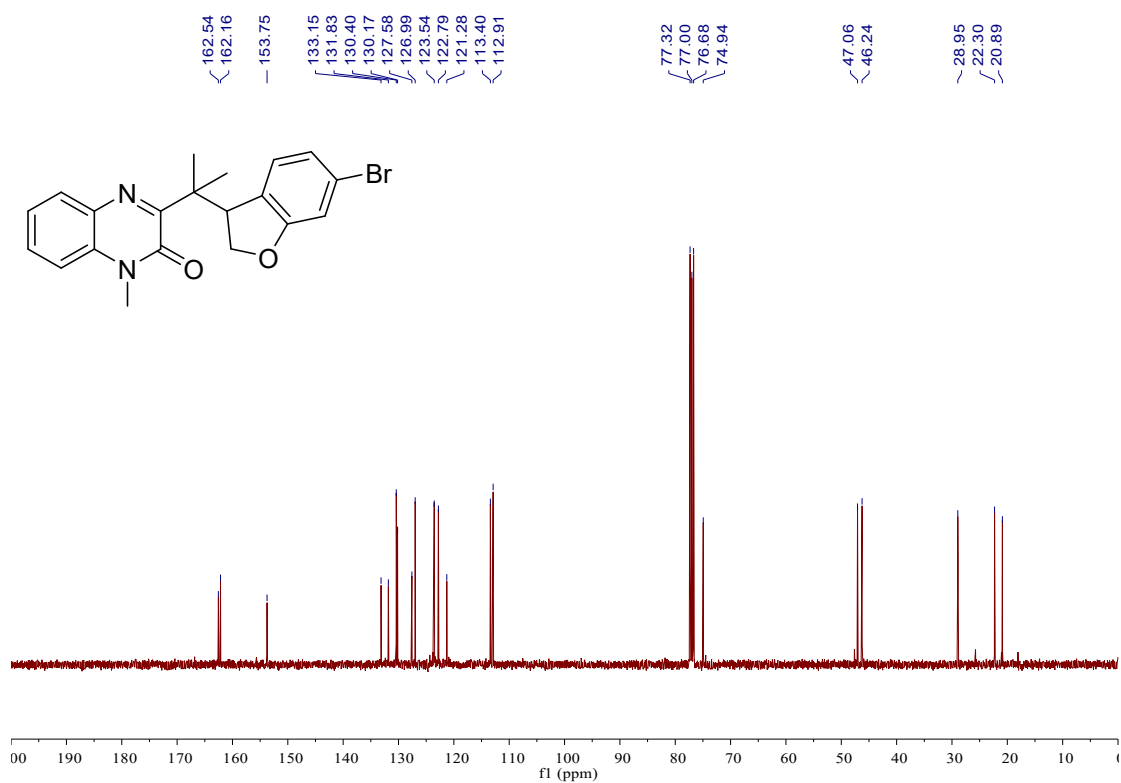
¹³C NMR spectrum of **4g** (100 MHz, CDCl₃)



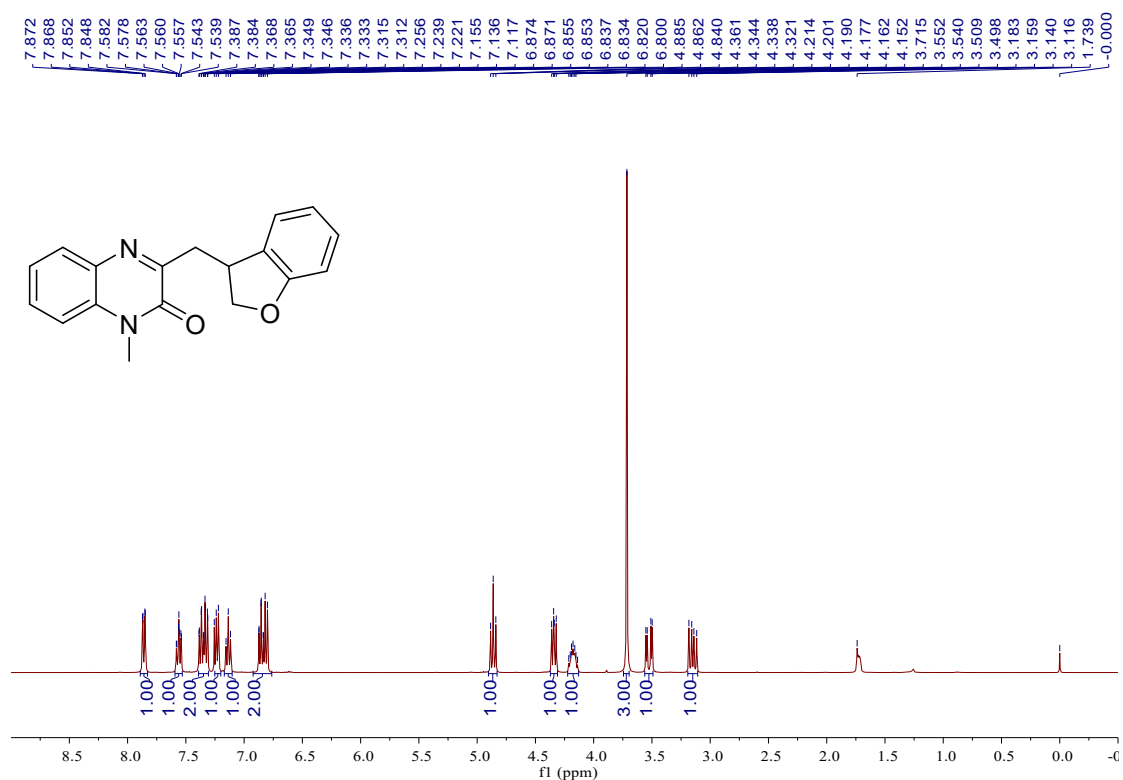
¹H NMR spectrum of **4h** (400 MHz, CDCl₃)



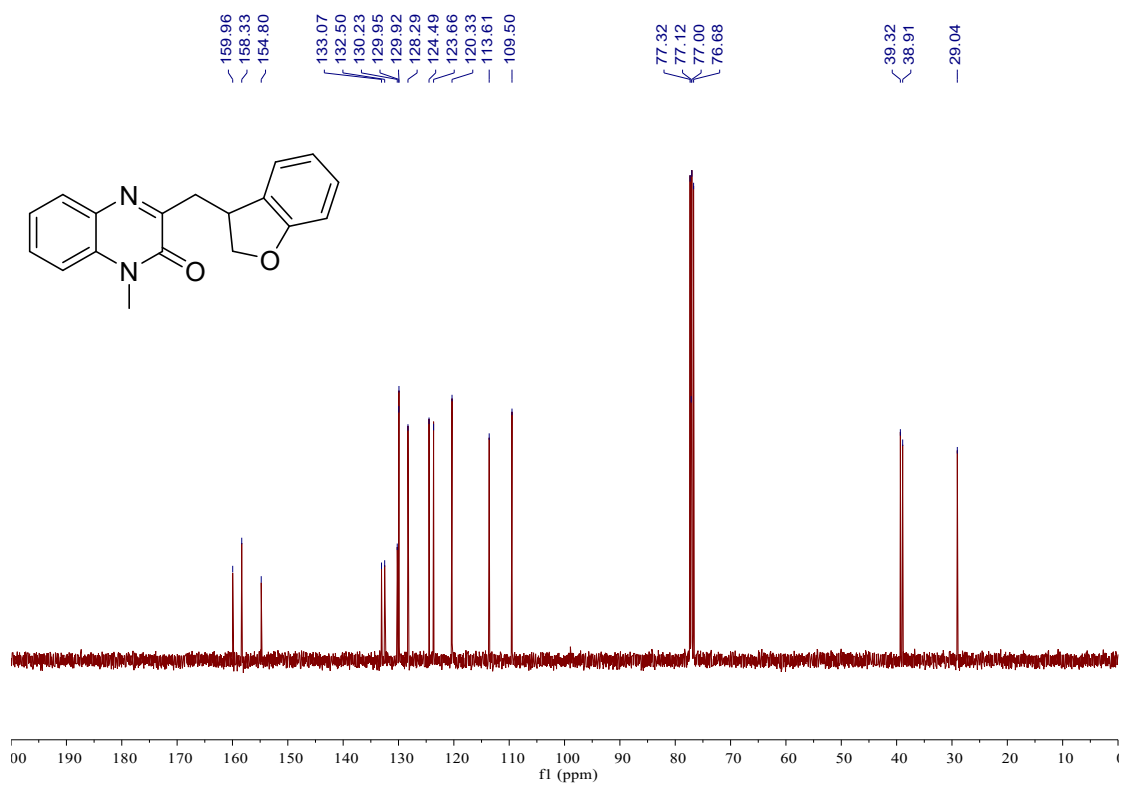
¹³C NMR spectrum of **4h** (100 MHz, CDCl₃)



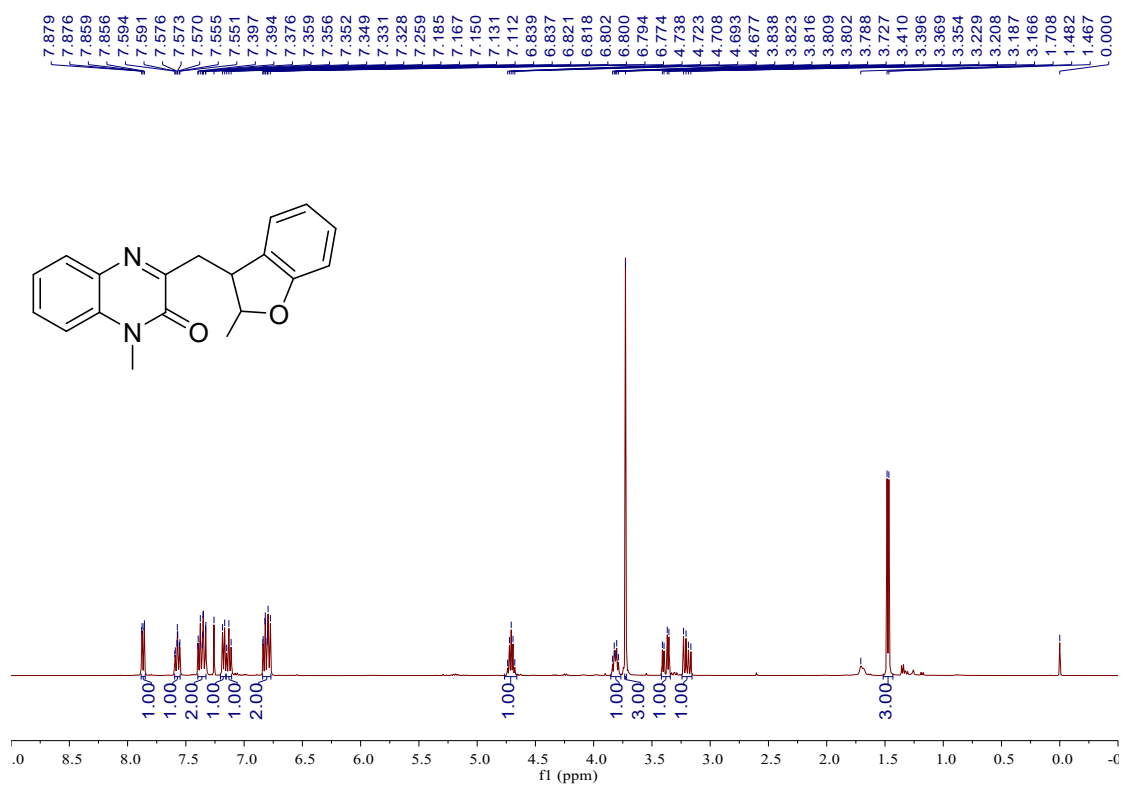
¹H NMR spectrum of **4i** (400 MHz, CDCl₃)



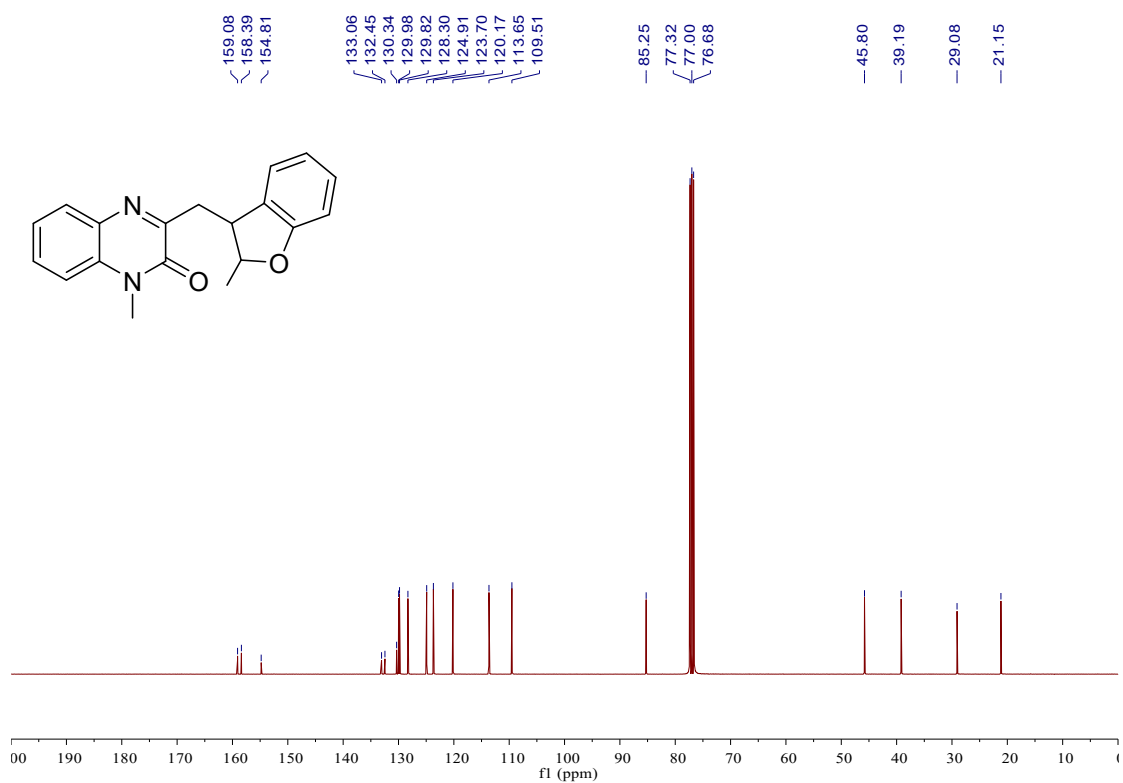
¹³C NMR spectrum of **4i** (100 MHz, CDCl₃)



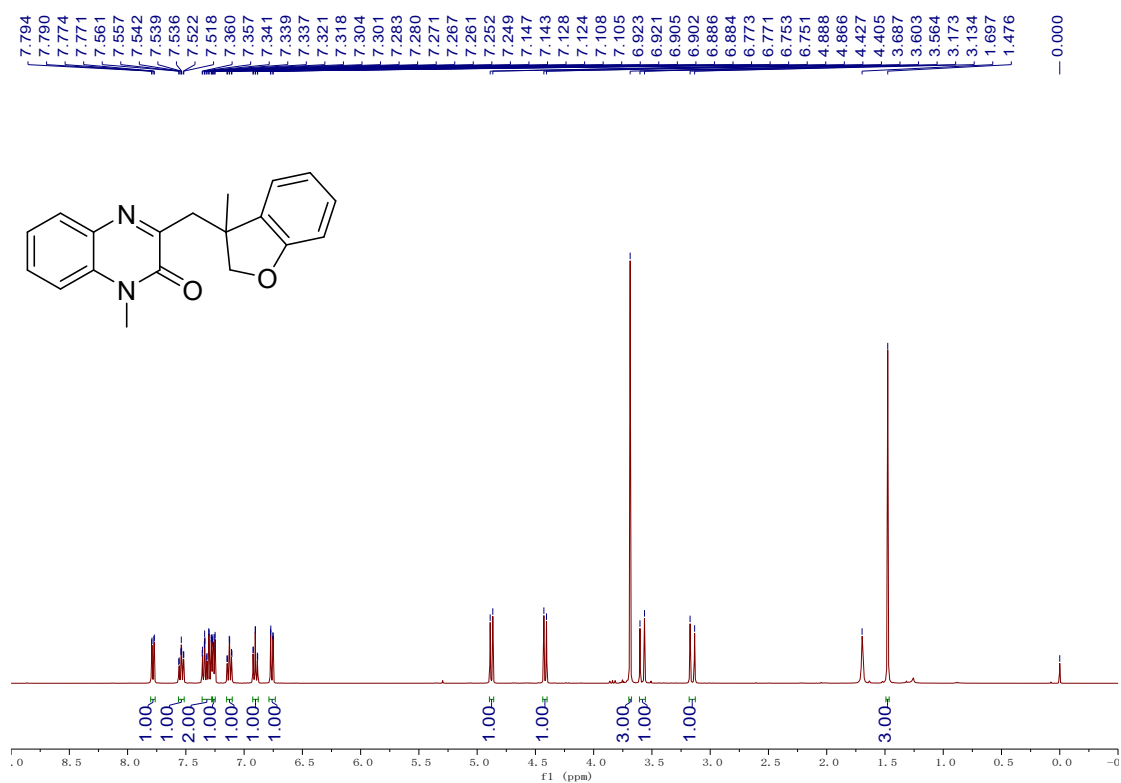
¹H NMR spectrum of **4j** (400 MHz, CDCl₃)



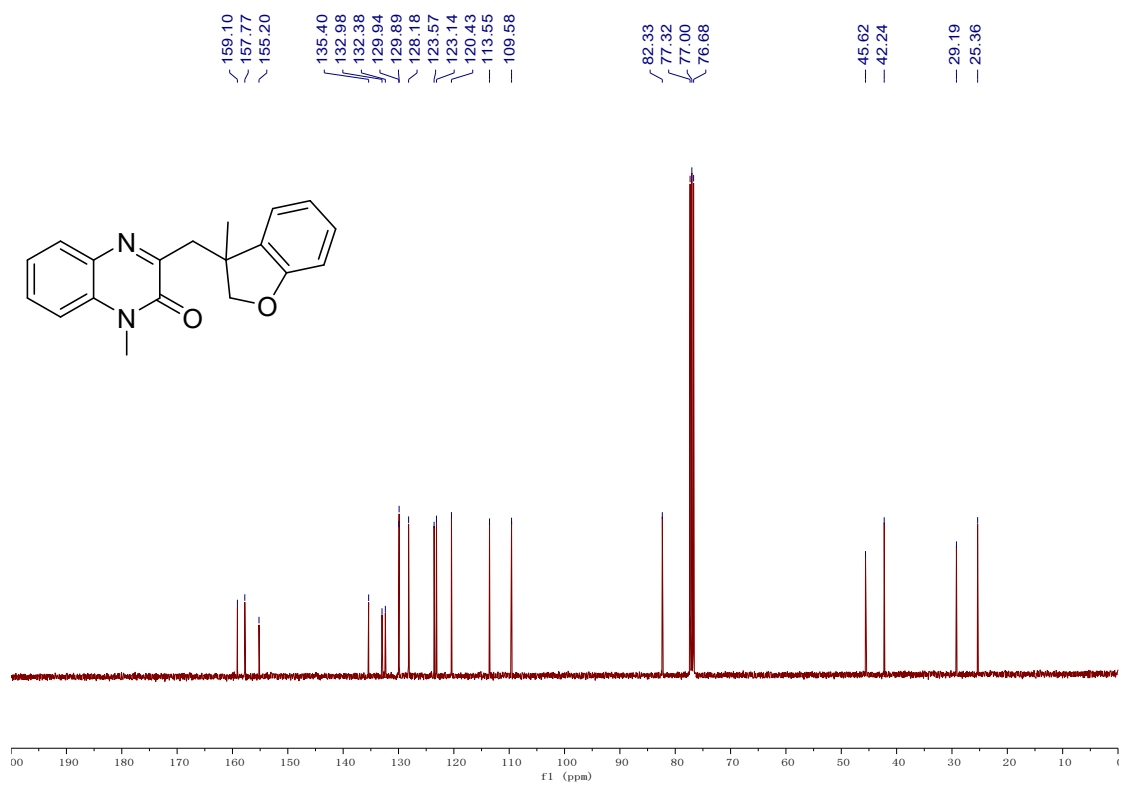
¹³C NMR spectrum of **4j** (100 MHz, CDCl₃)



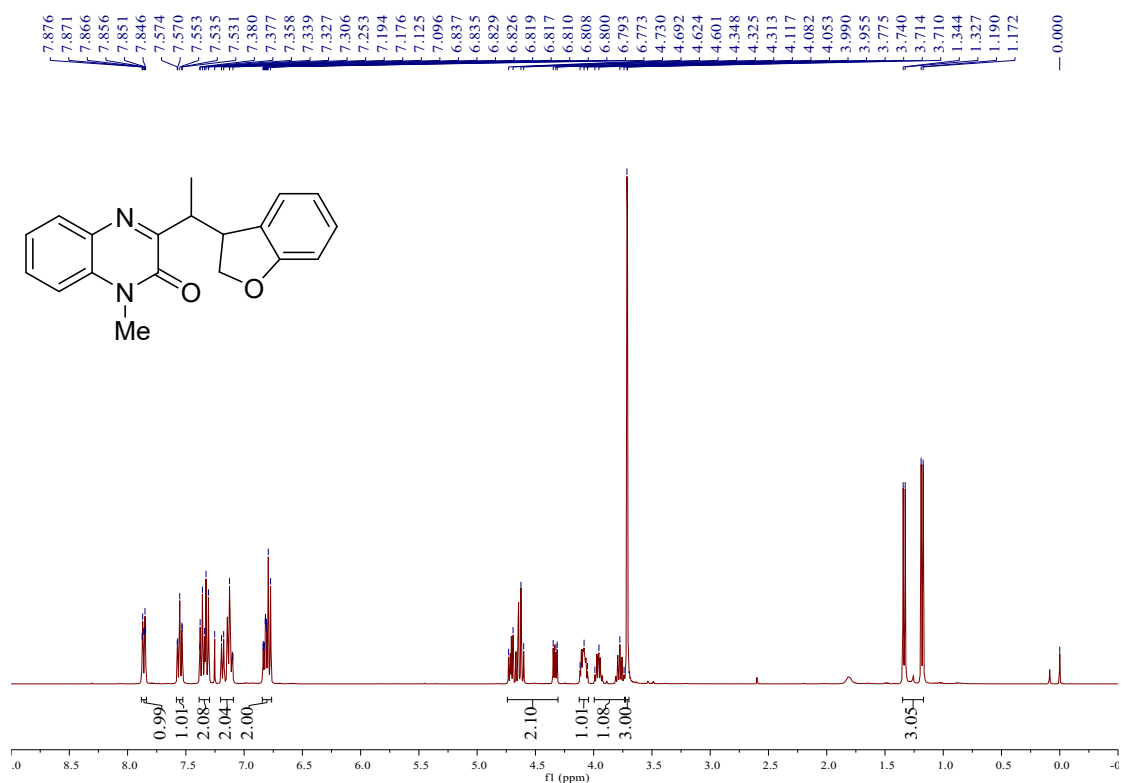
¹H NMR spectrum of **4k** (400 MHz, CDCl₃)



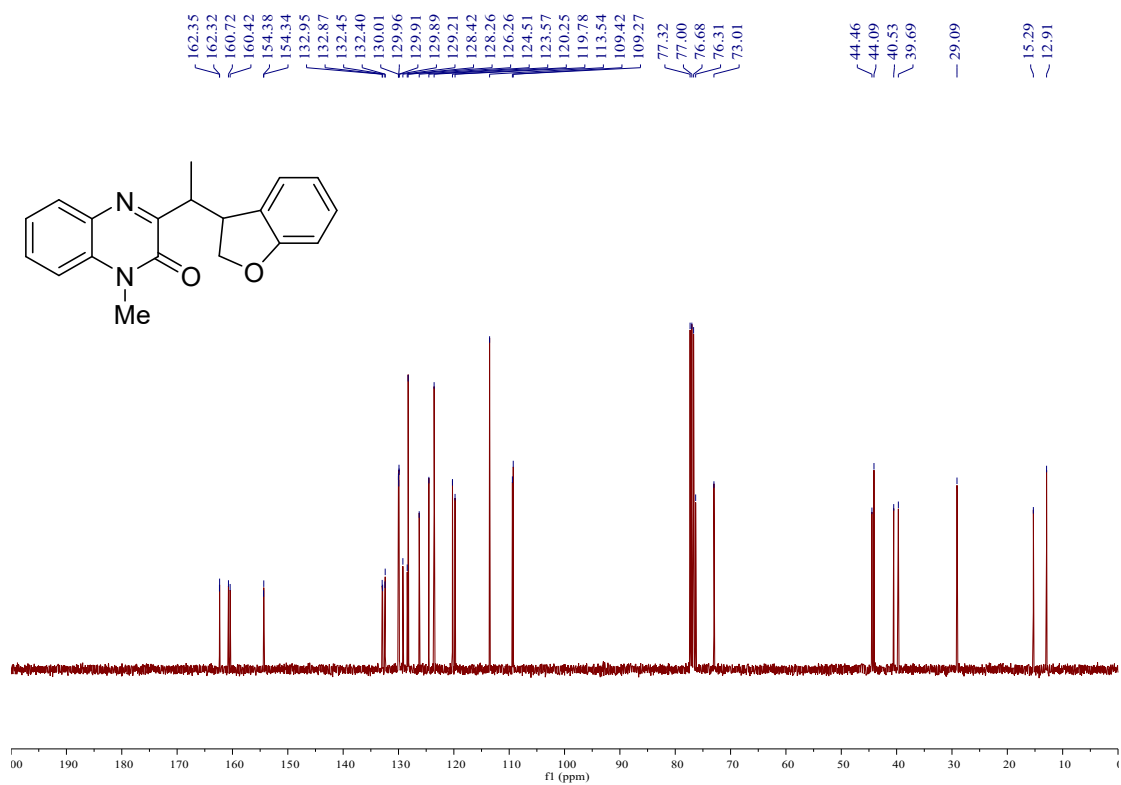
¹³C NMR spectrum of **4k** (100 MHz, CDCl₃)



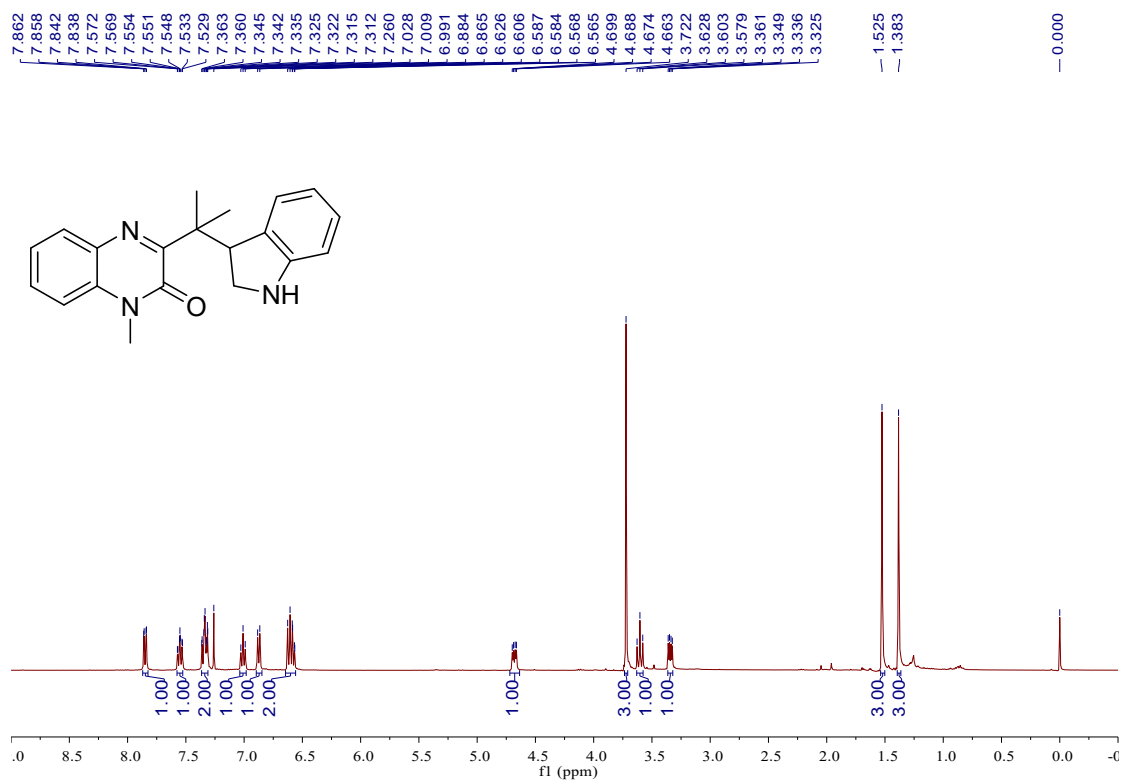
¹H NMR spectrum of **4l** (400 MHz, CDCl₃)



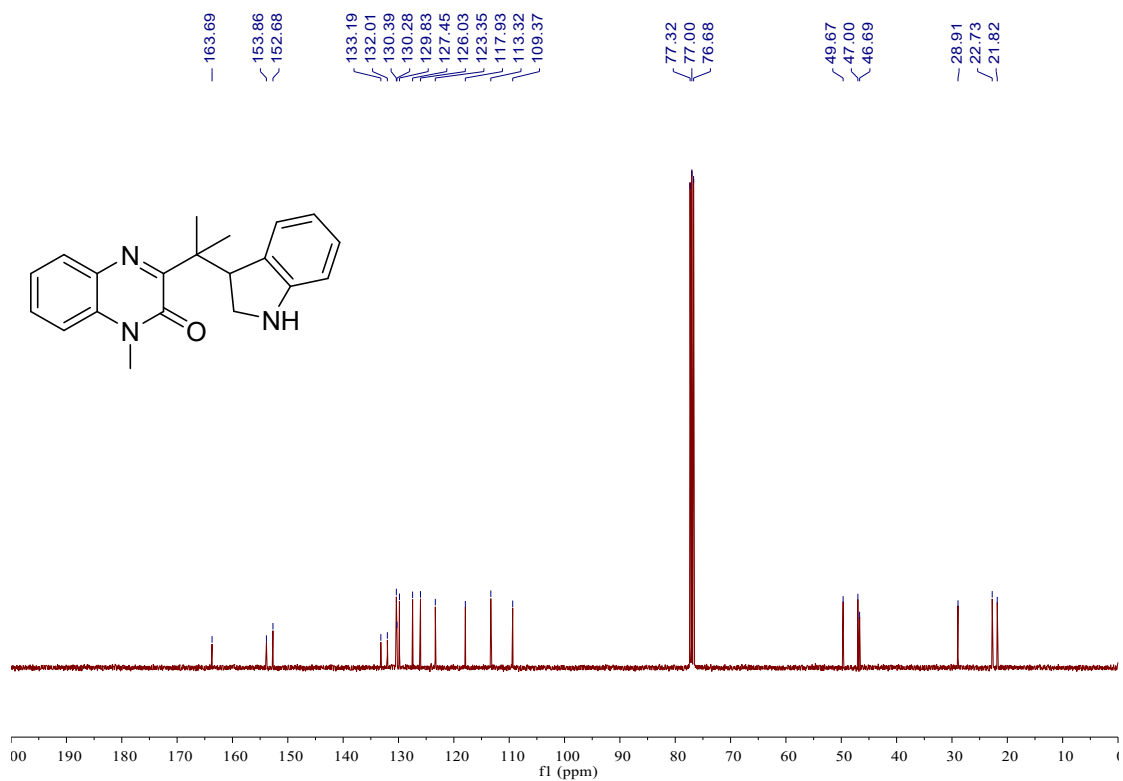
¹³C NMR spectrum of **4l** (100 MHz, CDCl₃)



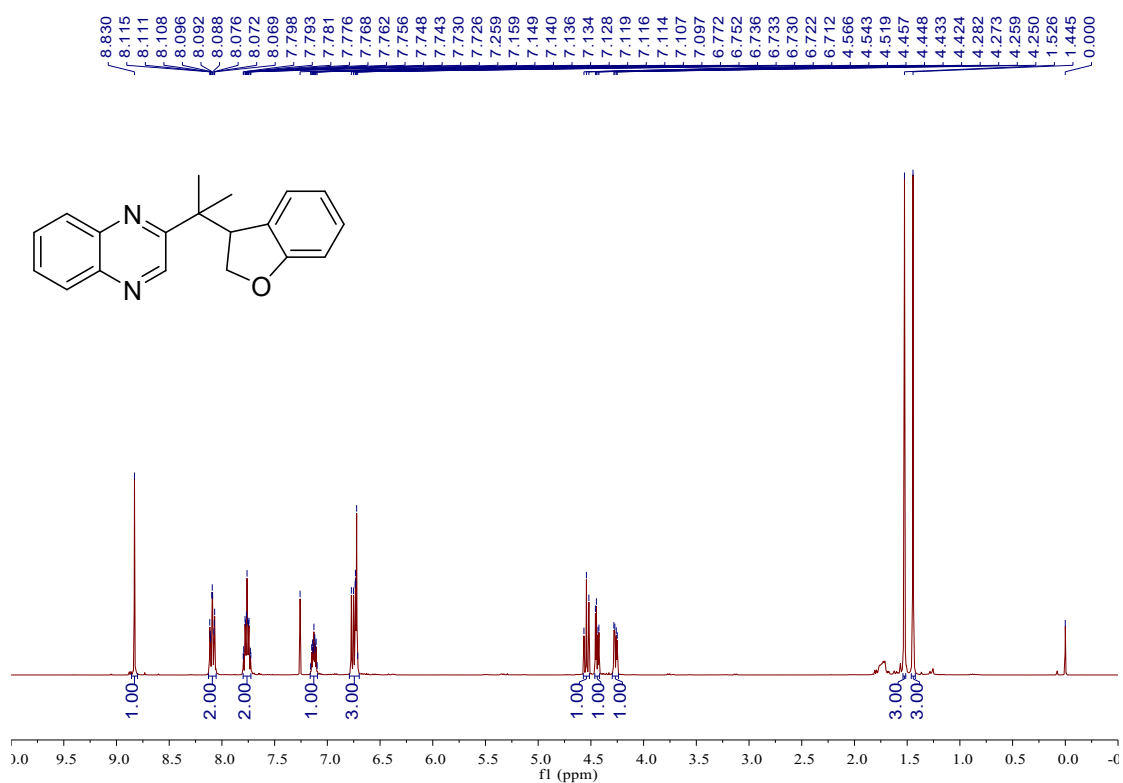
¹H NMR spectrum of **4m** (400 MHz, CDCl₃)



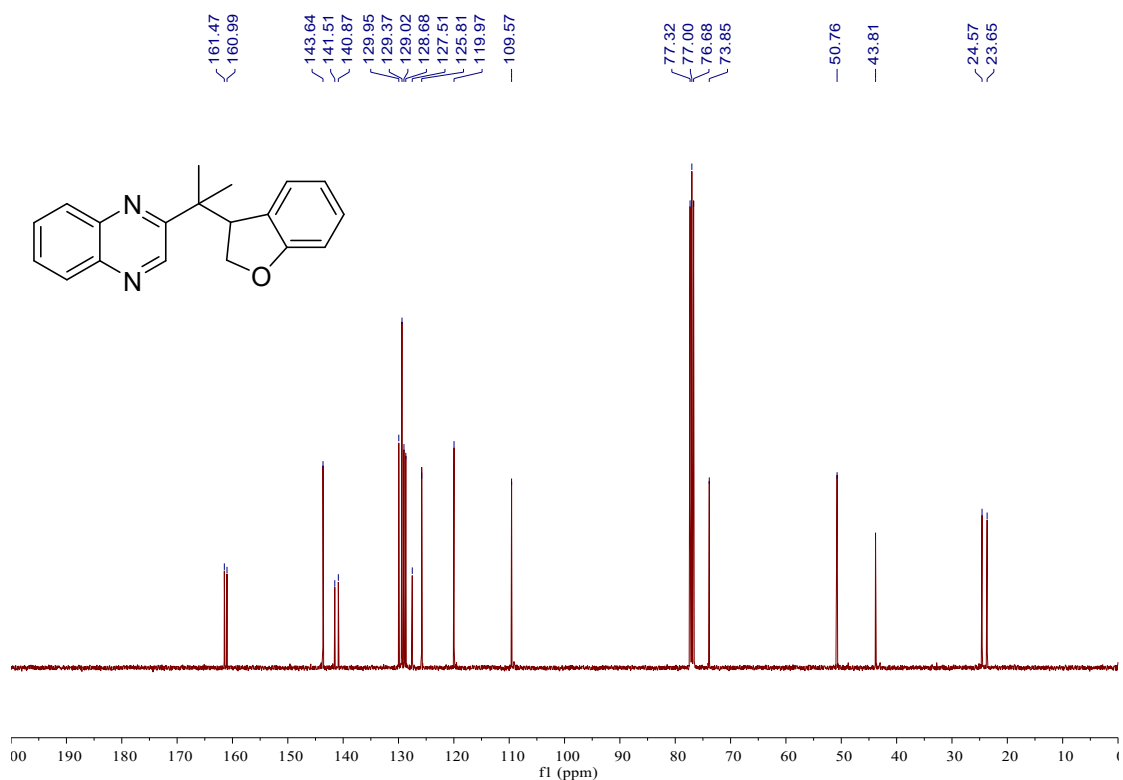
¹³C NMR spectrum of **4m** (100 MHz, CDCl₃)



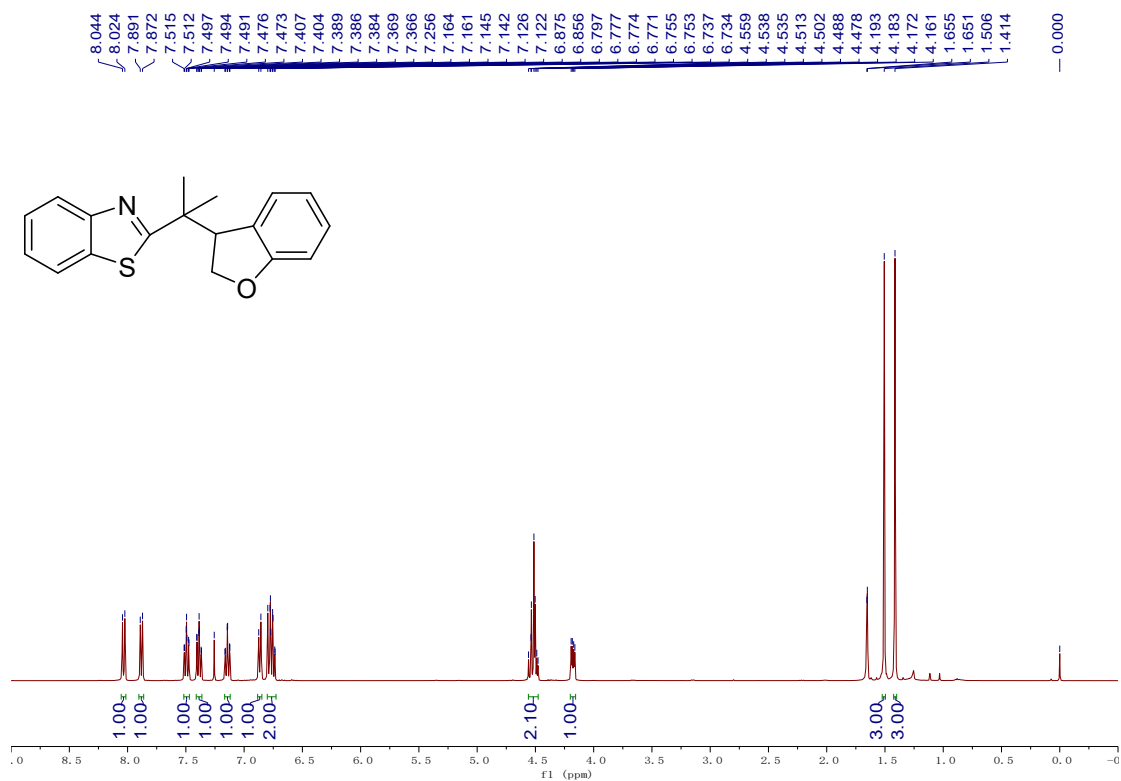
¹H NMR spectrum of **6a** (400 MHz, CDCl₃)



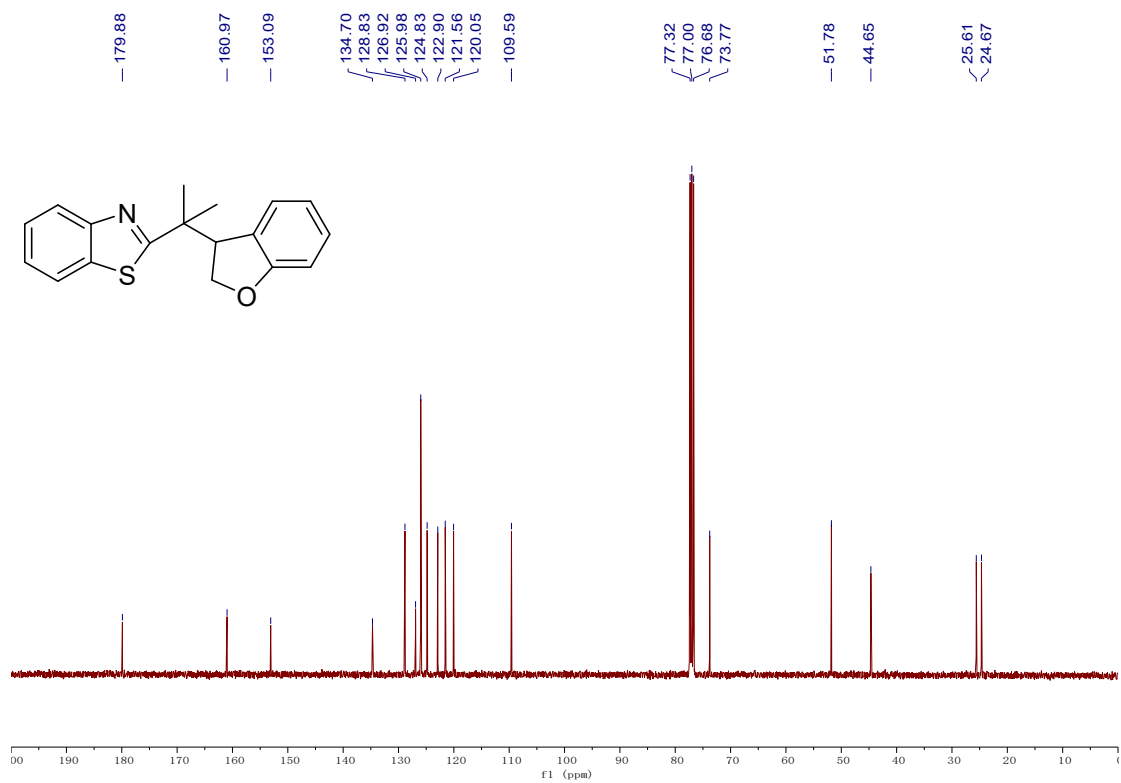
¹³C NMR spectrum of **6a** (100 MHz, CDCl₃)



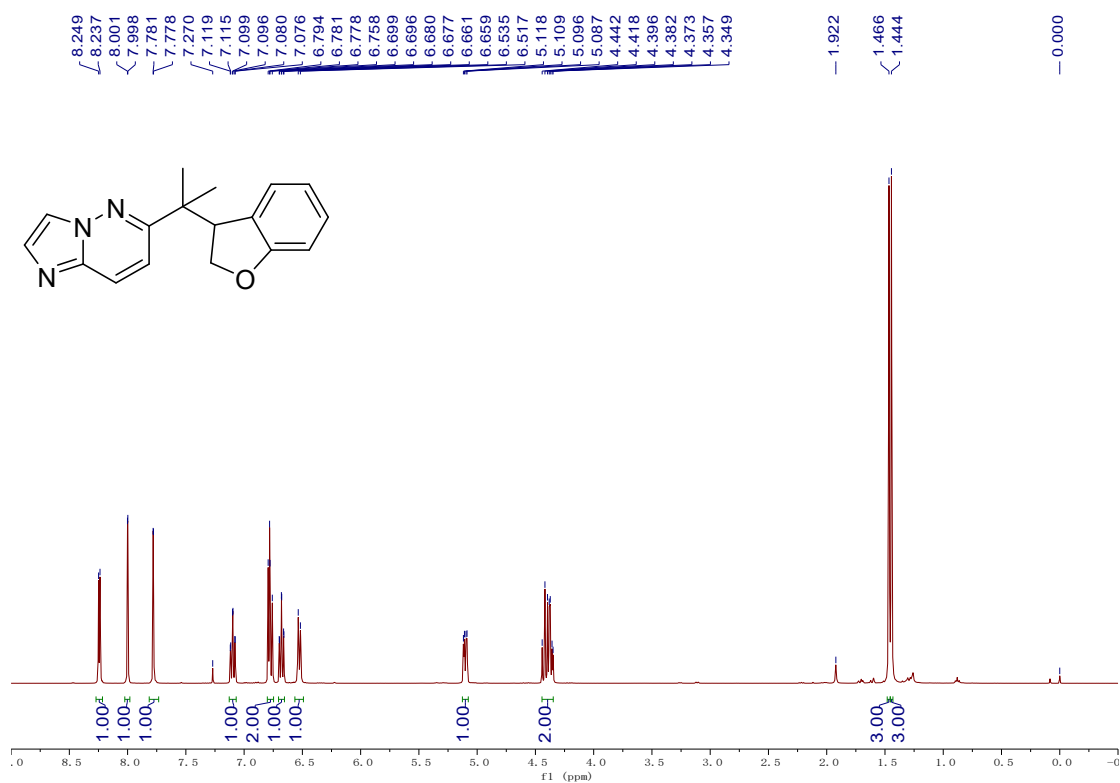
¹H NMR spectrum of **6b** (400 MHz, CDCl₃)



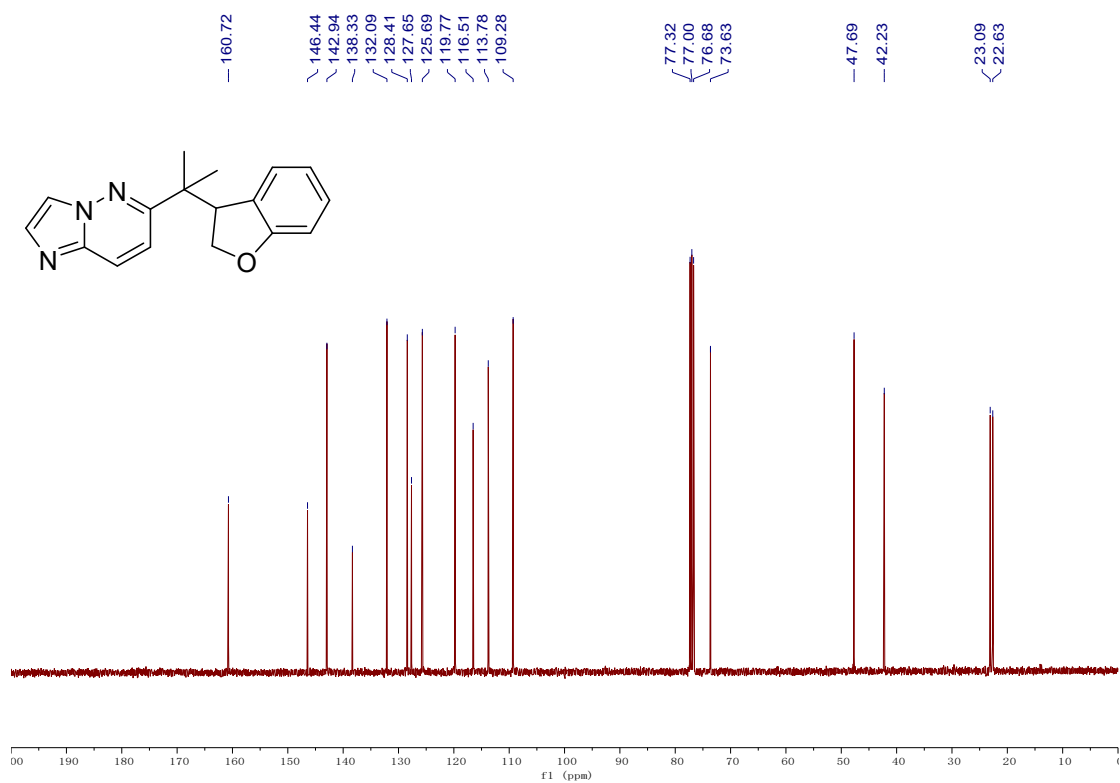
¹³C NMR spectrum of **6b** (100 MHz, CDCl₃)



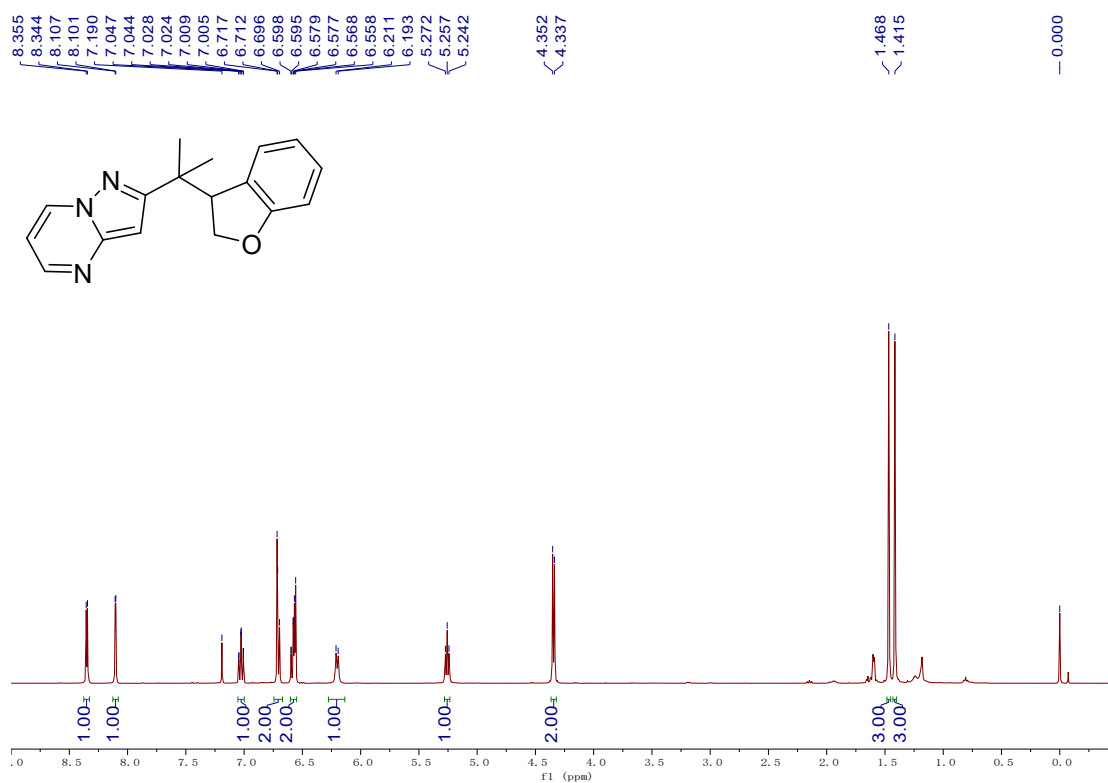
¹H NMR spectrum of **6c** (400 MHz, CDCl₃)



¹³C NMR spectrum of **6c** (100 MHz, CDCl₃)



¹H NMR spectrum of **6d** (400 MHz, CDCl₃)



¹³C NMR spectrum of **6d** (100 MHz, CDCl₃)

