

Supporting Information

Copper-Catalyzed Oxidative Functionalization of Benzylic C–H Bonds with Quinazoline 3-Oxides

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1. General considerations

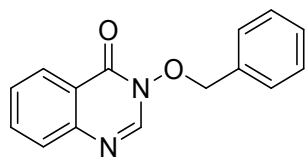
All reactions were carried out in oven-dried glassware. All methylarenes were obtained from commercial sources and used as received. All the reactions were monitored by thin-layer chromatography (TLC). products purification was done using silica gel column chromatography. $^1\text{H}/^{13}\text{C}$ NMR spectra were recorded on Bruker avance 400 MHz and Bruker AMX 400 MHz spectrometer at 400/100 MHz, respectively, in CDCl_3 unless otherwise stated, using either TMS or the undeuterated solvent residual signal as the reference. Chemical shifts are given in ppm and are measured relative to CDCl_3 or DMSO-d_6 as an internal standard. Mass spectra were obtained by the electrospray ionization time-of-flight (ESI-TOF) mass spectrometry. GC yields were obtained using biphenyl as an internal standard. Flash column chromatography purification of compounds was carried out by gradient elution using ethyl acetate (EA) in light petroleum ether (PE).

2. General experimental procedure for the synthesis of quinazolin-4-ones

A mixture of Quinazoline 3-oxides (0.2 mmol), alkyl arenes (4 mmol), CuSO_4 (0.006 mmol), TBAI (0.04 mmol), NaI (0.1 mmol) and TBHP (5.5 M in decane) (0.4 mmol) in DCM (2 mL) was stirred at 70 °C for 12 h. After the reaction was completion (monitored by TLC), the contents were cooled to room temperature and then extracted with ethyl acetate (3 x 10 mL). The combined organic phase was evaporated under reduced pressure to afford the crude product which was further purified by flash chromatography on silica gel gradient with elution of ethyl acetate in petroleum ether to obtain the quinazolin-4-ones.

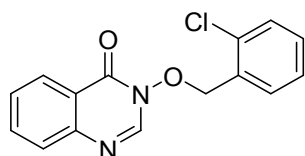
3. Characterization of products

3-(Benzyloxy)quinazolin-4(3H)-one (3a)



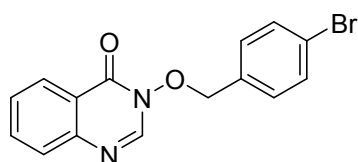
White solid (40.8 mg, 81 %); ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, 1H), 7.82–7.73 (m, 2H), 7.68 (d, J = 8.1 Hz, 1H), 7.56–7.50 (m, 1H), 7.45–7.34 (m, 5H), 5.32 (s, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 157.4, 146.9, 144.7, 134.3, 133.2, 130.0, 129.7, 128.9, 127.8, 127.3, 126.7, 123.5, 79.3; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 275.0796, found: 275.0795.

3-(2-Chlorobenzyloxy)quinazolin-4(3H)-one (3b)



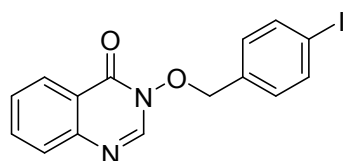
White solid (50.9 mg, 89%); ^1H NMR (400 MHz, CDCl_3) δ 8.37 (d, J = 8.0 Hz, 1H), 7.93 (s, 1H), 7.78 (t, J = 8.0 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.55 (t, J = 8.0 Hz, 1H), 7.46 (d, J = 7.9 Hz, 2H), 7.36 (t, J = 8.0 Hz, 1H), 7.32–7.23 (m, 1H), 5.49 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 147.0, 144.5, 135.3, 134.4, 132.6, 131.3, 131.1, 130.0, 127.9, 127.4 (2C), 126.7, 123.5, 76.3; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{11}\text{ClN}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 309.0407, found: 309.0403.

3-((4-Bromobenzyl)oxy)quinazolin-4(3H)-one (3c)



White solid (46.7 mg, 71 %); ^1H NMR (400 MHz, CDCl_3) δ 8.37–8.33 (m, 1H), 7.87 (s, 1H), 7.82–7.74 (m, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.57–7.49 (m, 3H), 7.33 (d, J = 8.3 Hz, 2H), 5.28 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.4, 147.0, 144.4, 134.4, 132.3, 132.2, 131.6, 128.0, 127.5, 126.7, 124.1, 123.5, 78.5; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{11}\text{BrN}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 331.0082, found: 331.0086.

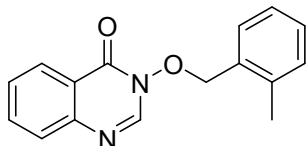
3-((4-Iodobenzyl)oxy)quinazolin-4(3H)-one (3d)



White solid (67.3 mg, 89 %); ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, J = 7.9 Hz, 1H), 7.87 (s, 1H), 7.82–7.76 (m, 1H), 7.76–7.69 (m, 3H), 7.58–7.52 (m, 1H), 7.19 (d, J = 7.9 Hz, 2H), 5.27 (s, 2H); ^{13}C

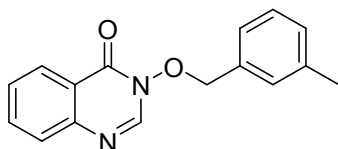
NMR (100 MHz, CDCl₃) δ 157.4, 146.9, 144.4, 138.2, 134.5, 132.9, 131.7, 127.9, 127.5, 126.7, 123.5, 96.0, 78.7; HRMS (ESI) calcd for C₁₅H₁₁N₂O₂ [M + H]⁺: 378.9943, found: 378.9938.

3-((2-Methylbenzyl)oxy)quinazolin-4(3H)-one (3e)



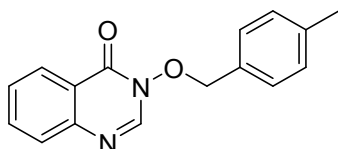
White solid (47.9 mg, 90 %); ¹H NMR (400 MHz, CDCl₃) δ 8.28–8.24 (m, 1H), 7.69 (s, 1H), 7.68–7.62 (m, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.45–7.39 (m, 1H), 7.23–7.12 (m, 3H), 7.08–7.02 (m, 1H), 5.28 (s, 2H), 2.43 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 147.0, 144.6, 138.5, 134.3, 131.5, 131.4, 130.9, 130.1, 127.9, 127.3, 126.7, 126.3, 123.5, 77.6, 19.0; HRMS (ESI) calcd for C₁₆H₁₄N₂O₂ [M + Na]⁺: 289.0953, found: 289.0952.

3-((3-Methylbenzyl)oxy)quinazolin-4(3H)-one (3f)



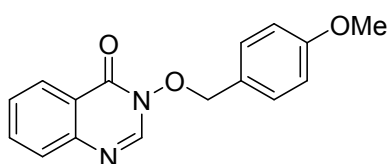
White solid (44.7 mg, 84 %); ¹H NMR (400 MHz, CDCl₃) δ 8.39–8.34 (m, 1H), 7.85–7.82 (m, 1H), 7.79–7.72 (m, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.57–7.49 (m, 1H), 7.29–7.17 (m, 4H), 5.28 (s, 2H), 2.34 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 147.0, 144.8, 138.8, 134.3, 133.2, 130.7, 130.5, 128.8, 127.8, 127.3, 127.1, 126.7, 123.6, 79.5, 21.3; HRMS (ESI) calcd for C₁₆H₁₄N₂O₂ [M + Na]⁺: 289.0953, found: 289.0952.

3-((4-Methylbenzyl)oxy)quinazolin-4(3H)-one (3g)



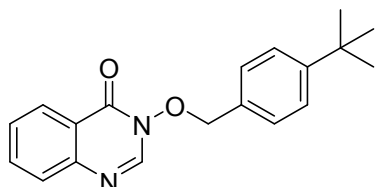
White solid (45.8 mg, 86 %); ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 8.0 Hz, 1H), 7.80–7.72 (m, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.56–7.49 (m, 1H), 7.32–7.25 (m, 2H), 7.18 (d, *J* = 7.7 Hz, 2H), 5.29 (s, 2H), 2.35 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 147.0, 144.9, 139.8, 134.3, 130.3, 130.2, 129.7, 127.8, 127.3, 126.7, 123.6, 79.2, 21.3; HRMS (ESI) calcd for C₁₆H₁₄N₂O₂ [M + Na]⁺: 289.0953, found: 289.0950.

3-((4-Methoxybenzyl)oxy)quinazolin-4(3H)-one (3h)



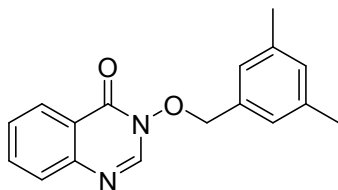
White solid (50.8 mg, 90 %); ^1H NMR (400 MHz, CDCl_3) δ 8.38–8.32 (m, 1H), 7.78–7.71 (m, 2H), 7.67 (d, $J = 7.4$ Hz, 1H), 7.55–7.47 (m, 1H), 7.36–7.30 (m, 2H), 6.90–6.85 (m, 2H), 5.25 (s, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.7, 157.5, 147.0, 144.9, 134.2, 131.7, 127.8, 127.2, 126.7, 125.4, 123.5, 114.3, 78.9, 55.3; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_3$ $[\text{M} + \text{Na}]^+$: 305.0902, found: 305.0901.

3-((4-(*tert*-Butyl)benzyl)oxy)quinazolin-4(3*H*)-one (3i)



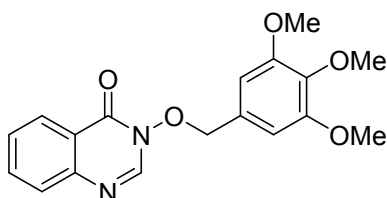
White solid (52.4 mg, 85 %); ^1H NMR (400 MHz, CDCl_3) δ 8.37 (d, $J = 8.0$ Hz, 1H), 7.85 (s, 1H), 7.79–7.73 (m, 1H), 7.69 (d, $J = 8.2$ Hz, 1H), 7.56–7.50 (m, 1H), 7.44–7.34 (m, 4H), 5.30 (s, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 152.9, 147.0, 144.9, 134.3, 130.3, 129.9, 127.8, 127.3, 126.7, 125.9, 123.6, 79.3, 34.8, 31.3; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 331.1422, found: 331.1418.

3-((3,5-Dimethylbenzyl)oxy)quinazolin-4(3*H*)-one (3j)



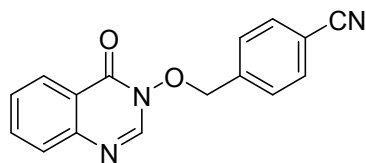
White solid (49.3 mg, 88 %); ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, $J = 7.9$ Hz, 1H), 7.86 (s, 1H), 7.80–7.71 (m, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.56–7.46 (m, 1H), 7.03 (d, $J = 10.6$ Hz, 3H), 5.24 (s, 2H), 2.29 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 147.0, 144.9, 138.6, 134.3, 133.1, 131.3, 127.8, 127.3, 126.7, 123.6, 79.6, 21.2; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 303.1109, found: 303.1110.

3-((3,4,5-Trimethoxybenzyl)oxy)quinazolin-4(3*H*)-one (3k)



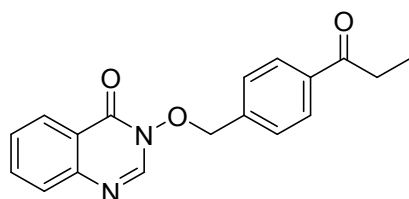
White solid (56.1 mg, 82%); ^1H NMR (400 MHz, CDCl_3) δ 8.37 (d, $J = 8.0$ Hz, 1H), 7.93 (s, 1H), 7.82–7.75 (m, 1H), 7.71 (d, $J = 8.1$ Hz, 1H), 7.58–7.51 (m, 1H), 6.66 (s, 2H), 5.26 (s, 2H), 3.85 (s, 3H), 3.82 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 153.6, 146.9, 144.6, 139.2, 134.4, 128.6, 127.9, 127.4, 126.6, 123.5, 107.1, 79.7, 60.9, 56.2; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_5$ $[\text{M} + \text{Na}]^+$: 365.1113, found: 365.1118.

4-(((4-Oxoquinazolin-3(4*H*)-yl)oxy)methyl)benzonitrile (3l)



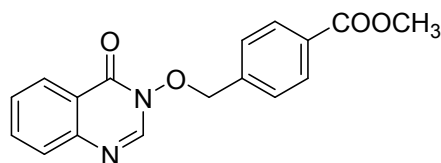
White solid (39.3 mg, 71 %); ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 7.8 Hz, 1H), 8.00 (s, 1H), 7.84–7.77 (m, 1H), 7.76–7.69 (m, 3H), 7.63 (d, *J* = 7.7 Hz, 2H), 7.60–7.52 (m, 1H), 5.39 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 157.3, 146.9, 144.0, 138.3, 134.6, 132.7, 130.1, 128.0, 127.7, 126.7, 123.5, 118.2, 113.5, 78.3; HRMS (ESI) calcd for C₁₆H₁₁N₃O₂ [M + H]⁺: 278.0930, found: 278.0926.

3-((4-Propionylbenzyl)oxy)quinazolin-4(3*H*)-one (3m)



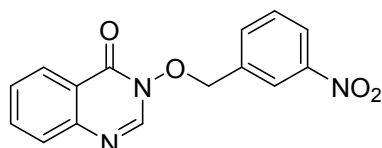
White solid (40.8 mg, 65 %); ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.91 (s, 1H), 7.81–7.75 (m, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.59–7.52 (m, 3H), 5.38 (s, 2H), 3.03 (q, *J* = 7.2 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 200.1, 157.4, 146.9, 144.4, 137.9, 137.8, 134.5, 130.0, 128.6, 127.9, 127.5, 126.7, 123.5, 78.6, 32.0, 8.1; HRMS (ESI) calcd for C₁₈H₁₆N₂O₃ [M + Na]⁺: 331.1059, found: 331.1062.

Methyl 4-(((4-oxoquinazolin-3(4*H*)-yl)oxy)methyl)benzoate (3n)



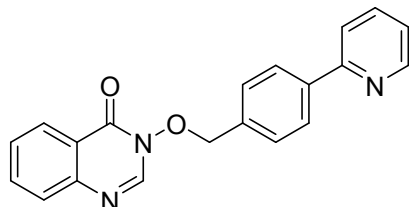
White solid (32.9 mg, 53 %); ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 7.9 Hz, 2H), 7.90 (s, 1H), 7.81–7.75 (m, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.57–7.50 (m, 3H), 5.38 (s, 2H), 3.93 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 166.4, 157.4, 146.9, 144.3, 138.0, 134.4, 131.3, 130.2, 129.7, 127.9, 127.5, 126.7, 123.5, 78.6, 52.3; HRMS (ESI) calcd for C₁₇H₁₄N₂O₄ [M + Na]⁺: 333.0851, found: 333.0850.

3-((3-Nitrobenzyl)oxy)quinazolin-4(3*H*)-one (3o)



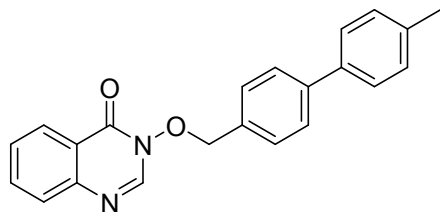
White solid (29.1 mg, 49 %); ^1H NMR (400 MHz, CDCl_3) δ 8.41–8.35 (m, 2H), 8.32–8.27 (m, 1H), 8.05 (s, 1H), 7.89 (d, $J = 7.6$ Hz, 1H), 7.84–7.78 (m, 1H), 7.74 (d, $J = 8.1$ Hz, 1H), 7.66–7.61 (m, 1H), 7.60–7.55 (m, 1H), 5.44 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.3, 148.5, 146.9, 143.9, 135.6, 135.3, 134.6, 130.1, 128.0, 127.7, 126.8, 124.5, 124.4, 123.5, 78.0; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{11}\text{N}_3\text{O}_4$ $[\text{M} + \text{H}]^+$: 298.0828, found: 298.0823.

3-((4-(Pyridin-2-yl)benzyl)oxy)quinazolin-4(3H)-one (3p)



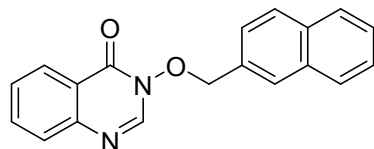
White solid (52.6 mg, 80 %); ^1H NMR (400 MHz, CDCl_3) δ 8.70 (d, $J = 4.7$ Hz, 1H), 8.37 (d, $J = 8.0$ Hz, 1H), 8.03 (d, $J = 8.2$ Hz, 2H), 7.86 (s, 1H), 7.79–7.71 (m, 3H), 7.68 (d, $J = 8.0$ Hz, 1H), 7.57–7.51 (m, 3H), 7.29–7.22 (m, 1H), 5.39 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 156.4, 149.8, 147.0, 144.7, 140.7, 136.9, 134.4, 133.9, 130.5, 127.9, 127.5, 127.4, 126.7, 123.5, 122.6, 120.7, 79.0; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{15}\text{N}_3\text{O}_2$ $[\text{M} + \text{Na}]^+$: 352.1062, found: 352.1060.

3-((4'-(4-Methylphenyl)-[1,1'-biphenyl]-4-yl)methoxy)quinazolin-4(3H)-one (3q)



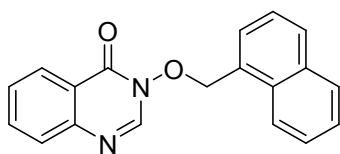
White solid (56.8 mg, 83 %); ^1H NMR (400 MHz, CDCl_3) δ 8.40–8.36 (m, 1H), 7.87 (s, 1H), 7.80–7.74 (m, 1H), 7.69 (d, $J = 7.8$ Hz, 1H), 7.60 (d, $J = 8.2$ Hz, 2H), 7.57–7.51 (m, 1H), 7.48 (d, $J = 8.2$ Hz, 4H), 7.28–7.23 (m, 2H), 5.36 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.6, 147.0, 144.8, 142.6, 137.6, 137.3, 134.4, 131.8, 130.6, 129.6, 127.9, 127.5, 127.4, 127.0, 126.8, 123.6, 79.2, 21.2; HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_2$, $[\text{M} + \text{Na}]^+$: 365.1266, found: 365.1268.

3-(Naphthalen-2-ylmethoxy)quinazolin-4(3H)-one (3r)



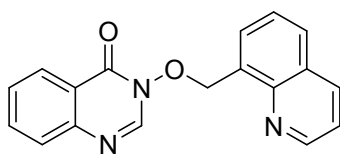
Yellow solid (48.3 mg, 80 %); ^1H NMR (400 MHz, CDCl_3) δ 8.38 (d, $J = 7.8$ Hz, 1H), 7.91–7.81 (m, 4H), 7.81–7.70 (m, 2H), 7.67–7.57 (m, 2H), 7.55–7.44 (m, 3H), 5.48 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 147.0, 144.7, 134.3, 133.7, 133.1, 130.7, 129.8, 129.0, 128.2, 127.9, 127.8, 127.3, 127.0, 126.7, 126.7, 126.6, 123.6, 79.6; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{14}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 325.0953, found: 325.0949.

3-(Naphthalen-1-ylmethoxy)quinazolin-4(3H)-one (3s)



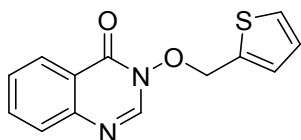
Yellow solid (52.5 mg, 87 %); ^1H NMR (400 MHz, CDCl_3) δ 8.47 (d, J = 8.4 Hz, 1H), 8.38 (d, J = 8.0 Hz, 1H), 7.92–7.85 (m, 2H), 7.76–7.49 (m, 6H), 7.41–7.31 (m, 2H), 5.79 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.6, 146.9, 144.6, 134.3, 133.9, 132.1, 130.9, 130.0, 129.0, 128.9, 127.9, 127.4, 127.3, 126.7, 126.5, 125.2, 124.0, 123.5, 77.5; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{14}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 325.0953, found: 325.0954.

3-(Quinolin-8-ylmethoxy)quinazolin-4(3H)-one (3t)



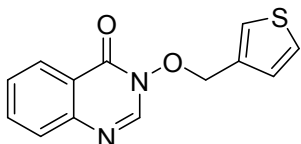
White solid (51.5 mg, 85%); ^1H NMR (400 MHz, CDCl_3) δ 8.91–8.82 (m, 1H), 8.40 (d, J = 7.6 Hz, 1H), 8.18 (d, J = 7.8 Hz, 1H), 8.02 (s, 1H), 7.91–7.80 (m, 2H), 7.78–7.70 (m, 1H), 7.66 (d, J = 7.7 Hz, 1H), 7.57–7.47 (m, 2H), 7.46–7.38 (m, 1H), 6.03 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.6, 150.4, 146.9, 146.6, 145.1, 136.3, 134.0, 132.1, 131.6, 130.0, 128.3, 127.6, 127.0, 126.6, 126.1, 123.6, 121.5, 75.8; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{O}_2$ $[\text{M} + \text{Na}]^+$: 326.0905, found: 326.0900.

3-(Thiophen-2-ylmethoxy)quinazolin-4(3H)-one (3u)



White solid (45.9 mg, 89 %); ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, J = 8.0 Hz, 1H), 7.80–7.73 (m, 2H), 7.69 (d, J = 8.1 Hz, 1H), 7.57–7.50 (m, 1H), 7.42 (d, J = 4.7 Hz, 1H), 7.06–7.03 (m, 1H), 7.01–6.95 (m, 1H), 5.52 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 147.0, 144.7, 134.9, 134.4, 130.9, 129.1, 127.9, 127.6, 127.3, 126.7, 123.5, 72.2; HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$: 281.0361, found: 281.0365.

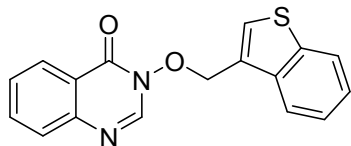
3-(Thiophen-3-ylmethoxy)quinazolin-4(3H)-one (3v)



White solid (36.1 mg, 70 %); ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, J = 8.0 Hz, 1H), 7.80–7.73 (m, 2H), 7.69 (d, J = 8.1 Hz, 1H), 7.56–7.50 (m, 1H), 7.41–7.36 (m, 1H), 7.33 (s, 1H), 7.20 (d, J = 4.9 Hz, 1H), 5.35 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.5, 147.0, 144.7, 134.4, 134.3, 128.1, 127.9, 127.7,

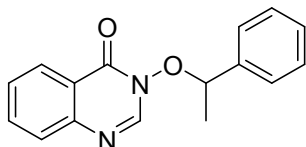
127.4, 127.3, 126.7, 123.5, 73.2; HRMS (ESI) calcd for C₁₃H₁₀N₂O₂S [M + Na]⁺: 281.0361, found: 281.0363.

3-(Benzo[b]thiophen-3-ylmethoxy)quinazolin-4(3H)-one (3w)



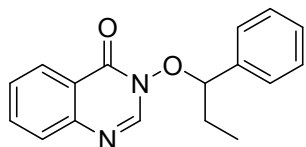
White solid (46.8 mg, 76 %); ¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, *J* = 7.9 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.79–7.72 (m, 1H), 7.68–7.63 (m, *J* = 8.2 Hz, 2H), 7.56–7.46 (m, 3H), 7.45–7.40 (m, 1H), 5.61 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 157.6, 147.0, 144.5, 140.6, 137.7, 134.4, 130.1, 128.7, 127.9, 127.4, 126.7, 125.2, 125.0, 123.5, 123.1, 122.1, 72.2; HRMS (ESI) calcd for C₁₇H₁₂N₂O₂S [M + Na]⁺: 331.0517, found: 331.0514.

3-(1-Phenylethoxy)quinazolin-4(3H)-one (3x)



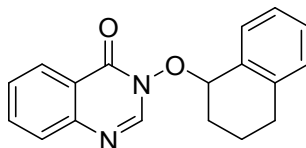
Colorless liquid (38.3 mg, 72 %); ¹H NMR (400 MHz, CDCl₃) δ 8.34 (d, *J* = 8.0 Hz, 1H), 7.75–7.68 (m, 1H), 7.64–7.59 (m, 2H), 7.53–7.46 (m, 1H), 7.40–7.30 (m, 5H), 5.59 (q, *J* = 6.5 Hz, 1H), 1.81–1.76 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.7, 146.8, 145.0, 138.3, 134.2, 129.6, 129.0, 127.7, 127.2, 126.7, 123.4, 84.7, 19.8; HRMS (ESI) calcd for C₁₆H₁₄N₂O₂ [M + Na]⁺: 289.0953, found: 289.0950.

3-(1-Phenylpropoxy)quinazolin-4(3H)-one (3y)



Colorless liquid (32.5 mg, 58%); ¹H NMR (400 MHz, CDCl₃) δ 8.25 (d, *J* = 7.8 Hz, 1H), 7.67–7.61 (m, 1H), 7.55–7.48 (m, 2H), 7.45–7.39 (m, 1H), 7.29–7.20 (m, 5H), 5.23 (t, *J* = 7.2 Hz, 1H), 2.31–2.19 (m, 1H), 1.97–1.86 (m, 1H), 0.97 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 157.7, 146.8, 145.1, 137.3, 134.2, 129.5, 129.0, 128.2, 127.7, 127.2, 126.6, 123.5, 90.3, 27.3, 10.1; HRMS (ESI) calcd for C₁₇H₁₆N₂O₂ [M + Na]⁺: 303.1109, found: 303.1107.

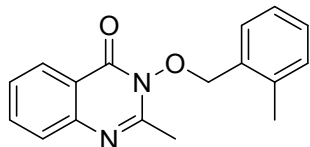
3-((1,2,3,4-Tetrahydronaphthalen-1-yl)oxy)quinazolin-4(3H)-one (3z)



Colorless liquid (42.0 mg, 72 %); ¹H NMR (400 MHz, CDCl₃) δ 8.40–8.36 (m, 1H), 7.81–7.70 (m, 3H), 7.58–7.51 (m, 1H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.32–7.25 (m, 1H), 7.21–7.11 (m, 2H), 5.58 (t, *J* = 3.3 Hz, 1H), 3.00–2.92 (m, 1H), 2.86–2.75 (m, 1H), 2.42–2.34 (m, 1H), 2.25–2.10 (m, 1H), 1.98–1.84 (m, 2H);

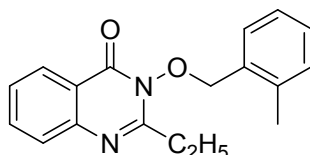
^{13}C NMR (100 MHz, CDCl_3) δ 158.0, 147.0, 145.5, 138.4, 134.3, 131.5, 131.2, 129.5, 129.3, 127.9, 127.3, 126.7, 126.1, 123.6, 81.6, 28.9, 26.7, 17.7; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 315.1109, found: 315.1108.

2-Methyl-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4a)



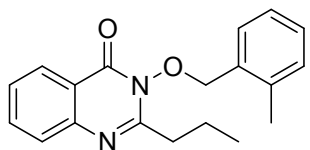
White solid (30mg, 83%); ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, $J = 7.6$ Hz, 1H), 7.68–7.62 (m, 1H), 7.55 (d, $J = 8.1$ Hz, 1H), 7.42–7.35 (m, 1H), 7.31–7.09 (m, 4H), 5.24 (s, 2H), 2.50 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.2, 153.9, 146.5, 138.6, 134.3, 131.8, 131.2, 130.8, 129.8, 127.1, 126.6, 126.5, 126.3, 122.6, 76.3, 20.3, 19.1; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 303.1109, found: 303.1107.

2-Ethyl-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4b)



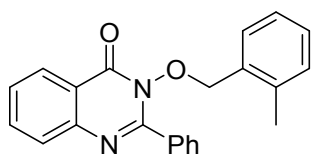
White solid (52.9 mg, 90 %); ^1H NMR (400 MHz, CDCl_3) δ 8.30 (d, $J = 7.6$ Hz, 1H), 7.77–7.70 (m, 1H), 7.68 (d, $J = 8.3$ Hz, 1H), 7.49–7.43 (m, 1H), 7.40 (d, $J = 7.4$ Hz, 1H), 7.34–7.28 (m, 1H), 7.28–7.18 (m, 3H), 5.32 (s, 1H), 2.83 (q, $J = 7.4$ Hz, 2H), 2.59 (s, 3H), 1.33 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.9, 156.9, 146.1, 138.0, 133.7, 131.4, 130.5, 130.2, 129.2, 126.8, 126.1, 125.9, 125.8, 122.0, 75.9, 25.6, 18.6, 10.3; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 317.1266, found: 317.1270.

3-((2-Methylbenzyl)oxy)-2-propylquinazolin-4(3H)-one (4c)



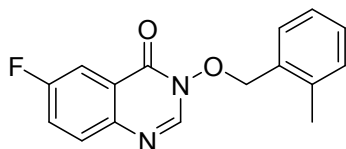
White solid (46.8 mg, 76 %); ^1H NMR (400 MHz, CDCl_3) δ 8.32–8.29 (m, 1H), 7.76–7.71 (m, 1H), 7.67 (d, $J = 7.6$ Hz, 1H), 7.49–7.43 (m, 1H), 7.40 (d, $J = 7.5$ Hz, 1H), 7.35–7.30 (m, 1H), 7.29–7.20 (m, 2H), 5.32 (s, 2H), 2.76 (t, $J = 7.6$ Hz, 2H), 2.59 (s, 3H), 1.87–1.76 (m, 2H), 0.99 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.4, 156.6, 146.6, 138.7, 134.2, 131.9, 131.0, 130.7, 129.7, 127.3, 126.6, 126.4, 126.3, 122.5, 76.4, 34.8, 20.1, 19.1, 13.9; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 331.1422, found: 331.1423.

3-((2-Methylbenzyl)oxy)-2-phenylquinazolin-4(3H)-one (4d)



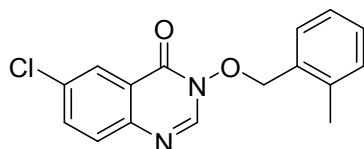
White solid (61.6 mg, 90 %); ^1H NMR (400 MHz, CDCl_3) δ 8.40 (d, $J = 8.0$ Hz, 1H), 7.79 (d, $J = 4.0$ Hz, 2H), 7.71 (d, $J = 8.0$ Hz, 2H), 7.59–7.47 (m, 2H), 7.42 (t, $J = 7.4$ Hz, 2H), 7.24–7.15 (m, 1H), 7.09–6.97 (m, 2H), 6.79 (d, $J = 7.2$ Hz, 1H), 4.98 (s, 2H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.3, 154.0, 146.6, 138.9, 134.5, 132.4, 131.5, 131.0, 130.5, 130.4, 129.6, 129.6, 128.2, 128.0, 127.0, 126.8, 125.9, 122.7, 76.0, 18.4; HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 365.1266, found: 365.1262.

6-Fluoro-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4e)



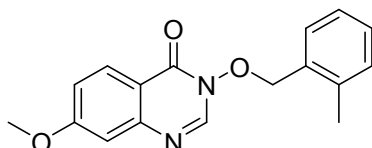
White solid (49.4 mg, 87 %); ^1H NMR (400 MHz, CDCl_3) δ 8.40–8.32 (m, 1H), 7.76 (s, 1H), 7.36–7.29 (m, 2H), 7.29–7.19 (m, 3H), 7.19–7.13 (m, 1H), 5.37 (s, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.4, 145.3, 138.0, 131.0, 130.7, 130.5, 129.7, 129.0, 128.9, 125.9, 119.7, 115.8, 112.9, 99.5, 77.2, 18.5; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{13}\text{FN}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 307.0859, found: 307.0850.

6-Chloro-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4f)



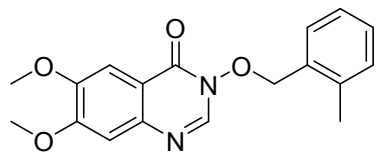
White solid (42.0 mg, 70 %); ^1H NMR (400 MHz, CDCl_3) δ 8.32 (s, 1H), 7.76–7.65 (m, 2H), 7.62 (d, $J = 8.6$ Hz, 1H), 7.34–7.19 (m, 3H), 7.19–7.11 (m, 1H), 5.37 (s, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.5, 145.5, 144.8, 138.5, 134.8, 133.4, 131.5, 131.2, 131.0, 130.2, 129.5, 126.4, 126.1, 124.6, 77.6, 19.0; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{13}\text{ClN}_2\text{O}_2$ $[\text{M} + \text{Na}]^+$: 323.0563, found: 323.0559.

7-Methoxy-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4g)



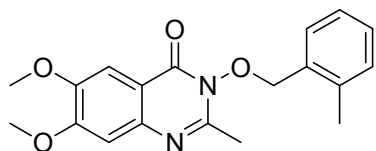
White solid (42.6 mg, 72 %); ^1H NMR (400 MHz, CDCl_3) δ 8.24 (d, $J = 8.9$ Hz, 1H), 7.73 (s, 1H), 7.33–7.21 (m, 3H), 7.18–7.12 (m, 1H), 7.11–7.03 (m, 2H), 5.36 (s, 2H), 3.90 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 164.5, 157.2, 149.2, 145.2, 138.5, 131.5 (2C), 130.9, 130.0, 128.2, 126.3, 117.3, 116.8, 108.6, 77.6, 55.7, 19.0; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_3$ $[\text{M} + \text{Na}]^+$: 319.1059, found: 319.1055.

6,7-Dimethoxy-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4h)



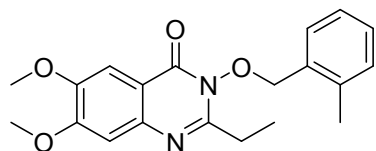
White solid (43.7 mg, 67 %); ^1H NMR (400 MHz, CDCl_3) δ 7.70 (s, 1H), 7.66 (s, 1H), 7.33–7.23 (m, 3H), 7.19–7.14 (m, 1H), 7.07 (s, 1H), 5.38 (s, 2H), 4.02 (s, 3H), 3.98 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.0, 154.9, 149.4, 143.3, 143.2, 138.5, 131.5 (2C), 130.9, 130.0, 126.3, 116.9, 108.2, 105.5, 77.6, 56.4, 56.3, 19.0; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4$ $[\text{M} + \text{Na}]^+$: 349.1164, found: 349.1166.

6,7-Dimethoxy-2-methyl-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4i)



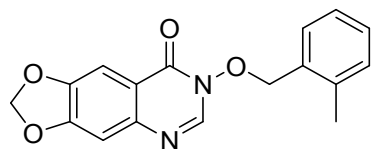
White solid (29.9 mg, 56%); ^1H NMR (400 MHz, CDCl_3) δ 7.60 (s, 1H), 7.37 (d, $J = 7.4$ Hz, 1H), 7.35–7.29 (m, 1H), 7.27 (d, $J = 8.2$ Hz, 1H), 7.24–7.19 (m, 1H), 7.04 (s, 1H), 5.33 (s, 2H), 4.04–3.93 (m, 6H), 2.60 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.7, 155.0, 152.4, 148.8, 142.8, 138.6, 131.9, 131.2, 130.7, 129.8, 126.3, 115.7, 107.5, 105.3, 76.3, 56.3 (2C), 20.1, 19.1; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_4$ $[\text{M} + \text{H}]^+$: 363.1321, found: 363.1325.

2-Ethyl-6,7-dimethoxy-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4j)



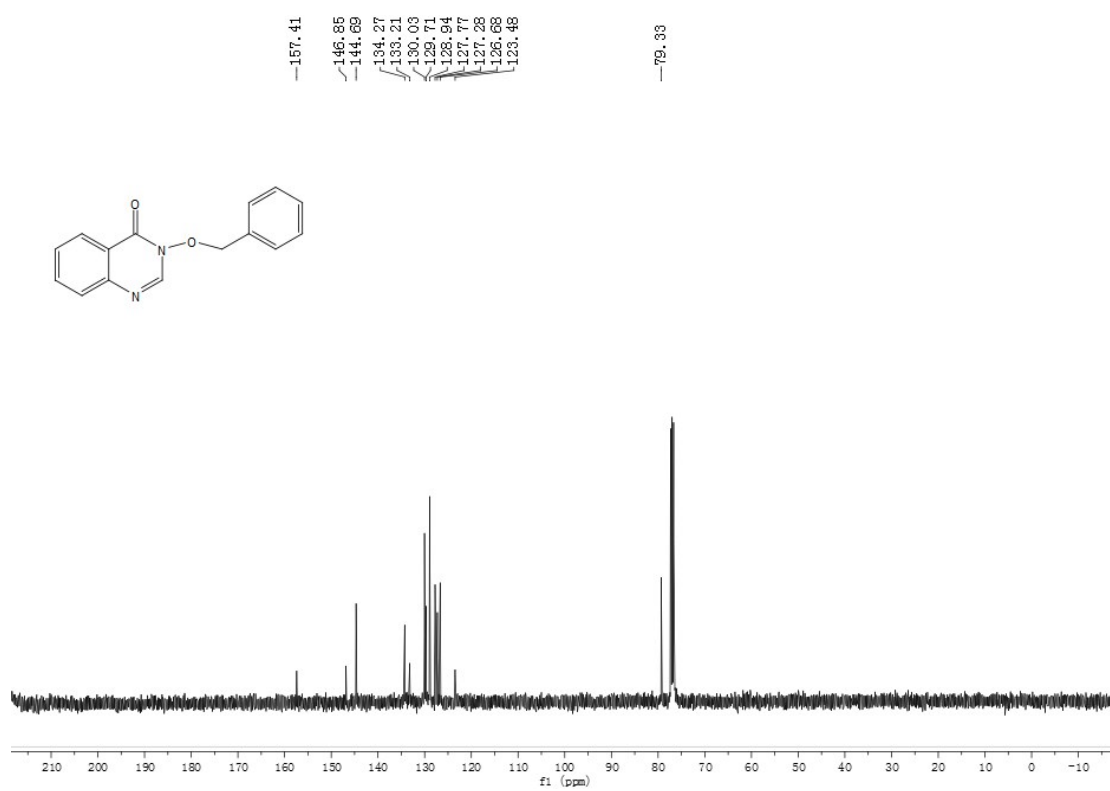
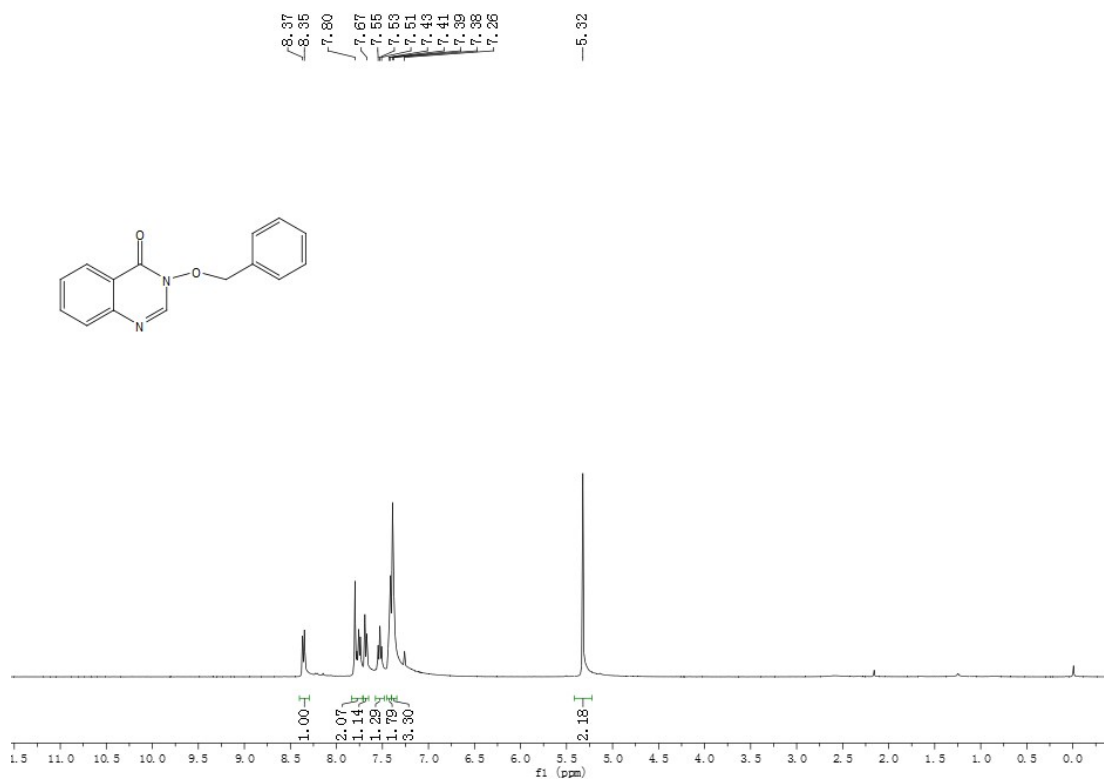
White solid (41.8 mg, 62 %); ^1H NMR (400 MHz, CDCl_3) δ 7.62 (s, 1H), 7.41 (d, $J = 7.4$ Hz, 1H), 7.36–7.31 (m, 1H), 7.30–7.21 (m, 2H), 7.09 (s, 1H), 5.33 (s, 2H), 4.01 (s, 6H), 2.82 (q, $J = 7.6$ Hz, 2H), 2.61 (s, 3H), 1.33 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.9, 156.0, 154.9, 148.8, 142.9, 138.6, 131.9, 131.0, 130.7, 129.7, 126.2, 115.7, 107.7, 105.3, 76.4, 56.3 (2C), 26.0, 19.1, 10.9; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_4$ $[\text{M} + \text{Na}]^+$: 377.1477, found: 377.1478.

7-((2-Methylbenzyl)oxy)-[1,3]dioxolo[4,5-g]quinazolin-8(7H)-one (4k)

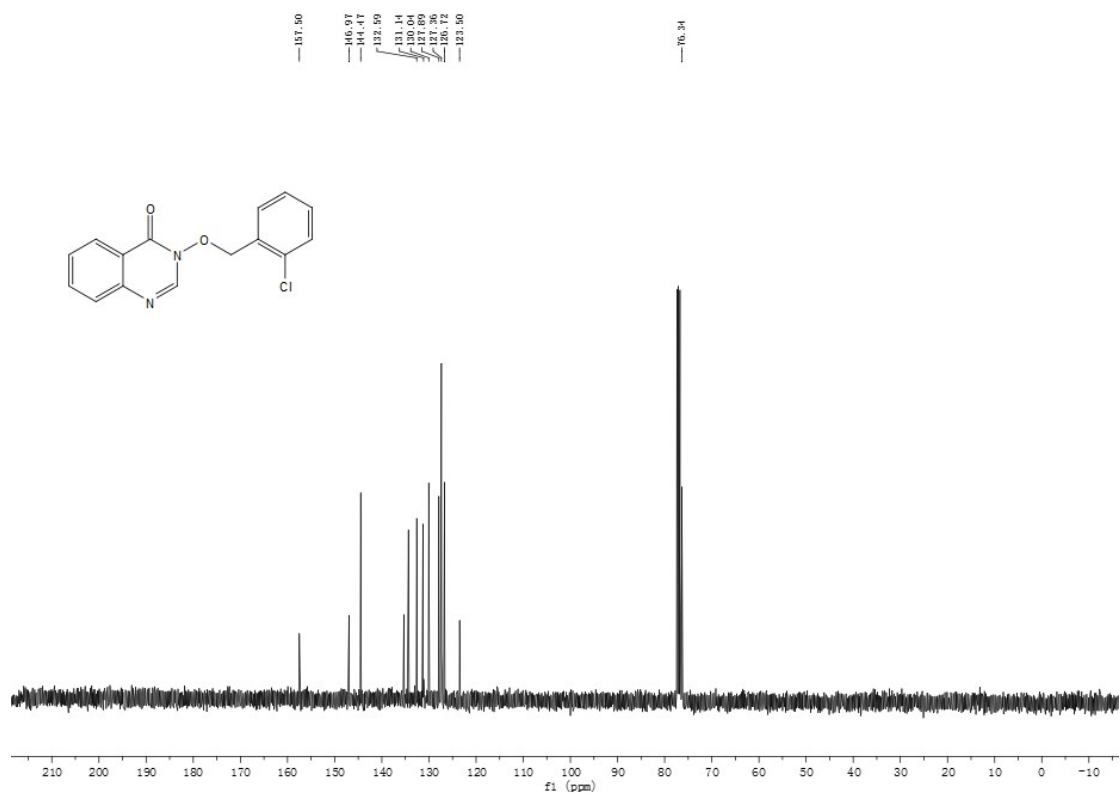
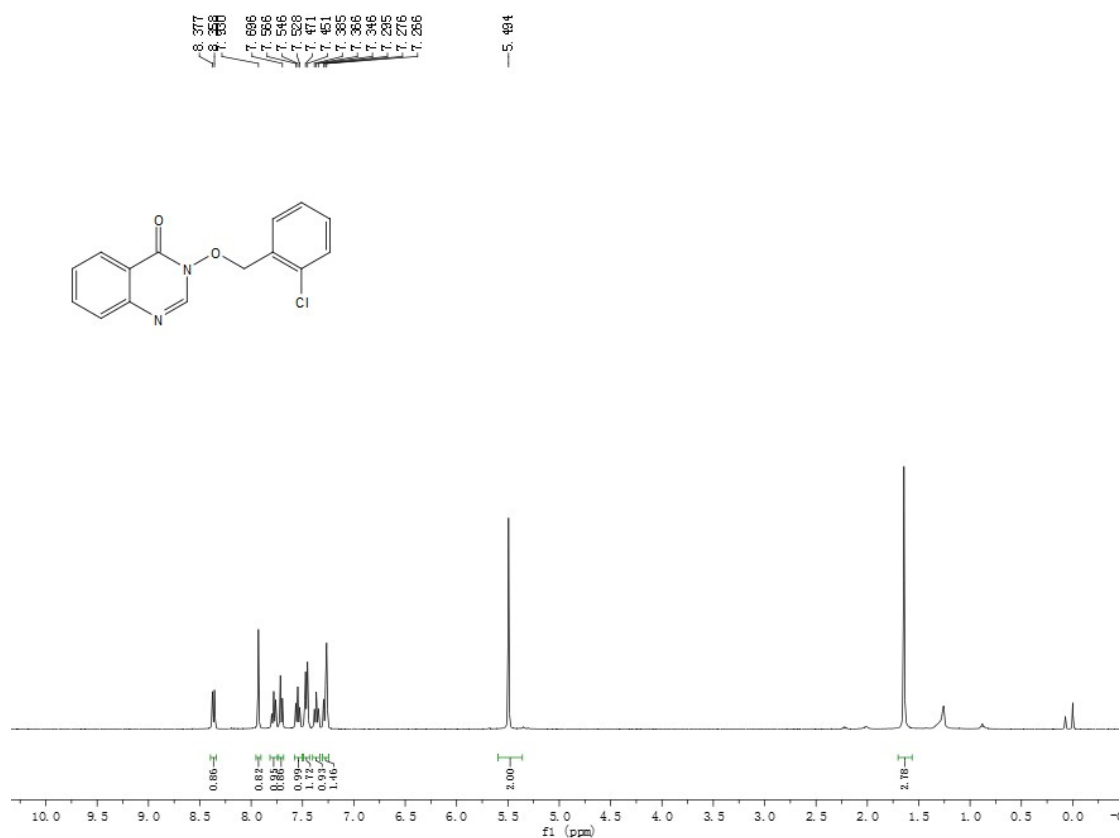


White solid (33.5, 54 %); ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, $J = 11.9$ Hz, 2H), 7.35–7.19 (m, 3H), 7.20–7.11 (m, 1H), 7.02 (s, 1H), 6.13 (s, 2H), 5.36 (s, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.9, 153.5, 147.9, 144.9, 143.2, 138.5, 131.5, 131.4, 130.9, 130.1, 126.3, 118.6, 106.2, 103.4, 102.5, 77.5, 19.0; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{14}\text{N}_2\text{O}_4$ $[\text{M} + \text{Na}]^+$: 333.0851, found: 333.0847.

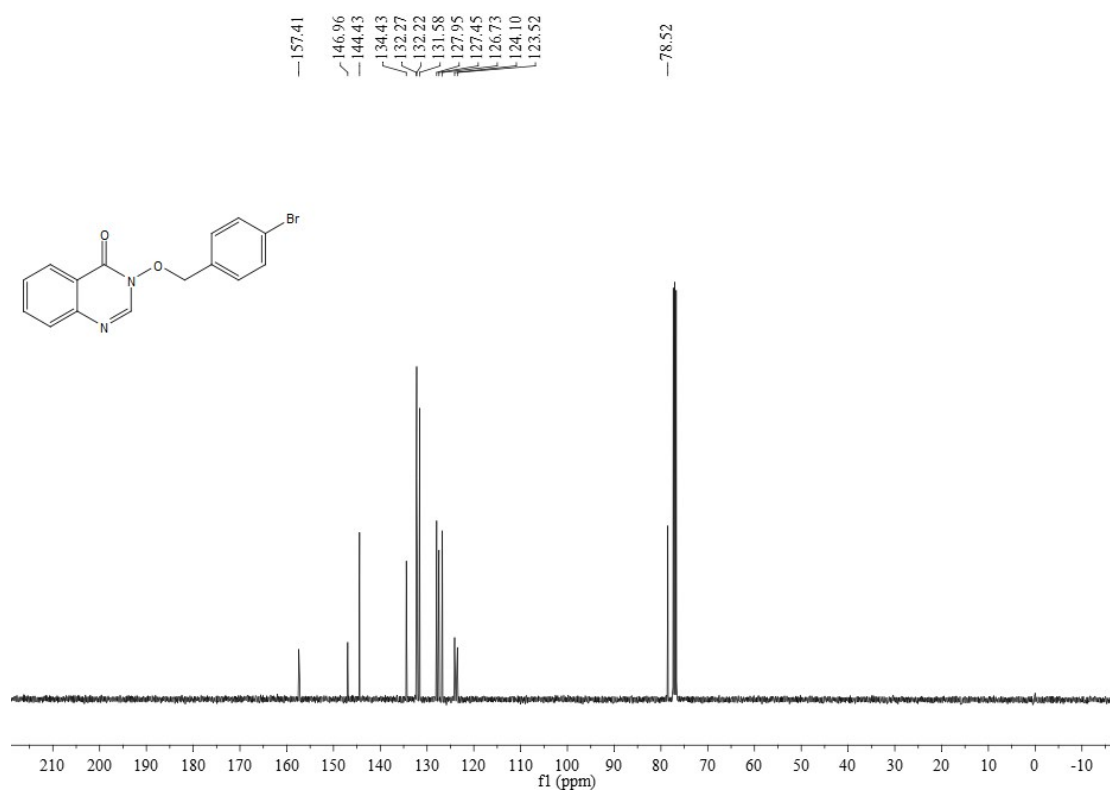
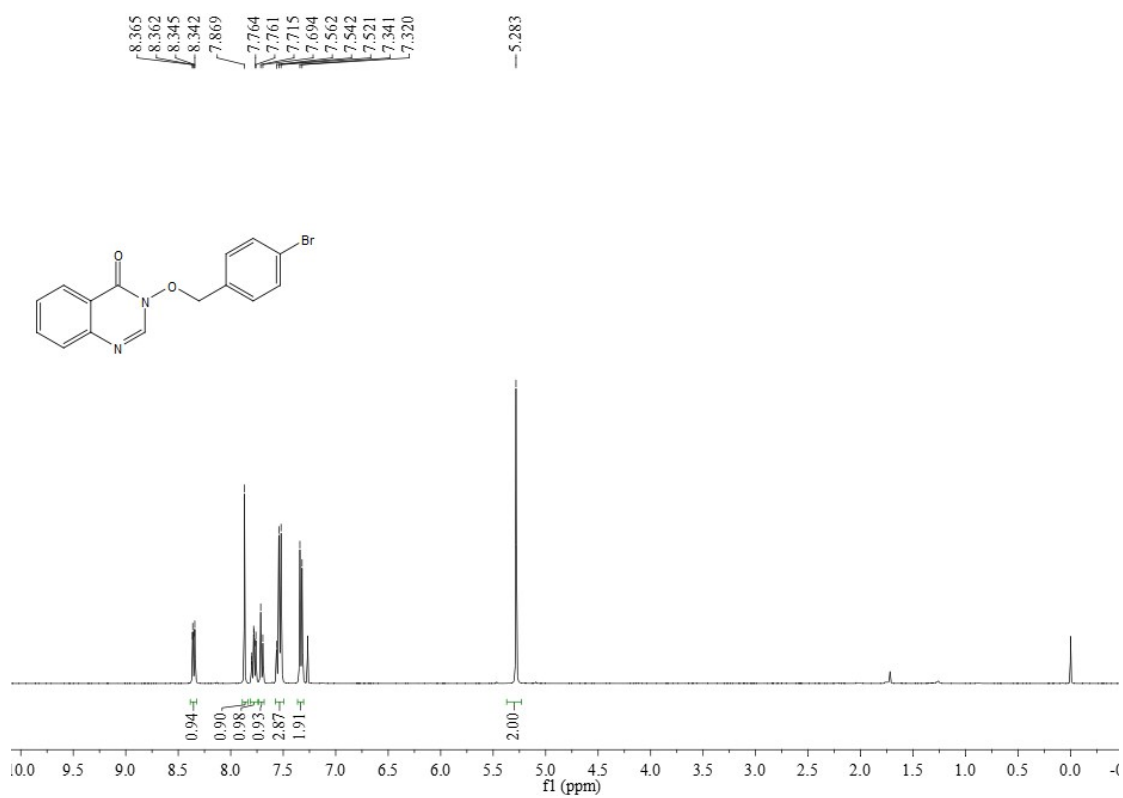
4. Copies of ^1H NMR & ^{13}C NMR Spectra



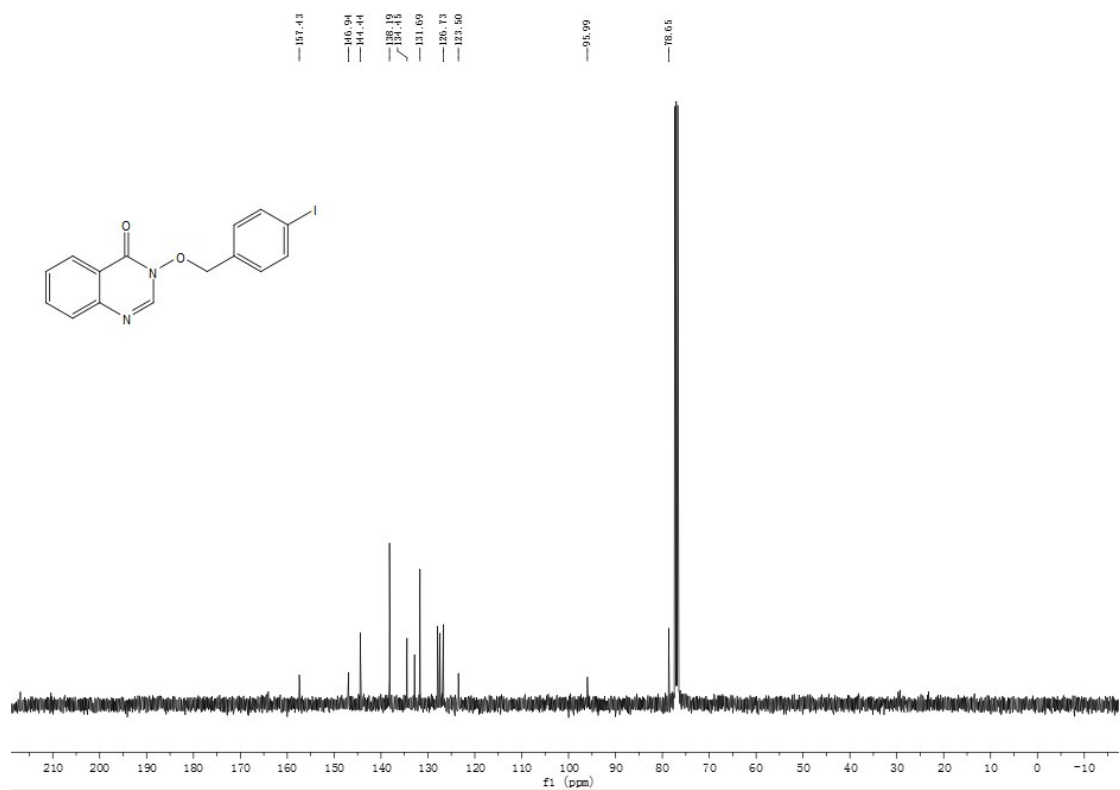
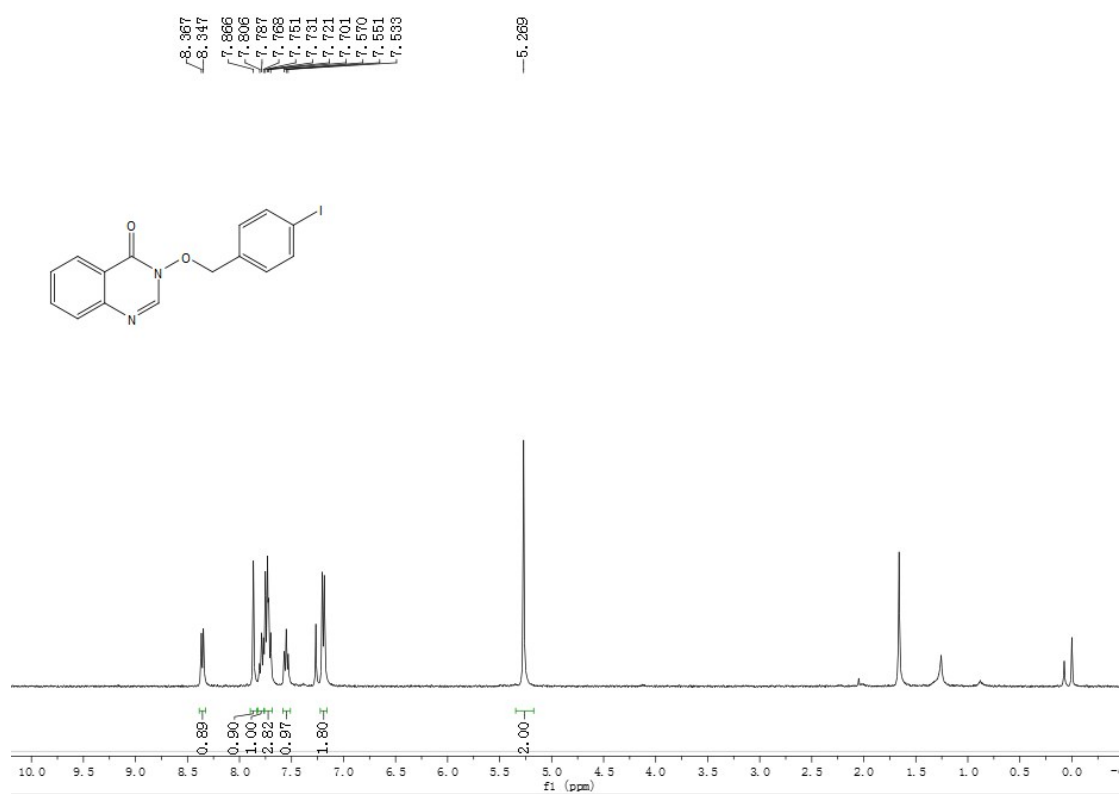
^1H NMR and ^{13}C NMR for compound **3a**



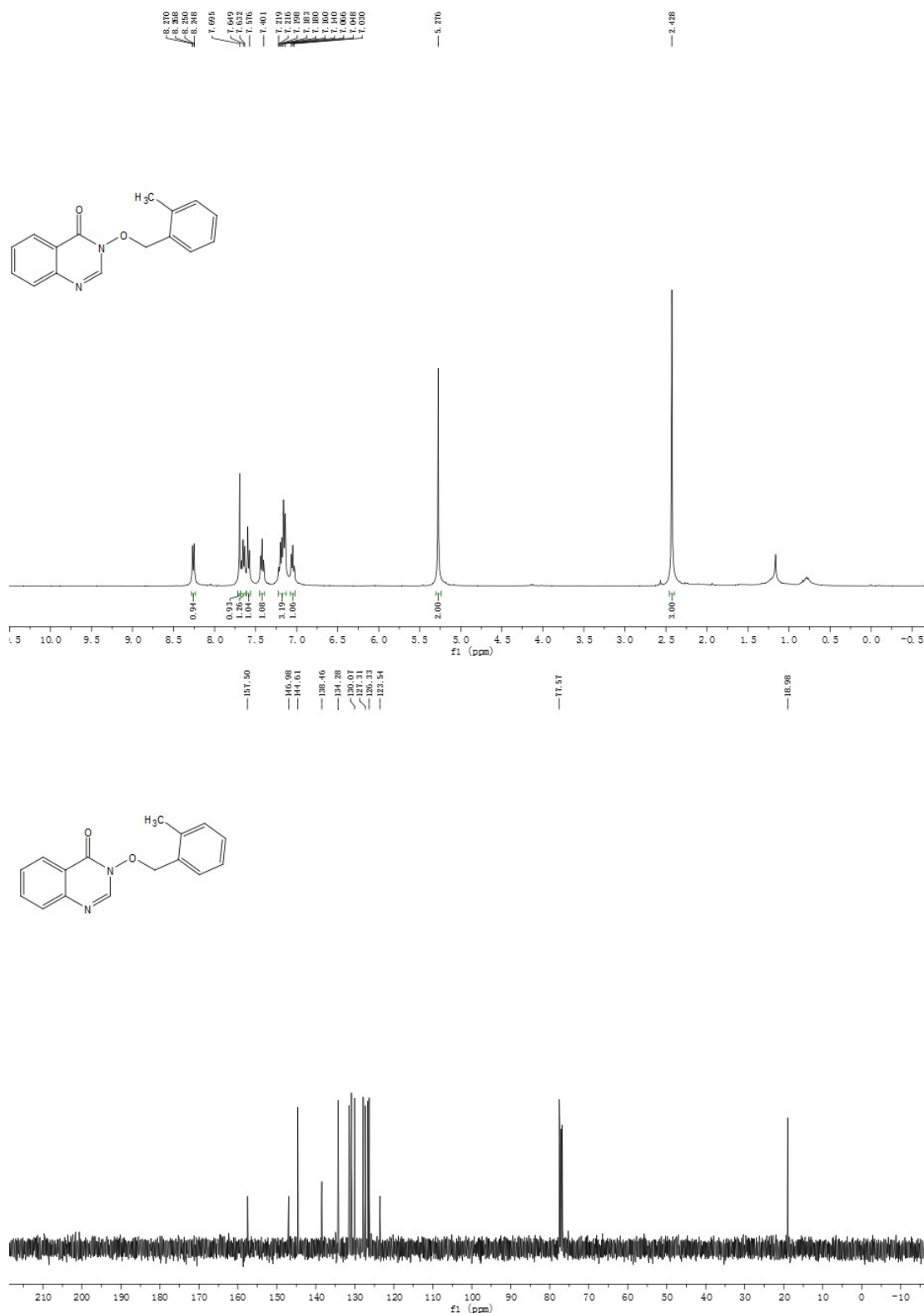
¹H NMR and ¹³C NMR for compound **3b**



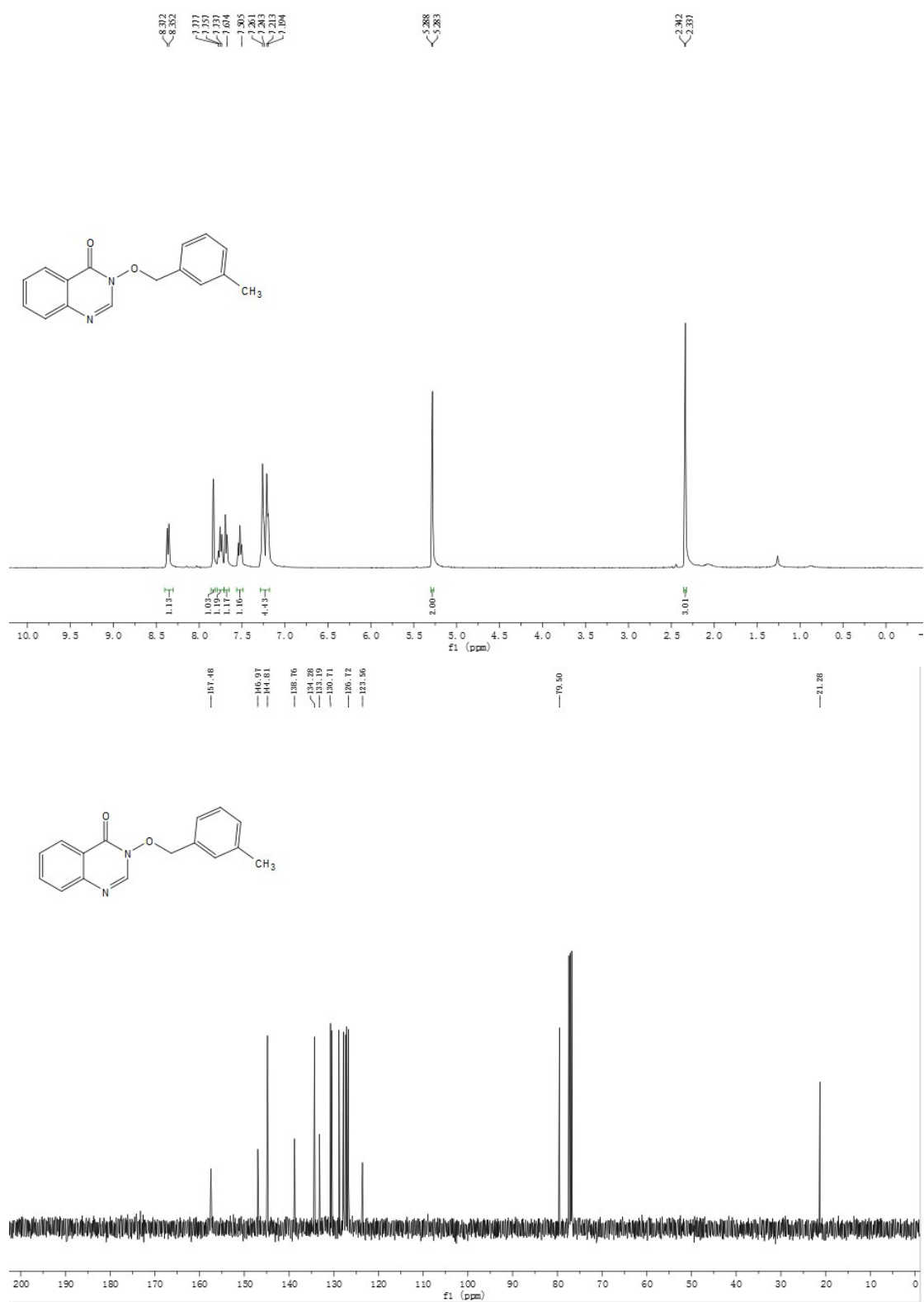
¹H NMR and ¹³C NMR for compound **3c**



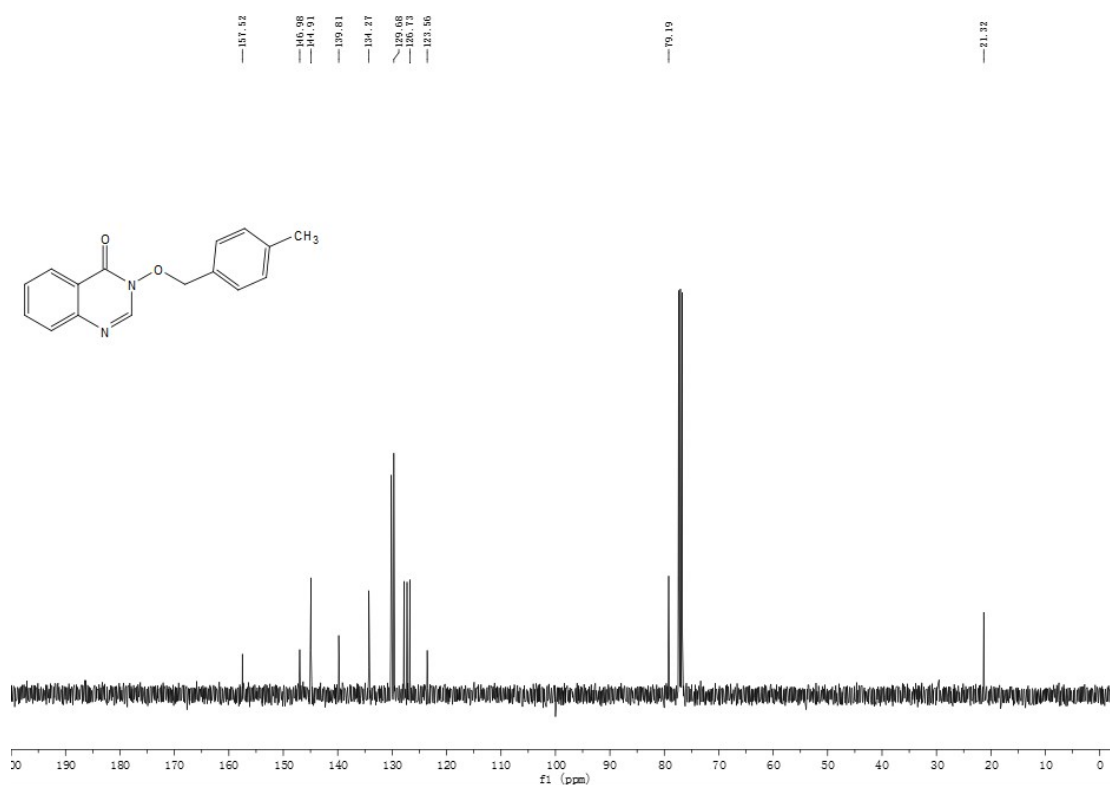
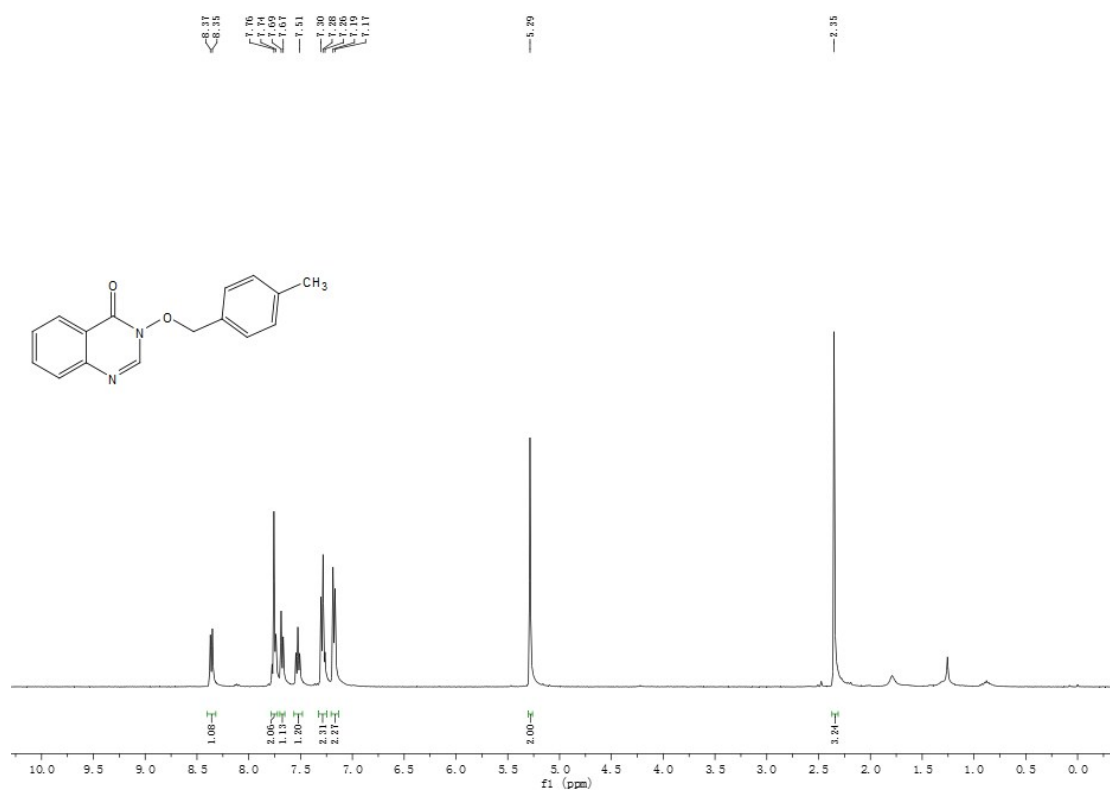
¹H NMR and ¹³C NMR for compound **3d**



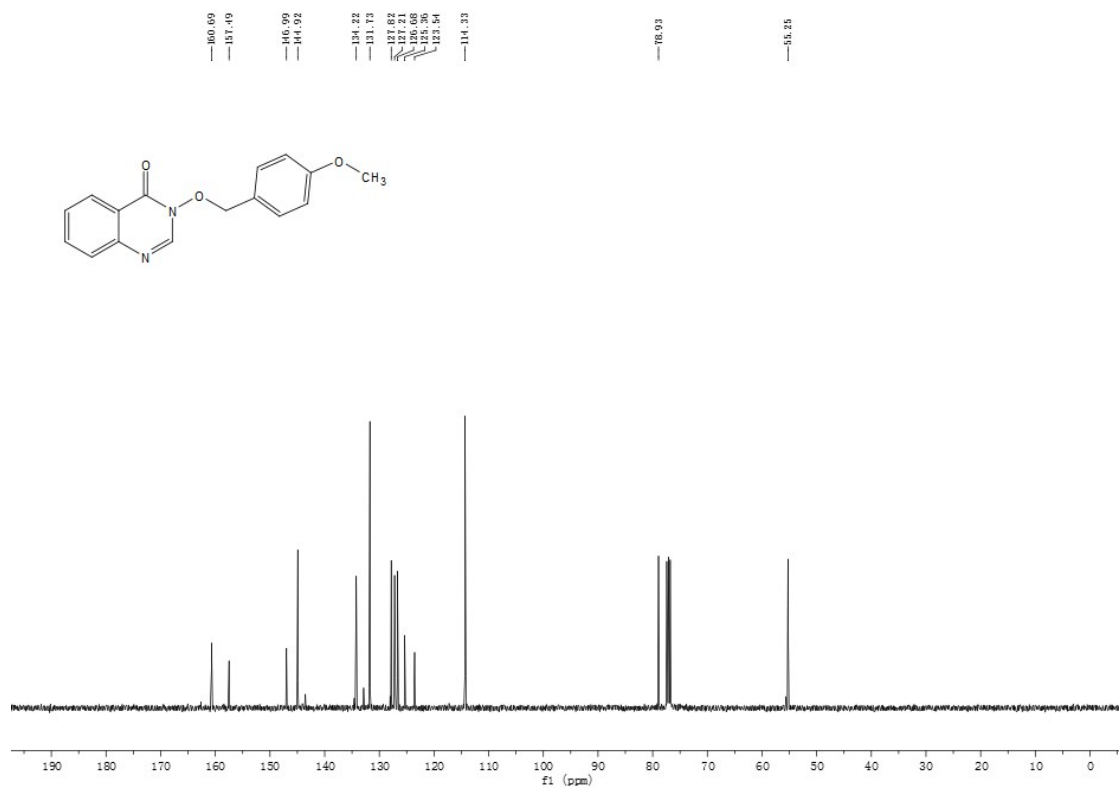
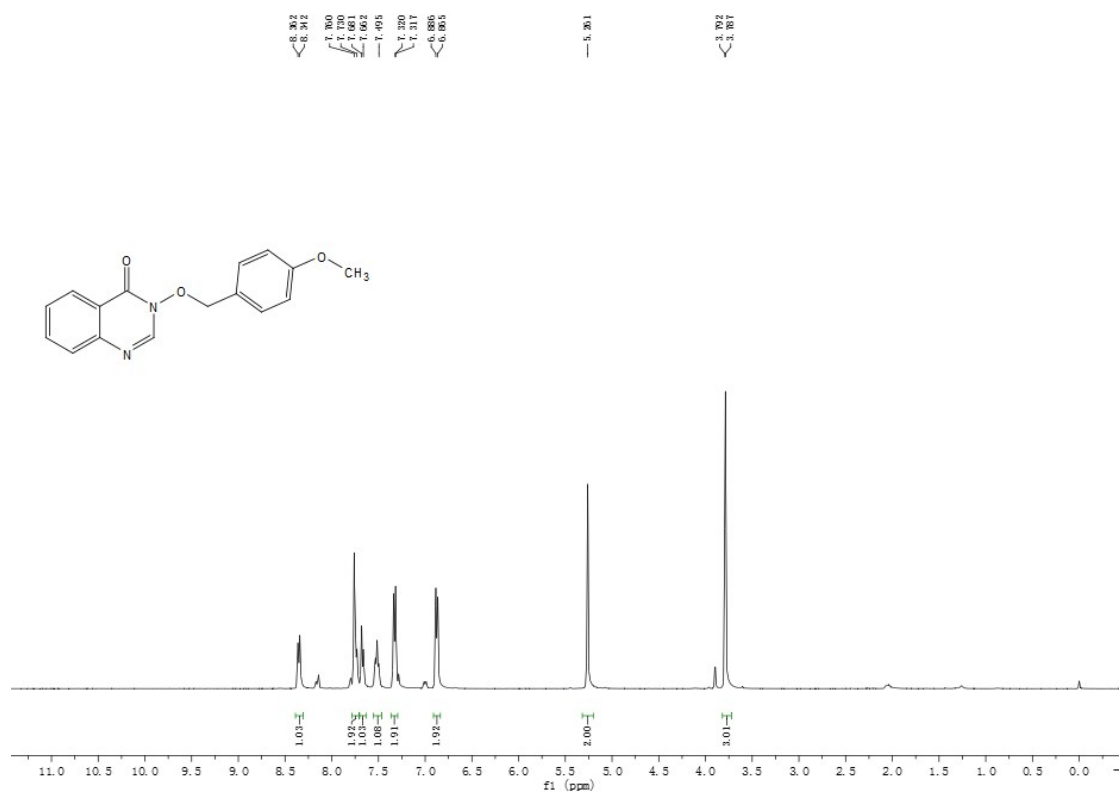
^1H NMR and ^{13}C NMR for compound **3e**



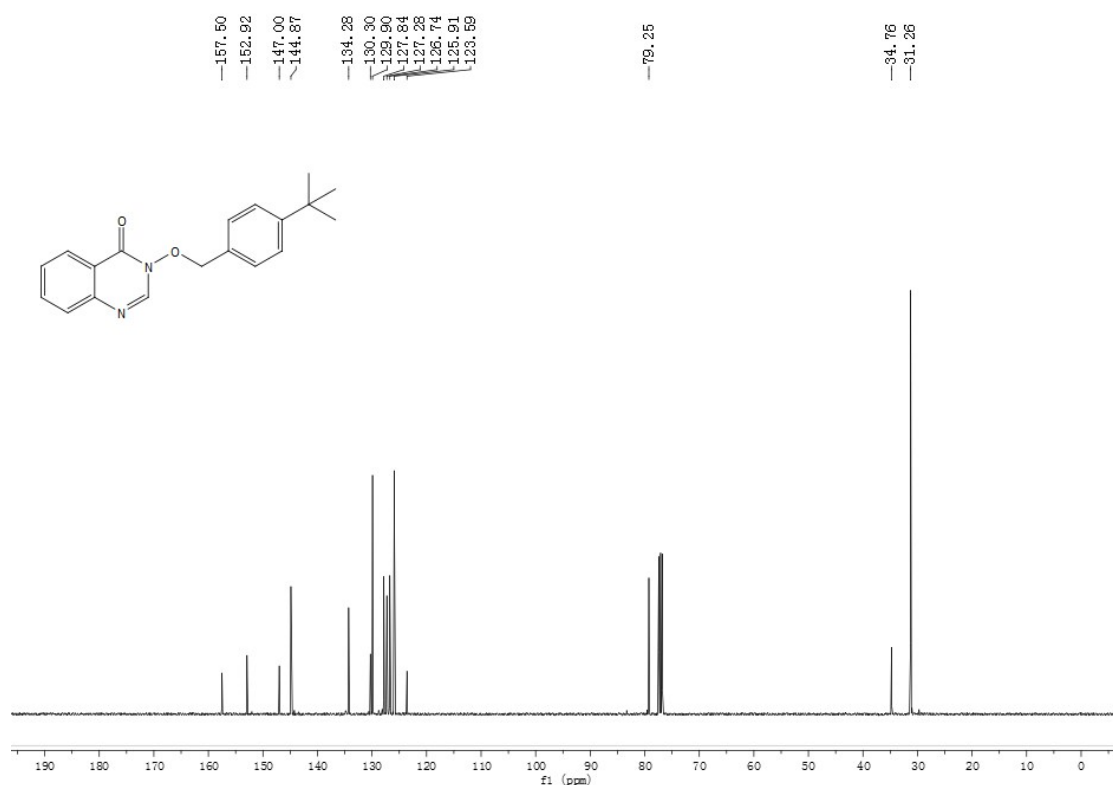
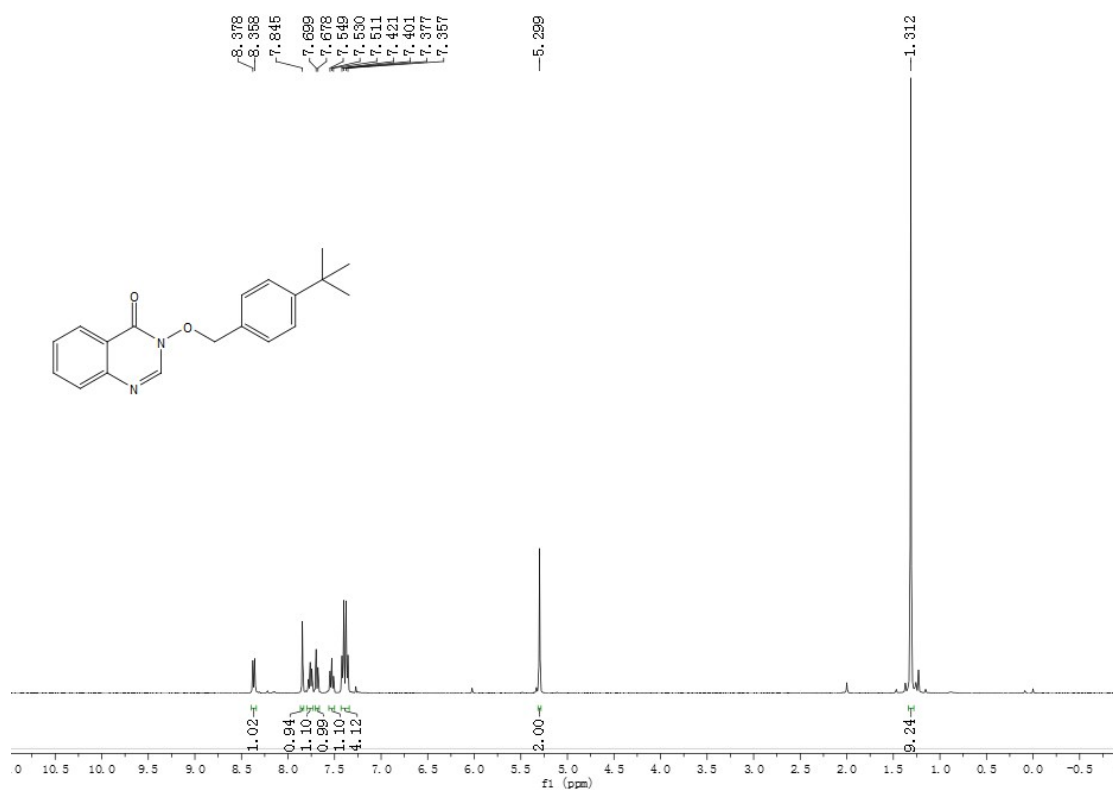
^1H NMR and ^{13}C NMR for compound **3f**



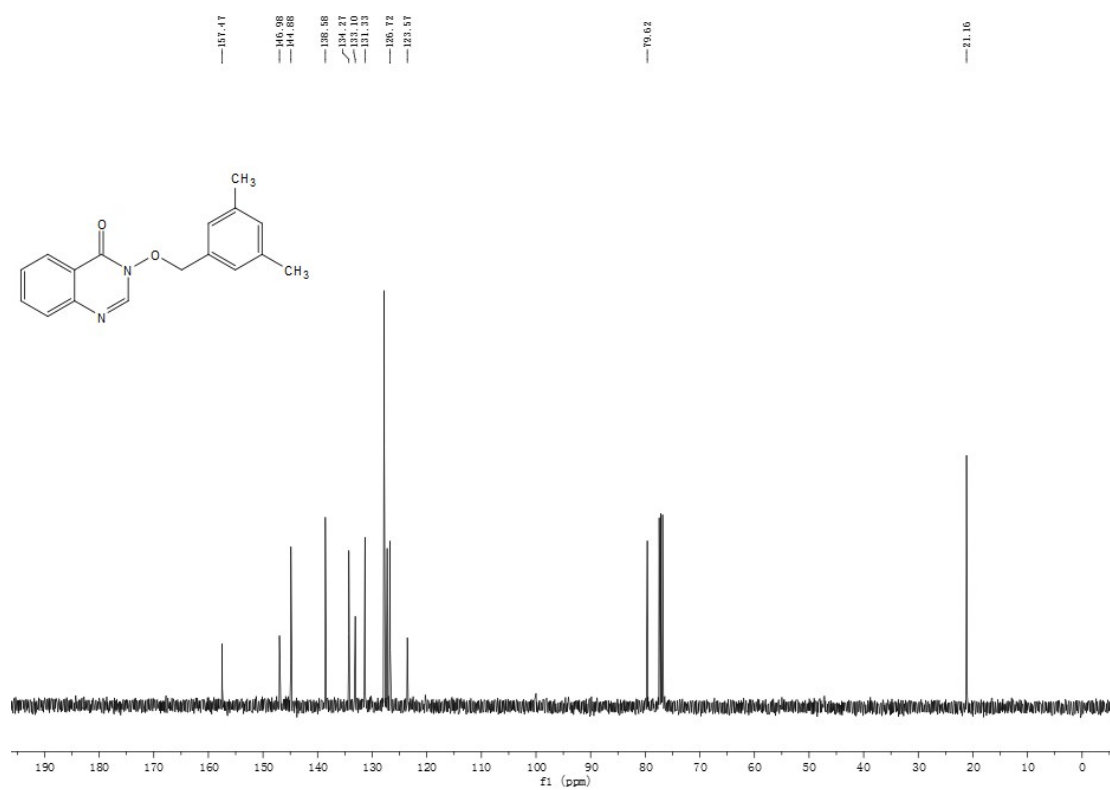
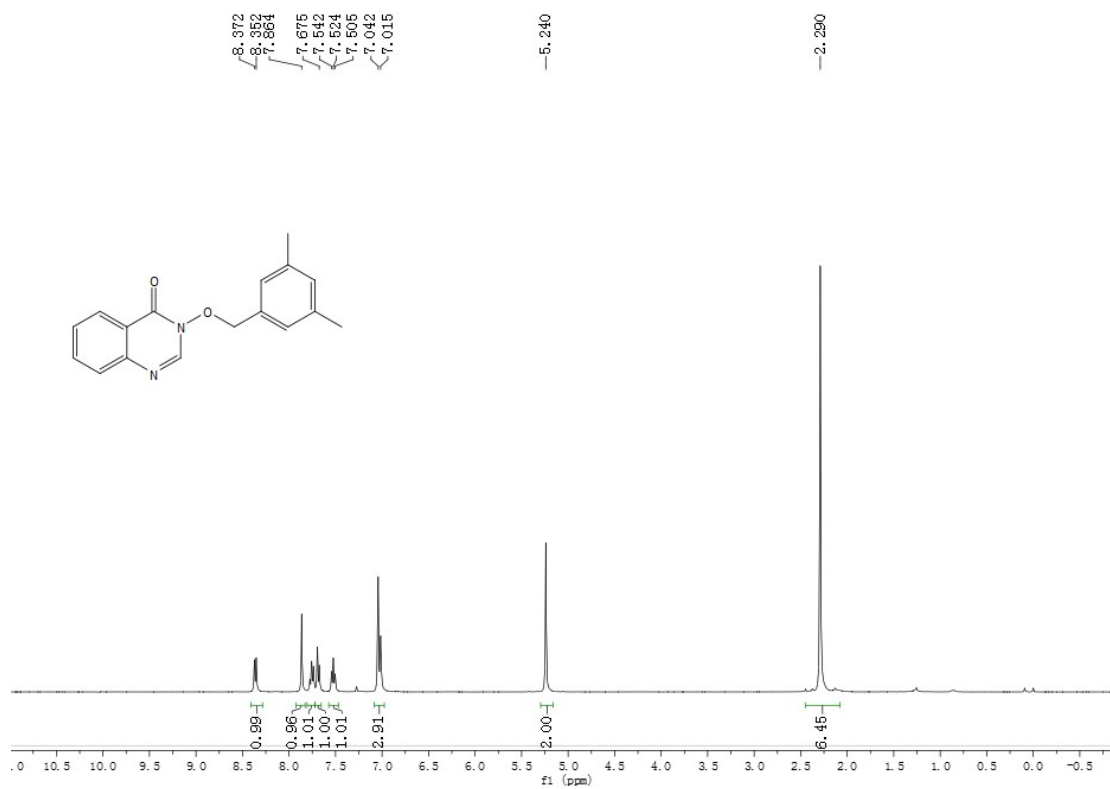
¹H NMR and ¹³C NMR for compound **3g**



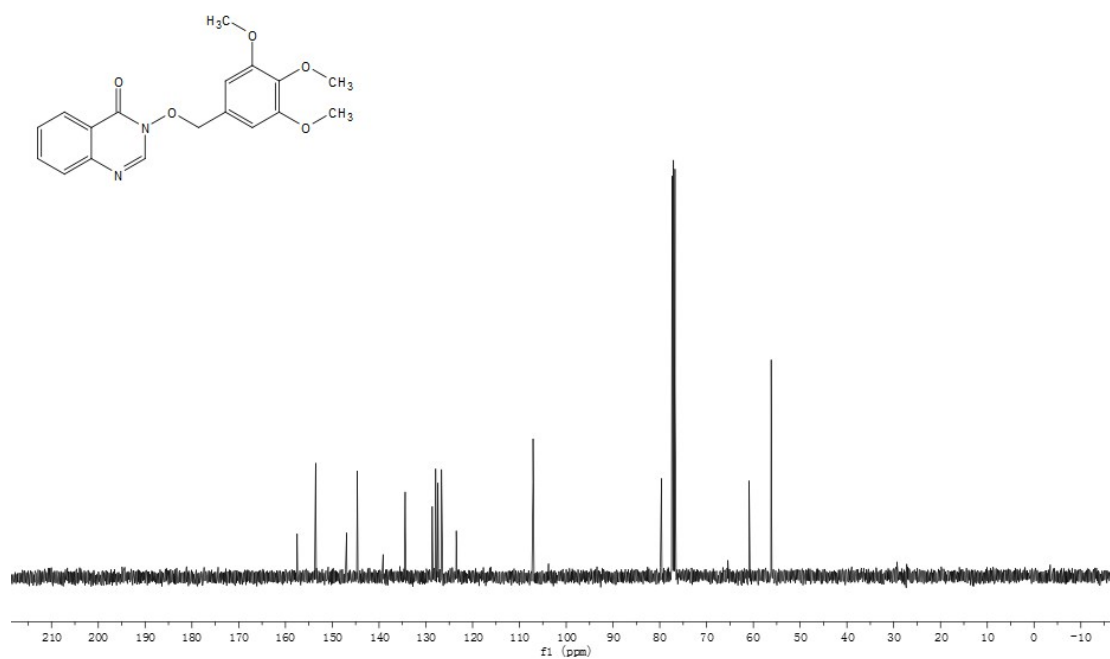
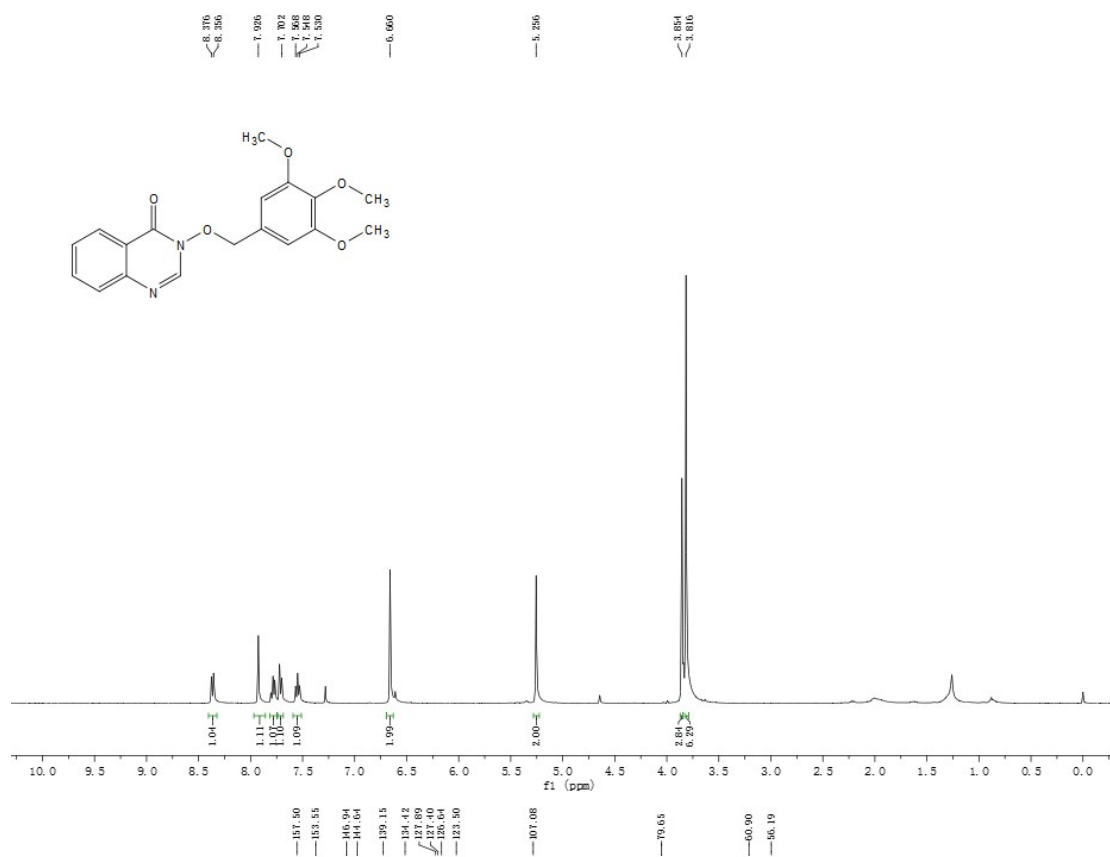
^1H NMR and ^{13}C NMR for compound **3h**



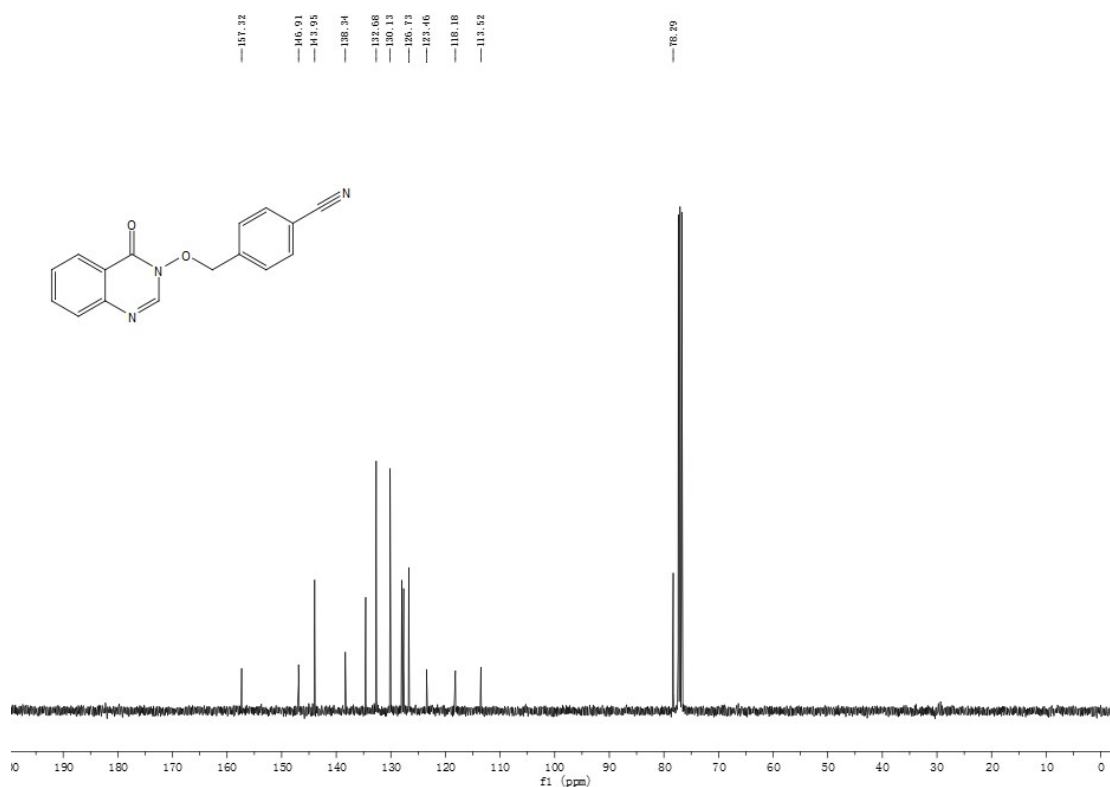
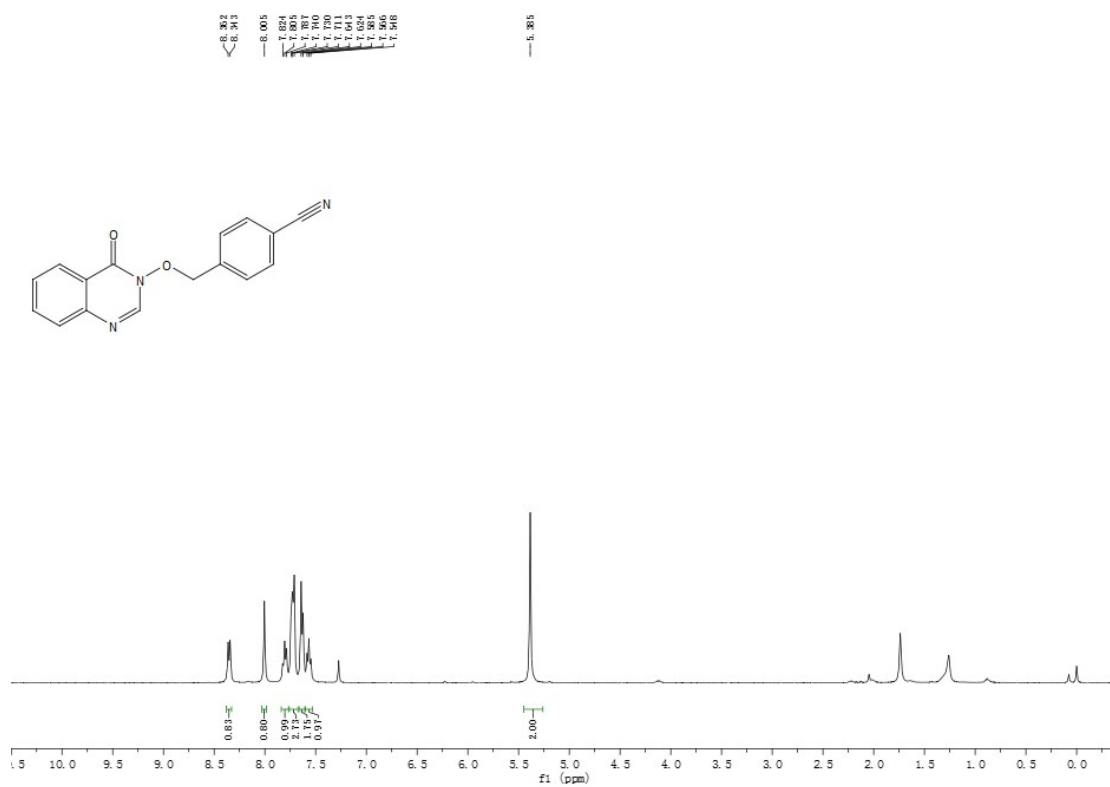
¹H NMR and ¹³C NMR for compound **3i**



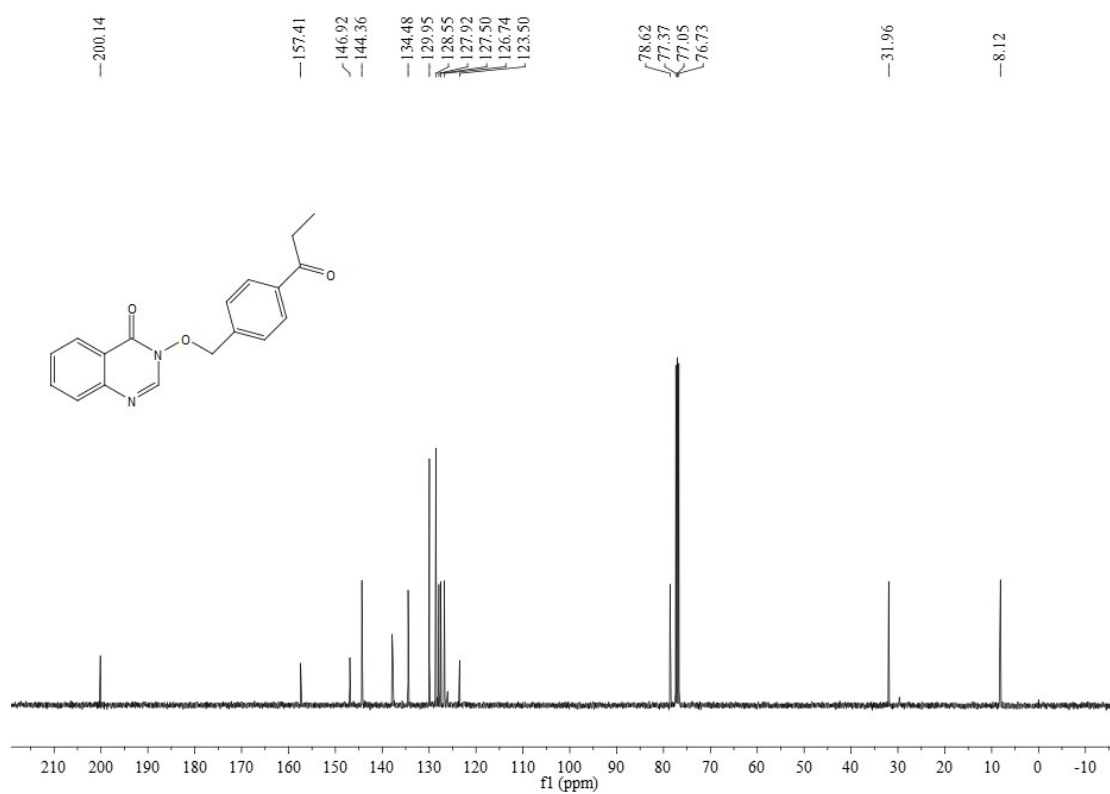
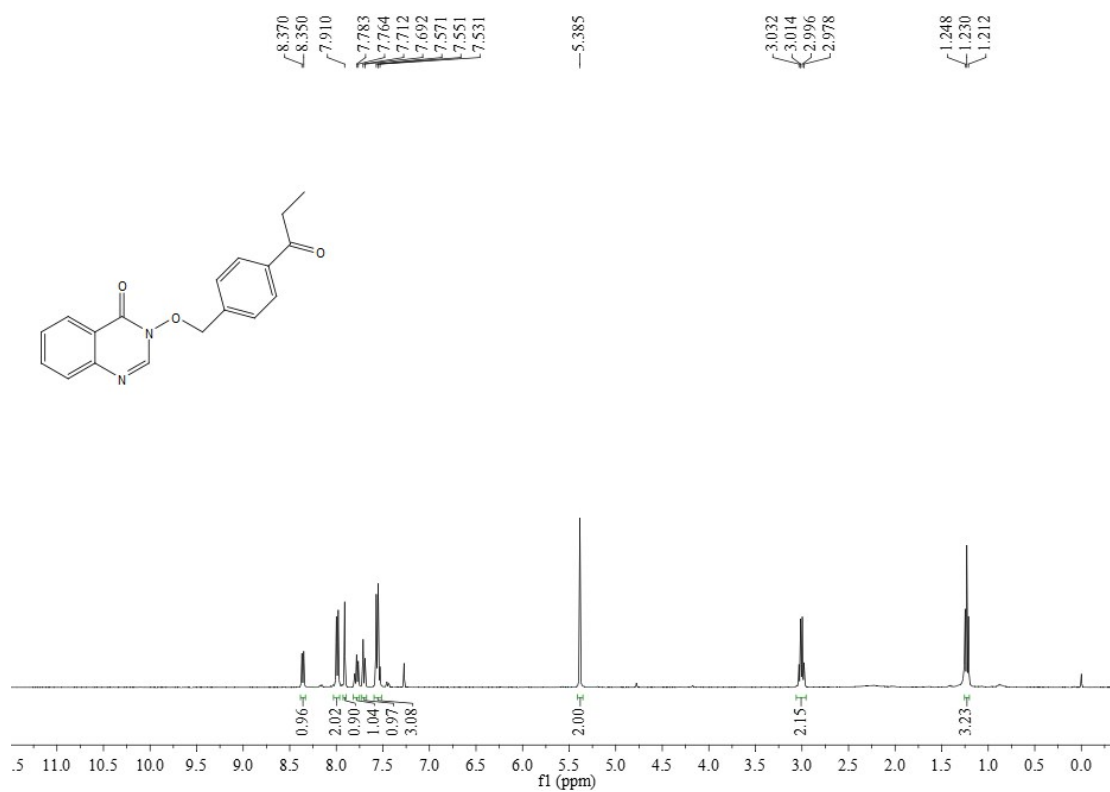
^1H NMR and ^{13}C NMR for compound **3j**



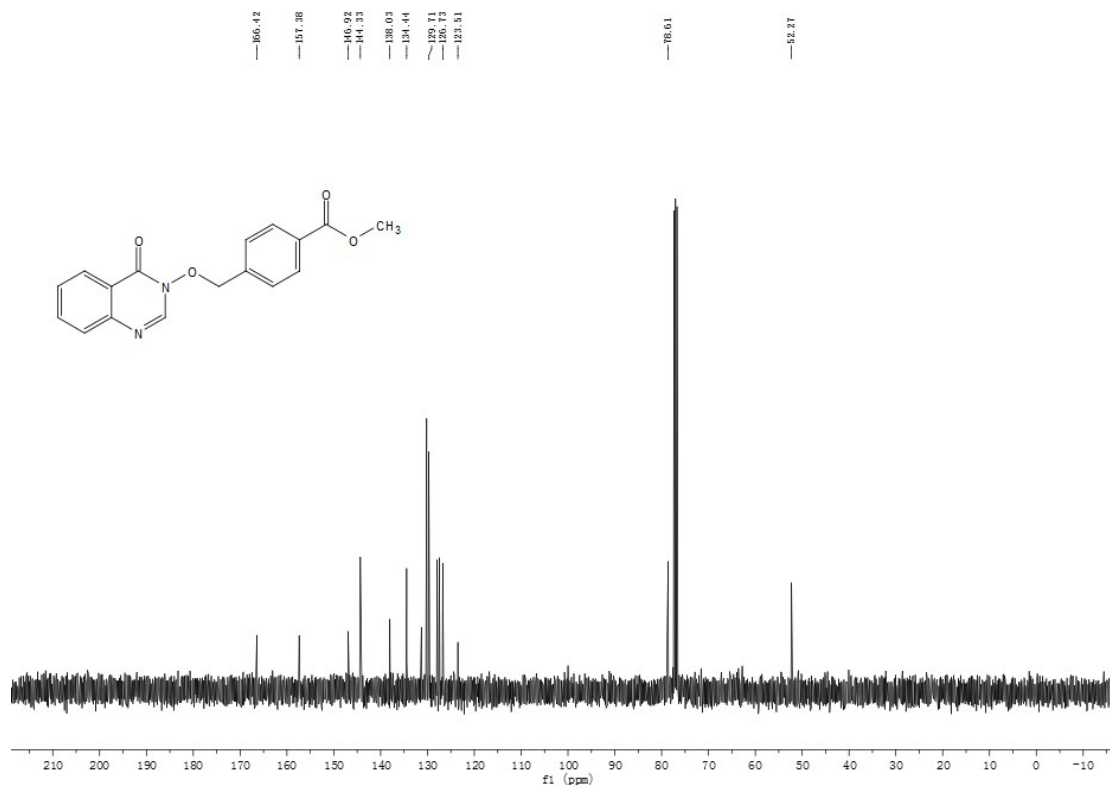
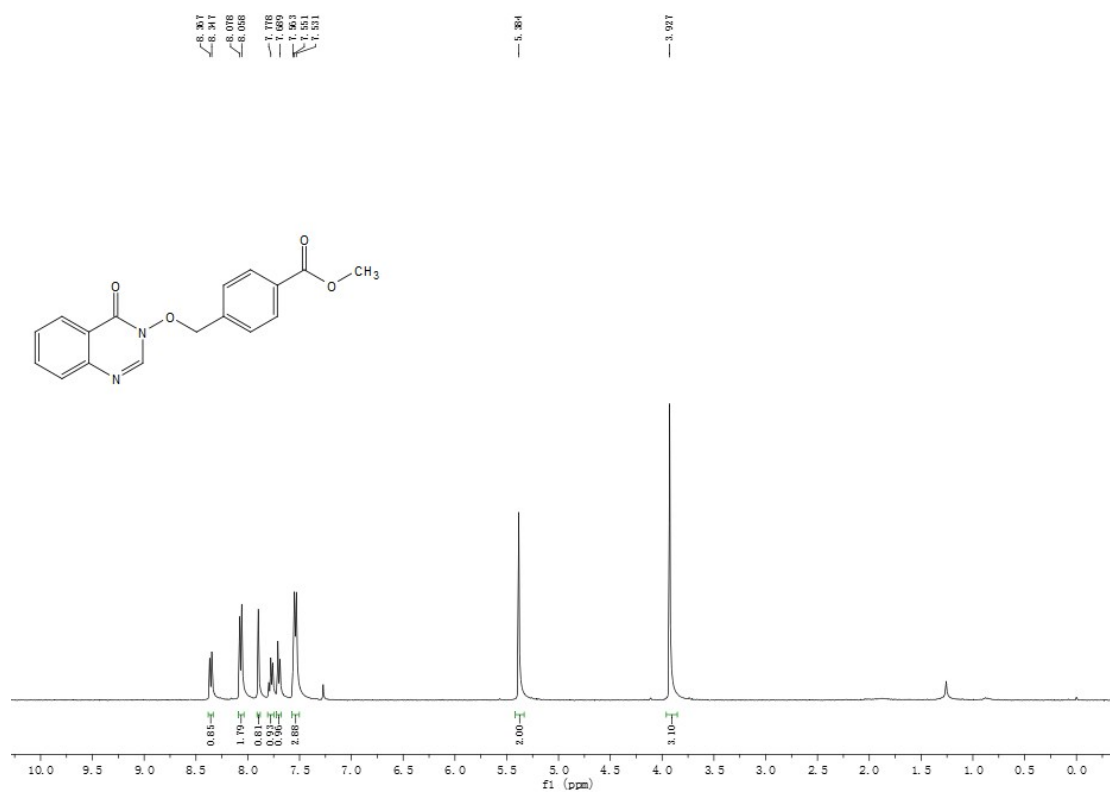
^1H NMR and ^{13}C NMR for compound **3k**



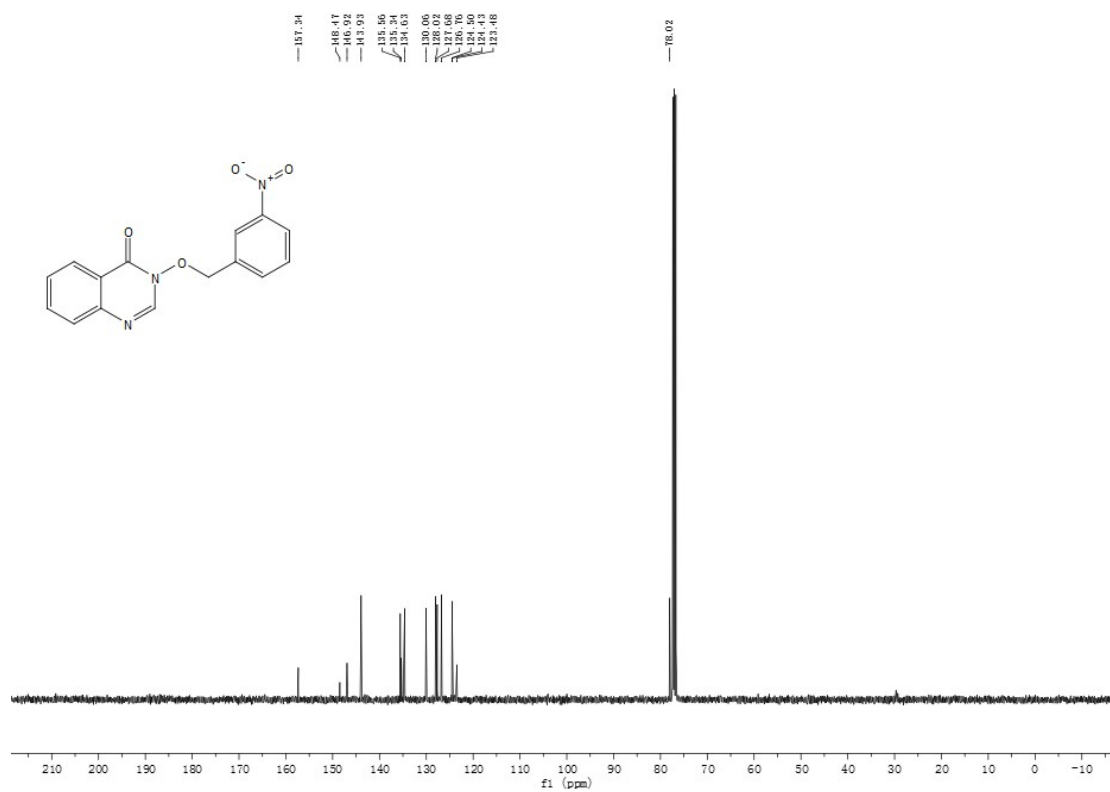
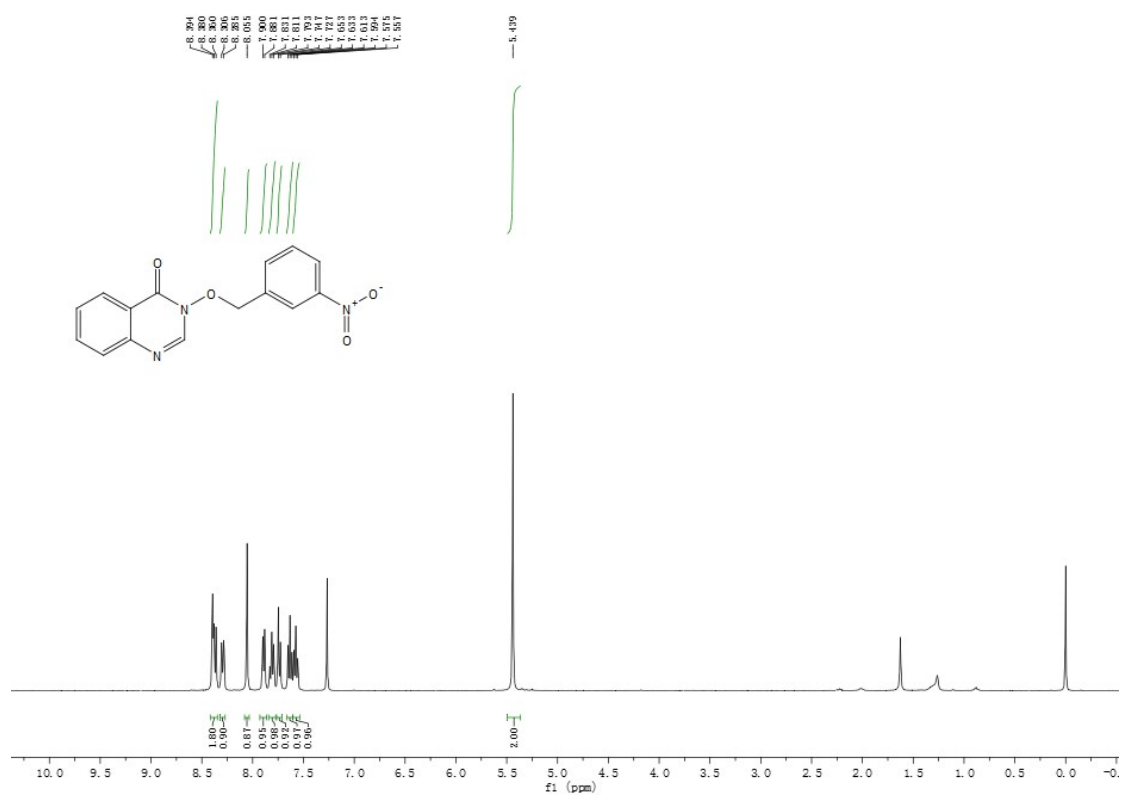
¹H NMR and ¹³C NMR for compound **31**



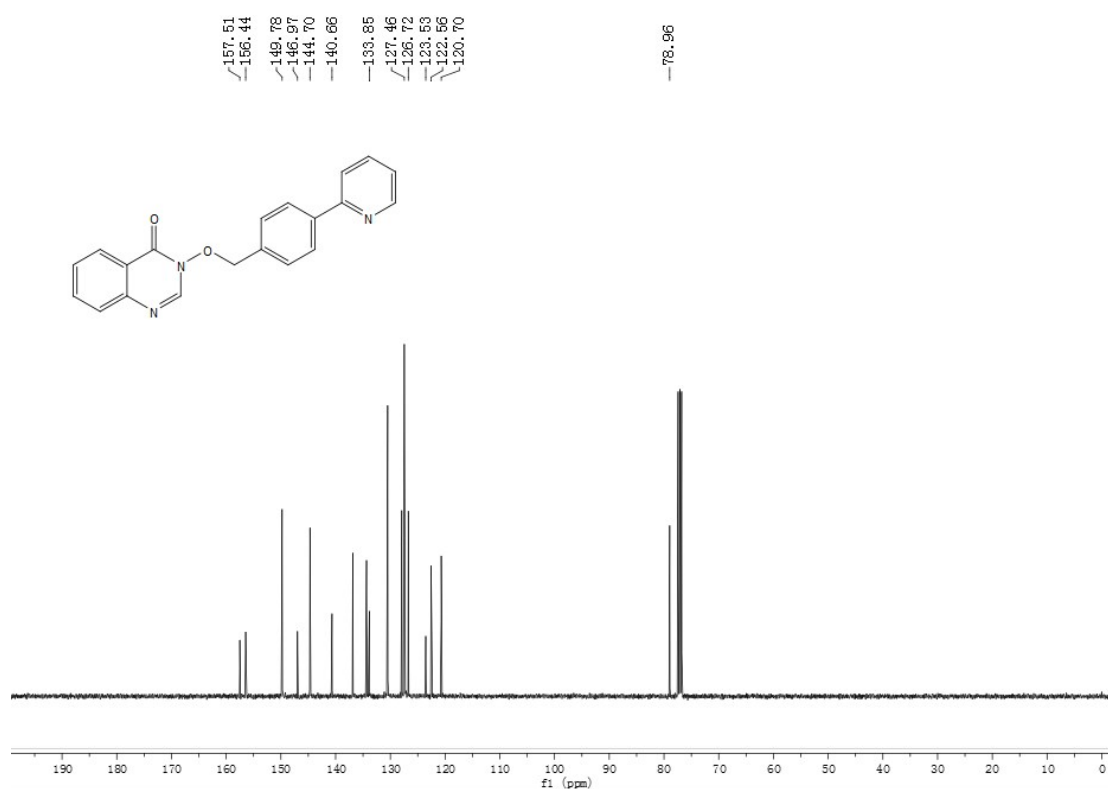
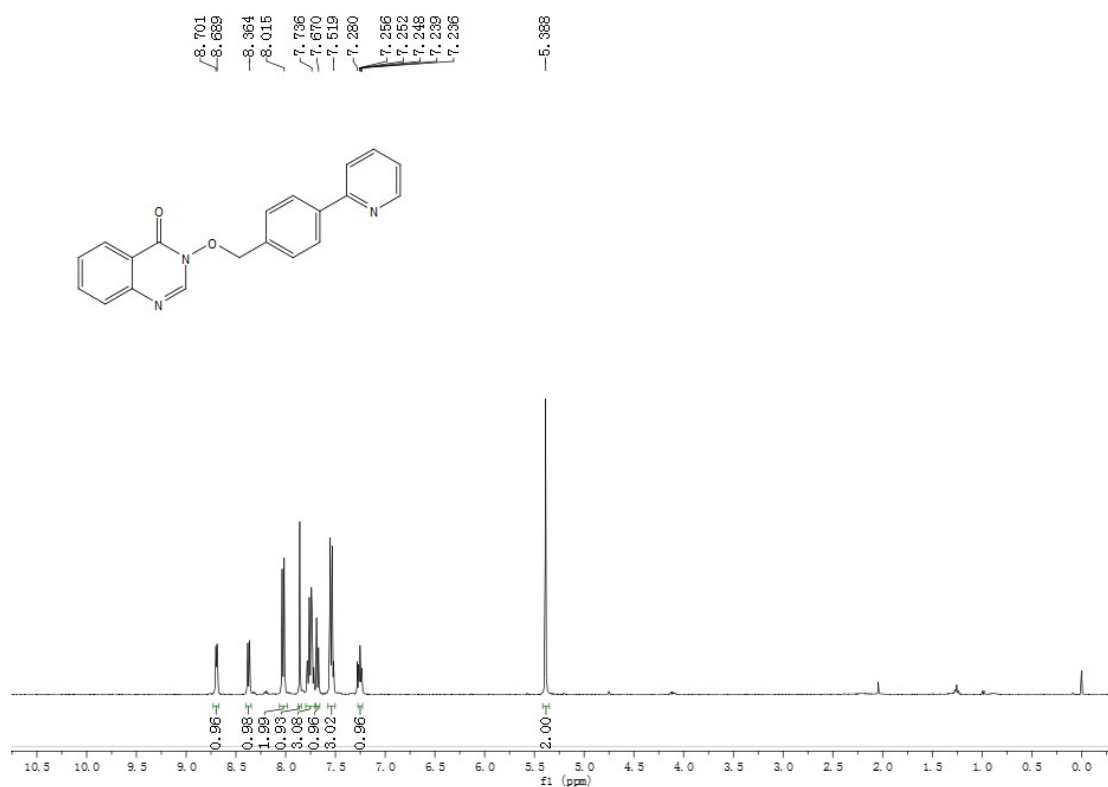
^1H NMR and ^{13}C NMR for compound **3m**



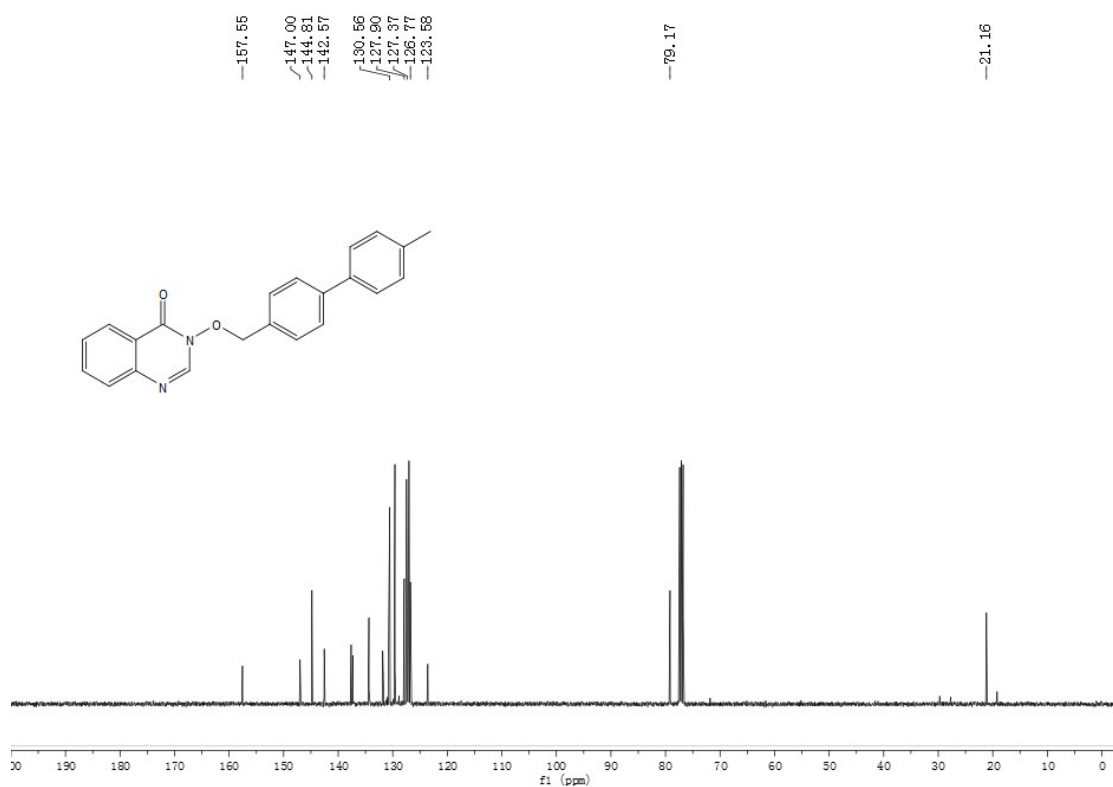
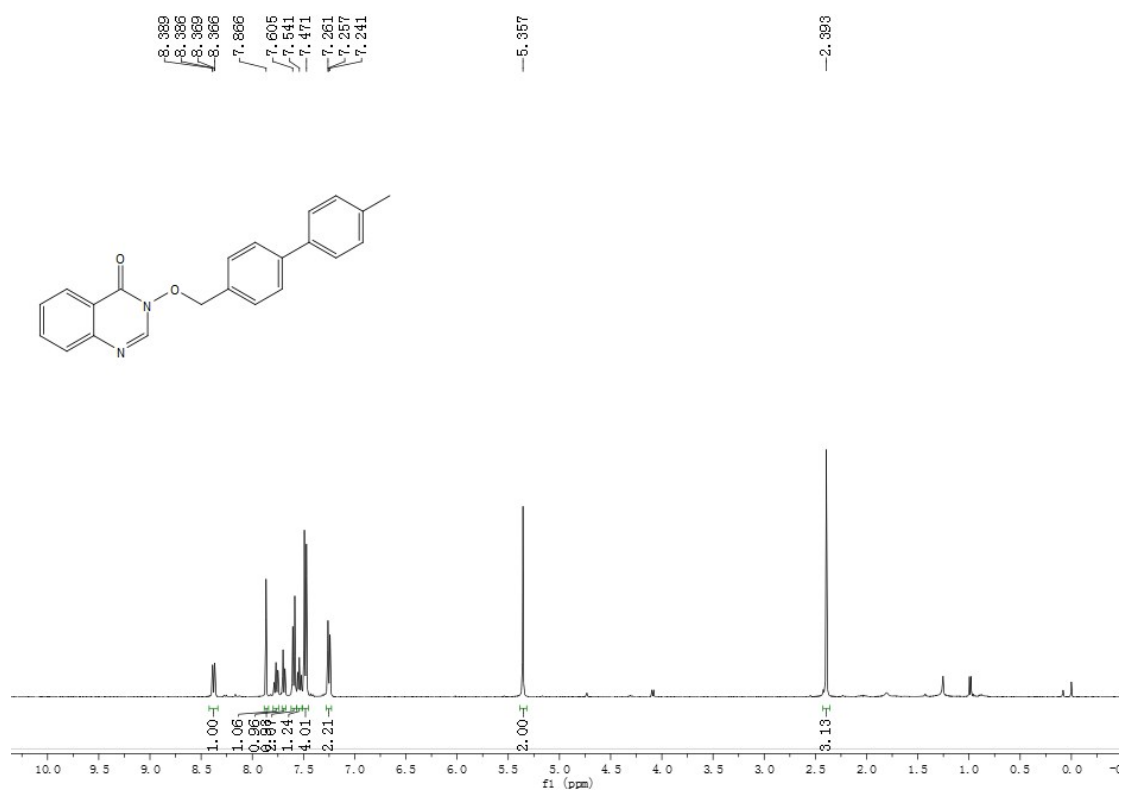
¹H NMR and ¹³C NMR for compound **3n**



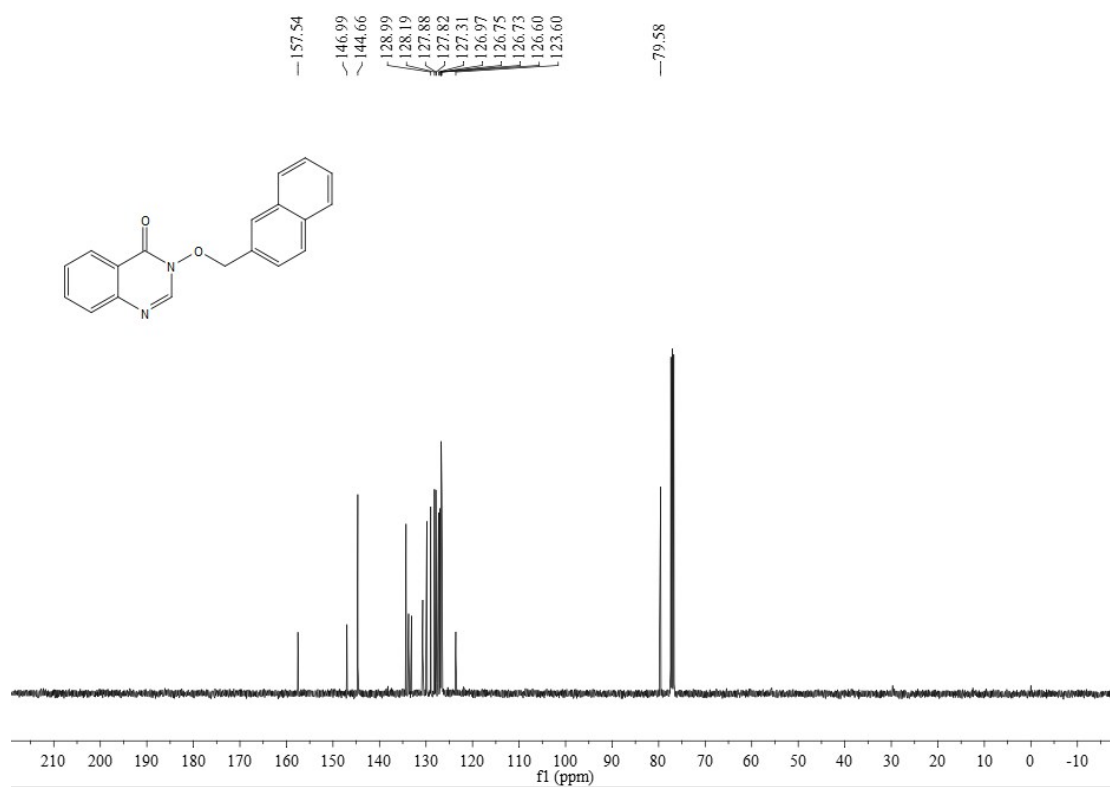
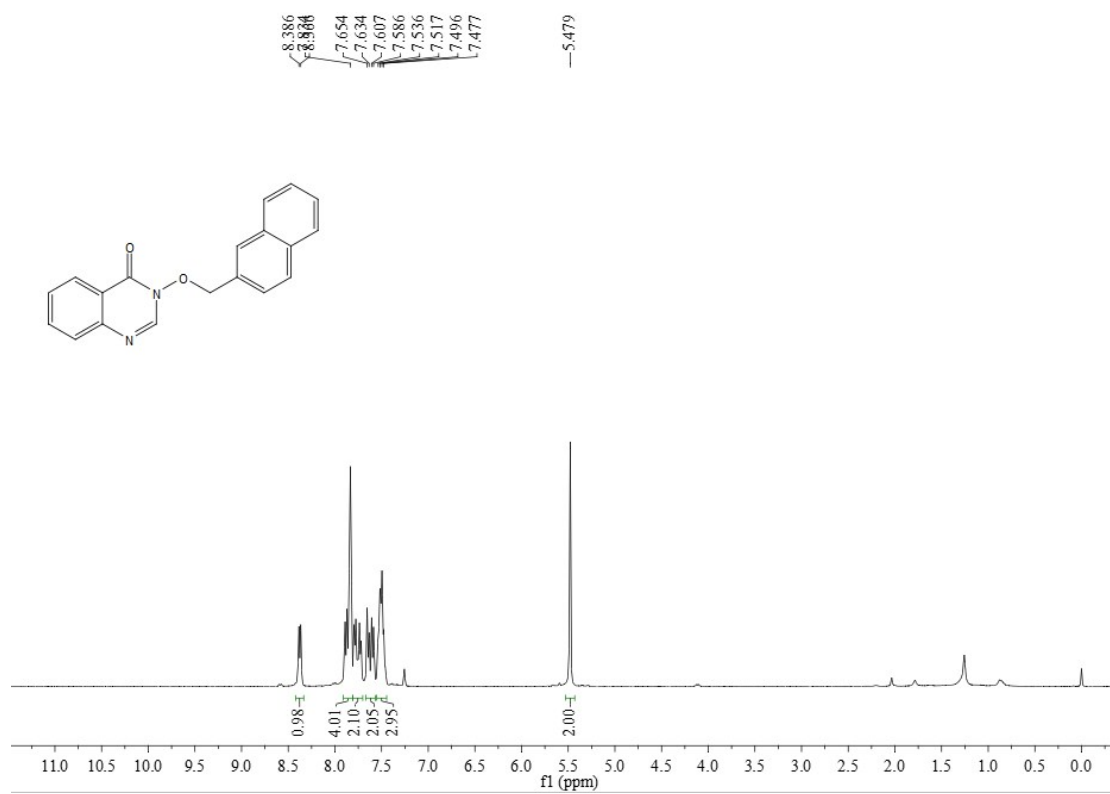
¹H NMR and ¹³C NMR for compound **3o**



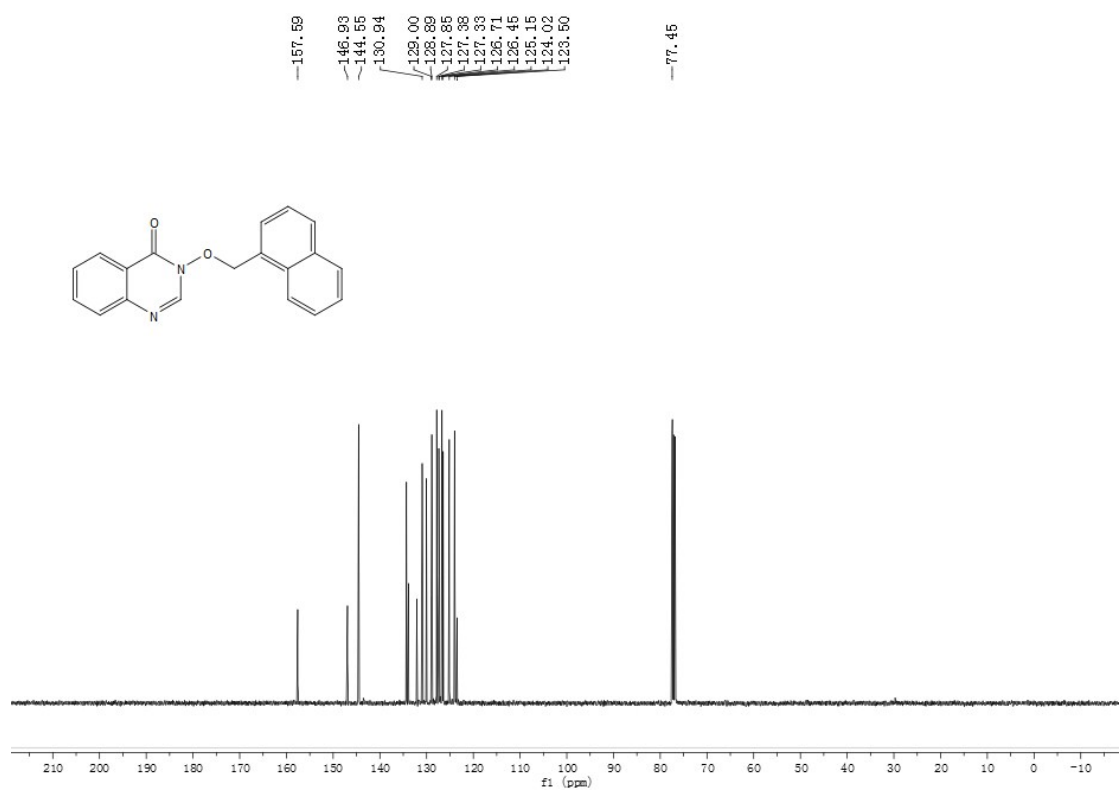
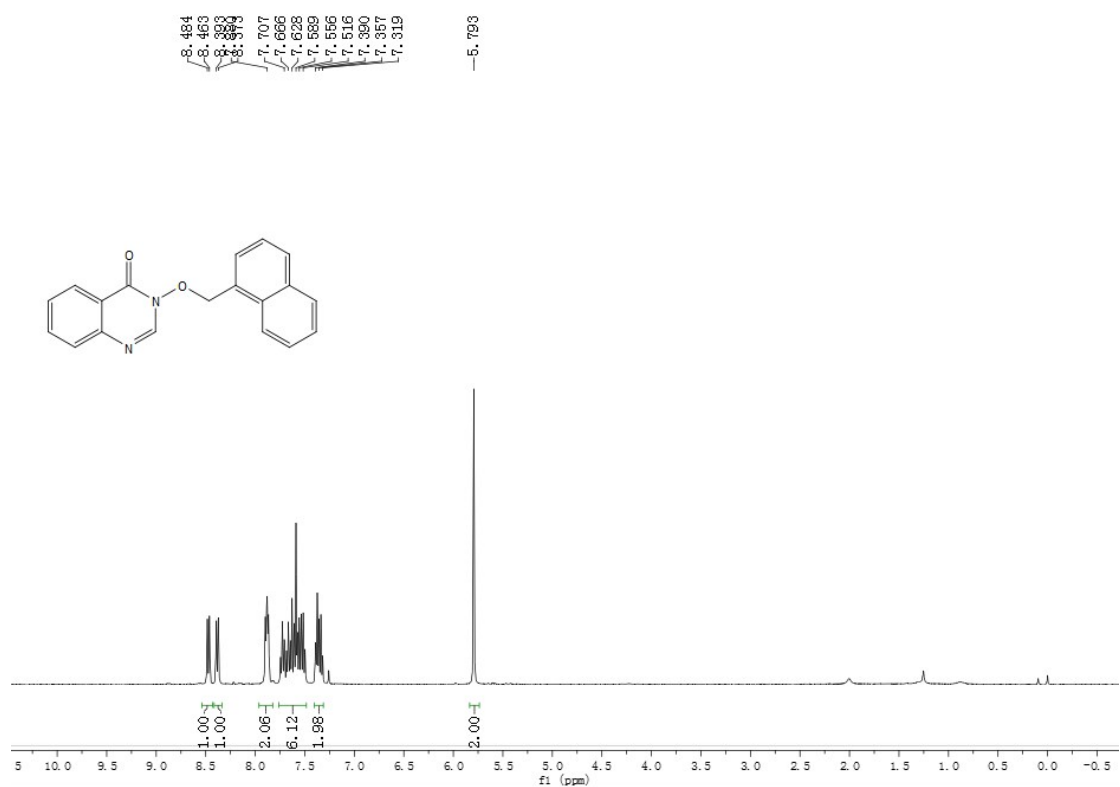
^1H NMR and ^{13}C NMR for compound **3p**



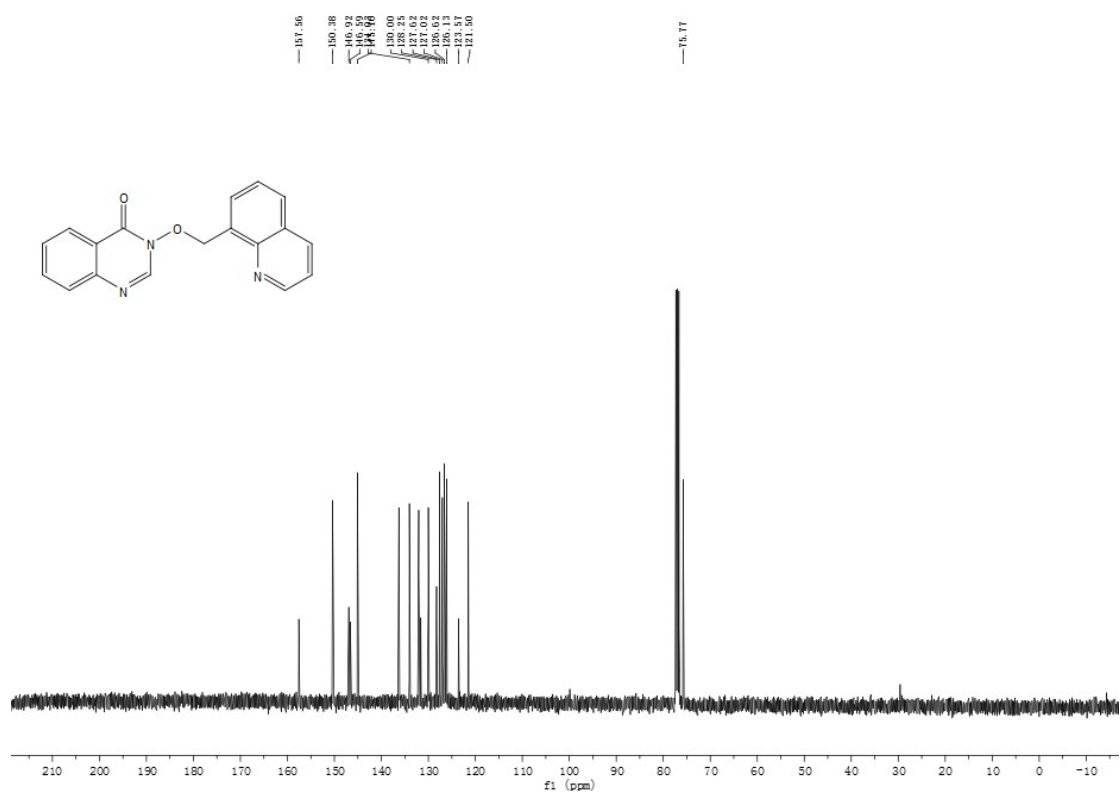
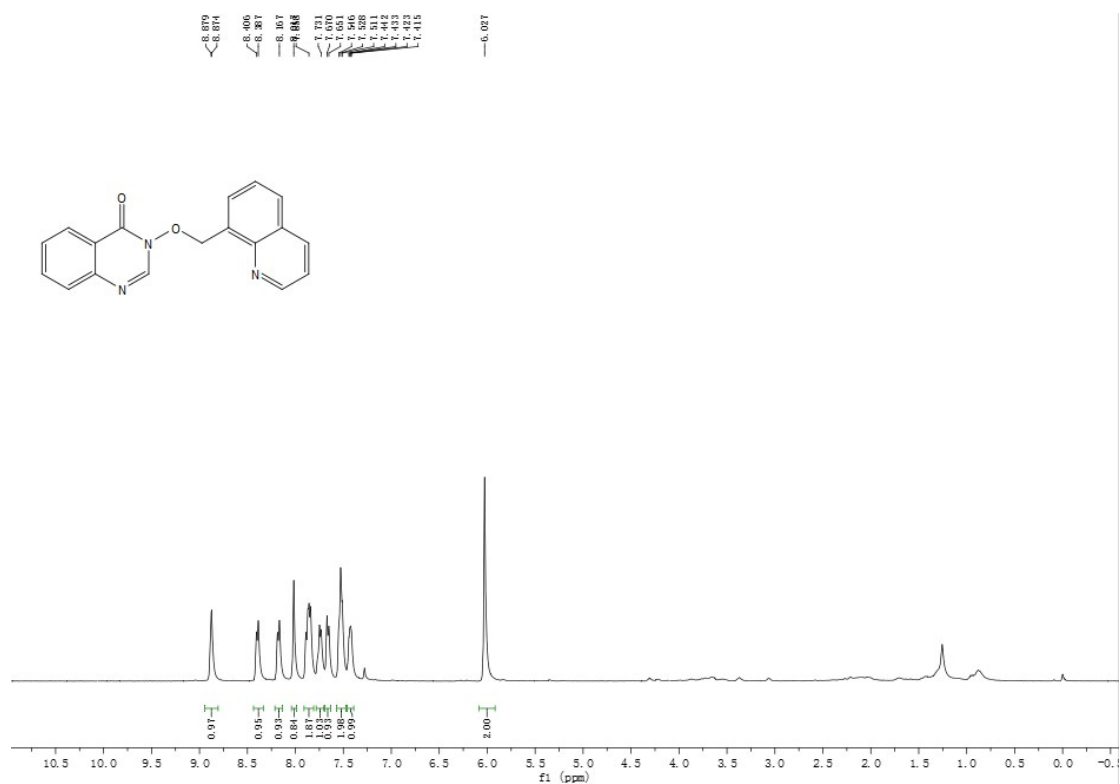
^1H NMR and ^{13}C NMR for compound **3q**



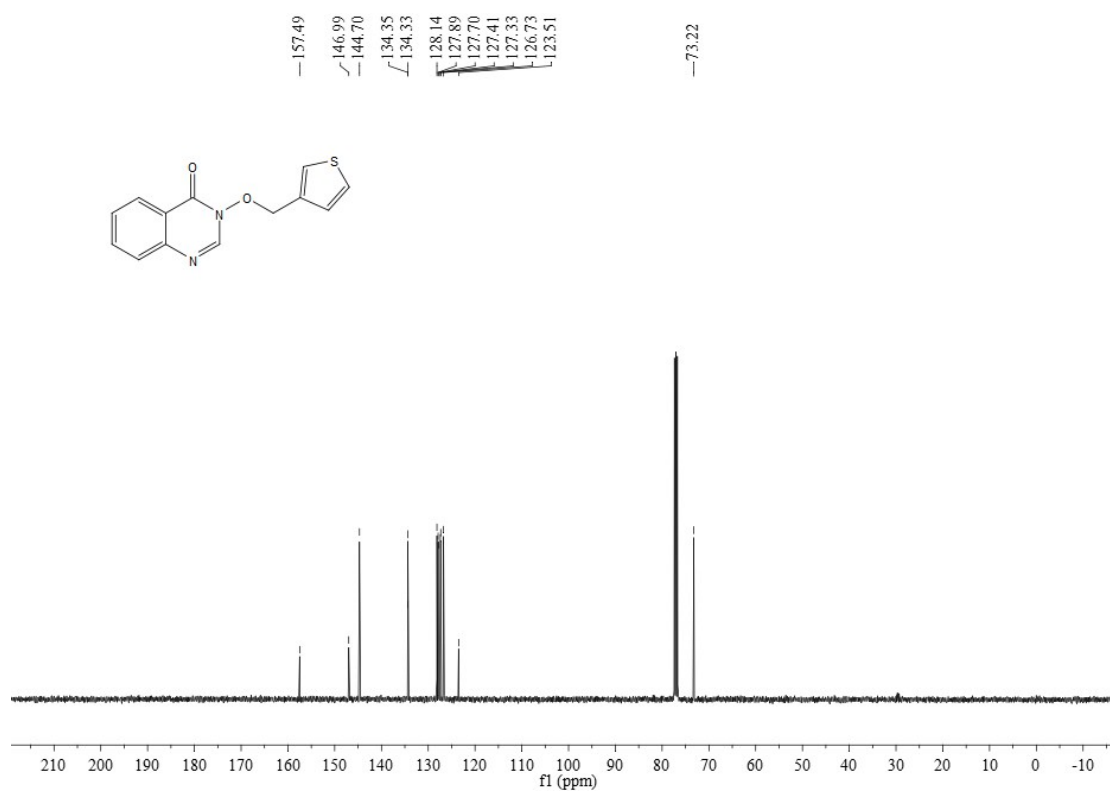
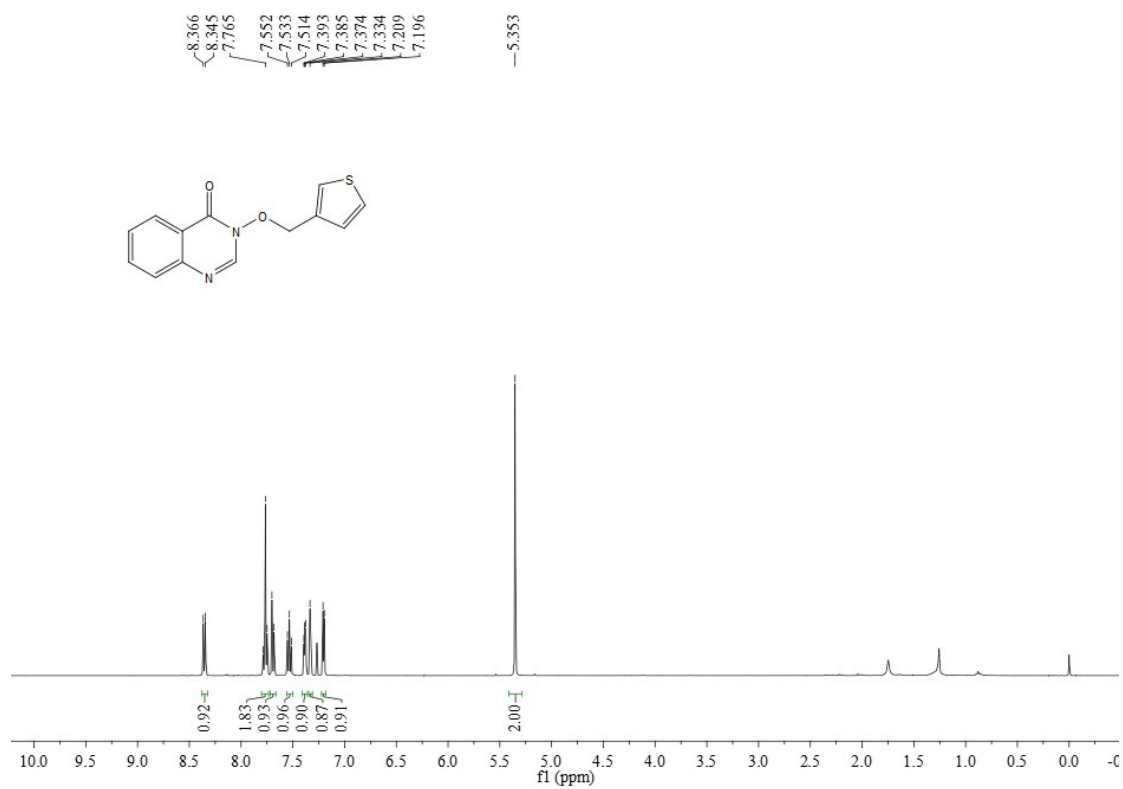
^1H NMR and ^{13}C NMR for compound **3r**



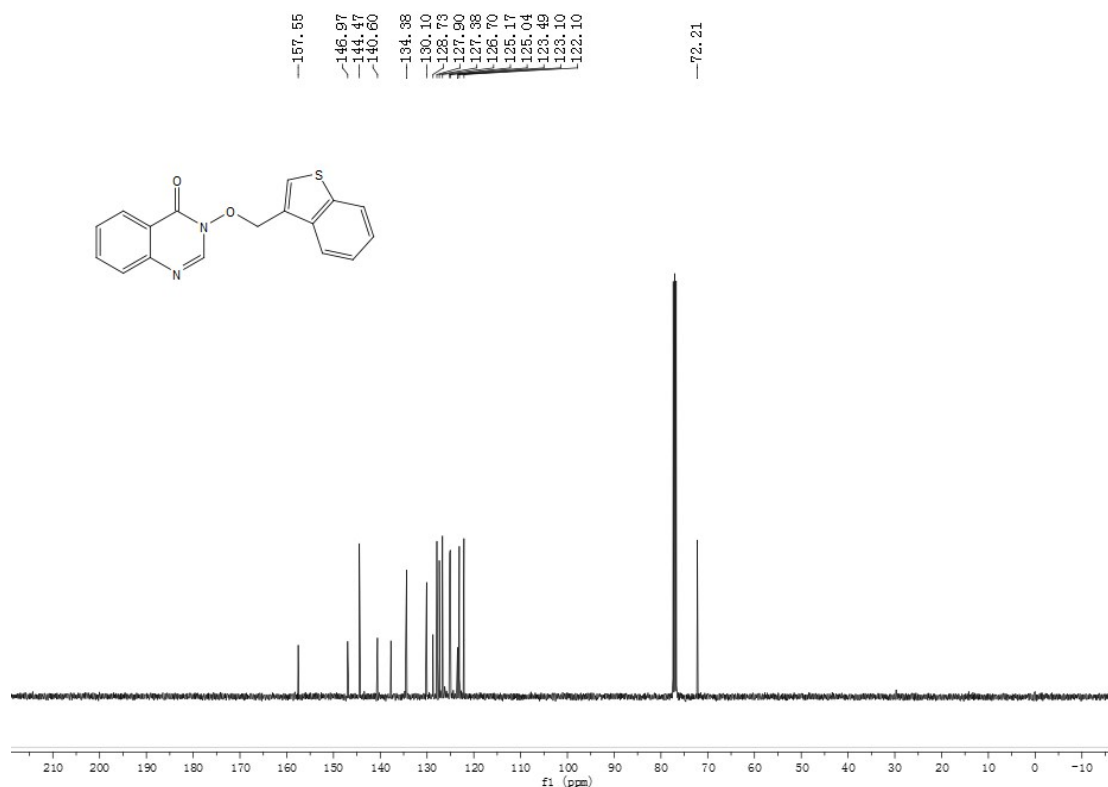
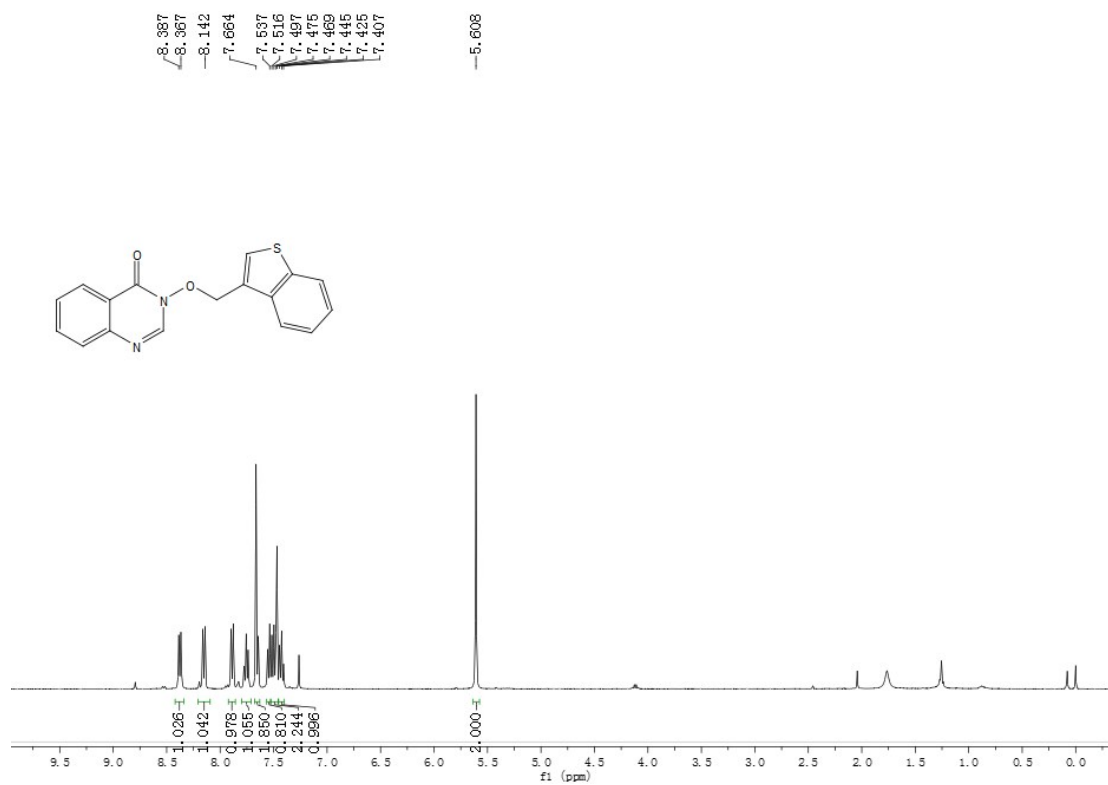
¹H NMR and ¹³C NMR for compound **3s**



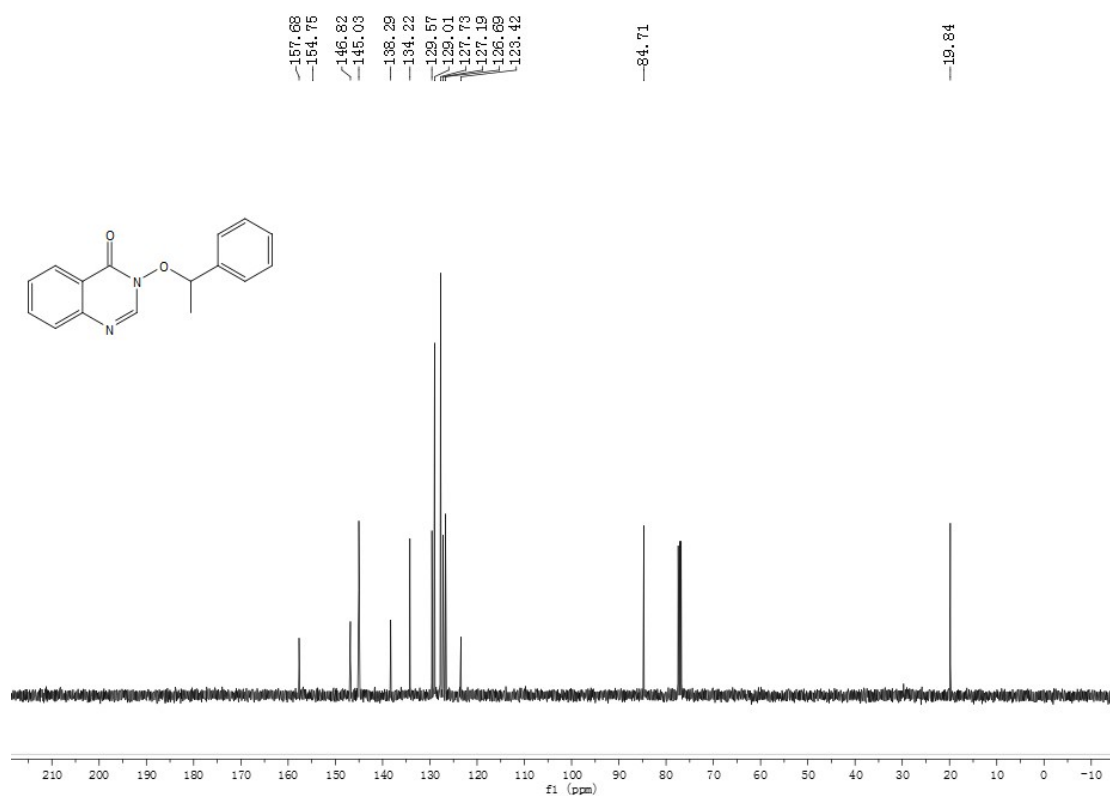
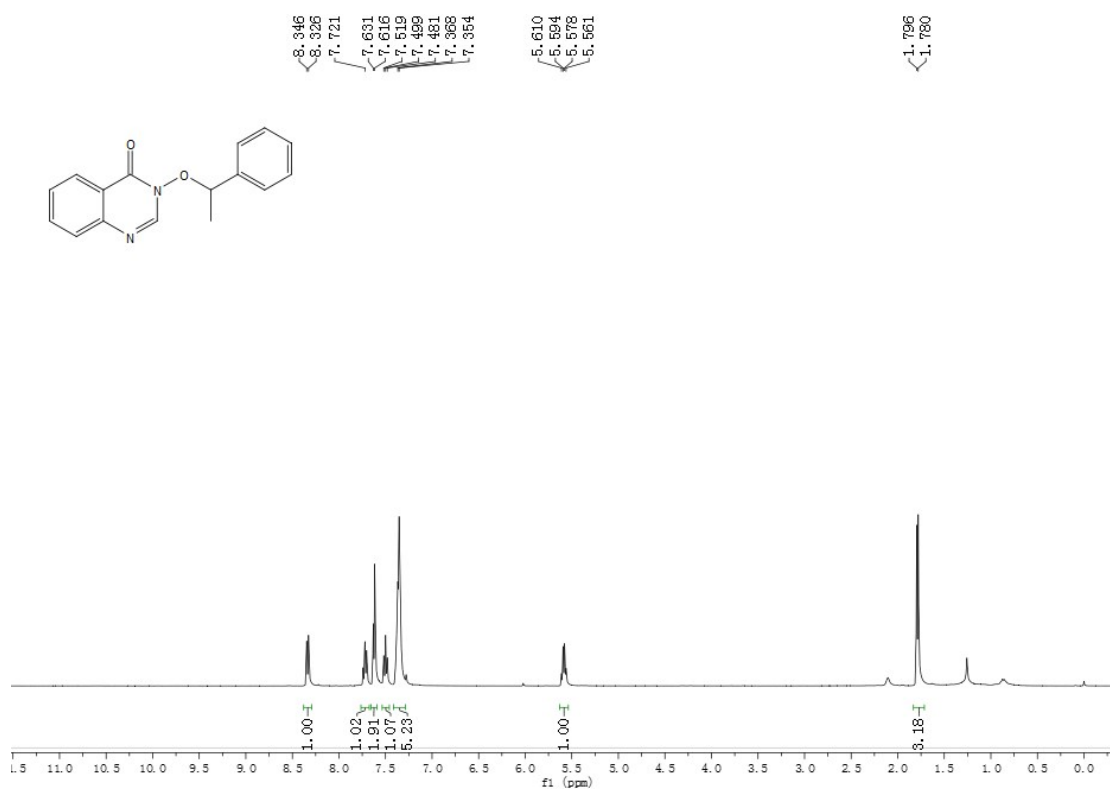
^1H NMR and ^{13}C NMR for compound **3t**



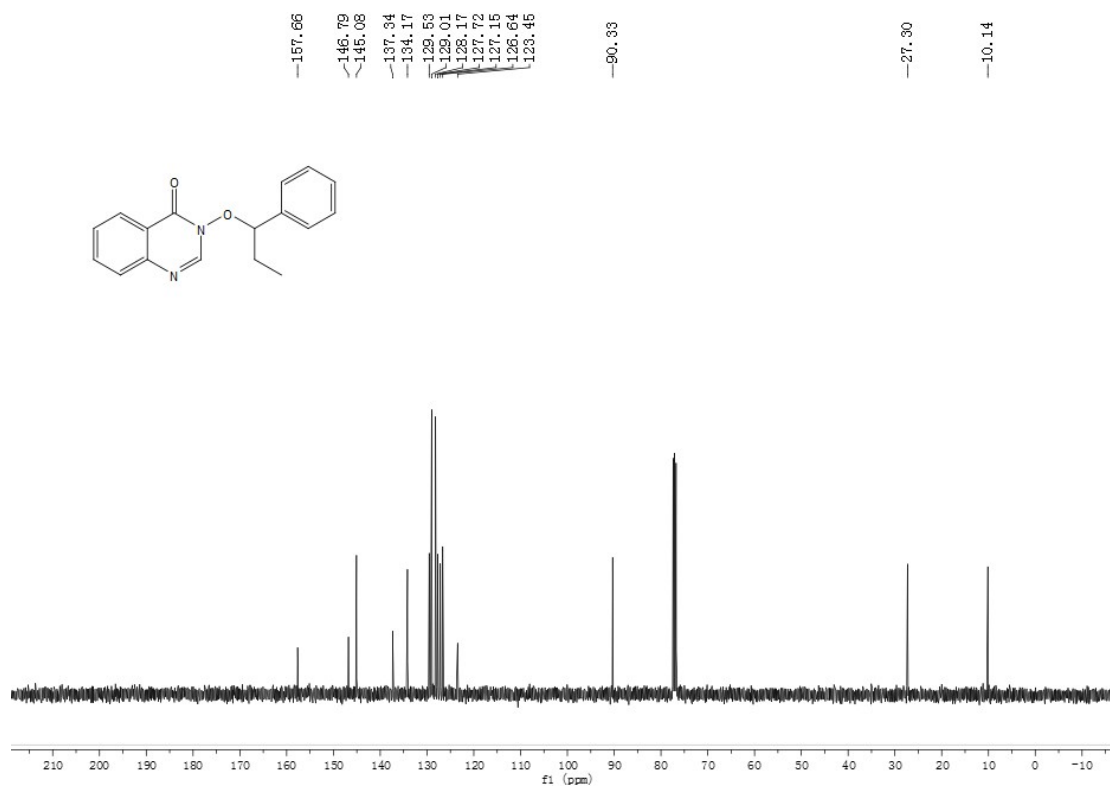
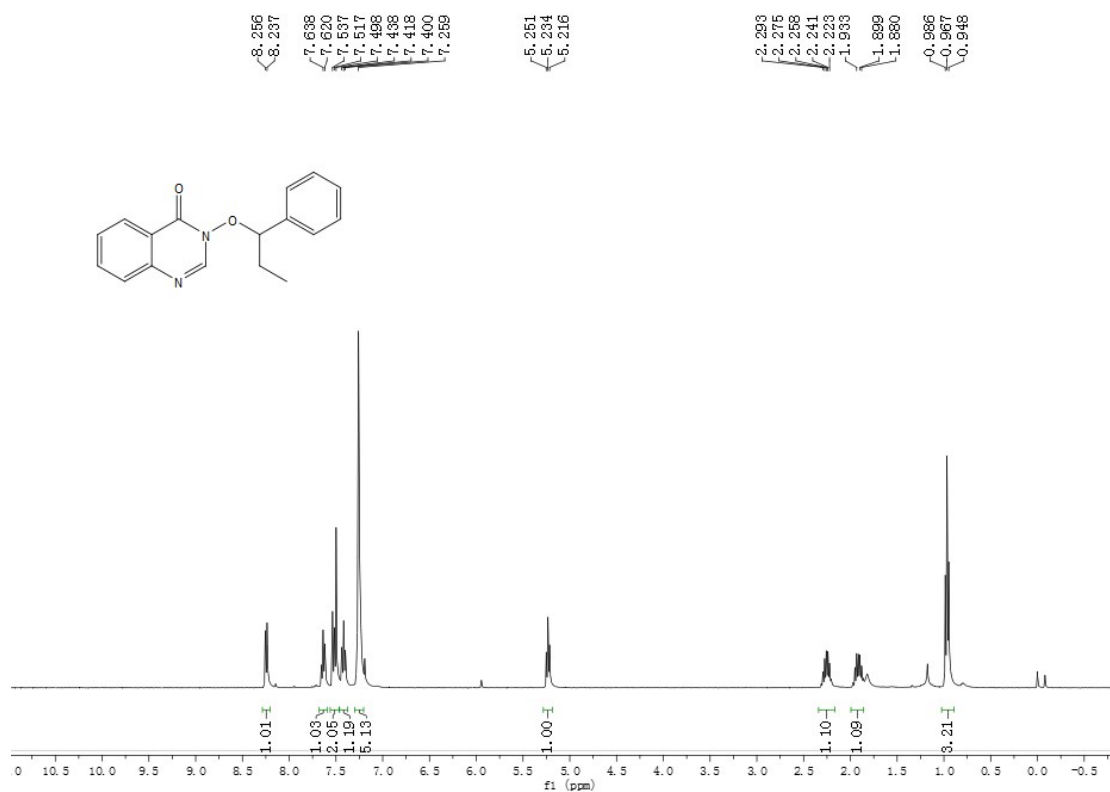
¹H NMR and ¹³C NMR for compound **3v**



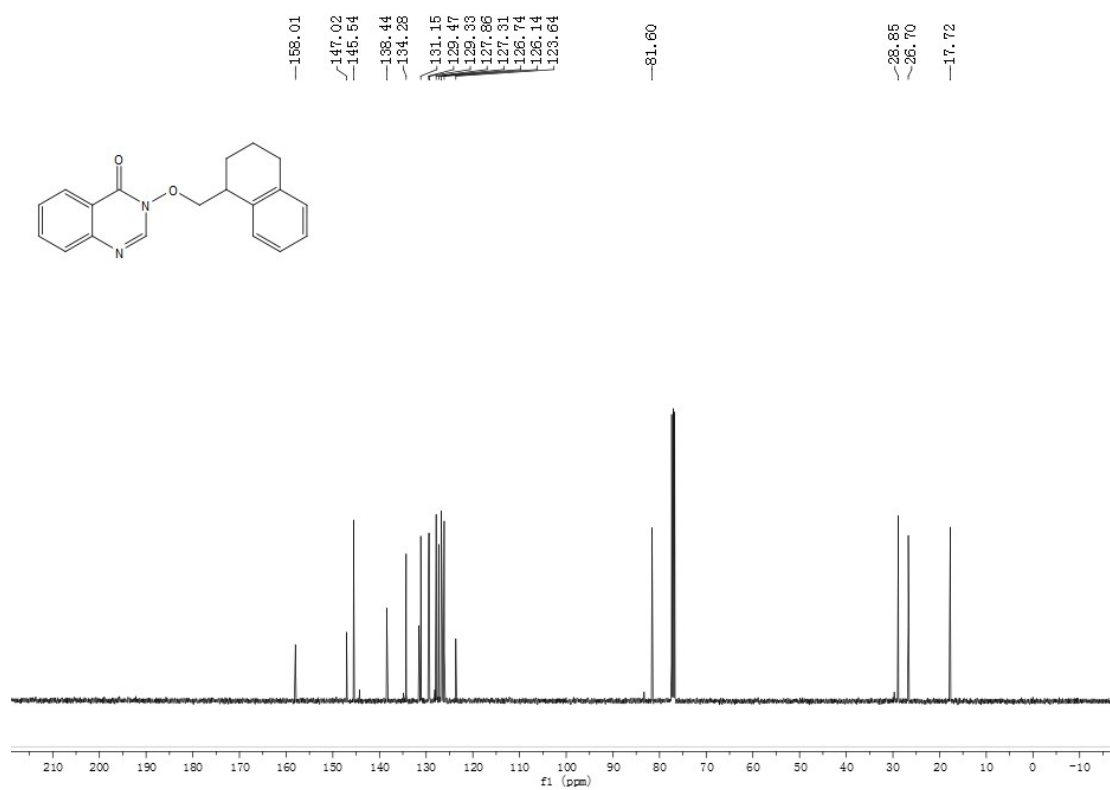
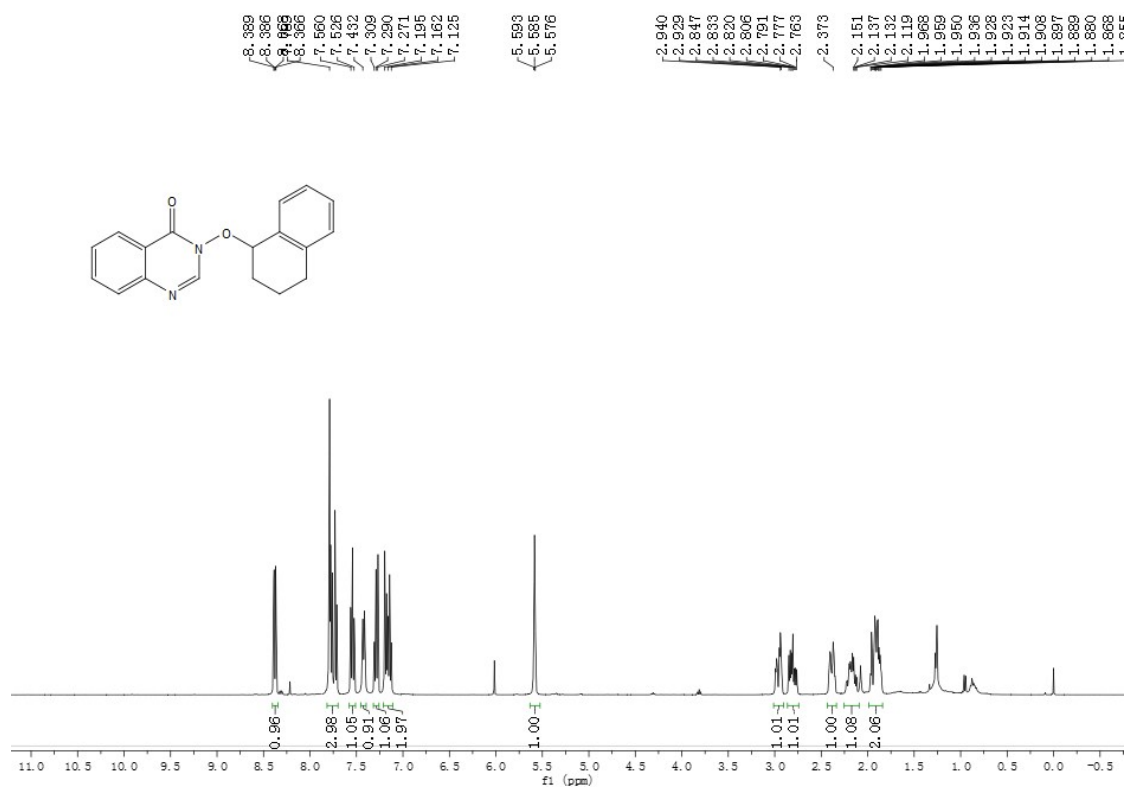
¹H NMR and ¹³C NMR for compound **3w**



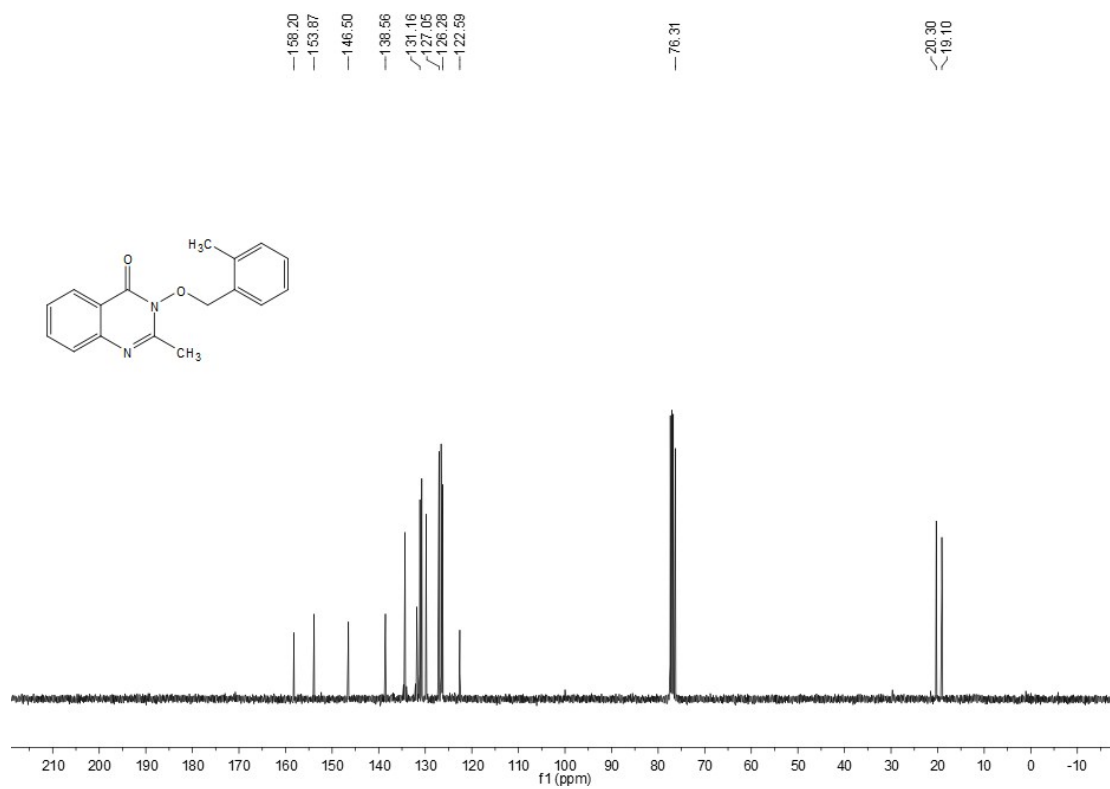
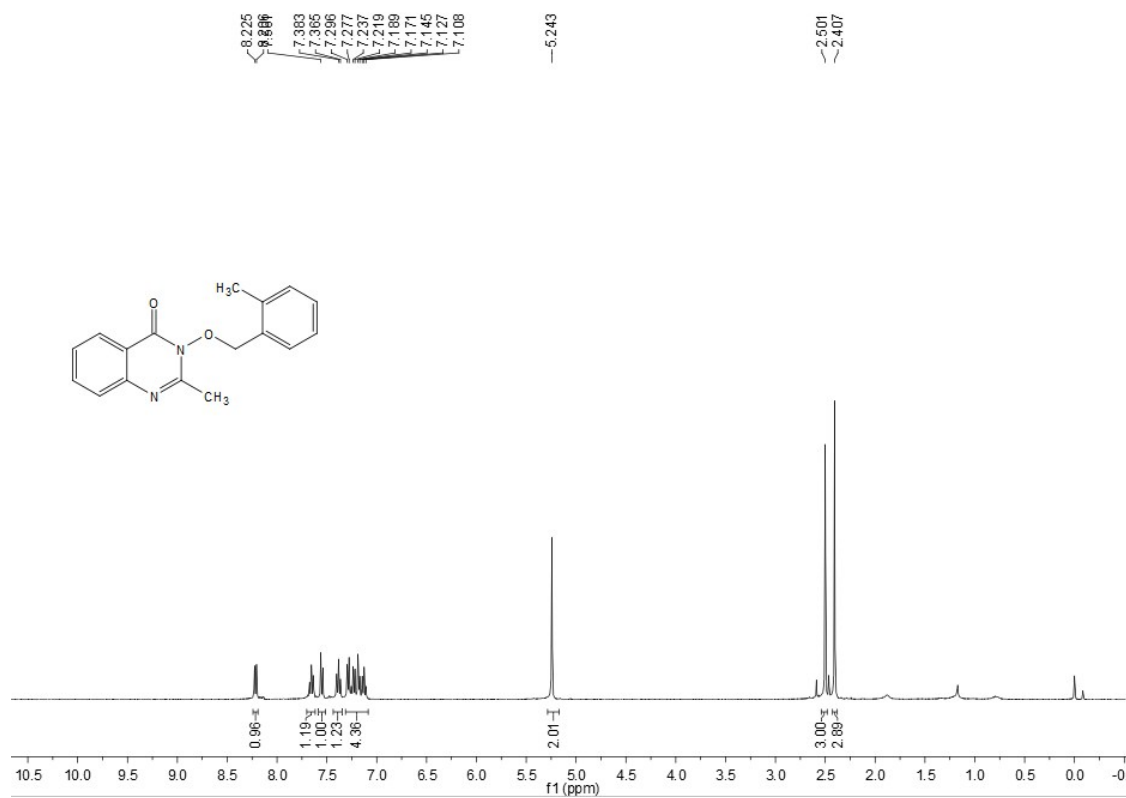
^1H NMR and ^{13}C NMR for compound **3x**



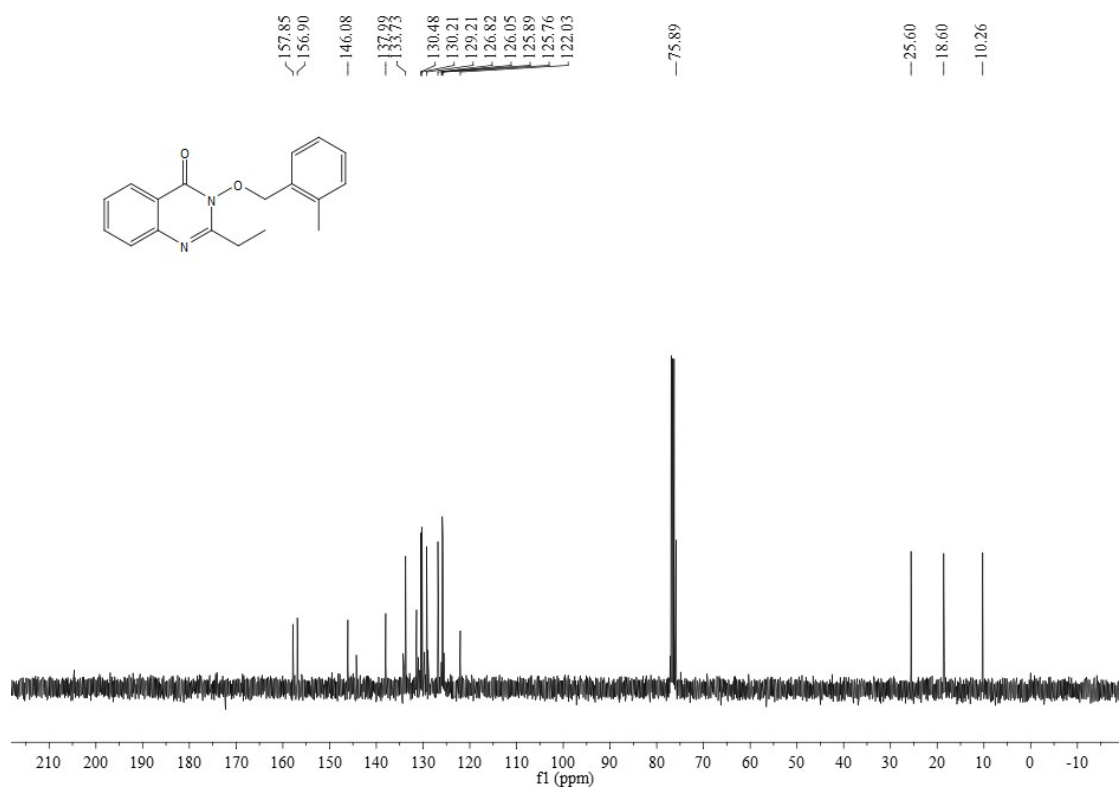
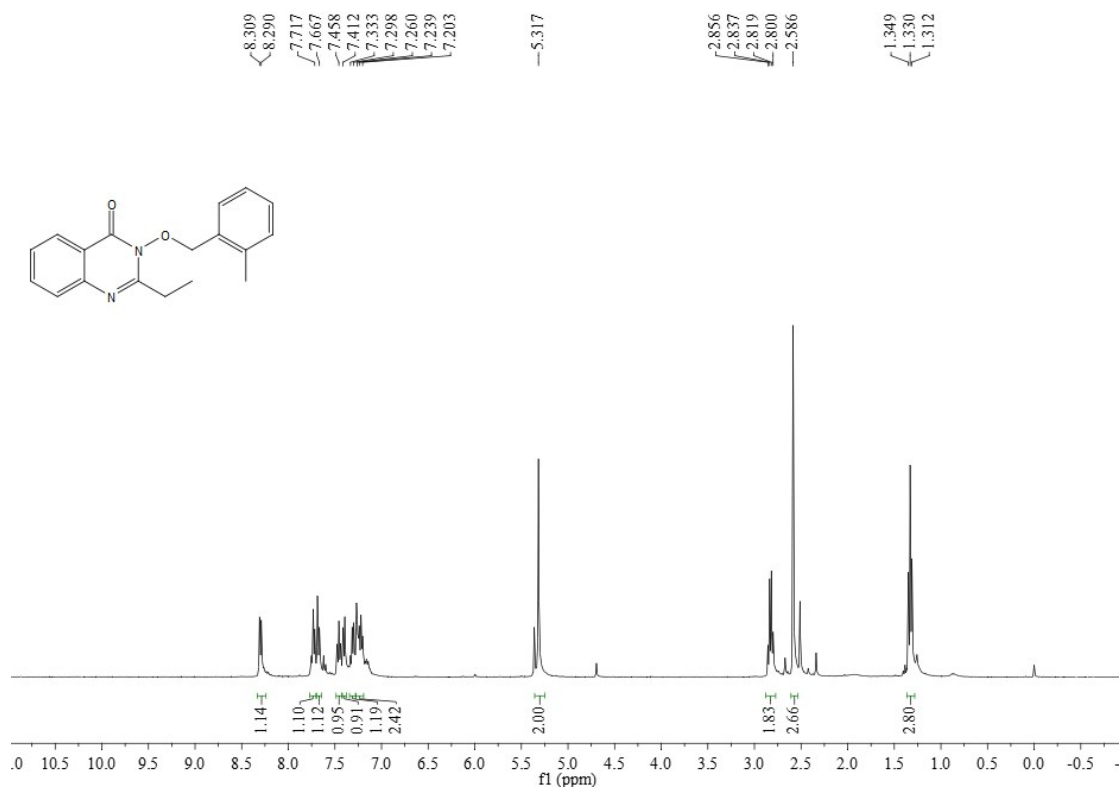
¹H NMR and ¹³C NMR for compound 3y



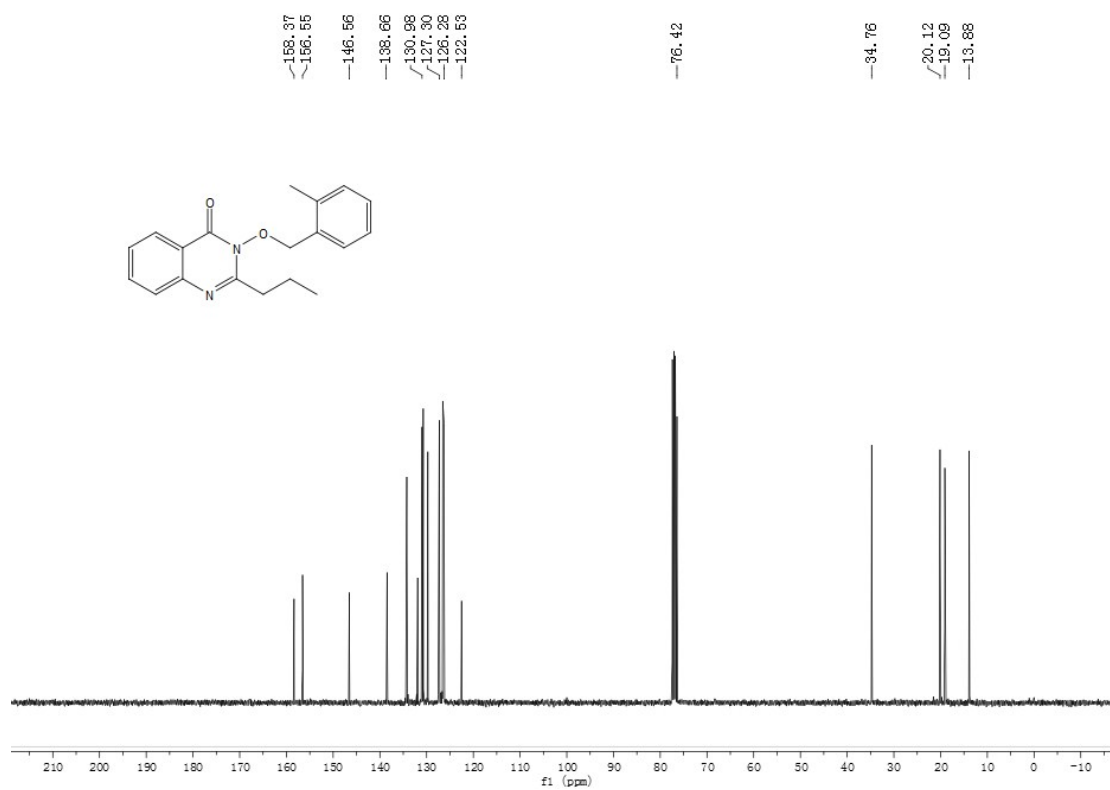
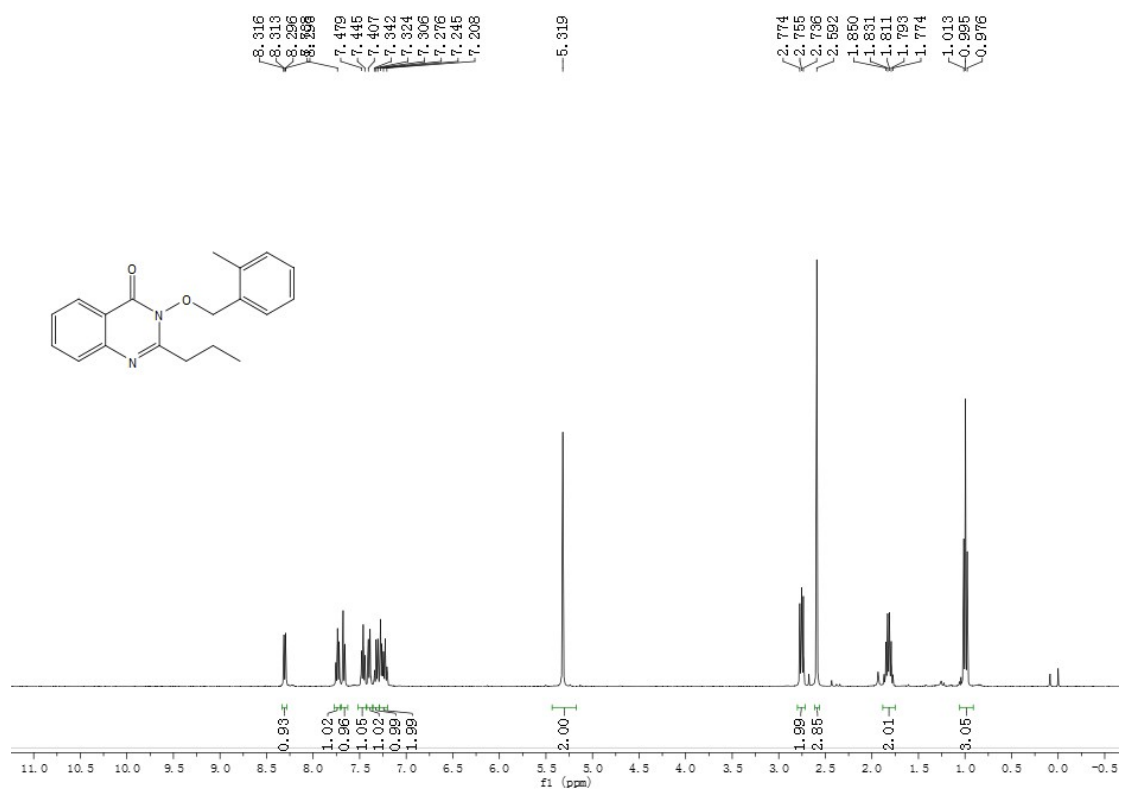
¹H NMR and ¹³C NMR for compound **3z**



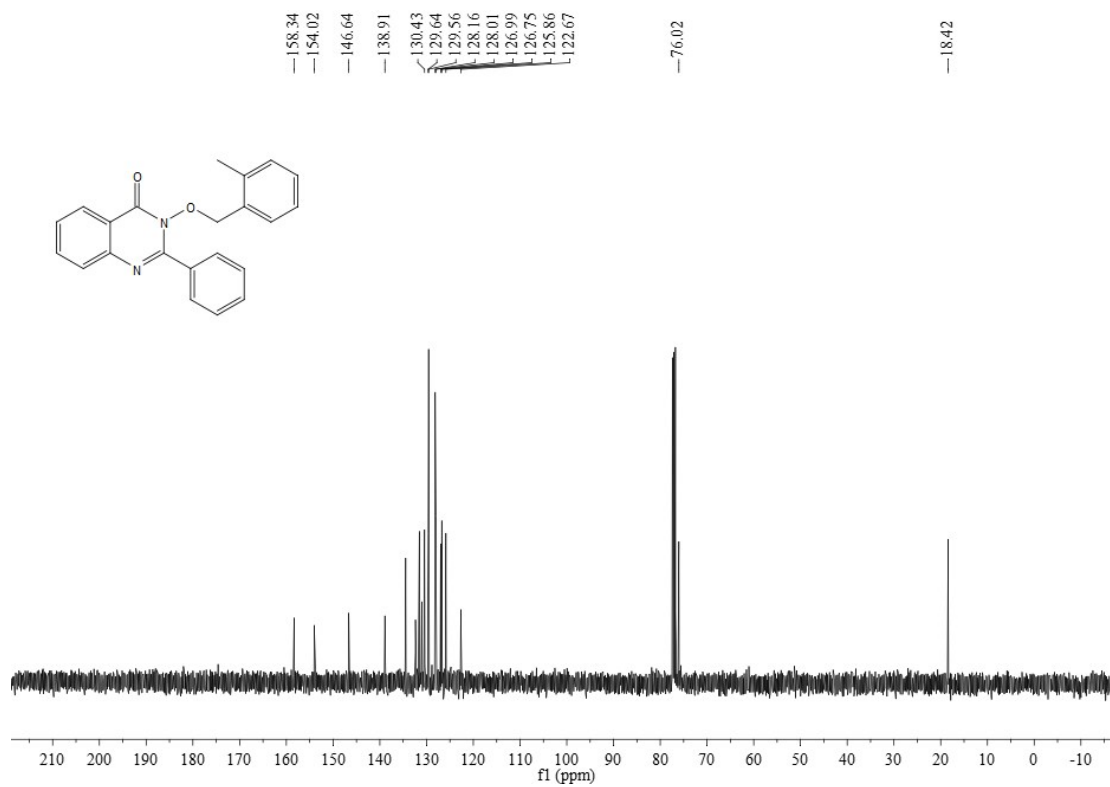
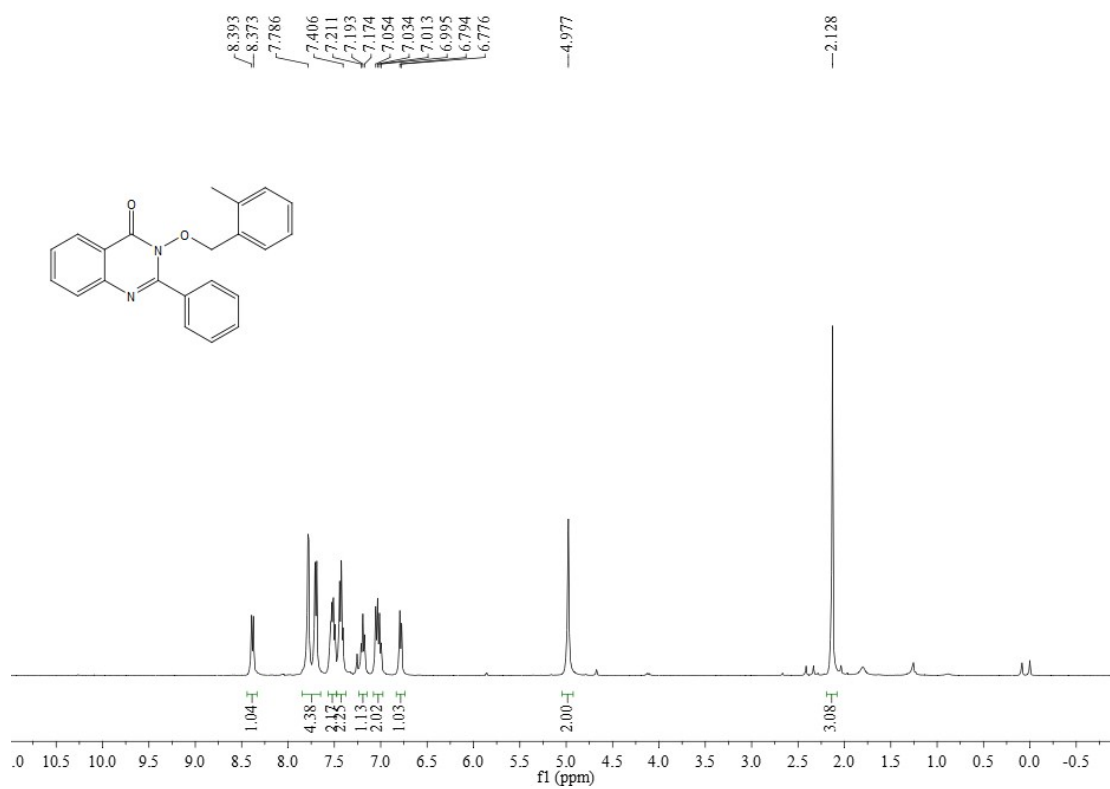
¹H NMR and ¹³C NMR for compound **4a**



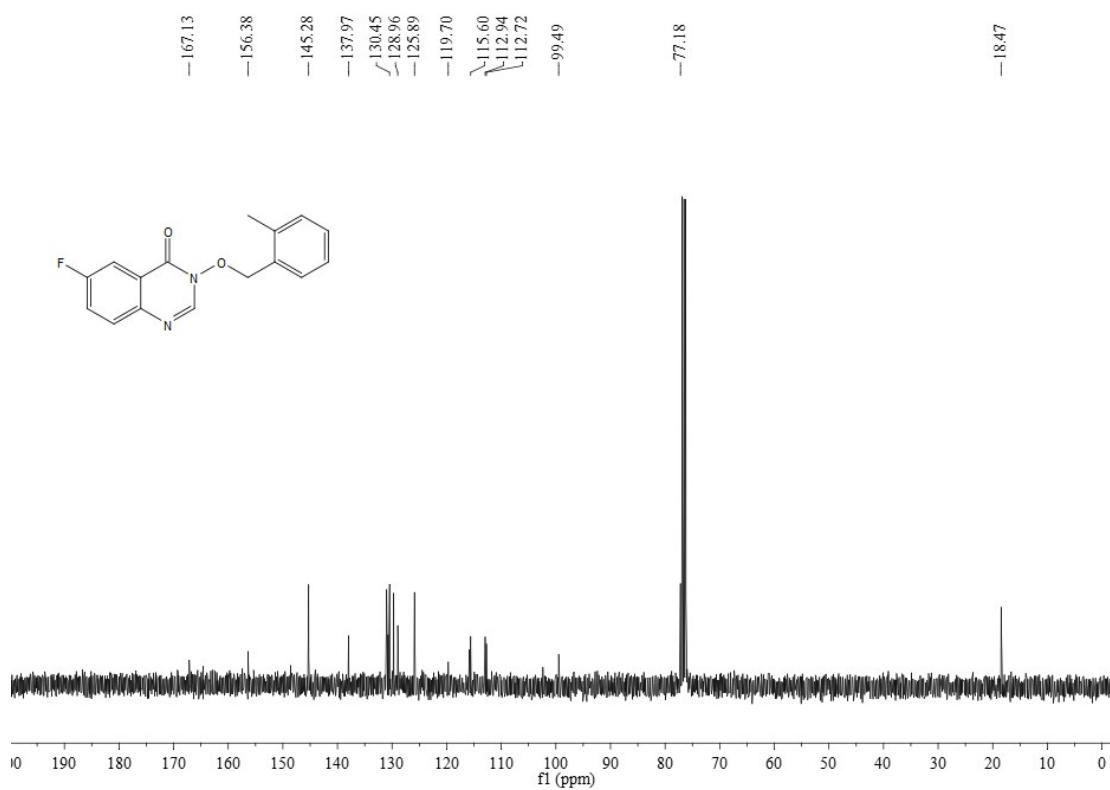
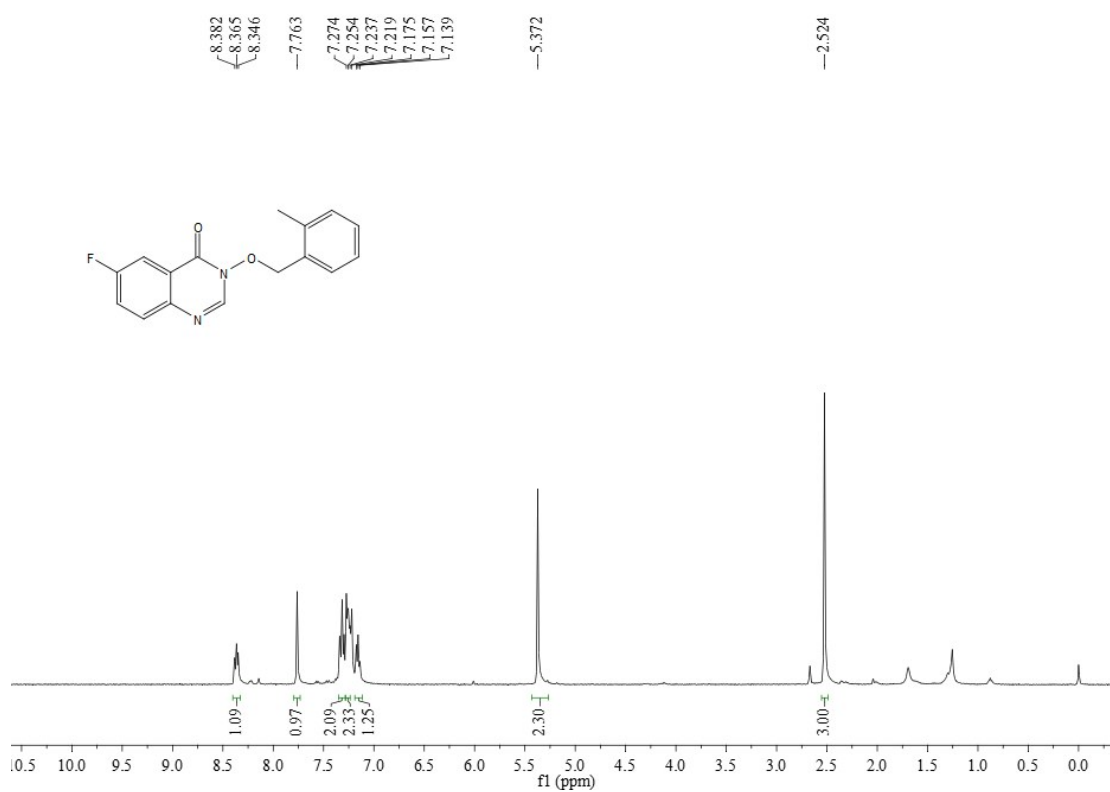
¹H NMR and ¹³C NMR for compound **4b**



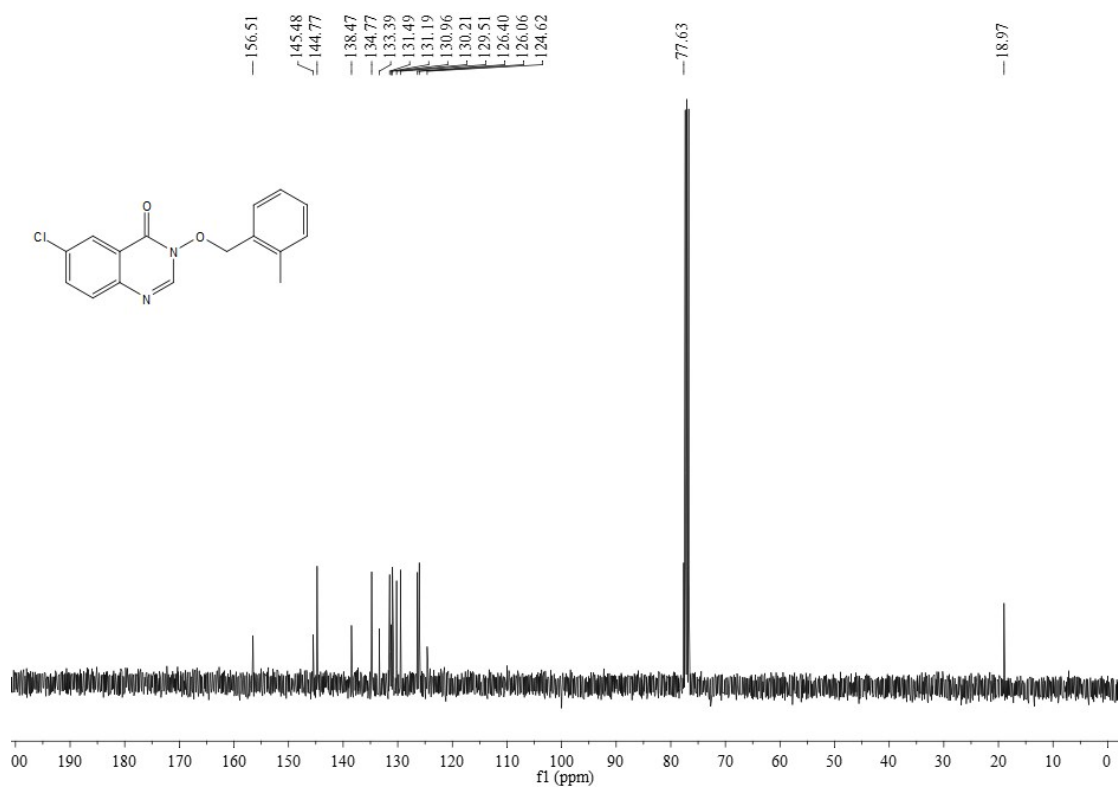
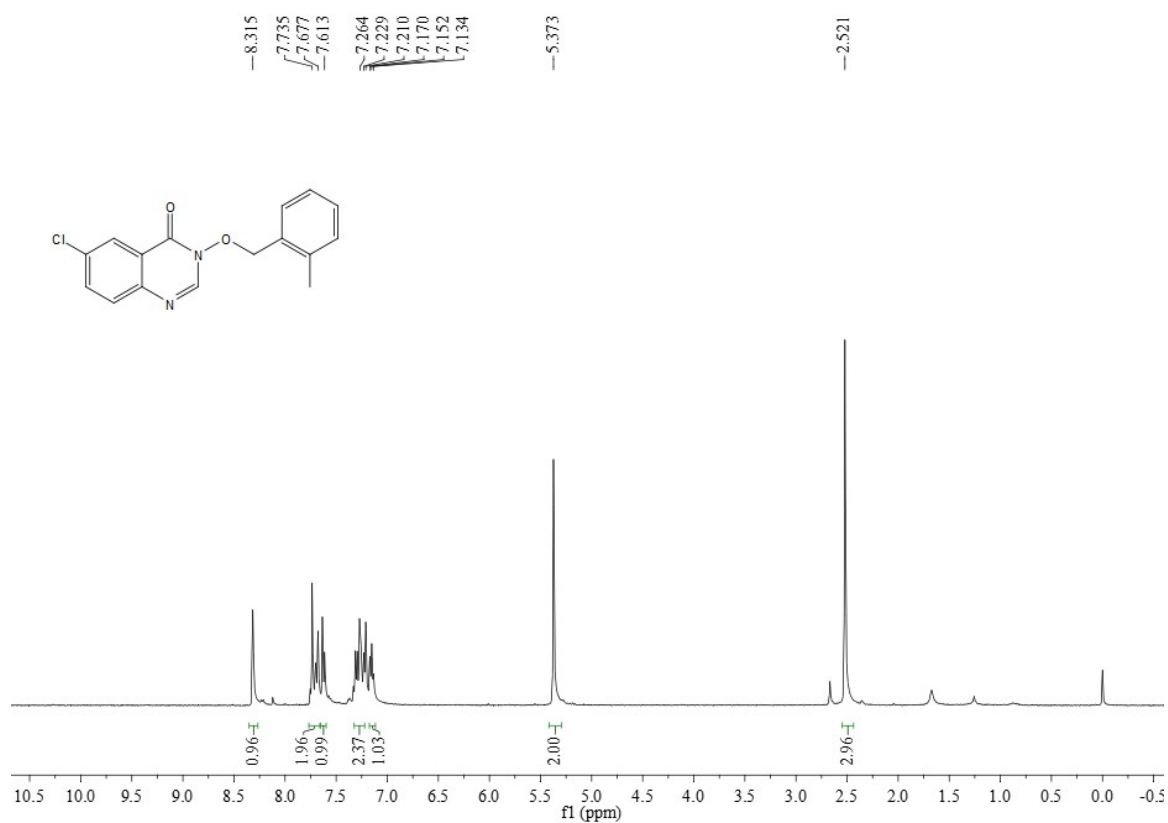
¹H NMR and ¹³C NMR for compound **4c**



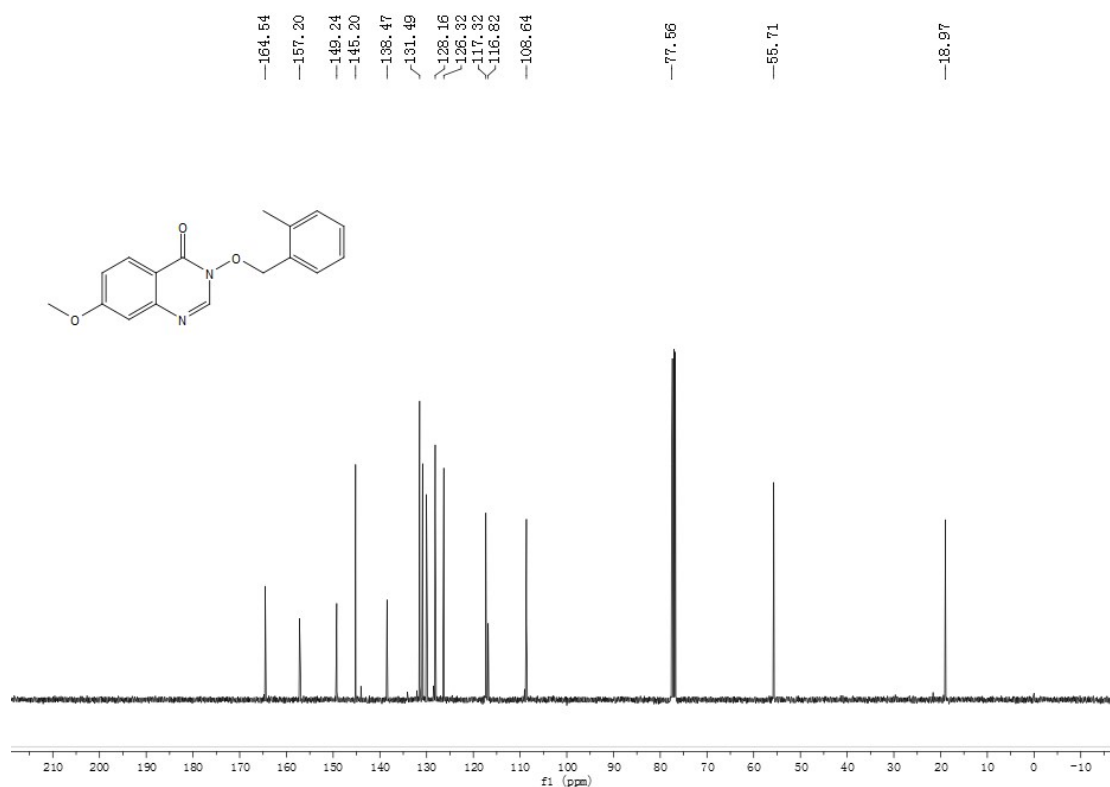
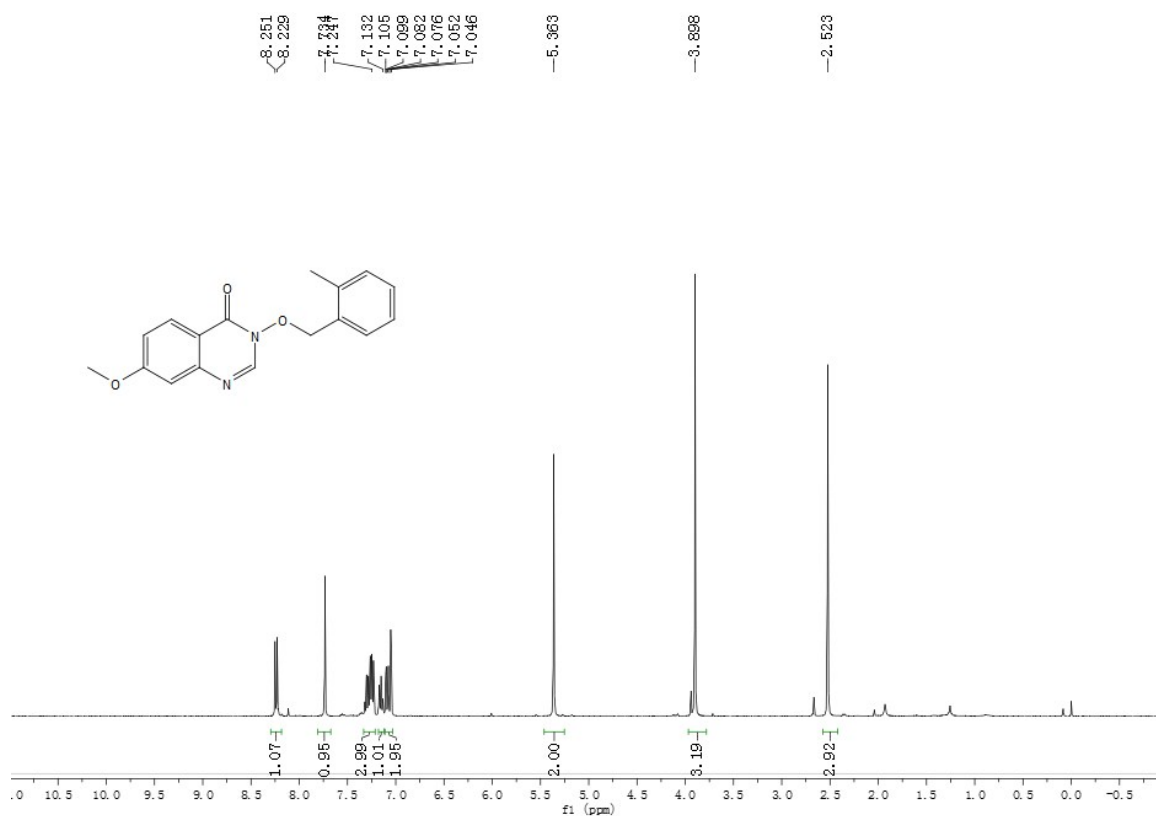
^1H NMR and ^{13}C NMR for compound **4d**



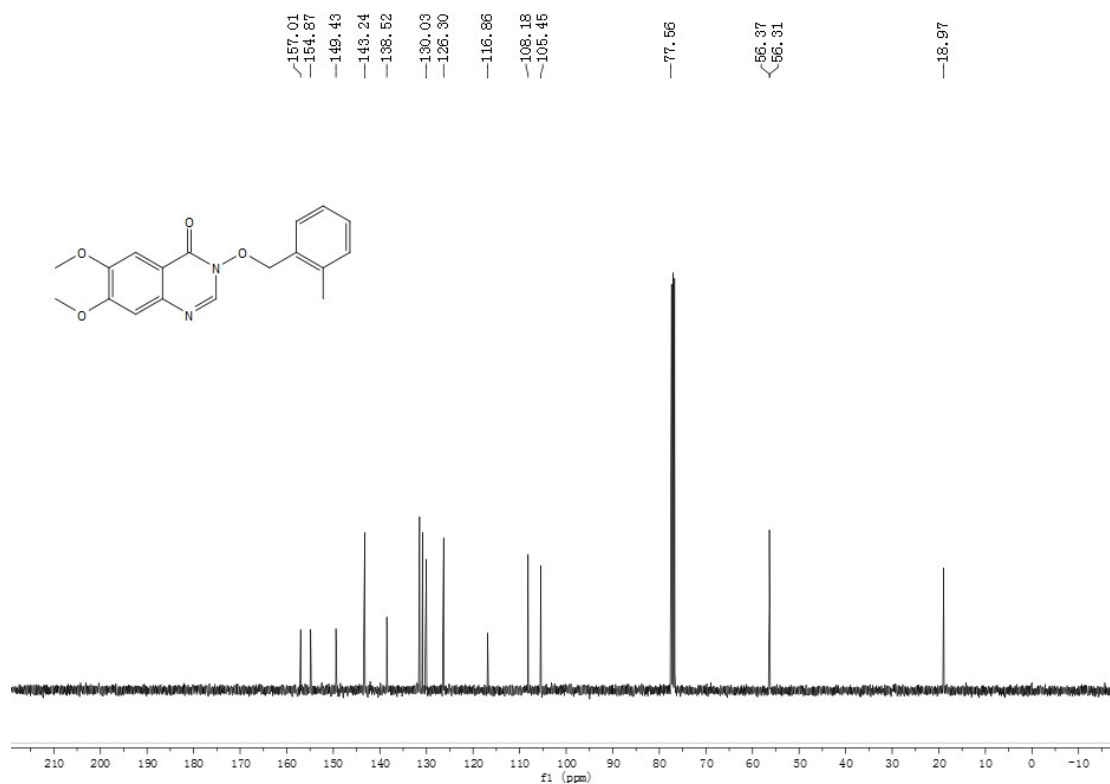
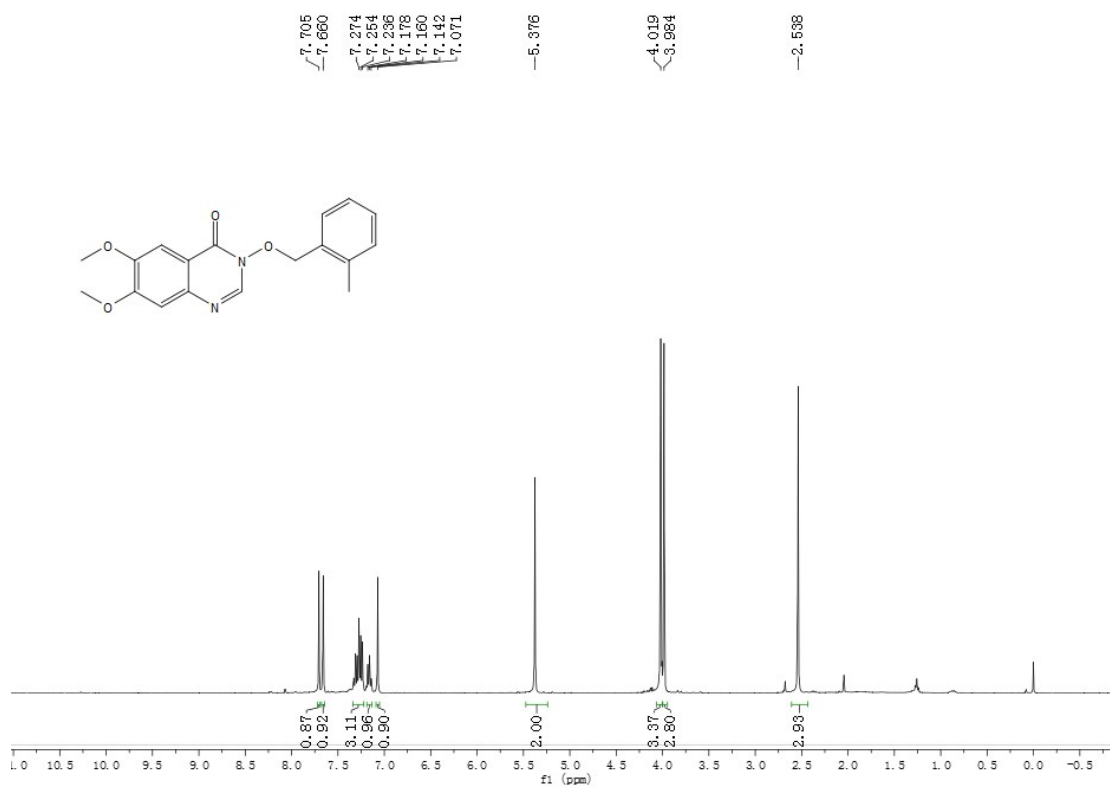
¹H NMR and ¹³C NMR for compound **4e**



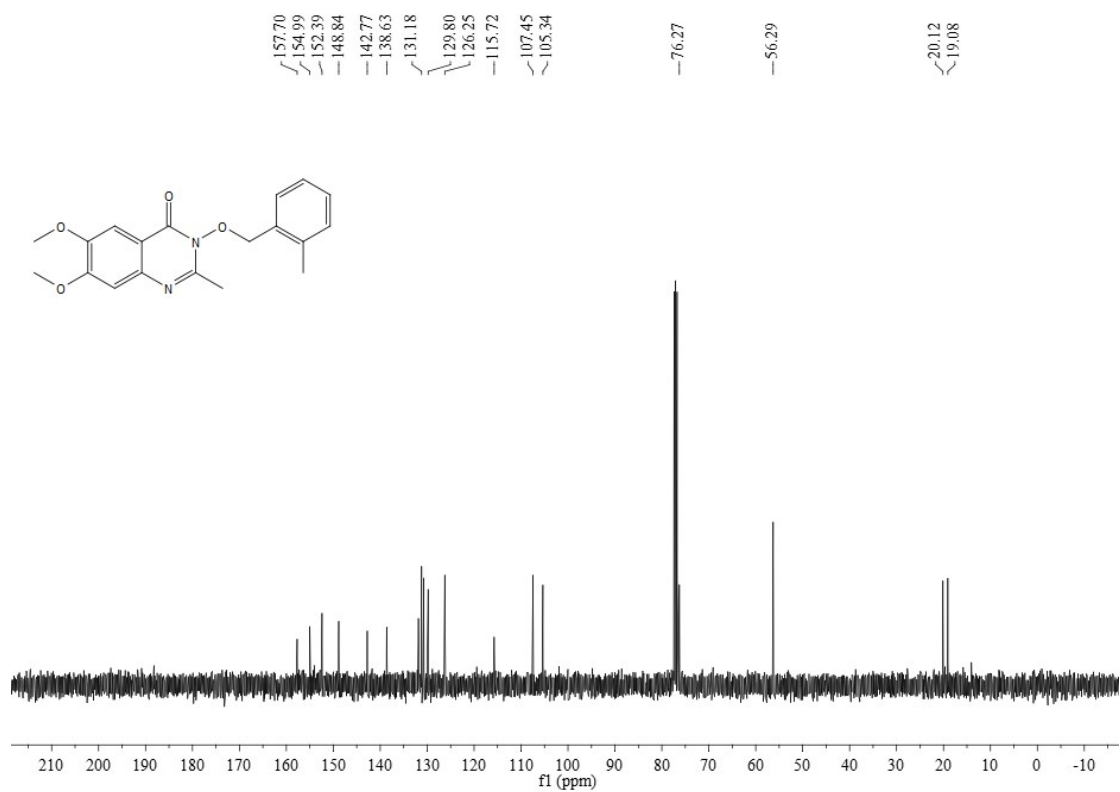
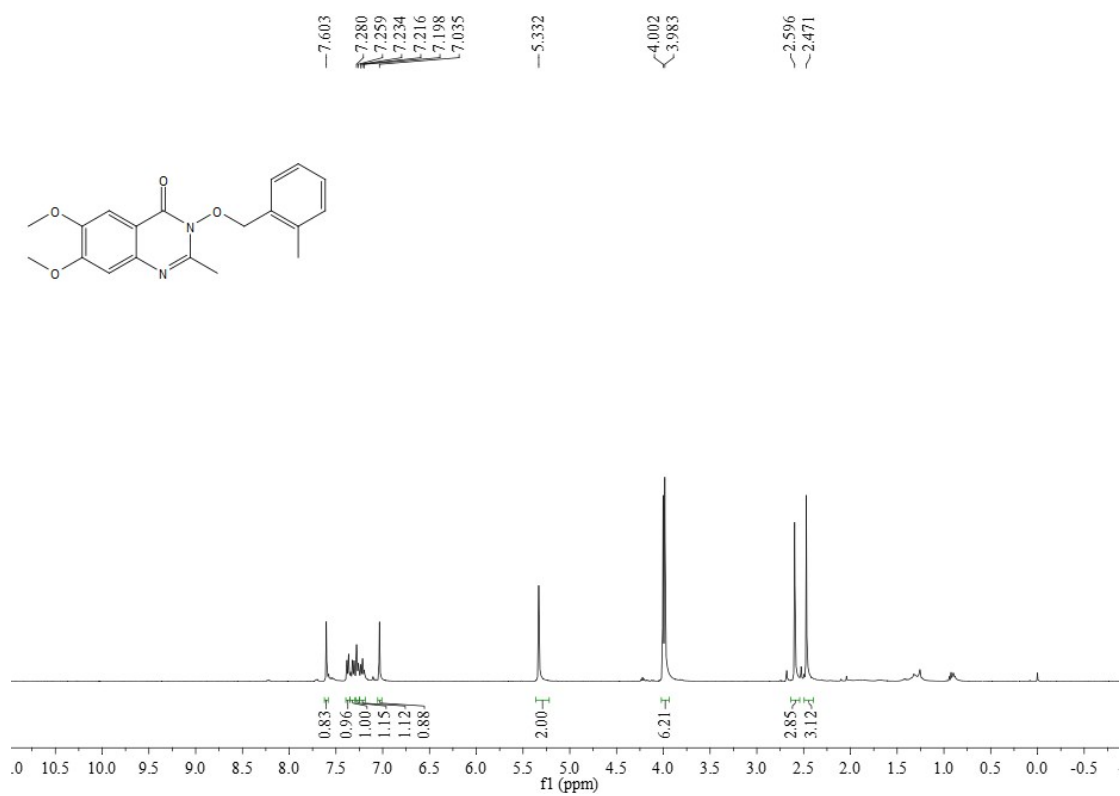
^1H NMR and ^{13}C NMR for compound **4f**



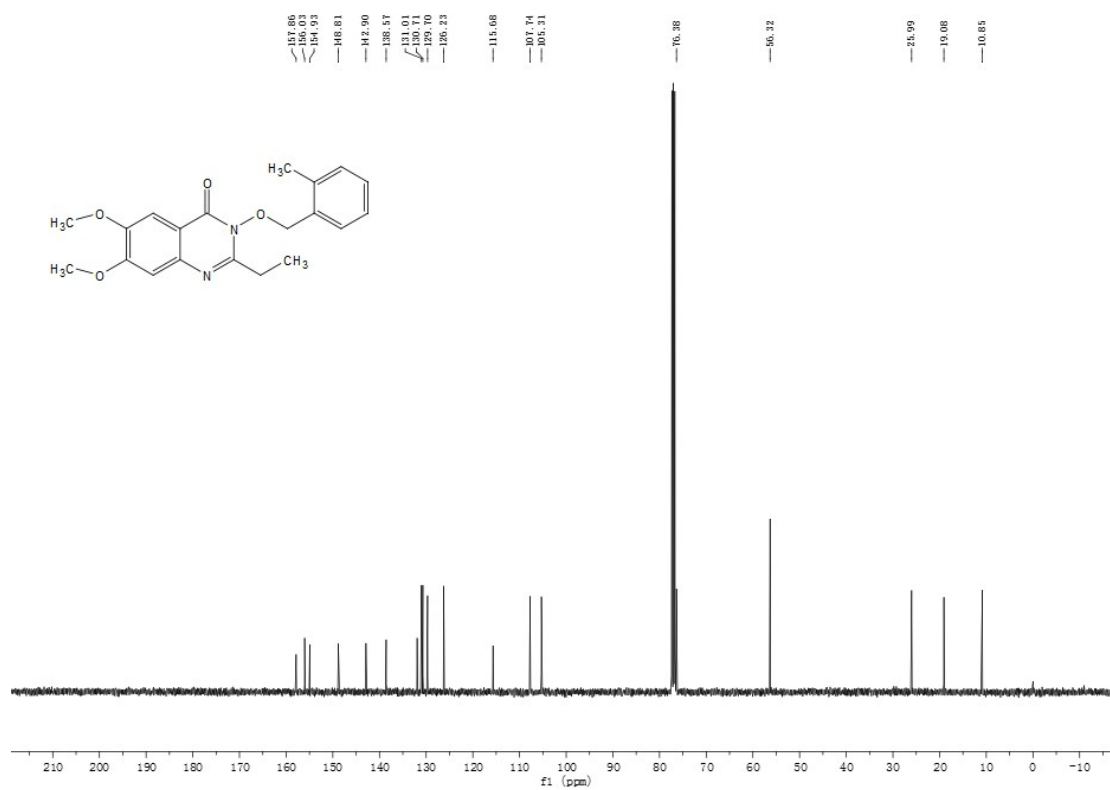
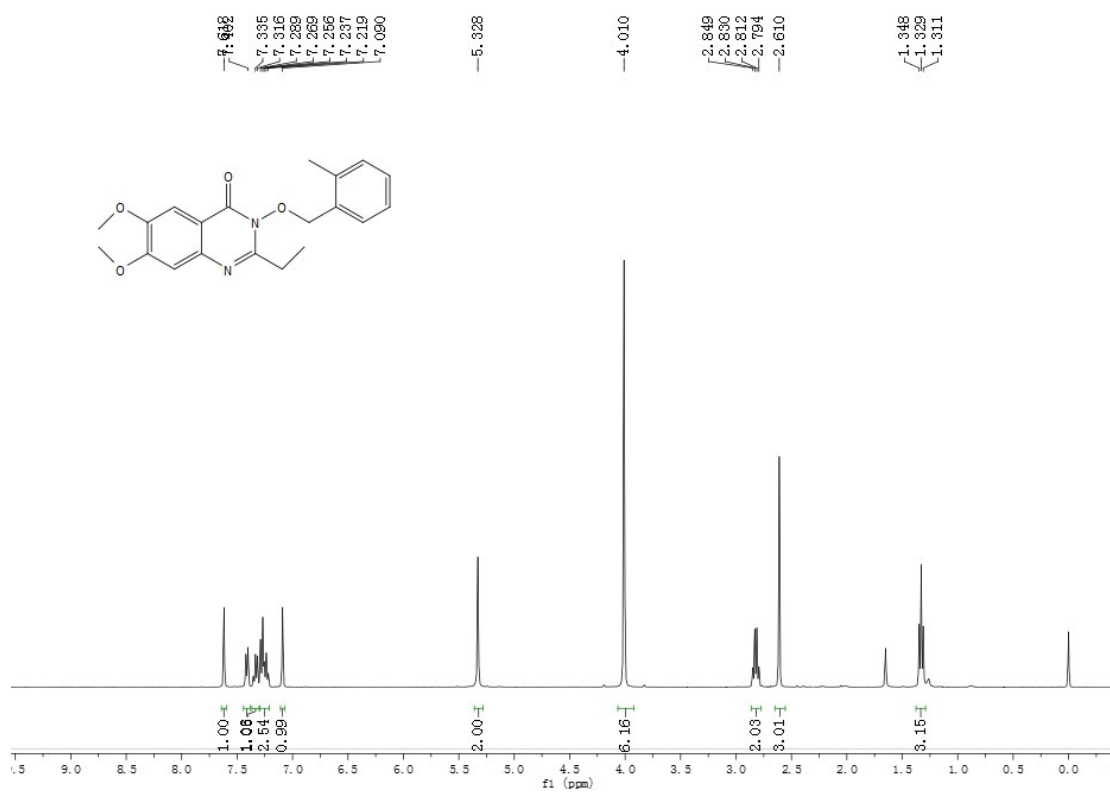
¹H NMR and ¹³C NMR for compound **4g**



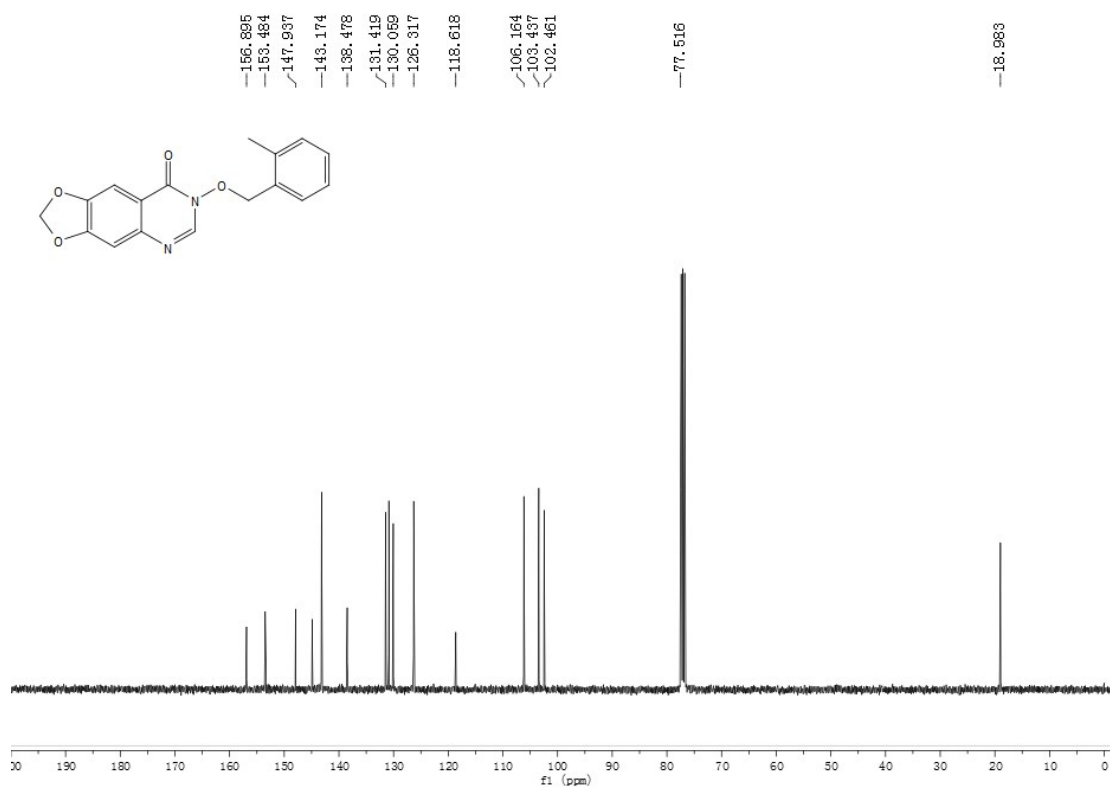
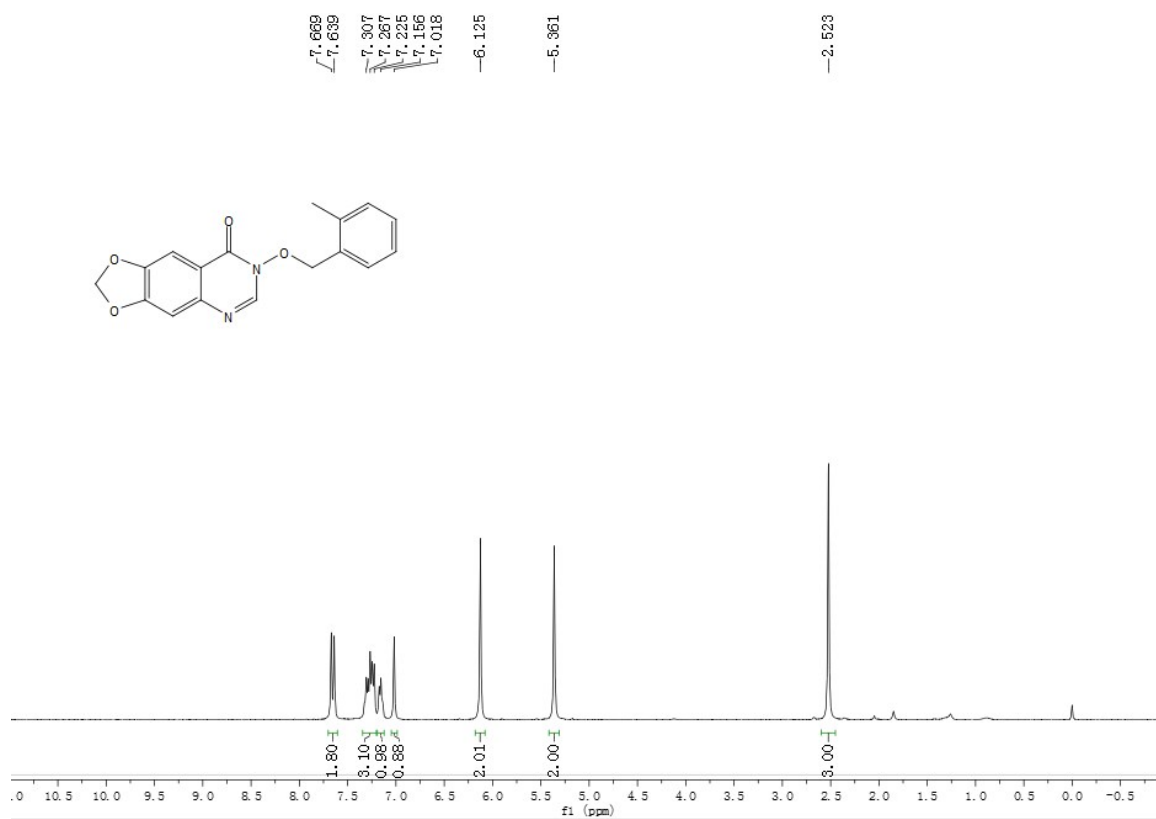
^1H NMR and ^{13}C NMR for compound **4h**



^1H NMR and ^{13}C NMR for compound **4i**



¹H NMR and ¹³C NMR for compound 4j



^1H NMR and ^{13}C NMR for compound **4k**