Supporting Information

Pd(II)-Catalyzed Cascade Annulation of *N*-Substituted Anilines with CO, NH_4OAc and Aldehydes to *N*1-Substituted 2,3-Dihydroquinazolin-4(1*H*)-ones

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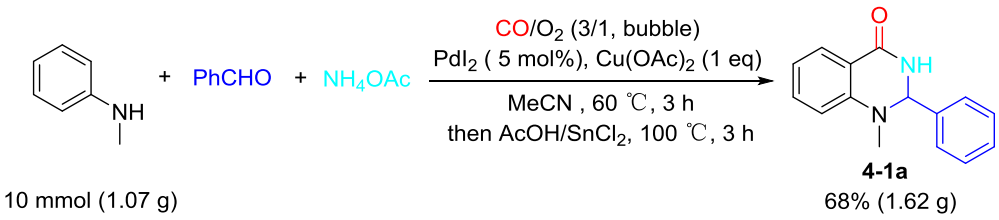
Contents

1. General Information

All reactions were carried out in a 50 mL three-necked round-bottom flask under continuous bubble of mixed oxygen and carbon monoxide with a balloon. Unless otherwise stated, all reagents and materials were obtained from commercial suppliers and used without further purification. 4-(Methylamino)phenol, 1-(4-(methylamino) phenyl)ethan-1-one, 4-bromo-*N*-methylaniline, *N*-isobutylaniline, *N*-(*tert*-butyl)aniline were prepared according to the reported method.[1] Reactions were monitored by thin layer chromatography (TLC) using silica gel plates (silica gel 60 F254) and components were visualized by observation under UV light. Flash column chromatography was performed with 200-300 mesh silica gel. Melting points were determined with a Yuhua X-5 apparatus (Gongyi, China) and were uncorrected. All new compounds were characterized by ^{1}H NMR, ^{13}C NMR and high resolution mass spectra (HRMS). The known compounds were characterized by ^{1}H NMR and ^{13}C NMR. ^{1}H and ^{13}C NMR data were recorded with Bruker Avance NEO 400 spectrometer and Bruker Avance III HD 600 spectrometer with tetramethylsilane (TMS) as an internal standard. All chemical shifts (δ) are reported in ppm and are referenced to residual solvent or TMS peaks. HRMS was performed on a Bruker Micro ToF II mass spectrometer.

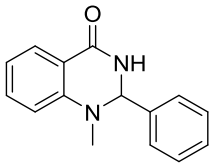
2. Gram-Scale Experiment



N-methylaniline (10 mmol, 1.07 g), PdI_2 (5 mol%, 0.5 mmol, 180.10 mg), $Cu(OAc)_2$ (1 equiv, 10 mmol, 1.82 g) and CH_3CN (25 mL) were charged into a oven-dried 50 mL three-necked round-bottom flask equipped with a stir bar and a T-branch tube connected with a CO/O_2 (3:1, bubble) balloon. The three-necked round-bottom flask was then placed in an oil bath preheated to 60 °C for 3 h. Next, the T-branch tube was removed and NH_4OAc (2 equiv, 20 mmol, 1.54 g), benzaldehyde (1.5 equiv, 15 mmol, 1.80 g), AcOH (5 mL) and $SnCl_2$ (0.5 equiv, 5 mmol, 948.10 mg) were added into the reactor equipped with a condenser to continue the reaction for a further 3 h at 100 °C. Then the reaction mixture was cooled to room temperature and was washed with brine (50 mL), and extracted with EtOAc (3 × 30 mL). The combined organic layers were

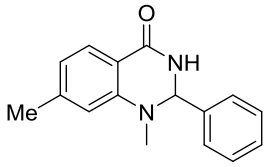
dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by column chromatography on silica gel to give the corresponding product with petroleum ether/ethyl acetate (PE/EA = 3/1) as the eluent.

3. Characterization Data of the Corresponding Products



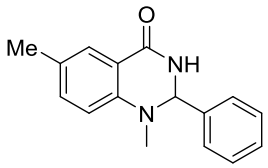
1-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1a)

White solid (37.17 mg, 78%); R_f = 0.33 (PE/EA = 1/1); melting point: 204 – 206 °C; CAS registry number: 1217-75-0; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.64 (d, J = 3.7 Hz, 1H), 7.71 (dd, J = 7.6, 1.6 Hz, 1H), 7.37 (td, J = 7.7, 1.7 Hz, 1H), 7.32 – 7.24 (m, 5H), 6.77 (t, J = 7.3 Hz, 1H), 6.67 (d, J = 8.2 Hz, 1H), 5.68 (d, J = 3.9 Hz, 1H), 2.81 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 147.7, 140.8, 134.4, 129.0, 128.9, 128.0, 126.7, 117.6, 116.5, 112.4, 72.8, 35.6.



1,6-dimethyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1b)

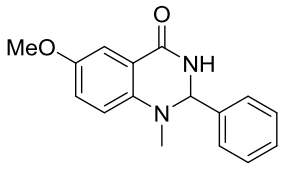
White solid (32.80 mg, 65%); R_f = 0.30 (PE/EA = 2/1); melting point: 200 –202 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.54 (d, J = 3.8 Hz, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.32 – 7.29 (m, 3H), 7.26 – 7.23 (m, 2H), 6.58 (d, J = 7.8 Hz, 1H), 6.49 (s, 1H), 5.64 (d, J = 3.9 Hz, 1H), 2.81 (s, 3H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.9, 147.6, 144.6, 140.8, 129.0, 128.8, 128.0, 126.6, 118.6, 114.1, 112.7, 72.9, 35.6, 22.2. **HRMS (ESI)** calcd for $C_{16}H_{16}N_2NaO^+$ $[M+Na]^+$: 275.1155; found: 275.1152.



1,7-dimethyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1c)

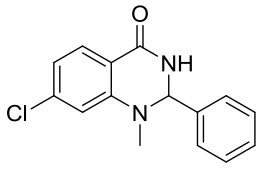
White solid (34.32 mg, 68%); R_f = 0.32 (PE/EA = 1/1); melting point: 211 – 213 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.59 (d, J = 3.8 Hz, 1H), 7.53 (d, J = 1.9 Hz, 1H),

7.31 – 7.18 (m, 6H), 6.58 (d, *J* = 8.3 Hz, 1H), 5.62 (d, *J* = 3.9 Hz, 1H), 2.77 (s, 3H), 2.21 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.0, 145.7, 140.6, 135.1, 129.0, 128.8, 128.1, 126.7, 126.4, 116.5, 112.6, 72.8, 35.6, 20.4. **HRMS (ESI)** calcd for $C_{16}H_{16}N_2NaO^+$ $[M+Na]^+$: 275.1155; found: 275.1154.



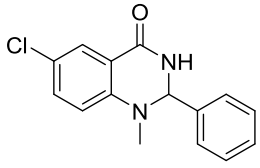
7-methoxy-1-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1d)

White solid (36.49 mg, 68%); R_f = 0.33 (PE/EA = 1/1); melting point: 164 – 166 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.66 (d, *J* = 3.7 Hz, 1H), 7.32 – 7.24 (m, 6H), 7.01 (dd, *J* = 8.9, 3.1 Hz, 1H), 6.66 (d, *J* = 8.9 Hz, 1H), 5.58 (d, *J* = 3.8 Hz, 1H), 3.71 (s, 3H), 2.75 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 152.0, 142.3, 140.4, 128.9, 128.8, 126.9, 121.3, 117.7, 114.5, 111.6, 72.9, 55.8, 36.1. **HRMS (ESI)** calcd for $C_{21}H_{18}N_2NaO^+$ $[M+H]^+$: 337.1311; found: 337.1305.



6-chloro-1-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1f)

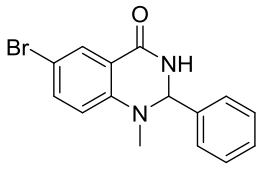
White solid (30.00 mg, 55%); R_f = 0.36 (PE/EA = 1/1); melting point: 235 – 236 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.75 (d, *J* = 3.8 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 1H), 7.35 – 7.31 (m, 3H), 7.25 – 7.23 (m, 2H),6.78 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.72 (d, *J* = 1.8 Hz, 1H), 5.72 (d, *J* = 3.9 Hz, 1H), 2.84 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.0, 148.6, 140.5, 139.2, 129.8, 129.2, 129.0, 126.5, 117.4, 115.0, 111.9, 72.8, 35.7. **HRMS (ESI)** calcd for $C_{15}H_{13}ClN_2NaO^+$ $[M+Na]^+$: 295.0609; found: 295.0605.



7-chloro-1-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1g)

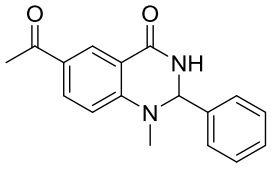
White solid (34.36 mg, 63%); R_f = 0.39 (PE/EA = 1/1); melting point: 194 – 195 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.83 (d, *J* = 3.7 Hz, 1H), 7.63 (d, *J* = 2.6 Hz, 1H),

7.40 (dd, *J* = 8.8, 2.7 Hz, 1H), 7.37 – 7.18 (m, 5H), 6.71 (d, *J* = 8.8 Hz, 1H), 5.72 (d, *J* = 3.9 Hz, 1H), 2.82 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.6, 146.4, 140.4, 134.0, 129.1, 129.1, 127.1, 126.6, 121.5, 117.6, 114.5, 72.6, 35.7. **HRMS (ESI)** calcd for $C_{15}H_{13}ClN_2NaO^+$ $[M+Na]^+$: 295.0609; found: 295.0604.



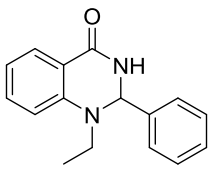
6-bromo-1-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1h)

White solid (33.62 mg, 53%); R_f = 0.39 (PE/EA = 1/1); melting point: 216 – 217 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.83 (d, *J* = 3.8 Hz, 1H), 7.75 (d, *J* = 2.5 Hz, 1H), 7.51 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.36 – 7.30 (m, 3H), 7.26 – 7.24 (m, 2H), 6.66 (d, *J* = 8.8 Hz, 1H), 5.72 (d, *J* = 3.9 Hz, 1H), 2.82 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.5, 146.7, 140.4, 136.7, 130.0, 129.1, 129.0, 126.5, 118.0, 114.9, 108.8, 72.6, 35.7. **HRMS (ESI)** calcd for $C_{15}H_{13}BrN_2NaO^+$ $[M+Na]^+$: 339.0104; found: 339.0104.



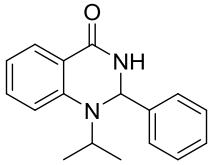
7-acetyl-1-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1i)

Yellow solid (20.74 mg, 37%)**;** R_f = 0.44 (PE/EA = 1/1); melting point: 195 – 196 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.86 (d, *J* = 3.7 Hz, 1H), 8.29 (d, *J* = 2.2 Hz, 1H), 7.96 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.37 – 7.32 (m, 3H), 7.26 – 7.24 (m, 2H), 6.78 (d, *J* = 8.8 Hz, 1H), 5.83 (d, *J* = 3.8 Hz, 1H), 2.94 (s, 3H), 2.49 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 195.8, 161.9, 150.7, 140.2, 134.5, 129.3, 129.1, 126.3, 114.8, 111.9, 72.8, 35.9, 26.6. **HRMS (ESI)** calcd for $C_{17}H_{16}N_2NaO^+$ $[M+H]^+$: 303.1104; found: 303.1100.



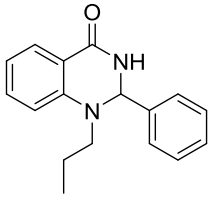
1-ethyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1l)

White solid (37.34 mg, 74%); R_f = 0.37 (PE/EA = 1/1); melting point: 138 – 139 °C; CAS registry number: 1221-29-0; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.61 (d, J = 3.3 Hz, 1H), 7.39 (dd, J = 7.7, 1.6 Hz, 1H), 7.37 (td, J = 7.7, 1.7 Hz, 1H), 7.32 – 7.28 (m, 5H), 6.82 (d, J = 8.3 Hz, 1H), 6.72 (t, J = 7.6 Hz, 1H), 5.74 (d, J = 3.8 Hz, 1H), 3.57 – 3.48 (m, 1H), 3.23 – 3.14 (m, 1H), 1.07 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.0, 146.8, 142.3, 134.3, 129.0, 128.7, 128.3, 126.7, 117.3, 116.8, 113.0, 70.9, 43.3, 12.8.



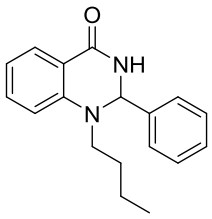
1-isopropyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1m)

White solid (4.79 mg, 9%); R_f = 0.44 (PE/EA = 1/1); melting point: 116 – 118 °C; CAS registry number: 1225-17-8; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.71 (d, J = 4.7 Hz, 1H), 7.65 (dd, J = 7.8, 1.6 Hz, 1H), 7.38 – 7.33 (m, 3H), 7.25 (t, J = 7.1 Hz, 2H), 7.20 – 7.16 (m, 2H), 6.81 (t, J = 7.1 Hz, 1H), 5.76 (d, J = 4.8 Hz, 1H), 4.14 – 4.08 (m, 1H), 1.26 (d, J = 6.8 Hz, 3H), 1.21 (d, J = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.4, 147.6, 144.0, 133.7, 128.6, 127.9, 127.7, 126.6, 120.7, 119.4, 118.8, 63.8, 53.7, 21.4, 21.1.



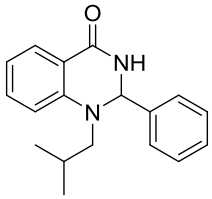
2-phenyl-1-propyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1n)

White solid (37.82 mg, 71%); R_f = 0.39 (PE/EA = 1/1); melting point: 119 – 120 °C; CAS registry number: 1225-62-3; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.65 (d, J = 3.9 Hz 1H) 7.67 (dd, J = 7.7, 1.6 Hz, 1H), 7.38 – 7.26 (m, 6H), 6.82 (d, J = 8.3 Hz, 1H), 6.70 (t, J = 7.5 Hz, 1H), 5.71 (d, J = 4.0 Hz, 1H), 3.54 – 3.47 (m, 1H), 3.11 – 3.04 (m, 1H), 1.61 – 1.48 (m, 2H), 0.88 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.1, 147.0, 142.4, 134.2, 128.9, 128.5, 128.3, 126.6, 117.1, 116.8, 112.9, 71.2, 50.6, 20.6, 11.5.



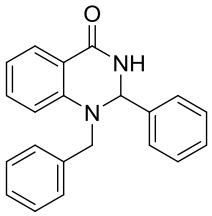
1-butyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1o)

White solid (36.74 mg, 66%); R_f = 0.44 (PE/EA = 1/1); melting point: 109 – 110 °C; CAS registry number: 1229-36-3; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.70 (d, J = 3.9 Hz, 1H), 7.72 (dd, J = 7.7, 1.6 Hz, 1H), 7.38 – 7.34 (m, 6H), 6.87 (d, J = 8.3 Hz, 1H), 6.76 (t, J = 7.2 Hz, 1H), 5.76 (d, J = 4.0 Hz, 1H), 3.57 – 3.50 (m, 1H), 3.15 – 3.07 (m, 1H), 1.59 – 1.54 (m, 1H), 1.47 – 1.43 (m, 1H), 1.34 – 1.29 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.1, 147.0, 142.3, 134.3, 128.9, 128.6, 128.3, 126.6, 117.2, 116.8, 113.0, 71.2, 48.6, 29.5, 20.0, 14.2.



1-isobutyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1p)

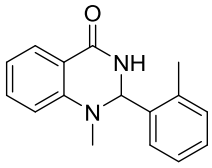
White solid (10.09 mg, 18%); R_f = 0.40 (PE/EA = 1/1); melting point: 125 – 126 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.73 (d, J = 4.5 Hz, 1H), 7.63 (dd, J = 7.7, 1.6 Hz, 1H), 7.37 – 7.23 (m, 7H), 6.84 (d, J = 8.3 Hz, 1H), 6.68 (t, J = 7.2 Hz, 1H), 5.65 (d, J = 4.5 Hz, 1H), 3.56 (dd, J = 14.4, 5.3 Hz, 1H), 2.84 (dd, J = 14.4, 9.2 Hz, 1H), 0.99 (d, J = 6.5 Hz, 3H), 0.90 (d, J = 6.7 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.2, 142.3, 134.2, 129.1, 128.9, 128.4, 126.5, 119.4, 117.0, 116.9, 113.0, 71.5, 56.4, 26.9, 20.3, 20.2.



1-benzyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4-1s)

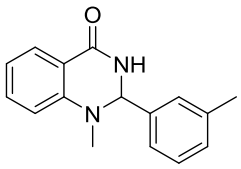
White solid (9.43 mg, 15%); R_f = 0.44 (PE/EA = 1/1); melting point: 118 – 120 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.77 (d, J = 4.2 Hz, 1H), 7.69 (dd, J = 7.6, 1.6 Hz, 1H), 7.37 – 7.25 (m, 11H), 6.74 – 6.70 (m, 2H), 5.82 (d, J = 4.2 Hz, 1H), 4.71 (d, J = 16.3 Hz, 1H), 4.48 (d, J = 16.4 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.1,

146.8, 141.9, 138.2, 134.1, 129.1, 129.0, 128.7, 128.2, 127.6, 127.5, 126.6, 117.8, 117.3, 113.7, 71.4, 52.3; **HRMS (ESI)** calcd for $C_{21}H_{18}N_2NaO^+$ $[M+H]^+$: 337.1311; found: 337.1311.



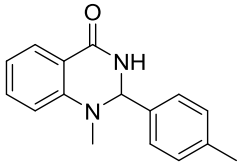
1-methyl-2-(*o*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2a)

White solid (36.84 mg, 73%); R_f = 0.36 (PE/EA = 2/1); melting point: 199 – 200 ℃; CAS registry number: 74374-99-5; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.45 (d, J = 2.4 Hz, 1H), 7.71 (dd, J = 7.6, 1.5 Hz, 1H), 7.42 (td, J = 8.6, 1.7 Hz, 1H), 7.22 – 7.09 (m, 4H), 6.81 – 6.76 (m, 2H), 5.90 (d, J = 2.9 Hz, 1H), 2.66 (s, 3H), 2.43 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 149.0, 138.4, 136.4, 134.5, 131.6, 128.9, 128.1, 126.8, 126.6, 117.6, 116.1, 112.2, 70.6, 34.9, 19.4.



1-methyl-2-(*m*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2b)

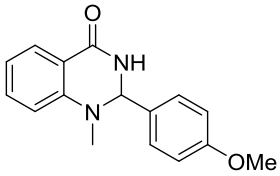
White solid (38.86 mg, 77%); R_f = 0.30 (PE/EA = 2/1); melting point: 139 – 140 ℃; CAS registry number: 930565-27-8; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.59 (d, J = 3.7 Hz, 1H), 7.71 (dd, J = 7.6, 1.6 Hz, 1H), 7.37 (ddd, J = 8.4, 7.3, 1.7 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 7.10 (d, J = 12.0 Hz, 2H), 7.02 (d, J = 7.6 Hz, 1H), 6.76 (td, J = 7.8, 0.8 Hz, 1H), 6.67 (d, J = 8.2 Hz, 1H), 5.62 (d, J = 3.8 Hz, 1H), 2.79 (s, 3H), 2.24 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 147.8, 140.7, 138.1, 134.4, 129.5, 128.9, 128.0, 127.4, 123.7, 117.5, 116.4, 112.3, 72.9, 35.6, 21.6.



1-methyl-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2c)

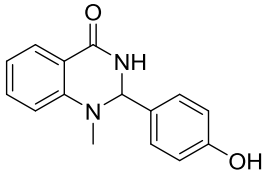
White solid (40.88 mg, 81%); R_f = 0.28 (PE/EA = 2/1); melting point: 169 – 170 °C; CAS registry number: 74374-96-2; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.61 (d, J = 3.7

Hz, 1H), 7.72 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.36 (ddd, *J* = 8.8, 7.4, 1.7 Hz, 1H), 7.13 (q, *J* = 8.3 Hz, 4H), 6.76 (td, *J* = 7.7, 0.6 Hz, 1H), 6.65 (d, *J* = 8.2 Hz, 1H), 5.63 (d, *J* = 3.8 Hz, 1H), 2.78 (s, 3H), 2.24 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.9, 147.7, 138.2, 137.7, 134.4, 129.5, 128.0, 126.6, 117.5, 116.5, 112.4, 72.7, 35.5, 21.1.



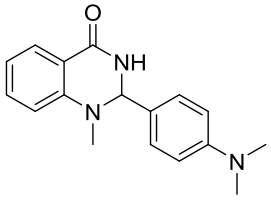
2-(4-methoxyphenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2d)

White solid (41.86 mg, 78%); R_f = 0.39 (PE/EA = 1/1); melting point: 136 – 138 ℃; CAS registry number: 74374-97-3; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.57 (d, *J* = 3.7 Hz, 1H), 7.71 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.36 (td, *J* = 8.6, 1.7 Hz, 1H), 7.18 (d, *J* = 8.7 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.76 (td, *J* = 7.7, 0.5 Hz, 1H), 6.65 (d, *J* = 8.2 Hz, 1H), 5.61 (d, *J* = 3.7 Hz, 1H), 3.70 (s, 3H), 2.76 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 159.8, 147.7, 134.4, 132.7, 128.0, 127.9, 117.6, 116.5, 114.3, 112.4, 72.5, 55.6, 35.4.



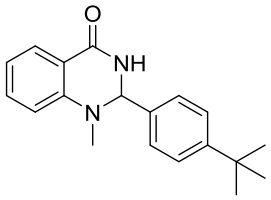
2-(4-hydroxyphenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2e)

White solid (40.69 mg, 80%); R_f = 0.20 (PE/EA = 1/1); melting point: 216 – 219 ℃; CAS registry number: 931606-36-9; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.51 (s, 1H), 8.50 (d, *J* = 3.5 Hz, 1H), 7.71 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.36 (td, *J* = 8.6, 1.7 Hz, 1H), 7.07 (d, *J* = 8.5 Hz, 2H), 6.75 (td, *J* = 7.5, 0.6 Hz, 1H), 6.70 – 6.68 (m, 2H), 6.65 (d, *J* = 8.2 Hz, 1H), 5.54 (d, *J* = 3.6 Hz, 1H), 2.74 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 158.0, 147.8, 134.3, 131.0, 128.0, 127.9, 117.5, 116.5, 115.6, 112.4, 72.7, 35.3.



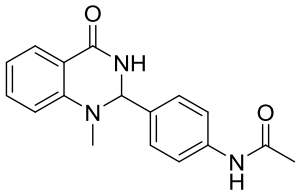
2-(4-(dimethylamino)phenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2f)

White solid (43.89 mg, 78%); R_f = 0.45 (PE/EA = 2/1); melting point: 167 – 168 ℃; CAS registry number: 421568-17-4; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.48 (d, J = 3.5 Hz, 1H), 7.72 (dd, J = 7.6, 1.6 Hz, 1H), 7.35 (td, J = 8.6, 1.7 Hz, 1H), 7.07 (d, J = 8.8 Hz, 2H), 6.75 (td, J =7.7, 0.6 Hz, 1H), 6.63 (dd, J = 8.5, 3.4 Hz, 3H), 5.52 (d, J = 3.6 Hz, 1H), 2.83 (s, 6H), 2.73 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.9, 150.9, 147.9, 134.3, 127.9, 127.8, 127.5, 117.4, 116.6, 112.4, 112.4, 72.9, 40.4, 40.4, 35.3.



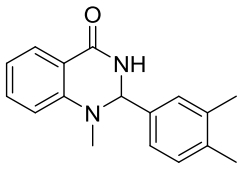
2-(4-(*tert*-butyl)phenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2g)

White solid (48.46 mg, 82%); R_f = 0.32 (PE/EA = 1/1); melting point: 149 – 151 ℃; CAS registry number: 2783565-60-4; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.59 (d, J = 3.8 Hz, 1H), 7.70 (dd, J = 7.6, 1.6 Hz, 1H), 7.39 – 7.32 (m, 3H), 7.16 (d, J = 8.4 Hz, 2H), 6.75 (td, J = 7.4, 0.7 Hz, 1H), 6.67 (d, J = 8.2 Hz, 1H), 5.63 (d, J = 3.9 Hz, 1H), 2.81 (s, 3H), 1.22 (s, 9H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 151.2, 147.7, 137.9, 134.4, 128.0, 126.4, 125.8, 117.5, 116.5, 112.3, 72.5, 35.7, 34.7, 31.5.



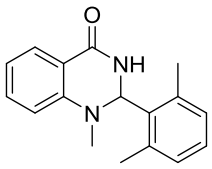
***N*-[4-(1,2,3,4-Tetrahydro-1-methyl-4-oxo-2-quinazolinyl)phenyl]acetamide (4-2h)**

White solid (46.07 mg, 78%); R_f = 0.19 (Pure EA); melting point: 211 – 212 ℃; CAS registry number: 930502-17-3; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.96 (s, 1H), 8.57 (d, J = 3.7 Hz, 1H), 7.71 (dd, J = 7.6, 1.6 Hz, 1H), 7.50 (d, J = 8.6 Hz, 2H), 7.37 (ddd, J = 8.8, 7.4, 1.7 Hz, 1H), 7.17 (d, J = 8.6 Hz, 2H), 6.76 (td, J = 6.8, 0.7 Hz, 1H), 6.66 (d, J = 8.2 Hz, 1H), 5.60 (d, J = 3.7 Hz, 1H), 2.77 (s, 3H), 2.01 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 168.8, 162.8, 147.7, 139.9, 135.1, 134.4, 128.0, 127.2, 119.4, 117.6, 116.5, 112.4, 72.6, 35.4, 24.4.



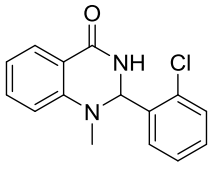
2-(3,4-dimethylphenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2i)

White solid (41.02 mg, 77%); R_f = 0.30 (PE/EA = 2/1); melting point: 138 – 139 ℃; CAS registry number; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.54 (d, J = 3.6 Hz, 1H), 7.71 (dd, J = 7.6, 1.6 Hz, 1H), 7.36 (td, J =8.6, 1.7 Hz,1H), 7.05 (d, J = 7.9 Hz, 2H), 6.95 – 6.93 (m, 1H), 6.76 (td, J = 7.4, 0.5 Hz, 1H), 6.65 (d, J = 8.2 Hz, 1H), 5.58 (d, J = 3.7 Hz, 1H), 2.77 (s, 3H), 2.15 (d, J = 3.2 Hz, 6H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 147.8, 138.1, 136.9, 136.7, 134.3, 130.0, 128.0, 127.9, 124.0, 117.5, 116.5, 112.4, 72.8, 35.5, 20.0, 19.5. **HRMS (ESI)** calcd for $C_{17}H_{18}N_2NaO^+$ $[M+Na]^+$: 289.1312; found: 289.1310.



2-(2,6-dimethylphenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2j)

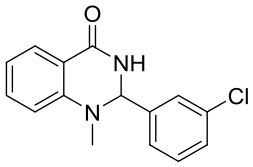
White solid (35.16 mg, 66%); R_f = 0.39 (PE/EA = 2/1); melting point: 229 – 231 ℃; CAS registry number; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.15 (s, 1H), 7.75 (dd, J = 7.8, 1.7 Hz, 1H), 7.40 (td, J = 8.7, 7.4, 1.7 Hz, 1H), 7.19 (dd, J = 7.9, 7.1 Hz, 1H), 7.08 (d, J = 7.6 Hz, 2H), 6.83 – 6.79 (m, 2H), 6.15 (s, 1H), 2.45 (s, 3H), 2.41 (s, 6H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.5, 149.9, 138.4, 134.3, 134.1, 130.0, 129.1, 128.1, 117.8, 116.4, 112.8, 69.8, 32.8, 20.8. **HRMS (ESI)** calcd for $C_{17}H_{18}N_2NaO^+$ $[M+Na]^+$: 289.1312; found: 289.1312.



2-(2-chlorophenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2k)

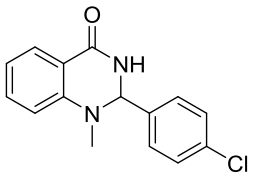
White solid (38.18 mg, 70%); R_f = 0.28 (PE/EA =3/1); melting point: 208 – 209 ℃; CAS registry number: 74375-00-1; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.58 (d, J = 3.4 Hz, 1H), 7.73 (dd, J = 7.6, 1.6 Hz, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.42 (ddd, J = 8.4, 7.4, 1.7 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.28 – 7.7.26 (m, 2H), 6.81 (td, J = 7.4, 0.7 Hz, 1H), 6.75 (d, J = 8.2 Hz, 1H), 6.09 (d, J = 3.7 Hz, 1H), 2.76 (s, 3H); **^{13}C NMR** (100

MHz, DMSO-d_6) δ 162.5, 147.9, 137.6, 134.7, 132.1, 130.8, 130.5, 128.2, 128.2, 128.1, 118.0, 116.1, 112.5, 69.8, 35.3.



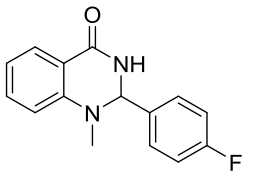
2-(3-chlorophenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2l)

White solid (40.91 mg, 75%); R_f = 0.26 (PE/EA = 3/1); melting point: 152 – 153 °C; CAS registry number: 2787027-27-2; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.70 (d, J = 3.9 Hz, 1H), 7.72 (dd, J = 7.6, 1.6 Hz, 1H), 7.41 – 7.32 (m, 4H), 7.18 (dt, J = 6.5, 1.8 Hz, 1H), 6.78 (td, J = 7.8, 0.6 Hz, 1H), 6.70 (d, J = 8.2 Hz, 1H), 5.73 (d, J = 4.0 Hz, 1H), 2.85 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.5, 143.3, 134.6, 133.6, 131.1, 128.8, 128.0, 126.7, 125.1, 117.9, 116.3, 112.5, 72.0, 35.7.



2-(4-chlorophenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2m)

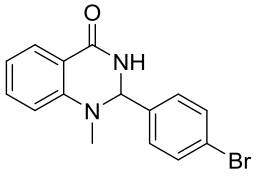
White solid (41.07 mg, 77%); R_f = 0.27 (PE/EA =2/1); melting point: 186 – 187 °C; CAS registry number: 74374-98-4; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.67 (d, J = 3.8 Hz, 1H), 7.71 (dd, J = 7.6, 1.5 Hz, 1H), 7.41 – 7.36 (m, 3H), 7.27 (d, J = 8.5 Hz, 2H), 6.78 (t, J = 7.4 Hz, 1H), 6.68 (d, J = 8.3 Hz, 1H), 5.71 (d, J = 3.9 Hz, 1H), 2.81 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.5, 139.6, 134.5, 133.5, 129.1, 128.5, 128.0, 117.8, 116.4, 112.5, 72.0, 35.6.



2-(4-fluorophenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2n)

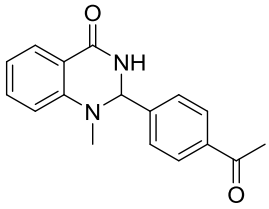
White solid (38.95 mg, 76%); R_f = 0.37 (PE/EA = 1/1); melting point: 187 – 188 °C; CAS registry number: 930504-64-6; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.66 (d, J = 3.7 Hz, 1H), 7.72 (dd, J = 7.6, 1.6 Hz, 1H), 7.38 (ddd, J = 8.8, 7.4, 1.7 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.19 – 7.14 (m, 2H), 6.77 (td, J =7.7, 0.6 Hz, 1H), 6.68 (d, J = 8.2 Hz,

1H), 5.71 (d, *J* = 3.8 Hz, 1H), 2.80 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.7, 162.7, 161.3, 147.6, 137.0, 137.0, 134.5, 128.8, 128.7, 128.0, 117.7, 116.4, 116.0, 115.7, 112.5, 72.1, 35.5.



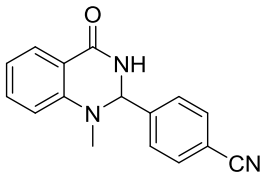
2-(4-bromophenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2o)

White solid (46.94 mg, 74%); R_f = 0.19 (PE/EA = 2/1); melting point: 194 – 196 ℃; CAS registry number: 1013308-89-8; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.68 (d, *J* = 3.9 Hz, 1H), 7.72 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.37 (td, *J* =8.6, 1.7 Hz, 1H), 7.21 (d, *J* = 8.5 Hz, 2H), 6.77 (td, *J* = 7.1, 0.6 Hz, 1H), 6.67 (d, *J* = 8.2 Hz, 1H), 5.70 (d, *J* = 3.9 Hz, 1H), 2.81 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.5, 140.0, 134.5, 132.0, 128.9, 128.0, 122.1, 117.8, 116.4, 112.5, 72.1, 35.6.



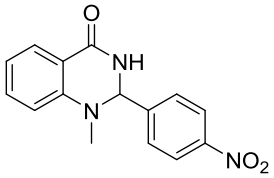
2-(4-acetylphenyl)-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2p)

White solid (37.56 mg, 67%); R_f = 0.18 (PE/EA = 1/1); melting point: 128 – 129 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.73 (d, *J* = 4.0 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.71 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.41 – 7.36 (m, 3H), 6.78 (td, *J* = 7.4, 0.7 Hz, 1H), 6.69 (d, *J* = 8.2 Hz, 1H), 5.78 (d, *J* = 4.1 Hz, 1H), 2.86 (s, 3H), 2.52 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 198.0, 162.8, 147.5, 145.5, 137.2, 134.5, 129.5, 129.0, 128.0, 126.9, 117.8, 116.5, 112.5, 72.1, 35.8, 27.2. **HRMS (ESI)** calcd for $C_{21}H_{18}N_2NaO^+$ $[M+H]^+$: 337.1311; found: 337.1305.



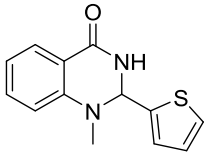
4-(1-methyl-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzonitrile (4-2q)

White solid (40.02 mg, 76%); R_f = 0.18 (PE/EA = 3/1); melting point: 158 – 160 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.77 (d, J = 4.1 Hz, 1H), 7.81 (d, J = 8.4 Hz, 2H), 7.70 (dd, J = 7.6, 1.6 Hz, 1H), 7.43 – 7.37 (m, 3H), 6.78 (td, J = 7.1, 4.0, 0.6 Hz, 1H), 6.70 (d, J = 8.2 Hz, 1H), 5.82 (d, J = 4.1 Hz, 1H), 2.86 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.3, 145.9, 134.7, 133.1, 128.1, 127.5, 119.0, 118.0, 116.3, 112.6, 111.6, 71.9, 35.8. **HRMS (ESI)** calcd for $C_{21}H_{18}N_2NaO^+$ $[M+H]^+$: 337.1311; found: 337.1305.



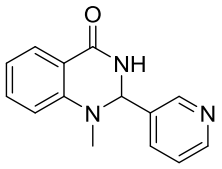
1-methyl-2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2r)

White solid (42.49 mg, 75%); R_f = 0.21 (PE/EA = 1/1); melting point: 176 – 177 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.80 (d, J = 4.1 Hz, 1H), 8.20 (d, J = 8.8 Hz, 2H), 7.71 (dd, J = 7.6, 1.6 Hz, 1H), 7.51 (d, J = 8.7 Hz, 2H), 7.40 (td, J = 8.6, 1.7 Hz, 1H), 6.79 (dd, J = 11.0, 3.9 Hz, 1H), 6.71 (d, J = 8.2 Hz, 1H), 5.89 (d, J = 4.1 Hz, 1H), 2.89 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.9, 147.8, 147.2, 134.7, 128.1, 127.9, 124.4, 118.1, 116.4, 112.7, 71.6, 35.8. **HRMS (ESI)** calcd for $C_{15}H_{13}N_3NaO_3^+$ $[M+Na]^+$: 306.0850; found: 306.0850.



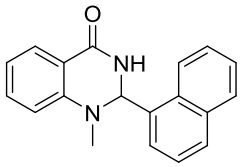
1-methyl-2-(thiophen-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2s)

White solid (36.65 mg, 75%); R_f = 0.27 (PE/EA = 1/1); melting point: 173 – 175 °C; CAS registry number: 1214-10-4; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.82 (d, J = 4.2 Hz, 1H), 7.73 (dd, J = 7.6, 1.6 Hz, 1H), 7.39 (td, J = 8.6, 1.6 Hz, 1H), 7.32 (dd, J = 5.0, 1.1 Hz, 1H), 7.02 (dd, J = 3.4, 0.7 Hz, 1H), 6.93 (dd, J = 5.0, 3.5 Hz, 1H), 6.81 (td, J = 7.8, 0.6 Hz, 1H), 6.67 (d, J = 8.2 Hz, 1H), 5.96 (d, J = 4.4 Hz, 1H), 2.84 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.2, 143.4, 134.4, 128.0, 126.8, 126.4, 126.1, 118.3, 116.9, 113.1, 69.0, 35.5.



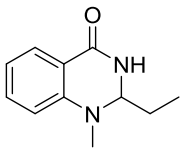
1-methyl-2-(pyridin-3-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2t)

White solid (36.85 mg, 77%); R_f = 0.20 (Pure EA); melting point: 175 – 177 °C; CAS registry number: 60868-36-2; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.73 (d, J = 3.9 Hz, 1H), 8.52 – 8.48 (m, 2H), 7.73 (dd, J = 7.6, 1.6 Hz, 1H), 7.62 (dt, J =7.9, 1.9 Hz, 1H), 7.42 – 7.33 (m, 2H), 6.80 (td, J =7.8, 0.7, 1H), 6.71 (d, J = 8.2 Hz, 1H), 5.80 (d, J = 4.0 Hz, 1H), 2.85 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 150.2, 148.0, 147.5, 136.0, 134.6, 134.3, 128.1, 124.3, 118.0, 116.5, 112.7, 70.7, 35.6.



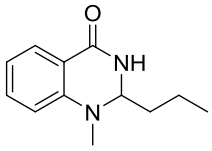
1-methyl-2-(naphthalen-1-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4-2u)

White solid (43.83 mg, 76%); R_f = 0.38 (PE/EA = 2/1); melting point: 238 – 239 °C; CAS registry number: 1013542-30-7; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.65 (d, J = 2.4 Hz, 1H), 8.55 – 8.53 (m, 1H), 8.0 – 7.93 (1H), 7.93 (d, J = 7.8 Hz, 1H), 7.76 (dd, J = 7.8, 1.6 Hz, 1H), 7.58 – 7.55 (m, 2H), 7.48 – 7.38 (m, 3H), 6.86 – 6.83 (m, 2H), 6.40 (d, J = 2.6 Hz, 1H), 2.68 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.1, 149.2, 134.9, 134.6, 134.4, 130.8, 129.9, 129.2, 128.3, 126.7, 126.4, 126.0, 125.7, 124.8, 118.0, 116.6, 112.6, 71.8, 35.1.



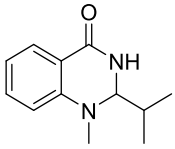
2-ethyl-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2v)

White solid (10.21 mg, 28%); R_f = 0.24 (PE/EA = 1/1); melting point: 126 – 127 °C; CAS registry number: 60868-26-0; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.31 (d, J = 3.7 Hz, 1H), 7.65 (dd, J = 7.6, 1.6 Hz, 1H), 7.34 (ddd, J = 8.4, 7.3, 1.7 Hz, 1H), 6.70 (td, J = 7.5, 0.8 Hz, 1H), 6.64 (d, J = 8.2 Hz, 1H), 4.48 (dt, J = 6.6, 4.7 Hz, 1H), 2.86 (s, 3H), 1.59 – 1.52 (m, 2H), 0.79 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.9, 147.9, 134.1, 127.8, 117.0, 116.5, 112.2, 71.9, 35.4, 25.6, 8.9.



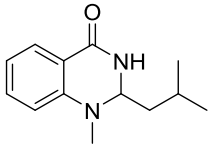
1-methyl-2-propyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2w)

White solid (6.13 mg, 15%); R_f = 0.39 (PE/EA = 1/1); melting point: 137 – 139 ℃; CAS registry number: 60868-27-1; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.34 (d, J = 4.2 Hz, 1H), 7.65 (dd, J = 7.6, 1.6 Hz, 1H), 7.34 (ddd, J = 8.4, 7.3, 1.7 Hz, 1H), 6.71 (td, J = 7.8, 0.7 Hz, 1H), 6.63 (d, J = 8.2 Hz, 1H), 4.54 – 4.50 (m, 1H), 2.85 (s, 3H), 1.54 – 1.47 (m, 2H), 1.32 – 1.19 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.9, 147.9, 134.0, 127.9, 117.1, 116.6, 112.3, 70.6, 35.5, 34.6, 17.5, 14.2.



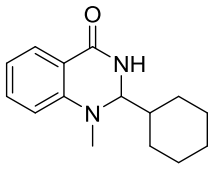
2-isopropyl-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2x)

White solid (10.21 mg, 25%); R_f = 0.26 (PE/EA = 1/1); melting point: 128 – 130 ℃; CAS registry number: 60868-28-2; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.22 (d, J = 4.0 Hz, 1H), 7.61 (dd, J = 7.6, 1.6 Hz, 1H), 7.32 (ddd, J = 8.4, 7.3, 1.7 Hz, 1H), 6.67 – 6.60 (m, 2H), 4.41 (t, J = 4.7 Hz, 1H), 2.95 (s, 3H), 1.99 (qd, J = 12.0, 6.8 Hz, 1H), 0.80 (d, J = 6.9 Hz, 3H), 0.69 (d, J = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.1, 147.8, 134.1, 127.7, 116.4, 116.3, 111.6, 75.5, 37.0, 34.0, 18.3, 17.1.



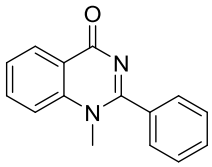
2-isobutyl-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2z)

White solid (7.86 mg, 25%); R_f = 0.35 (PE/EA = 1/1); melting point: 128 – 130 ℃; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.41 (d, J = 4.6 Hz, 1H), 7.64 (dd, J = 7.6, 1.6 Hz, 1H), 7.35 (dt, J =8.6, 1.6 Hz, 1H), 7.72 (dt, J =7.7, 0.6 Hz, 1H), 6.64 (d, J = 8.2 Hz, 1H), 4.56 – 4.52 (m, 1H), 2.85 (s, 3H), 1.70 – 1.61 (m, 1H), 1.51 – 1.45 (m, 1H), 1.30 – 1.23 (m, 1H), 0.85 (dd, J = 13.1, 6.6 Hz, 6H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 147.7, 134.0, 127.9, 117.2, 116.8, 112.7, 69.3, 35.6, 24.0, 23.3, 22.1.



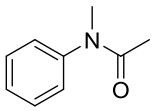
2-cyclohexyl-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (4-2cc)

White solid (29.32 mg, 60%); R_f = 0.23 (PE/EA = 1/1); melting point: 153 – 155 °C; CAS registry number: 60868-29-3; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.22 (d, J = 4.4 Hz, 1H), 7.60 (dd, J = 7.6, 1.6 Hz, 1H), 7.31 (ddd, J = 8.4, 7.3, 1.7 Hz, 1H), 6.65 (td, J = 7.8, 0.8 Hz, 1H), 6.60 (d, J = 8.2 Hz, 1H), 4.39 (t, J = 4.9 Hz, 1H), 2.96 (s, 3H), 1.67 – 1.43 (m, 7H), 1.08 – 1.01 (m, 4H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.0, 147.9, 134.0, 127.7, 116.4, 111.6, 75.0, 44.0, 37.3, 28.1, 27.3, 26.2, 25.9, 25.7.



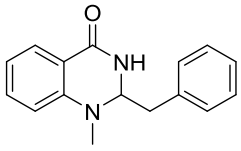
1-methyl-2-phenylquinazolin-4(1*H*)-one

Yellow solid (9.45 mg, 20%); R_f = 0.12 (DCM/EA = 3/1); melting point: 240 – 241 ℃; CAS registry number: 22686-80-2; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.13 (d, J = 7.5 Hz, 1H), 7.88 (t, J = 7.4 Hz, 1H), 7.76 (d, J = 8.5 Hz, 1H), 7.70 – 7.68 (m, 2H), 7.59 – 7.55 (m, 4H), 3.64 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 142.15, 135.64, 134.46, 130.77, 129.10, 128.89, 127.56, 126.52, 117.32, 38.39.



***N*-methyl-*N*-phenylacetamide**

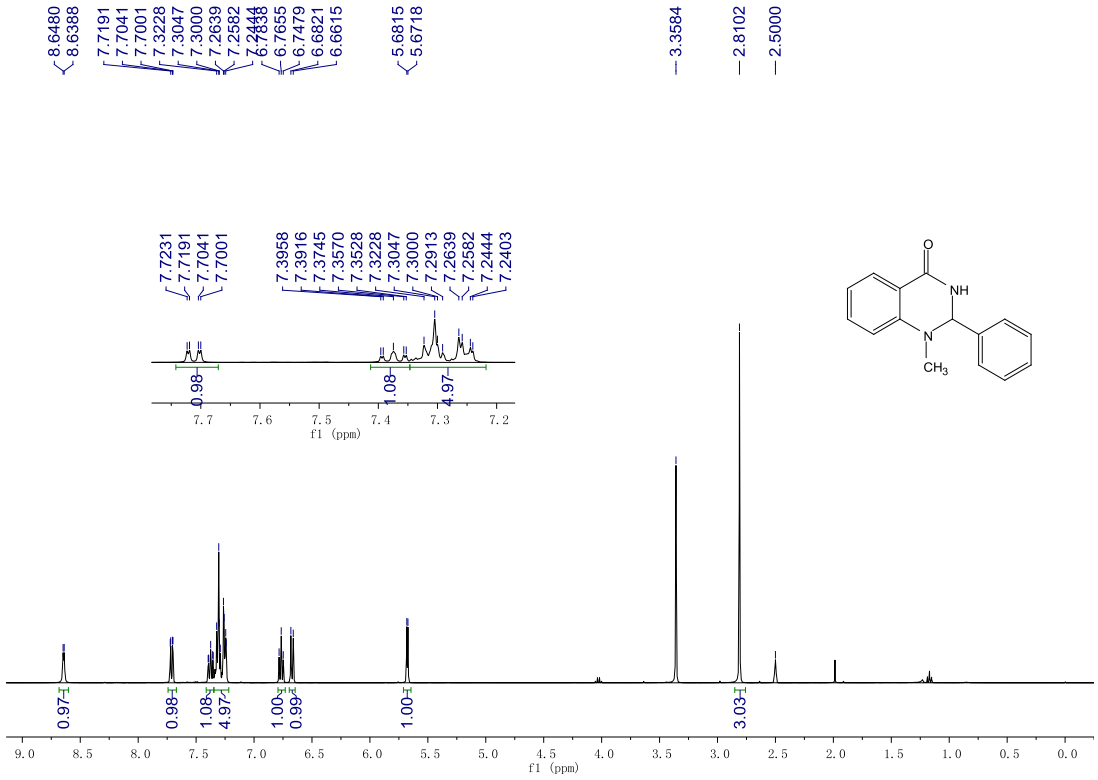
White solid (23.87 mg, 80%); R_f = 0.32 (PE/EA = 3/1); melting point: 104 – 105 ℃; CAS registry number: 579-10-2; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.3 Hz, 1H), 7.18 (d, J = 7.5 Hz, 2H), 3.25 (s, 3H), 1.86 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.61, 144.61, 129.73, 127.72, 127.08, 37.16, 22.40.



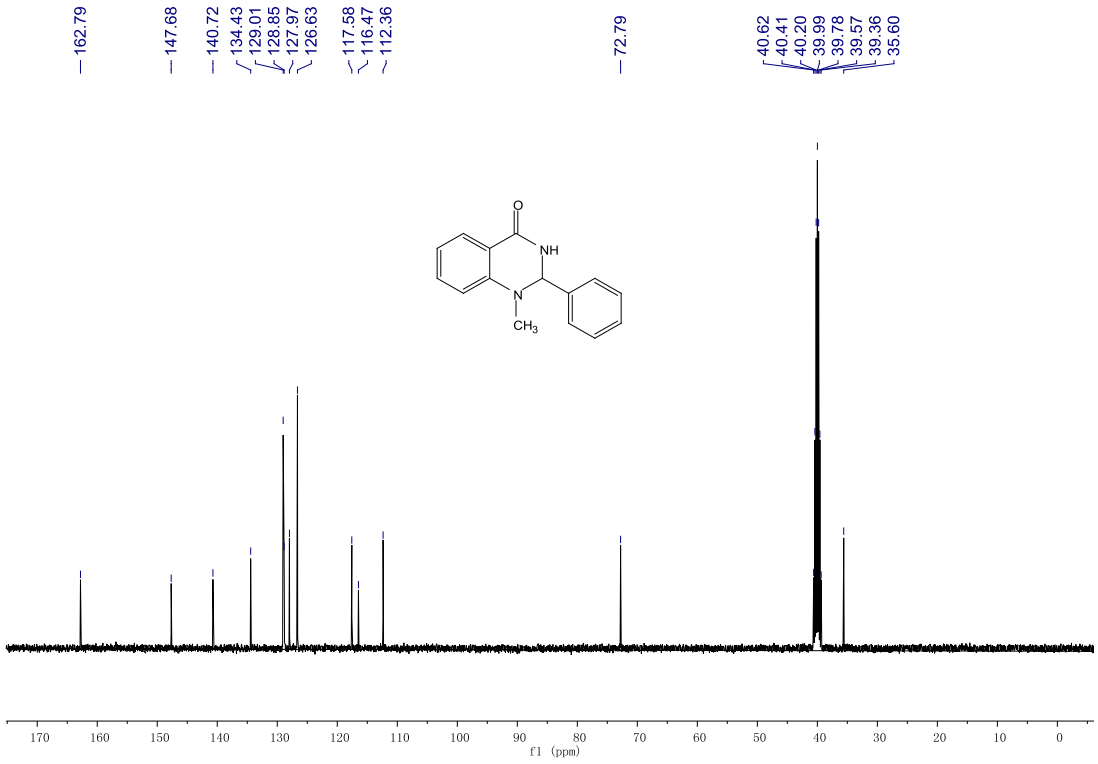
2-benzyl-1-methyl-2,3-dihydroquinazolin-4(1*H*)-one (Glycozolone A)

White solid (146.34 mg, 80%); R_f = 0.33 (PE/EA = 1/1), melting point: 195 – 196 ° C; CAS registry number: 26750-21-0; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.12 (d, J = 4.4 Hz, 1H), 7.63 (dd, J = 7.6, 1.5 Hz, 1H), 7.36 (td, J = 7.7, 1.6 Hz, 1H), 7.26 – 7.11 (m, 5H), 6.71 (t, J = 7.3 Hz, 1H), 6.64 (d, J = 8.2 Hz, 1H), 4.81 (dt, J = 9.8, 4.9 Hz, 1H), 2.91 – 2.74 (m, 5H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 147.3, 136.8, 134.1, 130.3, 128.6, 127.9, 126.8, 117.1, 116.7, 112.4, 71.9, 39.0, 36.1.

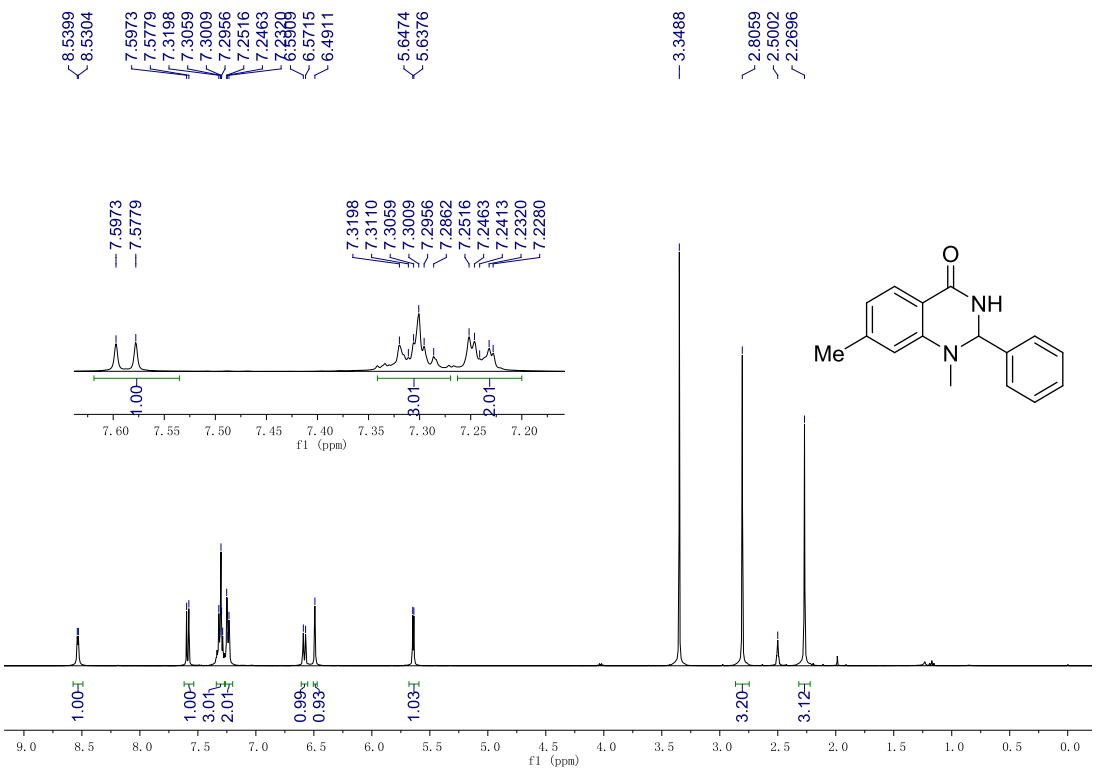
4. Copies of NMR Spectra for the Products



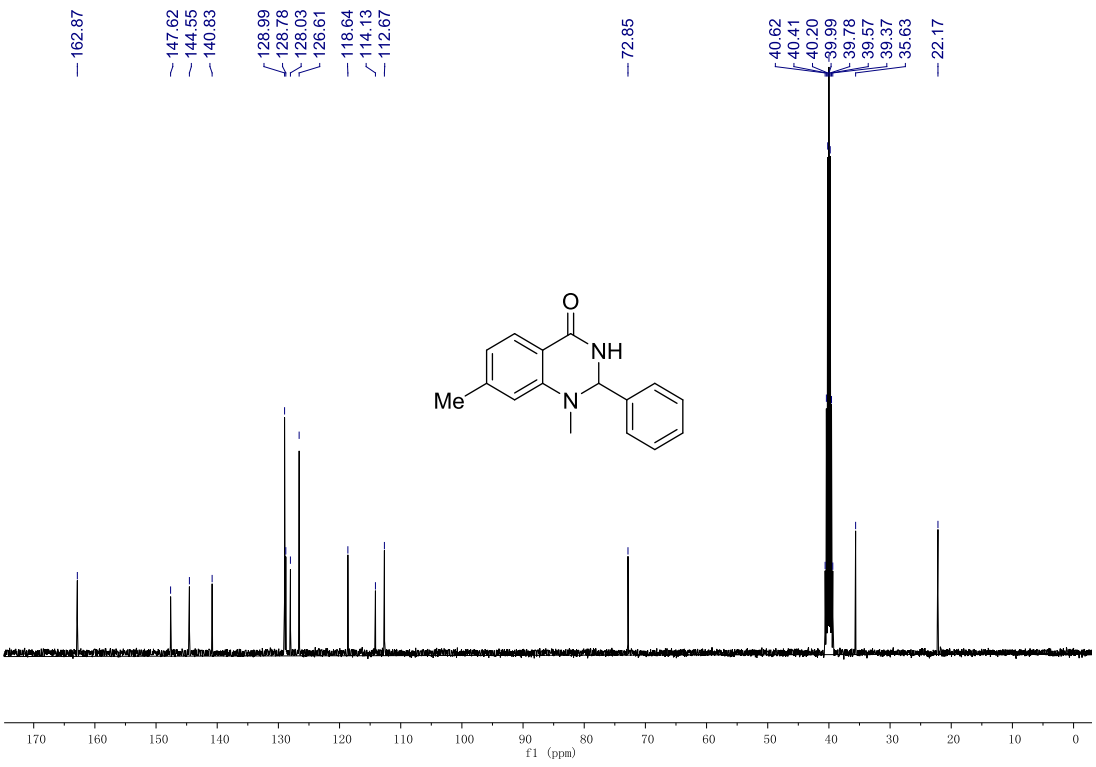
4-1a, ^{1}H NMR (400 MHz, DMSO-d_6)



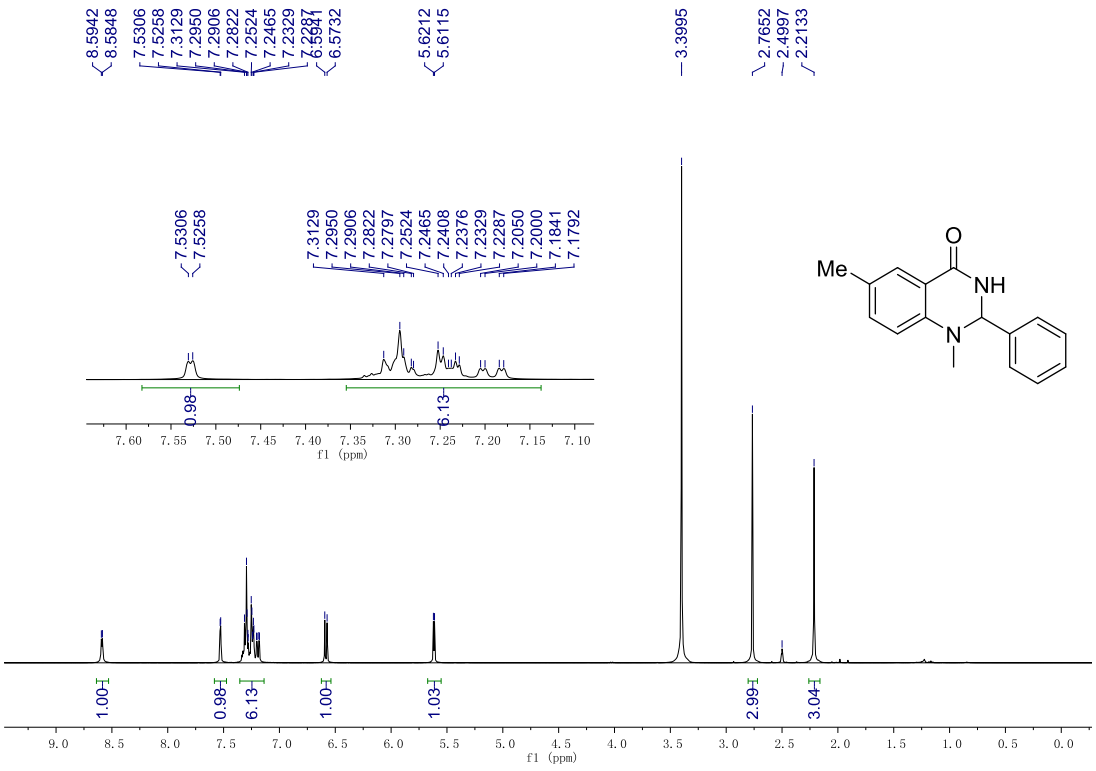
4-1a, ^{13}C NMR (100 MHz, DMSO-d_6)



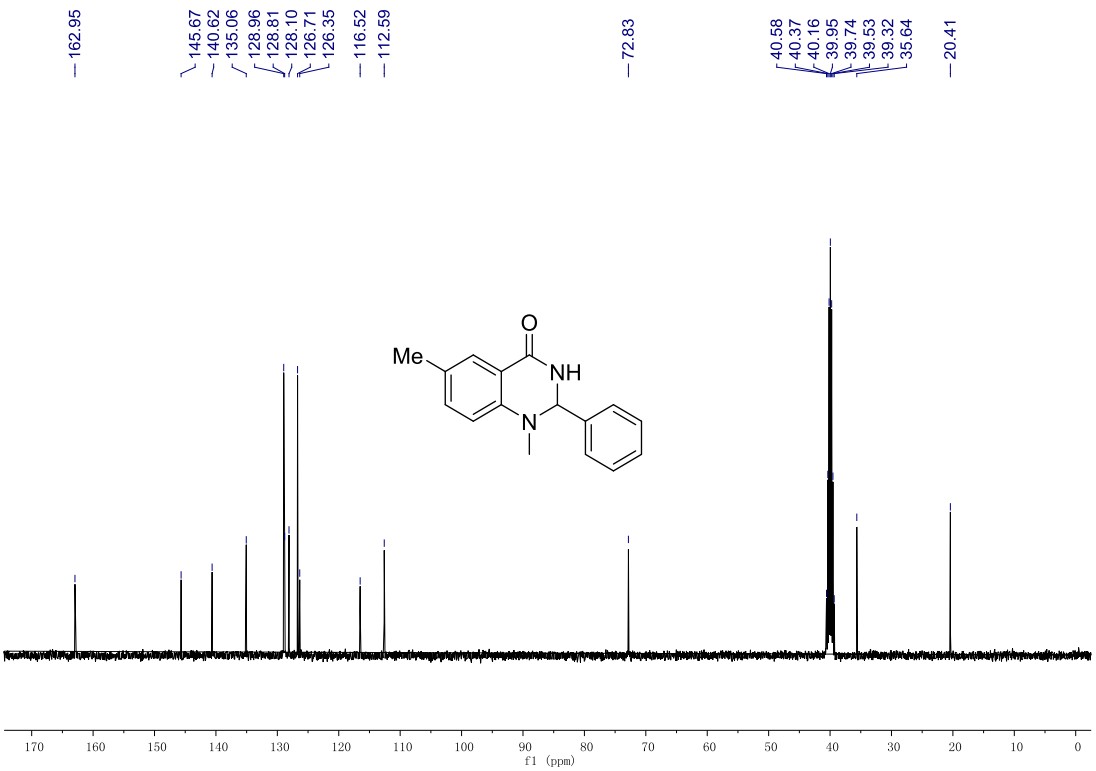
4-1b, ^{1}H NMR (400 MHz, DMSO-d_6)



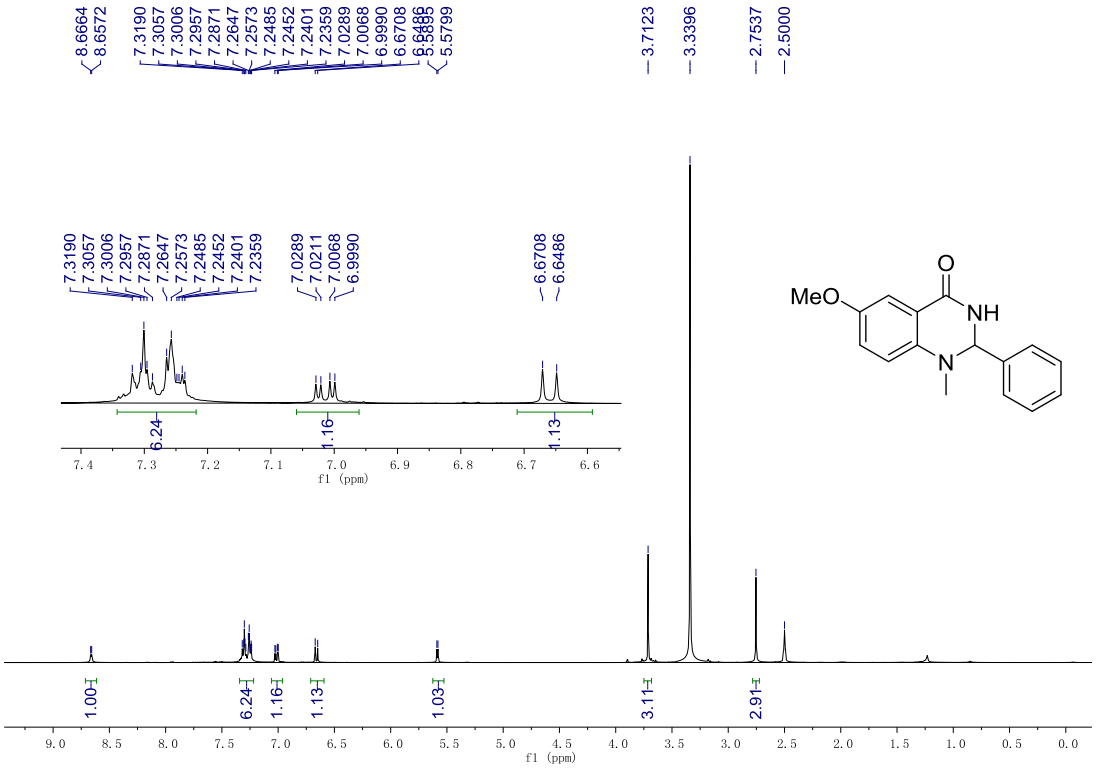
4-1b, ^{13}C NMR (100 MHz, DMSO-d_6)



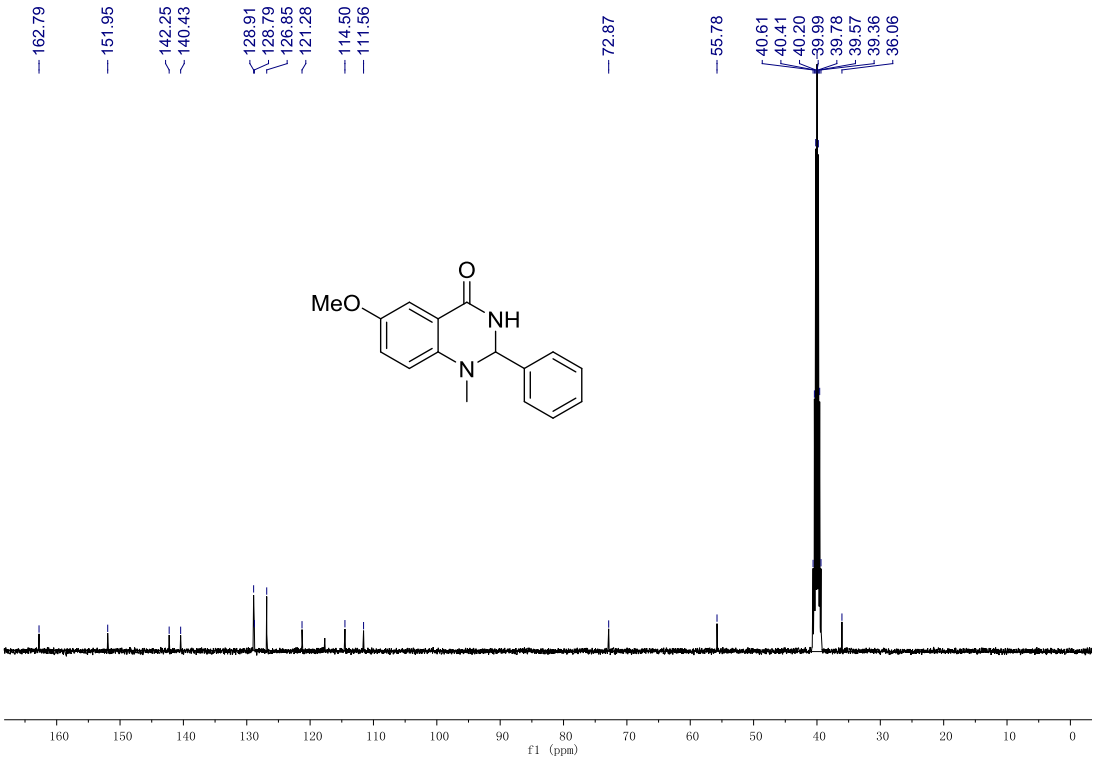
4-1c, ^{1}H NMR (400 MHz, DMSO-d_6)



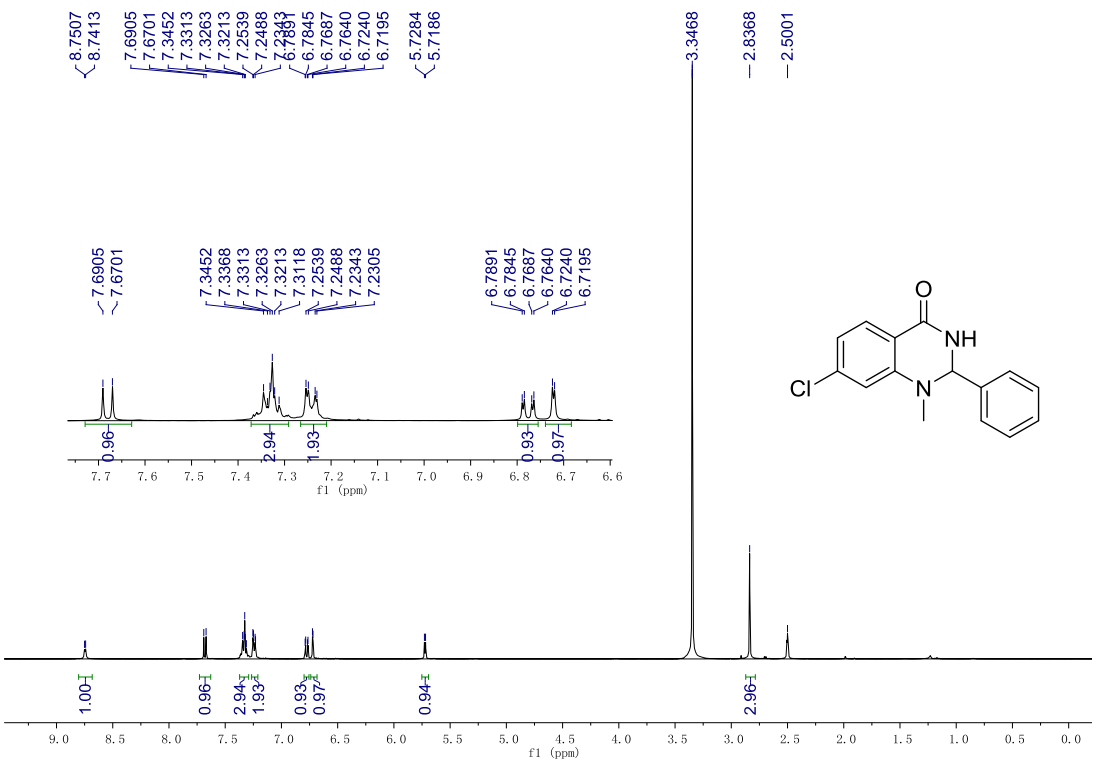
4-1c, ^{13}C NMR (100 MHz, DMSO-d_6)



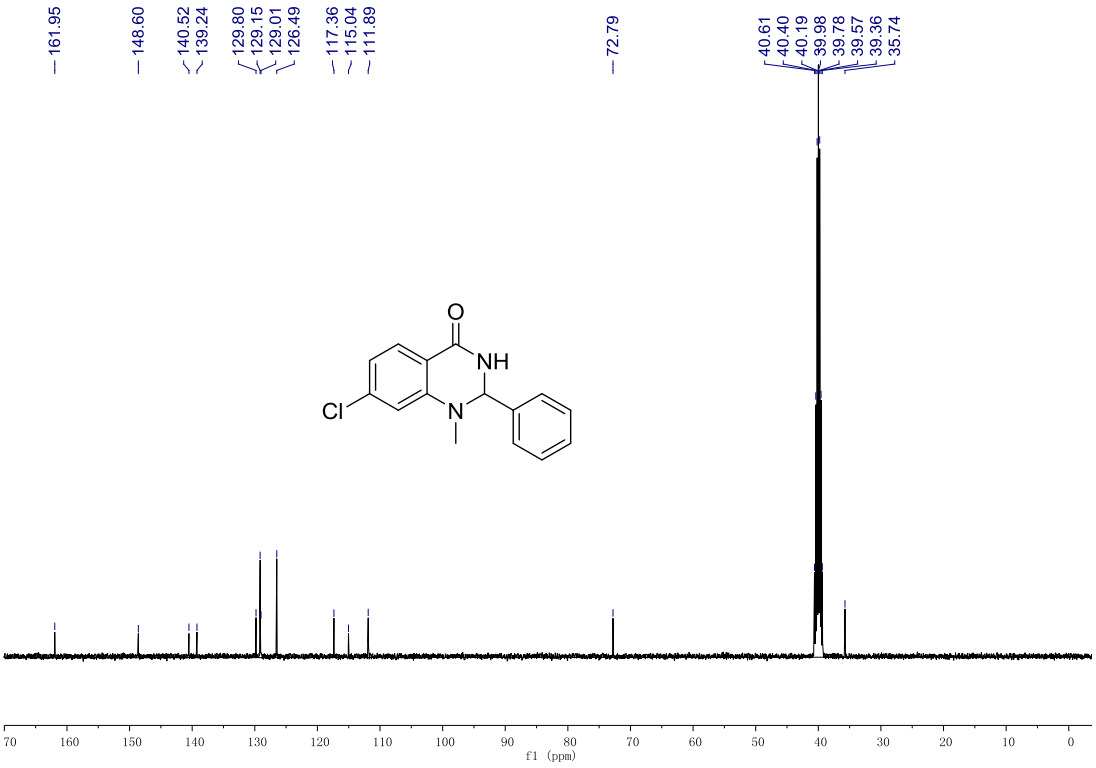
4-1d, ^{1}H NMR (400 MHz, DMSO-d_6)



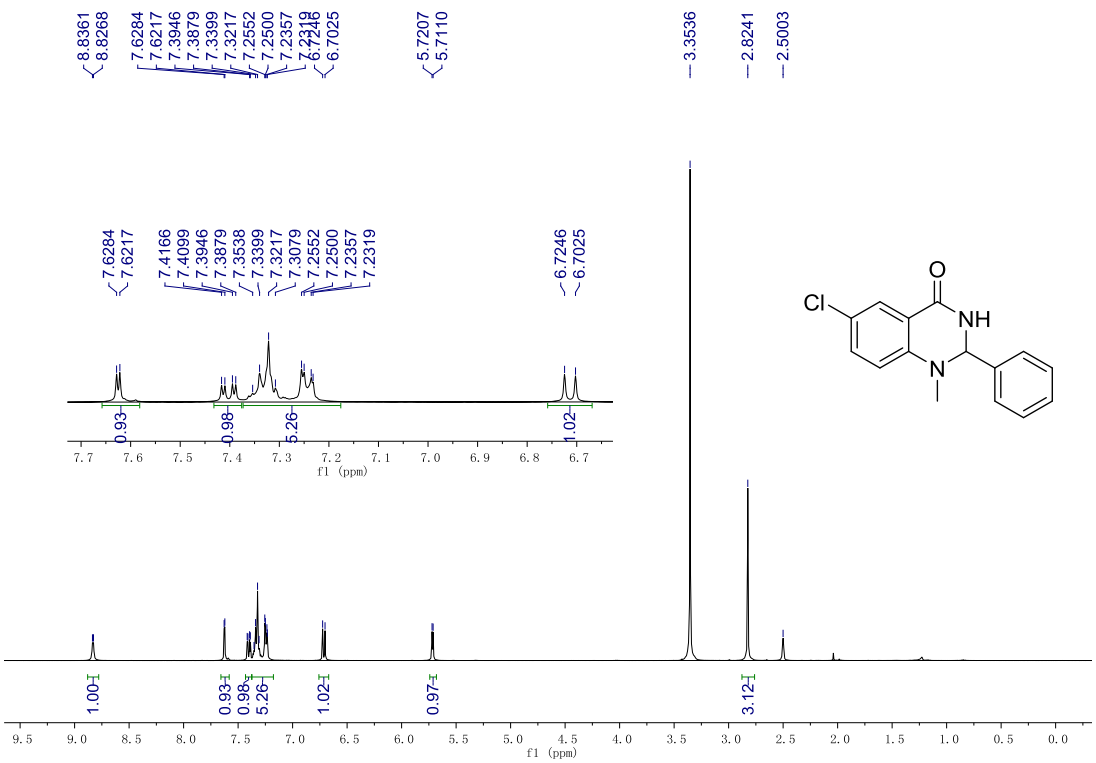
4-1d, ^{13}C NMR (100 MHz, DMSO-d_6)



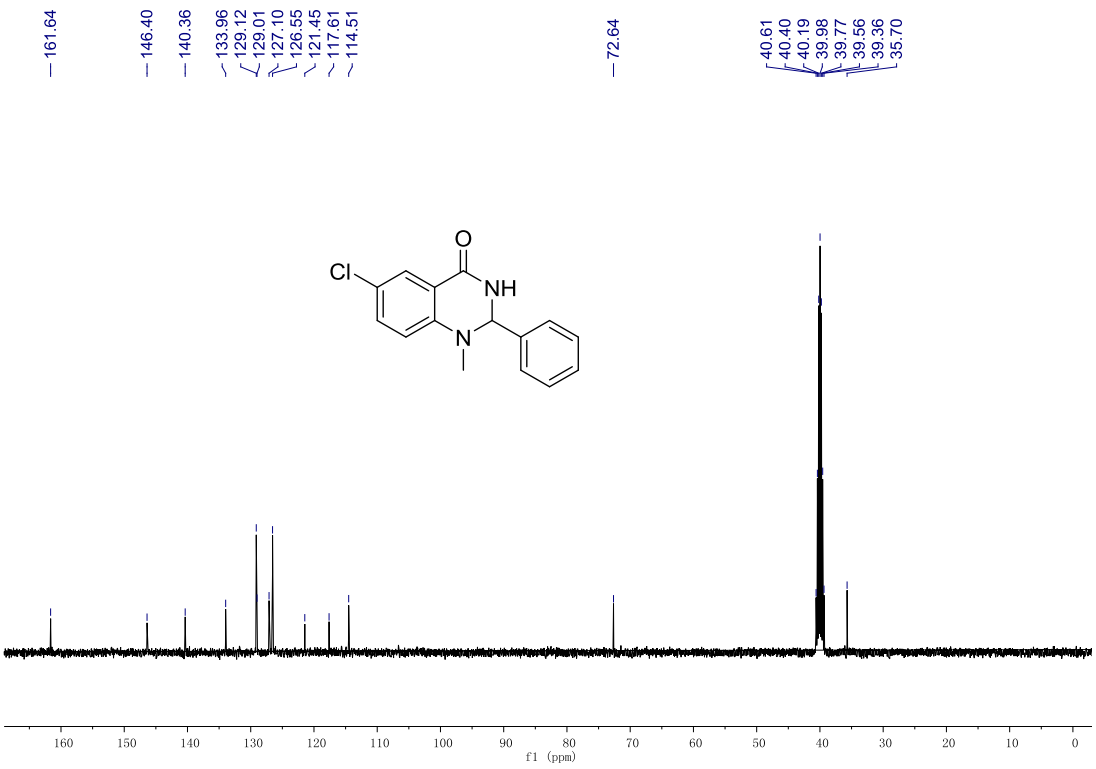
4-1f, ^{1}H NMR (400 MHz, DMSO-d_6)



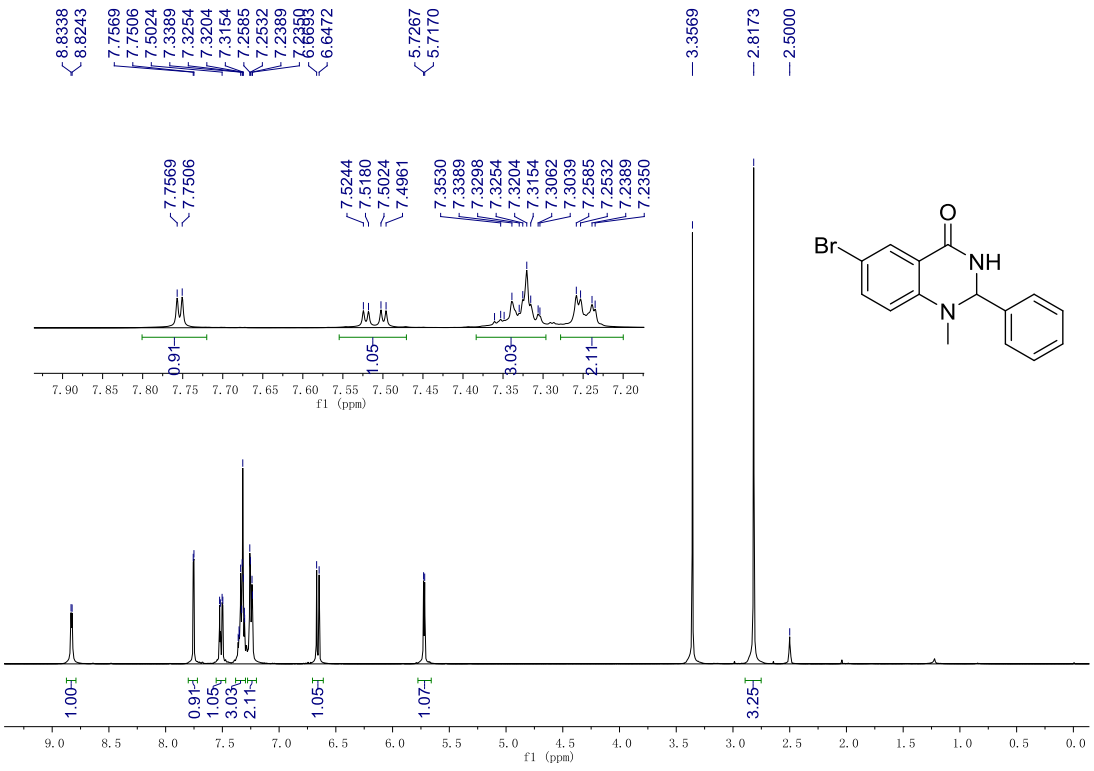
4-1f, ^{13}C NMR (100 MHz, DMSO-d_6)



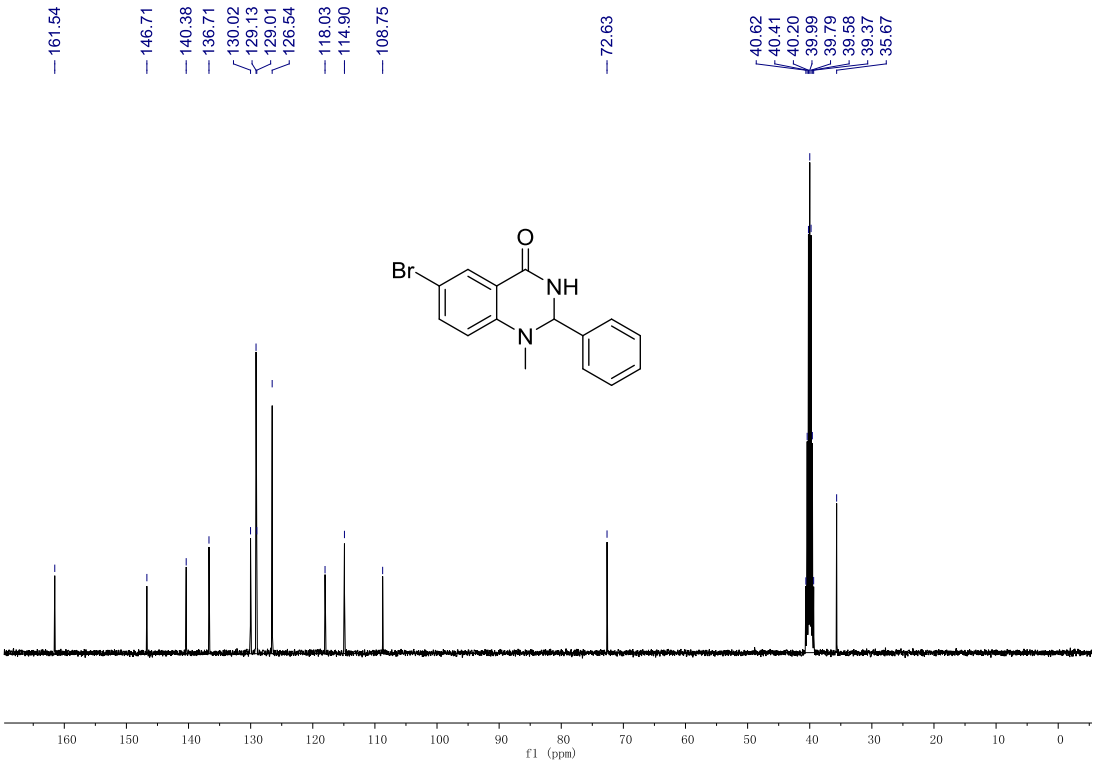
4-1g, ^{1}H NMR (400 MHz, DMSO-d_6)



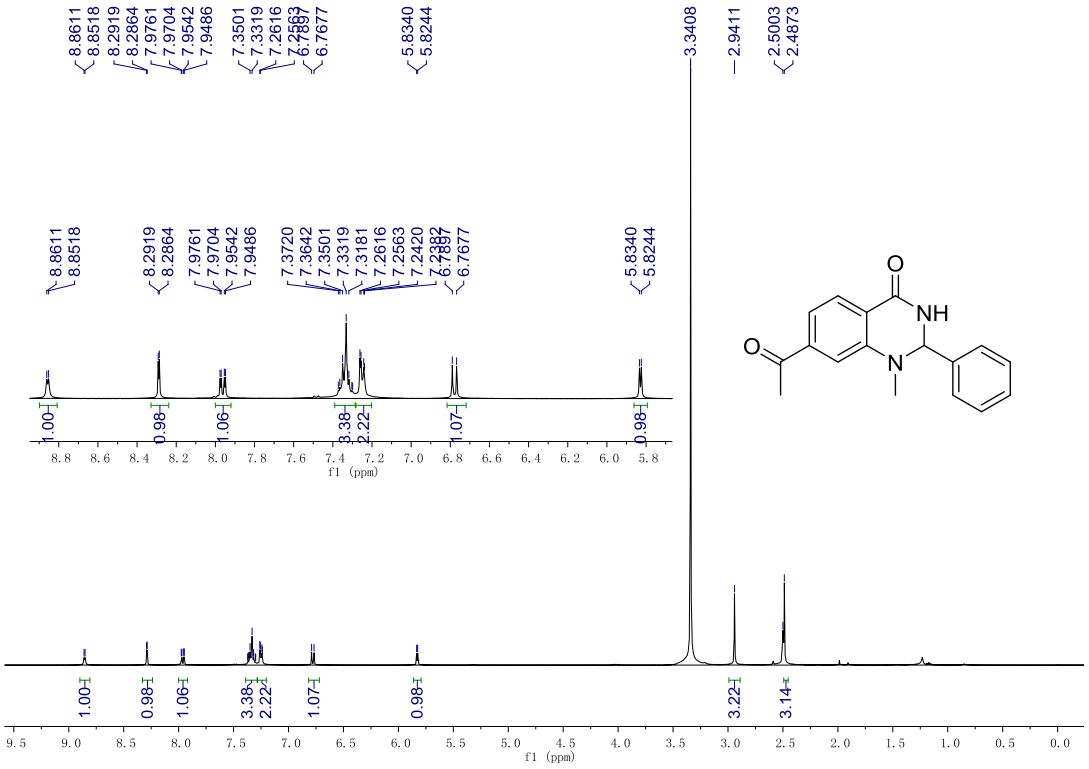
4-1g, ^{13}C NMR (100 MHz, DMSO-d_6)



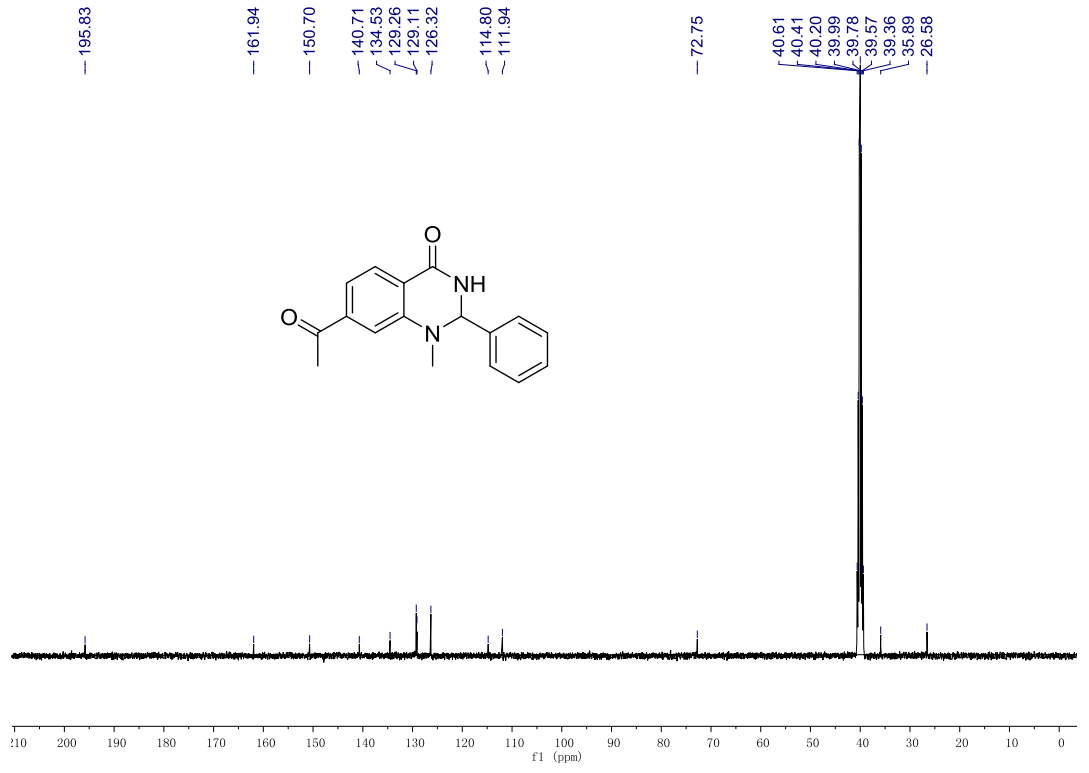
4-1h, ^{1}H NMR (400 MHz, DMSO-d_6)



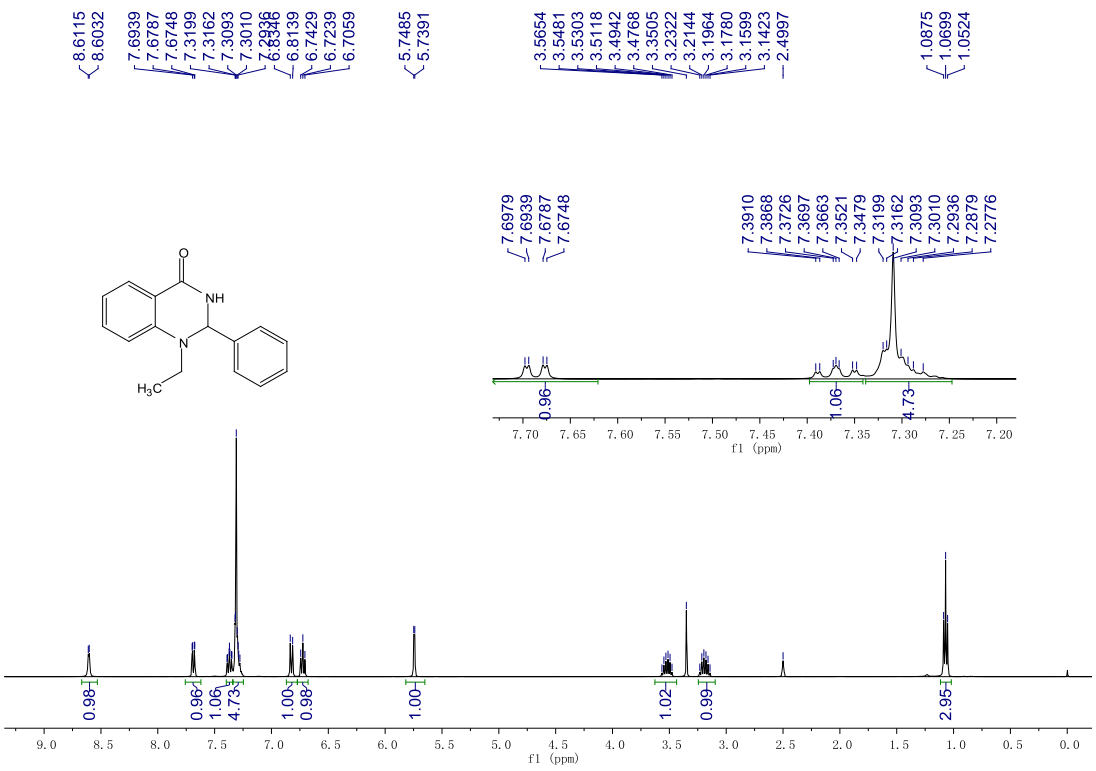
4-1h, ^{13}C NMR (100 MHz, DMSO-d_6)



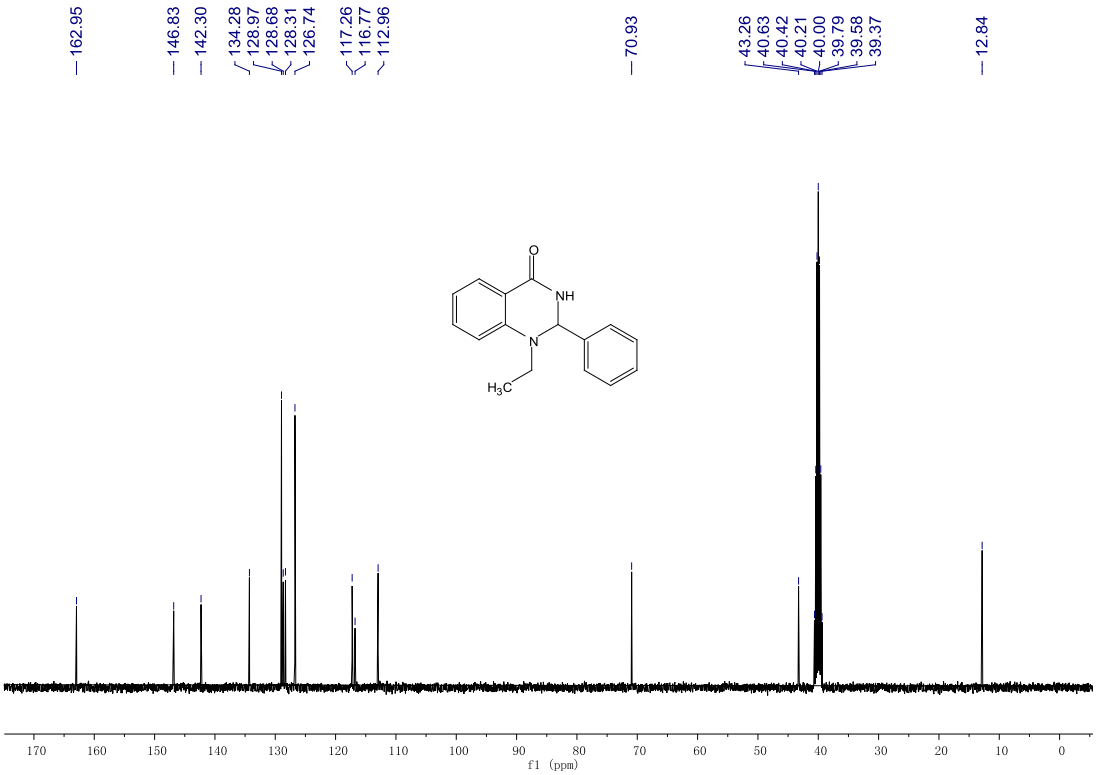
4-1i, ^{1}H NMR (400 MHz, DMSO-d_6)



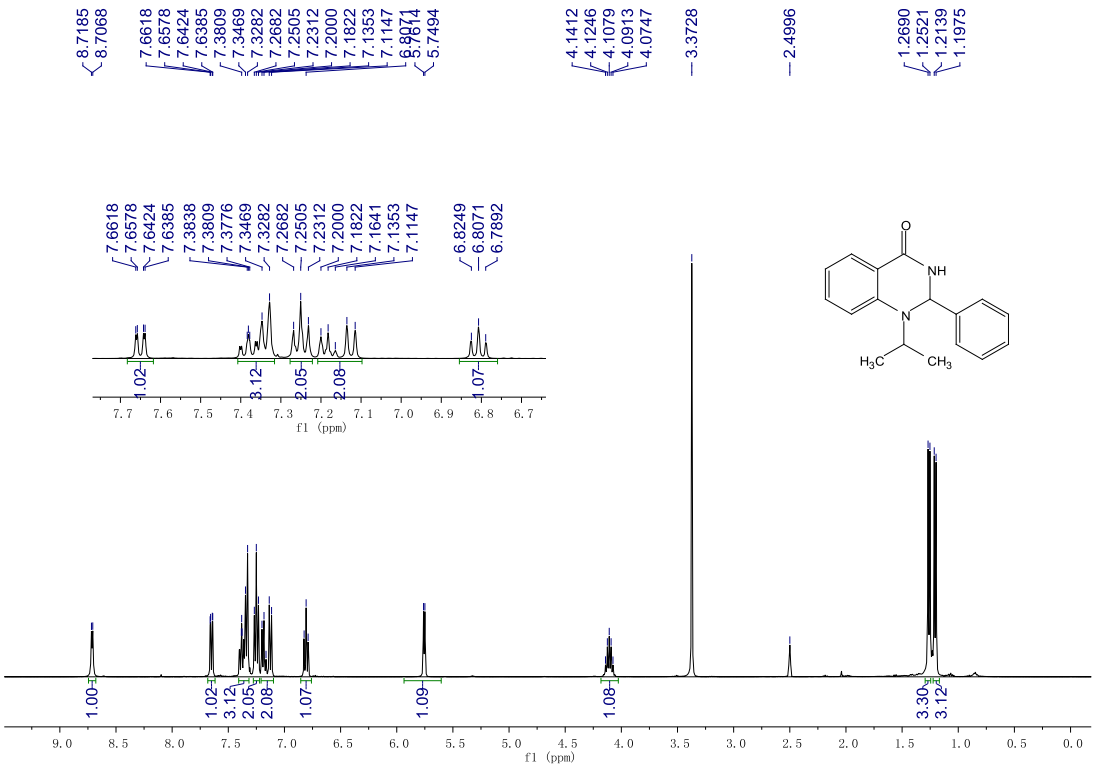
4-1i, ^{13}C NMR (100 MHz, DMSO-d_6)



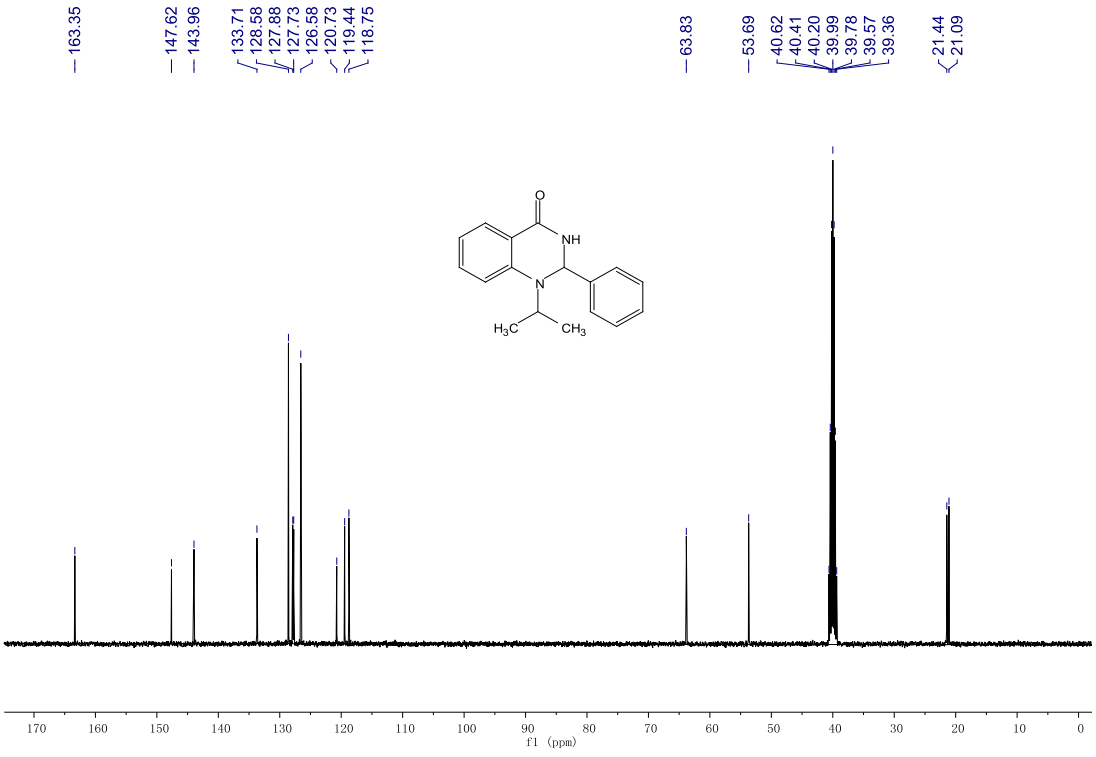
4-1l, ^{1}H NMR (400 MHz, DMSO-d_6)



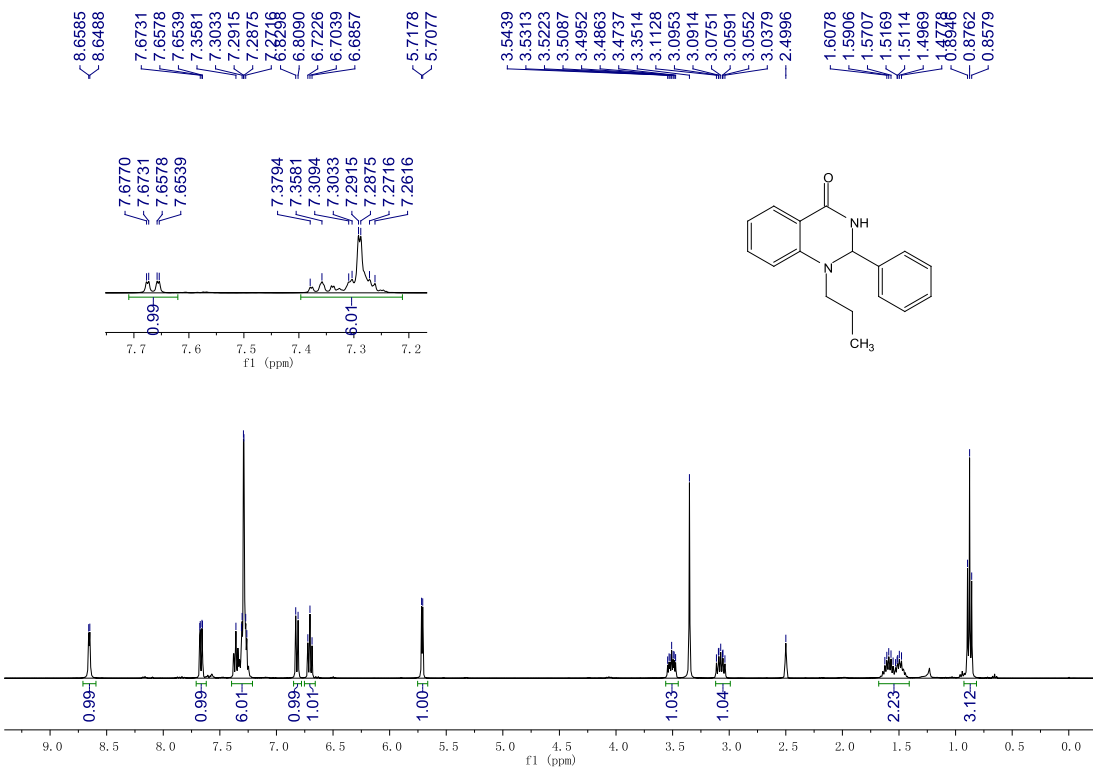
4-1l, ^{13}C NMR (100 MHz, DMSO-d_6)



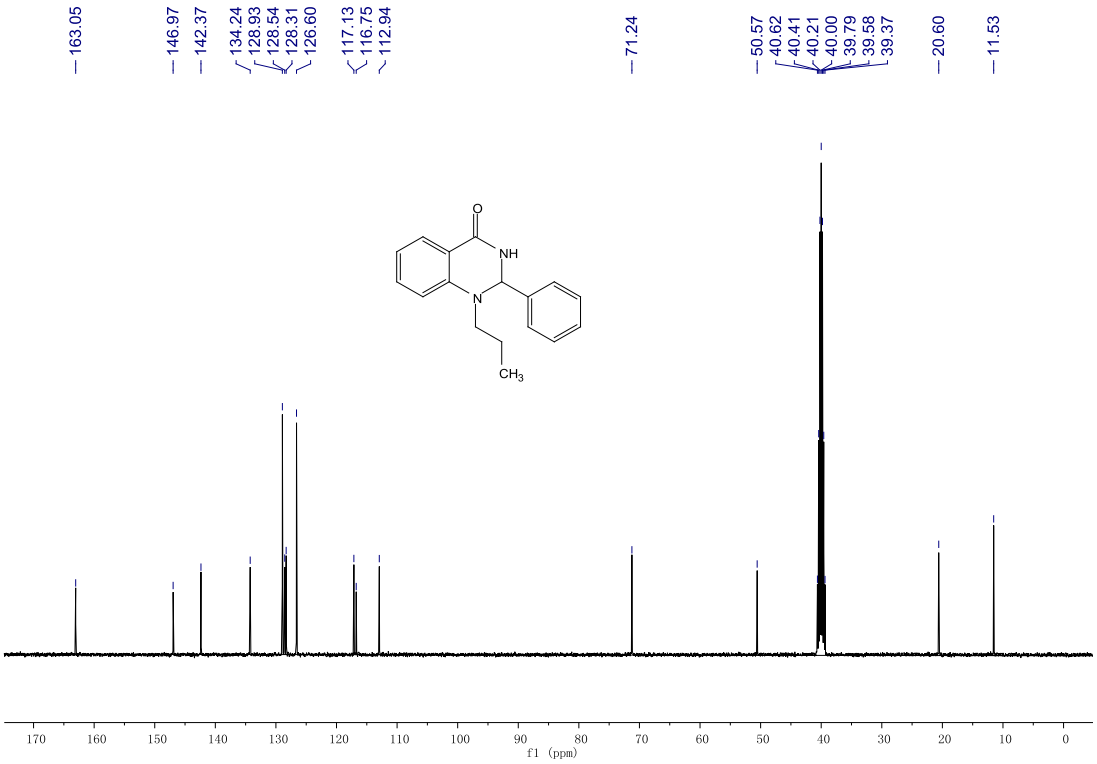
4-1m, ^{1}H NMR (400 MHz, DMSO-d_6)



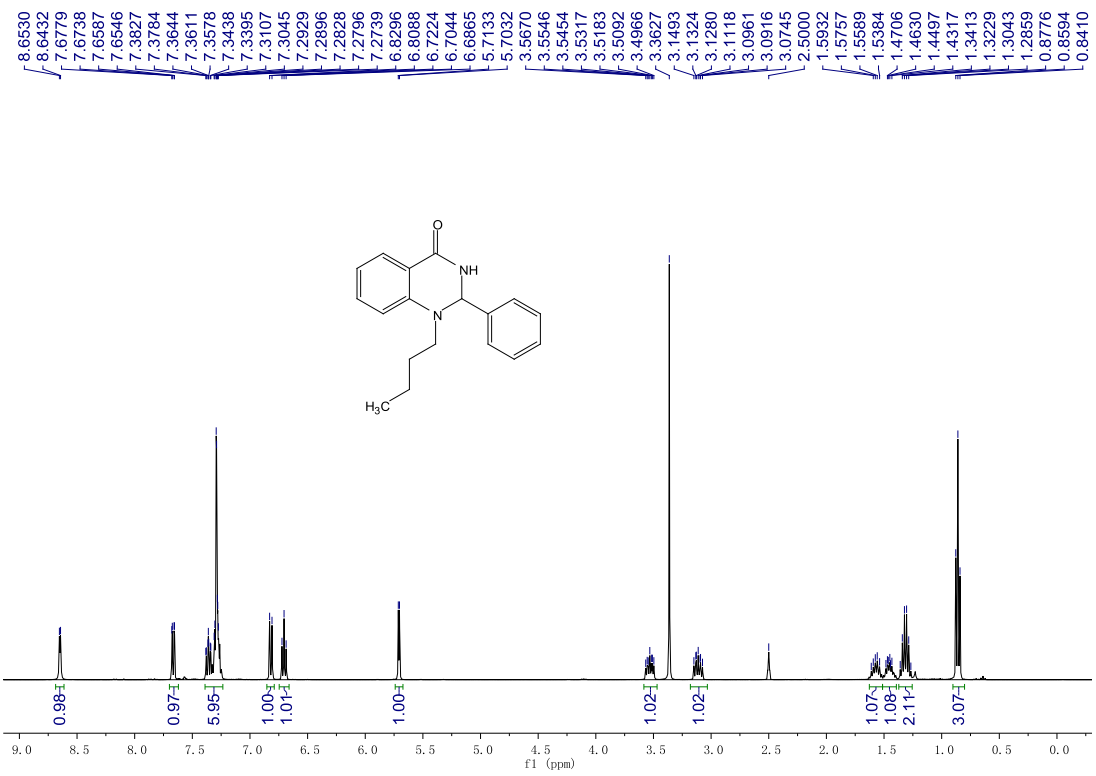
4-1m, ^{13}C NMR (100 MHz, DMSO-d_6)



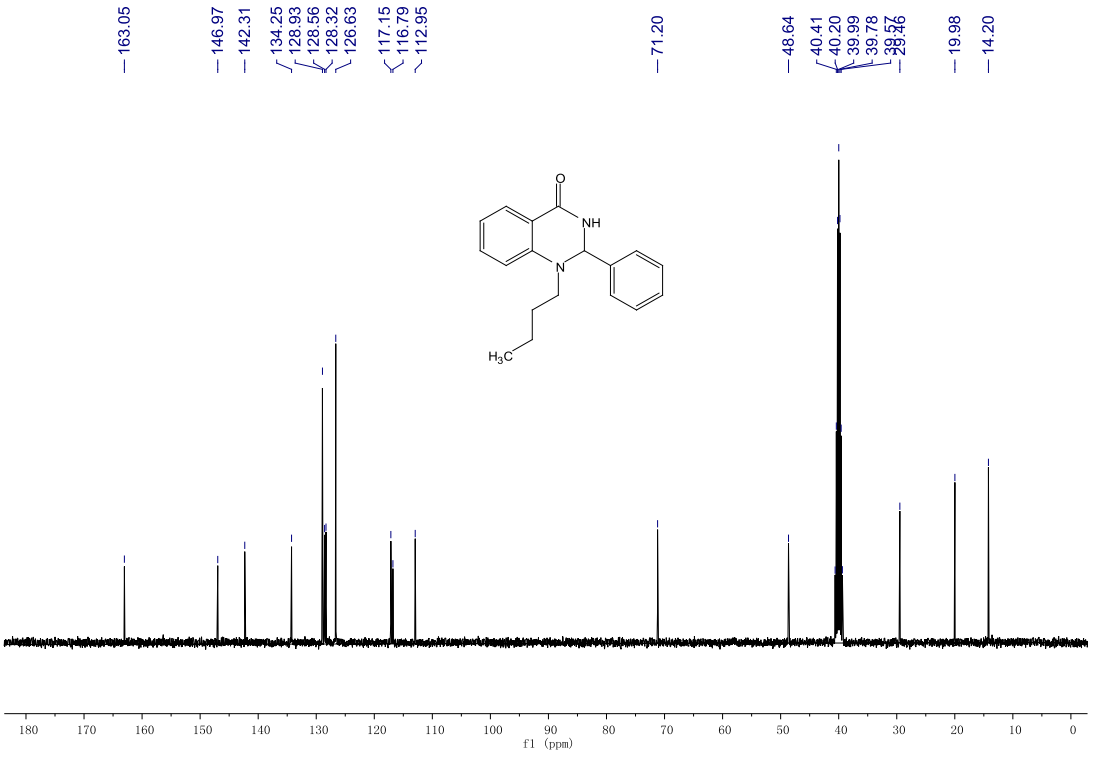
4-1n, ^{1}H NMR (400 MHz, DMSO-d_6)



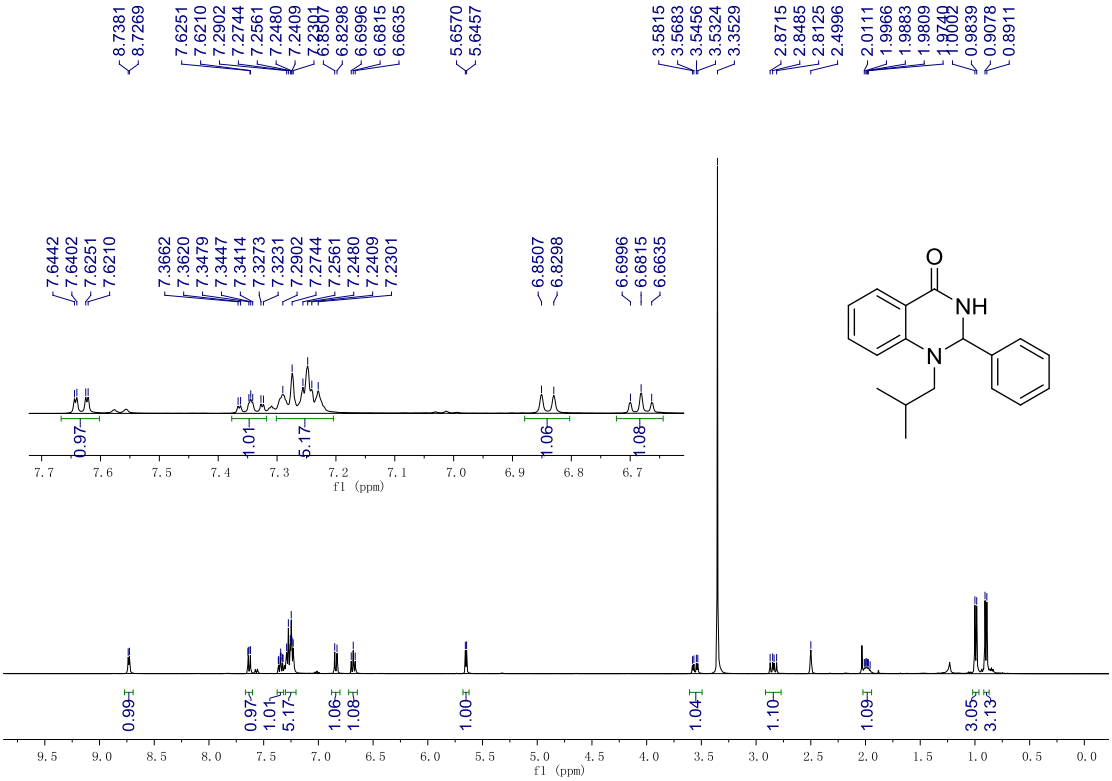
4-1n, ^{13}C NMR (100 MHz, DMSO-d_6)



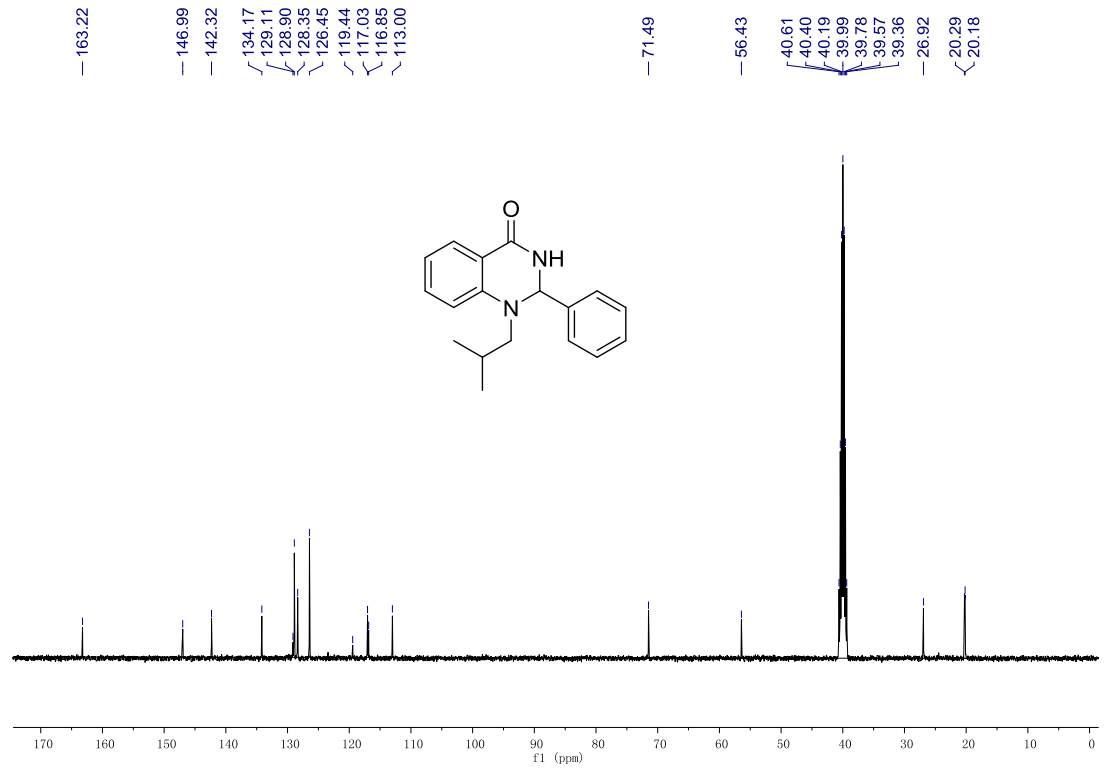
4-1o, ^{1}H NMR (400 MHz, DMSO-d_6)



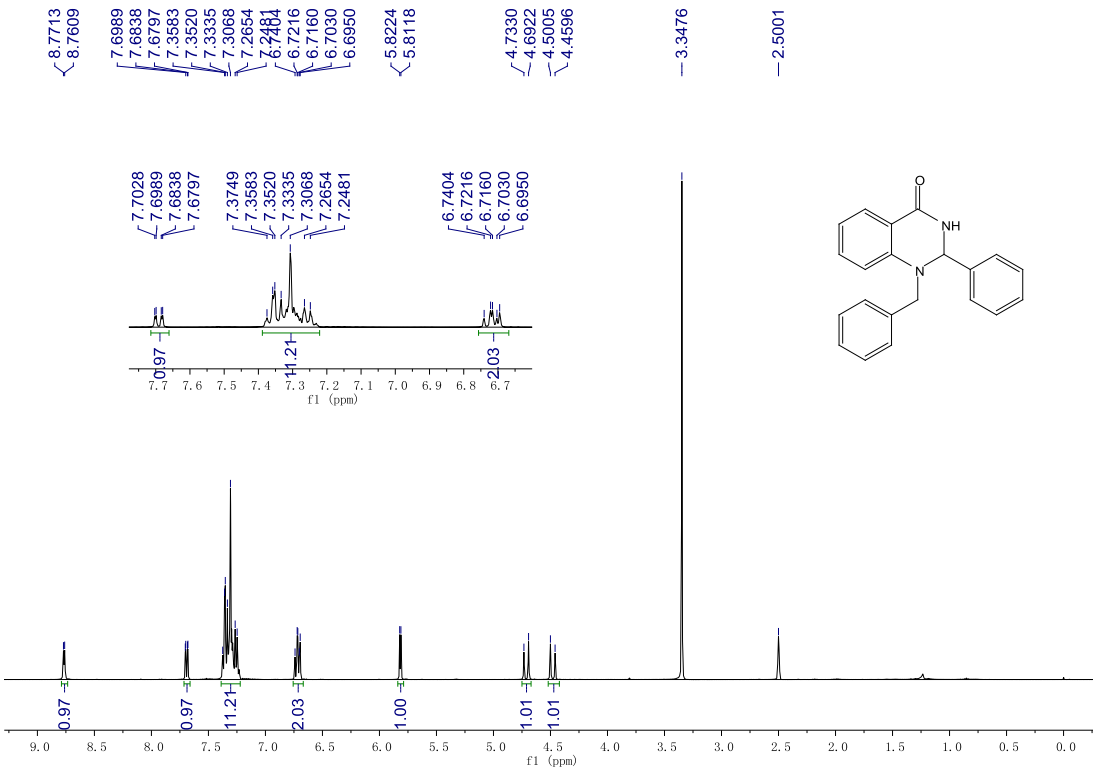
4-1o, ^{13}C NMR (100 MHz, DMSO-d_6)



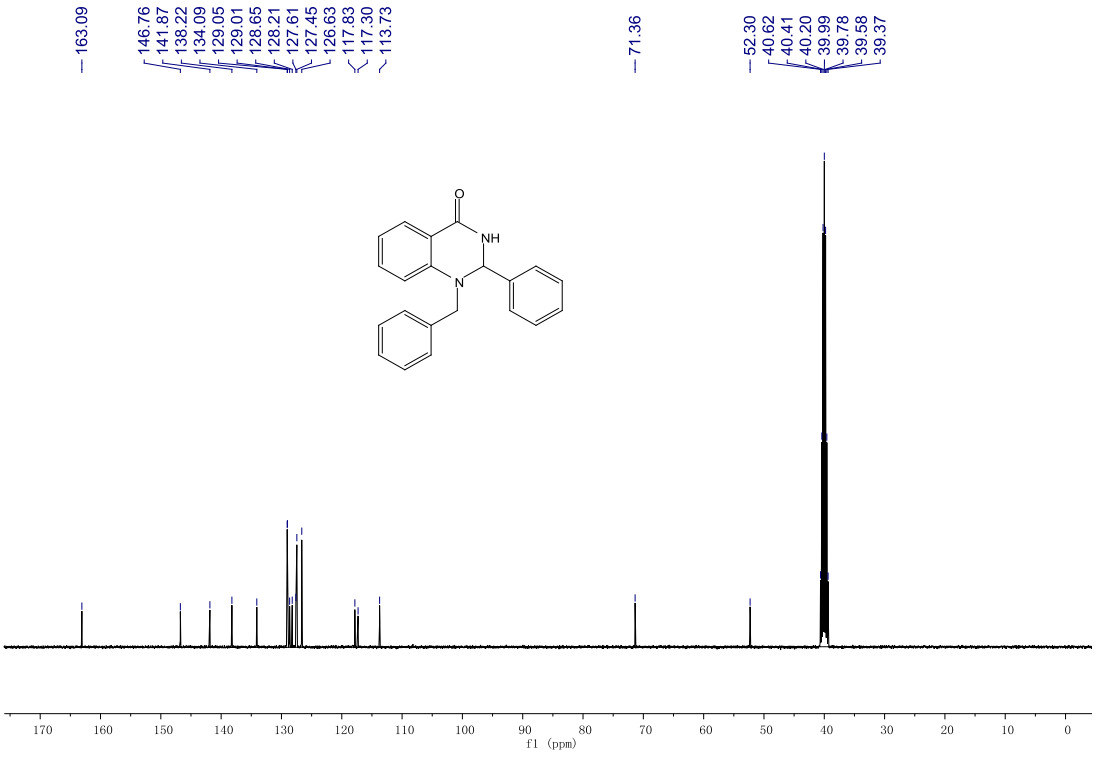
4-1p, ^{1}H NMR (400 MHz, DMSO-d_6)



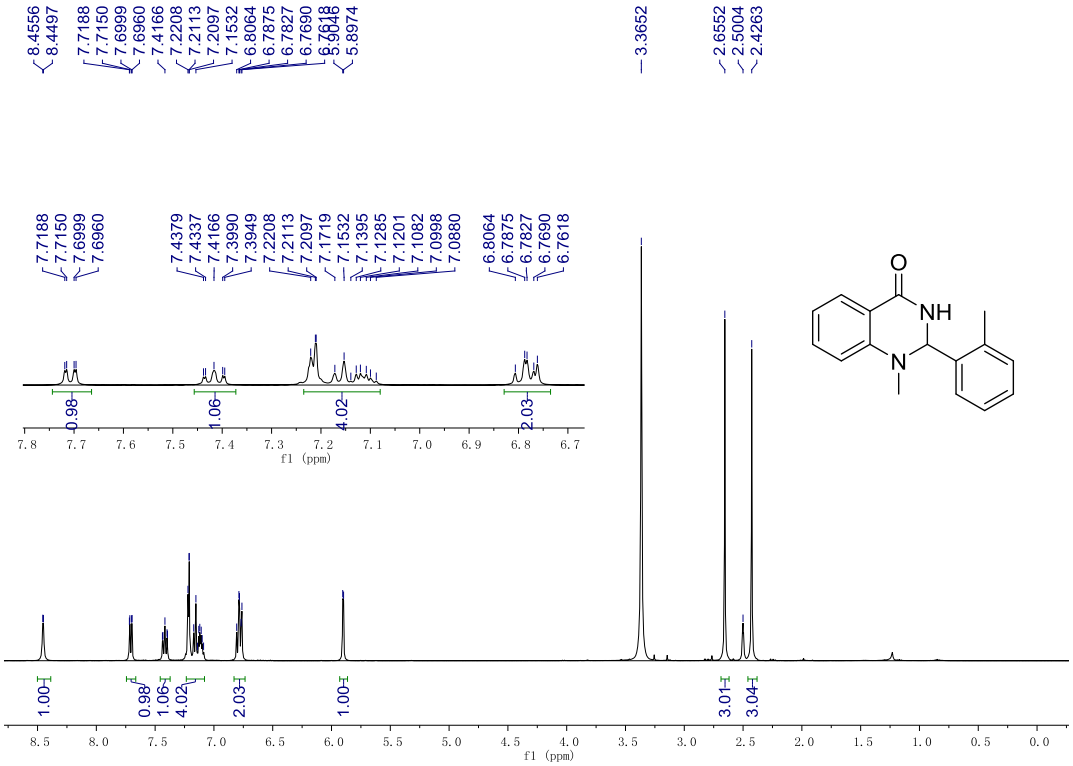
4-1p, ^{13}C NMR (100 MHz, DMSO-d_6)



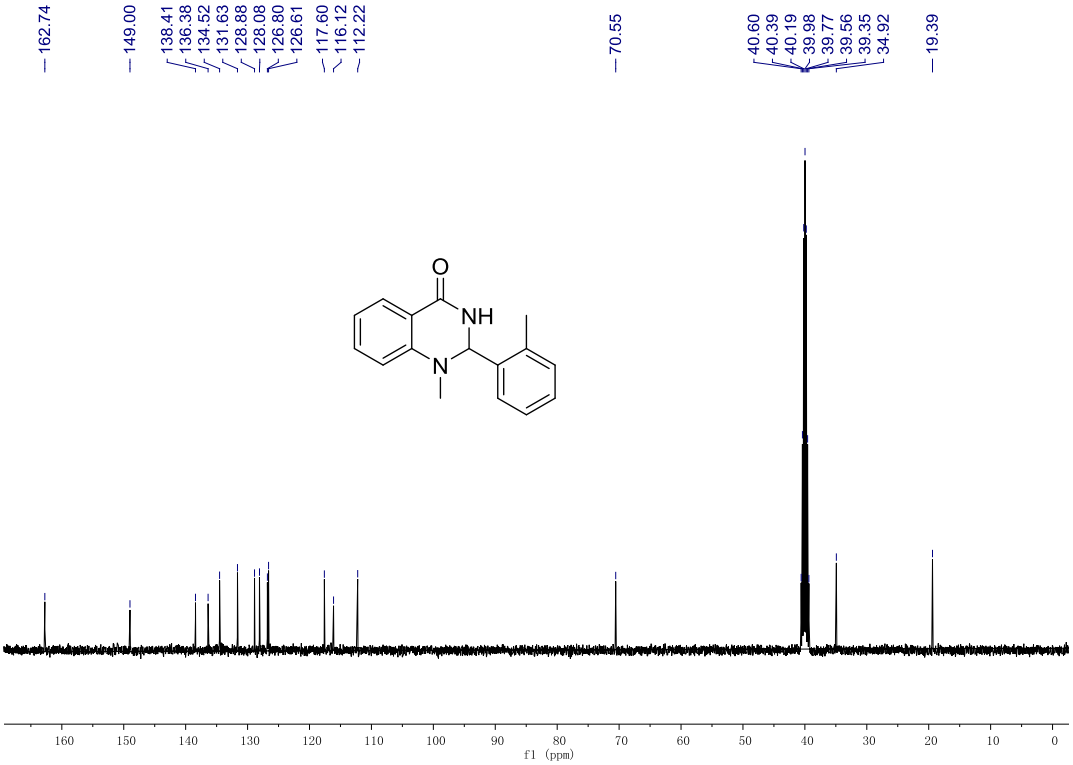
4-1s, ^{1}H NMR (400 MHz, DMSO-d_6)



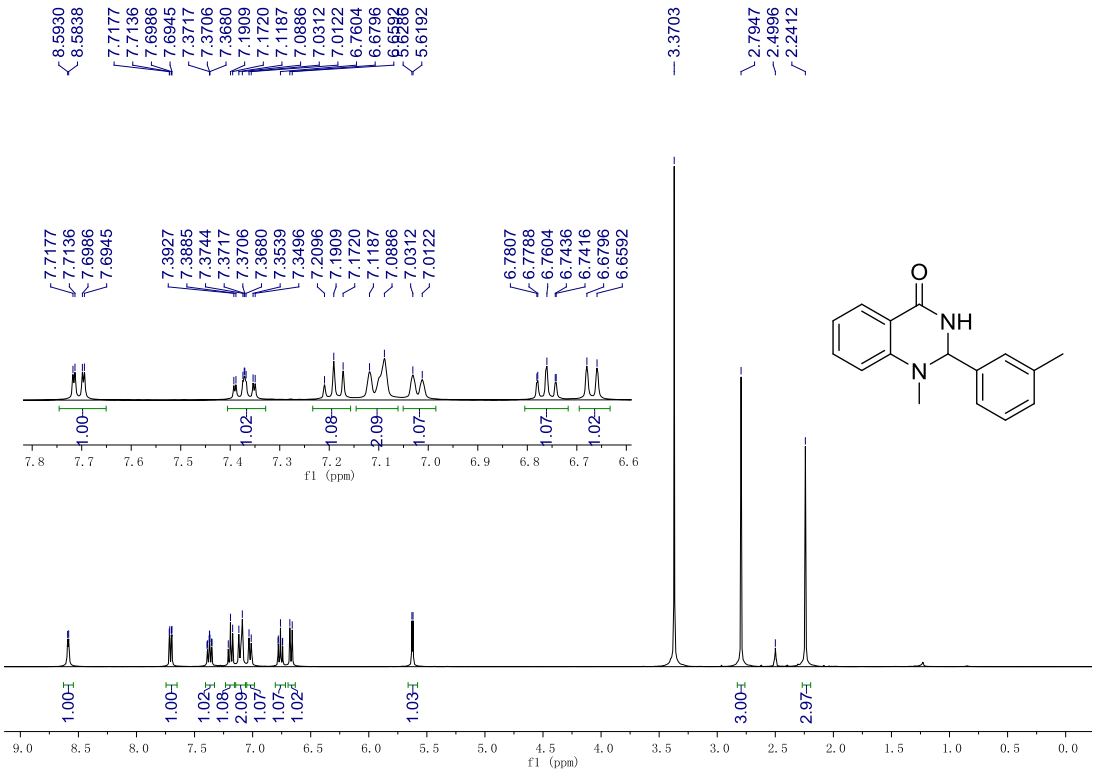
4-1s, ^{13}C NMR (100 MHz, DMSO-d_6)



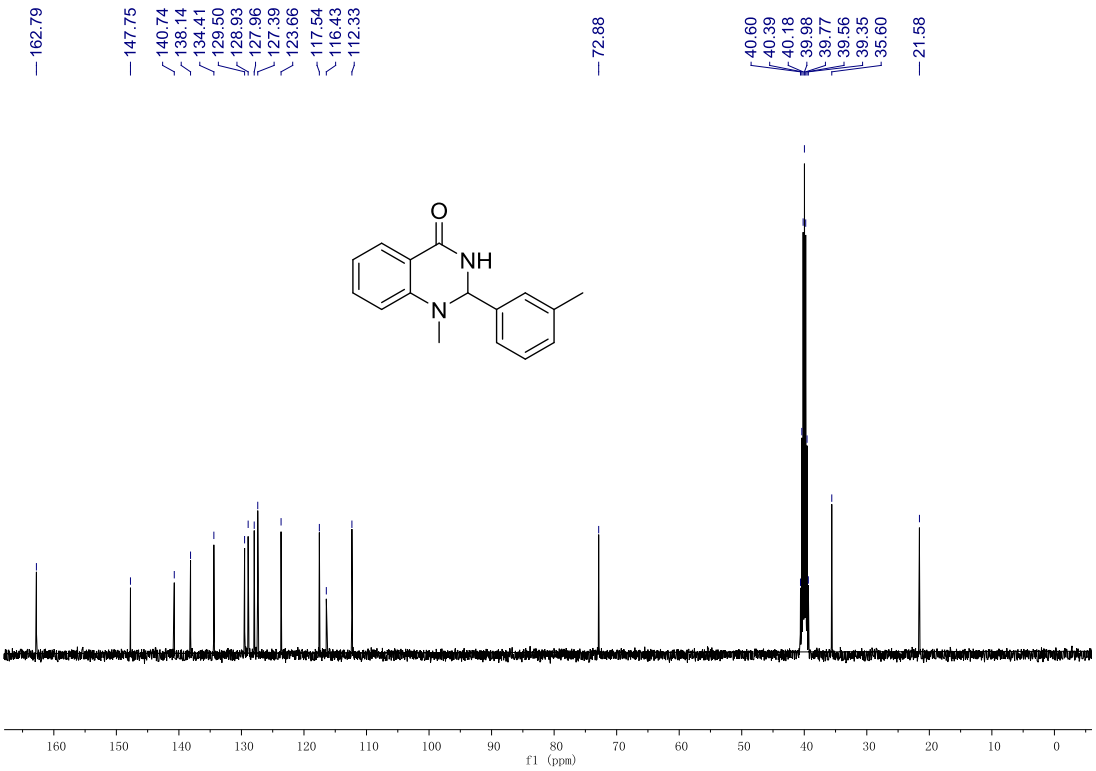
4-2a, ^{1}H NMR (400 MHz, DMSO-d_6)



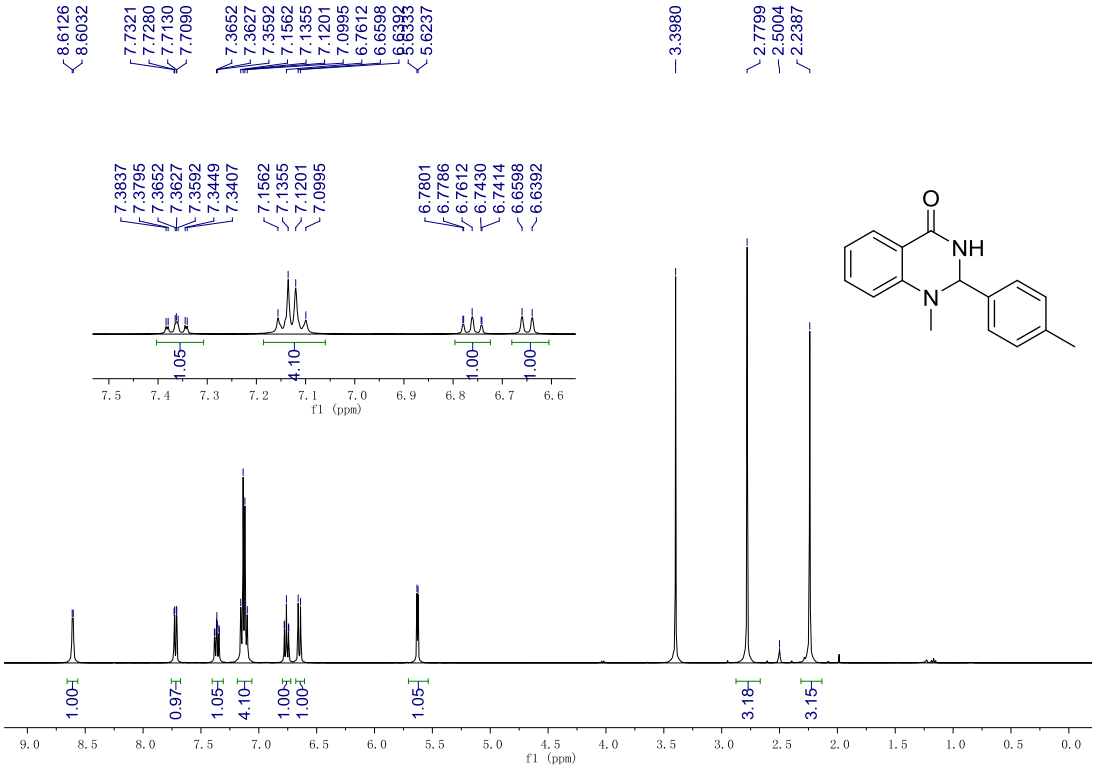
4-2a, ^{13}C NMR (100 MHz, DMSO-d_6)



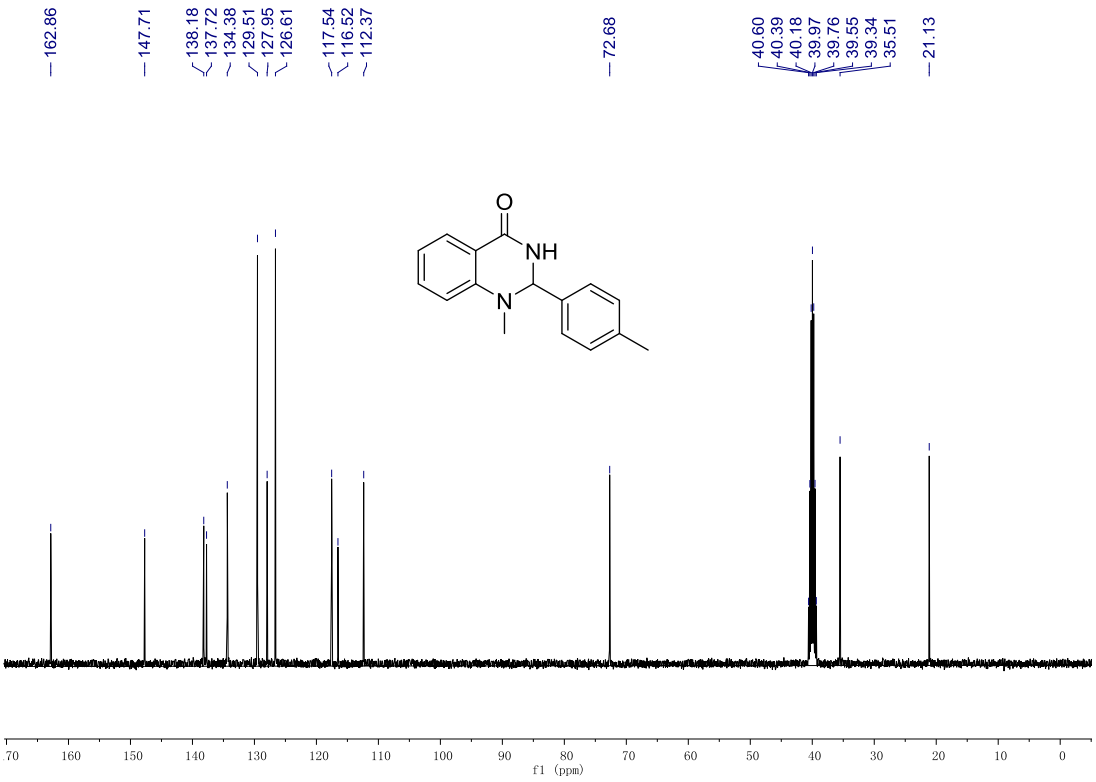
4-2b, ^{1}H NMR (400 MHz, DMSO-d_6)



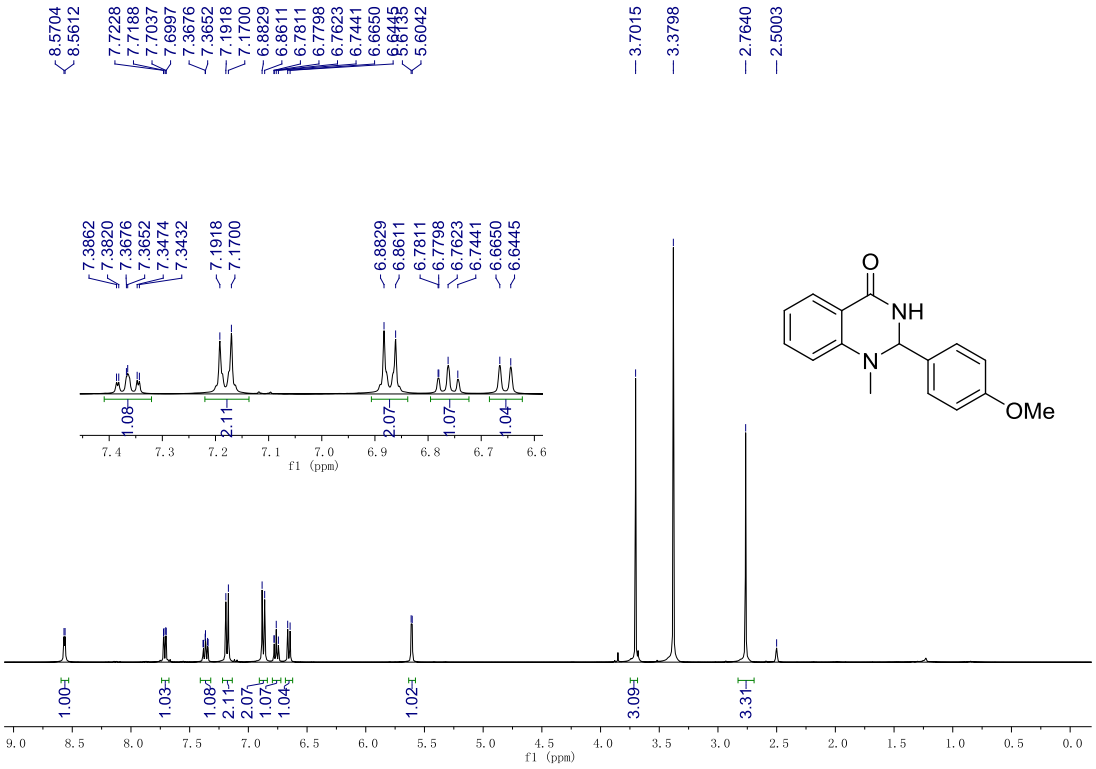
4-2b, ^{13}C NMR (100 MHz, DMSO-d_6)



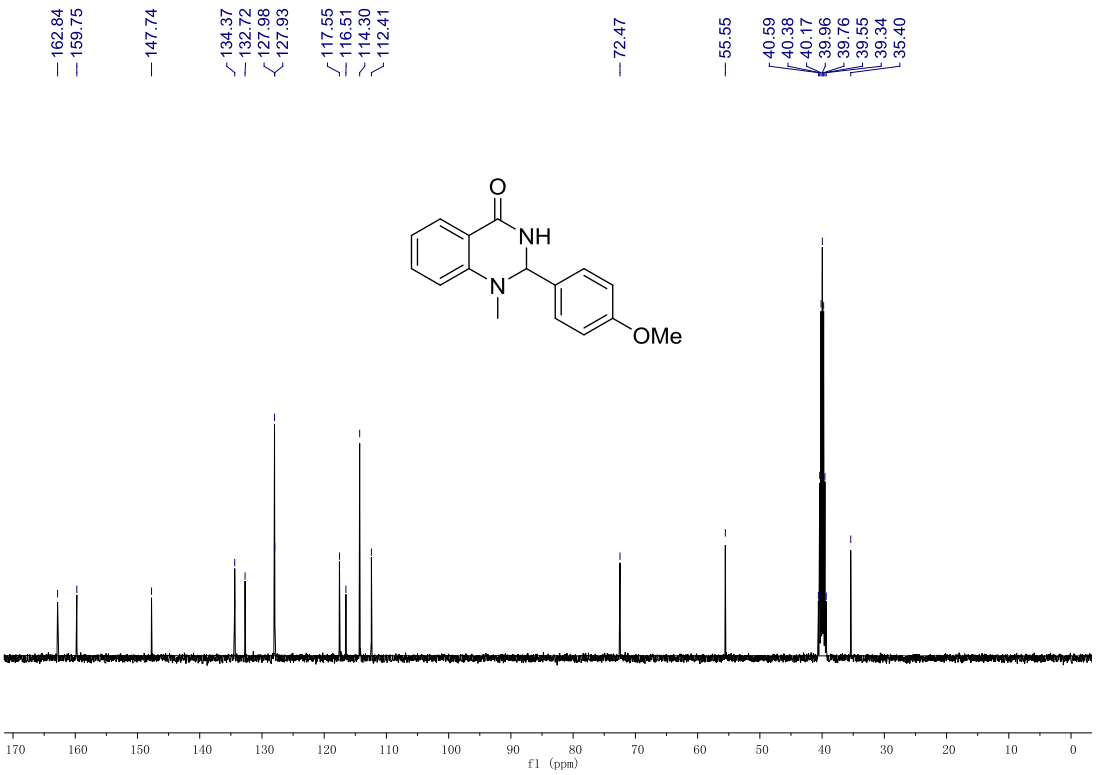
4-2c ^{1}H NMR (400 MHz, DMSO-d_6)



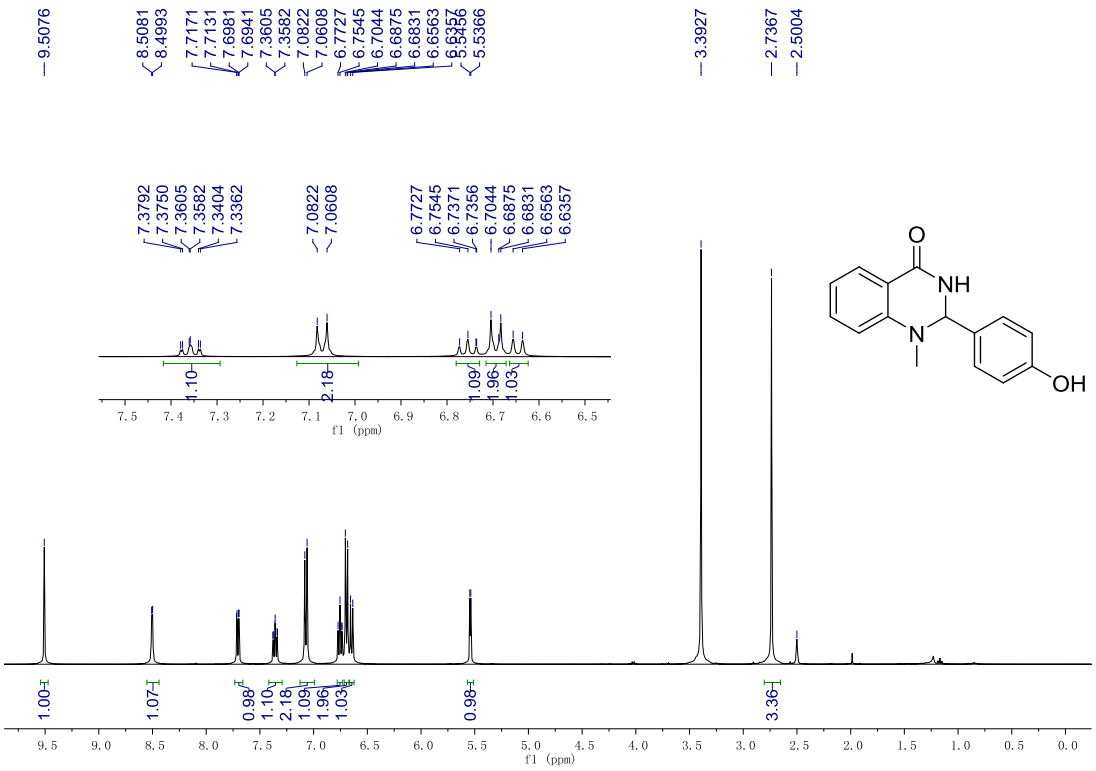
4-2c, ^{13}C NMR (100 MHz, DMSO-d_6)



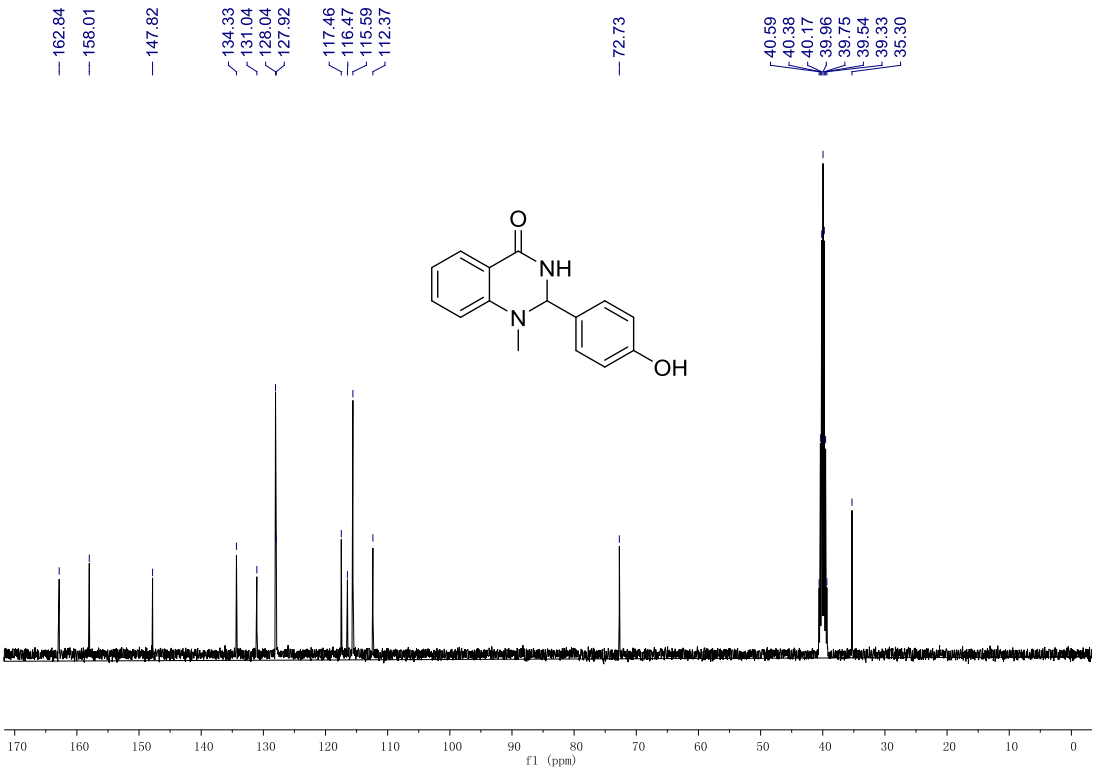
4-2d, ^{1}H NMR (400 MHz, DMSO-d_6)



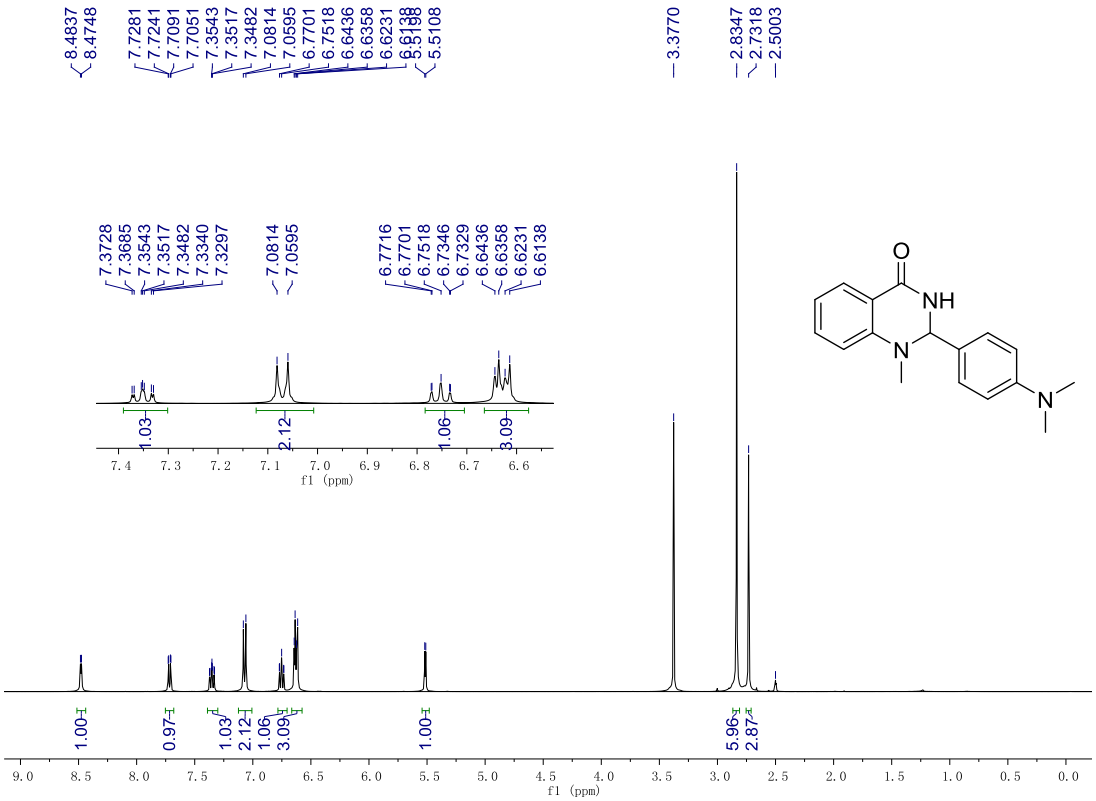
4-2d, ^{13}C NMR (100 MHz, DMSO-d_6)



4-2e, ^{1}H NMR (400 MHz, DMSO-d_6)



4-2e, ^{13}C NMR (100 MHz, DMSO-d_6)



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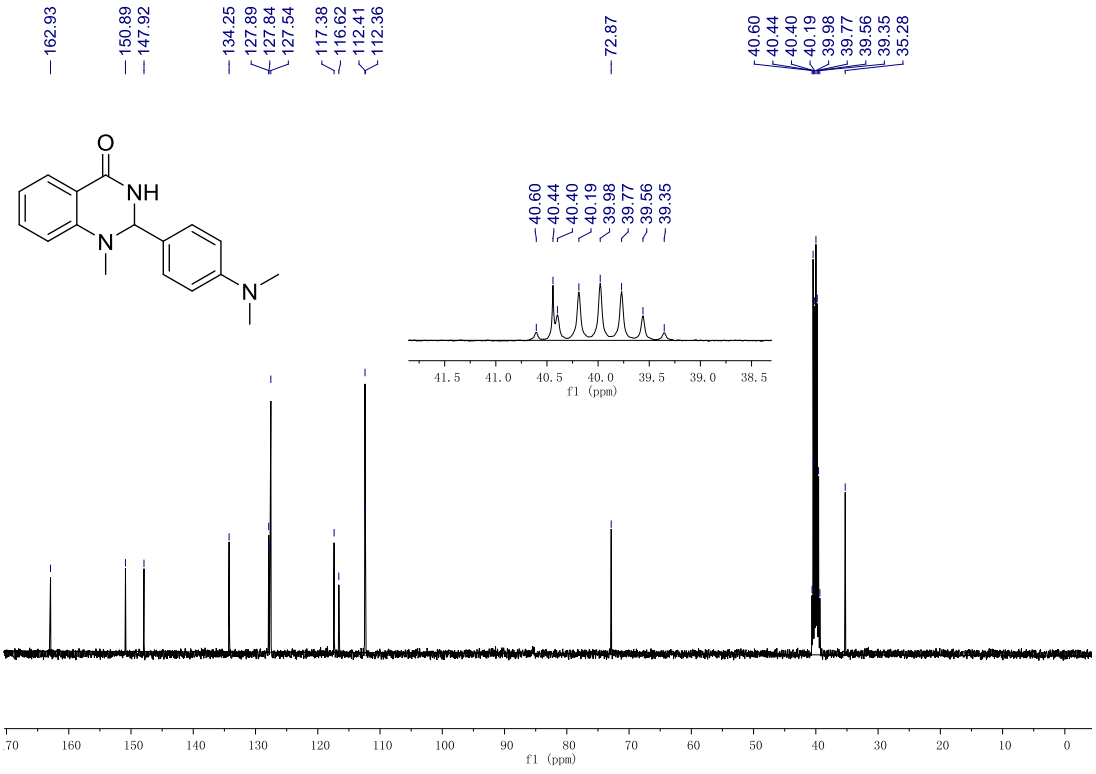
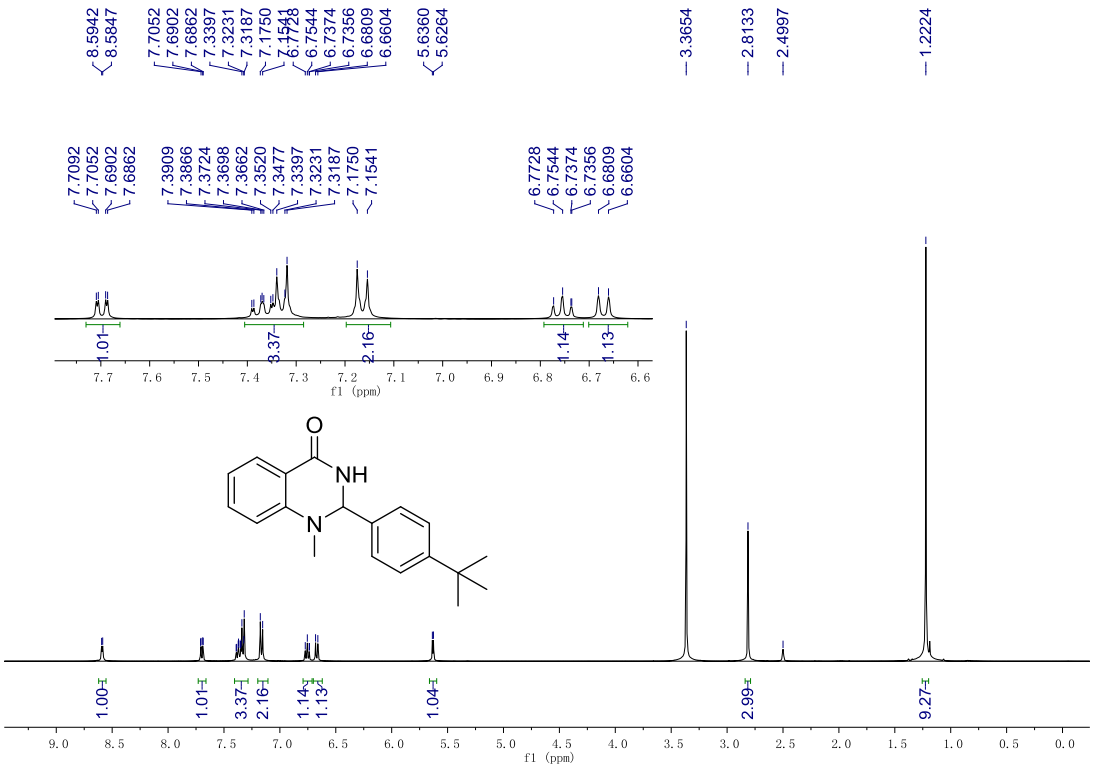
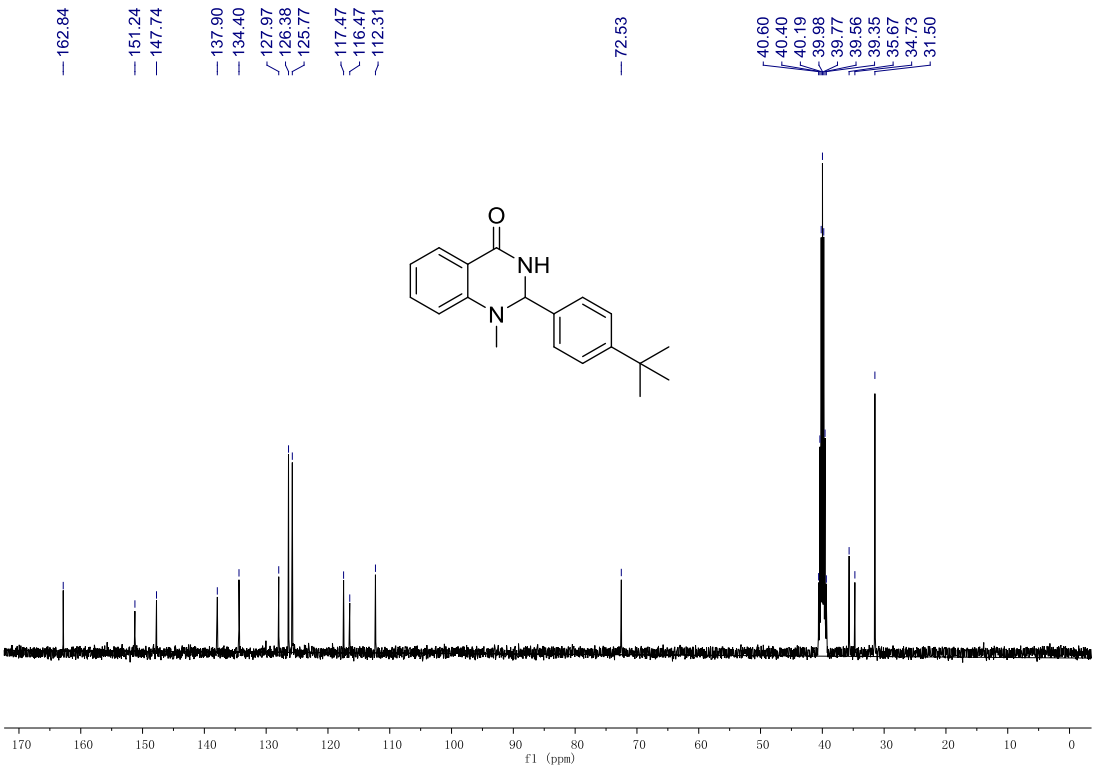


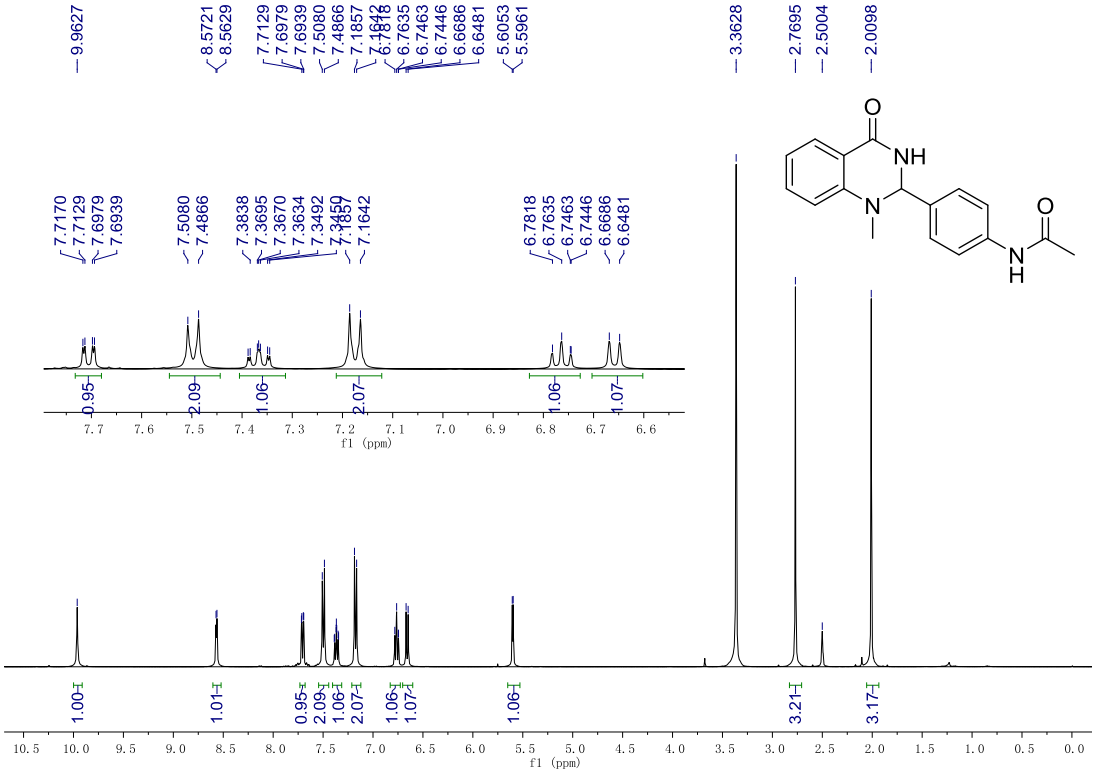
4-2f, ^{13}C NMR (100 MHz, DMSO-d_6)



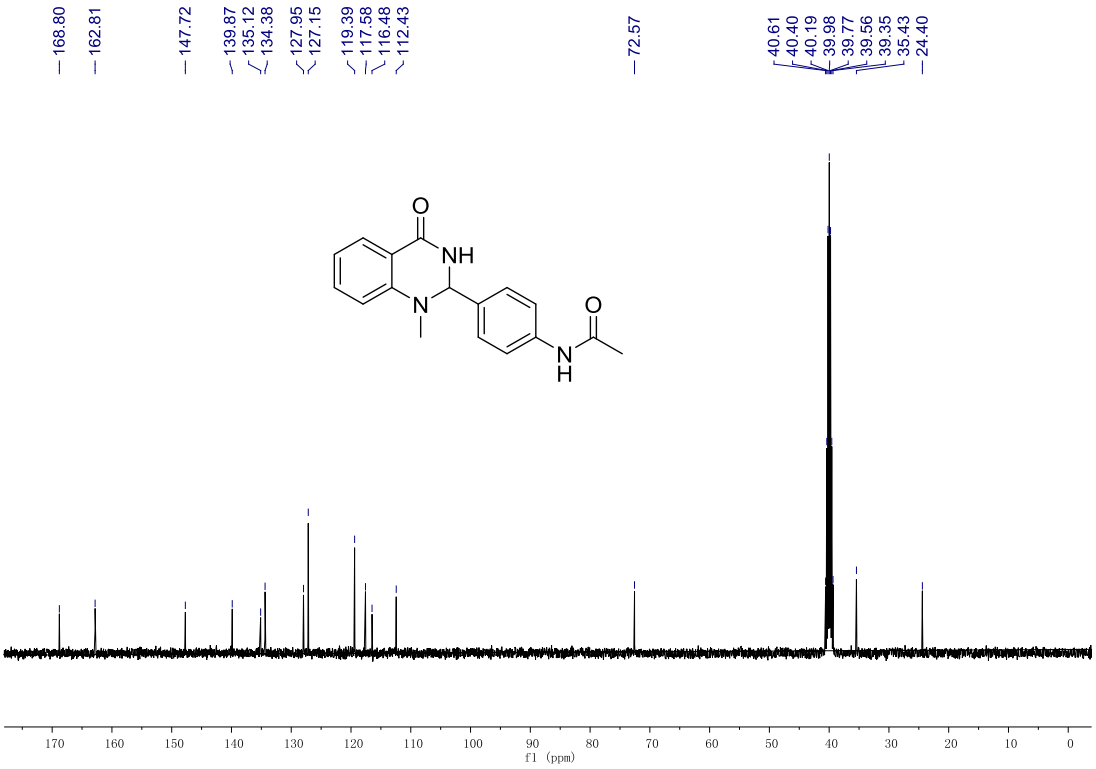
4-2g, ^{1}H NMR (400 MHz, DMSO-d_6)



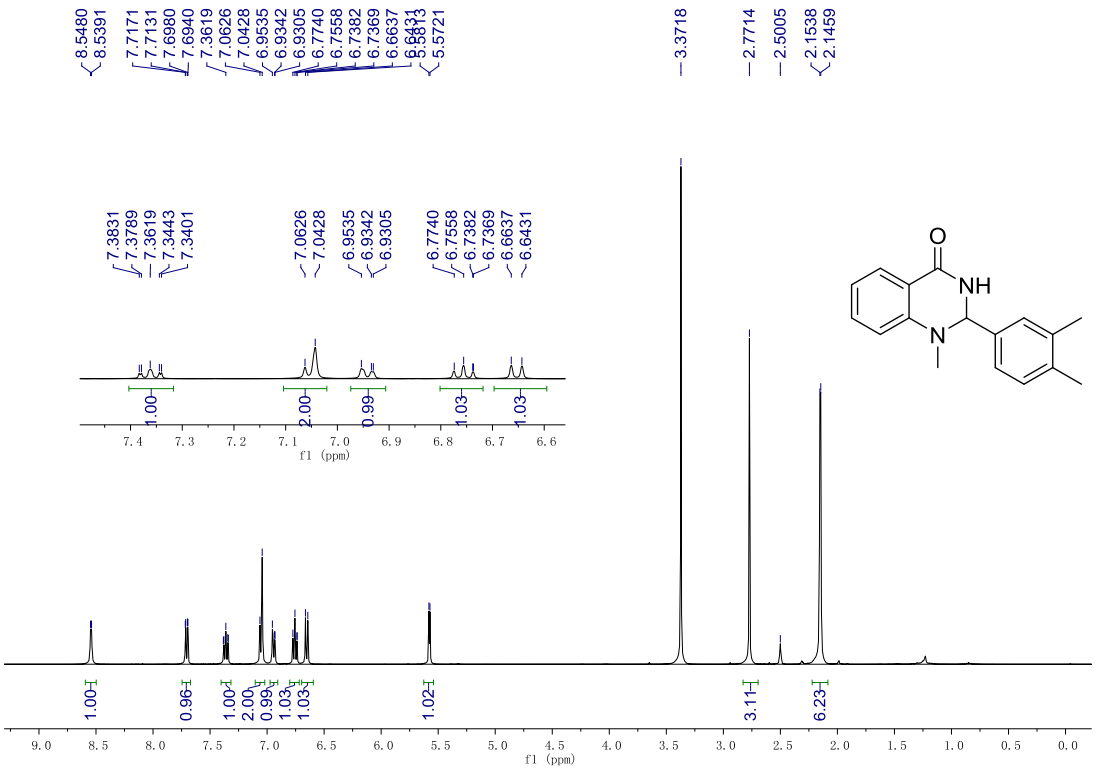
4-2g, ^{13}C NMR (100 MHz, DMSO-d_6)



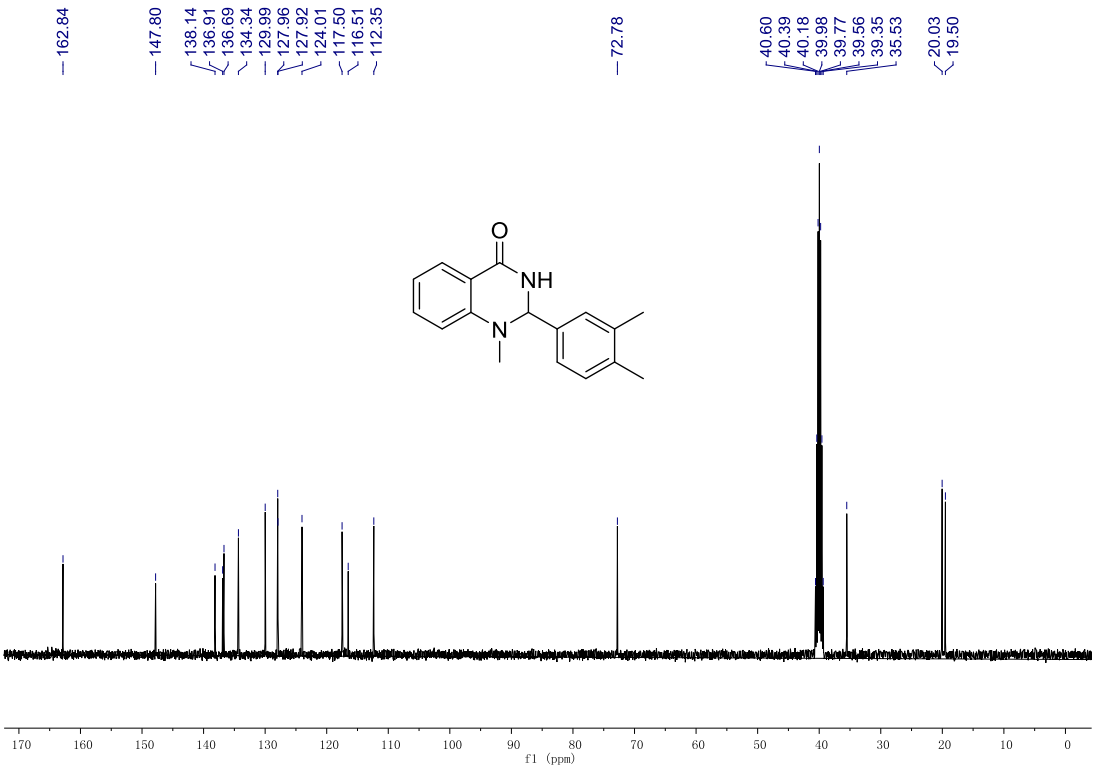
4-2h, ^{1}H NMR (400 MHz, DMSO-d_6)



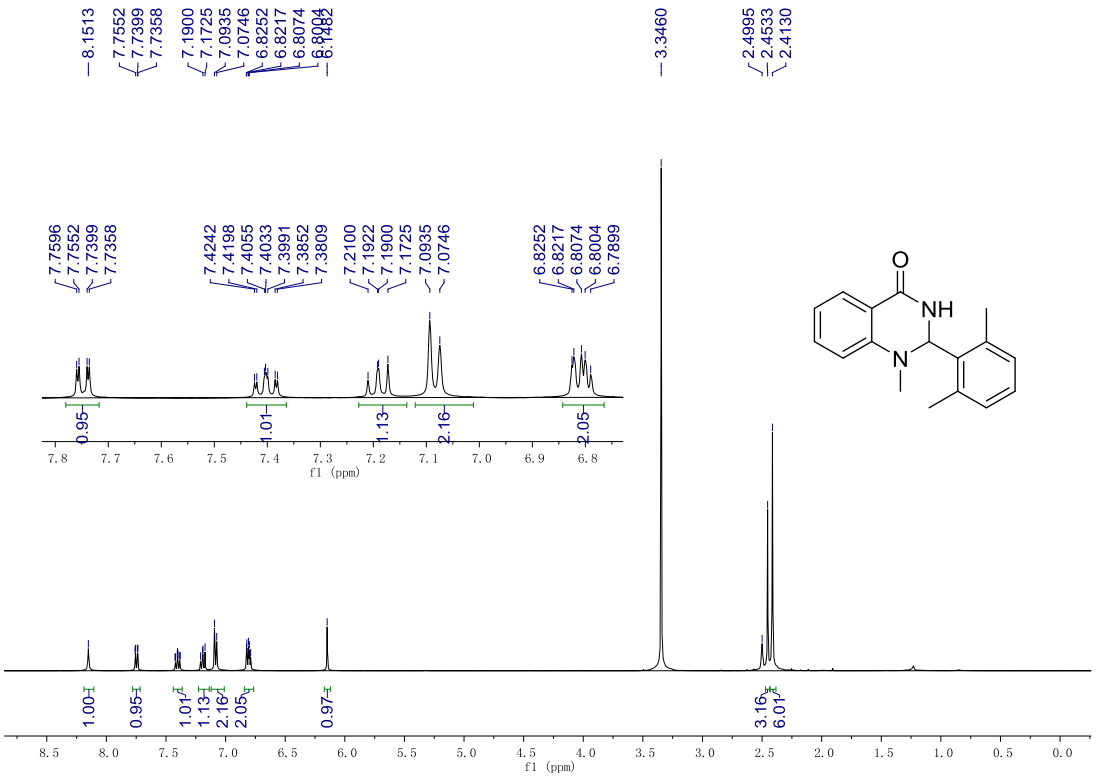
4-2h, ^{13}C NMR (100 MHz, DMSO-d_6)



4-2i, ^{1}H NMR (400 MHz, DMSO-d_6)



4-2i, ^{13}C NMR (100 MHz, DMSO-d_6)



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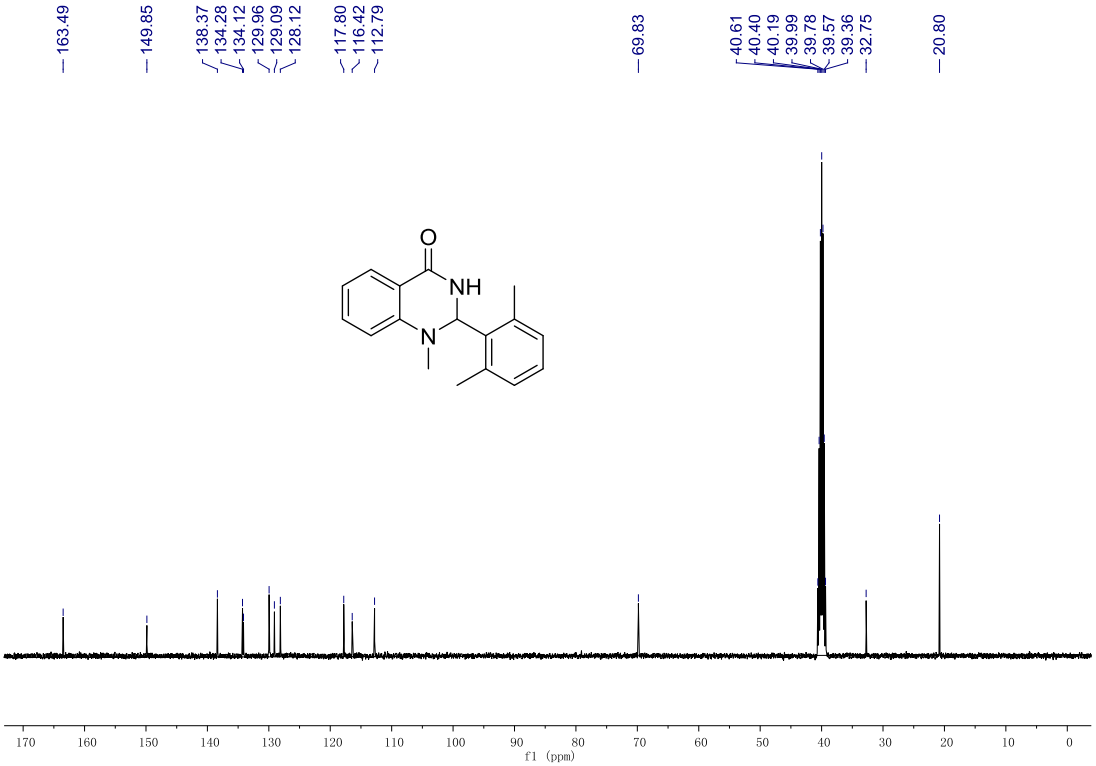

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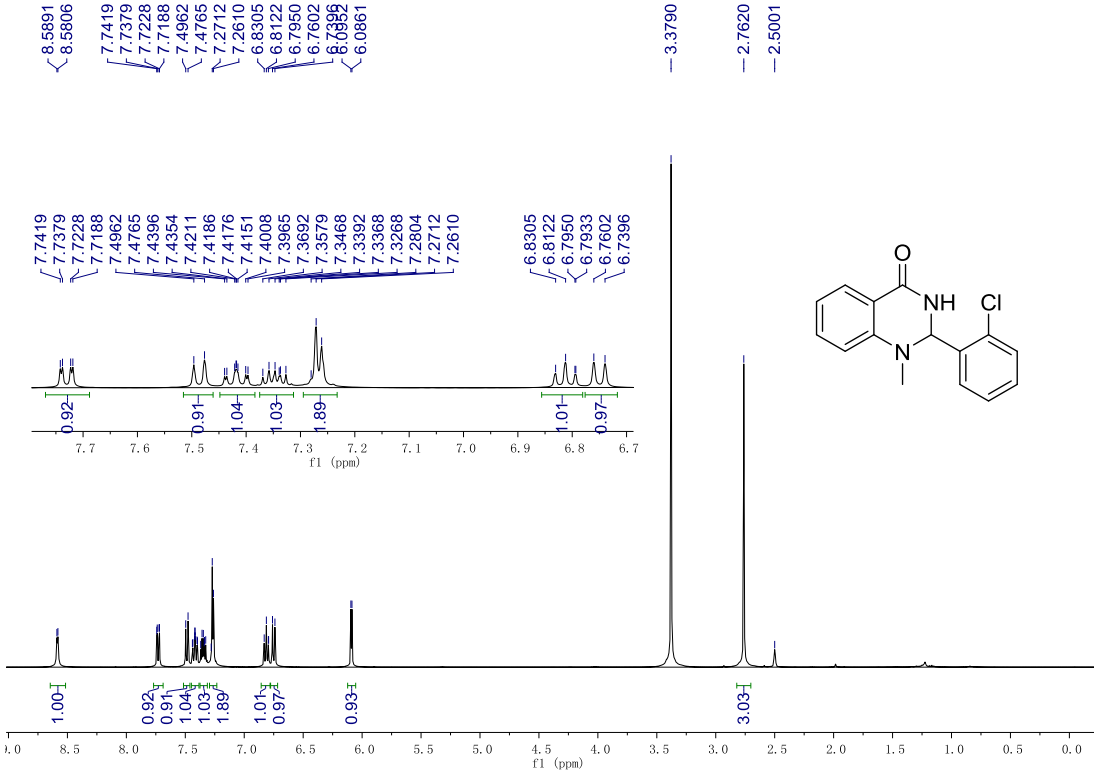
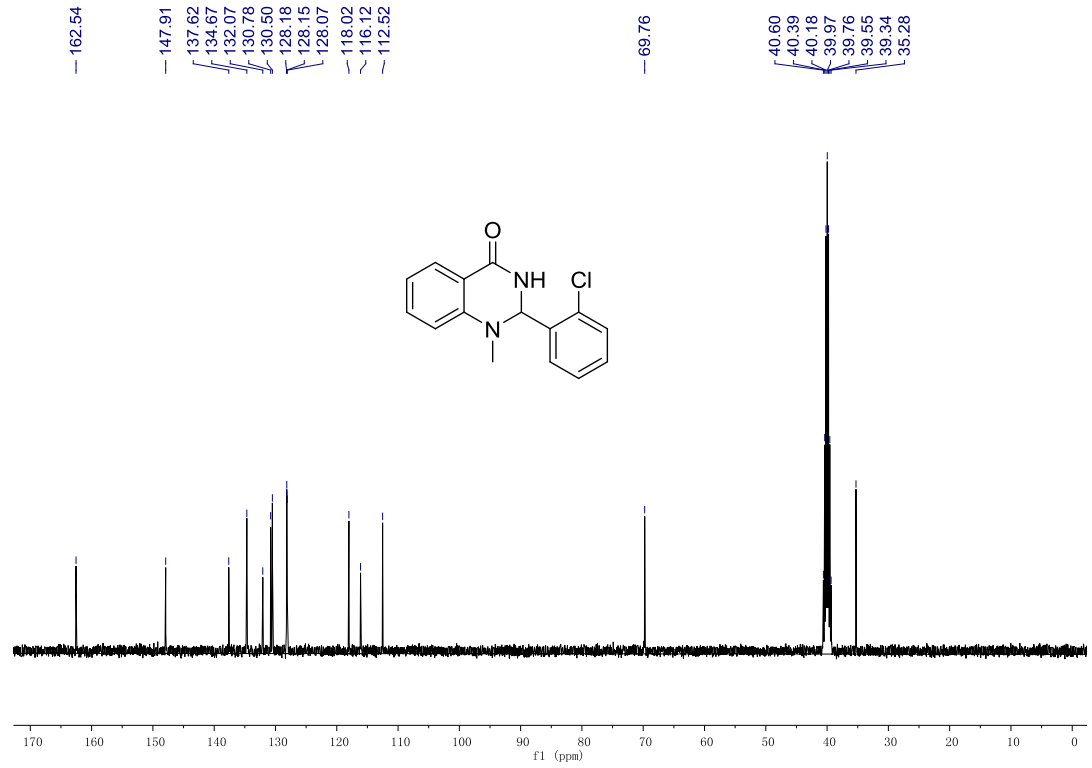


4-2k, ^{1}H NMR (400 MHz, DMSO-d_6)



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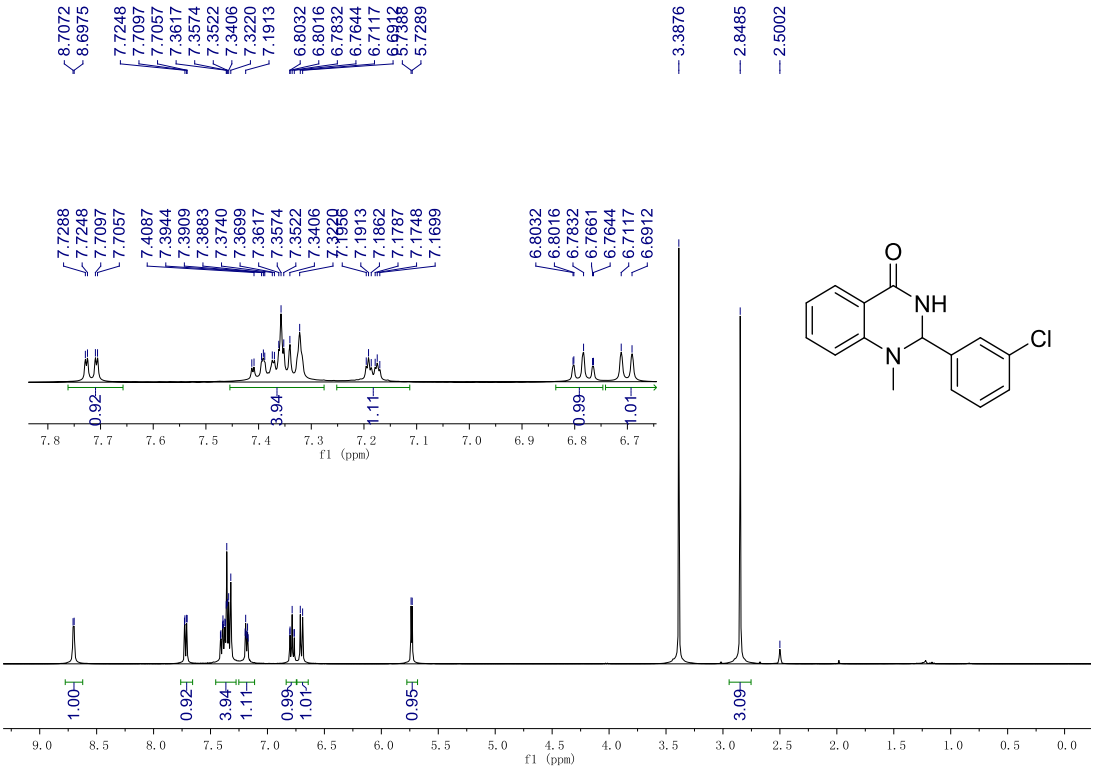
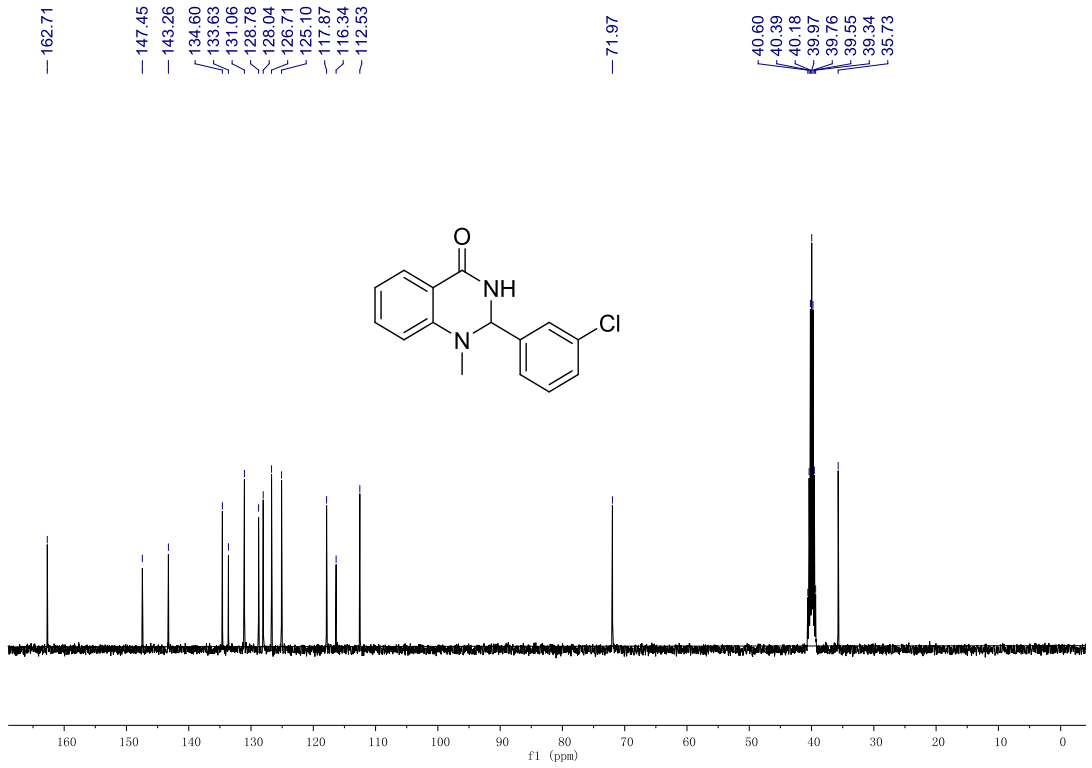


4-2l, ^{1}H NMR (400 MHz, DMSO-d_6)



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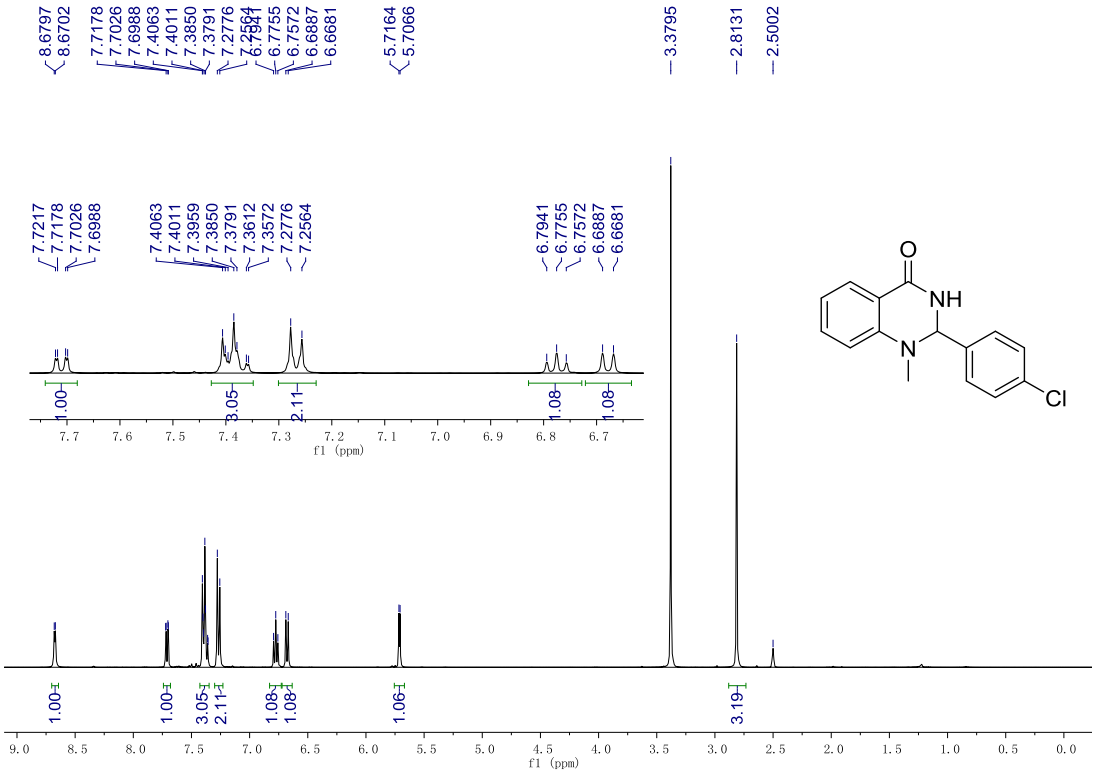
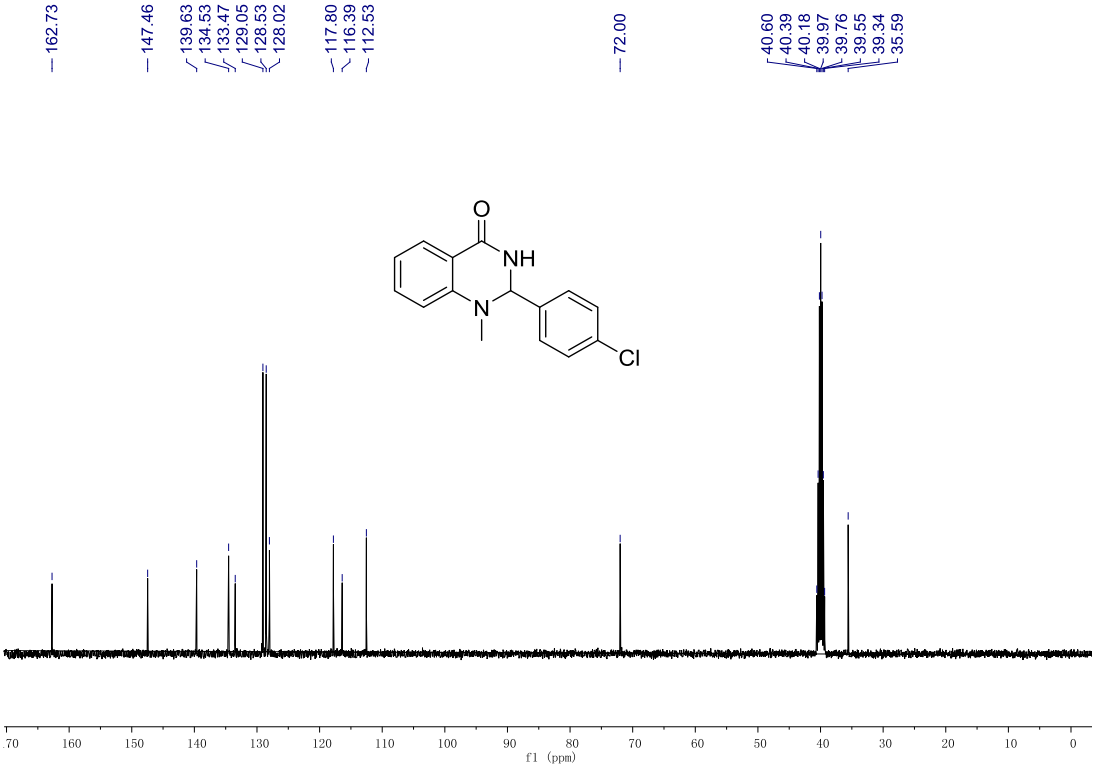
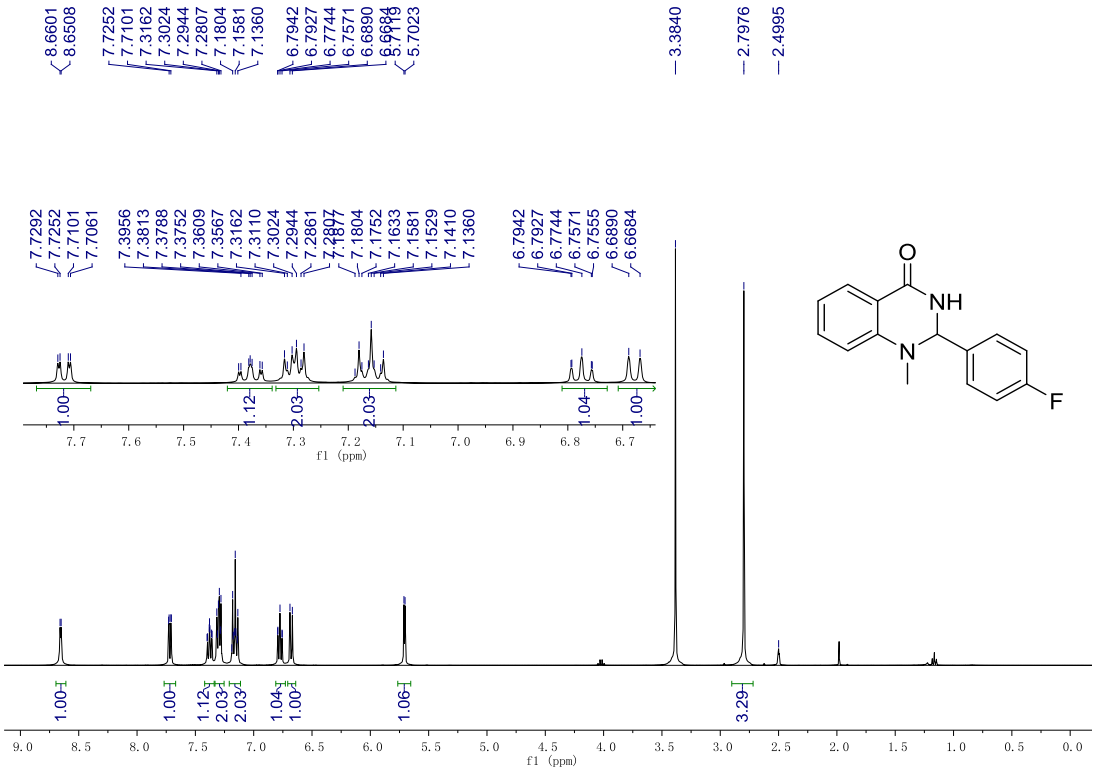


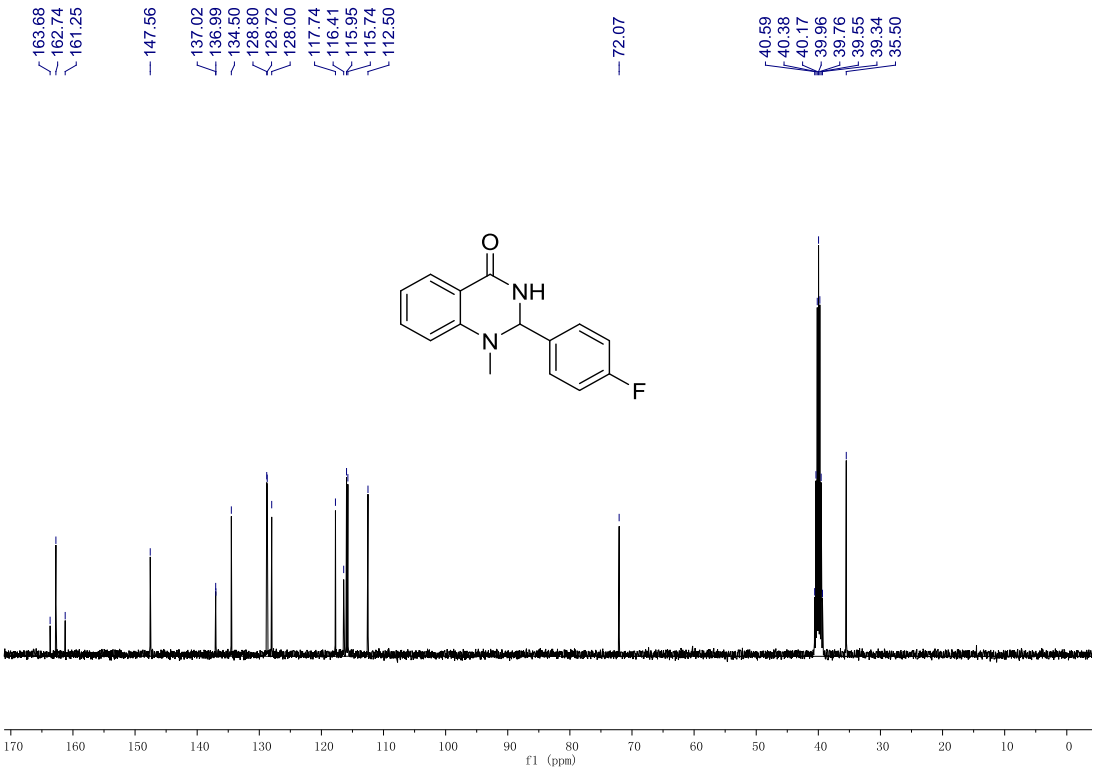
4-2m, ^{1}H NMR (400 MHz, DMSO-d_6)



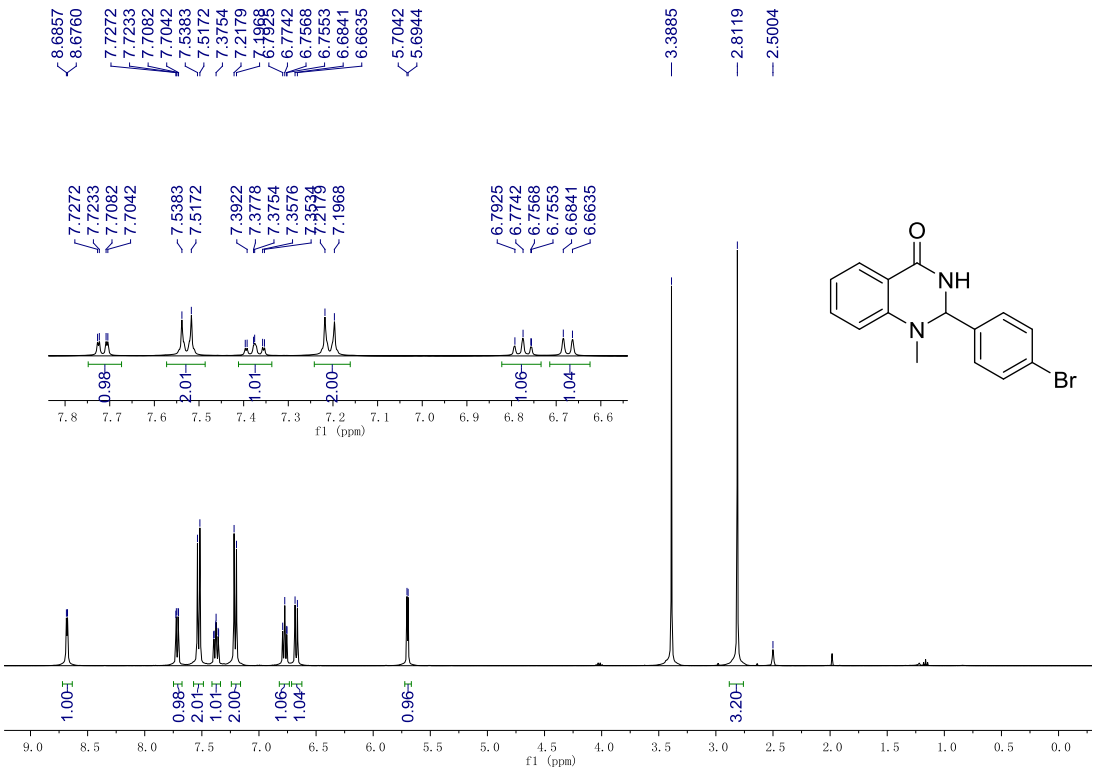
4-2m, ^{13}C NMR (100 MHz, DMSO-d_6)



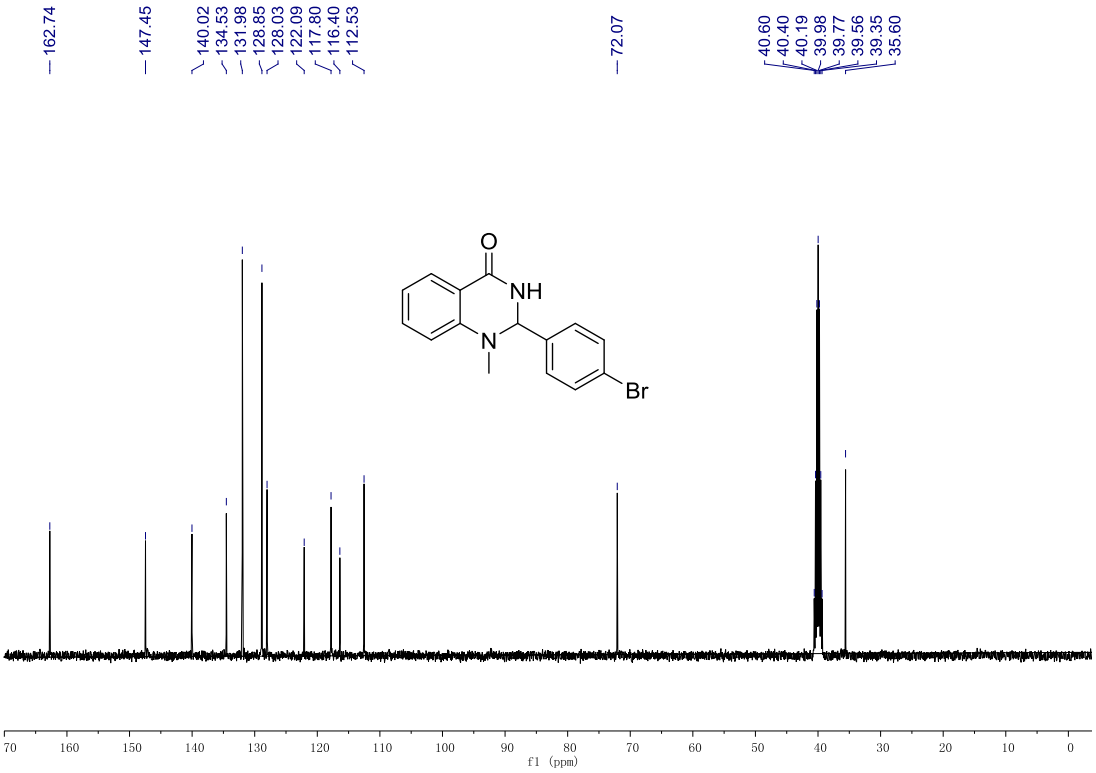
4-2n, ^{1}H NMR (400 MHz, DMSO-d_6)



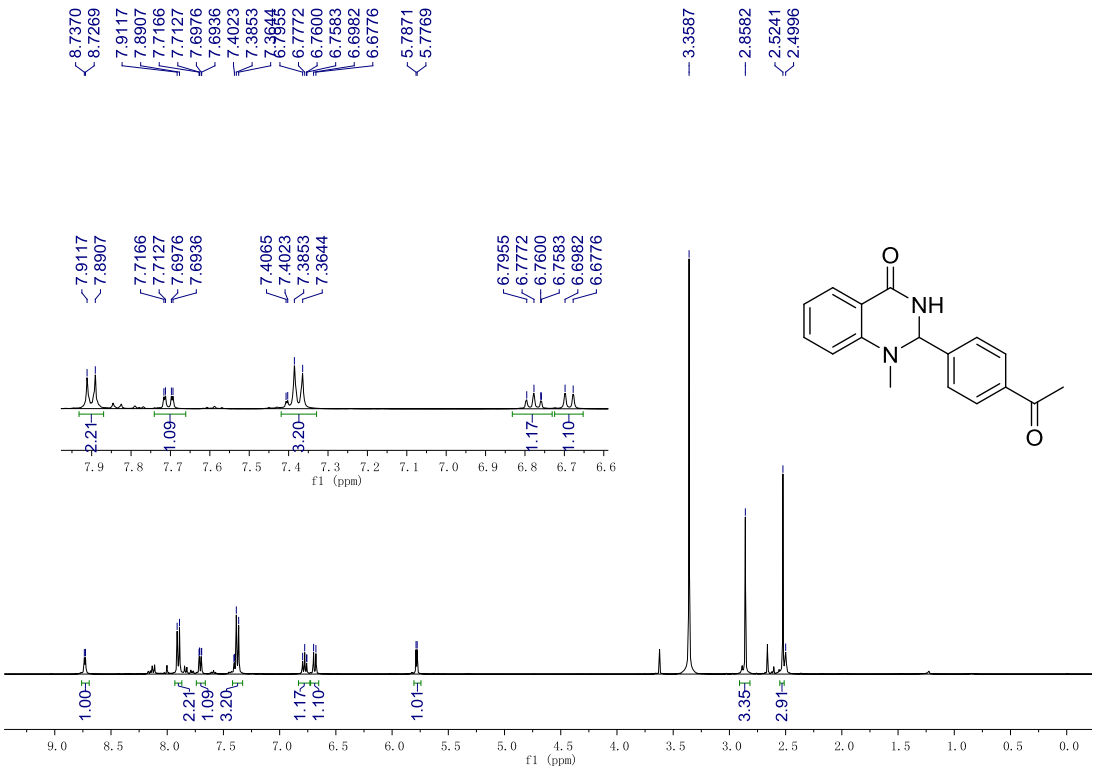
4-2n, ^{13}C NMR (100 MHz, DMSO-d_6)



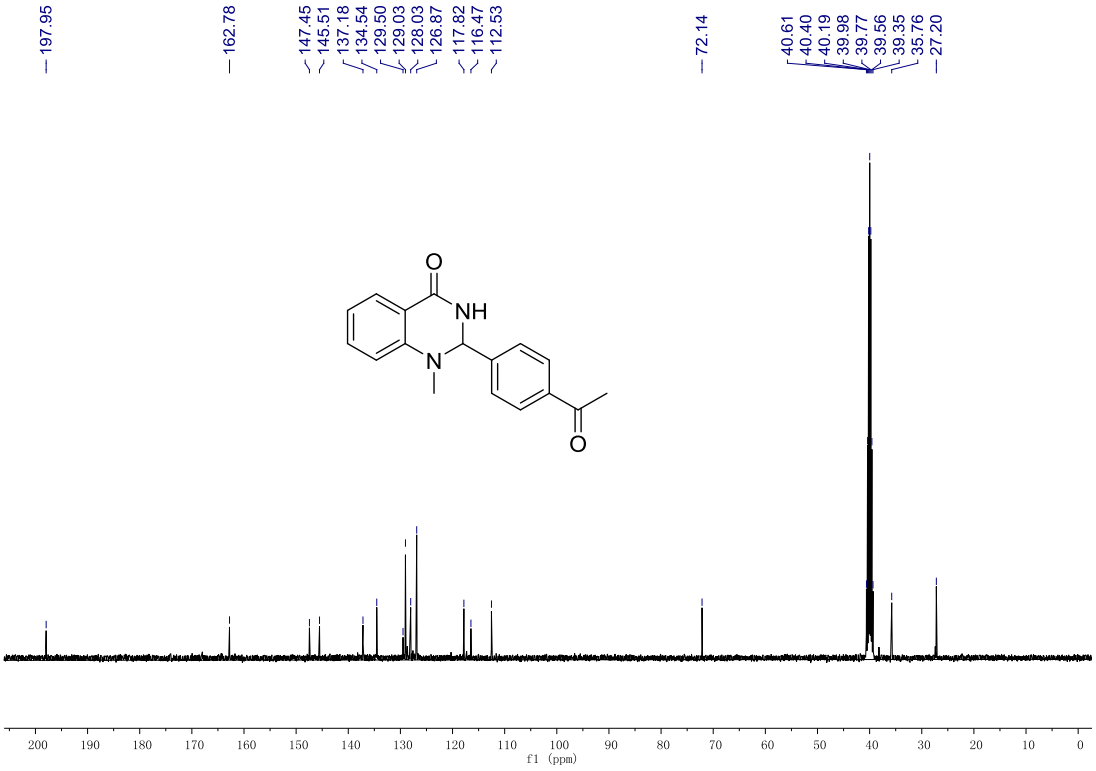
4-2o, ^{1}H NMR (400 MHz, DMSO-d_6)



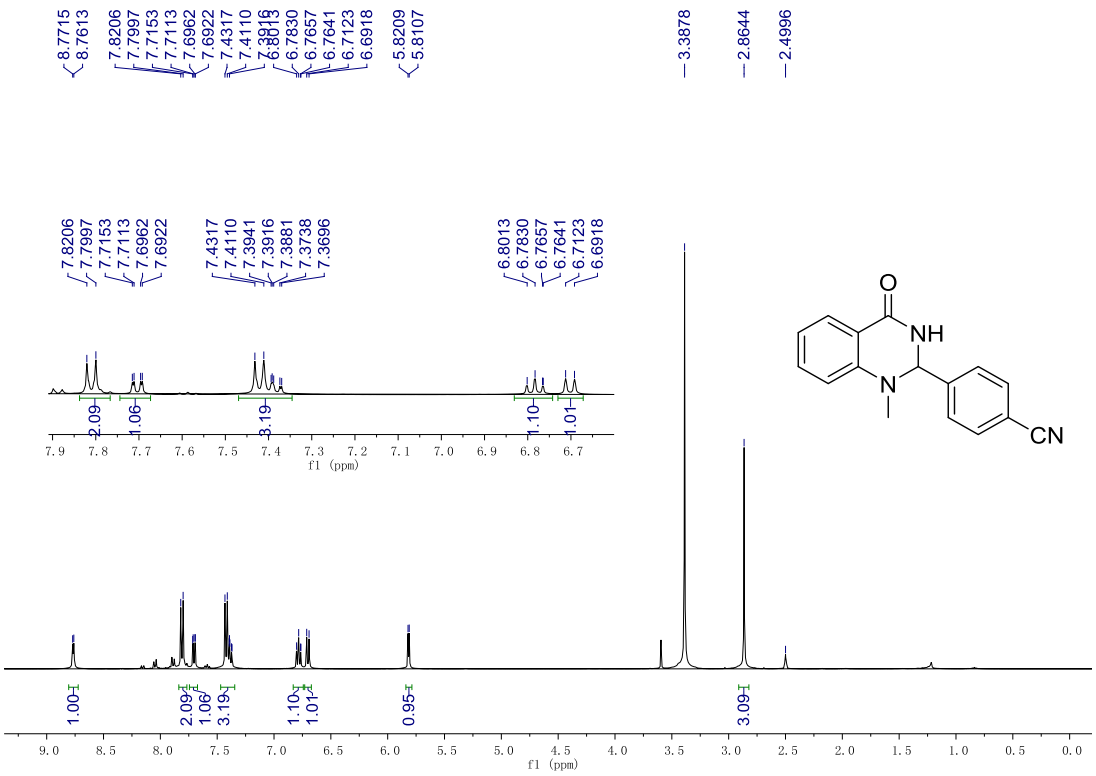
4-2o, ^{13}C NMR (100 MHz, DMSO-d_6)



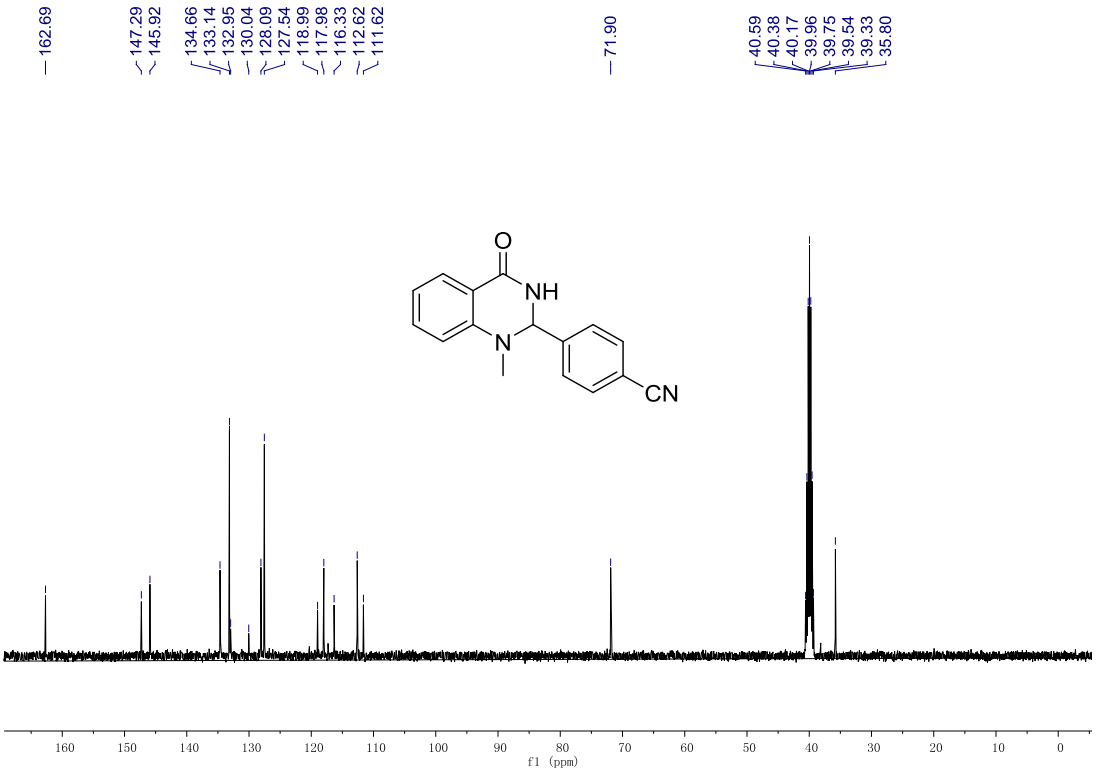
4-2p, ^{1}H NMR (400 MHz, DMSO-d_6)



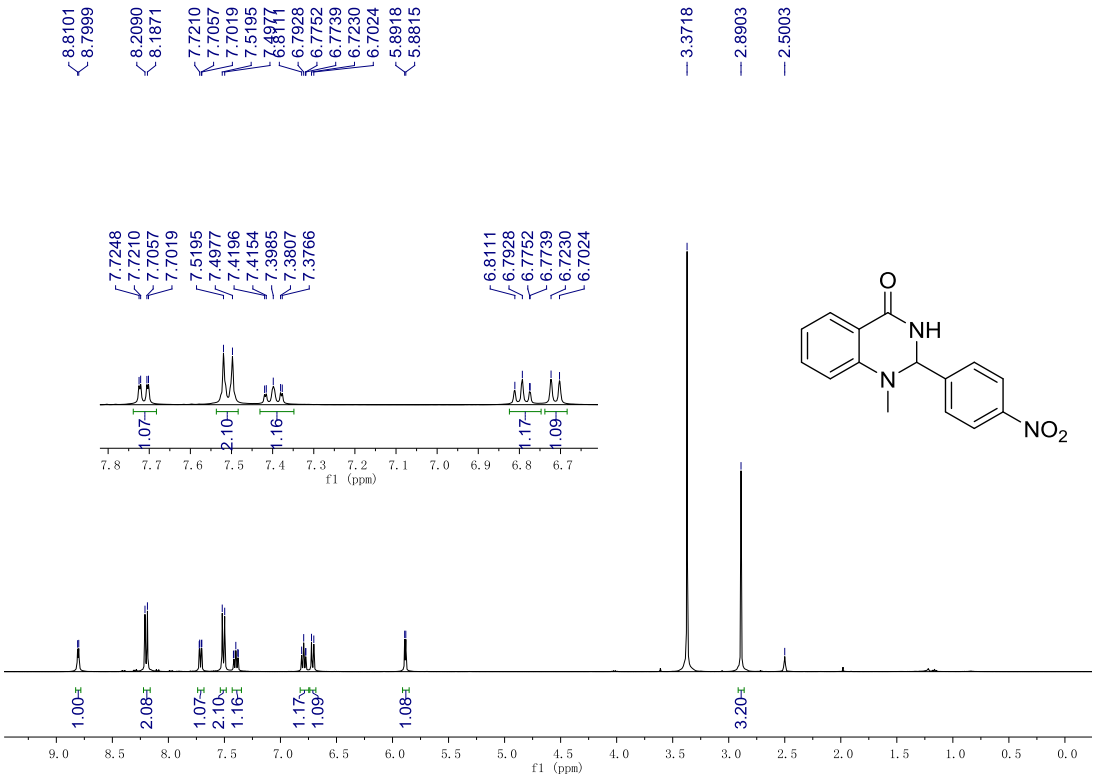
4-2p, ^{13}C NMR (100 MHz, DMSO-d_6)



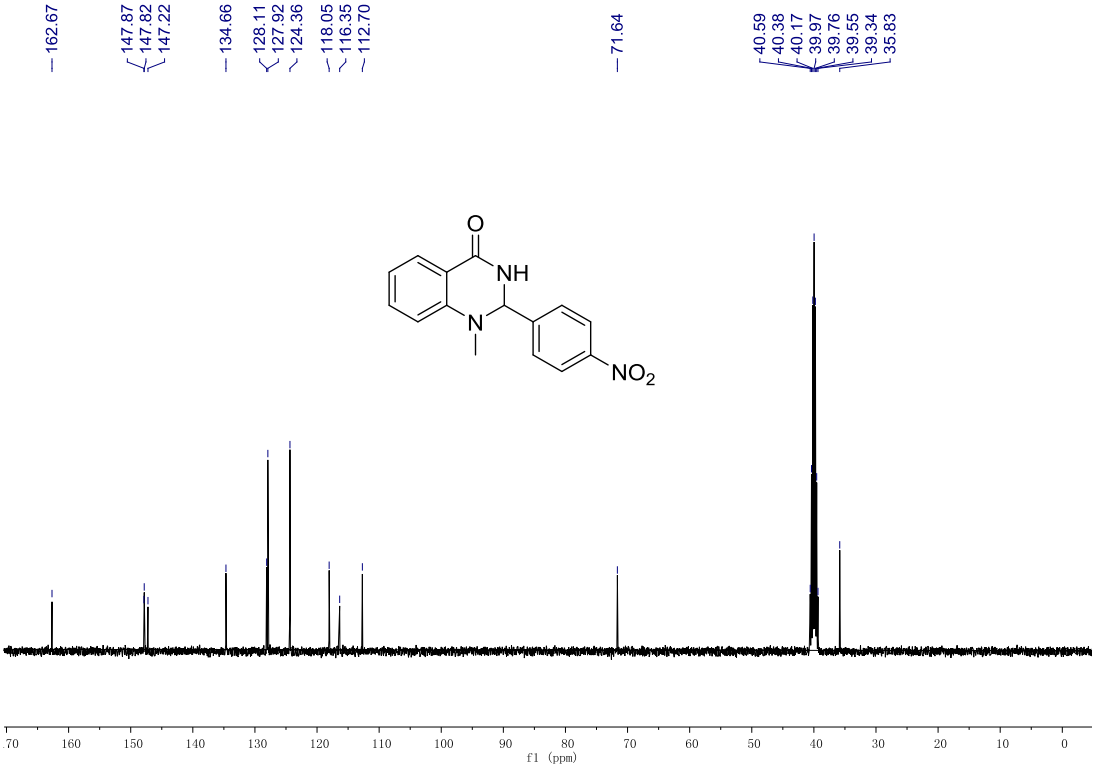
4-2q, ^{1}H NMR (400 MHz, DMSO-d_6)



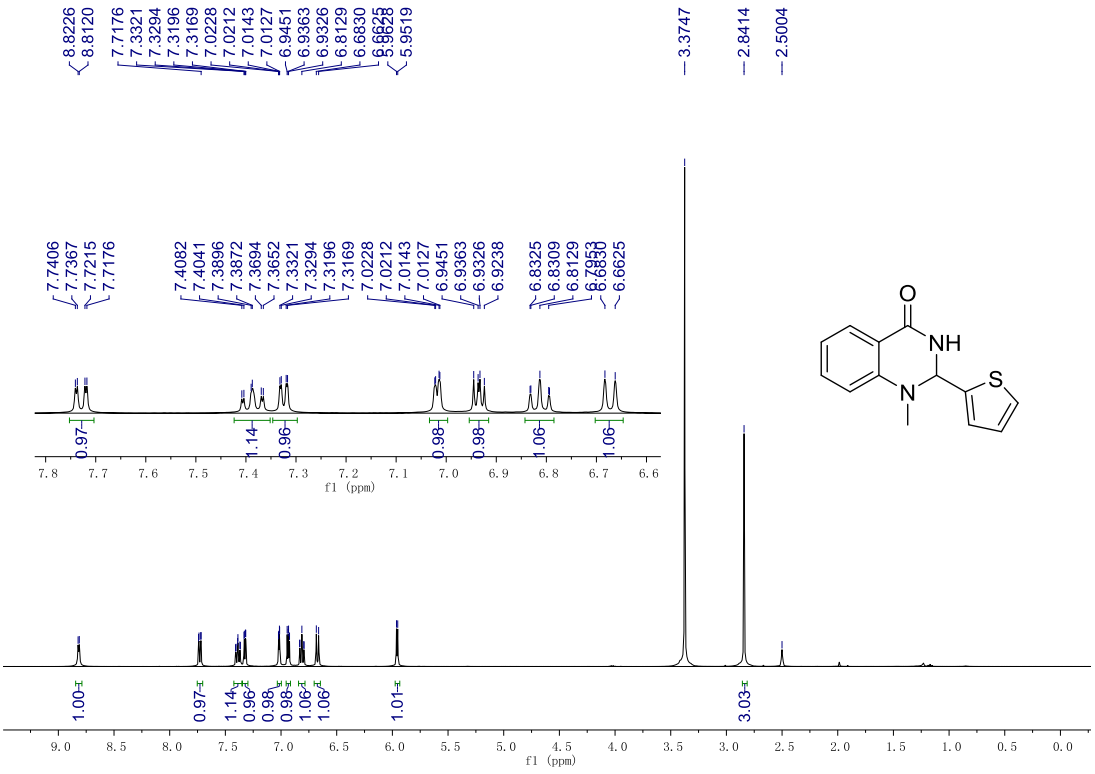
4-2q, ^{13}C NMR (100 MHz, DMSO-d_6)



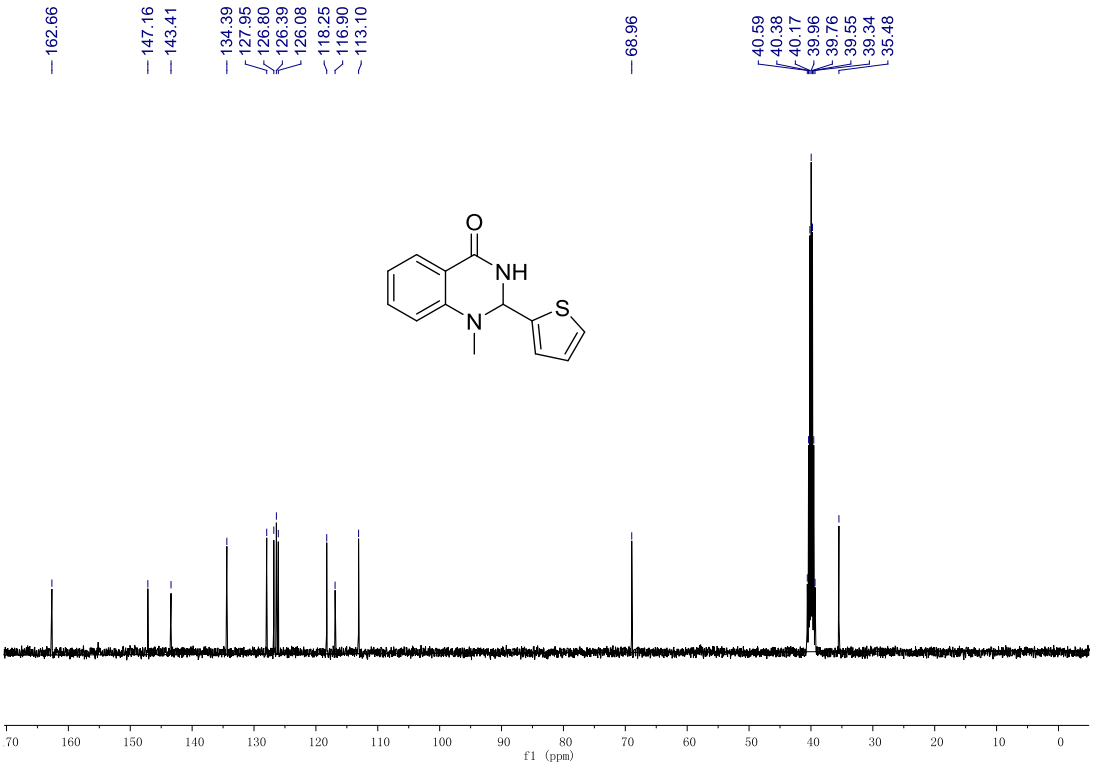
4-2r, ^{1}H NMR (400 MHz, DMSO-d_6)



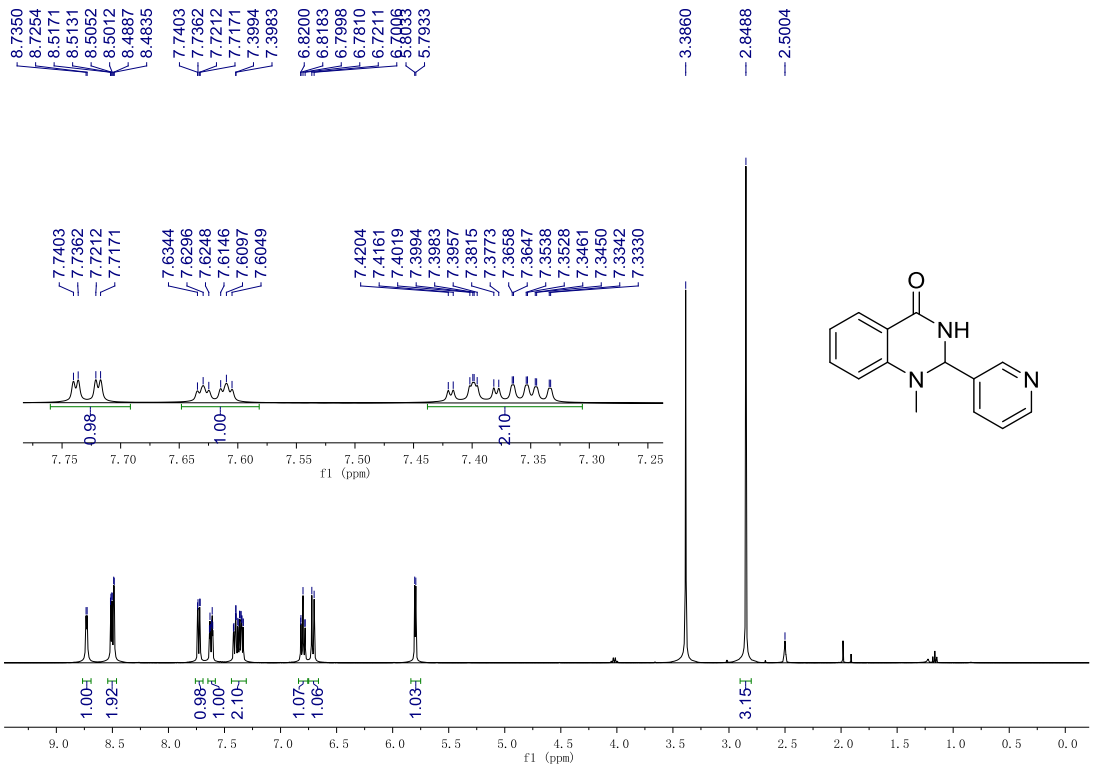
4-2r, ^{13}C NMR (100 MHz, DMSO-d_6)



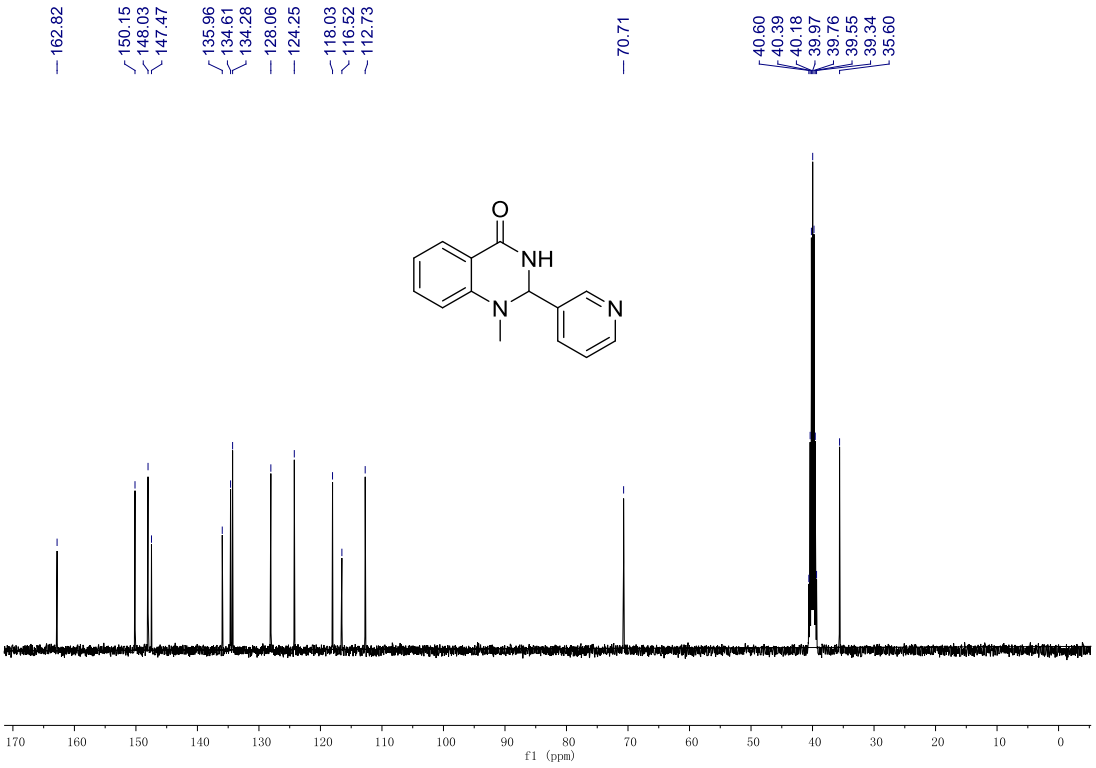
4-2s, ^{1}H NMR (400 MHz, DMSO-d_6)



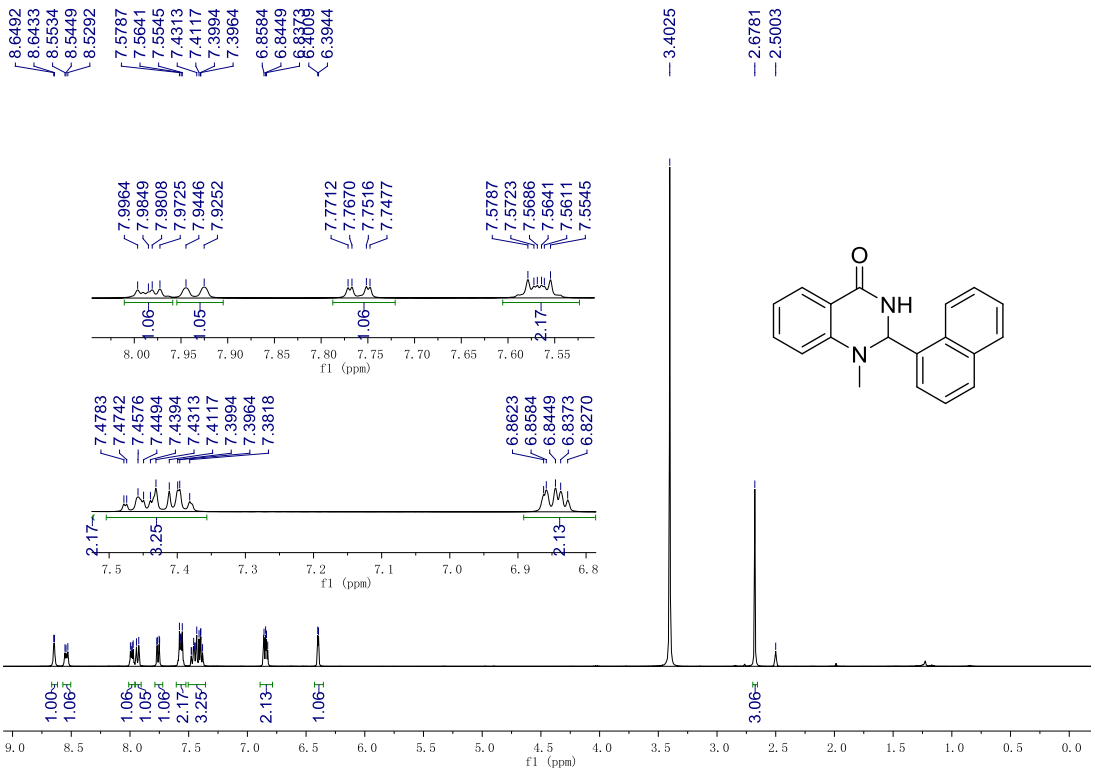
4-2s, ^{13}C NMR (100 MHz, DMSO-d_6)



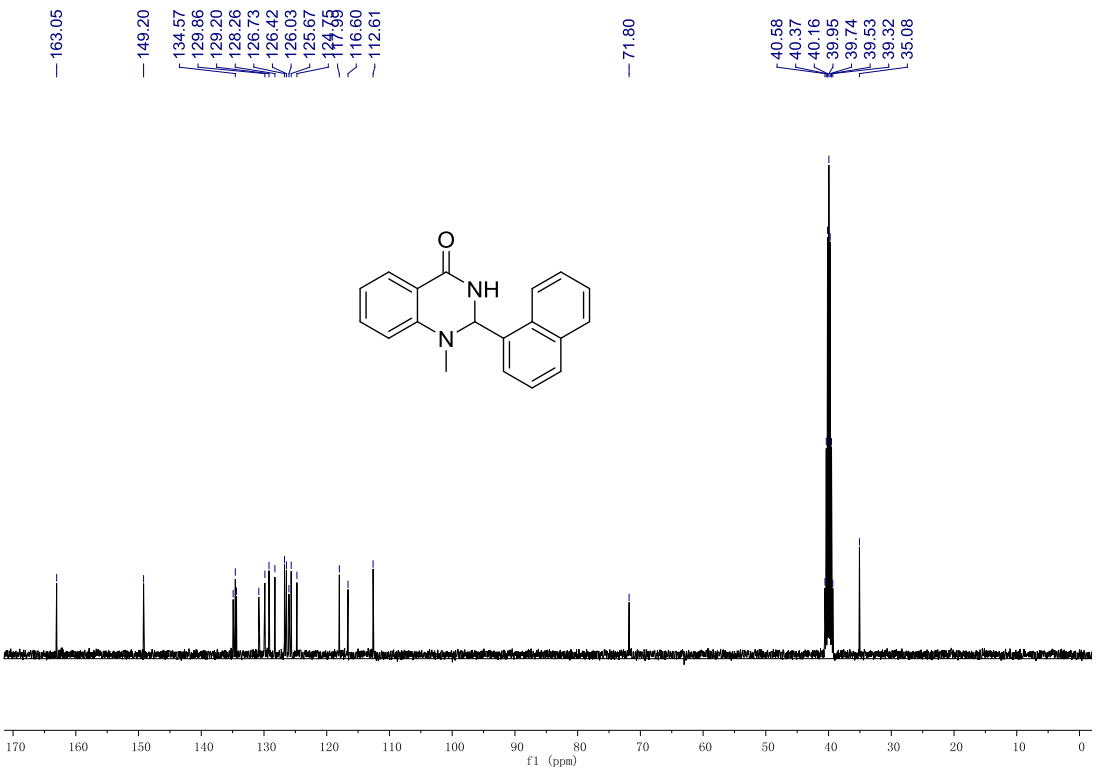
4-2t, ^{1}H NMR (400 MHz, DMSO-d_6)



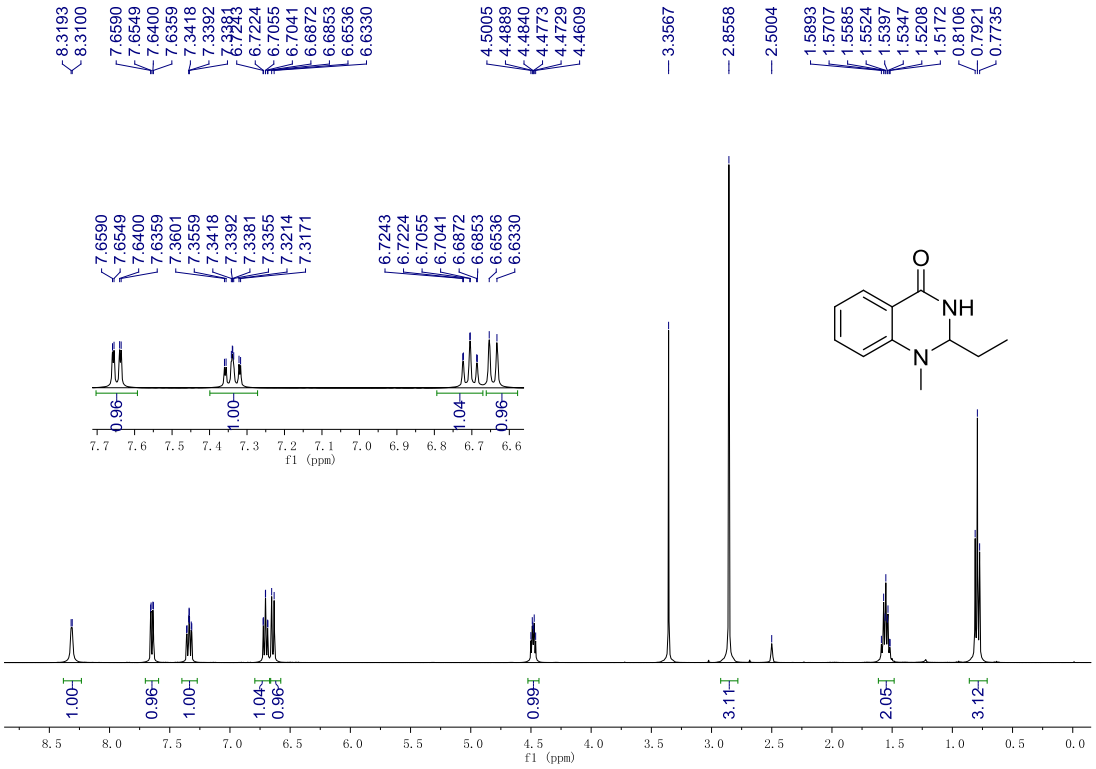
4-2t, ^{13}C NMR (100 MHz, DMSO-d_6)



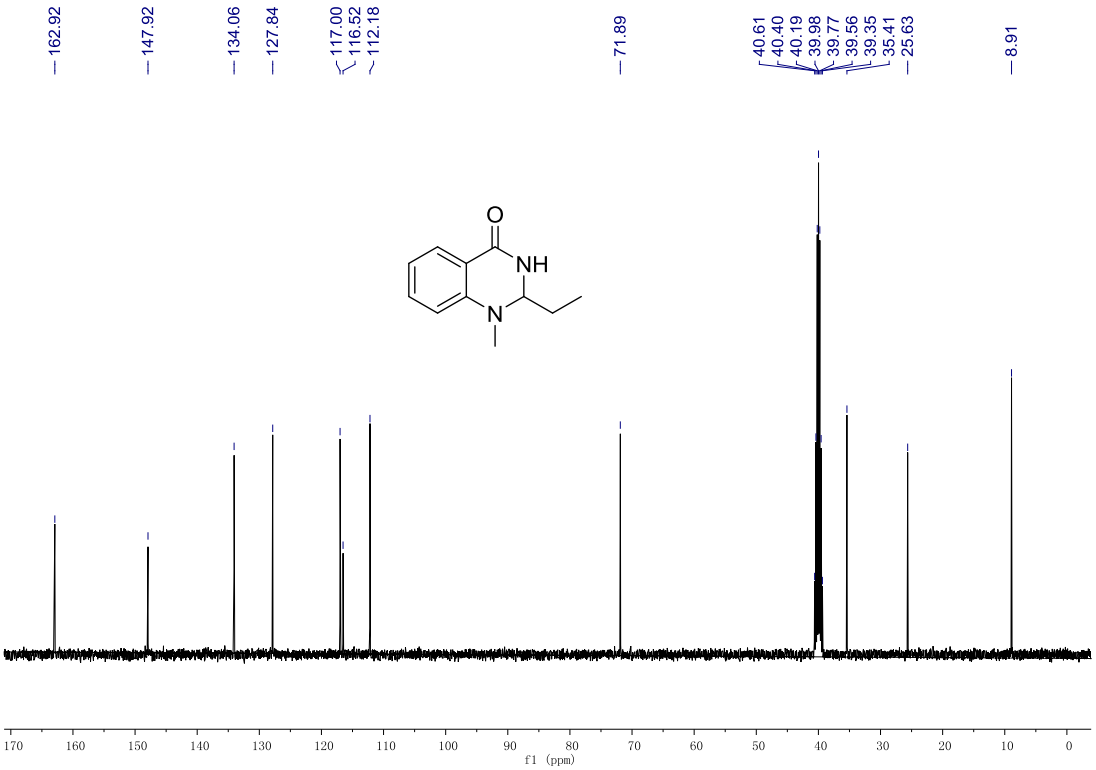
4-2u, ^{1}H NMR (400 MHz, DMSO-d_6)



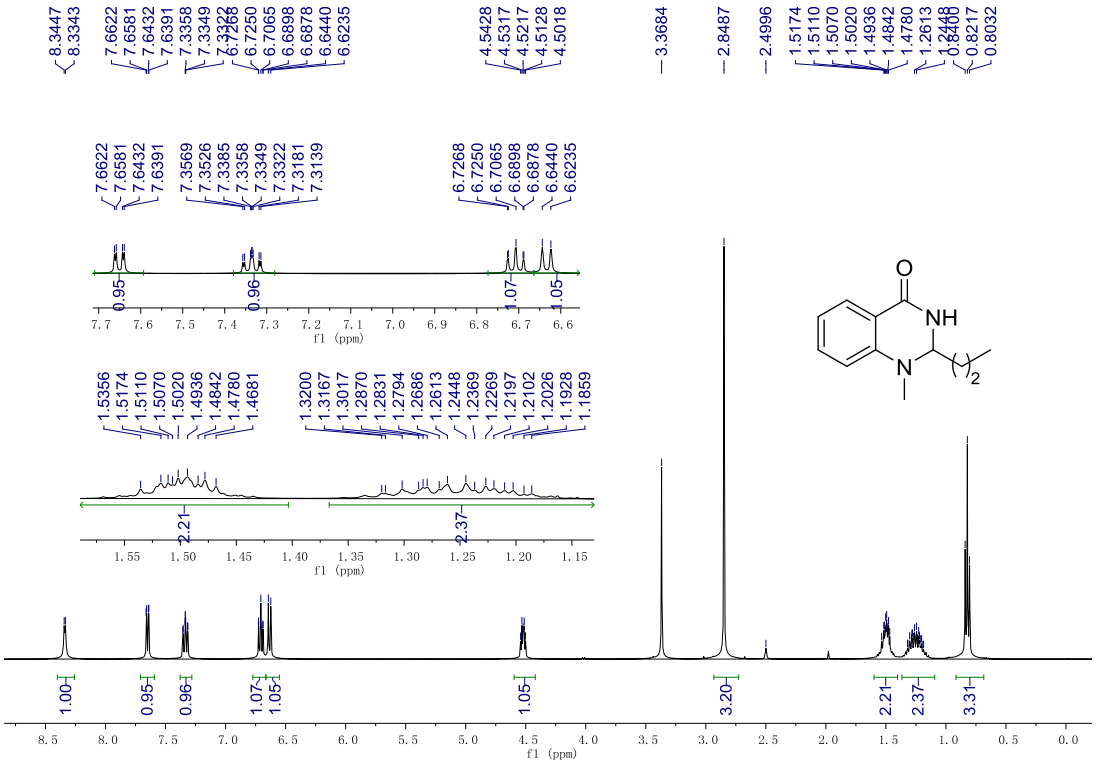
4-2u, ^{13}C NMR (100 MHz, DMSO-d_6)



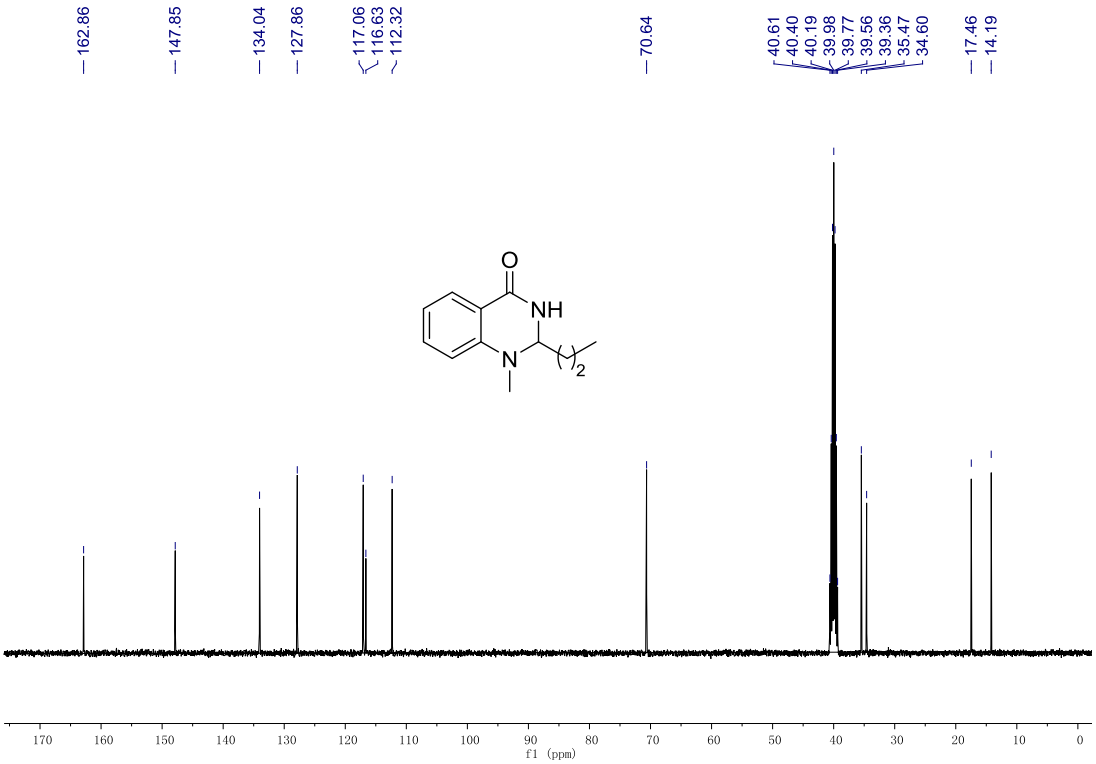
4-2v, ^{1}H NMR (400 MHz, DMSO-d_6)



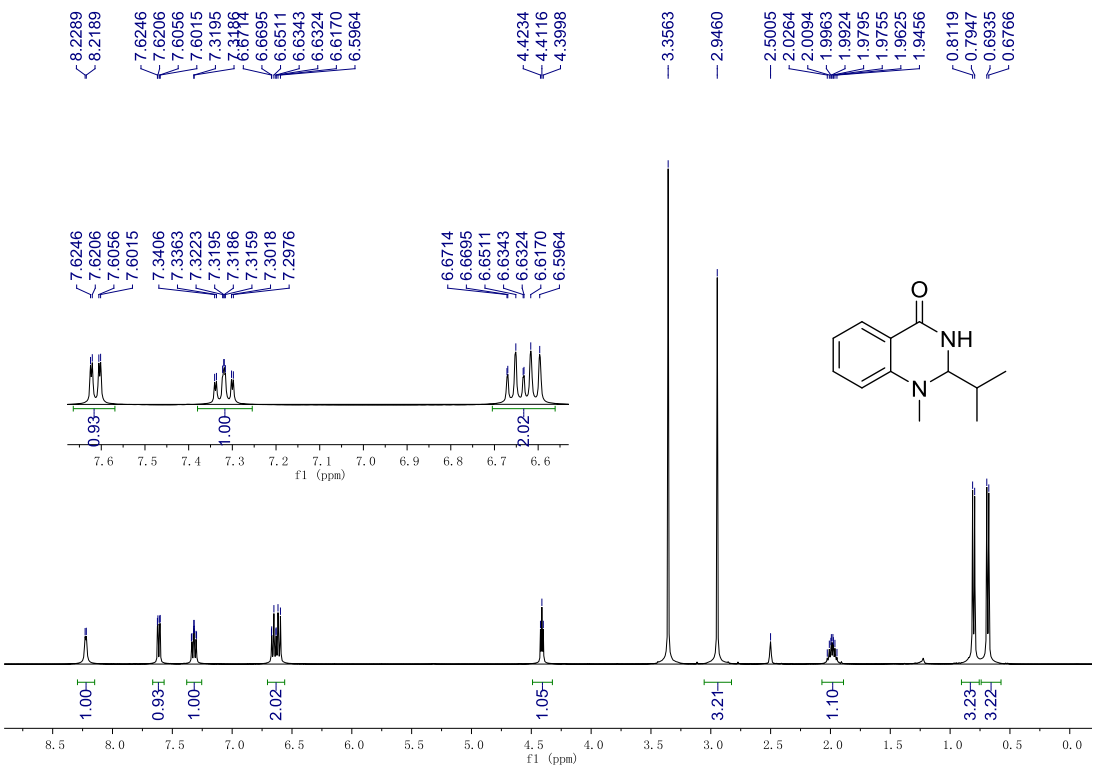
4-2v, ^{13}C NMR (100 MHz, DMSO-d_6)



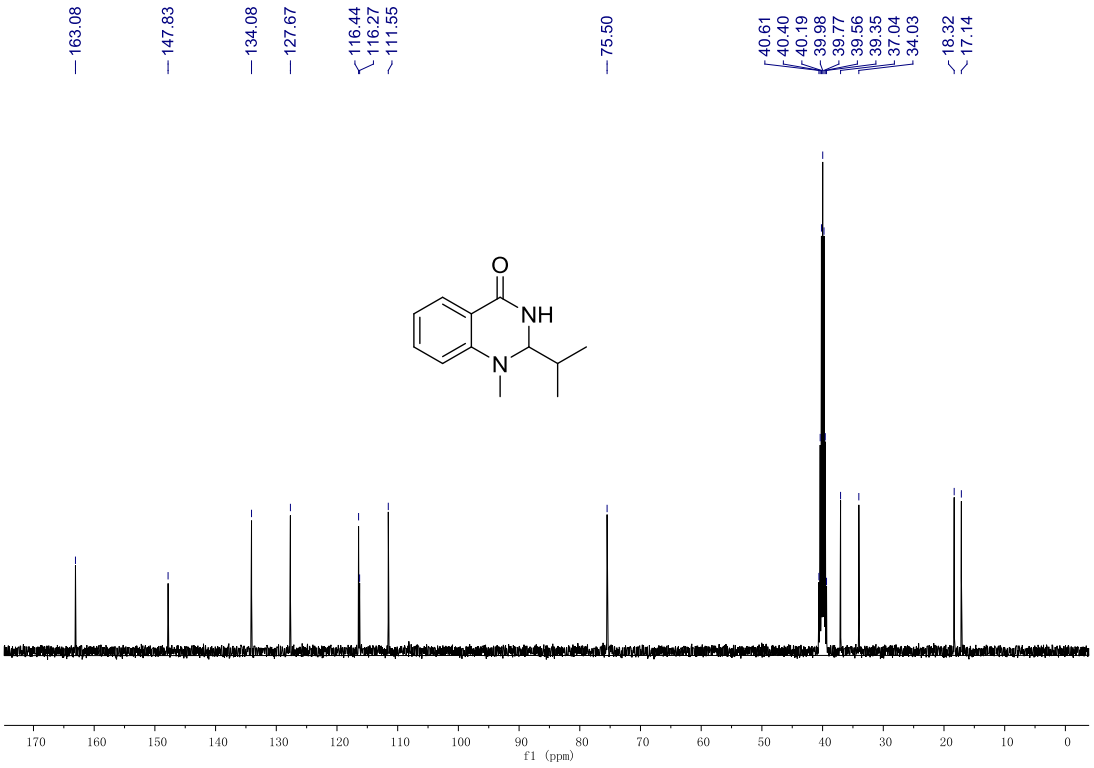
4-2w, ^{1}H NMR (400 MHz, DMSO-d_6)



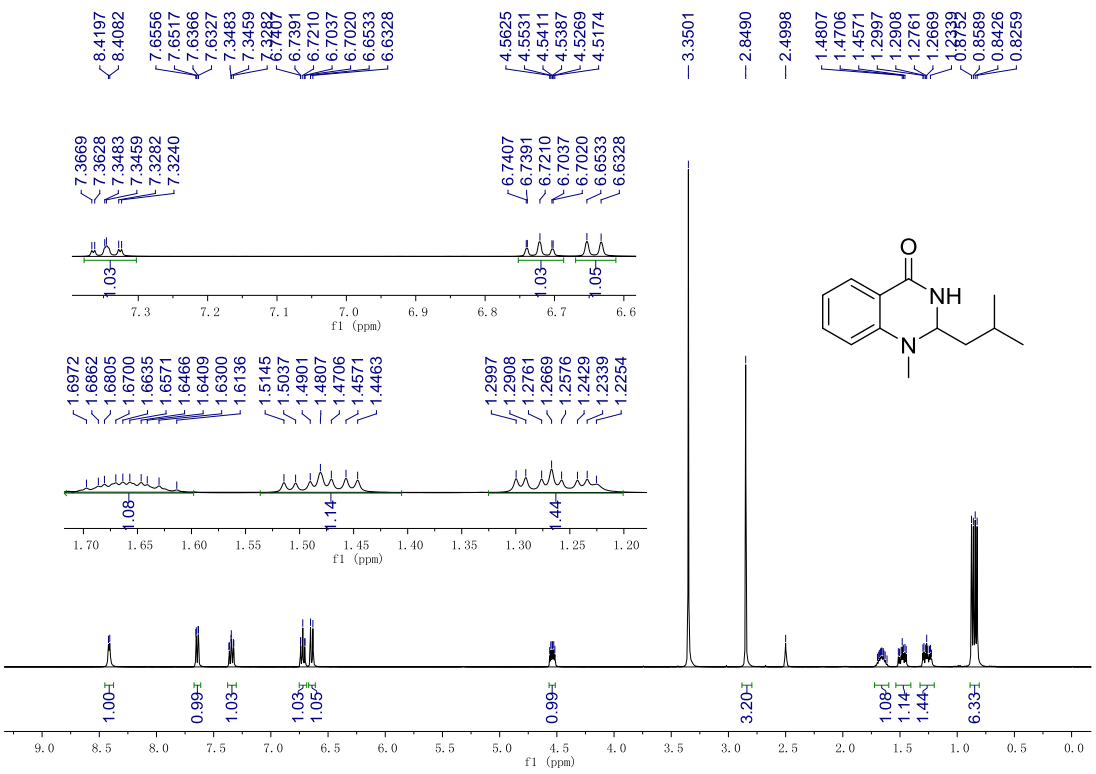
4-2w, ^{13}C NMR (100 MHz, DMSO-d_6)



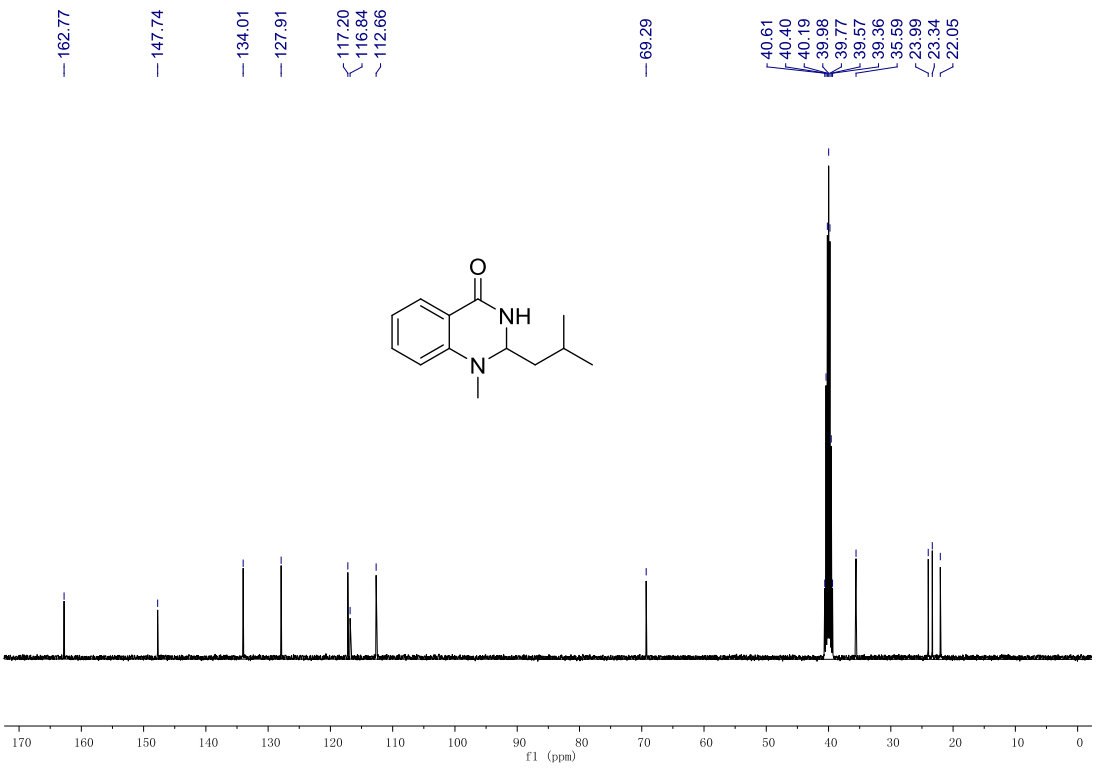
4-2x, ^{1}H NMR (400 MHz, DMSO-d_6)



4-2x, ^{13}C NMR (100 MHz, DMSO-d_6)



4-2z, ^{1}H NMR (400 MHz, DMSO-d_6)



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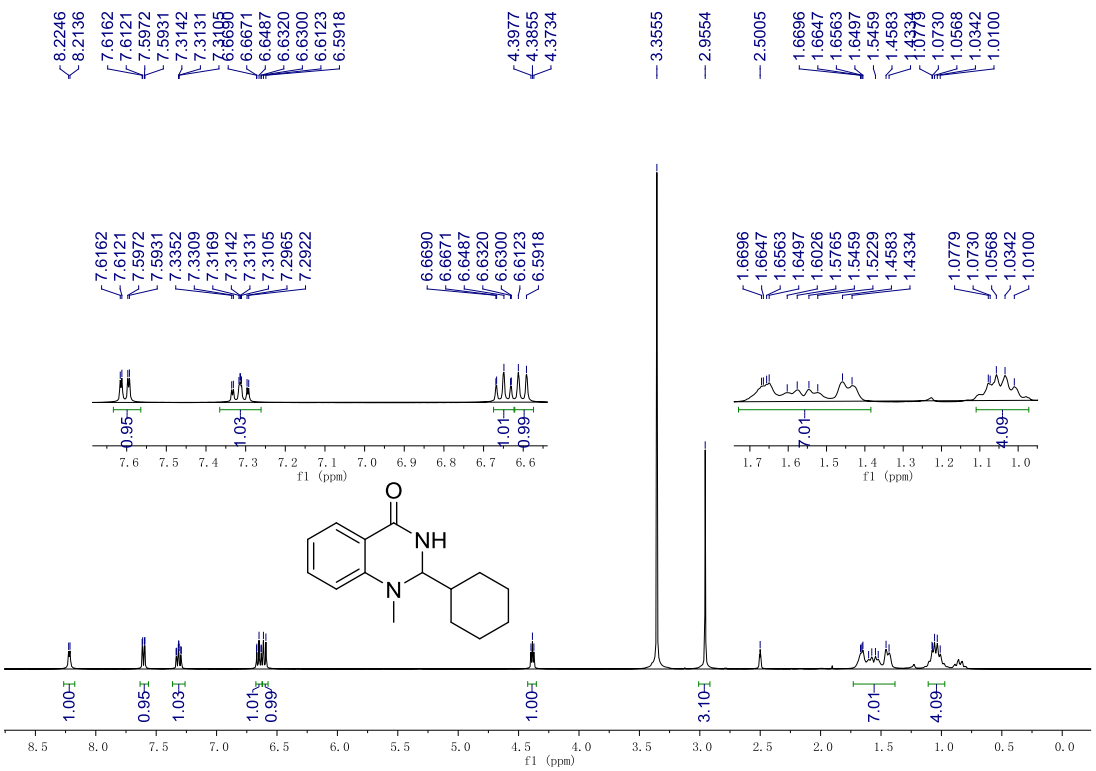
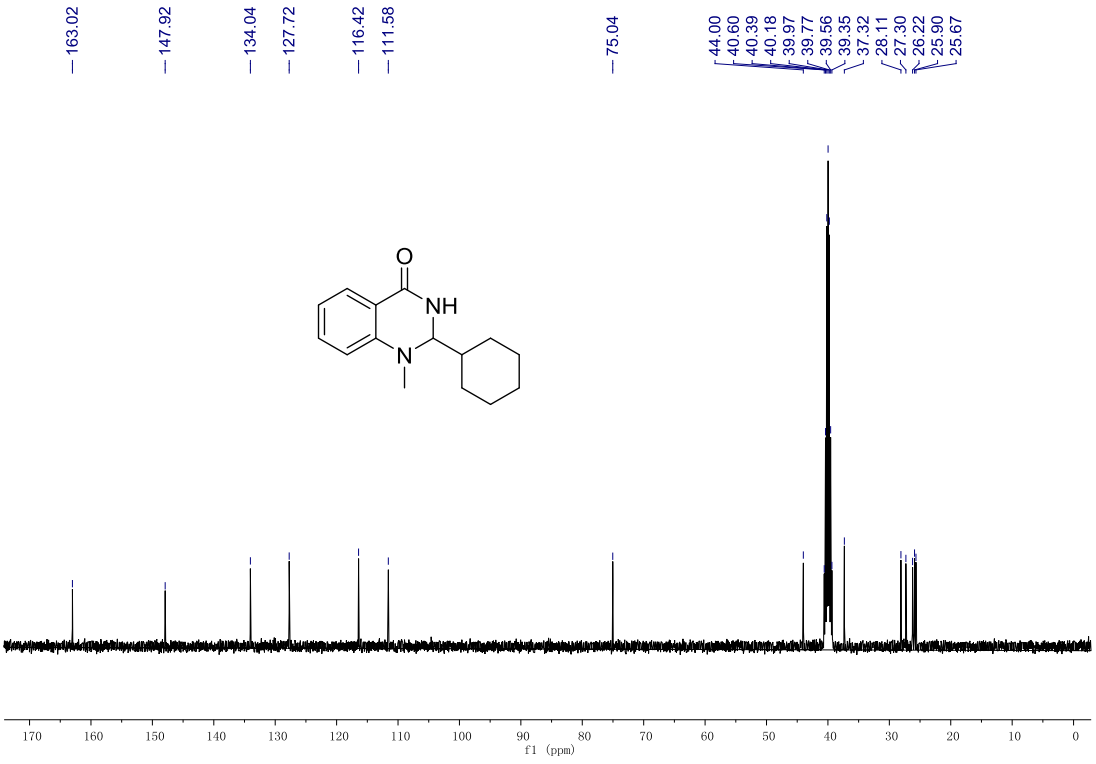
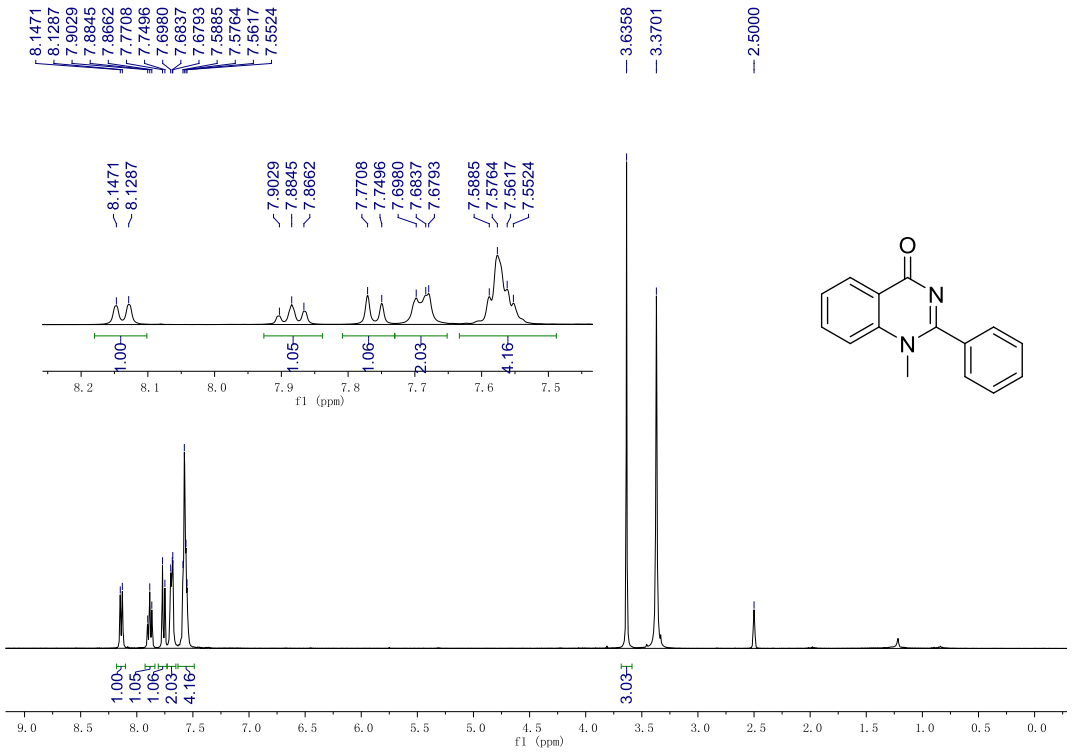


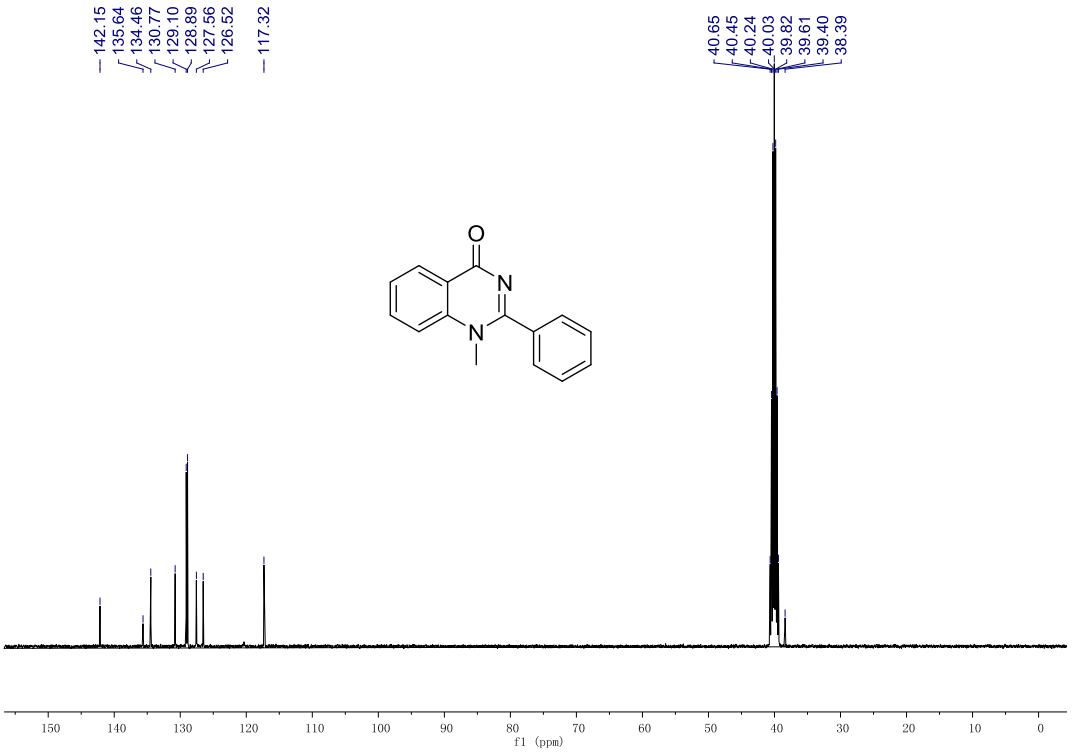
4-2cc, ^{1}H NMR (400 MHz, DMSO-d_6)



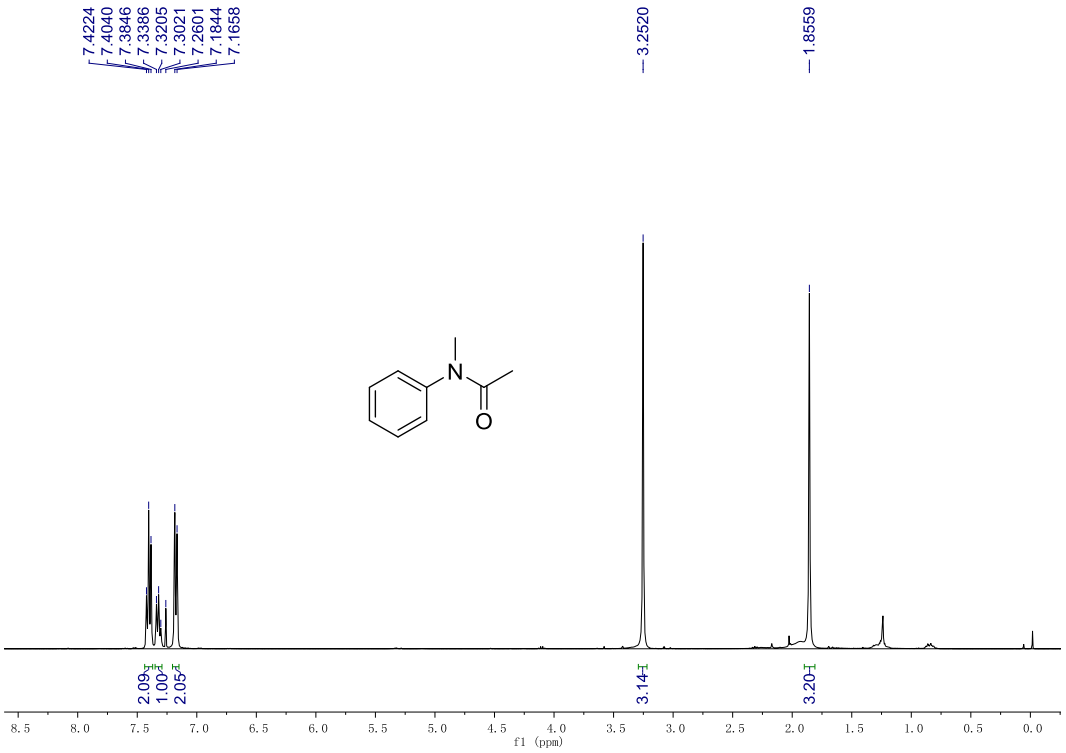
4-2cc, ^{13}C NMR (100 MHz, DMSO-d_6)



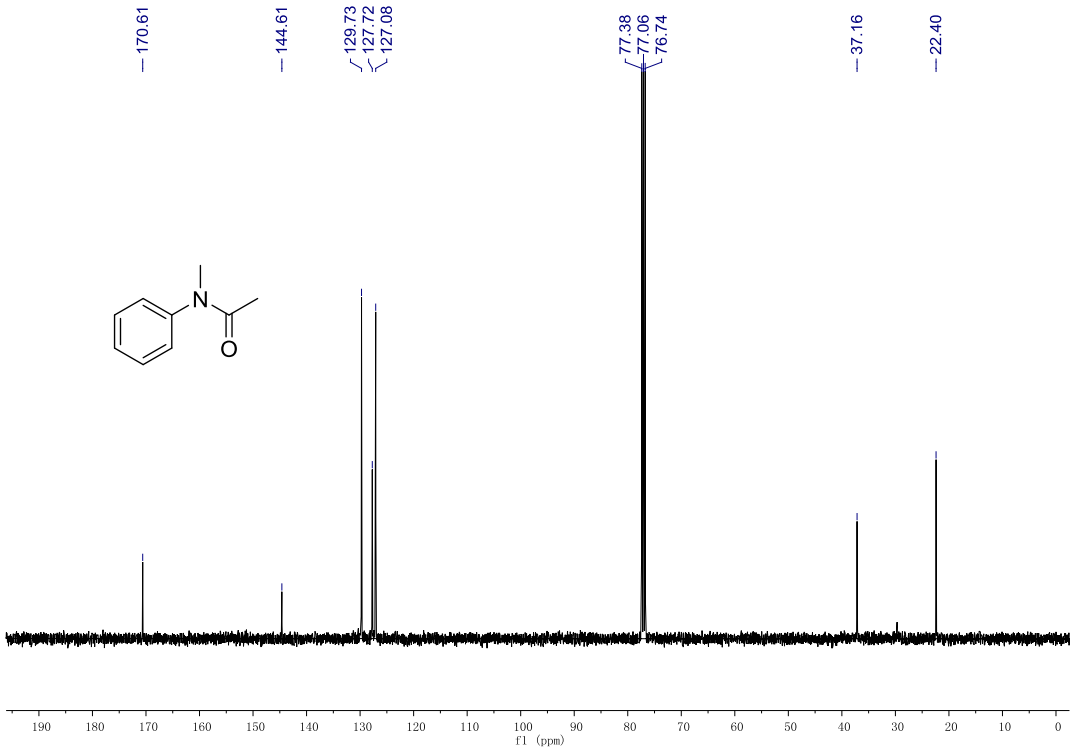
1-methyl-2-phenylquinazolin-4(1*H*)-one, ^{1}H NMR (400 MHz, DMSO-d_6)



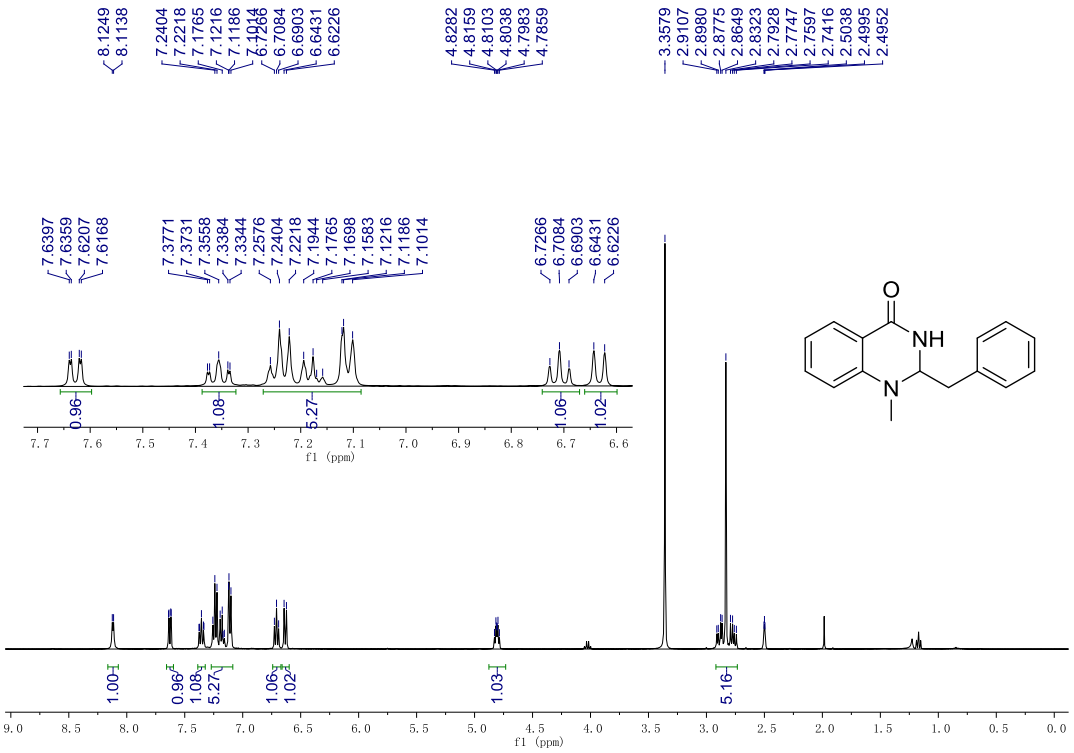
1-methyl-2-phenylquinazolin-4(1*H*)-one, ^{13}C NMR (100 MHz, DMSO-d_6)



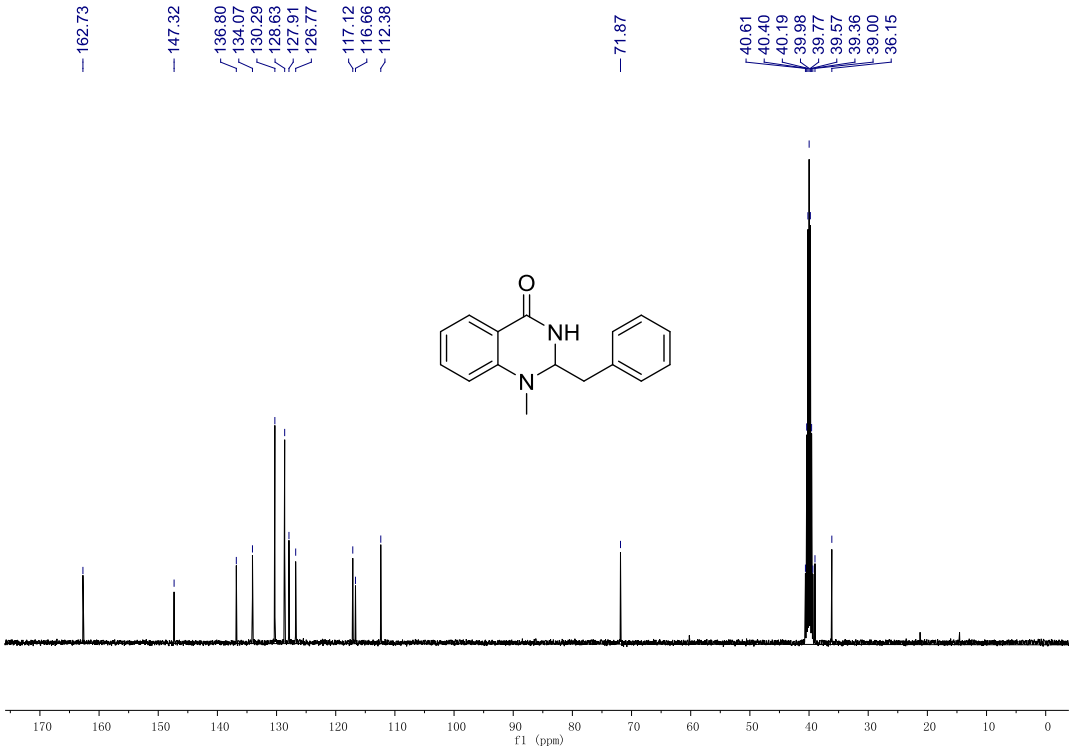
***N*-methyl-*N*-phenylacetamide**, ^{1}H NMR (400 MHz, CD_3Cl)



***N*-methyl-*N*-phenylacetamide**, ^{13}C NMR (100 MHz, CD_3Cl)

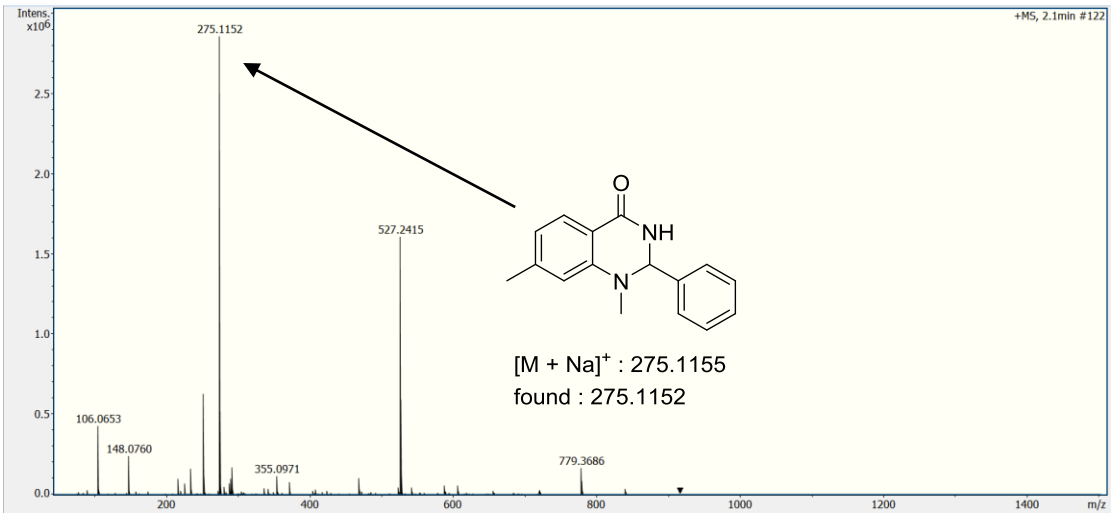


Glycozolone A, ^{1}H NMR (400 MHz, DMSO-d_6)

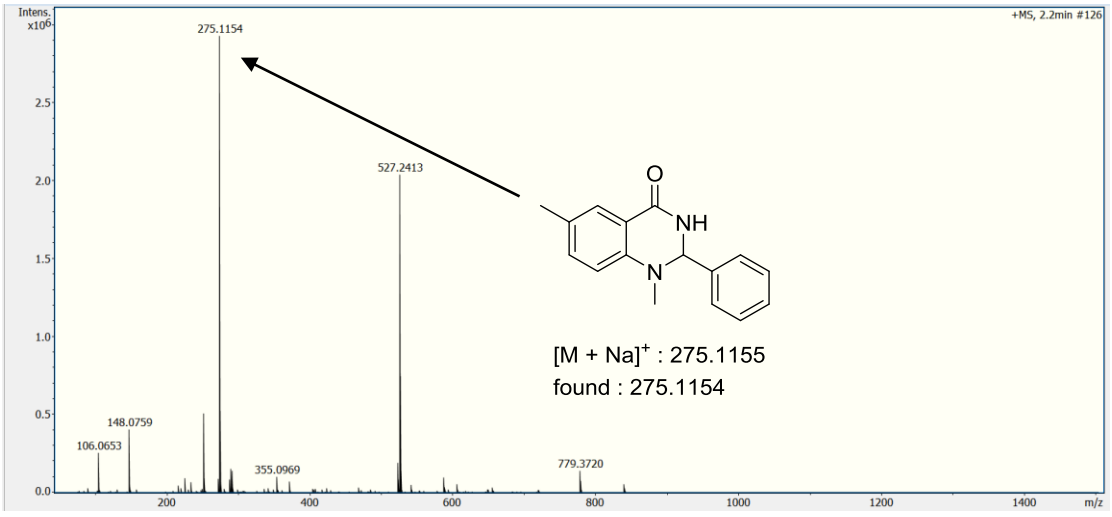


Glycozolone A, ^{13}C NMR (100 MHz, DMSO-d_6)

5. Copies of HRMS Spectra for the Products



HRMS Spectra of **4-1b**



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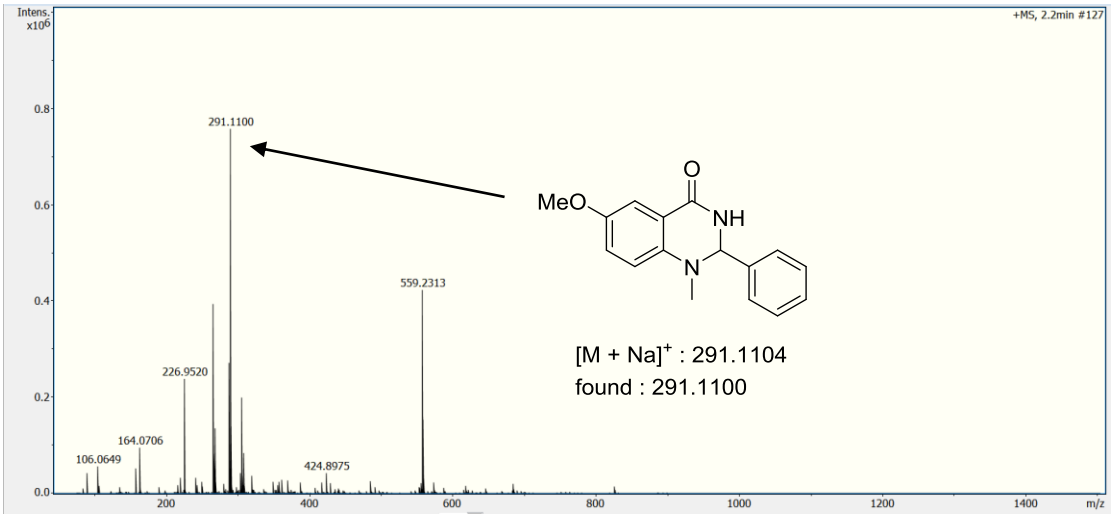

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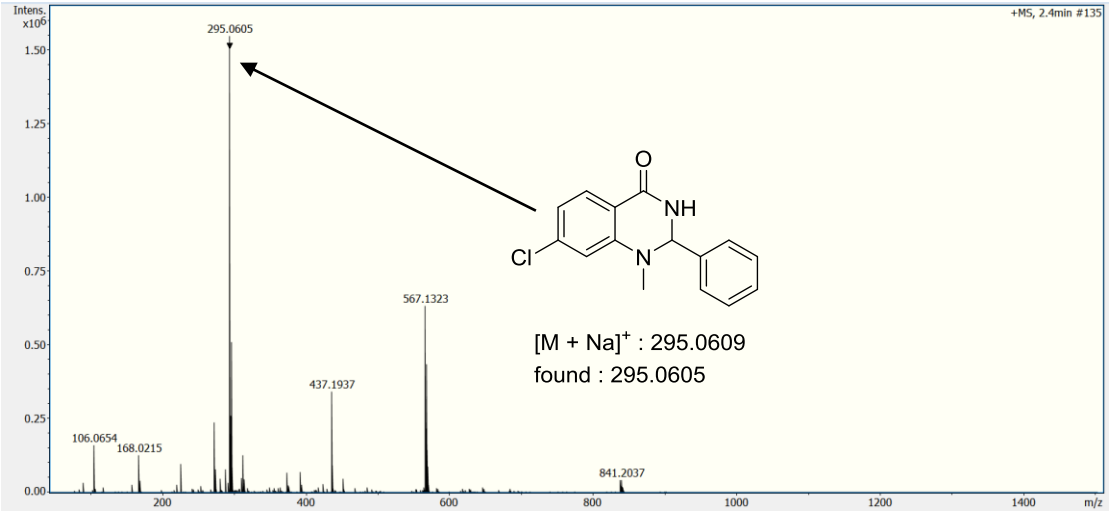

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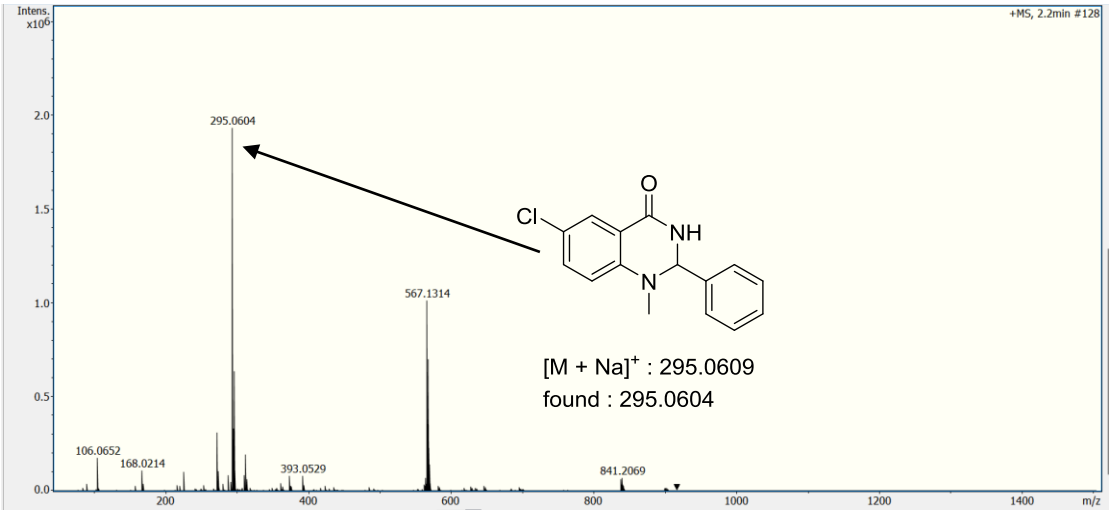

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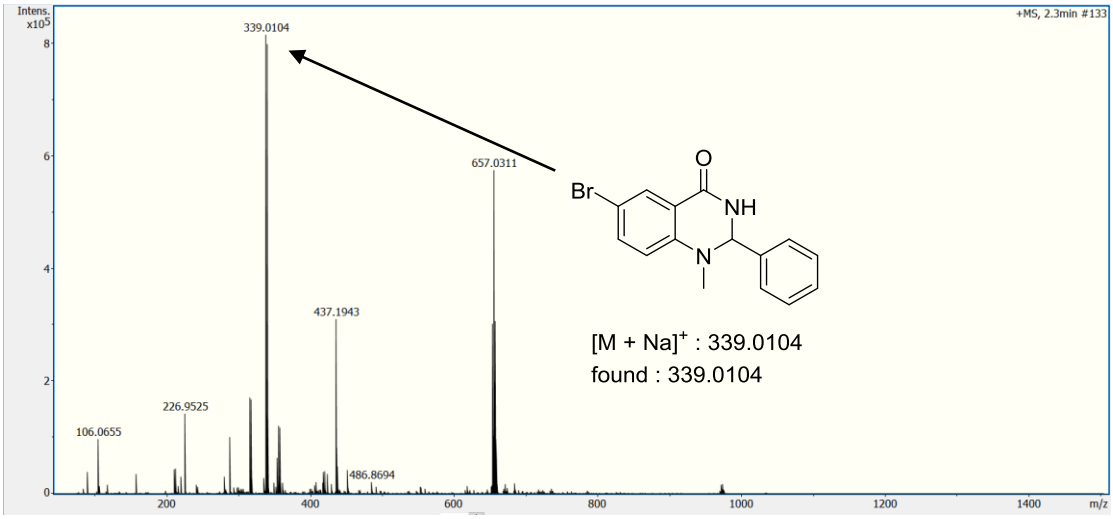

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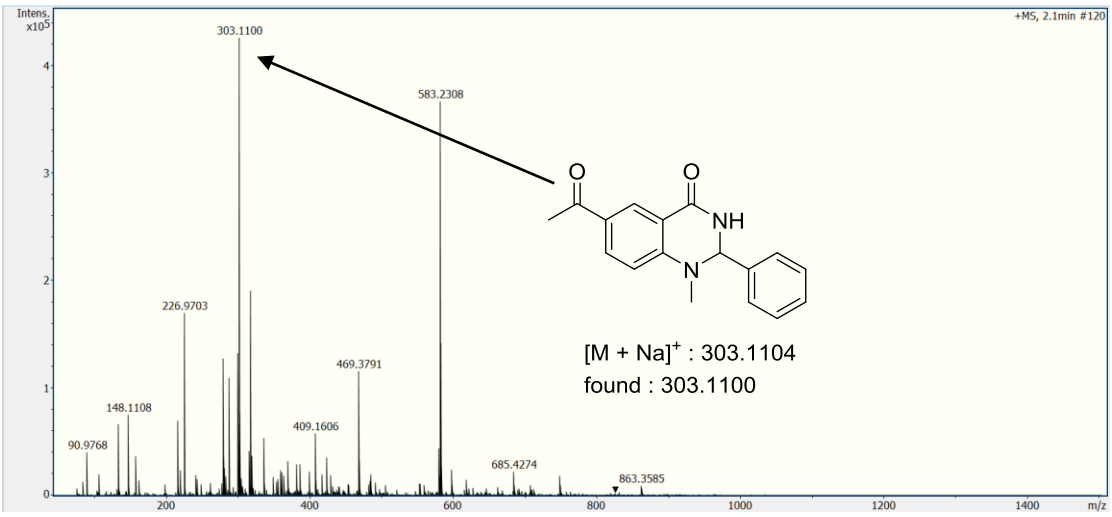
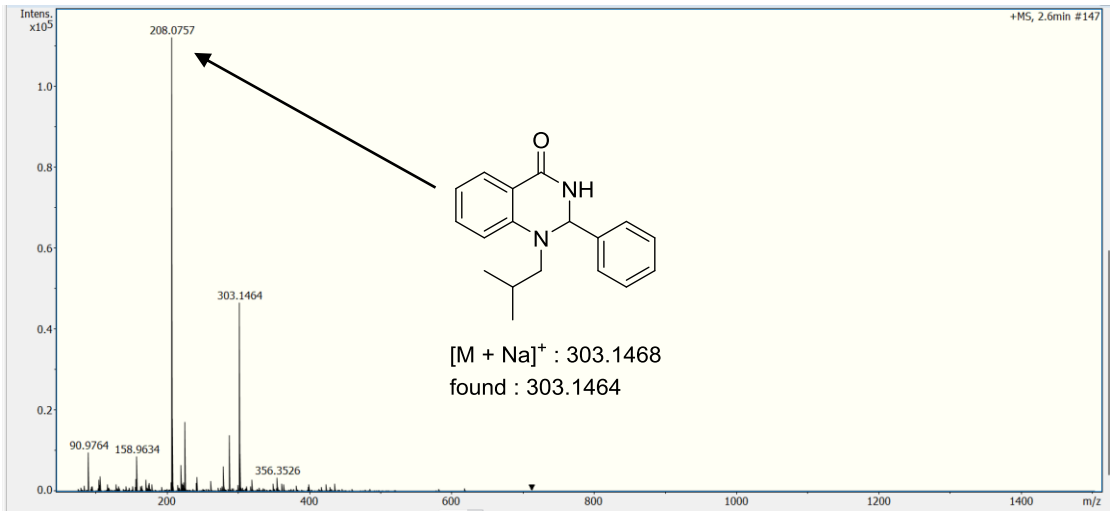
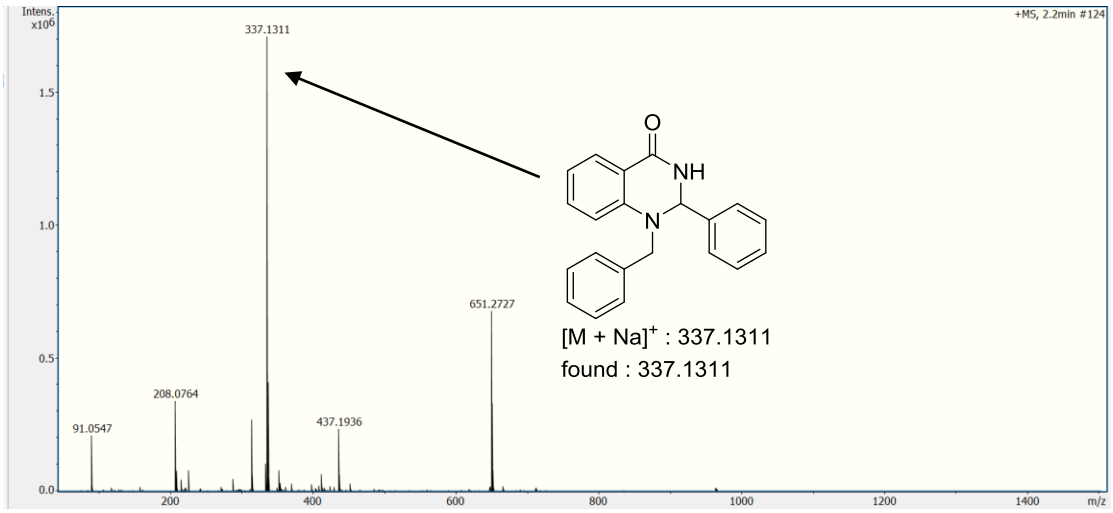


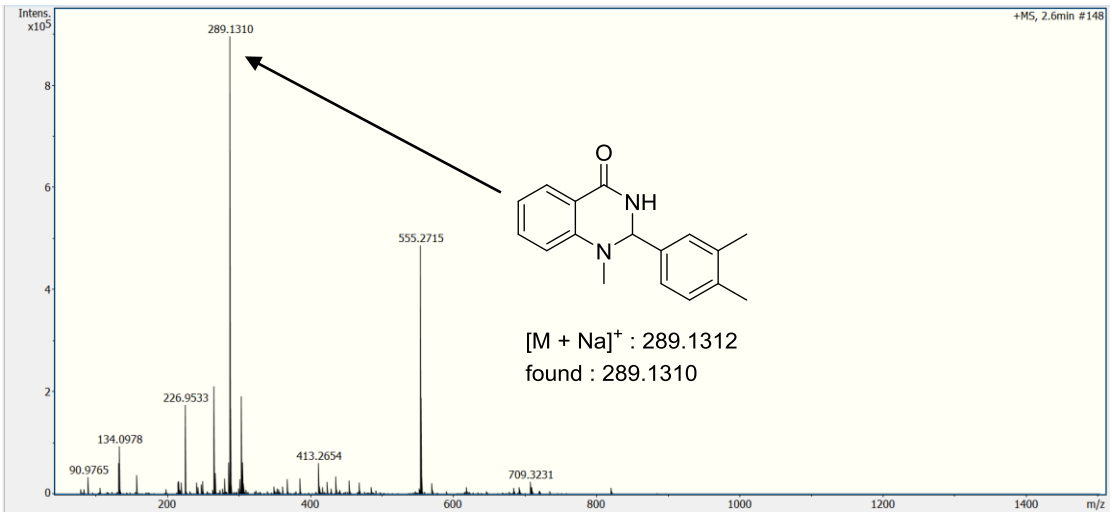
HRMS Spectra of **4-1i**



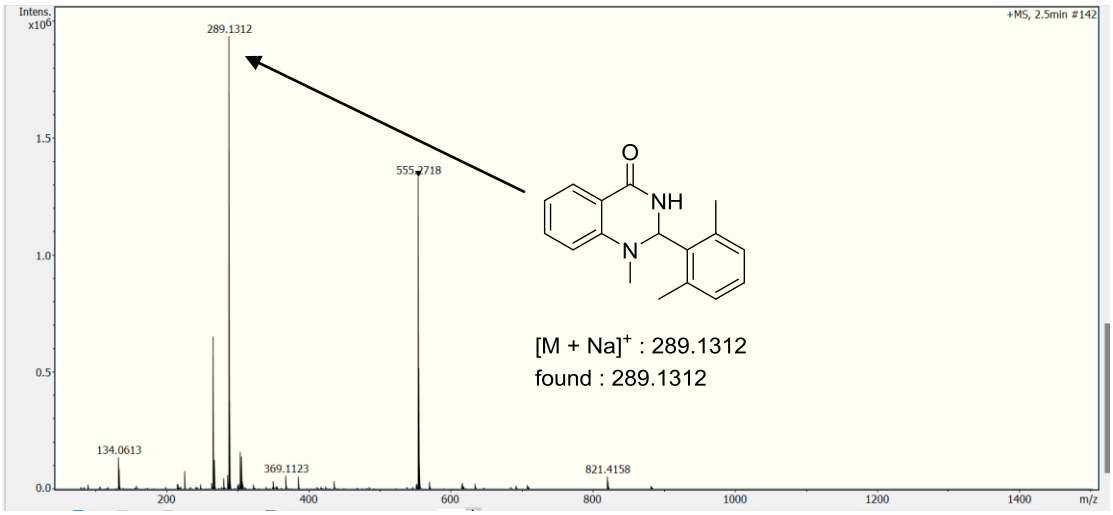
HRMS Spectra of **4-1p**



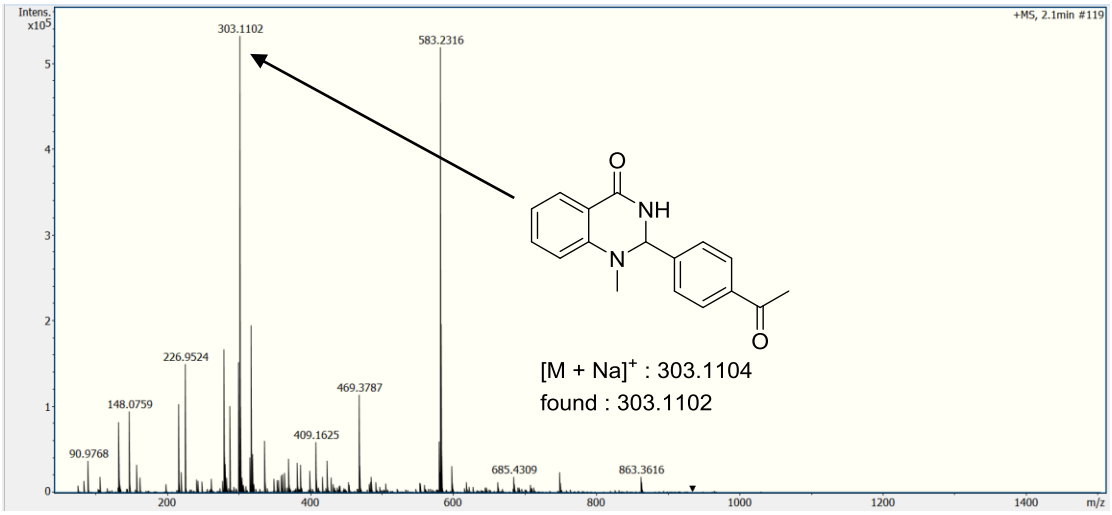
HRMS Spectra of **4-1s**



HRMS Spectra of **4-2i**



HRMS Spectra of **4-2j**



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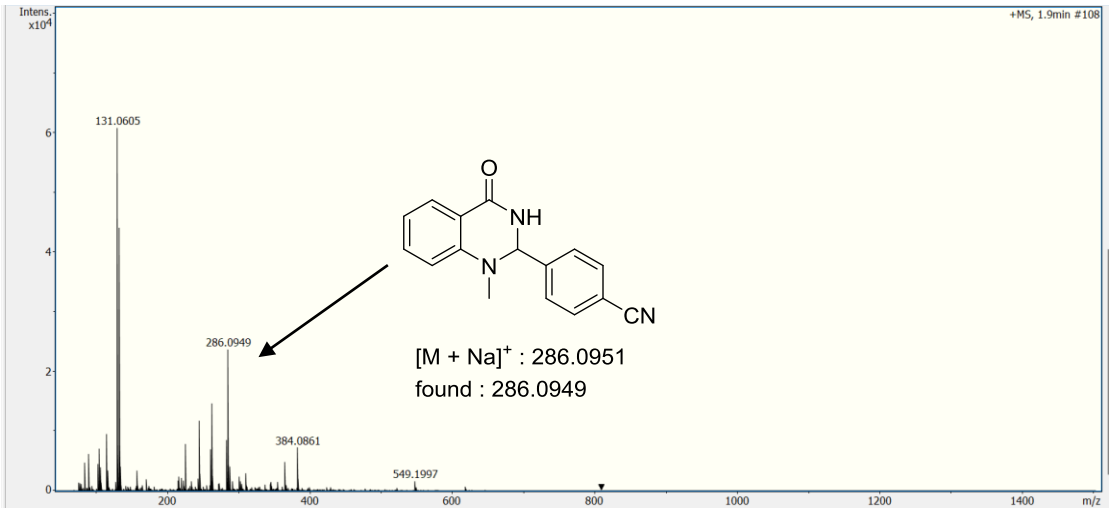
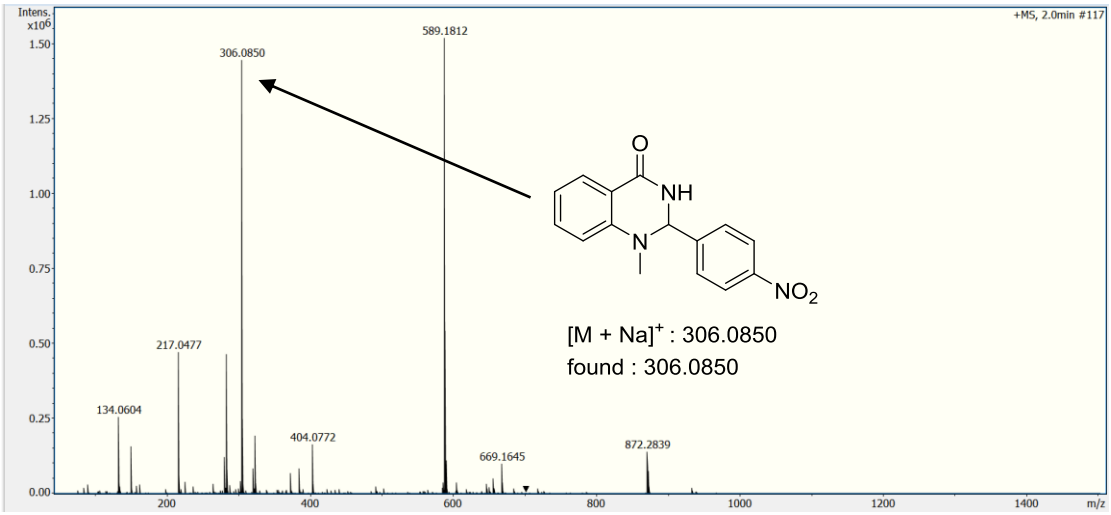


HRMS Spectra of **4-2q**



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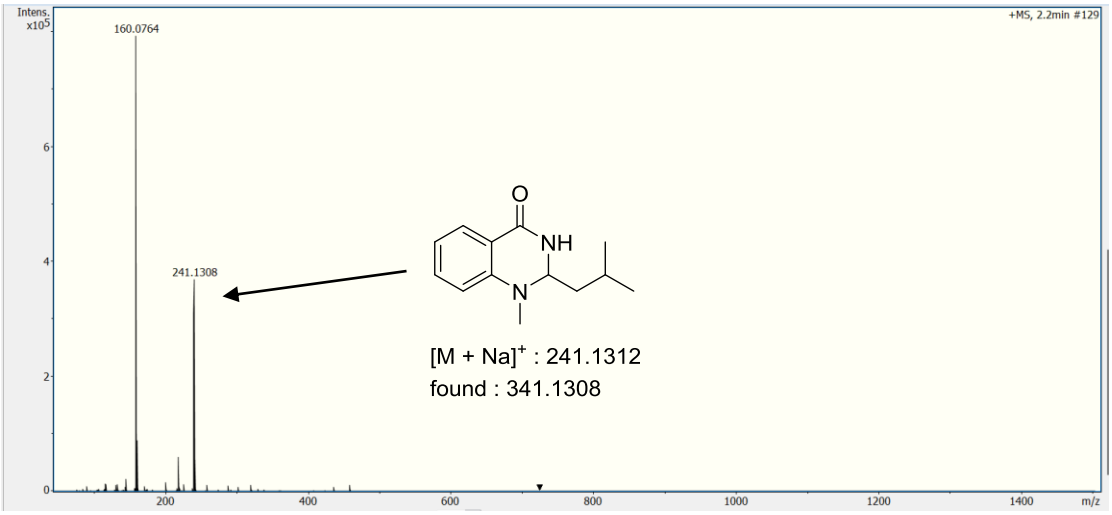

HRMS Spectra of **4-2z**

6. Reference

1. (a) V. Blanco, D. A. Leigh, V. Marcos, J. A. Morales-Serna and A. L. Nussbaumer, *J. Am. Chem. Soc*., 2014, **136**, 4905–4908; (b) J. Jiao, X.-R. Zhang, N.-H. Chang, J. Wang, J.-F. W, X.-Y. Shi and Z.-G. Chen, *J. Org. Chem*., 2011, **76**, 1180–1183; (c) Y. Peng, H. Liu, M. Min, L. Cai and V. Pike, *Chin. J. Chem*., 2009, **27**, 1339–1344; (d) L. Ke, G. Zhu, H. Qian, G. Xiang, Q. Chen and Z. Chen, *Org. Lett*., 2019, **21**, 4008–4 013.