Electronic Supplementary Material (ESI) for RSC Advances.

Palladium-Catalyzed One-Pot Synthesis of 2-Substituted Quinazolin-4(3H)-ones from *o*-Nitrobenzamide and Alcohols

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Supplementary Data

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1. General Information

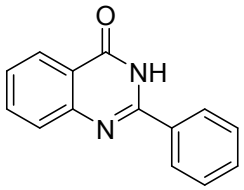
All materials were purchased from commercial suppliers and used without further purification, if not stated otherwise. All reactions involving air-sensitive reagents were performed under an argon atmosphere. Melting points were determined on an INESA SGW_R X-4A micro melting point apparatus and were uncorrected. ^1H NMR and ^{13}C NMR spectra were recorded on Varian Mercury 400 (1H, 400 MHz; 13C, 100 MHz) or Varian Mercury 500 (1H, 500 MHz; 13C, 125 MHz) spectrometers. Data for ^1H NMR are reported as follows: chemical shift (δ ppm), multiplicity, integration, and coupling constant (Hz). Data for ^{13}C NMR are reported in terms of chemical shift (δ ppm). The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, m = multiplet. High-resolution mass spectra (HRMS) was recorded on a Thermo Exactive Plus spectrometer. The ionization method was ESI and the mass analyzer type was orbitrap.

2. General Procedure for the Preparation of the Target Compounds

A 10 mL sealed tube was charged with catalyst (0.1 mmol), *o*-nitrobenzamides(1 mmol), solvent (1-2 mL) and benzyl alcohol (2.5 mmol), and purged with argon three times. The reaction was then heated to 140 ^oC for 8 h. After cooling to room temperature, the solvent was removed under vacumm and the residue was purified by flash column chromatography on silica gel, using petroleum ether and EtOAc as eluent to afford the target compound.

3. Analytical Data of the Target Compounds

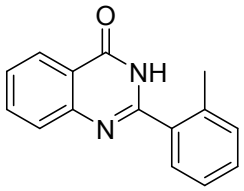
2-phenylquinazolin-4(3H)-one (3a)[1]



White solid, Yield: 87%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.22 – 8.15 (m, 3H), 7.88 – 7.81 (m, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.63 – 7.50 (m, 4H).^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 152.4 , 148.8 , 134.7 , 132.8 , 131.5 , 128.7 , 127.8 , 127.6 , 126.7 , 125.9 , 121.1 . HRMS (ESI) calcd for $C_{14}H_{11}N_2O[M+H]^+$ 223.0866, found 223.0866.

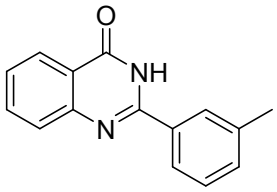
2-(o-tolyl)quinazolin-4(3H)-one (3b)[2]



White solid, Yield: 69%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.45 (s, 1H), 8.18 (dd, J = 7.9, 1.3 Hz, 1H), 7.94 – 7.78 (m, 1H), 7.70 (d, J = 7.9 Hz, 1H), 7.59 – 7.49 (m, 2H), 7.44 (td, J = 7.5, 1.3 Hz, 1H), 7.39 – 7.30 (m, 2H), 2.39 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ 162.2 , 154.8 , 149.2 , 136.6 , 134.9 , 134.7 , 131.0 , 130.3 , 129.6 , 127.8 , 127.1 , 126.2 , 126.1 , 121.4 , 20.0 . HRMS (ESI) calcd for $C_{15}H_{13}N_2O[M+H]^+$ 237.1022, found 237.1028.

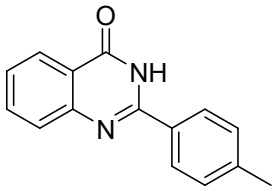
2-(m-tolyl)quinazolin-4(3H)-one (3c)[2]



White solid, Yield: 80%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.47 (s, 1H), 8.16 (d, J = 7.9 Hz, 1H), 8.03 (s, 1H), 7.98 (d, J = 7.3 Hz, 1H), 7.84 (t, J = 7.9 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.46 - 7.40 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 152.5 , 148.8 , 138.0 , 134.7 , 132.7 , 132.1 , 128.6 , 128.4 , 127.6 , 126.6 , 125.9 , 125.0 , 121.1 , 21.1 . HRMS (ESI) calcd for $C_{15}H_{13}N_2O[M+H]^+$ 237.1022, found 237.1028.

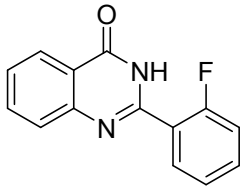
2-(p-tolyl)quinazolin-4(3H)-one (3d)[2]



White solid, Yield: 78%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.47 (s, 1H), 8.16 (dd, J = 7.9, 1.5 Hz, 1H), 8.04 (s, 1H), 7.98(d, J = 7.9, 1H), 7.87 – 7.81 (m, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.55 – 7.51(m, 1H), 7.36-7.40 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 152.4 , 148.8 , 138.0 , 134.6 , 132.7 , 132.1 , 128.6, 128.4, 127.6 , 126.6 , 125.9 , 125.0 , 121.1 , 21.0 . HRMS (ESI) calcd for $C_{15}H_{13}N_2O[M+H]^+$ 237.1022, found 237.1019.

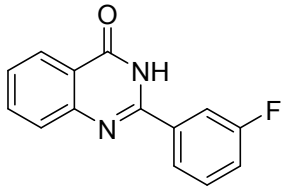
2-(2-fluorophenyl)quinazolin-4(3H)-one (3e)[3]



White solid, Yield: 46%.

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.19 (dd, J = 8.0, 1.6 Hz, 1H), 7.89-7.85 (m, 1H), 7.80 (td, J = 7.5, 1.8 Hz, 1H), 7.75 (dd, J = 8.2, 1.1 Hz, 1H), 7.66-7.62 (m, 1H), 7.60-7.56 (m, 1H), 7.45 – 7.34 (m, 2H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 161.6 , 159.7 (d, J = 250.8 Hz) , 150.1 , 148.8 , 134.8 , 133.0 (d, J = 8.7 Hz) , 131.2 , 127.6 , 127.2 , 126.0 , 124.8 (d, J = 3.4 Hz) , 122.3 (d, J = 13.0 Hz) , 121.2 , 116.2 (d, J = 21.3 Hz) . HRMS (ESI) calcd for $C_{14}H_{10}N_2OF[M+H]^+$ 241.0772, found 241.0770.

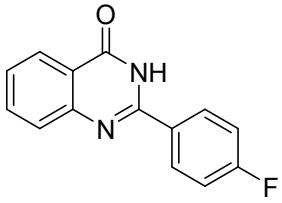
2-(3-fluorophenyl)quinazolin-4(3H)-one (3f)[3]



White solid, Yield: 82%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.17 (d, J = 7.9 Hz, 1H), 8.07 (d, J = 8.1 Hz, 1H), 8.02 (d, J = 10.4 Hz, 1H), 7.90 – 7.81 (m, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.64-7.53 (m, 2H), 7.48-7.43 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.2 , 162.2 (d, J = 244.2 Hz) , 151.1 , 148.6 , 135.1 (d, J = 8.1 Hz), 134.8 , 130.9 (d, J = 8.3 Hz), 127.7 , 127.1 , 126.0 , 124.1 , 121.2 , 118.3 (d, J = 21.1 Hz) , 114.7 (d, J = 24.0 Hz) . HRMS (ESI) calcd for $C_{14}H_{10}N_2OF[M+H]^+$ 241.0772, found 241.0769.

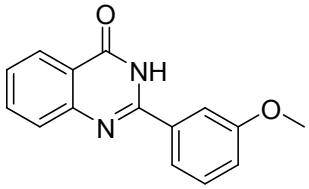
2-(4-fluorophenyl)quinazolin-4(3H)-one (3g)[2]



White solid, Yield: 82%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.30 – 8.23 (m, 2H), 8.16 (dd, J = 7.9, 1.2 Hz, 1H), 7.85 (td, J = 7.8, 7.2, 1.5 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.44 – 7.36 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.1 (d, J = 250.4 Hz), 162.3 , 151.4 , 148.7 , 134.7 ， 130.4 (d, J = 9.1 Hz) ， 129.3 (d, J = 2.9 Hz)， 127.5 , 126.7 , 125.9 , 121.0 , 115.7 (d, J = 22.0 Hz) .HRMS (ESI) calcd for $C_{14}H_{10}N_2OF[M+H]^+$ 241.0772, found 241.0771.

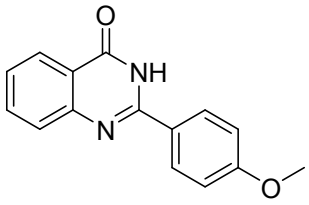
2-(3-methoxyphenyl)quinazolin-4(3H)-one (3h)[2]



White solid, Yield: 76%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.17 (dd, J = 7.9, 1.2 Hz, 1H), 7.88 – 7.73 (m, 4H), 7.57 – 7.51 (m, 1H), 7.47 (t, J = 8.0 Hz, 1H), 7.16 (dd, J = 8.1, 2.2 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 159.4 , 152.1 , 148.7 , 134.7 , 134.1 , 129.8 , 127.6 , 126.7 , 125.9 , 121.1 , 120.2 , 117.7 , 112.6 , 55.5 . HRMS (ESI) calcd for $C_{15}H_{13}N_2O_2[M+H]^+$ 253.0972, found 253.0978.

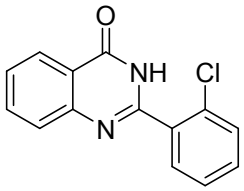
2-(4-methoxyphenyl)quinazolin-4(3H)-one (3i)[2]



White solid, Yield: 75%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 (s, 1H), 8.21 (d, J = 8.9 Hz, 2H), 8.15 (d, J = 7.4 Hz, 1H), 7.82 (t, J = 7.6 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.49 (t, J = 7.2 Hz, 1H), 7.10 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 161.9 , 151.9 , 148.9 , 134.5 , 129.5 , 127.3 , 126.1 , 125.8 , 124.8 , 120.7 , 114.0 , 55.5 . HRMS (ESI) calcd for $C_{15}H_{13}N_2O_2[M+H]^+$ 253.0972, found 253.0968.

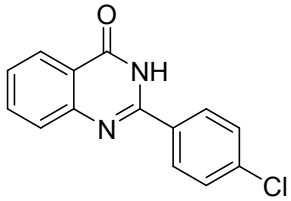
2-(2-chlorophenyl)quinazolin-4(3H)-one (3j)[2]



White solid, Yield: 60%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.63 (s, 1H), 8.18 (dd, J = 7.9, 1.4 Hz, 1H), 7.86 (dt, J = 7.8, 1.5 Hz, 1H), 7.75 – 7.65 (m, 2H), 7.65 – 7.53 (m, 3H), 7.50 (dt, J = 7.4, 1.3 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.5 , 152.3 , 148.8 , 134.7 , 133.9 , 131.7 , 131.5 , 131.0 , 129.7 , 127.5 , 127.3 , 127.2 , 125.9 , 121.3 . HRMS (ESI) calcd for $C_{14}H_{10}N_2OCl[M+H]^+$ 257.0476, found 257.0478.

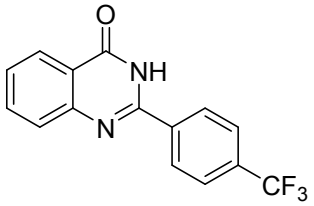
2-(4-chlorophenyl)quinazolin-4(3H)-one (3k)[2]



White solid, Yield: 73%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.21 (d, J = 8.3 Hz, 2H), 8.16 (d, J = 7.8 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.63 (d, J = 8.2 Hz, 2H), 7.55 (d, J = 7.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 152.4 , 148.6 , 136.4 , 134.8 , 131.6 , 129.7 , 128.8 , 127.6 , 126.9 , 126.0 , 121.1 . HRMS (ESI) calcd for $C_{14}H_{10}N_2OCl[M+H]^+$ 257.0476, found 257.0476.

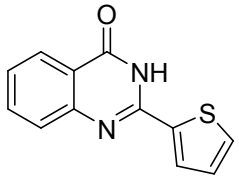
2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one (3l)[4]



White solid, Yield: 76%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.36 (s, 1H), 8.23-8.17 (m, 3H), 7.63-7.51 (m, 4H), 7.39 (t, J = 7.0 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.1 , 151.1 , 148.4 , 136.6 , 134.7 , 131.1 (q, J = 35.0 Hz) , 128.7 , 127.6 , 127.1 , 125.9 , 125.5 (q, J = 3.5 Hz) , 123.9 (q, J = 270.8 Hz) , 121.2 . HRMS (ESI) calcd for $C_{15}H_{10}N_2OF_3[M+H]^+$ 291.0740, found 291.0731.

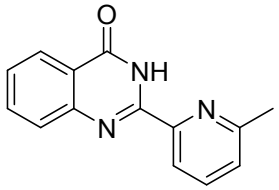
2-(thiophen-2-yl)quinazolin-4(3H)-one (3m)[2]



White solid, Yield: 66%.

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.66 (s, 1H), 8.24 (d, J = 3.8 Hz, 1H), 8.16 – 8.10 (m, 1H), 7.88 (d, J = 5.0 Hz, 1H), 7.85 – 7.77 (m, 1H), 7.66 (d, J = 8.2 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.24 (t, J = 4.4 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.9 , 148.7 , 147.9 , 137.4 , 134.8 , 132.3 , 129.5, 128.6 , 127.0 , 126.4 , 126.1 , 121.0 . HRMS (ESI) calcd for $C_{12}H_9N_3OS[M+H]^+$ 229.0430, found 229.0428.

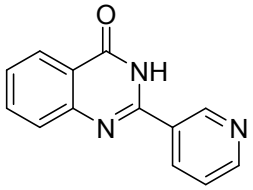
2-(6-methylpyridin-2-yl)quinazolin-4(3H)-one (3n)[5]



White solid, Yield: 83%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 8.25 (d, J = 7.8 Hz, 1H), 8.19 (d, J = 7.8 Hz, 1H), 7.95 (t, J = 7.8Hz, 1H), 7.88 (t, J = 8.1, 1H), 7.80 (d, J = 8.1 Hz, 1H), 7.57 (t, J = 7.8 Hz, 1H), 7.51 (d, J = 7.7 Hz, 1H), 2.63 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.8 , 157.9 , 150.0 , 148.6 , 147.7 , 138.2 , 134.8 , 127.8 , 127.3 , 126.2 , 122.1, 119.2 , 23.8 . HRMS (ESI) calcd for $C_{14}H_{12}N_3O[M+H]^+$ 238.0975, found 238.0989.

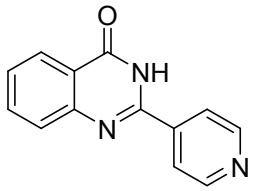
2-(pyridin-3-yl)quinazolin-4(3H)-one[2] (3o)[4]



White solid, Yield: 54%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.74 (s, 1H), 9.30 (d, J = 1.8 Hz, 1H), 8.76 (dd, J = 4.8, 1.5 Hz, 1H), 8.50 (dt, J = 8.2, 1.8 Hz, 1H), 8.18 (d, J = 8.7 Hz, 1H), 7.89 – 7.85 (m, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.61 – 7.54 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.2 , 151.9 , 150.8 , 149.8 , 148.6 , 135.5 , 134.8 , 127.7 , 127.0 , 126.0 , 123.6 , 121.2 . HRMS (ESI) calcd for $C_{13}H_{10}N_3O[M+H]^+$ 224.0818, found 224.0815.

2-(pyridin-4-yl)quinazolin-4(3H)-one (3p)[3]

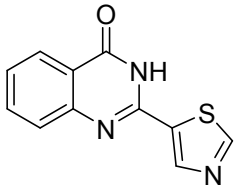


White solid, Yield: 48%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.76 (s, 1H), 8.78 (d, J = 6.0 Hz, 2H), 8.18 (d, J = 7.9 Hz, 1H), 8.11 (d, J = 6.0 Hz, 2H), 7.89 - 7.85 (m, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.61 – 7.54 (m, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.1 , 150.6 , 150.3 , 148.3 ,

140.0 , 134.9 , 127.9 , 127.5 , 126.0 , 121.7 , 121.6 . HRMS (ESI) calcd for $C_{13}H_{10}N_3O[M+H]^+$ 224.0818, found 224.0811.

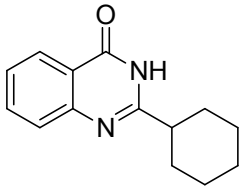
2-(thiazol-5-yl)quinazolin-4(3H)-one (3q)



White solid, Yield: 78%, mp 293-294°C

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.87 (s, 1H), 9.32 (s, 1H), 8.91 (s, 1H), 8.14 (d, J = 7.9 Hz, 1H), 7.83 (t, J = 6.5 Hz, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.53 (t, J = 7.1 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.7 , 159.1 , 148.5 , 146.5 , 144.5 , 134.9 , 133.9 , 127.2 , 127.0 , 126.1 , 121.1 . HRMS (ESI) calcd for $C_{11}H_8N_3OS[M+H]^+$ 230.0383, found 230.0380.

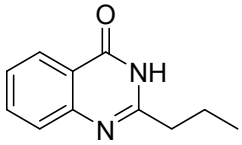
2-cyclohexylquinazolin-4(3H)-one (3r)[6]



White solid, Yield: 64%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.09 (s, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.77 (t, J = 7.7 Hz, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 2.58 (t, J = 11.7 Hz, 1H), 1.91 (d, J = 12.1 Hz, 2H), 1.80 (d, J = 12.2 Hz, 2H), 1.72 – 1.51 (m, 3H), 1.38 – 1.19 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.0 , 160.8 , 149.0 , 134.3 , 127.0 , 126.0 , 125.72 , 121.0 , 32.9 , 30.3 , 25.6 , 25.4 . HRMS (ESI) calcd for $C_{14}H_{17}N_2O[M+H]^+$ 229.1335, found 229.1334.

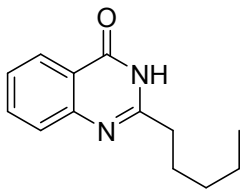
2-propylquinazolin-4(3H)-one (3s)[3]



White solid, Yield: 31%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.16 (s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.77 (t, J = 7.9 Hz, 1H), 7.60 (d, J = 8.2 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 2.58 (t, J = 7.6 Hz, 2H), 1.80 - 1.70 (m, 2H), 0.94 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.7 , 157.2 , 148.9 , 134.2 , 126.7 , 125.8 , 125.6 , 120.7 , 36.3 , 20.1 , 13.4 . HRMS (ESI) calcd for $C_{11}H_{13}N_2O[M+H]^+$ 189.1022, found 189.1019.

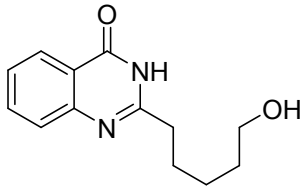
2-pentylquinazolin-4(3H)-one (3t)[6]



White solid, Yield: 42%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.16 (s, 1H), 8.08 (dd, J = 7.9, 1.5 Hz, 1H), 7.78-7.74 (m, 1H), 7.59 (d, J = 8.0, 1H), 7.49 – 7.38 (m, 1H), 2.59 (t, J = 7.5, 2H), 1.76 - 1.68 (m, 2H), 1.33 - 1.26 (m, 4H), 0.86 (t, J = 6.8, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.9 , 157.6 , 149.0 , 134.3 , 126.9 , 125.9 , 125.7 , 120.8 , 34.5 , 30.8 , 26.6 , 21.9 , 13.9 . HRMS (ESI) calcd for $C_{13}H_{17}N_2O[M+H]^+$ 217.1335, found 217.1331.

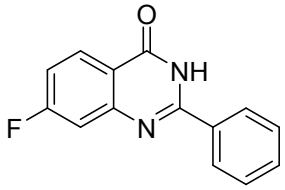
2-(5-hydroxypentyl)quinazolin-4(3H)-one (3u)



White solid, Yield: 48%, mp 152-153 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.16 (s, 1H), 8.08 (d, J = 7.9 Hz, 1H), 7.77 (t, J = 7.7 Hz, 1H), 7.59 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 4.35 (t, J = 5.2 Hz, 1H), 3.41 - 3.37 (m, 2H), 2.60 (t, J = 6.0 Hz, 2H), 1.76 - 1.69 (m, 2H), 1.48 - 1.43 (m, 2H), 1.38 - 1.32 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 , 158.0 , 149.5 , 134.8 , 127.3 , 126.4 , 126.2 , 121.3 , 121.2 , 61.1 , 35.1 , 32.7 , 27.2 , 25.6 . HRMS (ESI) calcd for $C_{13}H_{17}N_2O_2[M+H]^+$ 233.1285, found 233.1292.

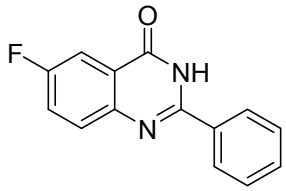
7-fluoro-2-phenylquinazolin-4(3H)-one (3bb)[7]



White solid, Yield: 87%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.64 (s, 1H), 8.26 – 8.15 (m, 3H), 7.66 – 7.47 (m, 4H), 7.38 (td, J = 8.7, 2.6 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.9 (d, J = 251.9 Hz) , 161.6 , 153.8 , 150.9 (d, J = 13.5 Hz) , 132.5 , 131.7 , 129.1 (d, J = 40.1 Hz) , 128.7 , 128.0 , 118.1, 115.3 (d, J = 23.7 Hz) , 112.7 (d, J = 21.6 Hz) .HRMS (ESI) calcd for $C_{14}H_{10}N_2OF[M+H]^+$ 241.0772, found 241.0770.

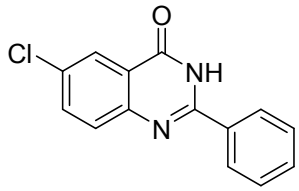
6-fluoro-2-phenylquinazolin-4(3H)-one (3bc)[8]



White solid, Yield: 85%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.17 (d, J = 7.6 Hz, 2H), 7.82 (dd, J = 8.7, 5.2 Hz, 2H), 7.75 - 7.71 (m, 1H), 7.60 - 7.56 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.7 , 160.0 (d, J = 245.9 Hz) , 151.9 , 145.7 , 132.6 , 131.5 , 130.3 , 128.7 , 127.8 , 123.1 (d, J = 24.2 Hz) , 122.3 (d, J = 9.8 Hz) , 110.6 (d, J = 23.4 Hz) . HRMS (ESI) calcd for $C_{14}H_{10}N_2OF[M+H]^+$ 241.0772, found 241.0780.

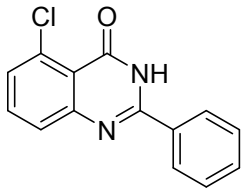
6-chloro-2-phenylquinazolin-4(3H)-one (3bd)[8]



White solid, Yield: 84%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.72 (s, 1H), 8.18 (d, J = 7.2 Hz, 2H), 8.09 (d, J = 2.5 Hz, 1H), 7.86 (dd, J = 8.7, 2.6 Hz, 1H), 7.76 (d, J = 8.7 Hz, 1H), 7.63 – 7.54 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.2 , 152.7 , 147.4 , 134.6 , 132.3 , 131.5 , 130.7 , 129.6 , 128.5 , 127.7 , 124.8 , 122.1 . HRMS (ESI) calcd for $C_{14}H_{10}N_2OCl$ $[M+H]^+$ 257.0476, found 257.0476.

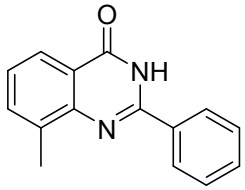
5-chloro-2-phenylquinazolin-4(3H)-one (3be)[7]



White solid, Yield: 85%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.18 (d, J = 7.5 Hz, 2H), 7.75 (t, J = 7.8 Hz, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.77 - 7.51 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.4 , 153.0 , 151.3 , 134.4 , 132.6 , 132.2 , 131.7 , 128.9 , 128.7 , 127.9 , 127.2 , 118.0 . HRMS (ESI) calcd for $C_{14}H_{10}N_2OCl[M+H]^+$ 257.0476, found 257.0477.

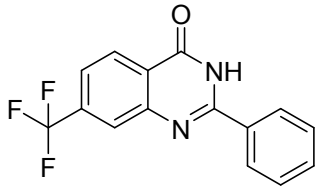
8-methyl-2-phenylquinazolin-4(3H)-one (3bf)[2]



White solid, Yield: 86%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.53 (s, 1H), 8.24 (d, J = 6.8 Hz, 2H), 8.01 (d, J = 7.9 Hz, 1H), 7.70 (d, J = 7.3 Hz, 1H), 7.60 - 7.55 (m, 3H), 7.40 (t, J = 7.6 Hz, 1H), 2.63 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.6 , 151.1 , 147.2 , 135.7 , 135.1 , 133.0 , 131.4 , 128.7 , 127.8 , 126.1 , 123.6 , 121.0 , 17.3 . HRMS (ESI) calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1022, found 237.1023.

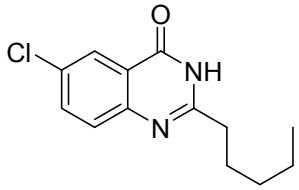
2-phenyl-7-(trifluoromethyl)quinazolin-4(3H)-one (3bg)[9]



White solid, Yield: 87%.

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.83 (s, 1H), 8.35 (d, J = 8.3 Hz, 1H), 8.21 (d, J = 7.4 Hz, 2H), 8.05 (s, 1H), 7.81 (d, J = 8.3 Hz, 1H), 7.60 (dt, J = 26.2, 7.4 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.6 , 154.0 ,148.9 , 134.3 (q, J = 31.9 Hz) , 132.4 , 131.9 , 128.7 , 128.1 , 127.8 , 125.0, 124.7 (q, J = 3.4 Hz) , 123.9 , 123.5 (q, J = 240.4 Hz) , 122.3 (q, J = 3.1 Hz). HRMS (ESI) calcd for $C_{15}H_{10}N_2OF_3$ $[M+H]^+$ 291.0740, found 291.0732.

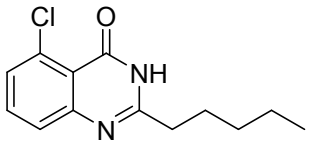
6-chloro-2-pentylquinazolin-4(3H)-one (3bh)[6]



White solid, Yield: 46%.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.35 (s, 1H), 8.01 (d, J = 2.5 Hz, 1H), 7.79 (dd, J = 8.7, 2.5 Hz, 1H), 7.62 (d, J = 8.7 Hz, 1H), 2.59 (t, J = 7.8 Hz, 2H), 1.72 (p, J = 7.3 Hz, 2H), 1.39 – 1.24 (m, 4H), 0.87 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.9 , 158.2 , 147.7 , 134.4 , 130.2 , 129.1 , 124.7 , 122.1 , 34.5 , 30.8 , 26.5 , 21.9 , 13.9 . HRMS (ESI) calcd for $C_{13}H_{16}N_2OCl$ $[M+H]^+$ 251.0946, found 251.0944.

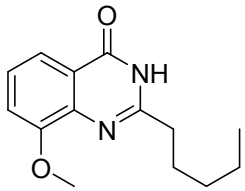
5-chloro-2-pentylquinazolin-4(3H)-one (3bi)



White solid, Yield: 53%, mp 177-178 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.21 (s, 1H), 7.67 (t, J = 8.0 Hz, 1H), 7.53 (dd, J = 8.3, 1.2 Hz, 1H), 7.45 (dd, J = 7.8, 1.2 Hz, 1H), 2.56 (t, J = 8.0 H, 2H), 1.79 – 1.62 (m, 2H), 1.39 – 1.23 (m, 4H), 0.96 – 0.79 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.0 , 158.5 , 151.6 , 134.1 , 132.4 , 128.3 , 126.5 , 117.8 , 34.2 , 30.8 , 26.4 , 21.9 , 13.9 . HRMS (ESI) calcd for $C_{13}H_{16}N_2OCl$ $[M+H]^+$ 251.0946, found 251.0945.

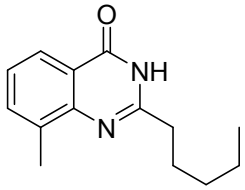
8-methoxy-2-pentylquinazolin-4(3H)-one (3bj)



White solid, Yield: 42%, mp 206-207 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.19 (s, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.37 (t, J = 7.9 Hz, 1H), 7.31 (d, J = 7.9 Hz, 1H), 3.89 (s, 3H), 2.58 (t, J = 7.6 Hz, 2H), 1.71 (p, J = 7.4 Hz, 2H), 1.31 (t, J = 7.1 Hz, 4H), 0.88 (t, J = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.8 , 156.3 , 154.3 , 139.6 , 126.1 , 121.9 , 116.8 , 114.9 , 55.9 , 34.9 , 30.9 , 27.0 , 21.9 , 13.9 . HRMS (ESI) calcd for $C_{14}H_{19}N_2O_2$ $[M+H]^+$ 247.1441, found 247.1441.

8-methyl-2-pentylquinazolin-4(3H)-one (3bk)



White solid, Yield: 54%, mp 139-140 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.14 (s, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.62 (d, J = 7.2 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 2.61 (t, J = 7.6 Hz, 2H), 2.51 (s, 3H), 1.75 (p, J = 7.2 Hz, 2H), 1.36 - 1.30 (m, 4H), 0.88 (t, J = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.2 , 156.3 , 147.4 , 134.9 , 134.6 , 125.4 , 123.4 , 120.7 , 34.6 , 30.8 , 26.4 , 21.9 , 17.2 , 13.9 . HRMS (ESI) calcd for $C_{14}H_{19}N_2O$ $[M+H]^+$ 231.1492, found 231.1492.

4. References

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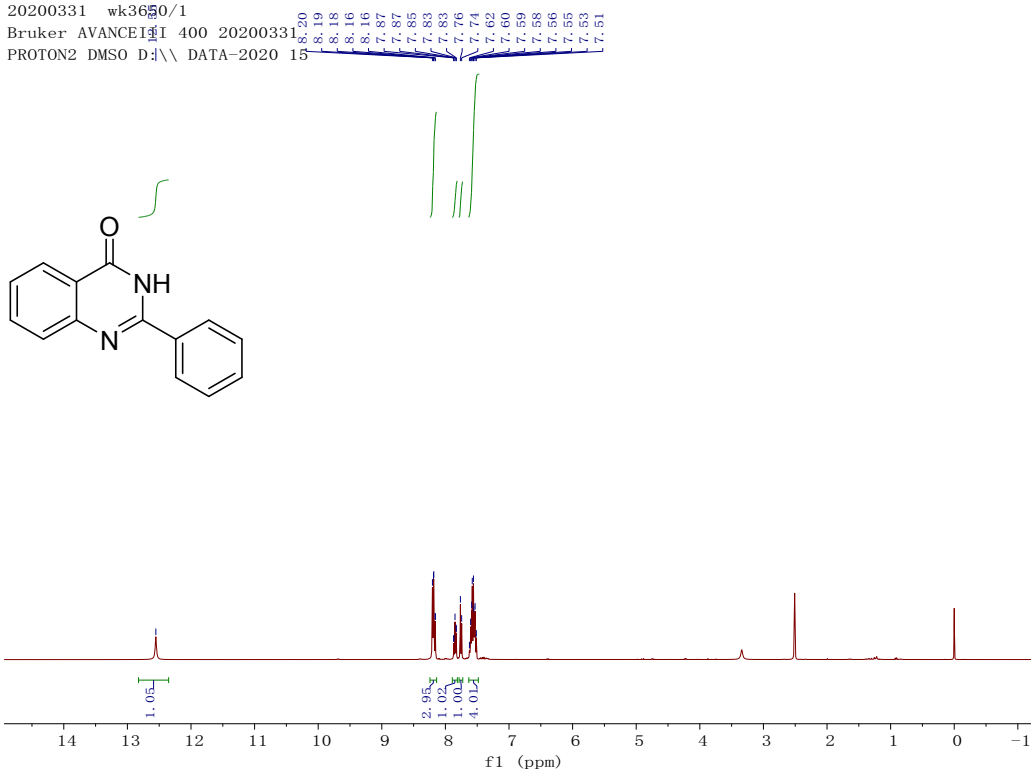
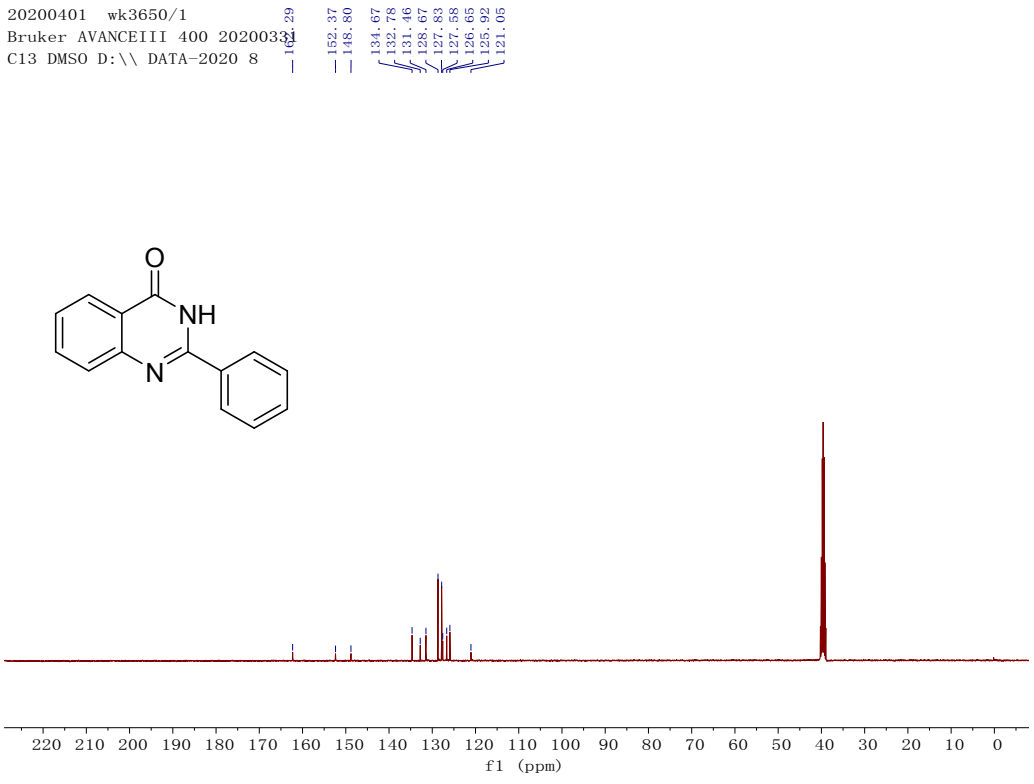
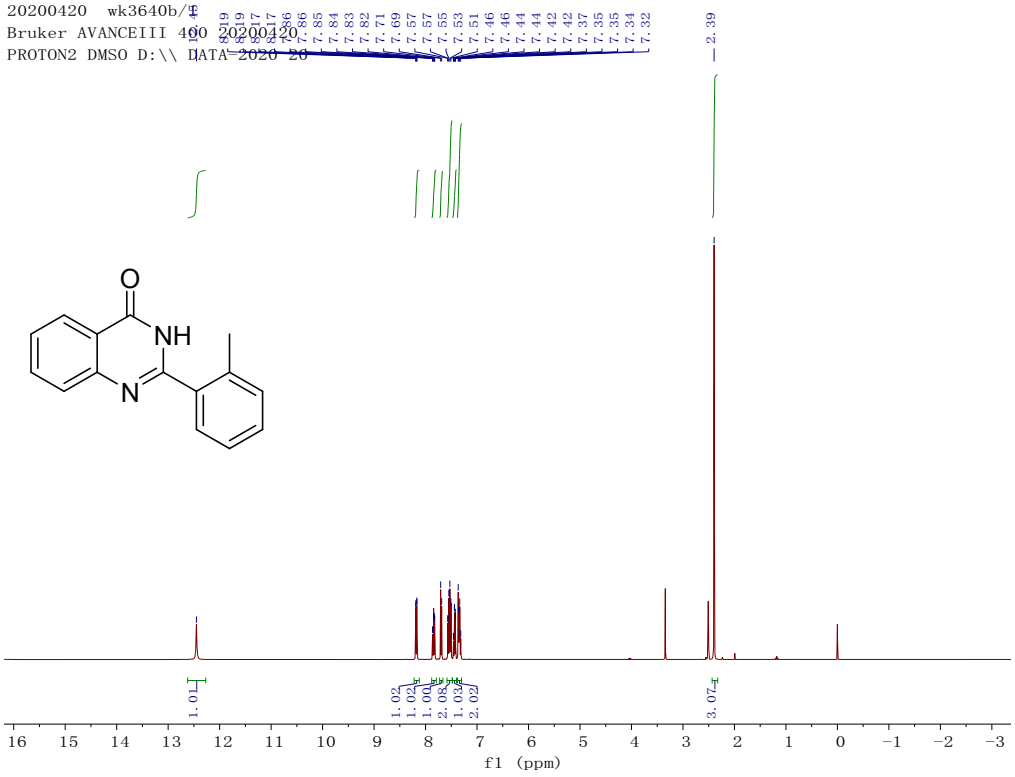
5. ^{1}H NMR and ^{13}C NMR Spectra of the Target Compounds



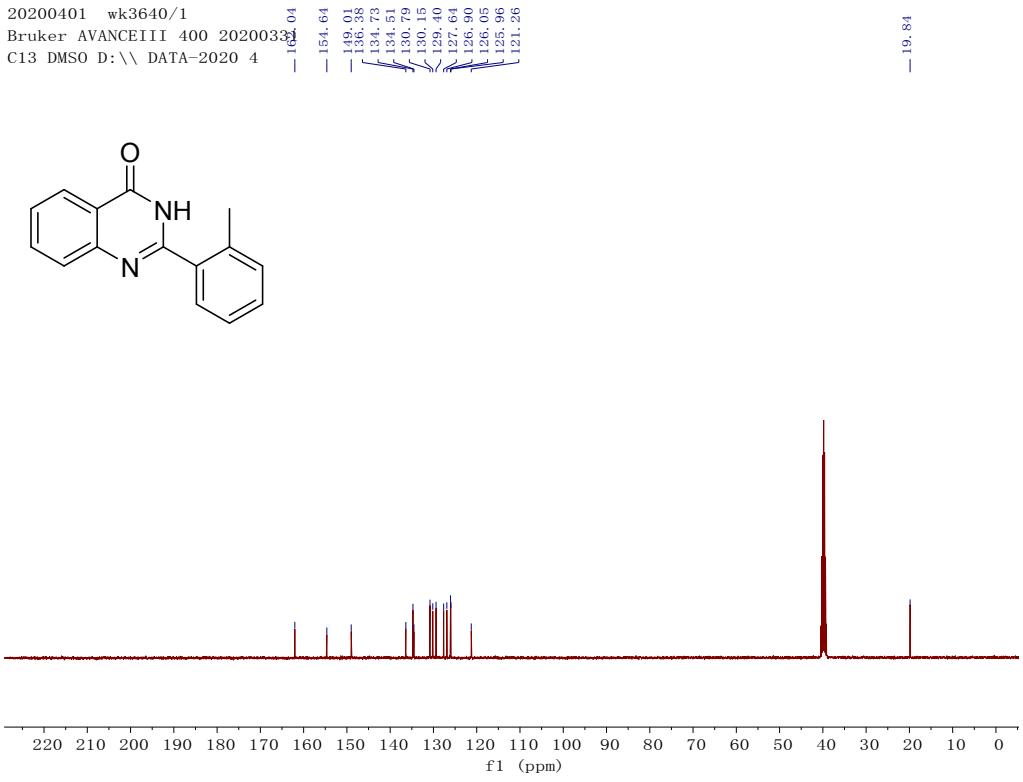
^{1}H NMR spectrum of 3a



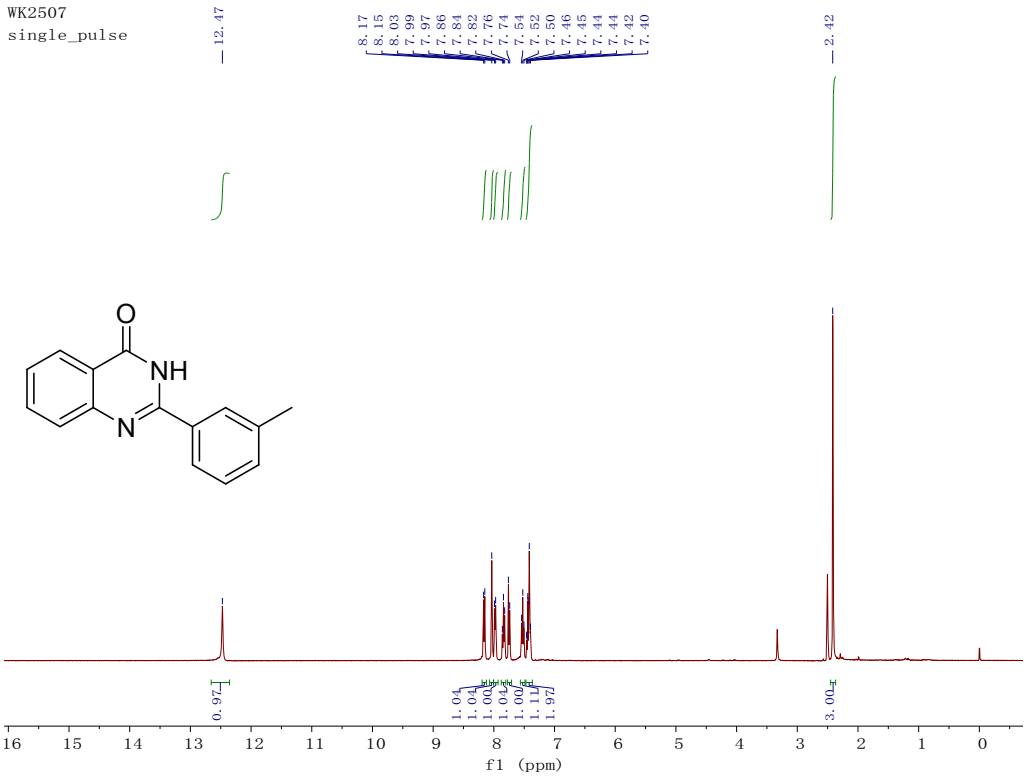
^{13}C NMR spectrum of 3a



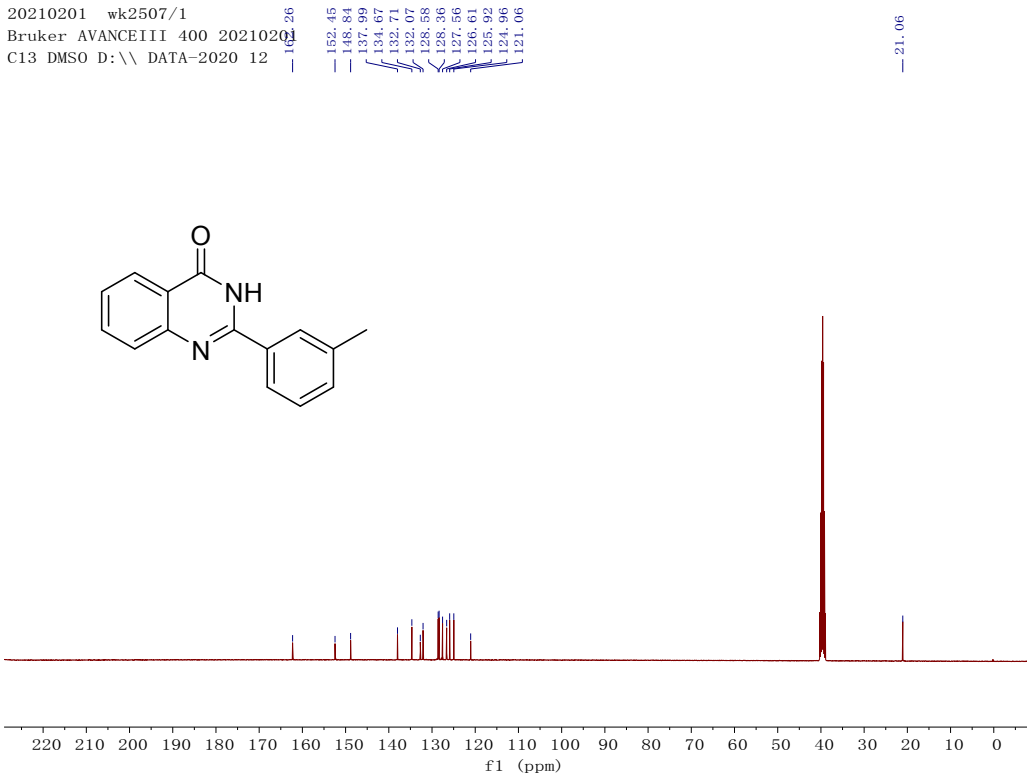
^{1}H NMR spectrum of 3b



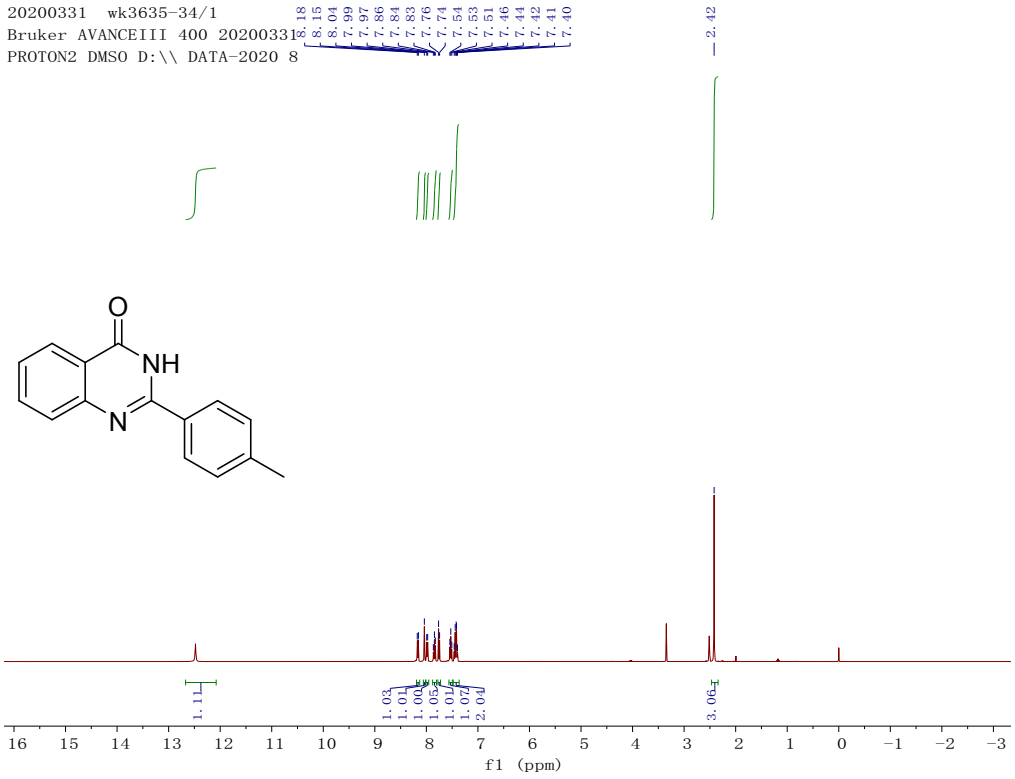
^{13}C NMR spectrum of 3b



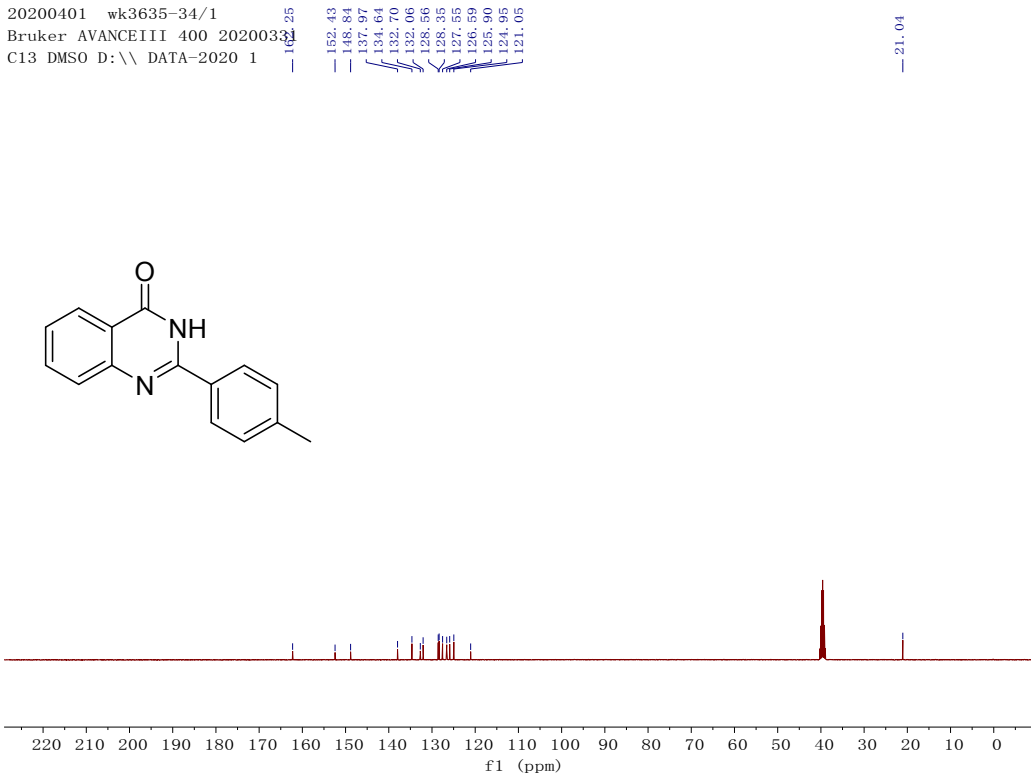
^{1}H NMR spectrum of 3c



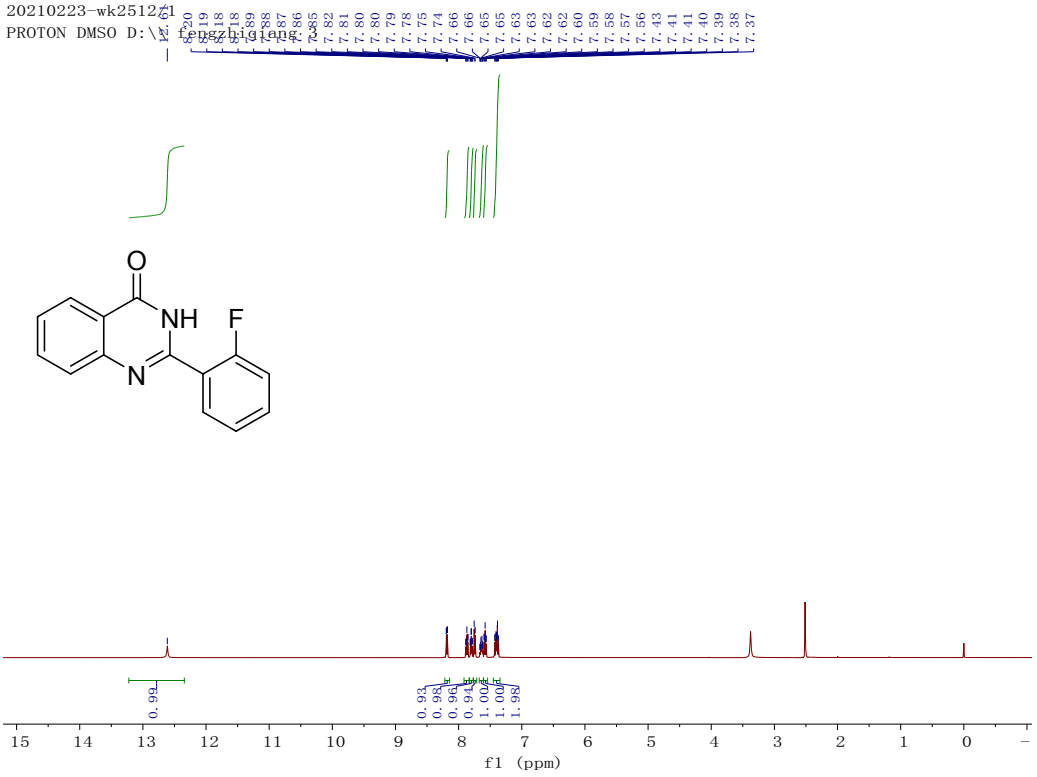
^{13}C NMR spectrum of 3c



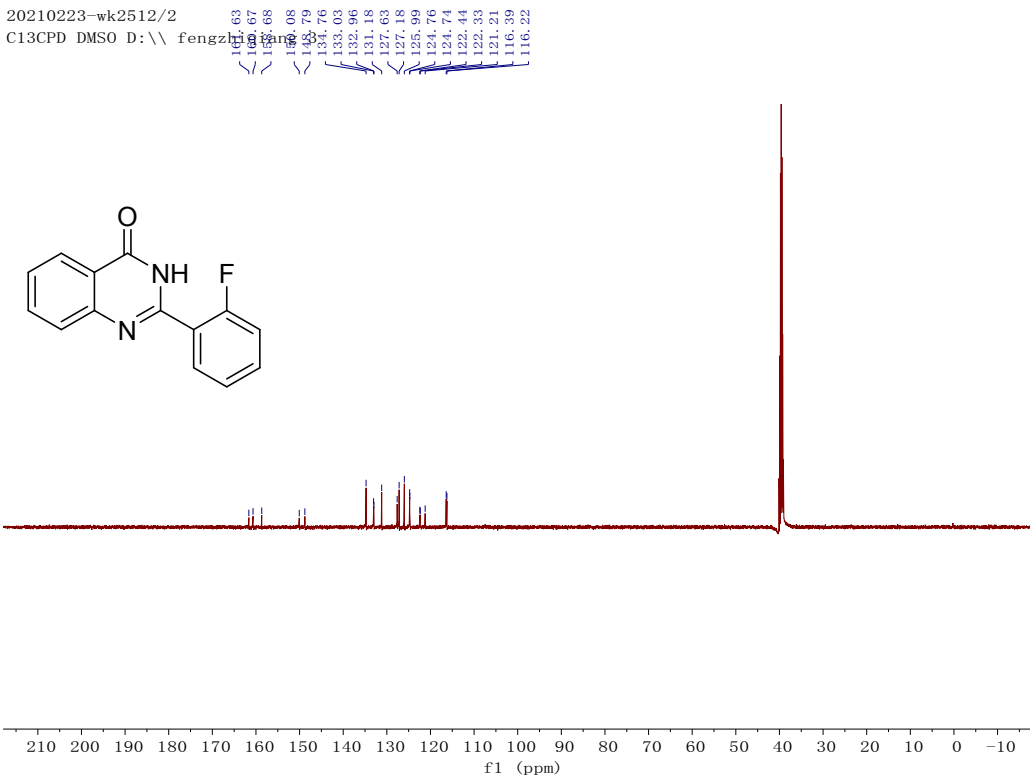
^{1}H NMR spectrum of 3d



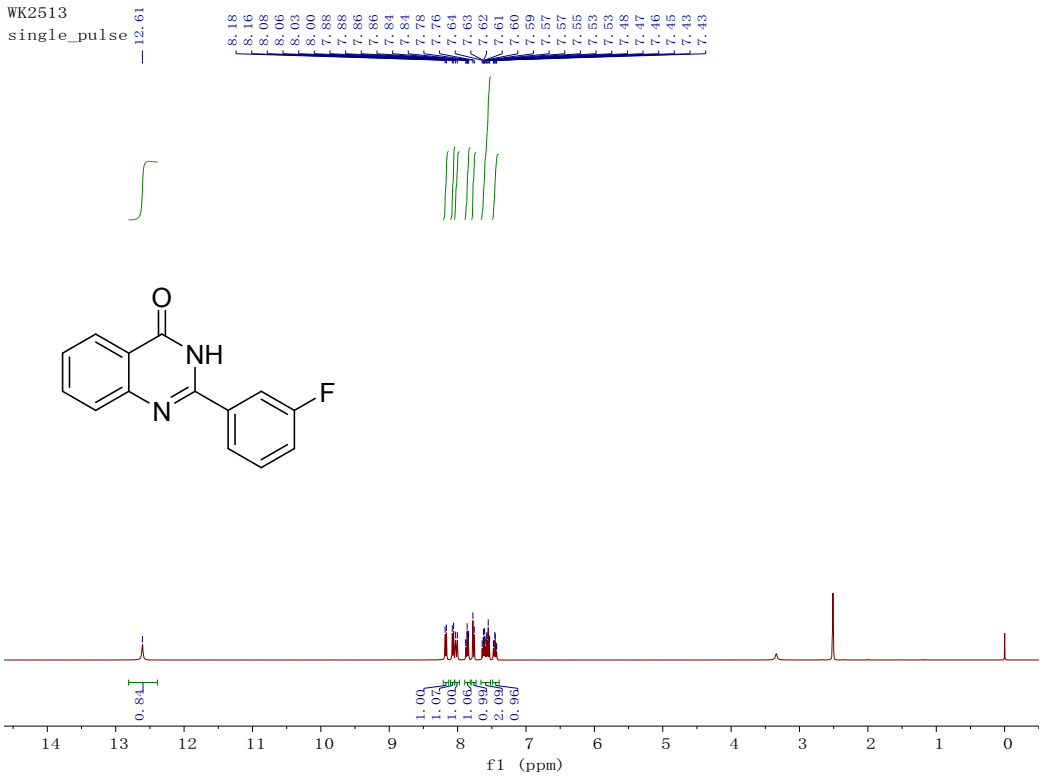
^{13}C NMR spectrum of 3d



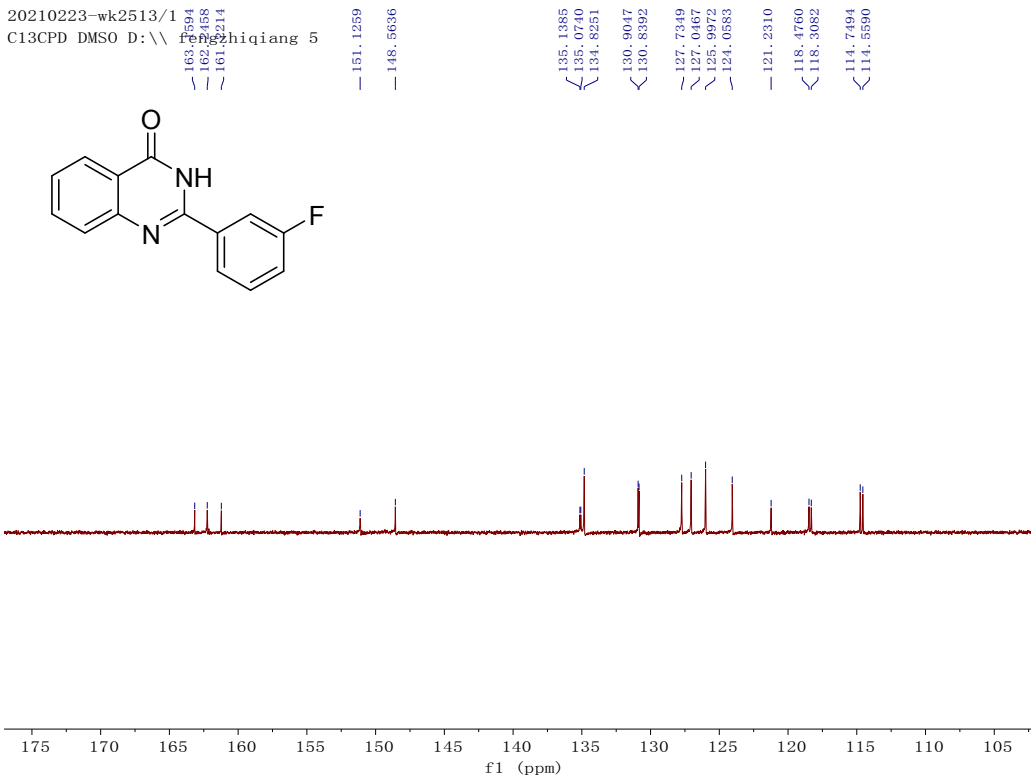
^{1}H NMR spectrum of 3e



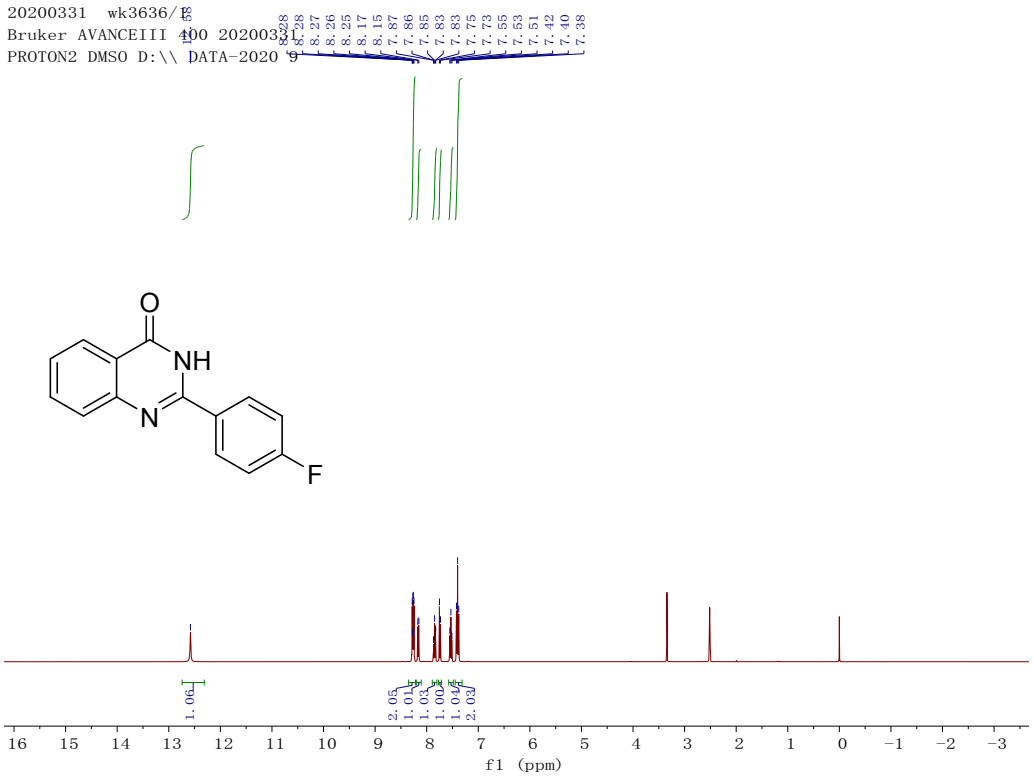
^{13}C NMR spectrum of 3e



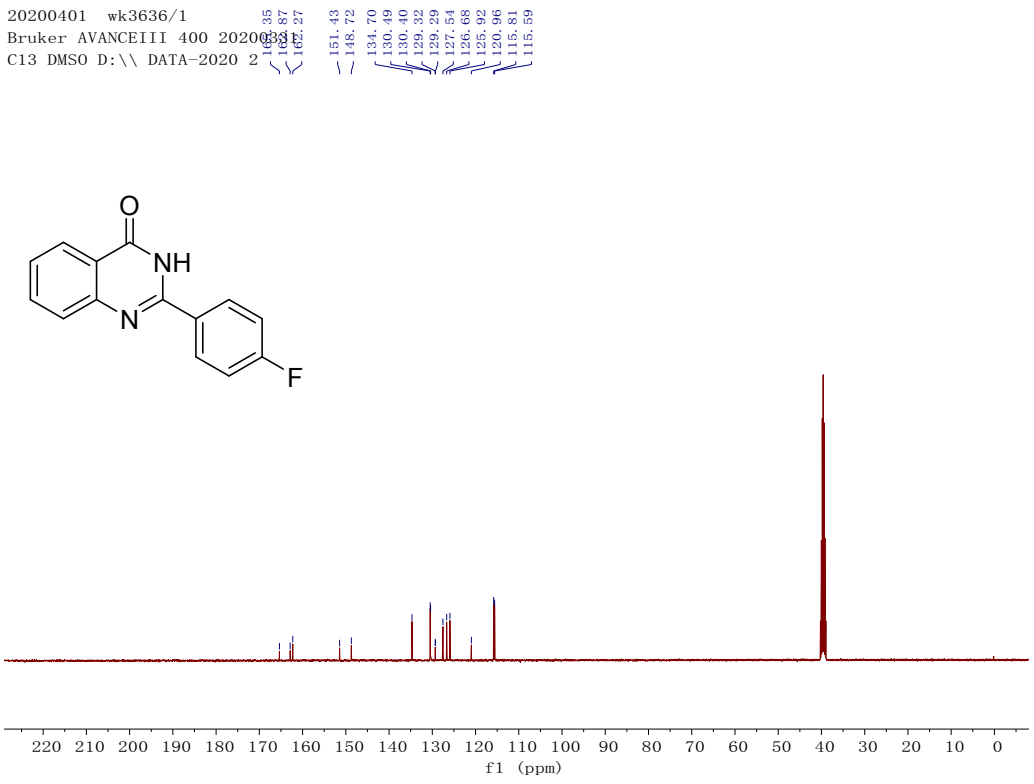
^{1}H NMR spectrum of 3f



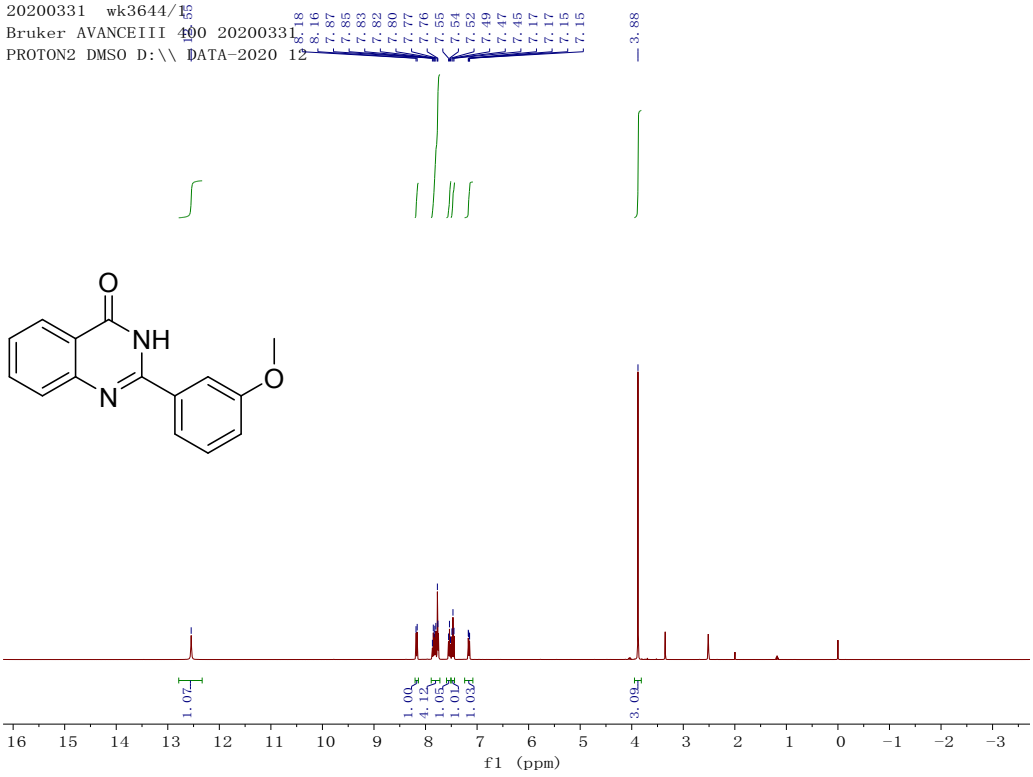
^{13}C NMR spectrum of 3f



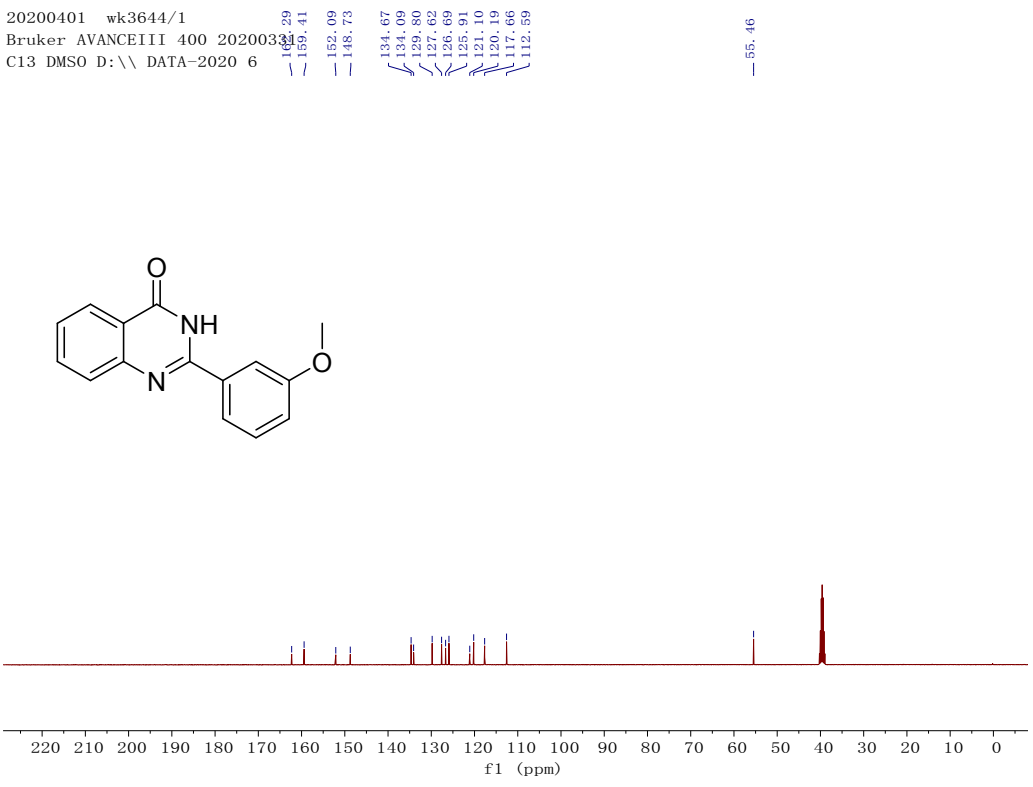
^{1}H NMR spectrum of 3g



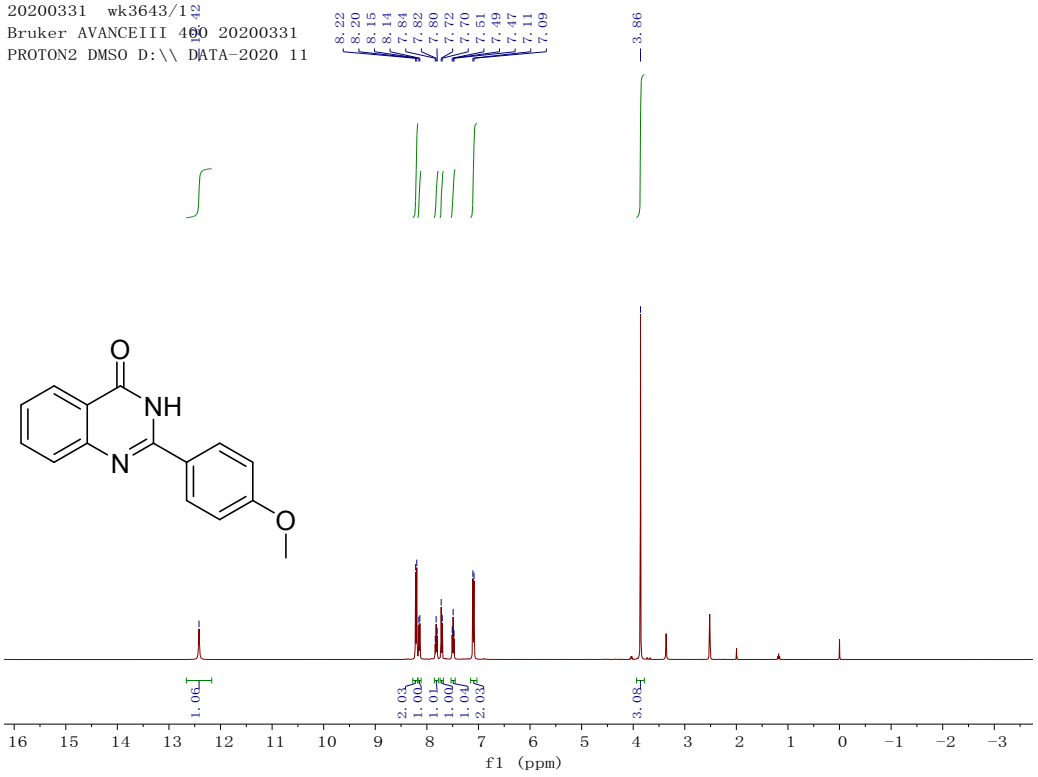
^{13}C NMR spectrum of 3g



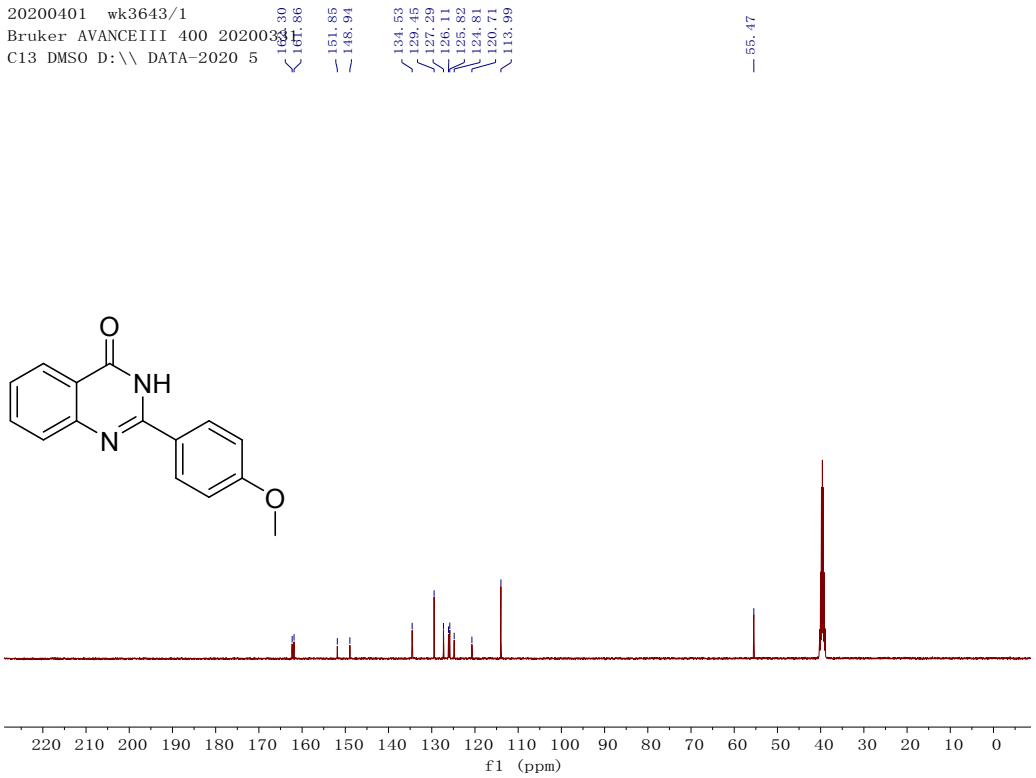
^{1}H NMR spectrum of 3h



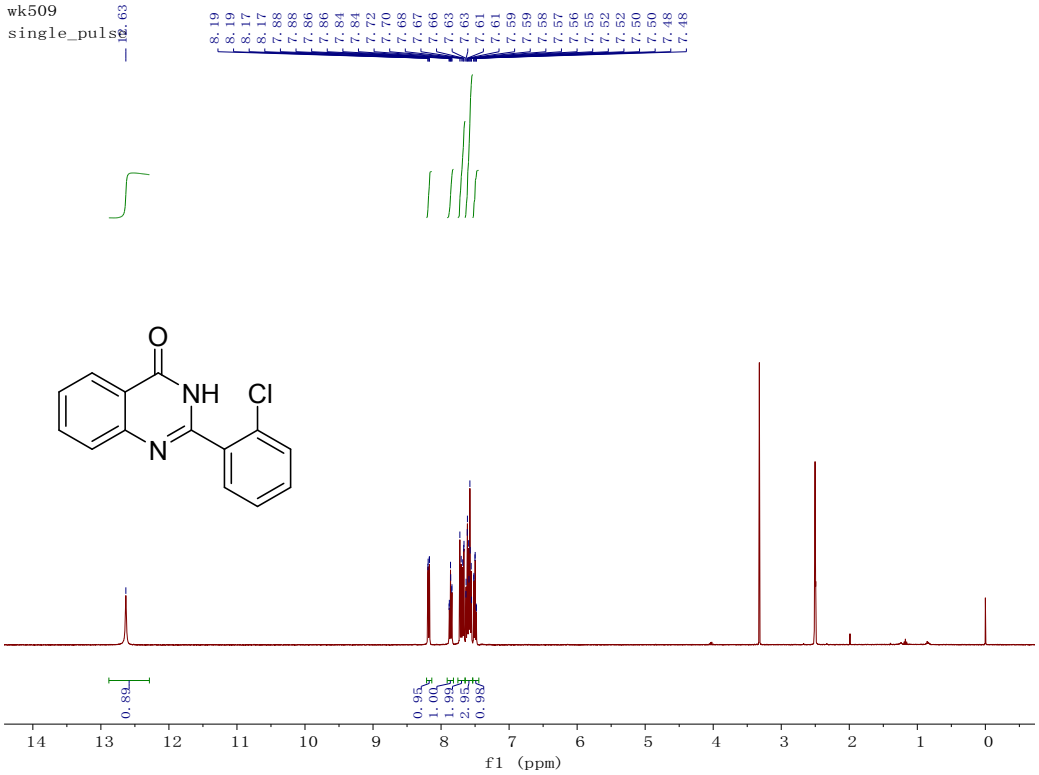
^{13}C NMR spectrum of 3h



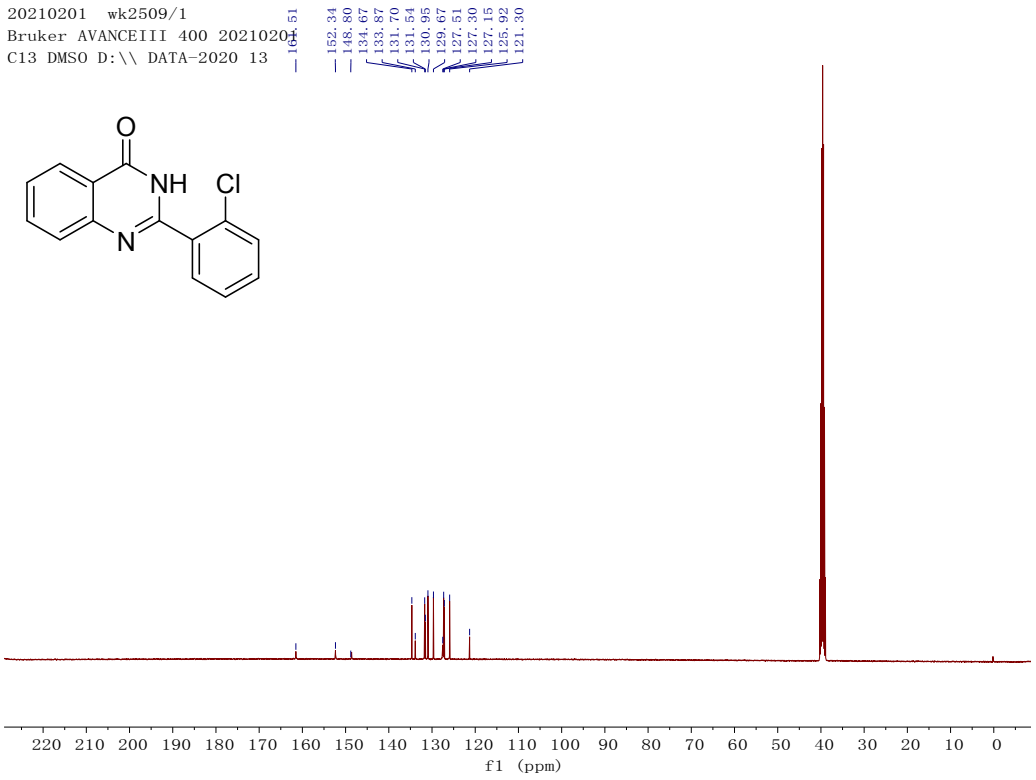
^{1}H NMR spectrum of 3i



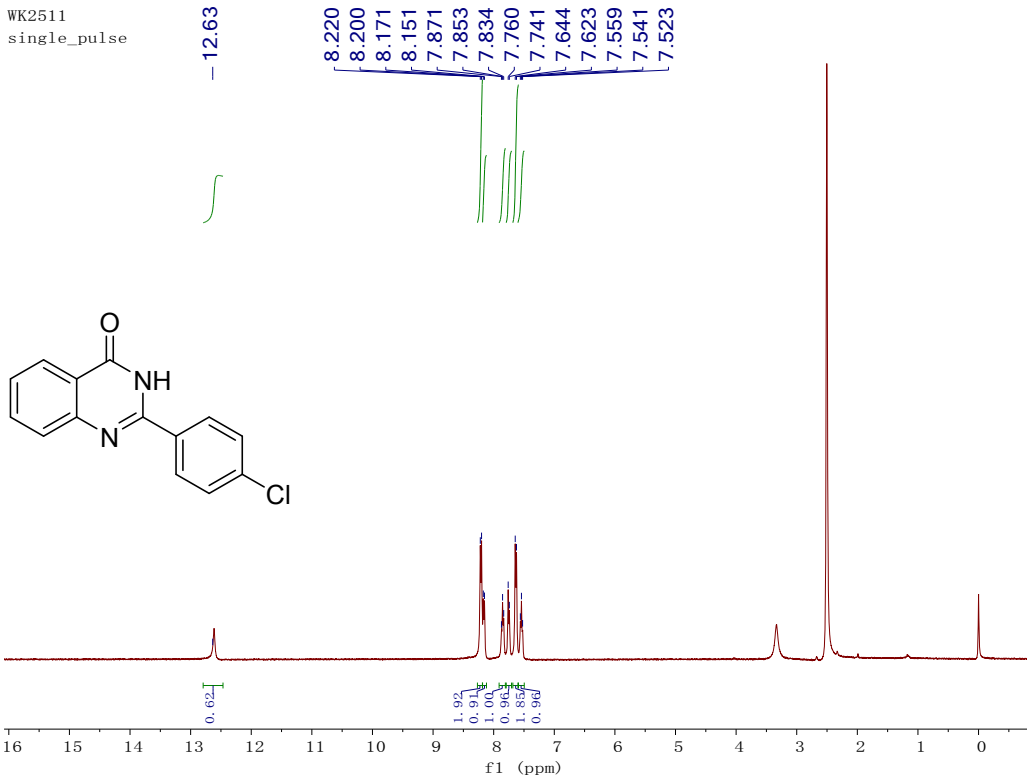
^{13}C NMR spectrum of 3i



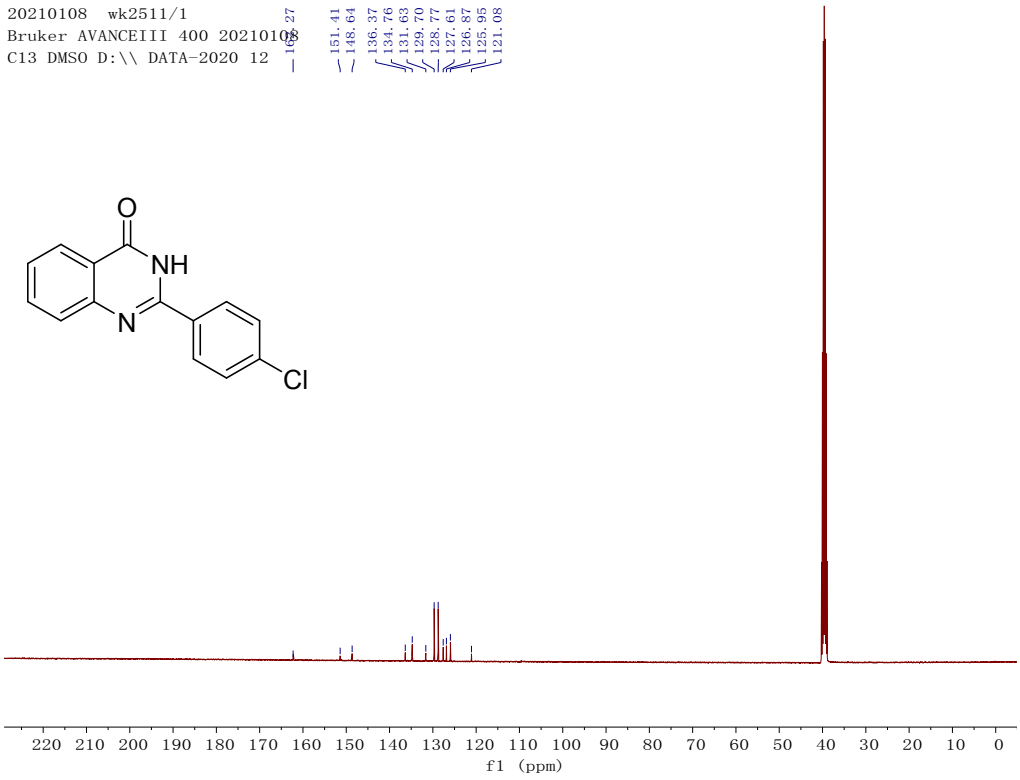
^{1}H NMR spectrum of 3j



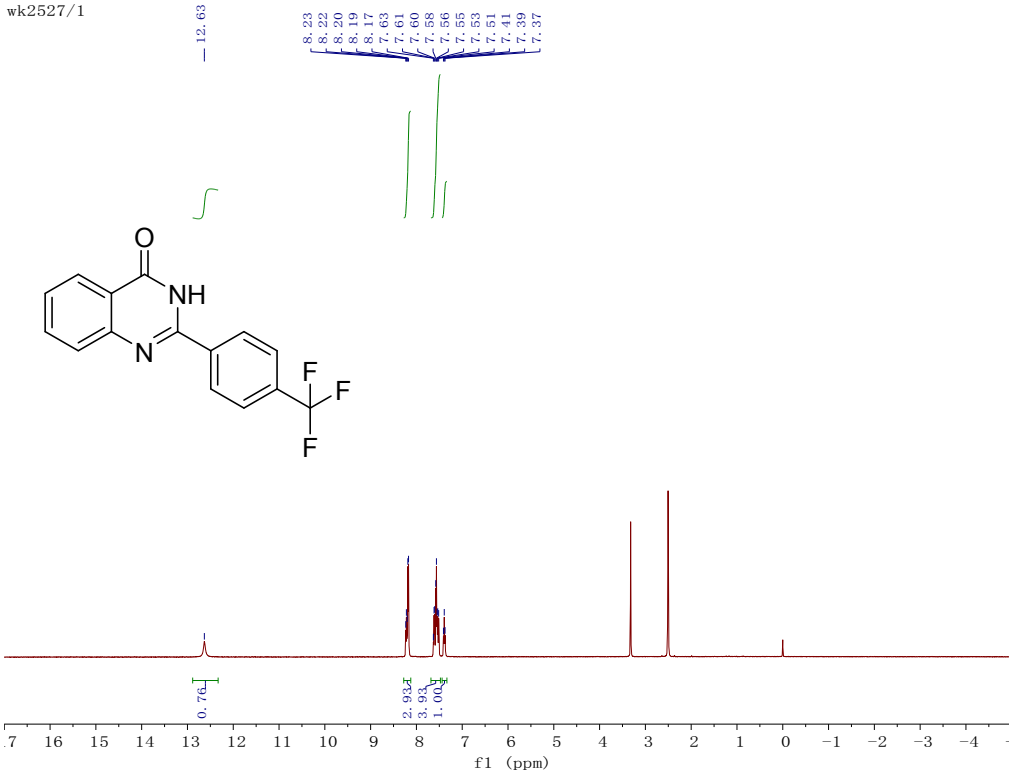
^{13}C NMR spectrum of 3j



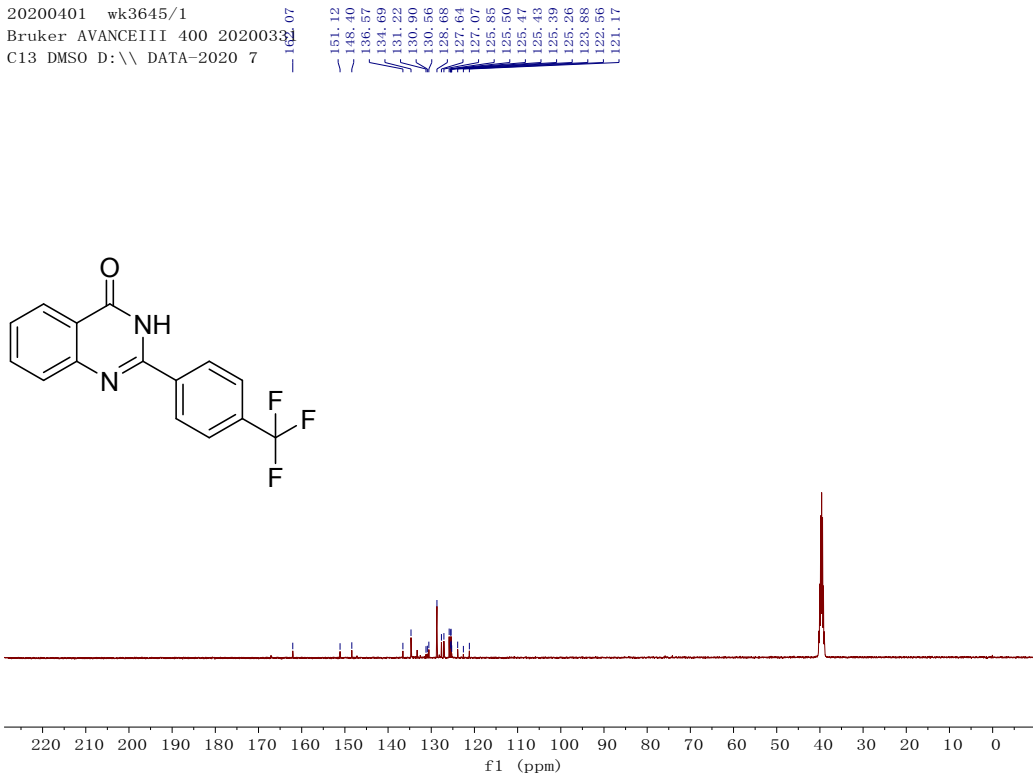
^{1}H NMR spectrum of 3k



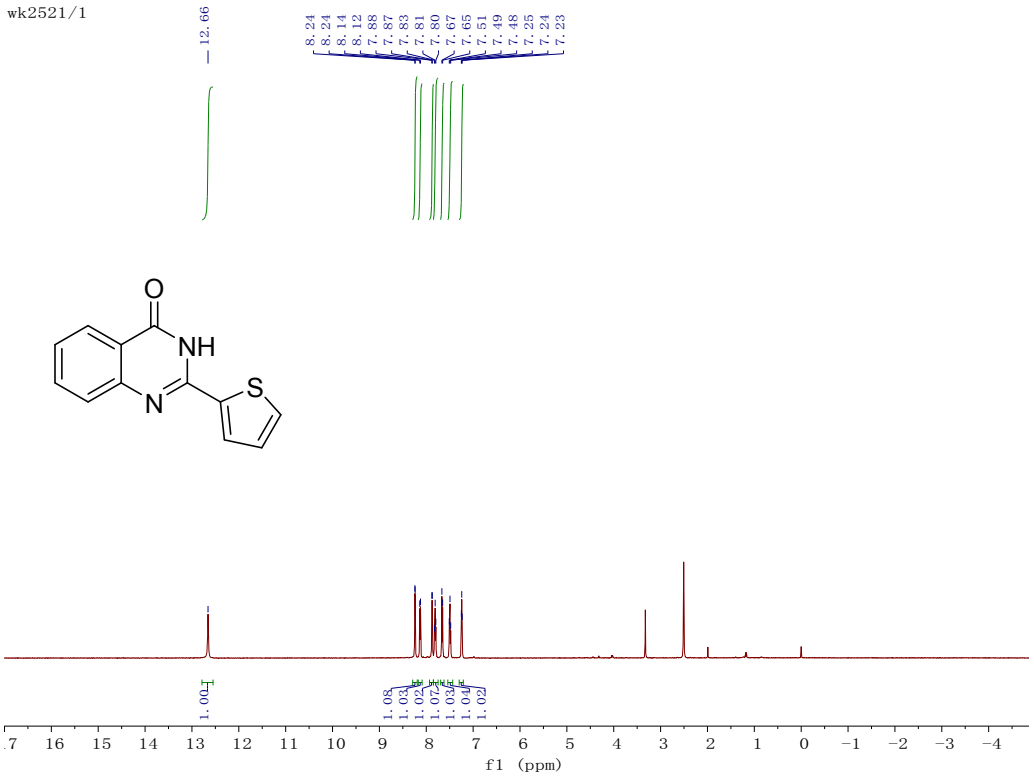
^{13}C NMR spectrum of 3k



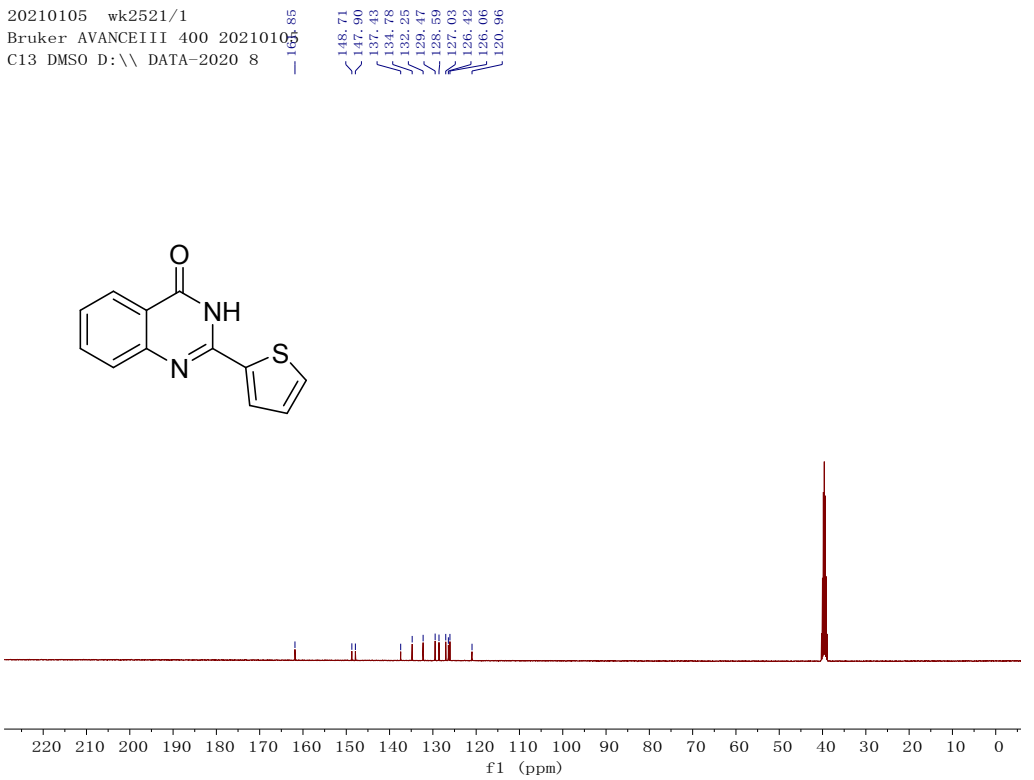
^{1}H NMR spectrum of 3l



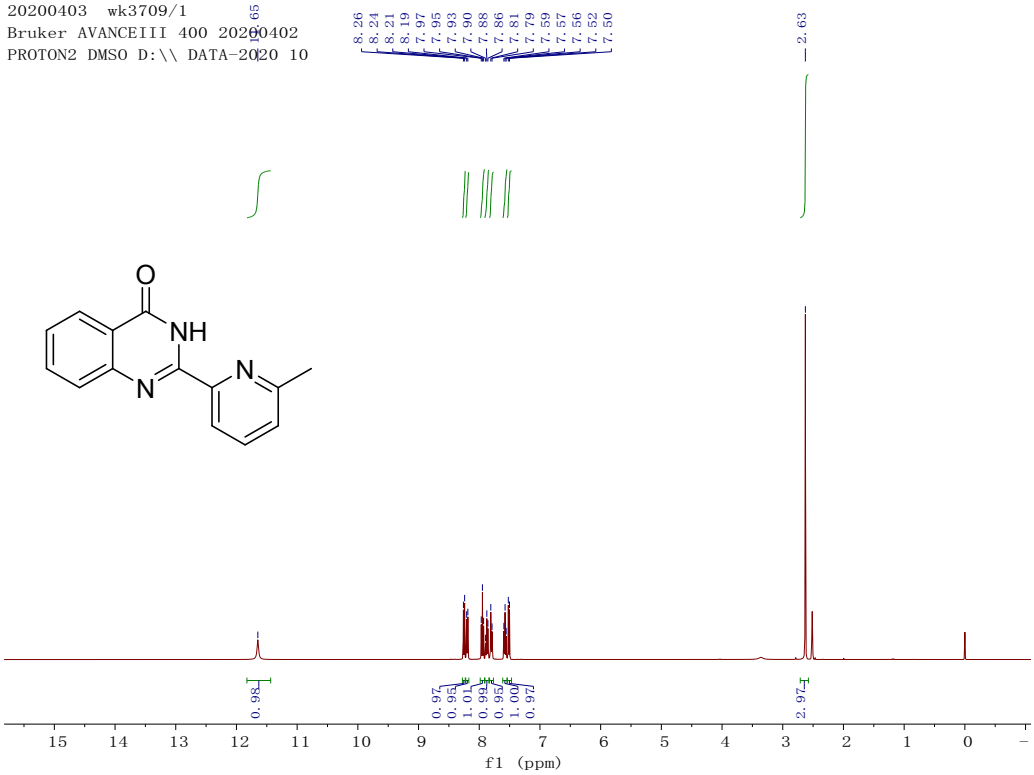
^{13}C NMR spectrum of 3l



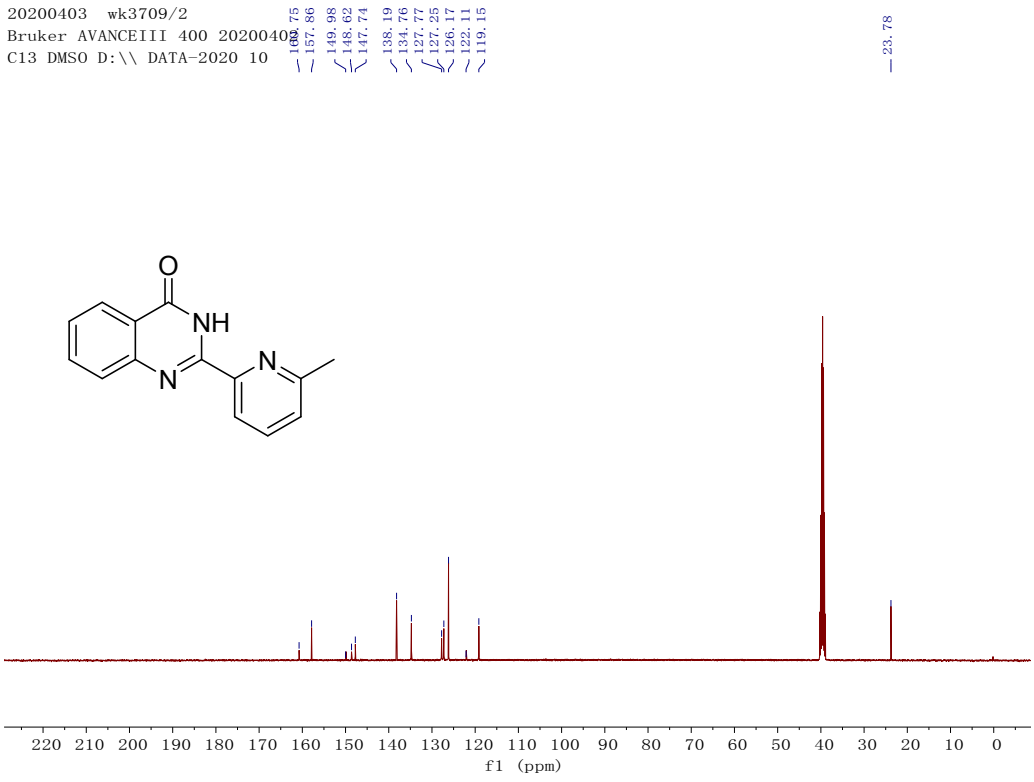
^{1}H NMR spectrum of 3m



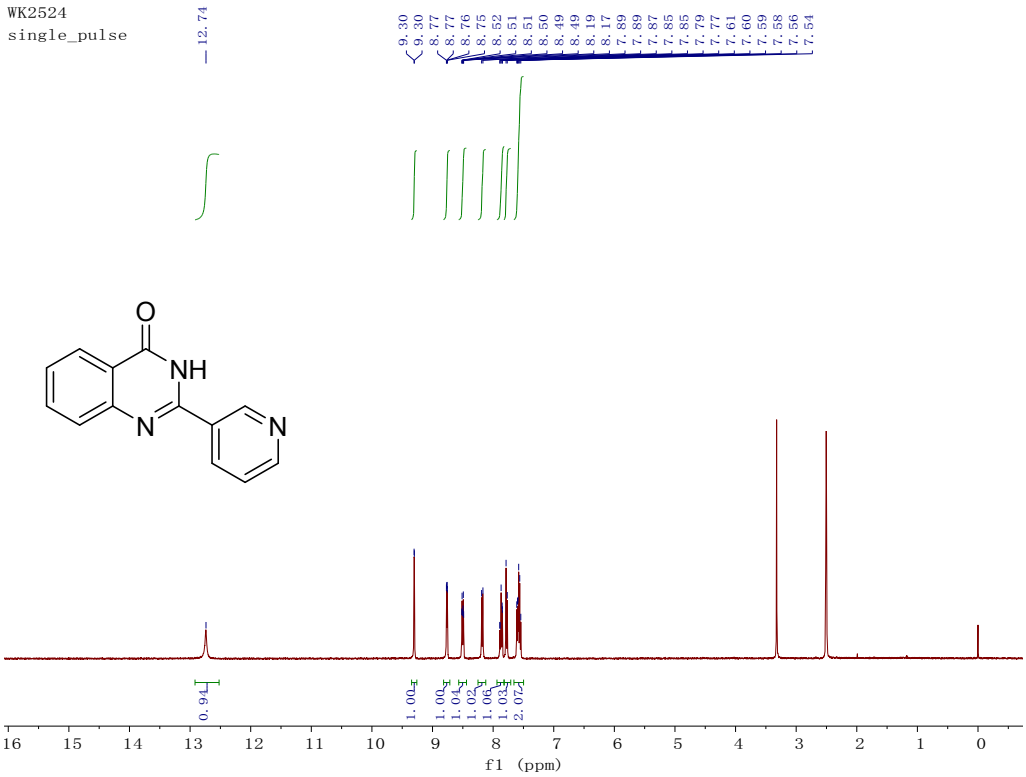
^{13}C NMR spectrum of 3m



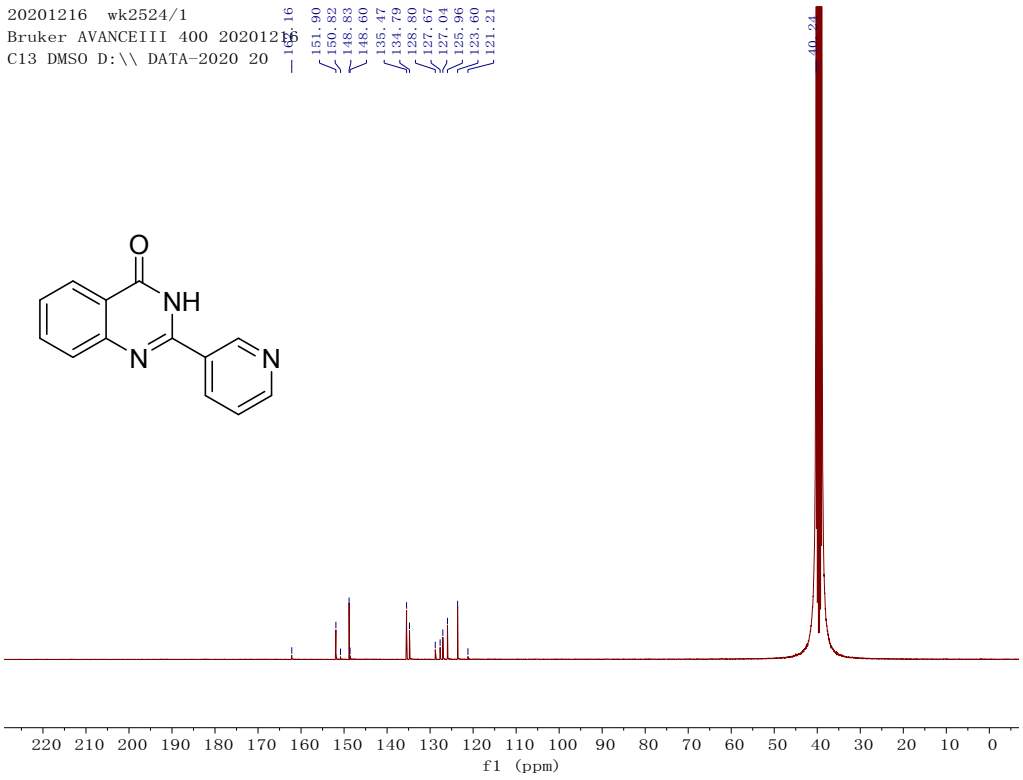
^{1}H NMR spectrum of 3n



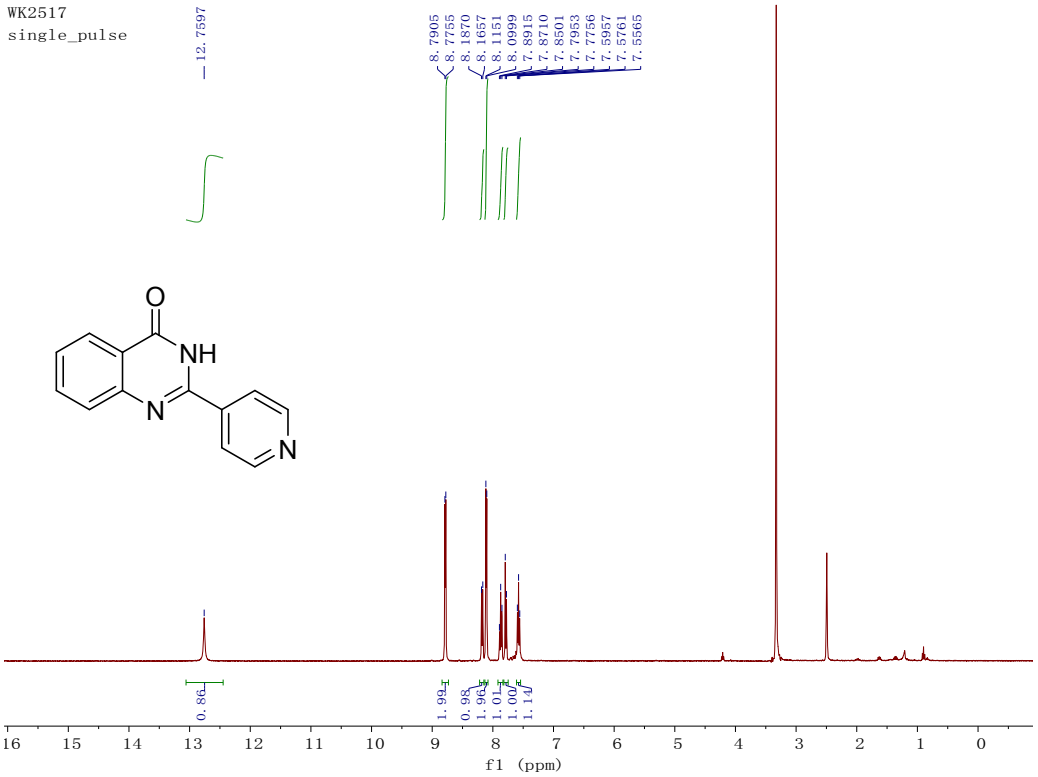
^{13}C NMR spectrum of 3n



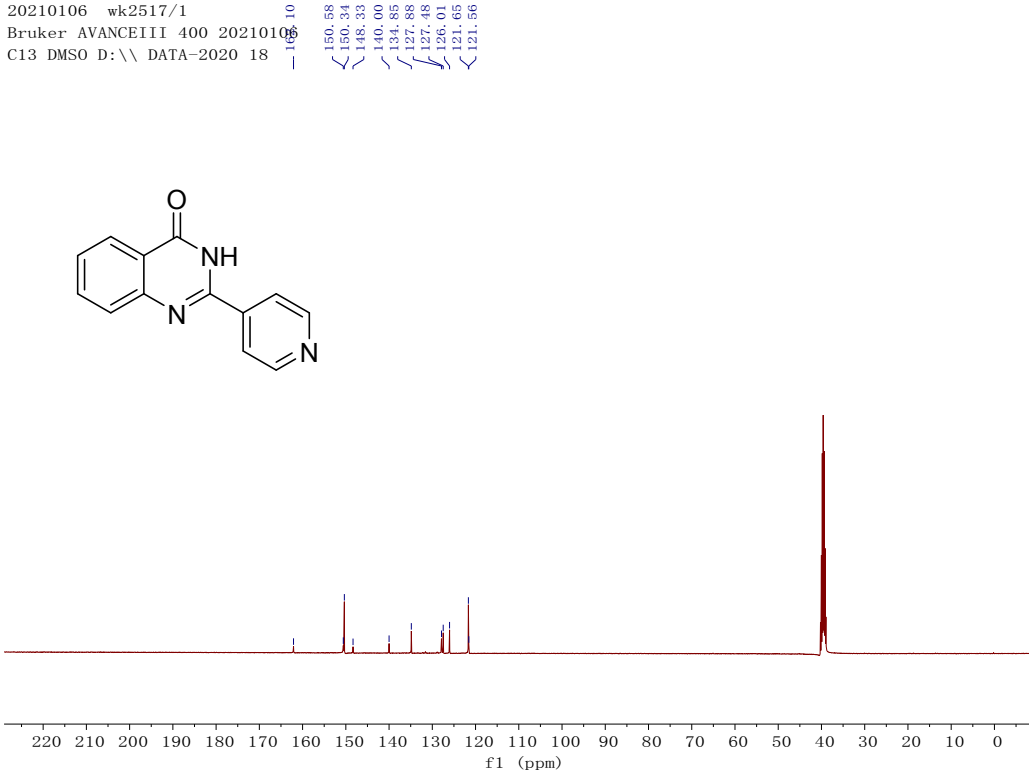
^{1}H NMR spectrum of 3o



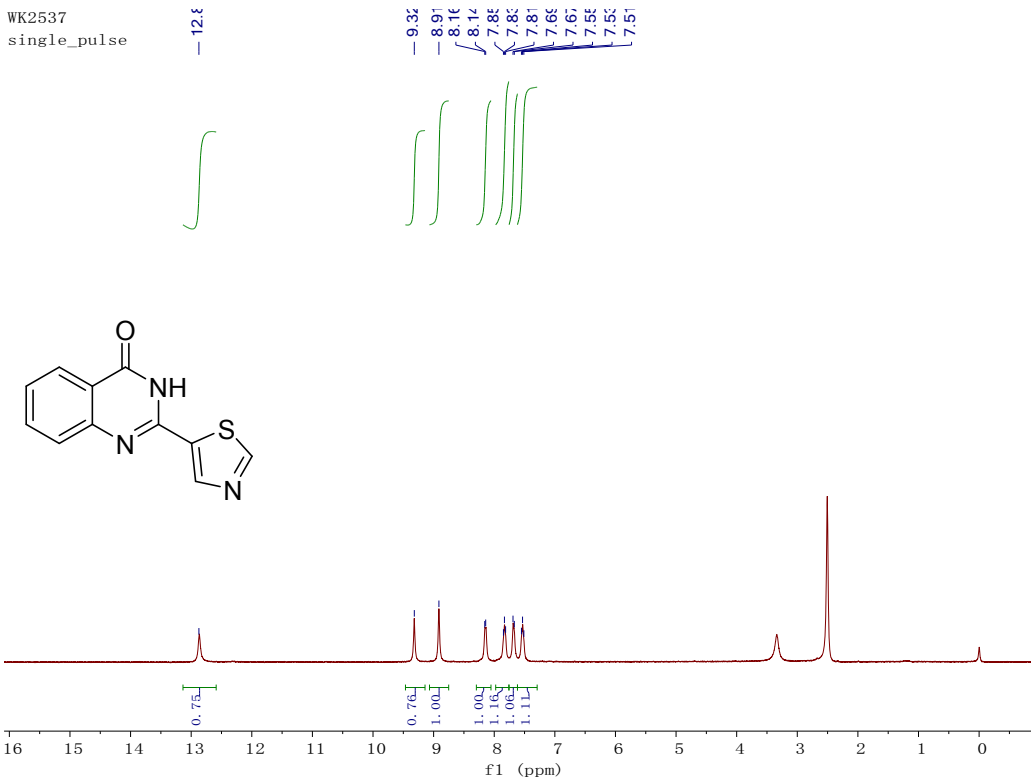
^{13}C NMR spectrum of 3o



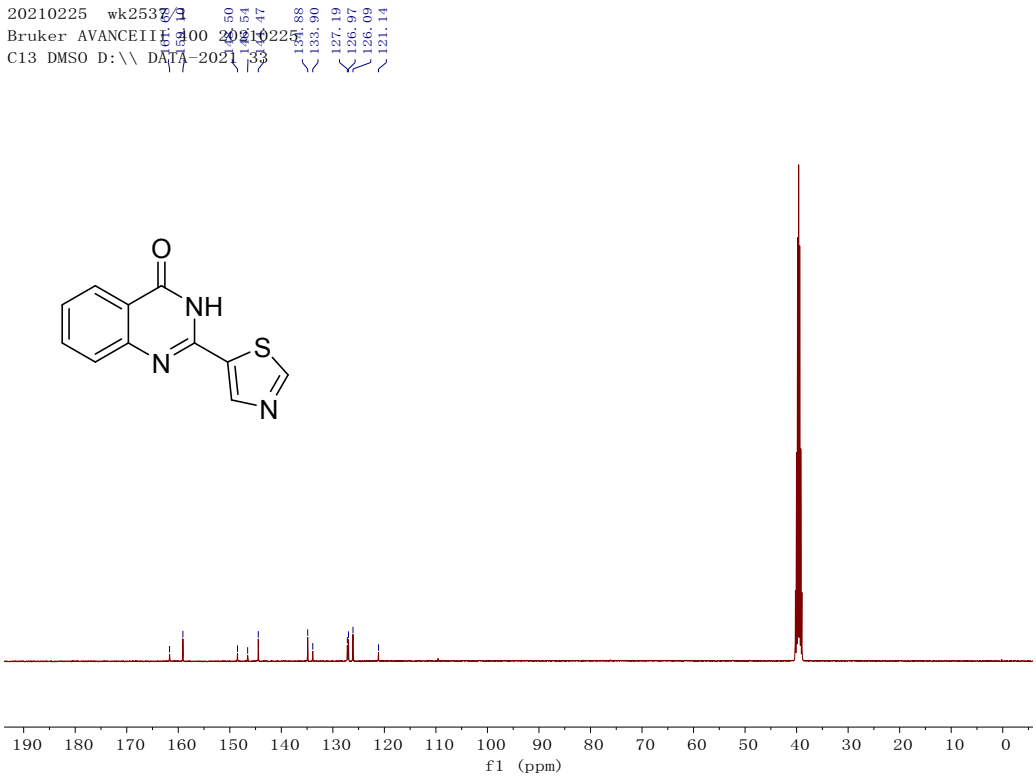
^{1}H NMR spectrum of 3p



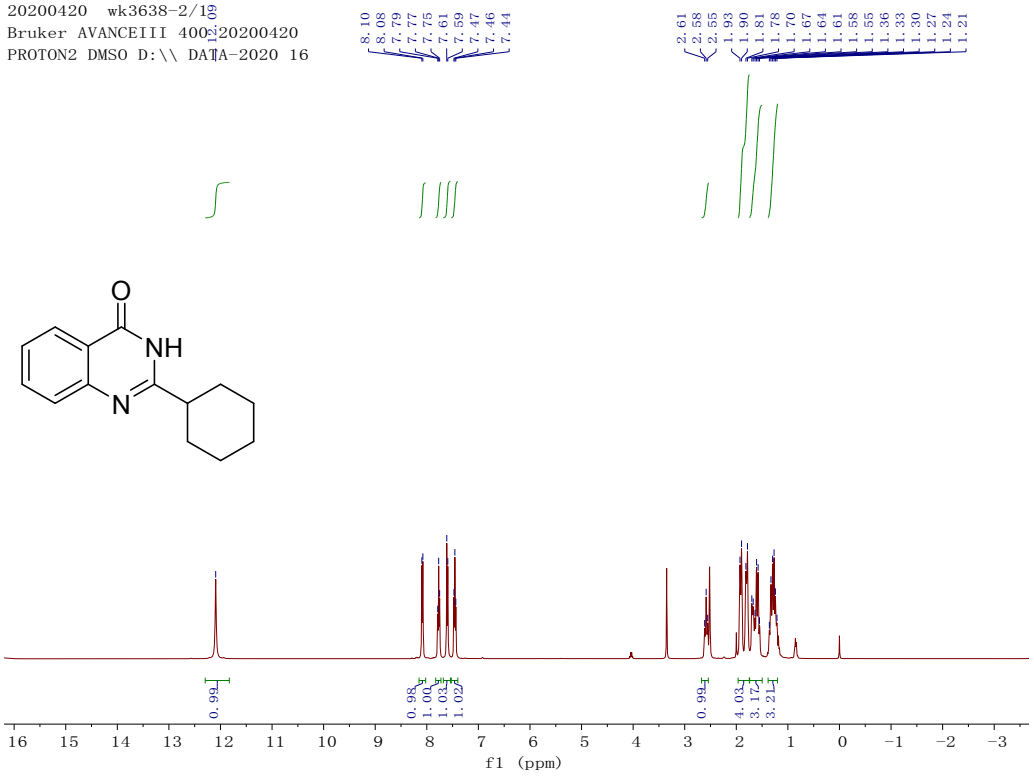
^{13}C NMR spectrum of 3p



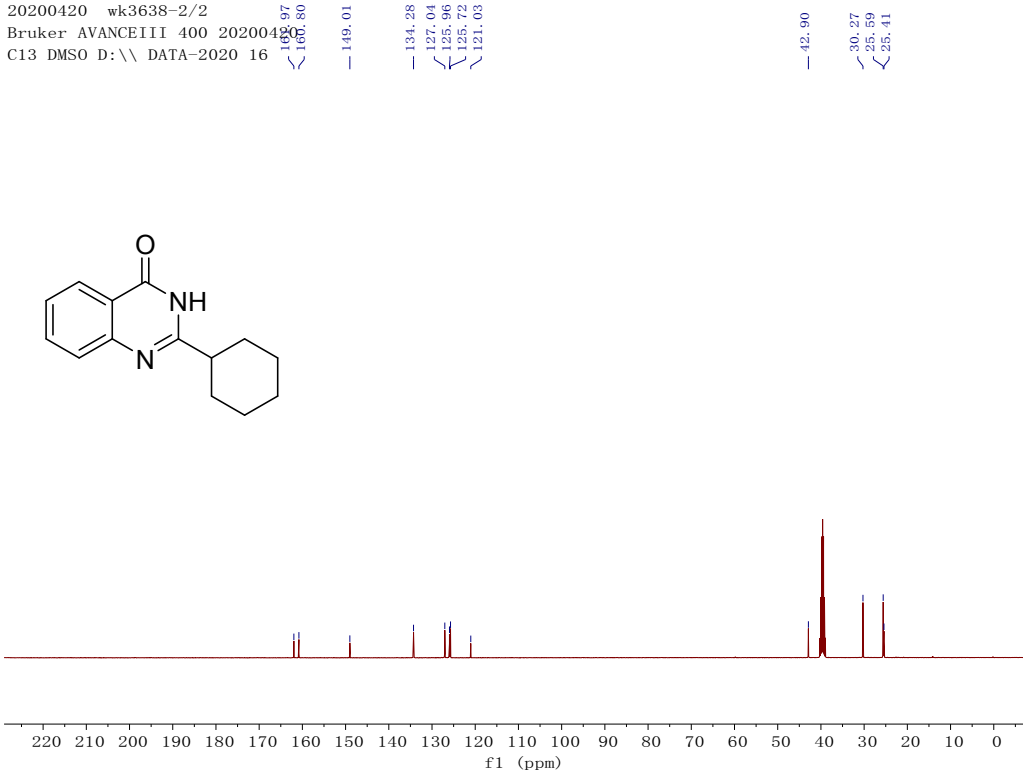
^{1}H NMR spectrum of 3q



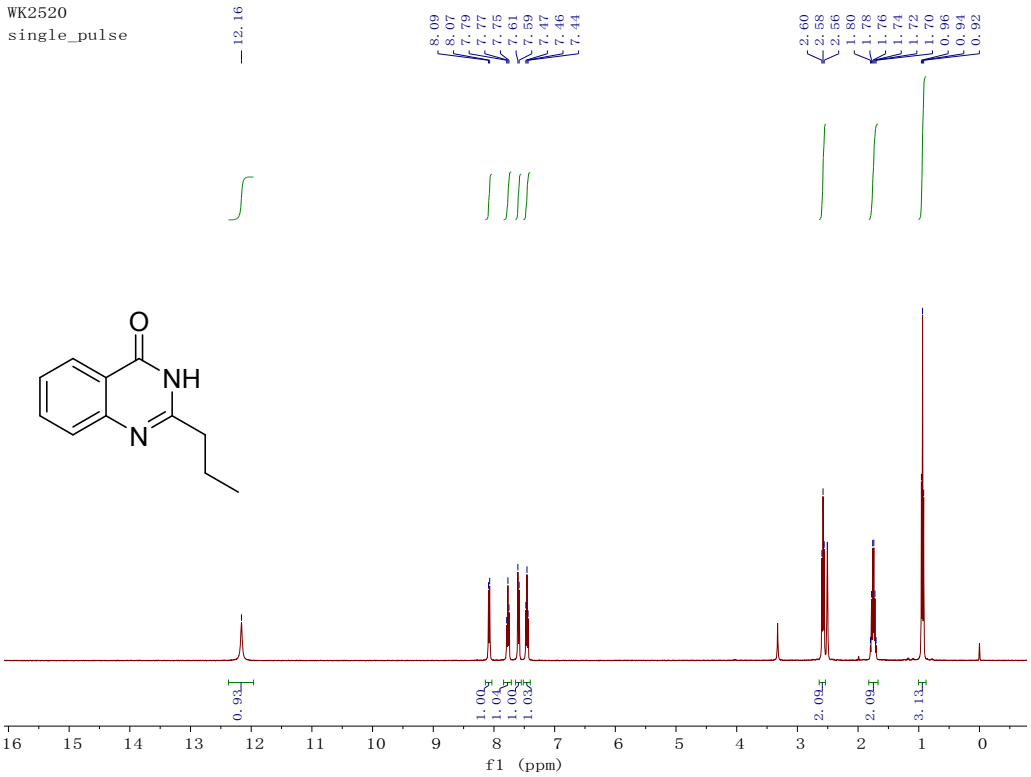
^{13}C NMR spectrum of 3q



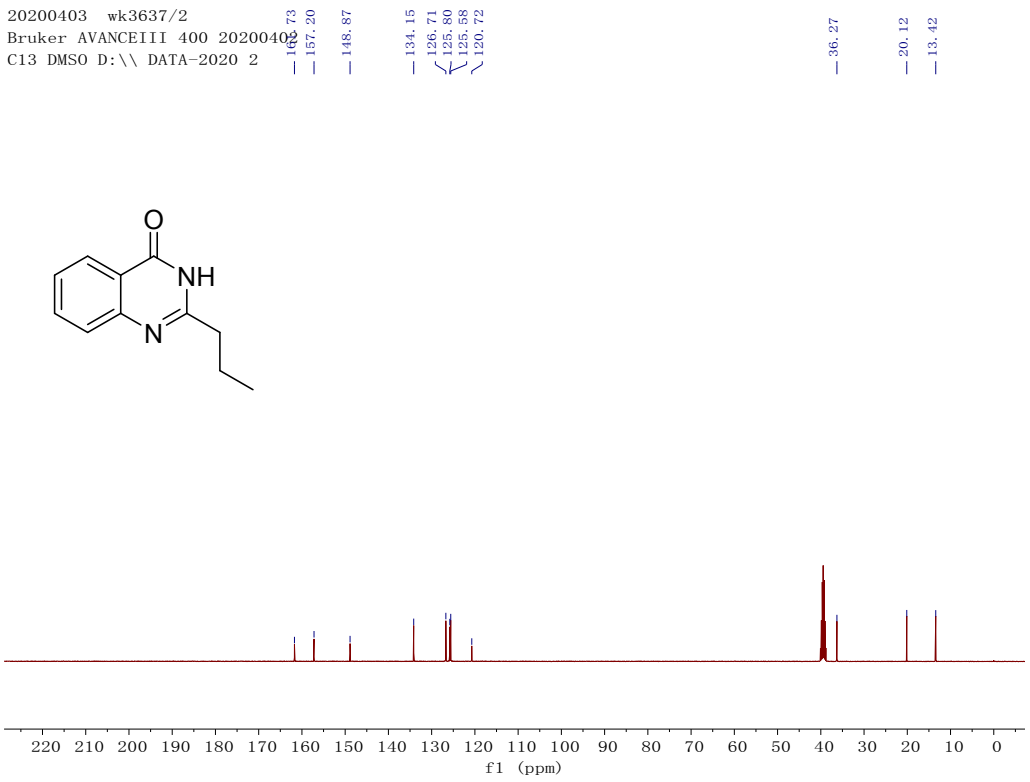
^{1}H NMR spectrum of 3r



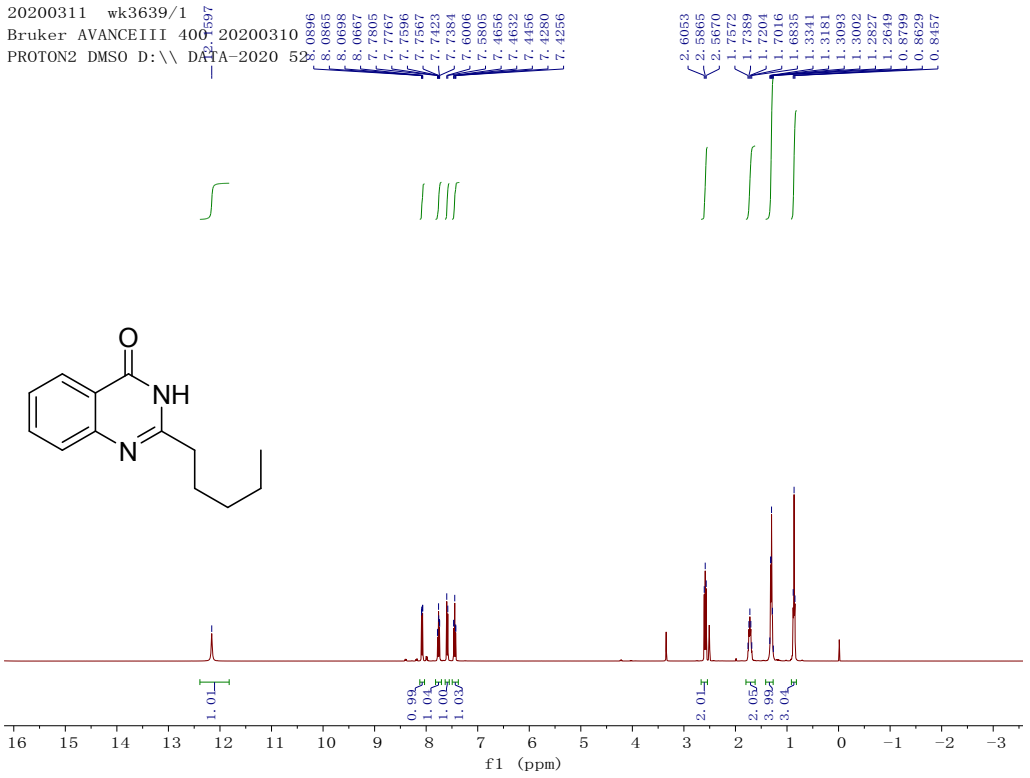
^{13}C NMR spectrum of 3r



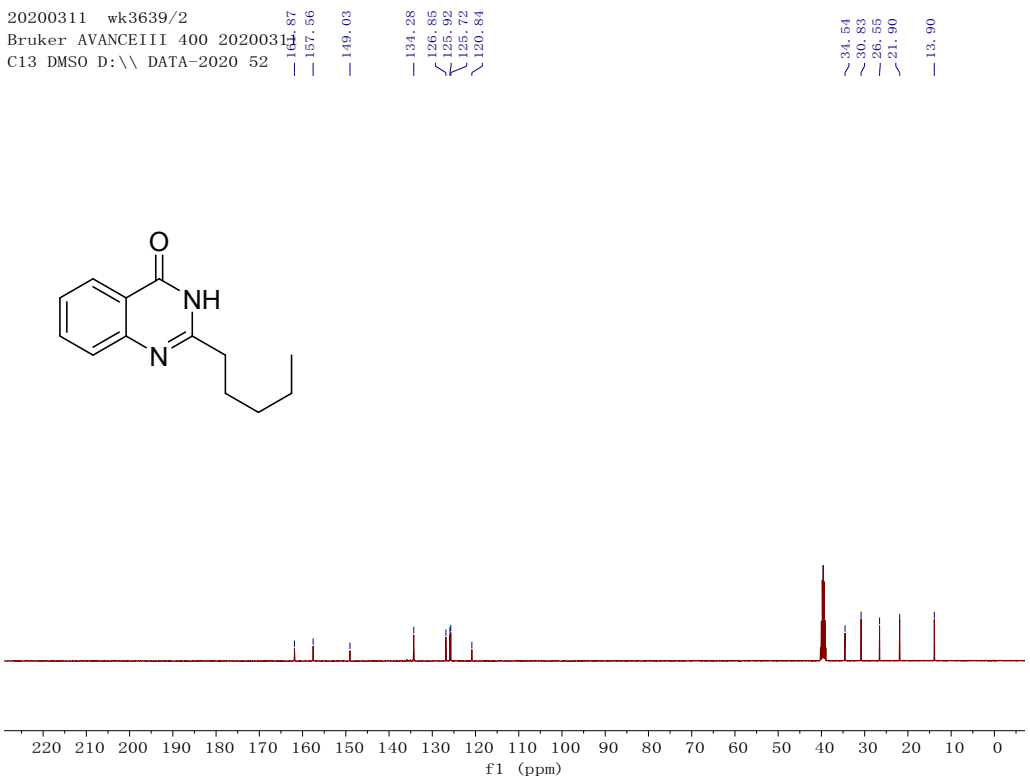
^{1}H NMR spectrum of 3s



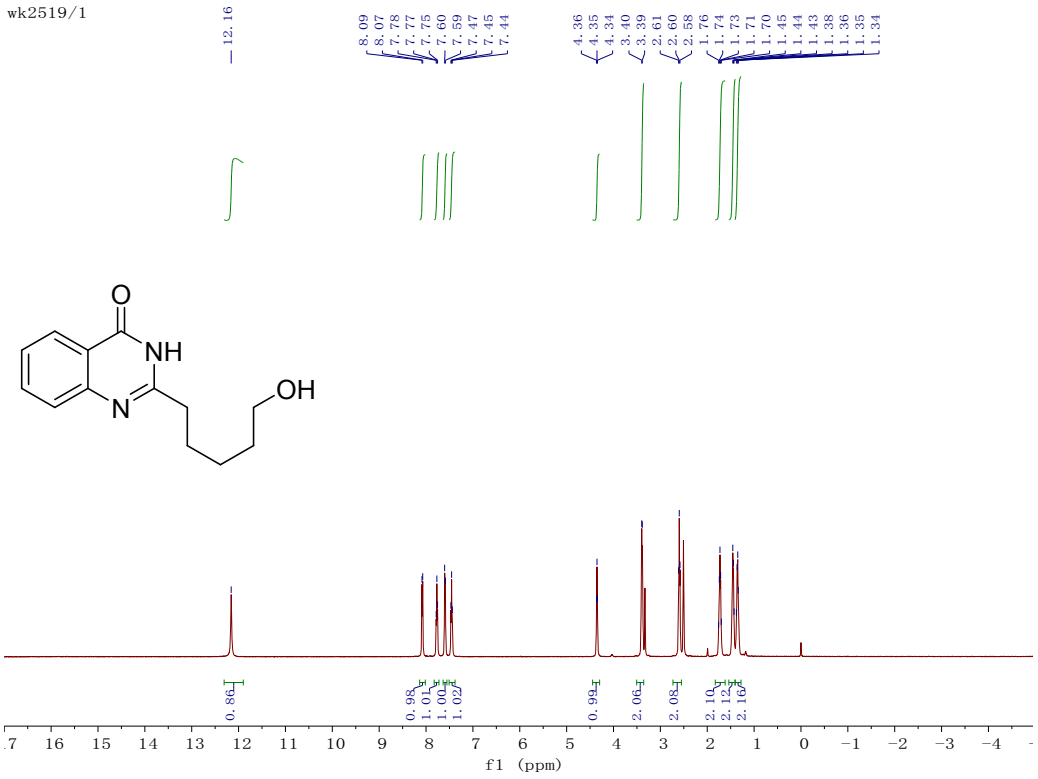
^{13}C NMR spectrum of 3s



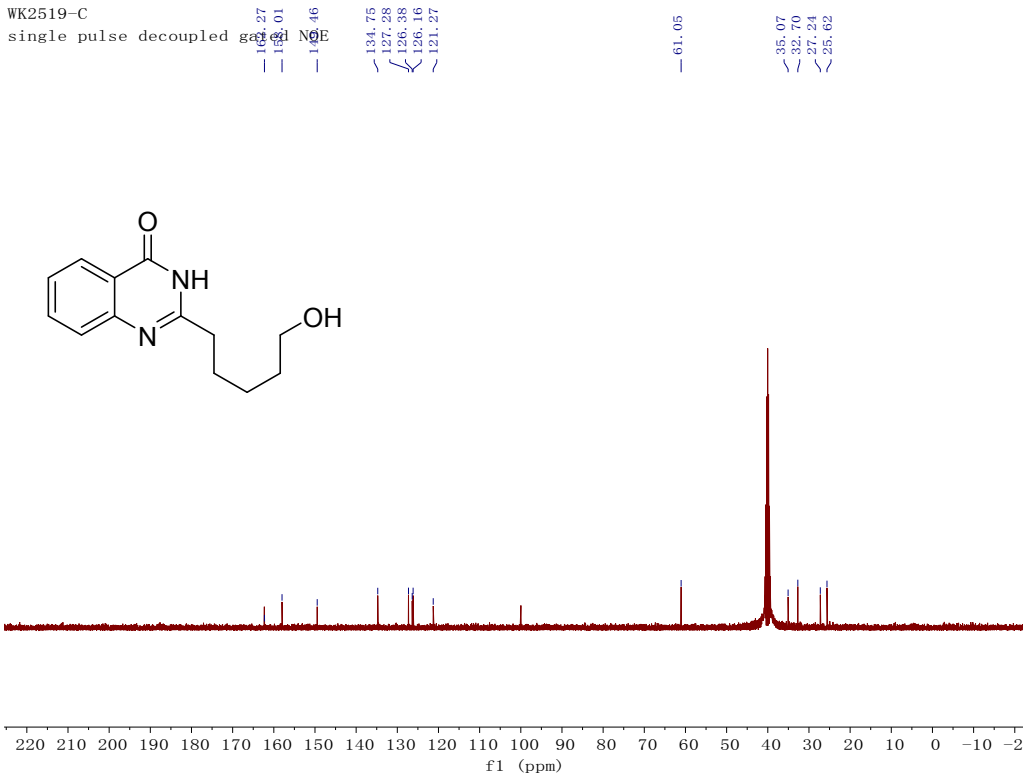
^{1}H NMR spectrum of 3t



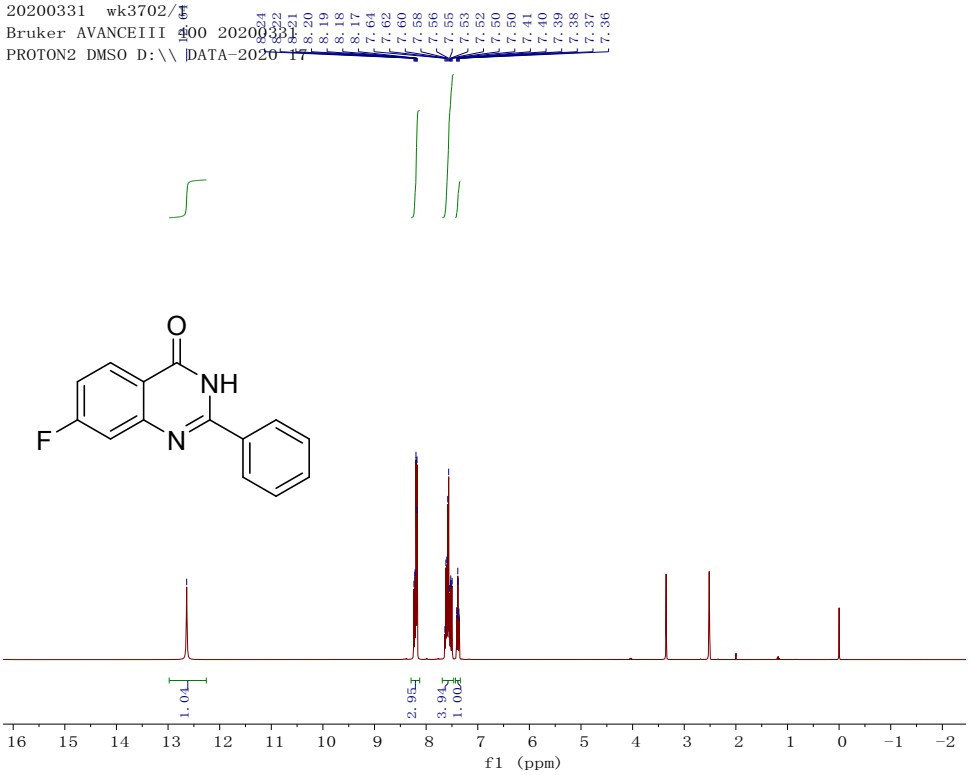
^{13}C NMR spectrum of 3t



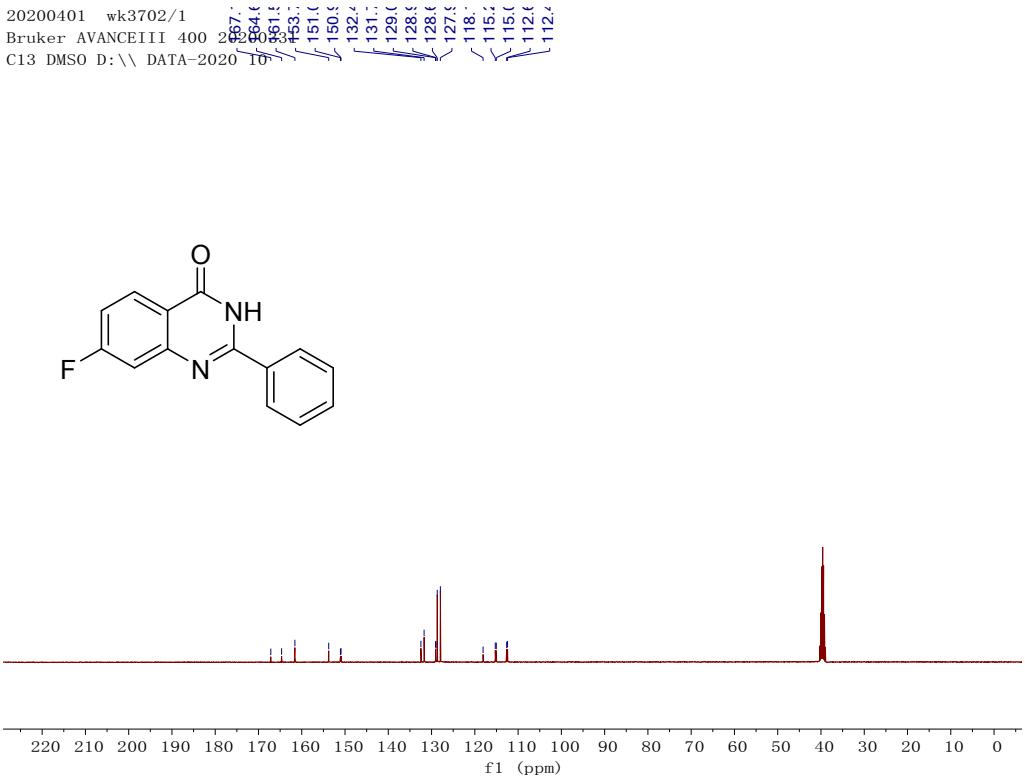
^{1}H NMR spectrum of 3u



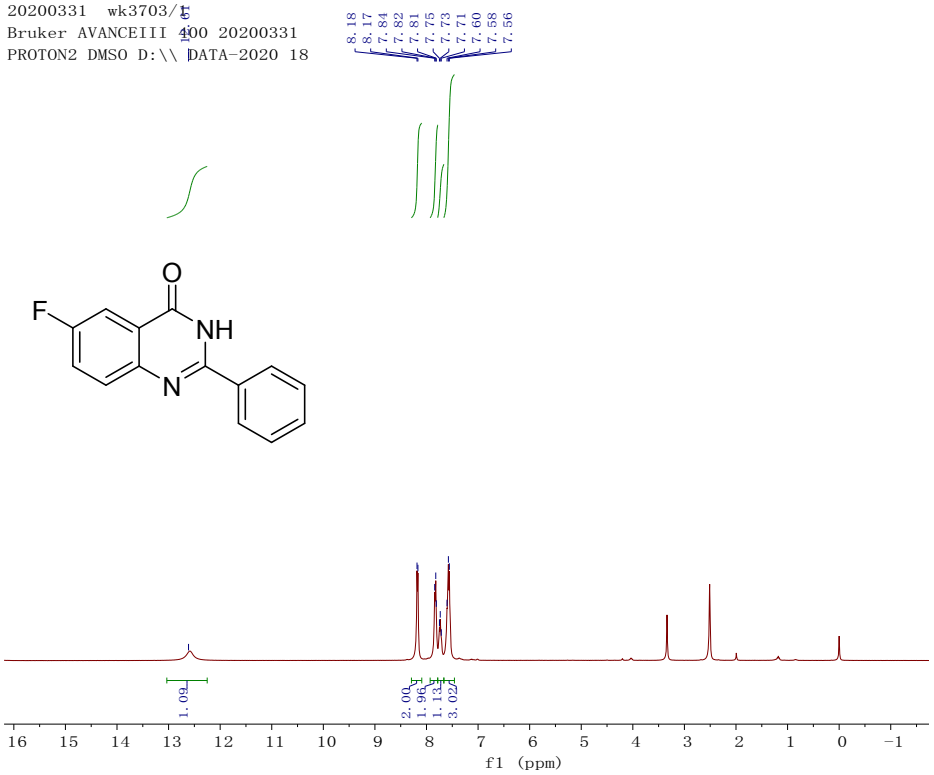
^{13}C NMR spectrum of 3u



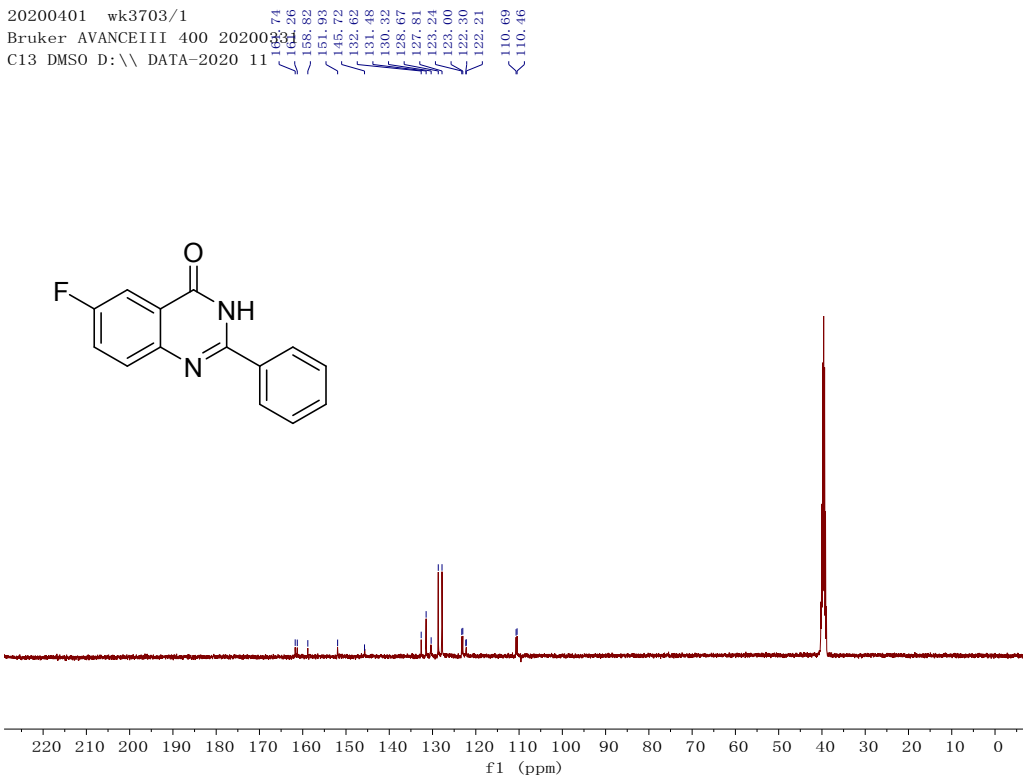
^{1}H NMR spectrum of 3bb



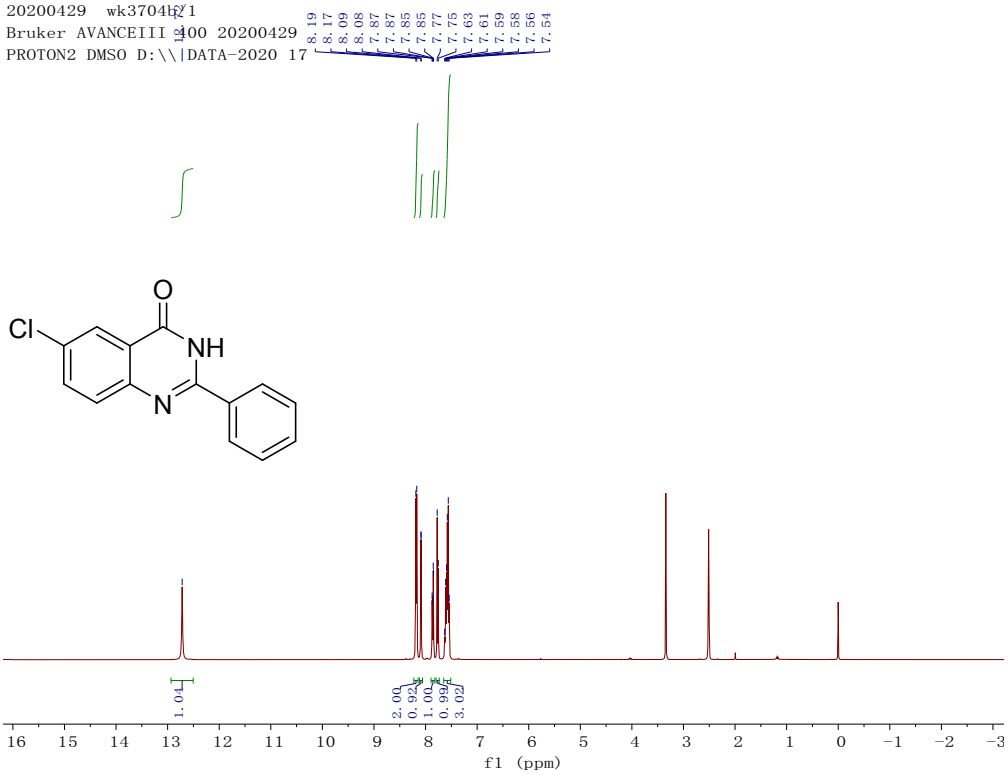
^{13}C NMR spectrum of 3bb



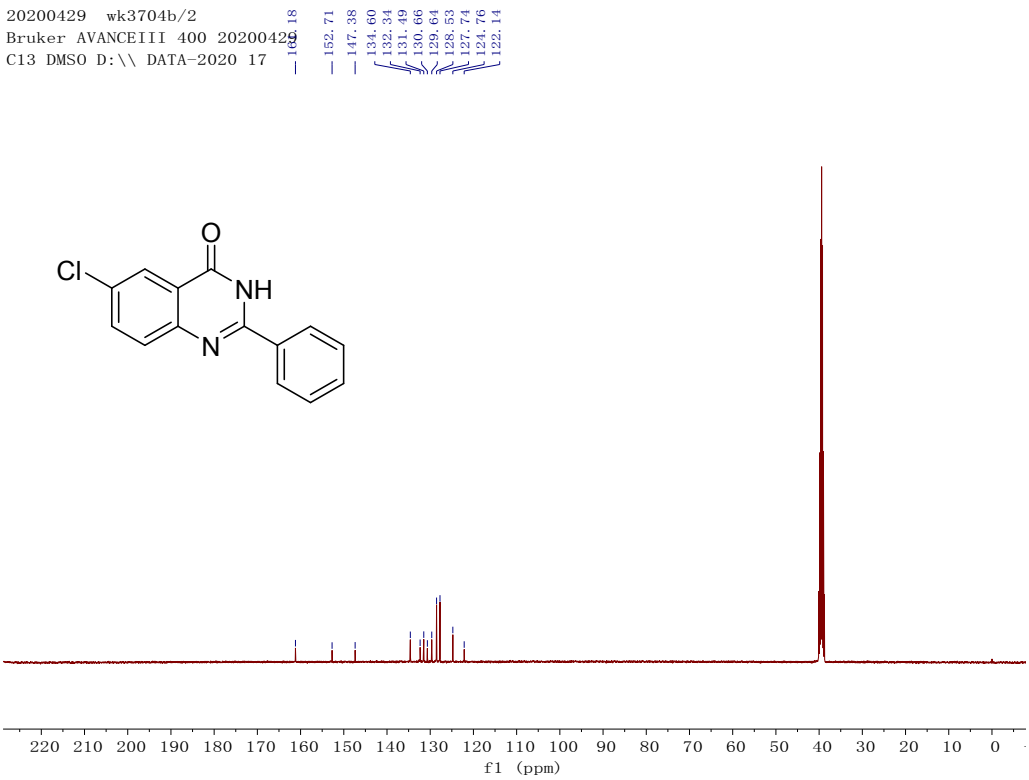
^{1}H NMR spectrum of 3bc



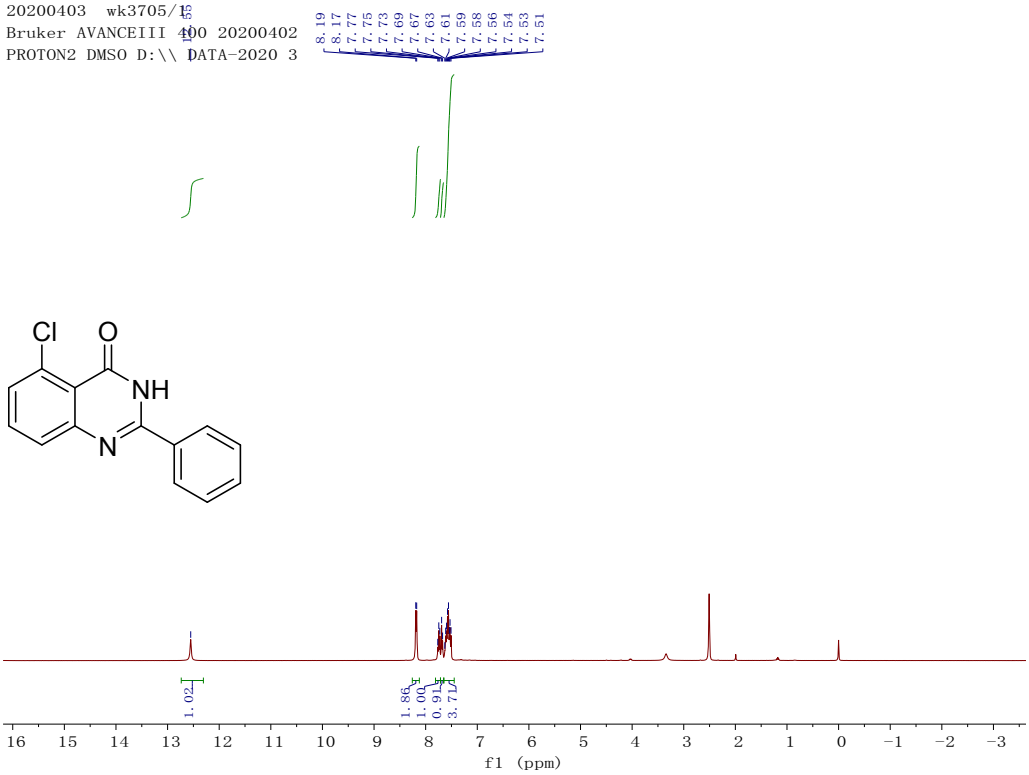
^{13}C NMR spectrum of 3bc



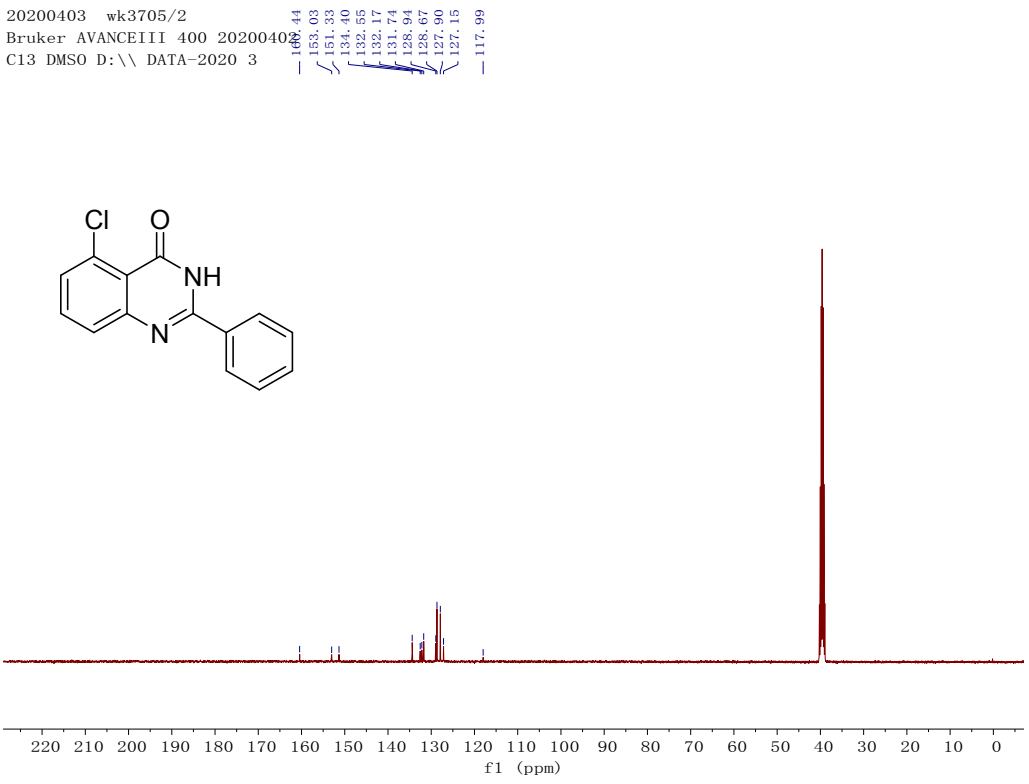
^{1}H NMR spectrum of 3bd



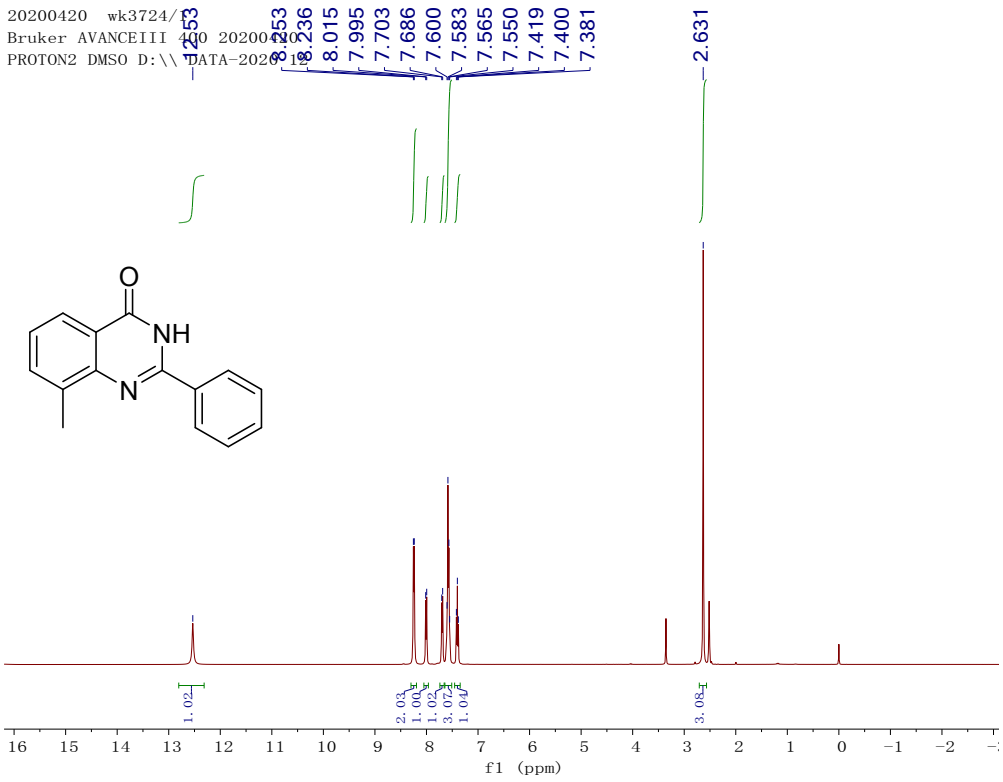
^{13}C NMR spectrum of 3bd



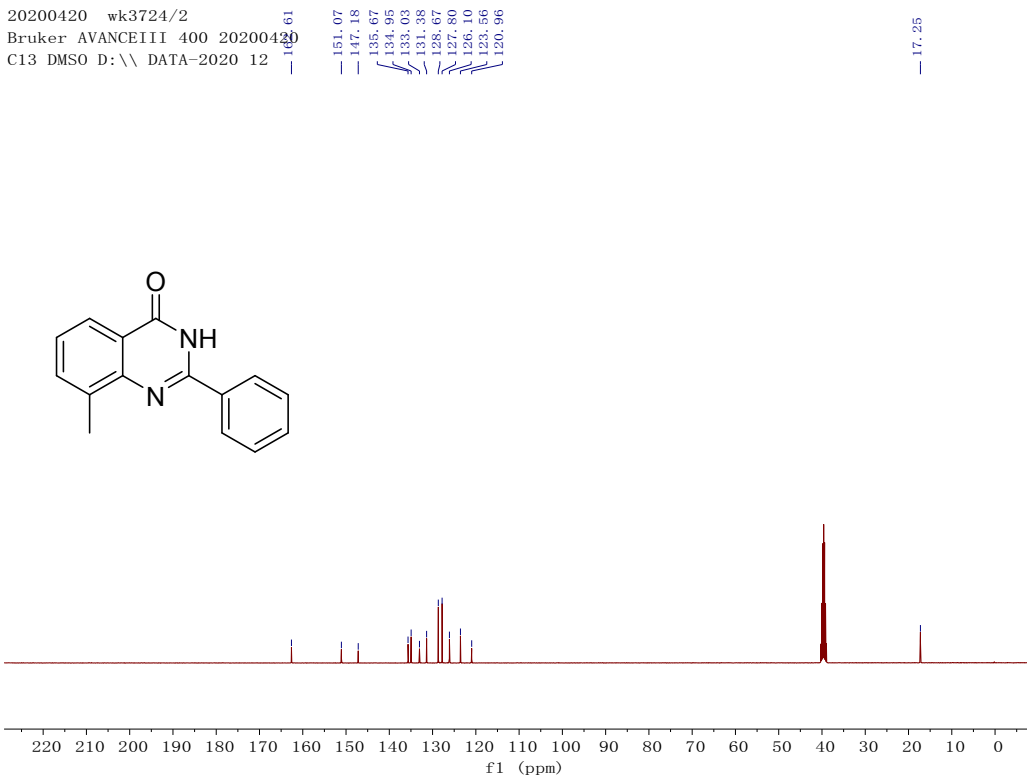
^{1}H NMR spectrum of 3be



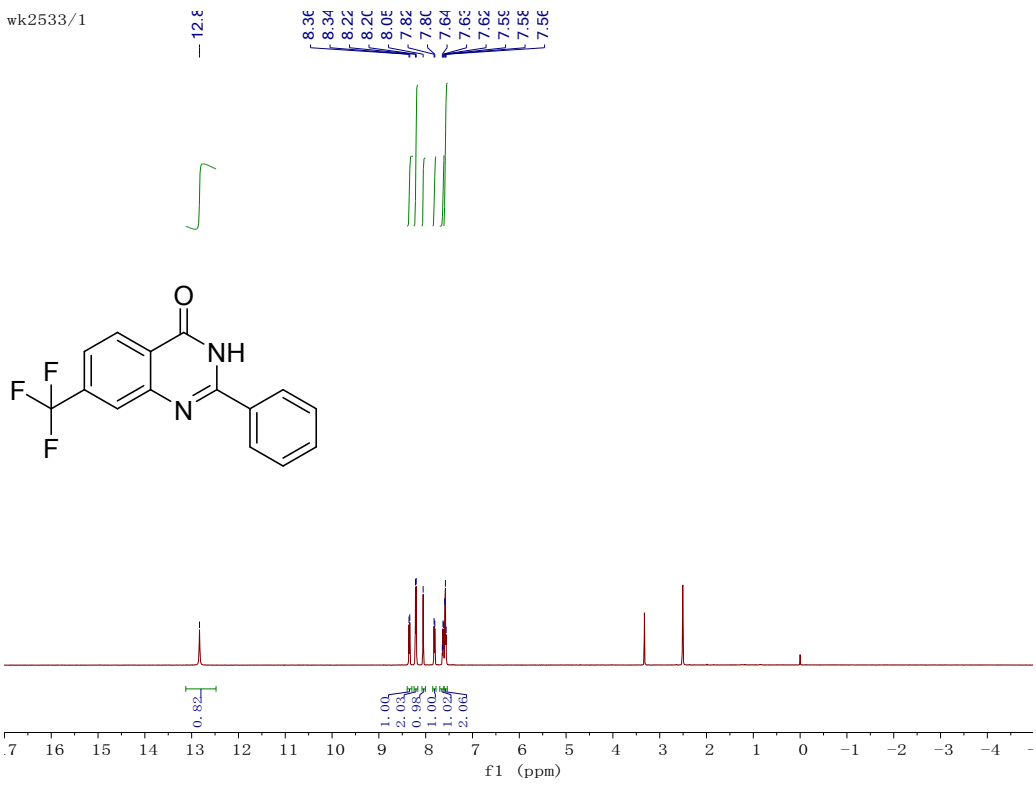
^{13}C NMR spectrum of 3be



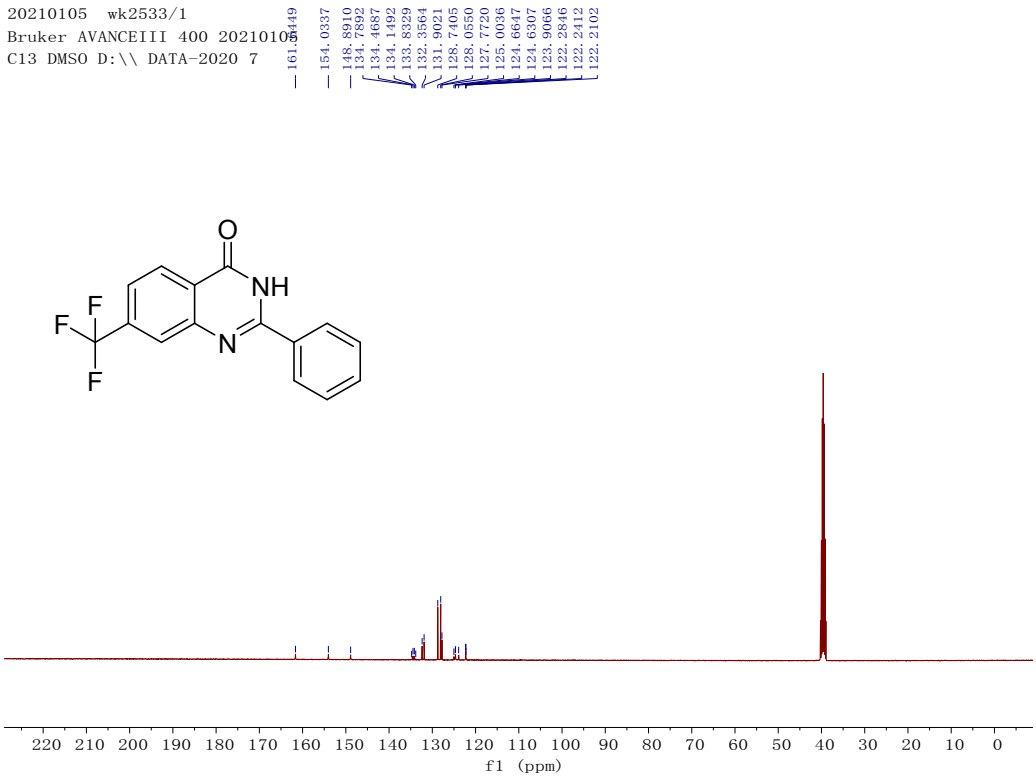
^{1}H NMR spectrum of 3bf



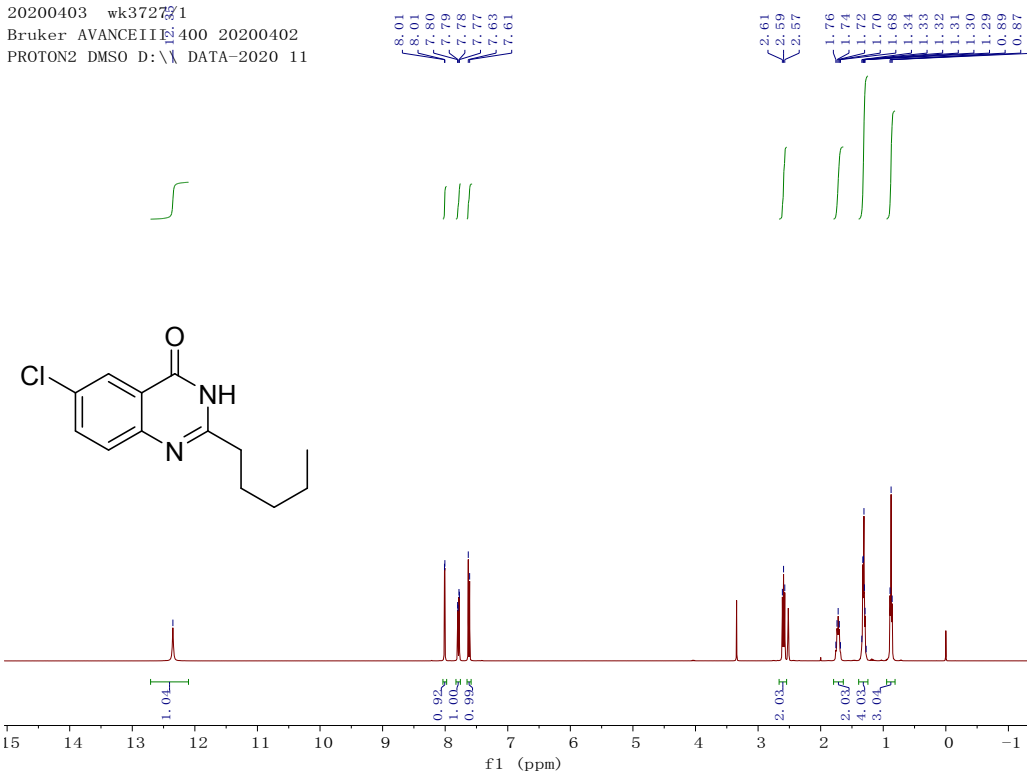
^{13}C NMR spectrum of 3bf



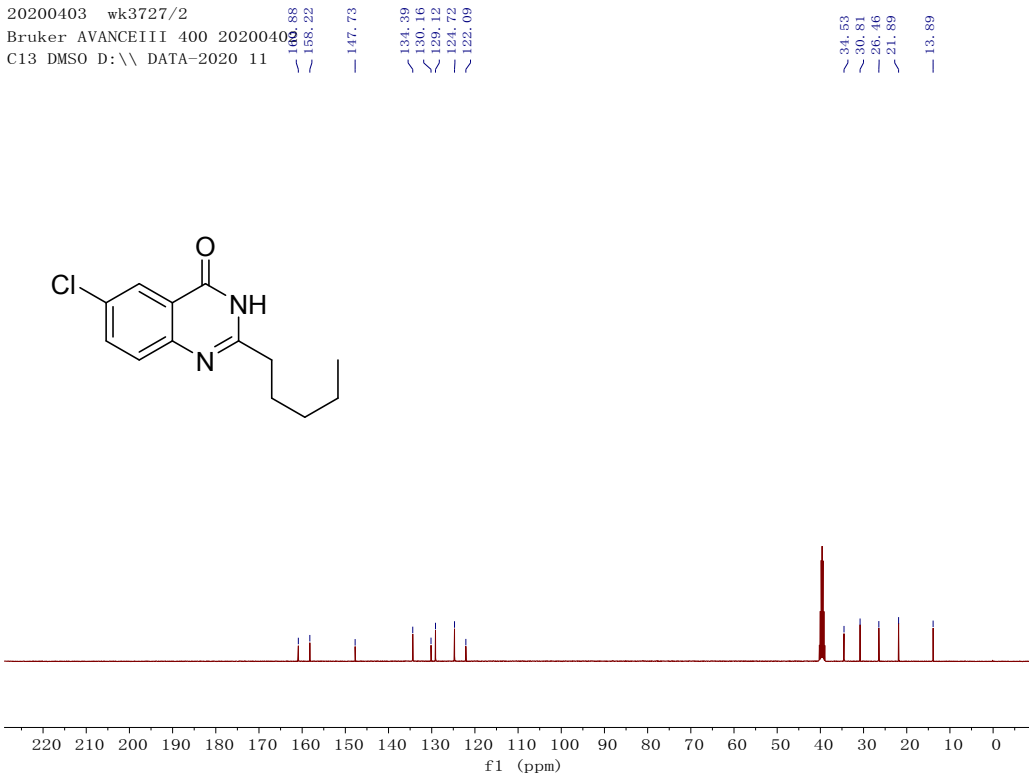
^{1}H NMR spectrum of 3bg



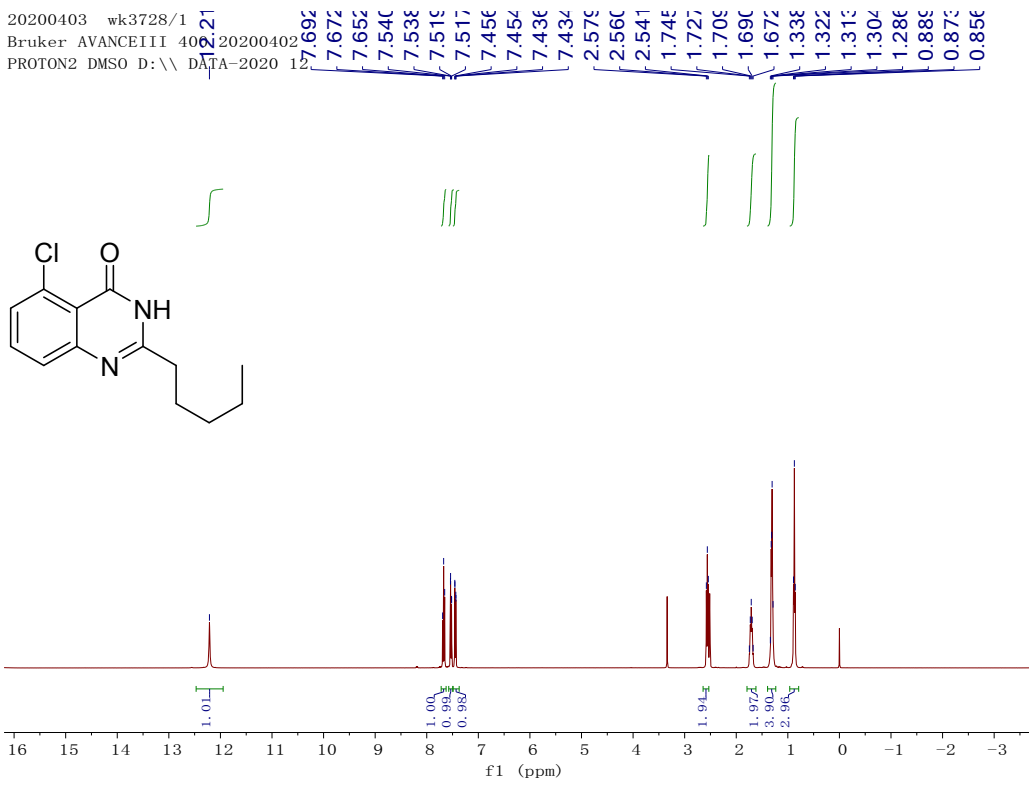
^{13}C NMR spectrum of 3bg



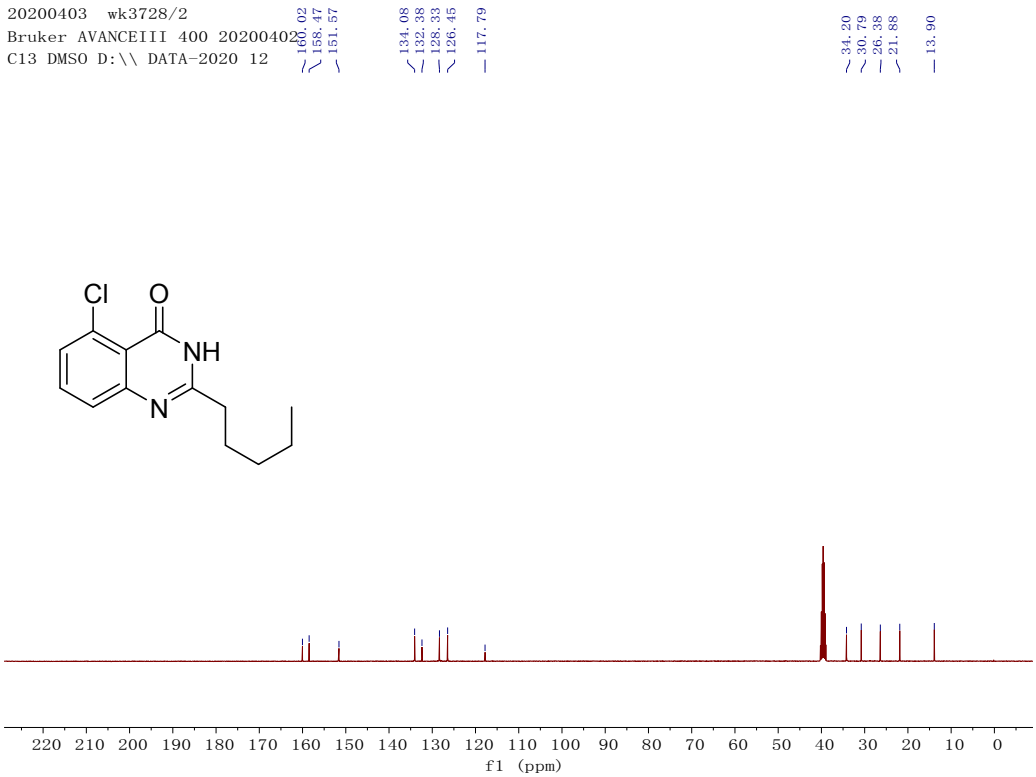
^{1}H NMR spectrum of 3bh



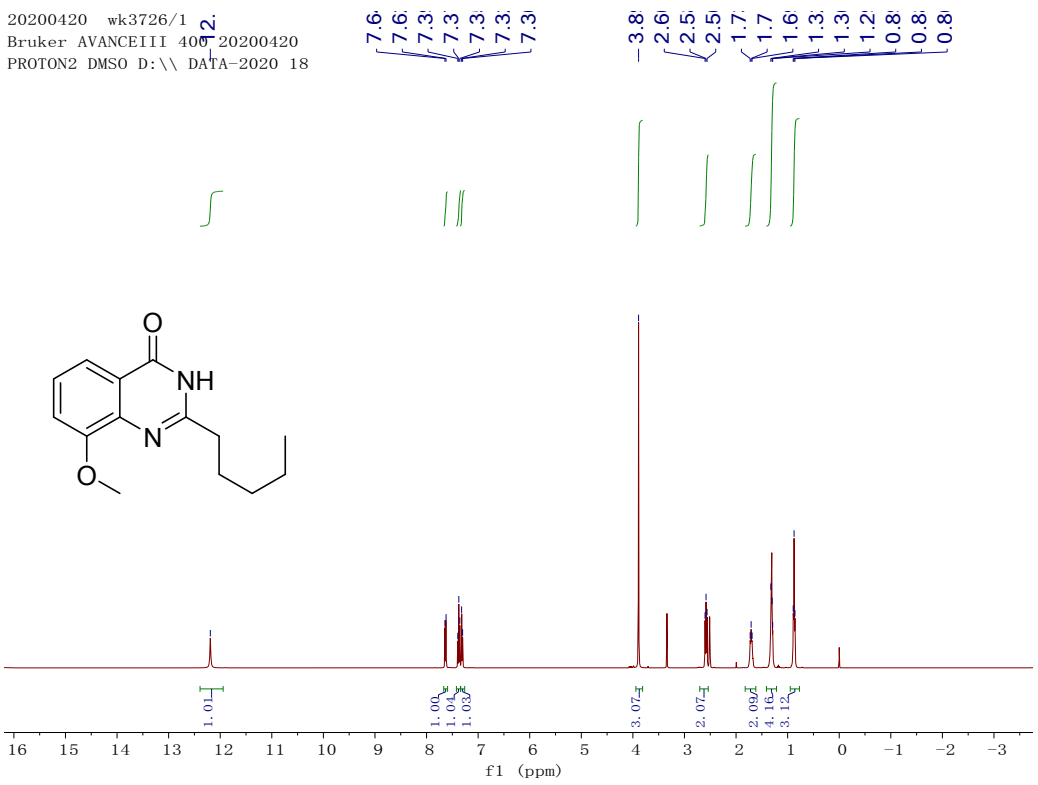
^{13}C NMR spectrum of 3bh



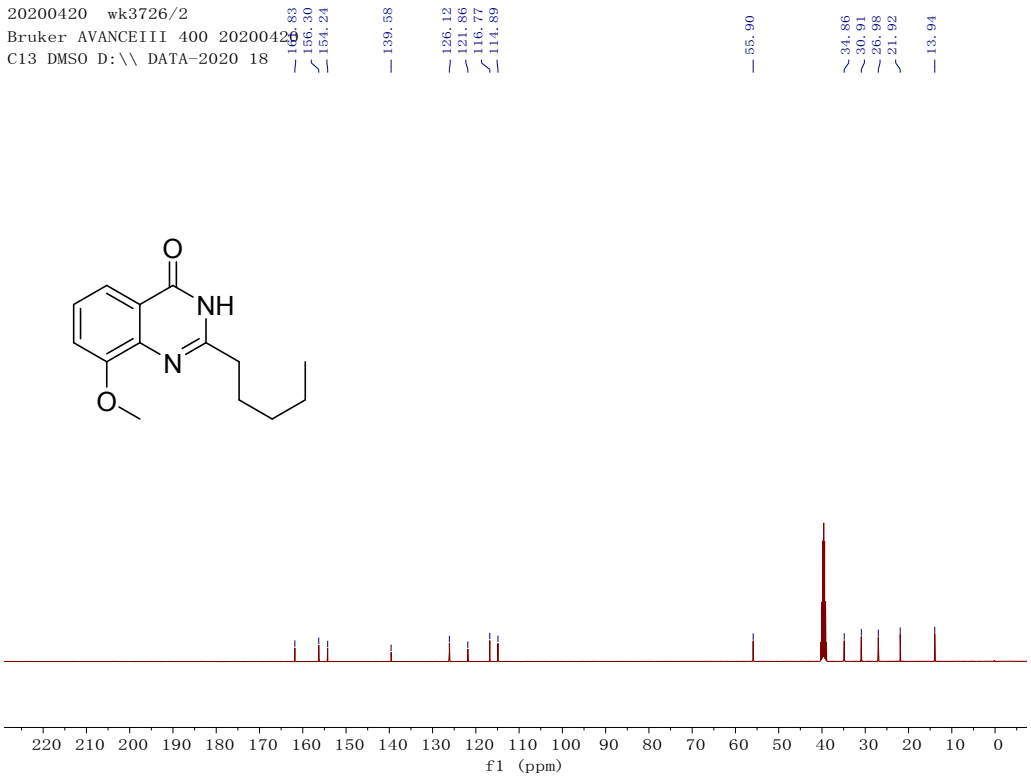
^{1}H NMR spectrum of 3bi



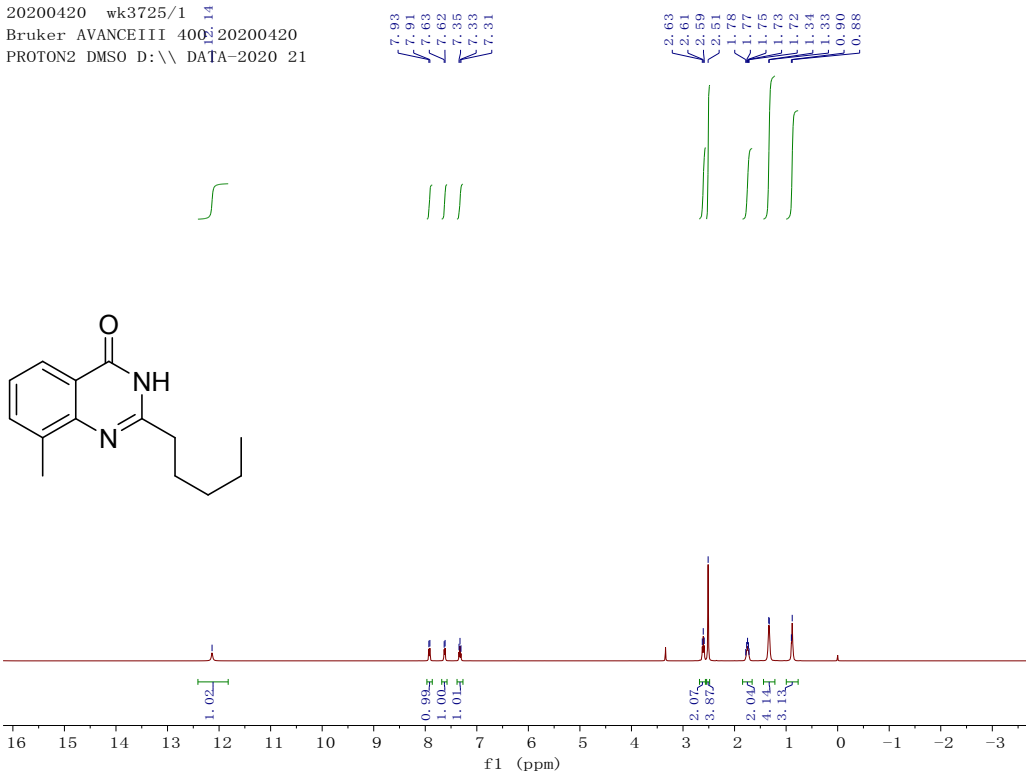
^{13}C NMR spectrum of 3bi



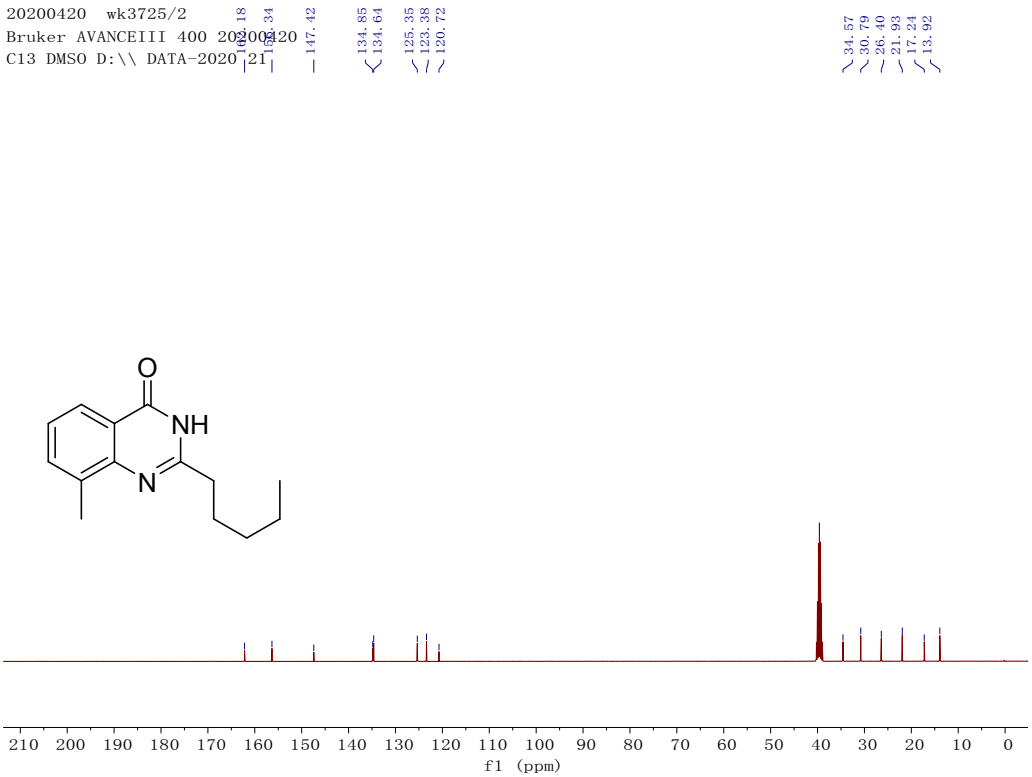
^{1}H NMR spectrum of 3bj



^{13}C NMR spectrum of 3bj



^{1}H NMR spectrum of 3bk



^{13}C NMR spectrum of 3bk