

Supporting Information

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An efficient zinc acetate dihydrate-catalyzed green protocol for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones

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Spectral data (3a-m)

2-Phenyl-2,3-dihydroquinazolin-4(1H)-one (3a): White solid; IR (KBr): 3301, 3176, 3062, 1653, 1610, 1509, 1482 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ = 7.99 (d, 1H, J = 7.5 Hz), 7.67-7.58 (m, 2H), 7.47-7.44 (m, 2H), 7.37-7.31 (m, 2H), 6.96 (t, 1H, J = 6.7 Hz), 6.71 (d, 1H, J = 7.5 Hz), 5.92 (s, 1H), 5.80 (s, 1H, br), 4.44 (s, 1H, br); ^{13}C NMR (100 MHz, CDCl_3) δ = 164.7, 147.2, 138.5, 134.0, 130.1, 129.1, 128.7, 127.4, 119.7, 114.6, 69.1; MS (ESI): m/z = 225 $[\text{M} + \text{H}]^+$.

2-(p-Tolyl)-2,3-Dihydroquinazolin-4(1H)-one (3b): White solid; IR (KBr): 3310, 3192, 3060, 2924, 2855, 1908, 1662, 1607, 1509 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ = 7.95 (d, 1H, J = 7.2 Hz), 7.46 (d, 2H, J = 8.3 Hz), 7.34-7.23 (m, 3H), 6.89 (t, 1H, J = 7.2 Hz), 6.65 (d, 1H, J = 7.2 Hz), 5.86 (s, 1H), 5.77 (s, 1H, br), 4.34 (s, 1H, br), 2.39 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ = 164.1, 148.4, 139.1, 138.2, 133.7, 129.3, 127.8, 127.3, 117.5, 115.5, 114.9, 66.8, 21.2; MS (ESI): m/z = 239 $[\text{M} + \text{H}]^+$.

(4-Methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3c): Light-yellow solid; mp 182-184 $^{\circ}\text{C}$. IR (KBr): 3448, 3315, 3183, 2923, 1676 cm^{-1} . ^1H NMR (400 MHz, DMSO- d_6) δ : (in ppm) 3.75 (s, 3H), 5.72 (s, 1H), 6.68 (s, 1H), 6.75 (d, J = 8.1 Hz, 1H), 6.96 (s, 2H), 7.02 (s, 1H), 7.25 (s, 1H), 7.43 (d, J = 8.6 Hz, 2H), 7.62 (d, J = 7.6 Hz, 1H), 8.25 (s, 1H); ^{13}C NMR (100 MHz, DMSO- d_6) δ : (in ppm) 57.1, 68.2, 115.5, 116.3, 116.9, 119.0, 129.2, 130.1, 135.1, 135.4, 149.9, 161.3, 165.6; MS (ESI): m/z = 255 $[\text{M} + \text{H}]^+$.

2-(2-Chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3d): White solid; IR (KBr): 3358, 3183, 3065, 1643, 1608, 1500, 1431, 1122, 1032, 742 cm^{-1} . ^1H NMR (400 MHz, DMSO) δ = 8.24 (s, 1H), 7.70-7.66 (m, 2H), 7.54-7.49 (m, 1H), 7.44-7.40 (m, 2H), 7.28 (dt, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.04 (s, 1H), 6.77 (d, J = 8.0 Hz, 1H), 6.72 (t, J = 7.2 Hz, 1H), 6.15 (s, 1H); ^{13}C NMR (100 MHz, DMSO) δ = 164.1, 148.1, 138.3, 133.9, 132.3, 130.8, 130.0, 129.2, 127.9, 127.8, 117.9, 115.1, 115.0, 64.1.

2-(4-Hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3e): White solid; IR (KBr): 3302, 3187, 3068, 2932, 1668, 1612, 1509, 1486 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ = 9.33 (s, 1H, br), 7.75 (d, 1H, J = 7.7 Hz), 7.37 (d, 3H, J = 7.1 Hz), 7.22 (t, 1H, J = 7.3 Hz), 6.83-6.69 (m, 4H), 6.28 (s, 1H, br), 5.72 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ = 160.98, 156.32, 146.66, 132.71, 128.07, 118.90, 115.65, 113.89, 65.59; MS (ESI): m/z = 241 $[\text{M} + \text{H}]^+$.

2-(4-Nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (3f): Yellow solid; mp 204-206 $^{\circ}\text{C}$. IR (KBr): 3278, 3174, 3032, 2922, 2855, 1647, 1608, 1520, 1461 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ = 8.31 (d, 1H, J = 8.3 Hz), 7.96 (m, 1H), 7.83-7.79 (m, 2H), 7.41-7.35 (m, 1H), 7.27 (s, 1H), 6.98-6.92 (m, 1H), 6.70 (d, 1H, J = 7.5 Hz), 6.15 (s, 1H, br), 6.05 (s, 1H), 4.43 (s, 1H, br); ^{13}C NMR (100 MHz, CDCl_3) δ = 162.96, 147.60, 146.50, 145.97, 132.46, 126.78, 126.49, 122.25, 116.70, 113.70, 64.89; MS (ESI): m/z = 270 $[\text{M} + \text{H}]^+$.

2-(2-(Trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one(3g): White solid; mp: 173-176°C; IR ($\nu_{\text{max}}/\text{cm}^{-1}$, KBr): 3276, 2923, 2852, 2367, 1663, 1488, 1313, 1121; ^1H NMR (400 MHz, DMSO-*d*₆): δ = 8.27 (s, 1H), 8.08 (d, J = 7.6 Hz, 1H), 7.75-7.80 (m, 2H), 7.60-7.66 (m, 2H), 7.27 (t, J = 8.4 Hz, 1H), 6.97 (s, 1H), 6.72-6.76 (m, 2H), 6.04 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-*d*₆): δ = 163.55, 148.08, 138.70, 133.47, 132.98, 129.82, 129.52, 127.46, 126.60, 125.31, 122.73, 117.77, 114.71, 114.54, 63.22 ppm; HRMS (ES): Calcd 293.0896, found 293.0902.

2-(Pyridin-2-yl)-2,3-dihydroquinazolin-4(1H)-one (3h): White solid, ^1H NMR (400 MHz, DMSO) δ = 8.76 (t, J = 6.0 Hz, 1H), 8.56 (dd, J_1 = 4.8 Hz, J_2 = 1.6 Hz, 1H), 7.87 (brs, 1H), 7.76 (dt, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.62 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.35 (d, J = 8.0 Hz, 1H), 7.30-7.27 (m, 1H), 7.22 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.19 (brs, 1H), 6.60 (d, J = 7.6 Hz, 1H), 6.53 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 172.0, 159.4, 149.7, 149.5, 137.2, 132.9, 129.5, 122.6, 121.6, 115.0, 114.8, 111.9, 48.4.

2,2-Dimethyl-2,3-dihydroquinazolin-4(1H)-one (3i): White solid, ^1H NMR (400 MHz, DMSO) δ = 7.95 (s, 1H), 7.59 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.23 (dt, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 6.67-6.61 (m, 3H), 1.39 (s, 6H). ^{13}C NMR (100 MHz, DMSO) δ = 163.5, 147.5, 133.7, 127.6, 116.9, 114.7, 114.3, 67.3, 29.5.

2-Methyl-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3k): White solid, ^1H NMR (400 MHz, DMSO) δ = 8.77 (d, J = 1.6 Hz, 1H), 7.64 (d, J = 1.6 Hz, 1H), 7.50-7.46 (m, 3H), 7.26 (dt, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 2H), 7.23-7.17 (m, 2H), 6.76 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 6.56 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 1.63 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ = 164.3, 148.2, 147.7, 133.8, 128.4, 127.7, 127.5, 125.6, 117.3, 115.5, 114.8, 70.6, 31.2.

1'H-Spiro[cyclohexane-1,2'-quinazolin]-4'(3'H)-one (3l): White solid, IR ($\nu_{\text{max}}/\text{cm}^{-1}$, KBr): 3365, 3163, 3021, 2923, 2851, 1644, 1607, 1502, 1480, 1379, 756. ^1H NMR (400 MHz, DMSO) δ = 7.93 (s, 1H), 7.58 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.21 (dt, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.81 (d, J = 8.0 Hz, 1H), 6.65-6.61 (m, 2H), 1.79-1.73 (m, 2H), 1.66-1.53 (m, 6H), 1.45-1.41 (m, 1H), 1.29-1.20 (m, 1H). ^{13}C NMR (100 MHz, DMSO) δ = 163.9, 148.0, 133.5, 127.7, 117.0, 115.0, 114.8, 100.0, 77.5, 22.5.

1'H-spiro[cyclopentane-1,2'-quinazolin]-4'(3'H)-one (3m): White solid, IR (KBr): 3289, 3161, 2972, 1634, 1611, 1515, 1482, 1382, 778 cm^{-1} . ^1H NMR (400 MHz, DMSO) δ = 8.11 (s, 1H), 7.58 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.21 (dt, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.76 (s, 1H), 6.70 (d, J = 8.0 Hz, 1H), 6.64 (t, J = 7.6 Hz, 1H), 1.82-1.78 (m, 4H), 1.69-1.65 (m, 4H). ^{13}C NMR (100 MHz, DMSO) δ = 163.9, 148.0, 133.5, 127.7, 117.0, 115.0, 114.8, 100.0, 77.5, 22.5.

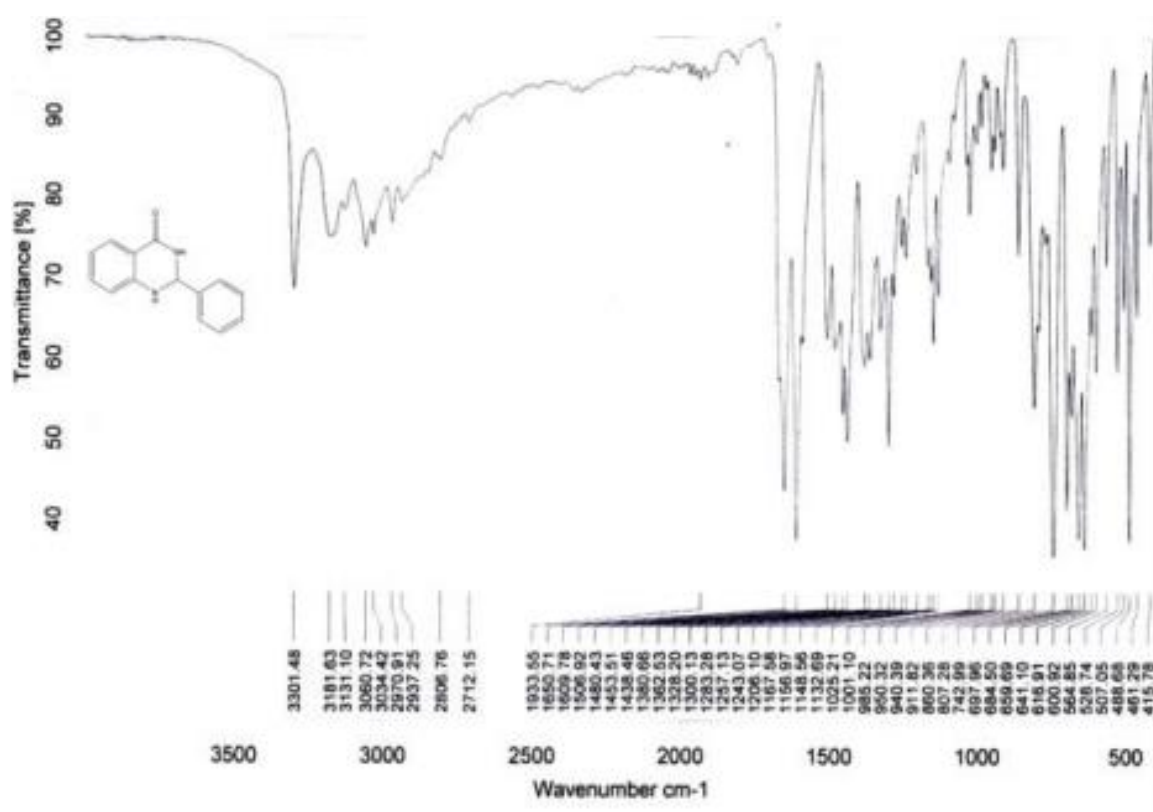


Figure S1: IR Spectrum of 3a

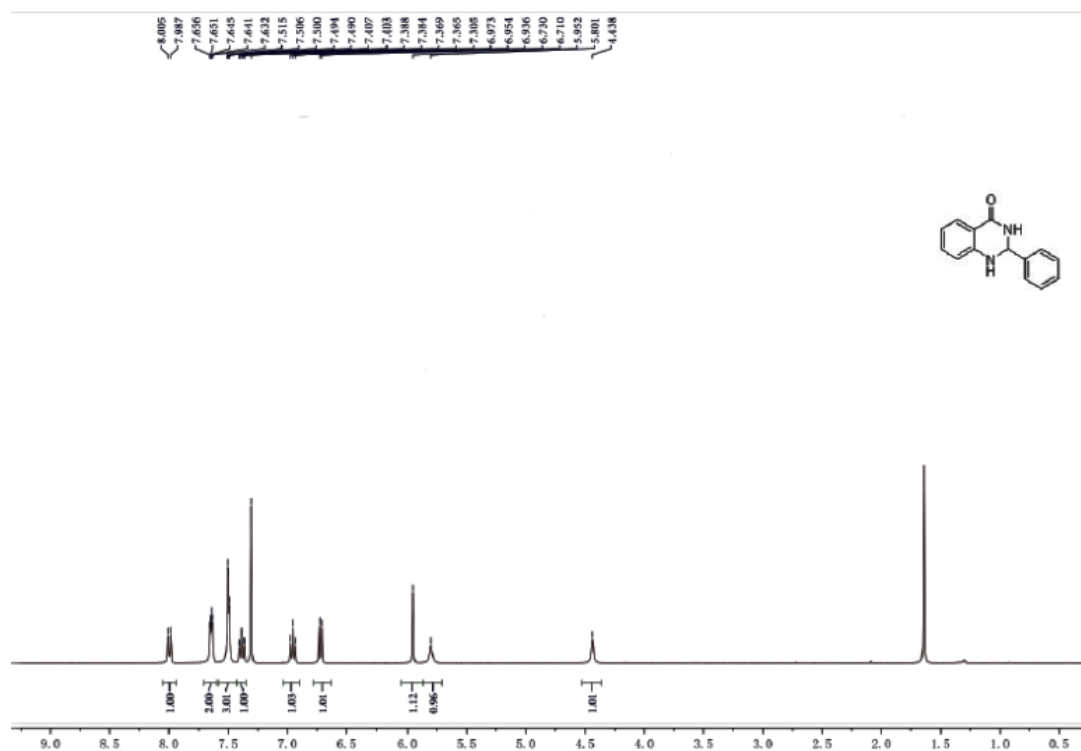


Figure S2: ^1H -NMR (400 MHz, CDCl_3) Spectrum of 3a

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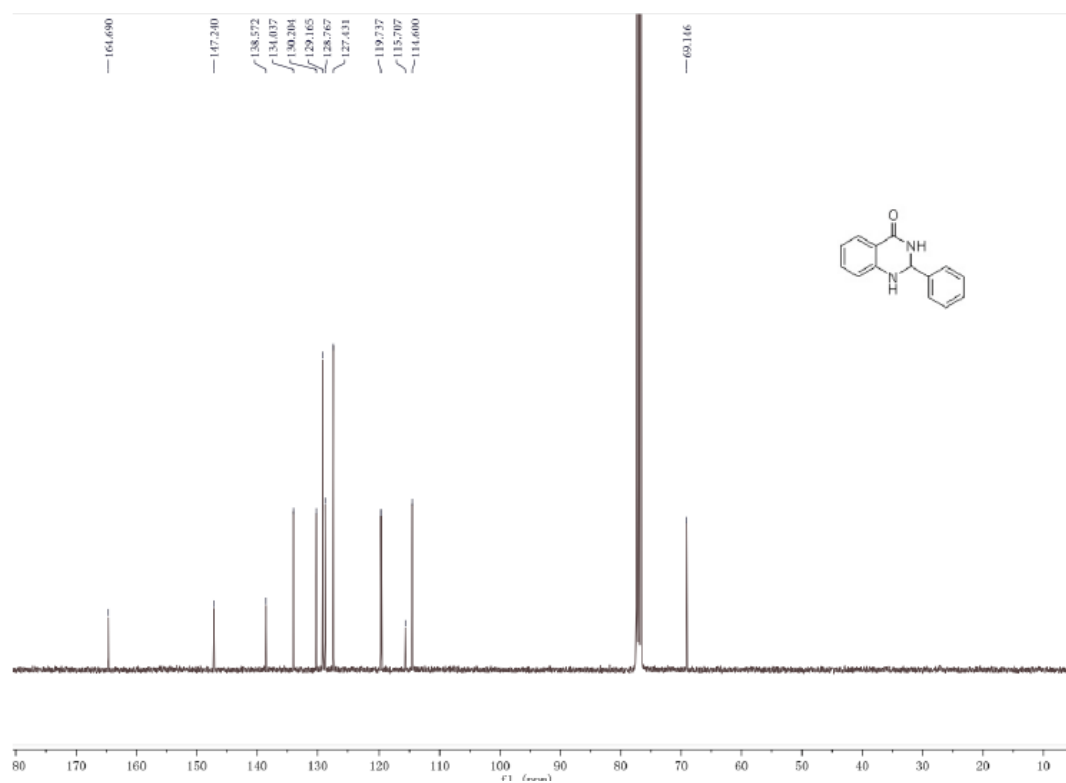


Figure S3: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of **3a**

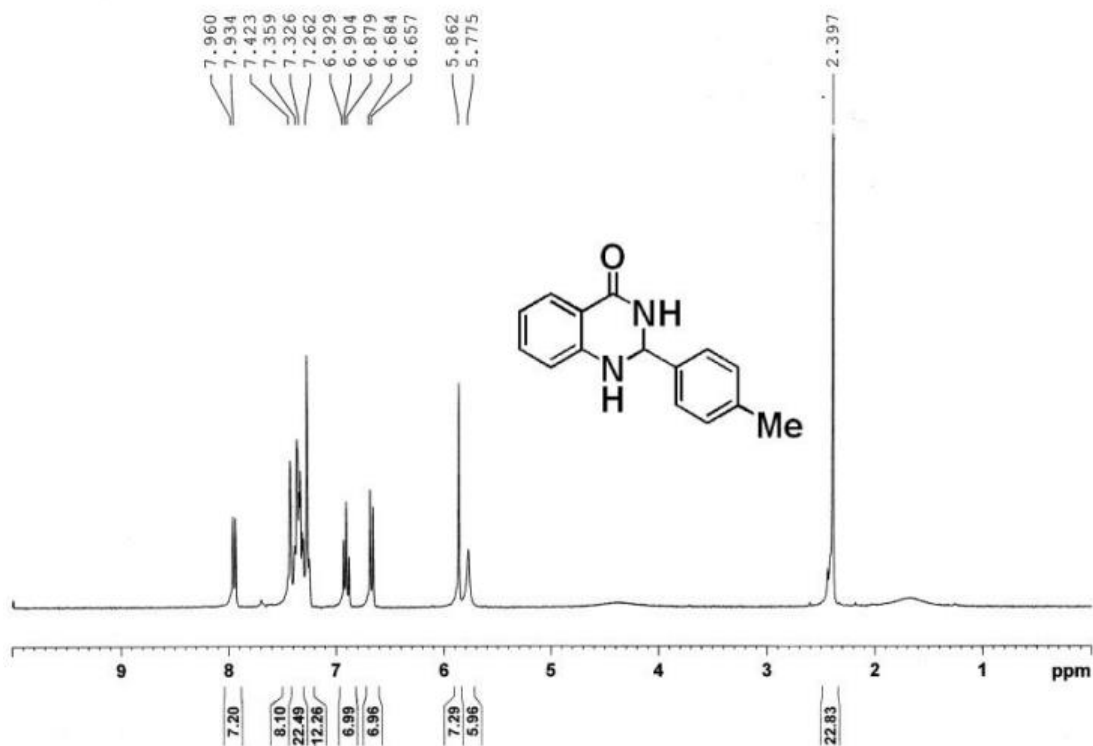


Figure S4: ¹H-NMR (400 MHz, CDCl₃) Spectrum of **3b**

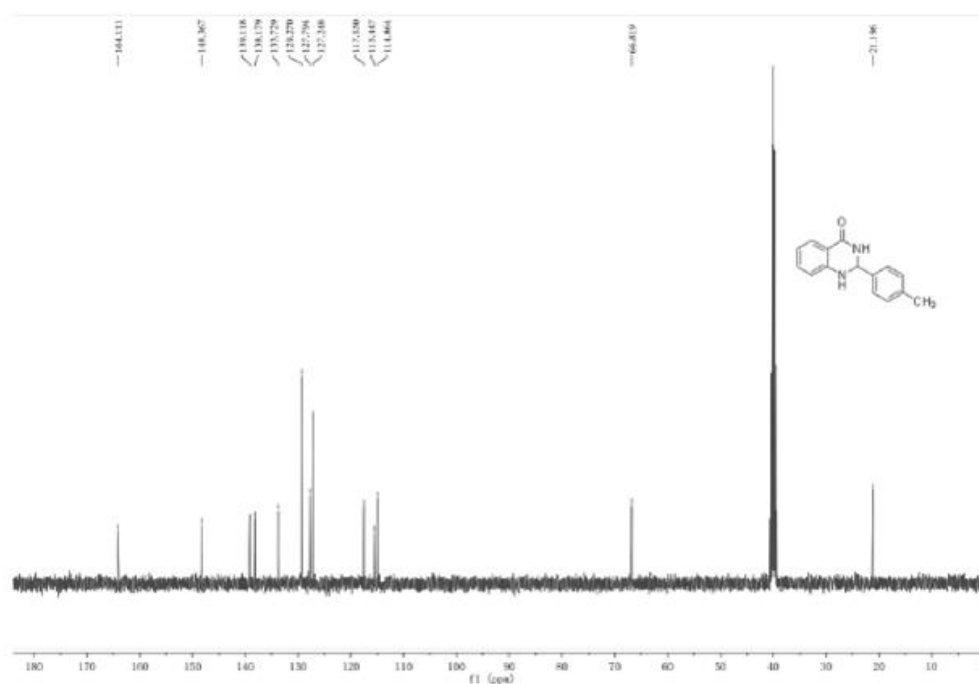


Figure S5: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of 3b

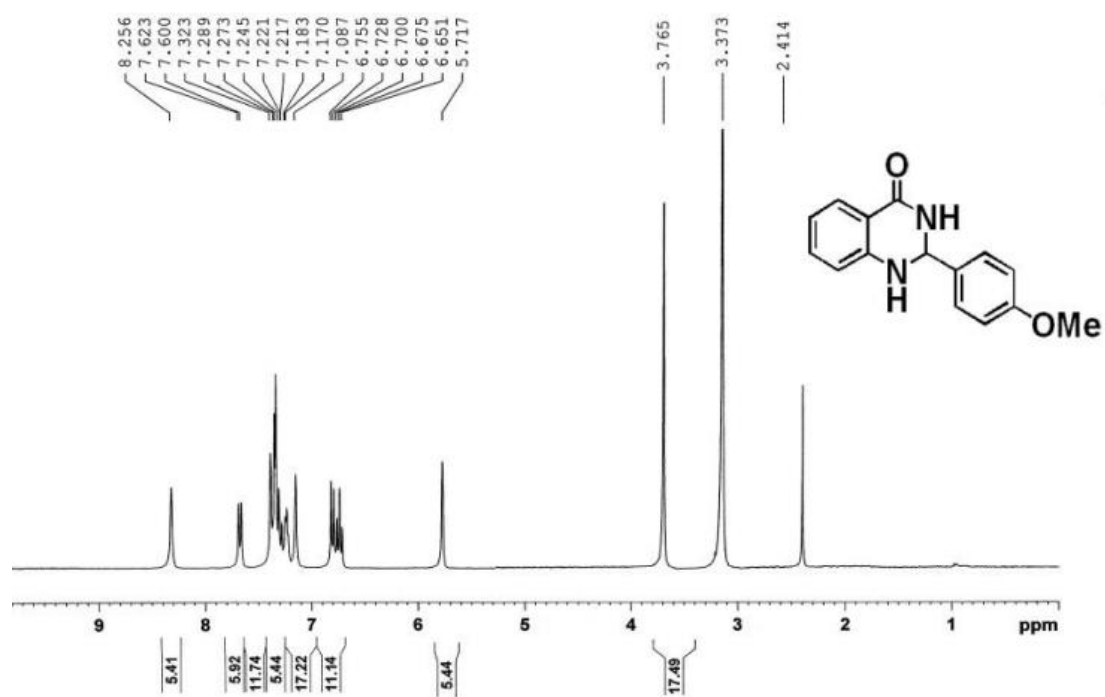


Figure S6: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 3c

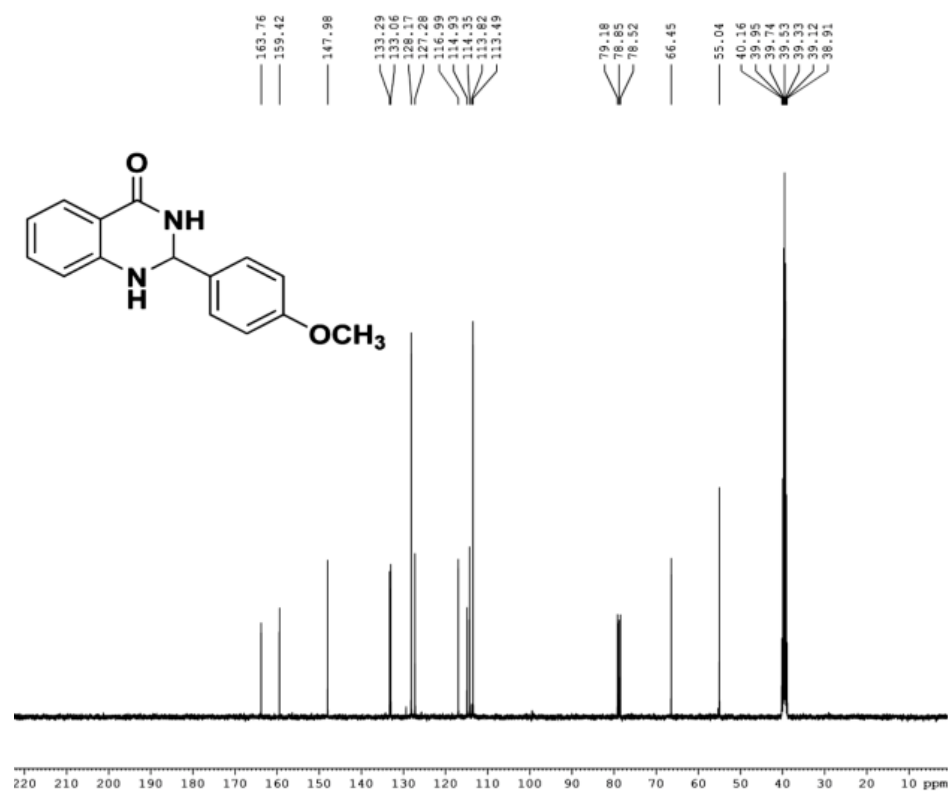


Figure S7: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of 3c

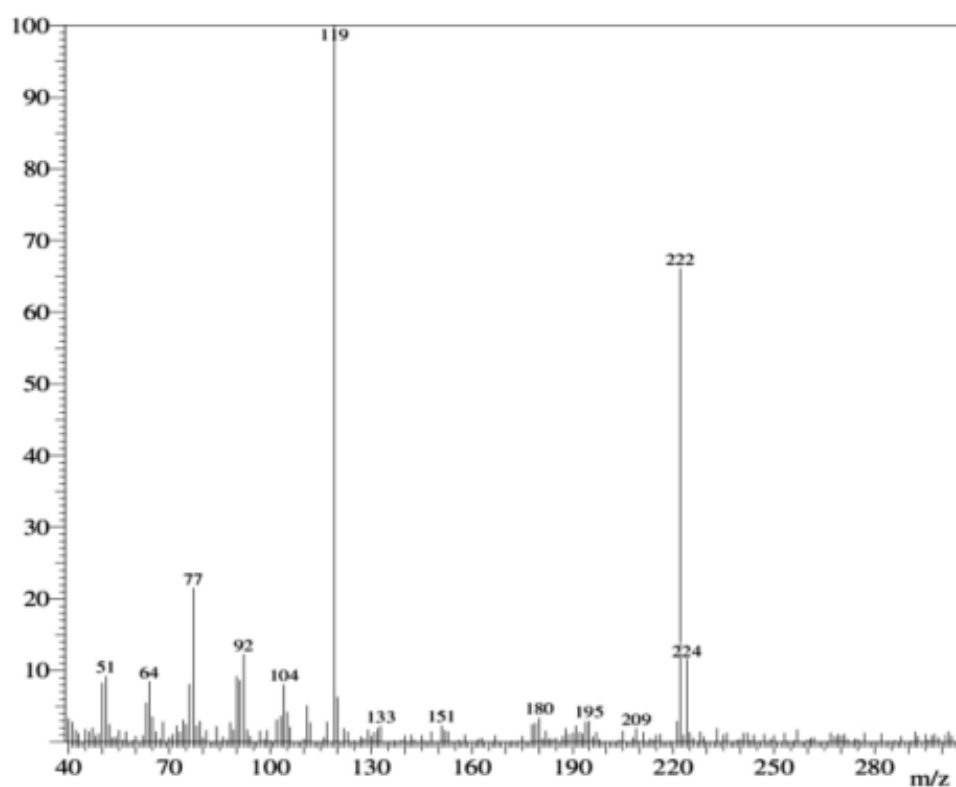


Figure S8: Mass Spectrum of 3c

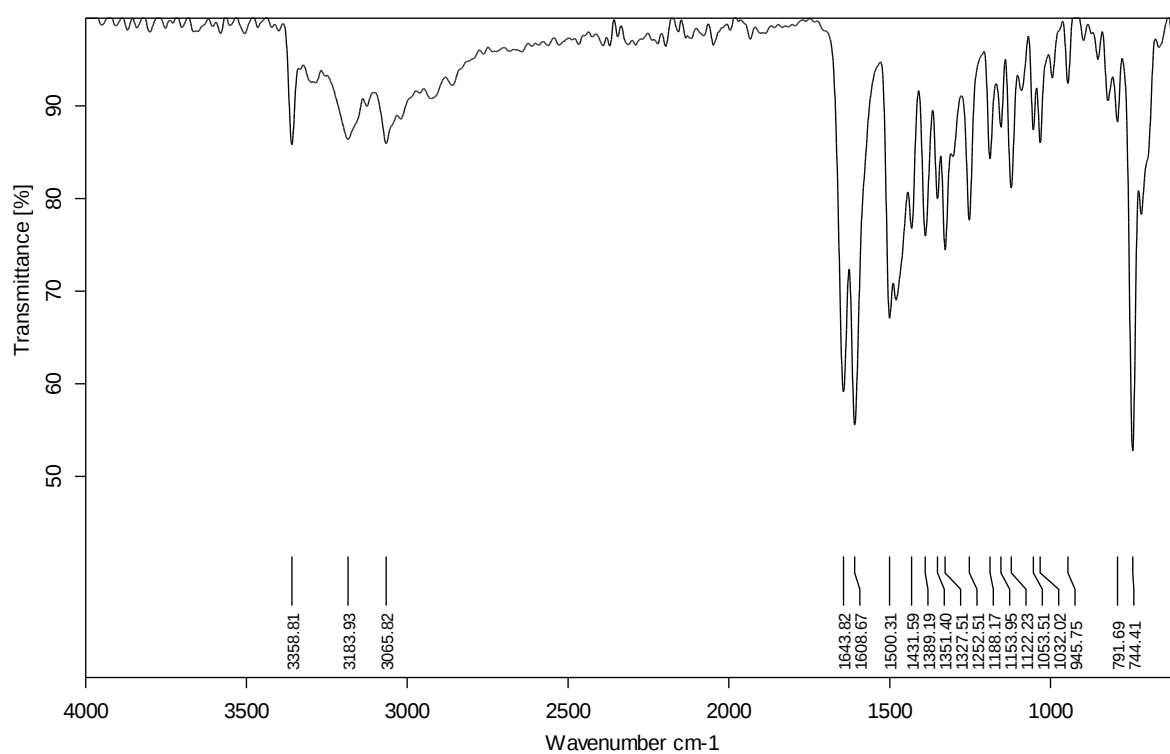


Figure S9: IR Spectrum of 3d

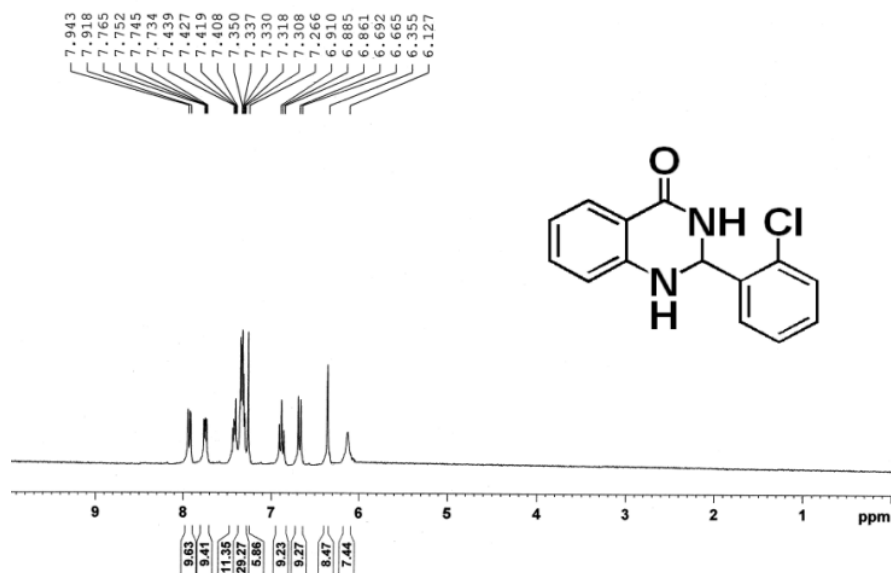


Figure S10: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 3d

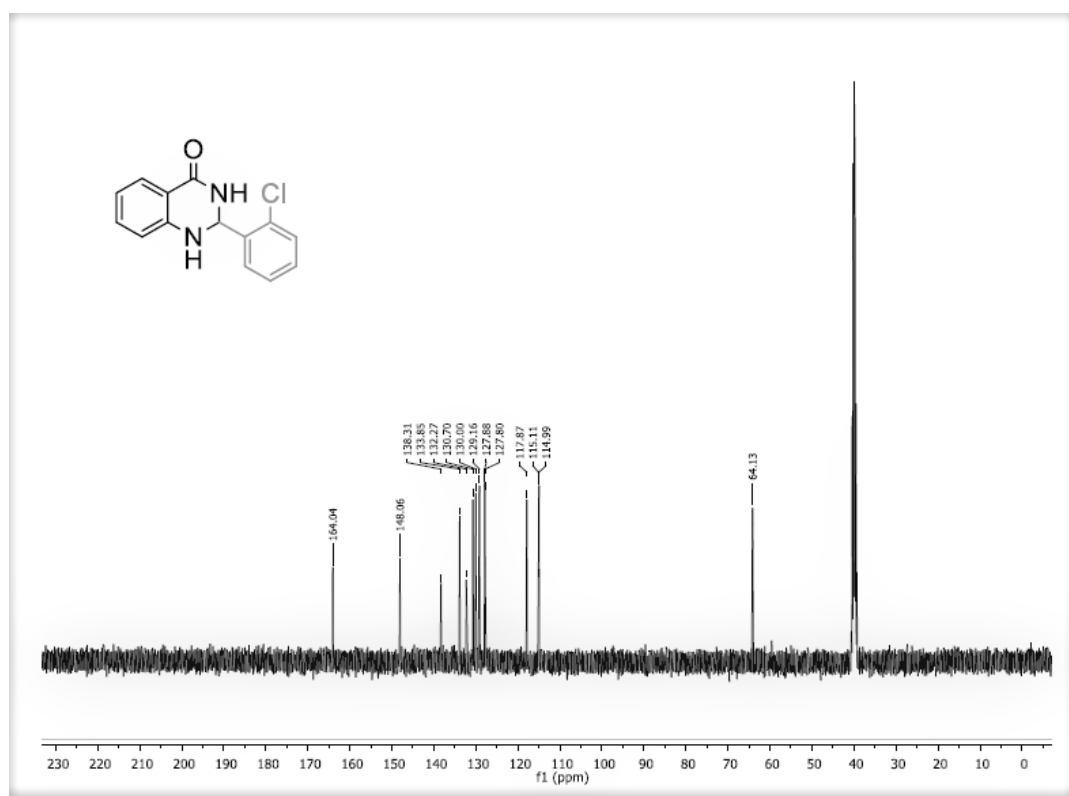


Figure S11: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of 3d

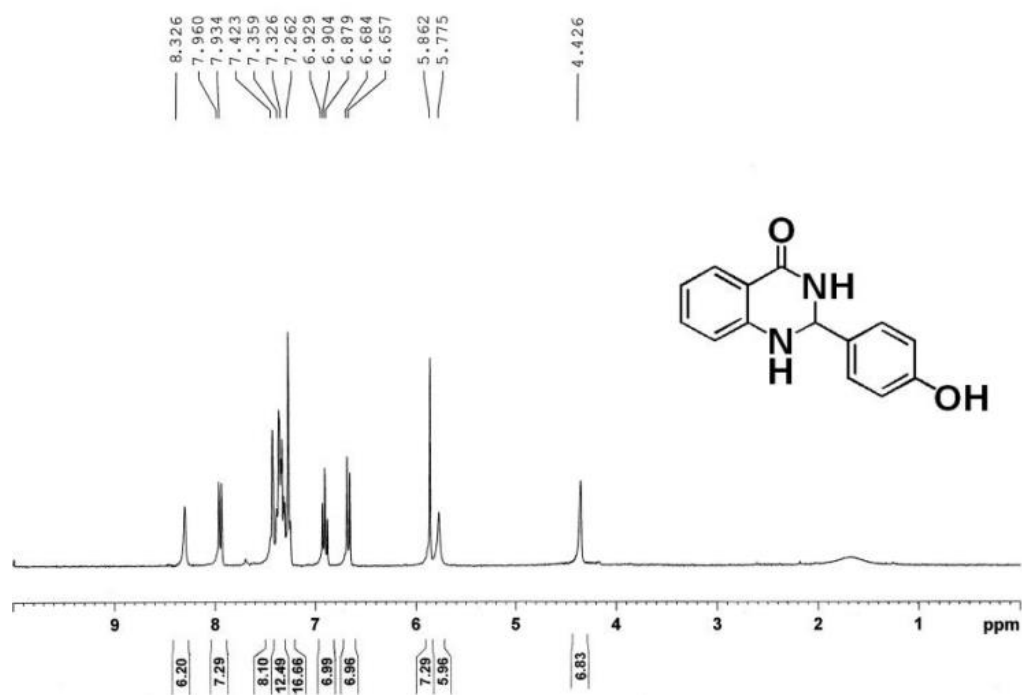


Figure S12: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 3e

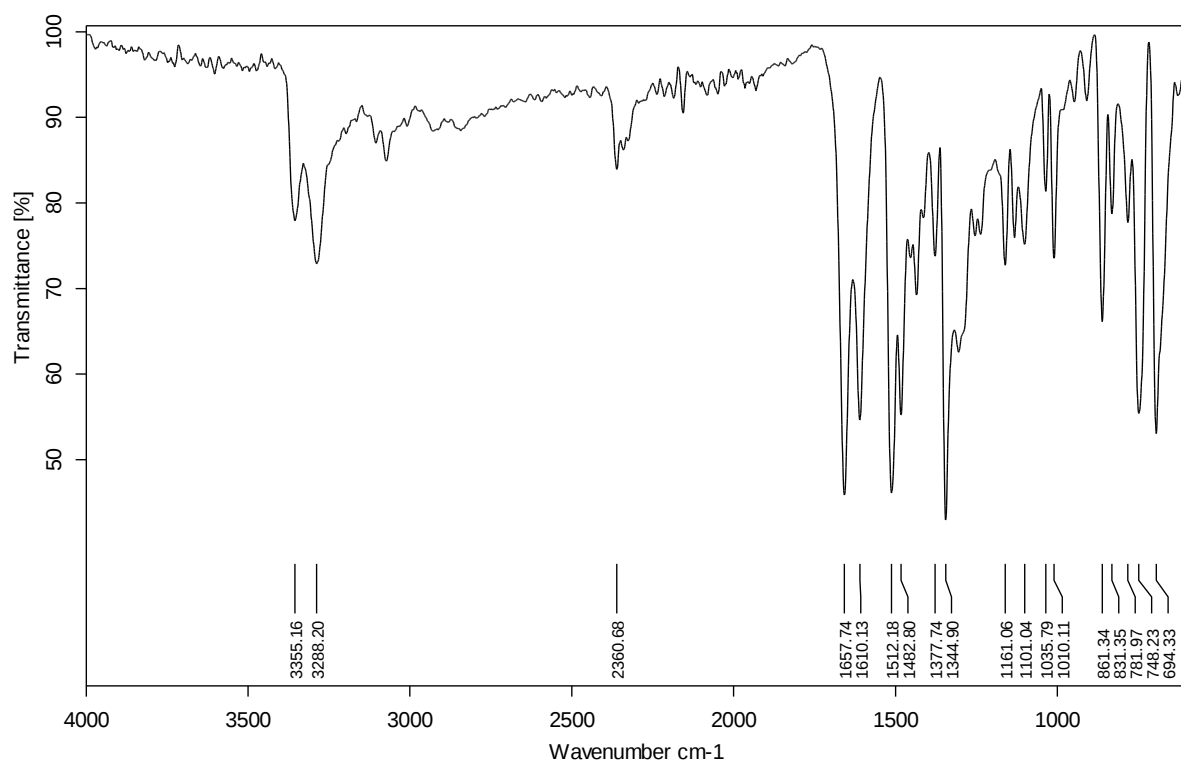


Figure S13: IR Spectrum of 3f

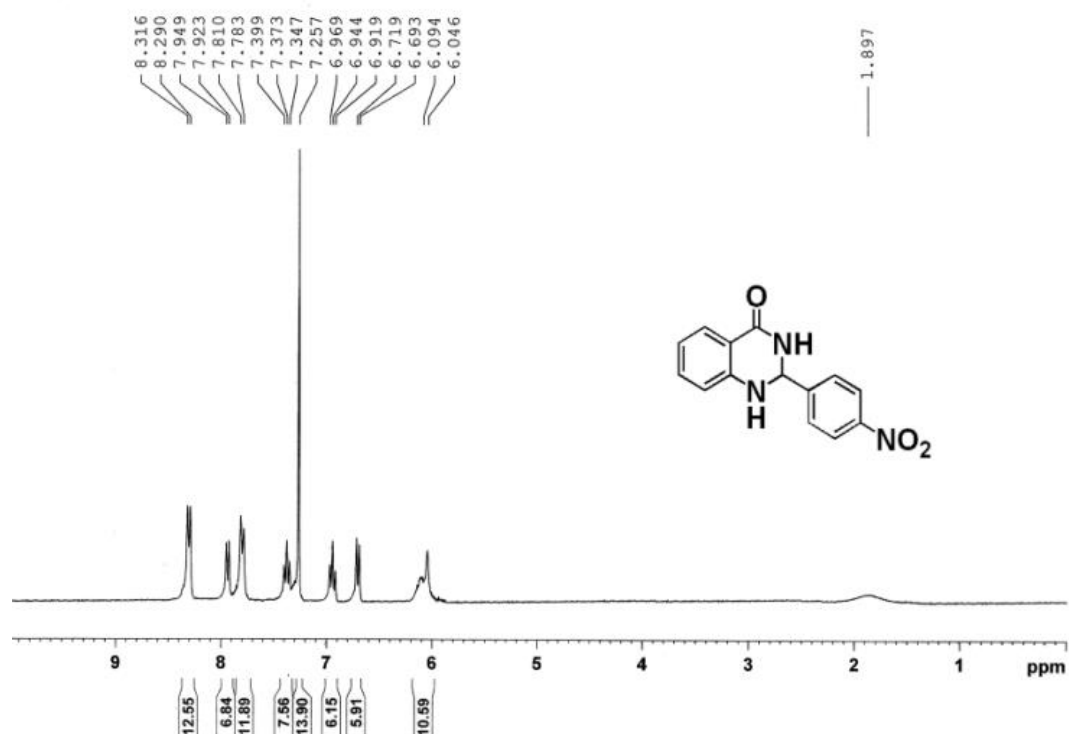


Figure S14: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 3f

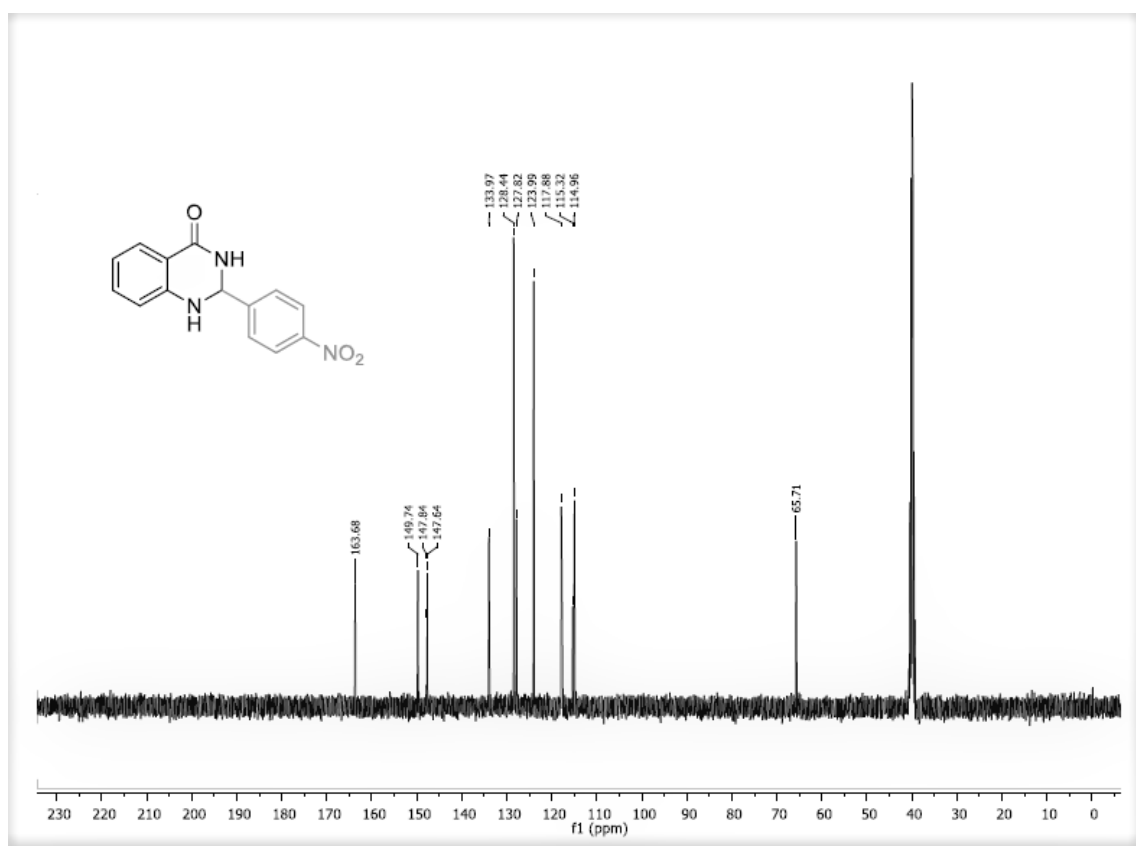


Figure S15: ^{13}C -NMR (100 MHz, CDCl_3) Spectrum of **3f**

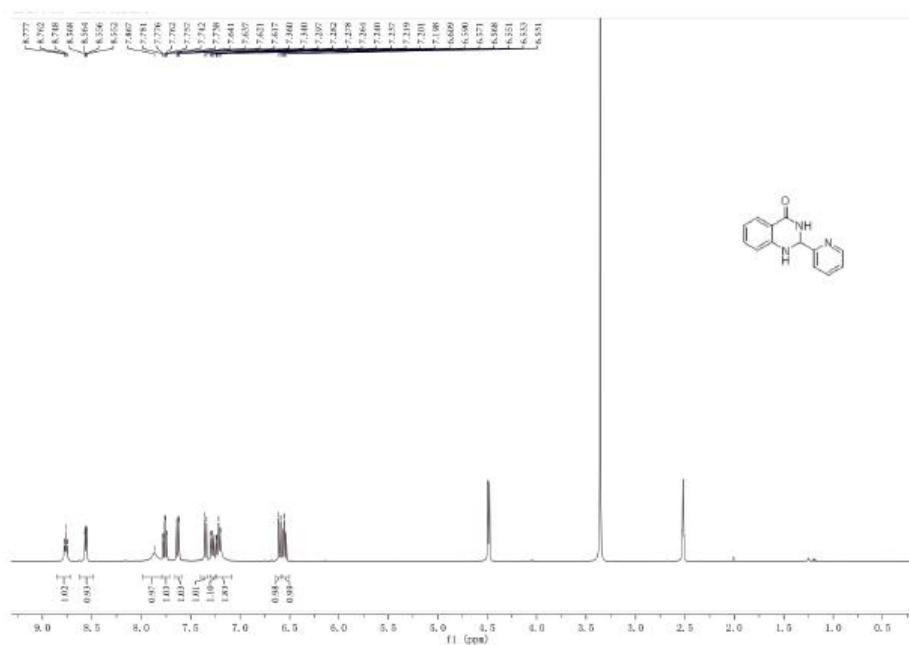


Figure S16: ^1H -NMR (400 MHz, CDCl_3) Spectrum of **3h**

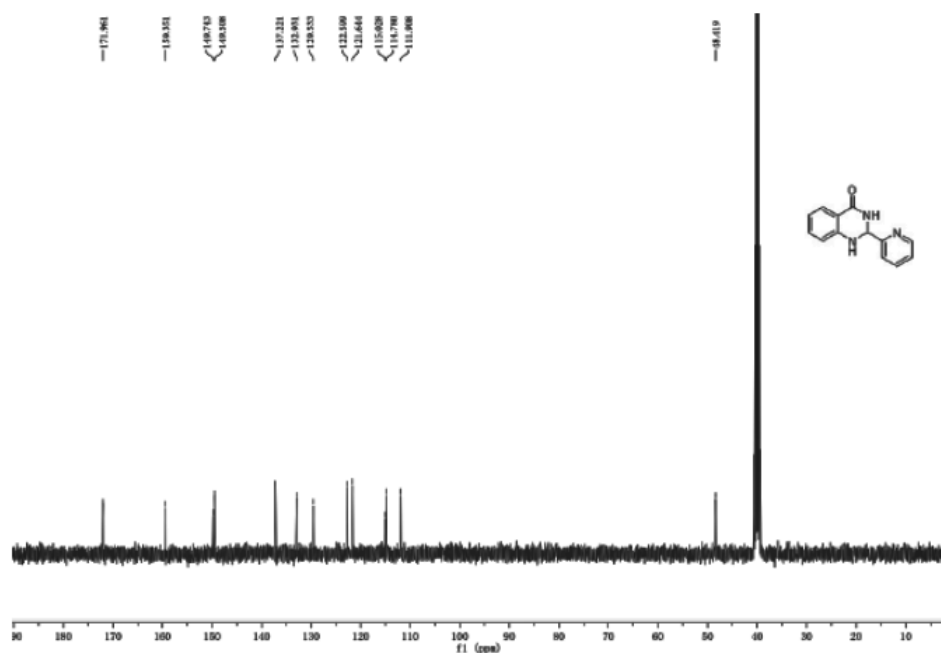


Figure S17: ^{13}C -NMR (100 MHz, CDCl_3) Spectrum of **3h**

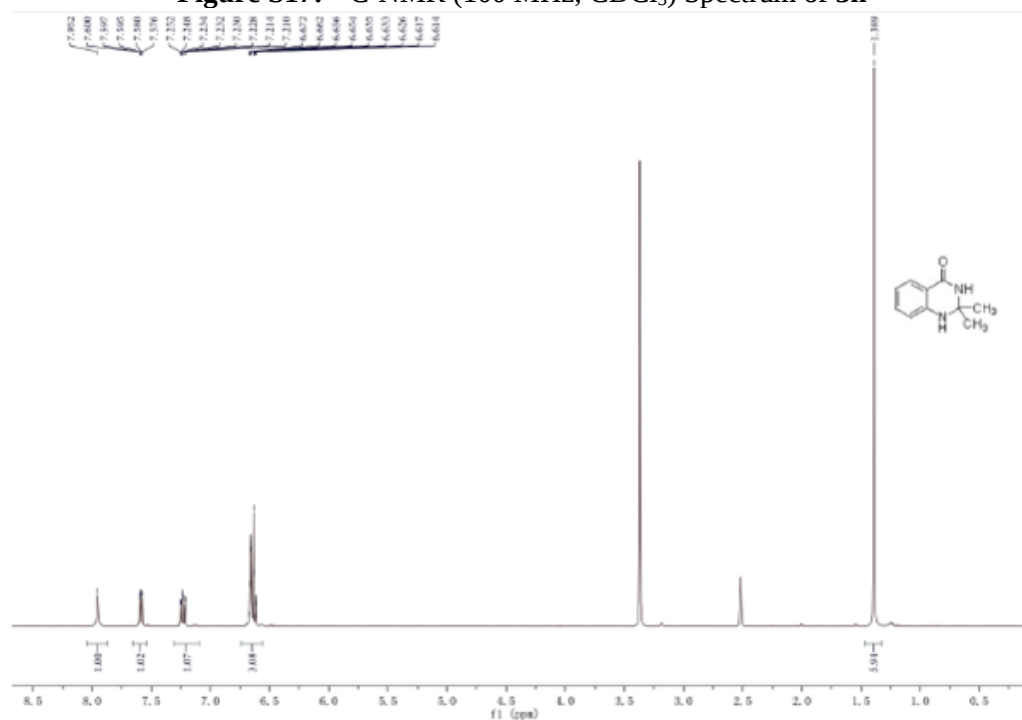


Figure S18: ^1H -NMR (400 MHz, CDCl_3) Spectrum of **3i**

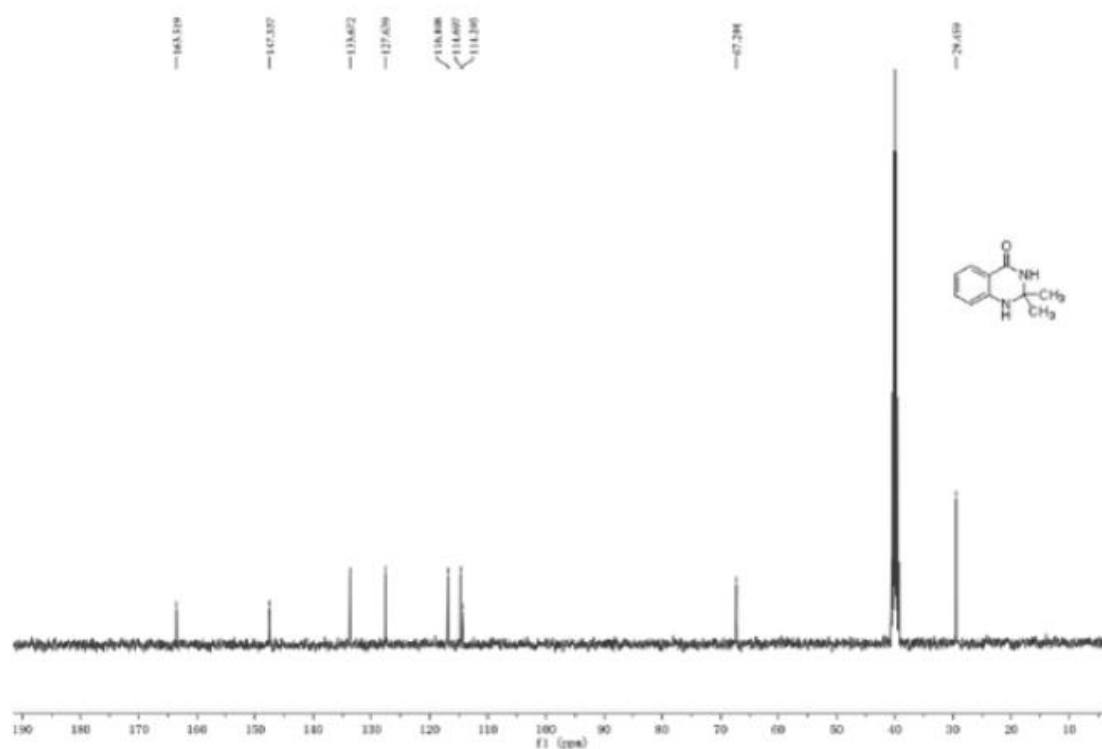


Figure S19: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of **3i**

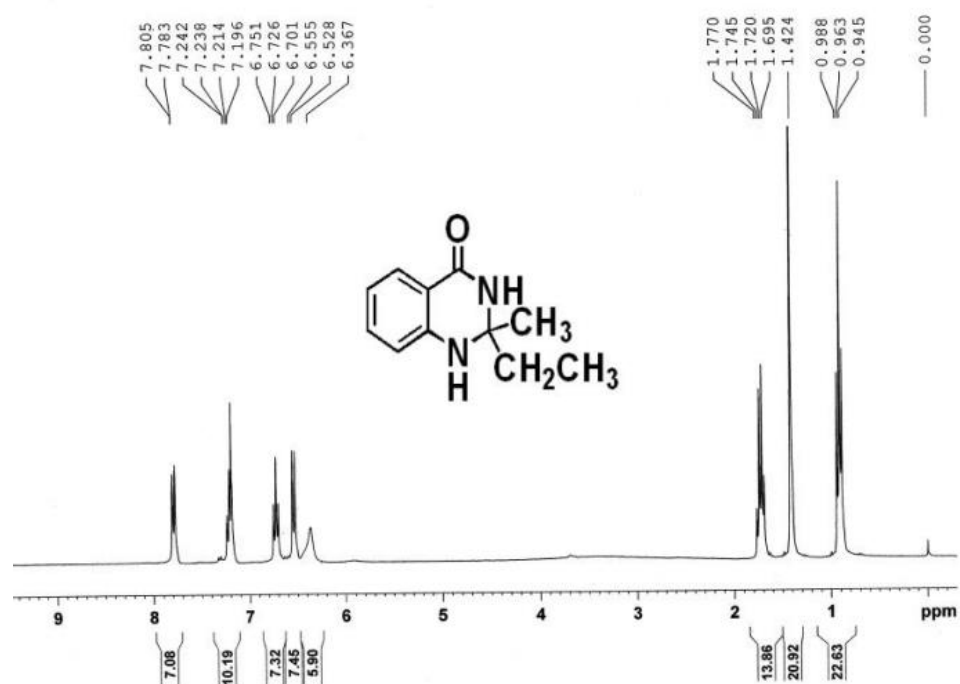


Figure S20: ¹H-NMR (400 MHz, CDCl₃) Spectrum of **3j**

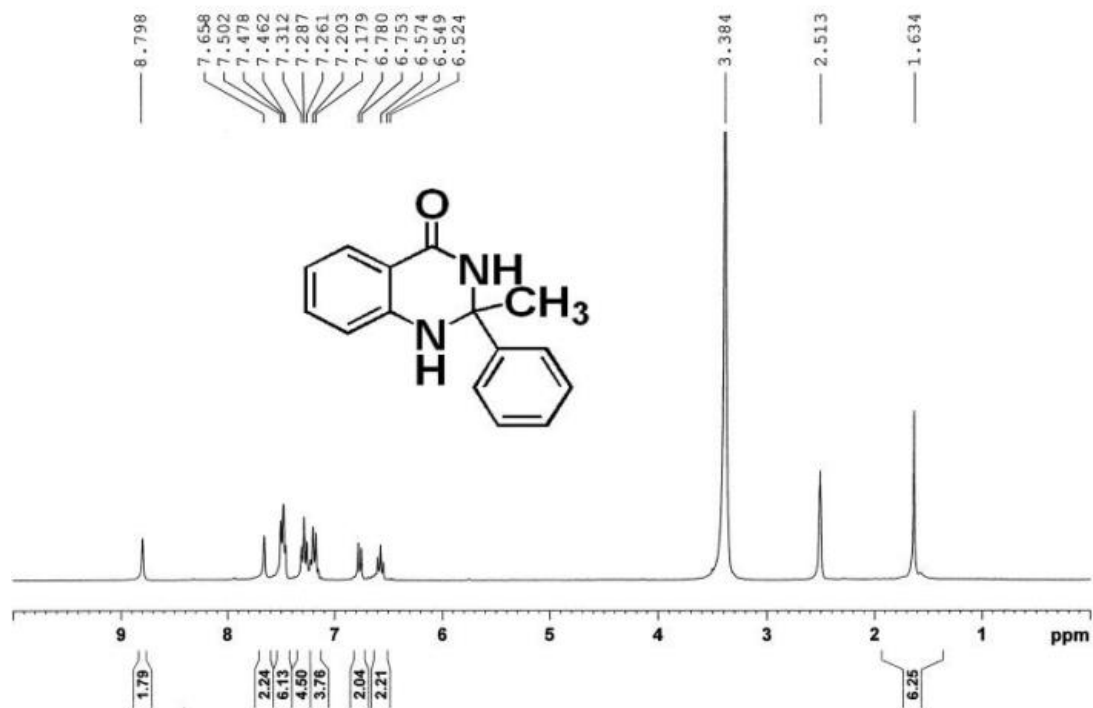


Figure S21: ¹H-NMR (400 MHz, CDCl₃) Spectrum of **3k**

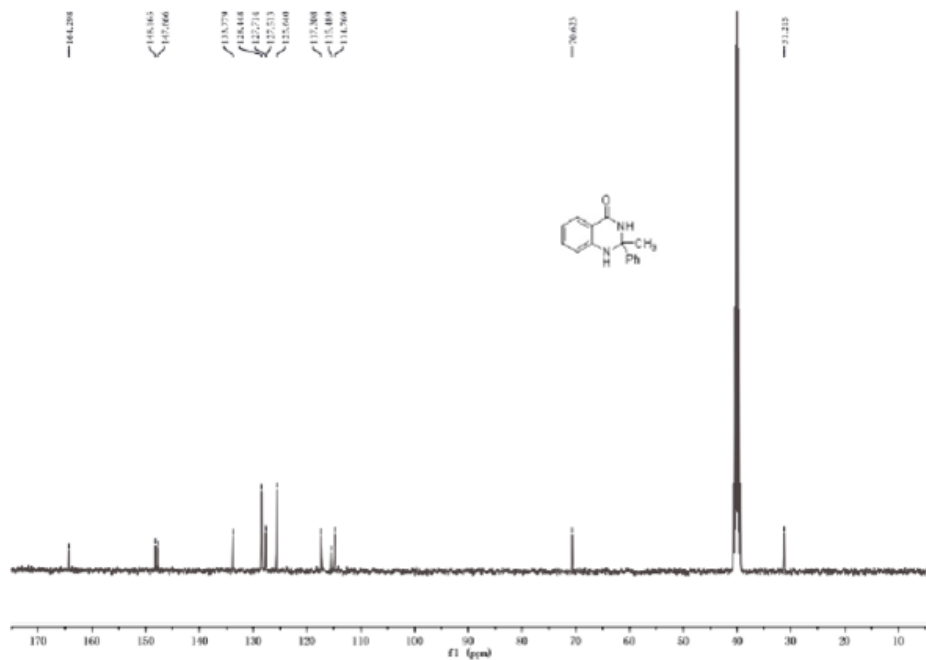


Figure S22: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of **3k**

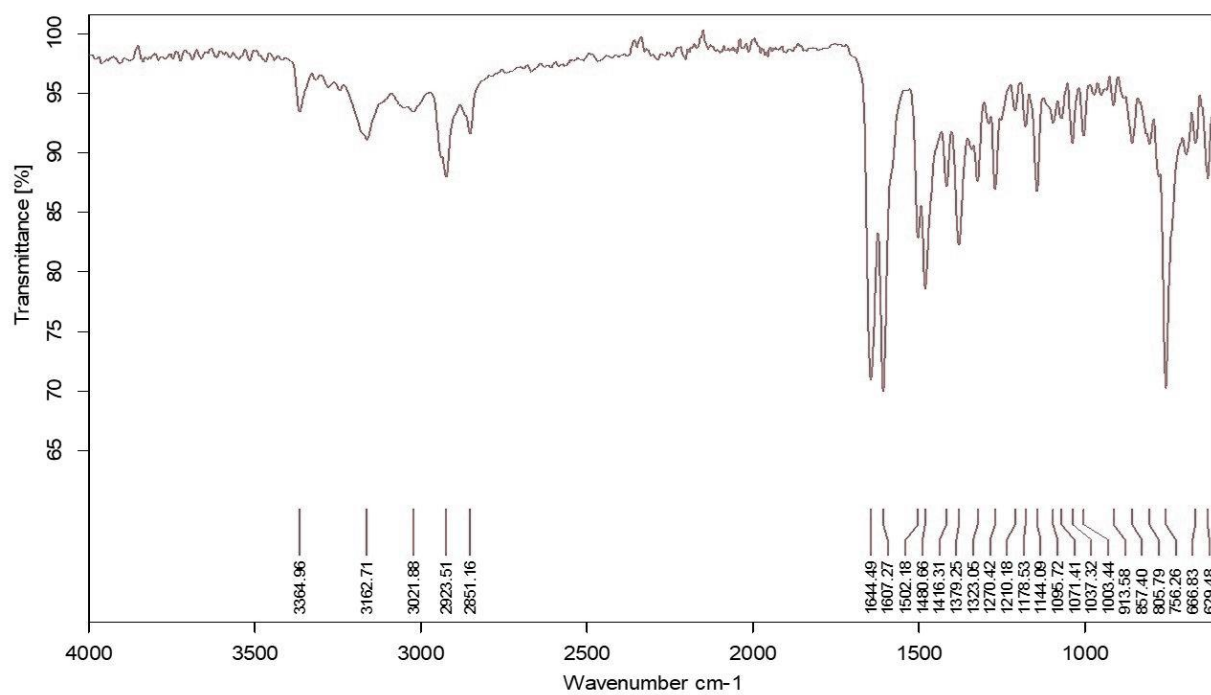


Figure S23: IR Spectrum of 3l

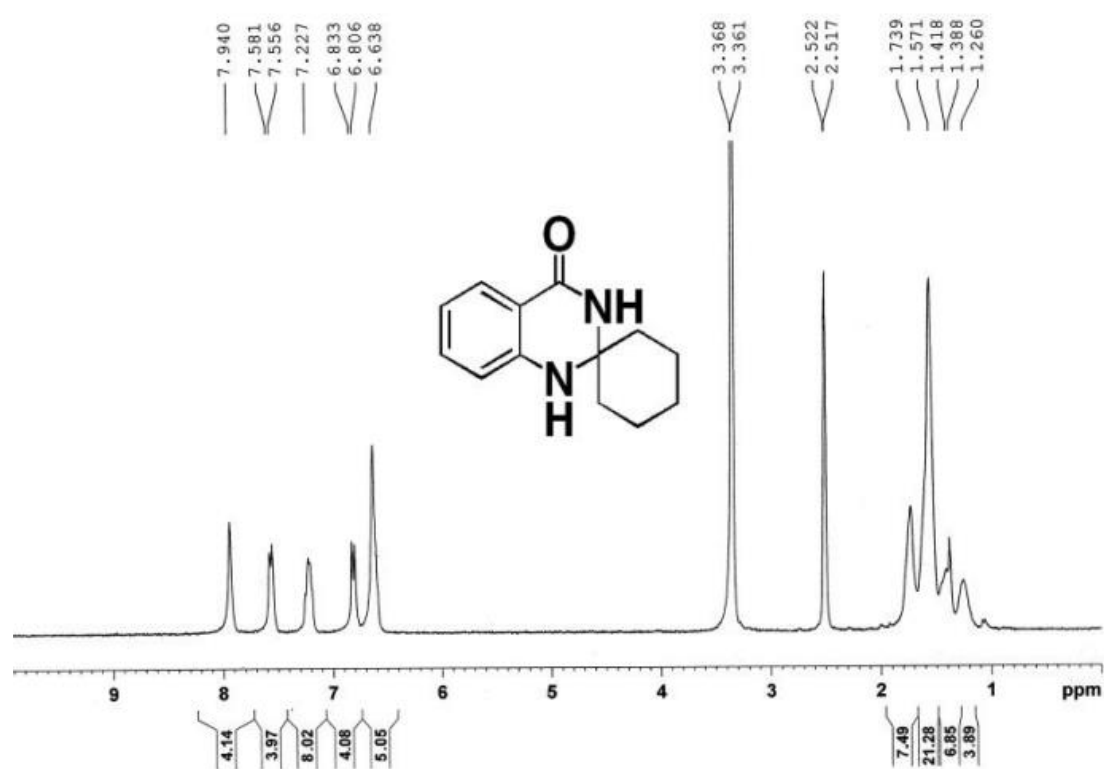


Figure S24: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 3l

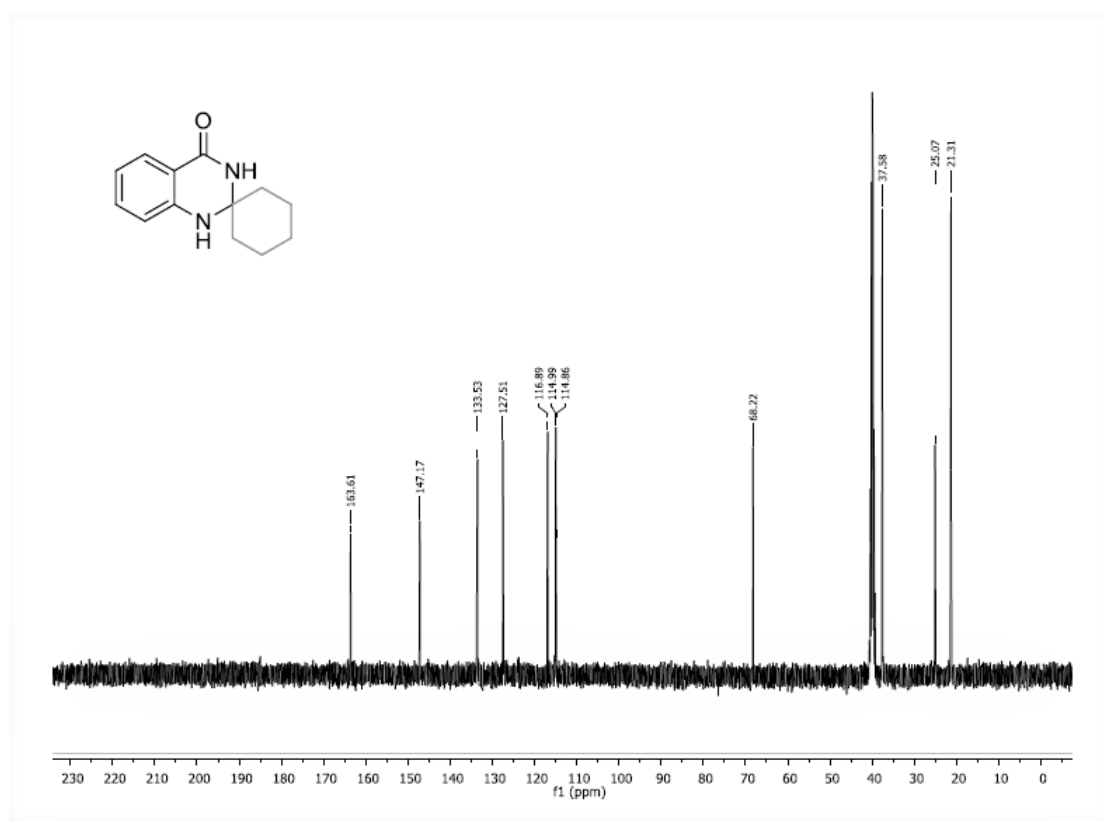


Figure S25: ^{13}C -NMR (100 MHz, CDCl_3) Spectrum of **3l**

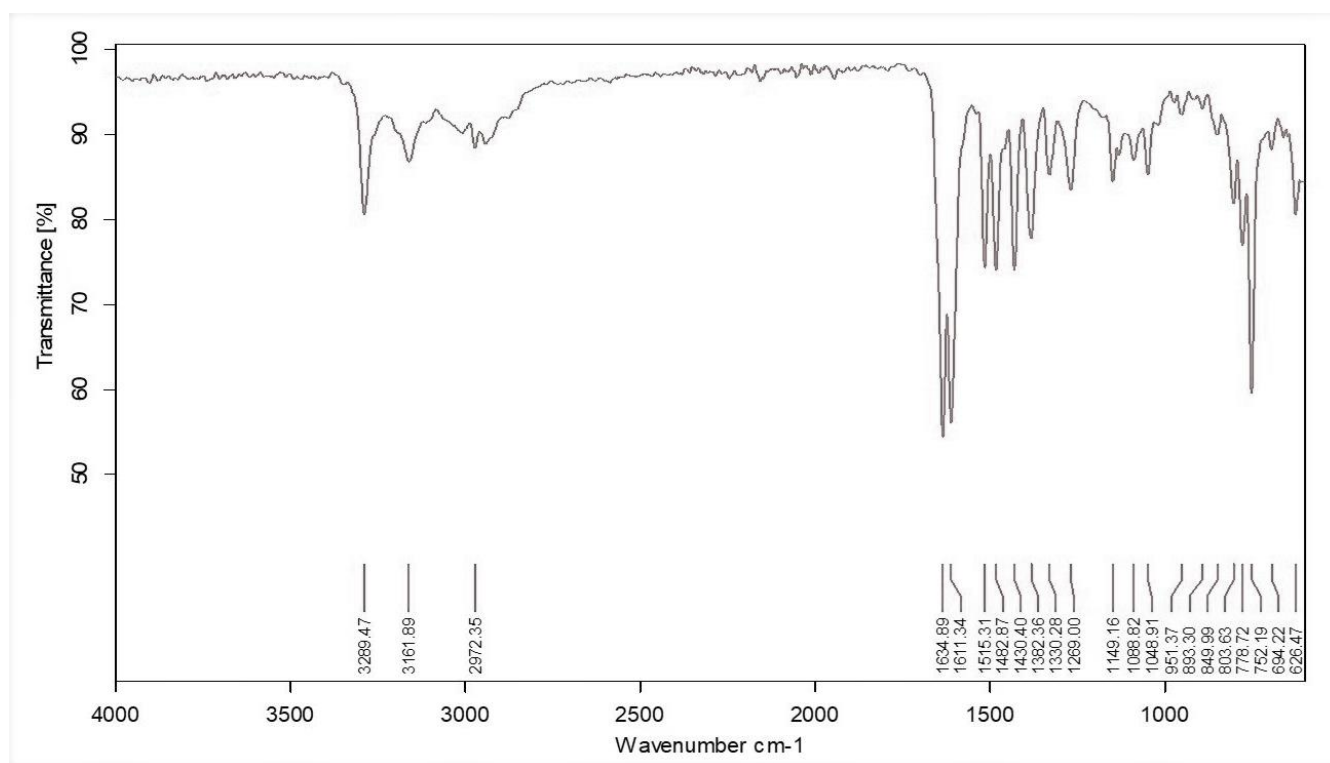


Figure S26: IR spectrum of **3m**

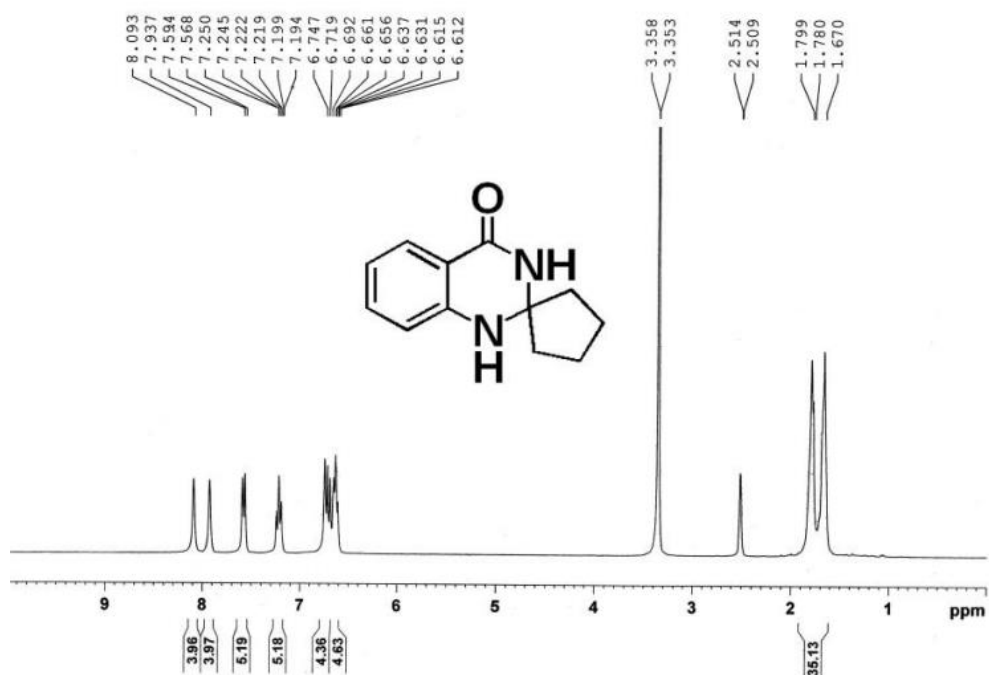


Figure S27: ¹H-NMR (400 MHz, CDCl₃) Spectrum of **3m**

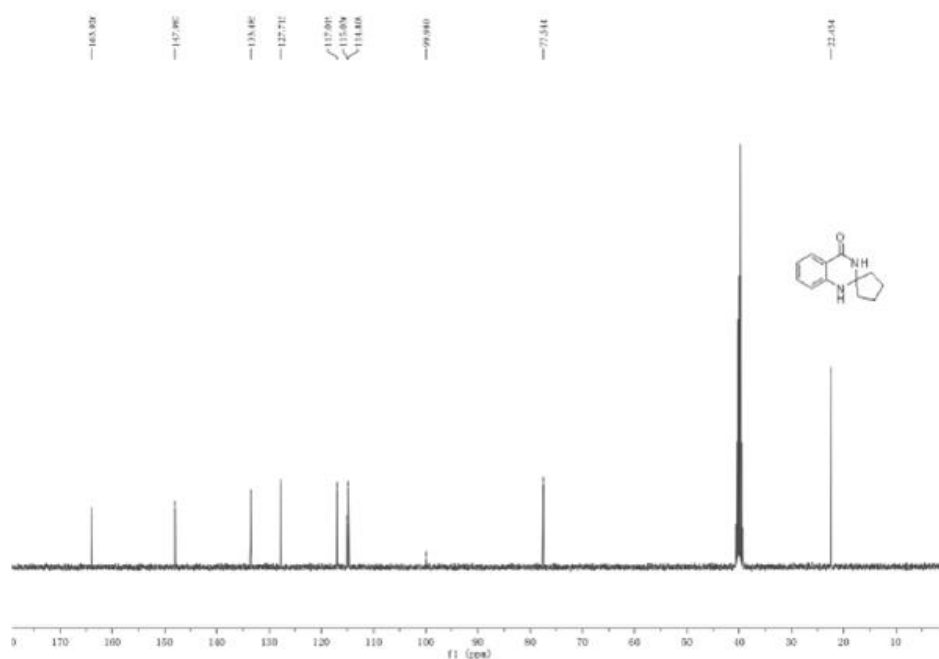


Figure S28: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of **3m**

