

Supporting Information

A Choline hydroxide catalyzed synthesis of 2,3-dihydroquinazolin-4(1H)-ones in an aqueous medium

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Detailed Characterization of compounds:

- 1) **2-phenyl-2,3-dihydroquinazolin-4(1H)-one:** White Solid; m.p. 226-228°C; IR (in cm⁻¹): 3295, 3162, 3051, 2924, 1651, 1600, 1436, 1294, 1157, 739, 630; ¹H NMR (δ in ppm 500 MHz, dmso) δ 8.25 (s, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.49 (d, J = 7.9 Hz, 2H), 7.38-7.31 (m, 3H), 7.23 (t, J = 7.6 Hz, 1H), 7.08 (s, 1H), 6.74 (d, J = 8.1 Hz, 1H), 6.66 (t, J = 7.5 Hz, 1H), 5.74 (s, 1H). ESI-MS : m/z (%) 222
Calculated for C₁₄H₁₂N₂O: 224
- 2) **2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one:** White Solid; m.p. 204-206°C; IR (in cm⁻¹): 3299, 3173, 3055, 2928, 1652, 1597, 1471, 1426, 1374, 1288, 1080, 790, 746, 658; ¹H NMR (δ in ppm 500 MHz, dmso) δ 8.30 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.49 (d, J = 8.4 Hz, 2H), 7.44 (d, J = 8.1 Hz, 2H), 7.24 (t, J = 7.6 Hz, 1H), 7.11 (s, 1H), 6.73 (d, J = 8.1 Hz, 1H), 6.67 (t, J = 7.5 Hz, 1H), 5.75 (s, 1H). ESI-MS : m/z (%) 258, Calculated C₁₄H₁₁ClN₂O: 258
- 3) **2-(4-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one:** White Solid; m.p. 277-279°C; IR (in cm⁻¹): 3296, 3162, 3012, 2904, 1641, 1602, 1504, 1453, 1246, 1160, 824, 736, 676; ¹H NMR (500 MHz, dmso) δ 9.47 (s, 1H), 8.06 (s, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.29 (d, J = 7.7 Hz, 2H), 7.22 (t, J = 7.6 Hz, 1H), 6.91 (s, 1H), 6.75 (d, J = 7.8 Hz, 2H), 6.72 (d, J = 8.1 Hz, 1H), 6.66 (t, J = 7.4 Hz, 1H), 5.64 (s, 1H). ESI-MS : m/z (%) 238
Calculated C₁₄H₁₂N₂O₂: 240
- 4) **2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one:** Yellowish Solid; m.p. 202-204°C; IR (in cm⁻¹): 3290, 3160, 3021, 2879, 1671, 1594, 1515, 1454, 1338, 1283, 1138, 940, 845, 760; ESI-MS : m/z (%) 269, Calculated C₁₄H₁₁ClN₂O: 269
- 5) **2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one:** White Solid; m.p. 192-194°C; IR (in cm⁻¹): 3292, 3171, 3042, 2938, 1731, 1651, 1603, 1497, 1299, 1242, 1167, 1026, 795, 751, 667; ¹H NMR (500 MHz, dmso) δ 8.18 (s, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.40 (d, J = 8.3 Hz, 2H), 7.22 (t, J = 7.6 Hz, 1H), 7.00 (s, 1H), 6.93 (d, J = 8.2 Hz, 2H), 6.72 (d, J = 8.1 Hz, 1H), 6.66 (t, J = 7.5 Hz, 1H), 5.69 (s, 1H), 3.73 (s, 3H). ESI-MS : m/z (%) 254, Calculated C₁₅H₁₄N₂O₂: 254
- 6) **2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one:** White Solid; m.p. 228-230°C; IR (in cm⁻¹): 3304, 3178, 3058, 2854, 1655, 1599, 1431, 1371, 1291, 1162, 1013, 741, 647, 600; ¹H NMR (500 MHz, dmso) δ 8.19 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.36 (d, J = 7.4 Hz, 2H), 7.22 (t, J = 7.7 Hz, 1H), 7.17 (d, J = 7.6 Hz, 2H), 7.02 (s, 1H), 6.72 (d, J = 8.0 Hz, 1H), 6.65 (t, J = 7.4 Hz, 1H), 5.69 (s, 1H), 2.28 (s, 3H). ESI-MS : m/z (%) 237, Calculated C₁₅H₁₄N₂O: 238
- 7) **2-(4-(dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1H)-one:** White Solid; m.p. 216-218°C; IR (in cm⁻¹): 3287, 3172, 3041, 2886, 2791, 1651, 1603, 1492, 1427, 1339, 1292, 1153, 803, 741, 657; ¹H NMR (500 MHz, dmso) δ 8.07 (s, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.21 (t, J

- = 7.6 Hz, 1H), 6.91 (s, 1H), 6.72 (d, $J = 7.6$ Hz, 1H), 6.70 (d, $J = 7.6$ Hz, 2H), 6.65 (t, $J = 7.4$ Hz, 1H), 5.62 (s, 1H), 2.87 (s, 6H). ESI-MS : m/z (%) 265, Calculated $C_{16}H_{17}N_3O$: 267
- 8) **2-(2-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 173-175°C; IR (in cm^{-1}): 3395, 3295, 3066, 2949, 1643, 1598, 1471, 1360, 1238, 1154, 1092, 1016, 817, 750, 681, 579; ESI-MS : m/z (%) 254, Calculated $C_{15}H_{14}N_2O_2$: 254
- 9) **2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 204-206°C; IR (in cm^{-1}): 3352, 3284, 3176, 3056, 2914, 1601, 1463, 1383, 1315, 1248, 1182, 1111, 1035, 805, 737, 610; ESI-MS : m/z (%) 258, Calculated $C_{14}H_{11}ClN_2O$: 258
- 10) **2-(3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 148-150°C; IR (in cm^{-1}): 3283, 3184, 3023, 2915, 1640, 1601, 1477, 1444, 1384, 1246, 1135, 1045, 931, 736, 688; ESI-MS : m/z (%) 254, Calculated $C_{15}H_{14}N_2O_2$: 254
- 11) **2-(3-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 185-186°C; IR (in cm^{-1}): 3283, 3184, 3060, 1647, 1602, 1475, 1430, 1375, 1328, 1160, 938, 868, 798, 749, 696, 651; ESI-MS : m/z (%) 258, Calculated $C_{14}H_{11}ClN_2O$: 258
- 12) **2-isopropyl-2,3-dihydroquinazolin-4(1H)-one**: White Solid; mp 160-170°C; IR (in cm^{-1}): 3275, 3181, 3065, 2963, 1639, 1607, 1514, 1447, 1385, 1299, 1150, 1029, 744, 610; 1H NMR (500 MHz, dmsO) δ 7.85 (s, 1H), 7.54 (d, $J = 7.7$ Hz, 1H), 7.20 (t, $J = 7.6$ Hz, 1H), 6.74 (d, $J = 8.1$ Hz, 1H), 6.61 (t, $J = 7.4$ Hz, 1H), 6.50 (s, 1H), 4.50 (s, 1H), 1.85 (tq, $J = 13.3, 6.5$ Hz, 1H), 0.91 (dd, $J = 11.5, 6.9$ Hz, 6H). ESI-MS : m/z (%) 190, Calculated $C_{11}H_{14}N_2O$: 190
- 13) **2-ethyl-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 120-122°C; IR (in cm^{-1}): 3285, 3181, 3072, 2965, 1639, 1606, 1440, 1383, 1294, 1244, 1147, 1034, 744, 659, 652; 1H NMR (500 MHz, dmsO) δ 7.88 (s, 1H), 7.56 (d, $J = 7.6$ Hz, 1H), 7.21 (t, $J = 7.6$ Hz, 1H), 6.71 (d, $J = 8.1$ Hz, 1H), 6.63 (t, $J = 7.4$ Hz, 1H), 6.55 (s, 1H), 4.64 (t, $J = 4.7$ Hz, 1H), 1.67 – 1.59 (m, 2H), 0.92 (t, $J = 7.4$ Hz, 3H). ESI-MS : m/z (%) 174, Calculated $C_{10}H_{12}N_2O$: 176
- 14) **2-hexyl-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 156-158°C; IR (in cm^{-1}): 3316, 3203, 3070, 2921, 2850, 1632, 1610, 1495, 1434, 1379, 1309, 1151, 1105, 1024, 751, 639, 573; 1H NMR (500 MHz, dmsO) δ 7.84 (s, 1H), 7.56 (d, $J = 7.6$ Hz, 1H), 7.21 (t, $J = 7.6$ Hz, 1H), 6.71 (d, $J = 8.1$ Hz, 1H), 6.63 (t, $J = 7.4$ Hz, 1H), 6.53 (s, 1H), 4.66 (t, $J = 5.0$ Hz, 1H), 1.60 (dd, $J = 15.1, 5.9$ Hz, 2H), 1.44–1.34 (m, 2H), 1.26 (s, 6H), 0.85 (t, $J = 6.5$ Hz, 3H). ESI-MS : m/z (%) 232, Calculated $C_{14}H_{20}N_2O$: 232
- 15) **2-(thiophen-2-yl)-2,3-dihydroquinazolin-4(1H)-one**: Off white Solid; m.p. 212-216°C; IR (in cm^{-1}): 3282, 3166, 3028, 2930, 1649, 1601, 1511, 1433, 1374, 1296, 1166, 1033, 808, 756, 693, 570; 1H NMR (500 MHz, dmsO) δ 8.41 (s, 1H), 7.60 (d, $J = 7.7$ Hz, 1H), 7.44 (d, $J = 5.0$ Hz, 1H), 7.28 – 7.20 (m, 2H), 7.11 (s, 1H), 6.97 (t, $J = 4.2$ Hz, 1H), 6.75 (d, $J = 8.1$ Hz, 1H), 6.69 (t, $J = 7.5$ Hz, 1H), 6.00 (s, 1H). ESI-MS : m/z (%) 230.70, Calculated $C_{12}H_{10}N_2OS$: 230.05
- 16) **2-(furan-2-yl)-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 165-167°C; IR (in cm^{-1}): 3241, 3178, 3022, 2913, 1606, 1516, 1457, 1388, 1306, 1248, 1125, 999, 817, 720, 587; 1H NMR (500 MHz, dmsO) δ 8.36 (s, 1H), 7.60 (d, $J = 5.2$ Hz, 2H), 7.22 (t, $J = 7.5$ Hz, 1H), 7.17 (s, 1H), 6.73 (d, $J = 8.0$ Hz, 1H), 6.66 (t, $J = 7.4$ Hz, 1H), 6.36 (m, 1H), 6.25 (d, $J = 3.8$ Hz, 1H), 5.73 (s, 1H). ESI-MS : m/z (%) 214, Calculated $C_{13}H_{11}N_3O$: 214
- 17) **2-(pyridin-2-yl)-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 184-186°C. IR (in cm^{-1}): 3282, 3177, 3033, 2917, 2856, 1655, 1602, 1501, 1455, 1383, 1307, 1245, 1168, 1121, 993, 810, 740, 670, 623; 1H NMR (500 MHz, DMSO- d_6) δ 8.54 (d, $J = 5.4$ Hz, 1H), 8.37 (s, 1H), 7.81 (td, $J = 7.7, 1.8$ Hz, 1H), 7.58 (d, $J = 7.7$ Hz, 1H), 7.48 (d, $J = 7.9$ Hz, 1H), 7.33 (ddd, $J = 7.5, 4.8, 0.9$ Hz, 1H),

7.26 (s, 1H), 7.23 – 7.18 (m, 1H), 6.73 (d, $J = 8.1$ Hz, 1H), 6.64 (t, $J = 7.8$ Hz, 1H), 5.69 (s, 1H). ESI-MS : m/z (%) 225, Calculated $C_{13}H_{11}N_3O$: 225

18) **7-chloro-2-phenyl-2,3-dihydroquinazolin-4(1H)-one**: White Solid; m.p. 185-187°C; IR (in cm^{-1}): 3287, 3169, 3038, 1651, 1597, 1511, 1460, 1413, 1355, 1295, 1125, 1071, 1012, 864, 809, 764, 682; 1H NMR (500 MHz, dmsO) δ 8.38 (s, 1H), 7.59 (d, $J = 8.3$ Hz, 1H), 7.47 (d, $J = 7.3$ Hz, 2H), 7.42 – 7.32 (m, 5H), 6.77 (s, 1H), 6.67 (d, $J = 8.3$ Hz, 1H), 5.79 (s, 1H). ESI-MS : m/z (%) 258, Calculated $C_{14}H_{11}ClN_2O$: 258

19) **Intermediate (E)-2-(benzylideneamino)benzotrile (Schiff Base)**: White Solid; 1H NMR (500 MHz, dmsO) δ 8.71 (s, 1H), 7.98 (d, $J = 6.8$ Hz, 2H), 7.85 (dd, $J = 7.7, 0.9$ Hz, 1H), 7.73 (td, $J = 8.2, 1.3$ Hz, 1H), 7.58 (m, 3H), 7.45 (d, $J = 8.1$ Hz, 1H), 7.40 (t, $J = 7.6$ Hz, 1H). ESI-MS : m/z (%) 206, Calculated $C_{14}H_{10}N_2$: 206

Figure S1: FT-IR of ChOH catalyst:

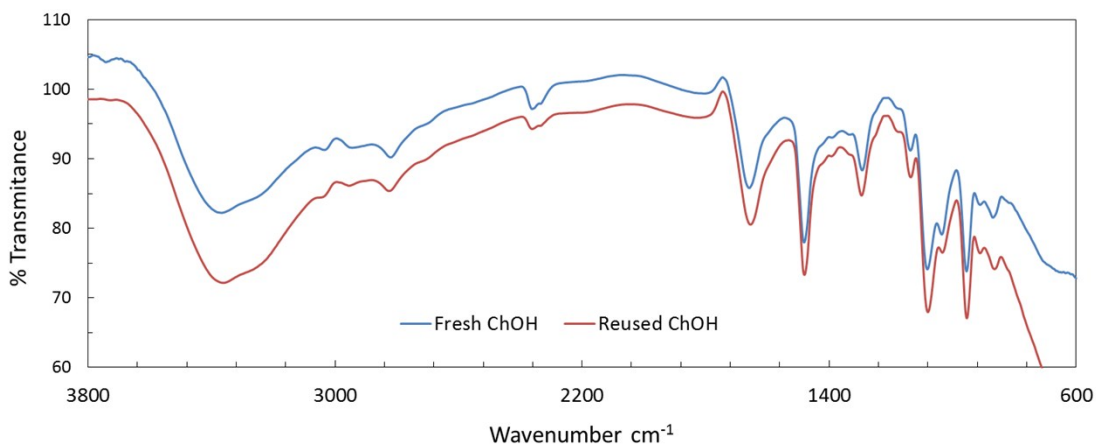


Figure S2: ¹H-NMR spectra of Intermediate Schiff base (*E*)-2-(benzylideneamino)benzonitrile:

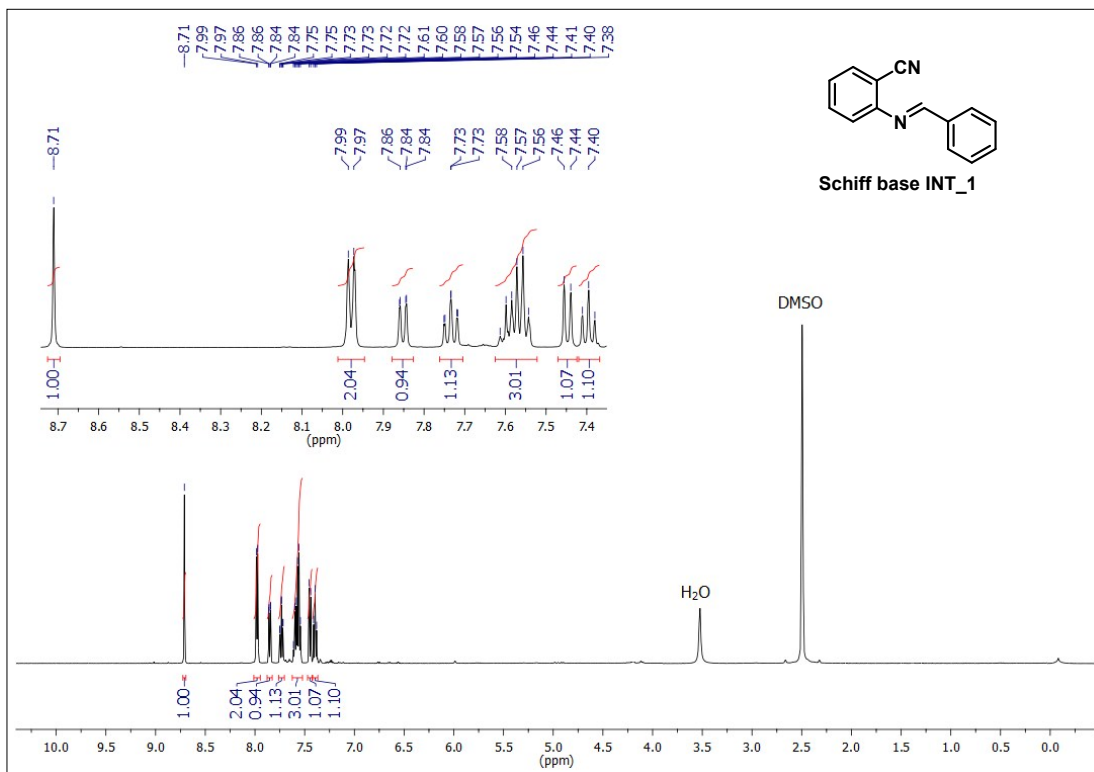


Figure S3: ¹H-NMR spectra of 2-phenyl-2,3-dihydroquinazolin-4(1H)-one:

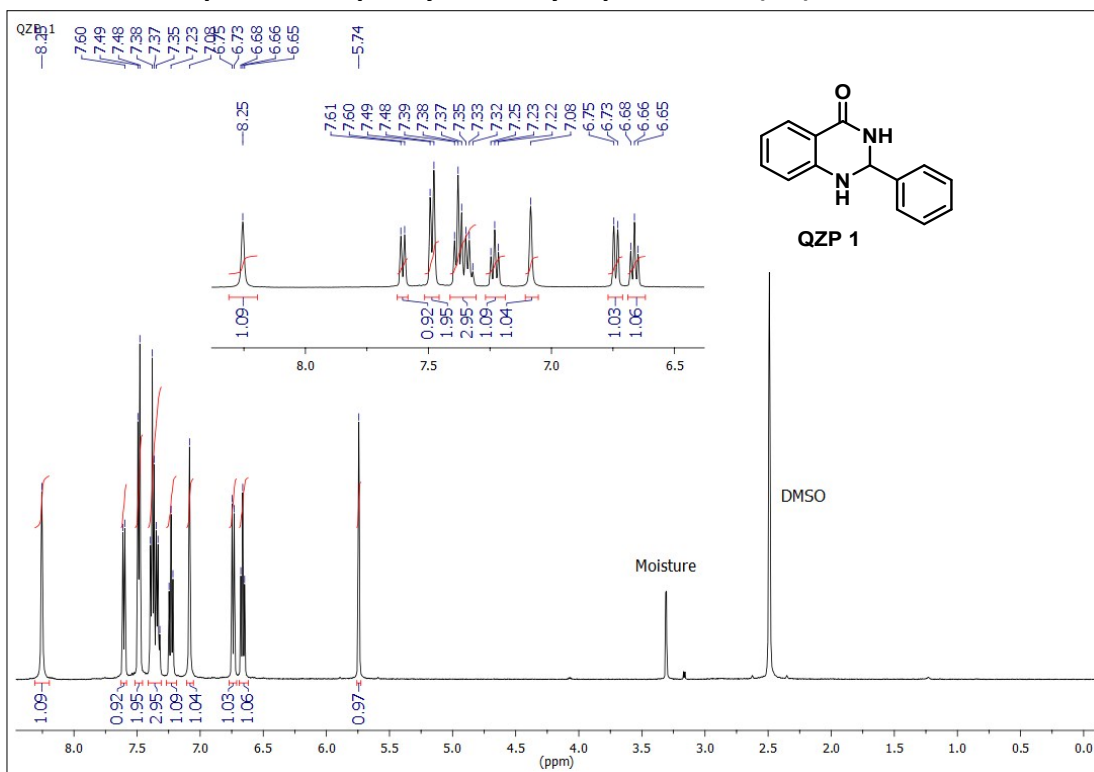


Figure S4: $^1\text{H-NMR}$ spectra of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one:

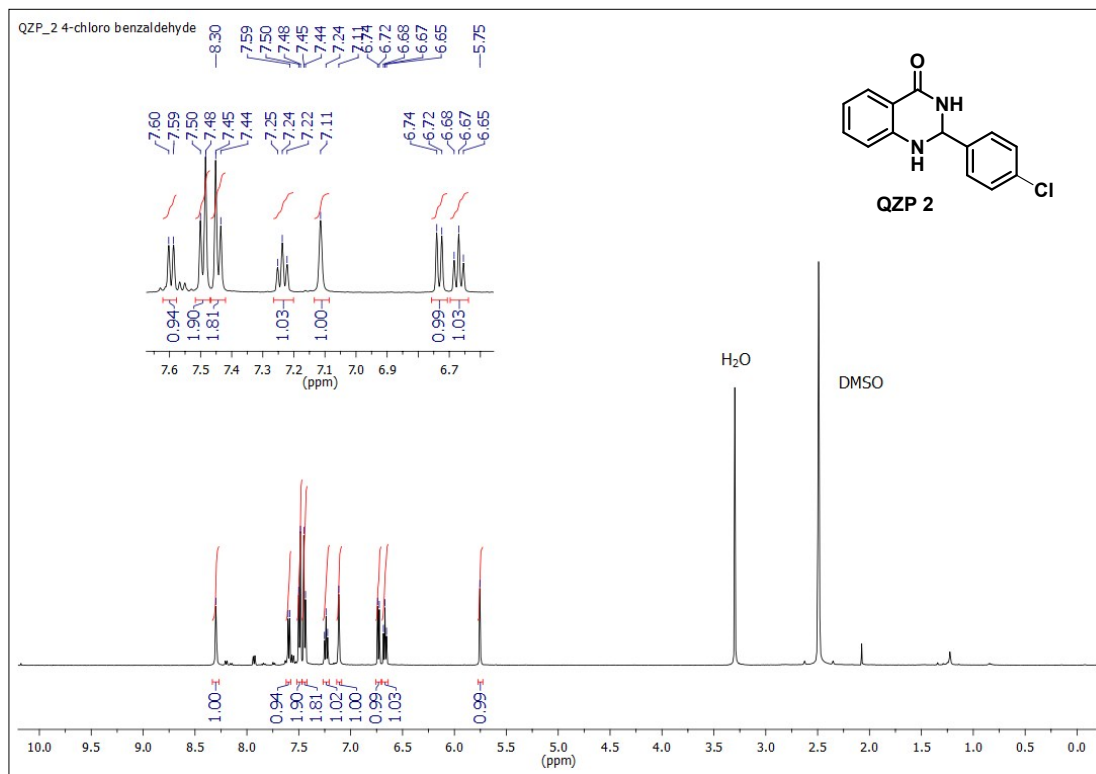


Figure S5: $^1\text{H-NMR}$ spectra of 2-(4-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one:

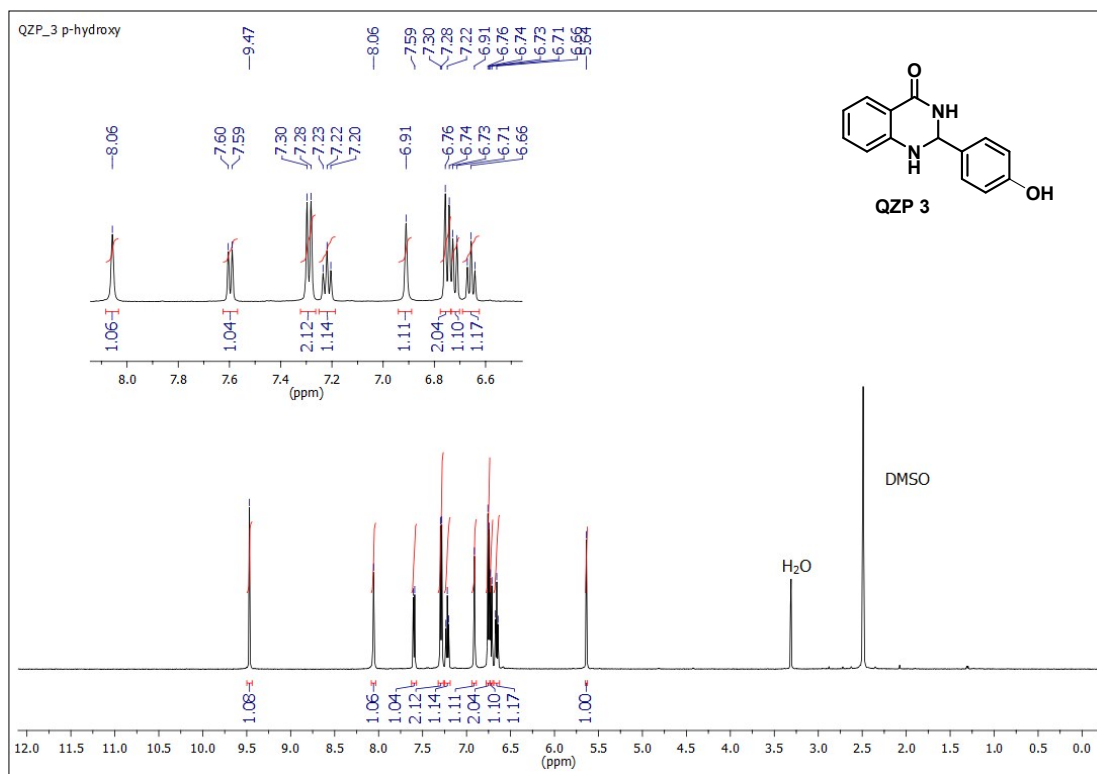


Figure S6: ¹H-NMR spectra of 2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one:

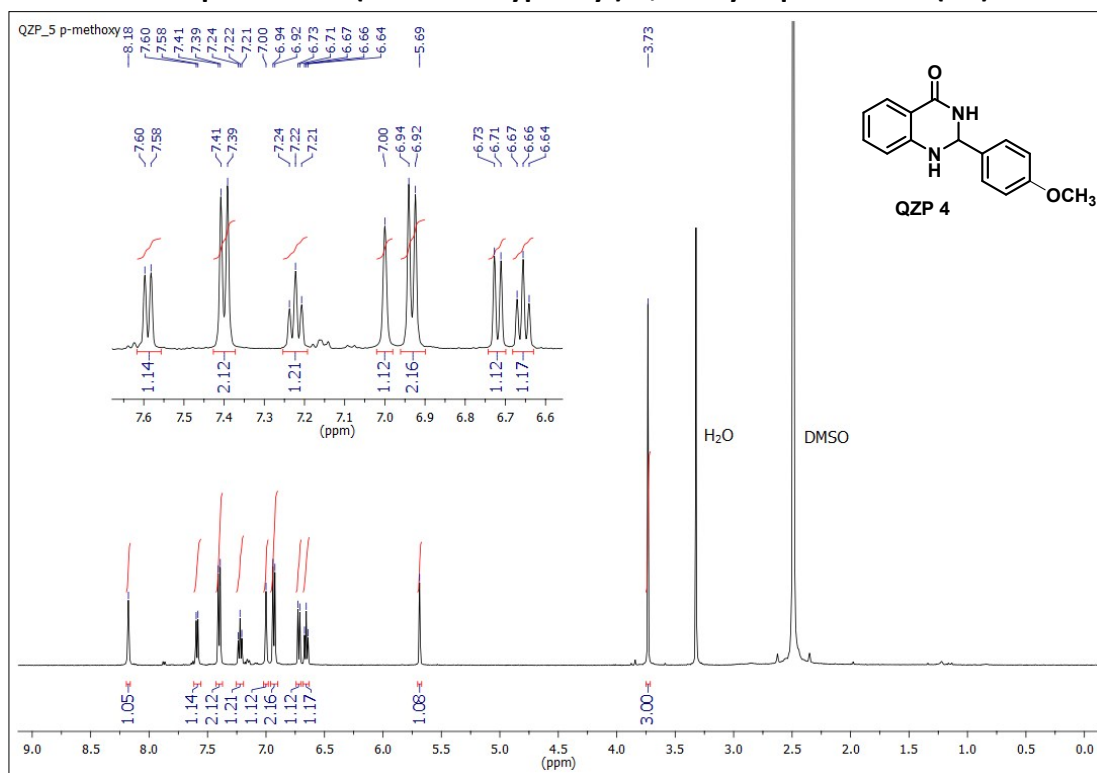


Figure S7: ¹H-NMR spectra of 2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one:

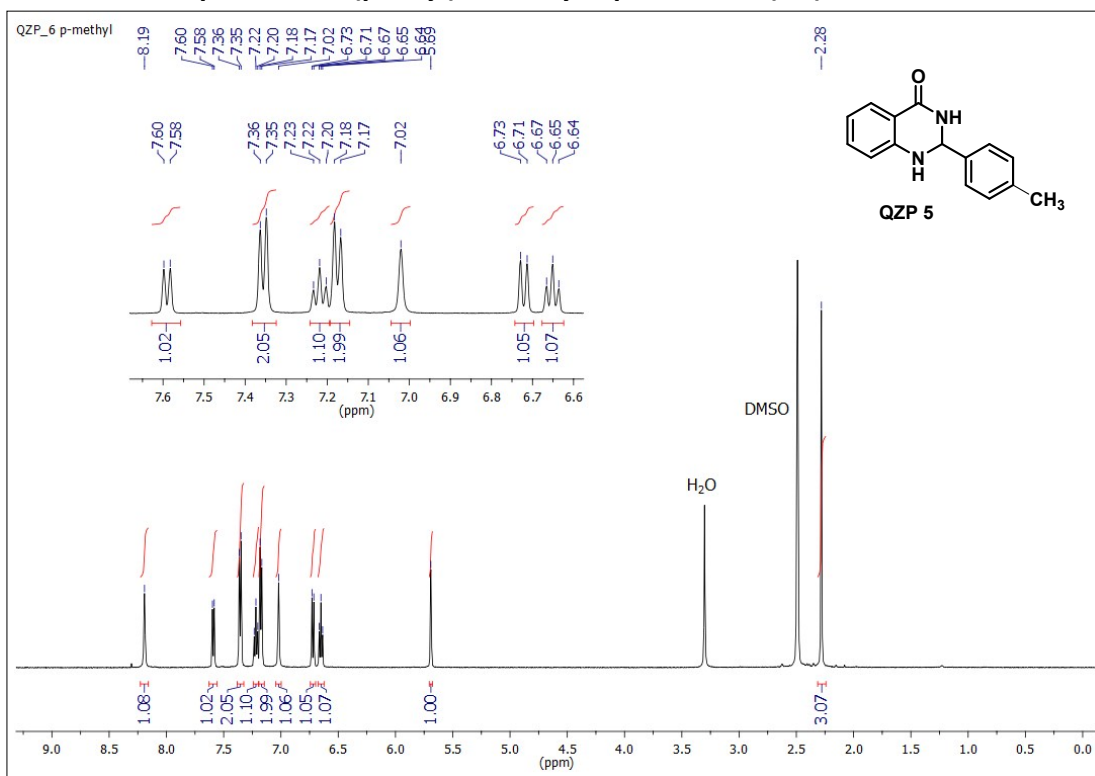


Figure S8: ¹H-NMR spectra of 2-(4-(dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1H)-one:

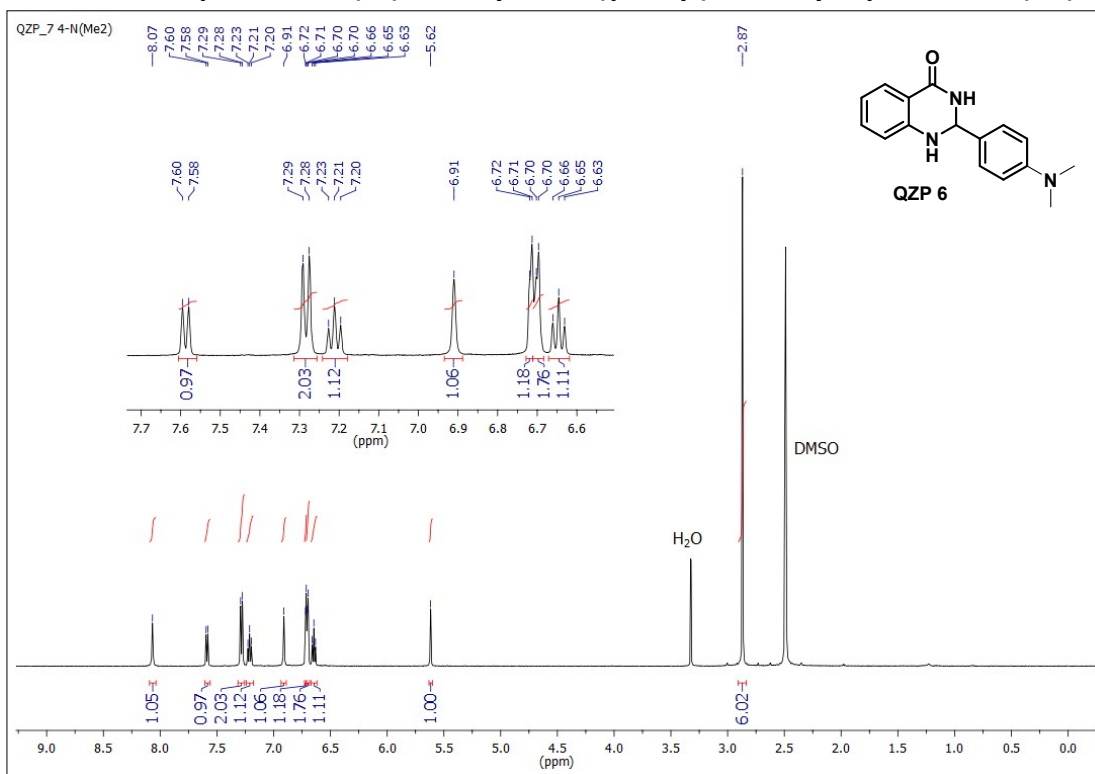


Figure S9: ¹H-NMR spectra of 2-isopropyl-2,3-dihydroquinazolin-4(1H)-one:

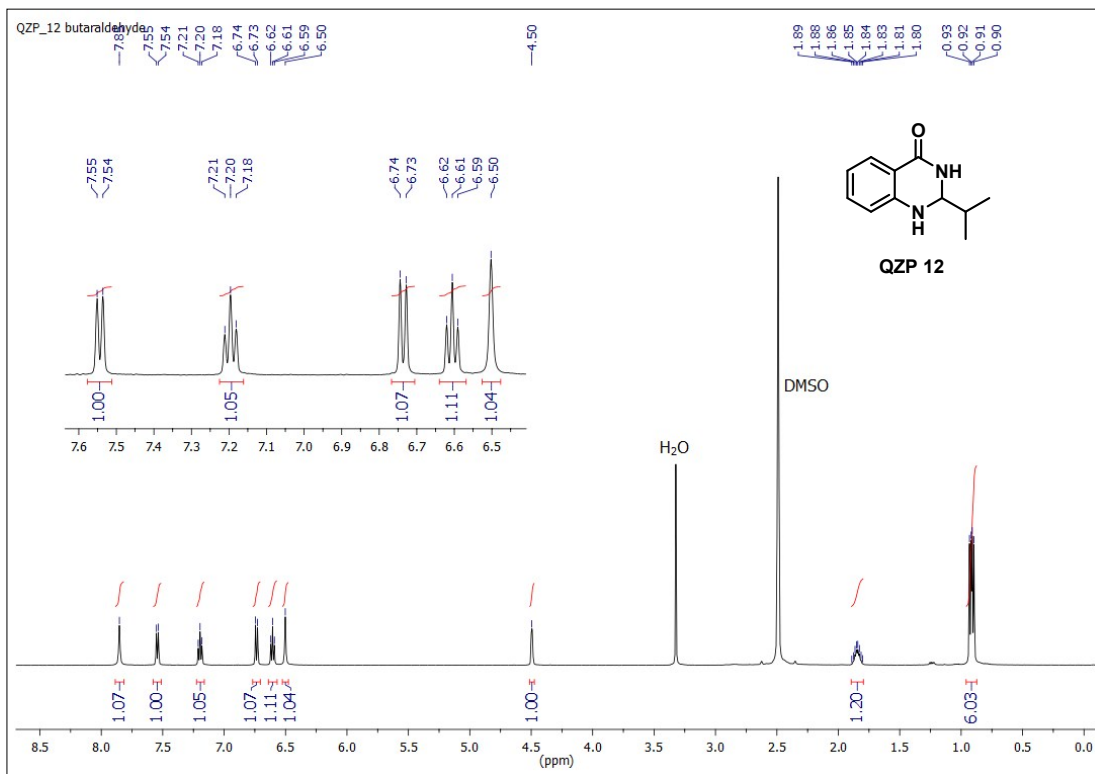


Figure S10: ¹H-NMR spectra of 2-ethyl-2,3-dihydroquinazolin-4(1H)-one:

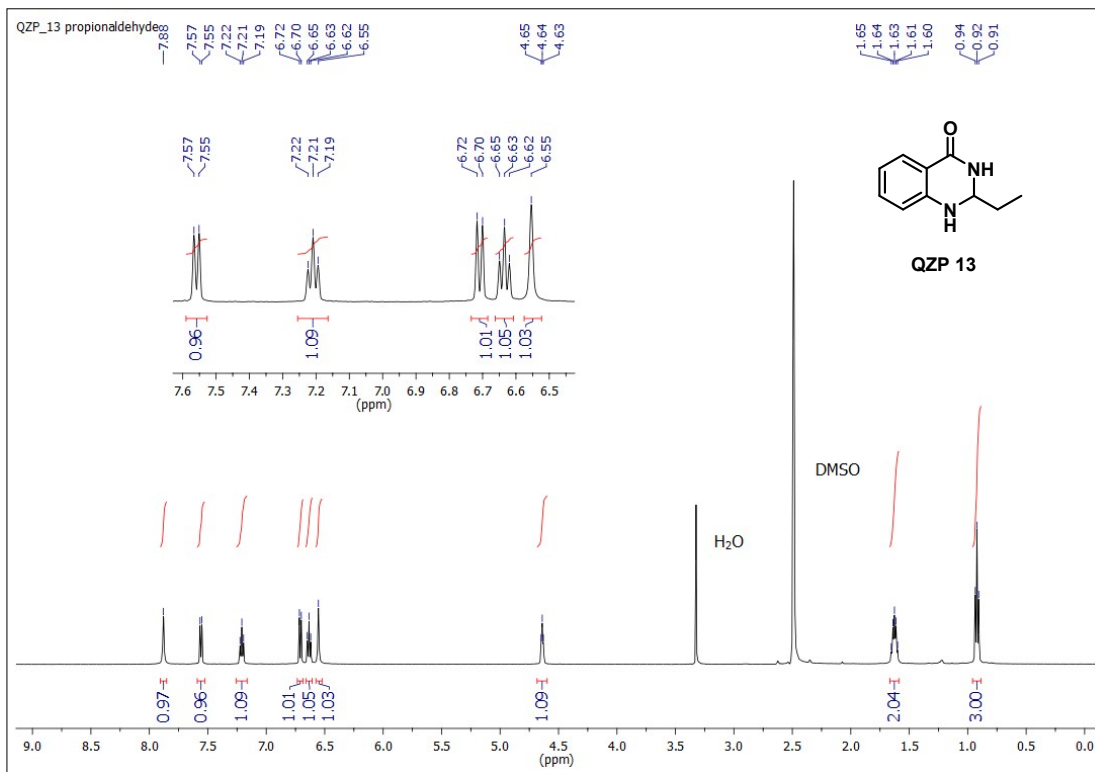


Figure S13: $^1\text{H-NMR}$ spectra of 2-(furan-2-yl)-2,3-dihydroquinazolin-4(1H)-one:

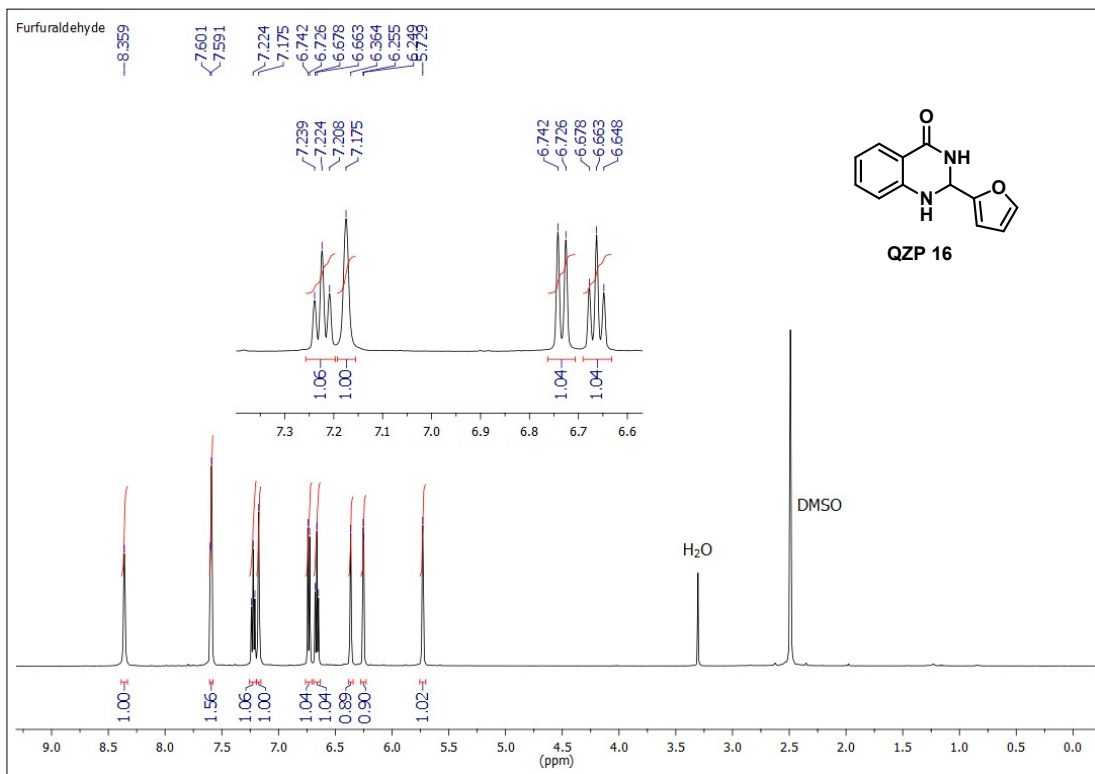


Figure S14: $^1\text{H-NMR}$ spectra of 2-(pyridin-2-yl)-2,3-dihydroquinazolin-4(1H)-one:

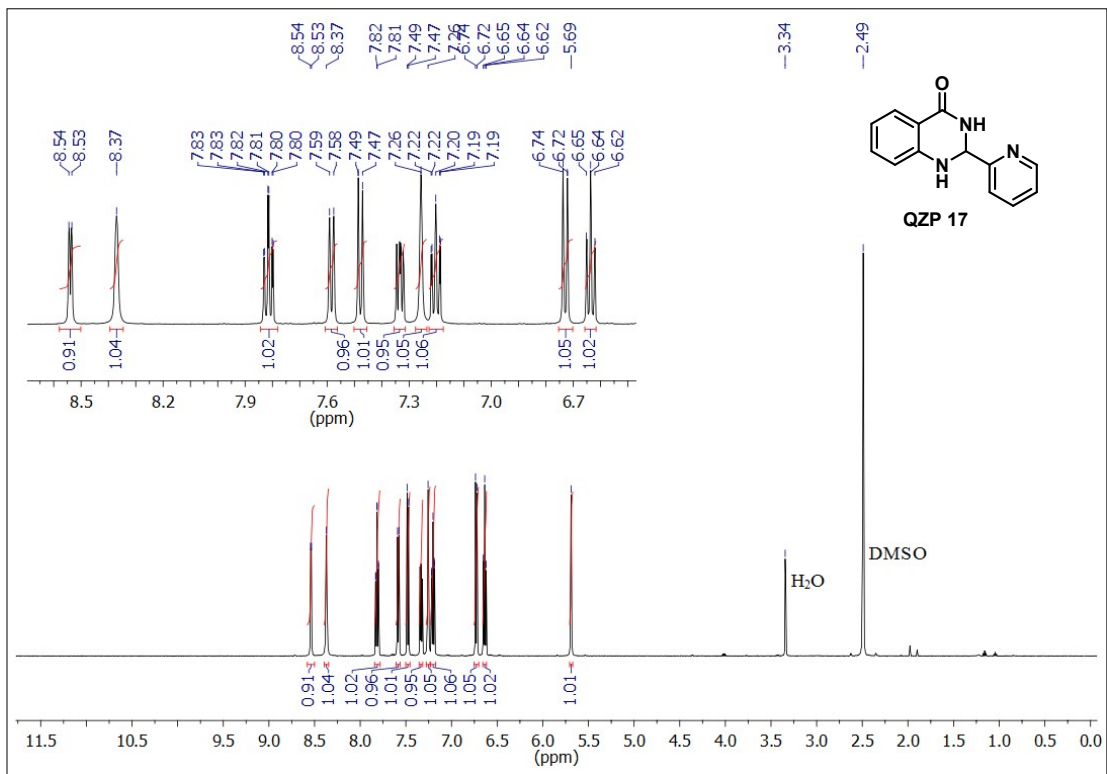


Figure S15: ¹H-NMR spectra of 7-chloro-2-phenyl-2,3-dihydroquinazolin-4(1H)-one:

