Supporting Information

1. General Methods.

NMR spectra were recorded on Bruker Avance 300 (300 MHz. Chemical shifts (ppm) are given relative to solvent: references for DMSO were 2.52 ppm (^{1}H-NMR) and 39.52 ppm (^{13}C-NMR). ^{13}C-NMR spectra were acquired on a broad band decoupled mode. Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). Gas chromatography analysis was performed on an Agilent HP-5890 instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d., 0.25 μm film thickness) using argon as carrier gas.

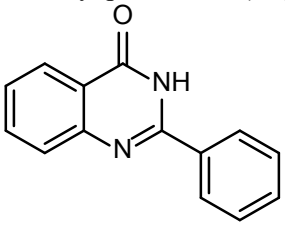
2. Materials and Methods.

All reactions were carried out under argon atmosphere. DMSO (anhydrous, 99.8%) and all the other chemicals were purchased from Sigma-Aldrich and used as received.

3. General Procedure for the Synthesis of 2-phenyl quinazolin-4(3*H*)-one.

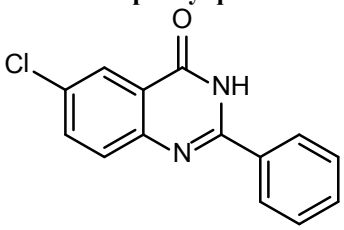
A 12 mL vial was charged with $Pd(OAc)_2$ (2 mol%), $BuPAd_2$ (6 mol%), 2-aminobenzonitrile (1 mmol), K_2CO_3 (2.5 mmol), and a stirring bar. Then, 1 mL DMSO, 1 mL H_2O, and 1.1 mmol of bromobenzene were injected by syringe under argon. The vial (or several vials) was placed in an alloy plate, which was transferred into a 300 mL autoclave of the 4560 series from Parr Instruments® under argon atmosphere. After flushing the autoclave three times with CO, a pressure of 10 bar CO was adjusted at ambient temperature. Then, the reaction was performed for 16 hours at 120 ^{o}C. After the reaction is finished, the autoclave was cooled down to room temperature and the pressure was released carefully. The pure product can be isolated by either washed with water, ethyl acetate and finally hexane or recrystallized from MeOH.

2-Phenylquinazolin-4(3*H*)-one:[1]



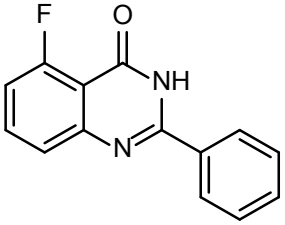
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.51 (s, 1H), 8.21 (s, 3H), 7.96 – 7.69 (m, 2H), 7.57 (h, *J*=7.2, 4H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.28, 152.30, 148.78, 134.65, 132.68, 131.43, 128.52, 127.82, 127.42, 126.41, 125.70, 120.99. **GC-MS (EI, 70eV):** m/z(%)=222 (M^+, 100).

6-Chloro-2-phenylquinazolin-4(3*H*)-one:[2]



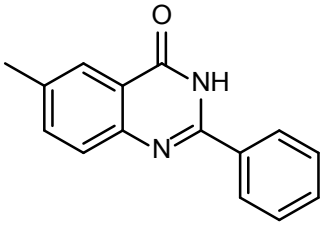
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.71 (s, br, 1H), 8.16 (d, 2H, *J* = 6.51 Hz), 8.09 (d, 1H, *J* = 2.4 Hz), 7.88-7.84 (dd, 1H, *J* = 8.9, 2.4 Hz), 7.75 (d, 1H, *J* = 8.7 Hz), 7.61-7.54 (m, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.9, 153.4, 147.9, 135.2, 133.0, 132.1, 131.3, 130.2, 129.2, 128.4, 125.4, 122.7. **GC-MS (EI, 70eV):** m/z(%)=256 (M^+, 100).

5-Fluoro-2-phenylquinazolin-4(3*H*)-one:[3]



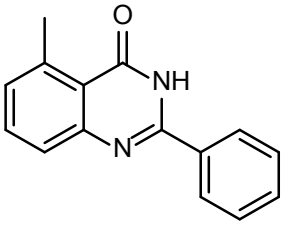
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.58 (s, br, 1H), 8.18 (d, 2H, J = 6.6Hz), 7.78–7.85 (m, 1H), 7.54–7.62 (m, 4H), 7.24–7.30 (m, 1H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.8, 159.5, 153.3, 150.9, 135.2, 135.1, 132.2, 131.7, 128.6, 127.9, 123.6, 113.0, 112.8, 110.5. **GC-MS (EI, 70eV):** m/z(%)=240 (M^+, 100).

6-Methyl-2-phenylquinazolin-4(3*H*)-one:[3]



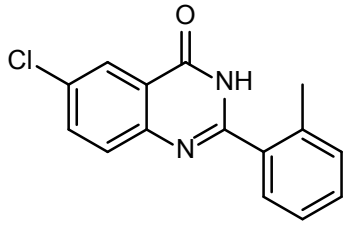
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.47 (s, br, 1H), 8.15 (d, 2H, J = 5.1 Hz), 7.94 (s, 1H), 7.63 (s, 2H), 7.51–7.56 (m, 3H) 2.44 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.1, 151.4, 146.7, 136.2, 135.8, 132.7, 131.1, 128.5, 127.6, 127.3, 125.2, 120.7, 20.8. **GC-MS (EI, 70eV):** m/z(%)=236 (M^+, 100).

5-Methyl -2-phenylquinazolin-4(3*H*)-one:[3]



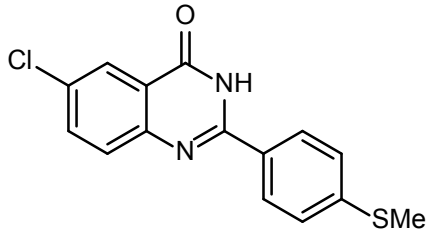
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.47 (s, br, 1H), 8.15 (d, 2H, J = 5.1 Hz), 7.94 (s, 1H), 7.63 (s, 2H), 7.51–7.56
(m, 3H) 2.44 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.1, 151.4, 146.7, 136.2, 135.8, 132.7, 131.1, 128.5, 127.6, 127.3, 125.2, 120.7, 20.8. **GC-MS (EI, 70eV):** m/z(%)=236 (M^+, 100).

6-Chloro-2-(o-tolyl)quinazolin-4(3*H*)-one:[4]



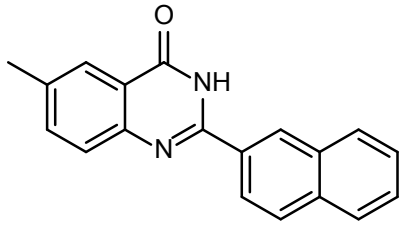
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.62 (s, br, 1H), 8.10 (s, 1H), 7.97-7.62 (m, 2H), 7.61-7.08(m, 4H), 7.51–7.56 (m, 3H) 2.38 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.3, 155.3, 147.9, 136.7, 134.9, 134.4, 131.3, 131.0, 130.5, 130.0, 129.6, 126.1, 125.2, 122.7, 20.0. **GC-MS (EI, 70eV):** m/z(%)=270 (M^+, 100).

6-Chloro-2-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one:



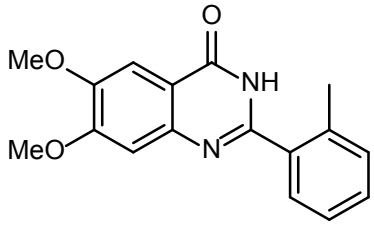
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.62 (s, br, 1H), 8.13 (d, 2H, J = 8.4 Hz), 8.06 (d, 1H, J = 2.4 Hz), 7.83 (dd, 1H, J = 8.8 Hz, 2.4 Hz), 7.73 (d, 1H, J = 8.8 Hz), 7.40 (d, 2H, J = 8.5 Hz), 2.55 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.8, 152.8, 147.9, 143.8, 135.1, 131.0, 130.0, 128.8, 128.6, 125.6, 125.3, 122.6, 14.5. **GC-MS (EI, 70eV):** m/z(%)=302 (M^+, 100).

6-Methyl-2-(naphthalen-2-yl)quinazolin-4(3*H*)-one:



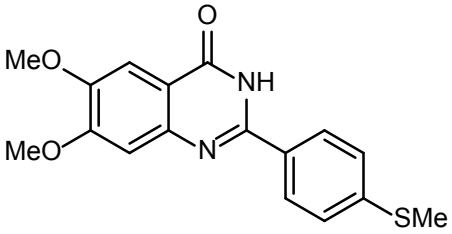
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.58 (s, br, 1H), 8.86-8.75 (m, 1H), 8.36-8.24 (m, 1H), 8.15-7.93 (m, 4H), 7.76-7.57 (m, 4H), 2.49 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.7, 151.9, 147.2, 136.8, 136.4, 134.5, 132.8, 130.5, 129.4, 128.6, 128.4, 128.3, 128.1, 127.8, 127.3, 125.8, 124.9, 121.3, 21.3. **GC-MS (EI, 70eV):** m/z(%)=286 (M^+, 100).

6,7-Dimethoxy-2-(o-tolyl)quinazolin-4(3*H*)-one:



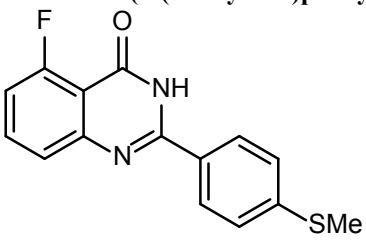
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.25 (s, br, 1H), 7.52-7.44 (m, 2H), 7.43-7.36 (m, 1H), 7.35-7.24 (m, 2H), 7.15 (s, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 2.38 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.2, 155.0, 154.1, 148.9, 145.5, 136.5, 135.3, 130.9, 123.0, 129.6, 126.1, 114.4, 108.5, 105.4, 56.4, 56.2, 20.1. **GC-MS (EI, 70eV):** m/z(%)=296 (M^+, 100).

6,7-Dimethoxy-2-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one:



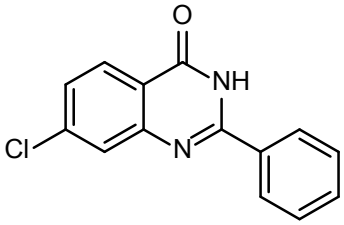
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.311 (s, br, 1H), 8.12 (d, 2H, J = 8.4 Hz), 7.46 (s, 1H), 7.37 (d, J = 8.57 Hz), 7.17 (s, 1H), 3.92 (s, 3H), 3.88 (s, 3H), 2.54 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.1, 155.2, 150.8, 148.9, 145.3, 142.9, 129.3, 128.2, 125.6, 114.3, 108.6, 105.5, 56.4, 56.2, 14.6. **GC-MS (EI, 70eV):** m/z(%)=328 (M^+, 100).

5-Fluoro-2-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one:



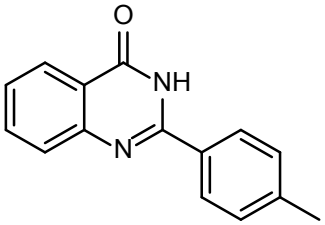
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.47 (s, br, 1H), 8.14 (d, 2H, J = 8.1 Hz), 7.80-7.70 (m, 1H), 7.50 (d, 1H, J = 8.29 Hz), 7.37 (d, J = 8.1 Hz), 7.23-7.15 (m, 1H), 2.54 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.1 (d, J = 261.5 Hz), 160.5 (d, J = 3.7 Hz), 159.3, 153.64, 151.57, 143.74, 135.33 (d, J = 10.8 Hz), 129.0, 128.6, 125.5, 123.8 (d, J = 3.7 Hz), 112.9 (d, J = 20.9 Hz), 110.8 (d, J = 6.3 Hz), 14.6. **GC-MS (EI, 70eV):** m/z(%)=286 (M^+, 100).

7-Chloro-2-phenylquinazolin-4(3*H*)-one:[3]



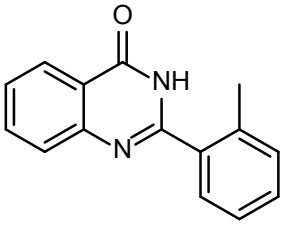
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.71 (s, br, 1H), 8.17 (m, 3H), 7.81 (m, 1H), 7.63 – 7.52 (m, 4H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.2, 154.4, 150.4, 139.6, 132.9, 132.2, 129.1, 128.4, 128.4, 127.2, 127.0, 120.3. **GC-MS (EI, 70eV):** m/z(%)=256 (M^+, 100).

2-(*p*-Tolyl)quinazolin-4(3*H*)-one: [5]



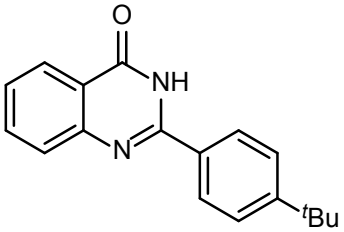
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.44 (s, 1H), 8.15 (d, J = 7.6 Hz, 1H), 8.11 (d, J = 8.0 Hz, 2H), 7.83 (t, J= 7.6 Hz, 1H),
7.73 (d, J = 8.4 Hz, 1H), 7.51 (t, J = 8.0 Hz, 1H), 7.36 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 163.0, 153.0, 149.3, 141.8, 134.9, 130.6, 129.6, 128.1, 127.7, 126.7, 126.3, 121.4, 21.4. **GC-MS (EI, 70eV):** m/z(%)=236 (M^+, 100).

2-(*o*-Tolyl)quinazolin-4(3*H*)-one:[3]



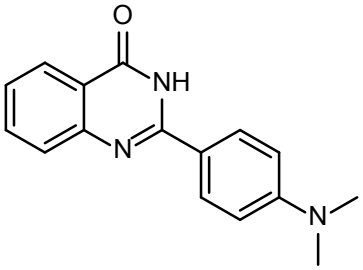
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.46 (s, br, 1H), 8.19-8.10 (m, 3H), 7.85-7.76 (m, 1H), 7.74-7.67 (m, 1H), 7.53-7.45 (m, 1H), 7.42-7.35 (m, 2H), 2.54 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.8, 152.3, 149.2, 143.5, 135.0, 129.2, 128.5, 127.8, 126.8, 126.3, 125.6, 121.4, 14.6. **GC-MS (EI, 70eV):** m/z(%)=236 (M^+, 100).

2-(4-(*tert*-Butyl)phenyl)quinazolin-4(3*H*)-one:[3]



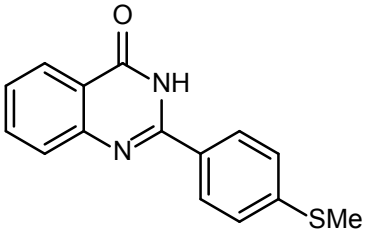
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.47 (s, br, 1H), 8.25-8.02 (m, 3H), 7.88-7.76 (m, 1H), 7.75-7.63 (m, 1H), 7.62-7.42 (m, 3H), 1.32 (s, 9H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.9, 154.7, 152.8, 149.3, 135.0, 130.5, 128.0, 127.8, 126.8, 126.3, 125.9, 121.4, 35.1, 31.4. **GC-MS (EI, 70eV):** m/z(%)=278 (M^+, 100).

2-(4-(Dimethylamino)phenyl)quinazolin-4(3*H*)-one:[1]



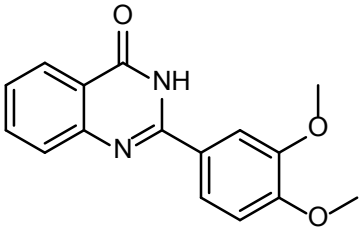
^{1}H NMR (300 MHz, DMSO-d_6) δ = ^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.17 (s, 1H), 8.10 (s, 3H), 7.86 – 7.34 (m, 3H), 6.78 (d, 2H, J = 3.1Hz), 2.99 (s, 6H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = ^{13}C NMR (75 MHz, DMSO) δ = 162.4, 152.2, 149.4, 134.4, 128.9, 127.0, 125.8, 125.4, 120.4, 118.8, 39.7. **GC-MS (EI, 70eV):** m/z(%)=265 (M^+, 100).

2-(4-(Methylthio)phenyl)quinazolin-4(3*H*)-one:[1]



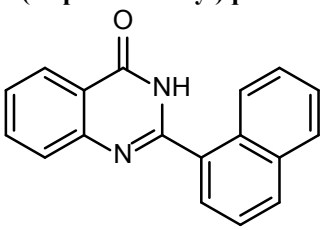
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.47 (s, 1H), 8.16 (d, *J*=8.4, 3H), 7.77 (dd, *J* = 26.5, 7.6, 2H), 7.50 (t, *J*=7.3, 1H), 7.40 (d, *J*=8.4, 2H), 2.55 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.8, 152.3, 149.2, 143.5, 135.0, 129.1, 128.5, 127.8, 126.8, 126.3, 125.6, 121.3, 14.6. **GC-MS (EI, 70eV):** m/z(%)=268 (M^+, 100).

2-(3,4-Dimethoxyphenyl)quinazolin-4(*3H*)-one:[1]



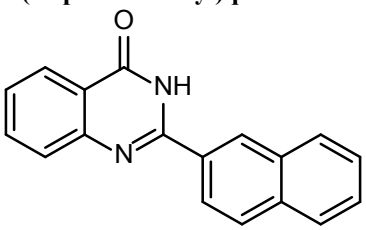
^{1}H NMR (300 MHz, DMSO-d_6) δ = ^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.42 (s, 1H), 8.15 (d, *J*=7.3, 1H), 7.98 – 7.61 (m, 4H), 7.47 (t, *J*=6.7, 1H), 7.07 (s, 1H), 3.90 (s, 3H), 3.85 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.41, 151.84, 151.57, 148.95, 148.54, 134.44, 127.25, 126.05, 125.83, 124.76, 121.15, 120.70, 111.30, 110.67, 55.63. **GC-MS (EI, 70eV):** m/z(%)=282 (M^+, 100).

2-(Naphthalen-1-yl)quinazolin-4(3*H*)-one:[1]



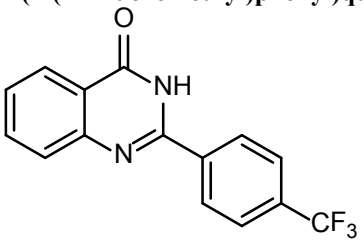
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.68 (s, 1H), 8.82 (s, 1H), 8.21 (d, *J*=7.7, 2H), 8.04 (dd, *J*=17.5, 8.7, 3H), 7.84 (dt, *J*=14.5, 7.3, 2H), 7.70 – 7.50 (m, 3H)
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.2, 152.3, 148.7, 134.6, 134.1, 132.3, 123.0, 130.0, 129.0, 128.1, 128.1, 128.0, 127.6, 127.6, 126.9, 126.6, 125.9, 124.5, 121.1. **GC-MS (EI, 70eV):** m/z(%)=272 (M^+, 100).

2-(Naphthalen-2-yl)quinazolin-4(3*H*)-one:[1]



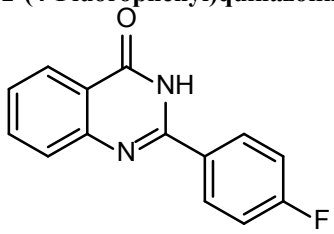
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.69 (s, 1H), 8.85 (s, 1H), 8.33 (dd, *J*=8.7, 1.8, 1H), 8.21 (d, *J*=6.9, 1H), 8.15 – 7.96 (m, 3H), 7.92 – 7.75 (m, 2H), 7.73 – 7.49 (m, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.2, 152.2, 148.8, 132.3, 129.9, 128.9, 128.1, 128.1, 127.9, 127.6, 127.6, 126.9, 126.6, 125.9, 124.5, 121.1. **GC-MS (EI, 70eV):** m/z(%)=272 (M^+, 100).

2-(4-(Trifluoromethyl)phenyl)quinazolin-4(3*H*)-one:[1]



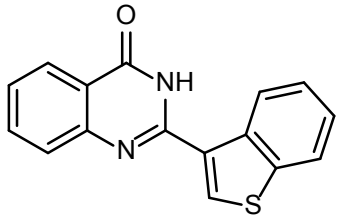
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.75 (s, 1H), 8.38 (d, *J*=8.2, 2H), 8.18 (d, *J*=7.9, 1H), 8.00 – 7.70 (m, 4H), 7.56 (t, *J*=7.4, 1H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.13, 151.19, 148.38, 136.58, 134.67, 131.53 (q, *J*= 34.5Hz), 130.88, 127.61, 127.06, 125.87, 125.45 (q, *J*= 3.7Hz), 123.94 (q, *J*= 270.2Hz), 121.18. **GC-MS (EI, 70eV):** m/z(%)=290 (M^+, 100).

2-(4-Fluorophenyl)quinazolin-4(3*H*)-one:[1]



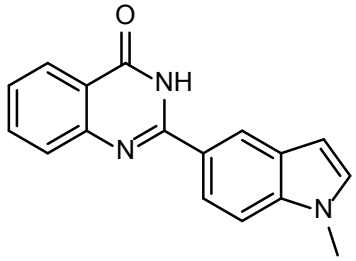
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.59 (s, 1H), 8.42 – 8.06 (m, 3H), 8.00 – 7.67 (m, 2H), 7.64 – 7.31 (m, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 164.0 (d, *J*= 243.0 Hz), 162.3, 151.4, 148.6, 134.6, 130.3 (d, *J*= 9.2 Hz), 129.2 (d, *J*=3.1 Hz), 127.4, 126.6, 125.8, 120.9, 115.6 (d, *J*= 21.8 Hz). **GC-MS (EI, 70eV):** m/z(%)=240 (M^+, 100).

2-(Benzo[*b*]thiophen-3-yl)quinazolin-4(3*H*)-one:



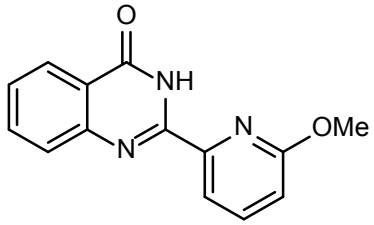
^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.52 (s, br, 1H), 9.03-9.00 (d, 1H, J = 8.1 Hz), 8.80 (s, 1H), 8.18 (d, 1H, J = 8.10 Hz), 8.10 (d, 1H, J = 7.5 Hz), 7.93-7.76 (m, 2H), 7.64-7.42 (m, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 162.5, 149.2, 149.1, 140.2, 137.0, 135.1, 132.9, 128.6, 128.0, 127.2, 126.3, 125.9, 125.7, 125.6, 123.4, 121.7. **GC-MS (EI, 70eV):** m/z(%)=278 (M^+, 100).

2-(1-Methyl-1*H*-indol-5-yl)quinazolin-4(3*H*)-one:[1]



^{1}H NMR (300 MHz, DMSO-d_6) δ = 12.40 (s, br, 1H), 8.51 (s, 1H), 8,23-7.97 (m, 2H), 7.88-7.64 (m, 2H), 7.63-7.52 (m, 1H), 7.52-7.36 (m, 2H), 6.59 (m, 1H), 3.84 (s, 3H).
^{13}C NMR (75 MHz, DMSO-d_6) δ = 163.0, 154.0, 149.6, 138.4, 134.9, 131.7, 128.2, 127.6, 126.3, 124.0, 121.4, 121.3, 121.1, 110.3, 102.2, 33.2. **GC-MS (EI, 70eV):** m/z(%)=275 (M^+, 100).

2-(6-Methoxypyridin-2-yl)quinazolin-4(3*H*)-one:



^{1}H NMR (300 MHz, DMSO-d_6) δ = 11.81 (s, br, 1H), 8.20 (d, 1H, J = 8.2 Hz), 8.06 (d, 1H, J = 7.5 Hz), 7.99-7.91 (m, 1H), 7.91-7.83 (m, 1H), 7.79 (d, 1H, J = 8.2 Hz), 7.61-7.53 (m, 1H), 7.07 (d, J = 8.2 Hz), 4.09 (s, 3H).

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