Supporting Information

1. General Methods

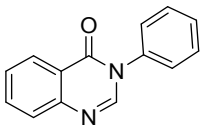
NMR spectra were recorded on Bruker Avance 300 and Bruker ARX 400 spectrometers. Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (*m/z*). 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. The products were isolated from the reaction mixture by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck).

2. General Procedure for the Synthesis of Quinazolinone:

A 12 mL vial was charged with $Pd(OAc)_2$ (2 mol%), $BuPAd_2$ (6 mol%), 2'-Bromoformanilide (1 mmol), $Mo(CO)_6$ (1 mmol) and a stirring bar. Then, nitro compounds (1.1 mmol), NEt_3 (2 mmol) and dioxane (2 mL) 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 N_2, a pressure of 10 bar N_2 was adjusted at ambient temperature. Then, the reaction was performed for 16 h at 140 ^oC. After the reaction finished, the autoclave was cooled down to room temperature and the pressure was released carefully. The solution was extracted 3-5 times with 2-3 ml of ethyl acetate. After evaporation of the organic solvent the residue was adsorbed on silica gel and the crude product was purified by column chromatography.

3. Characterization of Product

3-Phenylquinazolin-4(3*H*)-one:



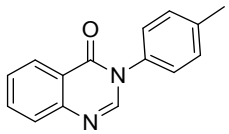
^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.38 (s, 1H), 8.24 (d, *J* = 8.35, 1H), 7.94-7.90 (m, 1H), 780-7.77 (m, 1H), 7.66- 7.54 (m, 6H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 160.9, 152.4, 148.70, 148.13, 138.60, 135.60, 130.25, 129.73, 128.51, 127.42, 122.87.

GC-MS (EI, 70eV): m/z(%)=222 (M^+, 99), 221 (100), 193 (10) , 119 (13), 77 (31).

HRMS (ESI): calcd. for $[C_{14}H_{10}N_2O + H]^+$: 223.08659; found: 223.0866.

3-(*p*-Tolyl)quinazolin-4(3*H*)-one:



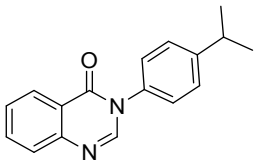
^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.36 (s, 1H), 8.23 (d, *J*=8.1, 1H), 7.94-7.90 (m, 1H), 7.80-7.76 (m, 1H), 7.65-7.60 (m, 1H), 7.48-7.38 (m, 4H), 2.43 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 160.88, 148.60, 148.11, 139.18, 135.92, 135.44, 128.22, 128.15, 128.06, 127.27, 122.77, 21.55.

GC-MS (EI, 70eV): m/z(%)=236 (M^+, 100), 235 (95), 221 (6), 207 (13), 119(14), 91 (22).

HRMS (ESI): calcd. for $[C_{15}H_{12}N_2O]$: 236.09441; found: 236.09465.

3-(4-Isopropylphenyl)quinazolin-4(3*H*)-one:



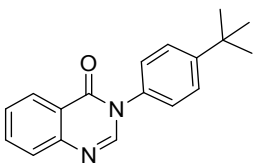
^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.38 (s, 1H), 8.23 (d, *J*=8.3, 1H), 7.94-7.88 (m, 1H), 7.79-7.76 (m, 1H), 7.65-7.60 (m, 1H), 7.51-7.44 (m, 4H), 3.02 (Hept. 1H), 1.30 (s, 3H), 1.28 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 160.96, 149.91, 148.63, 148.17, 136.22, 135.50, 128.26, 128.18, 127.98, 127.32, 122.79, 34.09, 24.69.

GC-MS (EI, 70eV): m/z(%)=264 (M^+, 68), 250 (19), 249 (100), 121 (11), 77 (8).

HRMS (ESI): calcd. for $[C_{17}H_{16}N_2O_1]$: 264.12571; found: 264.12533.

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

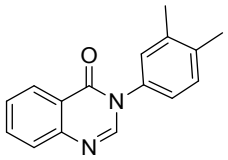


^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.39 (s, 1H), 8.24 (d, *J*=8.2, 1H), 7.95-7.89 (m, 1H), 7.79-7.76 (m, 1H), 7.63-7.59 (m, 3H), 7.52-7.48 (m, 2H), 1.37 (s, 9H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 160.95, 152.11, 148.63, 148.17, 135.93, 135.52, 128.27, 128.19, 127.85, 127.33, 126.92, 122.78, 35.39, 31.96.

GC-MS (EI, 70eV): m/z(%)=278 (M^+, 37), 264 (19), 263 (100).

3-(3,4-Dimethylphenyl)quinazolin-4(3*H*)-one:

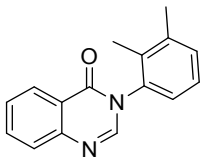


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.31-8.26 (m, 1H), 8.01 (s, 1H), 7.74-7.65 (m, 2H), 7.49-7.43 (m, 1H), 7.23-7.19 (m, 1H), 7.11-7.02 (m, 2H), 2.24 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 161.17, 148.22, 146.56, 135.78, 135.75, 134.66, 129.64, 128.91, 127.65, 127.59, 127.29, 122.60, 19.93, 19.60.

GC-MS (EI, 70eV): m/z(%)=250 (M^+, 100), 235 (10), 119 (10), 77 (8).

3-(2,3-Dimethylphenyl)quinazolin-4(3*H*)-one:

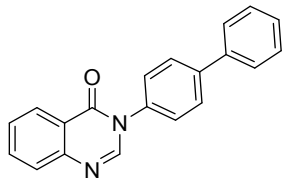


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.46-8.42 (m, 1H), 7.93 (s, 1H), 7.89-7.84 (m, 2H), 7.64-7.58 (m, 1H), 7.39-7.33 (m, 1H), 7.29-7.25 (m, 2H), 2.19 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 161.02, 147.97, 146.95, 138.31, 138.02, 135.16, 134.53, 130.74, 127.98, 127.59, 127.22, 124.20, 122.46, 18.00.

GC-MS (EI, 70eV): m/z(%)=250 (M^+, 55), 233 (100), 218 (10), 77 (8).

3-([1,1'-Biphenyl]-4-yl)quinazolin-4(3*H*)-one:

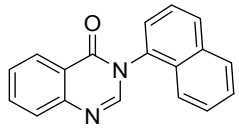


^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.20 (s, 1H), 8.17-8.14 (m, 1H), 7.88-7.84 (m, 1H), 7.70-7.58 (m, 7H), 7.31-7.25 (m, 4H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.19, 148.46, 148.34, 140.70, 138.56, 136.07, 135.52, 131.62, 130.59, 130.21, 129.53, 129.26, 129.13, 128.50, 128.27, 128.15, 127.25, 122.47.

GC-MS (EI, 70eV): m/z(%)=298 (M^+, 84), 297 (100), 282 (20), 281 (92), 152 (28), 76 (28).

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

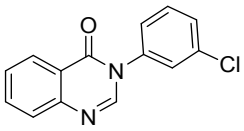


^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.26 (s, 1H), 8.19 (d, *J*=83 Hz, 1H), 8.16-8.14 (m, 2H), 8.00-7.96 (m, 1H), 7.80-7.78 (m, 1H), 7.76-7.57 (m, 6H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.24, 148.91, 148.59, 135.67, 135.13, 134.61, 130.60, 133.30, 129.27, 128.42, 128.37, 127.65, 126.65, 123.11, 122.79.

GC-MS (EI, 70eV): m/z(%)=272 (M^+, 79), 271 (100), 255 (12), 243 (14), 127 (20), 76 (5).

3-(3-Chlorophenyl)quinazolin-4(3*H*)-one:



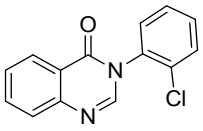
^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.40 (s, 1H), 8.20 (d, *J*=8.0, 1H), 7.96-7.91 (m, 1H), 7.83-7.80 (m, 2H), 7.67-7.60 (m, 4H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 160.73, 148.53, 147.68, 139.69, 135.63, 134.09, 131.64, 129.68, 128.34, 128.21, 127.31, 124.2, 122.68.

GC-MS (EI, 70eV): m/z(%)=256 (M^+, 9+7), 255 (100), 111 (23), 76 (15).

HRMS (ESI): calcd. for [$C_{14}H_9ClN_2O$]: 256.03979; found: 256.03924.

3-(2-Chlorophenyl)quinazolin-4(3*H*)-one:

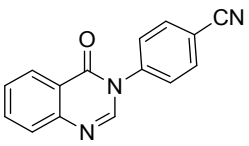


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.32-8.28 (m, 1H), 7.89 (s, 1H), 7.77-7.69 (m, 2H), 7.56-7.45 (m, 2H), 7.41-7.35 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.28, 147.89, 145.92, 135.04, 134.85, 132.50, 131.05, 130.77, 129.88, 128.16, 127.80, 127.72, 127.30, 122.41.

GC-MS (EI, 70eV): m/z(%)=256 (M^+, 3), 221 (100), 111 (5), 75 (3).

4-(4-Oxoquinazolin-3(4*H*)-yl)benzonitrile:

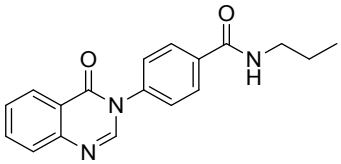


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.32-8.25 (m, 1H), 8.04 (s, 1H), 7.80-7.70 (m, 3H), 7.58-7.47 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.34, 147.53, 144.78, 141.14, 135.21, 133.95, 133.20, 128.26, 127.96, 127.79, 127.30, 119.79, 113.16.

GC-MS (EI, 70eV): m/z(%)=247 (M^+, 100), 219 (15), 119 (10), 75 (5).

4-(4-Oxoquinazolin-3(4*H*)-yl)-*N*-propylbenzamide:

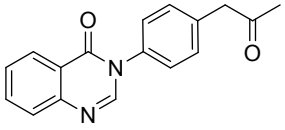


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.26-8.21 (m, 1H), 8.00 (s, 1H), 7.86-7.64 (m, 3H), 7.58-7.32 (m, 4H), 3.36-3.24 (m, 2H), 1.59-1.49 (m, 2H), 0.91-0.85 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 166.48, 160.70, 147.81, 145.47, 139.71, 135.66, 134.90, 128.59, 128.41, 127.93, 127.75, 127.12, 122.17, 114.12, 41.98, 22.88, 11.50.

GC-MS (EI, 70eV): m/z(%)=307 (M^+, 30), 265 (20), 249 (100), 121 (10).

3-(4-(2-oxopropyl)phenyl)quinazolin-4(3*H*)-one:

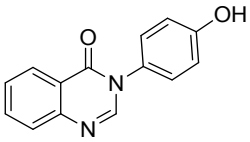


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.27-8.23 (m, 1H), 8.03 (s, 1H), 7.73-7.63 (m, 2H), 7.47-7.41 (m, 1H), 3.69 (s, 2H), 2.13 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 205.44, 161.79, 147.87, 146.04, 136.35, 134.67, 130.24, 129.98, 127.72, 127.63, 127.25, 127.16, 122.33, 50.19, 29.74.

GC-MS (EI, 70eV): m/z(%)=278 (M^+, 20), 236 (100), 129 (15), 107 (20).

3-(4-Hydroxyphenyl)quinazolin-4(3*H*)-one:



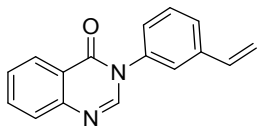
^{1}H NMR (300 MHz, DMSO-d_6) δ = 9.90 (s, 1H), 8.32 (s, 1H), 8.23 (d, *J*=8.1, 1H), 7.93-7.87 (m, 1H), 7.78-7.74 (m, 1H), 7.65-7.59 (m, 1H), 7.37-7.34 (m, 2H), 6.96-6.93 (m, 2H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 161.15, 158.57, 148.68, 148.52, 135.41, 129.73, 129.49, 128.20, 128.17, 127.31, 122.84, 116.50.

GC-MS (EI, 70eV): m/z(%)=238 (M^+, 100), 257 (56), 129 (9), 65 (12).

HRMS (ESI): calcd. for $[C_{15}H_{12}N_2O + H]^+$: 239.0815; found: 239.0819.

3-(3-Vinylphenyl)quinazolin-4(3*H*)-one:



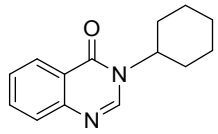
^{1}H NMR (300 MHz, DMSO-d_6) δ = 8.41 (s, 1H), 8.22 (d, *J*=8.3, 1H), 7.95-7.91 (m, 1H), 7.81-7.78 (m, 1H), 7.72-7.67 (m, 1H), 7.65-7.60 (m, 2H), 7.58-7.56 (m, 1H), 7.51-7.47 (m, 1H), 6.83 (q, 1H), 6.00 (d, *J*=12, 1H), 5.40 (d, *J*=8.3, 1H).

^{13}C NMR (75 MHz, DMSO-d_6) δ = 159.88, 147.02, 138.27, 137.89, 135.54, 134.57, 129.34, 127.31, 127.21, 126.78, 126.46, 126.31, 124.92, 121.78, 115.70.

GC-MS (EI, 70eV): m/z(%)=248 (M^+, 95), 247 (100), 103 (12).

HRMS (ESI): calcd. for $[C_{16}H_{12}N_2O_1 + H]^+$: 249.10224; found: 249.10257.

3-Cyclohexylquinazolin-4(3H)-one:

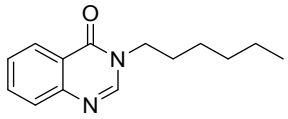


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.28-8.20 (m, 1H), 8.04 (s, 1H), 7.74-7.36 (m, 3H), 2.62-2.32 (m, 2H), 1.99-1.42 (m, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.78, 147.53, 143.98, 134.17, 127.33, 127.17, 127.03, 122.02, 53.42, 32.69, 25.97, 25.35.

GC-MS (EI, 70eV): m/z(%)=228 (M^+, 30), 147 (100), 118 (5).

3-Hexylquinazolin-4(3*H*)-one:

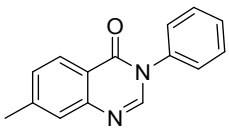


^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.25-8.21 (m, 1H), 7.95 (s, 1H), 7.61-7.51 (m, 2H), 7.45-7.39 (m, 1H), 3.91 (t, *J*=7.51 Hz, 2H), 1.76-1.65 (m, 2H), 1.35-1.16 (m, 6H), 0.84-0.76 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 161.12, 148.17, 146.69, 134.20, 127.40, 127.28, 126.77, 122.26, 47.17, 31.41, 29.42, 26.40, 22.55, 14.05.

GC-MS (EI, 70eV): m/z(%)=230 (M^+, 35), 160 (70), 146 (100), 129 (15), 77 (10).

7-Methyl-3-phenylquinazolin-4(3*H*)-one:



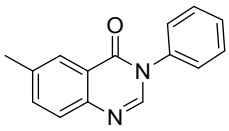
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.13 (d, *J*=23.2, 1H), 8.02 (s, 1H), 7.49-7.39 (m, 4H), 7.36-7.32 (m, 2H), 7.31-7.26 (m, 1H), 2.53 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.73, 147.96, 146.22, 145.75, 137.58, 129.65, 129.65, 129.08, 127.34, 127.07, 127.05, 119.93, 21.98.

GC-MS (EI, 70eV): m/z(%)= 236(M^+, 100), 221 (15), 207 (20), 133 (25), 77(30).

HRMS (ESI): calcd. for $[C_{15}H_{12}N_2O + H]^+$: 237.10224; found: 237.10228.

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



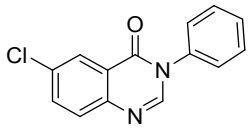
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.06 (d, *J*=8.1, 1H), 8.09 (s, 1H), 7.59-7.32 (m, 7H), 2.42 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.81, 145.83, 145.40, 138.03, 137.66, 136.06, 129.68, 129.10, 127.40, 127.08, 126.64, 122.12, 21.44.

GC-MS (EI, 70eV): m/z(%)=236(M^+, 100), 207 (10), 133 (30), 77(40).

HRMS (ESI): calcd. for $[C_{15}H_{12}N_2O + H]^+$: 237.10224; found: 237.10279.

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



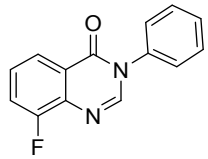
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.23 (d, *J*=2.1, 1H), 8.20 (s, 1H), 7.66-7.64 (m, 2H), 7.51- 7.43 (m, 3H), 7.36-7.32 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 159.71, 146.29, 146.25, 137.14, 135.00, 133.56, 129.72, 129.31, 129.20, 126.88, 126.52, 123.41.

GC-MS (EI, 70eV): m/z(%)=256(M^+, 100), 228 (10), 192 (5), 153(10), 77 (25).

HRMS (ESI): calcd. for $[C_{14}H_9ClN_2O + H]^+$: 257.04762; found: 257.04772.

8-Fluoro-3-phenylquinazolin-4(3*H*)-one:



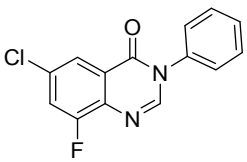
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.07-8.03 (m, 2H), 7.51-7.32 (m, 7H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 159.89, 157.02 (d, *J*= 250.0), 146.61, 137.38, 137.19, 129.79, 129.39, 127.80(d, *J*=8.3), 126.99, 124.26, 122.73 (d, *J*=4.5), 120.10 (d, *J*= 18.5).

GC-MS (EI, 70eV): m/z(%)=m/z(%)=240(M^+, 100), 212 (20), 192 (5), 137(15), 77 (35).

HRMS (ESI): calcd. for $[C_{14}H_9FN_2O + H]^+$: 241:07717; found: 241:07726.

6-Chloro-8-fluoro-3-phenylquinazolin-4(3*H*)-one:



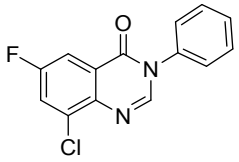
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.08 (s, 1H), 8.05- 8.02 (m, 1H), 7.53- 7.42 (m, 4H), 7.36- 7.29 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 158.86, 155.40 (d, *J*= 259.), 146.78, 136.93, 133. 10 (d, *J*= 12.0), 129.10 (d, *J*= 9.8), 124.81, 122.40, 121.29 (d, *J*= 4.5), 121.07 (d, *J*= 21.8).

GC-MS (EI, 70eV): m/z(%)=274(M^+, 100), 246 (10), 171 (15), 77 (40)

HRMS (ESI): calcd. for $[C_{14}H_8ClFN_2O + H]^+$: 275.0382; found: 275.03868.

8-Chloro-6-fluoro-3-phenylquinazolin-4(3*H*)-one:



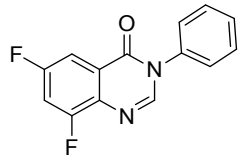
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.11 (s, 1H), 7.87-7.84 (m, 1H), 7.59- 7.55 (m, 1H), 7.52- 7.31 (m, 5H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 159.63, 158.40 (d, *J*= 260.), 146.17, 136.94, 133.75 (d, *J*= 12.0), 129.10 (d, *J*= 9.8), 124.81, 122.40, 121.29 (d, *J*= 4.5).

GC-MS (EI, 70eV): m/z(%)=274(M^+, 100), 246 (10), 171 (15), 77 (40).

HRMS (ESI): calcd. for $[C_{14}H_8ClFN_2O + H]^+$: 275.0382; found: 275.03831.

6,8-Difluoro-3-phenylquinazolin-4(3*H*)-one:



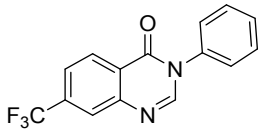
^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.04 (s, 1H), 7.75-7.70 (m, 1H), 7.51-7.42 (m, 3H), 7.35- 7.19 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 160.41(dd, *J*= 239.0, 15.0), 159.19, 157.13 (dd, *J*= 239.0 15.0), 146.01, 136.96, 129.88, 129.57, 126.91, 110.35(dd, *J*=27.8, 3.0), 108.99 (dd, *J*=23.3, 3.0).

GC-MS (EI, 70eV): m/z(%)=258(M^+, 100), 230 (10), 155 (10), 77 (35).

HRMS (ESI): calcd. for $[C_{14}H_8F_2N_2O + H]^+$: 259.06775; found: 259.06767.

3-Phenyl-7-(trifluoromethyl)quinazolin-4(3*H*)-one:



^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.40-8.39 (m, 1H), 8.11 (s, 1H), 7.96 (s, 1H), 7.65-7.33 (m, 6H).

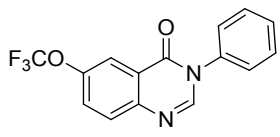
^{13}C NMR (75 MHz, $CDCl_3$) δ = 159.94, 147.88, 147.40, 137.07, 136.24 (q, *J*=33.88), 129.90, 129.56, 128.47, 126.95, 125.18 (q, *J*=3.79), 124.75, 123.79, 123.15 (q, *J*=246.64).

GC-MS (EI, 70eV): m/z(%)=290(M^+, 100), 262 (10), 187 (5), 77 (25).

HRMS (ESI): calcd. for $[C_{15}H_9F_3N_2O + H]^+$: 291.07397; found: 291.07418.

^{19}F NMR (75 MHz, $CDCl_3$) δ = -62.78

3-Phenyl-6-(trifluoromethoxy)quinazolin-4(3*H*)-one:



^{1}H NMR (300 MHz, $CDCl_3$) δ = 8.12-8.10 (m, 2H), 7.76-7.58 (m, 1H), 7.51-7.32 (m, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ = 159.97, 148.01, 146.52, 146.37, 137.17, 129.83, 129.44, 127.88, 126.95, 123.52 (q, *J*=272), 122.44, 118.54.

GC-MS (EI, 70eV): m/z(%)= 306(M^+, 100), 278 (10), 203 (10), 77 (25).

HRMS (ESI): calcd. for $[C_{15}H_9F_3N_2O_2 + H]^+$: 307.06889; found: 307.06908.