Research Article

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An efficient and green synthesis of 2-phenylquinazolin-4(3*H*)-ones *via* *t*-BuONa-mediated oxidative condensation of 2-aminobenzamides and benzyl alcohols under solvent- and transition metal-free conditions

Supplementary material

S1 Experimental procedure for the synthesis of 2-phenylquinazolin-4(3*H*)-one on a 2-mmol scale

In an experiment on a 2-mmol scale, 2-aminobenzamide (272.3 mg, 2 mmol), benzyl alcohol (6.6 mL, 32 equiv.) and *t*-BuONa (288.3 mg, 1.5 equiv.) were sequentially added to a 50-mL vial. After the reaction mixture was purged with oxygen in 15 min, the vial was tightly sealed. The reaction was performed at 120°C for 24 h under vigorously stirring. Upon completion of the reaction, the resulting mixture was cooled to room temperature, then diluted with ethyl acetate (100 mL) and quenched with brine (60 mL). The obtained organic layer was dried over anhydrous Na_2SO_4, filtered through a thin cotton layer, and evaporated under a reduced pressure, yielding a solid product. The raw product was further purified by washing with *n*-hexane (4 × 50 mL), affording 2-phenylquinazolin-4(3*H*)-one in a white solid (310 mg, 70%).

S2 Experimental procedure for the control experiments

S2.1 Reaction between 2-aminobenzamide and benzyl alcohol under O_2-free conditions

A mixture of 2-aminobenzamide (40.8 mg, 0.3 mmol), benzyl alcohol (1 mL, 32 equiv.), and *t*-BuONa (43.2 mg, 1.5 equiv.) were sequentially added to an 8-mL vial. The reaction mixture was purged with argon in 2 min before being tightly sealed. Subsequently, this mixture was vigorously stirred at 120°C for 24 h. Upon completion, the vial was cooled down to room temperature and added with diphenyl ether (51.1 mg, 0.3 mmol) as an internal standard. Ethyl acetate (3 mL) was then added to dilute the reaction mixture. An aliquot withdrawn from the resulting mixture was quenched with brine (2 mL), extracted with ethyl acetate (2 mL), dried over anhydrous sodium sulfate, and filtered through a cotton layer. The final organic sample was analyzed with GC and GC-MS.

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S2.2 Reaction between 2-aminobenzamide and benzyl alcohol in the absence of *t*-BuONa

A mixture of 2-aminobenzamide (40.8 mg, 0.3 mmol) and benzyl alcohol (1 mL, 32 equiv.) were added to an 8-mL vial. The reaction mixture was purged with oxygen in 2 min before being tightly sealed. Subsequently, this mixture was vigorously stirred at 120°C for 24 h. The reaction mixture was cooled to ambient temperature and then added with diphenyl ether as the internal standard (51.1 mg, 0.3 mmol). Ethyl acetate (3 mL) was then added to dilute the reaction mixture. An aliquot was withdrawn from this mixture and quenched with brine (2 mL). The organic phase was extracted with ethyl acetate (2 mL), dried over anhydrous Na_2SO_4, filtered through a cotton layer, and analyzed with GC and GC-MS.

S2.3 Reaction in the absence of 2-aminobenzamide

A mixture of benzyl alcohol (1 mL) and *t*-BuONa (43.2 mg, 1.5 equiv.) was stirred at 120°C for 24 h under an oxygen atmosphere in a tightly sealed 8-mL vial. The solution was diluted with ethyl acetate (3 mL) and quenched with brine (2 mL). An aliquot withdrawn from the organic layer was dried over anhydrous Na_2SO_4, filtered through a cotton layer, and analyzed with GC-MS.

S2.4 Reaction between 2-aminobenzamide and benzyl alcohol under standard conditions for 5 h

A mixture of 2-aminobenzamide (40.8 mg, 0.3 mmol), benzyl alcohol (1 mL, 32 equiv.) and *t*-BuONa (43.2 mg, 1.5 equiv.) was stirred at 120°C for 5 h under an oxygen atmosphere in a tightly sealed 8-mL vial. The reaction mixture was cooled to ambient temperature and then added with diphenyl ether as the internal standard (51.1 mg, 0.3 mmol). Ethyl acetate (3 mL) was then added to dilute the reaction mixture. An aliquot was withdrawn from this mixture and quenched with brine (2 mL). The organic phase was extracted with ethyl acetate (2 mL), dried over anhydrous Na_2SO_4, filtered through a cotton layer, and analyzed with GC and GC-MS.

S2.5 Reaction between 2-aminobenzamide and benzaldehyde in the absence of *t*-BuONa

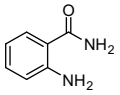
A mixture of 2-aminobenzamide (40.8 mg, 0.3 mmol) and benzaldehyde (1 mL) was stirred at 120 °C for 24 h under an oxygen atmosphere in a tightly sealed 8-mL vial. The reaction mixture was cooled to ambient temperature and then added with diphenyl ether as the internal standard (51.1 mg, 0.3 mmol). Ethyl acetate (3 mL) was then added to dilute the reaction mixture. An aliquot was withdrawn from this mixture and quenched with brine (2 mL). The organic phase was extracted with ethyl acetate (2 mL), dried over anhydrous Na_2SO_4, filtered through a cotton layer, and analyzed with GC and GC-MS.

S2.6 Reaction between 2-aminobenzamide and benzaldehyde under O_2-free conditions

A mixture of 2-aminobenzamide (40.8 mg, 0.3 mmol) and benzaldehyde (1 mL) was stirred at 120°C for 24 h under an argon atmosphere in a tightly sealed 8-ml vial. The reaction mixture was cooled to ambient temperature and then added with diphenyl ether as the internal standard (51.1 mg, 0.3 mmol). Ethyl acetate (3 mL) was then added to dilute the reaction mixture. An aliquot was withdrawn from this mixture and quenched with brine (2 mL). The organic phase was extracted with ethyl acetate (2 mL), dried over anhydrous Na_2SO_4, filtered through a cotton layer, and analyzed with GC and GC-MS.

S3 Results of the effect of benzyl alcohol amount and additional solvent on the product yield

Table S1: Screening of the reaction conditions with respect to benzyl alcohol amount and additional solvent

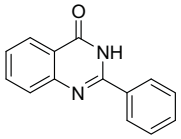


Entry	Benzyl alcohol amount (mL)	Additional solvent	GC yield (%)
1	0.25	None	57
2	0.5	None	70
3	0.75	None	76
4	1	None	84
5	1.25	None	81
6	1.5	None	79
7	1	H_2O	Trace
8	1	DMF	15
9	1	DMSO	39
10	1	DCB	55
11	1	Toluene	58

General conditions: 2-aminobenzamide (0.5 mmol), benzyl alcohol, *t*-BuONa (1.5 equiv.) and additional solvent (if any, 0.5 mL) at 120°C under an O_2 atmosphere for 24 h.

S4 Detailed synthesis conditions and NMR analysis of 2-phenylquinazolin-4(3*H*)-one derivatives

S4.1 2-Phenylquinazolin-4(3*H*)-one



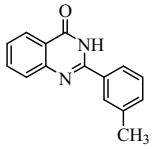
Prepared as the described procedure using 2-aminobenzamide (40.8 mg, 0.3 mmol), benzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.22 (ethyl acetate:hexane = 1:3 (v/v). Purified by washing with hexane (3 × 15 mL), yielding a white solid (50.0 mg, yield = 75%), mp 230–232°C. This compound is known [1].

^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 12.53 (s, 1H), 8.20–8.14 (m, 3H), 7.83 (ddd, J = 8.4, 7.1, 1.6 Hz, 1H), 7.77–7.72 (m, 1H), 7.61–7.50 (m, 4H).

^{13}C NMR (151 MHz, DMSO-d_6) δ (ppm) = 162.26, 152.34, 148.69, 134.58, 132.71, 131.38, 128.59, 127.75, 127.45, 126.57, 125.84, 120.95.

EI-MS m/z (% relative intensity, ion): 119 (100), 222 (63, M^+).

S4.2 2-(3-Methylphenyl)-quinazolin-4(3*H*)-one



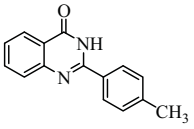
Prepared as the described procedure using 2-aminobenzamide (40.8 mg, 0.3 mmol), 3-methylbenzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.22 (ethyl acetate:hexane = 1:7 (v/v). Purified by column chromatography on silica gel (230–400 mesh or 37–63 µm, ethyl acetate/hexane = 1:7 (v/v), yielding a white solid (47.3 mg, yield = 67%), mp 208–210°C. This compound is known [2].

^{1}H NMR (600 MHz, DMSO-d_6) δ 12.44 (s, 1H), 8.15 (dd, J = 7.9, 1.6 Hz, 1H), 8.02 (d, J = 1.9 Hz, 1H), 7.97 (m, 1H), 7.83 (ddd, J = 8.4, 7.0, 1.5 Hz, 1H), 7.74 (dd, J = 8.2, 1.1 Hz, 1H), 7.51 (ddd, J = 8.1, 7.1, 1.2 Hz, 1H), 7.47–7.35 (m, 2H), 2.41 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 162.20, 152.39, 148.71, 137.87, 134.52, 132.62, 131.95, 128.45, 128.24, 127.40, 126.47, 125.81, 124.85, 120.93, 20.92.

EI-MS m/z (% relative intensity, ion): 119 (100), 236 (57, M^+).

S4.3 2-(4-Methylphenyl)-quinazolin-4(3*H*)-one



Prepared as the described procedure using 2-aminobenzamide (40.8 mg, 0.3 mmol), 4-methylbenzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.20 (ethyl acetate/hexane = 1:4 (v/v). Purified

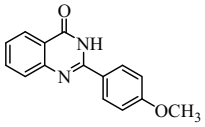
by column chromatography on silica gel (230–400 mesh or 37–63 μm, ethyl acetate:hexane = 1:4 (v/v), yielding a white solid (48.7 mg, yield = 69%), mp 230–232°C. This compound is known [3].

^{1}H NMR (600 MHz, DMSO-d_6) δ 12.43 (s, 1H), 8.14 (dd, J = 7.9, 1.6 Hz, 1H), 8.11–8.06 (m, 2H), 7.82 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.72 (dd, J = 8.2, 1.1 Hz, 1H), 7.50 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.34 (d, J = 8.0 Hz, 2H), 2.38 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 162.34, 152.30, 148.75, 141.45, 134.55, 129.90, 129.19, 127.68, 127.32, 126.38, 125.84, 120.87, 20.97.

EI-MS m/z (% relative intensity, ion): 119 (100), 236 (56, M^+).

S4.4 2-(4-Methoxyphenyl)-quinazolin-4(3*H*)-one



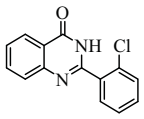
Prepared as the described procedure using 2-aminobenzamide (40.8 mg, 0.3 mmol), 4-methoxybenzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.20 (ethyl acetate/hexane = 1:2 (v/v). Purified by column chromatography on silica gel (230–400 mesh or 37–63 μm, ethyl acetate:hexane = 1:2 (v/v), yielding a white solid (50.1 mg, yield = 66%), mp 242–244°C. This compound is known [4].

^{1}H NMR (600 MHz, DMSO-d_6) δ 12.38 (s, 1H), 8.23–8.16 (m, 2H), 8.13 (dd, J = 8.0, 1.6 Hz, 1H), 7.81 (ddd, J = 8.5, 7.1, 1.6 Hz, 1H), 7.74–7.66 (m, 1H), 7.48 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 7.12–7.05 (m, 2H), 3.85 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) 162.30, 161.84, 151.86, 148.88, 134.47, 129.41, 127.22, 126.06, 125.78, 124.78, 120.64, 113.95, 55.42.

EI-MS m/z (% relative intensity, ion): 119 (100), 252 (82, M^+).

S4.5 2-(2-Chlorophenyl)-quinazolin-4(3*H*)-one



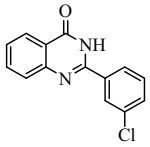
Prepared as the described procedure using 2-aminobenzamide (40.8 mg, 0.3 mmol), 2-chlorobenzyl alcohol (1369 mg, 32 equiv.), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.38 (ethyl acetate:hexane = 1:1 (v/v). Purified by washing with hexane (3 × 15 mL), yielding a white solid (23.5 mg, yield = 31%), mp 198–200°C. This compound is known [5].

^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 12.63 (s, 1H), 8.19 (dd, J = 7.9, 1.6 Hz, 1H), 7.84 (m, 1H), 7.74–7.69 (m, 1H), 7.67 (dd, J = 7.6, 1.7 Hz, 1H), 7.61 (dd, J = 8.1, 1.3 Hz, 1H), 7.59–7.53 (m, 2H), 7.49 (m, 1H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 161.47, 152.27, 148.60, 134.60, 133.82, 131.62, 131.52, 130.88, 129.62, 127.49, 127.24, 127.08, 125.87, 121.26.

EI-MS m/z (% relative intensity, ion): 119 (100), 256 (52, M^+), 258 (19).

S4.6 2-(3-Chlorophenyl)-quinazolin-4(3*H*)-one



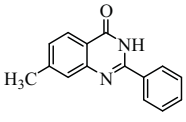
Prepared as the described procedure using 2-aminobenzamide (40.8 mg, 0.3 mmol), 3-chlorobenzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.32 (ethyl acetate:hexane = 1:3 (v/v). Purified by washing with hexane (3 × 15 mL), yielding a white solid (21.9 mg, yield = 29%), mp 298–300°C. This compound is known [2].

^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 12.60 (s, 1H), 8.25 (m, 1H), 8.16 (m, 2H), 7.86 (m, 1H), 7.77 (dd, J = 8.2, 1.1 Hz, 1H), 7.66 (ddd, J = 8.1, 2.2, 1.0 Hz, 1H), 7.62–7.49 (m, 2H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 162.12, 151.01, 148.37, 134.73, 134.62, 133.41, 131.09, 130.46, 127.50, 126.86, 126.38, 125.83, 121.08.

EI-MS m/z (% relative intensity, ion): 119 (100), 256 (54, M^+), 258 (20).

S4.7 7-Methyl-2-2-phenylquinazolin-4(3*H*)-one



Prepared as the described procedure using 2-amino-4-methylbenzamide (45.1 mg, 0.3 mmol), benzyl alcohol

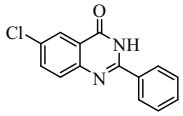
(1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.21 (ethyl acetate:hexane = 1:3 (v/v). Purified by washing with hexane (3 × 15 mL), yielding a light yellow solid (40.5 mg, yield = 57%), mp 236–238°C. This compound is known [6].

^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 12.42 (s, 1H), 8.23–8.13 (m, 2H), 8.04 (d, J = 8.1 Hz, 1H), 7.64–7.48 (m, 4H), 7.33 (dd, J = 8.0, 1.7 Hz, 1H), 2.47 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 162.09, 152.31, 148.78, 145.00, 132.75, 131.27, 128.54, 127.95, 127.65, 127.07, 125.66, 118.54, 21.31.

EI-MS m/z (% relative intensity, ion): 133 (100), 236 (68, M^+).

S4.8 6-Chloro-2-phenylquinazolin-4(3*H*)-one



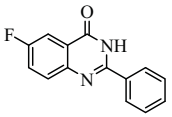
Prepared as the described procedure using 2-amino-5-chlorobenzamide (51 mg, 0.3 mmol), benzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.20 (ethyl acetate:hexane = 1:5 (v/v). Purified by column chromatography on silica gel (230–400 mesh or 37–63 µm, ethyl acetate/hexane = 1:5 (v/v), yielding a white solid (39.2 mg, yield = 51%), mp 291°C (decomposed). This compound is known [7].

^{1}H NMR (600 MHz, DMSO) δ (ppm) = 12.70 (s, 1H), 8.18 (dd, J = 7.1, 1.6 Hz, 2H), 8.09 (d, J = 2.5 Hz, 1H), 7.87 (dd, J = 8.7, 2.5 Hz, 1H), 7.77 (d, J = 8.7 Hz, 1H), 7.64–7.58 (m, 1H), 7.56 (m, 2H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 161.37, 152.90, 147.43, 134.67, 132.47, 131.57, 130.72, 129.69, 128.62, 127.83, 124.86, 122.21.

EI-MS m/z (% relative intensity, ion): 153 (100), 256 (79, M^+), 155 (33), 258 (26).

S4.9 6-Fluoro-2-phenylquinazolin-4(3*H*)-one



Prepared as the described procedure using 2-amino-5-fluorobenzamide (46.2 mg, 0.3 mmol), benzyl alcohol (1 mL), sodium *tert*-butoxide (43.2 mg, 1.5 equiv.) at 120°C under an O_2 atmosphere for 24 h. TLC silica gel 60 F_{254}, R_f = 0.21 (ethyl acetate:hexane = 1:5 (v/v). Purified by column chromatography on silica gel (230–400 mesh or 37–63 µm, ethyl acetate/hexane = 1:5 (v/v), yielding a clear solid (45.4 mg, yield = 63%), mp 254°C (decomposed). This compound is known [8].

^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 12.63 (s, 1H), 8.22–8.11 (m, 2H), 7.82 (m, 2H), 7.72 (m, 1H), 7.63–7.50 (m, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ (ppm) = 161.67, 160.95–159.01 (d, $J_{C\text{-}F}$ = 245.1 Hz), 151.87, 145.57, 132.55, 131.41, 130.30, 128.60, 127.73, 123.14–122.95 (d, $J_{C\text{-}F}$ = 23.9 Hz), 122.20–122.13 (d, $J_{C\text{-}F}$ = 8.6 Hz), 110.58–110.40 (d, $J_{C\text{-}F}$ = 23.9 Hz).

EI-MS m/z (% relative intensity, ion): 137 (100), 240 (64, M^+).

S5 ^{1}H- and ^{13}C-NMR spectra of 2-phenylquinazolin-4(3*H*)-one derivatives

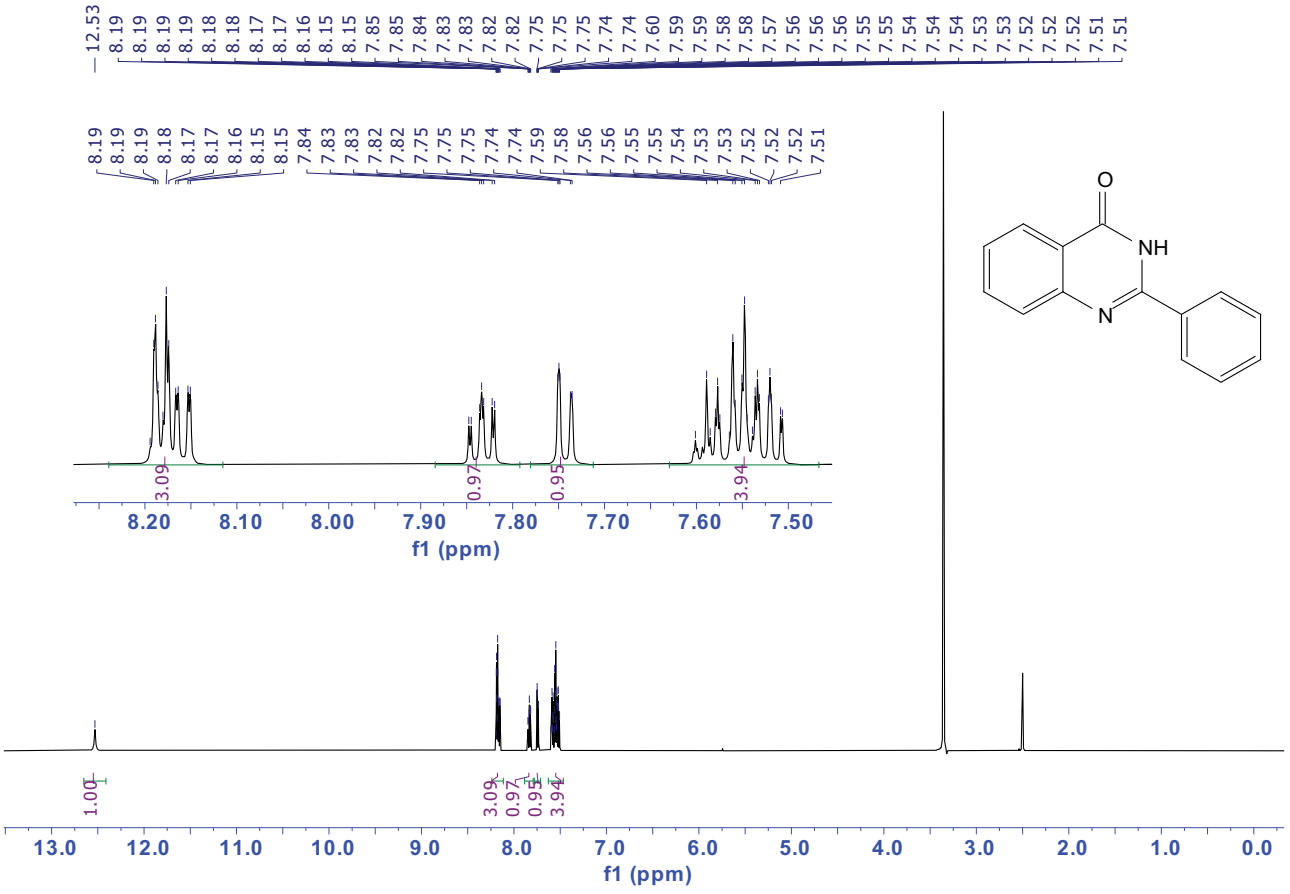


Figure S1: ^{1}H-NMR spectrum of 2-phenylquinazolin-4(3*H*)-one.

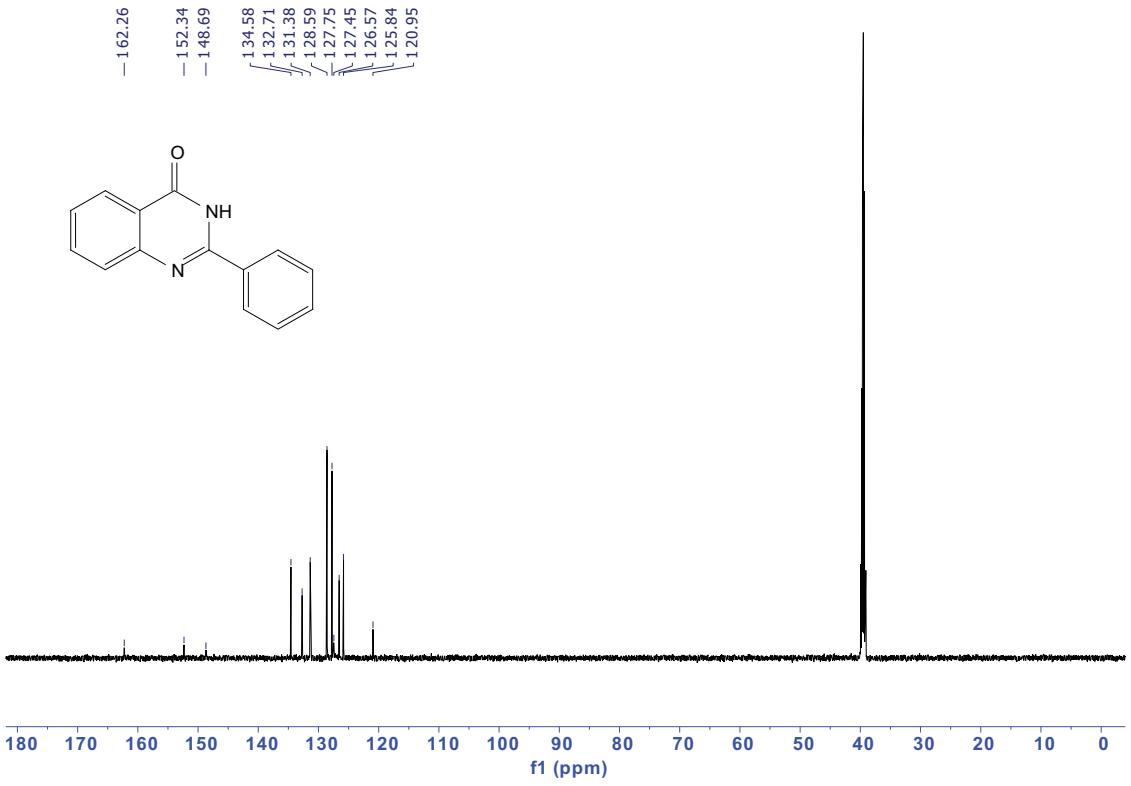


Figure S2: ^{13}C-NMR spectrum of 2-phenylquinazolin-4(3*H*)-one.

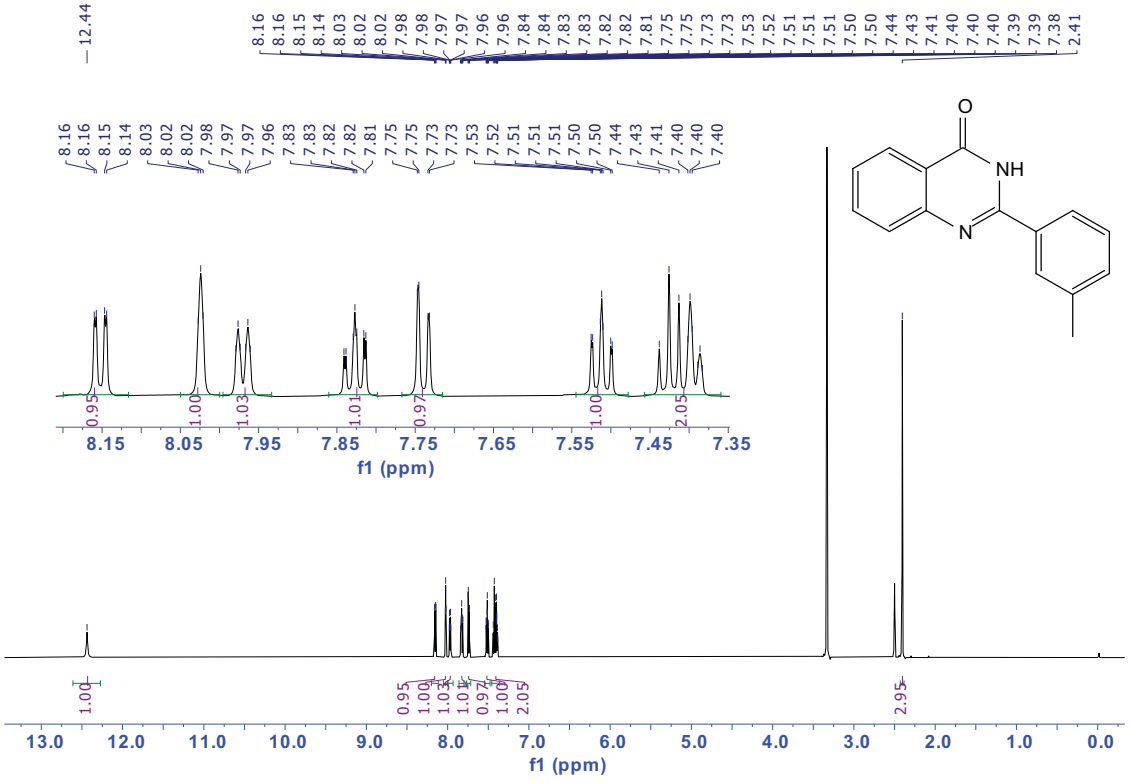


Figure S3: ^{1}H-NMR spectrum of 2-(3-methylphenyl)-quinazolin-4(3*H*)-one.

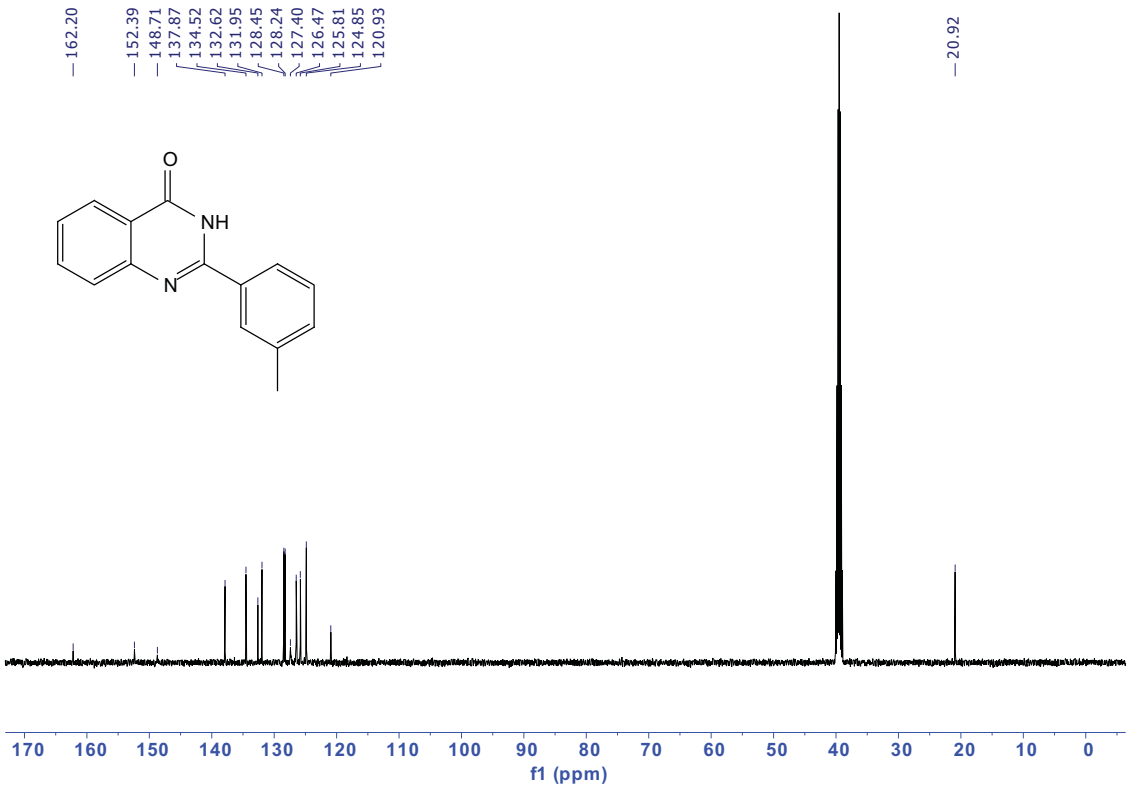


Figure S4: ^{13}C-NMR spectrum of 2-(3-methylphenyl)-quinazolin-4(3*H*)-one.

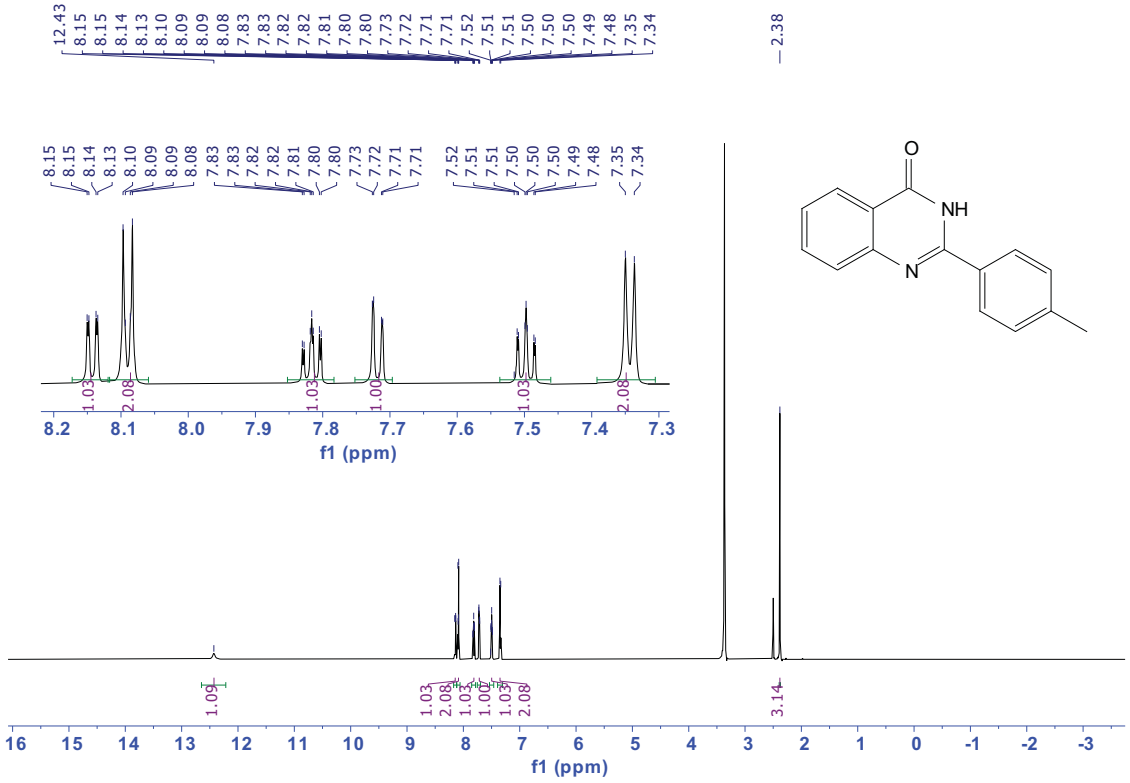


Figure S5: ^{1}H-NMR spectrum of 2-(4-methylphenyl)-quinazolin-4(3*H*)-one.

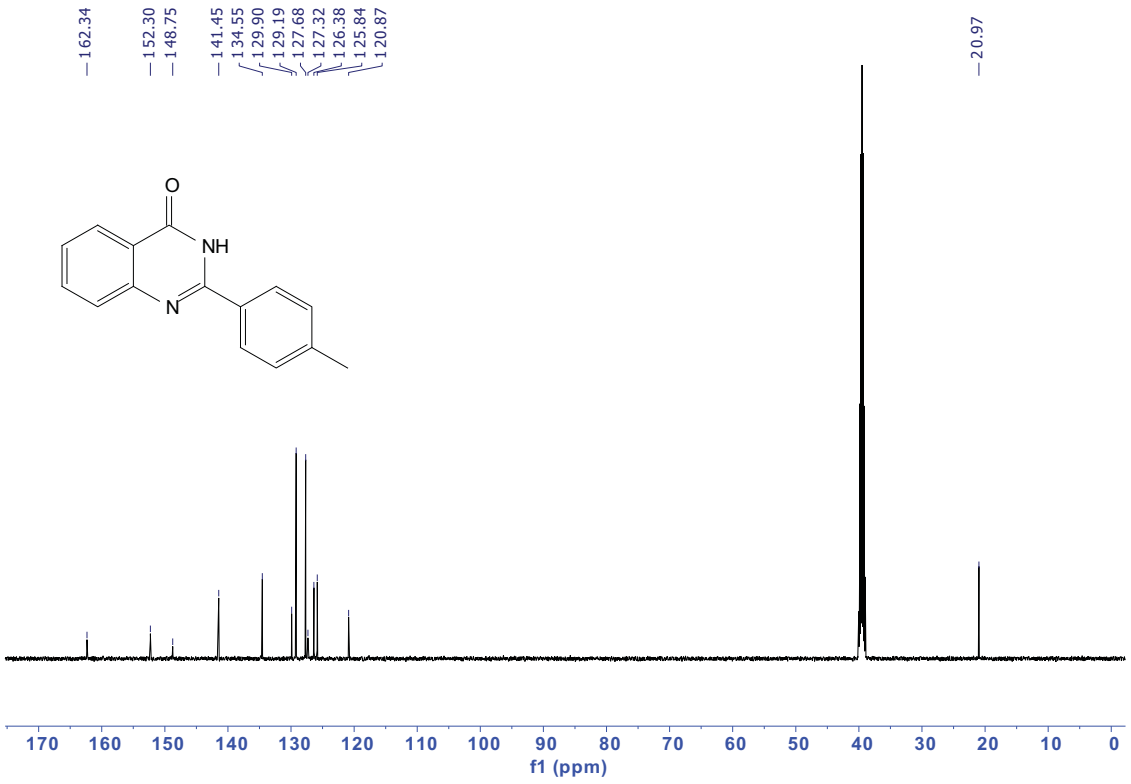


Figure S6: ^{13}C-NMR spectrum of 2-(4-methylphenyl)-quinazolin-4(3*H*)-one.

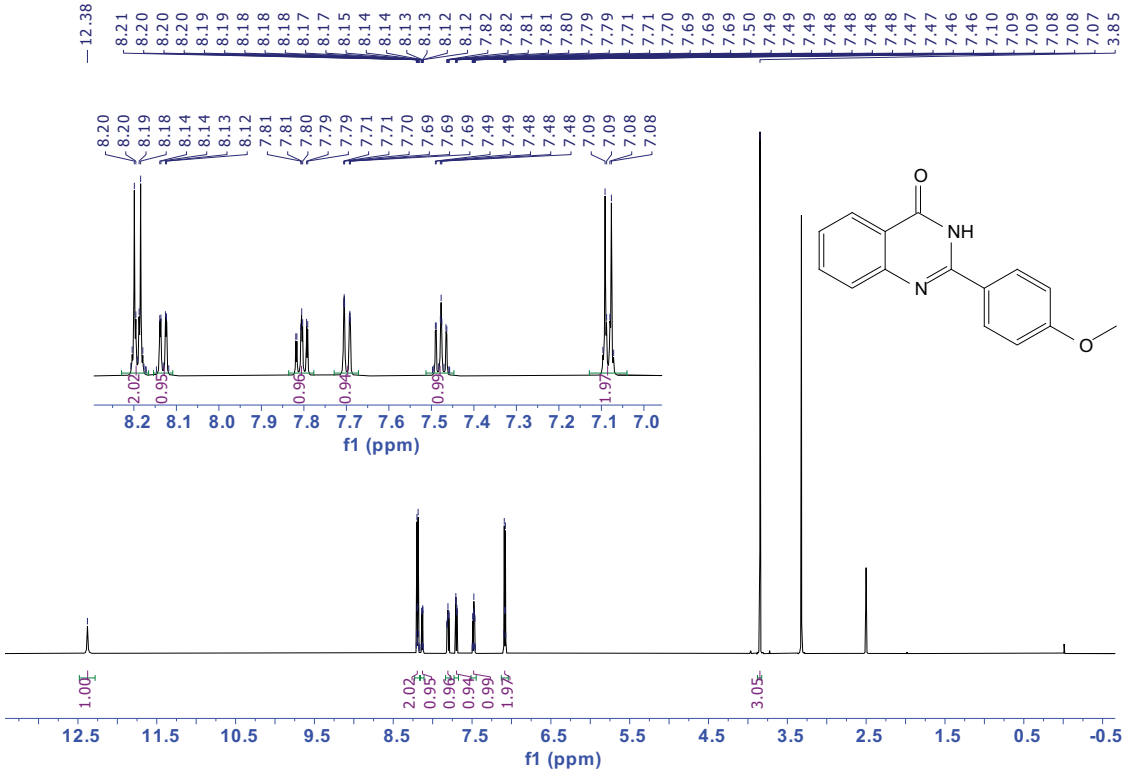


Figure S7: ^{1}H-NMR spectrum of 2-(4-methoxyphenyl)-quinazolin-4(3*H*)-one.

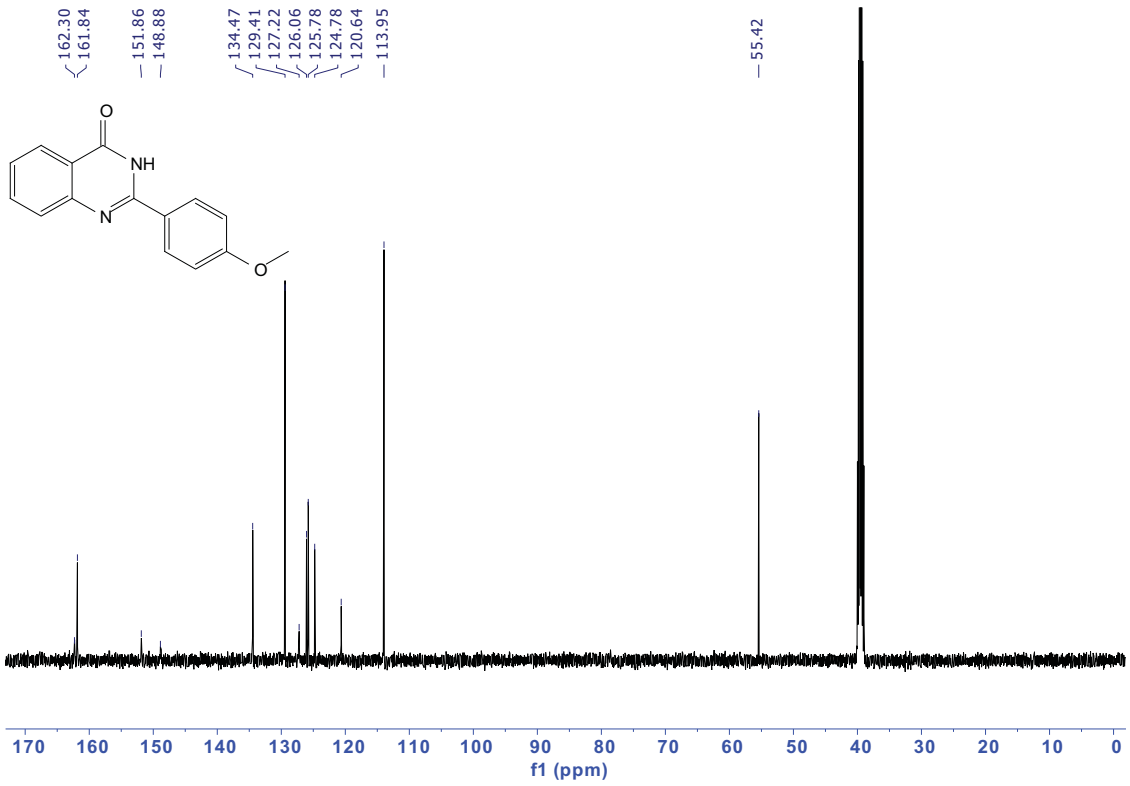


Figure S8: ^{13}C-NMR spectrum of 2-(4-methoxyphenyl)-quinazolin-4(3*H*)-one.

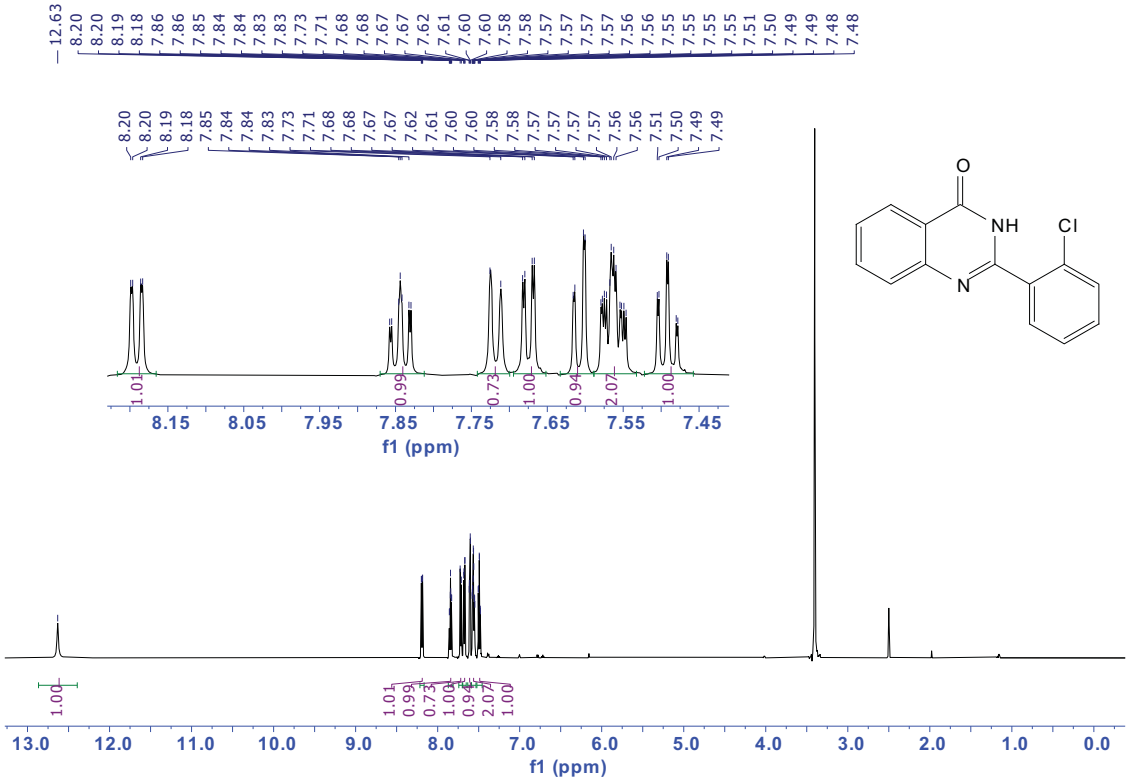


Figure S9: ^{1}H-NMR spectrum of 2-(2-chlorophenyl)-quinazolin-4(3*H*)-one.

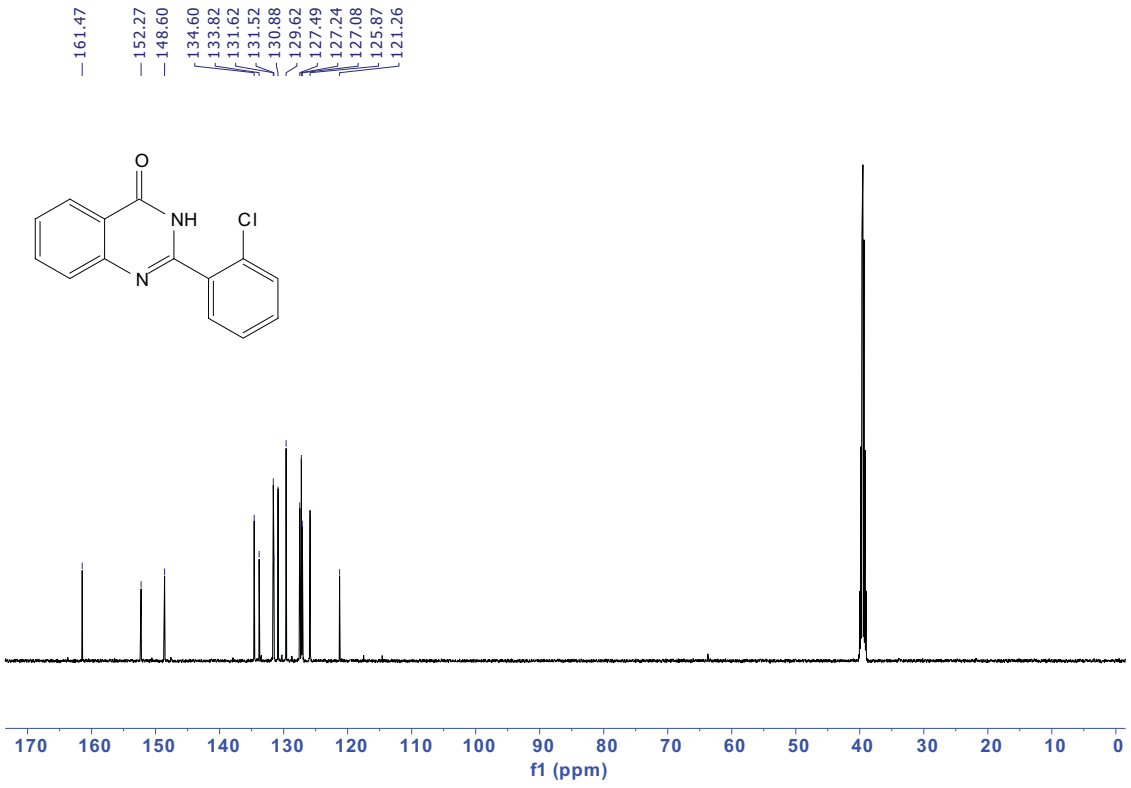


Figure S10: ^{13}C-NMR spectrum of 2-(2-chlorophenyl)-quinazolin-4(3*H*)-one.

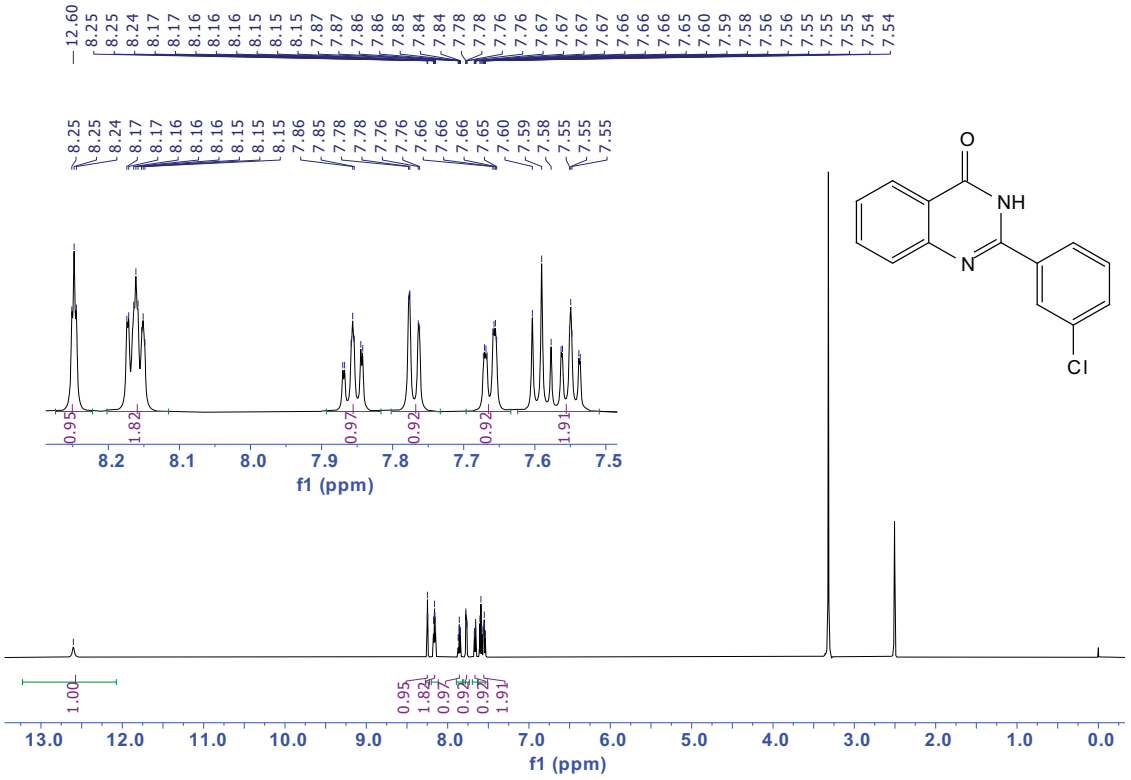


Figure S11: ^{1}H-NMR spectrum of 2-(3-chlorophenyl)-quinazolin-4(3*H*)-one.

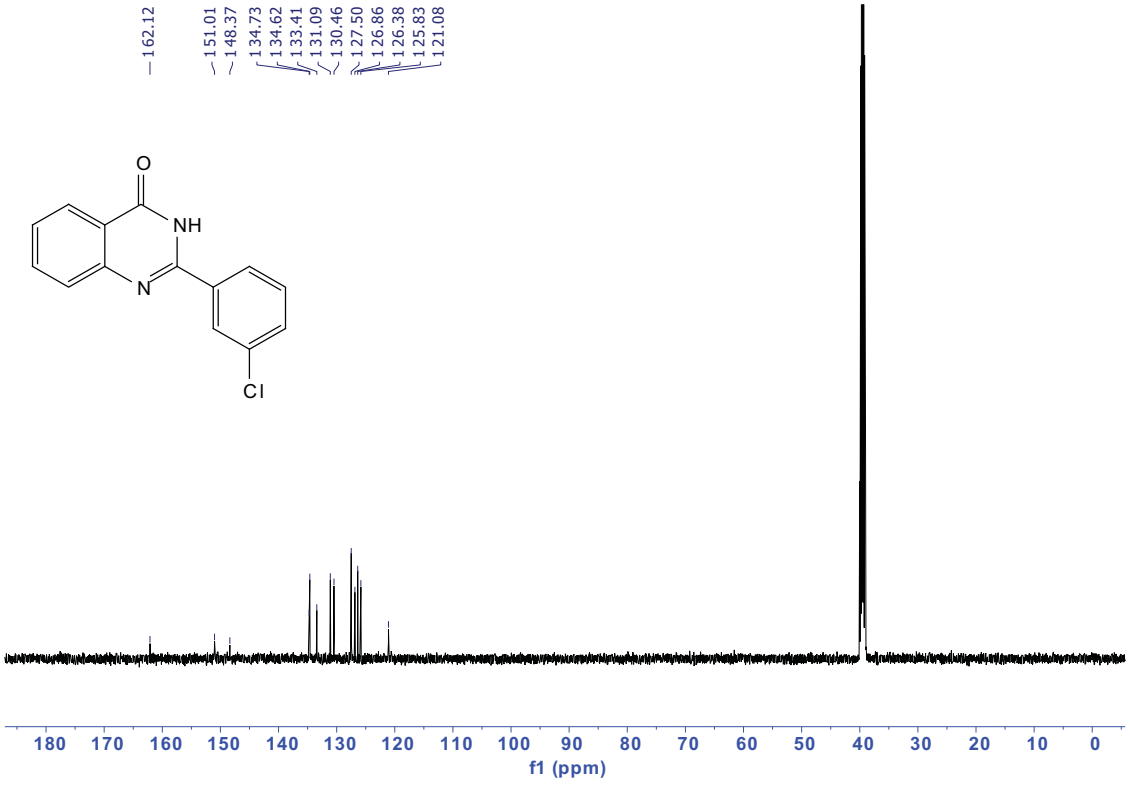


Figure S12: ^{13}C-NMR spectrum of 2-(3-chlorophenyl)-quinazolin-4(3*H*)-one.

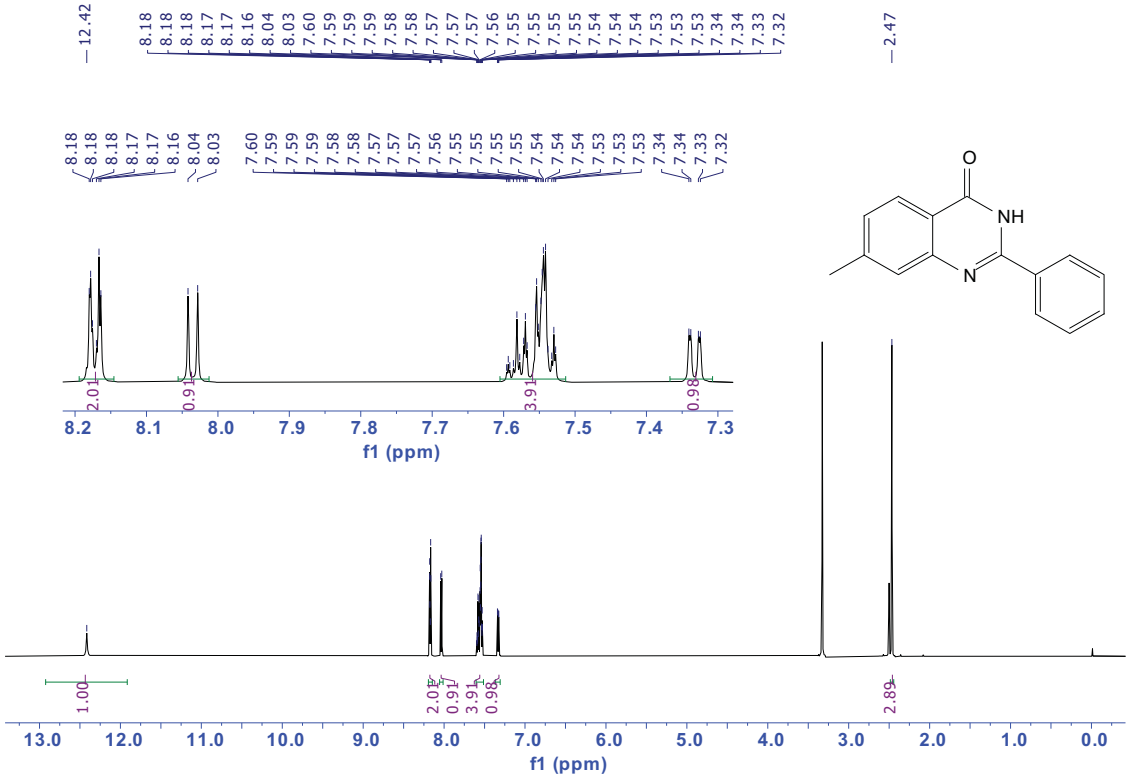


Figure S13: ^{1}H-NMR spectrum of 7-methyl-2-2-phenylquinazolin-4(3*H*)-one.

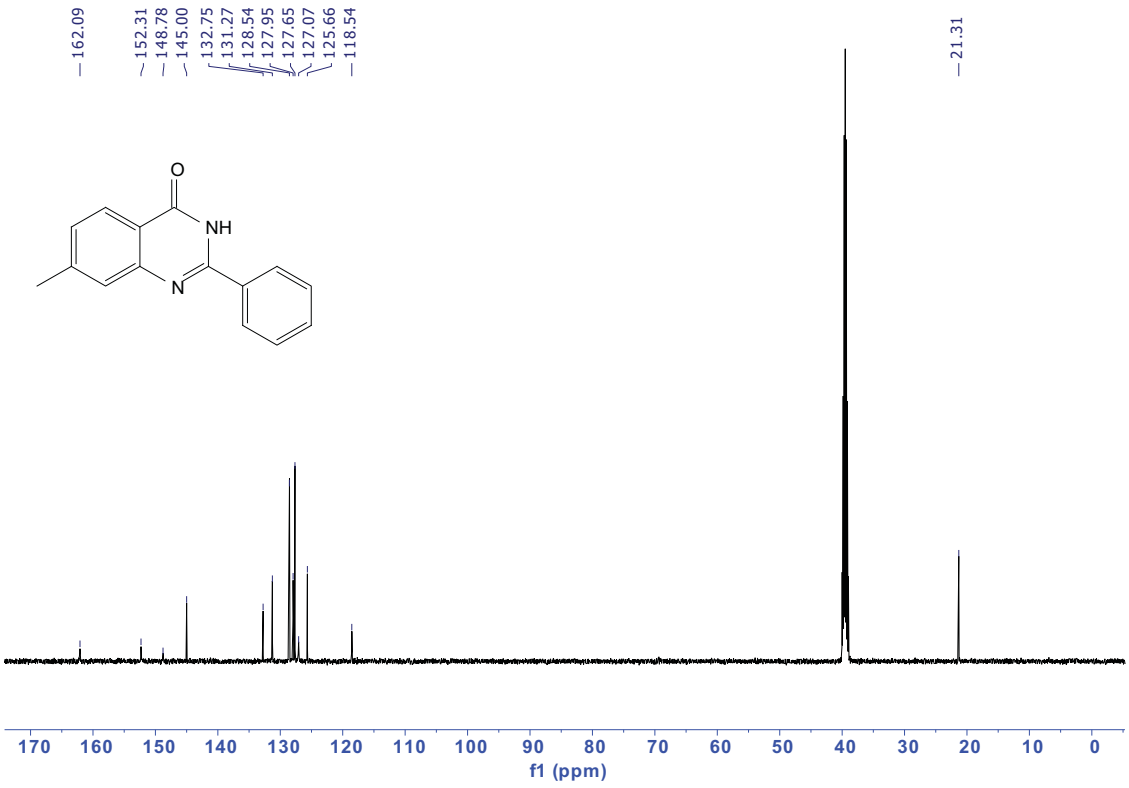


Figure S14: ^{13}C-NMR spectrum of 7-methyl-2-2-phenylquinazolin-4(3*H*)-one.

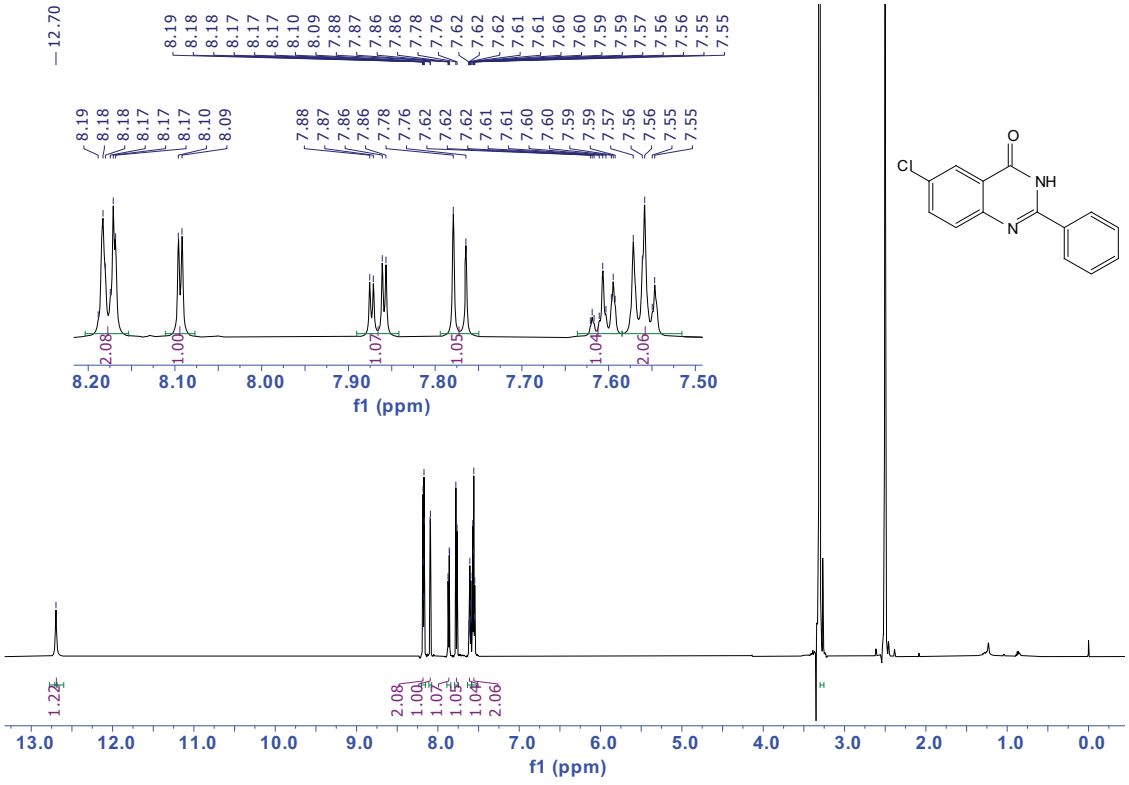


Figure S15: ^{1}H-NMR spectrum of 6-chloro-2-phenylquinazolin-4(3*H*)-one.

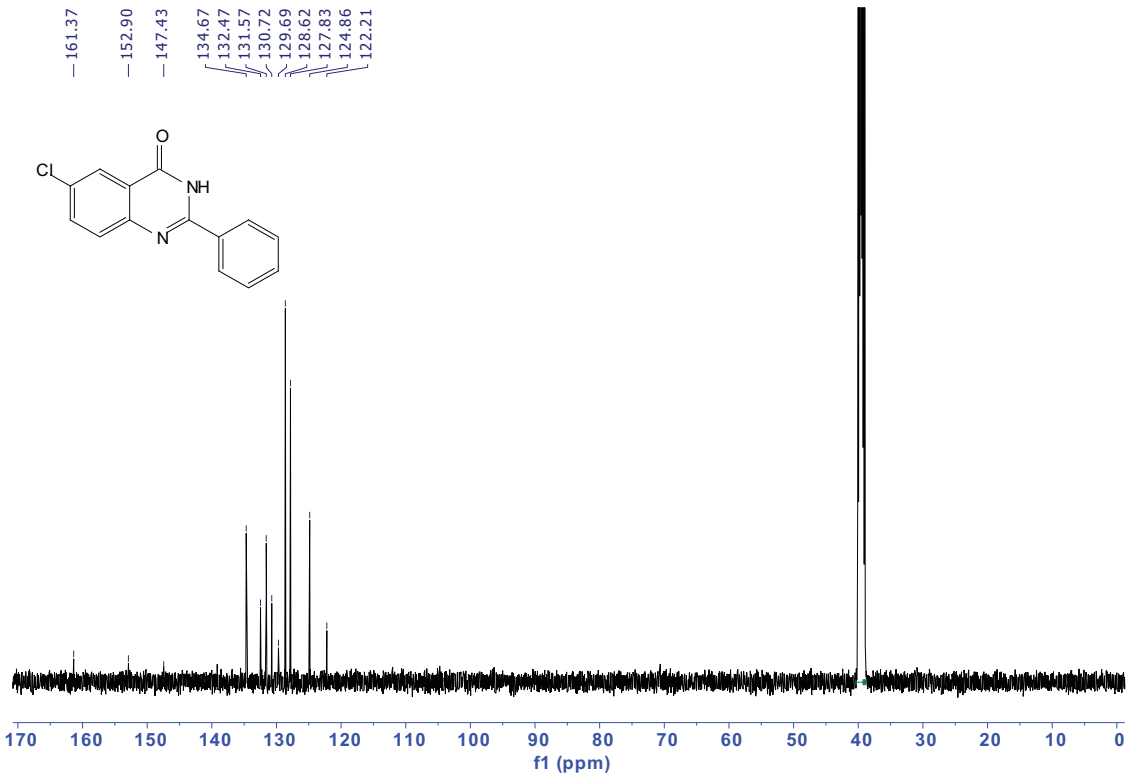


Figure S16: ^{13}C-NMR spectrum of 6-chloro-2-phenylquinazolin-4(3*H*)-one.

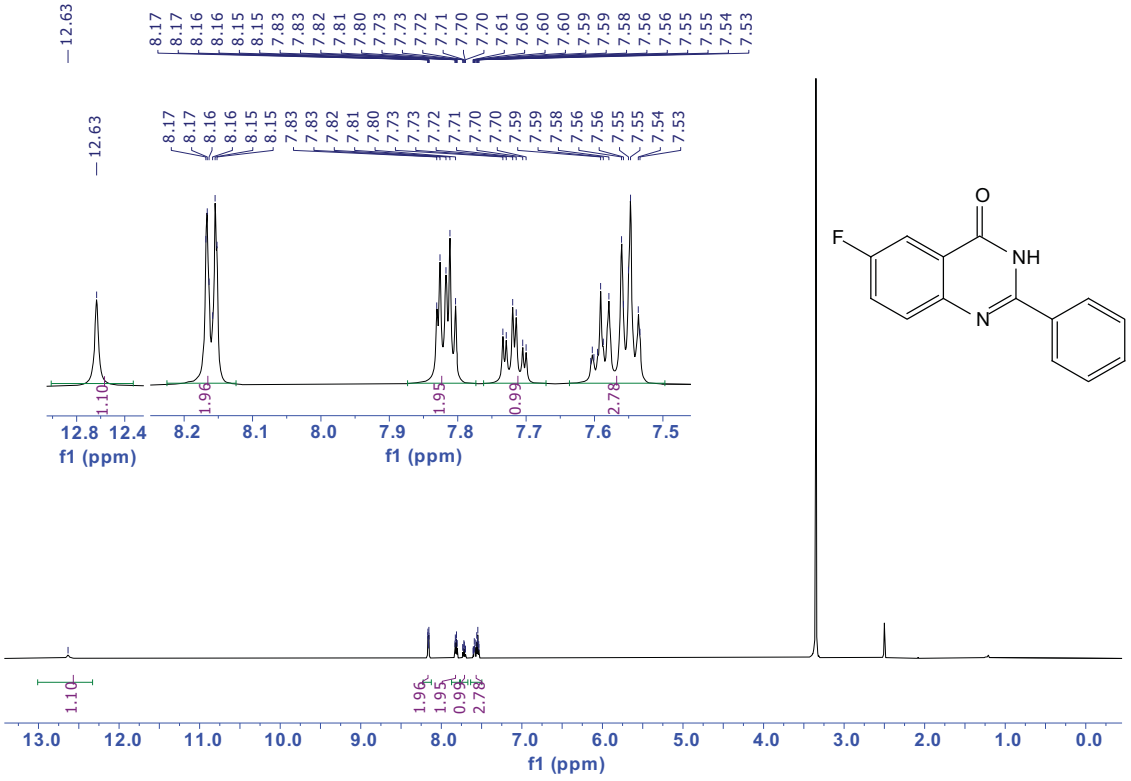


Figure S17: ^{1}H-NMR spectrum of 6-fluoro-2-phenylquinazolin-4(3*H*)-one.

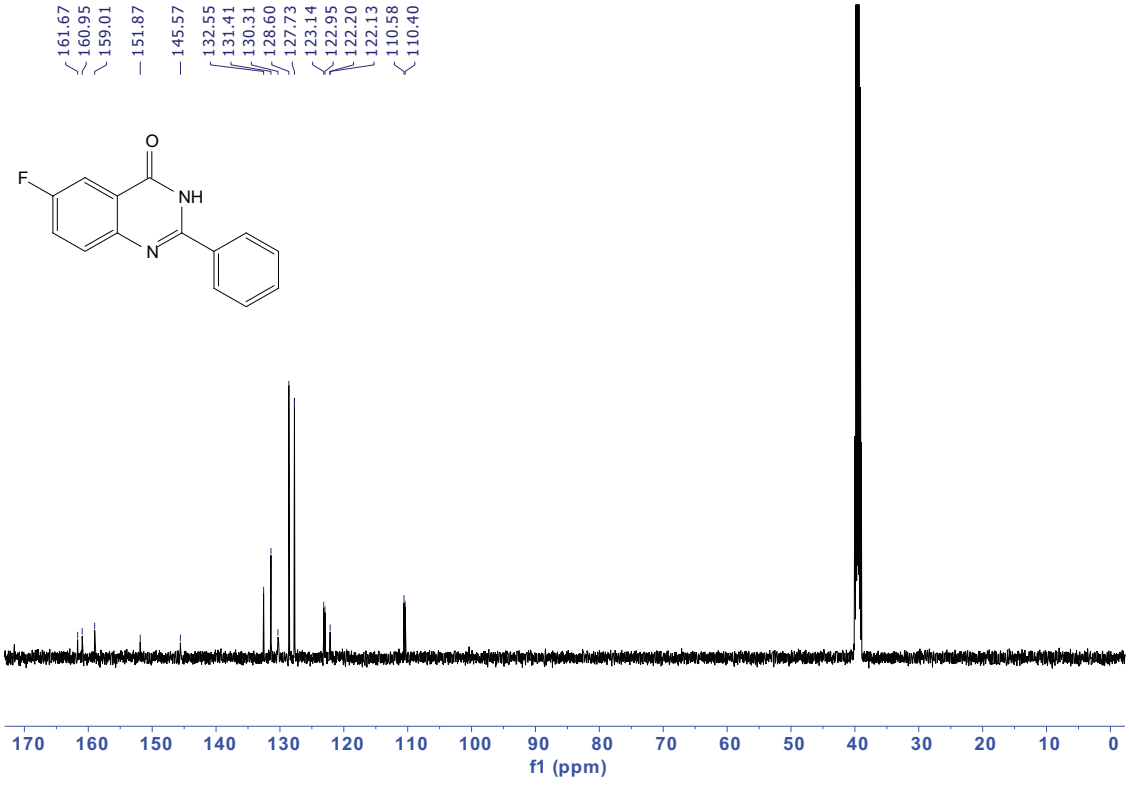


Figure S18: ^{13}C-NMR spectrum of 6-fluoro-2-phenylquinazolin-4(3*H*)-one.

S6 Mass spectrum results of 2-phenylquinazolin-4(3*H*)-one derivatives

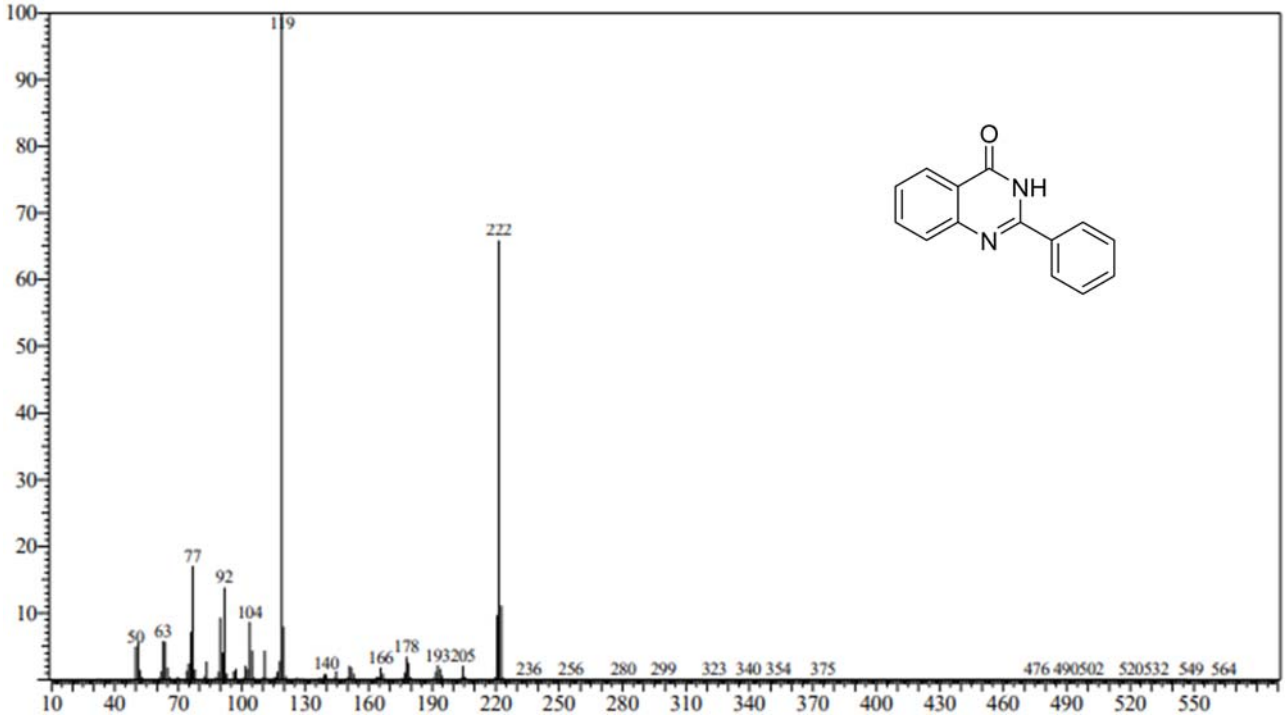


Figure S19: Mass spectrum of 2-phenylquinazolin-4(3*H*)-one.

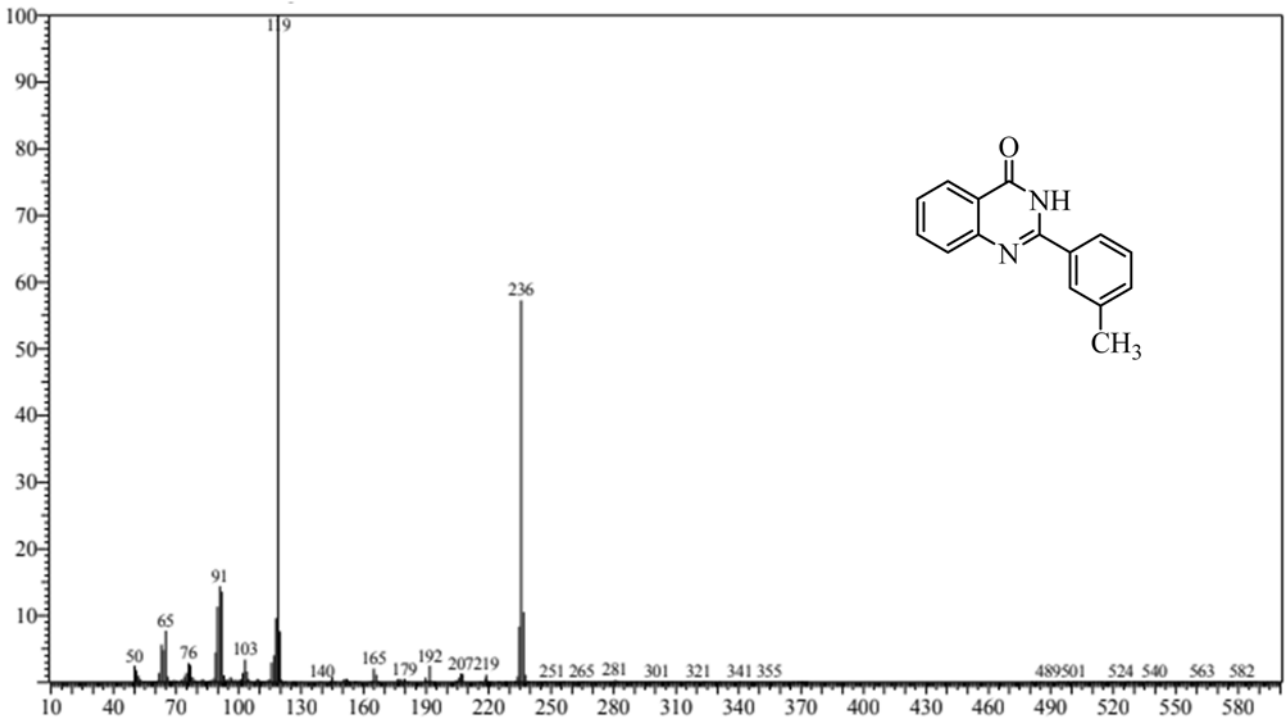


Figure S20: Mass spectrum of 2-(3-methylphenyl)-quinazolin-4(3*H*)-one.

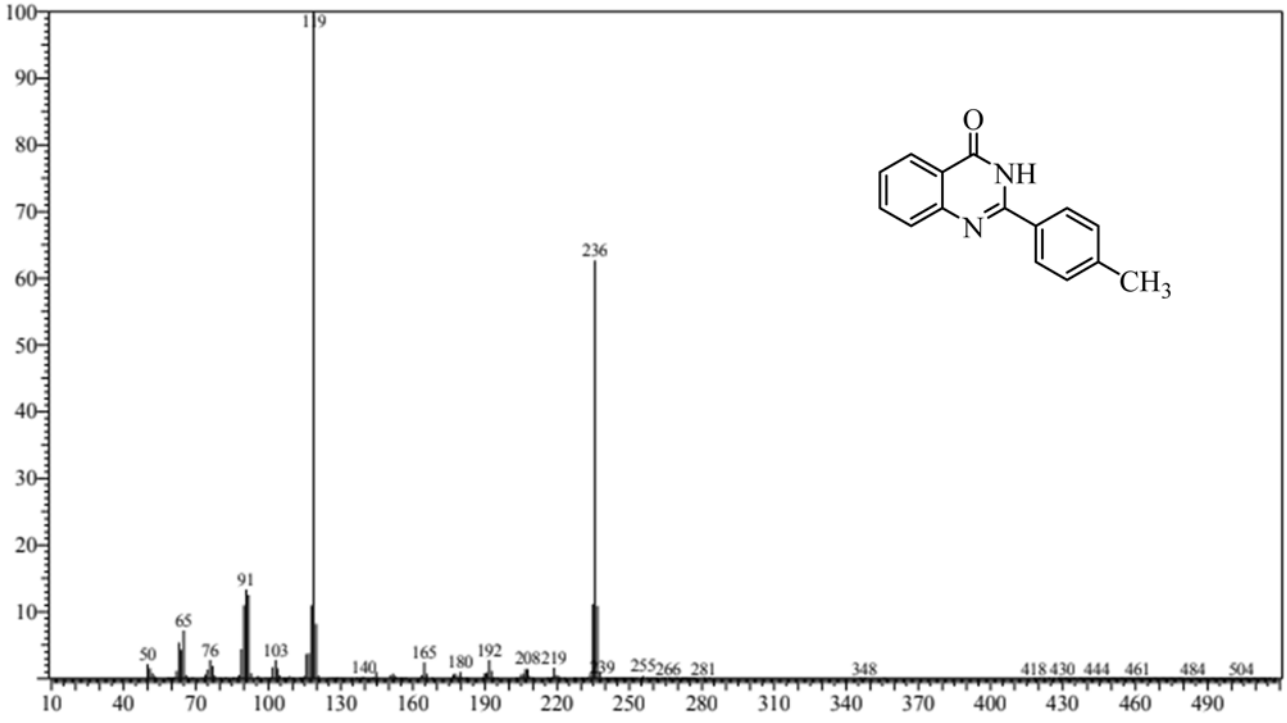


Figure S21: Mass spectrum of 2-(4-methylphenyl)-quinazolin-4(3*H*)-one.

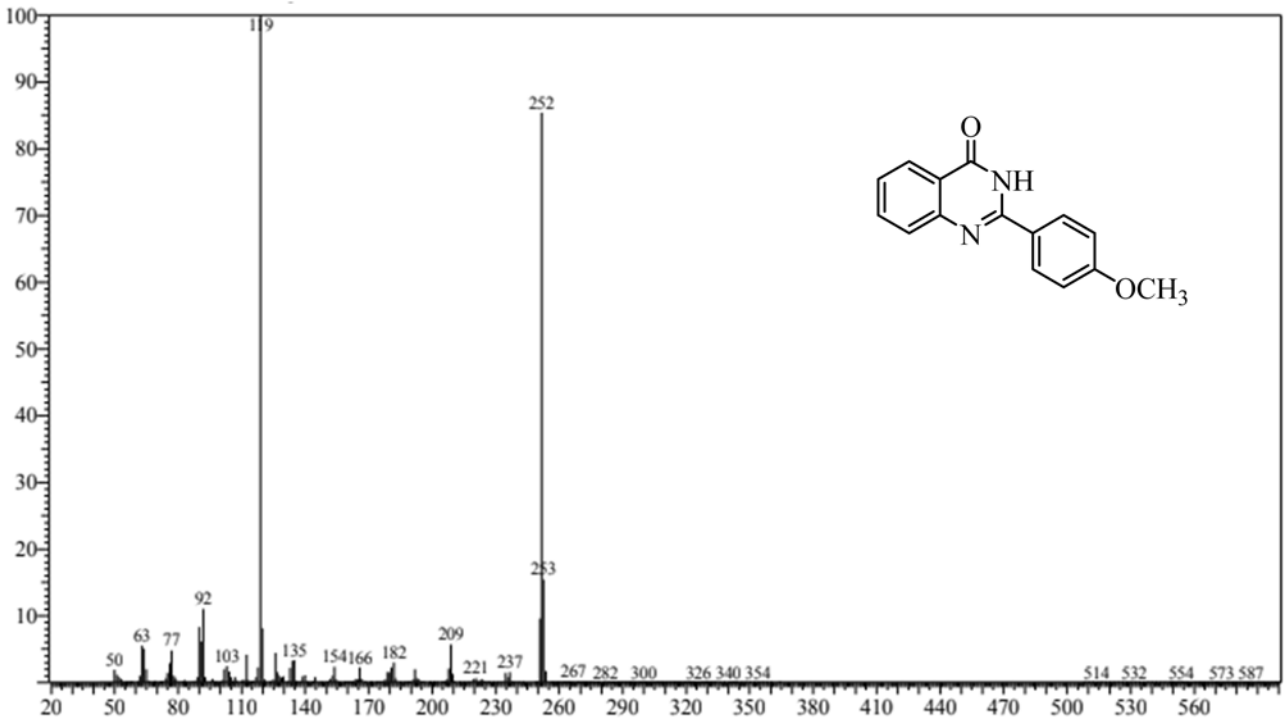


Figure S22: Mass spectrum of 2-(4-methoxyphenyl)-quinazolin-4(3*H*)-one.

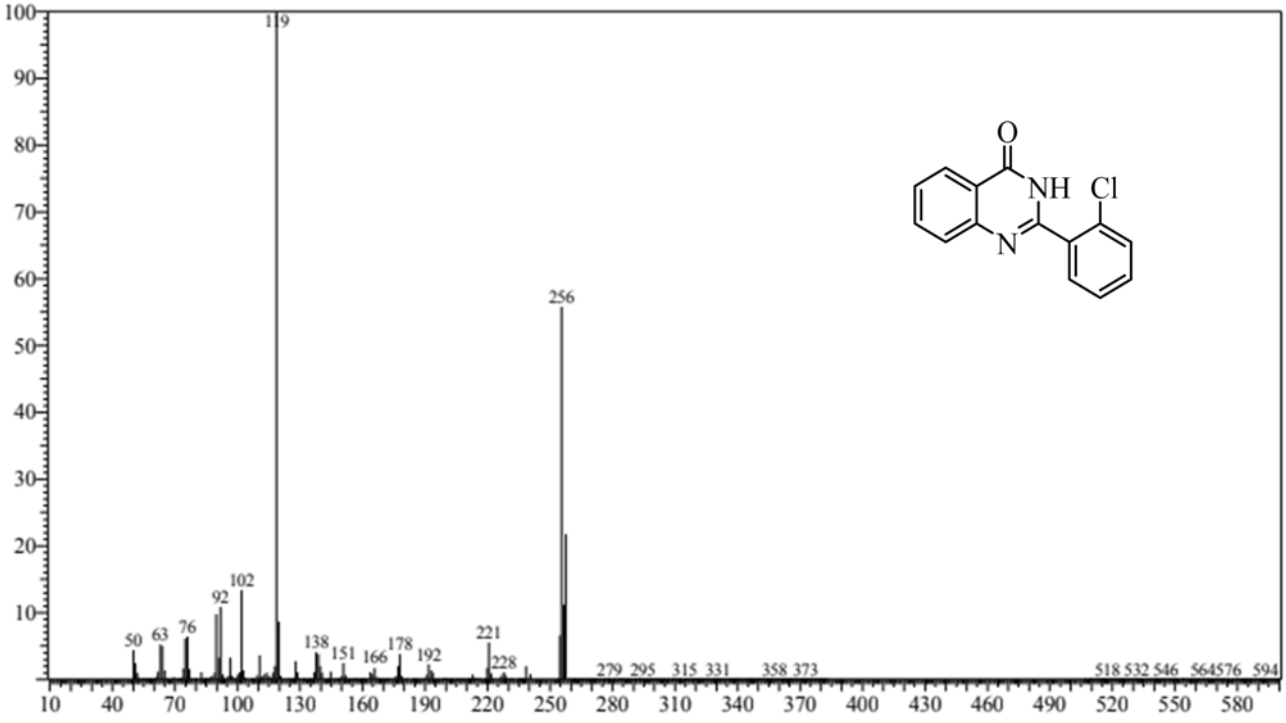


Figure S23: Mass spectrum of 2-(2-chlorophenyl)-quinazolin-4(3*H*)-one.

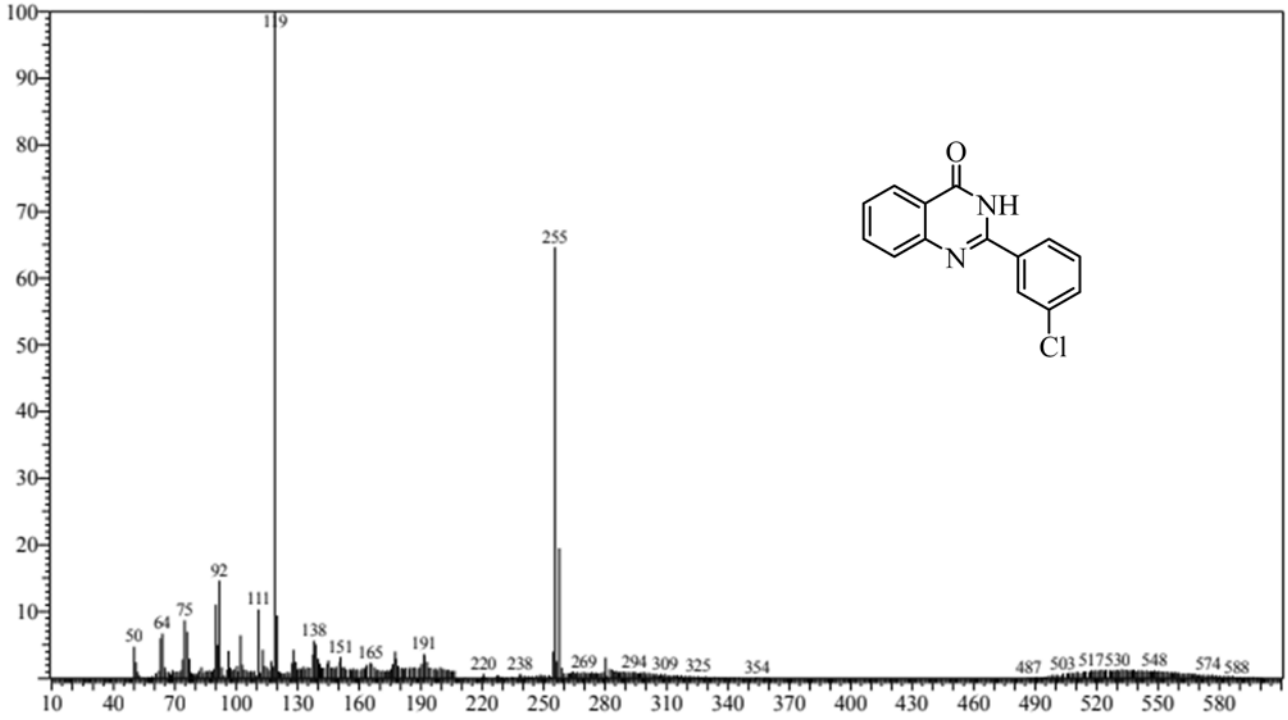


Figure S24: Mass spectrum of 2-(3-chlorophenyl)-quinazolin-4(3*H*)-one.

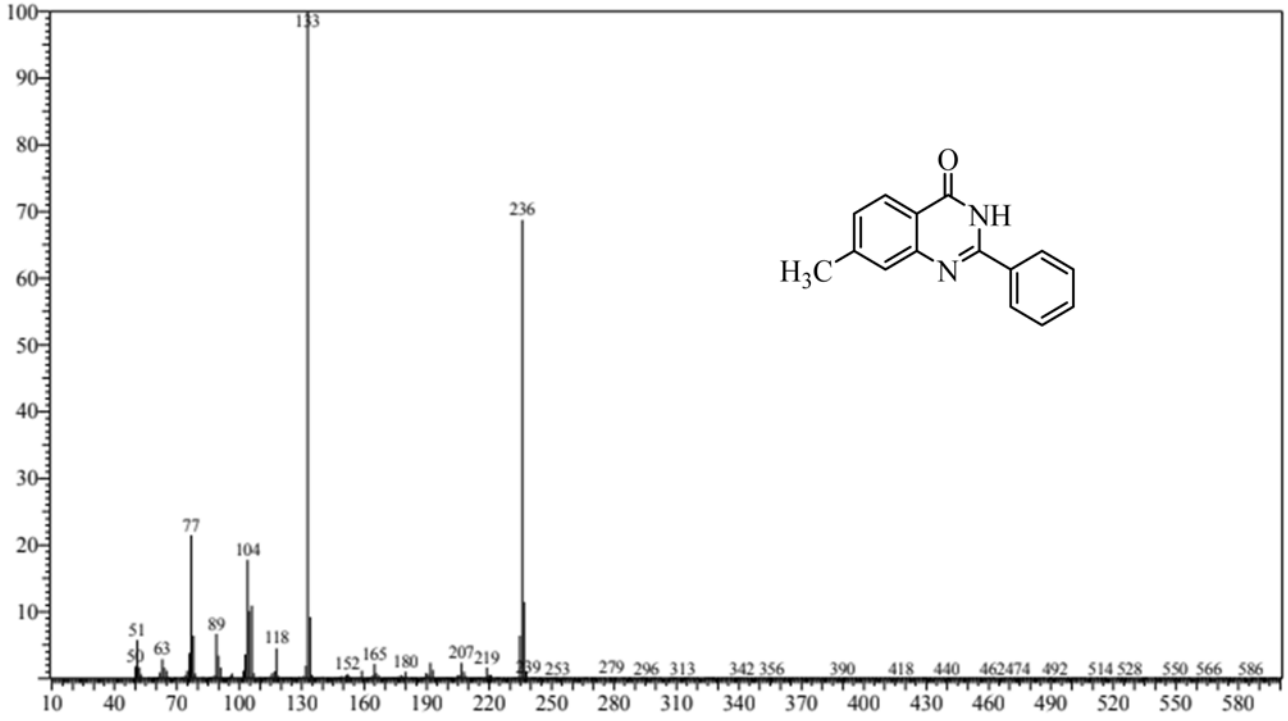


Figure S25: Mass spectrum of 7-methyl-2-2-phenylquinazolin-4(3*H*)-one.

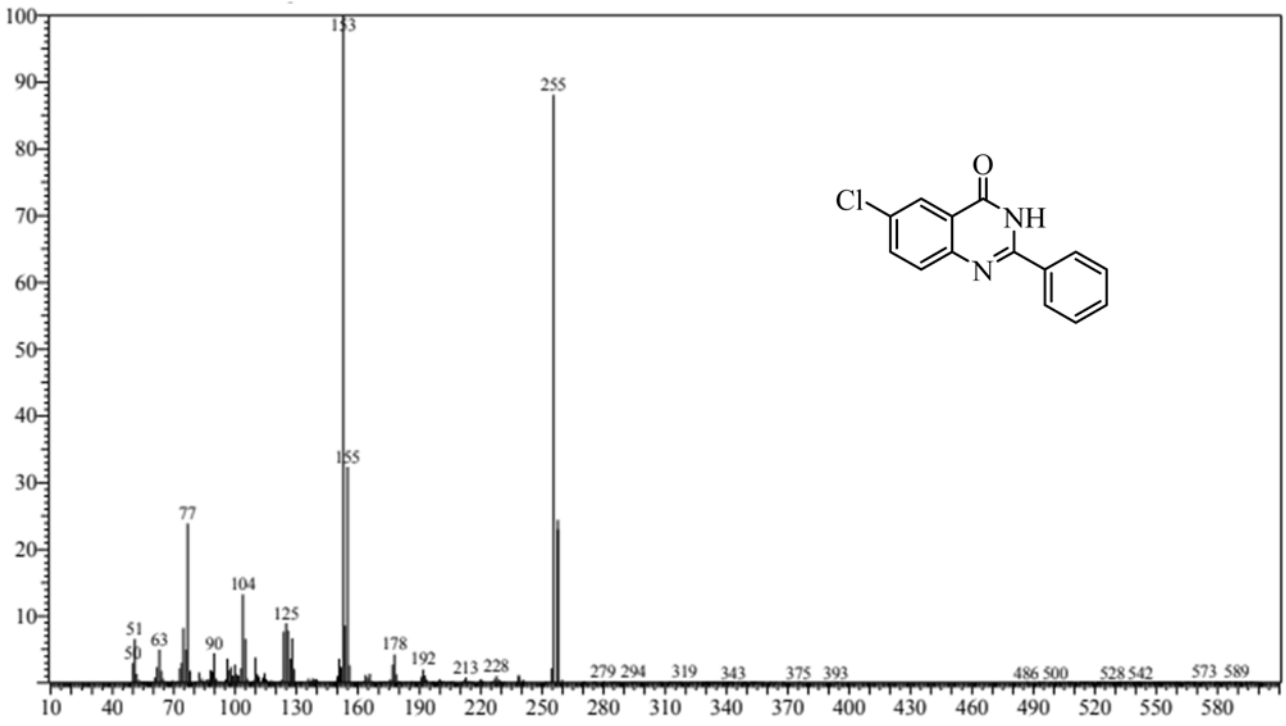


Figure S26: Mass spectrum of 6-chloro-2-phenylquinazolin-4(3*H*)-one.

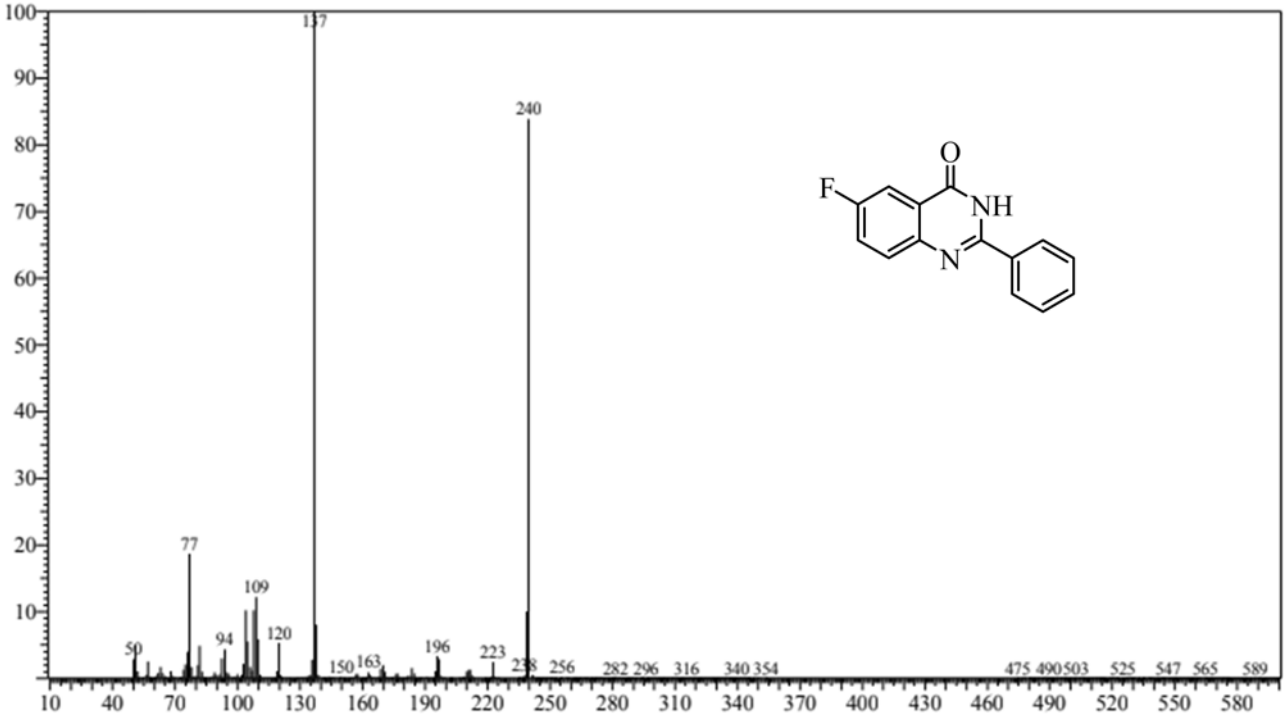


Figure S27: Mass spectrum of 6-fluoro-2-phenylquinazolin-4(3*H*)-one.

References

[1] Balaji S, Balamurugan G, Ramesh R, Semeril D. Palladium(II) N^O chelating complexes catalyzed one-pot approach for synthesis of quinazolin-4(3*H*)-ones via acceptorless dehydrogenative coupling of benzyl alcohols and 2-Aminobenzamide. Organometallics. 2021;40(6):725–34. doi: 10.1021/acs.organomet.0c00814.

[2] Parua S, Das S, Sikari R, Sinha S, Paul ND. One-pot cascade synthesis of quinazolin-4(3*H*)-ones via nickel-catalyzed dehydrogenative coupling of o-Aminobenzamides with alcohols. J Org Chem. 2017;82(14):7165–75. doi: 10.1021/acs.joc.7b00643.

[3] Liu W, Wu G, Gao W, Ding J, Huang X, Liu M, et al. Palladium-catalyzed oxidative C-C bond cleavage with molecular oxygen: one-pot synthesis of quinazolinones from 2-amino benzamides and alkenes. Org Chem Front. 2018;5(18):2734–8. doi: 10.1039/C8QO00670A.

[4] Sardar B, Jamatia R, Samanta A, Srimani D. Ru doped hydrotalcite catalyzed borrowing hydrogen-mediated N-alkylation of benzamides, sulfonamides, and dehydrogenative synthesis of quinazolinones. J Org Chem. 2022;87(9):5556–67. doi: 10.1021/acs.joc.1c02913.

[5] Sayahi MH, Bahadorikhalili S, Mahdavi M, Baghshirin L. Synthesis of quinazolin-4(3*H*)-ones via the reaction of isatoic anhydride with benzyl azides in the presence of potassium tert-butoxide in DMSO. Chem Heterocycl Compd. 2019;55:964+. doi: 10.1007/s10593-019-02563-w.

[6] Upadhyaya K, Thakur RK, Shukla SK, Tripathi RP. One-pot copper(I)-catalyzed ligand/base-free tandem cyclooxidative synthesis of quinazolinones. J Org Chem. 2016;81(12):5046–55. doi: 10.1021/acs.joc.6b00599.

[7] Pal D, Mondal A, Srimani D. Well-defined manganese complex catalyzed dehydrogenative synthesis of quinazolin-4(3*H*)-ones and 3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxides. Catal Sci Technol. 2022;12(10):3202–8. doi: 10.1039/D2CY00260D.

[8] Akbari A, Zahedifar M. Synthesis of Quinazolin-4(3*H*)-ones via a novel approach. J Saudi Chem Soc. 2023;27(2):101597. doi: 10.1016/j.jscs.2023.101597.