Biomass Derived Cu_2O Nanoparticles for N-atom insertion Reactions: A Base Free Synthesis of Quinazolinones with a Green Approach

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1.0. General considerations

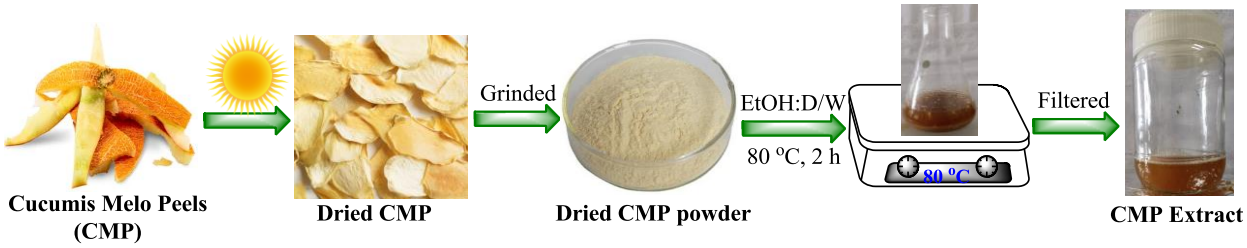
Unless otherwise specified, the reaction mixture was analyzed using GC-MS data which was performed in SHIMADZU GC-MS QP 2010SE system. The crystallographic nature and the phase of the Cu_2O NPs was examined and confirmed using powder X-ray diffraction spectroscopy (*P*-XRD) noted on a Rigaku X-Ray Diffraction Ultima IV (Rigaku Corporation, Japan) X-ray diffractometer using Ni filtered Cu Kα radiation (λ = 1.5406 Å) with a scan rate of 3º min^{-1} and theta value range of 0- 80° at 30 kV voltage and 15 mA current. The surface area analysis of Cu_2O NPs was performed using Brunauer Emmet and Teller (BET) method on Belsorp-Max (M/s. Microtrac BEL, Japan) under N_2 atmosphere at a temperature of -196 ºC. The corresponding pore size distribution of the catalysts was analyzed using Barrett Joyner Halenda (BJH) method. The catalyst was degassed at 80 ºC for 2h under vacuum prior to analysis in order to push out absorbed moisture. The thermal degradation of Cu_2O NPs was determined by a thermal analyser within the temperature window of 26 ºC to 900 ºC under continuous N_2 flow with a heating rate of 10 ºC min^{-1}. XPS analysis data is noted AXIS ULTRA DLD, KRATOS System with 200 um spot size.The surface morphology of Cu_2O NPs was investigated using Field Emission Scanning Electron Microscope (JEOL JSM-7100F, Singapore). The carbon tape on the aluminium metal stub was adequately covered with the powdered sample and subjected to sputtering using gold nanoparticles. To know more information about size, shape and surface morphology of Cu_2O NPs was investigated using HR-TEM analysis which was performed at SRM-University. All reactions were carried out in oven dried vials or sealed tubes with magnetic stirring under air atmosphere. All other reagents were directly used as purchased without further purification unless otherwise specified. All experiments were monitored by analytical thin layer chromatography (TLC) on pre-coated silica gel 60 F254 plates. Visualization on TLC was achieved by the use of UV light (254 nm). Column chromatography was undertaken on silica gel (60–120 mesh) using a proper eluent. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak (DMSO in d_6-DMSO: 2.5 ppm). Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), and multiplet (m). ^{13}C {^1H} NMR was recorded on Agilent Technologies DD2 (100 MHz) and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the centre of a multiplet at 40.0 ppm of DMSO. All analytical and spectral data are

given for newly synthesized products while for reported compounds; the corresponding references are cited.

2. Synthesis of Cu_2O NPs using *Cucumis melo* peels extract

2.1. Preparation of *Cucumis melo* (CM) peels extract

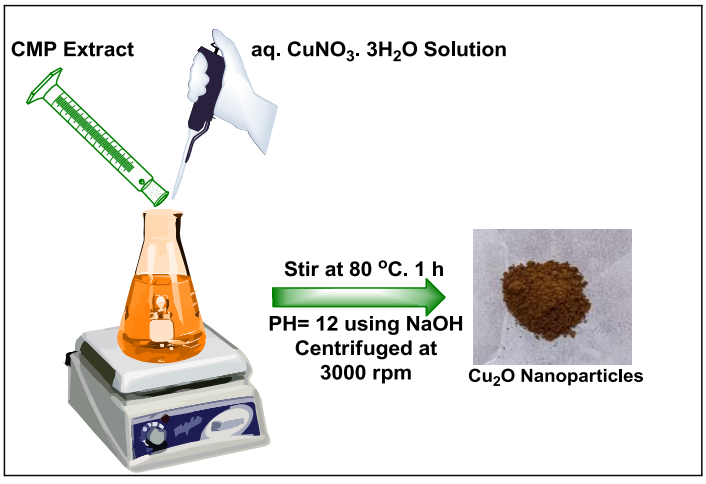
The peels of the Cucumis melo were obtained at a fruit store in Kanakapura, Karnataka, India. Then, 10 g of the powder was taken in 250 mL flask containing 100 mL of 1:1 (distilled water: ethanol) and the mixture was stirred at 80 ^oC for 2 h to extract the active chemical constituents exist in CMPE.[S1] Further, the mixture was cooled to room temperature, the residues were removed by filtration and stored at 4 ^oC (Scheme S1).



Scheme S1. Preparation of *Cucumis melo* peels (CMP) extract

2.2. Preparation of Cu_2O NPs using *Cucumis melo* peels (CMP) extract

The aqueous solution (0.05 M, 50 mL) of $Cu(NO_3)_2.3H_2O$ was taken in 100 mL round bottom flask at room temperature. Further, 30 mL of CMPE was added dropwise under stirring at 80 ^oC. The pH=12 of the solution was maintained by adding 0.5 M NaOH solution wherein the change



Scheme S2. Schematic representation of Copper oxide nanoparticles synthesis.

in color from blue to green followed by light orange was evidenced the formation of NPs. The reaction mixture was further allowed to stir for 1 h at 80 °C (Scheme S2). The mixture was then allowed to cool to room temperature followed by centrifugation at 3000 rpm for 10 minutes. Thus, formed NPs were further washed with the deionized water, ethanol, and acetone, and dried at 70 °C for 12 h and analyzed by different spectroscopic methods.[S2]

2.3 XPS spectra of Cu_2O NPs

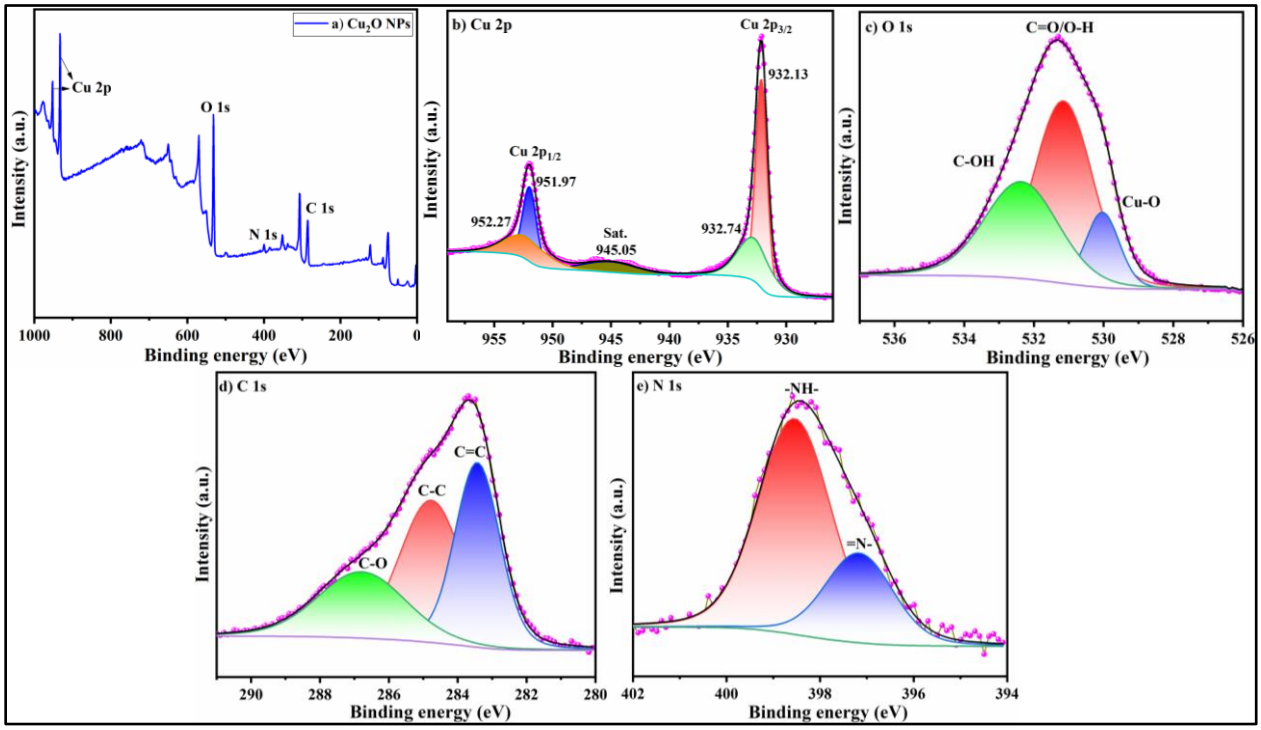
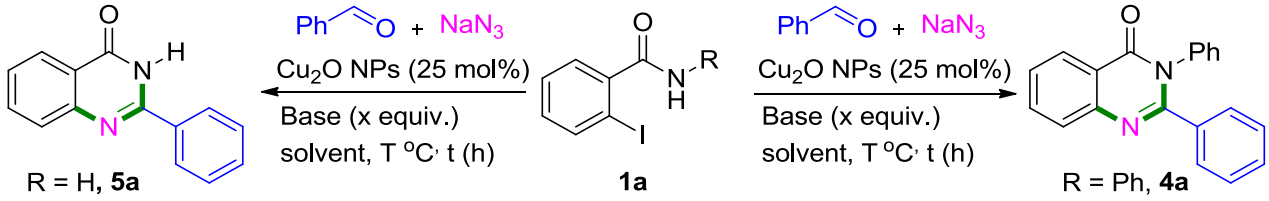


Figure. S1. XPS analysis (a) Survey spectra (b) Cu 2p (c) O 1s (d) C 1s (e) N 1s spectra of Cu_2O NPs

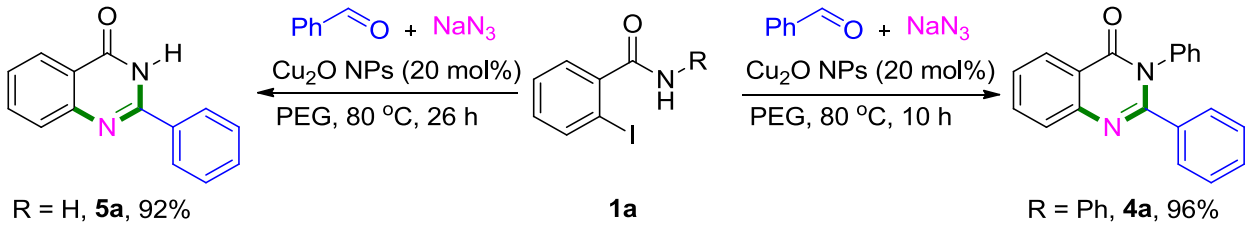
3. General experimental procedure for optimization study of Quinazolinones



The Cu_2O NPs (0-25 mol %, Cu content: 68.03% w/w) was added in an oven-dried 15 mL sealed tube containing compound **1a** (0.5 mmol, 1.0 equiv.), then the sodium azide (1.0 mmol, 2 equiv.) and solvent (1.0 mL) is added to the tube. Then, solution (1.0 mL) of compound **2a** (0.6 mmol,

1.2 equiv.) was added slowly. The reaction mixture was stirred at 60-100 °C for 8-26 h. After complete conversion of starting material (indicated by TLC), the reaction mixture was diluted with ethyl acetate and filtered. Further, filtrate was quenched with water and the organic layer was extracted with EtOAc (10×3). The combined organic layer was dried over anhydrous Na_2SO_4 then the solvent was evaporated under reduced pressure and crude compound was purified by column chromatography (eluent: 7-10% EA/Hexane) to get the compound **4a**. The reaction was repeated twice and product was isolated to determine the yield (by average of two run). Similar procedure was followed for the synthesis of 2-phenylquinazolin-4(3H)-one. The crude compound was purified by column chromatography (eluent: 14-18% EA/Hexane) to get the compound **5a**. The reaction was repeated twice and product was isolated to determine the yield (by average of two runs).

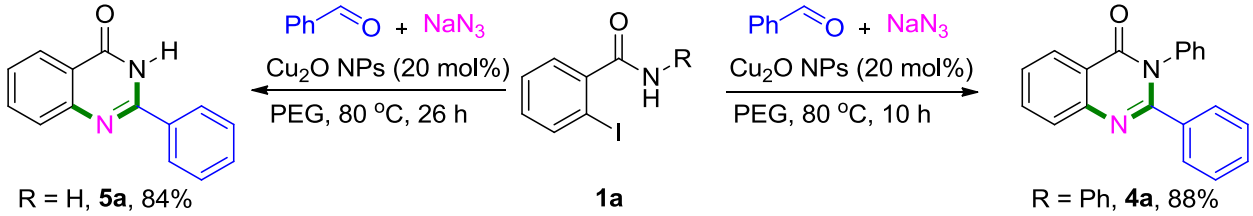
4. Exact experimental procedure for the synthesis of 2,3-diphenylquinazolin-4(3H)-one (4a) and 2-phenylquinazolin-4(3H)-one (5a)



The Cu_2O NPs (20 mol %, Cu content: 68.03% w/w) was added in an oven-dried 15 mL sealed tube containing compound **1a** (0.5 mmol, 1.0 equiv.), then the sodium azide (1.0 mmol, 2 equiv.) and solvent (1.0 mL) is added to the tube. Then, solution (1.0 mL) of compound **2a** (0.6 mmol, 1.2 equiv.) was added slowly. The reaction mixture was stirred at 60-100 °C for 8-26 h. After complete conversion of starting material (indicated by TLC), the reaction mixture was diluted with ethyl acetate and filtered. Further, filtrate was quenched with water and the organic layer was extracted with EtOAc (10×3). The combined organic layer was dried over anhydrous Na_2SO_4 then the solvent was evaporated under reduced pressure and crude compound was purified by column chromatography (eluent: 10-14% EA/Hexane) to get the compound **4a**. The reaction was repeated twice and product was isolated to determine the yield (by average of two run). Similar procedure was followed for the synthesis of 2-phenylquinazolin-4(3H)-one. The crude compound was purified by column chromatography (eluent: 14-18% EA/Hexane) to get

the compound **5a**. The reaction was repeated twice and product was isolated to determine the yield (by average of two runs).

5. Representative procedure of gram scale synthesis of 2,3-diphenylquinazolin-4(3H)-one (4a) and 2-phenylquinazolin-4(3H)-one (5a)

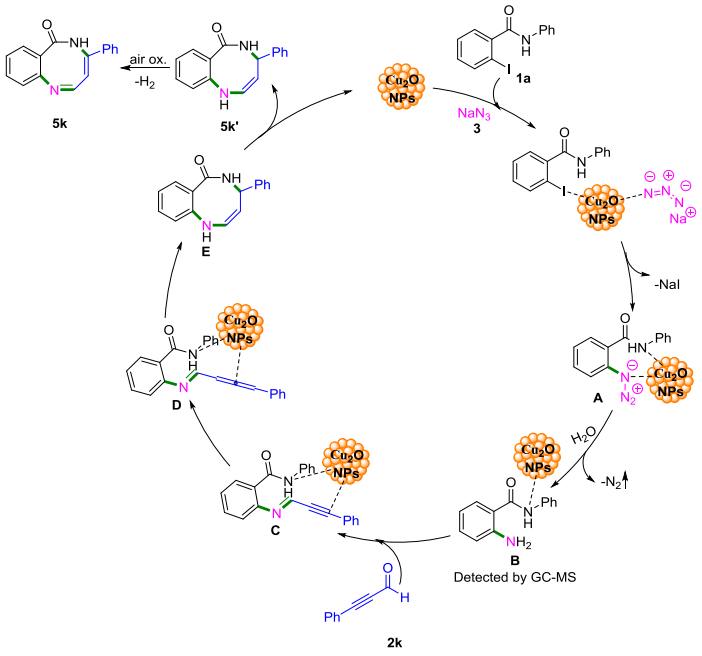


The Cu_2O NPs (20 mol %, Cu content: 68.03% w/w) was added in an oven-dried 15 mL sealed tube containing compound **1a** (0.5 mmol, 1.0 equiv.), then the sodium azide (1.0 mmol, 2 equiv.) and solvent (1.0 mL) is added to the tube. Then, solution (1.0 mL) of compound **2a** (0.6 mmol, 1.2 equiv.) was added slowly. The reaction mixture was stirred at 60-100 °C for 8-26 h. After complete conversion of starting material (indicated by TLC), the reaction mixture was diluted with ethyl acetate and filtered. Further, filtrate was quenched with water and the organic layer was extracted with EtOAc (10×3). The combined organic layer was dried over anhydrous Na_2SO_4 then the solvent was evaporated under reduced pressure and crude compound was purified by column chromatography (eluent: 10-14% EA/Hexane) to get the compound **4a**. The reaction was repeated twice and product was isolated to determine the yield (by average of two run). Similar procedure was followed for the synthesis of 2-phenylquinazolin-4(3H)-one. The crude compound was purified by column chromatography (eluent: 14-18% EA/Hexane) to get the compound **5a**. The reaction was repeated twice and product was isolated to determine the yield (by average of two runs).

6. Plausible mechanism for compound 5k

The proposed mechanistic route is based on the results of the control investigations and previous research in this area of interest. Initially, copper-catalyzed *S_NAr* reaction of 2-iodobenzamide (**1a**) with sodium azide produces intermediate **A**. Further, with the utility of trace amount of H_2O present in PEG-400, the Cu-mediated denitrogenation of **A** results in 2-aminobenzamide formation (**B**), which is detected by GC-MS analysis *via* Cu_2O NPs with the release of nitrogen as a by-product. Later, **B** undergoes condensation with aldehyde **2k**, leading to the formation of Schiff's base intermediate **C** which will further undergoes rearrangement to form allene

intermediate **D**. Subsequently, intramolecular nucleophilic attack of nitrogen in amide to allene carbon of **D** gives intermediate **5k**' via *8-exo-dig* cyclization process.[S5, S6] Finally, **5k**' undergoes aerial oxidation to form target molecule **5k (**Scheme S3).



Scheme S3. Plausible mechanism for compound **5k**.

7. Catalyst recyclability study for oxidation of 2,3-diphenylquinazolin-4(3H)-one (4a) synthesis

The recyclability of freshly synthesized Cu_2O NPs was examined for 2,3-diphenylquinazolin-4(3H)-one synthesis under optimized condition for fresh cycle after which the reactions were performed under external oxygen to facilitate the conversion of dihydro analogue (**4a'**) to yield the desired product **4a**. After the completion of reaction, the desired product is purified by column chromatography and yield was determined. Nevertheless, the heterogeneous Cu_2O NPs catalyst was separated from reaction mixture by centrifugation, washed with water (3 x 10 mL) followed by ethanol (3 x 10 mL) and dried at 70 °C for 12 h. It is then further used for second cycle and so on. As shown in Figure S2, Cu_2O NPs catalyst used up to seven consecutive cycle and the yield was determined. The recycled catalyst was further characterized wherein *P*-XRD analysis indicates that, the Cu_2O NPs was still remained unchanged which reveals the stability of catalyst (Figure S2 b) while FE-SEM images reveals, slight change in morphology figure S2 (c-e). However, the agglomeration was enhanced as compared to the fresh catalyst. EDX analysis

shows the presence of Carbon (C) and nitrogen (N) are still intact with the catalyst which represents the existence of the active functional groups along with metal center (Fig. S3).

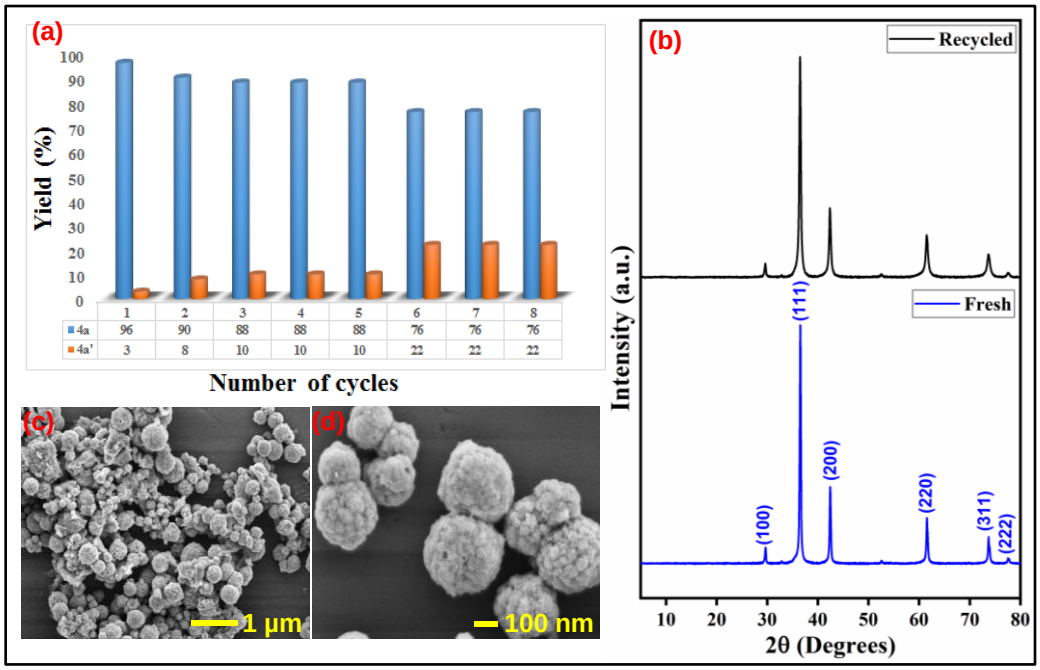


Figure S 2. a) Recycling efficiency of Cu_2O NPs in 2,3-diphenylquinazolin-4(3H)-one synthesis, b) *P*-XRD after 7th cycle c-d) FE-SEM after 7th cycle.

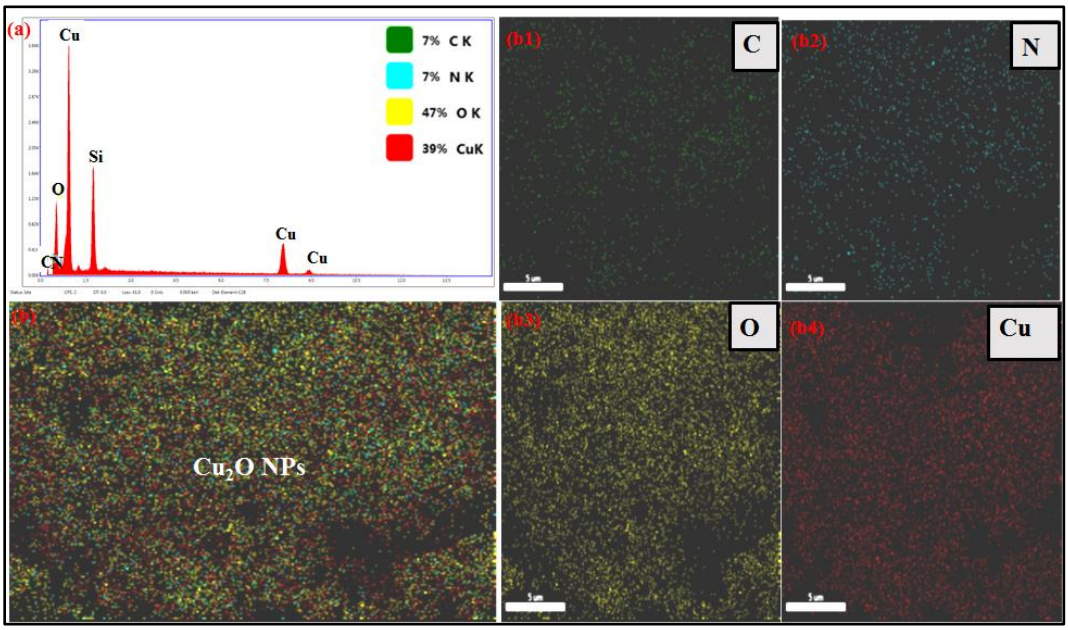


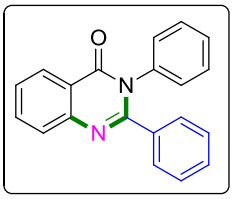
Figure S 3. a) EDX mapping, b) Elemental mapping of Cu_2O NPs, C, N, O and Cu of recycled catalyst after 7th cycle.

8. Hot filtration test

To determine the leaching of Cu_2O NPs catalyst in the reaction of quinazolinone synthesis, a hot filtration test was carried out under the standard reaction condition for 6 hours, following which it was halted and reaction mixture was filtered to eliminate the catalyst. Furthermore, the filtrate was stirred up to 12 hours, during which time the yield of the intended product increased marginally due to the presence of amine intermediate (**5**). This hot filtration test performed confirms the catalyst's heterogeneous character during the quinazolinone synthesis.

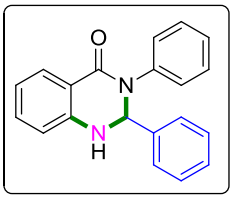
9. Spectroscopic data of newly obtained Products

2,3-diphenylquinazolin-4(3H)-one (**4a**)



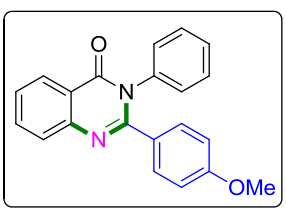
Purified by column chromatography (12% ethyl acetate in hexane), pale yellow solid. Melting point: 158 – 160 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.99 – 7.95 (m, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.44 – 7.42 (m, 2H), 7.40 – 7.36 (m, 4H), 7.35 – 7.26 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.9, 155.7, 147.7, 138.3, 136.1, 135.3, 130.0, 129.4, 129.0, 128.6, 128.0, 127.9, 127.7, 126.9, 121.2. HRMS *m/z* calcd for $C_{20}H_{15}N_2O$ $[M + H]^+$ 299.1179, found 299.1184.[S3]

(S)-2,3-diphenyl-2,3-dihydroquinazolin-4(1H)-one (**4a'**)



Purified by column chromatography (13% ethyl acetate in hexane), pale yellow solid. Melting point: 166 – 166 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.73 (d, *J* = 6.4 Hz, 1H), 7.66 (d, *J* = 2.4 Hz, 1H), 7.38 (d, *J* = 7.2 Hz, 2H), 7.33 – 7.19 (m, 8H), 7.19 (t, *J* = 7.2 Hz, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 7.4 Hz, 1H), 6.29 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 147.0, 141.3, 141.2, 134.2, 129.1, 128.9, 128.8, 128.4, 127.0, 126.7, 126.5, 118.0, 115.8, 115.3, 73.1. HRMS *m/z* calcd for $C_{20}H_{15}N_2O$ $[M + H]^+$ 301.1179, found 301.1184.[S3]

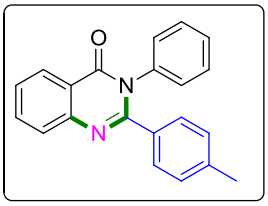
2-(4-methoxyphenyl)-3-phenylquinazolin-4(3H)-one (**4b**)



Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 152 – 154 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.19 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.91 – 7.88 (m, 1H), 7.76 (d, *J* = 8.0

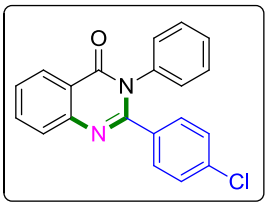
Hz, 1H), 7.60 – 7.57 (m, 1H), 7.35 – 7.29 (m, 7H), 6.79 – 6.76 (m, 2H), 3.70 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.0, 160.0, 155.4, 147.8, 135.2, 131.2, 129.9, 129.1, 128.6, 128.4, 127.8, 127.4, 126.9, 121.0, 113.0, 55.0. HRMS *m/z* calcd for $C_{21}H_{17}N_2O_2$ $[M+H]^+$ 329.1285, found 329.1290.[S3]

3-phenyl-2-(p-tolyl)quinazolin-4(3H)-one (**4c**)



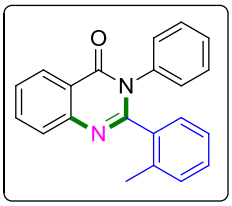
Purified by column chromatography (14% ethyl acetate in hexane), pale yellow solid. Melting point: 170 – 173 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.19 (d, *J* = 8.0 Hz, 1H), 7.89 (t, *J* = 7.5 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 4.5 Hz, 4H), 7.28 – 7.25 (m, 3H), 7.02 (d, *J* = 8.0 Hz, 2H), 2.21 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.9, 155.7, 147.8, 138.9, 138.4, 135.2, 133.3, 130.0, 129.4, 129.1, 128.6, 128.5, 127.9, 127.5, 126.9, 121.1, 21.3. HRMS *m/z* calcd for $C_{21}H_{17}N_2O$ $[M+H]^+$ 313.1335, found 313.1342. [S3]

2-(4-chlorophenyl)-3-phenylquinazolin-4(3H)-one (**4d**)



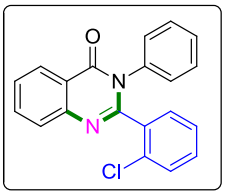
Purified by column chromatography (13% ethyl acetate in hexane), pale yellow solid. Melting point: 174 – 176 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.21 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.93 – 7.90 (m, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 7.75 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.37 – 7.34 (m, 4H), 7.33 – 7.29 (m, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.8, 154.7, 147.7, 138.2, 135.3, 135.0, 134.1, 131.3, 130.0, 129.2, 128.8, 128.1, 127.9, 127.8, 127.0, 121.3. HRMS *m/z* calcd for $C_{20}H_{14}ClN_2O$ [M+H]+ 333.0789, found 333.0794.[S3]

3-phenyl-2-(o-tolyl)quinazolin-4(3H)-one (**4e**)



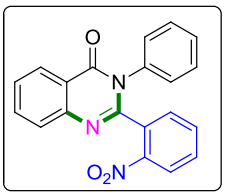
Purified by column chromatography (13% ethyl acetate in hexane), pale yellow solid. Melting point: 171 – 173 °C.^{1}H NMR (500 MHz, DMSO-d_6) δ 8.22 (d, *J* = 8.0 Hz, 1H), 7.92 – 7.88 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.60 (m, 1H), 7.31 – 7.20 (m, 6H), 7.14 – 7.11 (m, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 2.24 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.9, 155.4, 147.7, 137.8, 135.5, 135.4, 135.2, 130.1, 129.6, 129.2, 129.0, 128.8, 127.9, 127.7, 126.9, 125.2 121.5, 19.8. HRMS *m/z* calcd for $C_{21}H_{17}N_2O$ $[M+H]^+$ 313.1335, found 313.1342. [S3]

2-(2-chlorophenyl)-3-phenylquinazolin-4(3H)-one (4f)



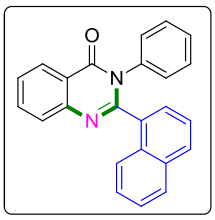
Purified by column chromatography (12% ethyl acetate in hexane), pale yellow solid. Melting point: 158 – 161 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.24 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.95 – 7.92 (m, 1H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.62 (dd, *J* = 7.25, 1.75 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.34 – 7.24 (m, 7H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.6, 153.1, 147.5, 137.2, 135.5, 134.9, 131.5, 131.3, 131.3, 130.2, 129.3, 129.2, 129.1, 128.1, 128.0, 127.0, 121.5. HRMS *m/z* calcd for $C_{20}H_{14}ClN_2O$ $[M+H]^+$ 333.0789, found 333.0794.[S3]

2-(2-nitrophenyl)-3-phenylquinazolin-4(3H)-one (4g)



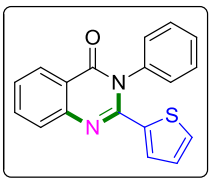
Purified by column chromatography (23% ethyl acetate in hexane), white solid. Melting point: 166 – 168 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.26 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.05 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.95 – 7.90 (m, 1H), 7.81 – 7.72 (m, 3H), 7.68 – 7.64 (m, 1H), 7.61 – 7.57 (m, 1H), 7.31 – 7.25 (m, 5H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.5, 152.8, 147.6, 146.4, 137.2, 135.5, 134.5, 132.2, 131.3, 130.7, 129.5, 129.4, 128.2, 127.9, 127.1, 124.7, 121.4. HRMS *m/z* calcd for $C_{20}H_{14}N_3O_3$ $[M+H]^+$ 344.1030, found 344.1037.[S3]

2-(naphthalen-1-yl)-3-phenylquinazolin-4(3H)-one (4h)



Purified by column chromatography (12% ethyl acetate in hexane), pale yellow solid. Melting point: 211 – 213 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.28 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.98 (d, *J* = 9.0 Hz, 1H), 7.94 – 7.91 (m, 1H), 7.84 – 7.80 (m, 2H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.67 – 7.64 (m, 1H), 7.60 (d, *J* = 7.0 Hz, 1H), 7.50 – 7.46 (m, 3H), 7.38 – 7.35 (m, 1H), 7.21 (t, *J* = 6.75, 1.75 Hz, 1H), 7.09 (d, *J* = 6.5 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 7.0 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.9, 154.9, 147.8, 137.9, 135.2, 133.3, 132.8, 130.6, 130.3, 129.5, 128.6, 128.5, 128.4, 128.0, 127.9, 127.8, 127.2, 127.0, 126.6, 126.1, 124.9, 121.8. HRMS *m/z* calcd for $C_{24}H_{17}N_2O$ $[M+H]^+$ 349.1335, found 349.1341.[S3]

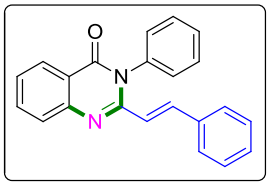
3-phenyl-2-(thiophen-2-yl)quinazolin-4(3H)-one (4i)



Purified by column chromatography (13% ethyl acetate in hexane), pale yellow solid. Melting point: 171 – 174 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ

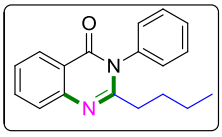
8.14 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.89 – 7.86 (m, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.68 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.57 – 7.53 (m, 4H), 7.51 – 7.49 (m, 2H), 6.86 – 6.84 (m,1H), 7.19 (dd, *J* = 7.25, 1.75 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.0, 148.9, 147.7, 138.5, 138.3, 135.4, 132.2, 131.4, 130.0, 129.9, 128.0, 127.6, 127.4, 127.0, 120.6. HRMS *m/z* calcd for $C_{18}H_{13}N_2OS$ $[M+H]^+$, 305.0743, found 305.0749.[S3]

(E)-3-phenyl-2-styrylquinazolin-4(3H)-one (**4j**)



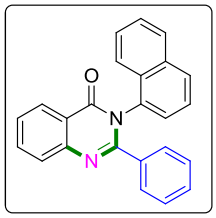
Purified by column chromatography (11% ethyl acetate in hexane), pale yellow solid. Melting point: 167 – 169 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.20 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.95 (t, *J* = 7.75 Hz, 2H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.70 – 7.65 (m, 3H), 7.63 – 7.59 (m, 2H), 7.56 – 7.53 (m, 2H), 7.41 (s, 4H), 6.38 (d, *J* = 15.5 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.7, 151.9, 147.8, 139.2, 137.5, 135.3, 130.2, 129.7, 129.5, 129.4, 127.9, 127.7, 127.1, 126.9, 121.2, 120.5. ESI-HRMS $[M + H]^+$; $C_{12}H_{16}N_2O$ Calculated: 324.1263.

2-butyl-3-phenylquinazolin-4(3H)-one (**4l**)



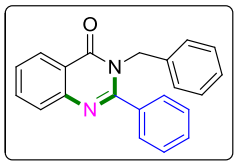
Purified by column chromatography (11% ethyl acetate in hexane), pale yellow solid. Melting point: 164 – 168 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.10 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.87 – 7.82 (m, 1H), 7.71 – 7.70 (m, 2H), 7.60 – 7.50 (m, 4H), 7.44 – 7.43 (m, 1H), 2.33 (t, *J* = 7.8 Hz, 2H), 1.65 – 1.56 (m, 2H), 1.12 – 1.15 (m, 2H), 0.81 – 0.72 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.0, 157.4, 147.7, 137.8, 135.1, 130.0, 129.1, 127.3, 127.0, 126.8, 121.0, 35.2, 28.6, 22.0, 14.0. GCMS (M+2H): 280.15

3-(naphthalen-1-yl)-2-phenylquinazolin-4(3H)-one (**4n**)



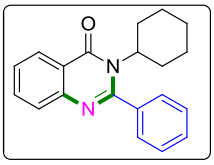
Purified by column chromatography (12% ethyl acetate in hexane), pale yellow solid. Melting point: 210 – 212 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28 (dd, *J* = 7.8, 1.4 Hz, 1H), 8.05 – 7.84 (m, 5H), 7.77 – 7.75 (m, 1H), 7.73 – 7.69 (m, 1H), 7.66 (dd, *J* = 7.2, 0.8 Hz, 1H), 7.60 – 7.58 (m, 2H), 7.52 – 7.49 (m, 1H), 7.35 – 7.33 (m, 2H), 7.23 – 7.19 (m, 1H), 7.12 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.0, 156.2, 147.9, 135.8, 135.5, 134.8, 133.8, 130.4, 129.6, 129.5, 129.3, 128.7, 128.7, 128.5, 128.1, 128.0, 127.9, 127.7, 127.0, 126.9, 125.7, 123.0, 121.1. HRMS *m/z* calcd for $C_{24}H_{17}N_2O$ $[M+H]^+$ 349.1335, found 349.1341.[S3]

3-benzyl-2-phenylquinazolin-4(3H)-one (**4o**)



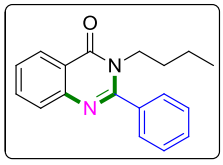
Purified by column chromatography (11% ethyl acetate in hexane), pale yellow solid. Melting point: 171 – 174 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 8.26 (d, *J* = 7.8 Hz, 1H), 7.96 – 7.91 (m, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.55 – 7.47 (m, 5H), 7.28 – 7.23 (m, 3H), 6.97 – 6.95 (m, 2H), 5.23 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d$_6$) δ 161.9, 156.6, 147.4, 137.2, 135.6, 135.2, 130.2, 128.9, 128.7, 128.4, 127.8, 127.7, 127.6, 126.9, 126.7, 120.8, 48.7. ESI-HRMS [M + H]$^+$; $C_{21}H_{16}N_2O$ Calculated: 312.1263.

3-cyclohexyl-2-phenylquinazolin-4(3H)-one (**4p**)



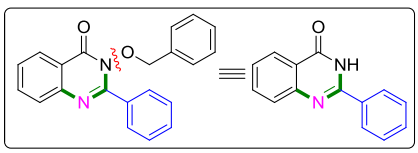
Purified by column chromatography (11% ethyl acetate in hexane), pale yellow solid. Melting point: 164 – 167 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 8.21 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.89 – 7.85 (m, 1H), 7.73 – 7.57 (m, 7H), 3.82 – 3.76 (m, 1H), 2.65 – 2.56 (m, 2H), 1.79 – 1.73 (m, 4H), 1.53 (d, *J* = 12.8 Hz, 1H), 1.17 – 1.08 (m, 1H), 0.93 – 0.83 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d$_6$) δ 162.1, 157.1, 146.9, 136.7, 134.8, 130.0, 129.0, 127.7, 127.4, 126.4, 122.1, 62.3, 28.6, 26.3, 25.2. ESI-HRMS [M + H]$^+$; $C_{20}H_{20}N_2O$ Calculated: 3043856.

3-butyl-2-phenylquinazolin-4(3H)-one (**4q**)



Purified by column chromatography (10% ethyl acetate in hexane), pale yellow solid. Melting point: 169 – 171 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 8.20 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.82 – 7.82 (m, 1H), 7.68 – 7.63 (m, 3H), 7.59 – 7.55 (m, 4H), 3.89 (t, *J* = 7.8 Hz, 2H), 1.52 – 1.45 (m, 2H), 1.12 – 1.09 (m, 2H), 0.66 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d$_6$) δ 162.1, 157.1, 146.9, 136.7, 134.8, 130.0, 129.0, 127.7, 127.4, 126.4, 122.1, 62.3, 28.6, 26.3, 25.2. ESI-HRMS [M + H]$^+$; $C_{18}H_{18}N_2O$ Calculated: 278.1419.

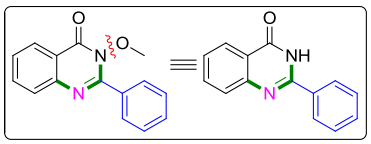
2-phenylquinazolin-4(3H)-one (**4r**)



Purified by column chromatography (15% ethyl acetate in hexane), pale yellow solid. Melting point: 236 – 238 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 12.55 (br-s, 1H), 8.21 – 8.16 (m, 3H), 7.87 – 7.83 (m, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.60 – 7.52 (m, 4H). ^{13}C NMR (100

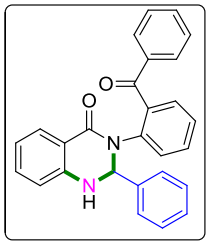
MHz, DMSO-d_6) δ 162.7, 152.8, 149.2, 135.1, 133.2, 131.9, 129.1, 128.2, 128.0, 127.1, 126.3, 121.5. HRMS *m/z* calcd for $C_{14}H_{11}N_2O$ $[M+H]^+$ 223.0866, found 223.0869.[S3]

2-phenylquinazolin-4(3H)-one (**4s**)



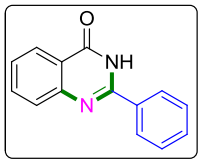
Purified by column chromatography (15% ethyl acetate in hexane), pale yellow solid. Melting point: 236 – 238 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.55 (br-s, 1H), 8.20 – 8.16 (m, 3H), 7.86 – 7.83 (m, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.52 (m, 4H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.7, 152.8, 149.2, 135.1, 133.2, 131.9, 129.1, 128.2, 128.0, 127.1, 126.3, 121.5. HRMS *m/z* calcd for $C_{14}H_{11}N_2O$ $[M+H]^+$ 223.0866, found 223.0869.[S3]

3-(2-benzoylphenyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (**4t**)



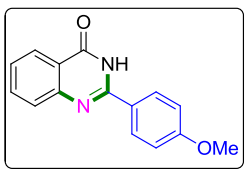
Purified by column chromatography (15% ethyl acetate in hexane), pale yellow solid. Melting point: 196 – 198 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.32 (s, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.89 (t, *J* = 7.25 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.58 – 7.43 (m, 12H), 7.31 (t, *J* = 7.25 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 195.1, 161.6, 155.1, 147.7, 137.0, 136.7, 135.8, 135.8, 135.5, 133.7, 132.3, 131.7, 130.7, 130.5, 129.9, 129.4, 128.8, 128.6, 128.2, 127.9, 127.7, 127.0, 120.6, 79.6. ESI-HRMS $[M + H]^+$; $C_{27}H_{20}N_2O$ Calculated: 404.1525.

2-phenylquinazolin-4(3H)-one (**5a**)



Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 236 – 238 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.54 (br-s, 1H), 8.20 – 8.17 (m, 3H), 7.86 – 7.84 (m, 1H), 7.75 (d, *J* = 6.5 Hz, 1H), 7.62 – 7.52 (m, 4H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.8, 152.8, 149.3, 135.1, 133.3, 131.9, 129.1, 128.2, 128.0, 127.1, 126.4, 121.5. HRMS *m/z* calcd for $C_{14}H_{11}N_2O$ $[M+H]^+$ 223.0866, found 223.0869.[S3]

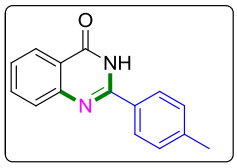
2-(4-methoxyphenyl)quinazolin-4(3H)-one (**5b**)



Purified by column chromatography (18% ethyl acetate in hexane), pale yellow solid. Melting point: 240 – 243 °C. ^{1}H NMR (400 MHz, DMSO-d_6)

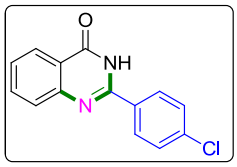
δ 12.41 (br-s, 1H), 8.21 (d, *J* = 9.2 Hz, 2H), 8.15 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.84 – 7.80 (m, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.51 – 7.47 (m, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 3.70 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 162.3, 152.3, 149.4, 135.0, 129.9, 127.8, 126.6, 126.3, 125.3, 121.2, 114.5, 55.9. HR-ESIMS: *m/z* 253.0967 calcd for $C_{15}H_{12}N_2O_2$ (253.0977).[S4]

2-(p-tolyl)quinazolin-4(3H)-one (**5c**)



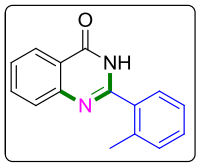
Purified by column chromatography (17% ethyl acetate in hexane), pale yellow solid. Melting point: 244 – 246 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.46 (br-s, 1H), 8.15 (d, *J* = 6.0 Hz, 1H), 8.10 (d, *J* = 6.5 Hz, 2H), 7.84 (t, *J* = 6.0 Hz, 1H), 7.73 (d, *J* = 6.5 Hz, 1H), 7.52 (t, *J* = 6.0 Hz, 1H), 7.36 (d, *J* = 6.5 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.8, 152.7, 149.3, 142.0, 135.1, 130.4, 129.7, 128.2, 127.9, 126.9, 126.4, 121.4, 21.5. $[M+H]^+$; HR-ESIMS: *m/z* 237.1029 calcd for $C_{15}H_{12}N_2O$ (237.1028).[S4]

2-(4-chlorophenyl)quinazolin-4(3H)-one (**5d**)



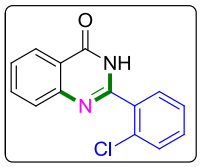
Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 260 – 264 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.61 (br-s, 1H), 8.21 (d, *J* = 6.0 Hz, 2H), 8.16 (d, *J* = 6.5 Hz, 1H), 7.85 (t, *J* = 6.0 Hz, 1H), 7.75 (d, *J* = 6.5 Hz, 1H), 7.63 (d, *J* = 6.0 Hz, 2H), 7.54 (t, *J* = 6.5 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 151.8, 149.1, 136.8, 135.1, 132.0, 130.1, 129.2, 128.0, 127.3, 126.3, 121.5. ESI-HRMS $[M + H]^+$; $C_{14}H_9ClN_2O$ Calculated: 256.0403.

2-(o-tolyl)quinazolin-4(3H)-one (**5e**)



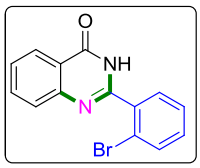
Purified by column chromatography (17% ethyl acetate in hexane), pale yellow solid. Melting point: 222 – 224 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.46 (br-s, 1H), 8.15 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.87 – 7.83 (m, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.87 – 7.83 (m, 2H), 7.46 – 7.42 (m, 1H), 7.37 – 7.32 (m, 2H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.2, 154.8, 149.2, 136.6, 134.9, 134.7, 131.0, 130.3, 129.6, 127.8, 127.1, 126.3, 126.2, 121.5, 20.0. $[M+H]^+$; HR-ESIMS: *m/z* 237.1029 calcd for $C_{15}H_{12}N_2O$ (237.1028).[S4]

2-(2-chlorophenyl)quinazolin-4(3H)-one (**5f**)



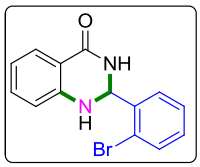
Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 194 – 196 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.51 (br-s, 1H), 8.20 – 8.18 (m, 2H), 7.87 – 7.83 (m, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.60 – 7.51 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 152.9, 149.3, 135.1, 133.2, 131.9, 129.1, 128.2, 128.0, 127.1, 126.3, 121.5. ESI-HRMS $[M + H]^+$; $C_{14}H_9ClN_2O$ Calculated: 256.0403.

2-(2-bromophenyl)quinazolin-4(3H)-one (**5g**)



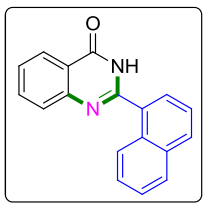
Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 298 – 300 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.56 (br-s, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.85 – 7.81 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.59 – 7.50 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 152.8, 149.2, 135.1, 133.2, 131.8, 129.1, 128.2, 128.0, 127.0, 126.3, 121.4. HR-ESIMS: *m/z* 300.9962 calcd for $C_{14}H_9BrN_2O$ (300.9976).[S4]

(S)-2-(2-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (**5g'**)



Purified by column chromatography (18% ethyl acetate in hexane), pale yellow solid. Melting point: 294 – 298 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.83 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.66 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.52 – 7.50 (m, 1H), 7.30 – 7.22 (m, 2H), 7.19 – 7.14 (m, 1H), 6.79 (t, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 6.38 (br-s, 1H), 6.22 (s, 1H), 4.67 (br-s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.9, 145.5, 137.2, 133.2, 132.3, 129.9, 128.0, 127.5, 127.5, 127.2, 121.2, 118.5, 114. 2, 113.6, 65.9. HR-ESIMS: *m/z* 302.9962 calcd for $C_{14}H_9BrN_2O$ (302.9976).[S4]

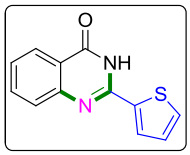
2-(naphthalen-1-yl)quinazolin-4(3H)-one (**5h**)



Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 164 – 166 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.69 (br-s, 1H), 8.23 (d, *J* = 7.6 Hz, 1H), 8.18 (d, *J* = 7.2 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 8.06 (dd, *J* = 6.6, 2.2 Hz, 1H), 7.90 – 7.86 (m, 1H), 7.80 (d, *J* =

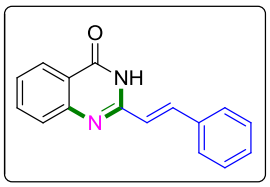
6.8 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H),7.67 – 7.57 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 154.1, 149.3, 135.0, 133.6, 132.2, 130.9, 130.7, 128.8, 128.2, 127.9, 127.5, 127.3, 126.8, 126.3, 125.7, 125.5, 121.8. HR-ESIMS: *m/z* 273.1040 calcd for $C_{18}H_{12}N_2O$ (273.1028).[S4]

2-(thiophen-2-yl)quinazolin-4(3H)-one (**5h**)



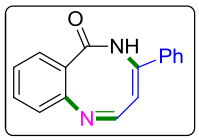
Purified by column chromatography (15% ethyl acetate in hexane), pale yellow solid. Melting point: 271 – 273 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.66 (br-s, 1H), 8.23 (dd, *J* = 8.0, 0.8 Hz, 1H), 8.13 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.86 (dd, *J* = 5.2, 0.8 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.46 (m, 1H), 8.25 – 7.22 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 149.1, 148.3, 137.8, 135.2, 132.6, 129.9, 129.0, 127.4, 126.8, 126.5, 121.3. ESI-HRMS $[M + H]^+$; $C_{12}H_{18}N_2OS$ Calculated: 228.0357.

(E)-2-styrylquinazolin-4(3H)-one (**5j**)



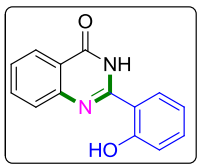
Purified by column chromatography (14% ethyl acetate in hexane), pale yellow solid. Melting point: 184 – 186 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.33 (br-s, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 16.0 Hz, 1H), 7.83 – 7.79 (m, 1H), 7.68 (t, *J* = 7.2 Hz, 3H), 7.50 – 7.42 (m, 4H), 6.99 (d, *J* = 16.0 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 151.9, 149.5, 138.7, 135.5, 135.0, 130.2, 129.5, 128.1, 127.6, 126.7, 126.3, 121.6. ESI-HRMS $[M + H]^+$; $C_{16}H_{12}N_2O$ Calculated: 248.0950.

(1Z,3Z)-4-phenylbenzo[b][1,5]diazocin-6(5H)-one (**5k**)



Purified by column chromatography (12% ethyl acetate in hexane), pale yellow solid. Melting point: 162 – 164 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.55 (br-s, 1H), 8.18 (t, *J* = 8.8 Hz, 3H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.49 (m, 5H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 152.8, 149.2, 135.1, 133.2, 131.9, 129.3, 129.1, 128.2, 128.0, 127.1, 127.1, 126.3, 121.5. ESI-HRMS $[M + H]^+$; $C_{16}H_{12}N_2O$ Calculated: 248.0950.

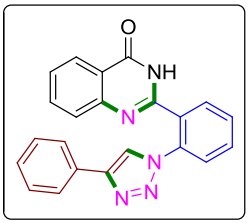
2-(2-hydroxyphenyl)quinazolin-4(3H)-one (**5l**)



Purified by column chromatography (16% ethyl acetate in hexane), pale yellow solid. Melting point: 249 – 252 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.77

(br-s, 1H), 12.48 (br-s, 1H), 8.22 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.16 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.89 – 7.85 (m, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.49 – 7.44 (m, 1H), 7.03 – 6.95 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.5, 146.7, 135.5, 134.2, 128.2, 127.5, 126.5, 121.2, 119.4, 118.4, 114.2. HRMS *m/z* calcd for $C_{14}H_{11}N_2O$ $[M+H]^+$ 238.0738, found 239.0821.[S4]

2-(2-(4-phenyl-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (**5m**)



Purified by column chromatography (38% ethyl acetate in hexane), pale yellow solid. Melting point: 184 – 186 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.60 (br-s, 1H), 9.14 (s, 1H), 8.15 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.95 – 7.92 (m, 3H), 7.88 – 7.85 (m, 2H), 7.83 – 7.75 (m, 2H), 7.56 – 7.48 (m, 4H), 7.40 – 7.36 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 152.5, 149.1, 146.8, 135.4, 134.9, 131.9, 131.6, 130.7, 129.9, 129.8, 129.5, 128.6, 127.7, 127.3, 126.2, 125.7, 125.3, 123.3, 121.5. ESI-HRMS $[M + H]^+$; $C_{22}H_{15}N_5O$ Calculated: 365.1277.

10. References

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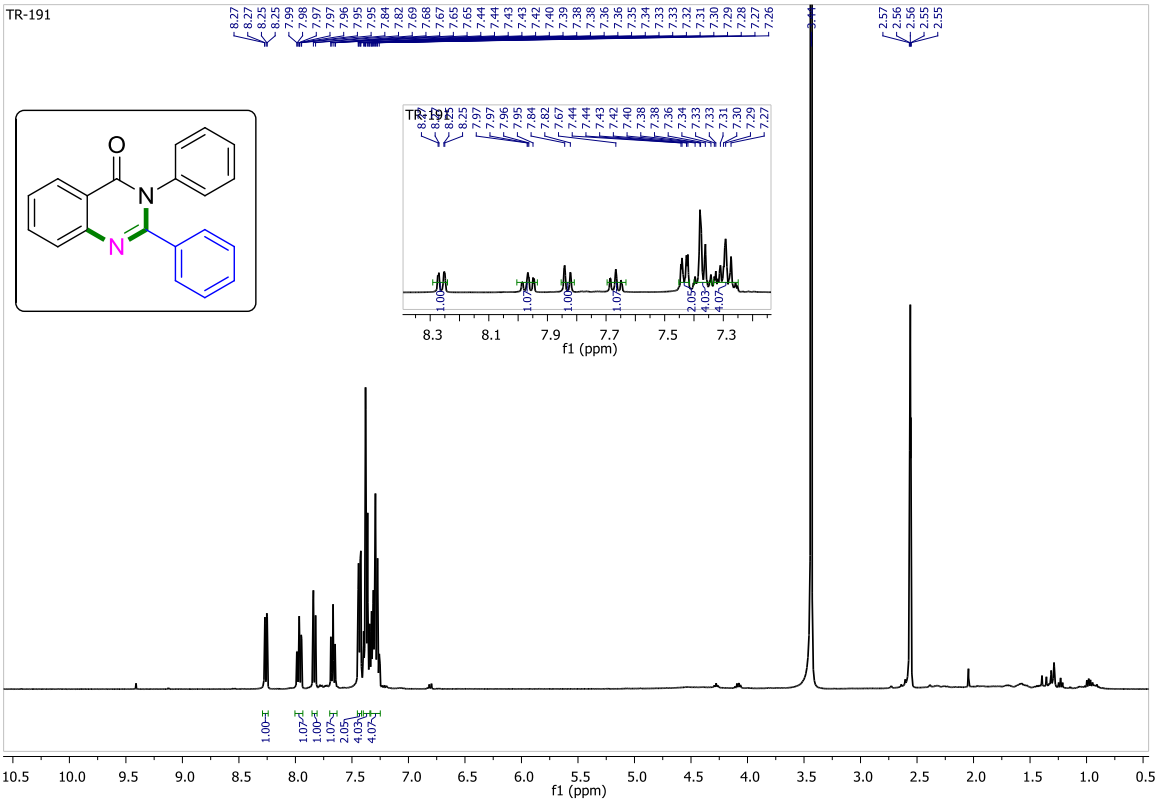
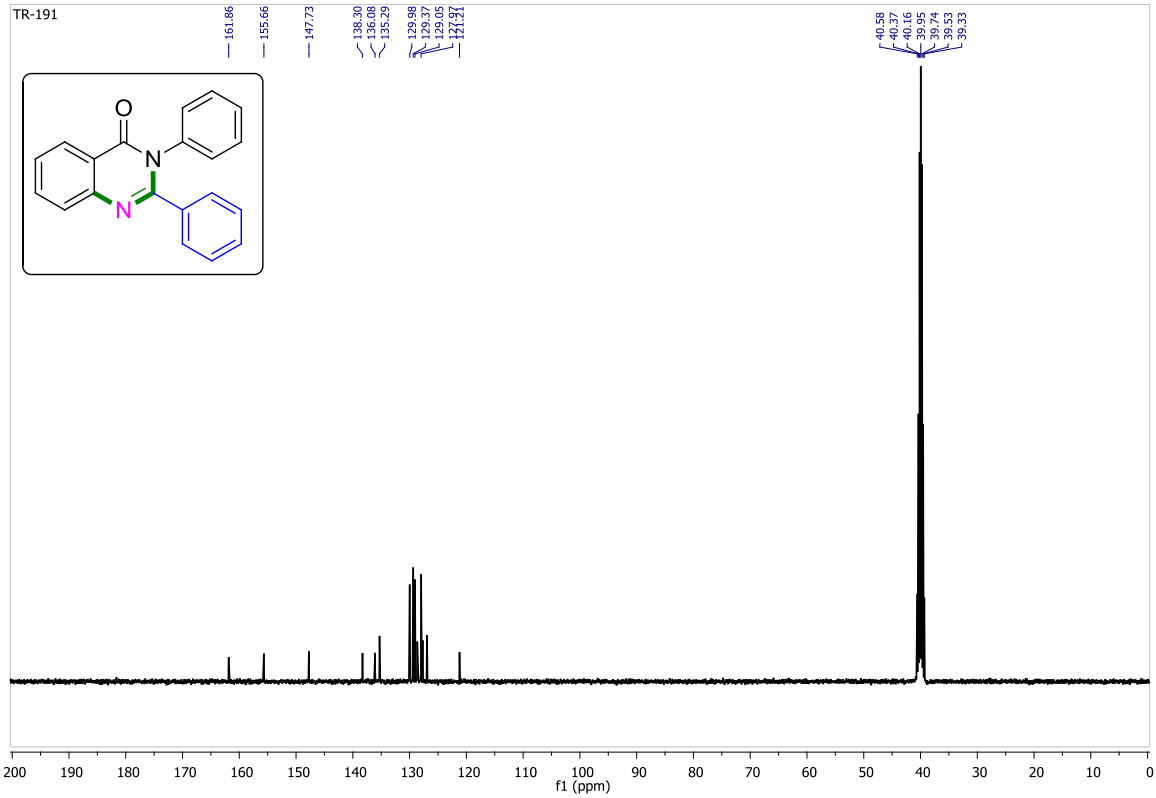
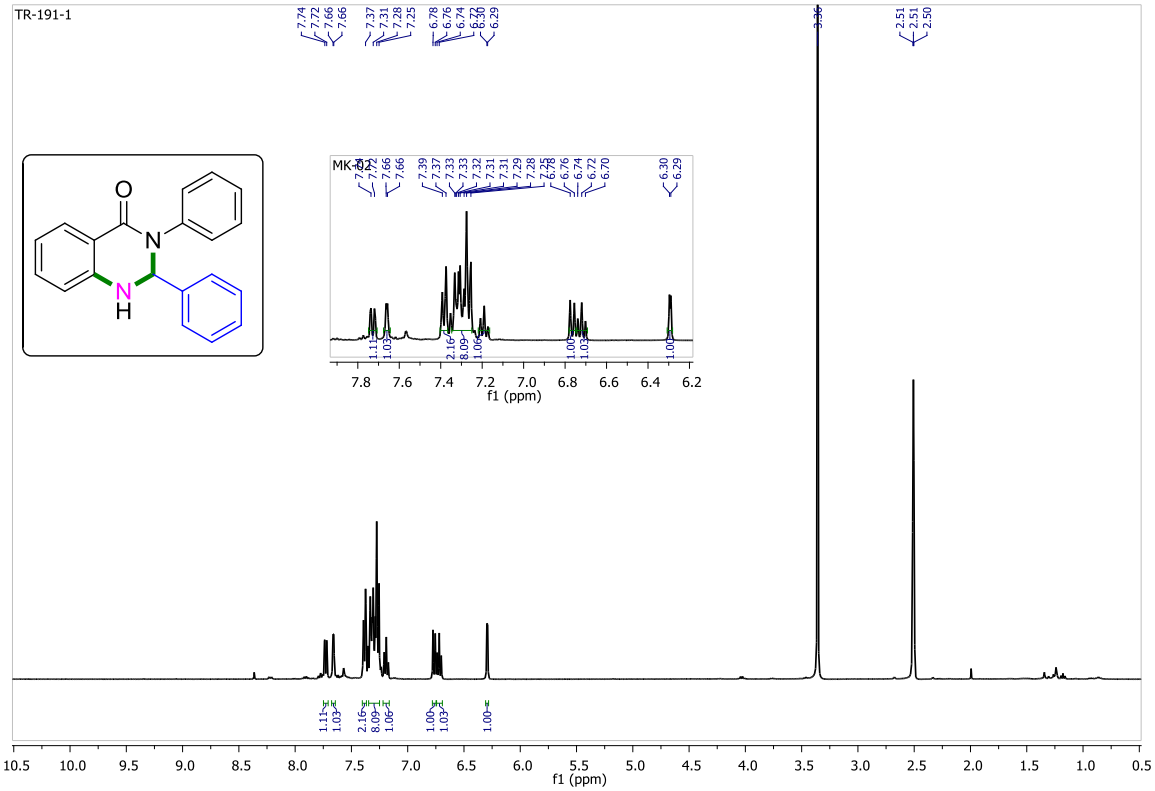
Appendix I: **Spectral copies of ^{1}H and ^{13}C NMR of compounds obtained in this study**

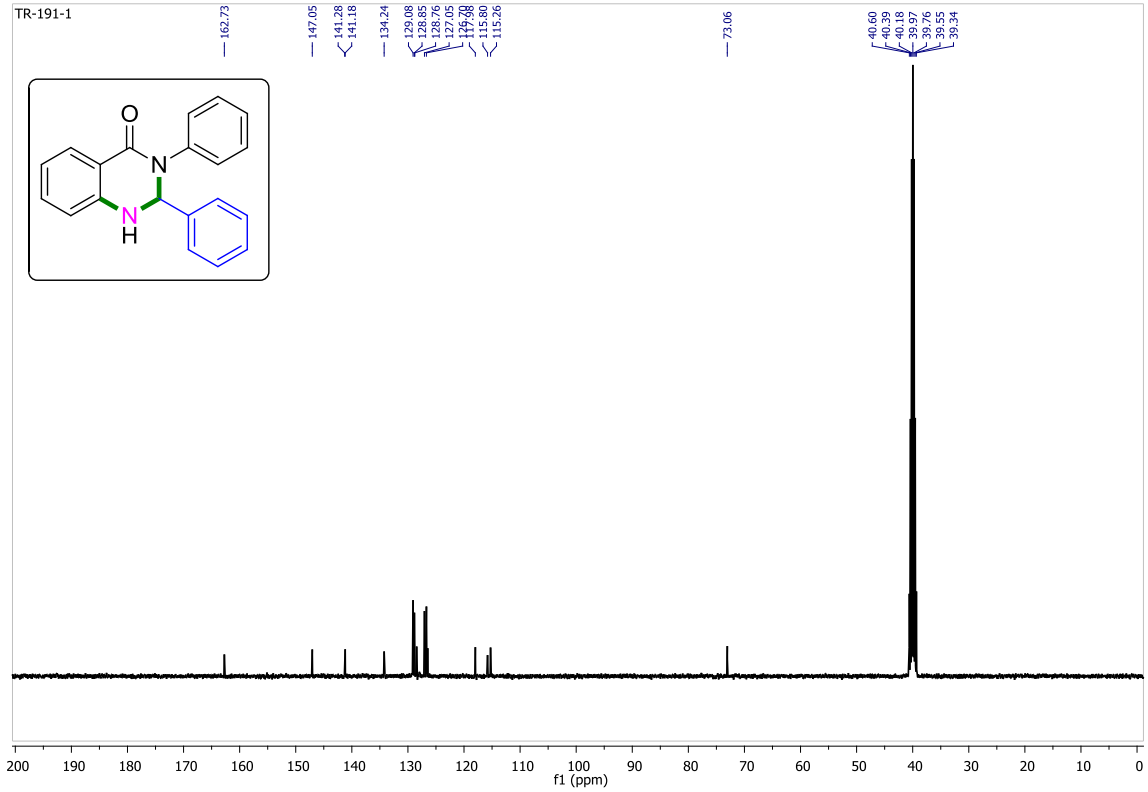
2,3-diphenylquinazolin-4(3H)-one (4a)



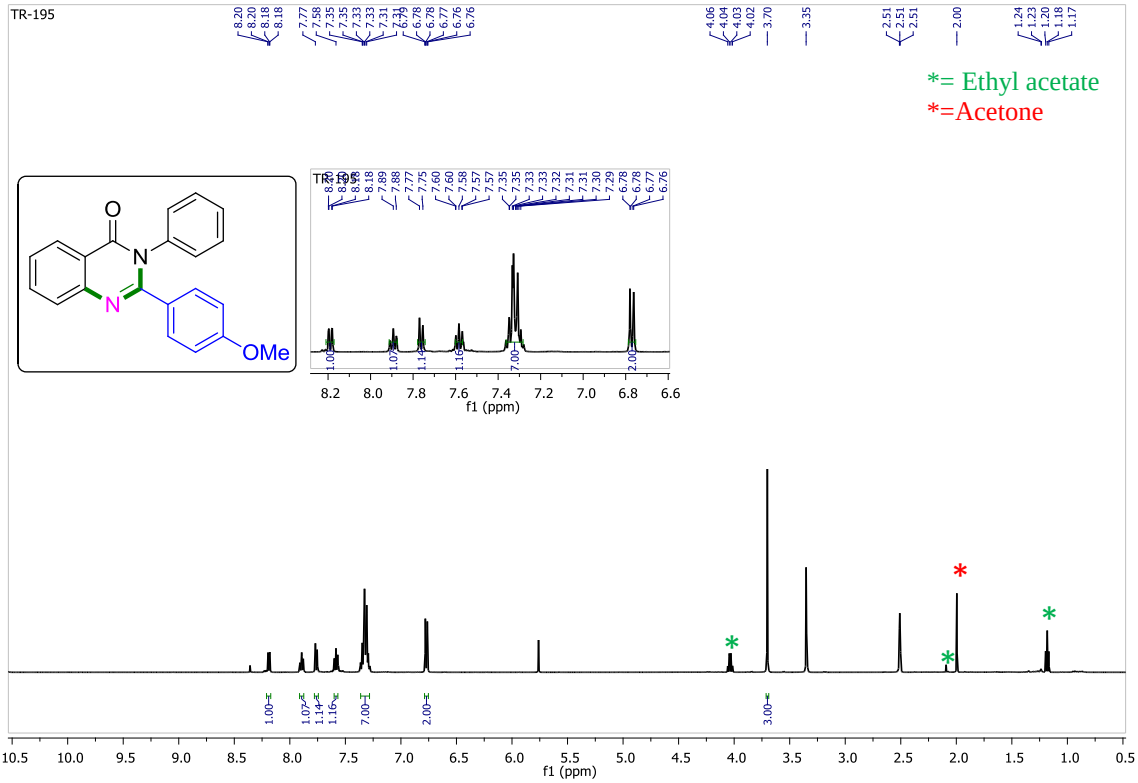


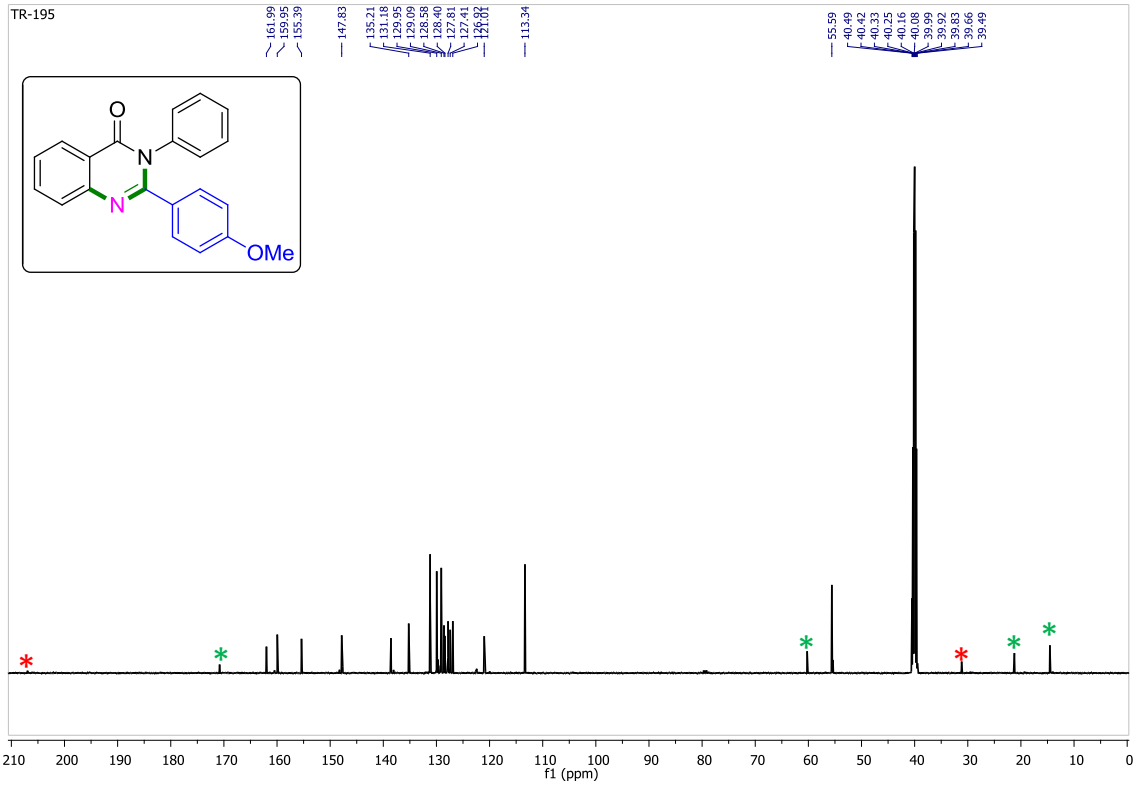
(S)-2,3-diphenyl-2,3-dihydroquinazolin-4(1H)-one (4a')



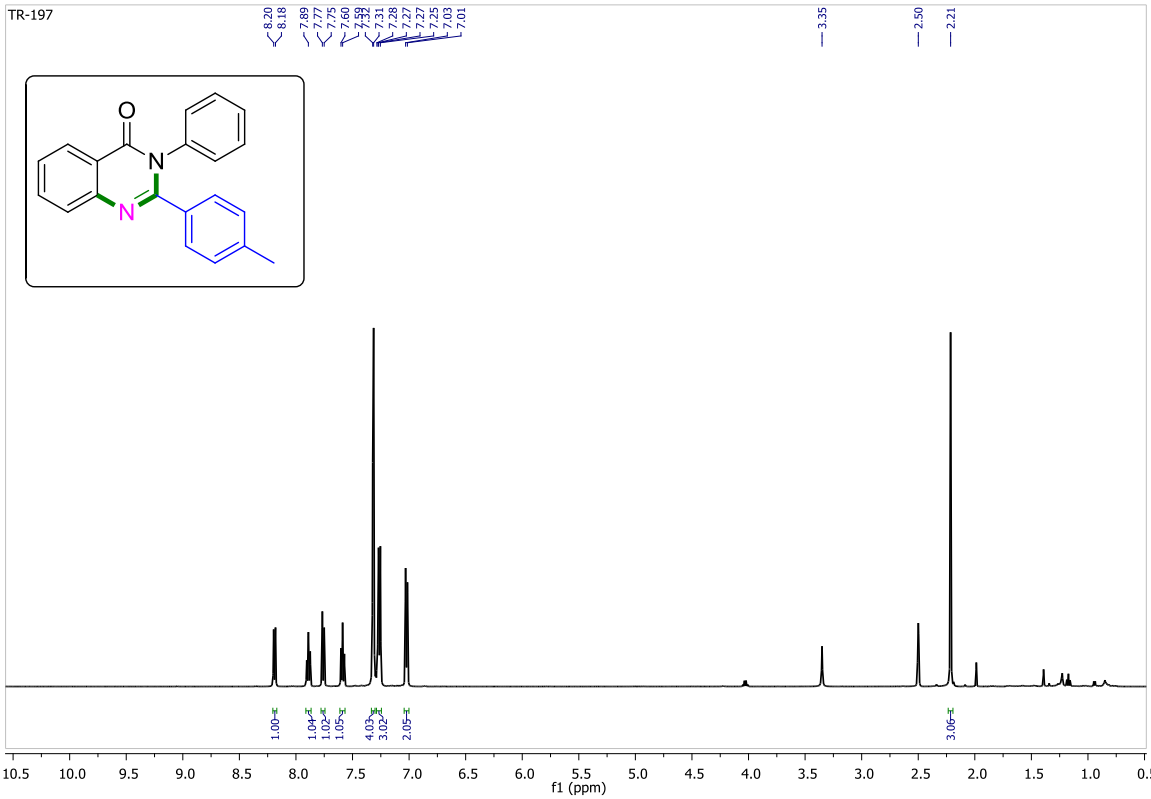


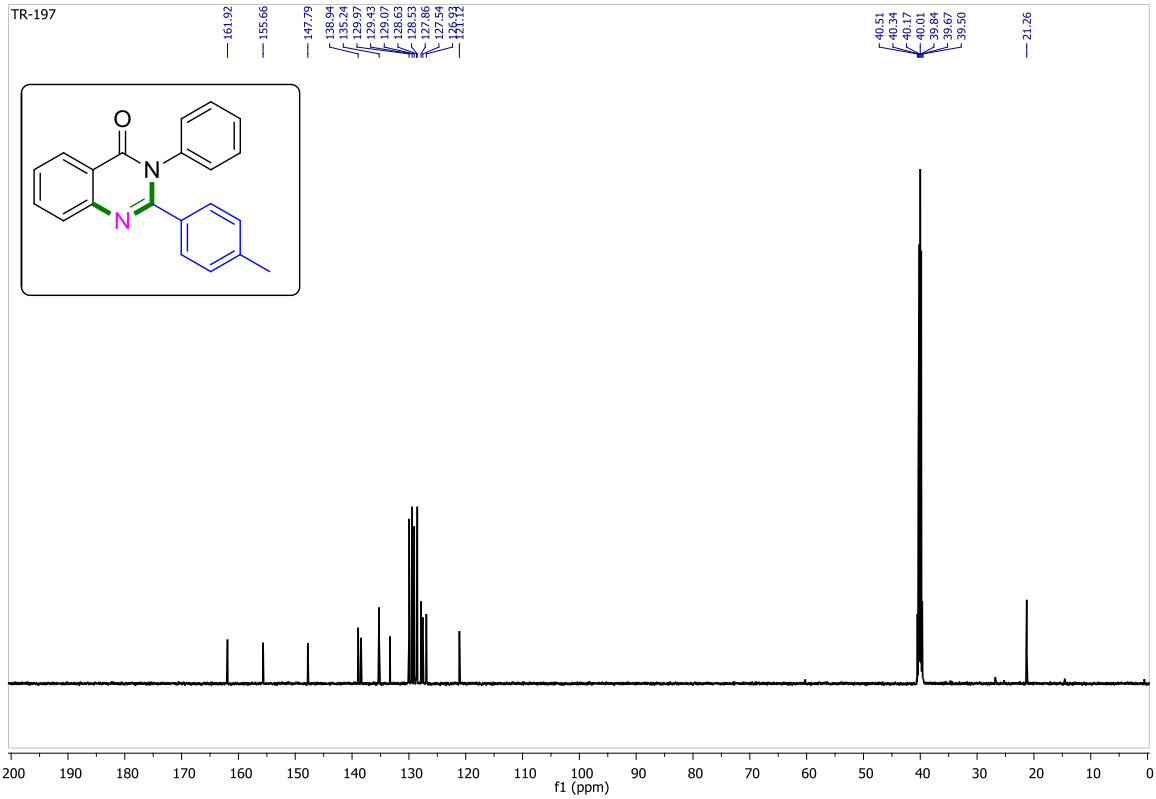
2-(4-methoxyphenyl)-3-phenylquinazolin-4(3H)-one (4b)



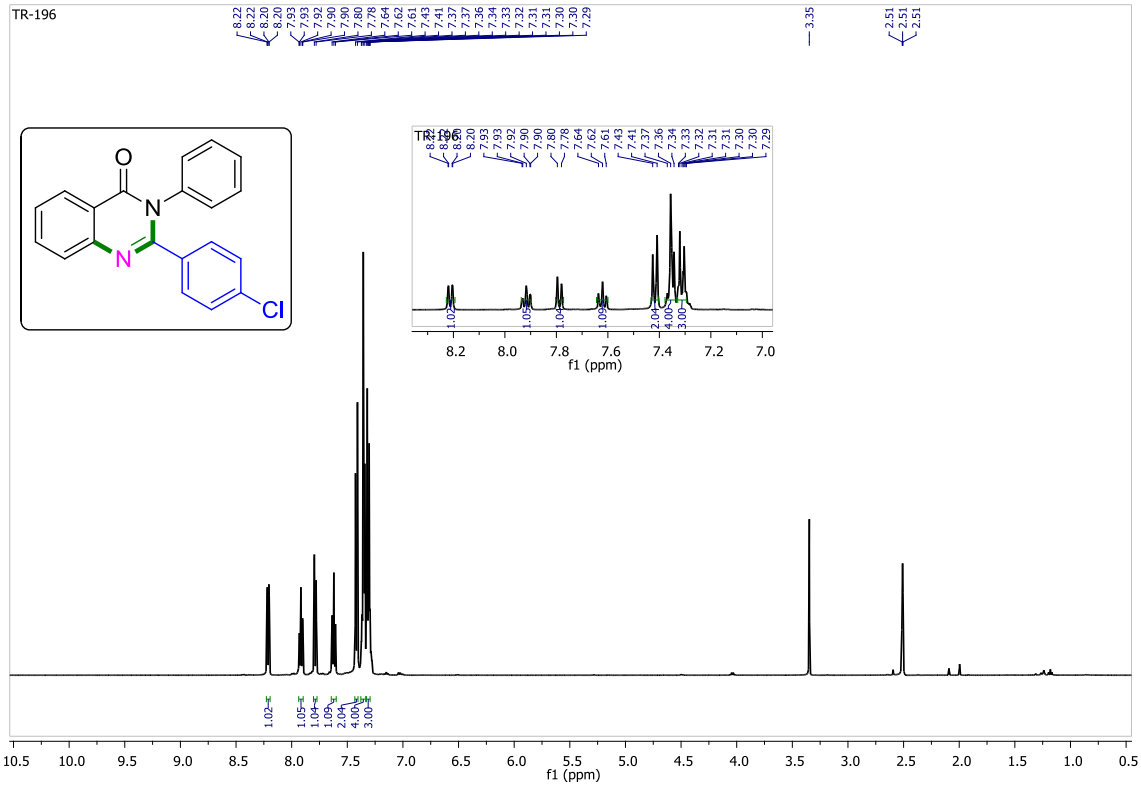


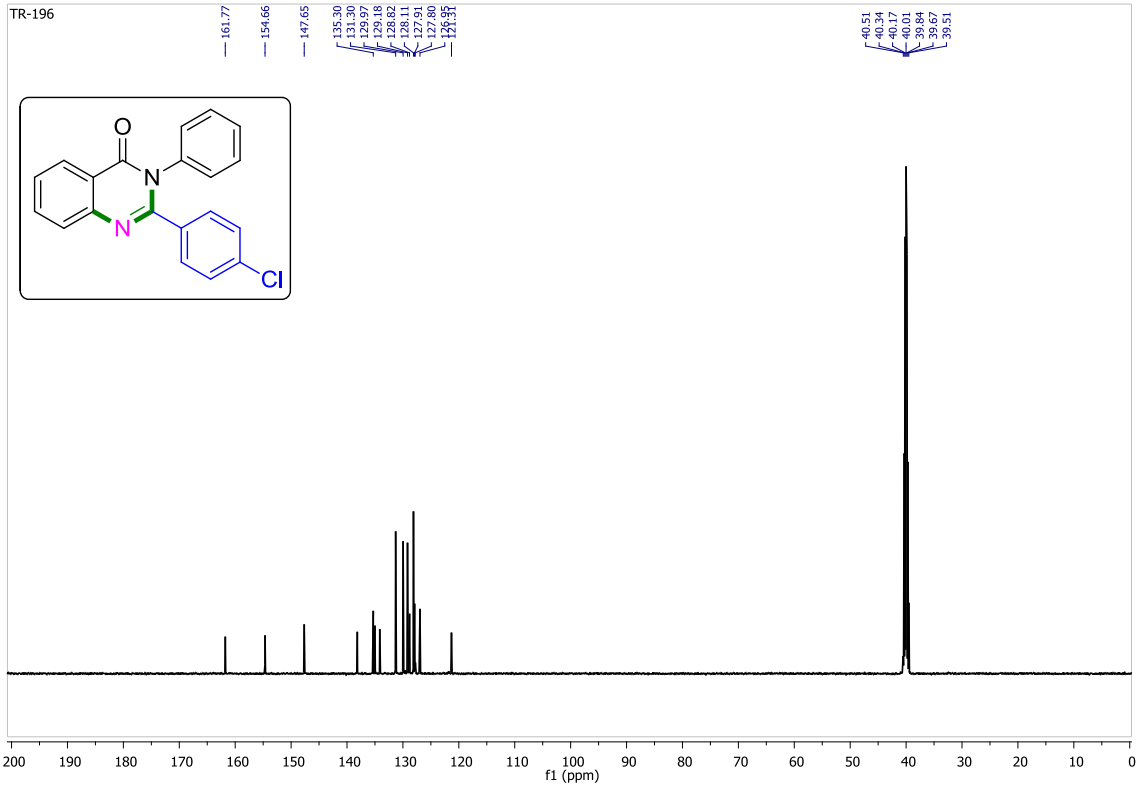
3-phenyl-2-(p-tolyl)quinazolin-4(3H)-one (4c)



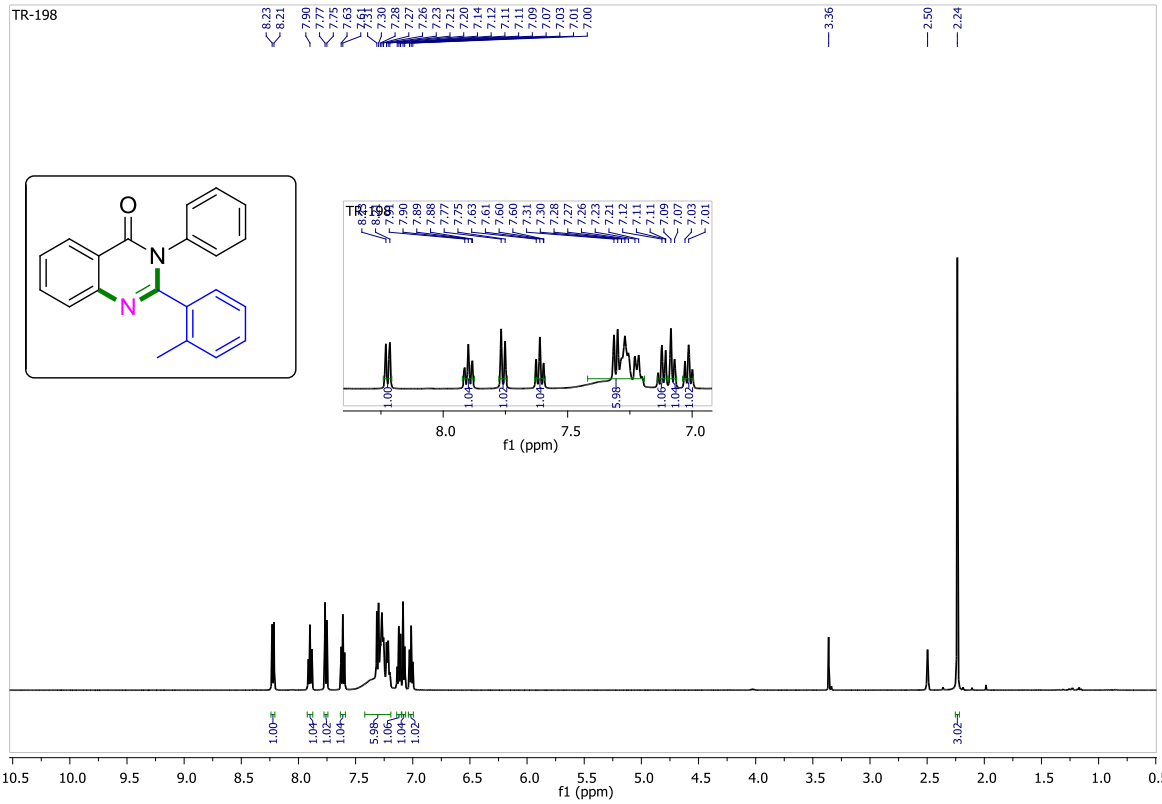


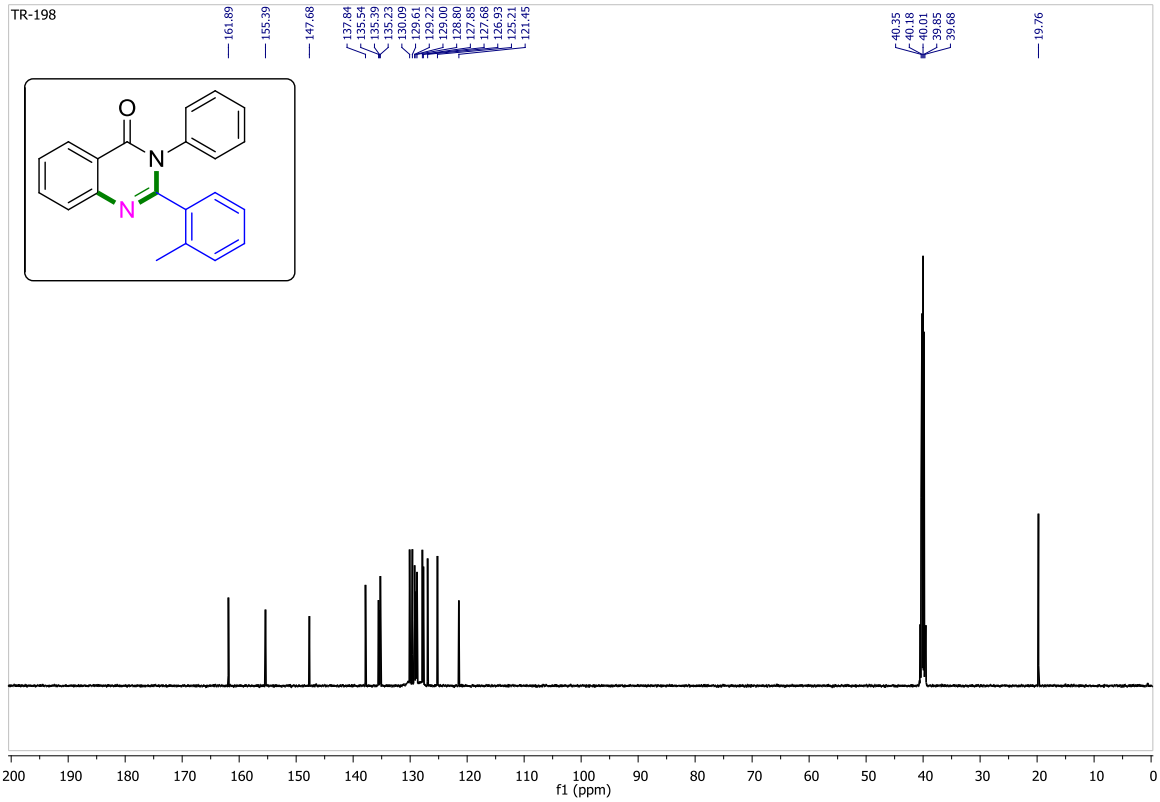
2-(4-chlorophenyl)-3-phenylquinazolin-4(3H)-one (4d)



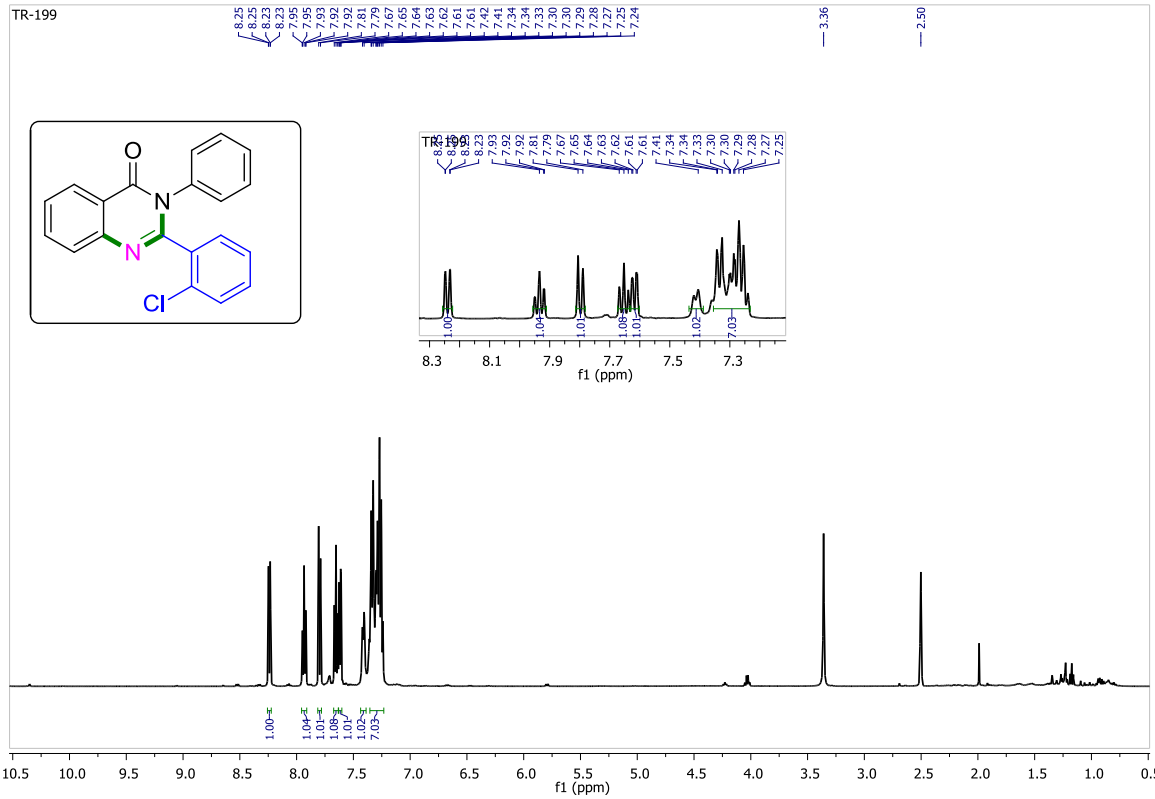


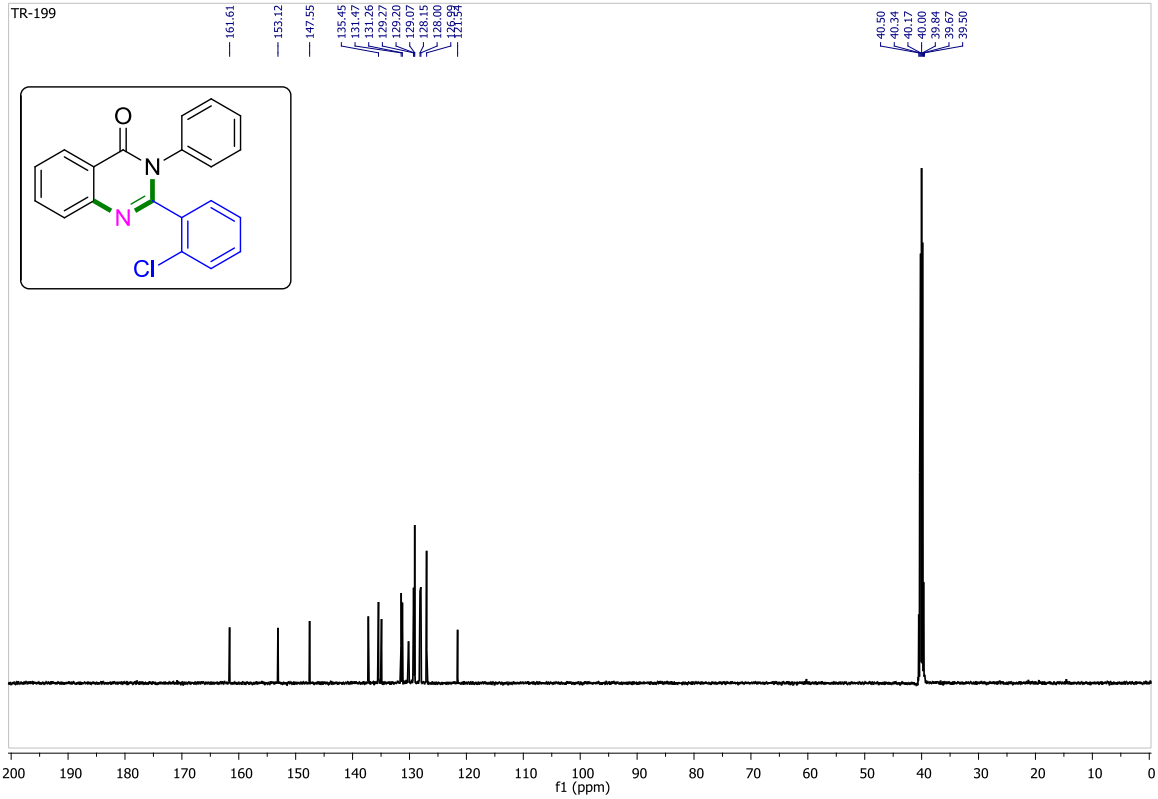
3-phenyl-2-(o-tolyl)quinazolin-4(3H)-one (4e)



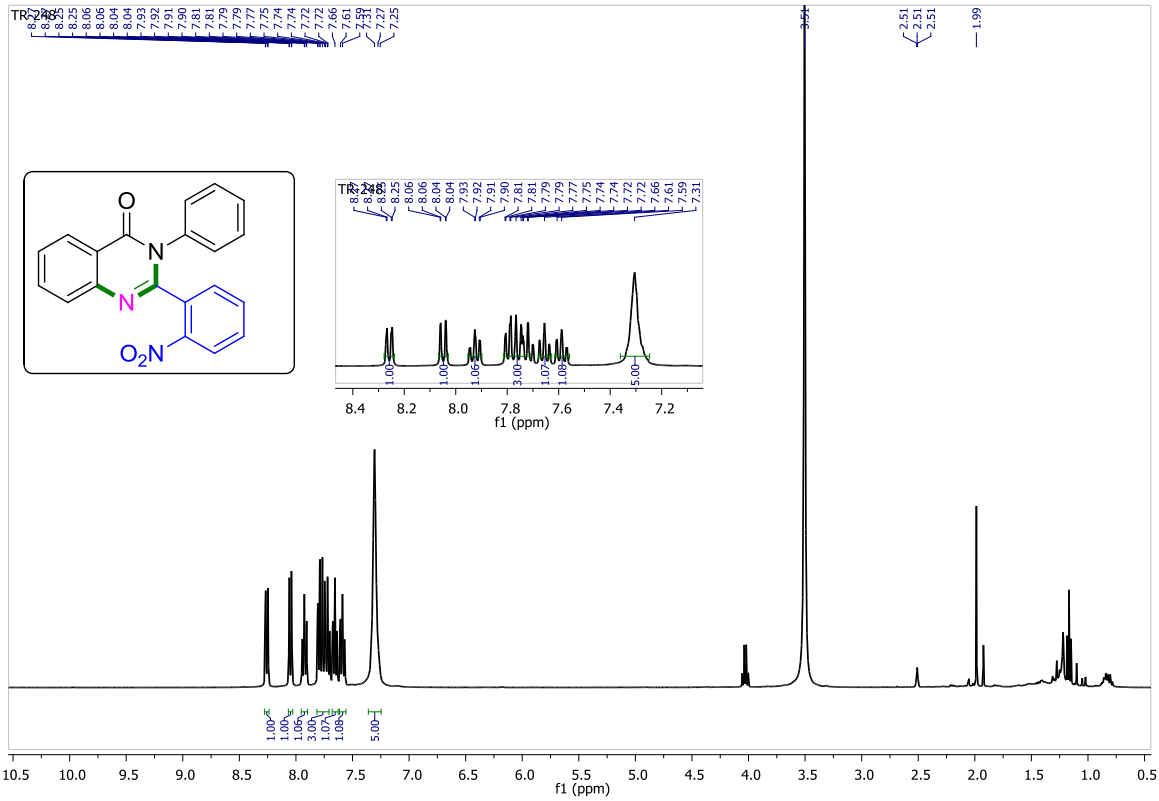


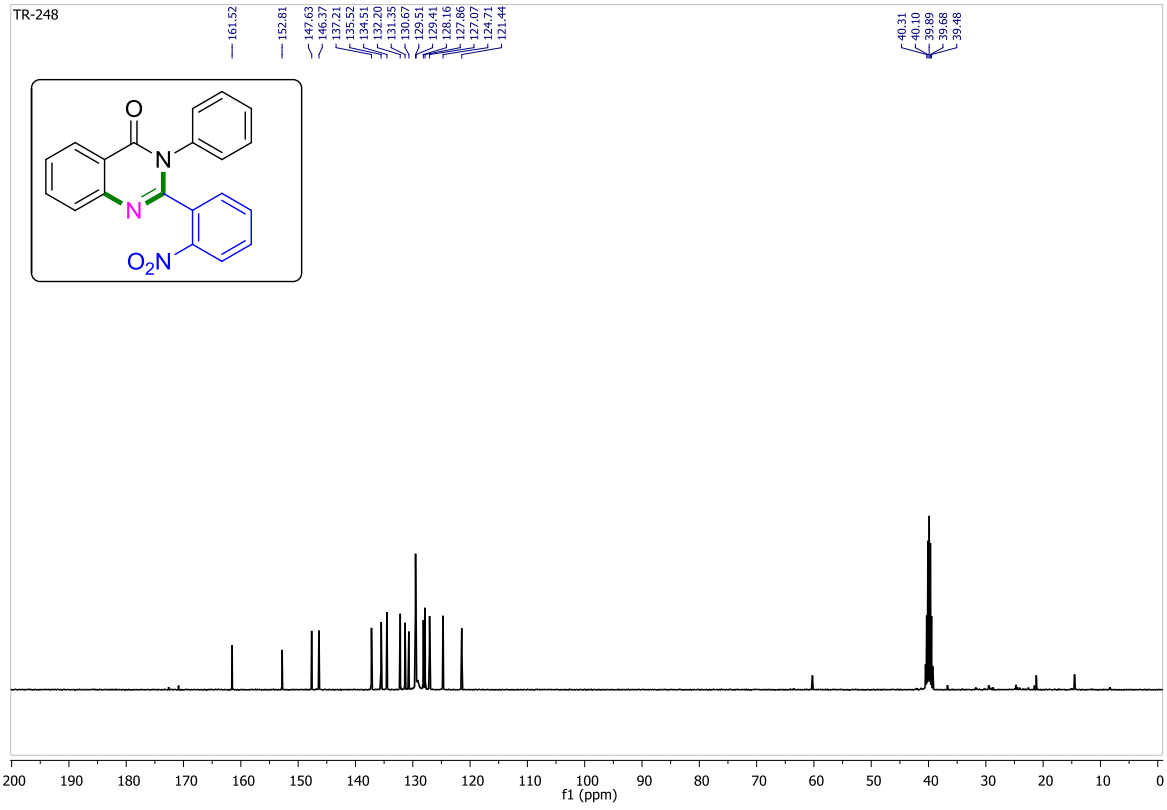
2-(2-chlorophenyl)-3-phenylquinazolin-4(3H)-one (4f)



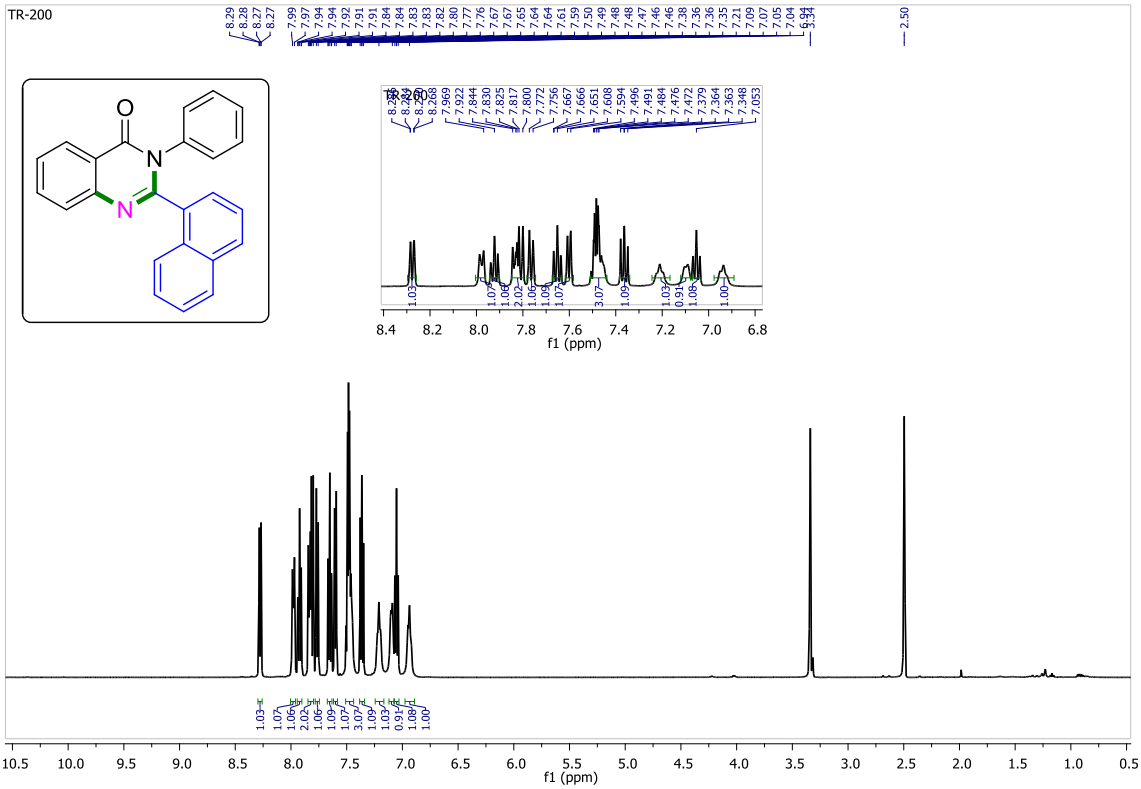


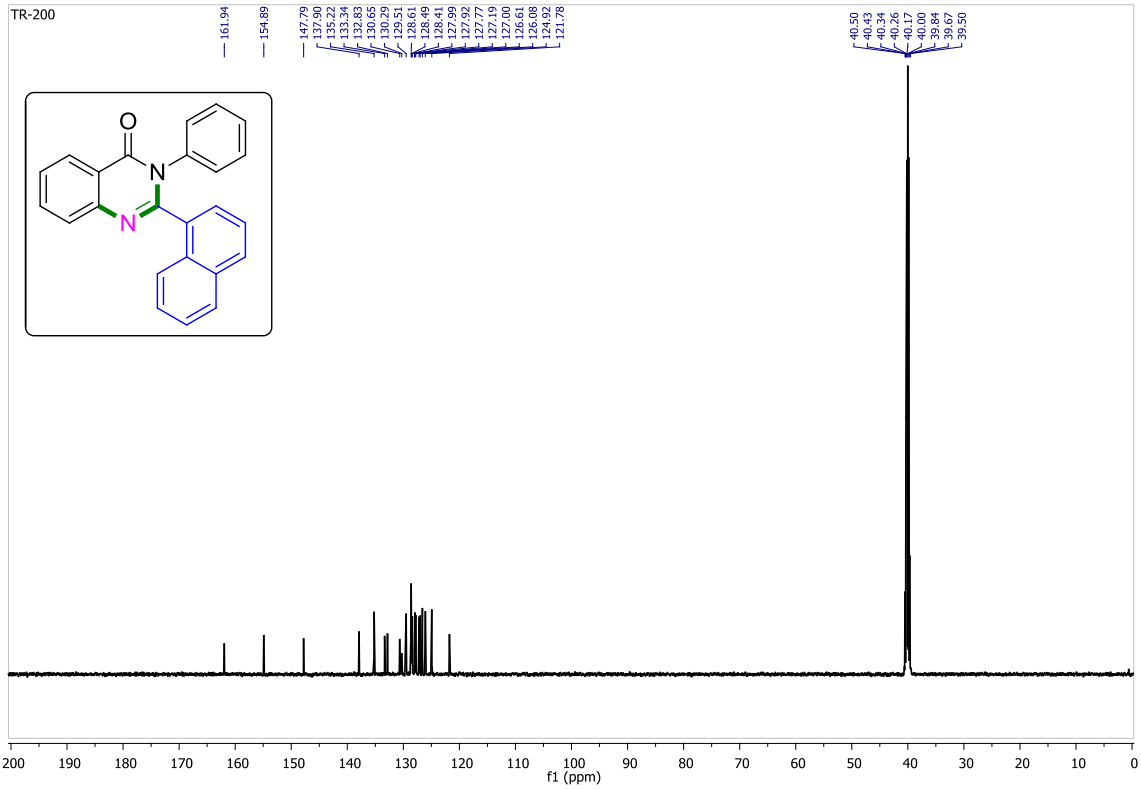
2-(2-nitrophenyl)-3-phenylquinazolin-4(3H)-one (4g)



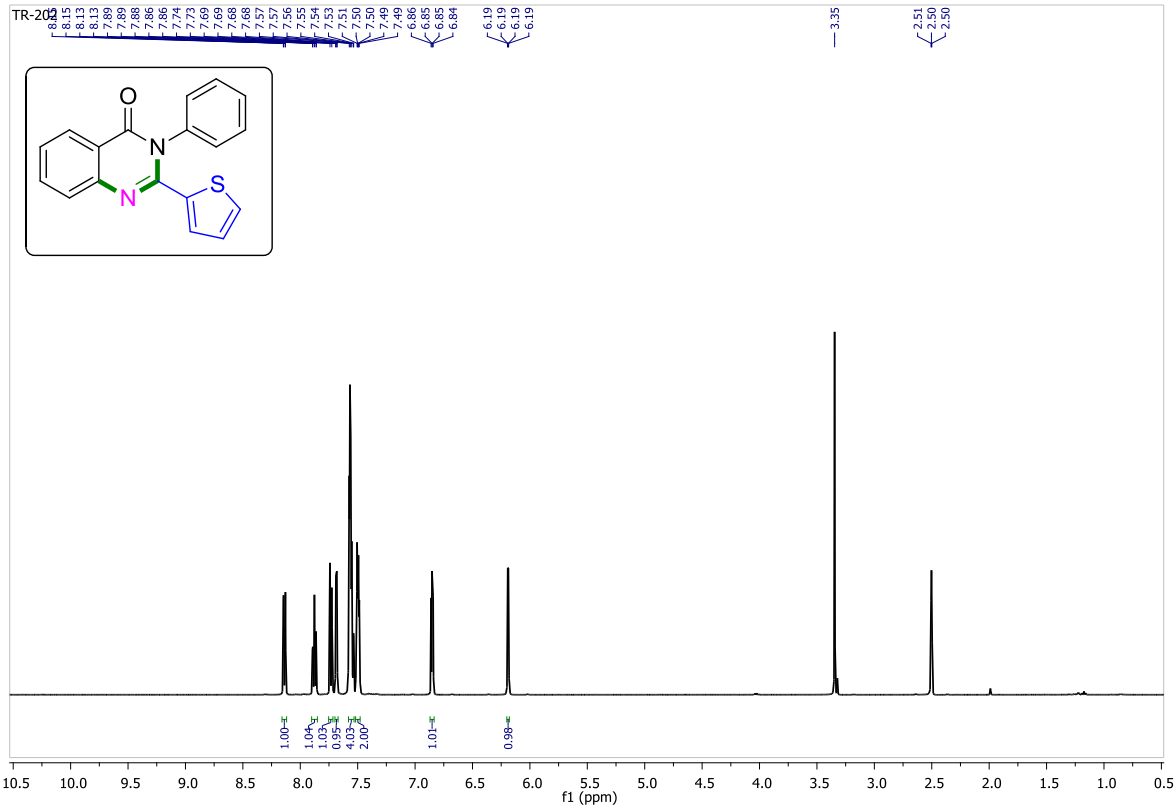


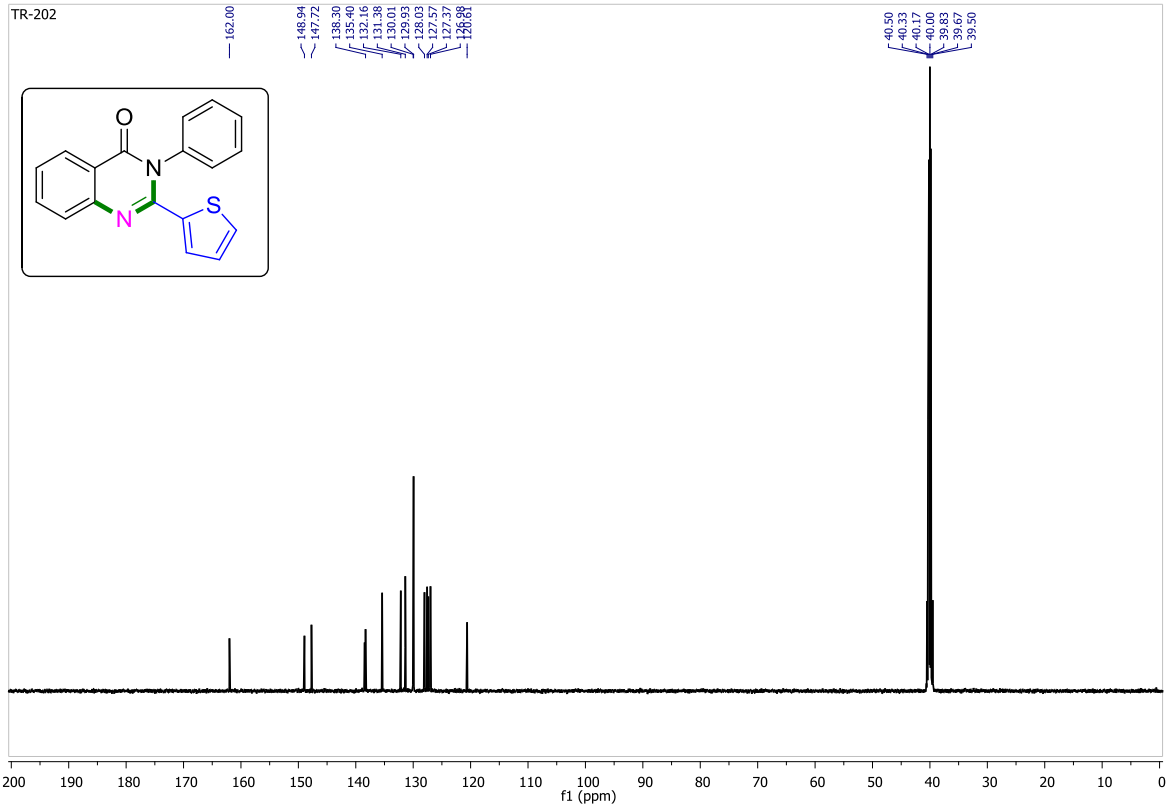
2-(naphthalen-1-yl)-3-phenylquinazolin-4(3H)-one (4h)



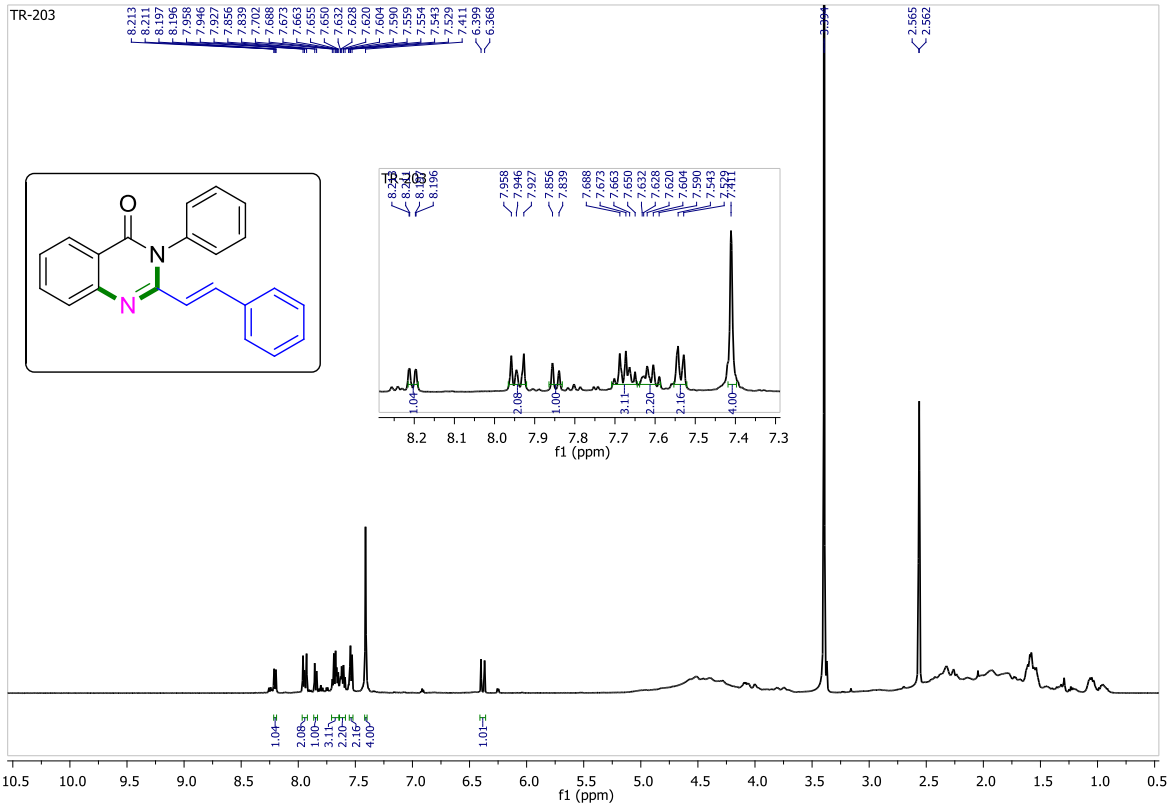


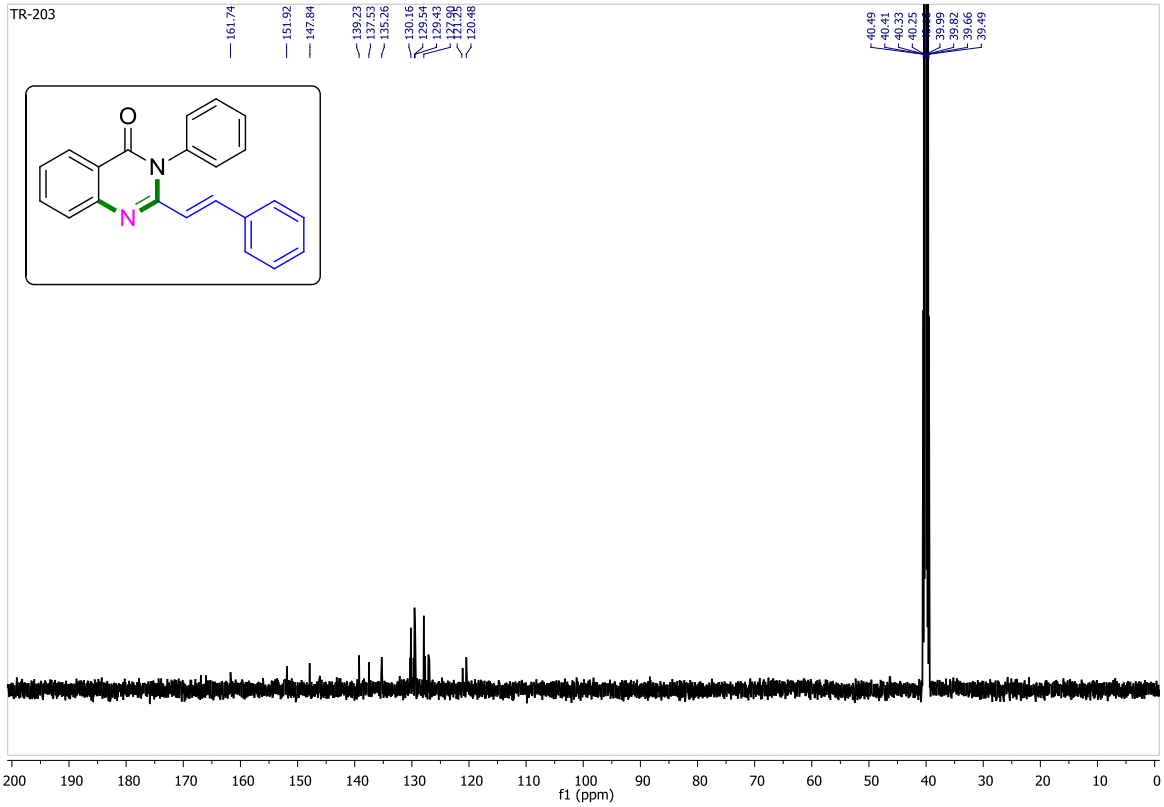
3-phenyl-2-(thiophen-2-yl)quinazolin-4(3H)-one (4i)



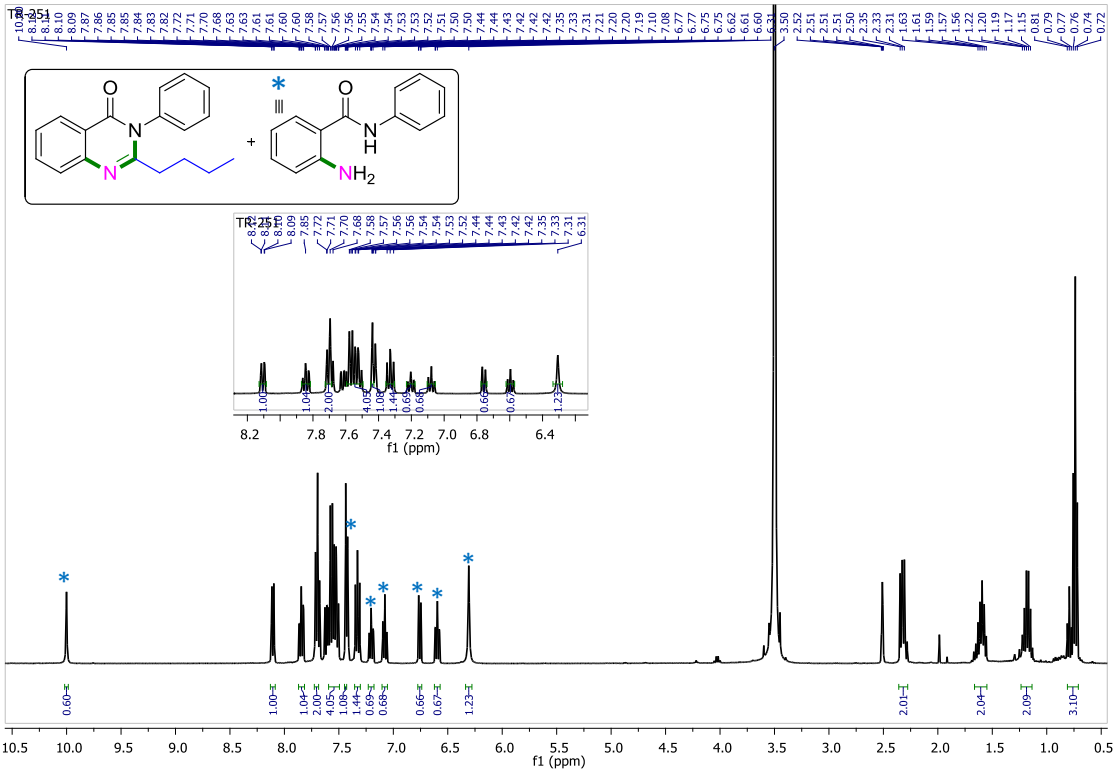


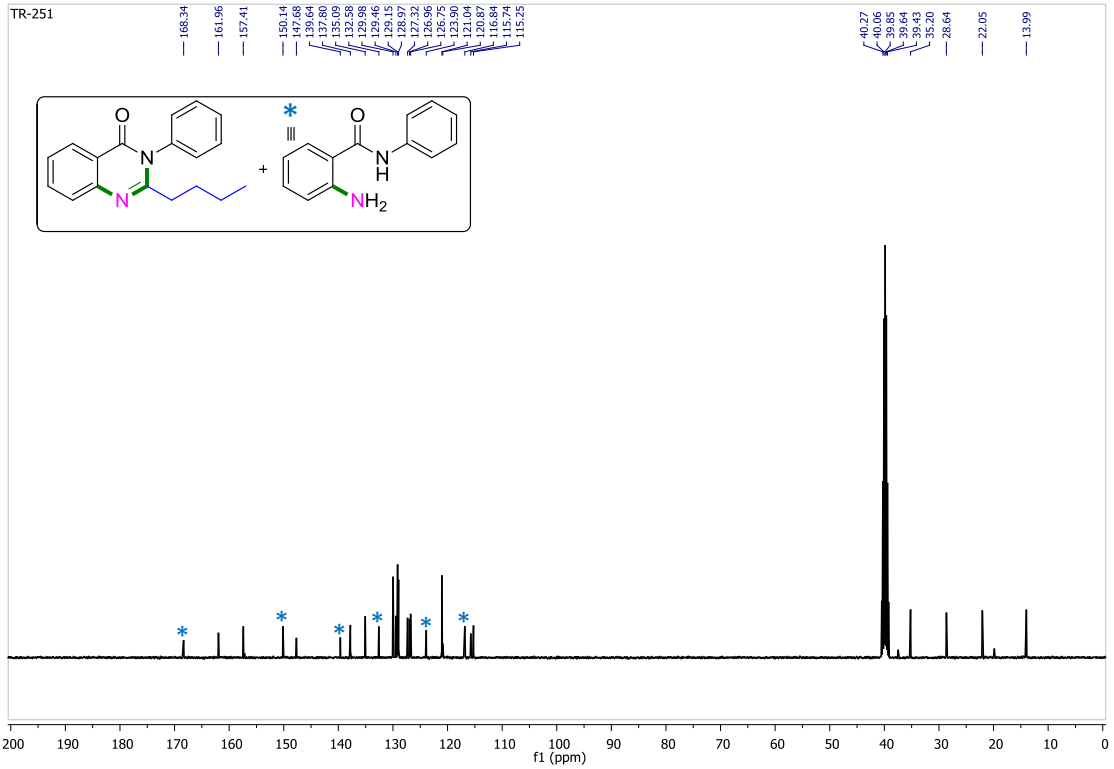
(E)-3-phenyl-2-styrylquinazolin-4(3H)-one (4j)



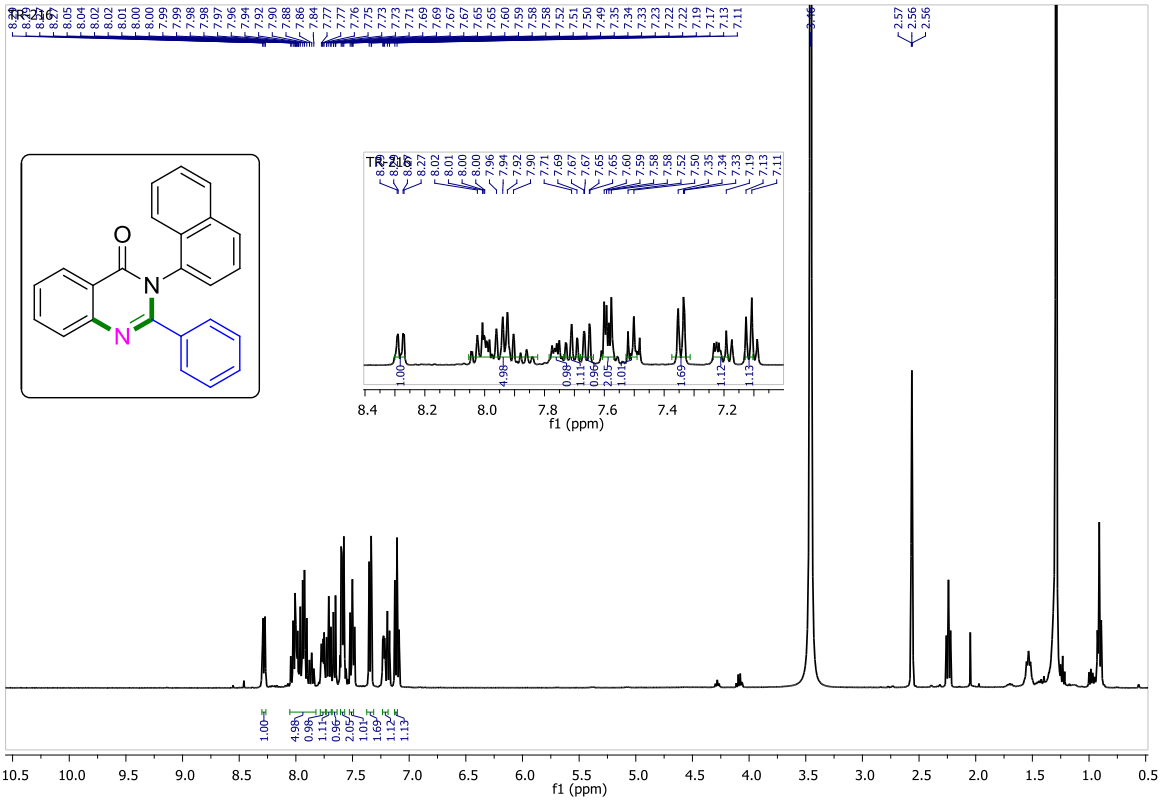


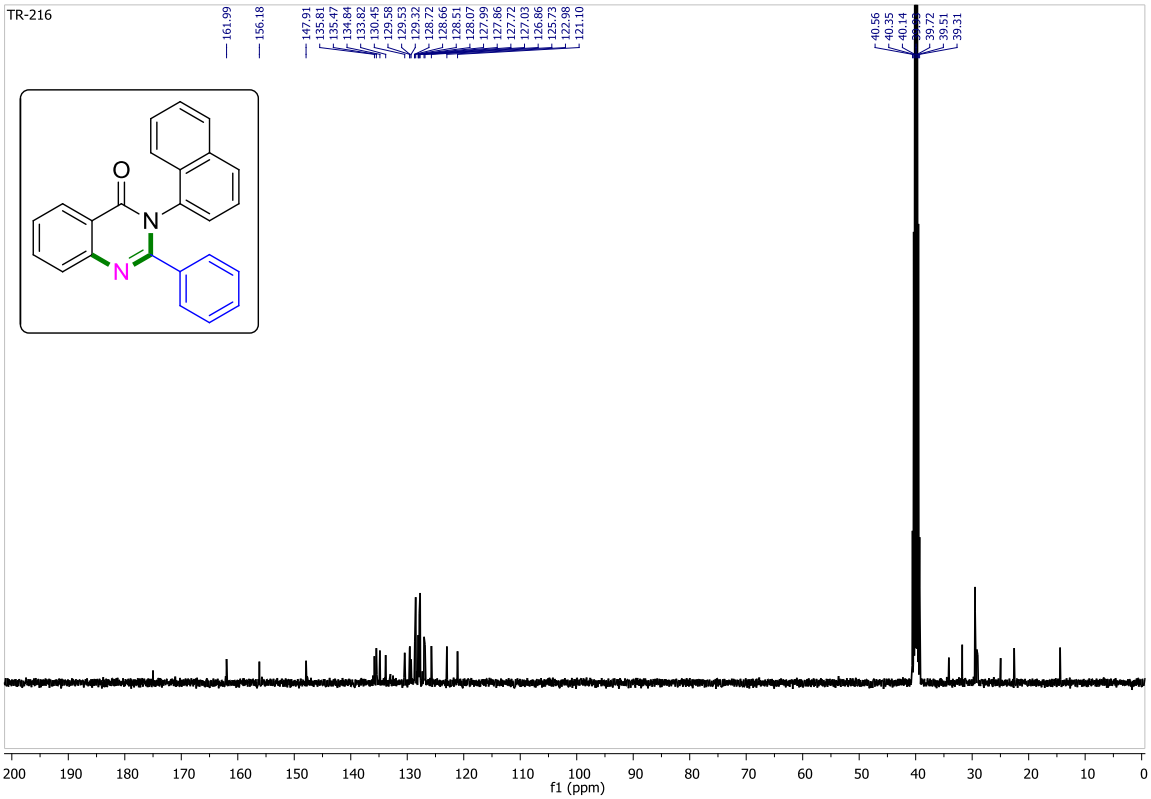
2-butyl-3-phenylquinazolin-4(3H)-one (4l)



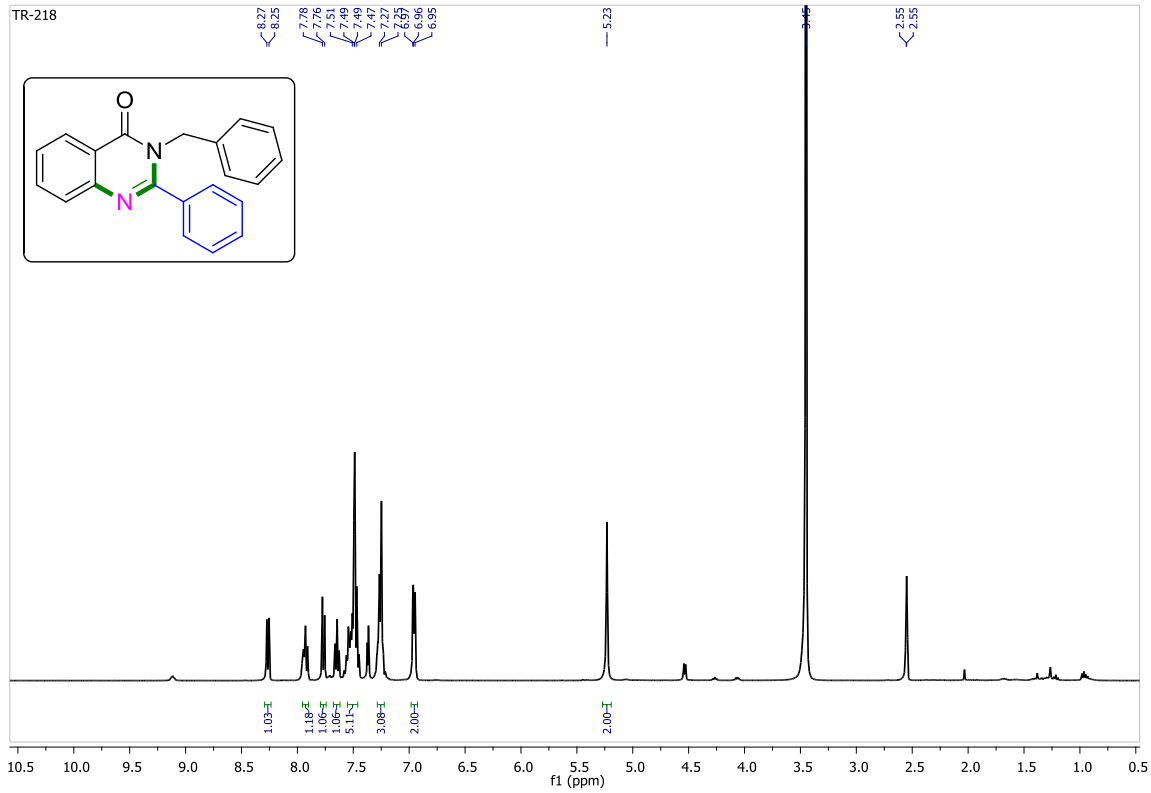


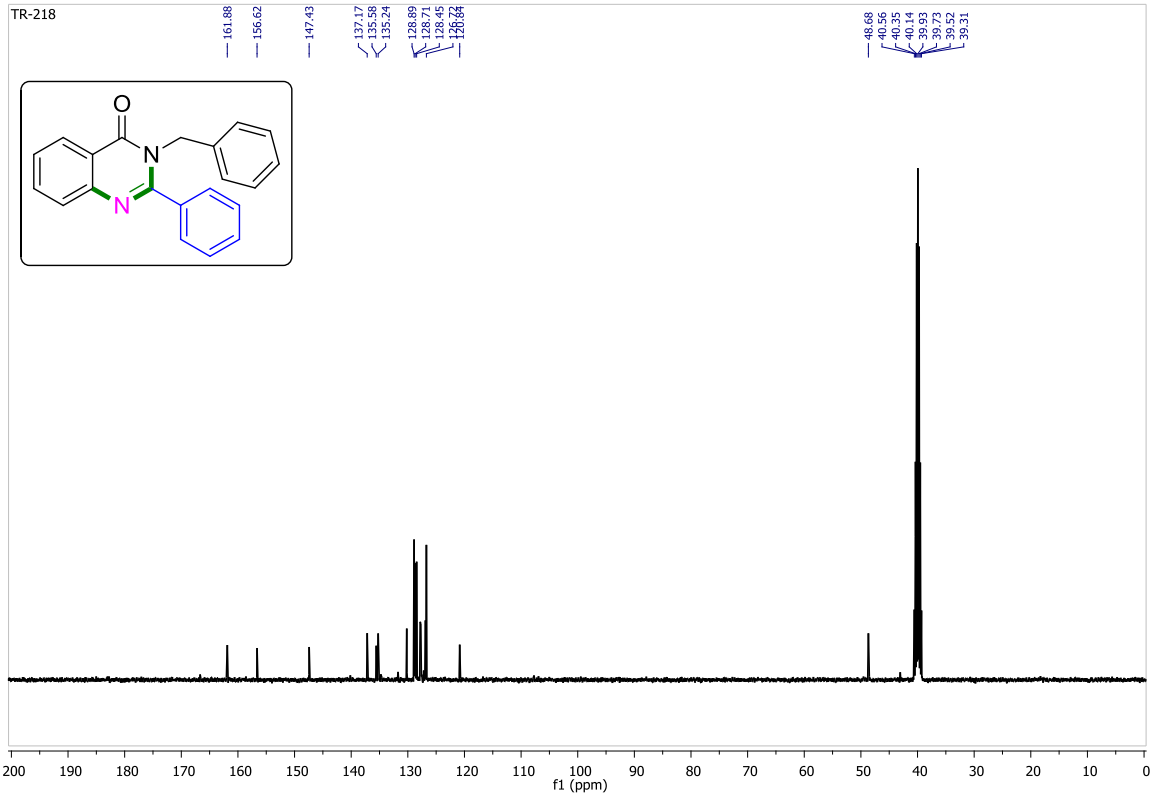
3-(naphthalen-1-yl)-2-phenylquinazolin-4(3H)-one (4n)



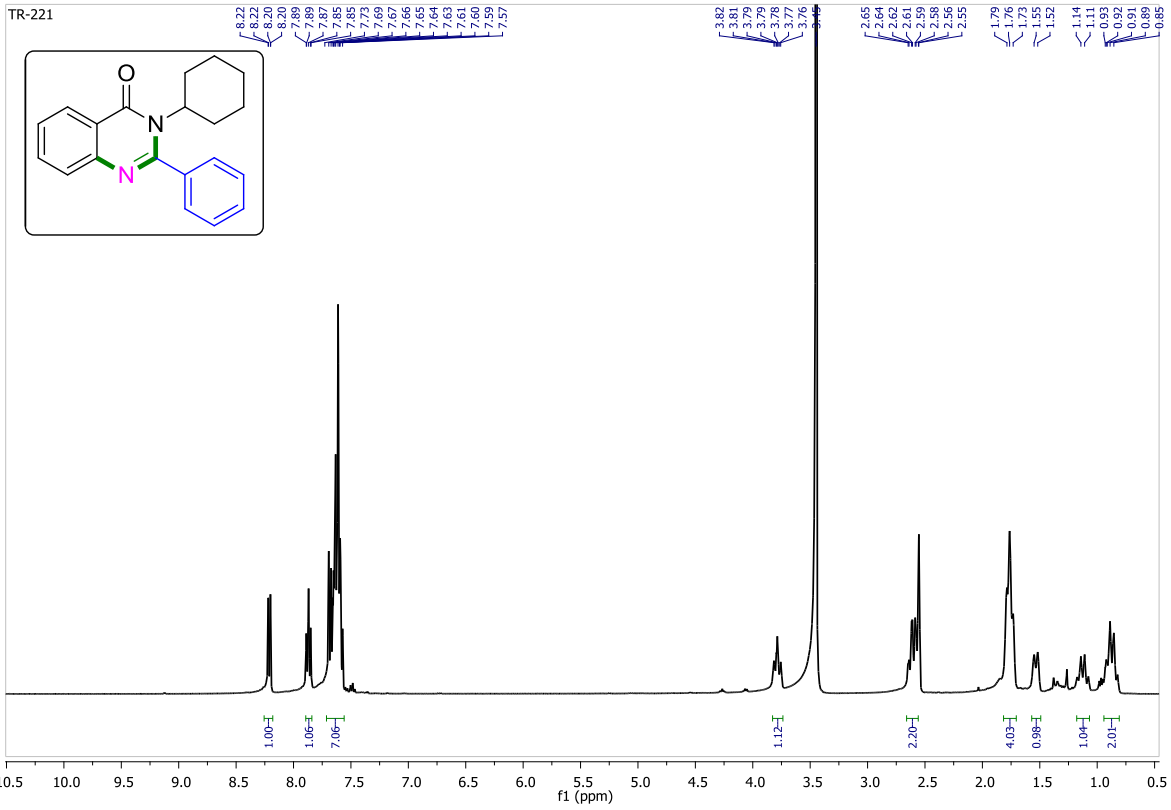


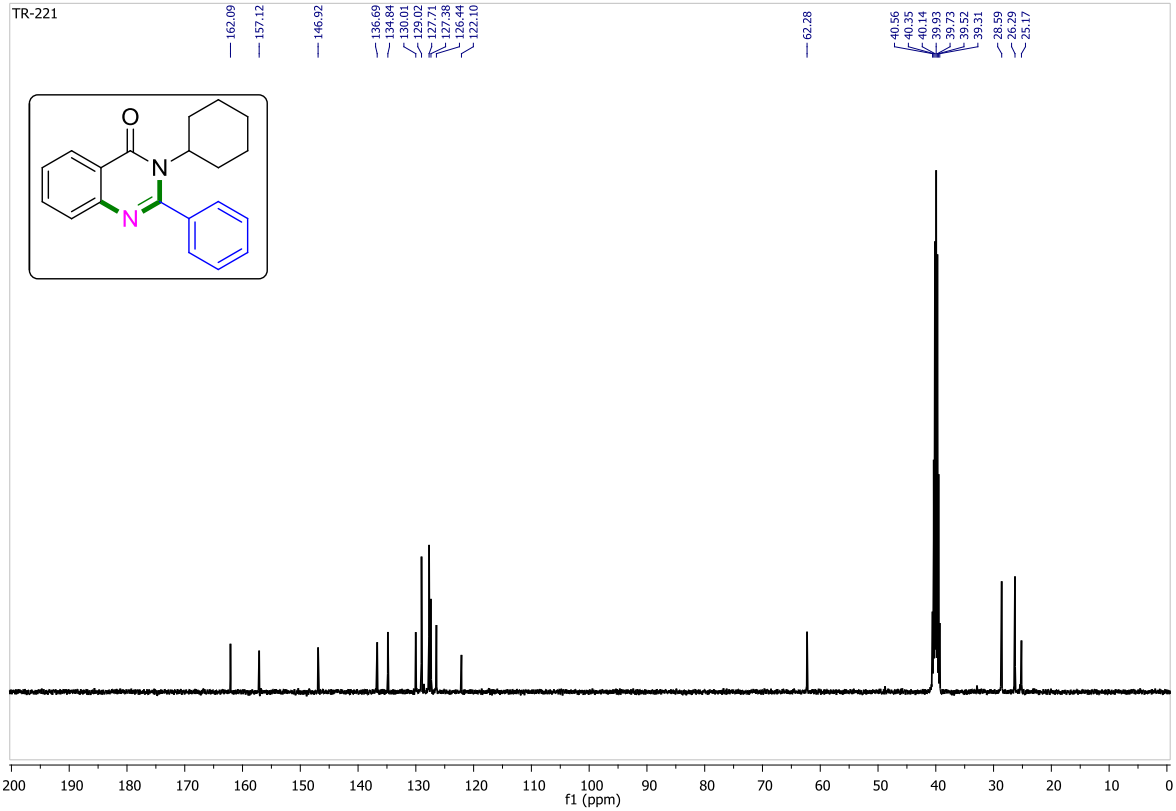
3-benzyl-2-phenylquinazolin-4(3H)-one (4o)



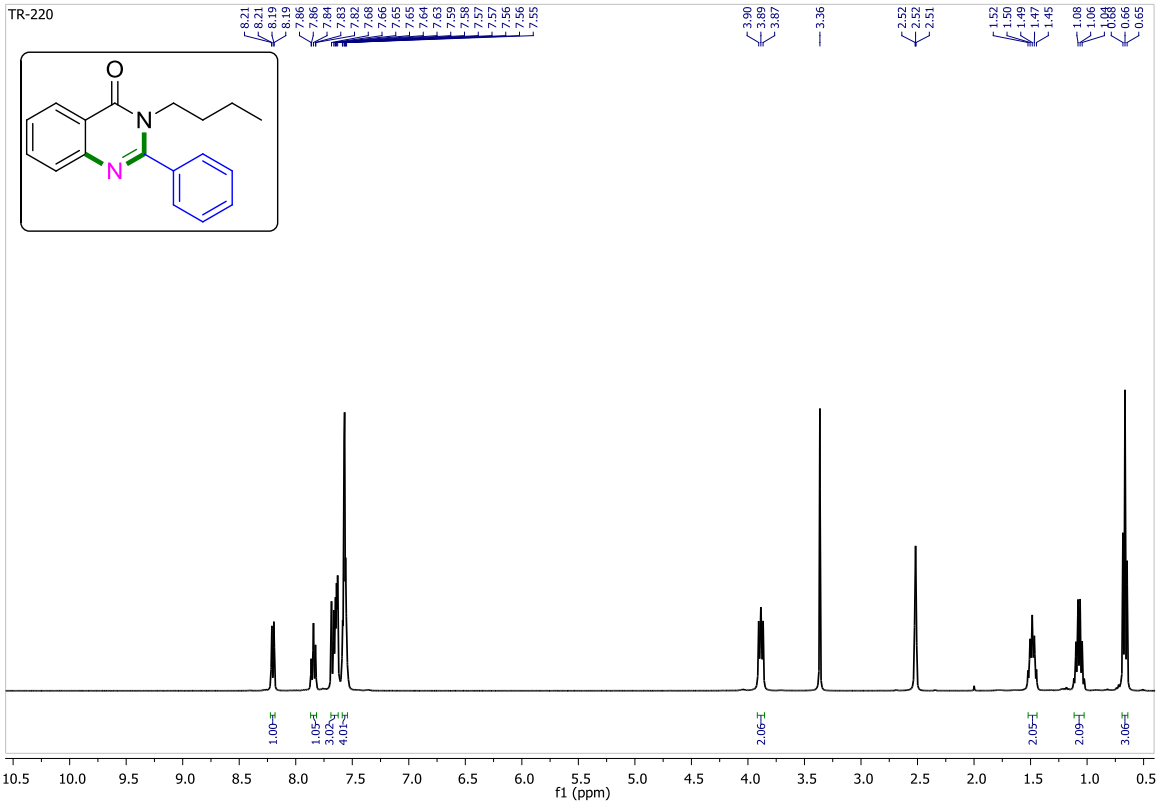


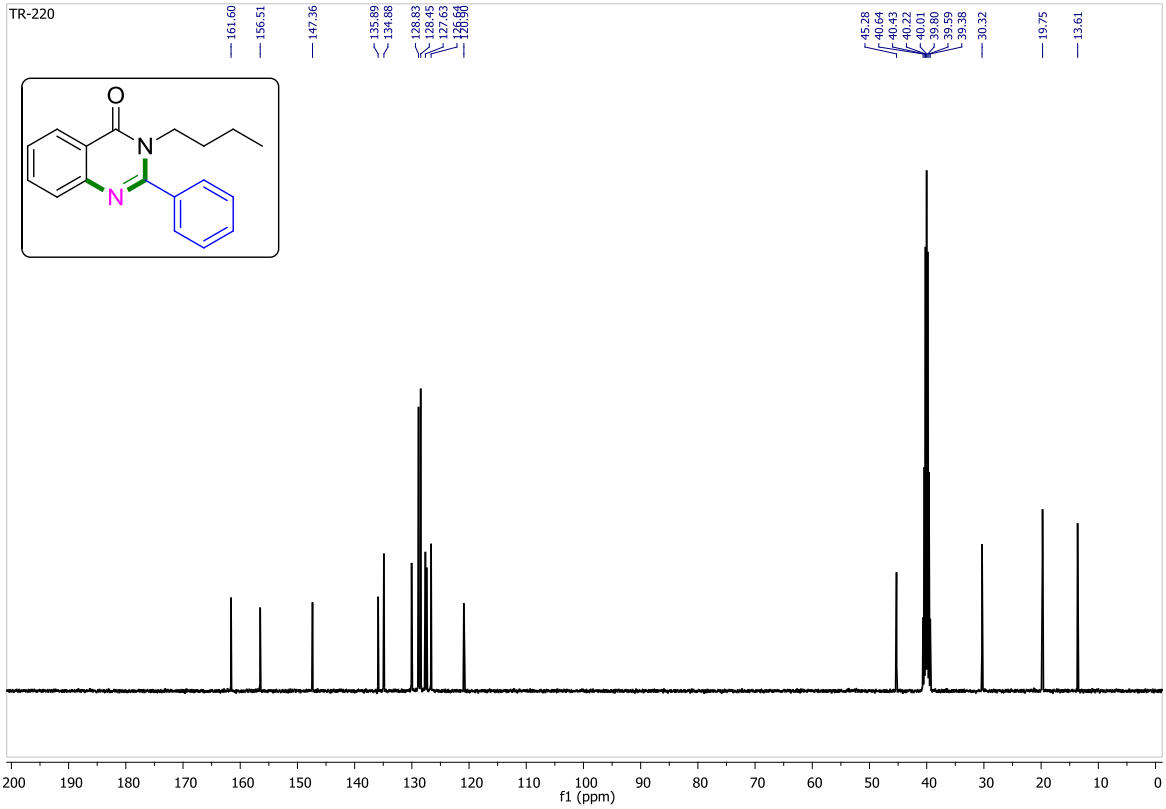
3-cyclohexyl-2-phenylquinazolin-4(3H)-one (4p)



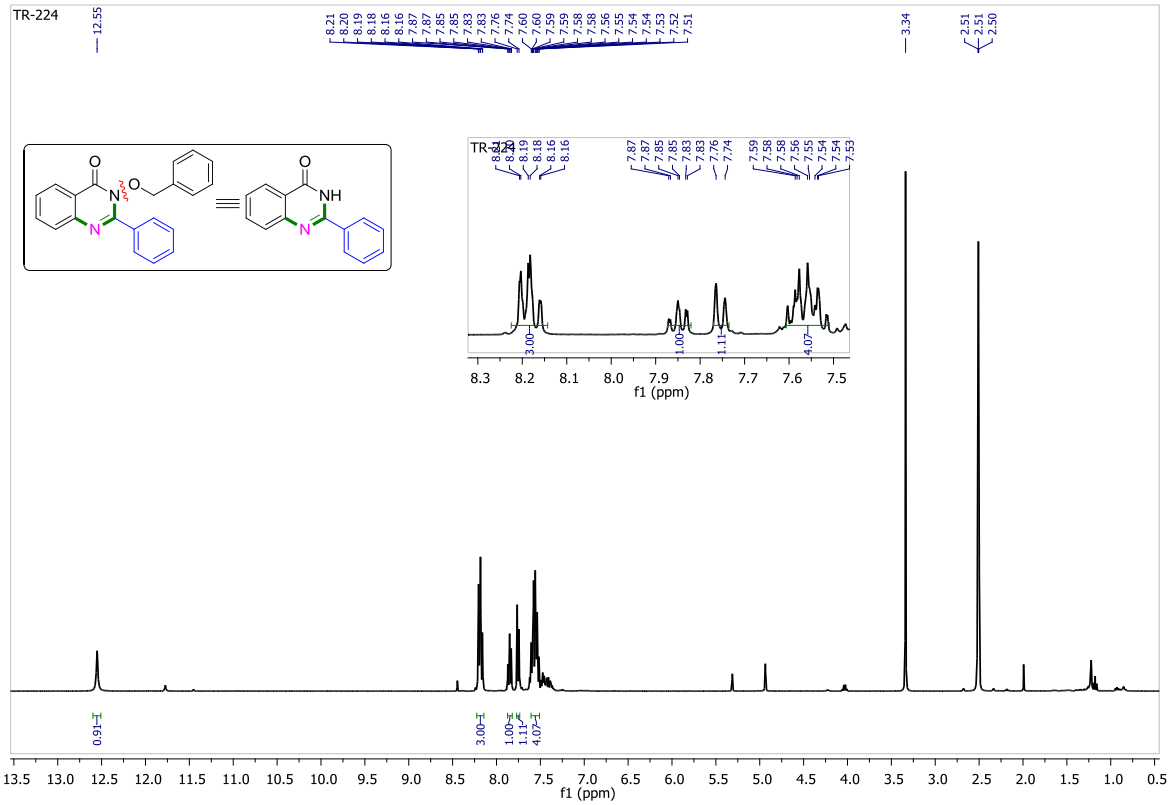


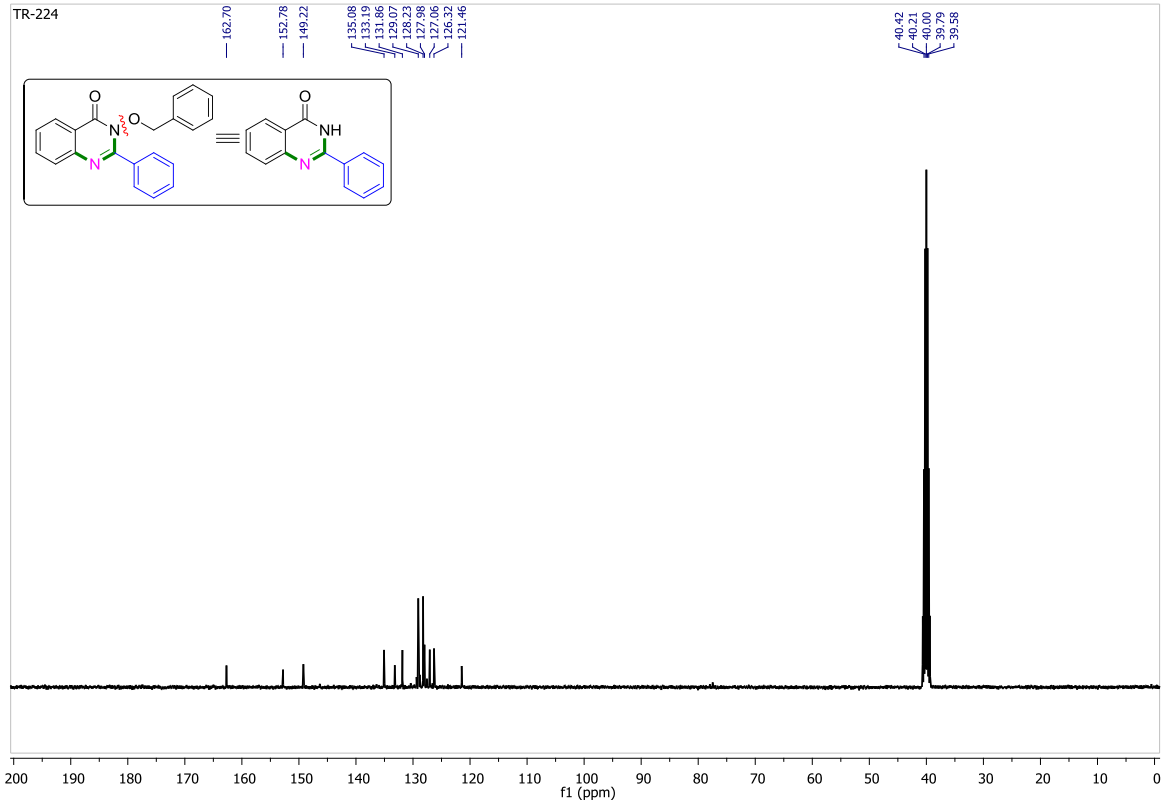
3-butyl-2-phenylquinazolin-4(3H)-one (4q)



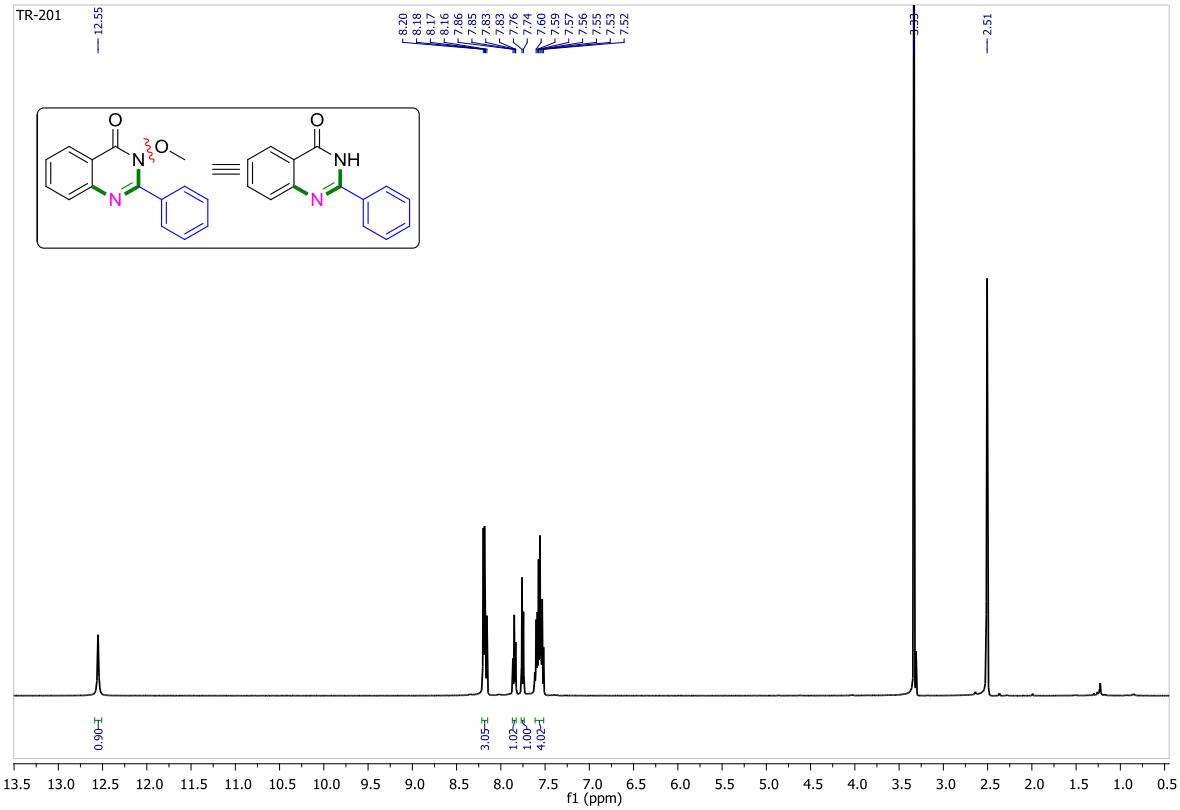


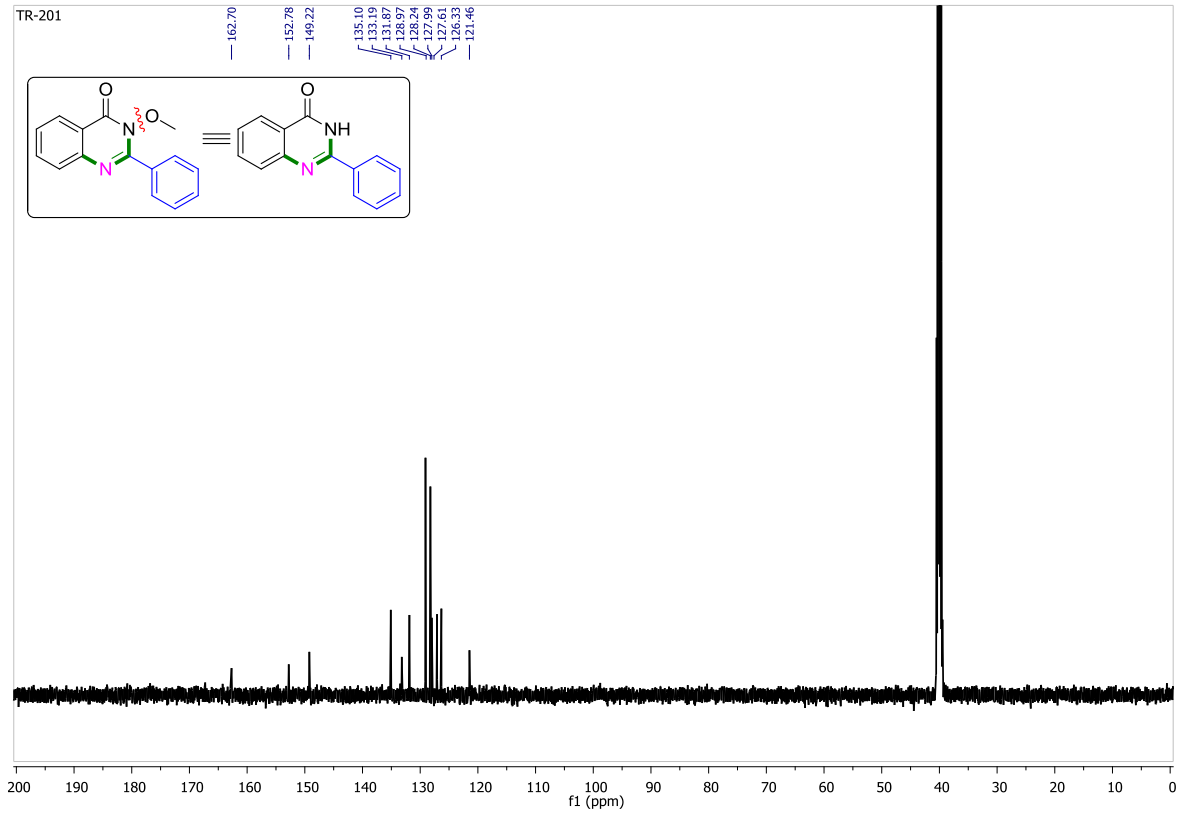
2-phenylquinazolin-4(3H)-one (4r)





2-phenylquinazolin-4(3H)-one (4s)





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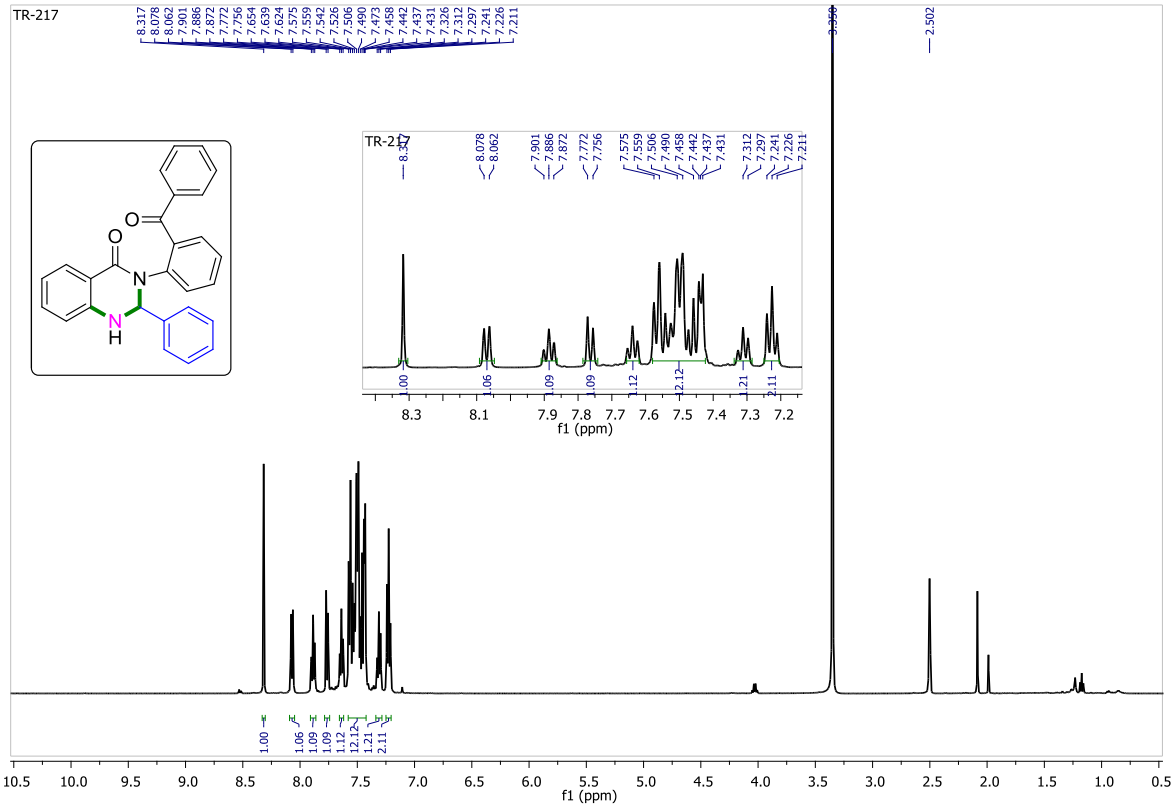
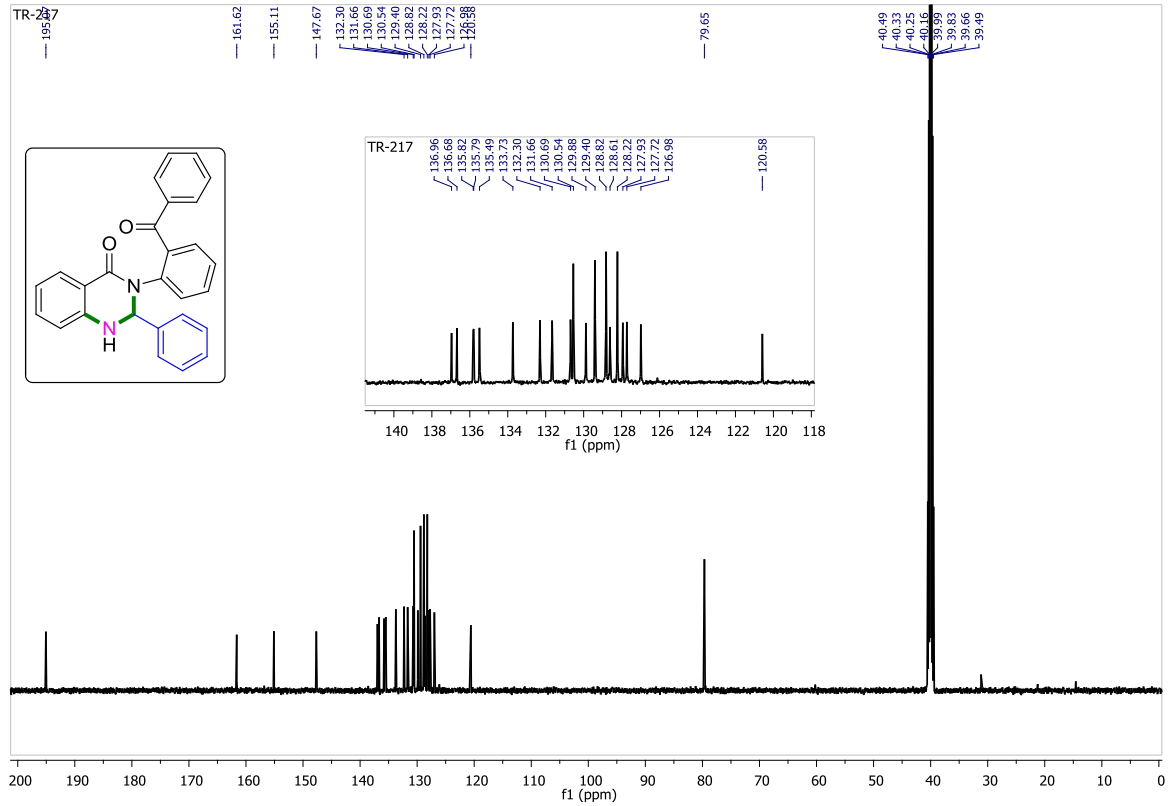
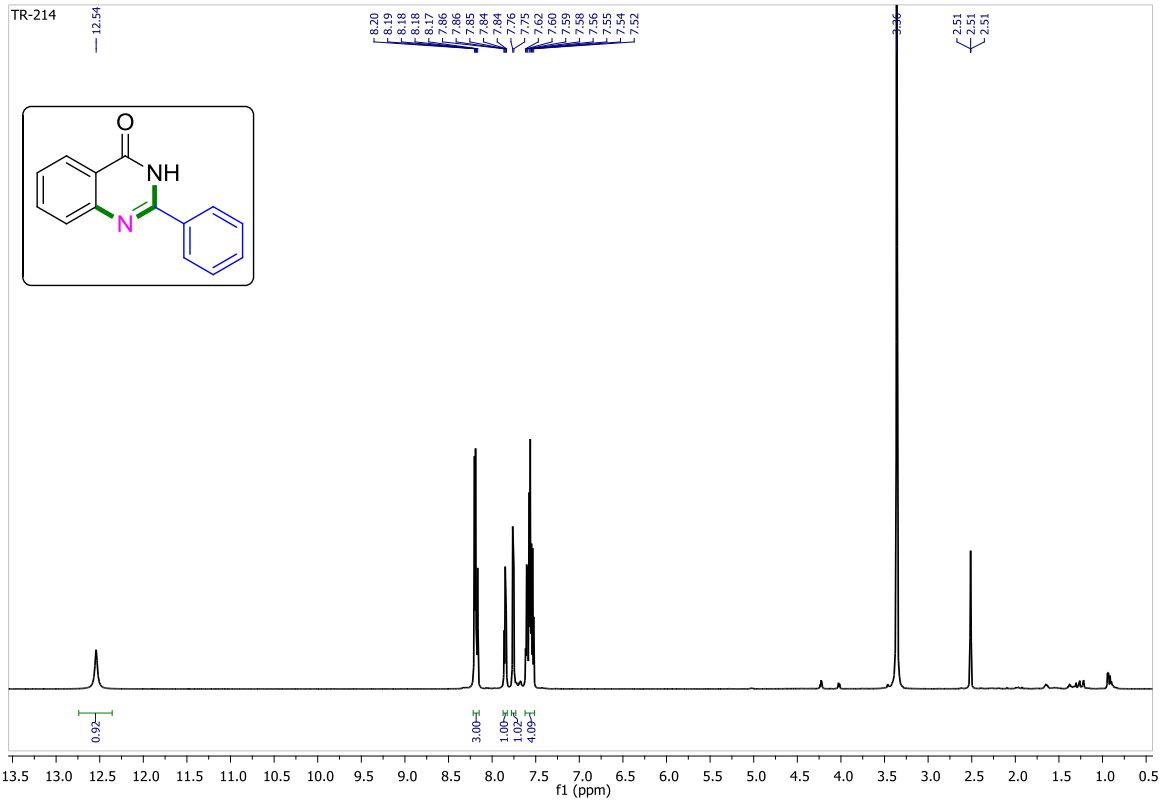
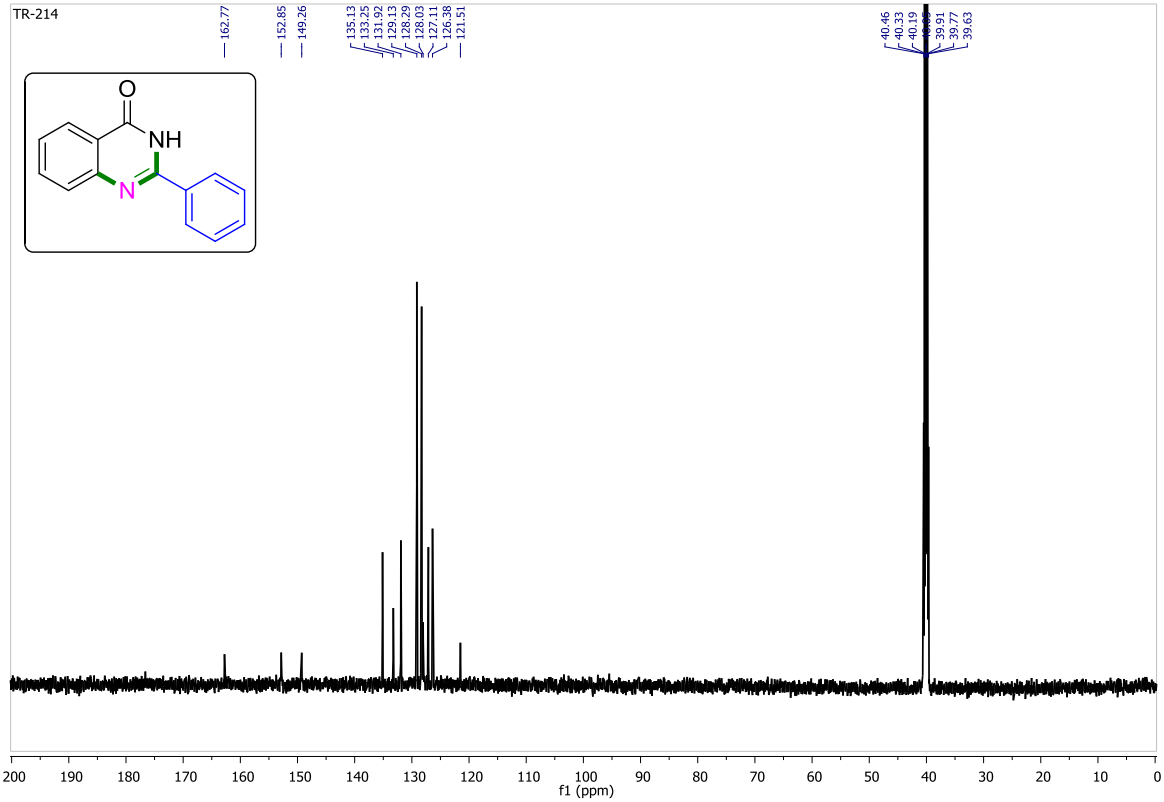




2-phenylquinazolin-4(3H)-one (5a)





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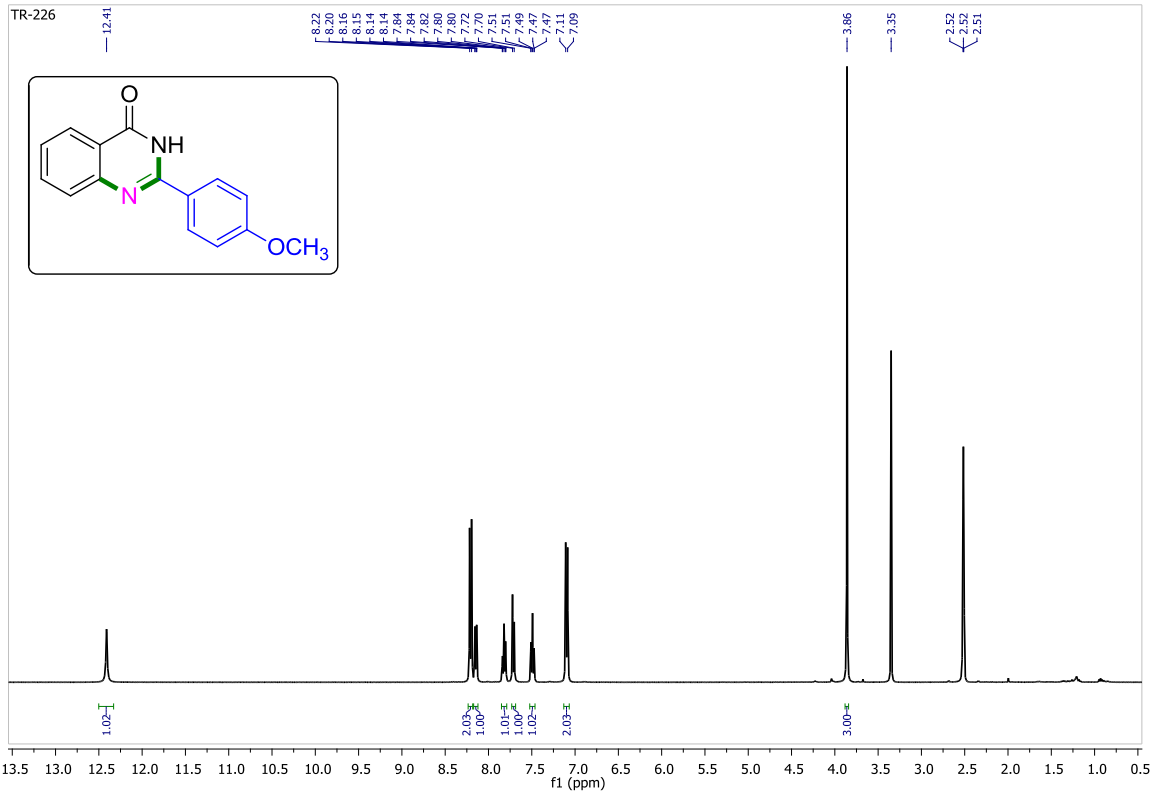
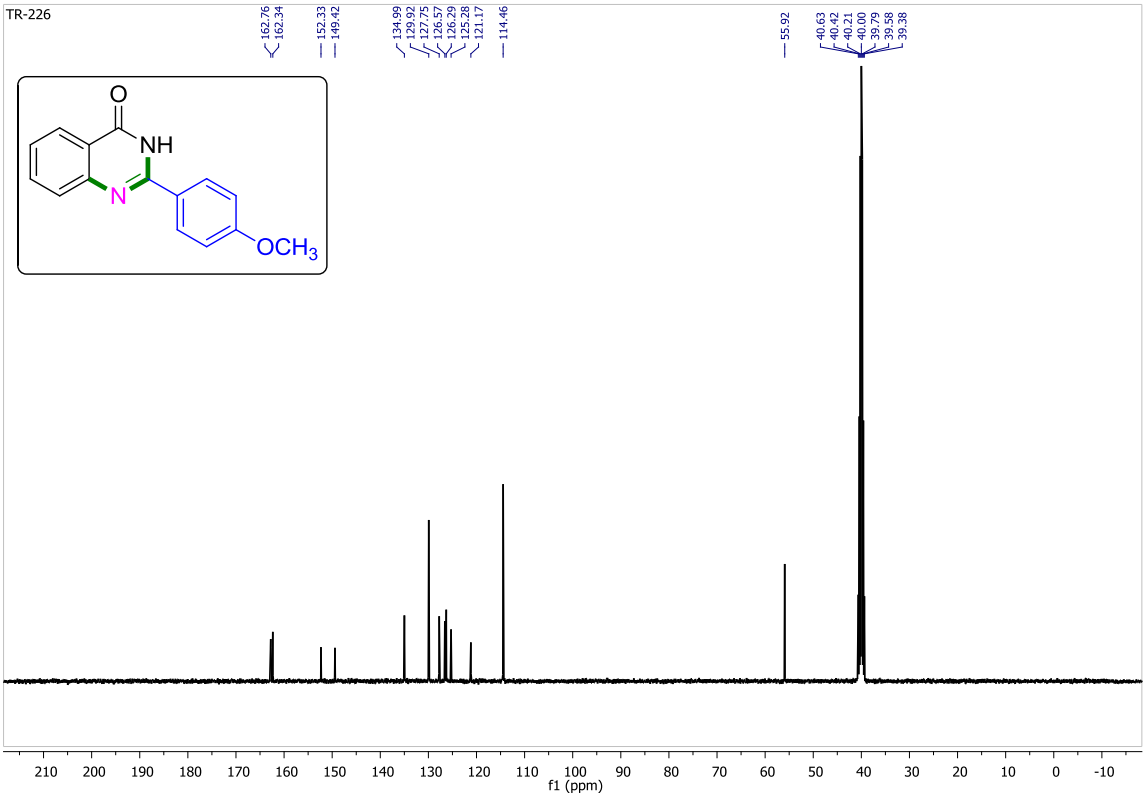
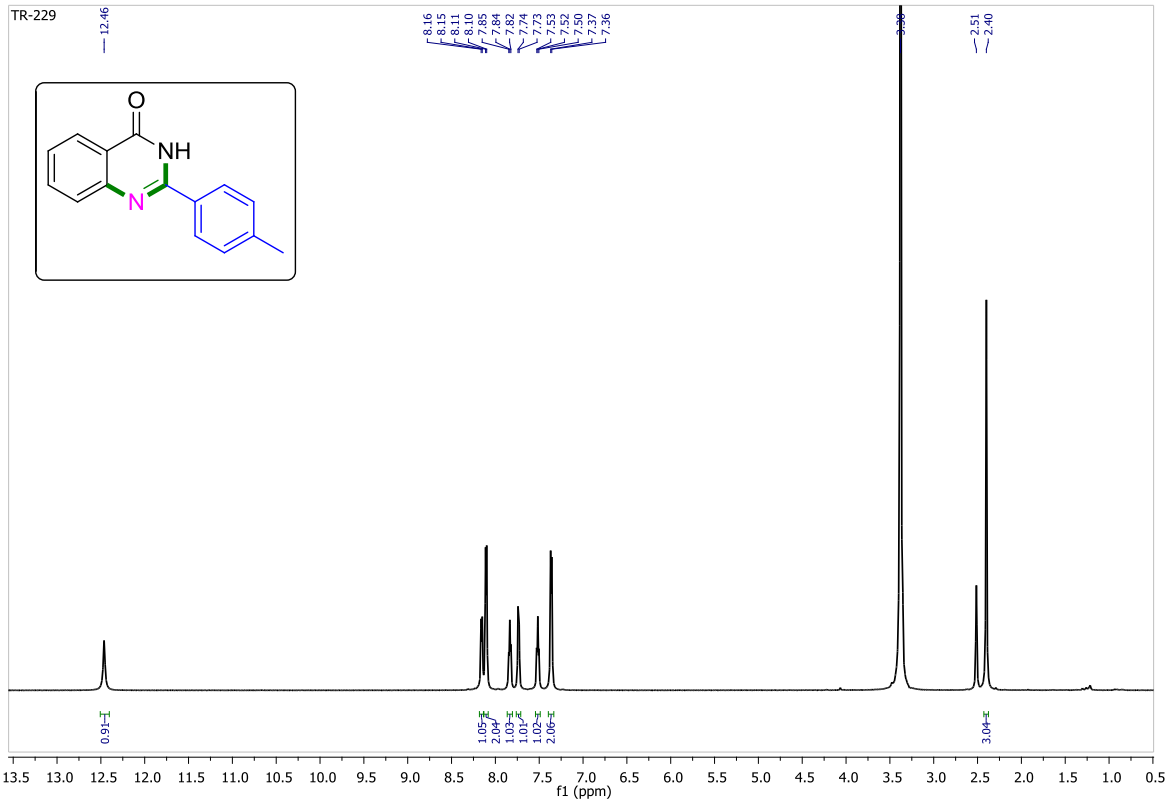
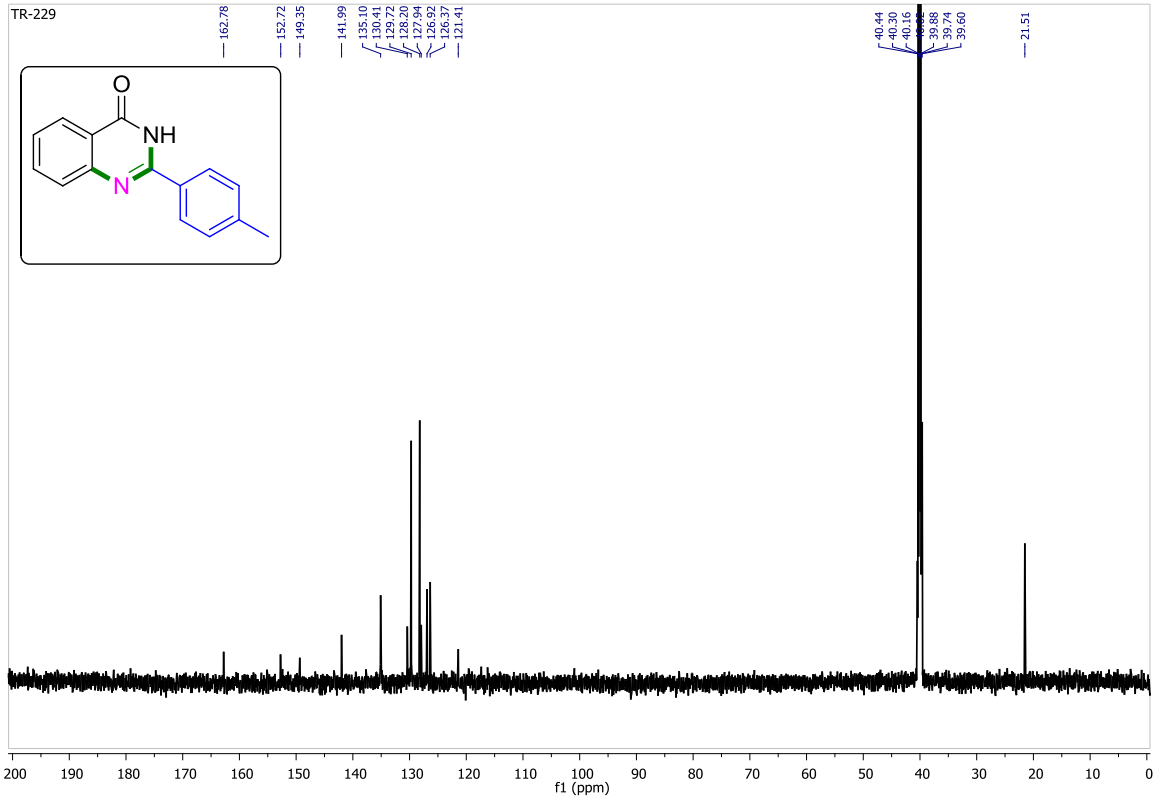


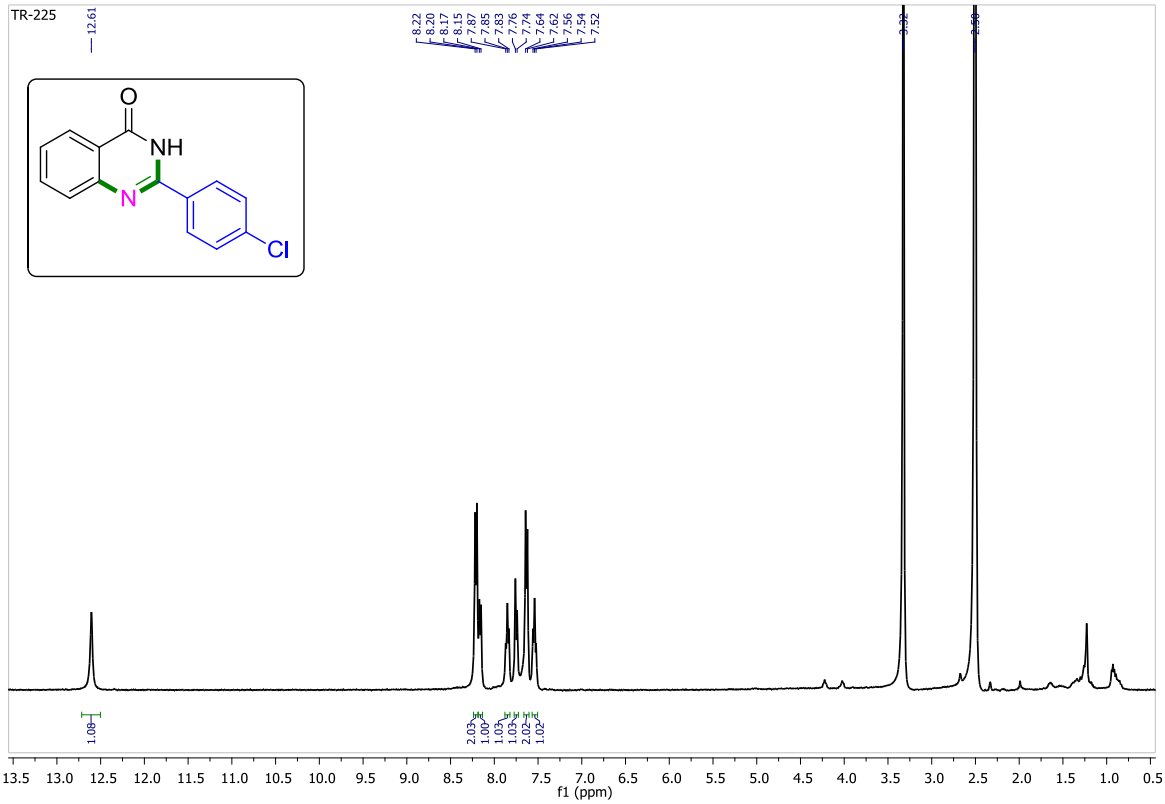


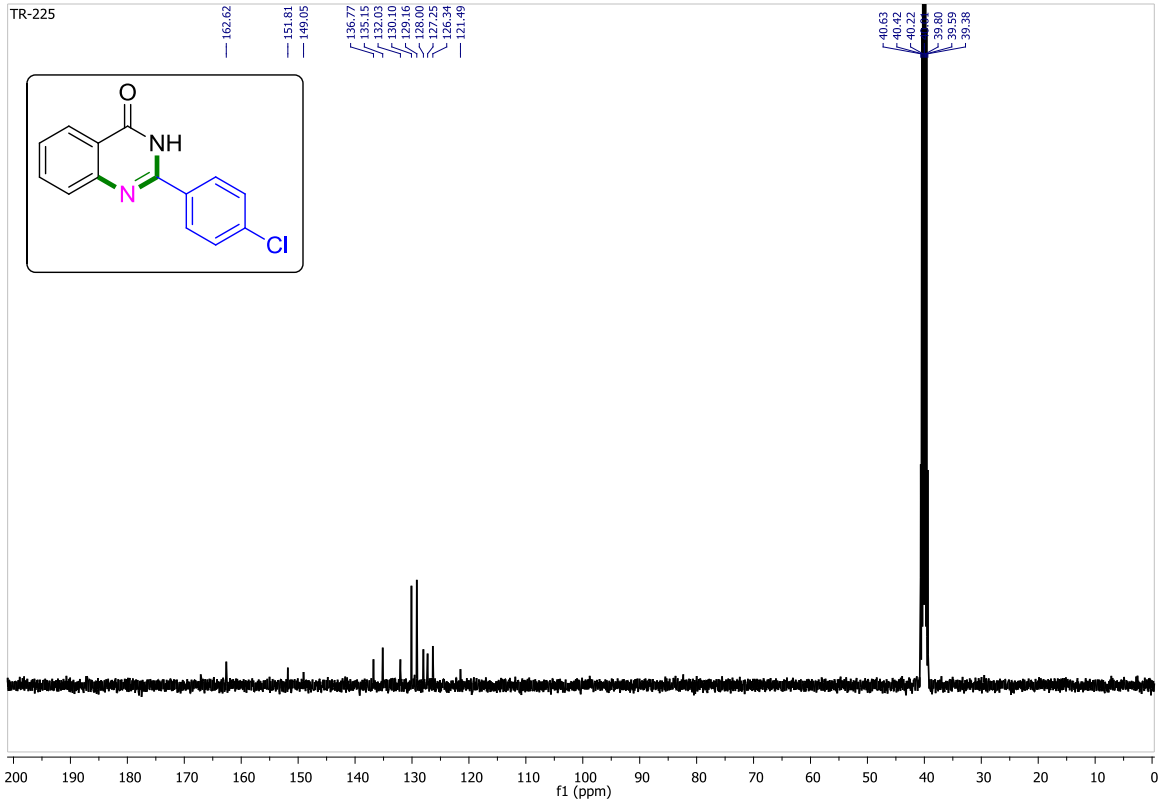
2-(p-tolyl)quinazolin-4(3H)-one (5c)





2-(4-chlorophenyl)quinazolin-4(3H)-one (5d)





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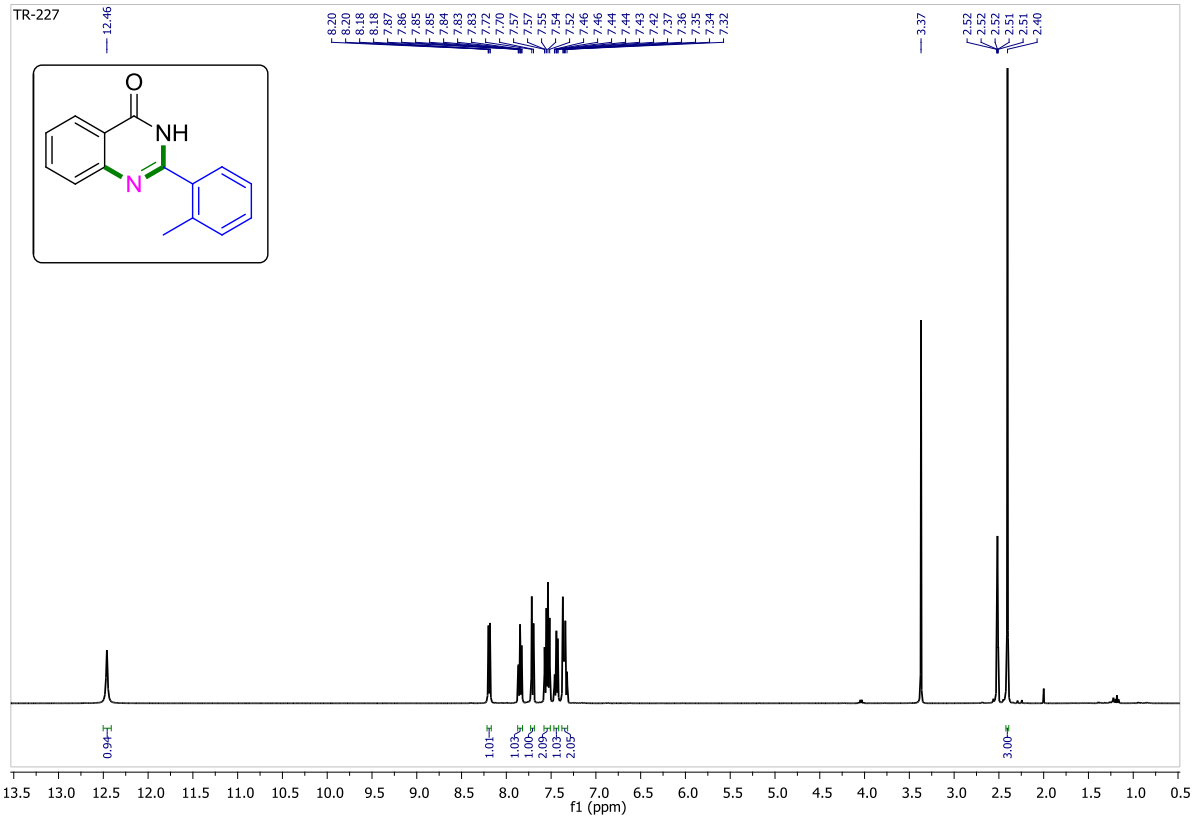
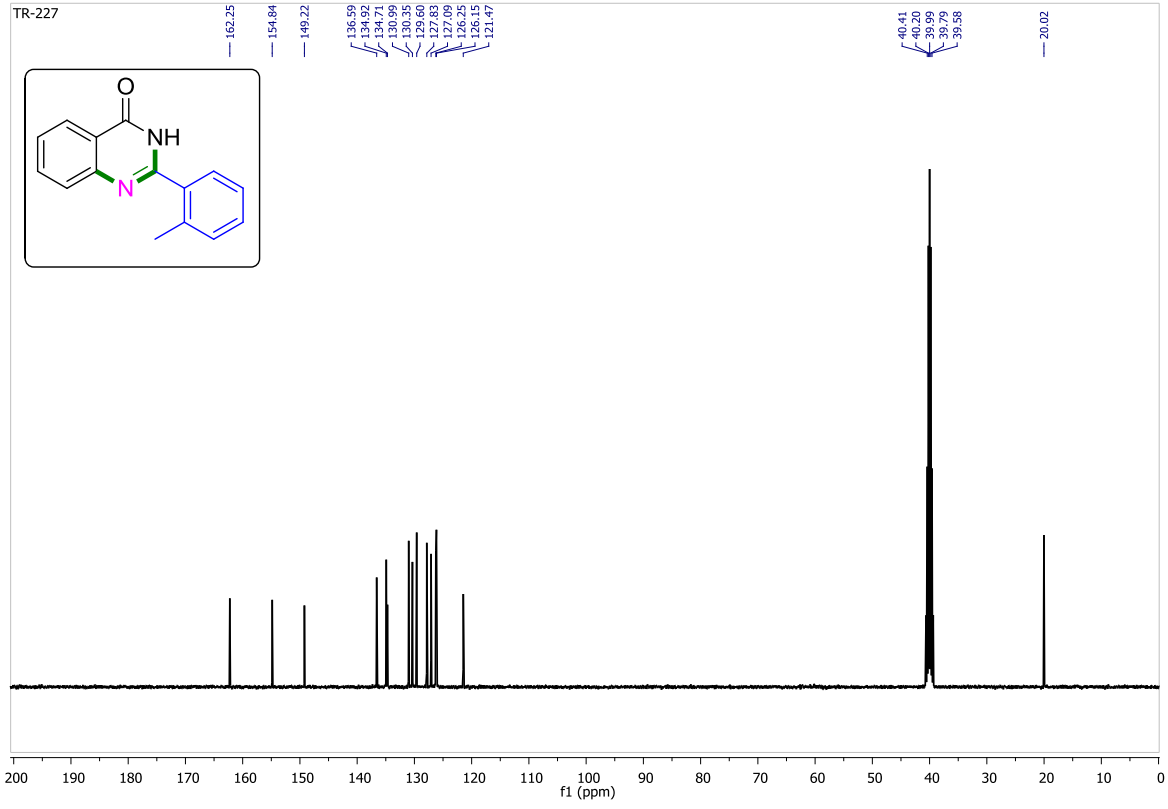
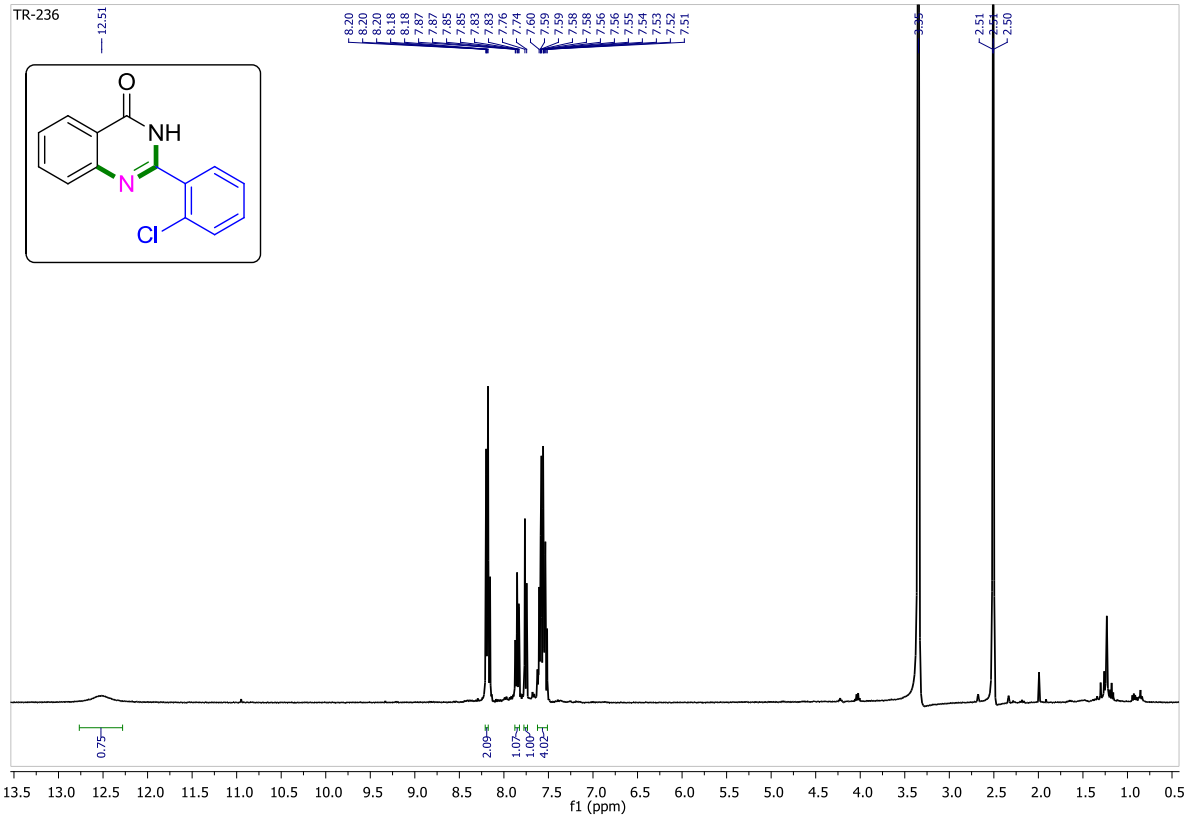
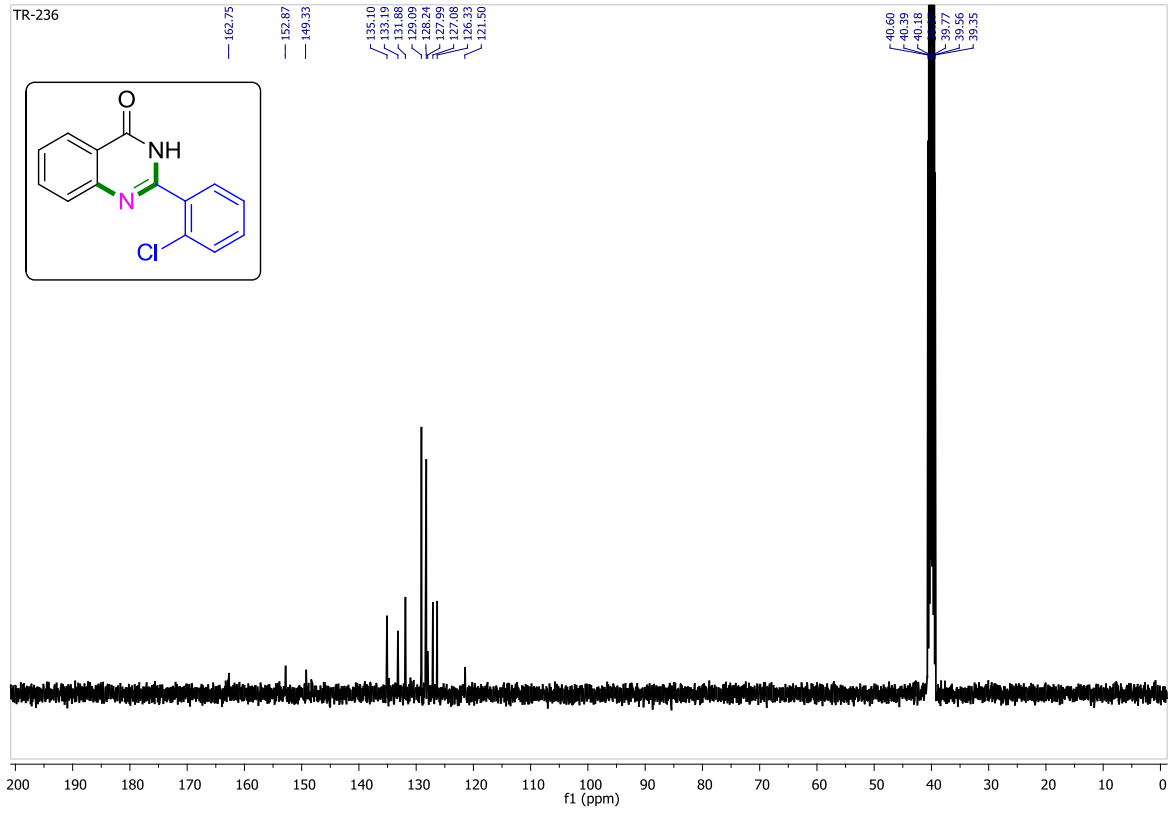


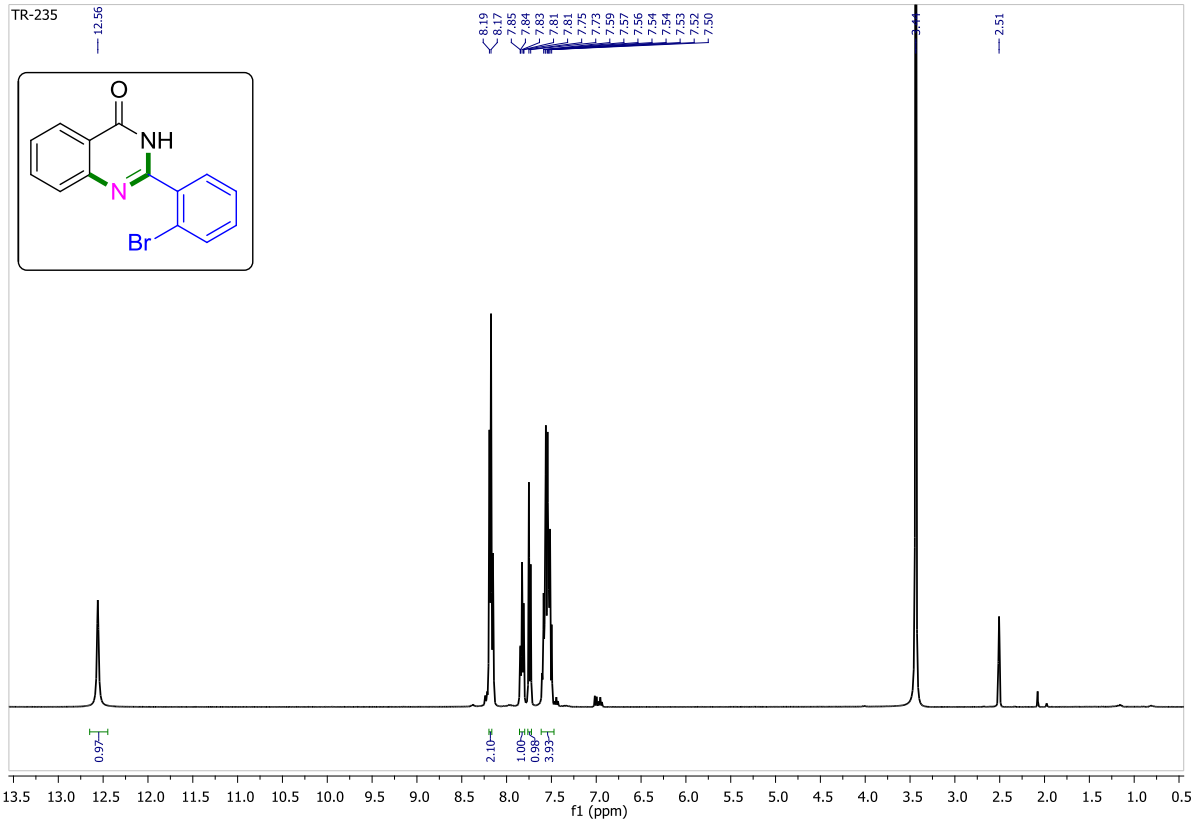


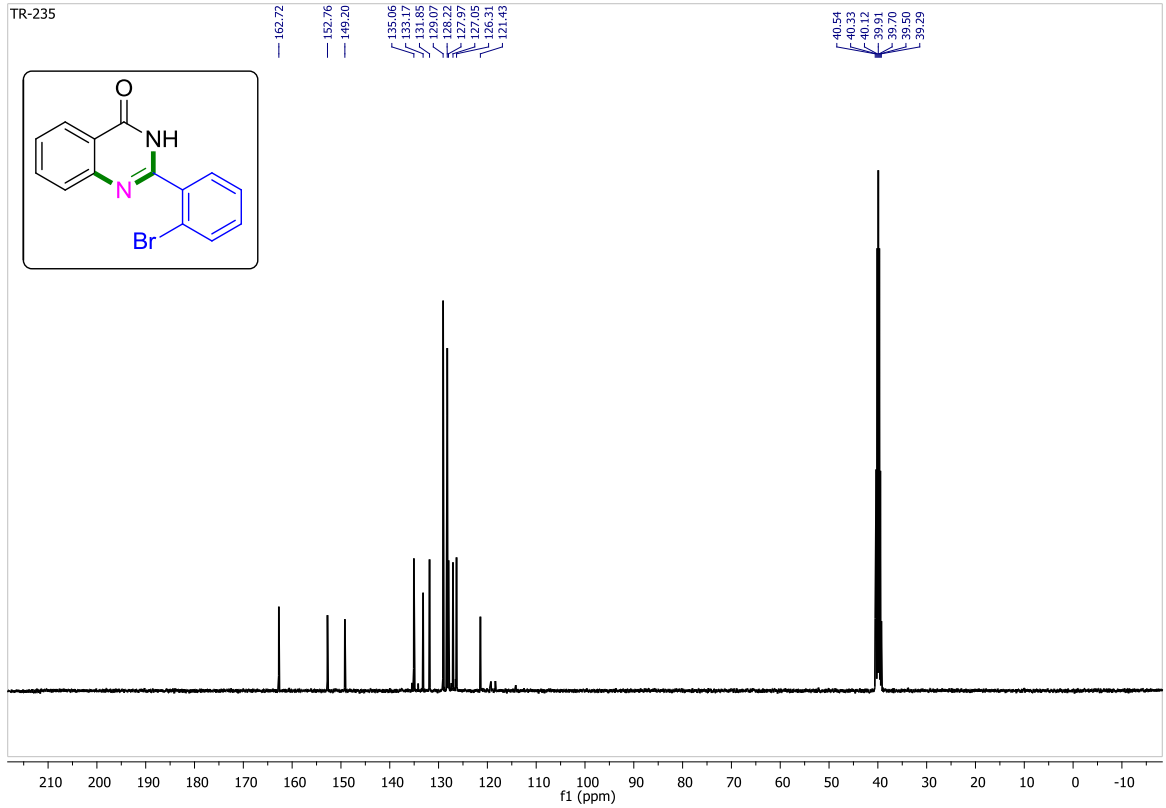
2-(2-chlorophenyl)quinazolin-4(3H)-one (5f)



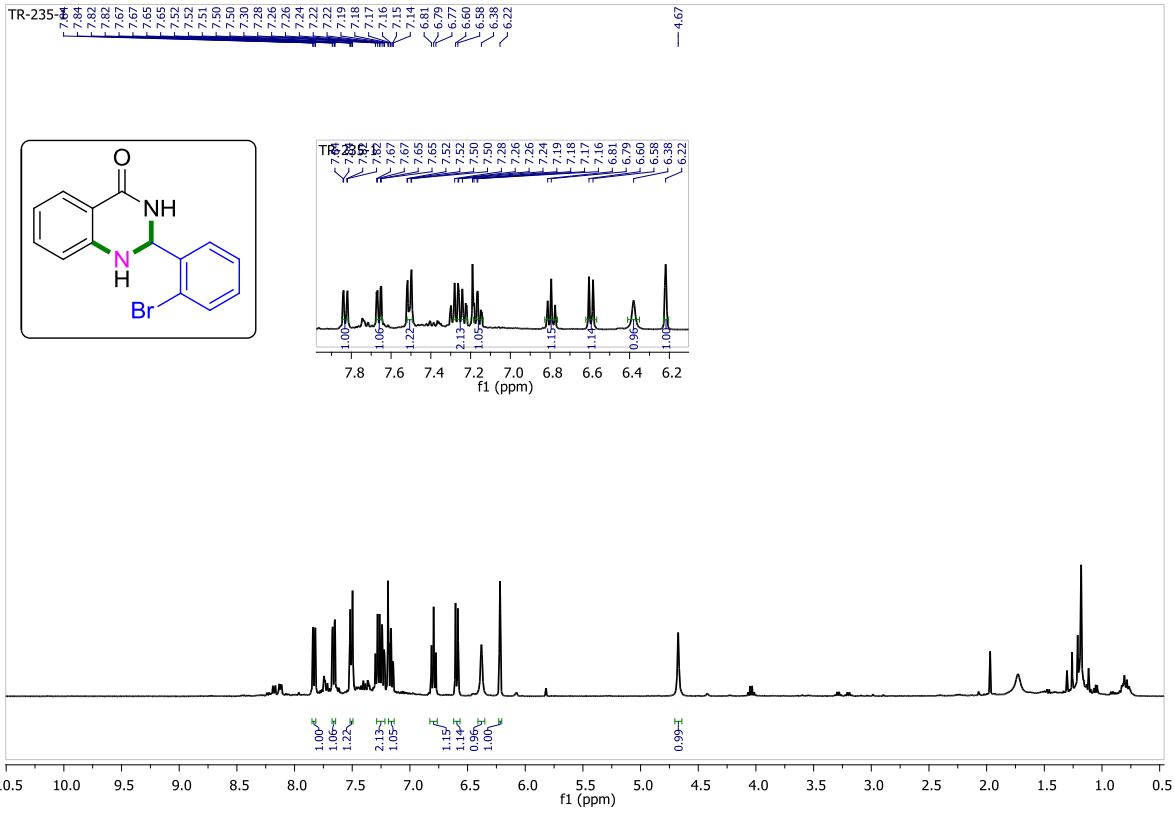


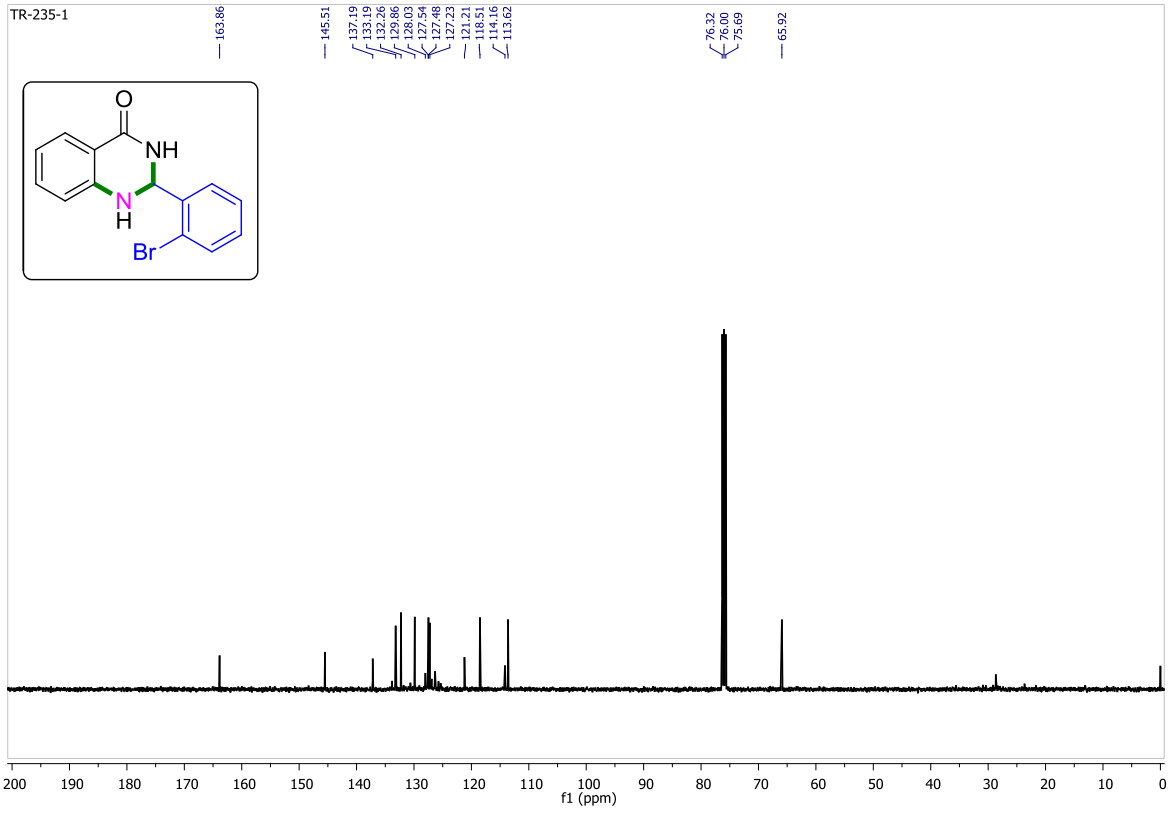
2-(2-bromophenyl)quinazolin-4(3H)-one (5g)



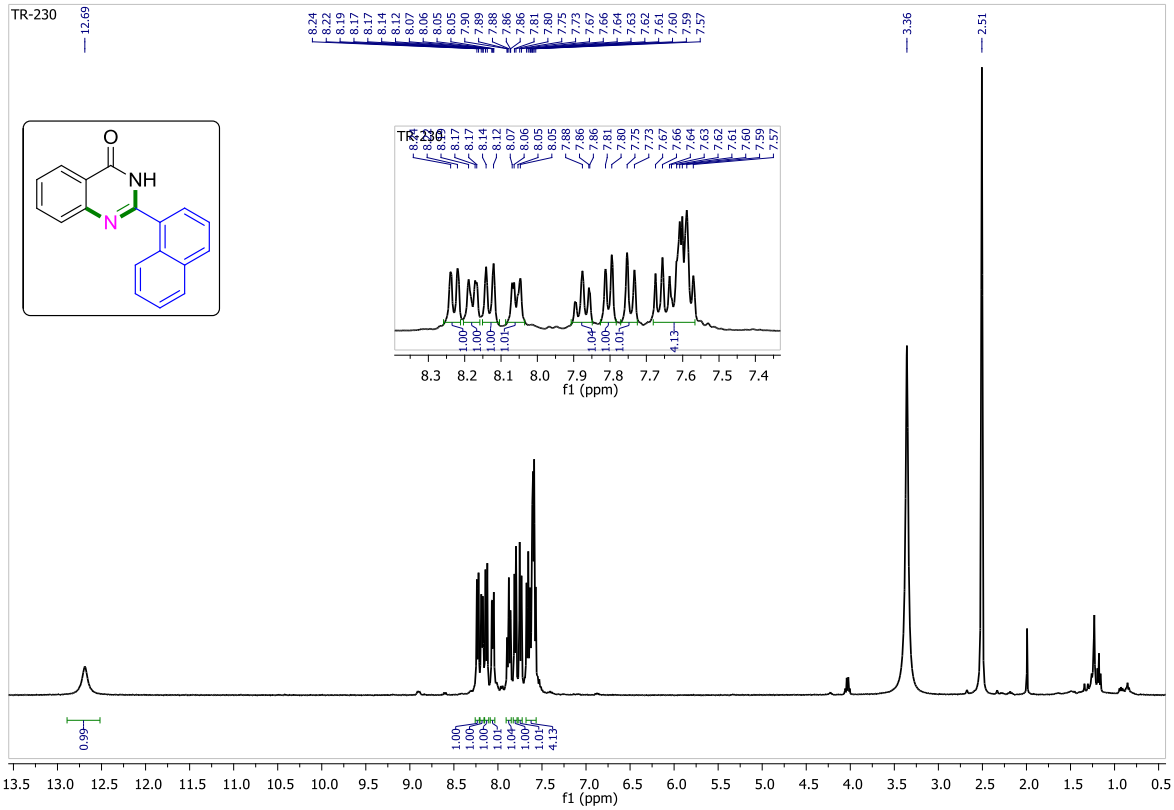


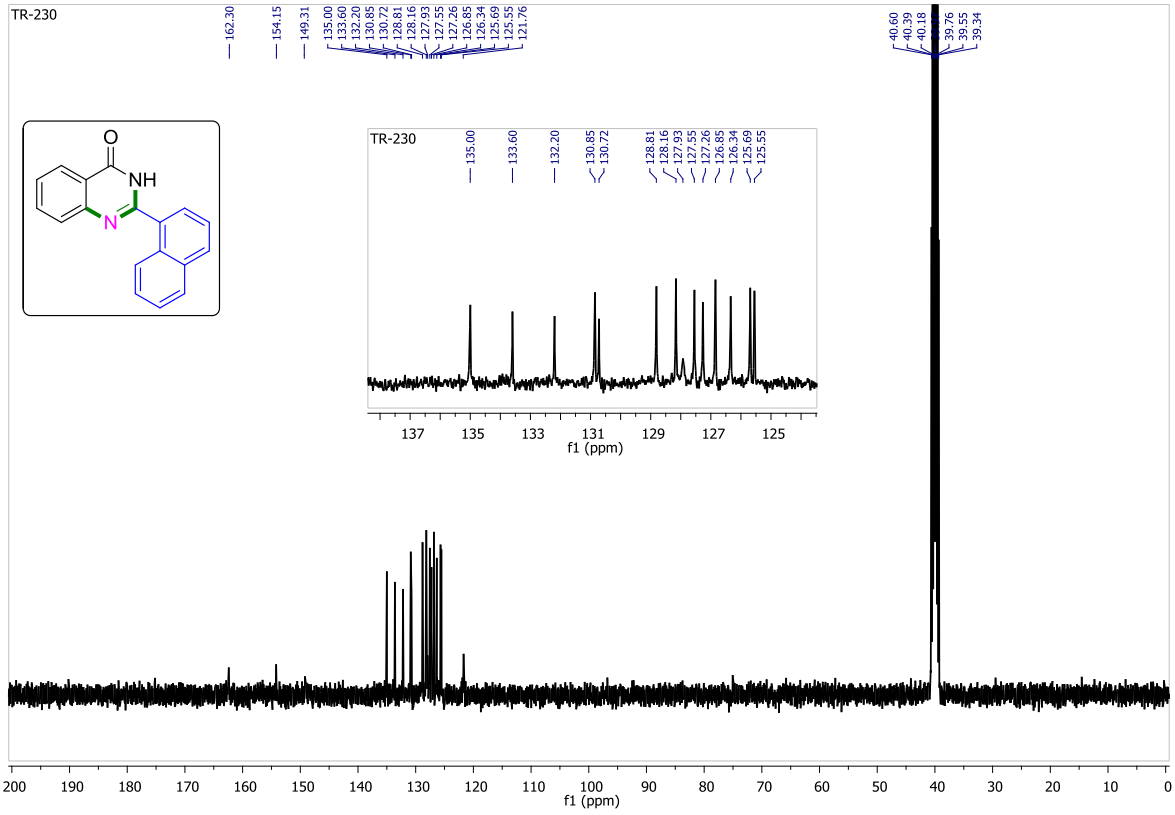
(S)-2-(2-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (5g')



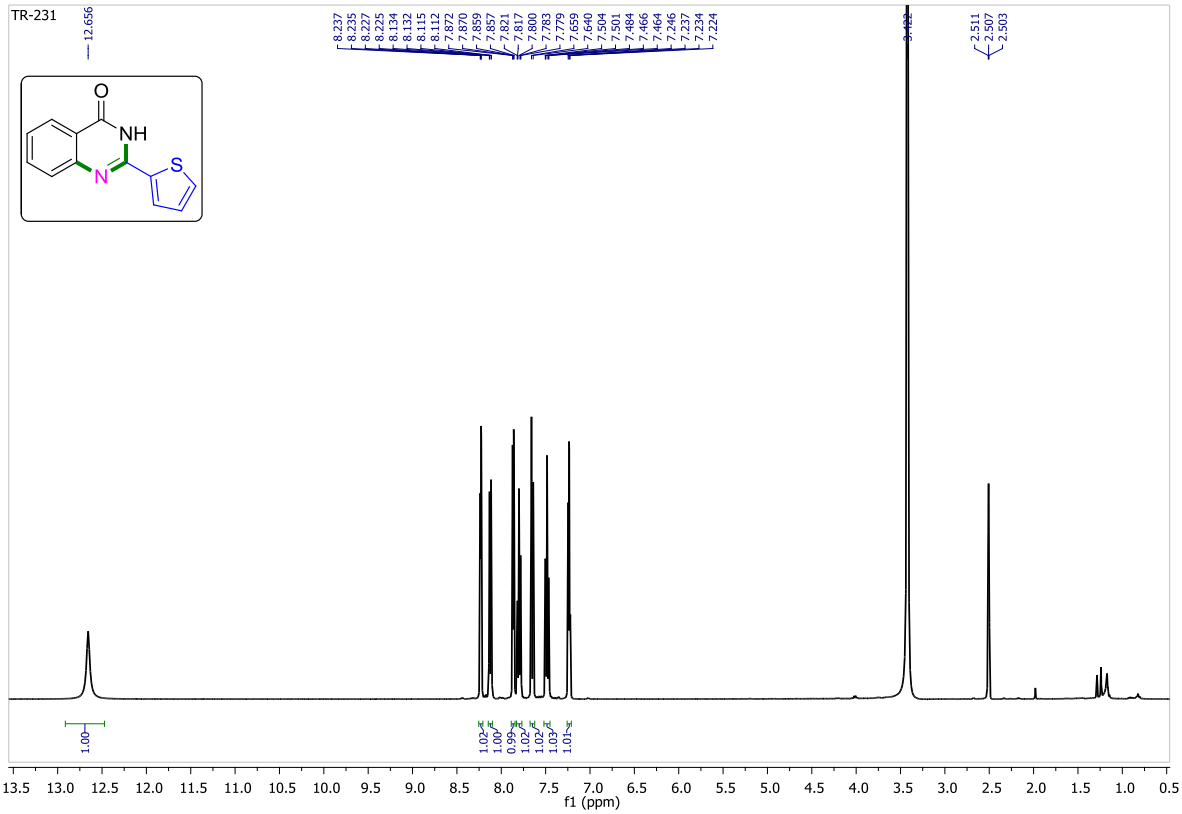


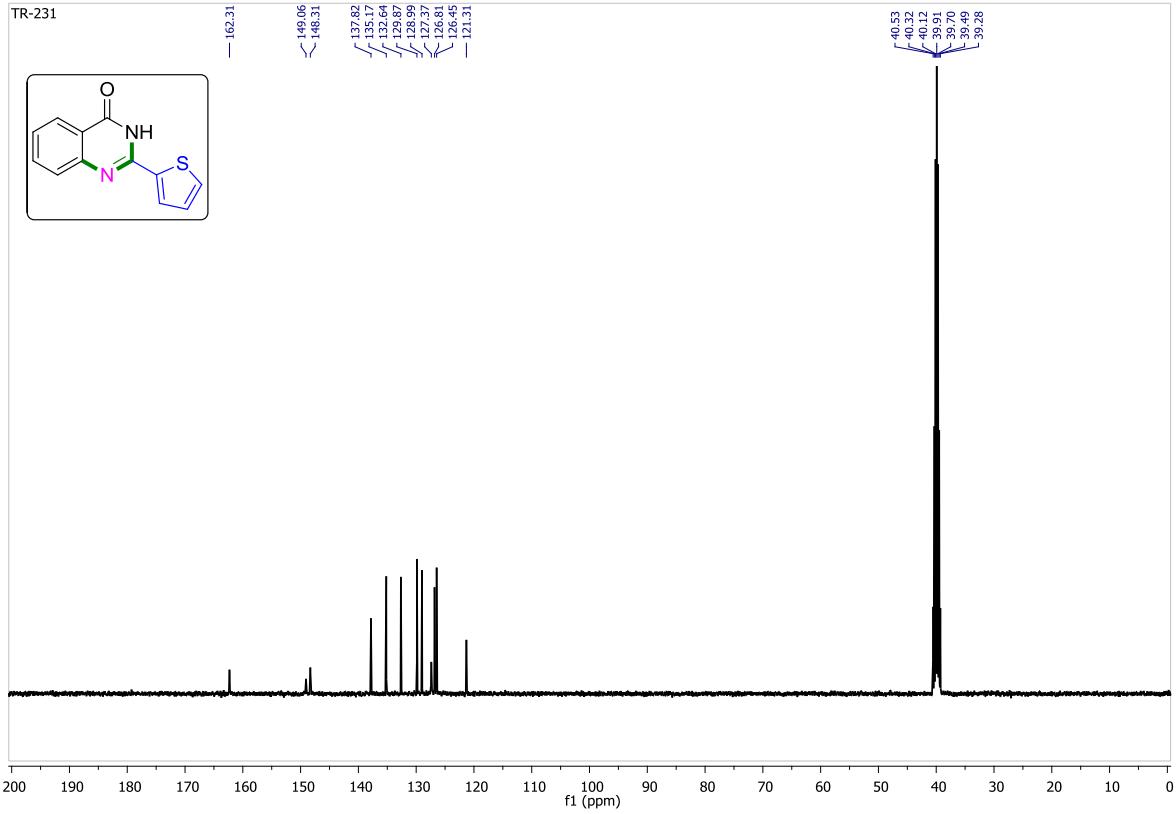
2-(naphthalen-1-yl)quinazolin-4(3H)-one (5h)



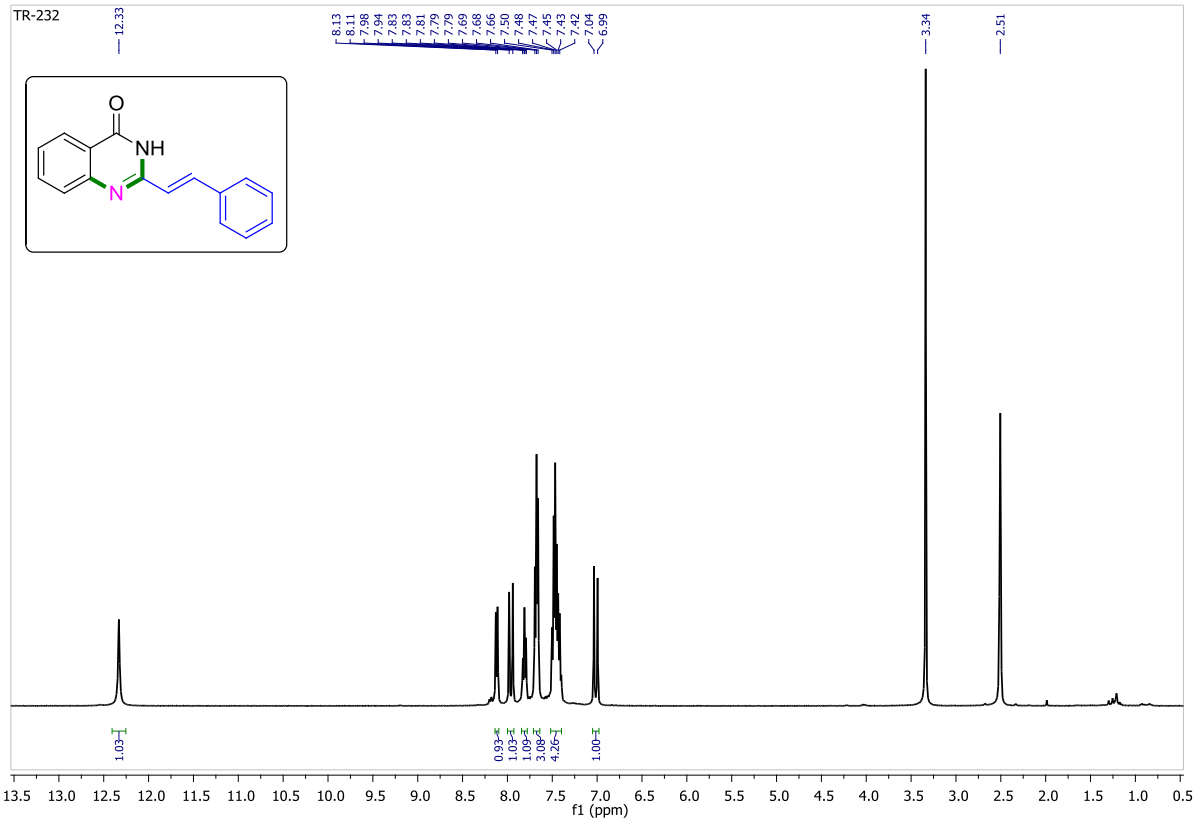


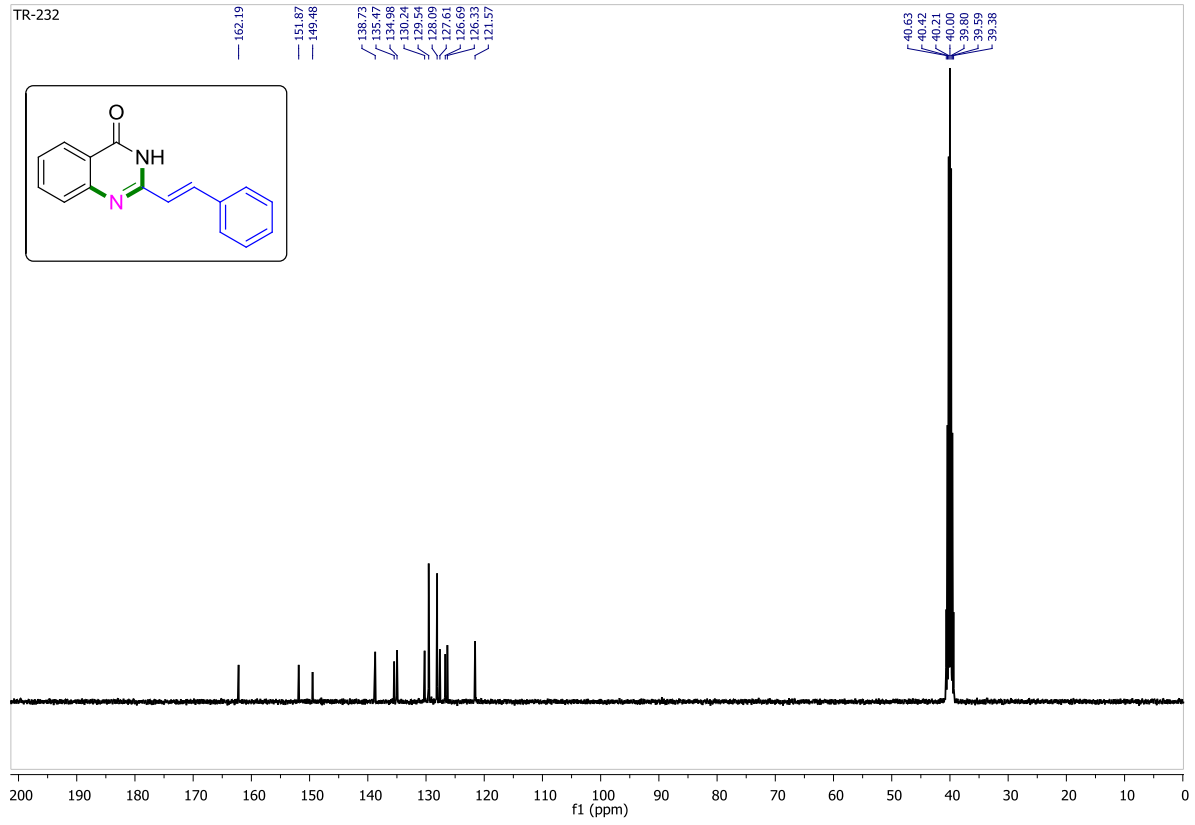
2-(thiophen-2-yl)quinazolin-4(3H)-one (5i)



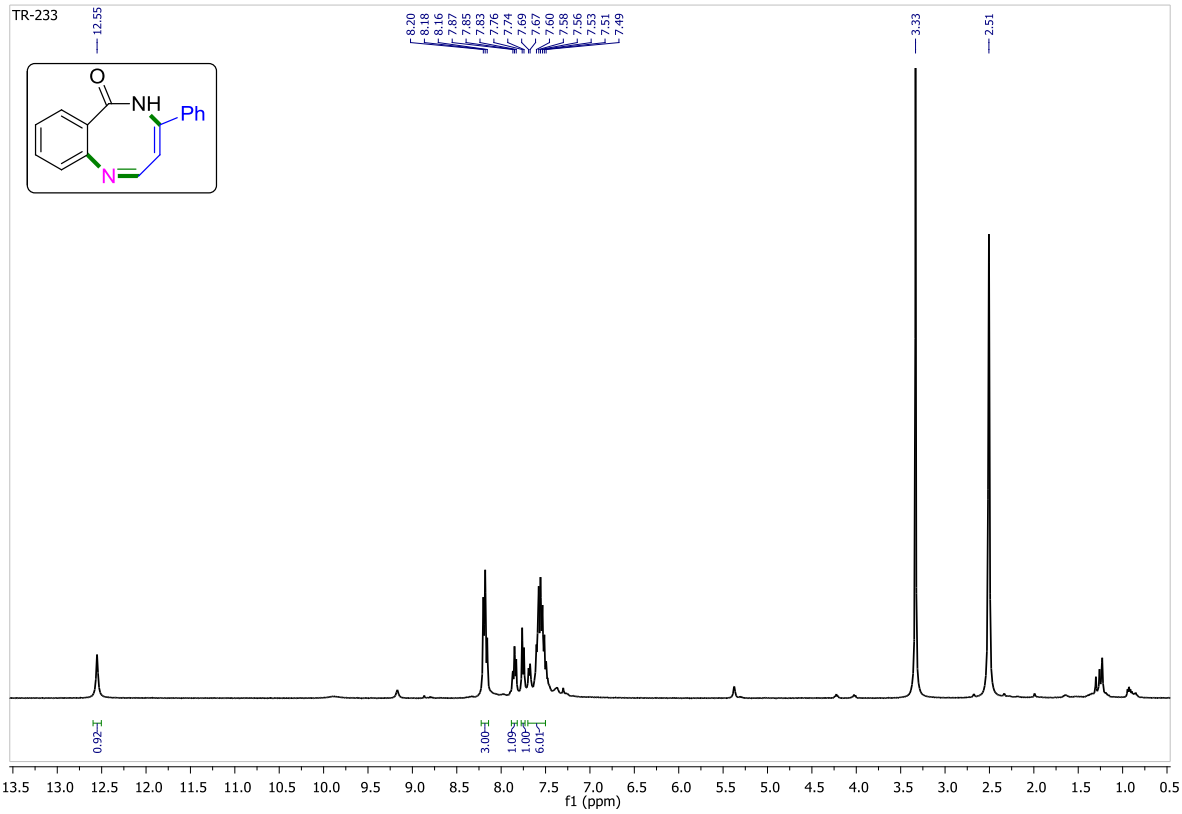


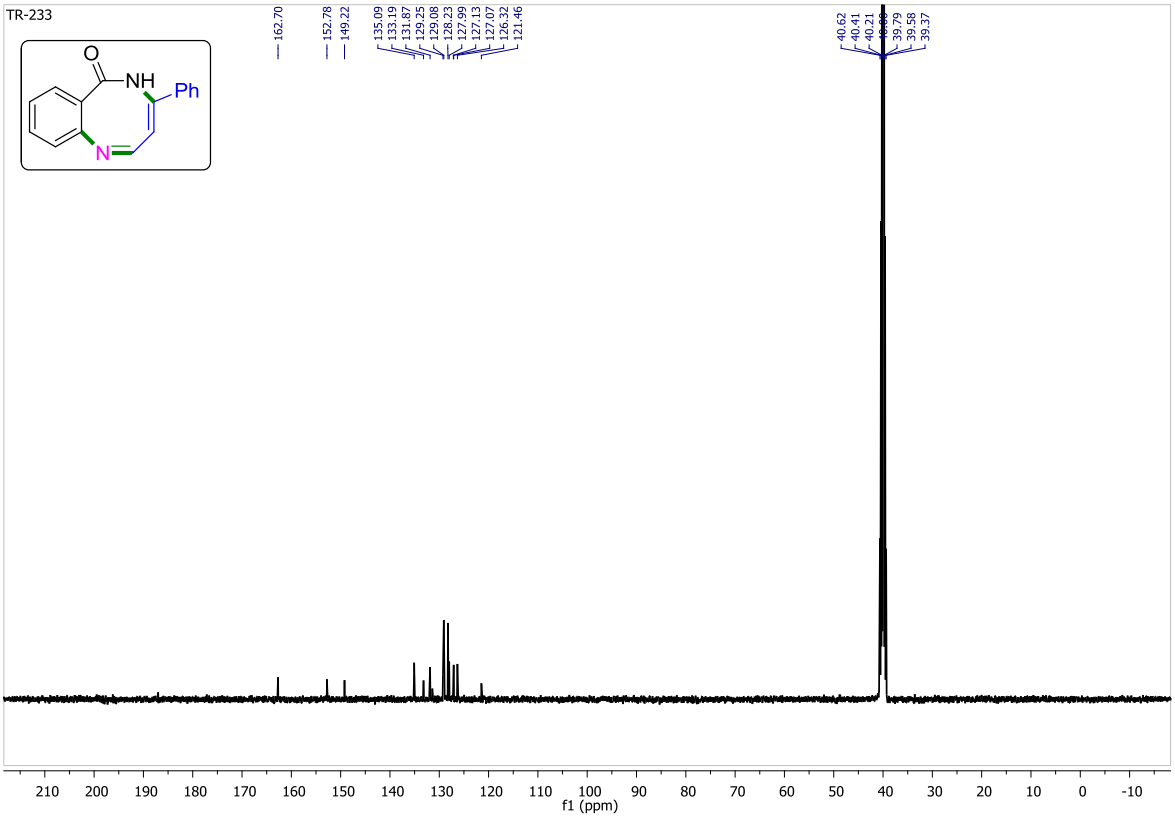
(E)-2-styrylquinazolin-4(3H)-one (5j)



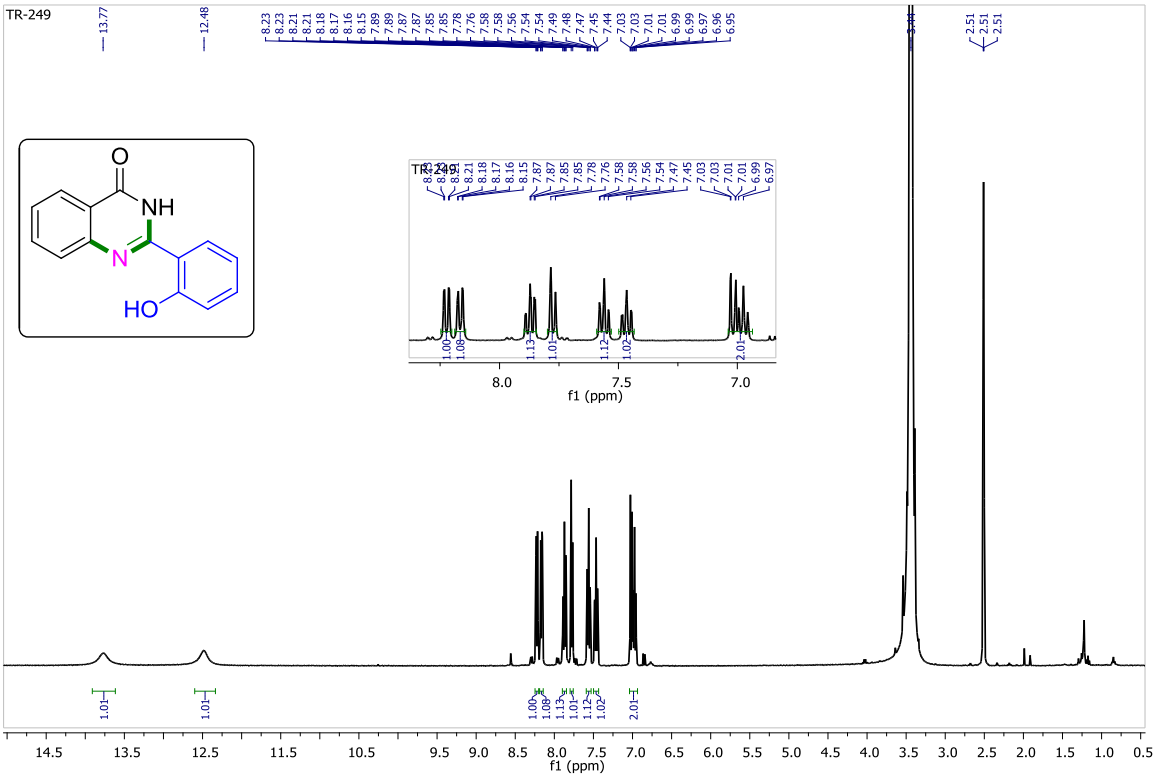


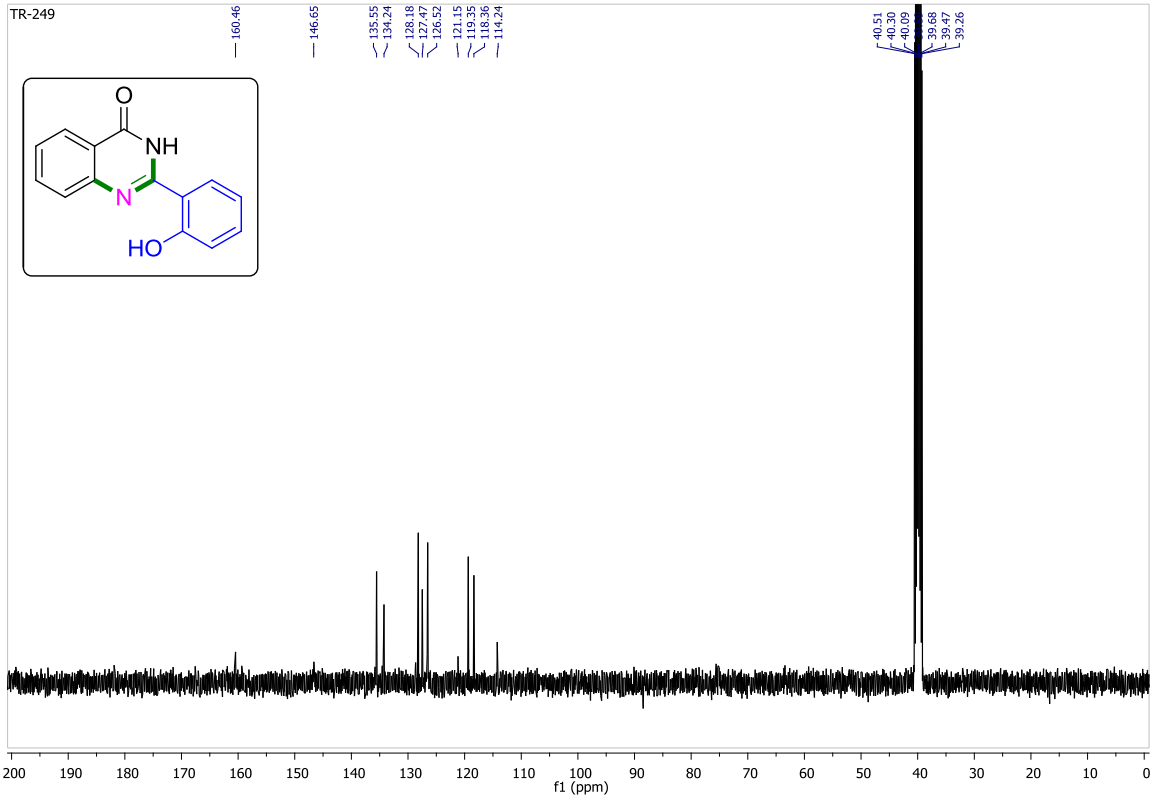
(1Z,3Z)-4-phenylbenzo[b][1,5]diazocin-6(5H)-one (5k)



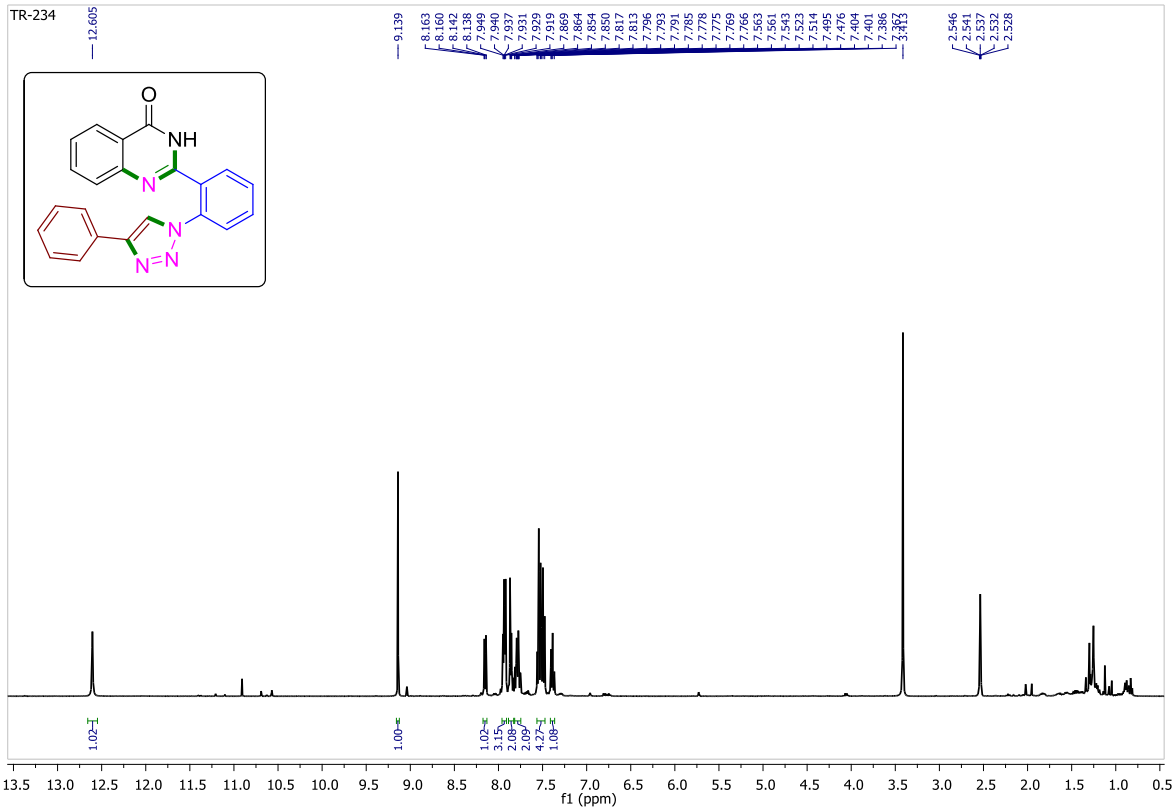


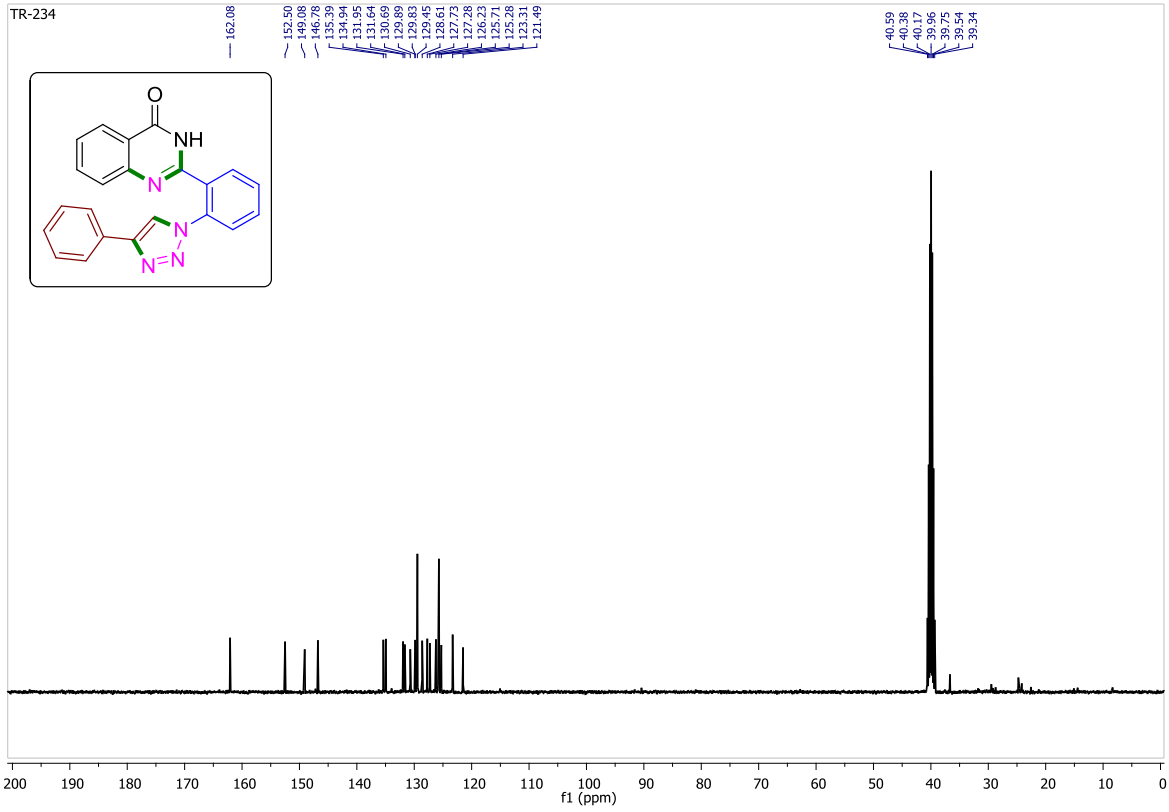
2-(2-hydroxyphenyl)quinazolin-4(3H)-one (5l)



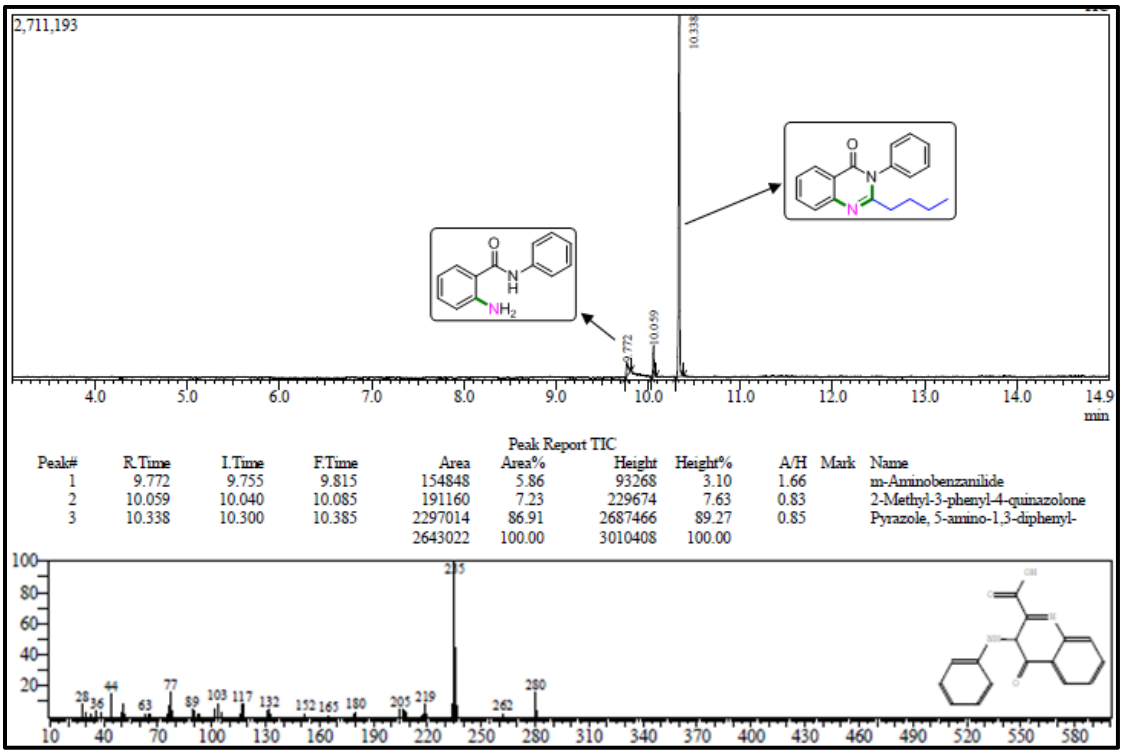


2-(2-(4-phenyl-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (5m)

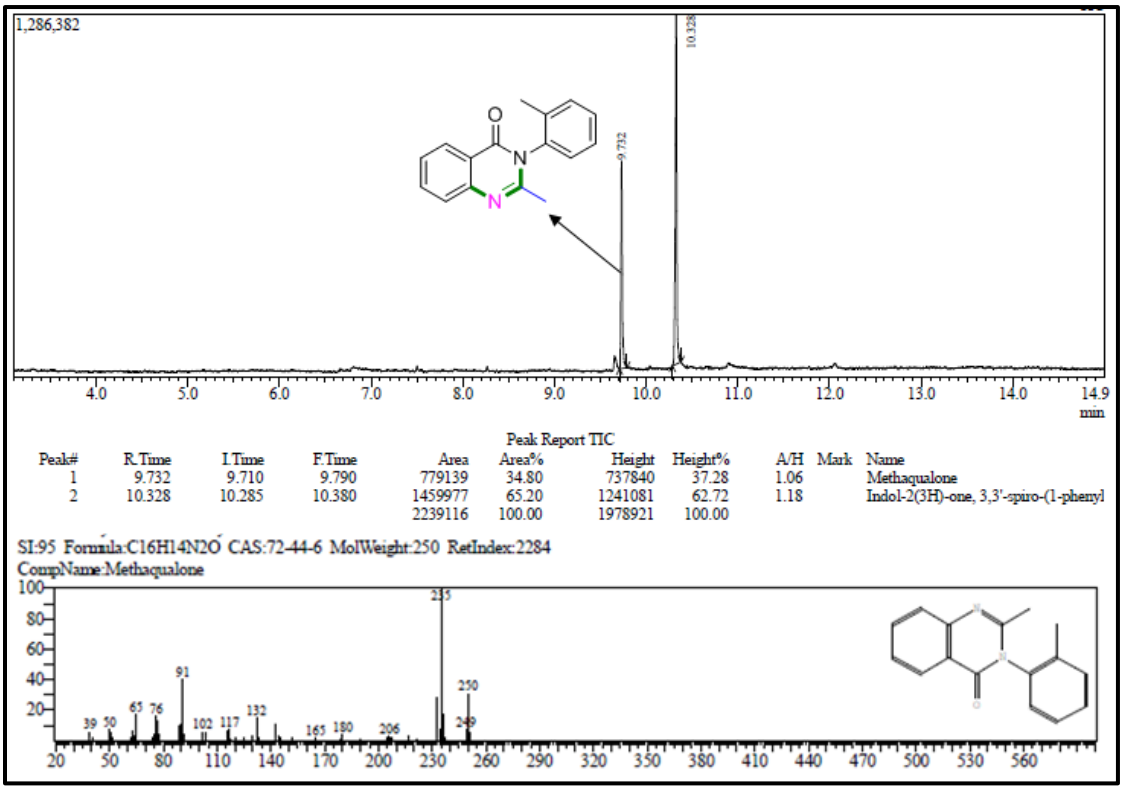




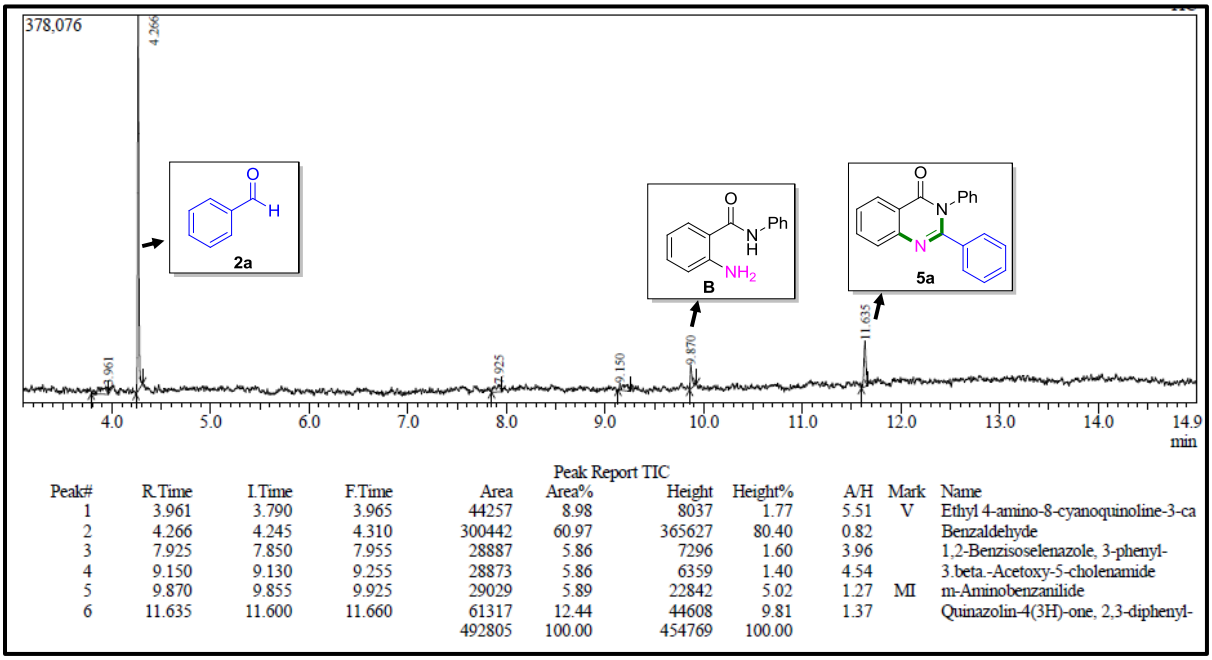
GCMS spectra of 2-butyl-3-phenylquinazolin-4(3H)-one (4l)



GCMS spectra of 2-methyl-3-(o-tolyl)quinazolin-4(3H)-one (4v)



GCMS spectra of intermediate **B**



Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	3.961	3.790	3.965	44257	8.98	8037	1.77	5.51	V	Ethyl 4-amino-8-cyanoquinoline-3-ca
2	4.266	4.245	4.310	300442	60.97	365627	80.40	0.82		Benzaldehyde
3	7.925	7.850	7.955	28887	5.86	7296	1.60	3.96		1,2-Benzisoselenazole, 3-phenyl-
4	9.150	9.130	9.255	28873	5.86	6359	1.40	4.54		3.beta.-Acetoxy-5-cholenamide
5	9.870	9.855	9.925	29029	5.89	22842	5.02	1.27	MI	m-Aminobenzanilide
6	11.635	11.600	11.660	61317	12.44	44608	9.81	1.37		Quinazolin-4(3H)-one, 2,3-diphenyl-
				492805	100.00	454769	100.00			

Appendix-II

Crystallographic data of compound 5b

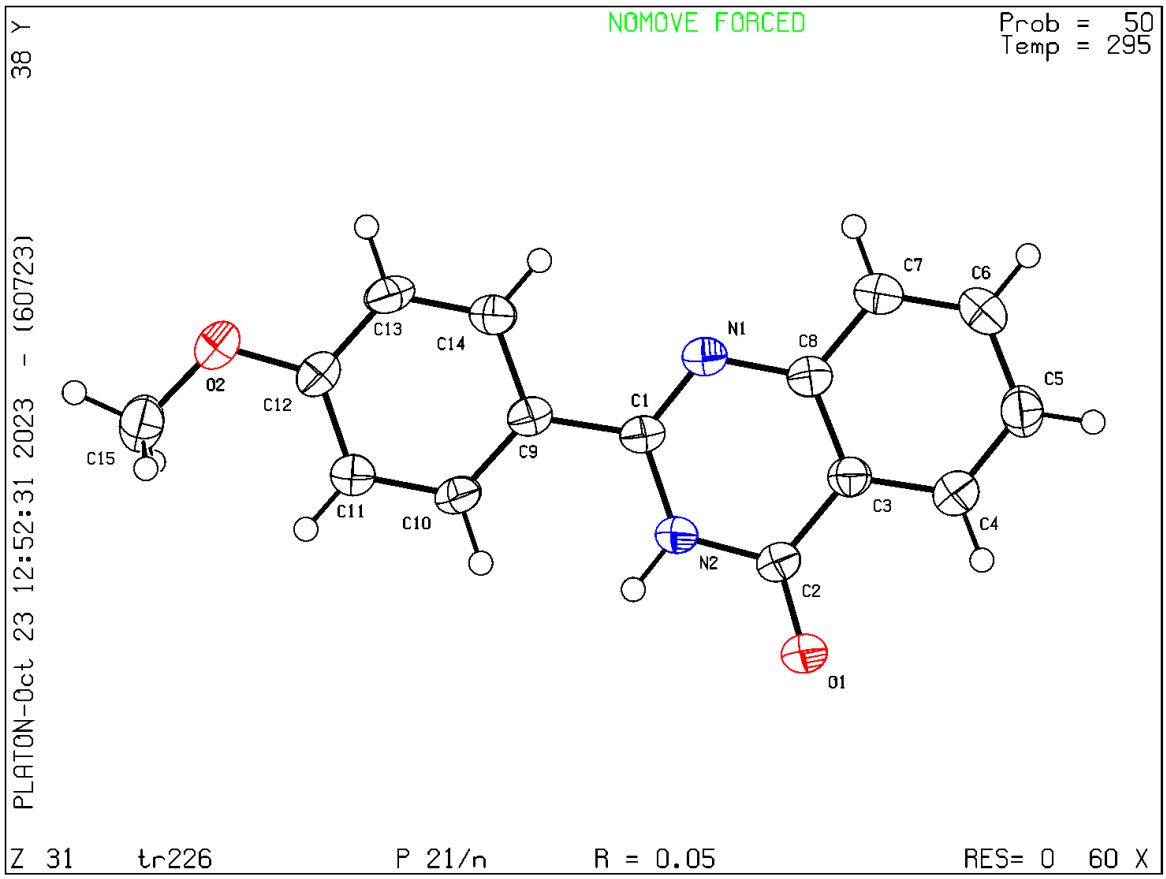


Figure S4. A view of **5b**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

The single crystal of compound **5b** (tr 226) have been obtained through X–ray analysis. The crystals were mounted on a Gemini A Ultra Oxford Diffraction automatic diffractometer. X–ray intensity data were collected with graphite monochromated MoKα radiation (λ=0.71073 Å) at a temperature of 295(2) K, with ω scan mode. Lorentz, polarization and empirical absorption correction using spherical harmonics implemented in SCALE3 ABSPACK scaling algorithm were applied. All the non–hydrogen atoms were refined anisotropically using full–matrix, least–squares technique. The hydrogen atoms were located in their calculated positions, and their temperature factors were constrained with the Uiso = 1.2Uiso for all H atoms joined to the aromatic C atoms, or Uiso = 1.5Uiso for the H atoms of the CH_2 or CH_3 groups. The structure of the compounds were solved by direct methods and refined by full–matrix least squares method on F2 using SHELXS, Mercury and Olex2 programs. The geometrical calculations were carried out using PLATON program. The molecular graphic designs and packing diagram were performed using Mercury software.

Crystal sample preparation of 5b

Crystal of **5b** was prepared using dimethyl sulphoxide, after the formation of crystals the solution was decanted and washed with pentane and single crystals were separated.

Crystal structure determination of 5b

Crystal Data for $C_{15}H_{12}N_2O_2$ (M =252.27 g/mol): orthorhombic, space group Pca21 (no. 29), a = 10.4760 (8) Å, b = 5.0246 (2) Å, c = 22.8902 (16) Å, V = 1193.86 (16) Å3, Z = 4, T = 295 K, Dcalc = 1.404 g/cm^3, 2859 unique which were used in all calculations. The final R1 was 0.0538 (I > 2σ(I)) and wR2 was 0.1467 (all data). CCDC 2306780 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk.

Datablock: 5b

Bond precision:	C-C = 0.0023 A	Wavelength=0.71073	
Cell:	a=10.4760(8)	b=5.0246(5)	c=22.8902(16)
	alpha=90	beta=97.761(7)	gamma=90
Temperature:	295 K		
Volume	1193.85(17)		
Space group	P 21/n		
Hall group	-P 2yn		
Moiety formula	C15 H12 N2 O2		
Sum formula	C15 H12 N2 O2		
Mr	252.27		
Dx,g cm-3	1.403		
Z	4		
Mu (mm-1)	0.095		
F000	528.0		
F000’	528.23		
h,k,lmax	14,6,31		

Nref 3285

Tmin,Tmax 0.981,0.996

Tmin' 0.966

Correction method= T Limits: Tmin=0.496 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.870 Theta(max)= 29.416

R(reflections)= 0.0538(1944) wR2(reflections)= 0.1467(2859)

S = 1.046 Npar= 177

IMPORTANT BOND LENGTHS:

Atom	Atom	Length/Å
C1	N1	1.294
C1	N2	1.381
N2	C2	1.372
C2	O1	1.235
N1	C8	1.387
C12	O2	1.363
O2	C15	1.416

IMPORTANT BOND ANGLES:

Atom	Atom	Atom	Angle (º)
C2	N1	C1	123.64
N1	C1	N2	122.48
C8	N1	C1	117.96
N2	C2	O1	120.64
N1	C1	C9	119.66
N2	C1	C9	117.86
C12	O2	C15	117.94