Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Pd/Fe_3O_4 supported on nitrogen doped reduced graphene oxide for room temperature isocyanide insertion reactions

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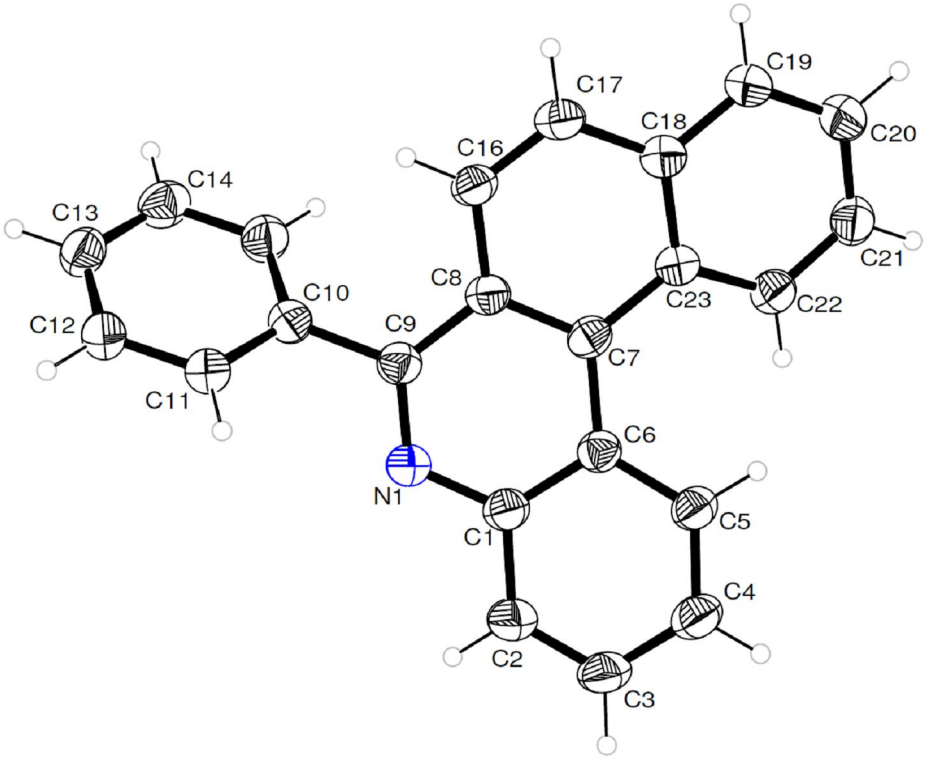
S1. Chemicals and characterization. All the reactions were carried out at room temperature, that is, 28-35^{0}C. Unless otherwise specified, all the reagents were purchased from Sigma-Aldrich Chemical Co., and were used directly without further any purification. NMR spectra were obtained using the Brucker 500 and 300 MHz spectrometers. Chemical shifts (δ) are given in parts per million relative to TMS, coupling constants (*J*) in hertz. Elemental analysis was performed using a Perkin Elmer Autosystem XL Analyzer. Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm silica gel plates visualized with UV light. For each and every experiment for the synthesis of catalyst deionized water (18.2 mS conductivity) was used. Wide angle X-ray diffractograms of the synthetic sample were recorded using Rigaku D/max 2500/PC X-ray diffractometer with Cu Kα (1.54056) radiation. The surface morphology of thoroughly dried sample was studied by a JEOL JEM 2100F transmission electron microscope (TEM). The JEOL JEM 2100F transmission electron microscope with tungsten, Electron source operated at an accelerating voltage of up to 120 kV. The TEM sample was prepared by dispersing dry powder of catalyst in ethanol solvent. For scanning electron microscopy (SEM), gold sputter coating were carried out on desired samples at pressure ranging in between 1 and 0.1 Pa. Sample was loaded in the machine, which was operated at 10^{-2} to 10^{-3} Pa with EHT 15.00 kv with 300 V collector bias using Philip XL30 SEMs were recorded. All XPS measurements were taken in a SIGMA PROBE (ThermoVG) using a monochromatic Al-Kα X-ray source at 100 W. The thermal stability of catalyst was investigated by thermo-gravimetric analyzer (SDTQ600) under a nitrogen atmosphere with 10 ^{o}C min^{-1} heating rate from 30 to 800 ^{o}C. Gyrogen 1236 MG for centrifugation, power sonic 405 for sonication were used.



Crystal data for product (6f).

Crystallographic parameters of **6-phenylbenzo[k]phenanthridine (6f).**

Compound Name	**6-phenylbenzo[k]phenanthridine**
CCDC No.	**1014399**
Formulae	$C_{23}H_{15}N$
Formula. wt.	305.36
Crystal system	orthorhombic
Space group	Pbca
a /Å	19.533(4)
b /Å	7.5052(15)
c /Å	21.247(4)
α/°	90.00
β/°	90.00
γ/°	90.00
V/ Å^3	3114.9(11)

Z	8
Density/Mgm^{-3}	1.302
Abs. Coeff. /mm^{-1}	0.075
F(000)	1280
Total no. of reflections	46038
Reflections, $I > 2\sigma(I)$	1741
Max. 2θ/°	50.00
Ranges (h, k, l)	$-25 \leq h \leq 25$ $-9 \leq k \leq 9$ $-27 \leq l \leq 27$
Complete to 2θ (%)	99.9
Data/ Restraints/Parameters	3606/ 0 / 219
Goof (F^2)	0.934
R indices [$I > 2\sigma(I)$]	0.0578
R indices (all data)	0.1231

S2. Synthesis of materials

Synthesis of graphene oxide (GO): GO was obtained by the oxidation of graphite powder using modified Hummer methods.[1-3] In general, 10 g of graphite powder was added into 500 ml concentrate H_2SO_4, stirred on ice bath for 1 h and then 40 g of $KMnO_4$ was slowly added. The reaction mixture was further stirred for 2 h then ice bath was removed and stirring was continued for 24 h. The reaction mixture was put back on ice bath and 500 ml deionized water was slowly added to dilute the reaction mixture, then hydrogen peroxide solution (30%) was added drop wise till to solution color changed to orange/gold. The orange color solution was centrifuged at 800 rpm (10 minute) to isolate unexploited graphite oxide, then the supernatant solution was transferred to other centrifuging tube and centrifuged at 4000 rpm for 30 minute to get golden color solid. The solid material was washed thoroughly by repeated centrifugation with deionized

water (till the pH of solution pH 6.6). Finally the solid material was dried under reduced pressure.

Synthesis of N-doped reduced graphene oxide (N-rGO): N-rGO was synthesized by the reported methods.[1, 3, 4] 2 g of synthesized GO powder was dispersed in 1000 ml deionized water in a beaker and sonicated for 3 h to make stable colloidal suspension. 15 ml hydrazine monohydrate (65% in water) was added into the beaker and heated at 90 ^{o}C with continuous stirring for 12 h to yield a black precipitate of N-rGO powder. After cooling to room temperature solution was centrifuged at 4000 rpm for 10 min. to collect the precipitate. The obtained black material was washed with deionized water and centrifuged, dried under vacuum oven at 120 ^{o}C for 24 h.

Synthesis of Pd/N-rGO:2 g GO powder was dispersed in 1000 ml deionized water in a beaker and sonicated for 3 h to make stable colloidal suspension. An aqueous solution of $PdNO_3.2H_2O$ (0.5 mmol in 25 mL water) was added drop wise into the GO colloidal solution. The reaction mixture was allowed to stir for 2 h, the solution was reduced by the adding 15 ml hydrazine monohydrate (65% in water), and then the beaker was immersed in oil bath at 90 ^{o}C and stirred on 12 h. After cooling the reaction mixture to room temperature the solution was centrifuged at 4000 rpm for 10 minute to collect black precipitate of Pd/N-rGO powder. The black material was washed with deionized water, centrifuged, and dried under vacuum oven at 120 ^{o}C for 24 h.

Synthesis of magnetite (Fe_3O_4).The magnetite was synthesized by reported oxidation methods. [5, 6] An aqueous solution of $FeCl_3$ and $FeCl_2$were mixed (2:1) ($FeCl_3$ = 0.810g /100 ml and $FeCl_2$ = 0.316 g/100 ml) and stirred for 1h. Ammonia solution was added drop wise to this solution till to solution pH =10. Then the temperature of solution was raised to 90 ^{o}C and stirred for 1h. The

resulting black solution was filtered, washed with water and acetone several times, and finally dried in vacuum at 120^{o}C for 24 h. The obtained Fe_3O_4 was characterized.

Synthesis of magnetite reduced graphene oxide (Fe_3O_4/N-rGO) composites: 2.0 g GO was first dispersed in 1000 ml water and sonicated for 3 h. Then the solution of $FeCl_3$ and $FeCl_2$($FeCl_3$ = 0.810g/25 ml and $FeCl_2$ = 0.316 g/25 ml) was added drop wise at RT.[7] Ammonia solution was added to this solution till to solution pH =10. The temperature of solution raised to 90^{o}C and 15 ml of hydrazine hydrate (65% in water) was added with constant stirring, resulting a black coloredsolution. After being rapidly stirred for 12 hour the solution was cooled to room temperature. The black solution was filtered, washed with waterand acetone several times, and finally dried in vacuum at 120 ^{o}C for 24 h to get Fe_3O_4/N-rGO composite powder.

Synthesis of Pd/Fe_3O_4/N-rGO catalyst: 2.0 g GO was first dispersed in 1000 ml water in a beaker and sonicated for 3 h.[7] Then the solution of $FeCl_3$ and $FeCl_2$($FeCl_3$ = 0.810g/25 ml and $FeCl_2$ = 0.316 g/25 ml) was added drop wise at RT. Then the aqueous solution of $Pd(NO_3)_2.xH_2O$ (0.5 mM, in 25 ml water) was added to colloidal solution at RT and reaction mixture was further stirred for 3 h for complete mixing. For making magnetite particles, ammonia solution was added to this solution till to solution pH =10. The temperature of solution raised to 90^{o}C and 15 ml of hydrazine hydrate (65% in water) was added with constant stirring, resulting in black color solution. After being rapidly stirred for 12 hour the solution was cooled to room temperature. The black solution was filtered, washed with waterand acetone several times, and finally dried in vacuum at 120 ^{o}C for 24 h. The obtained M/Fe_3O_4/N-rGO composite powder was analyzed characterized by different analytical tools.

Catalyst leaching studies: During this test, the catalyst was removed from the reaction mixture by external permanent magnet and the filtrate was monitored for catalytic activity. Removal of

the catalyst completely inhibits the reaction, indicating that no catalytically active Pd remained in the filtrate. In addition, supernatant was analysed by ICP-MS technique, and no detectable amount of Pd was found in the solution. It suggests a heterogeneous mechanism for the insertion reaction using Pd/Fe_3O_4/N-rGO as a catalyst.

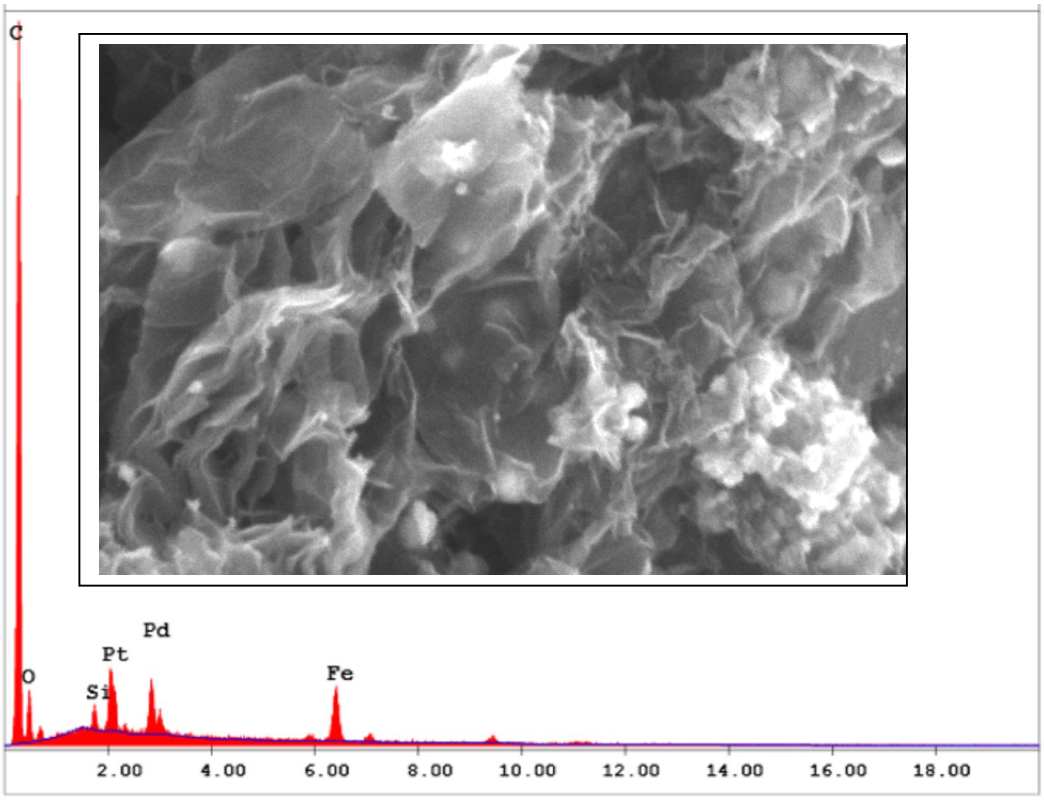


Figure S1- (a) SEM image of $Pd@Fe_3O_4$/N-rGO; (b) EDX image of $Pd@Fe_3O_4$/N-rGO.

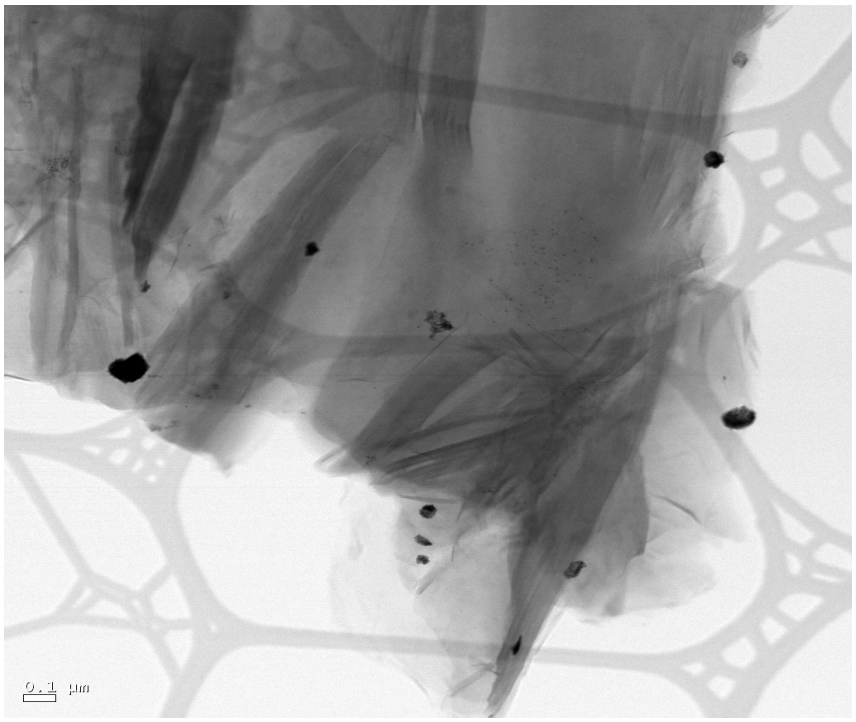


Figure S2. Low resolution TEM image

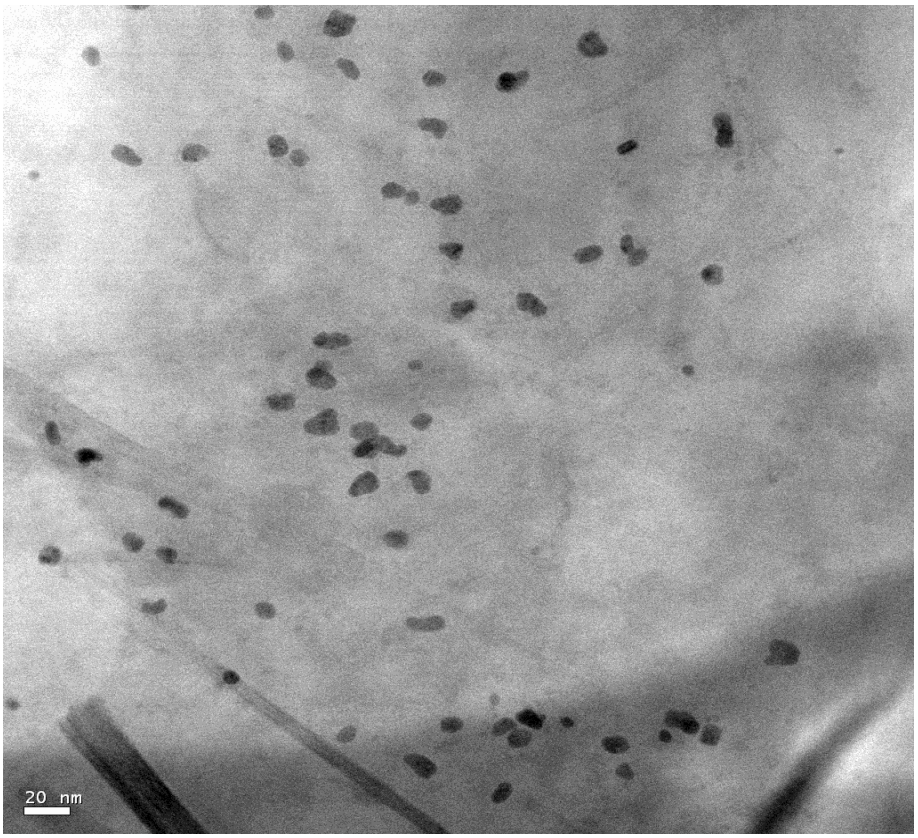


Figure S3. High resolution TEM image dark field.

Figure S4. High resolution TEM imagebright field.

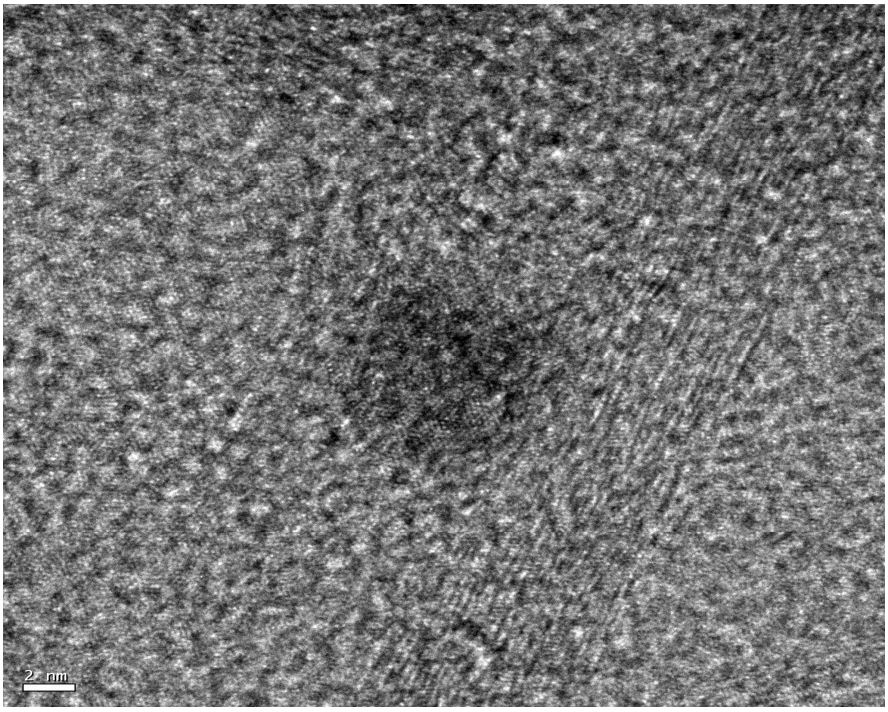


Figure S5. High resolution **c**onventional TEM image of Pd/Fe_3O_4/N-rGO.

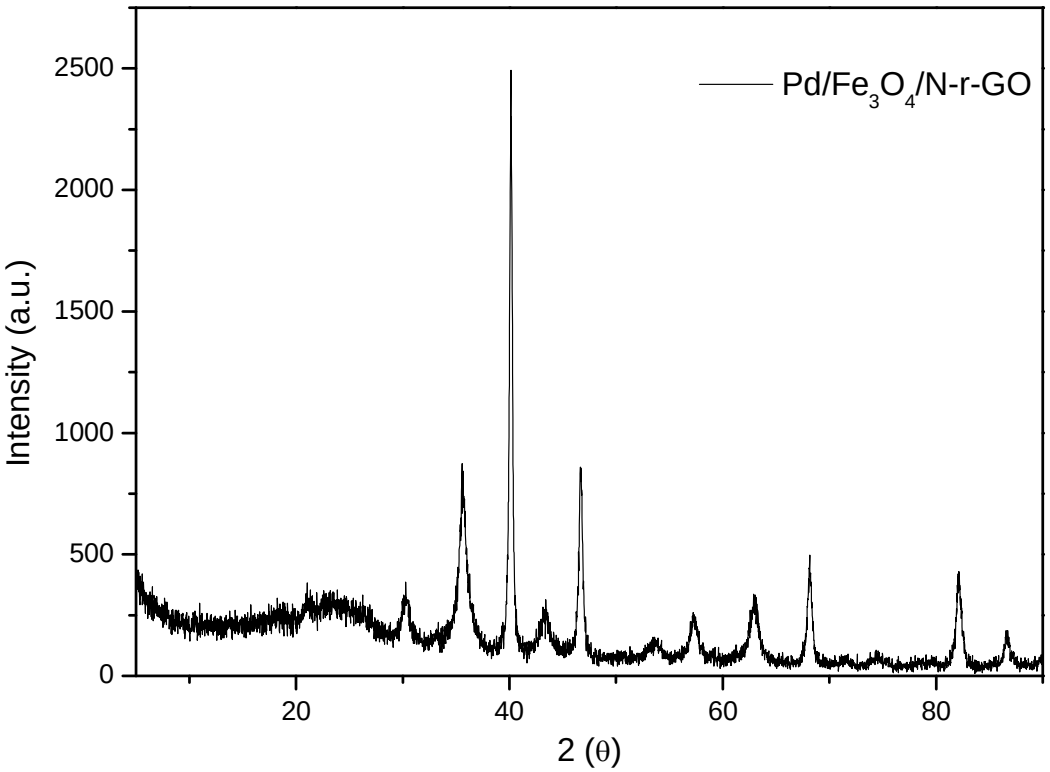


Figure S6-XRD peak patterns of Pd/Fe_3O_4/N-rGO.

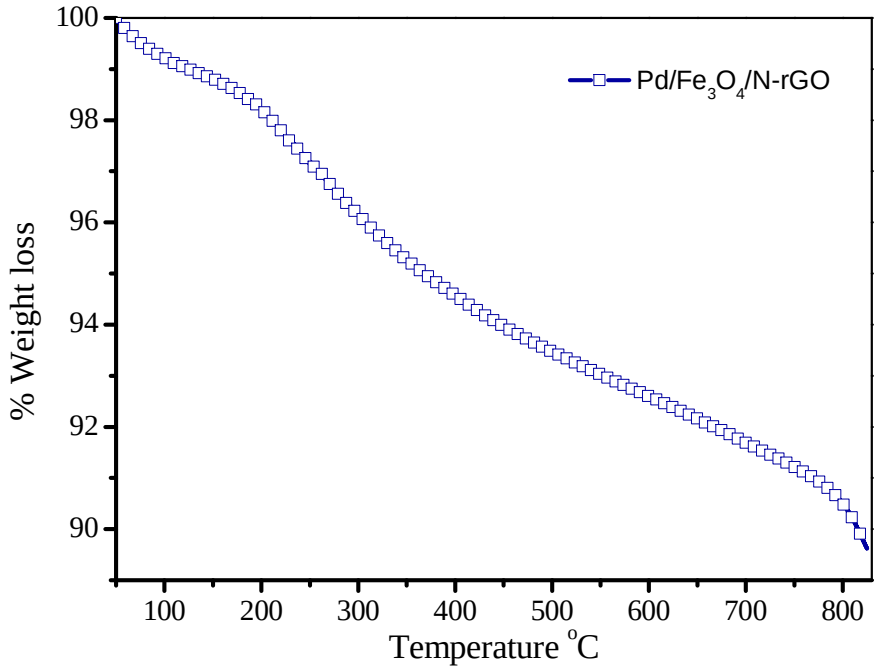


Fig.S7 TGA of the Pd/Fe_3O_4/N-rGO catalyst.

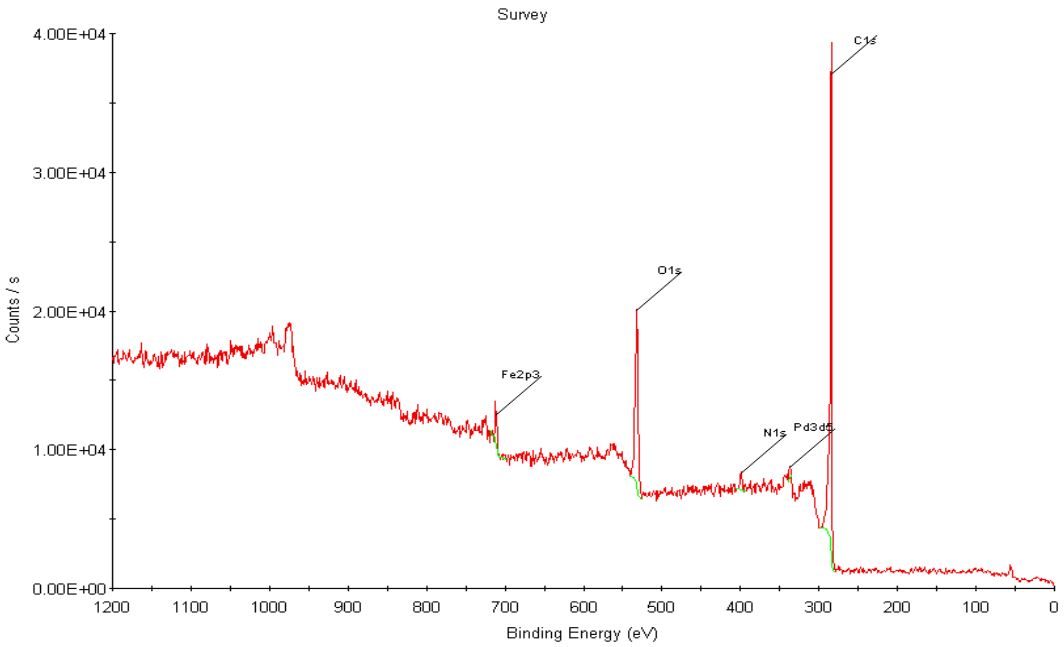


Figure S8-Full scan XPS spectra of Pd/Fe_3O_4/N-rGO.

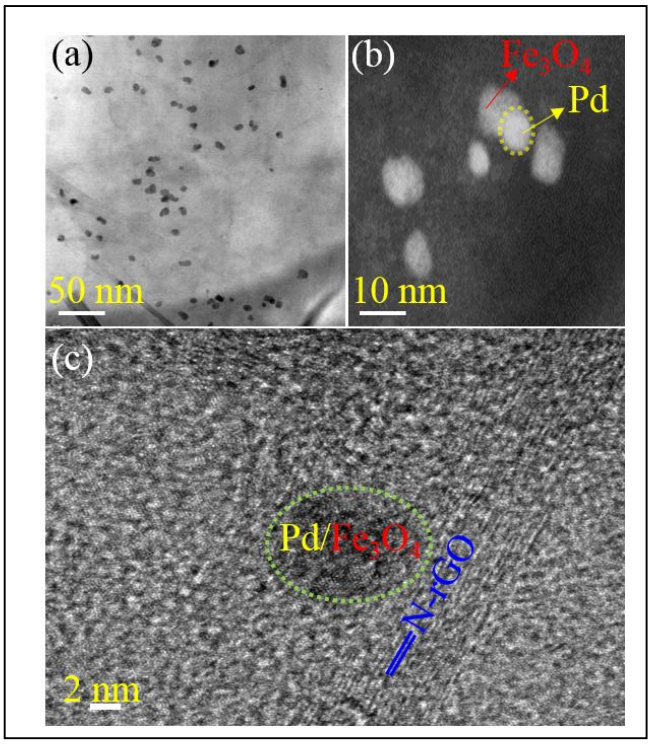


Figure S9. TEM image of Pd/Fe_3O_4/N-rGO; (a) low resolution; (b) Atomic sensitive HAADF image; (c) high resolution image.

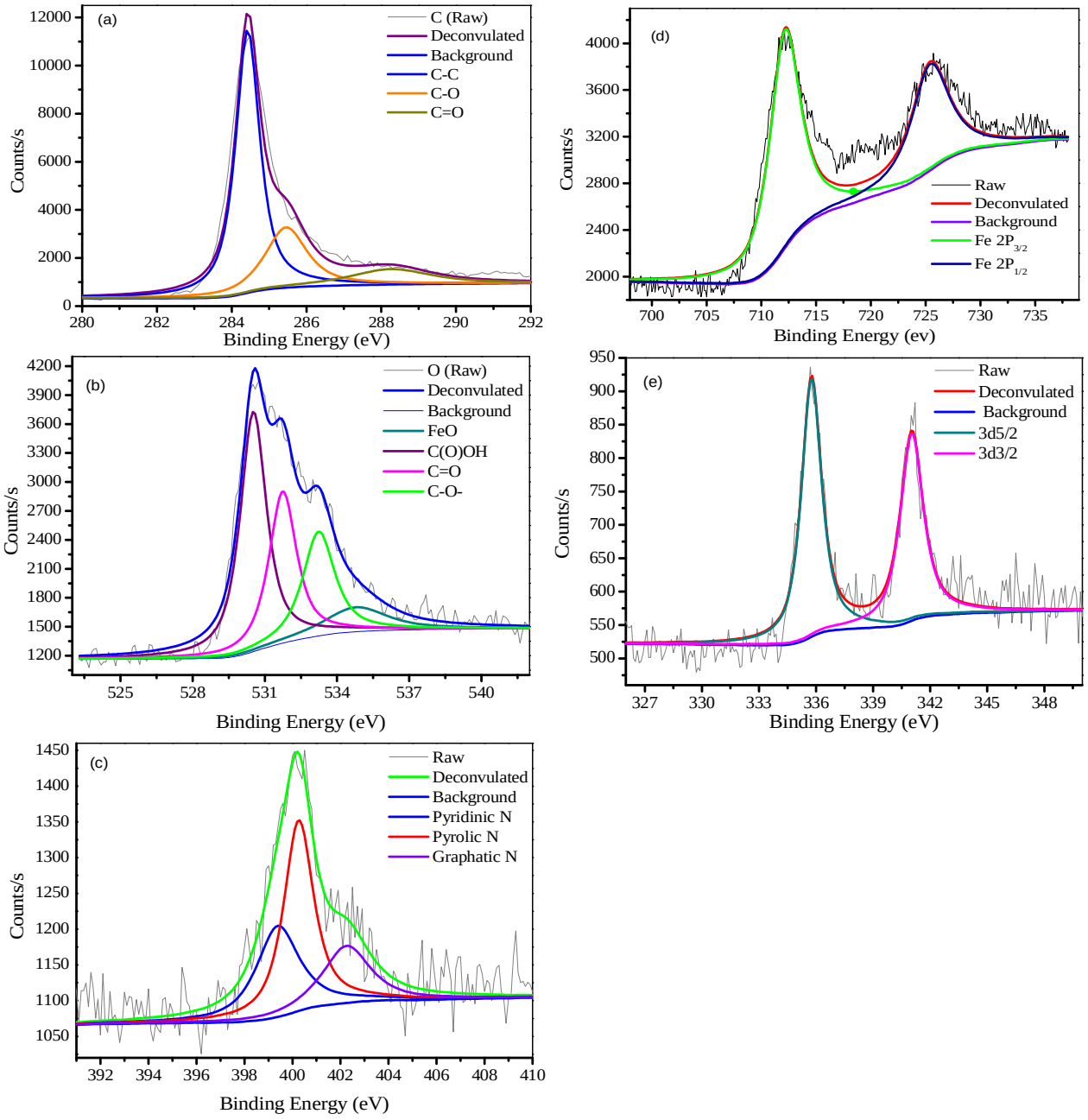


Figure S10 | Catalyst Pd/Fe_3O_4/N-rGO XPS analysis results. a. C1s spectra of catalyst. **b.** O1s XPS spectra.**c.** N1s XPS spectra.**d.** Fe 2p XPS spectra.**e.** Pd 3d XPS spectra.

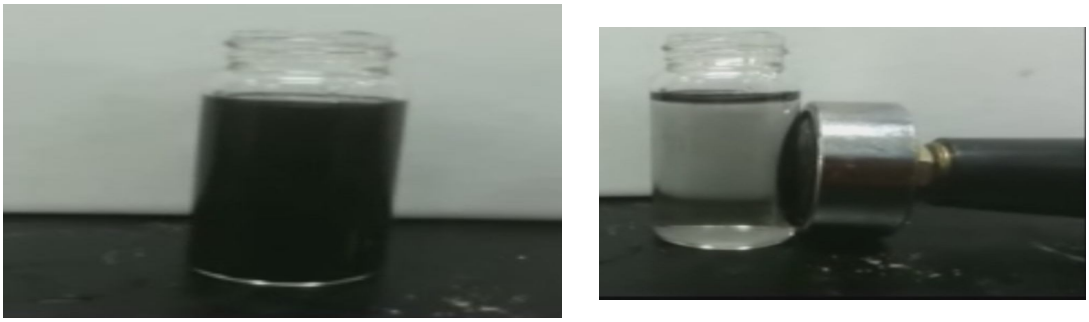


Figure S11. Magnetically separable catalyst (a) fully dispersed in reaction crude mixture; (b) catalyst separation with magnet.

Synthesis of 2-isocyanobenzamide (1a), ethyl 2-isocyanobenzoate (1b).

To a stirred solution of sodium formate (7.0 g, 103 mmol, 1.2 eq) in 6 ml of ethyl ether was added acetyl chloride(6.3 ml, 88.7 mmol, 1.0eq) quickly. The reaction mixture was stirred at room temperature for 5 hr. The upper ethyl ether layer was directly used for formylation reaction. Anthranilamide (33.3 mmol), ethyl 2-aminobenzoate (33.3) was dissolved in 100 ml of THF, then the solution of acetic formic anhydride was added at 0^0C. The reaction mixture warmed at room temperature and stirred overnight. The solvent was evaporated and residue was worked up with ethyl acetate and water. Ethylacetate layer dried on sodium sulfate and evaporated to give a crude product, which was pure enough for the next step (Confirmed by TLC and GC-MS). This N-formylated product and DIPEA (4.0 ml, 22.8 mmol, 2.7 eq.) were dissolved in DCM and cooled to 0^0C. $POCl_3$ (0.87 ml, 9.3 mmol, 1.1 eq) was slowly added and stirred at room temperature for 60 min. A solution of sodium carbonate (1.7 g, 16.0 mmol, 1.9 eq) in 8 ml of water was added at room temperature. Water and DCM layer was separated and washed with water and the solvent removed at room temperature under vacuum to obtain 2-isocyanobenzamide at 86% yield (by NMR) (**1a**) (Isolated yield after chromatography on silica gel was 53%) and ethyl 2-isocyanobenzoate (**1b**) in 84% yield.

Synthesis of of 2-Isocyanobiaryl compounds (**1c-1f**). Compounds were prepared according to the reported procedure(See NMR below)[8]

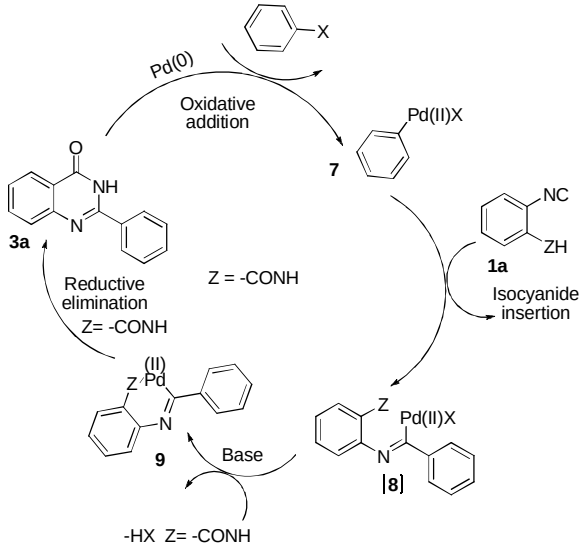
General procedure for the synthesis 2-substituted quinazolinones (3a-l) and 8: An oven-dried round bottom flask charged with heterogeneous catalyst Pd-Fe_3O_4/N-rGO (1.0 mol%, 40mg for 1 mmol reaction by weight), Cs_2CO_3 (2 mmol) using inert atmosphere. Then aryl halide (1.0 mmol) in 2 mL dioxane was added. After the mixture was stirred at room temperature for 15 min, solution of 2-isocyanobenzamide (**1a**) (1.2 mmol) in 5mL dioxane was added dropwise for 1h min. The reaction mixture was stirred until aryl halides was completely consumed (as determined by TLC). Catalyst was removed by the use of external magnate, washed with ether and dried for further use. The reaction solution was diluted with ethyl acetate (15 mL) and water (15 mL x 3). The layers were separated and the organic layer was dried over Na_2SO_4, and then concentrated under reduced pressure. The material obtained was of enough purity for spectroscopic analysis. Obtained compound was recrystallized from MeOH.

General procedure for the synthesis 3-substituted quinazolinones (5a-n) and 10:

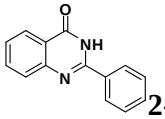
An oven-dried round-bottom flask charged with heterogeneous catalyst Pd-Fe_3O_4/N-rGO (1.0 mol%, 40mg for 1 mmol reaction by weight), Cs_2CO_3 (2 mmol). Then amines (1.0 mmol) in 2 mL dioxane was added. Solution of 2-isocyanobenzoate (**1b**) (1.2 mmol) in 5mL dioxane was added after 5 min. The reaction mixture was stirred in open atmosphere at room temperature until amines had been completely consumed (as determined by TLC). Catalyst was removed by the use of external magnate, washed with ether and dried for further use. The reaction solution was diluted with ethyl acetate (15 mL) and water (15 mL x 3). The layers were separated and the organic layer was dried over Na_2SO_4, and then concentrated under reduced pressure. The material obtained was of enough purity for spectroscopic analysis. Obtained compound was recrystallized from MeOH.

Synthesis of fused nitrogen heterocycles (6a-6j):

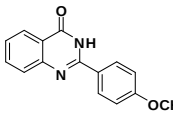
Round bottom flask charged with heterogeneous catalyst Pd-Fe_3O_4/N-rGO (1.0 mol%, 40mg for 1 mmol reaction by weight), Cs_2CO_3 (2 mmol) and the tube was refilled with N_2 3 times. Then aryl halides (**2a-q)** (1.0 mmol) in 2 mL dioxane was added. After the mixture was stirred at room temperature for 15 min, solution of (**1c-f**) (1.2 mmol) in 5mL dioxane was added dropwise for 1h. The reaction mixture was stirred until aryl halides had been completely consumed (as determined by TLC). Catalyst was removed by the use of external magnate, washed with ether and dried for further use. The reaction solution was diluted with ethyl acetate (15 mL) and water (15 mL x 3). The layers were separated and the organic layer was dried over Na_2SO_4, and then concentrated under reduced pressure. The crude material obtained was then purified by using flash chromatography with ethylacetate/ hexane as eluent on silica gel.

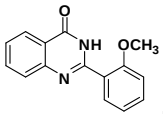


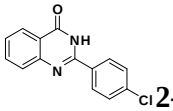
Scheme S1. Proposed mechanism for the synthesis of 2-substituted quinazolinones (3a-3m).

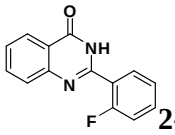


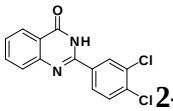
2-Phenylquinazolin-4(3H)-one 3a:[9] White solid, Yield 81% (180 mg), ESI MS (*m/z*) = 223 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.50-7.60 (m, 4H), 7.73-7.86 (m, 2H), 8.15-8.20 (m, 3H), 12.52 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.4, 126.3, 127.0, 127.8, 128.2, 129.0, 131.8, 133.1, 135.0, 149.1, 152.8, 162.8.


2-(4-Methoxyphenyl)quinazolin-4(3H)-one 3b:[10] White solid, Yield 73% (184 mg), ESI MS (*m/z*) = 253 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.85 (s, 3H), 7.07 (d, *J* = 8.8 Hz, 2H), 7.46 (t, *J* = 7.05 Hz, 1H), 7.69 (d, *J* = 7.95 Hz, 1H), 7.79 (t, *J* = 6.93 Hz, 1H), 8.12-8.21 (m, 3H), 12.38 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 55.5, 114.0, 120.6, 124.4, 125.9, 126.2, 126.8, 129.6, 134.6, 148.4, 152.1, 162.0, 162.3.

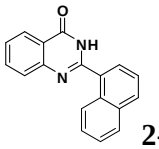

2-(2-Methoxyphenyl)quinazolin-4(3H)-one 3c: White solid, Yield 67% (169 mg), ESI MS (*m/z*) = 253 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.87 (s, 3H), 7.07 (t, *J* = 7.47 Hz, 1H), 7.18 (d, *J* = 8.28 Hz, 1H), 7.51-7.55 (m, 2H), 7.69-7.73 (m, 2H), 7.81 (t, *J* = 7.02 Hz, 1H), 8.14 (d, *J* = 7.6 Hz, 1H), 12.07 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 56.4, 112.3, 120.9, 121.6, 123.3, 126.3, 127.1, 128.0, 131.0, 132.9, 135.0, 149.6, 152.8, 157.8, 161.7.


2-(4-Chlorophenyl)quinazolin-4(3H)-one 3d: White solid, Yield 70% (180 mg), ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.51 (t, *J* = 7.0 Hz, 1H), 7.61 (d, *J* = 8.6 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.82-7.87 (m, 1H), 8.14-8.22 (m, 3H), 12.55 (s, 1H) ; ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.0, 125.9, 126.7, 127.5, 128.7, 129.6, 131.5, 134.6, 136.3, 148.4, 151.3, 162.1; Analysis calculated for $C_{14}H_9ClN_2O$ C, 65.51; H, 3.53; N, 10.91; Found: C, 65.58; H, 3.51; N, 10.92.

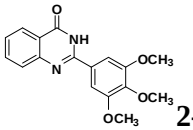

2-(2-Fluorophenyl)quinazolin-4(3H)-one 3e: White solid, Yield 72% (173 mg), ESI MS (m/z) = 241 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.35-7.42 (m, 2H), 7.54-7.66 (m, 2H), 7.72-7.88 (m, 3H), 8.16 (d, *J* = 7.0 Hz, 1H), 12.57 (s, br, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 102.1, 107.7, 113.4, 113.9, 114.4, 115.9, 119.0, 122.4, 124.2, 126.1, 127.3, 133.1, 134.7, 135.2, 150.2; Analysis calculated for $C_{14}H_9FN_2O$ C, 69.99; H, 3.78; N, 11.66; Found: 70.03; H, 3.71; N, 11.62.



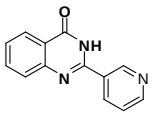
2-(3,4-Dichlorophenyl)quinazolin-4(3H)-one 3f: White solid, Yield 86% (250 mg), ESI MS (m/z) = 291 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.56-7.61 (m, 2H), 7.70 (d, *J* = 8.34, 2H), 7.82-7.89 (m, 2H), 8.17 (d, *J* = 7.86, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.7, 126.2, 127.6, 127.9, 129.5, 132.6, 133.1, 135.1, 135.9, 148.8, 151.8, 161.9; Analysis calculated for $C_{14}H_8Cl_2N_2O$ C, 57.76; H, 2.77; N, 9.62; Found: C, 57.78; H, 2.83; N, 9.67.



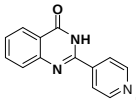
2-(Naphthalen-1-yl)quinazolin-4(3H)-one 3g:[11] White solid, Yield 79% (215 mg), ESI MS (m/z) = 273 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.56-7.68 (m, 4H), 7.74 (d, *J* = 8.3 Hz, 1H), 7.81 (d, *J* = 7.2 Hz, 1H), 7.86 (t, *J* = 7.6 Hz, 1H), 8.06-8.23 (m, 4H), 12.6 (s, br, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.2, 125.1, 125.2, 125.9, 126.4, 126.8, 127.1, 127.4, 127.7, 128.3, 130.2, 130.4, 131.7, 133.1, 134.5, 148.8, 153.7, 161.9.



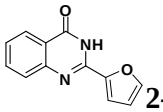
2-(3,4,5-Trimethoxyphenyl)quinazolin-4(3H)-one 3h: White solid, Yield 63% (197 mg), ESI MS (m/z) = 313 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.51 (s, 3H), 3.90 (s, 6H), 7.49-7.56 (m, 3H), 7.74-7.86 (m, 2H), 8.14 (d, *J* = 6.9 Hz, 1H), 12.45 (s, br, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 56.5, 60.6, 105.7, 121.2, 126.3, 126.9, 127.4, 127.8, 128.1, 135.2, 149.1, 152.3, 153.4, 162.9; Analysis calculated for $C_{17}H_{16}N_2O_4$ C, 65.38; H, 5.16; N, 8.97; Found: C, 65.43; H, 5.11; N, 9.00.



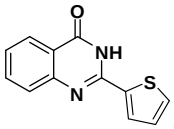
2-(Pyridin-3-yl)quinazolin-4(3H)-one 3i: White solid, Yield 65% (145 mg), ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.55 (t, *J* = 7.5 Hz, 1H), 7.71-7.90 (m, 3H), 8.17 (d, *J* = 7.6 Hz, 1H), 8.63 (d, *J* = 7.8 Hz, 1H), 8.82-8.84 (m, 1H), 9.35 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.1, 123.5, 125.9, 127.0, 127.6, 128.7, 134.7, 135.3, 148.5, 148.7, 150.7, 151.8, 162.1.



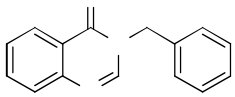
2-(Pyridin-4-yl)quinazolin-4(3H)-one 3j: White solid, Yield 72% (161 mg), ESI MS (m/z) = 224 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.56 (t, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.86-7.91 (m, 1H), 8.10 (d, *J* = 6.12 Hz, 2H), 8.17 (d, *J* = 6.7 Hz, 1H), 8.78 (m, 2H), 12.76 (s, br, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.6, 125.1, 126.3, 127.6, 127.9, 130.0, 135.2, 138.7, 146.9, 148.5, 149.5, 150.4, 162.5.



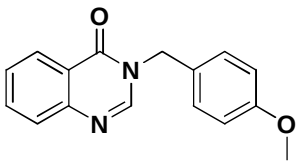
2-(Furan-2-yl)quinazolin-4(3H)-one 3k:[11] White solid, Yield 68% (144 mg), ESI MS (m/z) = 213 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.47 (t, *J* = 7.05 Hz, 1H), 7.62-7.63 (m, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.74-7.76 (m, 1H), 7.79 (t, *J* = 6.99 Hz, 1H), 8.00 (m, 1H), 8.11(d, *J* = 7.8 Hz, 1H), 12.46 (s, br, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 113.0, 115.0, 121.7, 126.5, 127.0, 127.7, 135.1, 144.5, 146.6, 147.0, 149.1, 162.1.



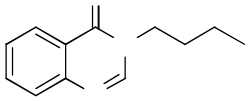
2-(Thiophen-2-yl)quinazolin-4(3H)-one 3l:[12] White solid, Yield 72% (164 mg), ESI MS (m/z) = 229 $(M+H)^+$; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.22 (t, *J* = 3.9 Hz, 1H), 7.46 (t, *J* = 7.02 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.78-7.88 (m, 2H), 8.11(d, *J* = 7.8 Hz, 1H), 8.22 (d, *J* = 3.7 Hz, 1H), 12.63 (s, br, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 121.3, 126.4, 126.7, 127.3, 128.9, 129.8, 132.5, 135.0, 137.8, 148.2, 149.1, 162.2.



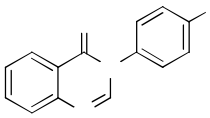
3-Benzylquinazolin-4(3H)-one (5a): White solid, Yield 73% (172 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.21 (s, 2H), 7.36-7.31 (m, 5H), 7.53-7.49 (m, 1H), 7.78-7.70 (m, 2H), 8.11 (s, 1H), 8.34 (dd, *J* = 1.2 Hz, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 49.7, 122.2, 126.9, 127.4, 127.6, 128.1, 128.4, 129.1, 134.4, 135.8, 146.4, 148.1, 161.1. HRMS-ESI: m/z calcd for $C_{15}H_{13}N_2O$ $[M + H]^+$, 237.1028, found 237.1013.



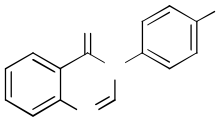
3-(4-Methoxybenzyl)quinazolin-4(3H)-one (5b): White solid, Yield 84 % (224 mg) ^{1}H NMR ($CDCl_3$, 500 MHz): δ 3.77 (s, 3H), 5.10 (s, 2H), 6.85–6.90 (m, 2H), 7.29-7.33 (m, 2H), 7.47–7.51 (m, 1H), 7.66–7.69 (m, 1H), 7.72–7.77 (m, 1H), 8.11 (s, 1H), 8.26–8.29 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 49.7, 55.8, 114.7, 122.9, 127.1, 127.7, 128.0, 128.7, 130.1, 134.6, 147.1, 148.8, 160.1, 161.4. HRMS (ESI): calcd. for $C_{16}H_{14}N_2O_2H$ 267.1128; found 267.1129. $C_{16}H_{14}N_2O_2$ (266.29): calcd. C 72.16, H 5.30, N 10.52; found C 71.99, H 5.59, N 10.14.



3-Butylquinazolin-4(3H)-one (5c): White solid, Yield 82% (166 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.99−0.96 (t, 3H), 1.45−1.39 (s, 2H), 1.82−1.75 (q, 2H), 4.03−4.00 (t, 2H), 7.53−7.49 (m, 1H), 7.78−7.71 (m, 2H), 8.10 (s, 1H), 8.33−8.30 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.6, 19.9, 31.4, 46.9, 122.1, 126.7, 127.1, 127.3, 134.2, 146.7, 147.7,160.9.

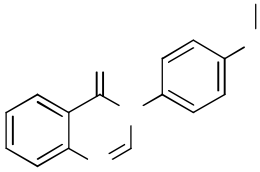


3-(4-Fluorophenyl)quinazolin-4(3H)-one (5d): White solid,Yield 56% (134 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (t, *J* = 8.4 Hz, 2H), 7.43-7.21 (m, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.82-7.75 (m, 2H), 8.09 (s, 1H), 8.36 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 116.9, 122.3, 127.2, 127.7, 127.9, 129.0, 133.5, 134.8, 145.9, 147.9, 160.9,163.9. HRMS-ESI: m/z calcd for $C_{14}H_{10}FN_2O$ $[M + H]^+$: 241.0777, found 241.0777.

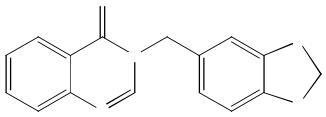


3-p-Tolylquinazolin-4(3H)-one (5e): White solid,Yield 66% (156 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.43 (s, 3H), 7.35-7.28 (m, 4H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.81-7.49

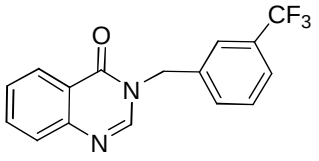
(m, 2H), 8.11 (s, 1H), 8.37 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.3, 122.5, 126.8, 127.3, 127.6, 130.3, 134.6, 135.0, 139.3, 146.4, 148.0,161.0. HRMS-ESI: m/z calcd for $C_{15}H_{13}N_2O$ $[M + H]^+$: 237.1028, found 237.1022.



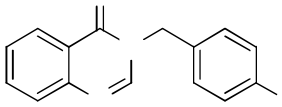
3-(4-Methoxyphenyl)quinazolin-4(3H)-one (5f): White solid, Yield 73% (184 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.87 (s, 3H), 7.05 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 2H), 7.56 (t, *J* = 6.4 Hz, 1H), 7.80-7.77 (m, 2H), 8.11 (s, 1H), 8.37 (dd, *J* = 0.4 Hz, *J* = 8.0 Hz, 1H),; ^{13}C NMR (125 MHz, $CDCl_3$) δ 55.7, 114.9, 122.4, 127.2, 127.6, 127.7, 128.2, 130.2, 134.6, 146.5, 147.4, 148.0, 160.0,. HRMS-ESI: m/z calcd for $C_{15}H_{13}N_2O_2$ $[M + H]^+$: 253.0977, found 253.0979.



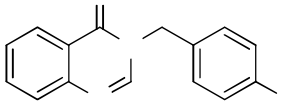
3-((Benzo[d][1,3]dioxol-5-yl)methyl)quinazolin-4(3H)-one (5g): White solid, Yield 68% (190mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.09 (s, 2H), 5.93 (s, 2H), 6.75 (d, *J*= 8 Hz,1H), 6.83-6.86 (m,2H), 7.48 (t, *J* = 7.50 Hz, 1H), 7.68-7.76 (m, 2H), 8.08 (s, 1H), 8.31 (d, *J*= 7.95 Hz, 1H); 13C NMR (500 MHz, $CDCl_3$) δ 49.4, 108.5, 108.6, 121.7, 122.2, 126.8, 127.3, 127.5, 129.5, 134.3, 146.1, 147.7, 148.0, 148.2,161.0.



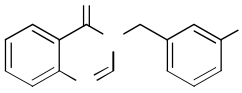
3-(3-(Trifluoromethyl)benzyl)quinazolin-4(3H)-one (5h): White Solid, Yield 77% (234mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.24 (s, 2H), 7.46-7.59 (m, 4H), 7.63 (s, 1H), 7.71-7.79 (m, 2H), 8.12 (s, 1H), 8.31 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 49.3, 122.1, 122.6,124.60-124.77, 124.8, 125.20-125.28, 126.9, 127.61-127.66, 129.6, 131.3, 131.5, 134.5, 136.7, 145.9, 148.0, 161.0.



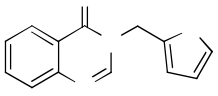
3-(4-Chlorobenzyl)quinazolin-4(3H)-one (5i): White solid, Yield 66% (179 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.11 (s, 2H), 7.26 (s, 4H), 7.40-7.50 (m, 1H), 7.79-7.59 (m, 2H), 8.07 (s, 1H), 8.26 (d, *J* = 10.0, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 48.9, 121.9, 126.6, 127.3, 127.4, 128.9, 129.2, 134.0, 134.1, 134.2, 145.9, 147.8, 160.8.



3-(4-(Trifluoromethyl)benzyl)quinazolin-4(3H)-one (5j): White solid, Yield 77% (234 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.24 (s, 2H), 7.46 (d, *J* = 8.05 Hz,2H), 7.51 (t, *J* = 7.52 Hz, 1H), 7.60 (d, *J* = 8.15 Hz, 2H), 7.72-7.79 (m, 2H), 8.11 (s, 1H), 8.32 (d, *J* = 8 Hz, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 49.3, 122.1, 122.7, 124.9, 125.90-126.07, 126.9, 126.65-127.68, 127.8, 128.1, 130.5, 130.7, 134.5, 139.6, 145.9, 148.0, 161.0.

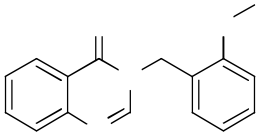


3-(3-Chlorobenzyl)quinazolin-4(3H)-one (5k): White solid, Yield 64% (173 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.16 (s, 2H), 7.22-7.24 (m, 2H), 7.27-7.28 (m, 2H), 7.34(s, 1H), 7.50(td, *J*= 1.3 Hz, *J* = 6.85 Hz, 1H), 7.70 (dd, *J* =0.8 Hz, *J* = 8.15 Hz, 1H), 7.75 (td, *J* = 1.5 Hz, *J* = 6.95 Hz, 1H), 8.09 (s, 1H), 8.31 (dd, *J* =1.45 Hz, *J* = 8.45 Hz, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 49.1, 122.1, 126.0, 126.9, 127.5, 127.6, 128.0, 128.5, 130.3, 134.4, 134.9, 137.7, 146.0, 148.0, 161.0.

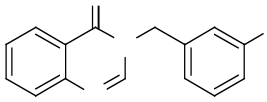


3-((Furan-2-yl)methyl)quinazolin-4(3H)-one (5l): White solid, Yield 74% (167 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.18 (s, 2H), 6.34-6.35 (m, 1H), 6.46 (d, *J*= 3.15, 1H), 7.38 (d, *J* = 1.05 Hz, 1H), 7.48 (td, *J* = 1.2 Hz, *J* = 8.05 Hz, 2H), 7.69-7.76 (m, 2H), 8.16 (s, 1H),

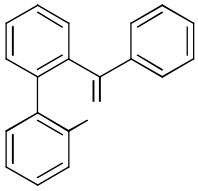
8.30 (dd, *J* =1.0 Hz, *J* = 7.95 Hz, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 42.1, 109.9, 110.7, 122.1, 126.8, 127.3, 127.5, 134.3, 143.1, 146.0, 148.0, 148.4, 160.7



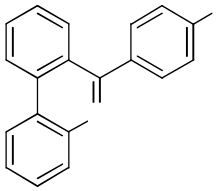
3-(2-Methoxybenzyl)quinazolin-4(3H)-one (5m): White solid, Yield 74% (167 mg), 1H NMR (500 MHz, $CDCl_3$) δ 3.86 (s, 3H), 5.15 (s, 2H), 6.87 (d, *J*= 8.25 Hz, 1H), 6.93 (t, *J*=7.45 Hz, 1H), 7.26-7.30 (m, 1H), 7.44-7.51 (m, 2H), 7.66-7.73 (m, 2H), 8.28-8.29 (m, 2H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 45.7, 55.3, 110.4, 120.7, 122.3, 123.4, 126.7, 126.9, 127.3, 129.9, 131.6, 134.0, 147.4, 148.0, 157.5, 161.2.



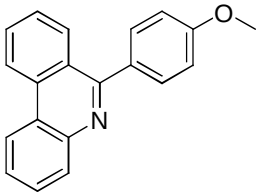
3-(3-Fluorobenzyl)quinazolin-4(3H)-one (5n): White solid, Yield 84% (213 mg), ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.10 (s, 2H), 6.98 (td, *J* = 2.5 Hz, *J* = 8.35 Hz, 1H), 7.04 (dt, *J* = 1.85 Hz, *J* = 9.35, 1H), 7.11 (dd, *J* =0.55 Hz, *J*= 7.45, 1H), 7.29 (q, *J*= 8 Hz, 1H), 7.50 (td, *J*= 1.25 Hz, *J*= 6.90 Hz, 1H), 7.71 (dd, *J*= 0.75 Hz, *J*= 8.1 Hz, 1H) 7.75 (td, *J*= 1.5 Hz, *J*= 6.95 Hz, 1H), 8.09 (s, 1H), 8.31 (dd, *J*=1.45 Hz, *J*= 8 Hz, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 49.1, 114.8-115.06, 115.26-115.43, 122.1, 123.43-123.46, s126.9, 127.54, 127.61, 130.61-130.67, 134.4, 138.13, 138.18, 146.0, 148.0, 161.0.



6-Phenylphenanthridine (6a): White solid, Yield (181 mg, 71%), ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.58–7.52 (m, 3H), 7.62 (td, *J* = 7.8, *J* = 0.6 Hz, 1H), 7.70 (td, *J* = 7.8, *J* = 1.2 Hz, 1H), 7.78–7.74 (m, 3H), 7.87 (td, *J* = 7.8, *J* = 1.2 Hz, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 8.25 (dd, *J* = 7.8, *J* = 1.2 Hz, 1H), 8.63 (d, *J* = 8.4 Hz, 1H), 8.72 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 121.9, 122.2, 123.7, 125.3, 126.9, 127.1, 128.4, 128.7, 128.8, 128.9, 129.7, 130.4, 130.5, 133.5, 139.8, 143.8, 161.3,; HRMS: $C_{19}H_{13}N$ calculated 255.1048, found 255.1045

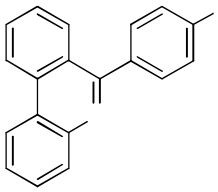


6-(4-Nitrophenyl)phenanthridine (6b): White solid, Yield 62% (186 mg), ^{1}H NMR: (500 MHz, DMSO-d_6) δ 7.66 (t, *J* = 7.6 Hz, 1 H), 7.75 (t, *J* = 7.4 Hz, 1 H), 7.80 (t, *J* = 7.2 Hz, 1 H), 7.95-7.89 (m, 3 H), 7.99 (d, *J* = 8.4 Hz, 1 H), 8.24 (d, *J* = 7.6 Hz, 1 H), 8.43 (d, *J* = 8.4 Hz, 2 H), 8.65 (d, *J* = 7.6 Hz, 1 H), 8.75 (d, *J* = 8.4 Hz, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 122.1, 122.6, 123.7, 123.9, 124.6, 127.5, 127.7, 127.9, 129.2, 130.4, 130.9, 131.0, 133.5, 143.6, 146.1, 148.1,158.7.

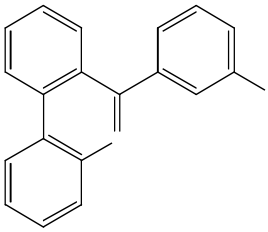


6-(4-Methoxyphenyl)phenanthridine (6c): White solid, Yield (214 mg, 75%), ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.92 (s, 3H), 7.10 (d, *J* = 8.4 Hz, 2H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.75 (t, *J* = 7.8 Hz, 1H), 7.85 (t, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 8.61 (d, *J* = 7.8 Hz, 1H), 8.69 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 55.4, 113.9, 121.9, 122.2, 123.6, 125.4, 126.7,

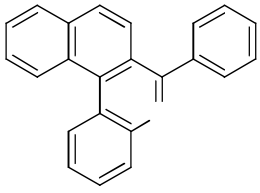
127.0, 128.8, 128.9, 130.3, 130.4, 131.2, 132.3, 133.5, 143.9, 160.1, 160.9. HRMS: $C_{20}H_{15}NO$ calculated 285.1154, found 285.1156.



6-(4-Chlorophenyl)phenanthridine (6d): White solid, Yield (188 mg, 65%), ^{1} H NMR (500 MHz, DMSO-d_6): δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.70 (m, *J* = 8.4 Hz, 3H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.62 (d, *J* = 7.8 Hz, 1H), 8.71 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 122.0, 122.3, 123.8, 125.0, 127.1, 127.3, 128.5, 128.7, 129.0, 130.3, 130.7, 131.1, 133.5, 134.9, 138.2, 143.7, 160.0. HRMS: $C_{19}H_{12}ClN$ calculated 289.0658, found 289.0654;

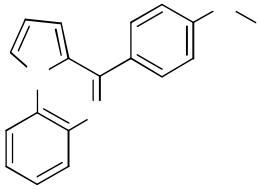


6-(3-Nitrophenyl)phenanthridine (6e): Yield 53% (159 mg), ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.67 (t, *J* = 7.6 Hz, 1H), 7.92 (t, *J* = 7.5 Hz, 1H), 8.01 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 8.41 (d, *J* = 7.8 Hz, 1H), 8.66-8.64 (m, 2H), 8.76 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 122.1, 122.6, 123.6, 123.9, 124.6, 124.9, 127.6, 127.9, 129.2, 129.5, 130.4, 131.1, 133.6, 135.9, 141.4, 143.6, 148.3, 158.4. MS (m/z): HRMS (ESI) Calcd for $C_{19}H_{12}N_2O_2$ $[M + H]^+$: 301.0978, found 301.0981.

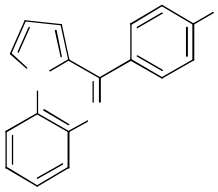


6-Phenylbenzo[k]phenanthridine (6f): yellow solid, Yield 69% (211 mg), ^{1}H (500MHz, DMSO-d_6) δ 7.22 (t, *J* = 7.9, 1H), 7.30-7.60 (m, 4H), 7.65 (m, 2H), 7.70 (t, *J* = 7.7, 1H), 7.80 (m, 2H), 7.93 (d, *J* = 7.9, 1H), 8.15 (d, *J* = 8.9, 1H), 8.29 (d, *J* = 8.2, 1H), 8.63

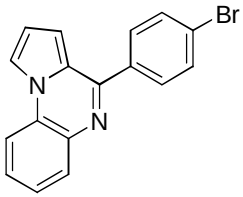
(d, *J* = 8.9, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 119.8, 121.4, 122.4, 123.5, 125.8, 126.3, 126.8, 128.3, 128.4, 128.6, 128.8, 129.0, 129.9, 130.2, 132.2, 133.1, 134.3, 144.0, 144.5, 159.2.



4-(4-Methoxyphenyl)pyrrolo(1,2-a)quinoxaline (6g): Light yellow solid, Yield 68% (186 mg), ^{1}H (500MHz, DMSO-d_6) δ 3.89 (s, 3H), 6.88 (t, *J* = 3.2 Hz, 1H), 7.00 (d, J = 2.9 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.49-7.44 (m, 2H), 7.86 (d, J = 8.4 Hz, 1H), 8.03-7.97 (m, 4H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 55.4, 108.5, 113.6, 113.8, 113.9, 114.4, 125.2, 125.4, 127.1, 130.0, 131.0, 136.3, 150.0, 153.8, 161.0.

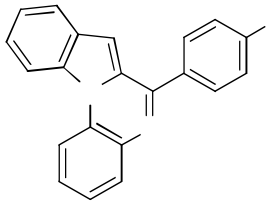


4-(4-Chlorophenyl)pyrrolo(1,2-a)quinoxaline (6h): Light yellow solid, Yield 57% (159 mg), ^{1}H (500MHz, $CDCl_{3,}$) δ 6.92 (t, *J* = 3.2 Hz, 1H), 6.96 (d, *J* = 3.2 Hz, 1H), 7.56-7.45 (m, 4H), 7.89 (dd, *J* = 6.8, *J* = 1.2 Hz, 1H), 7.97 (d, *J* = 6.8 Hz, 2H), 8.63 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 108.4, 113.6, 114.1, 114.8, 125.1, 125.4, 127.1, 127.7, 128.8, 129.9, 130.2, 135.8, 136.1, 136.9, 153.1.

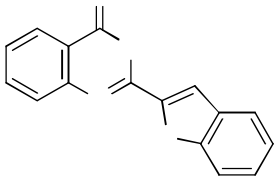


4-(4-Bromophenyl)pyrrolo[1,2-a]quinoxaline (6i): White solid, Yield 37% (120 mg), ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.00–7.90 (m, 2 H), 7.90–7.80 (m, 3 H), 7.70–7.60 (m, 2 H), 7.50 (td, *J* = 8.7, *J* = 1.5 Hz, 1 H), 7.50 (td, *J* = 8.0, *J* = 1.4 Hz, 1H), 6.94 (t, *J* = 3 Hz, 1

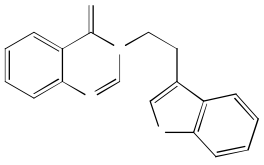
H), 6.93 (t, *J* = 2.9 Hz, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 153.0, 137.2, 136.0, 131.7, 130.2, 127.7, 127.0, 125.3, 124.9, 124.1, 114.8, 114.1, 113.6, 108.5.



6-(4-Bromophenyl)indolo[1,2-a]quinoxaline (6j): Yellow solid, Yield 56% (209 mg), ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.23 (s, 1H), 7.48 (t, *J* = 7.9 Hz, 2H), 7.68–7.57 (m, 2H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.95–7.93 (m, 3H), 8.09 (dd, *J* = 1.2, *J* = 7.9 Hz, 1H), 8.54 (t, *J* = 8.3 Hz, 2H),; ^{13}C NMR (125 MHz, $CDCl_3$): δ 114.7, 114.9, 115.8, 117.2, 123.1, 124.4, 125.1, 125.9, 126.5, 127.5, 129.4, 129.5, 130.1, 130.2, 130.9, 131.6, 133.0, 135.8,154.0.



2-(1H-Indol-2-yl)quinazolin-4(3H)-one (8): White solid, Yield 83% (217 mg), ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.06 (t, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.50-7.56 (m, 2H), 7.65 (d, *J* = 7.8 Hz, 2H), 7.69 (s, 1H), 7.75 (d, *J* = 7.8, 1H), 7.84-7.87 (m, 1H), 8.16 (d, *J* = 7.8 Hz, 2H), 11.81 (s, 1H), 12.63 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 105.4, 112.8, 120.4, 121.6, 122.0, 124.5, 126.5, 126.7, 127.4, 127.9, 130.5, 135.1, 138.1, 147.0, 149.2, 162.3.



3-(2-(1*H*-Indol-3-yl)ethyl)quinazolin-4(3*H*)-one (10): White solid, Yield 76% (220 mg), ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.25 (t, *J* = 6.7, 2H), 4.28 (t, *J* = 6.7, 2H), 6.82 (d, *J* = 2.2, 1H), 7.12 (t, = 6.9, 1H), 7.21 (d, = 7.8, 1H), 7.32 (d, *J* = 8.1, 1H), 7.47 (d, *J* = 6.1, 2H), 7.66 (d, *J* = 7.9, 2H), 7.71 (t, *J* = 8.4, 1H), 8.35 (d, *J* = 9.4, 2H); ^{13}C NMR (75 MHz,

$CDCl_3$) δ 24.8, 47.5, 111.1, 111.4, 118.2, 119.6, 123.0, 122.2, 122.7, 126.5, 126.7, 127.1, 127.2, 134.1, 136.4, 146.6, 147.9, 161.0.

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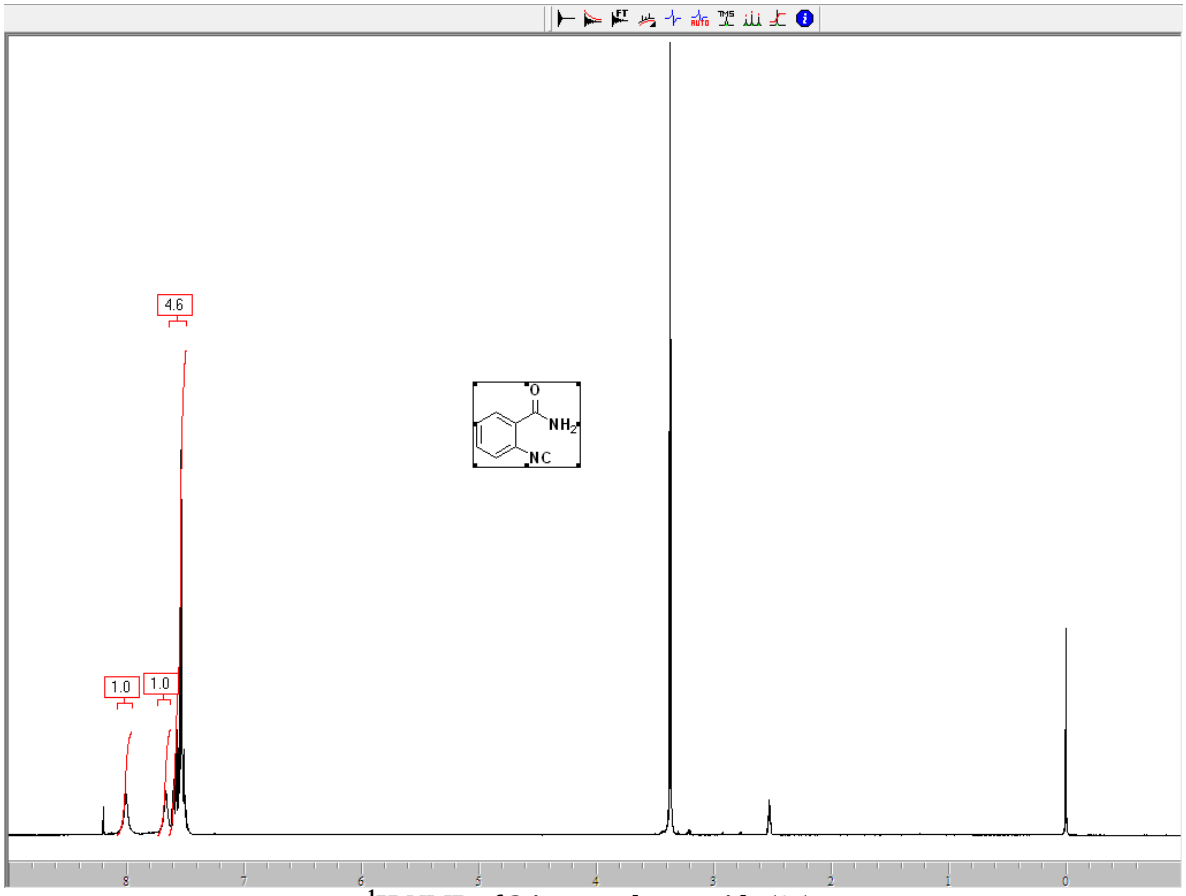
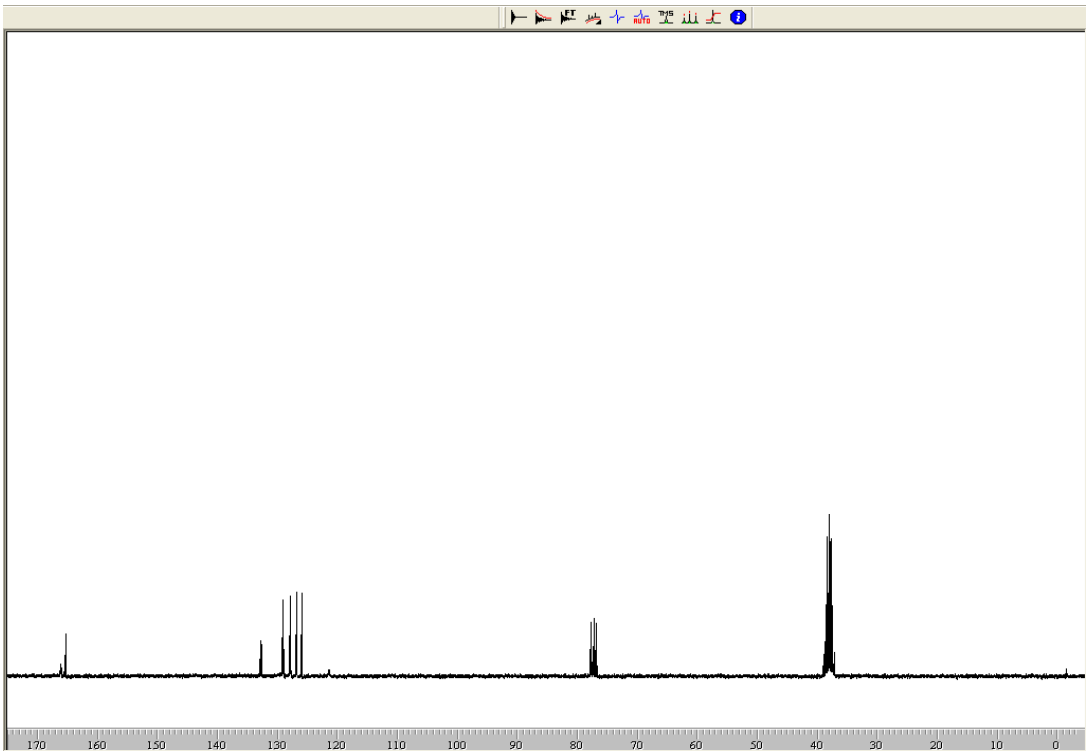
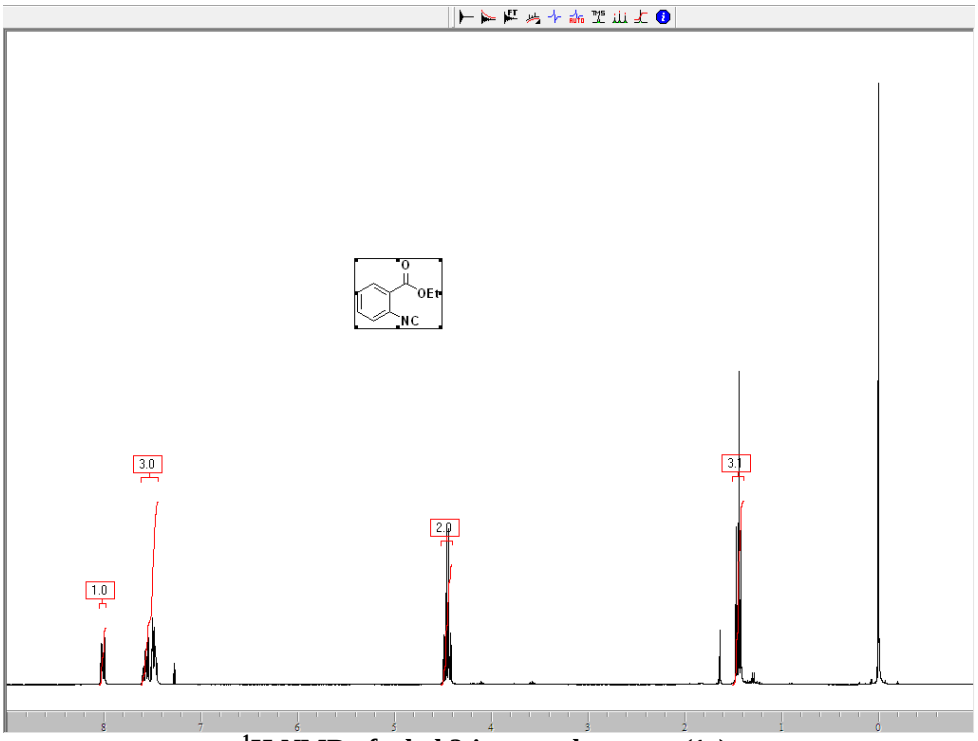


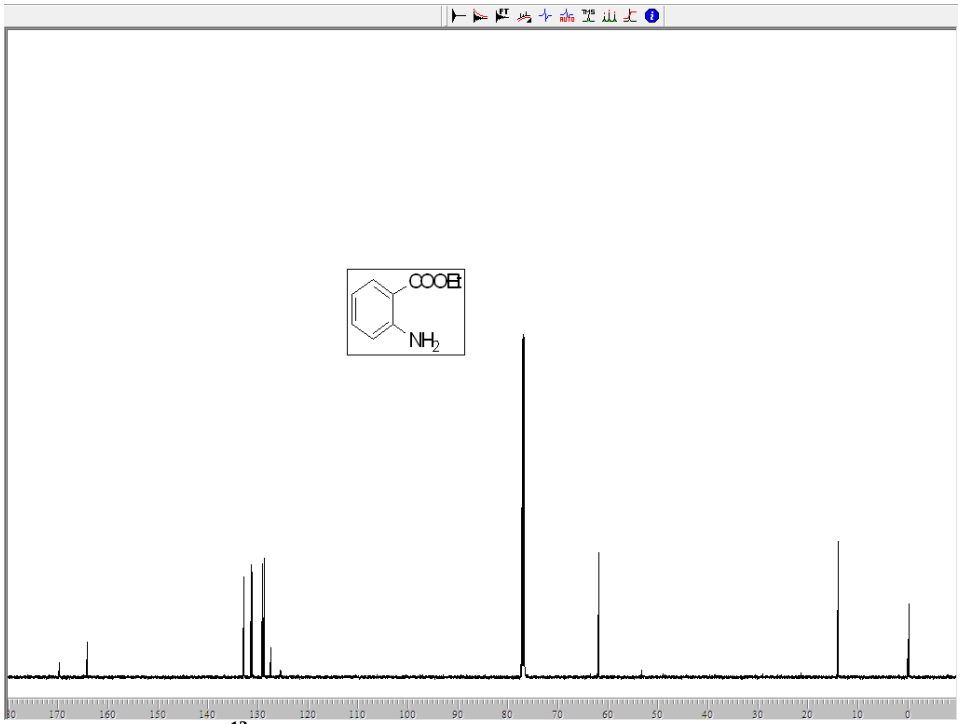
^{1}H-NMR of 2-isocyanobenzamide (1a).



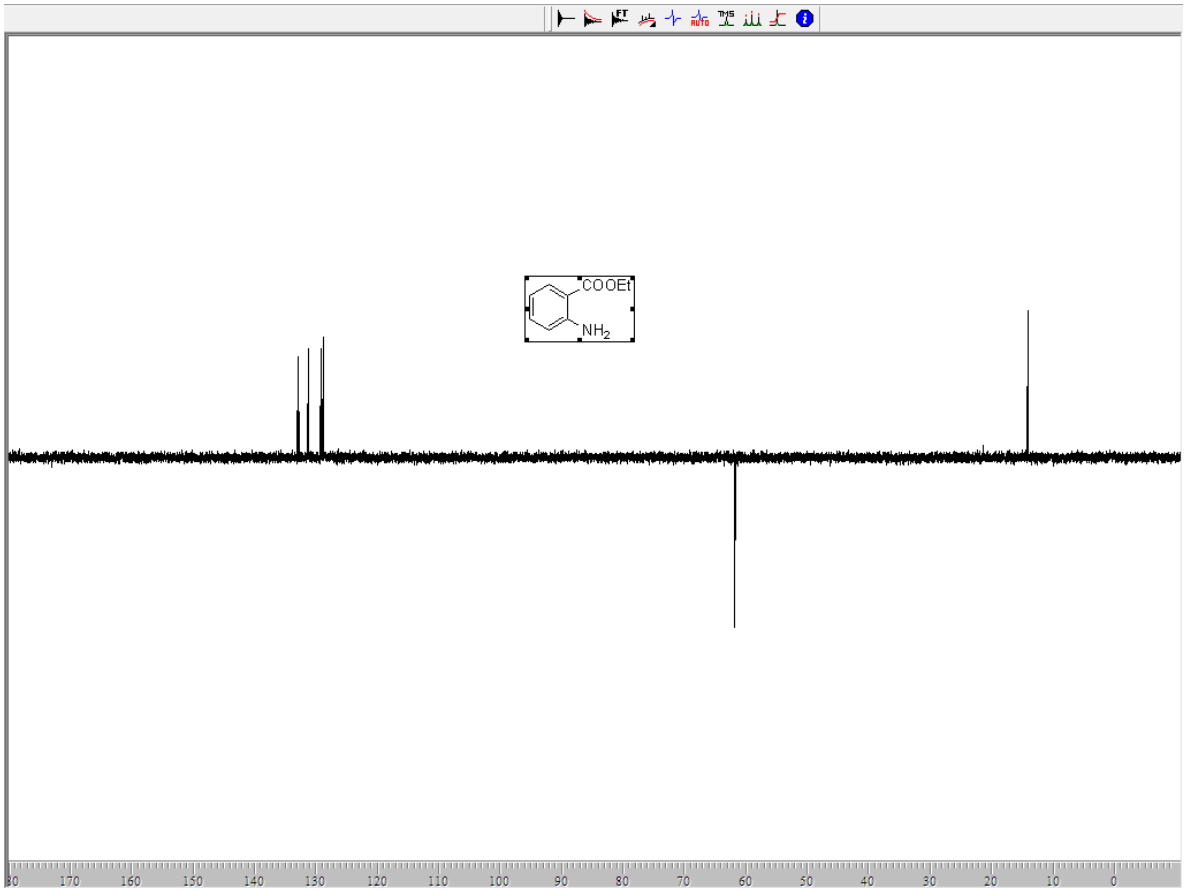
^{13}C-NMR of 2-isocyanobenzamide (1b).



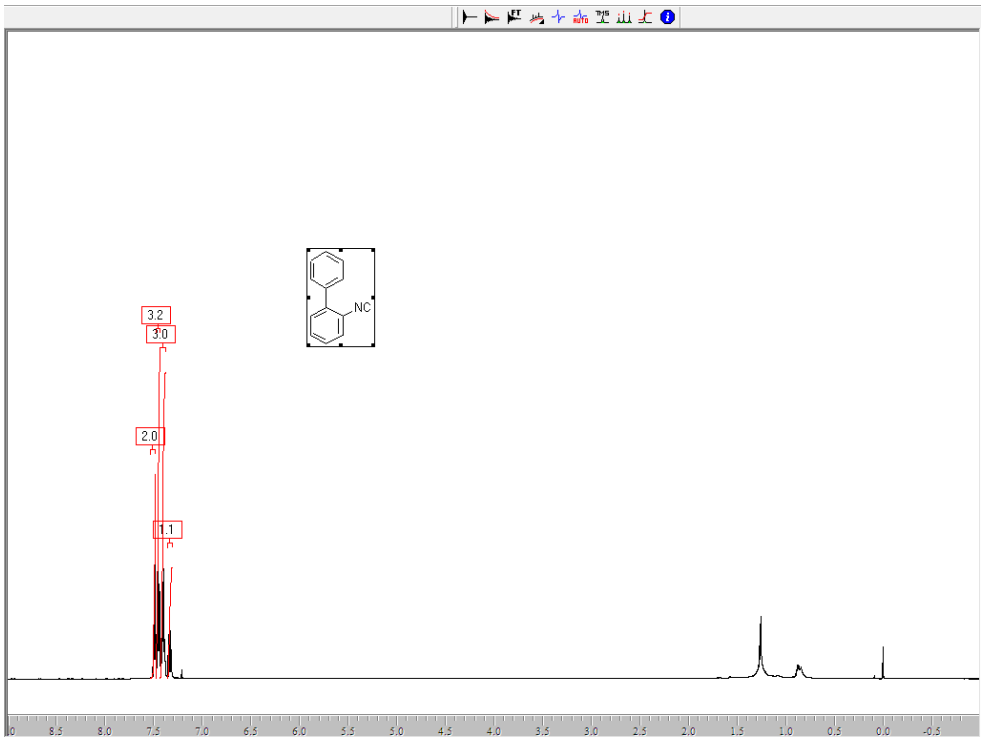
^{1}H-NMR of ethyl 2-isocyanobenzoate (1c).



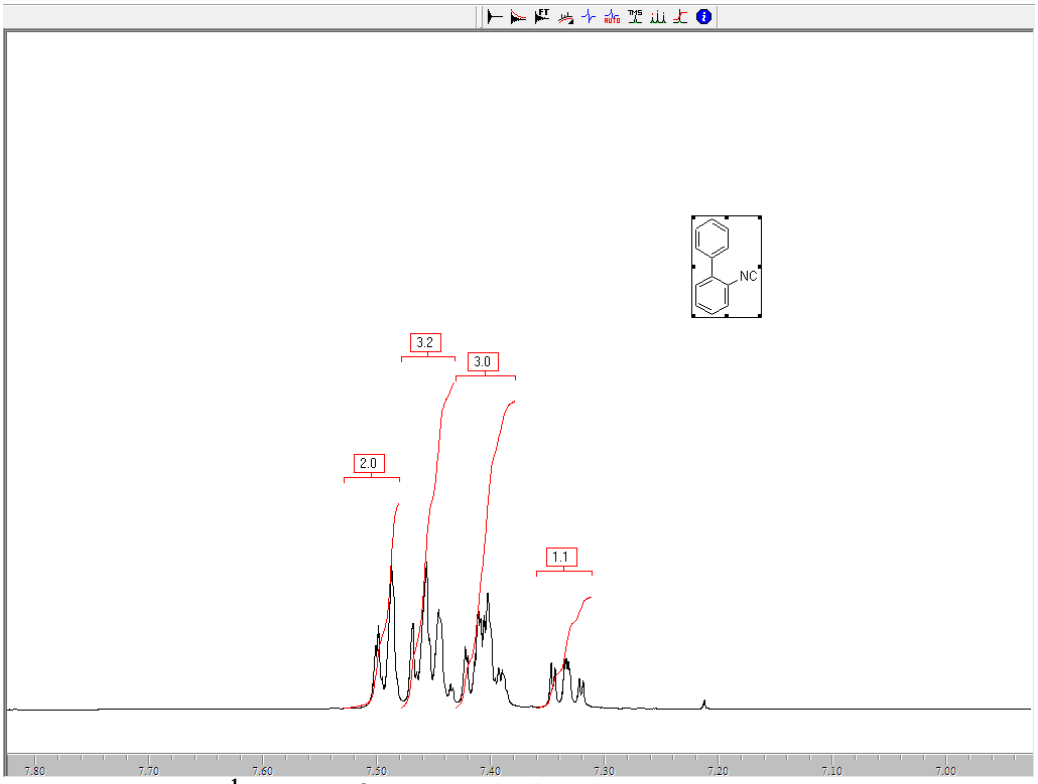
^{13}C-NMR of ethyl 2-isocyanobenzoate (1c).



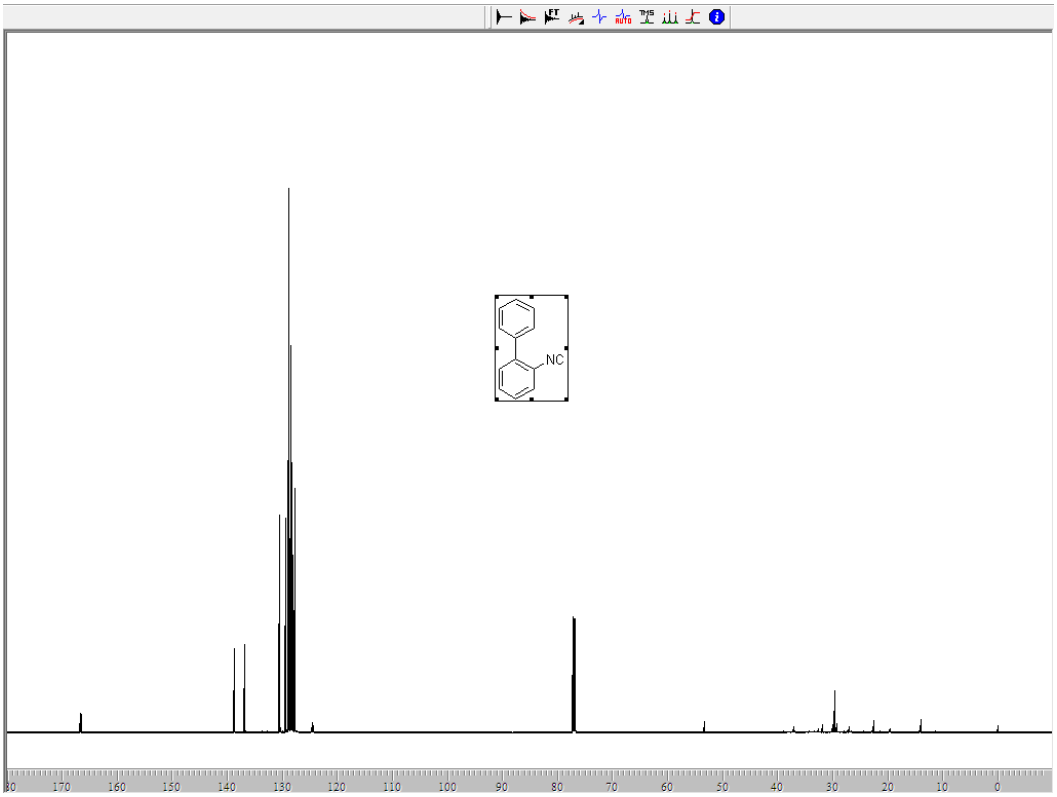
DEPT-135 NMR of ethyl 2-isocyanobenzoate (1c).



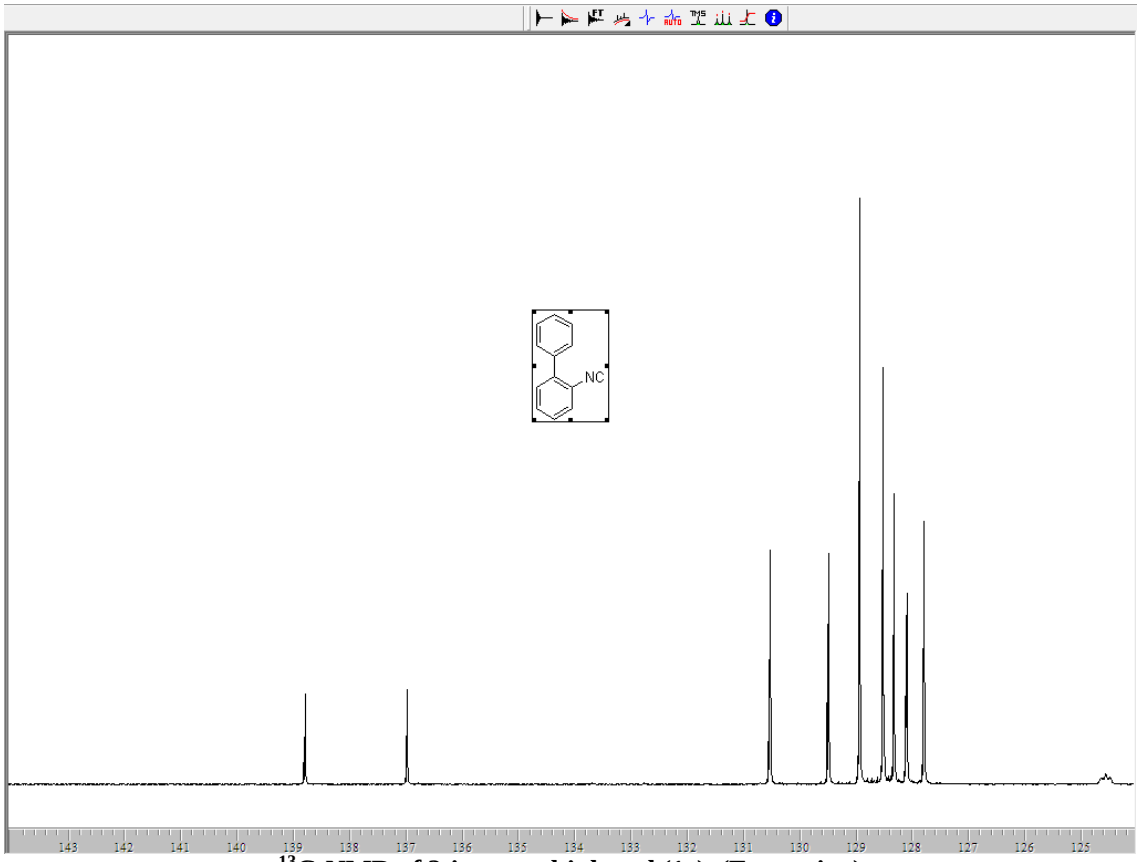
^{1}H-NMR of 2-isocyanobiphenyl (1c).



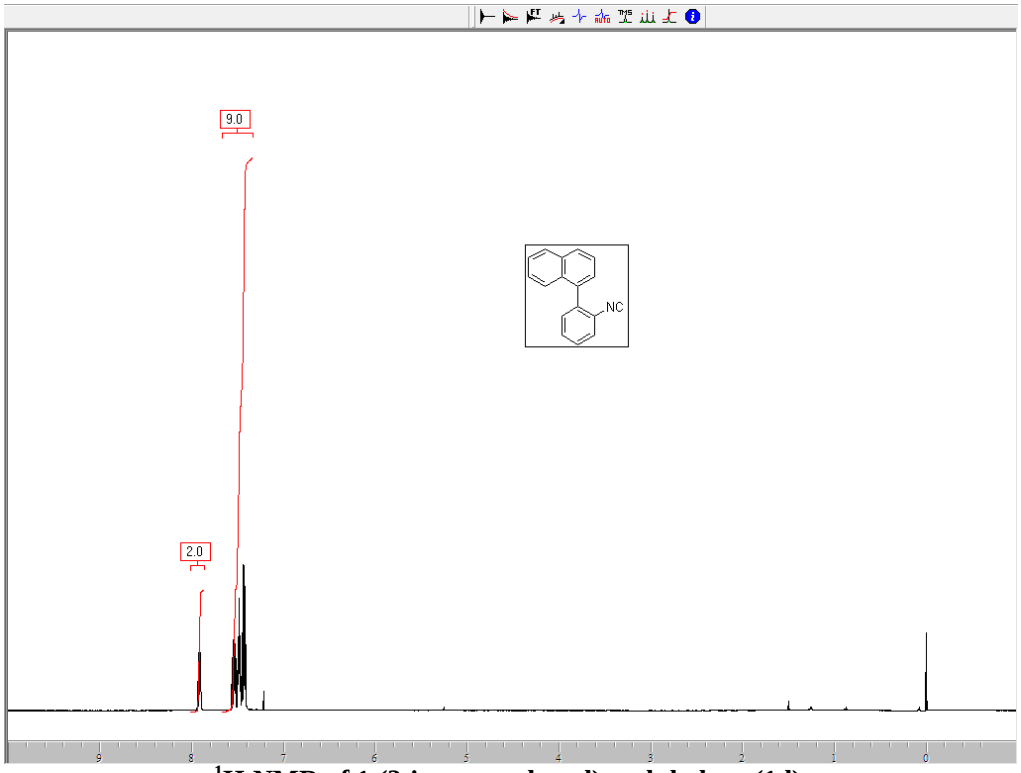
^{1}H-NMR of 2-isocyanobiphenyl (1c). (Expansion)



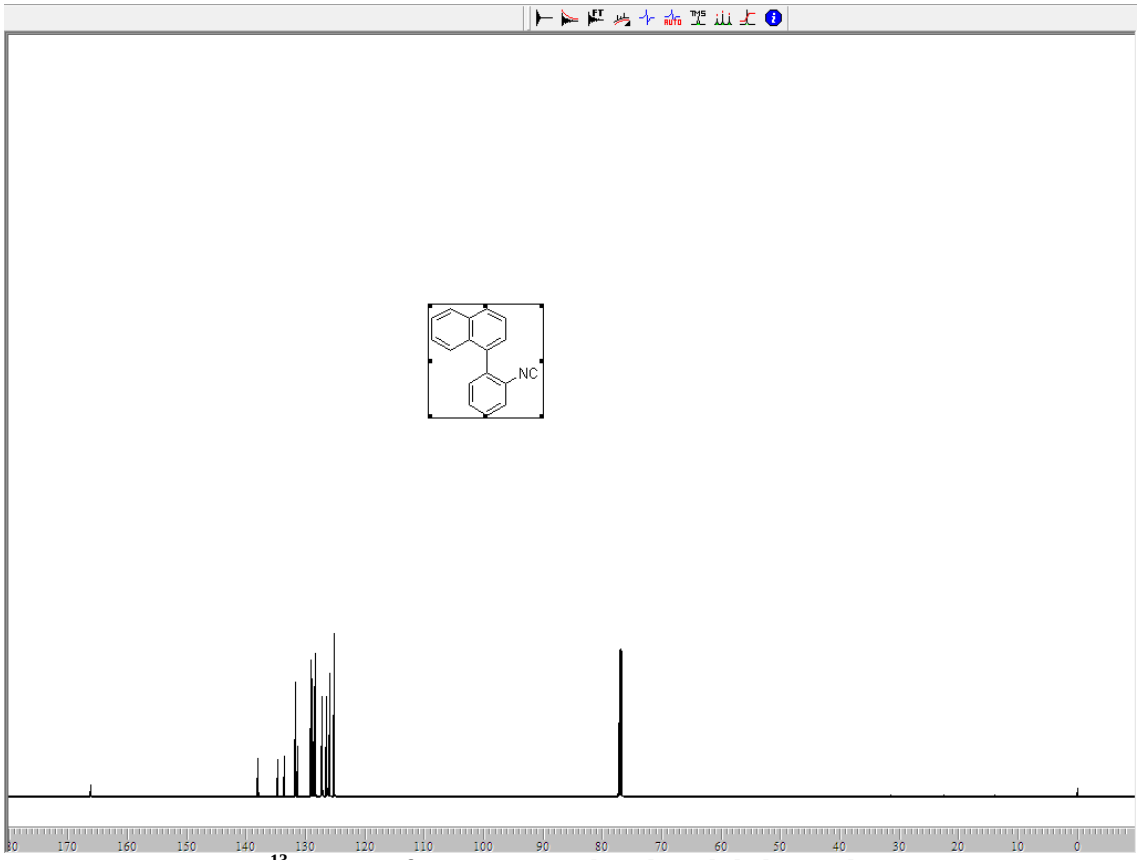
^{13}C-NMR of 2-isocyanobiphenyl (1c).



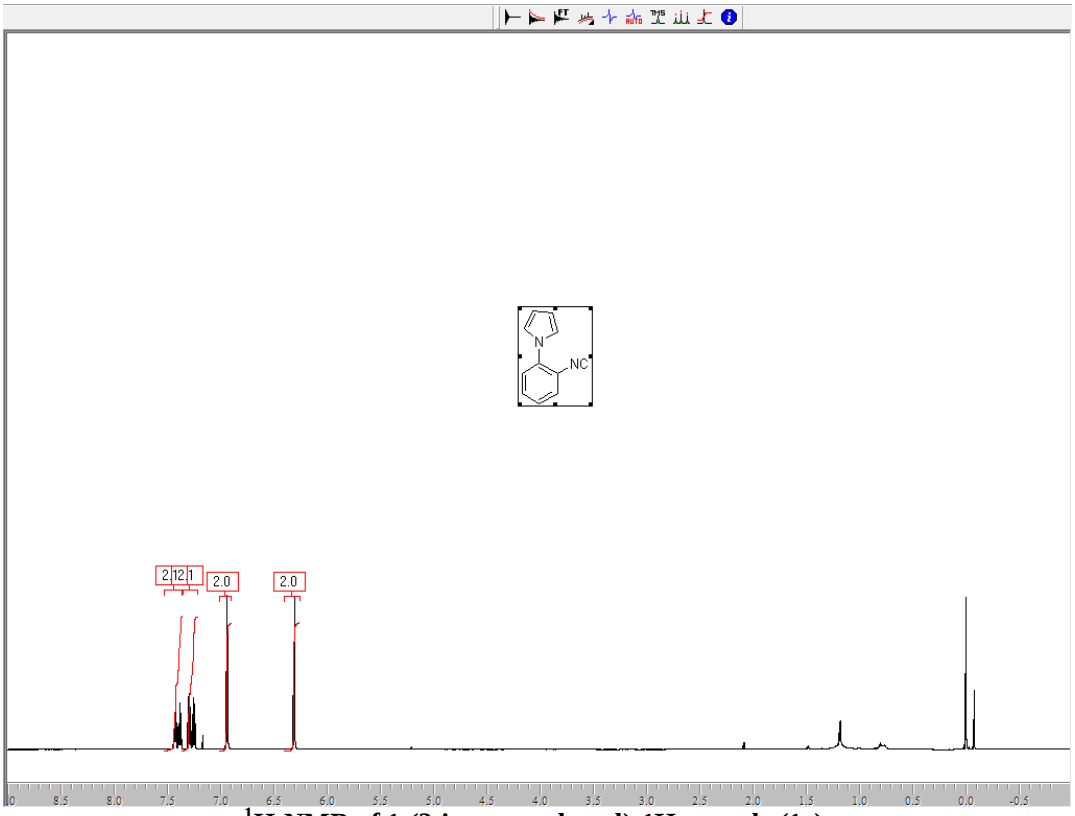
^{13}C-NMR of 2-isocyanobiphenyl (1c). (Expansion)



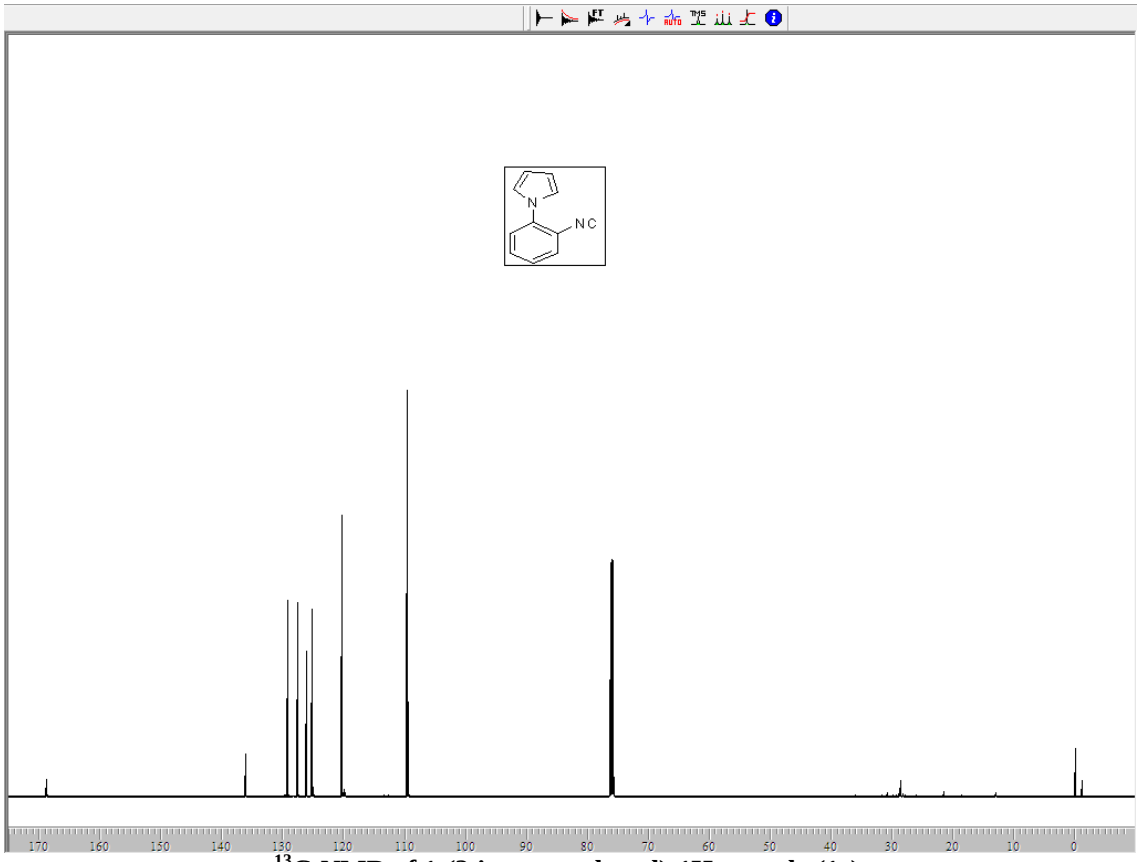
^{1}H-NMR of 1-(2-isocyanophenyl)naphthalene (1d).



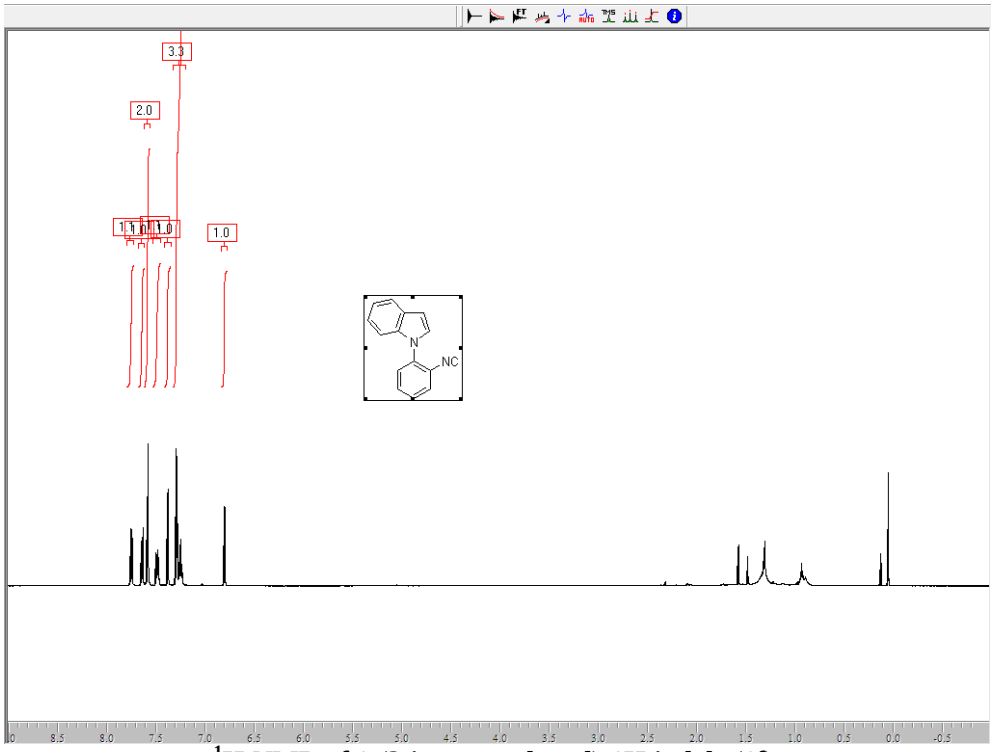
^{13}C-NMR of 1-(2-isocyanophenyl)naphthalene (1d).



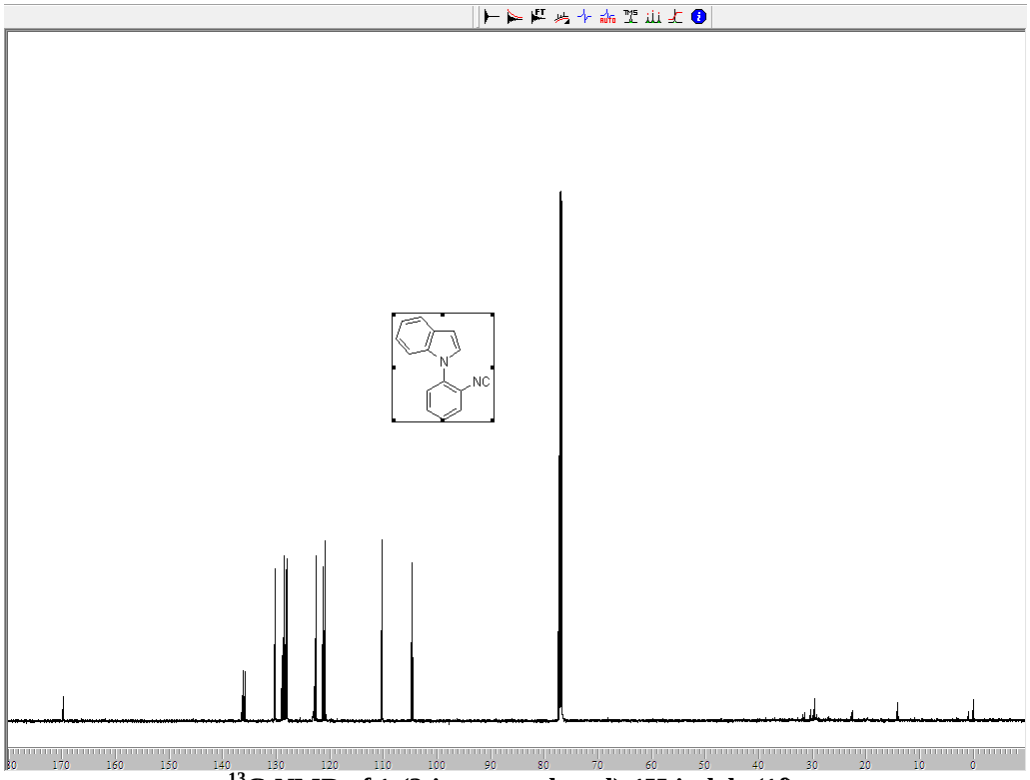
^{1}H-NMR of 1-(2-isocyanophenyl)-1H-pyrrole (1e).



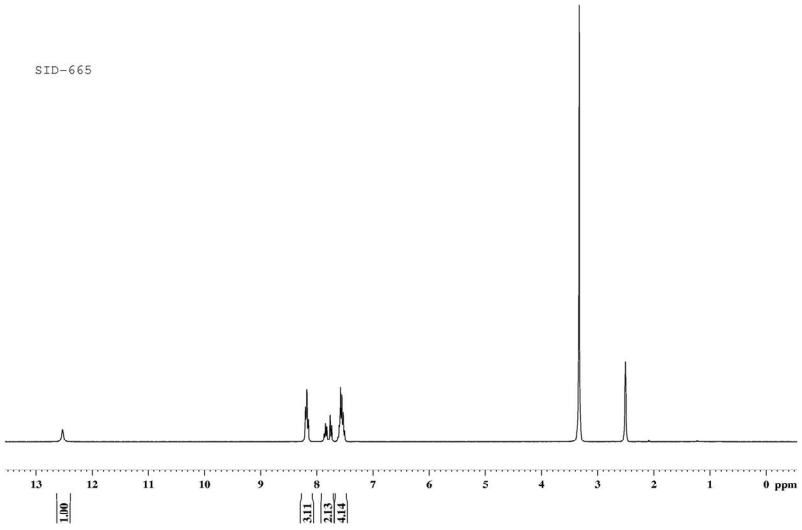
^{13}C-NMR of 1-(2-isocyanophenyl)-1H-pyrrole (1e).



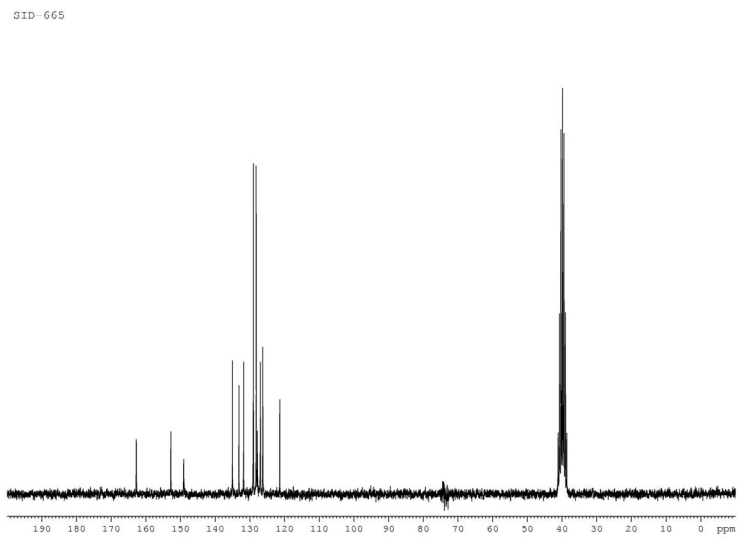
^{1}H-NMR of 1-(2-isocyanophenyl)-1H-indole (1f).



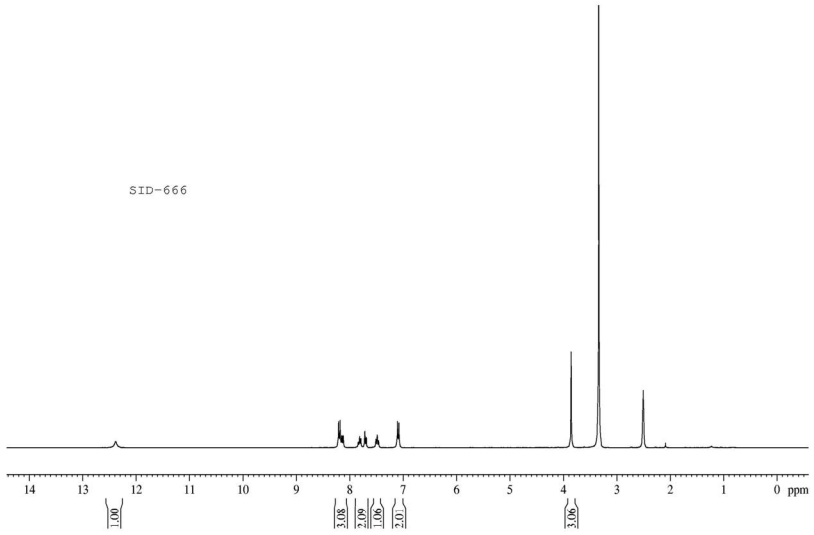
^{13}C-NMR of 1-(2-isocyanophenyl)-1H-indole (1f).



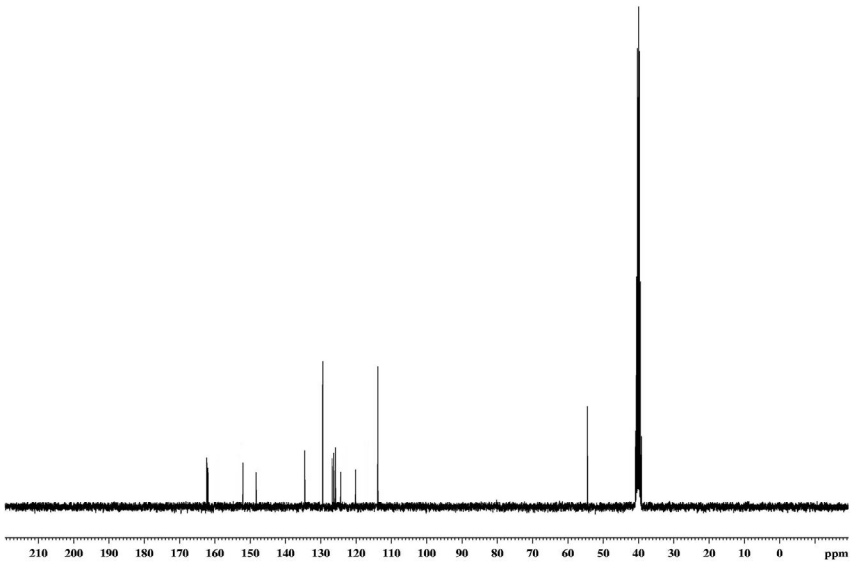
^{1}H NMR spectra of 2-Phenylquinazolin-4(3H)-one (3a).



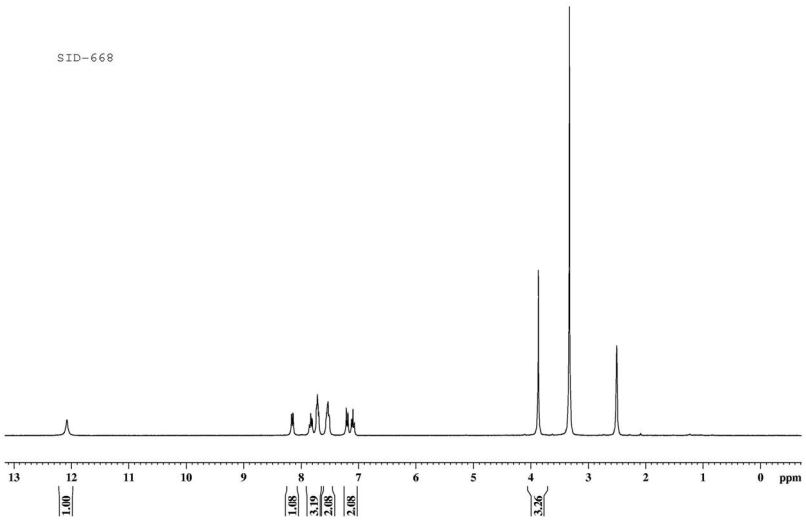
^{13}C NMR spectra of 2-Phenylquinazolin-4(3H)-one 3a.



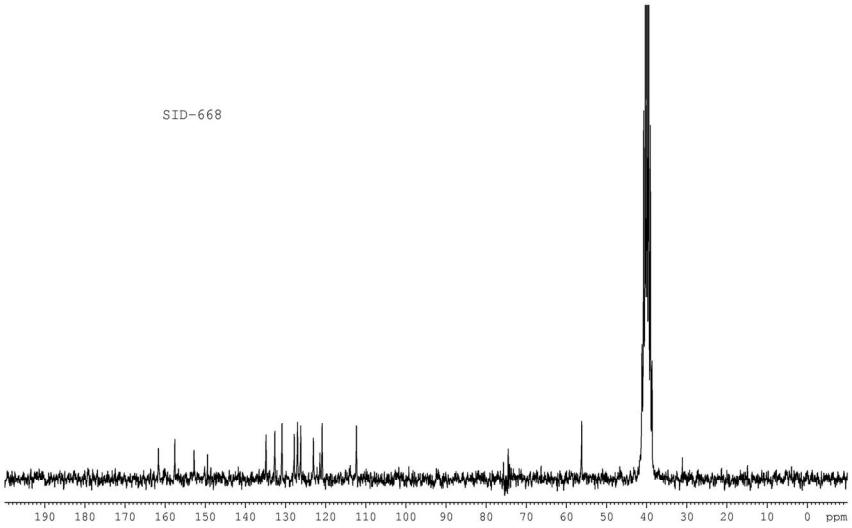
^{1}H NMR spectra of 2-(4-Methoxyphenyl)quinazolin-4(3H)-one 3b.



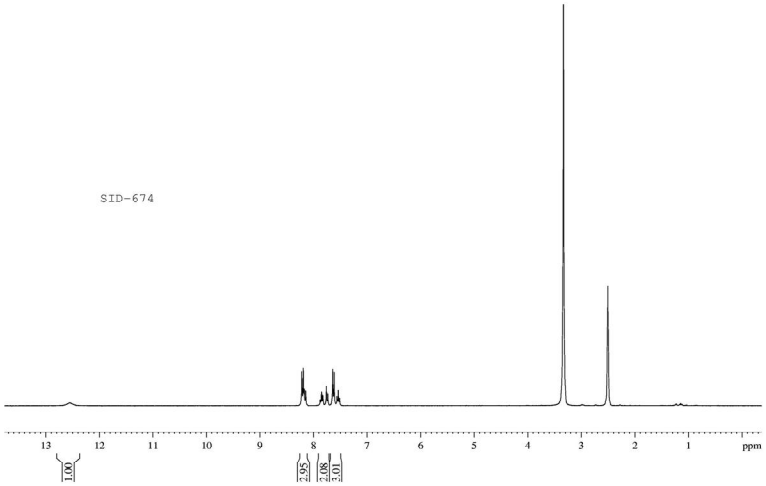
^{13}C NMR spectra of 2-(4-Methoxyphenyl)quinazolin-4(3H)-one 3b.



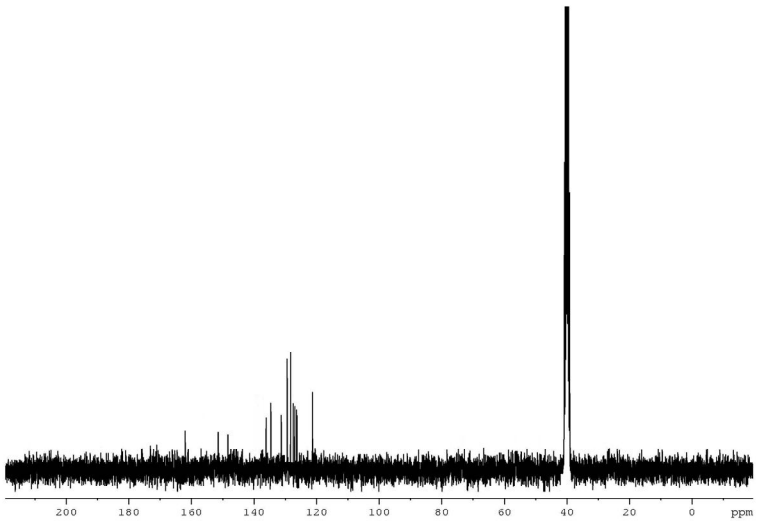
^{1}H NMR spectra of 2-(2-methoxyphenyl)quinazolin-4(3H)-one 3c.



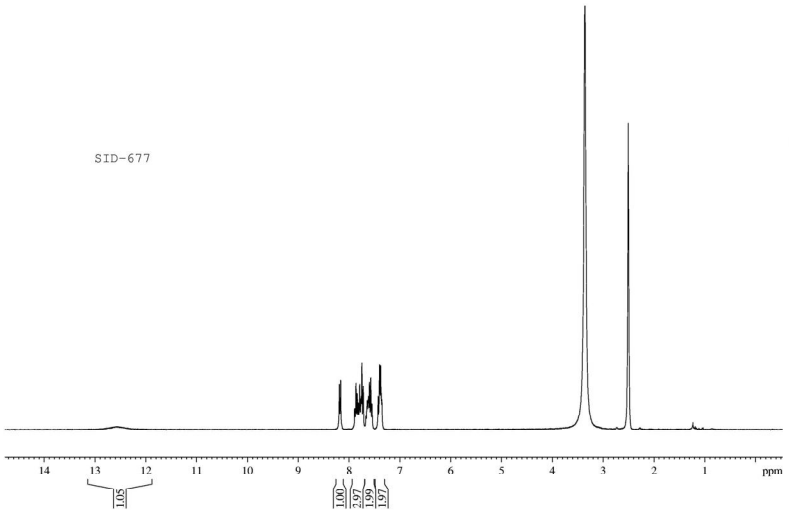
^{13}C NMR spectra of 2-(2-methoxyphenyl)quinazolin-4(3H)-one 3c.



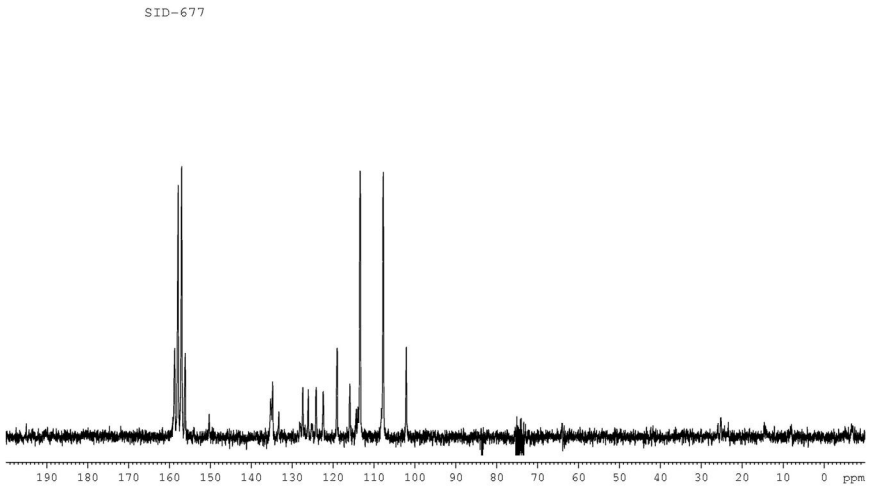
^{1}H NMR spectra of 2-(4-chlorophenyl)quinazolin-4(3H)-one 3d.



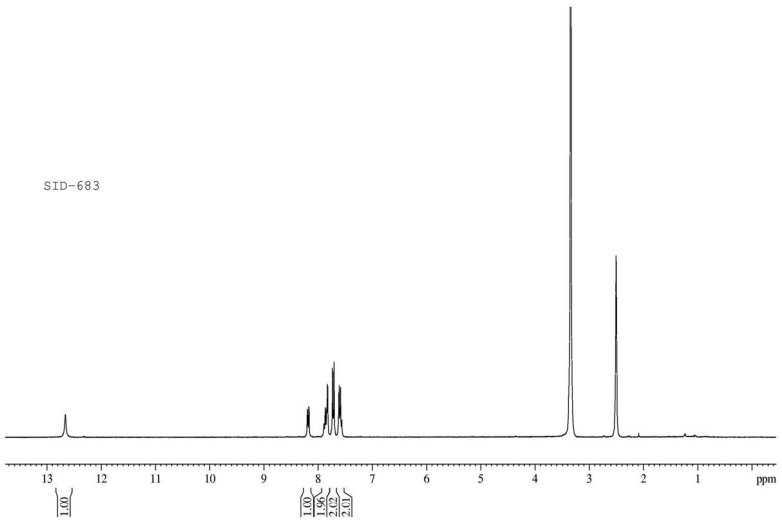
^{13}C NMR spectra of 2-(4-chlorophenyl)quinazolin-4(3H)-one 3d.



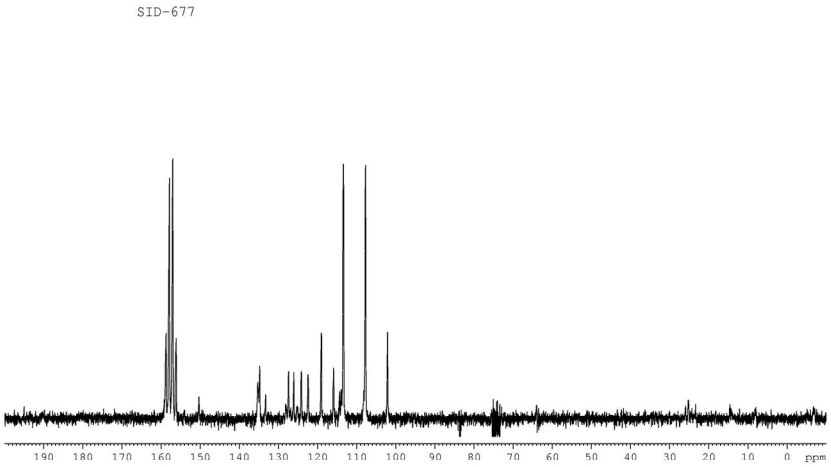
^{1}H NMR spectra of 2-(2-fluorophenyl)quinazolin-4(3H)-one 3e.



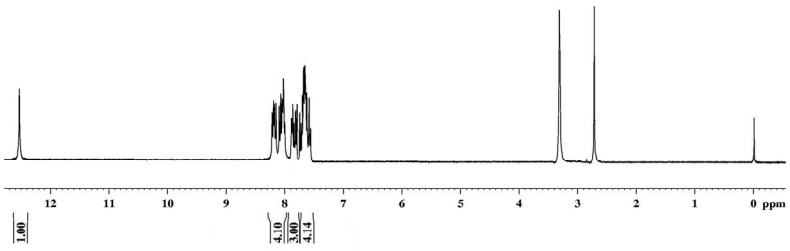
^{13}C NMR spectra of 2-(2-fluorophenyl)quinazolin-4(3H)-one 3e.



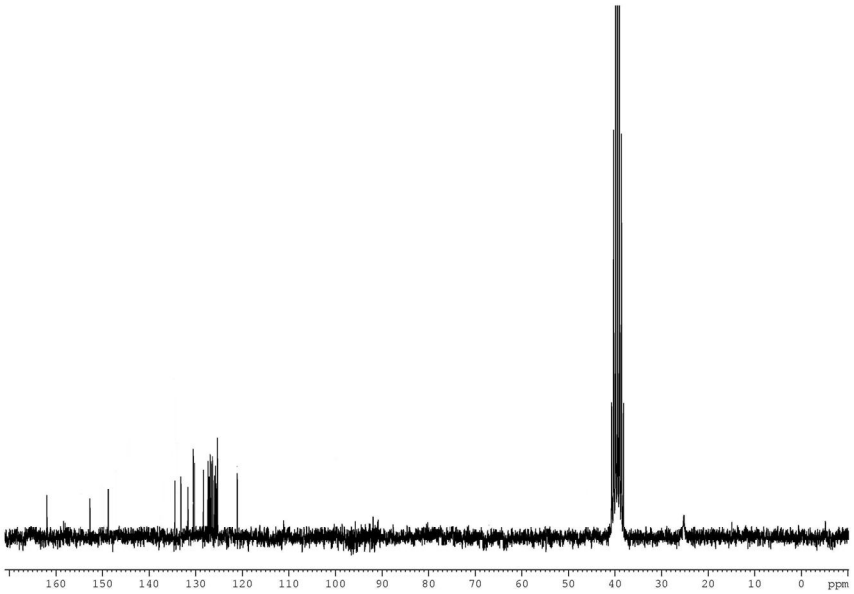
^{1}H NMR spectra of 2-(3,4-dichlorophenyl)quinazolin-4(3H)-one 3f.



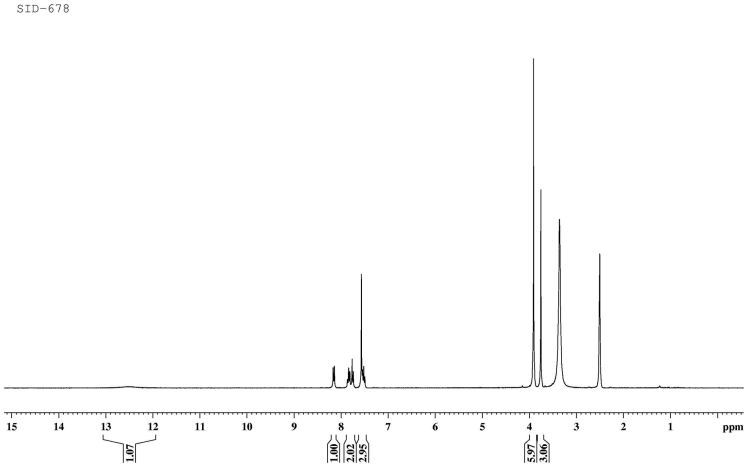
^{13}C NMR spectra of 2-(3,4-dichlorophenyl)quinazolin-4(3H)-one 3f.



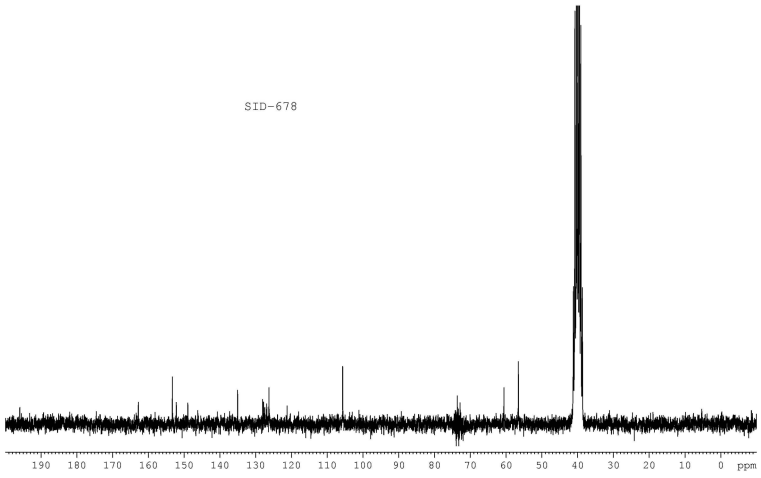
^{1}H NMR spectra of 2-(Naphthalen-1-yl)quinazolin-4(3H)-one 3g.



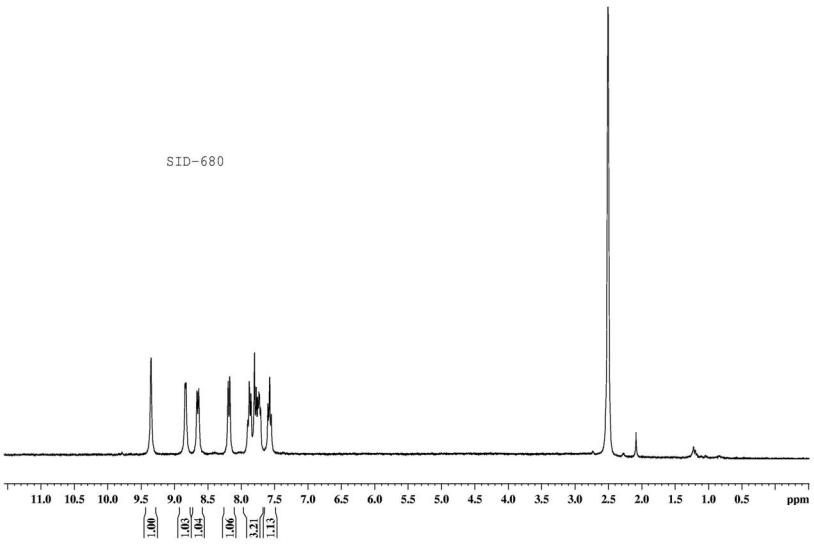
^{13}C NMR spectra of 2-(Naphthalen-1-yl)quinazolin-4(3H)-one 3g.



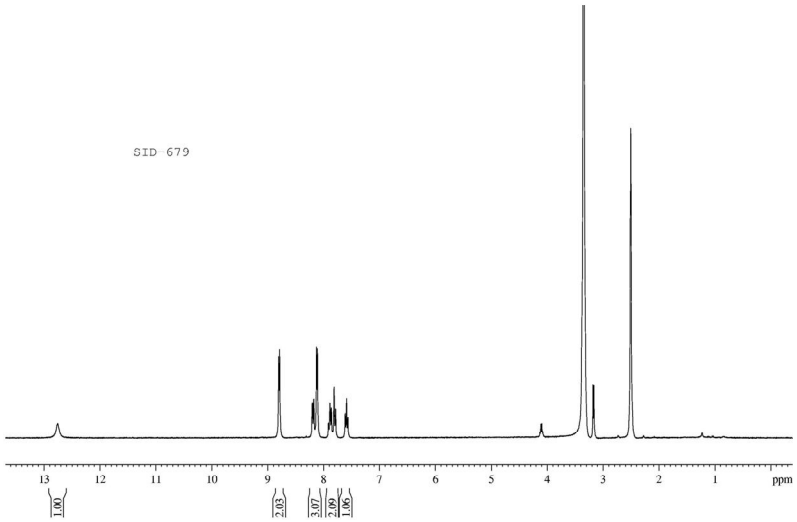
^{1}H NMR spectra of 2-(3,4,5-trimethoxyphenyl)quinazolin-4(3H)-one 3h.



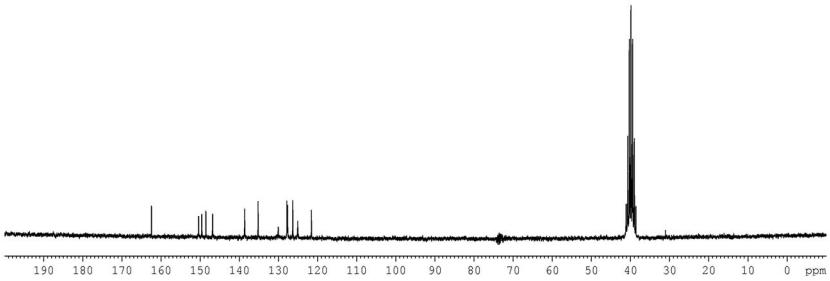
^{13}NMR spectra of 2-(3,4,5-trimethoxyphenyl)quinazolin-4(3H)-one 3h.



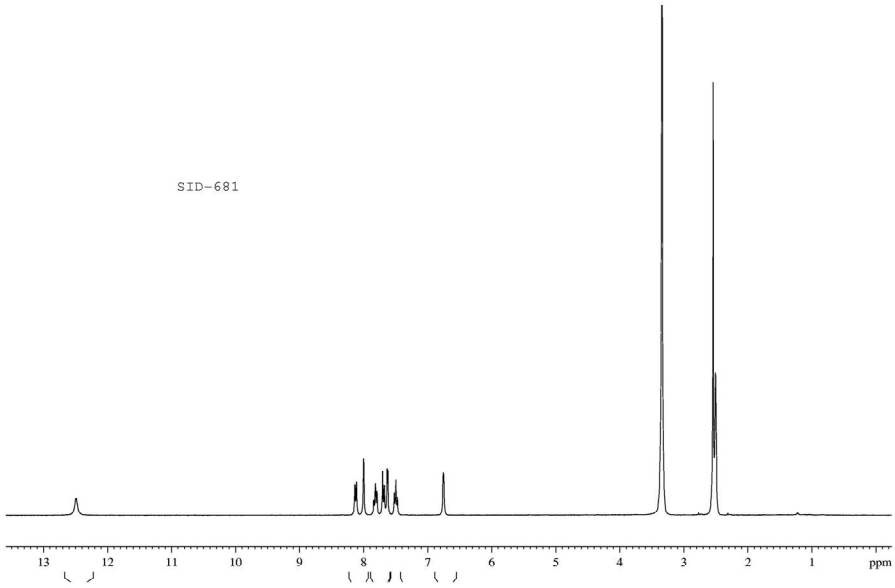
^{1}H NMR spectra of 2-(Pyridin-3-yl)quinazolin-4(3H)-one 3i.



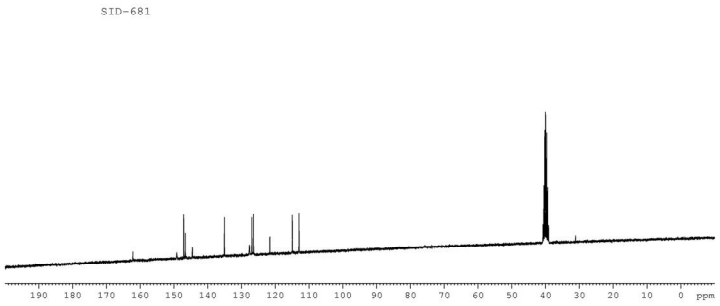
^{1}H NMR spectra of 2-(Pyridin-4-yl)quinazolin-4(3H)-one 3j.



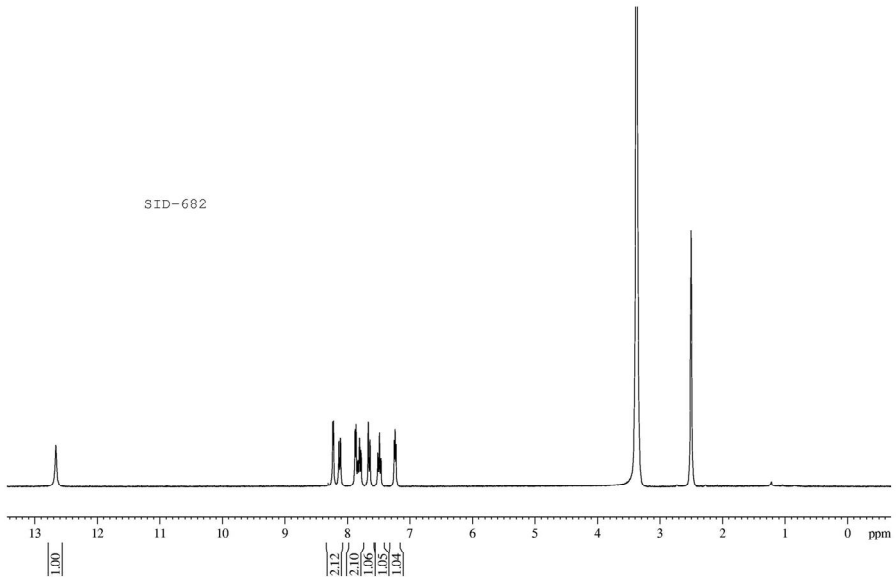
^{13}C NMR spectra of 2-(Pyridin-4-yl)quinazolin-4(3H)-one 3j.



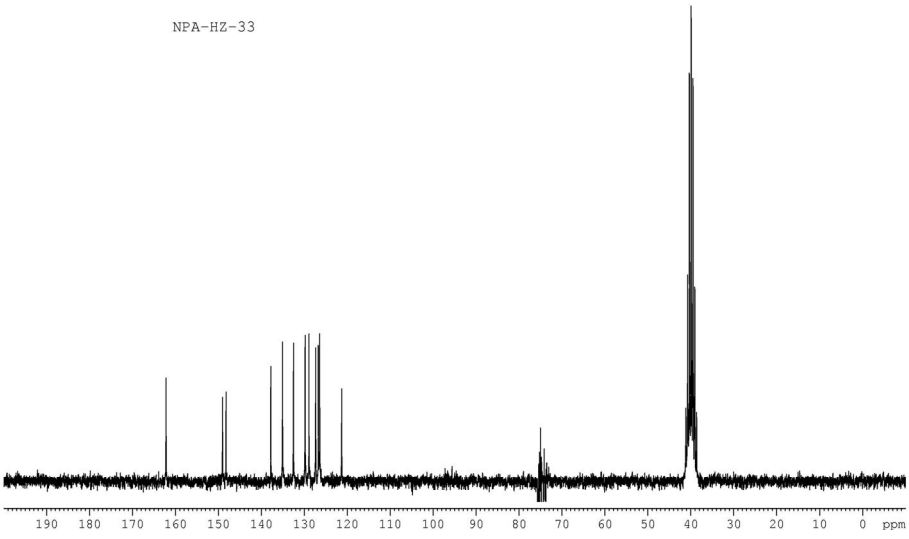
^{1}H NMR spectra of 2-(Furan-2-yl)quinazolin-4(3H)-one 3k.



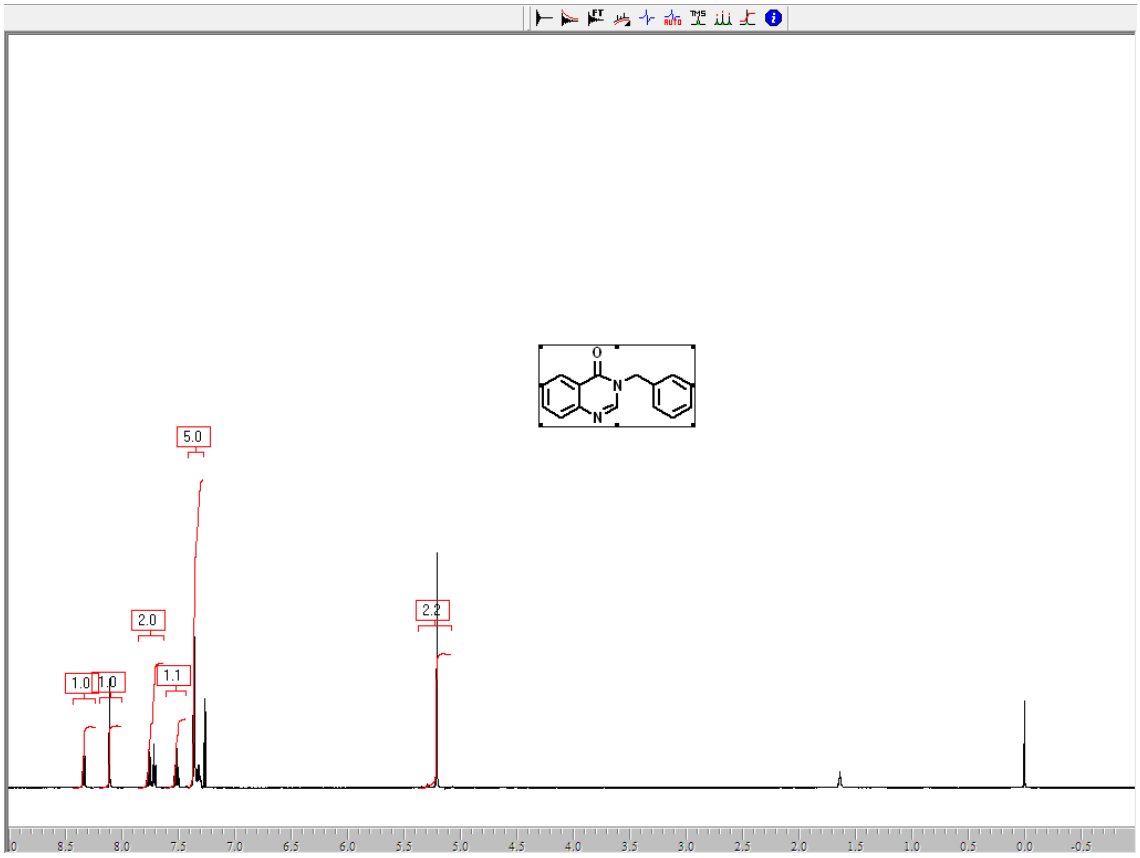
^{13}C NMR spectra of 2-(Furan-2-yl)quinazolin-4(3H)-one 3k.



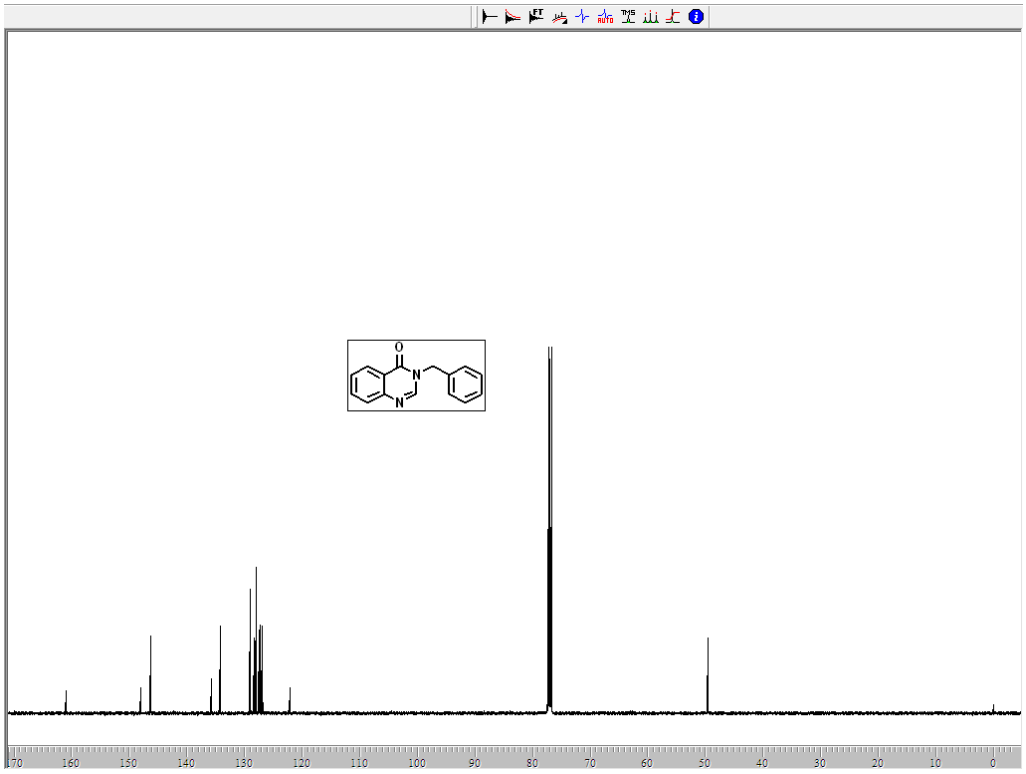
^{1}H NMR spectra of 2-(Thiophen-2-yl)quinazolin-4(3H)-one 3l.



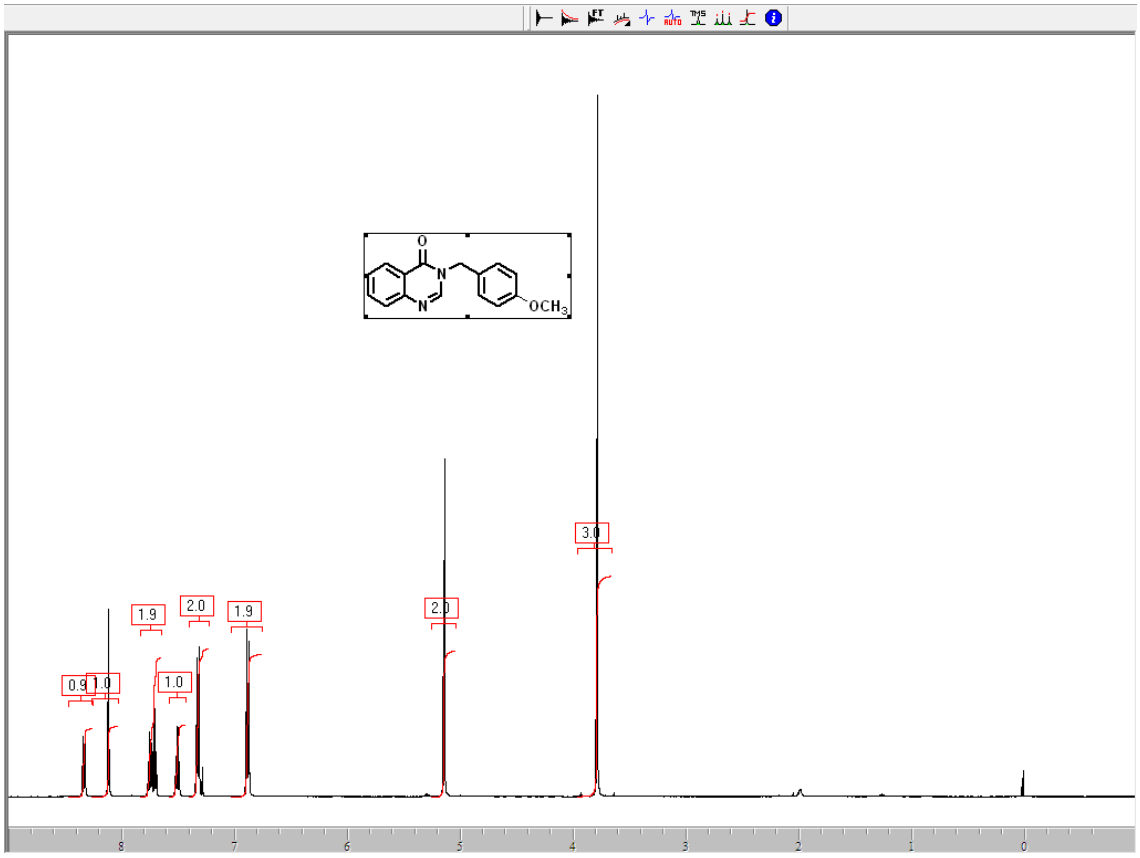
^{13}C NMR spectra of 2-(Thiophen-2-yl)quinazolin-4(3H)-one 3l.



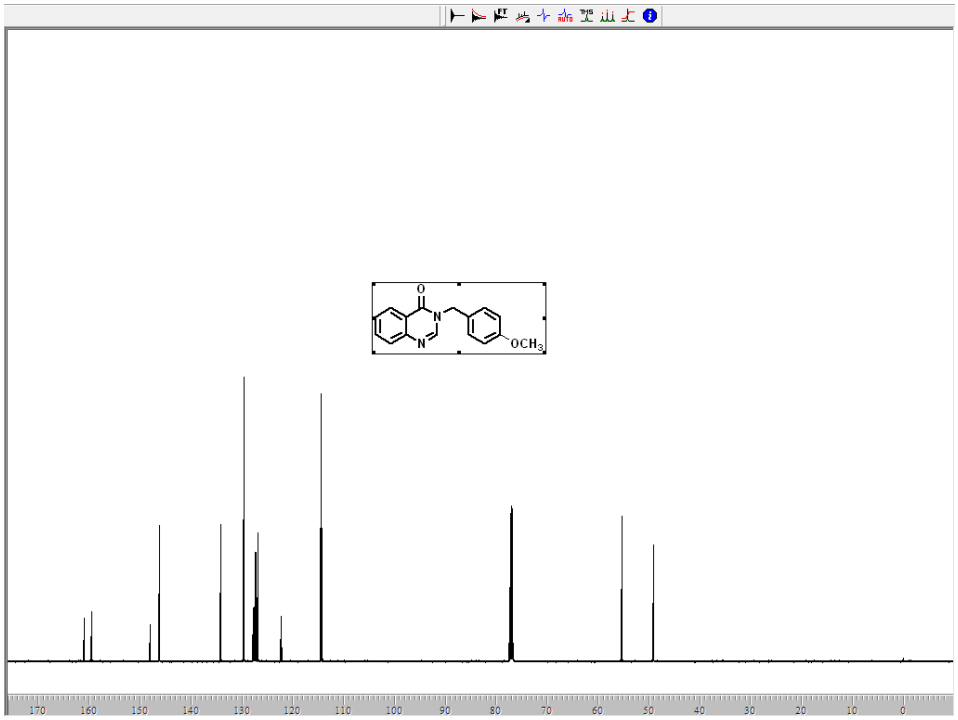
^{1}H NMR spectra of 3-benzylquinazolin-4(3H)-one 5a.



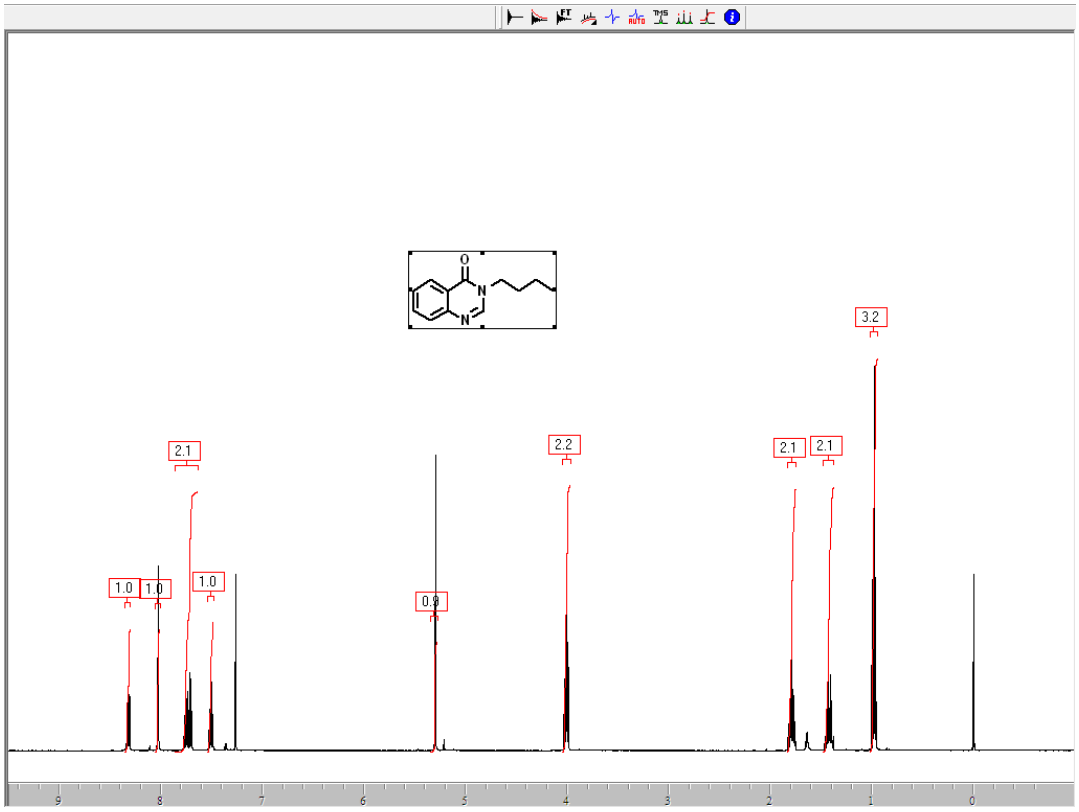
^{13}C NMR spectra of 3-benzylquinazolin-4(3H)-one 5a.



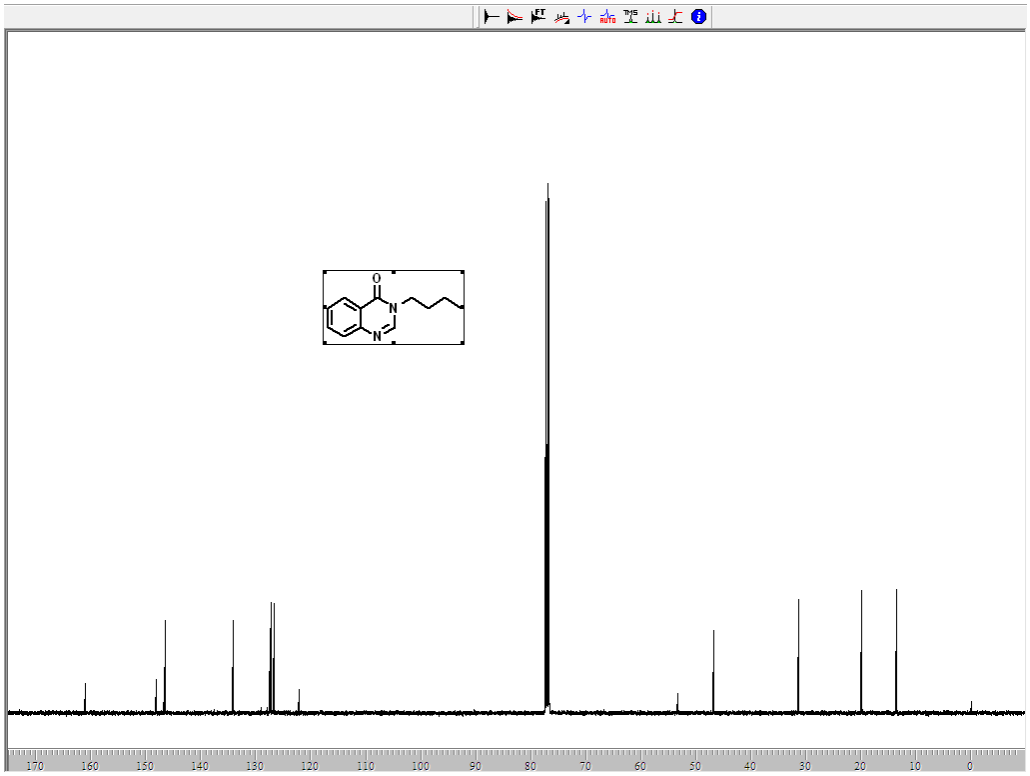
^{1}H NMR spectra of 3-(4-methoxybenzyl)quinazolin-4(3H)-one 5b.



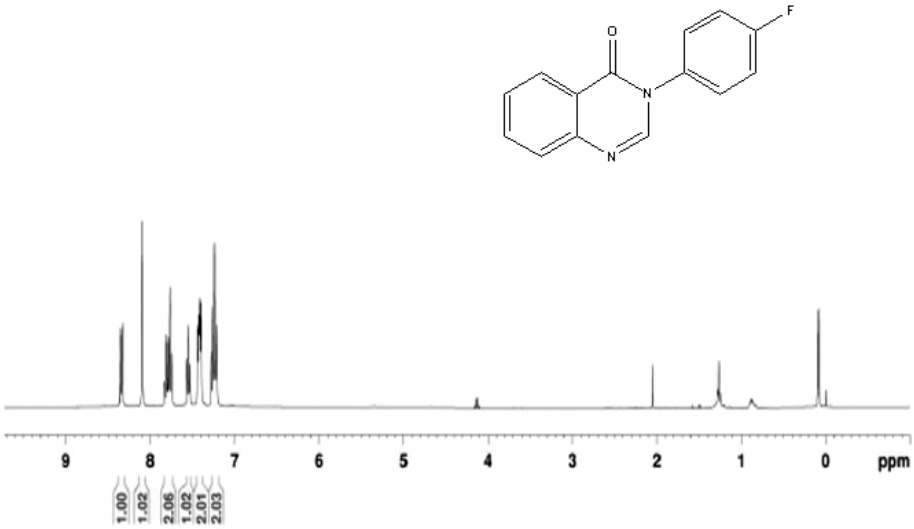
^{13}C NMR spectra of 3-(4-methoxybenzyl)quinazolin-4(3H)-one 5b.



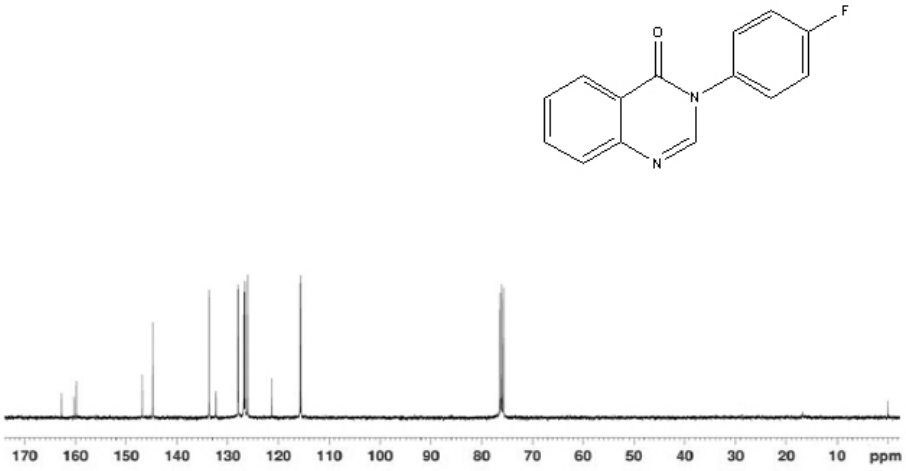
^{1}H NMR spectra of 3-butylquinazolin-4(3H)-one 5c:



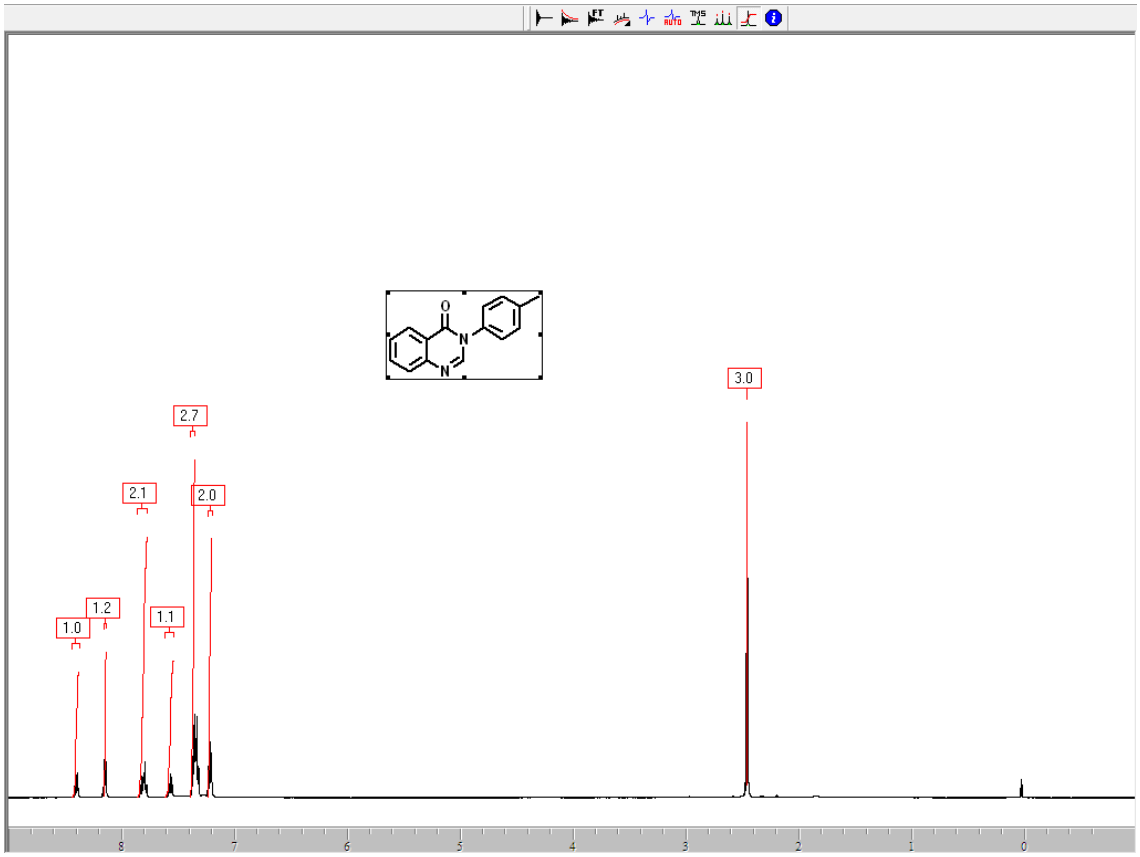
^{13}C NMR spectra of 3-butylquinazolin-4(3H)-one 5c:



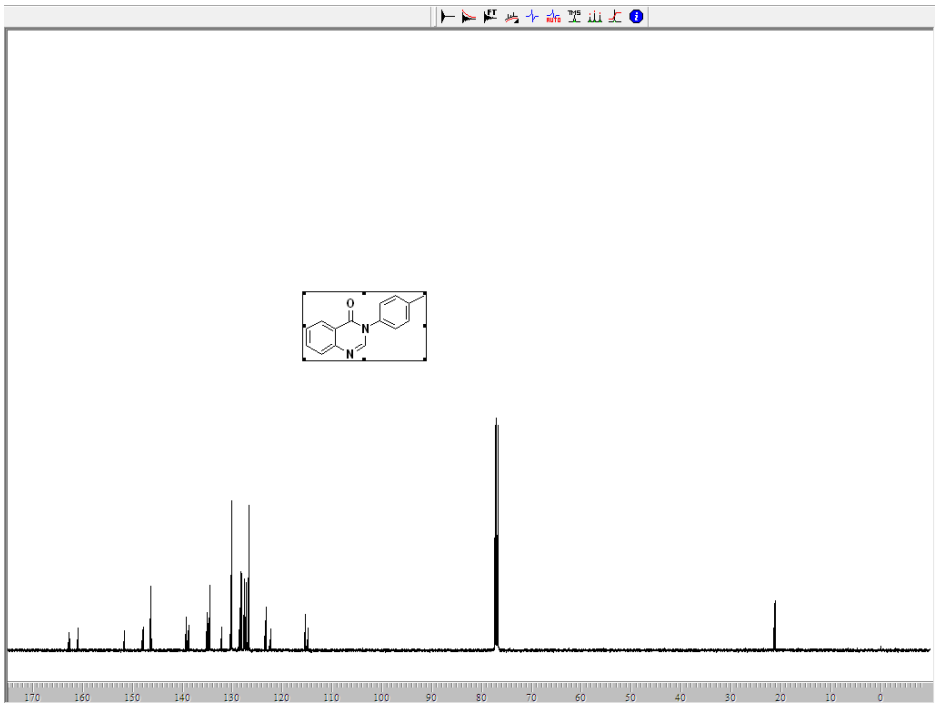
^{1}H NMR of 3-(4-fluorophenyl)quinazolin-4(3H)-one 5d.



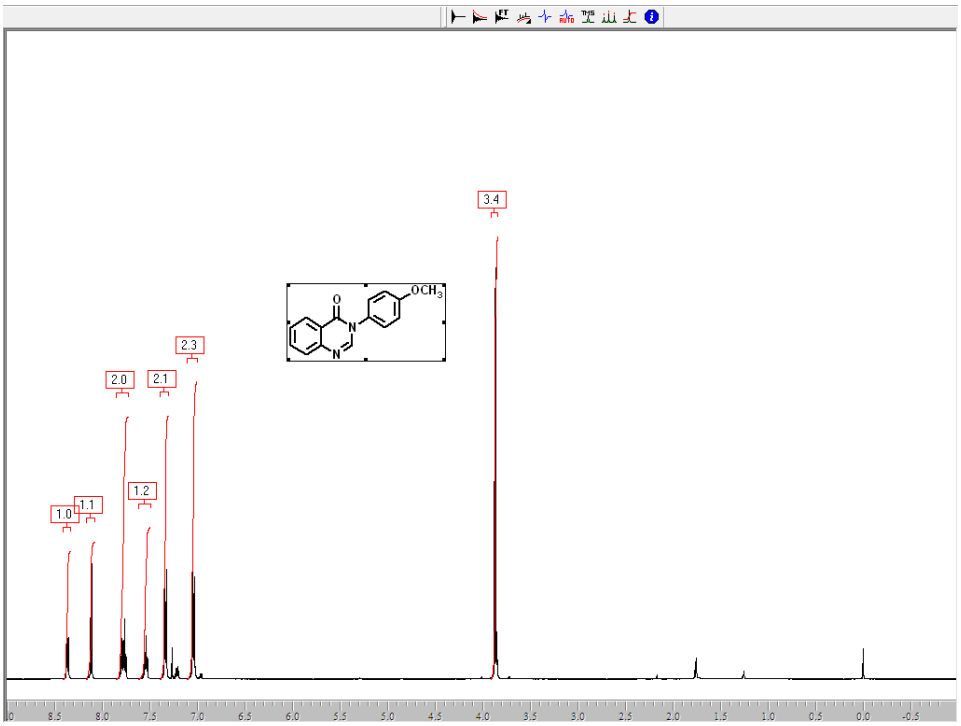
^{13}C NMR of 3-(4-fluorophenyl)quinazolin-4(3H)-one 5d.



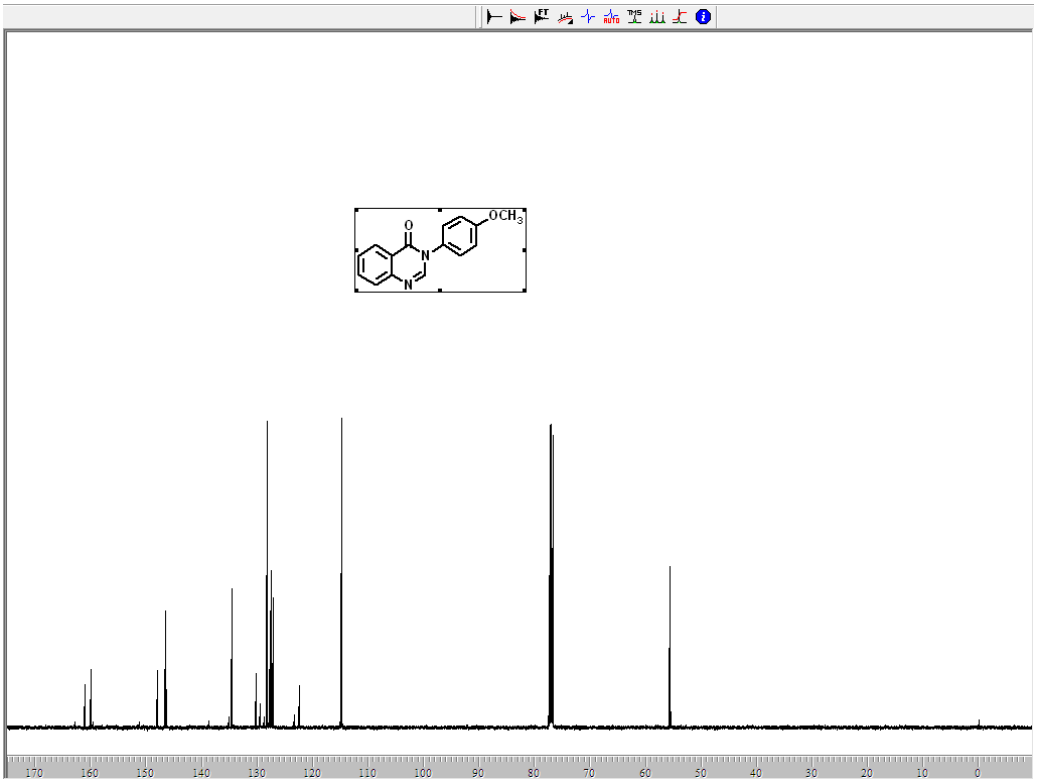
^{1}H NMR of 3-p-tolylquinazolin-4(3H)-one 5e.



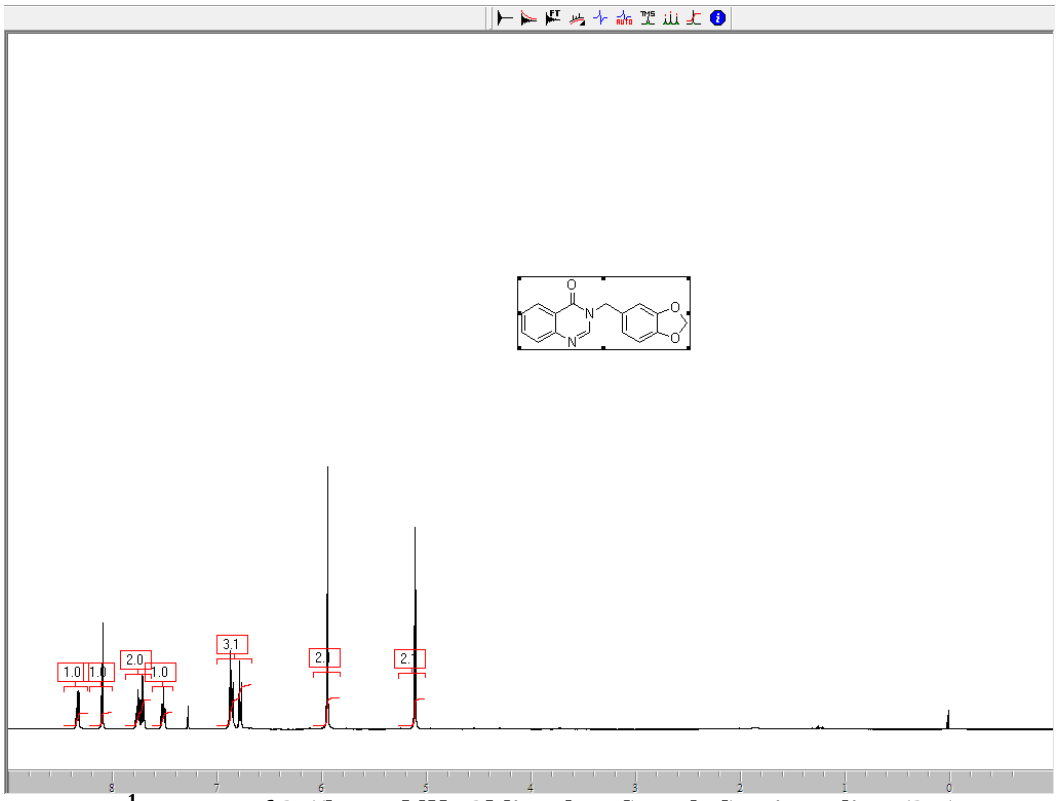
^{13}C NMR of 3-p-tolylquinazolin-4(3H)-one 5e.



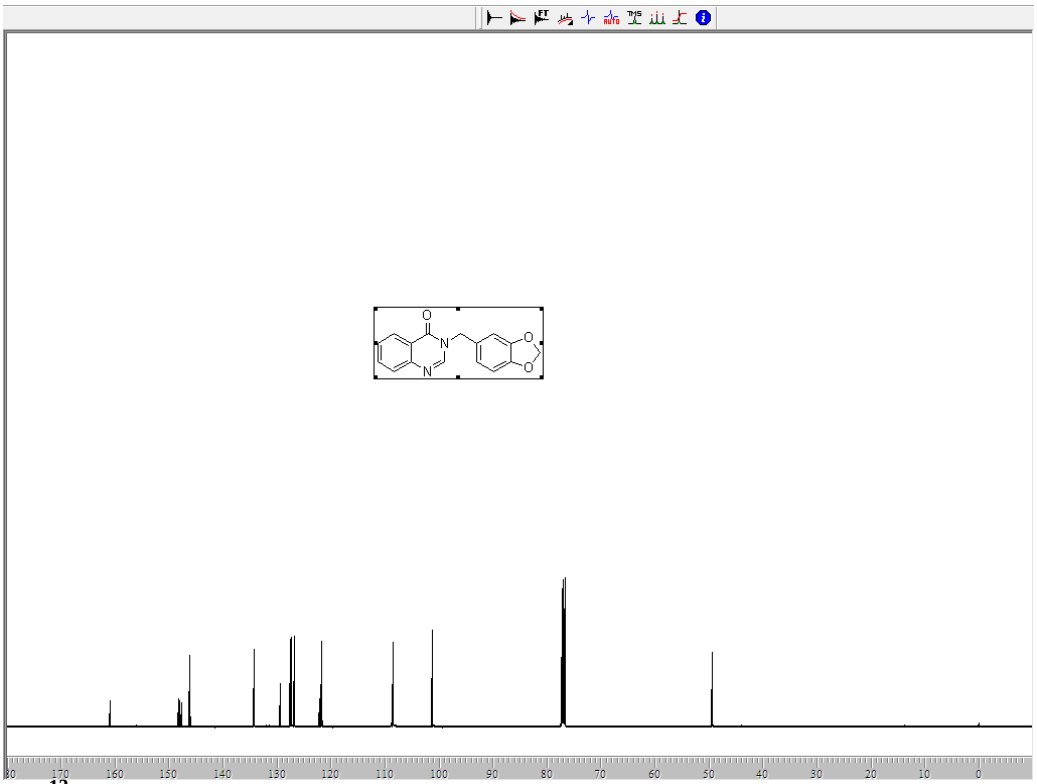
^{1}H NMR of 3-(4-Methoxyphenyl)quinazolin-4(3H)-one 5f.



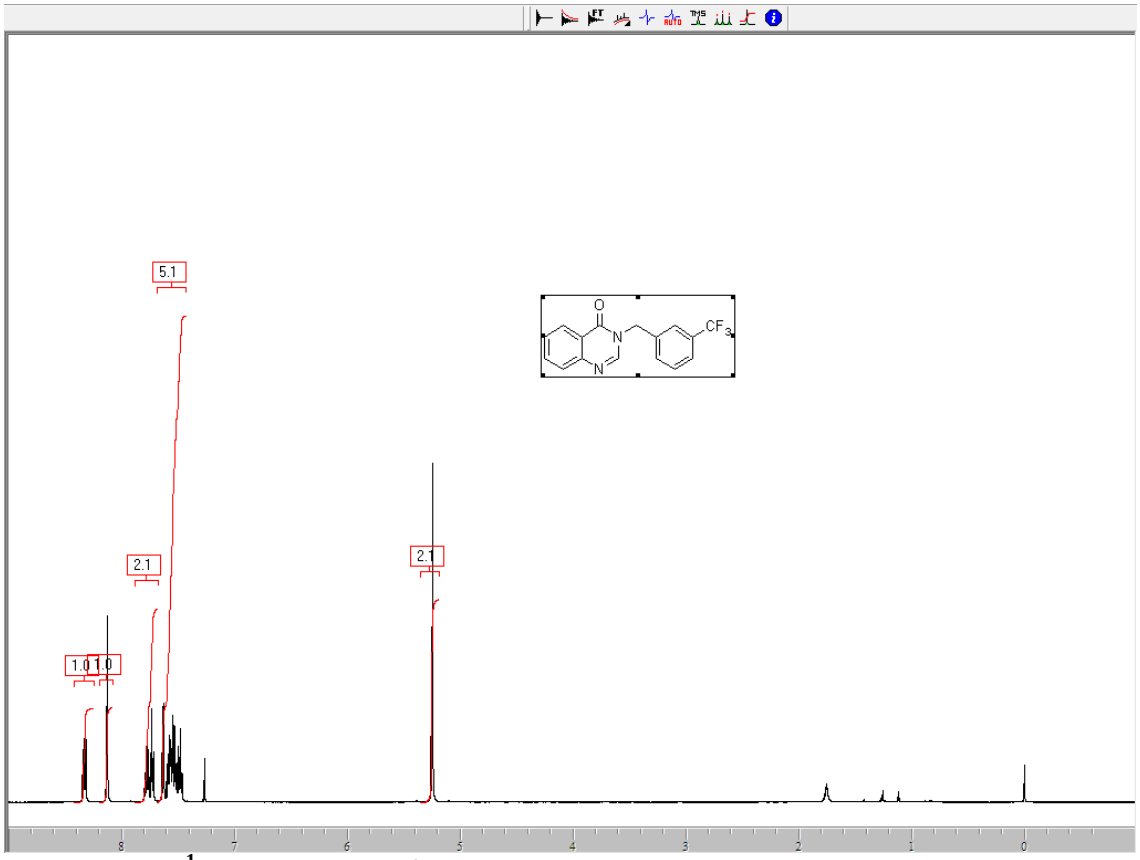
^{13}C NMR of 3-(4-Methoxyphenyl)quinazolin-4(3H)-one 5f.



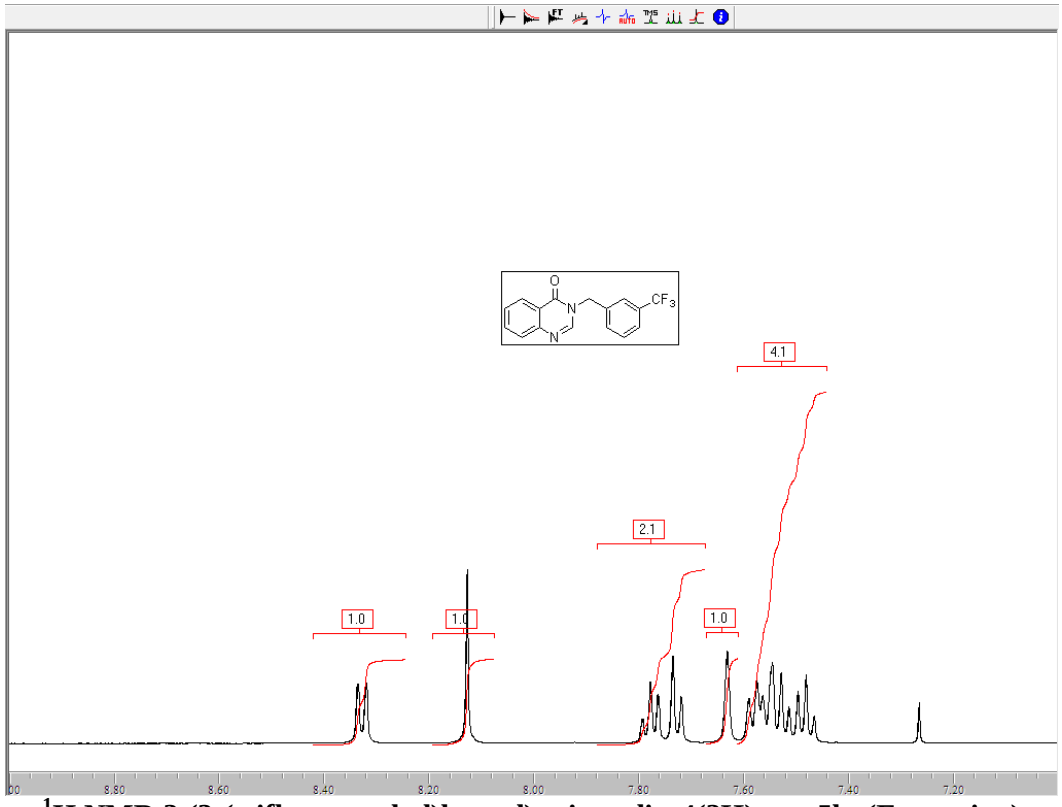
^{1}H NMR of 3-((benzo[d][1,3]dioxol-5-yl)methyl)quinazolin-4(3H)-one 5g.



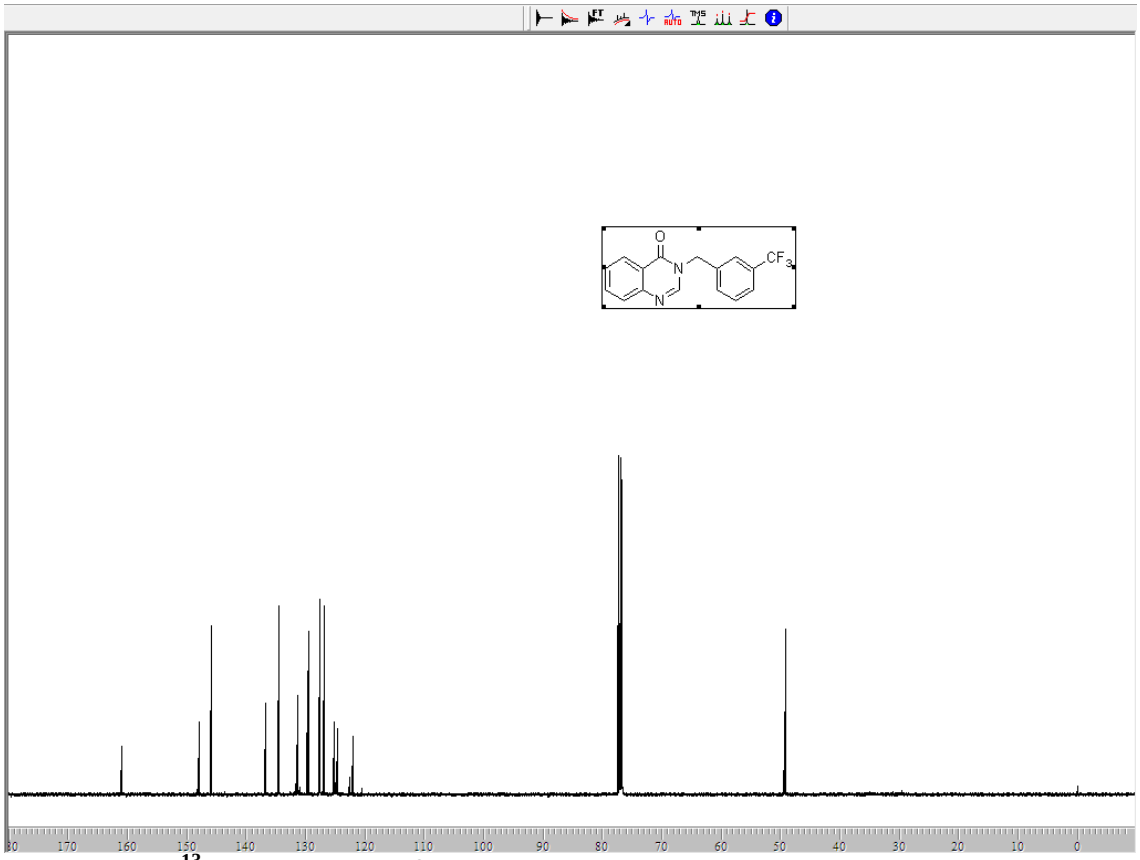
^{13}C NMR of 3-((benzo[d][1,3]dioxol-5-yl)methyl)quinazolin-4(3H)-one 5g.



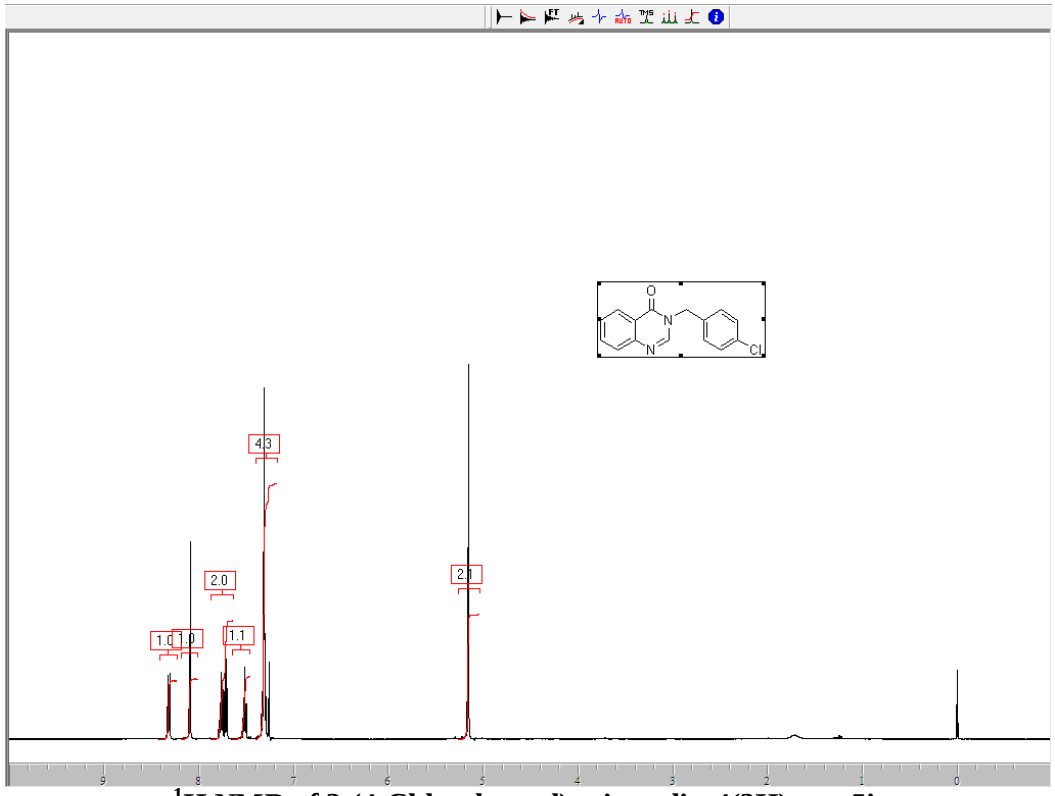
^{1}H NMR 3-(3-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5h:



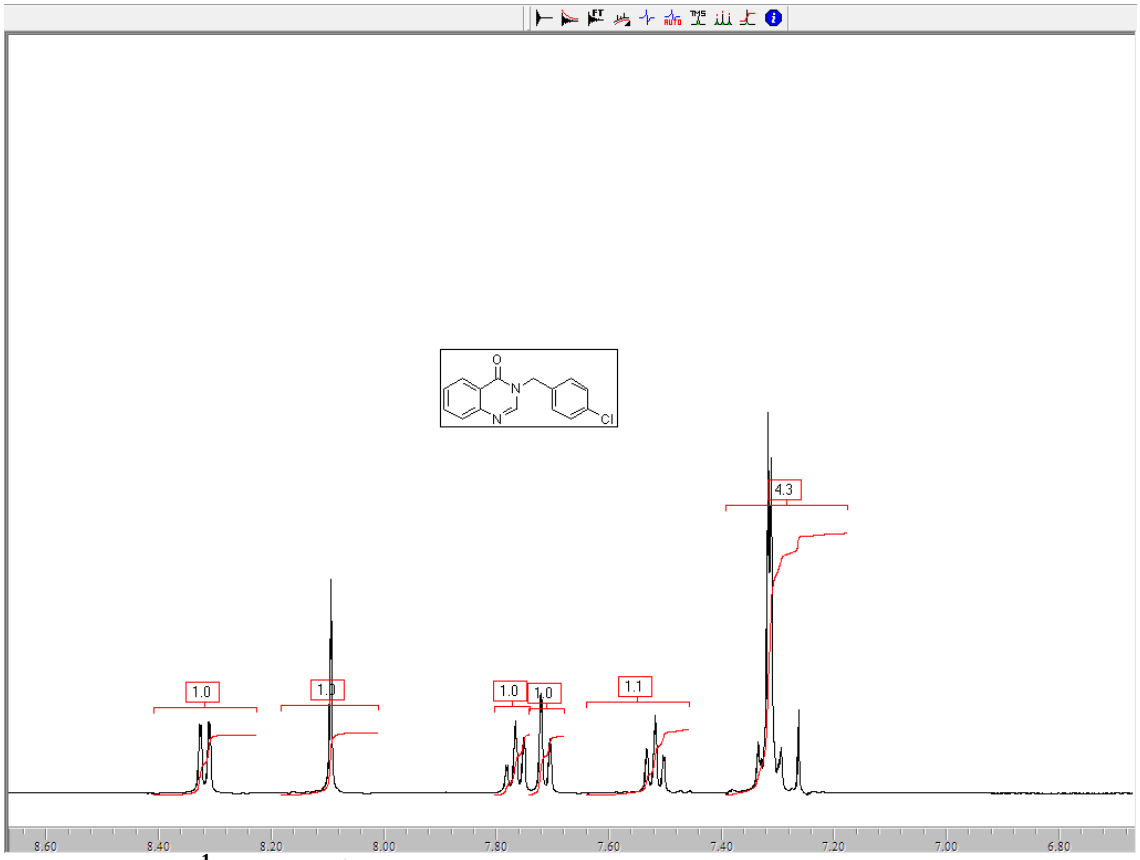
^{1}H NMR 3-(3-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5h: (Expansion)



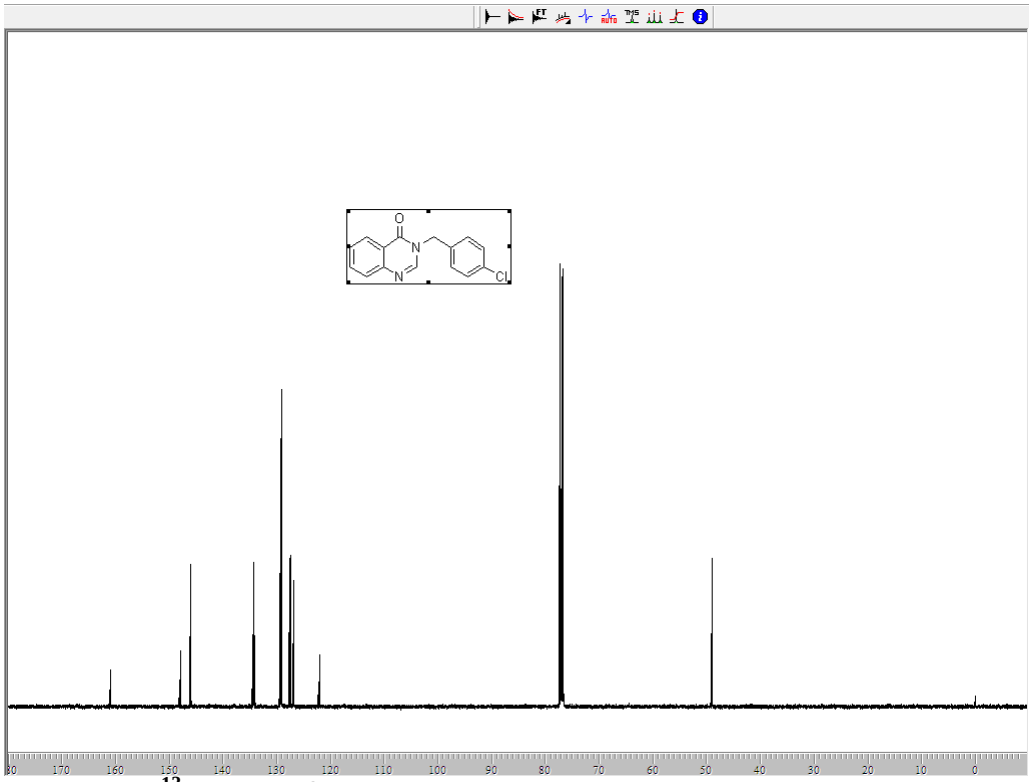
^{13}C NMR 3-(3-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5h:



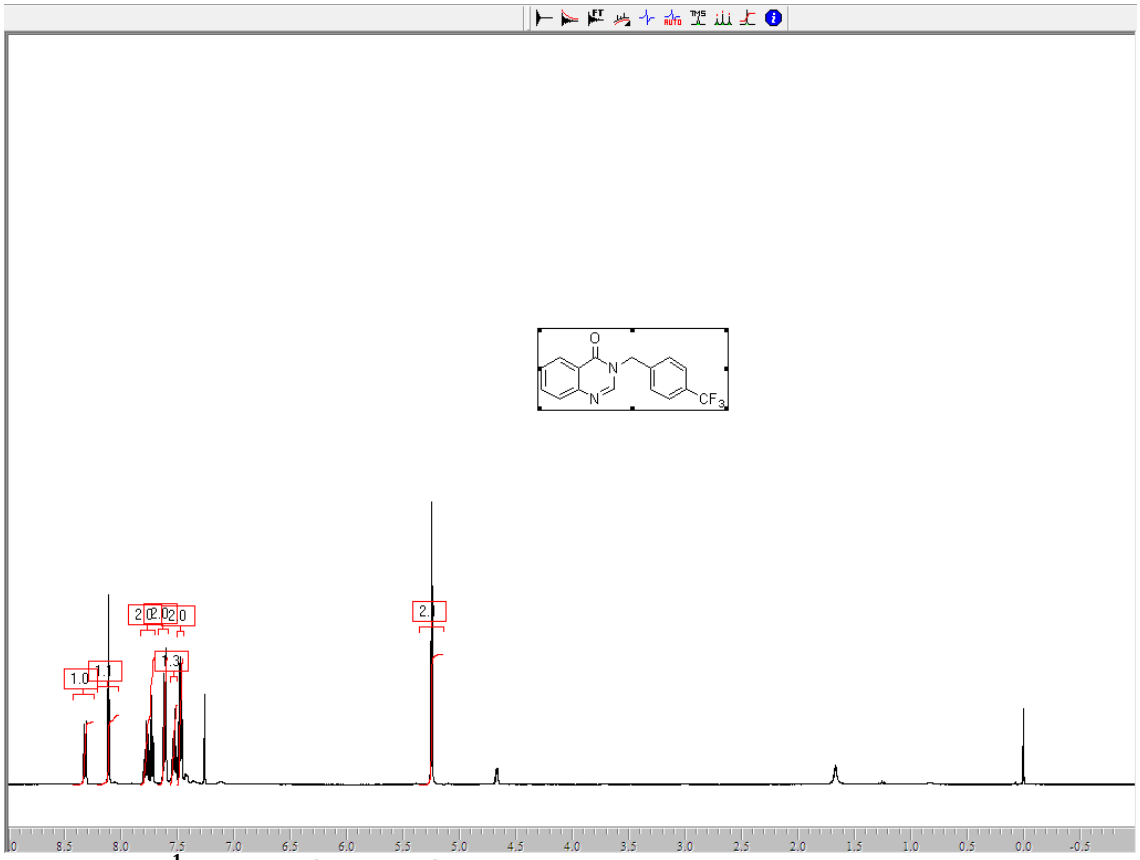
^{1}H NMR of 3-(4-Chlorobenzyl)quinazolin-4(3H)-one 5i:



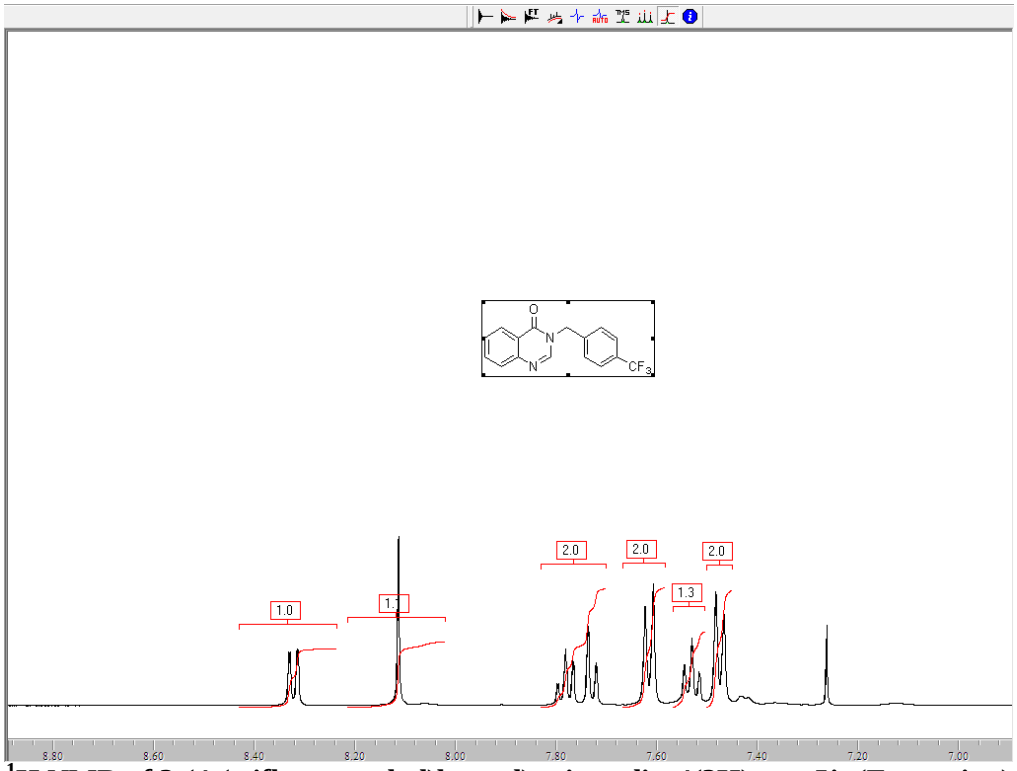
^{1}H NMR of 3-(4-Chlorobenzyl)quinazolin-4(3H)-one 5i: (Expansion)



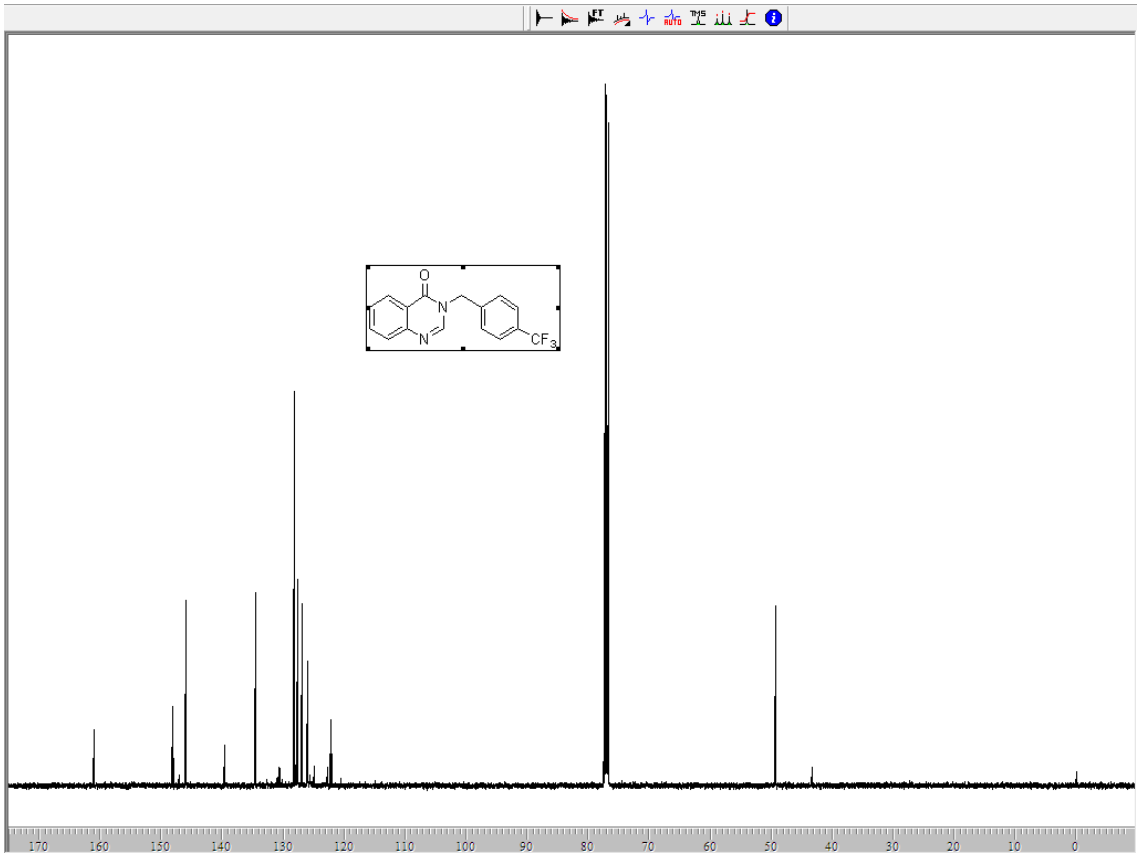
^{13}C NMR of 3-(4-chlorobenzyl)quinazolin-4(3H)-one 5i:



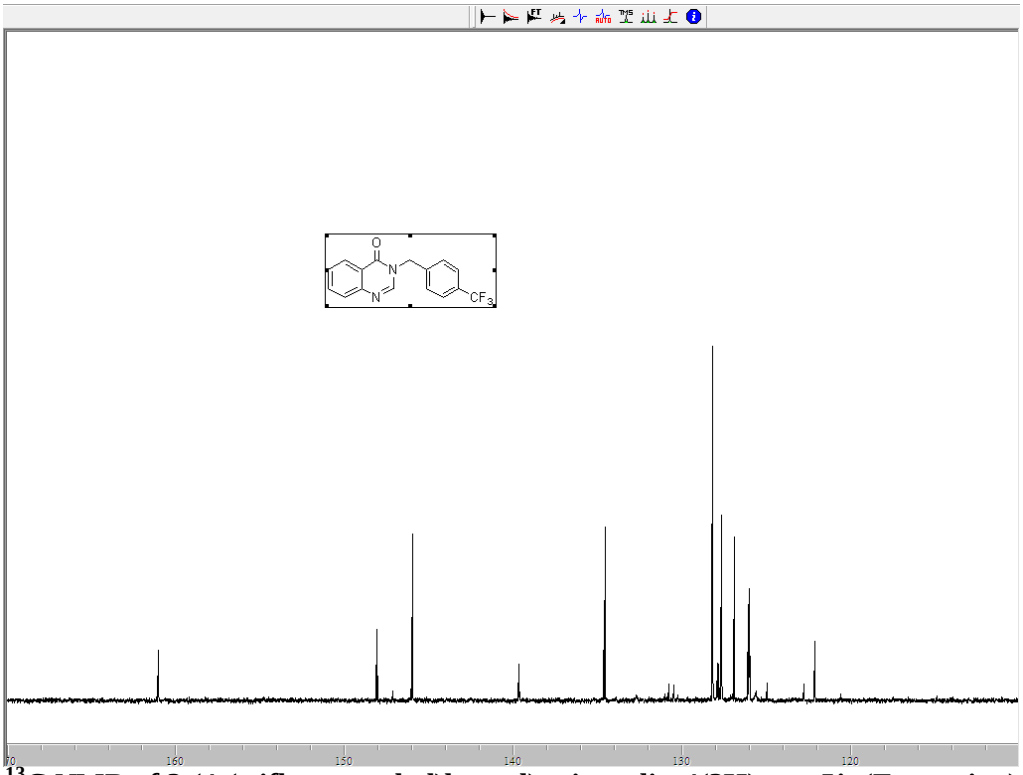
^{1}H NMR of 3-(4-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5j:



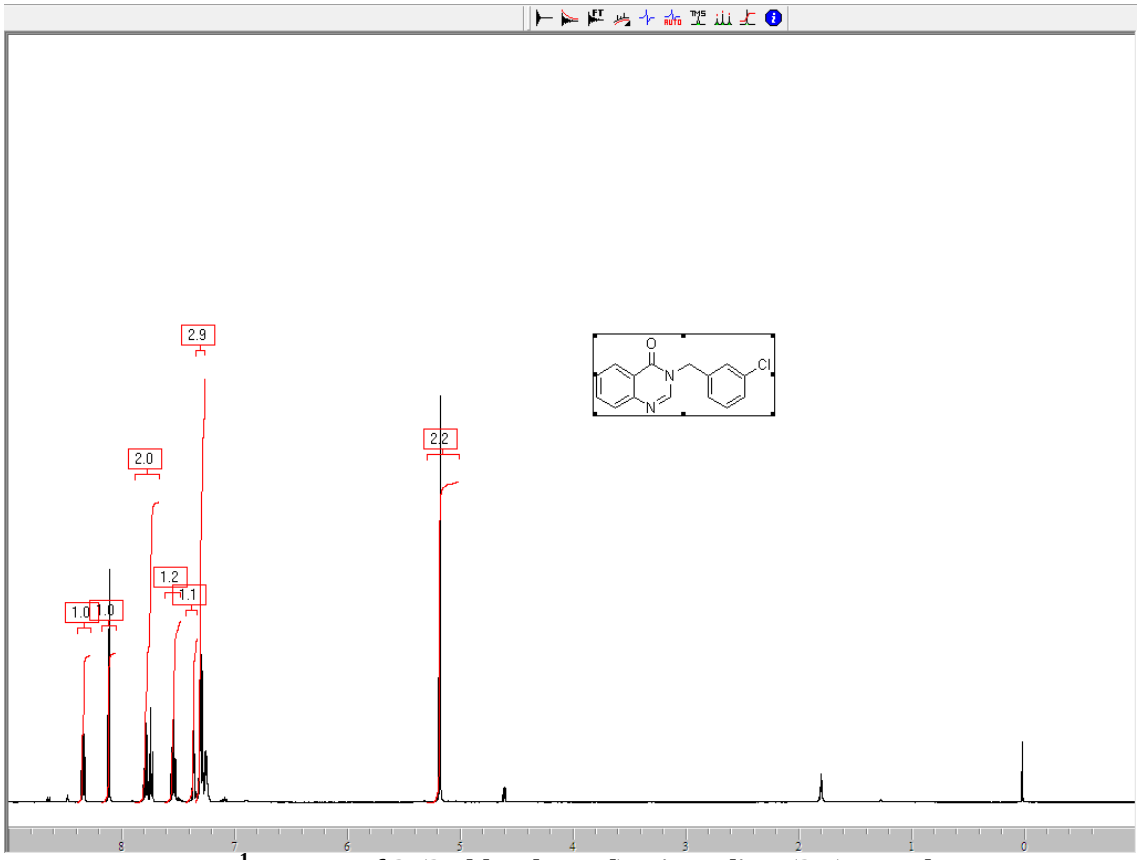
^{1}H NMR of 3-(4-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5j: (Expansion)



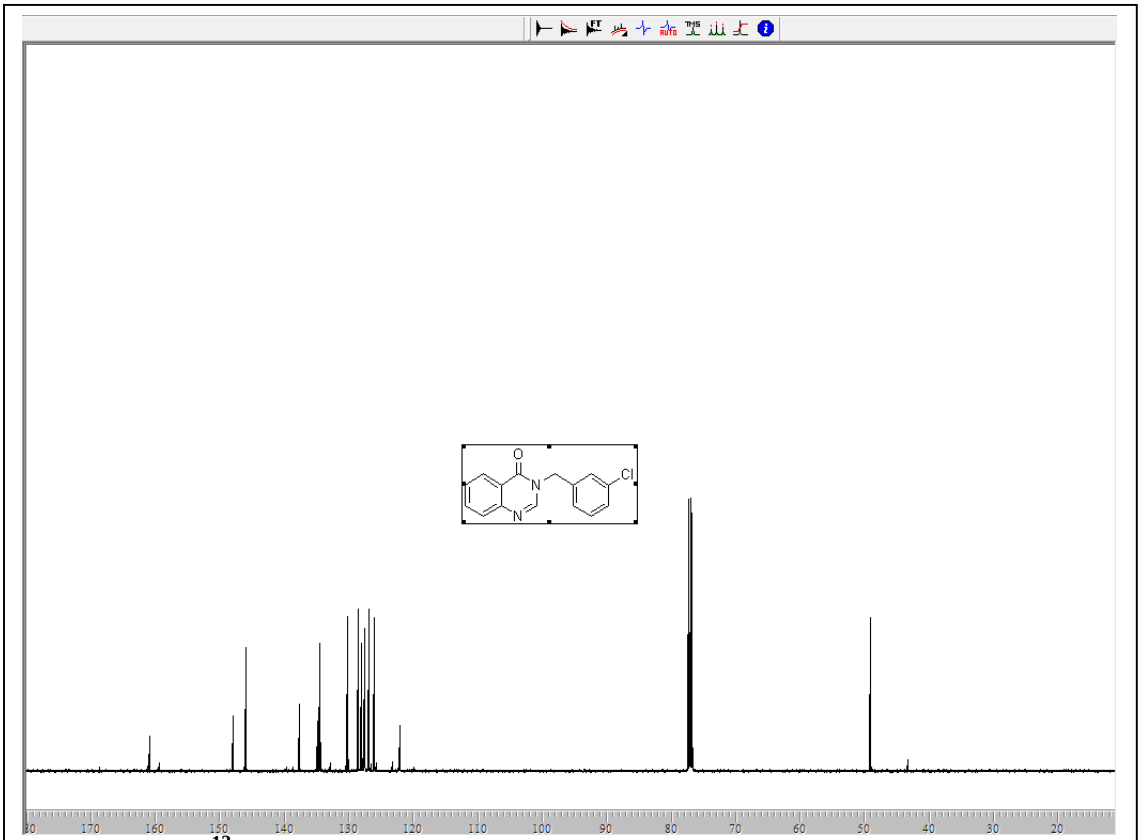
^{13}C NMR of 3-(4-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5j:



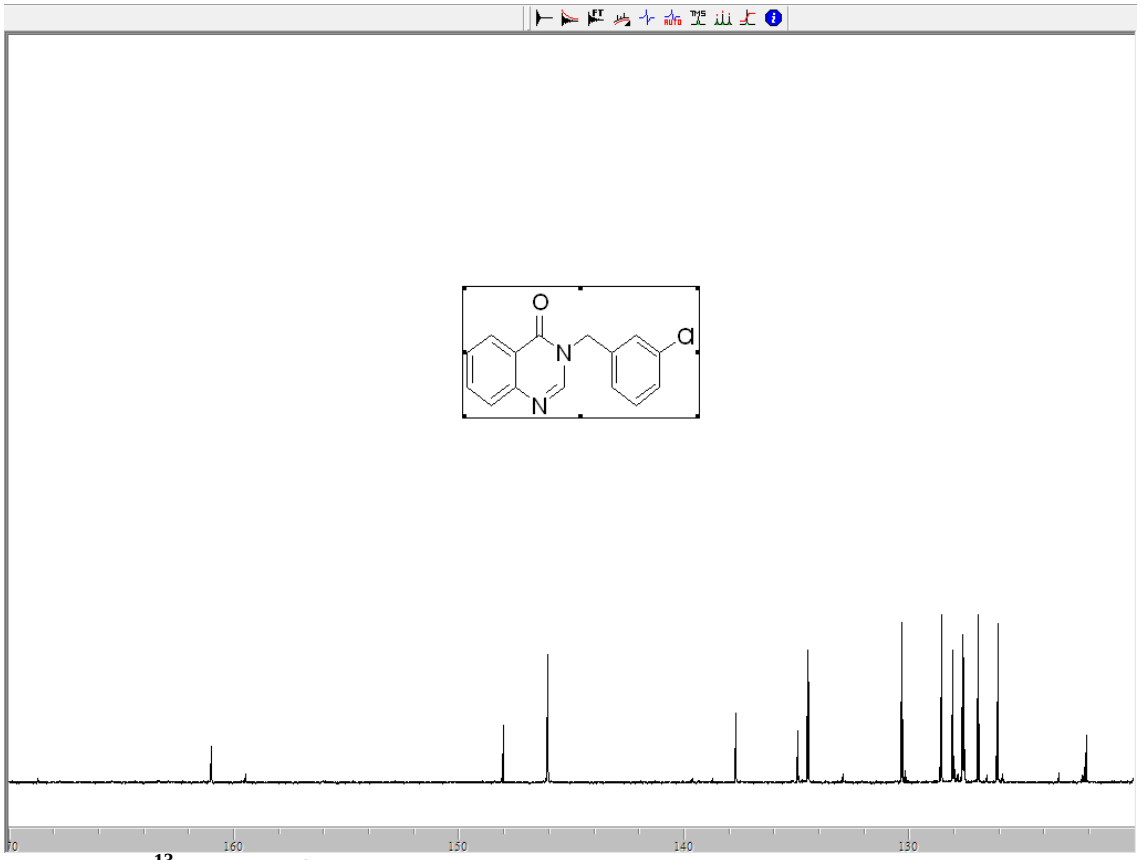
^{13}C NMR of 3-(4-(trifluoromethyl)benzyl)quinazolin-4(3H)-one 5j: (Expansion)



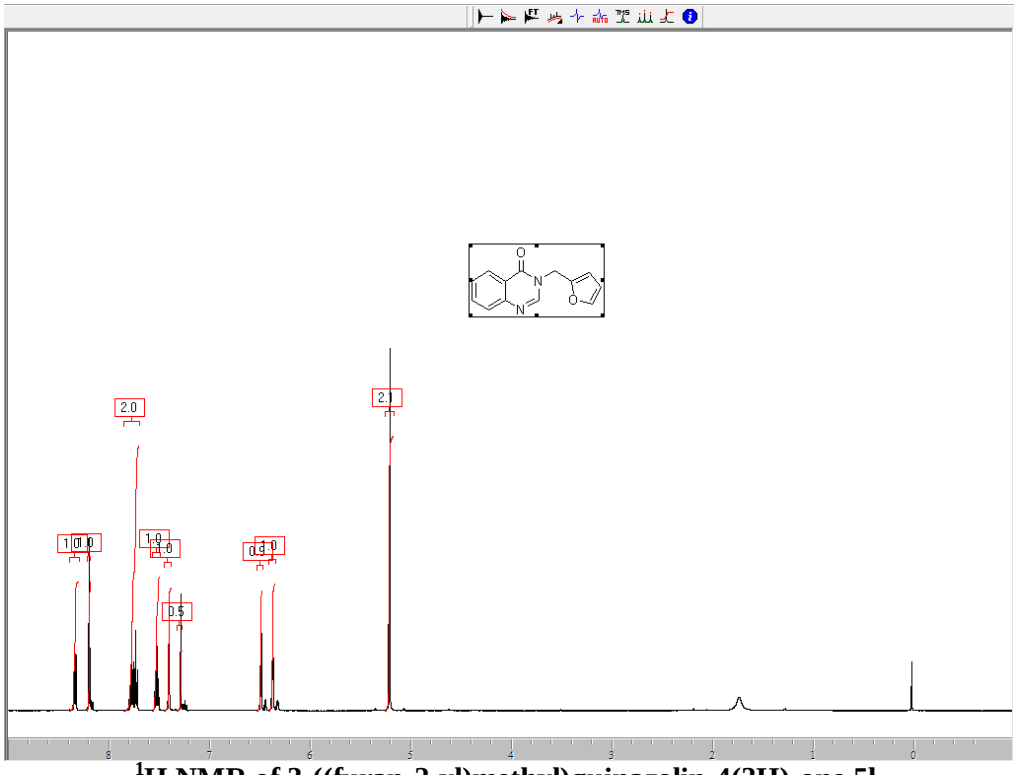
^{1}H NMR of 3-(3-chlorobenzyl)quinazolin-4(3H)-one 5k.



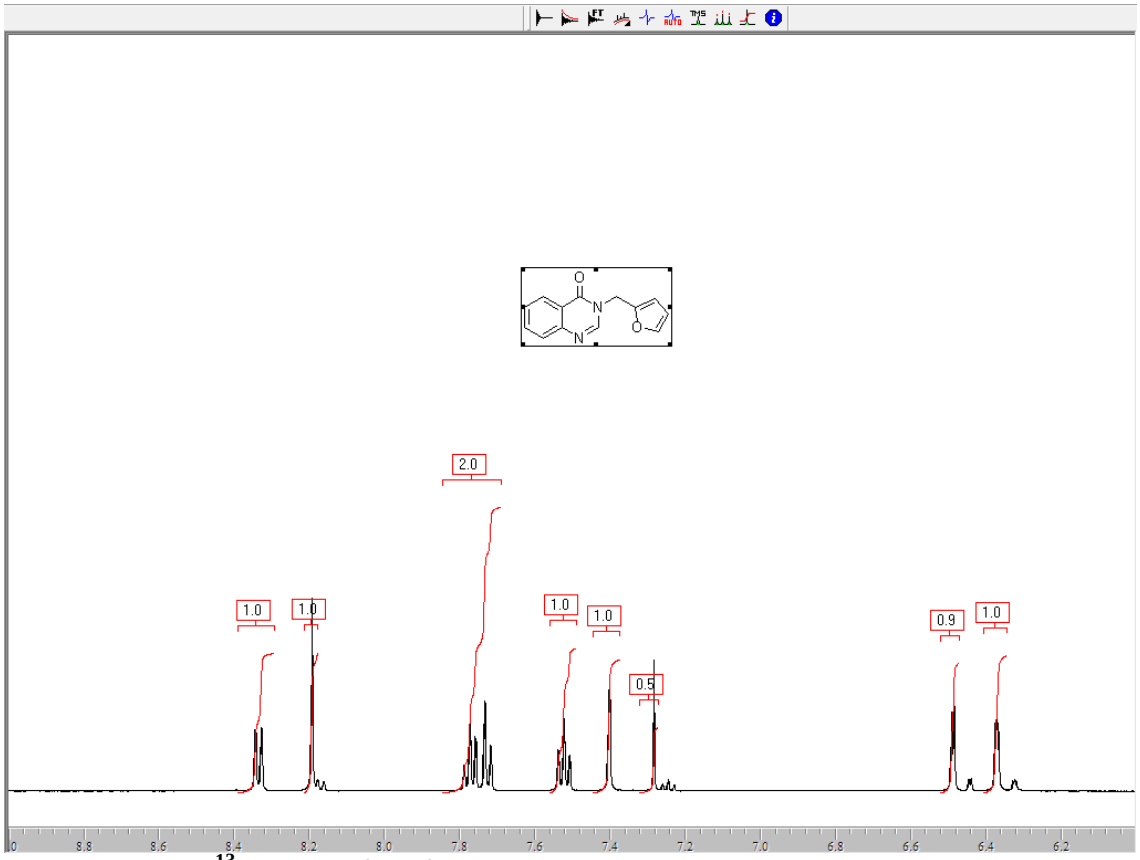
^{13}C NMR of 3-(3-chlorobenzyl)quinazolin-4(3H)-one 5k.



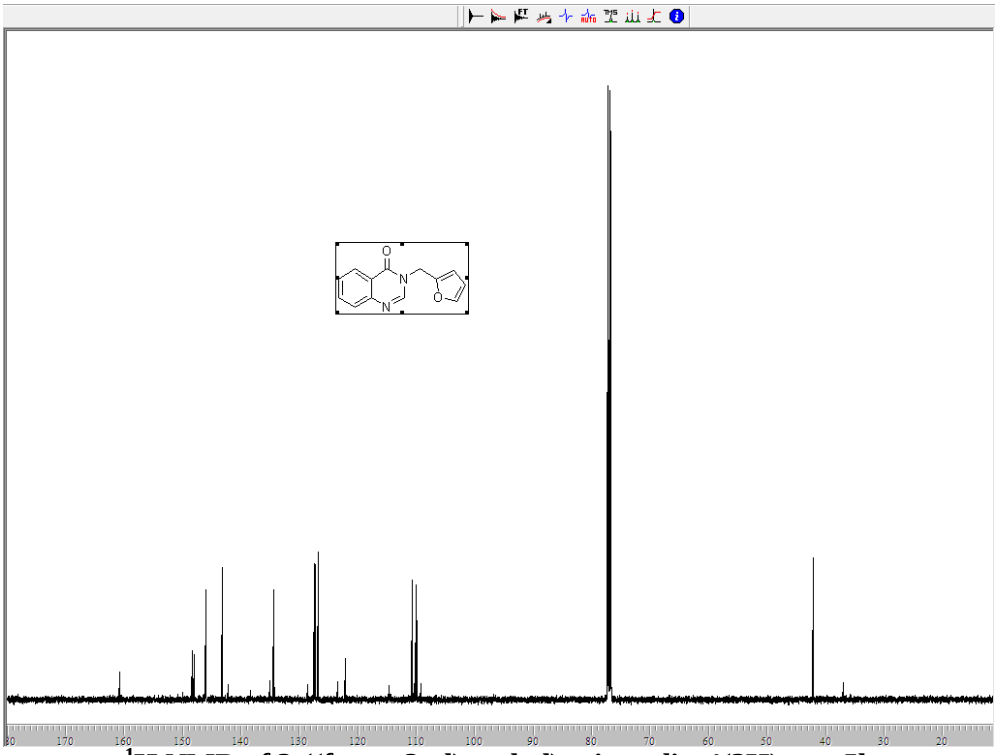
^{13}C NMR of 3-(3-chlorobenzyl)quinazolin-4(3H)-one 5k. (Expansion)



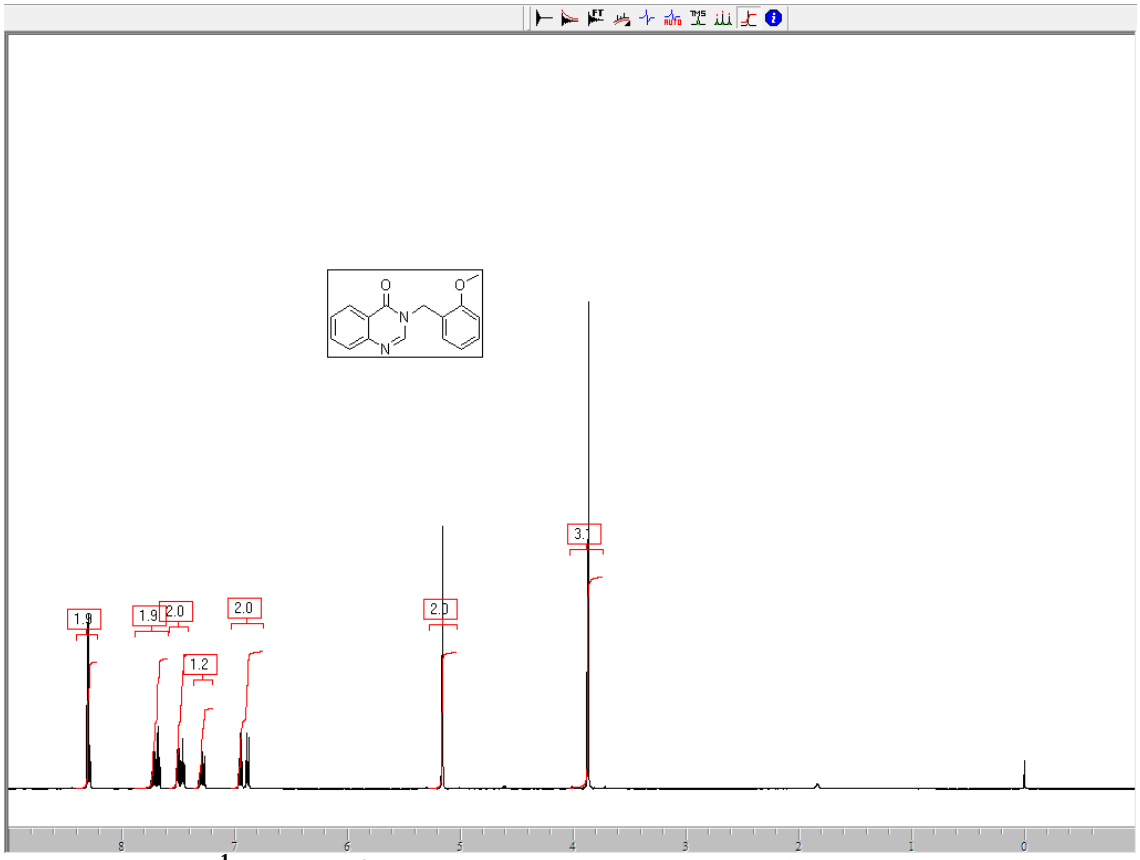
^{1}H NMR of 3-((furan-2-yl)methyl)quinazolin-4(3H)-one 5l.



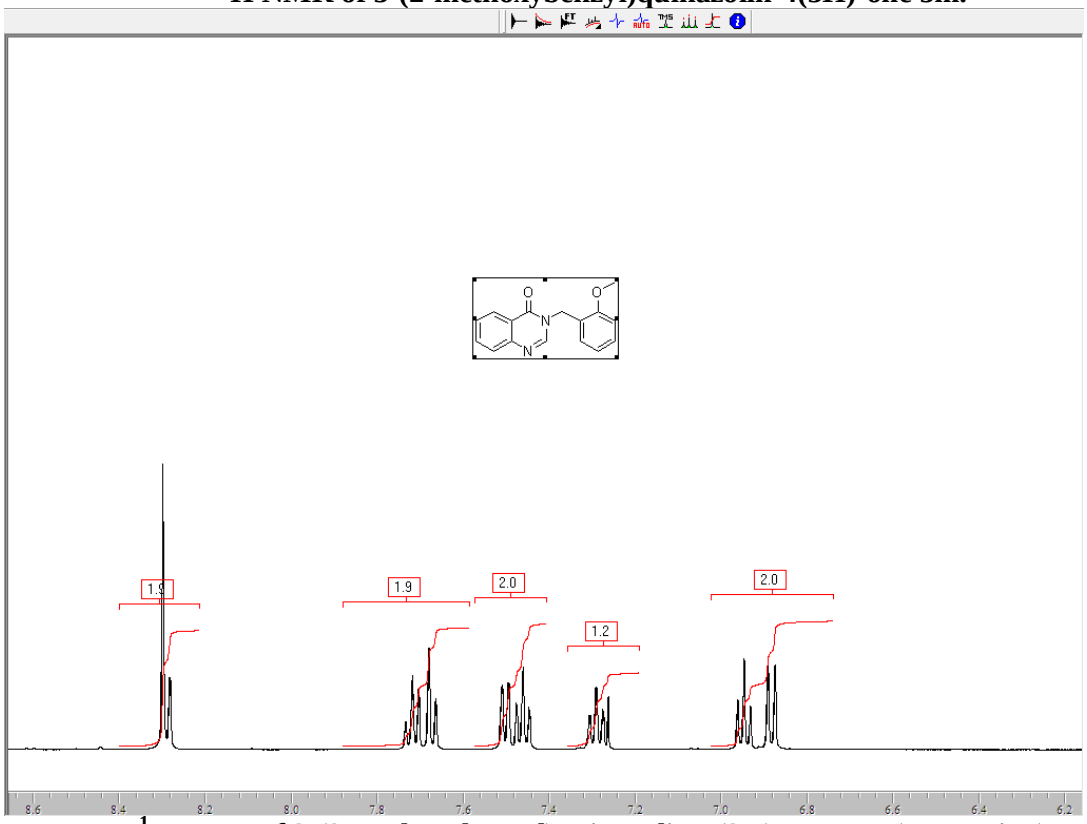
^{13}C NMR of 3-((furan-2-yl)methyl)quinazolin-4(3H)-one 5l.



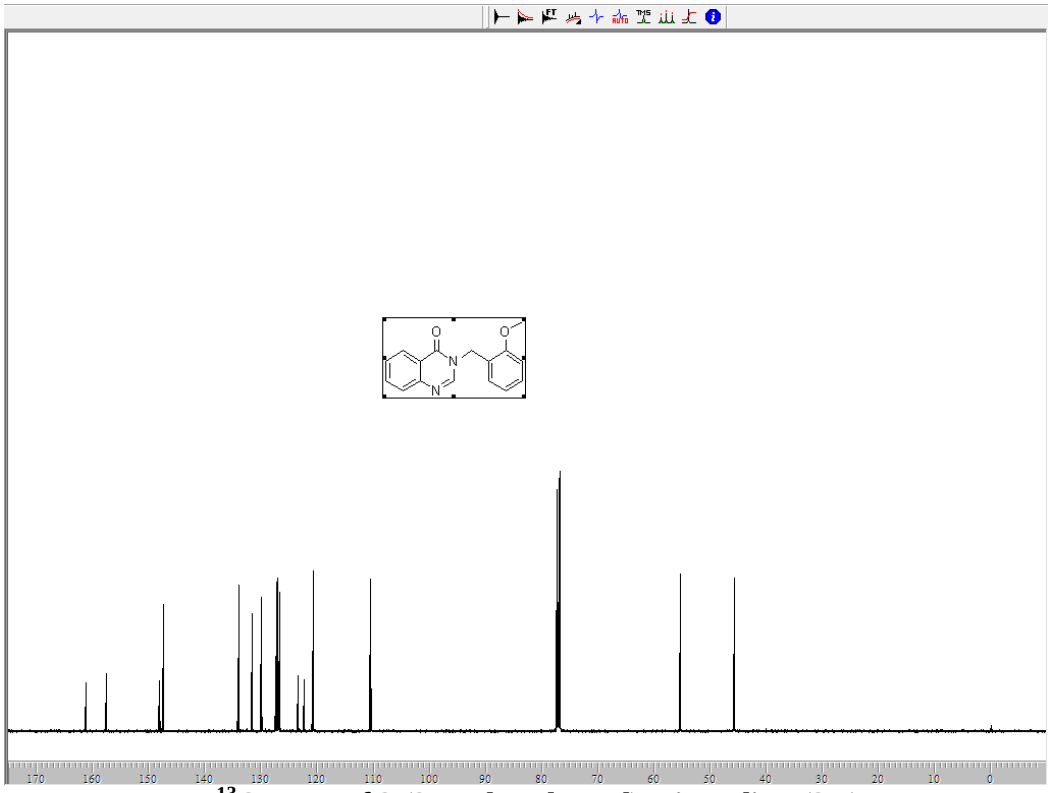
^{1}H NMR of 3-((furan-2-yl)methyl)quinazolin-4(3H)-one 5l.



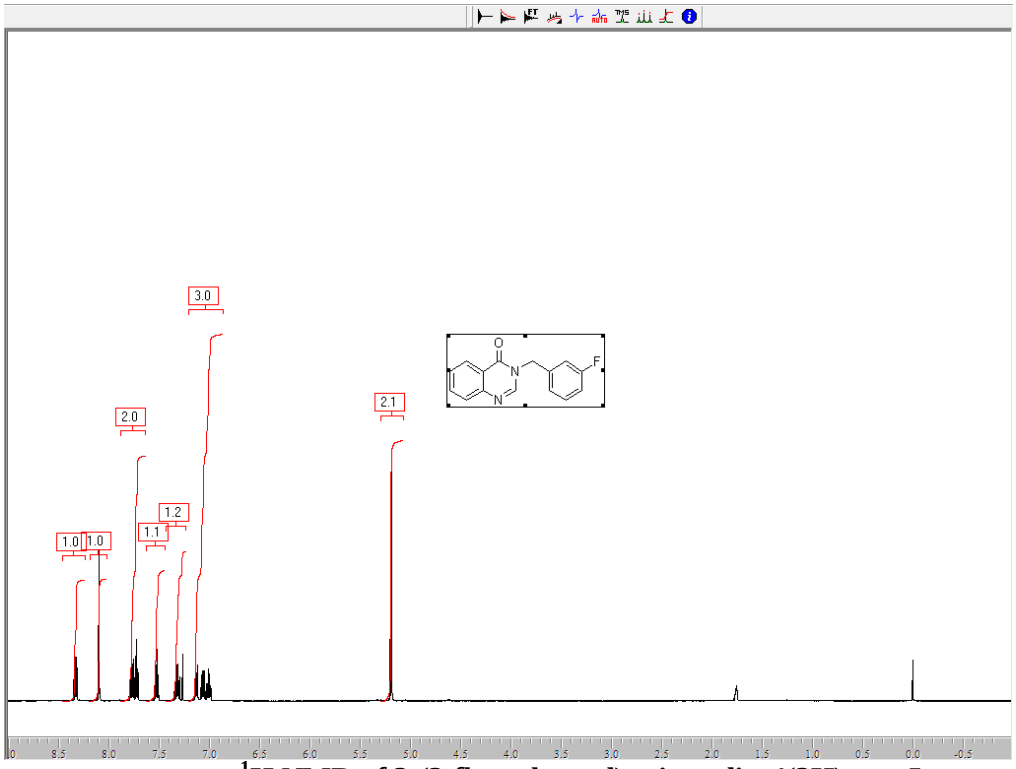
^{1}H NMR of 3-(2-methoxybenzyl)quinazolin-4(3H)-one 5m.



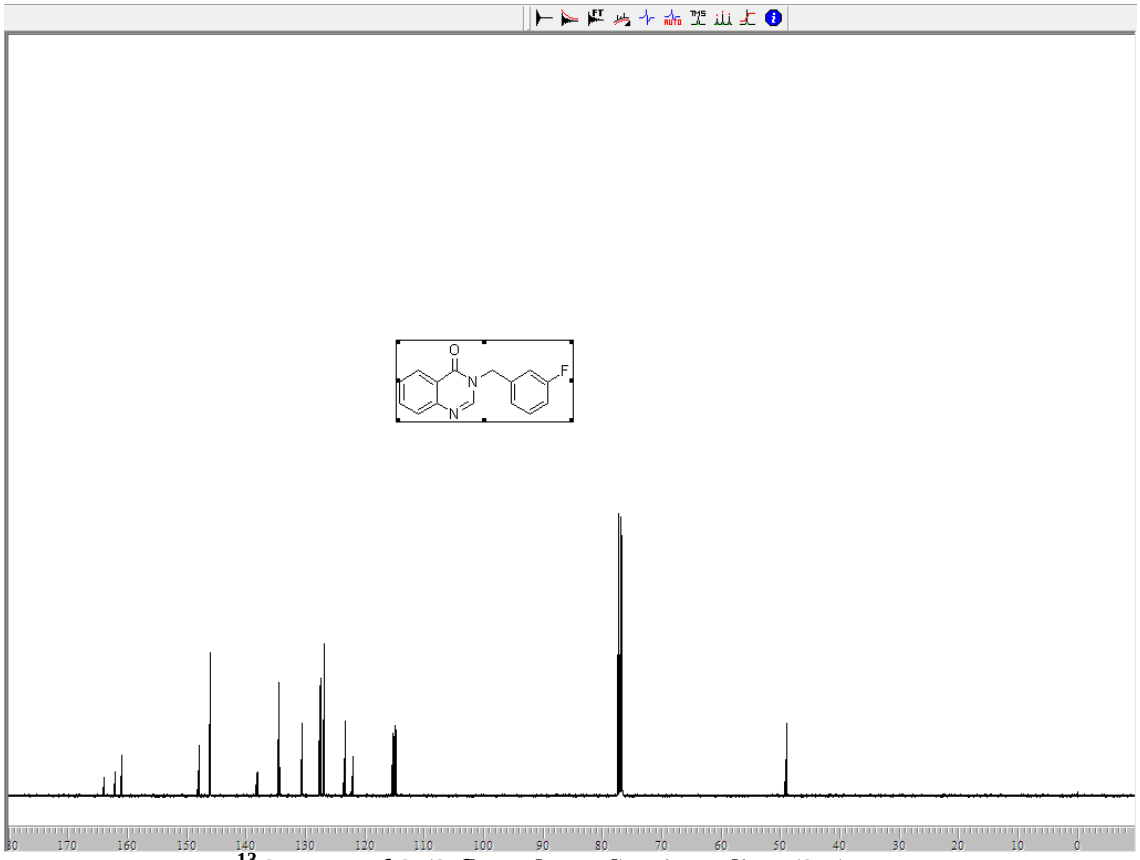
^{1}H NMR of 3-(2-methoxybenzyl)quinazolin-4(3H)-one 5m. (Expansion)



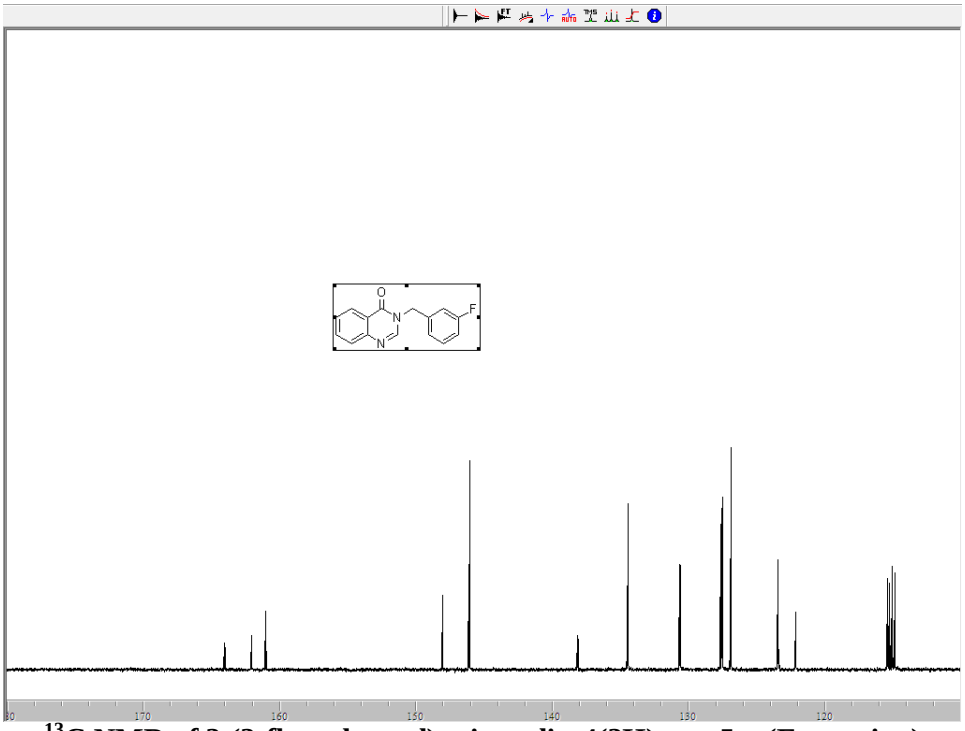
^{13}C NMR of 3-(2-methoxybenzyl)quinazolin-4(3H)-one 5m.



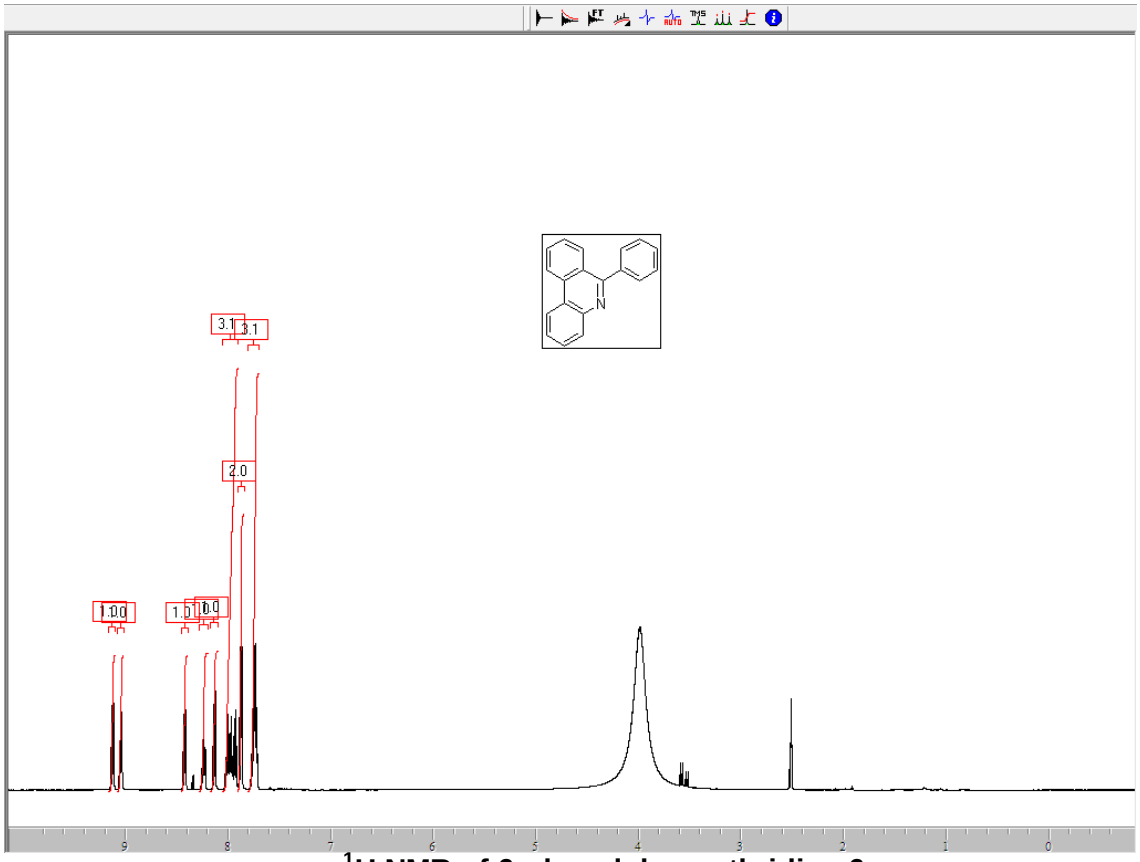
^{1}H NMR of 3-(3-fluorobenzyl)quinazolin-4(3H)-one 5n.



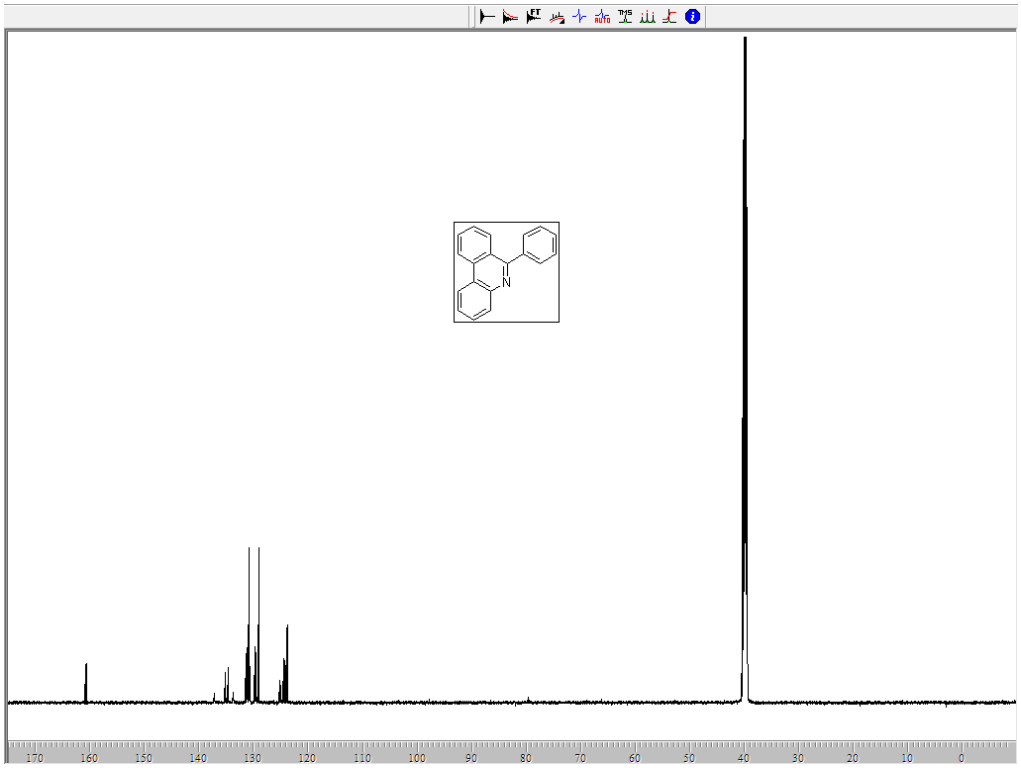
^{13}C NMR of 3-(3-fluorobenzyl)quinazolin-4(3H)-one 5n.



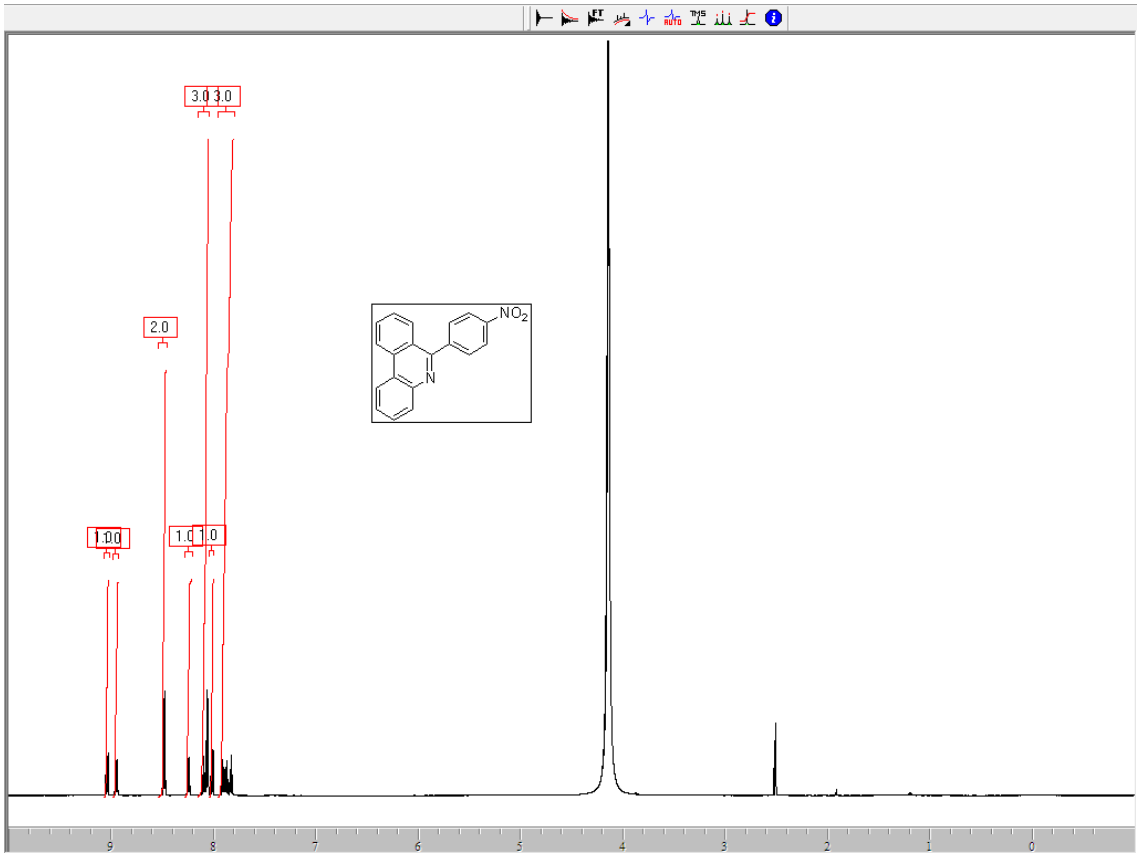
^{13}C NMR of 3-(3-fluorobenzyl)quinazolin-4(3H)-one 5n. (Expansion)



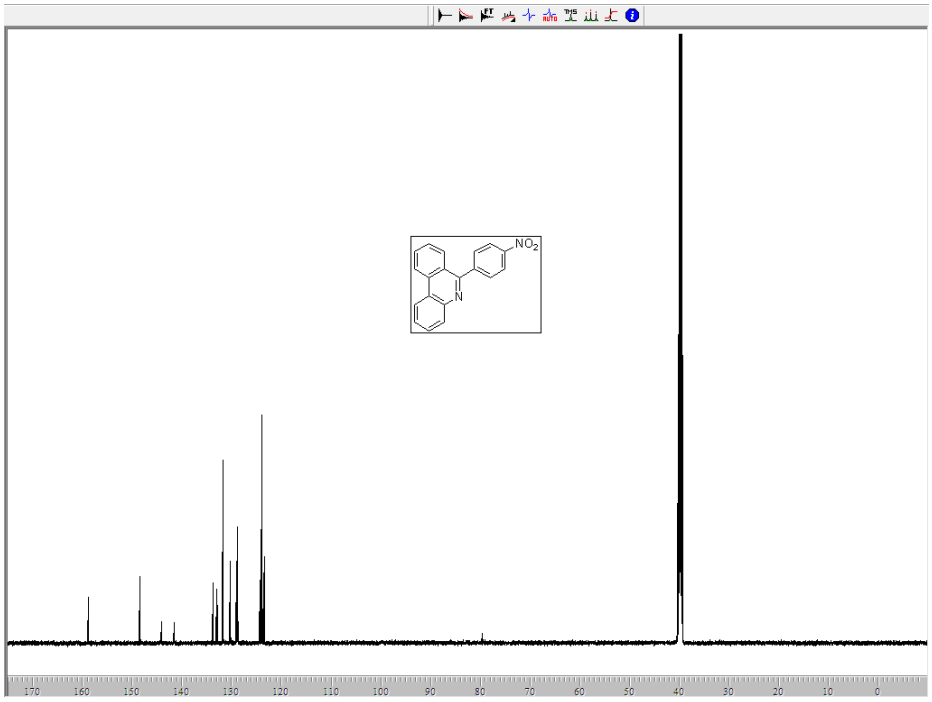
^{1}H NMR of 6-phenylphenanthridine 6a.



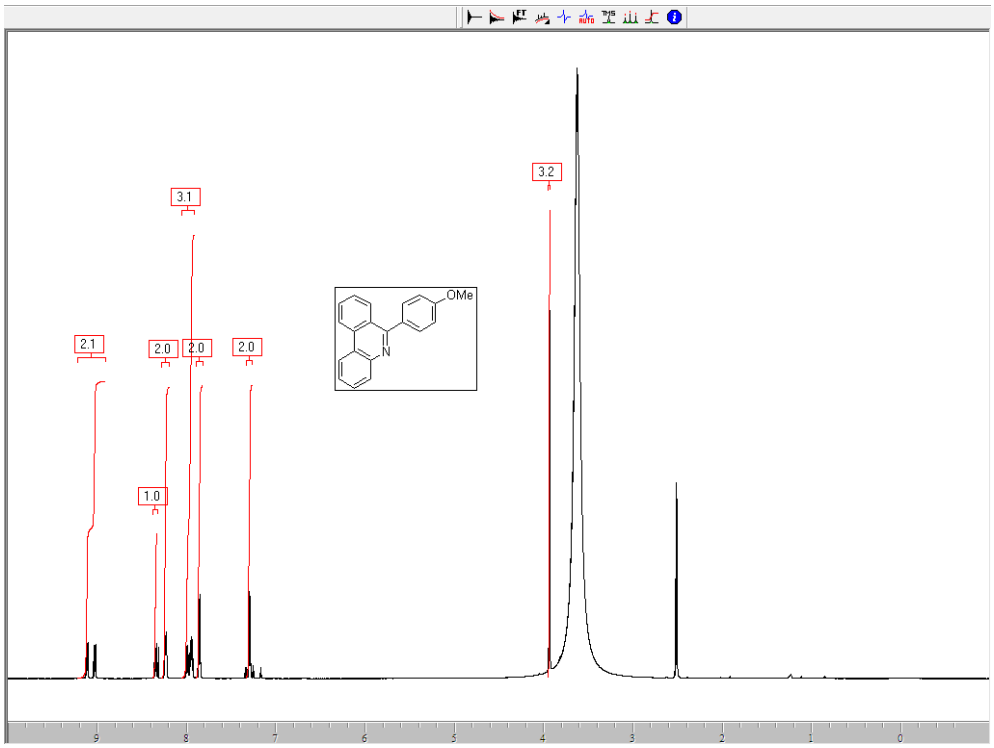
^{13}C NMR of 6-phenylphenanthridine 6a.



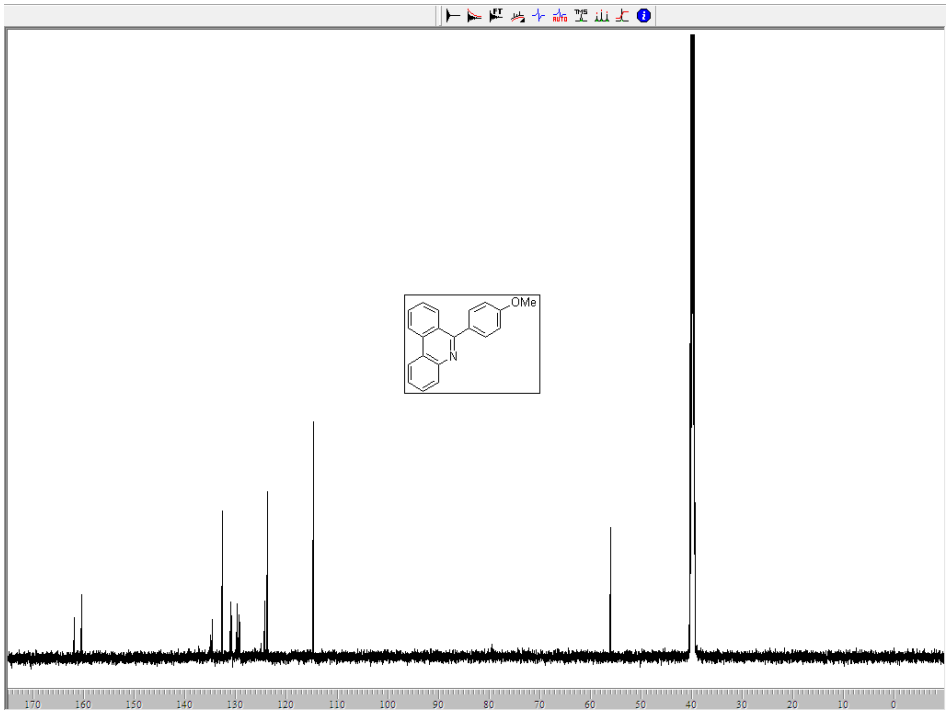
^{1}H NMR of 6-(4-Nitrophenyl)phenanthridine 6b.



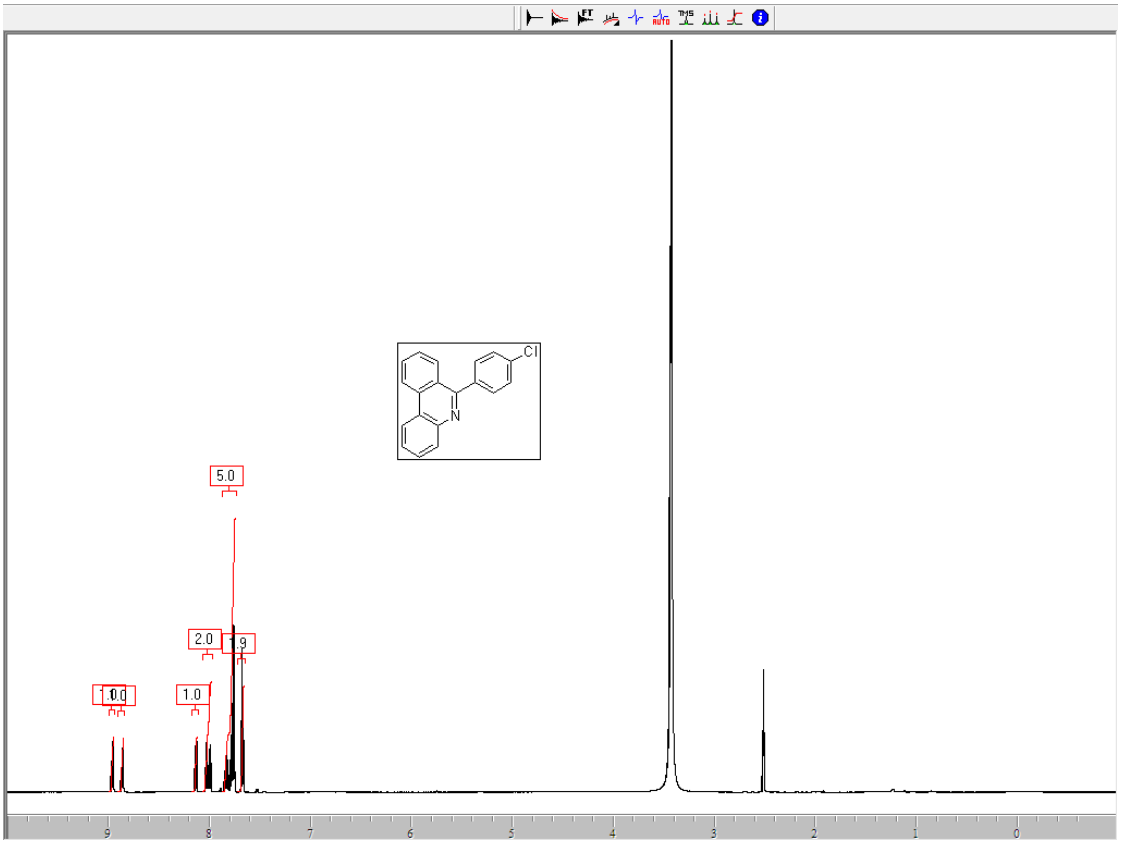
^{13}C NMR of 6-(4-Nitrophenyl)phenanthridine 6b.



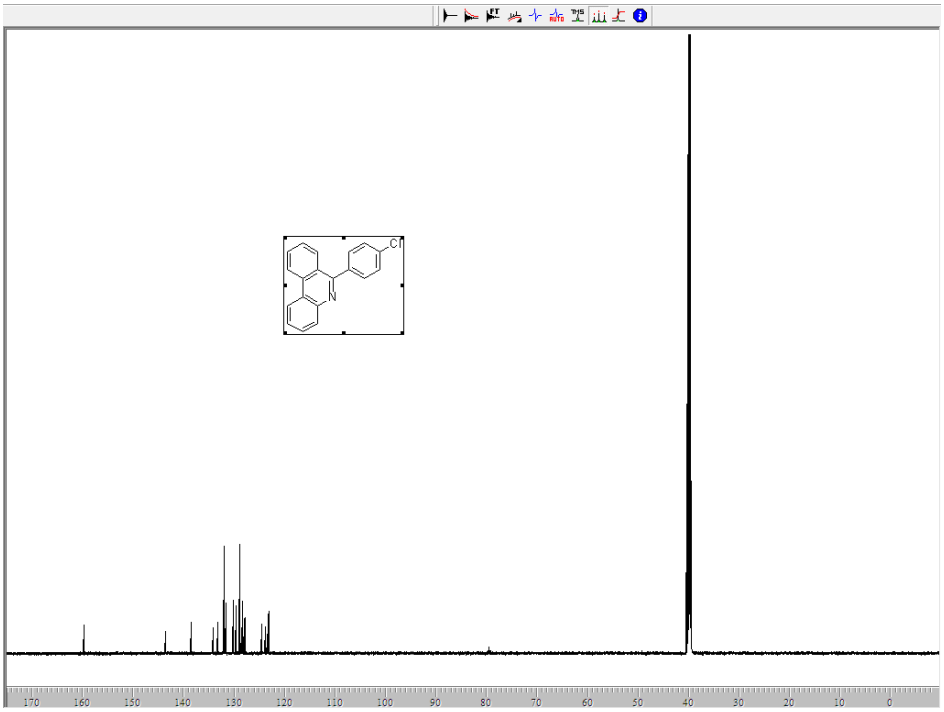
^{1}H NMR of 6-(4-Methoxyphenyl)phenanthridine 6c.



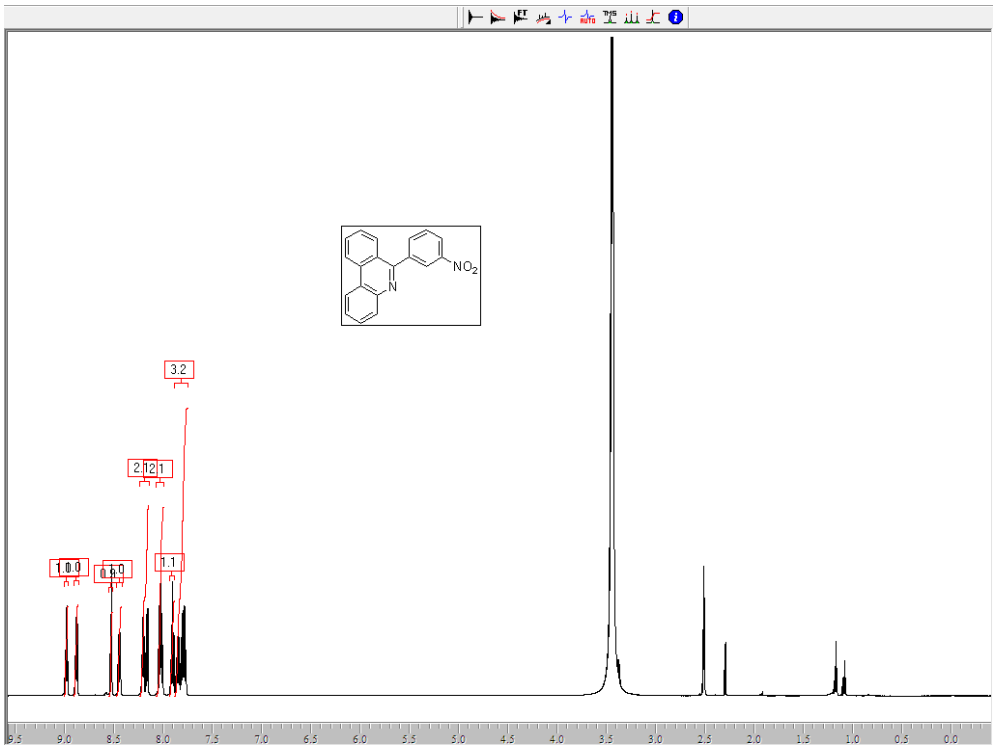
^{13}C NMR of 6-(4-Methoxyphenyl)phenanthridine 6c.



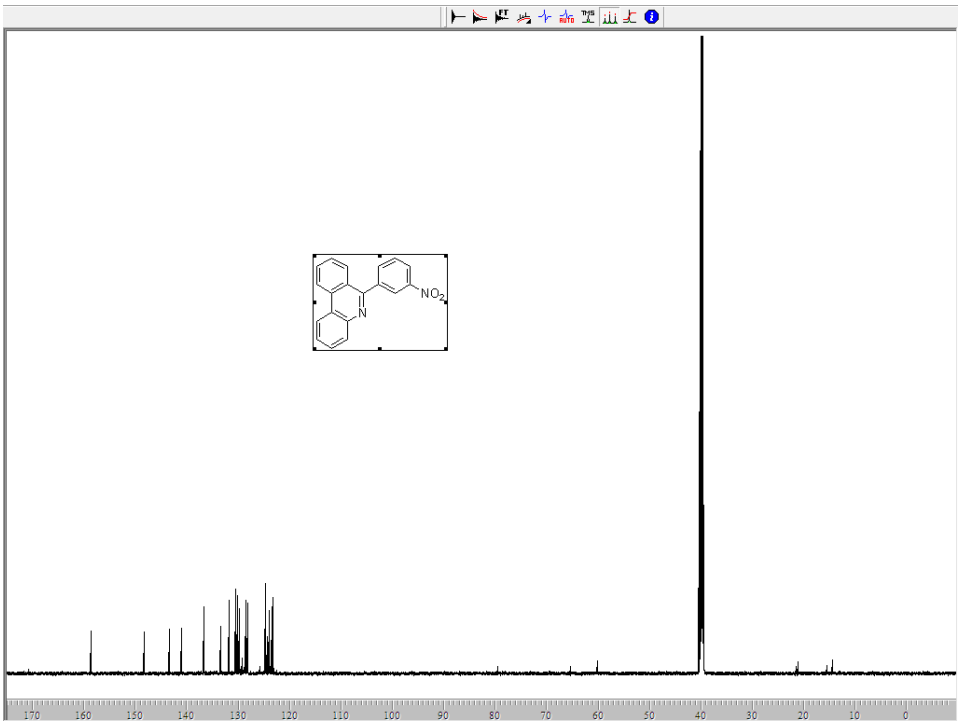
^{1}H NMR of 6-(4-Chlorophenyl)phenanthridine 6d.



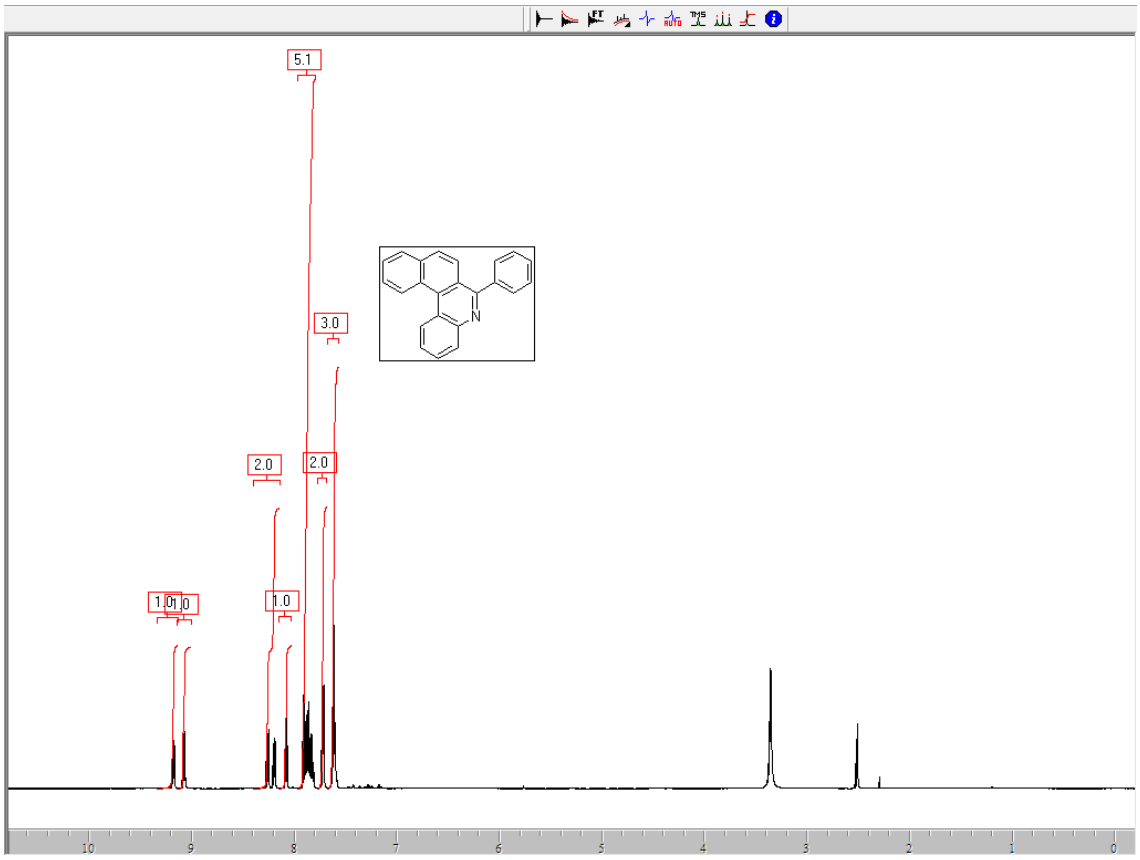
^{13}C NMR of 6-(4-Chlorophenyl)phenanthridine 6d.



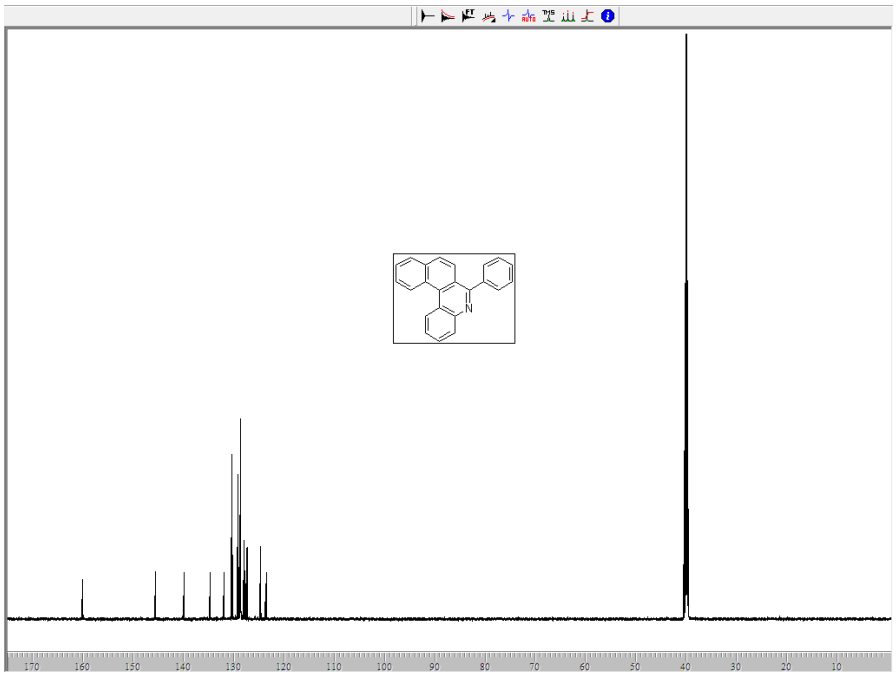
^{1}H NMR of 6-(3-nitrophenyl)phenanthridine 6e.



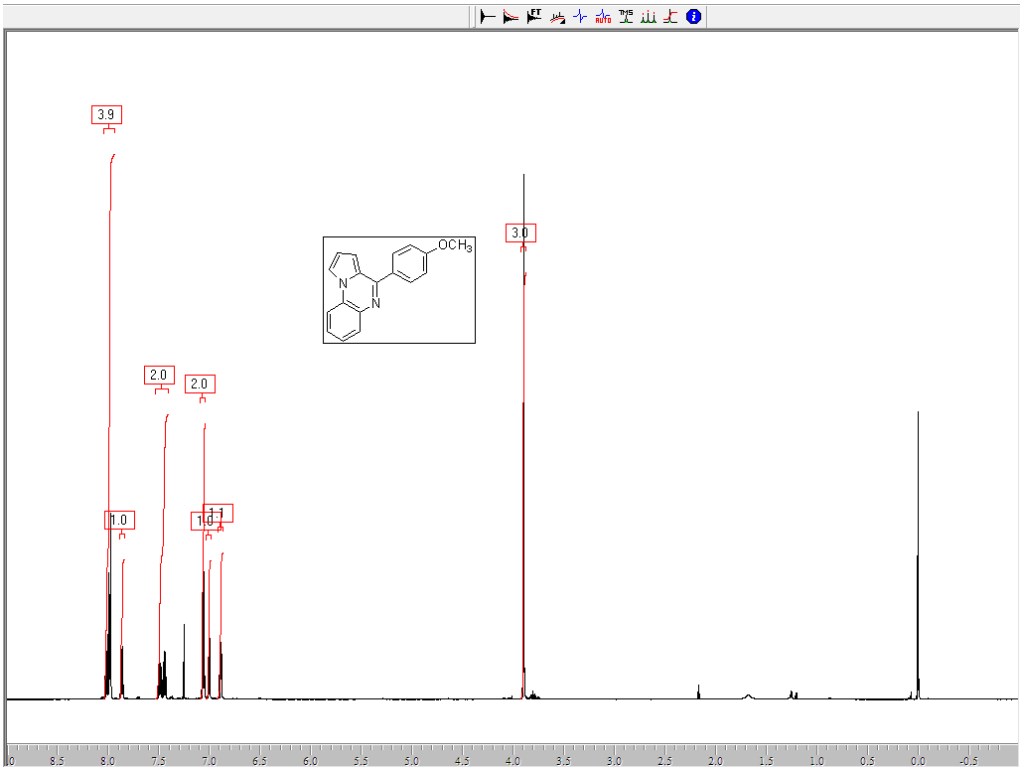
^{1}H NMR of 6-(3-nitrophenyl)phenanthridine 6e.



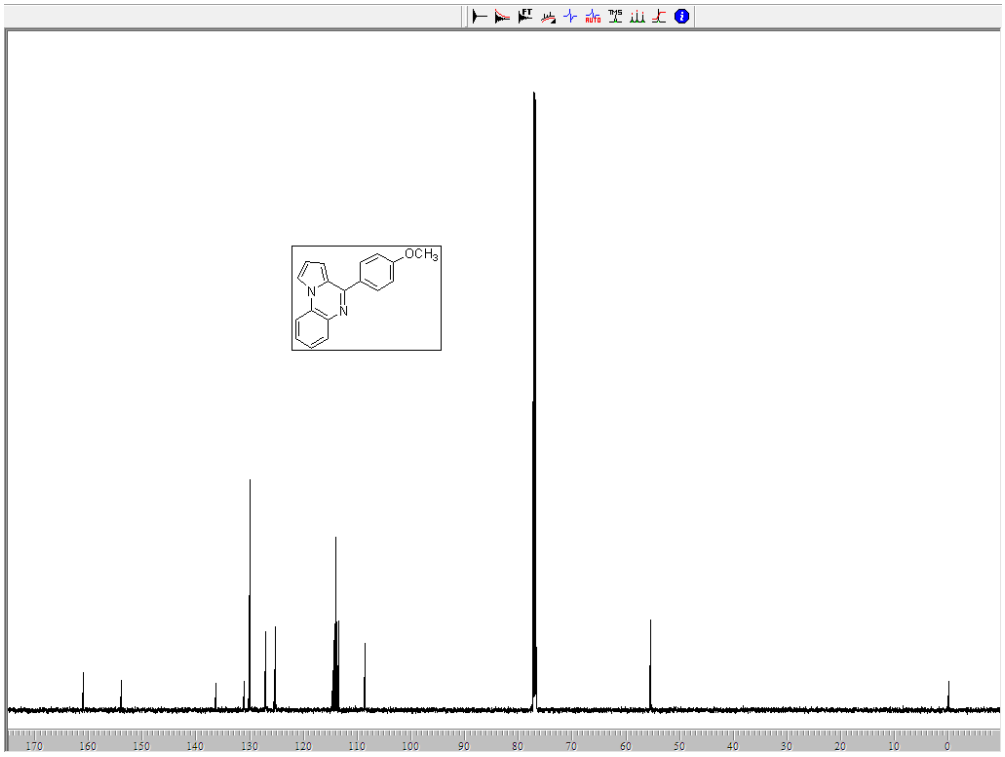
^{1}H NMR of 6-Phenylbenzo[k]phenanthridine 6f.



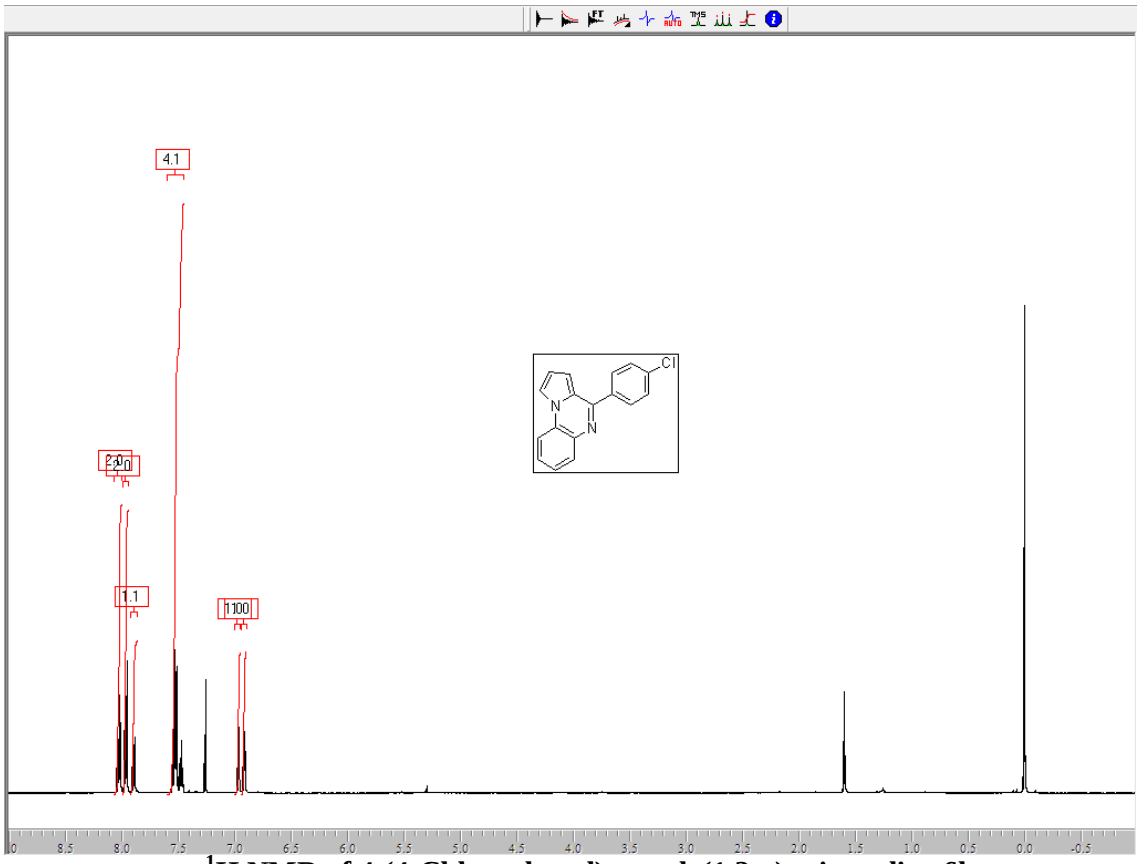
^{13}C NMR of 6-Phenylbenzo[k]phenanthridine 6f.



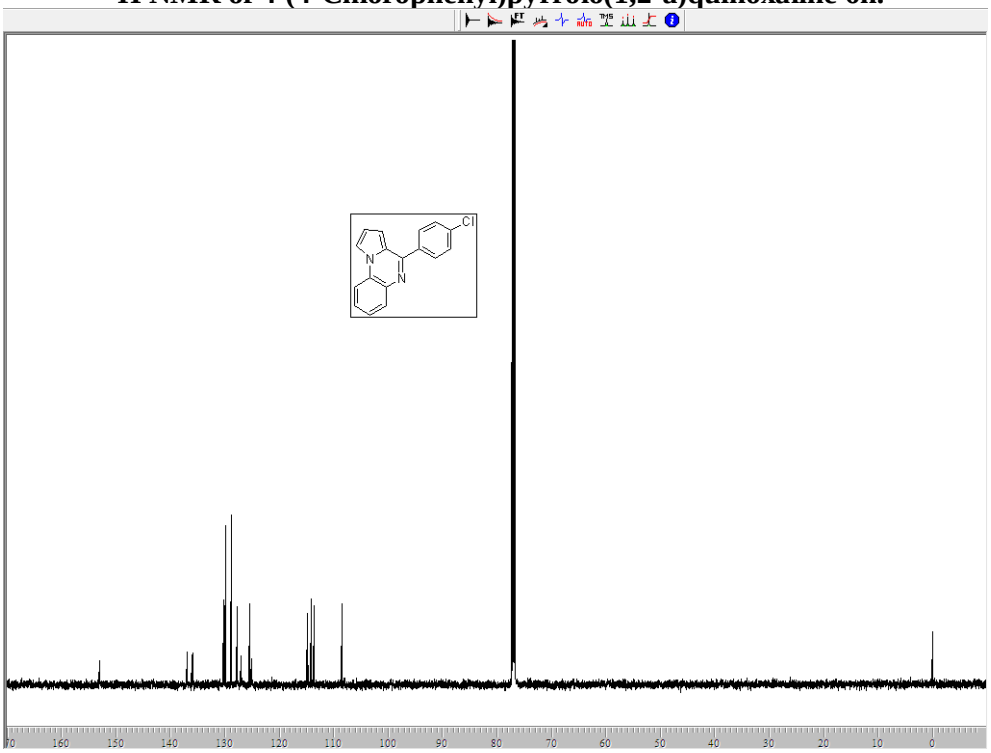
^{1}H NMR of 4-(4-Methoxyphenyl)pyrrolo(1,2-a)quinoxaline 6g.



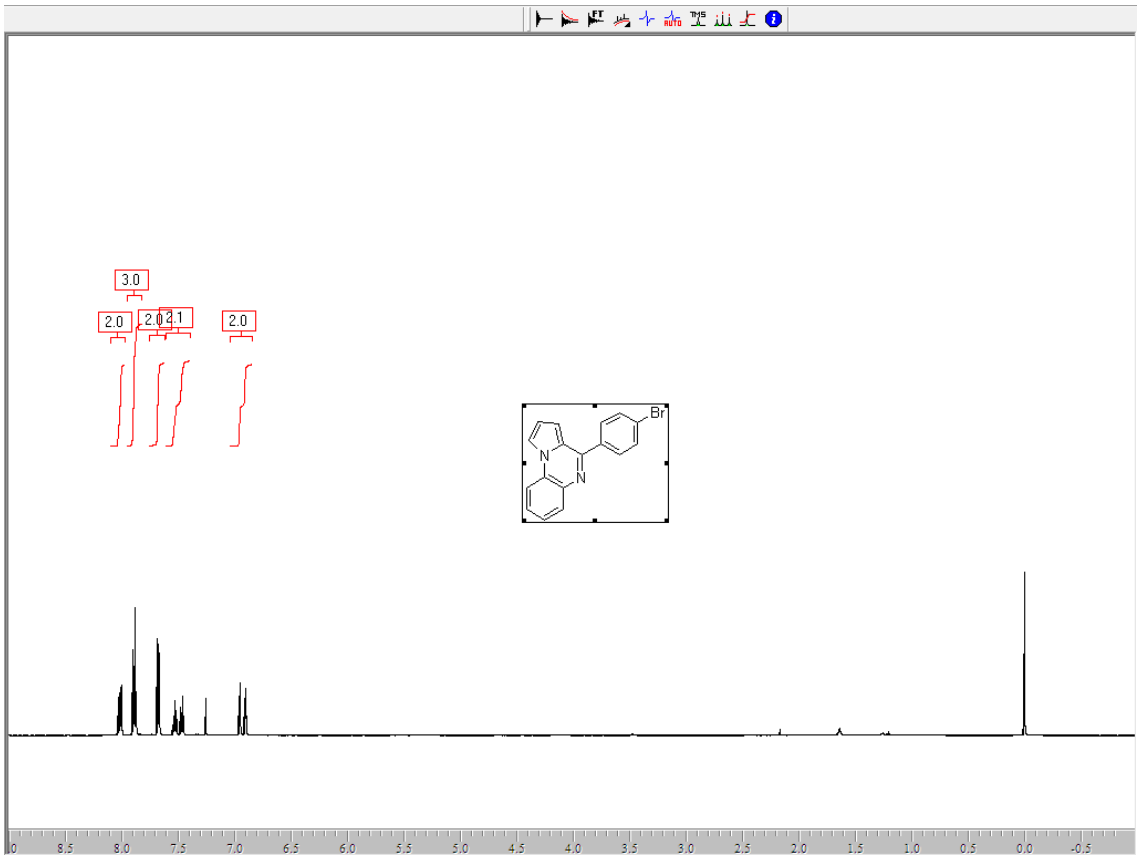
^{13}C NMR of 4-(4-Methoxyphenyl)pyrrolo(1,2-a)quinoxaline 6g.



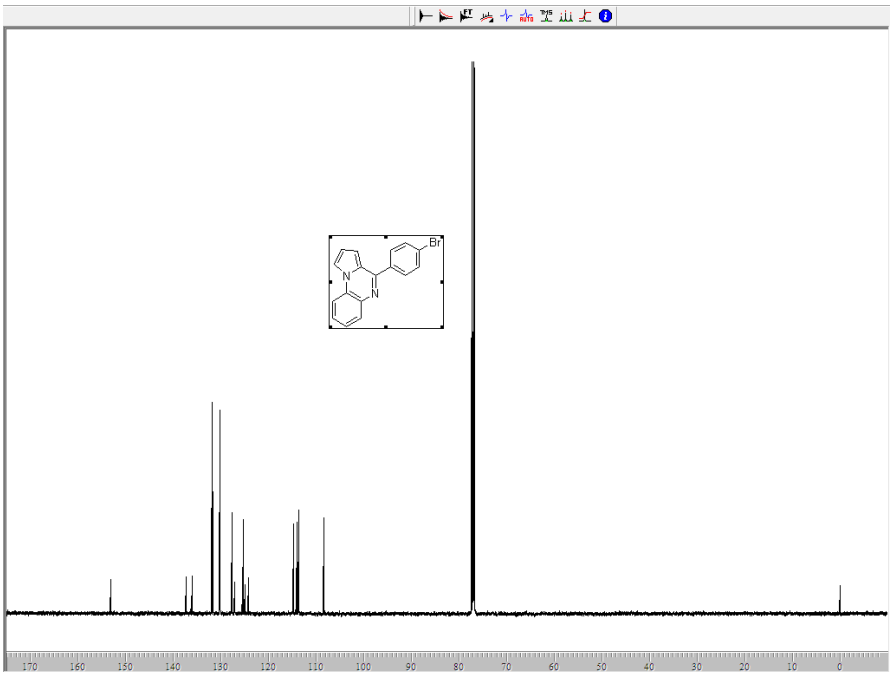
^{1}H NMR of 4-(4-Chlorophenyl)pyrrolo(1,2-a)quinoxaline 6h.



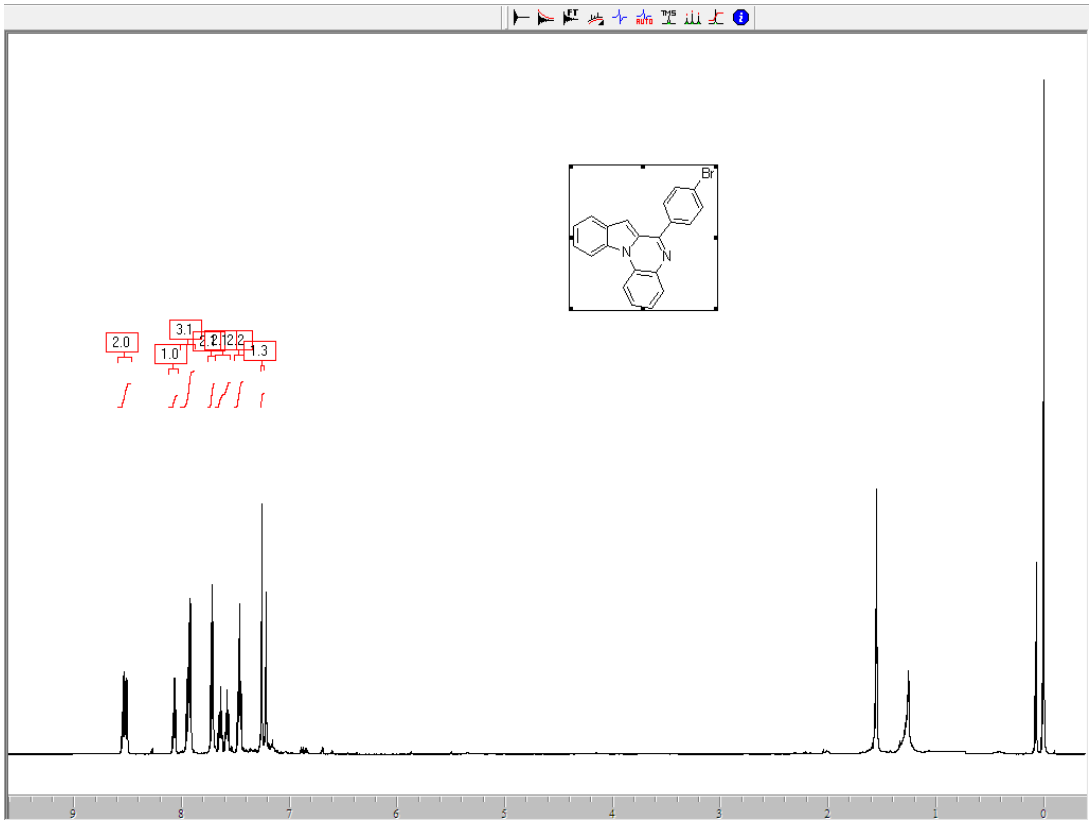
^{13}C NMR of 4-(4-Chlorophenyl)pyrrolo(1,2-a)quinoxaline 6h.



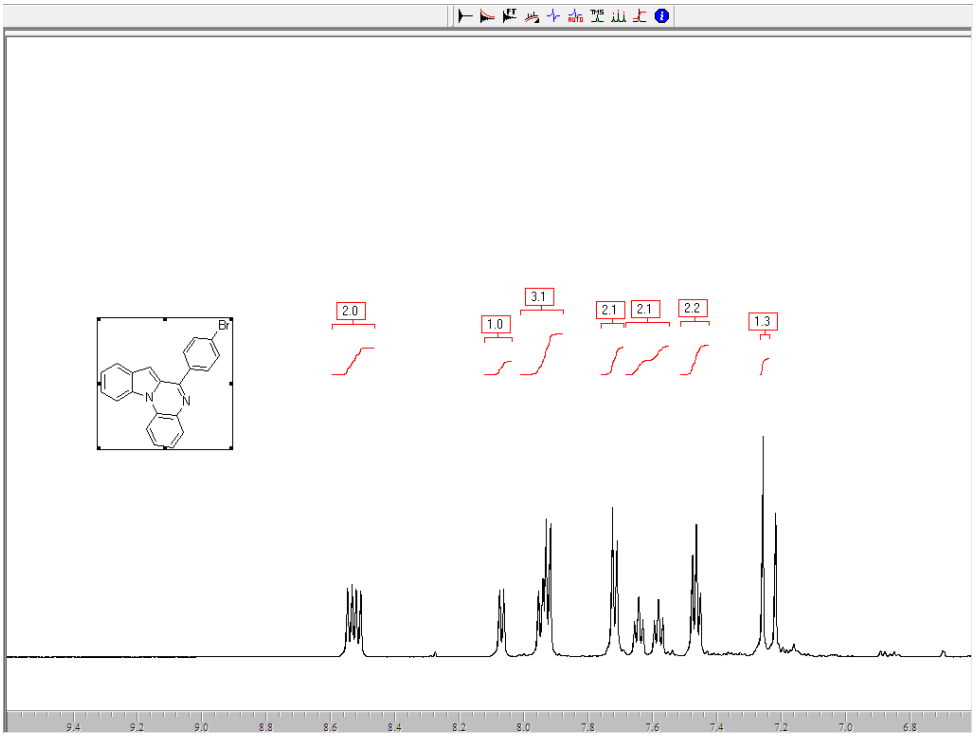
^{1}H NMR of 4-(4-Bromophenyl)pyrrolo[1,2-a]quinoxaline 6i.



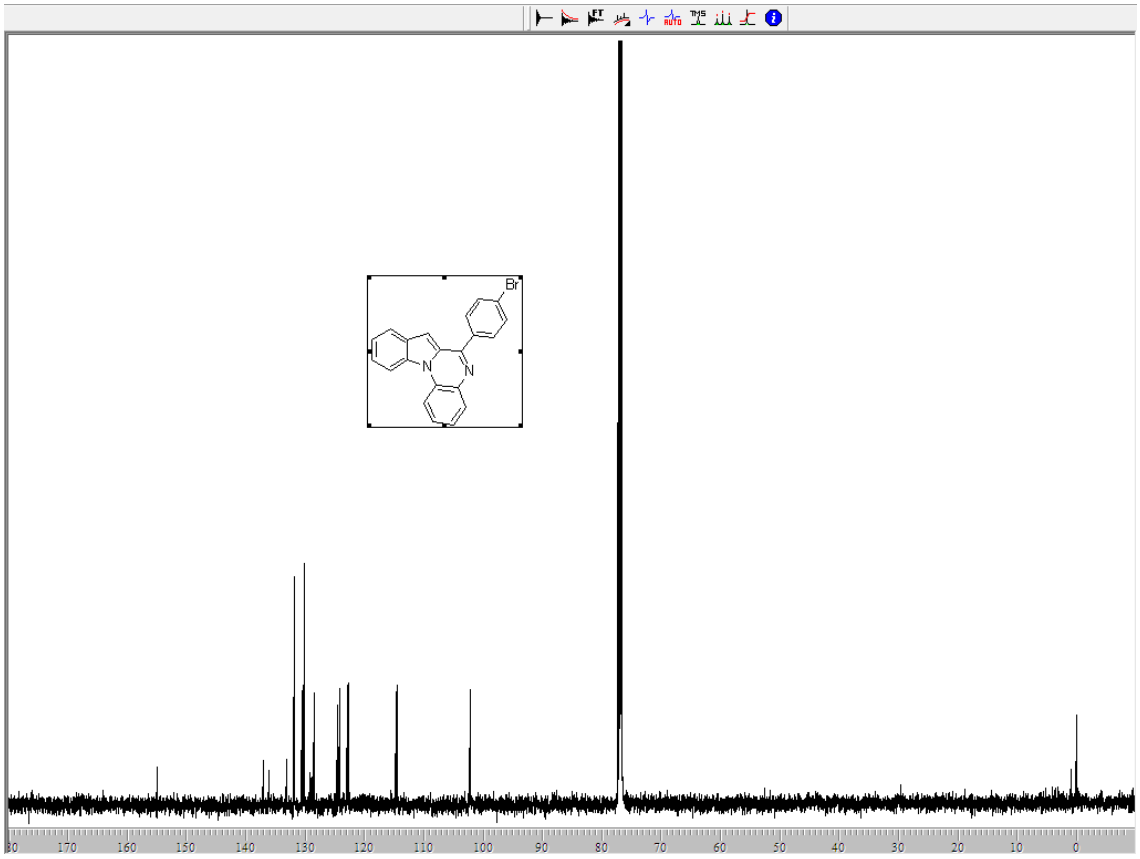
^{13}C NMR of 4-(4-Bromophenyl)pyrrolo[1,2-a]quinoxaline 6i.



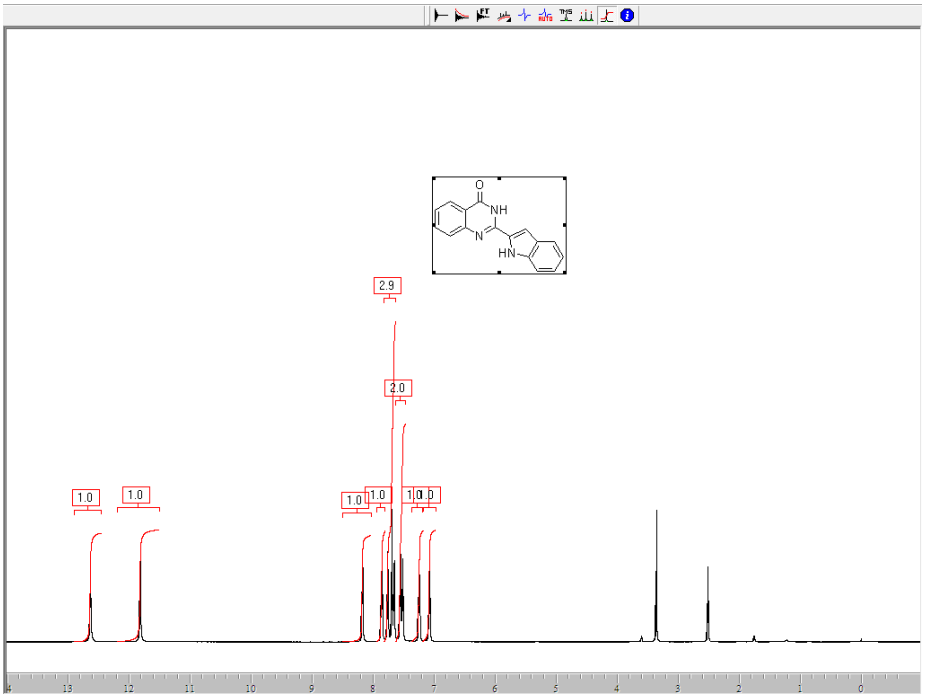
^{1}H NMR of 6-(4-Bromophenyl)indolo[1,2-a]quinoxaline 6i.



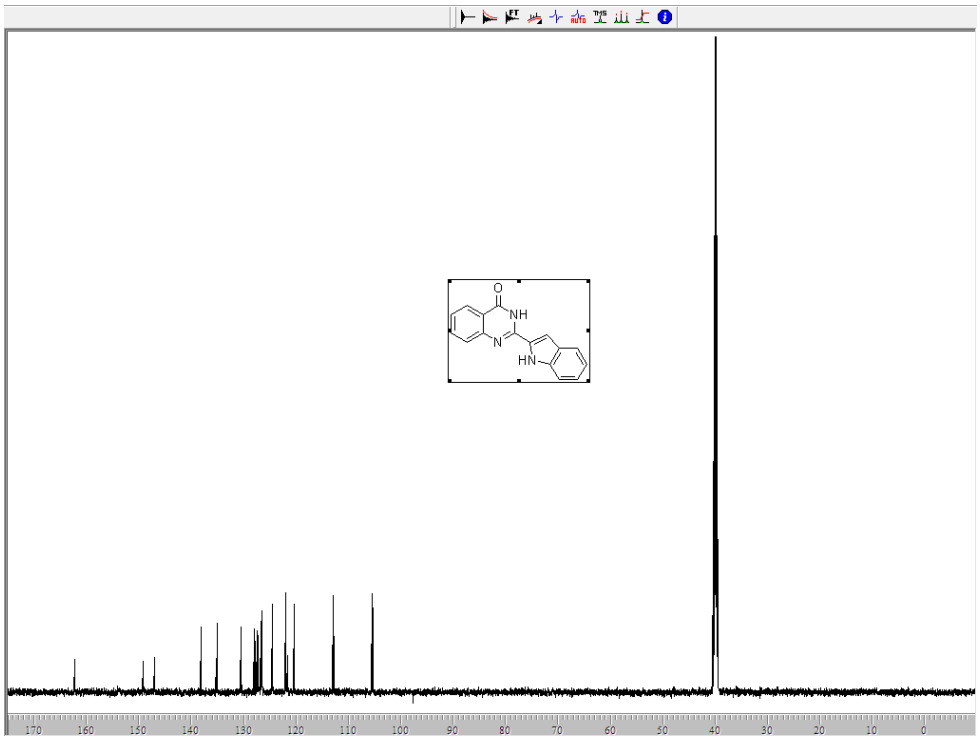
^{1}H NMR of 6-(4-Bromophenyl)indolo[1,2-a]quinoxaline 6i. (Expansion)



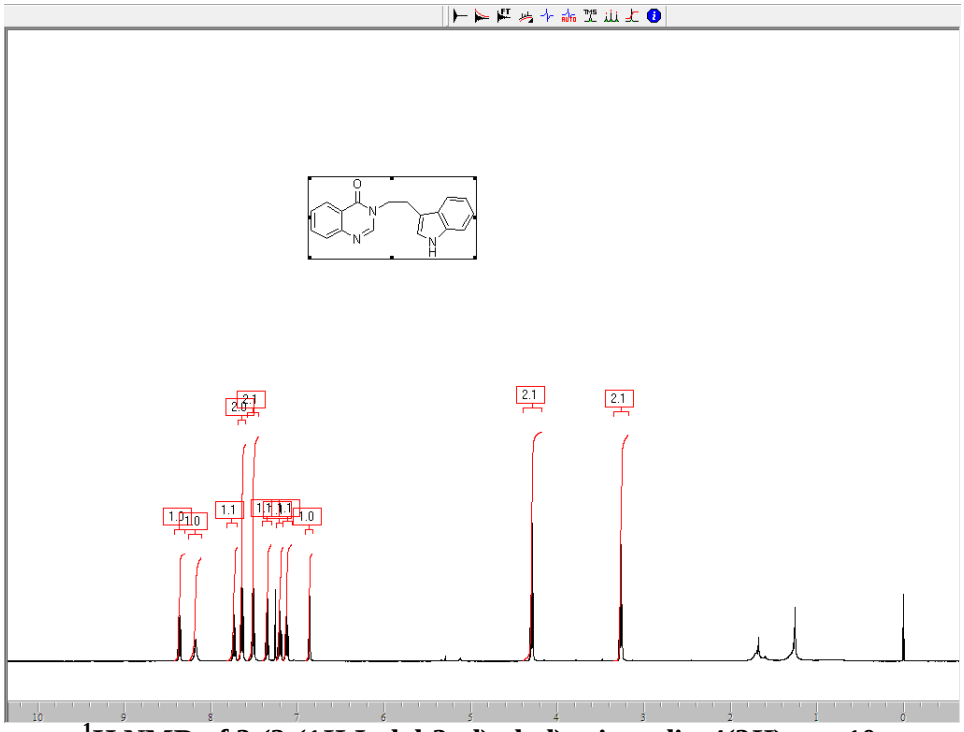
^{13}C NMR of 6-(4-Bromophenyl)indolo[1,2-a]quinoxaline 6i.



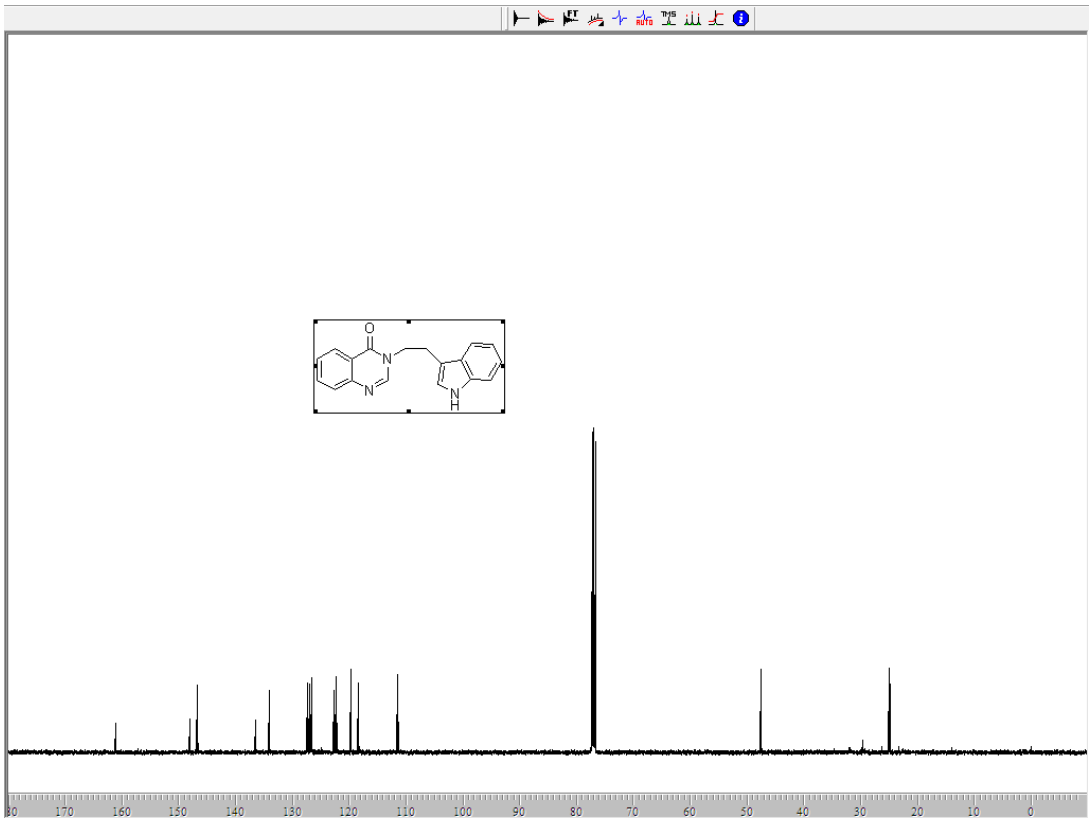
^{1}H NMR of 2-(1H-Indol-2-yl)quinazolin-4(3H)-one 8.



^{13}C NMR of 2-(1H-Indol-2-yl)quinazolin-4(3H)-one 8.



^{1}H NMR of 3-(2-(1*H*-Indol-3-yl)ethyl)quinazolin-4(3*H*)-one 10.



^{13}C NMR of 3-(2-(1*H*-Indol-3-yl)ethyl)quinazolin-4(3*H*)-one 10.