

Supplementary Information

Hydroxyapatite nanoparticles (HAP NPs): As a green and efficient heterogeneous catalyst for three-component one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)-one derivatives in aqueous media

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Experimental

General

The purity determinations of the products were accomplished by thin layer chromatography (preparative TLC was carried out using a Merck GF 254 silica gel on a glass support). The melting points of products were determined with an Electrothermal Type 9100 melting point apparatus. The FT-IR spectra were recorded on an Avatar 370 FT-IR Thermo Nicolet spectrometer. The NMR spectra were provided on Bruker Avance 300, 400 and 500 MHz instruments in DMSO- d_6 and $CDCl_3$. Elemental analyses were performed using a Thermo Finnegan Flash EA 1112 Series instrument. Mass spectra were recorded with a CH7A Varianmat Bremem instrument at 70 eV; in m/z (rel %).

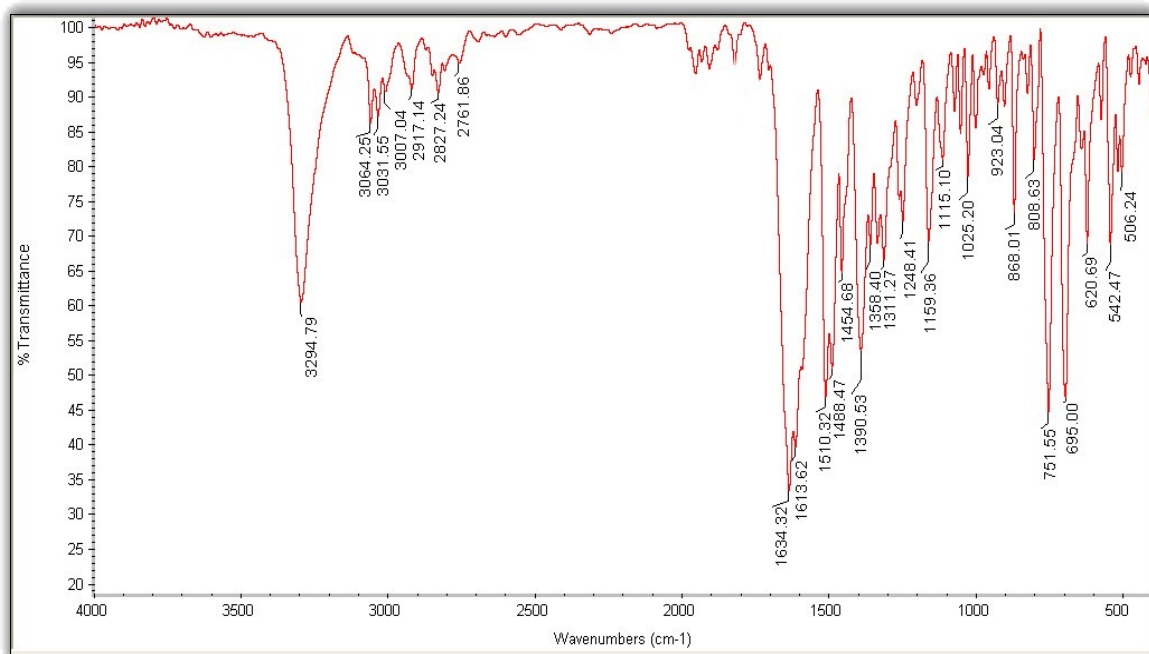
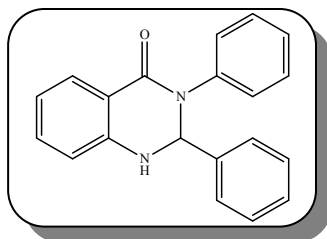


Figure 3a-A: FT-IR (KBr) of 2,3-Diphenylquinazolin-4(1H)-one (3a).

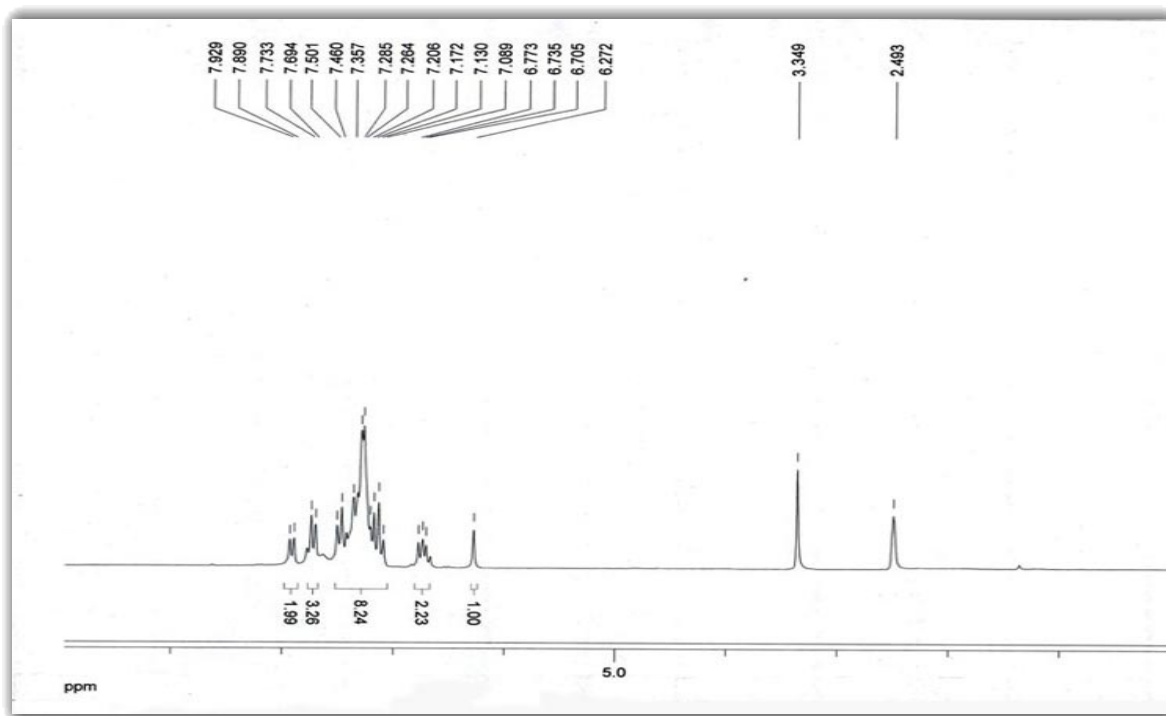


Figure 3a-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2,3-Diphenylquinazolin-4(1H)-one (3a).

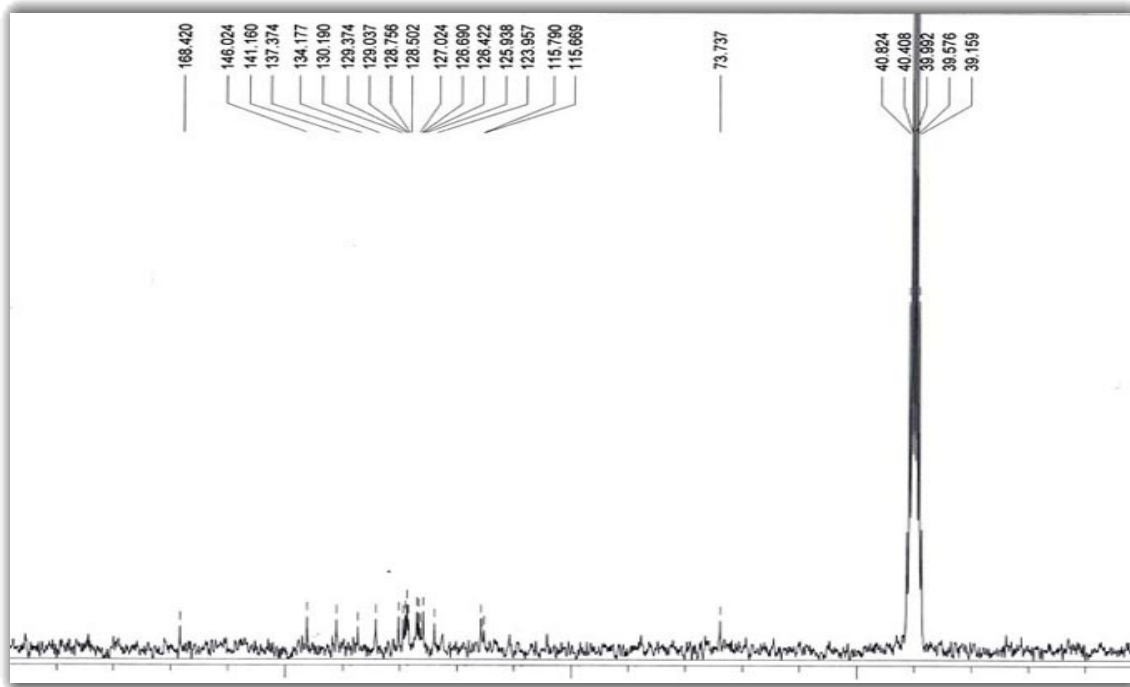


Figure 3a-C: ^{13}C NMR of 2,3-diphenylquinazolin-4(1H)-one (3a).

Figure 3a-D: Mass spectrum of 2,3-diphenylquinazolin-4(1H)-one (3a).

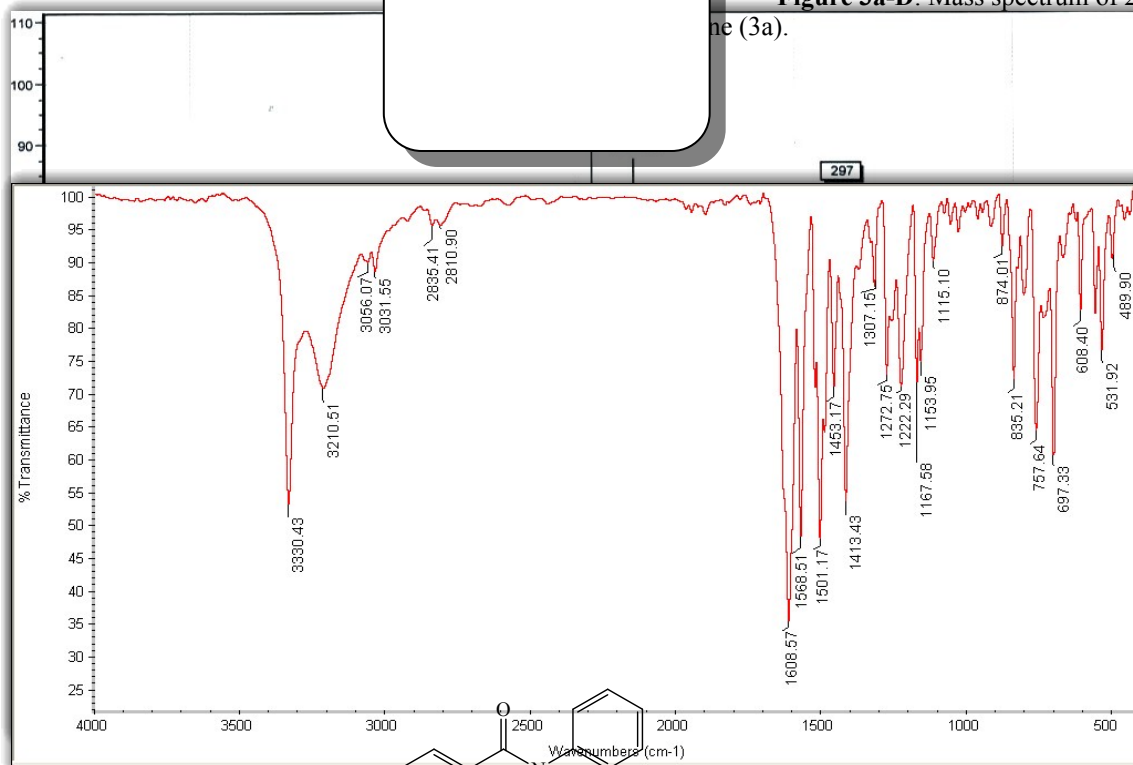
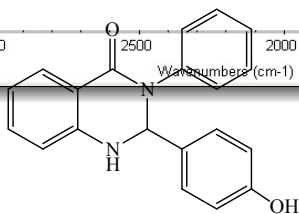


Figure 3b-A: FT-IR (KBr) of 2-(4-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3b).



Hydroxyphenyl)-3-phenyl-2,3-

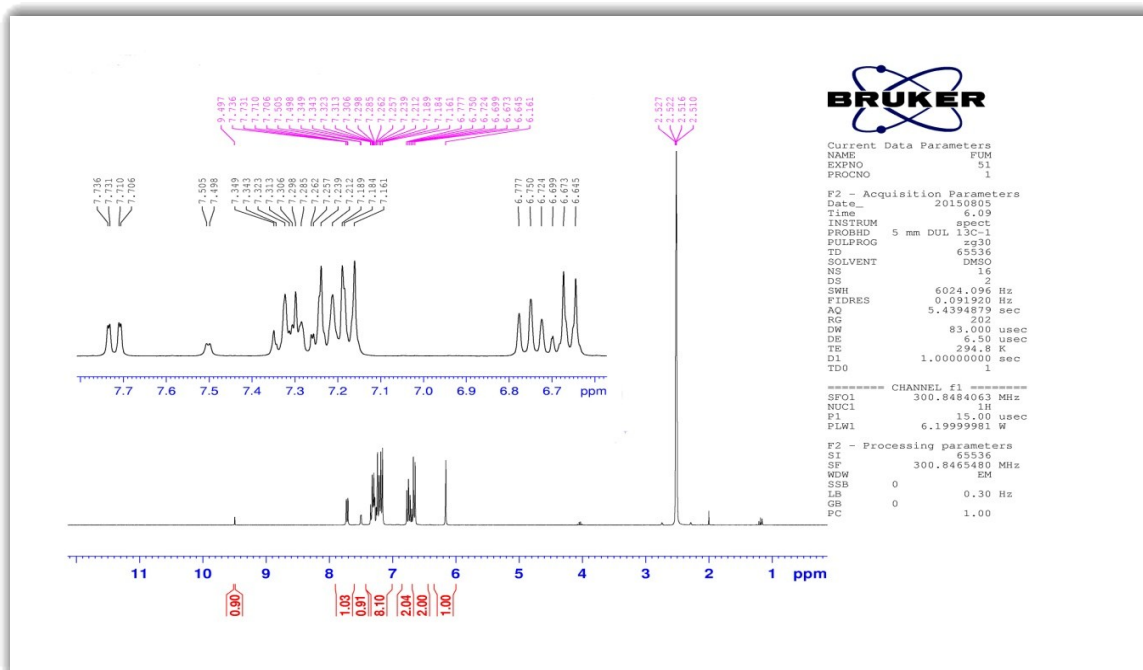


Figure 3b-B: ^1H NMR (300 MHz, $\text{DMSO}-d_6$) of 2-(4-Hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3b).

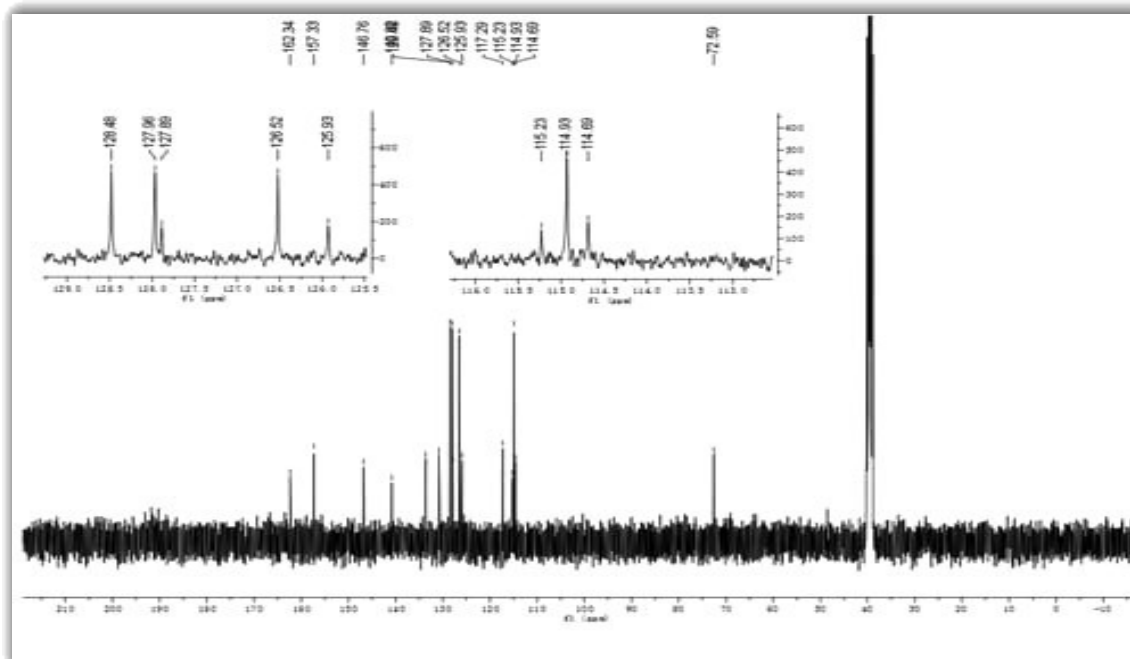


Figure 3b-C: ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of 2-(4-Hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3b).

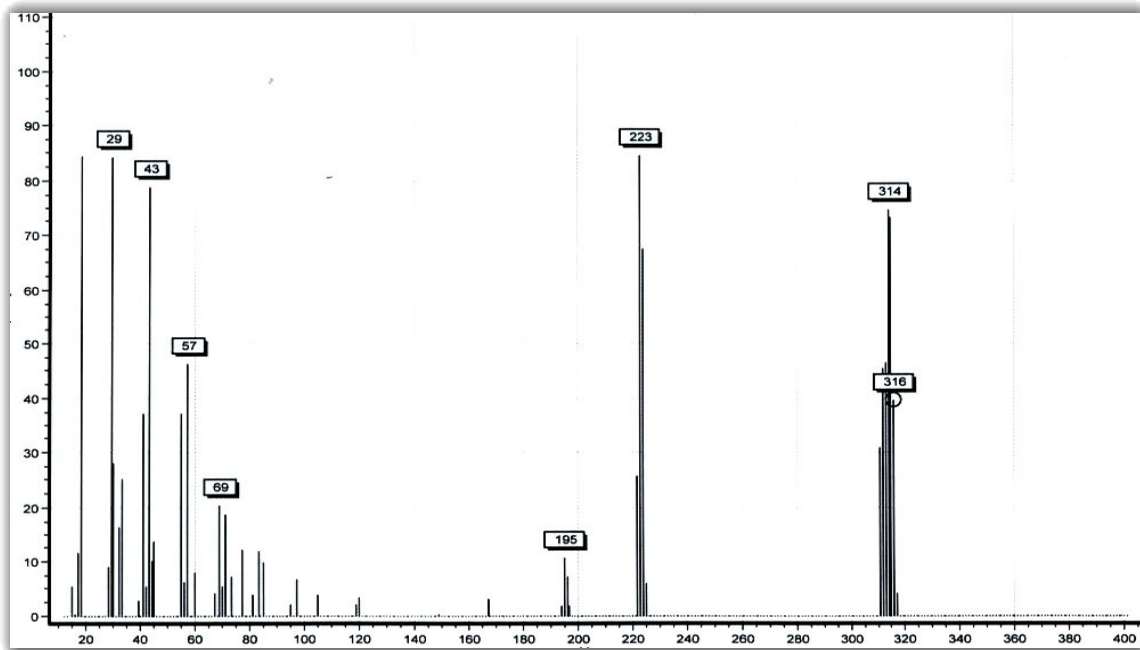


Figure 3b-D: Mass spectrum of 2-(4-Hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3b).

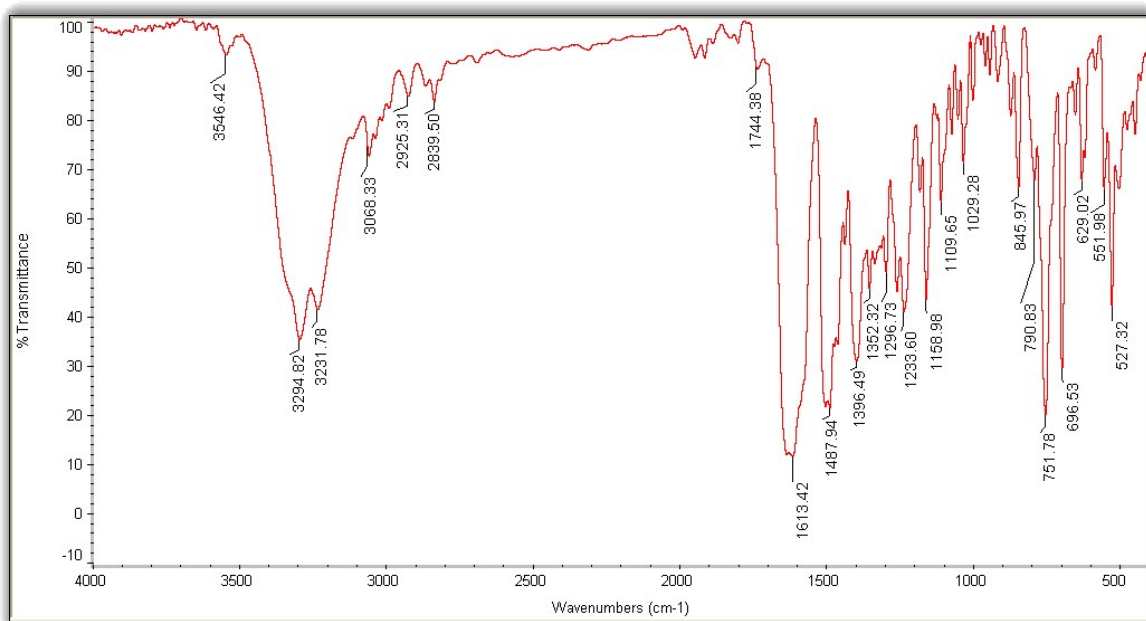
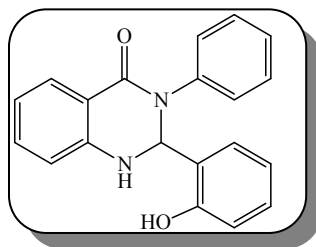


Figure 3c-A: FT-IR (KBr) of 2-(2-Hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3c).

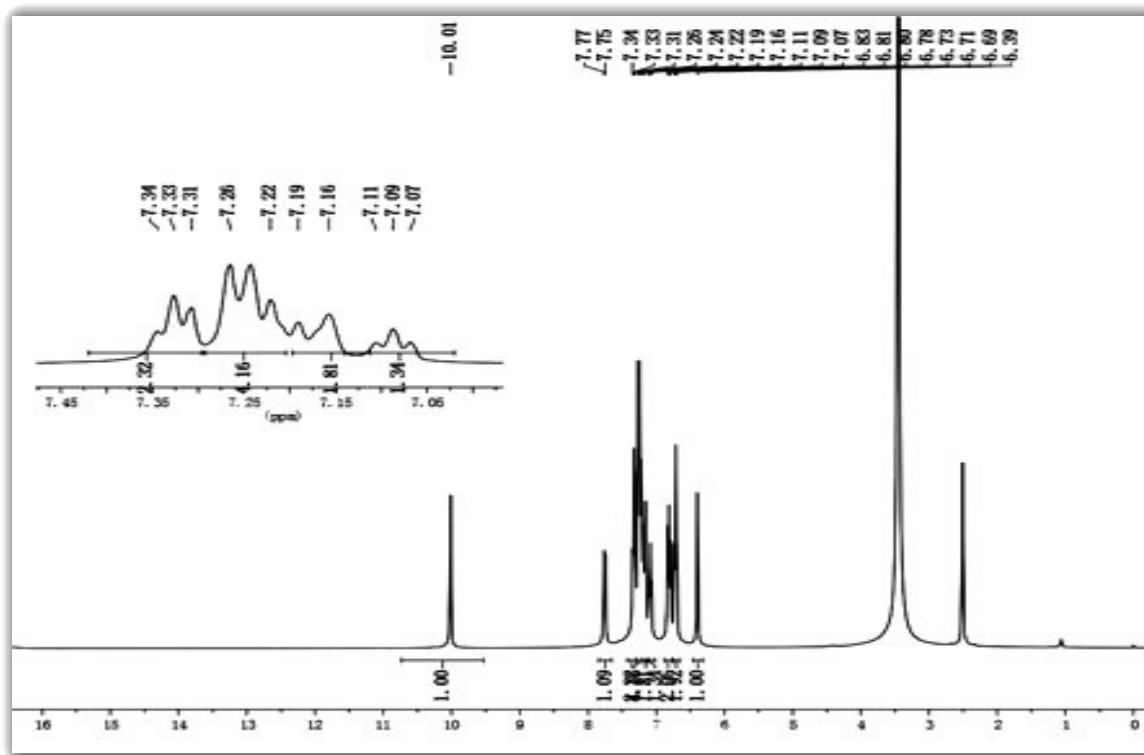


Figure 3c-B: ¹³C NMR (400 MHz, DMSO-*d*₆) of 2-(2-Hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3c).

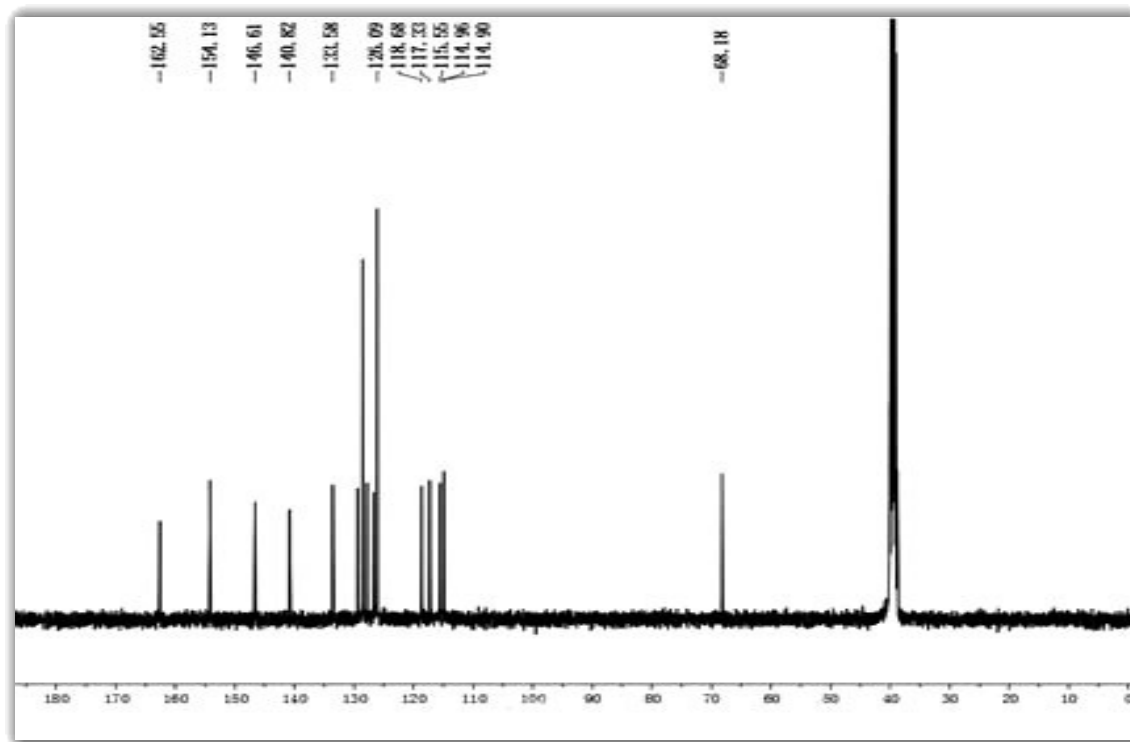


Figure 3c-C: ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) of 2-(2-Hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3c).

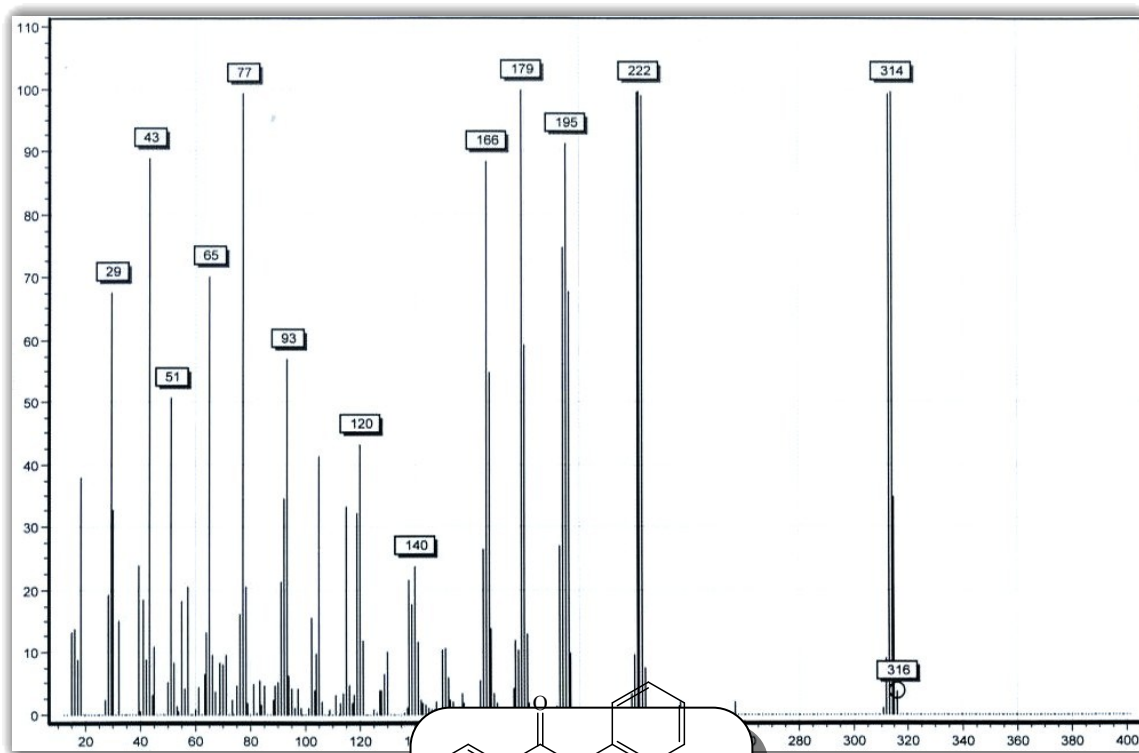
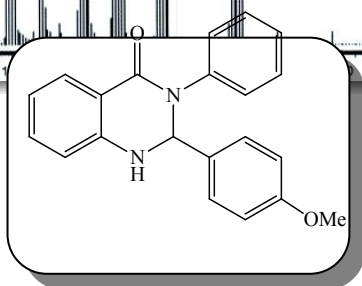


Figure 3c-D: Mass spectrum of 2-(4-



Hydroxyphenyl)-3-phenyl-2,3-

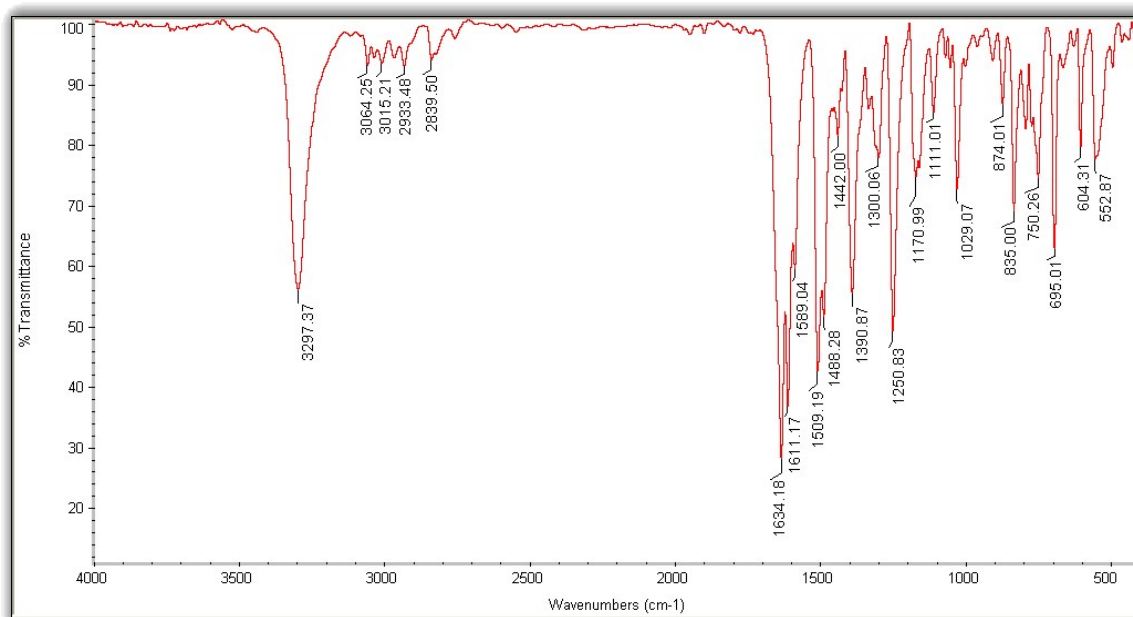


Figure 3d-A: FT-IR (KBr) of 2-(4-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3d).

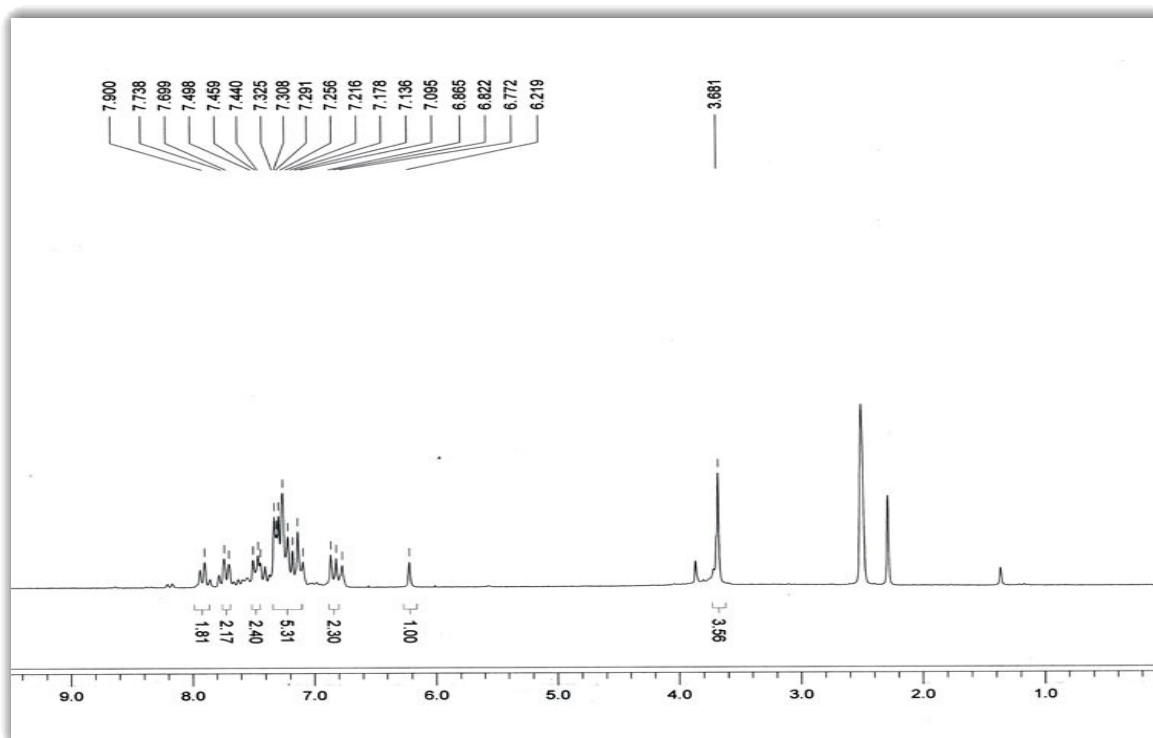


Figure 3d-B: ^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 2-(4-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3d).

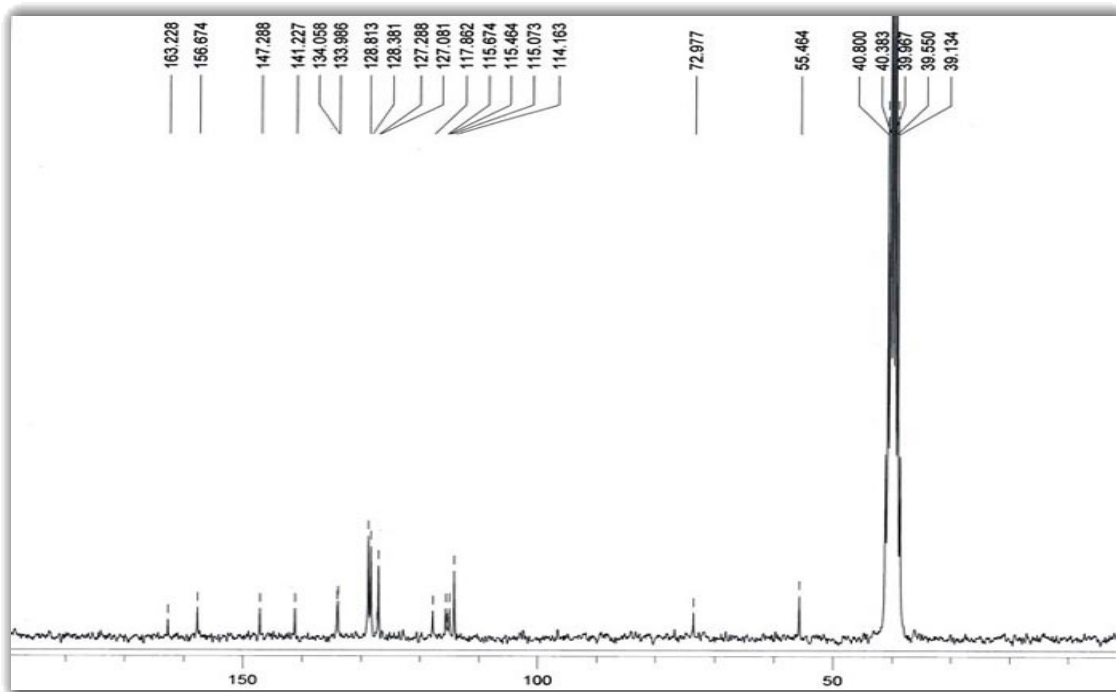


Figure 3d-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3d).

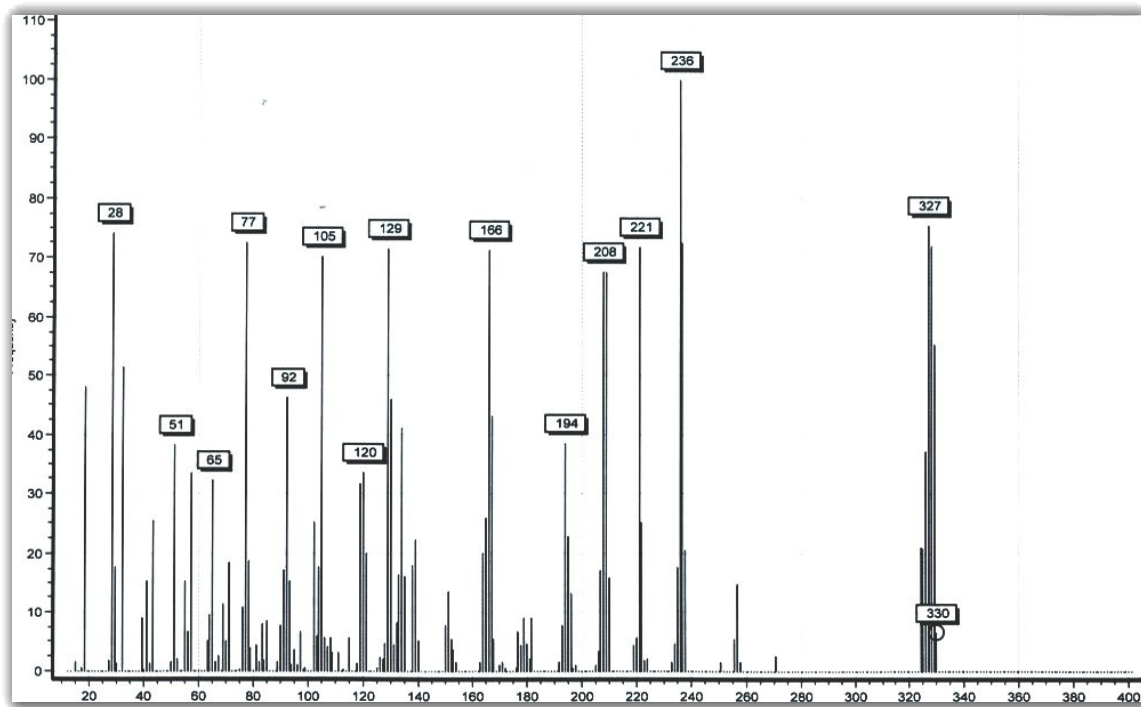


Figure 3d-D: Mass spectrum of 2-(4-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3d).

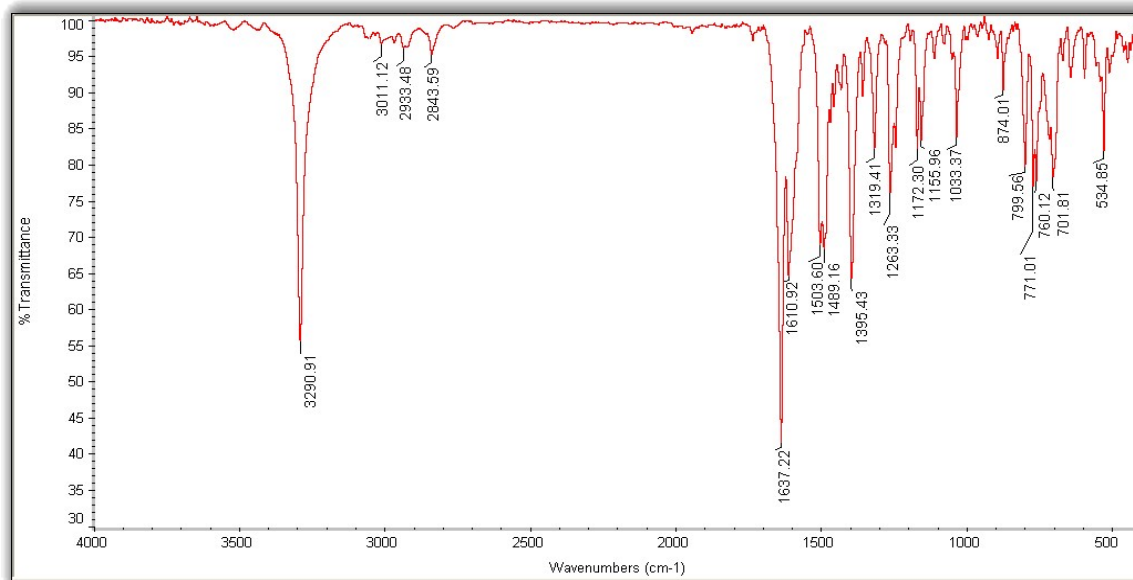
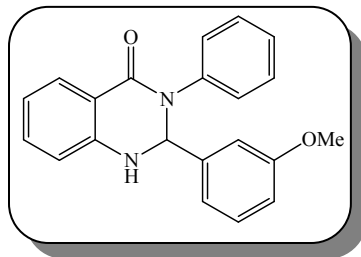


Figure 3e-A: FT-IR (KBr) of 2-(3-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3e).

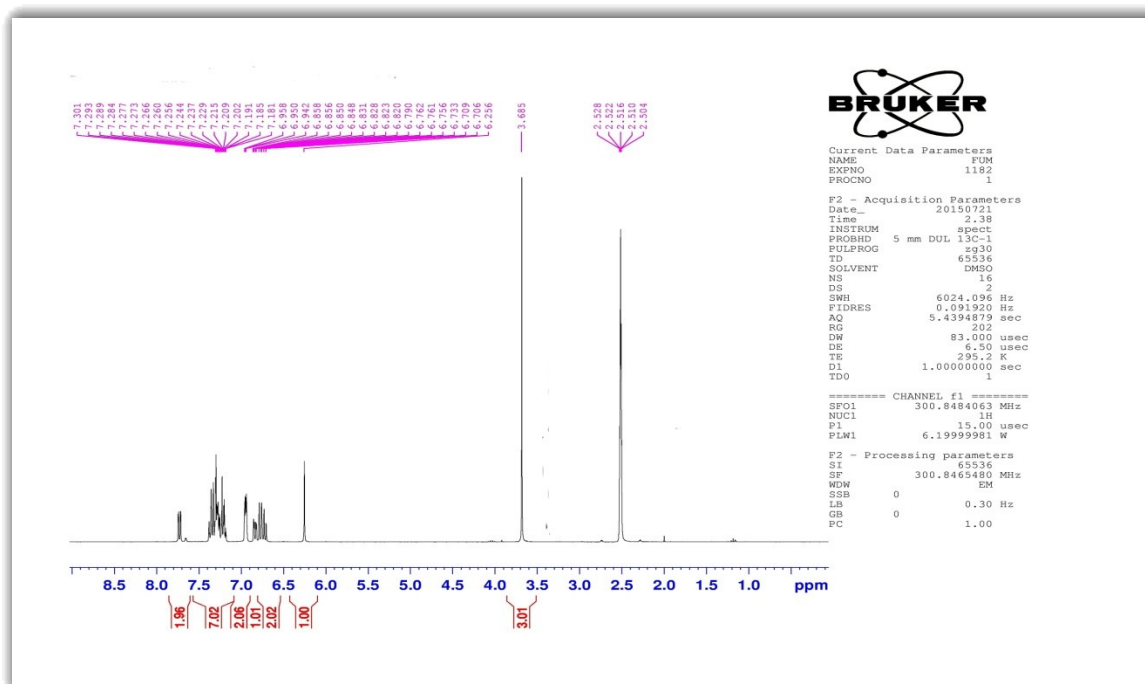


Figure 3e-B1: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(3-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3e).

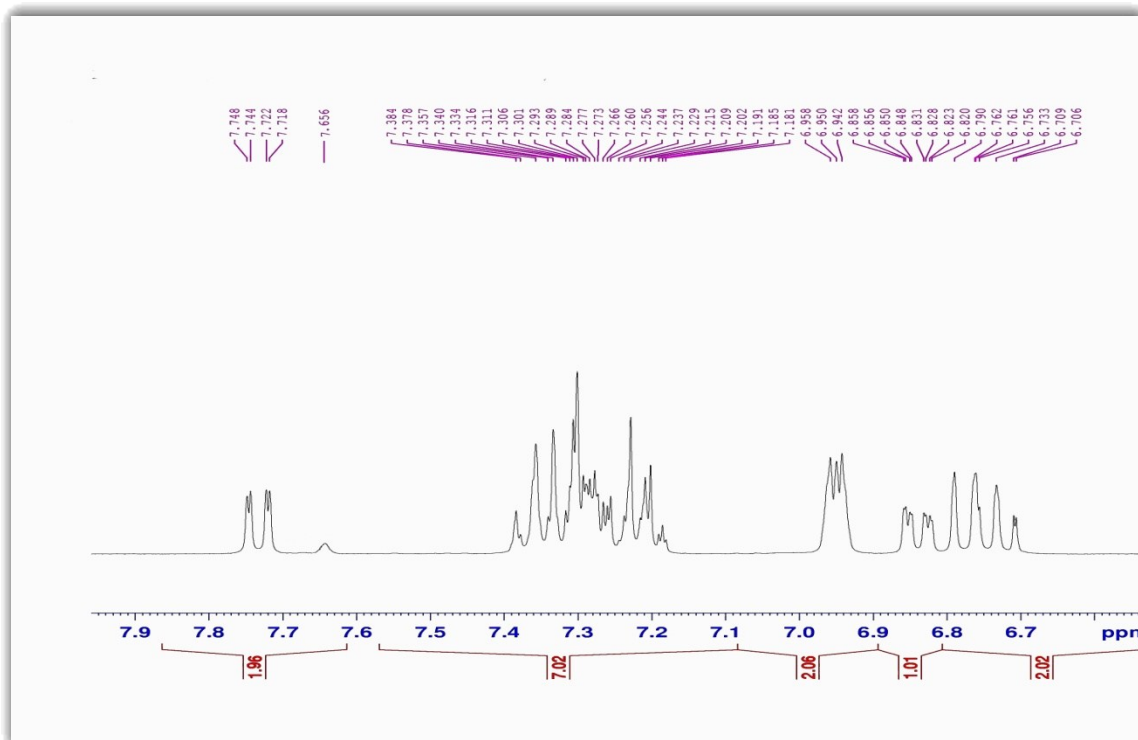


Figure 3e-B2: ^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 2-(3-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3e) expanded.

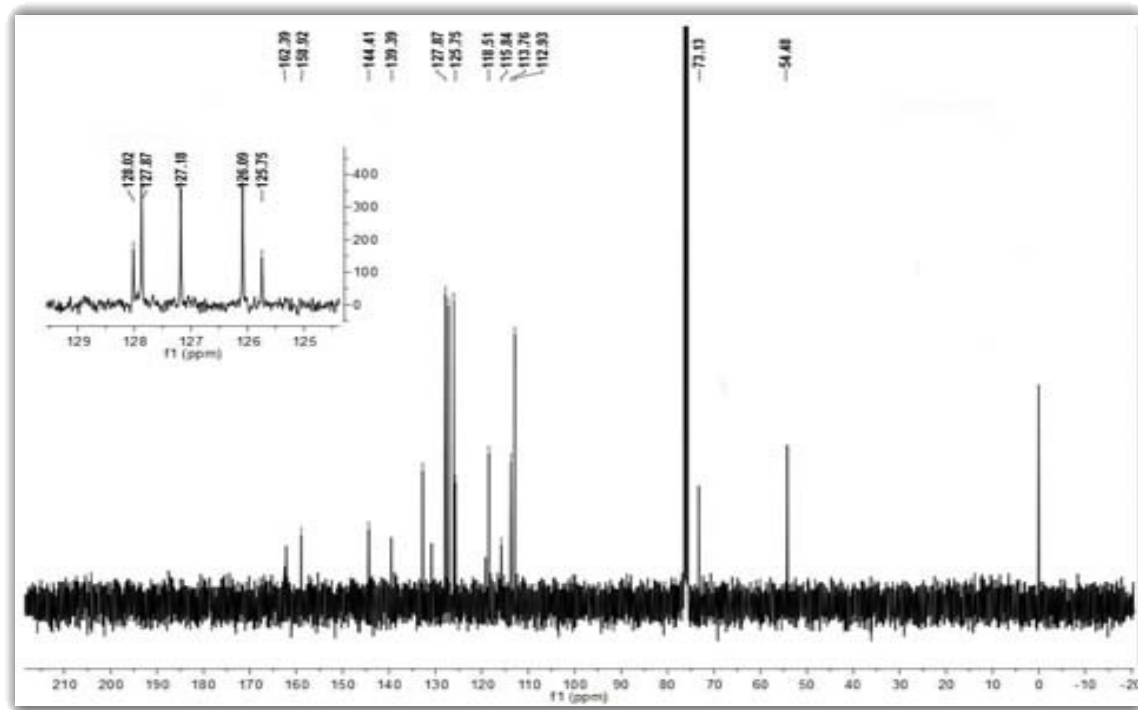


Figure 3e-C: ^{13}C NMR (100 MHz, CDCl_3) of 2-(3-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3e).

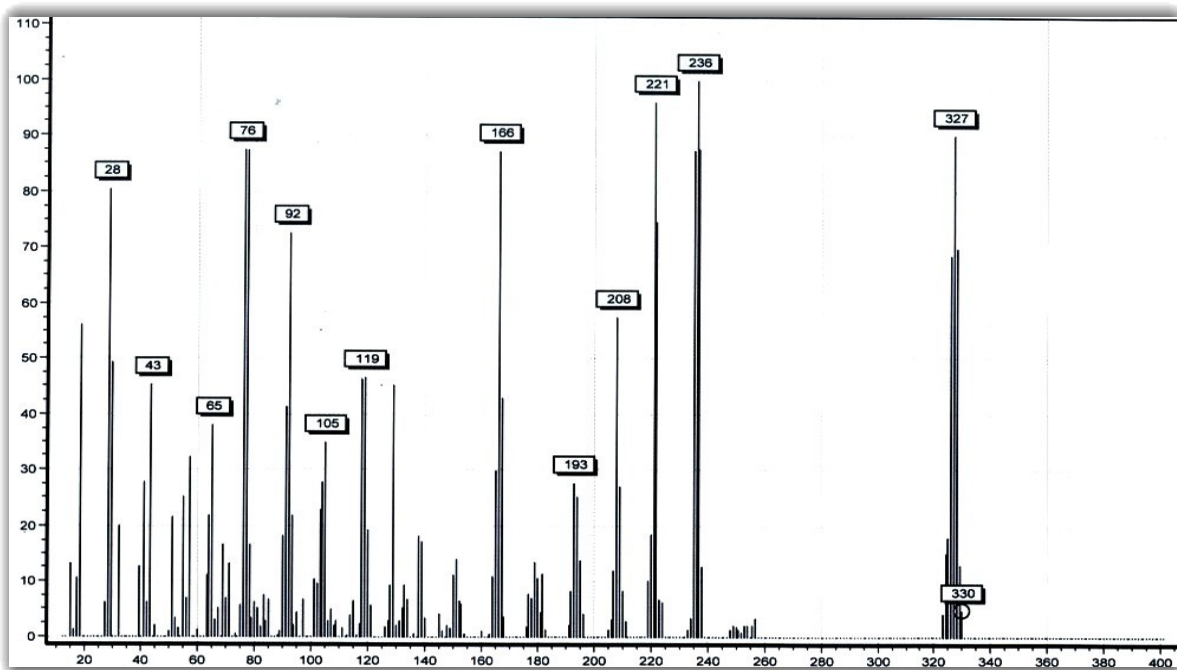


Figure 3e-D: Mass spectrum of 2-(3-Methoxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3c).

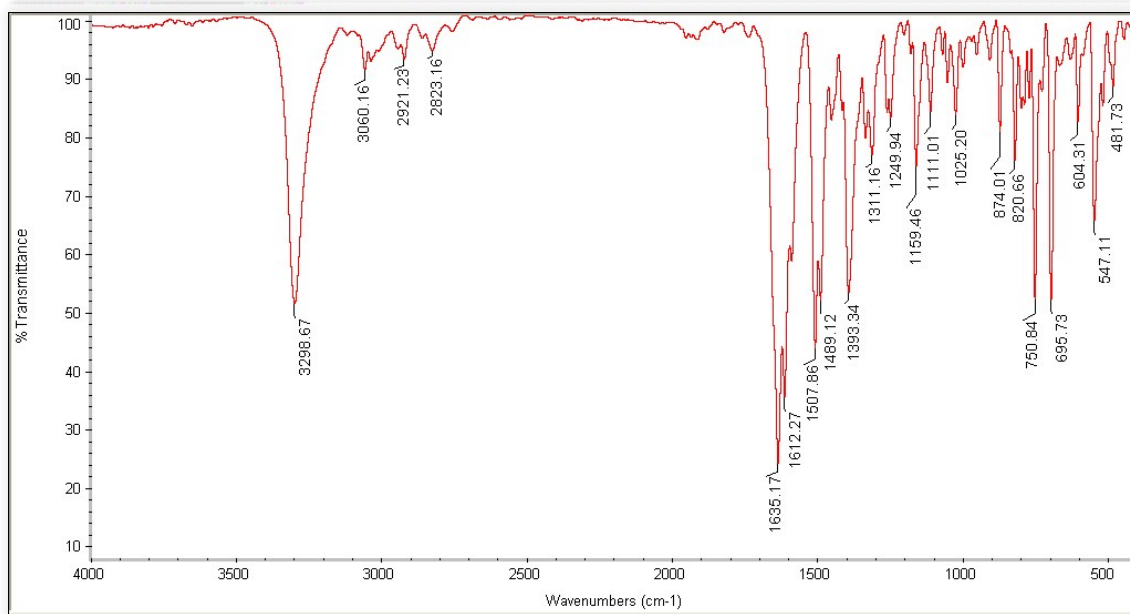
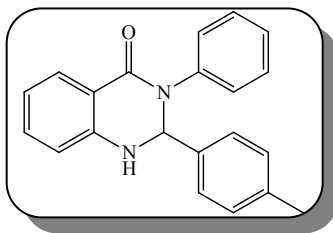


Figure 3f-A: FT-IR (KBr) of 2-(4-Methylphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3f).

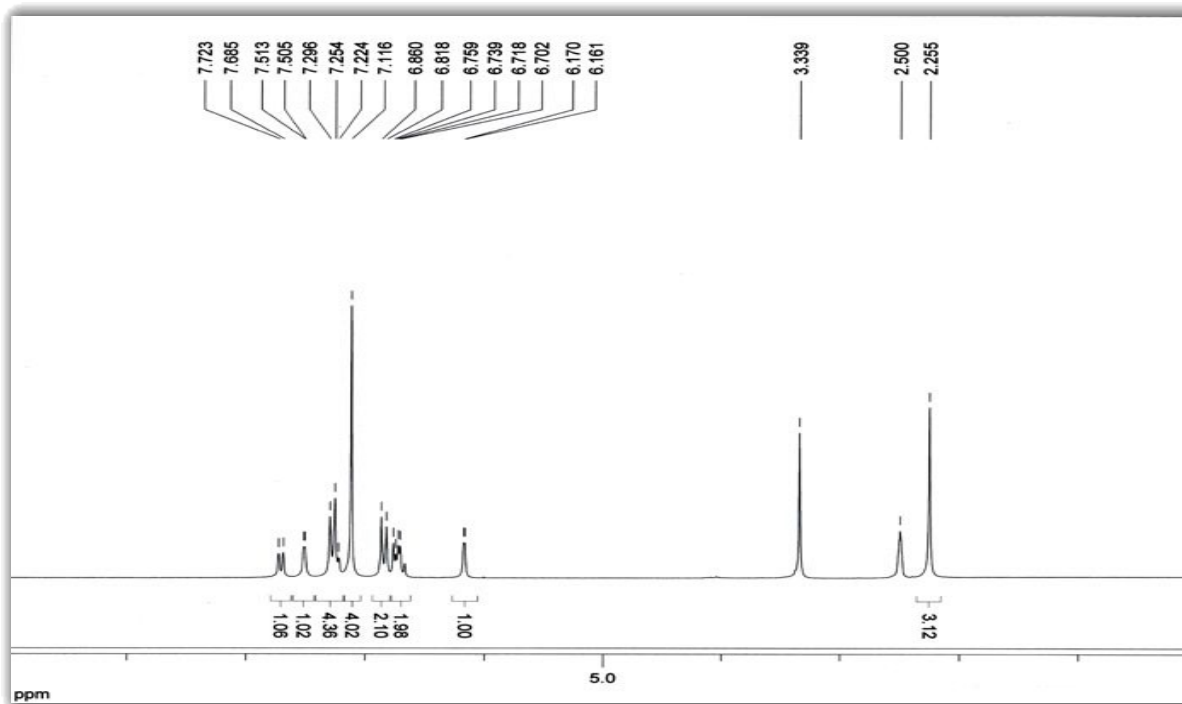


Figure 3f-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(4-Methylphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3f).

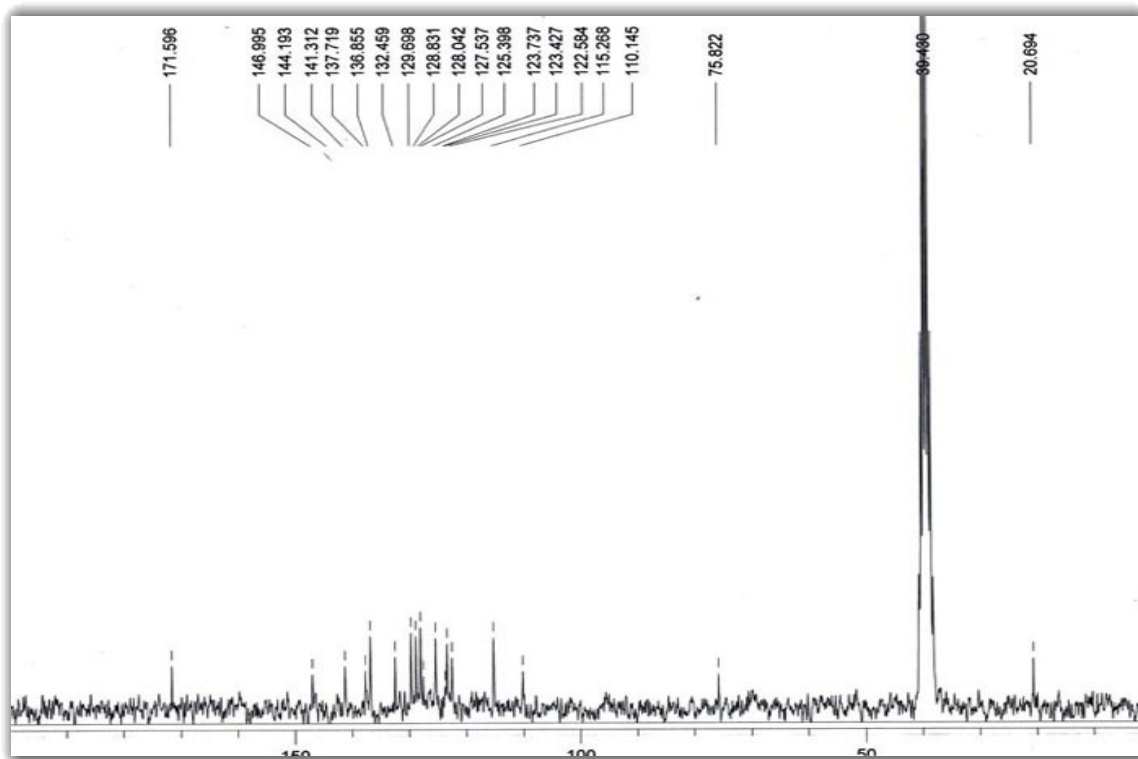


Figure 3f-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-Methylphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3f).

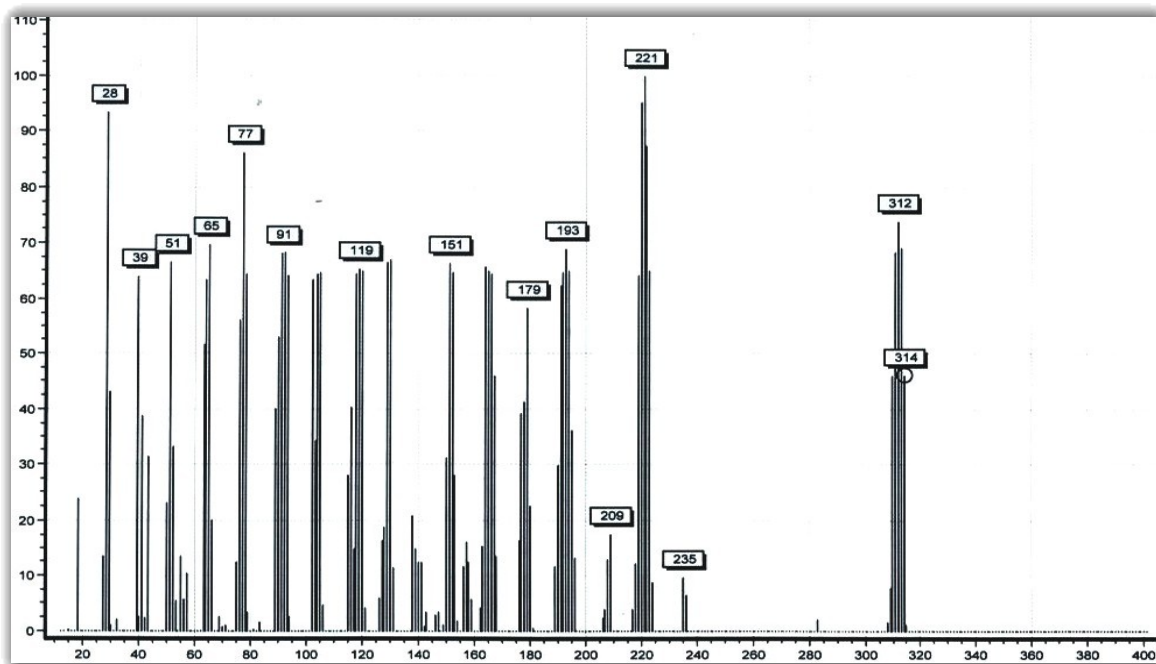


Figure 3f-D: Mass spectrum of 2-(4-Methylphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3f).

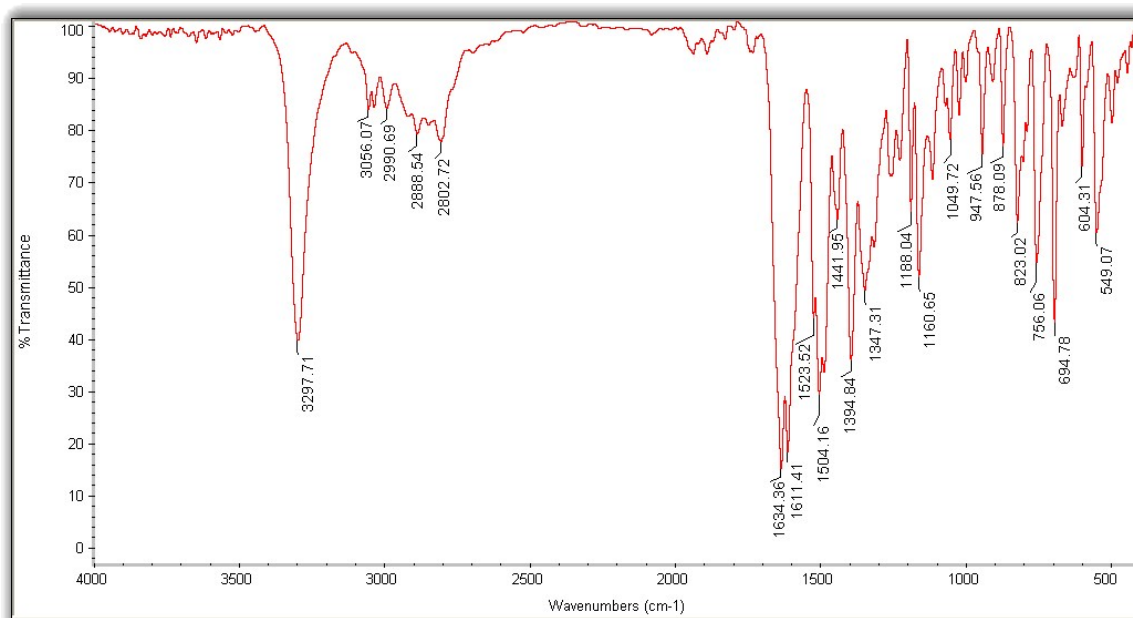
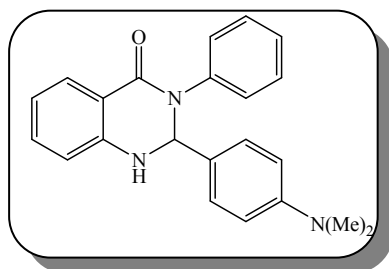


Figure 3g-A: FT-IR (KBr) of 2-(4-(Dimethylamino) phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3g).

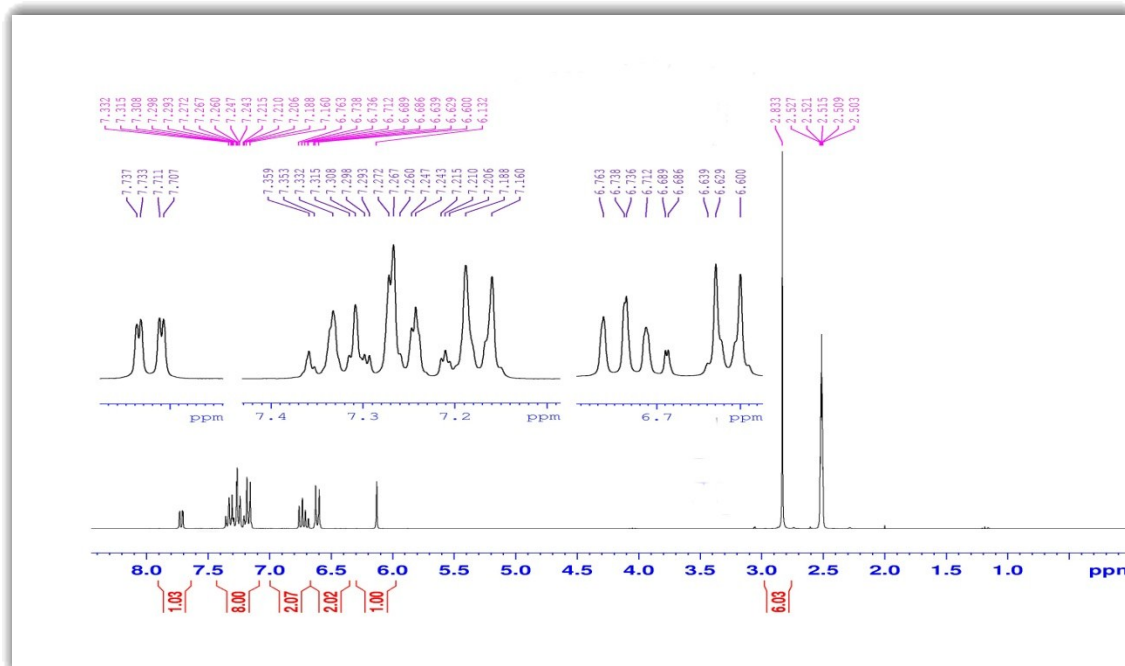


Figure 3g-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(4-(Dimethylamino) phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3g).

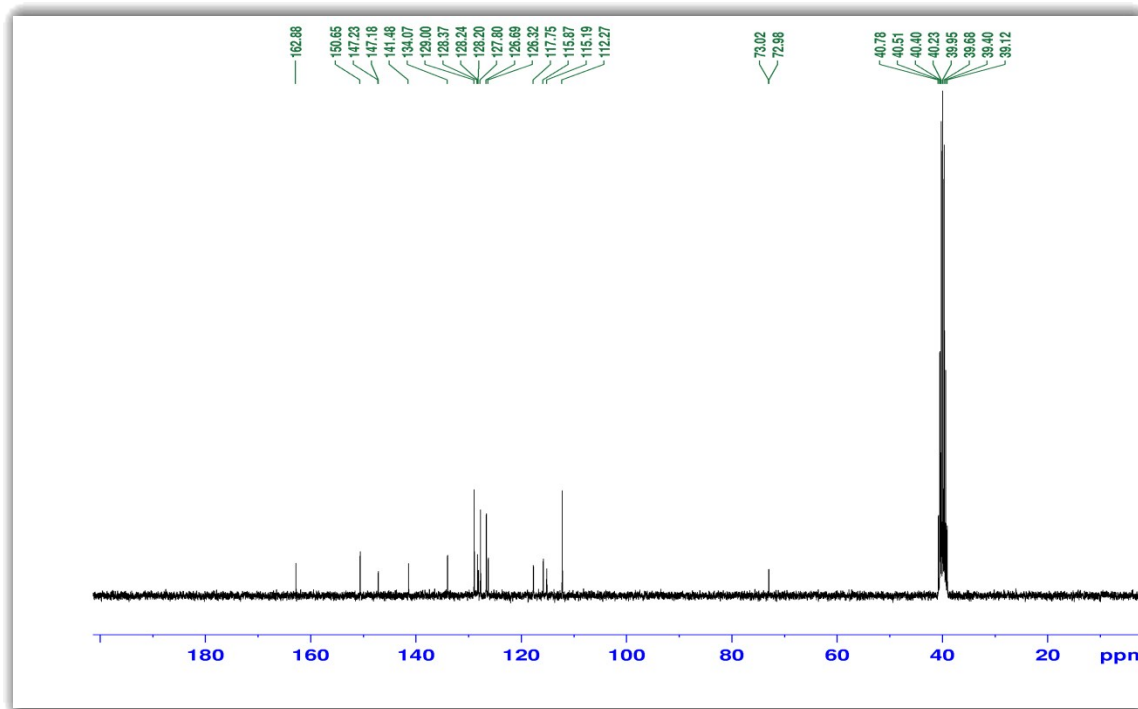


Figure 3g-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-(Dimethylamino) phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3g).

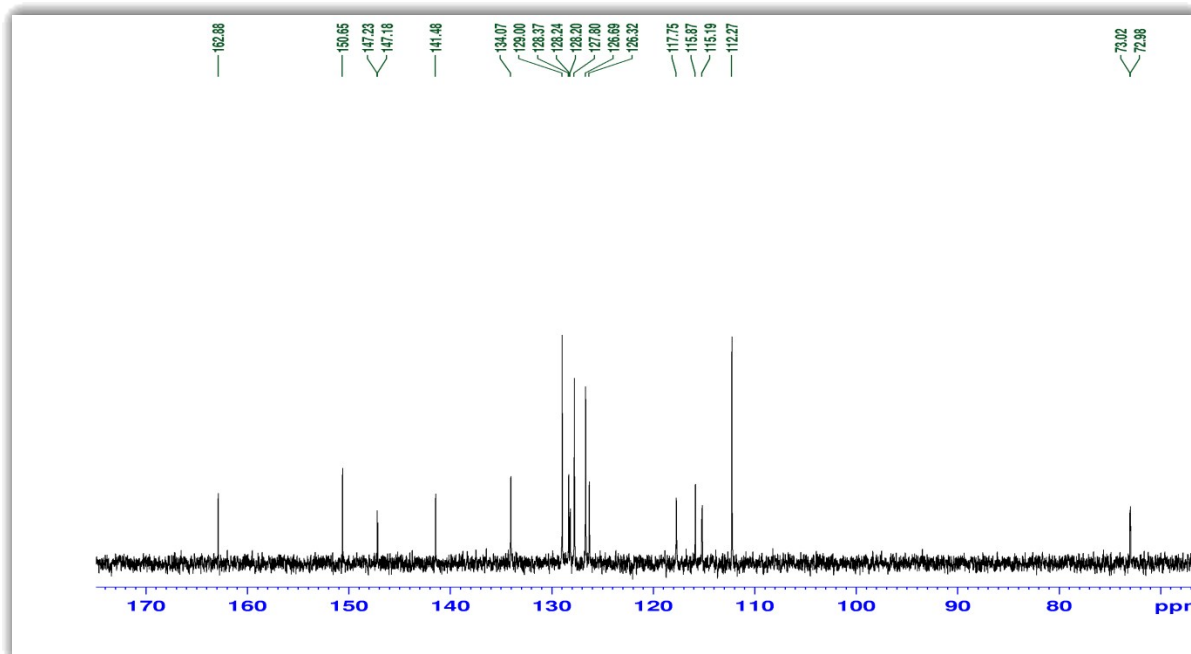


Figure 3g-C1: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-(Dimethylamino) phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3g) expanded.

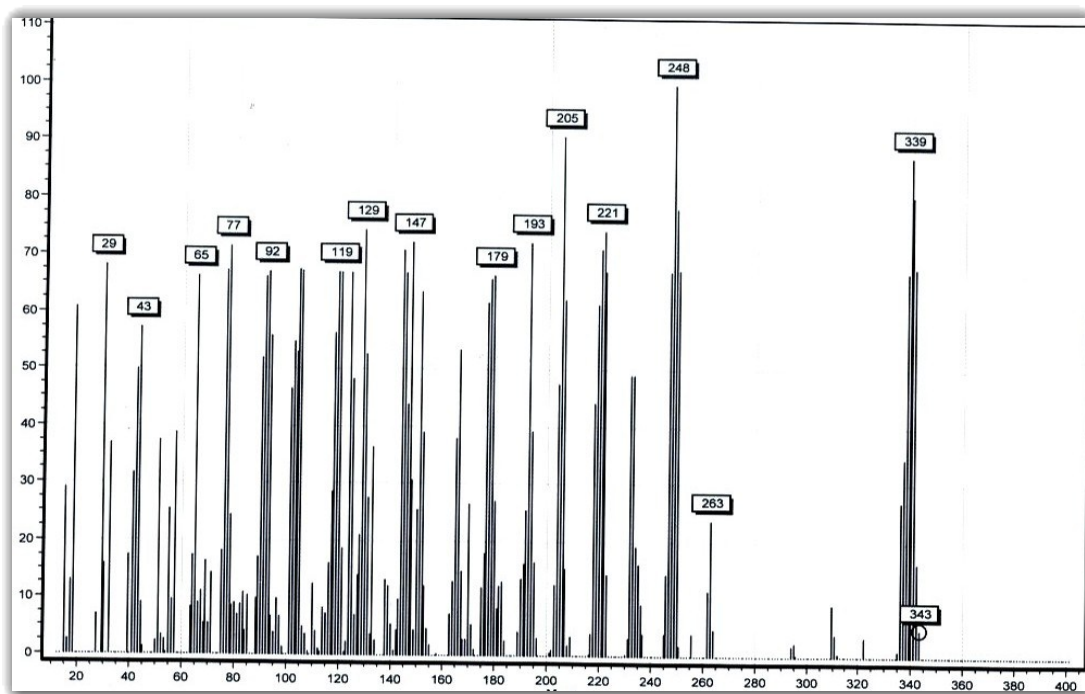


Figure 3g-D: Mass spectrum of 2-(4-(Dimethylamino) phenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3g).

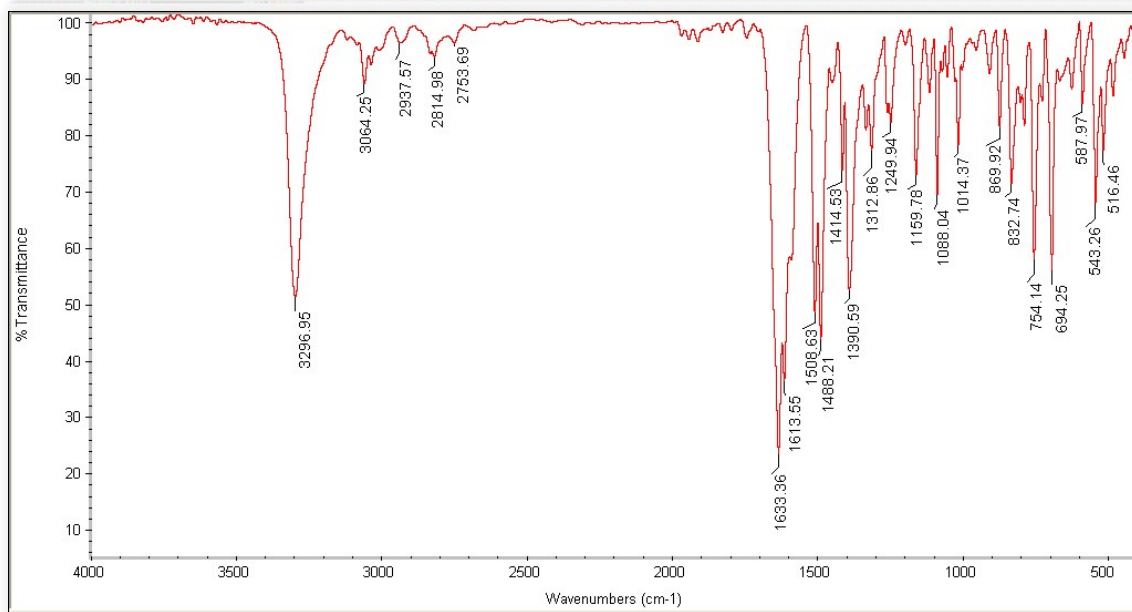
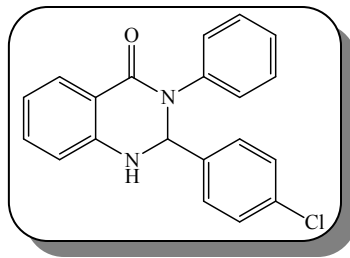


Figure 3h-A: FT-IR (KBr) of 2-(4-Chlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3h).

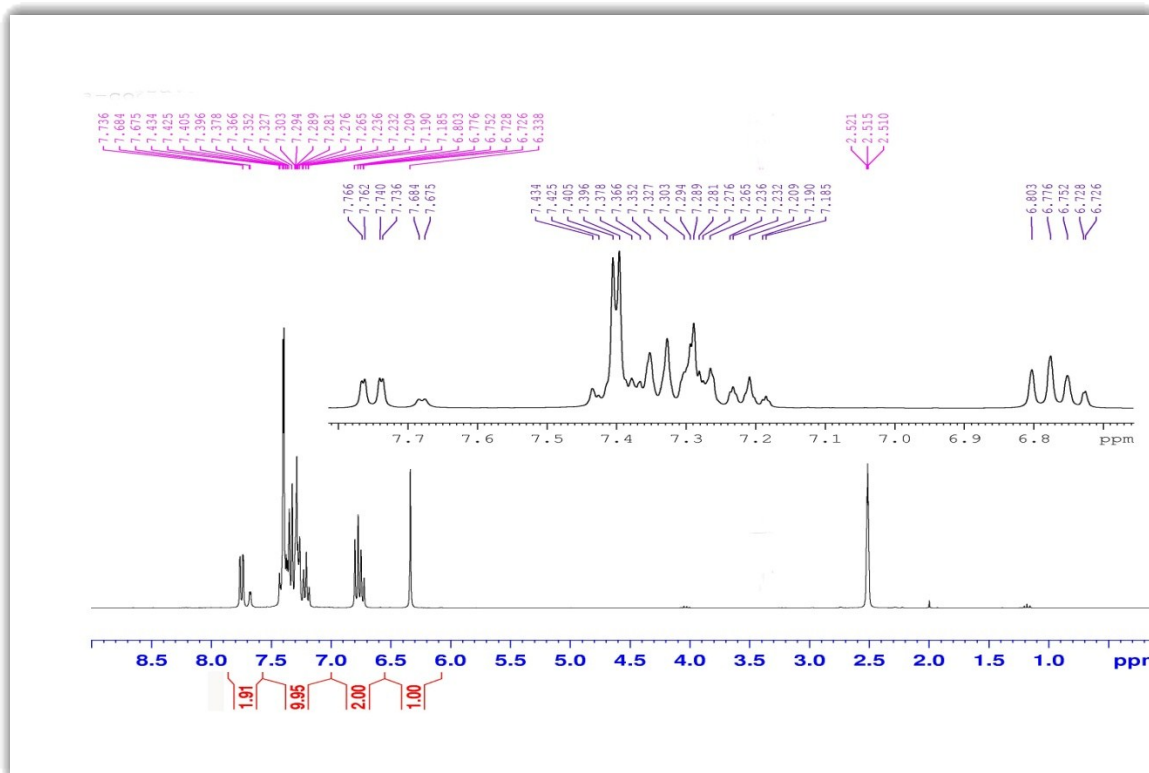


Figure 3h-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(4-Chlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1H)-one (3h).

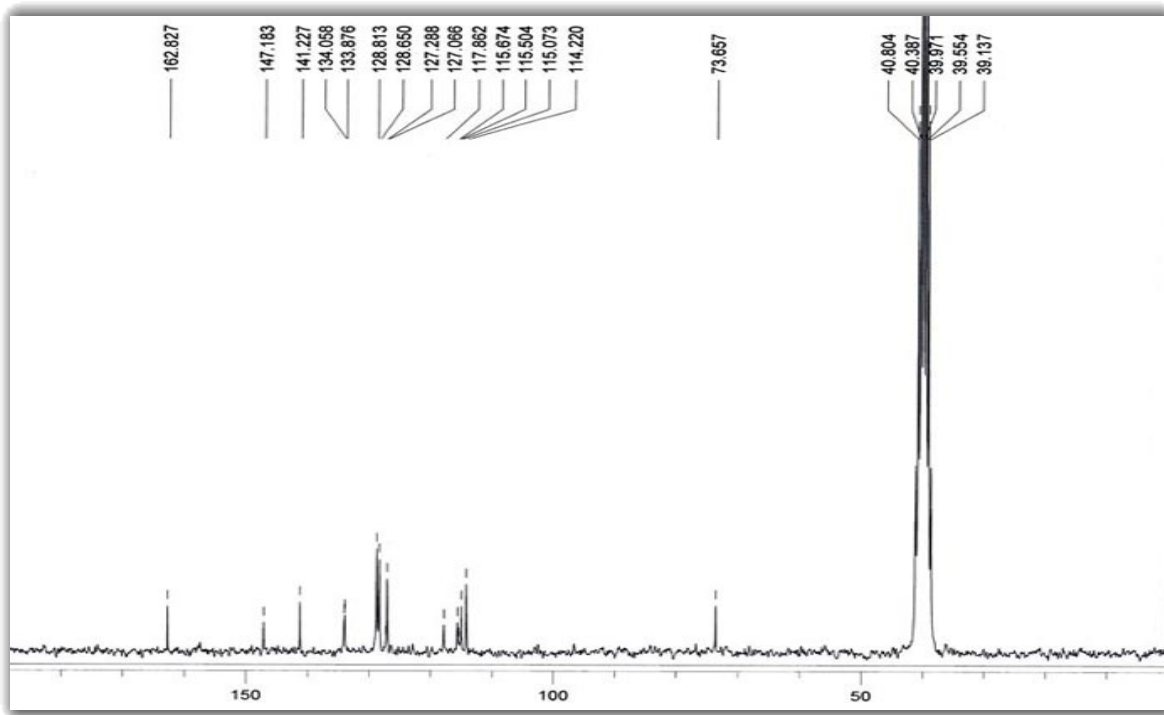


Figure 3h-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-Chlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3h).

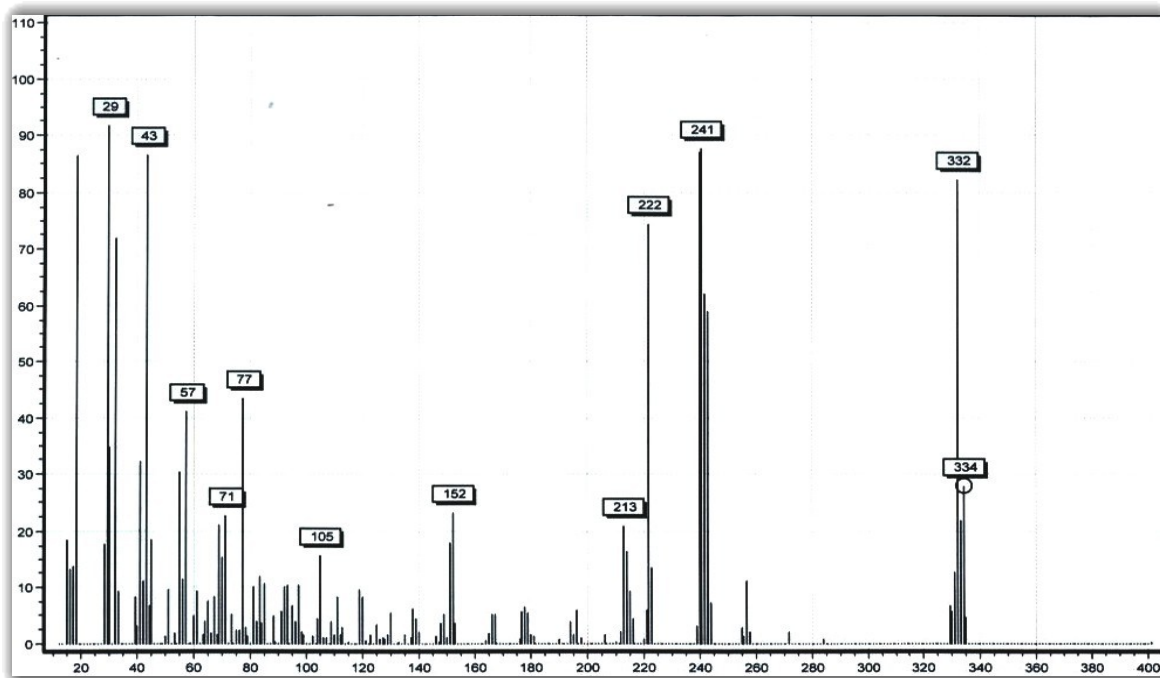


Figure 3h-D: Mass spectrum of 2-(4-Chlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3h).

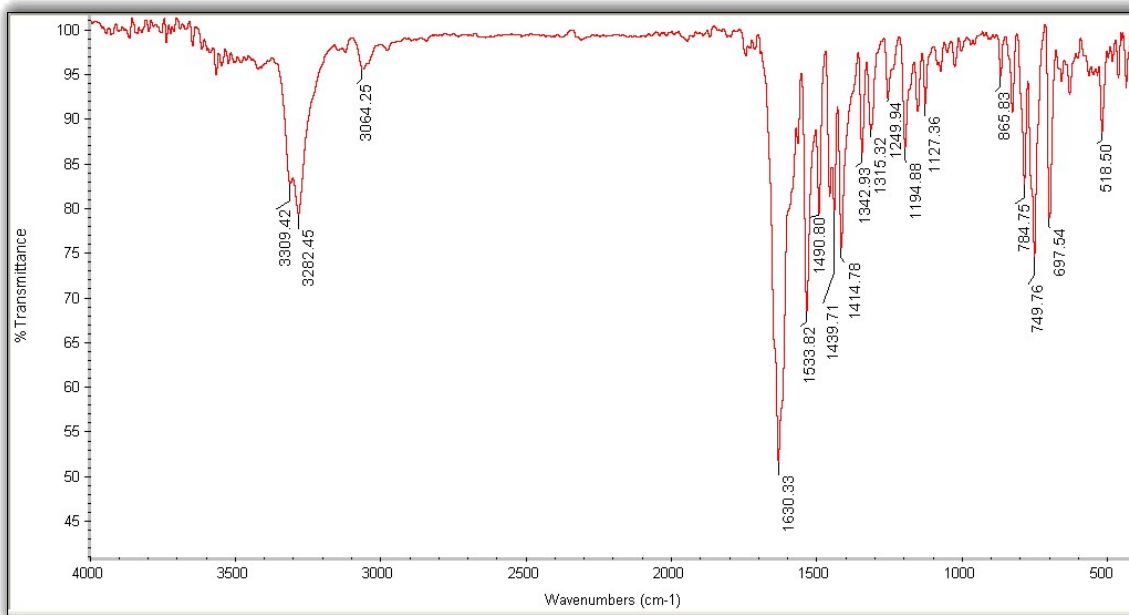
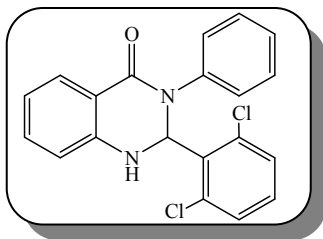


Figure 3i-A: FT-IR (KBr) of 2-(2,6-Dichlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3i).

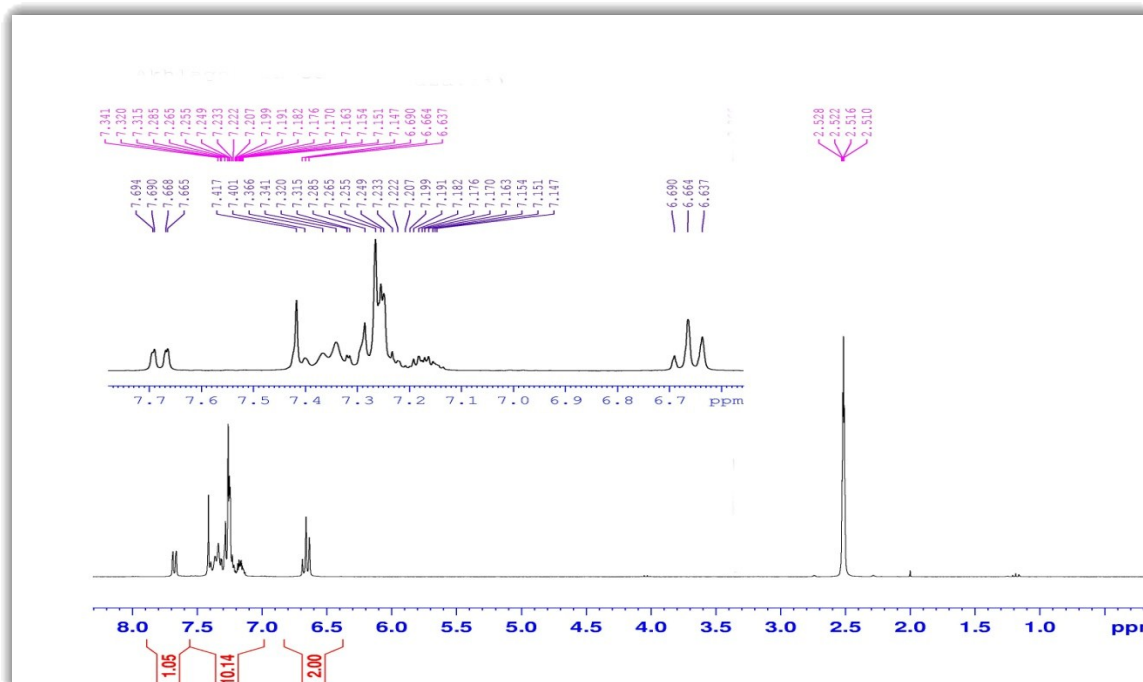


Figure 3i-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(2,6-Dichlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3i).

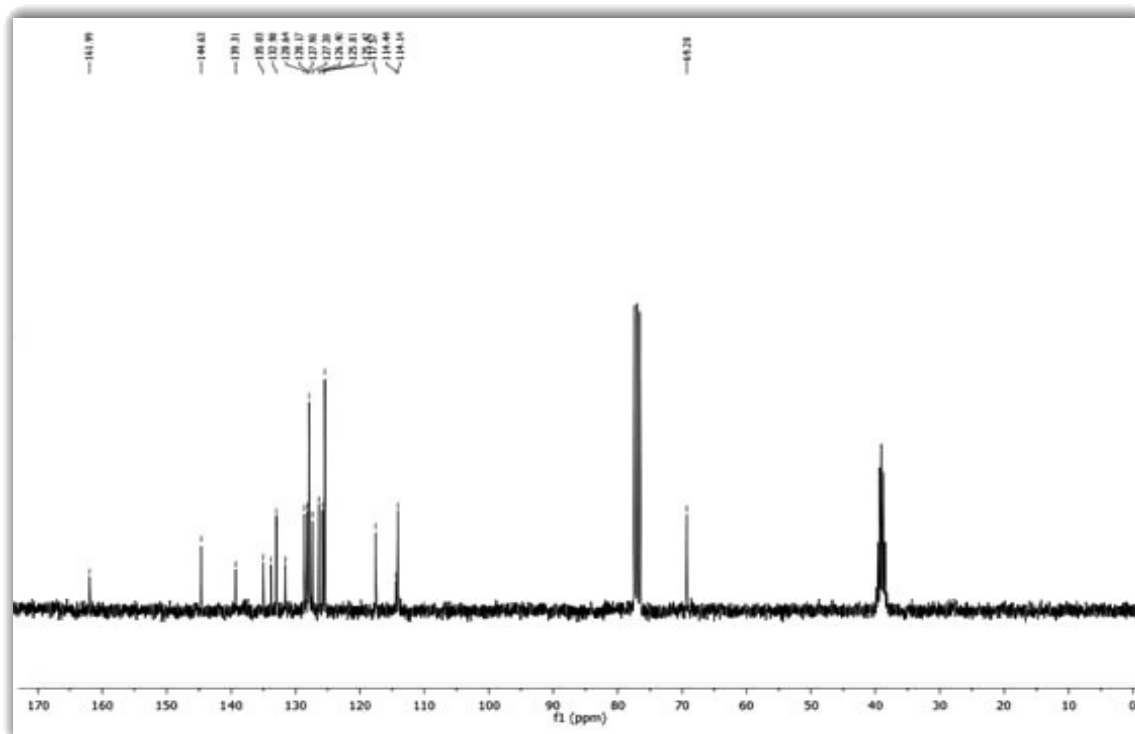


Figure 3i-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$, CDCl_3) of 2-(2,6-Dichlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3i).

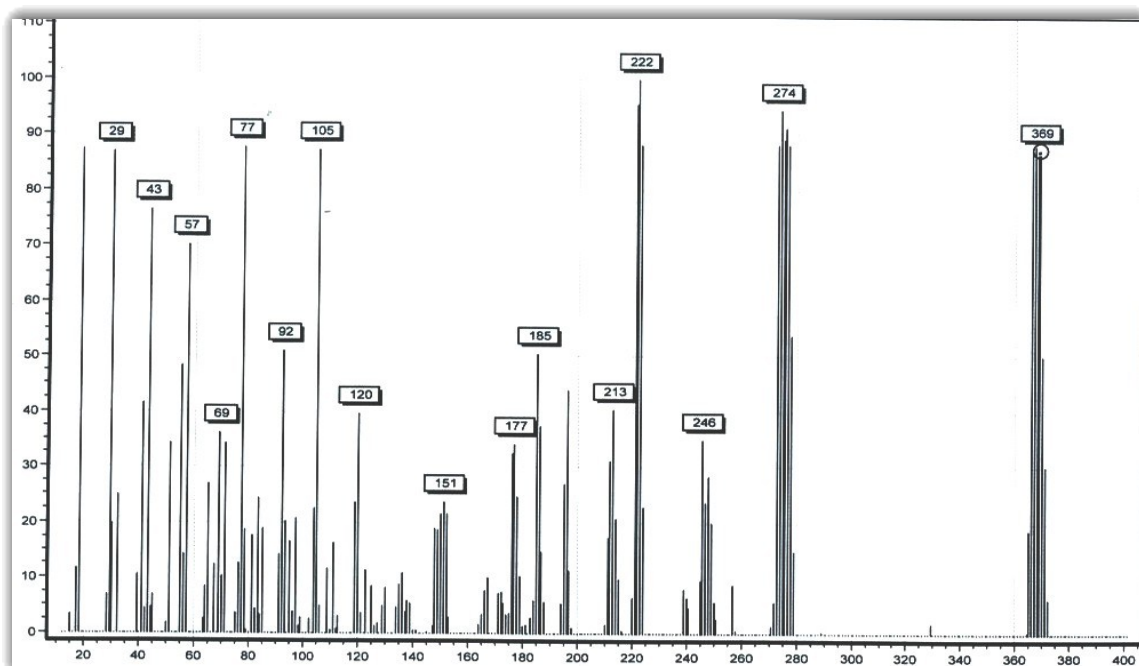


Figure 3i-D: Mass spectrum of 2-(2,6-Dichlorophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3i).

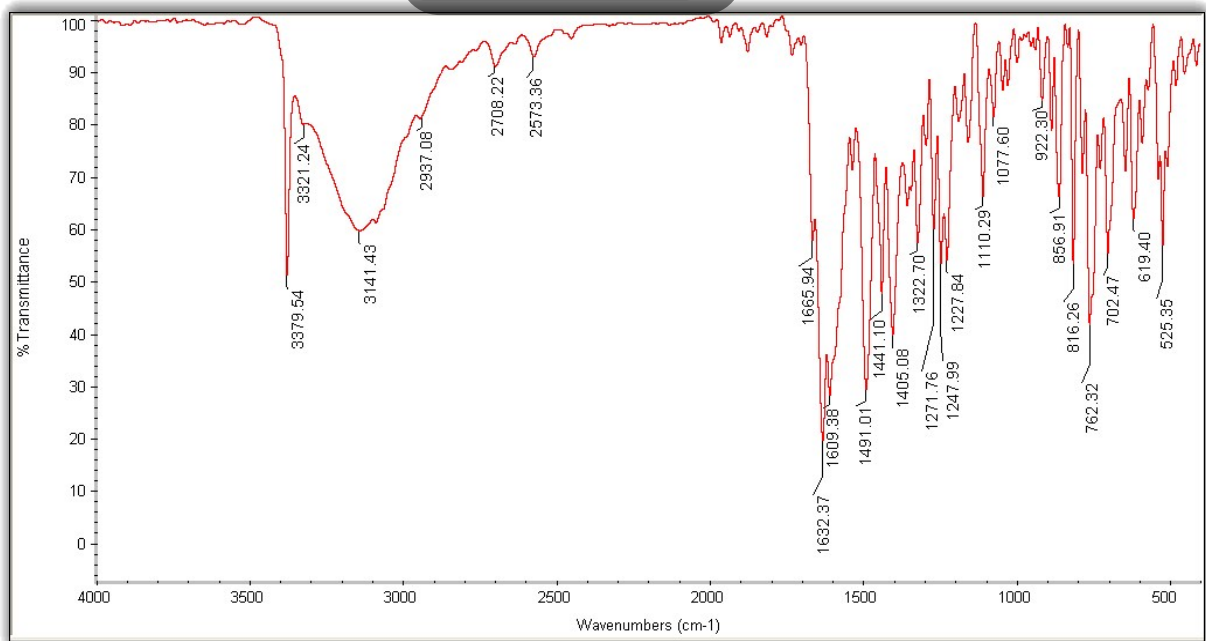
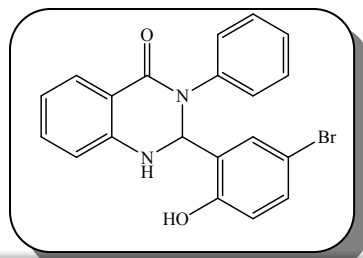


Figure 3j-A: FT-IR (KBr) of 2-(5-Bromo-2-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3j).

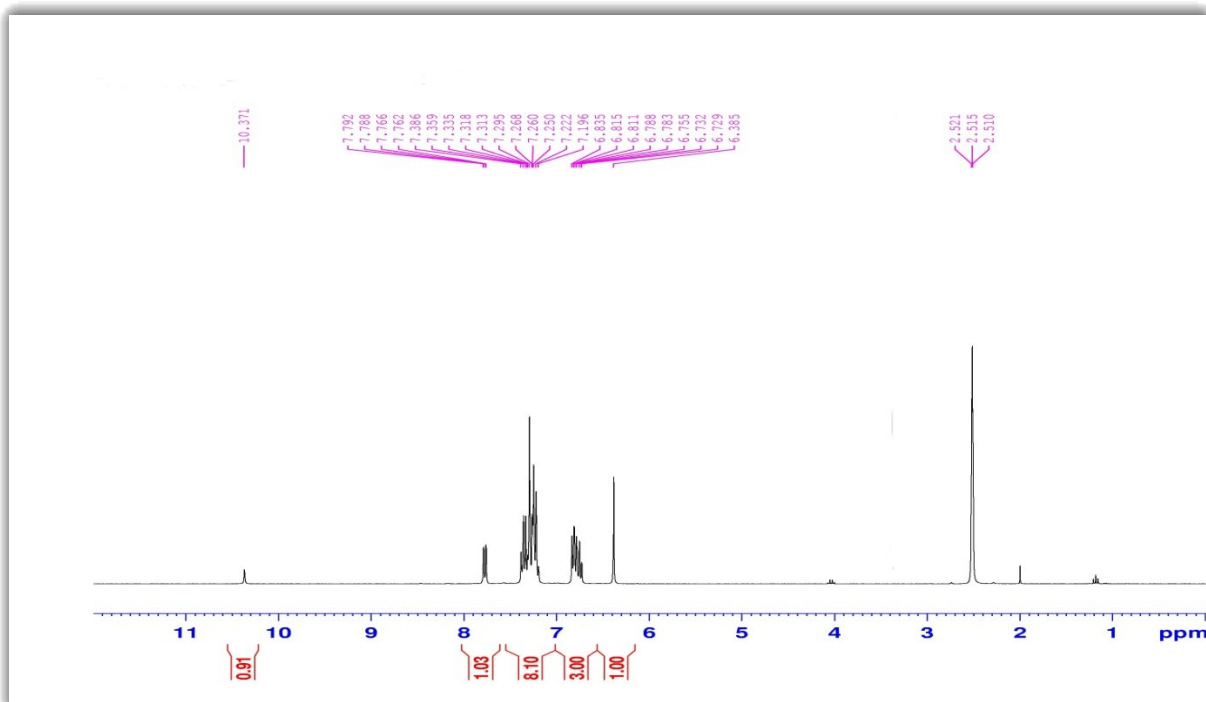


Figure 3j-B1: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(5-Bromo-2-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3j).

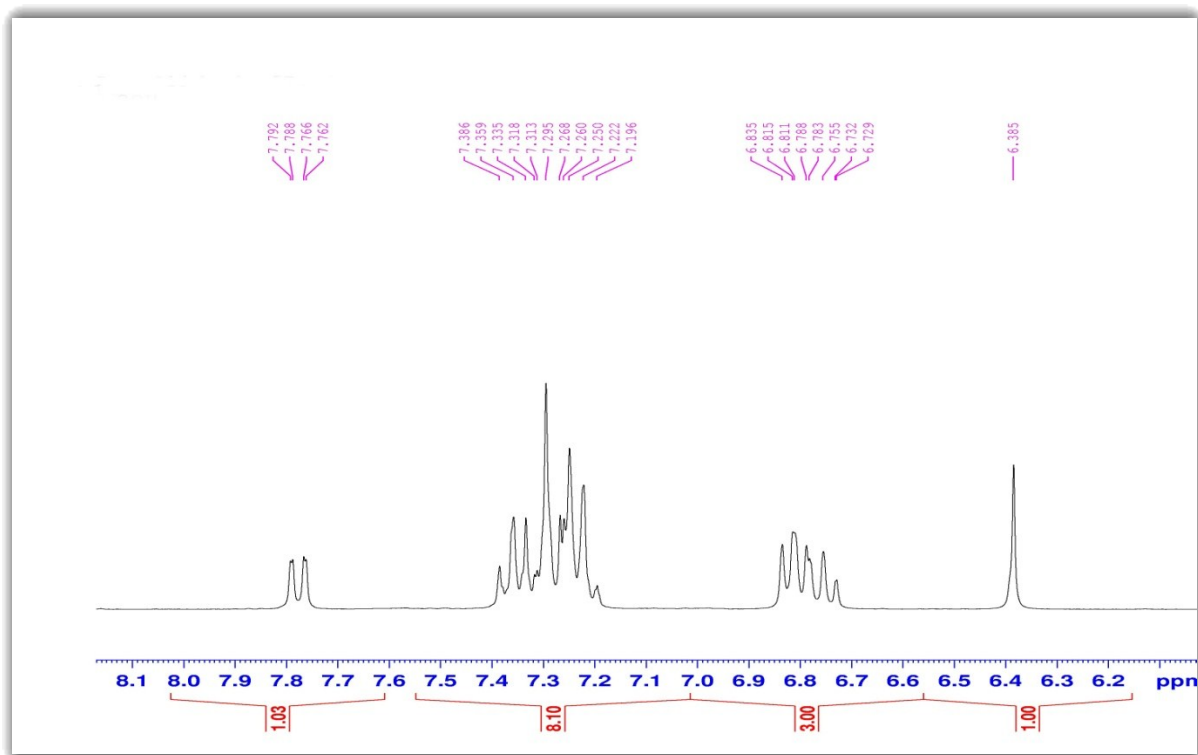


Figure 3j-B2: ^1H NMR (300 MHz, $\text{DMSO}-d_6$) of 2-(5-Bromo-2-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3j) expanded.

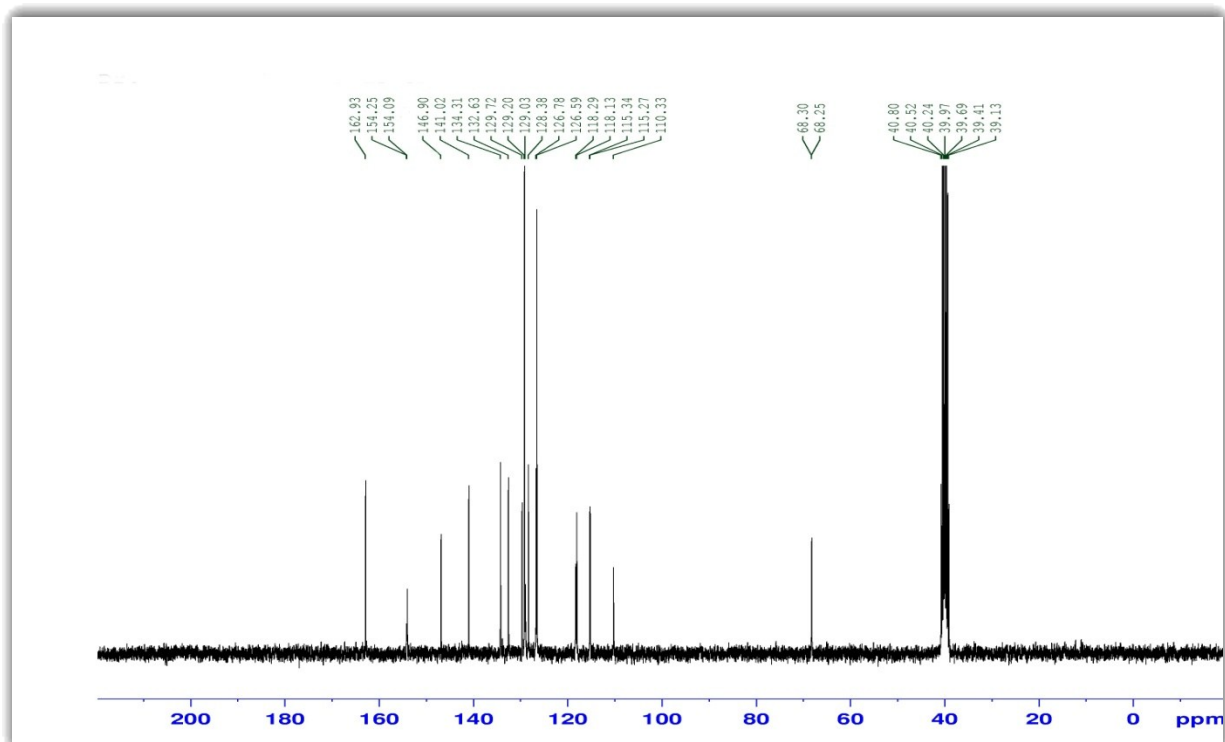


Figure 3j-C1: ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of 2-(5-Bromo-2-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3j).

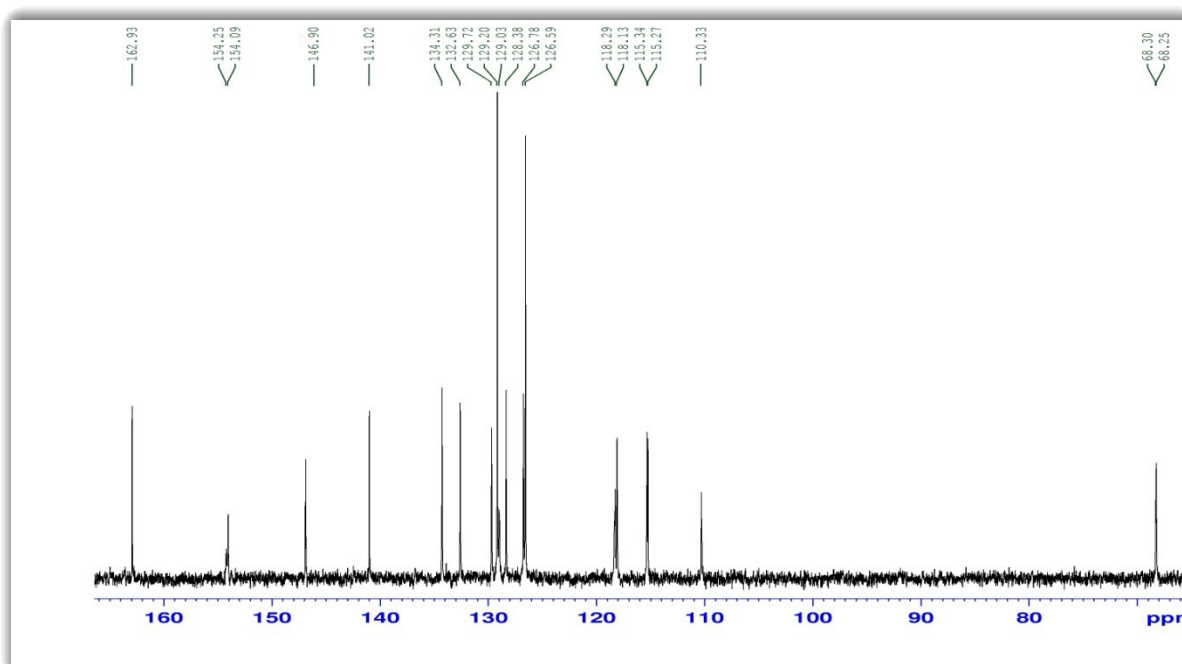


Figure 3j-C2: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(5-Bromo-2-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3j) expanded.

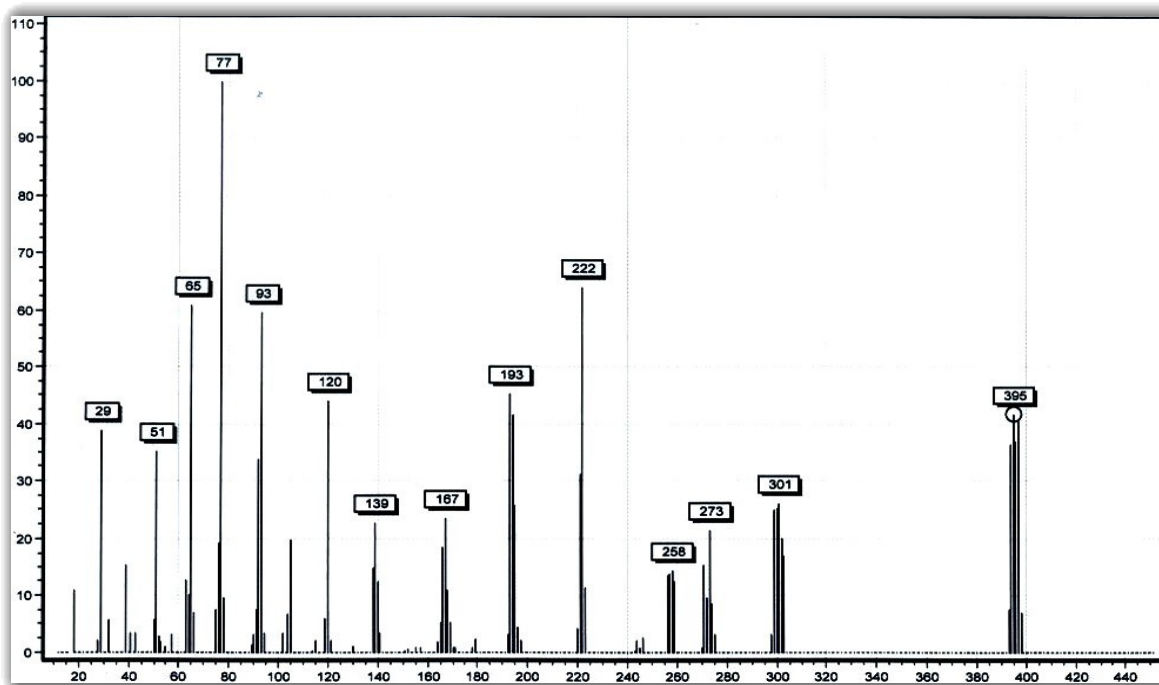


Figure 3j-D: Mass spectrum of 2-(5-Bromo-2-hydroxyphenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3j).

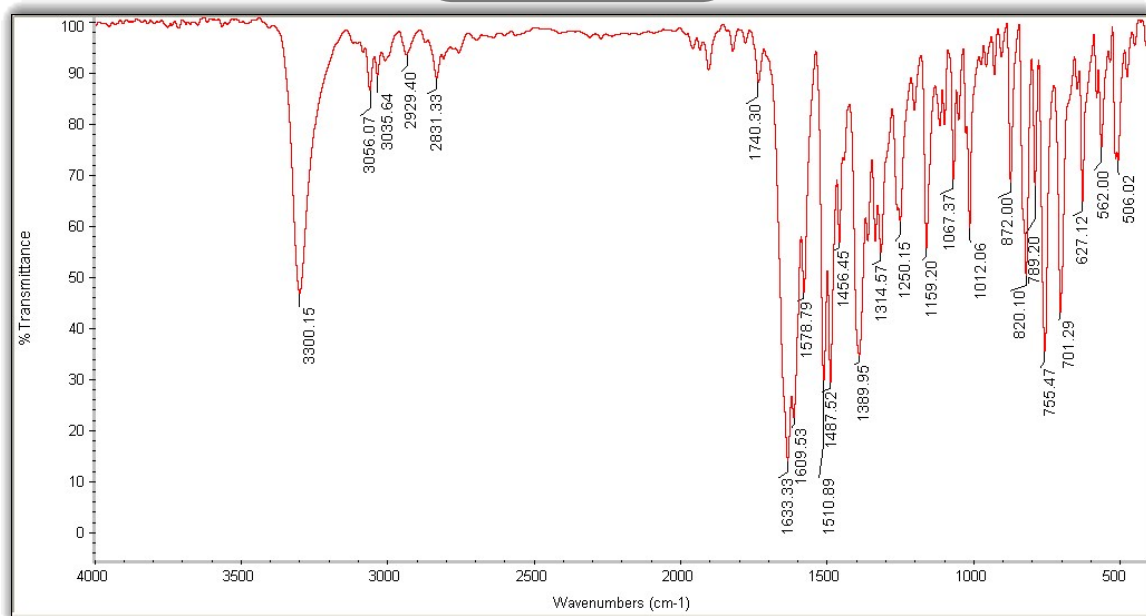
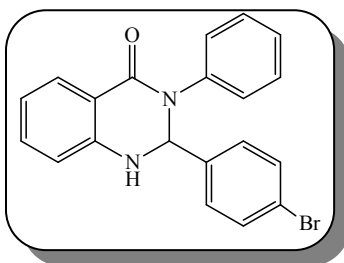


Figure 3k-A: FT-IR (KBr) of 2-(4-Bromophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3k).

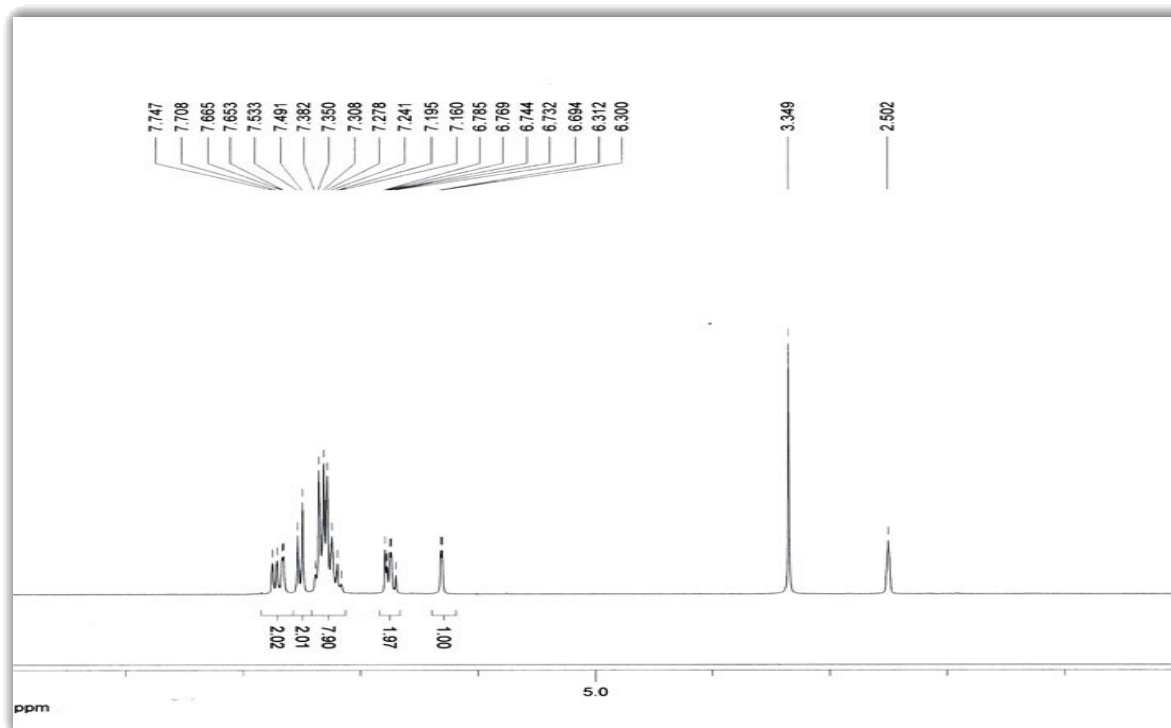


Figure 3k-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(4-Bromophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3k).

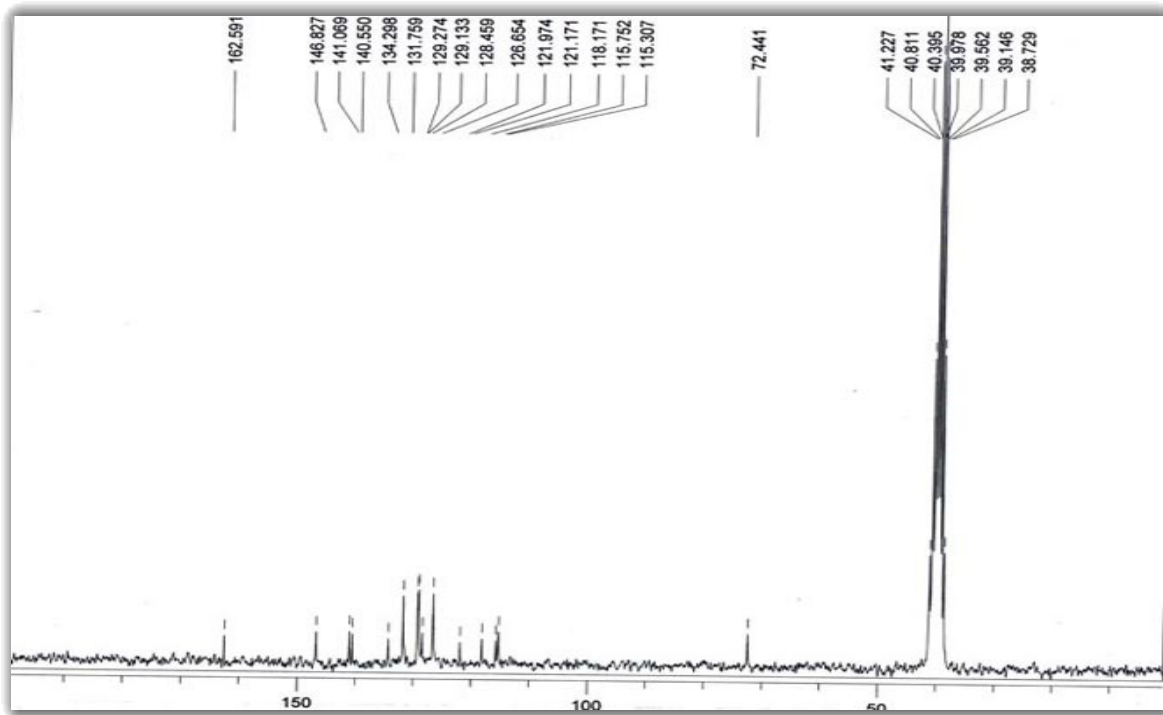


Figure 3k-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-Bromophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3k).

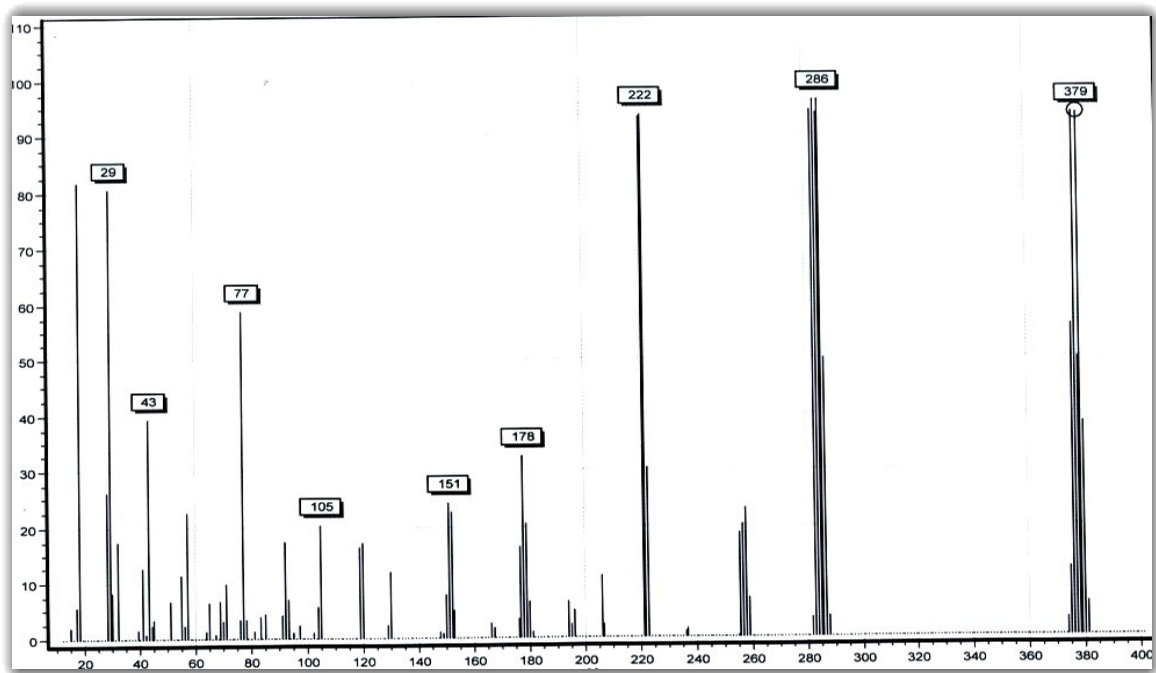


Figure 3k-D: Mass spectrum of 2-(4-Bromophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3k).

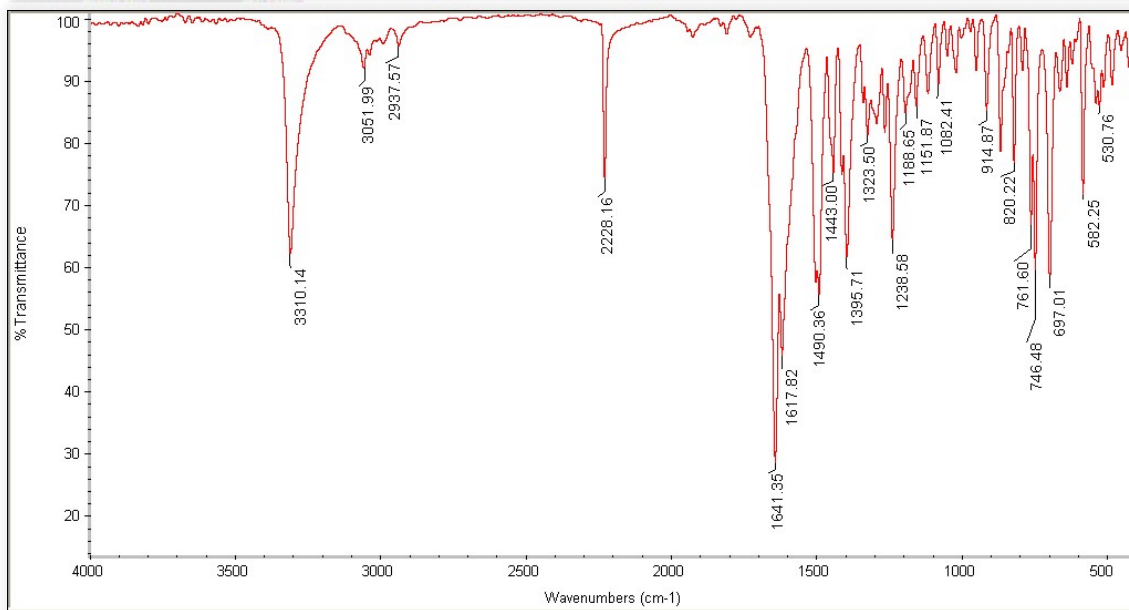
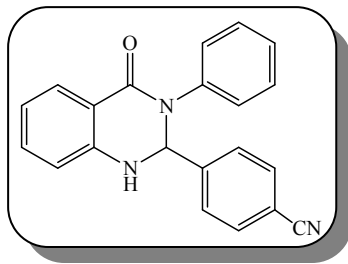


Figure 31-A: FT-IR (KBr) of 2-(4-Cyanophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (31).

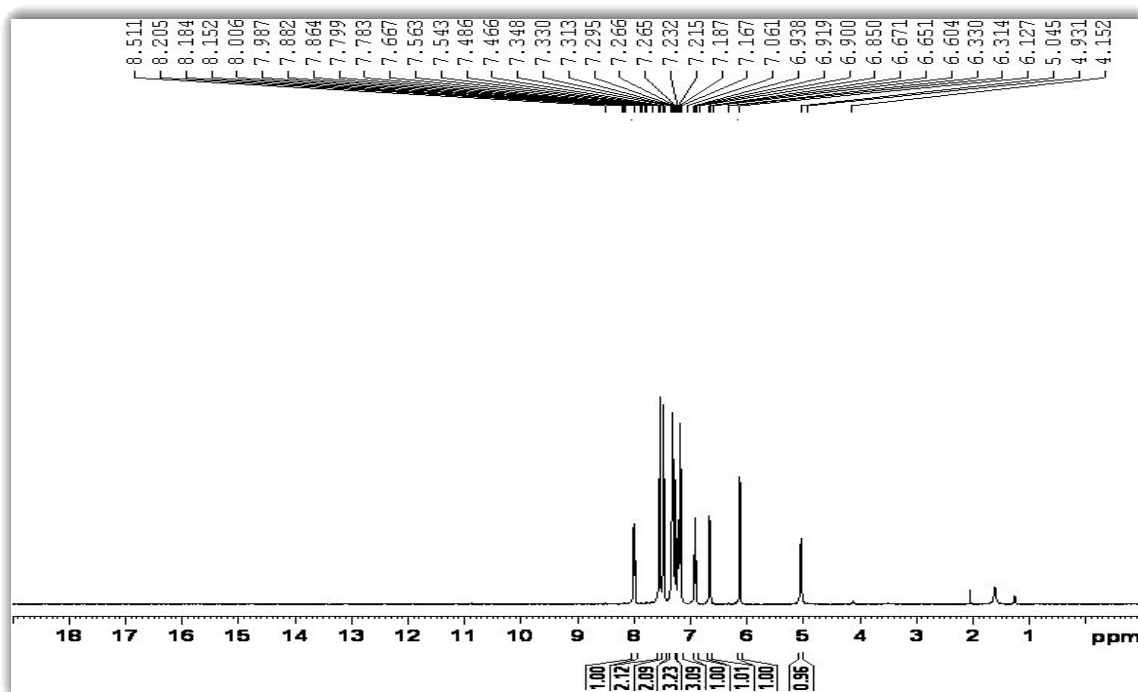


Figure 31-B1: ¹H NMR (400 MHz, CDCl₃) of 2-(4-Cyanophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (31).

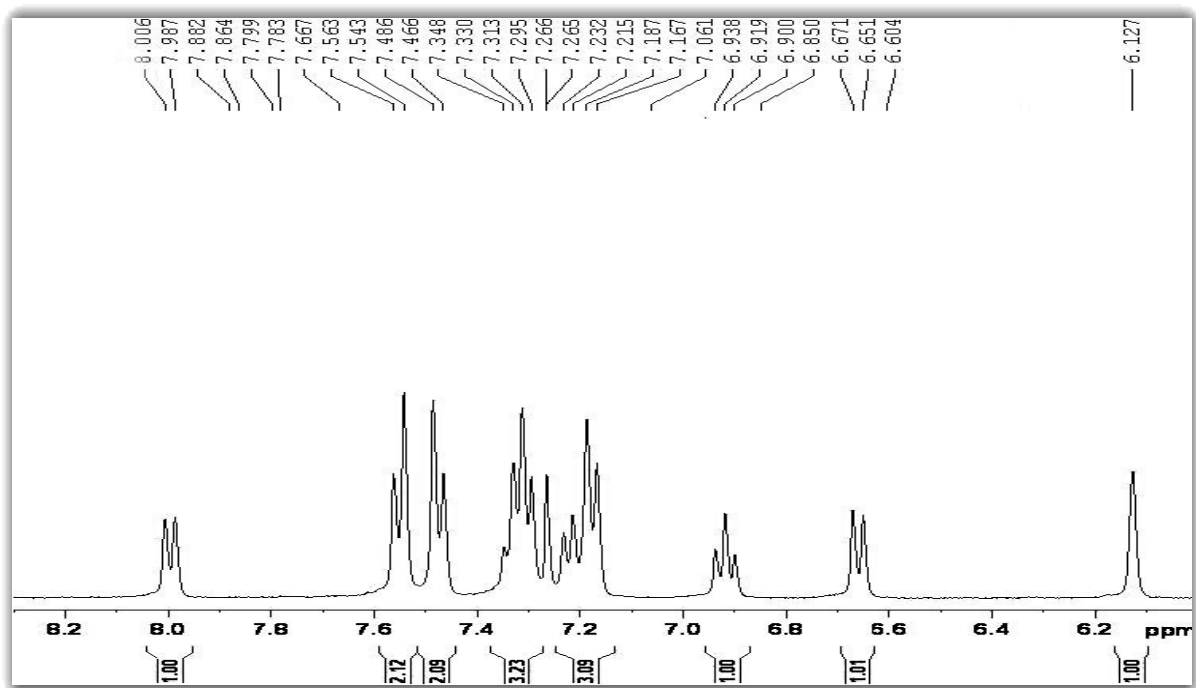


Figure 31-B2: ^1H NMR (400 MHz, CDCl_3) of 2-(4-Cyanophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (31) expanded.

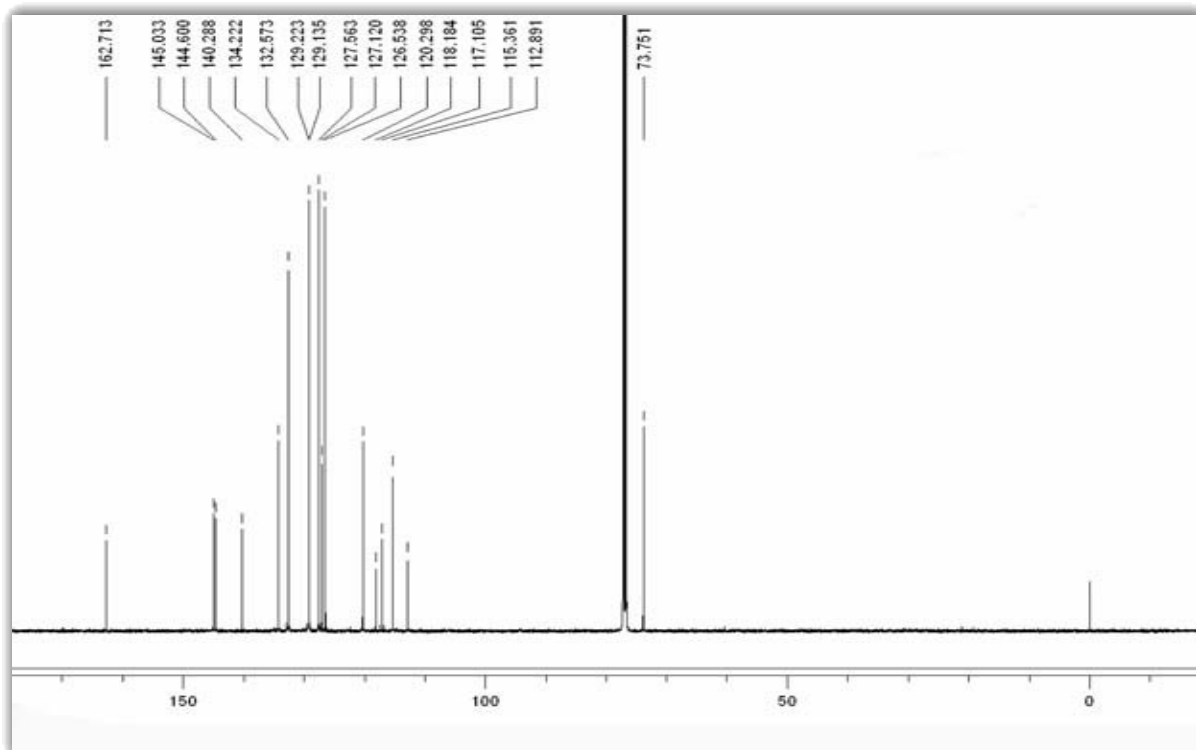


Figure 31-C: ^{13}C NMR (125 MHz, CDCl_3) of 2-(4-Cyanophenyl)-3-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (31).

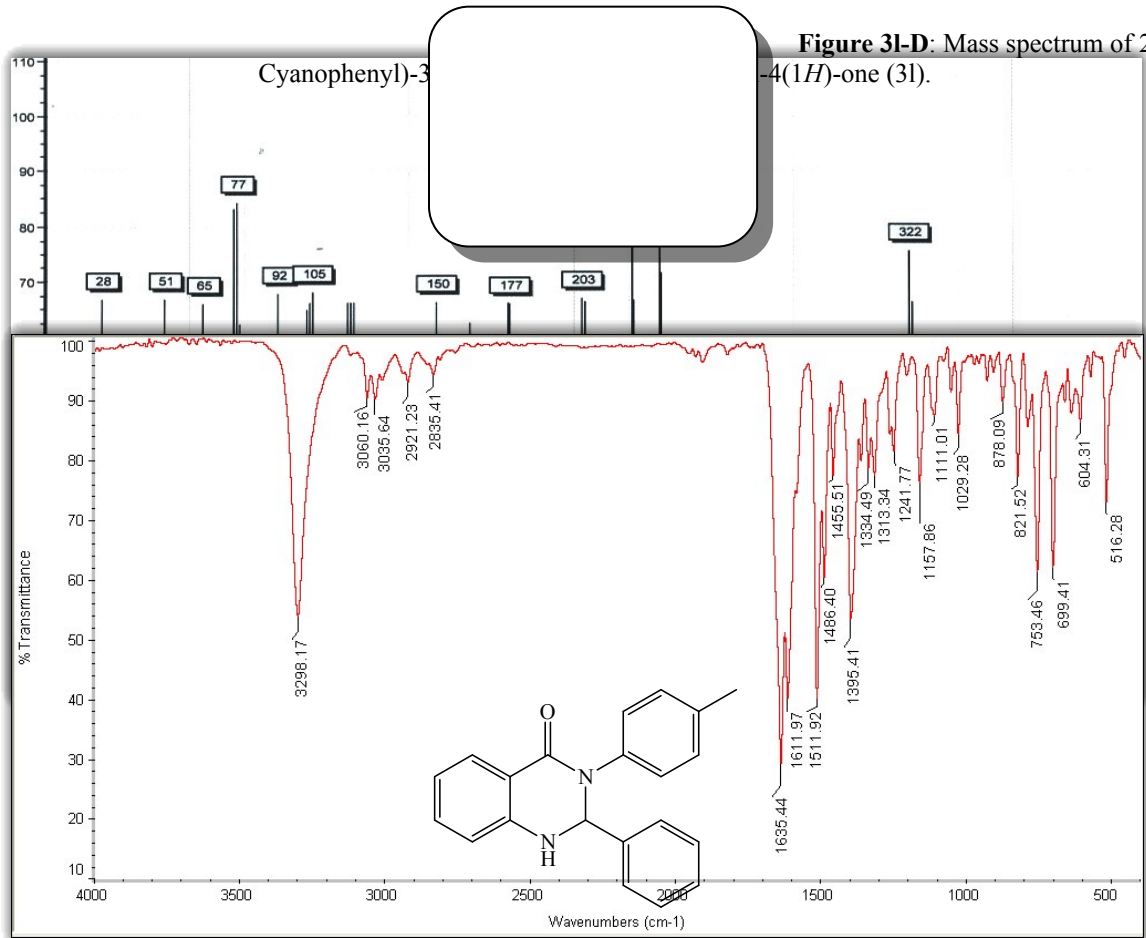


Figure 3m-A: FT-IR (KBr) of 3-(4-Methylphenyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3m).

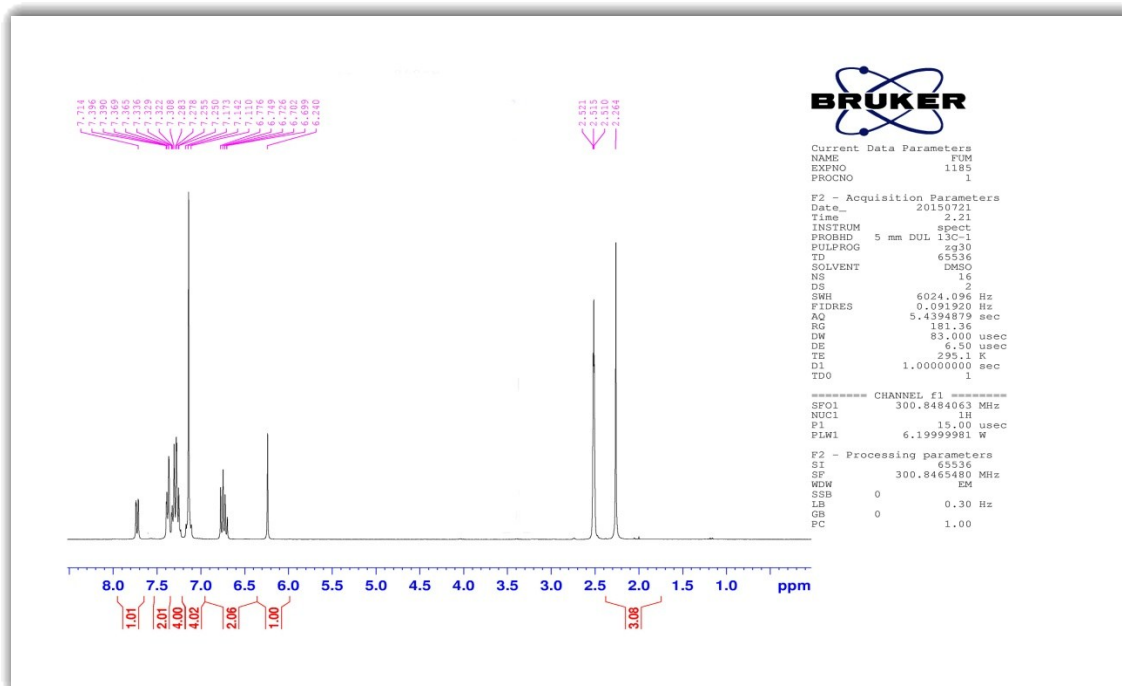


Figure 3m-B1: ^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 3-(4-Methylphenyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3m).

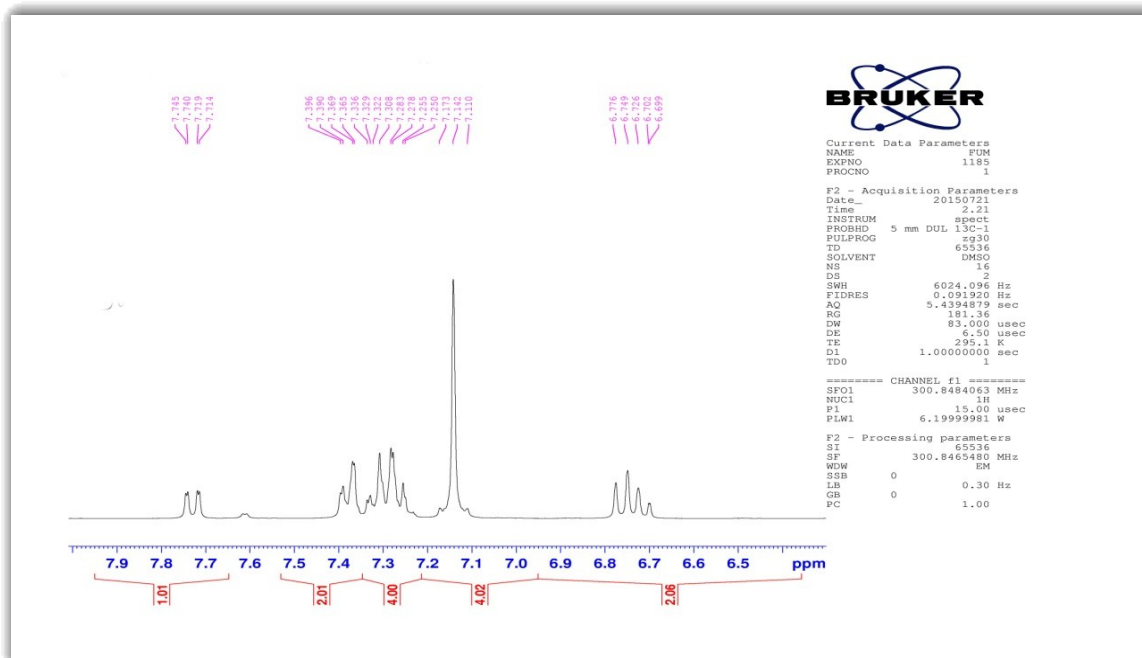


Figure 3m-B2: ^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 3-(4-Methylphenyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3m) expanded.

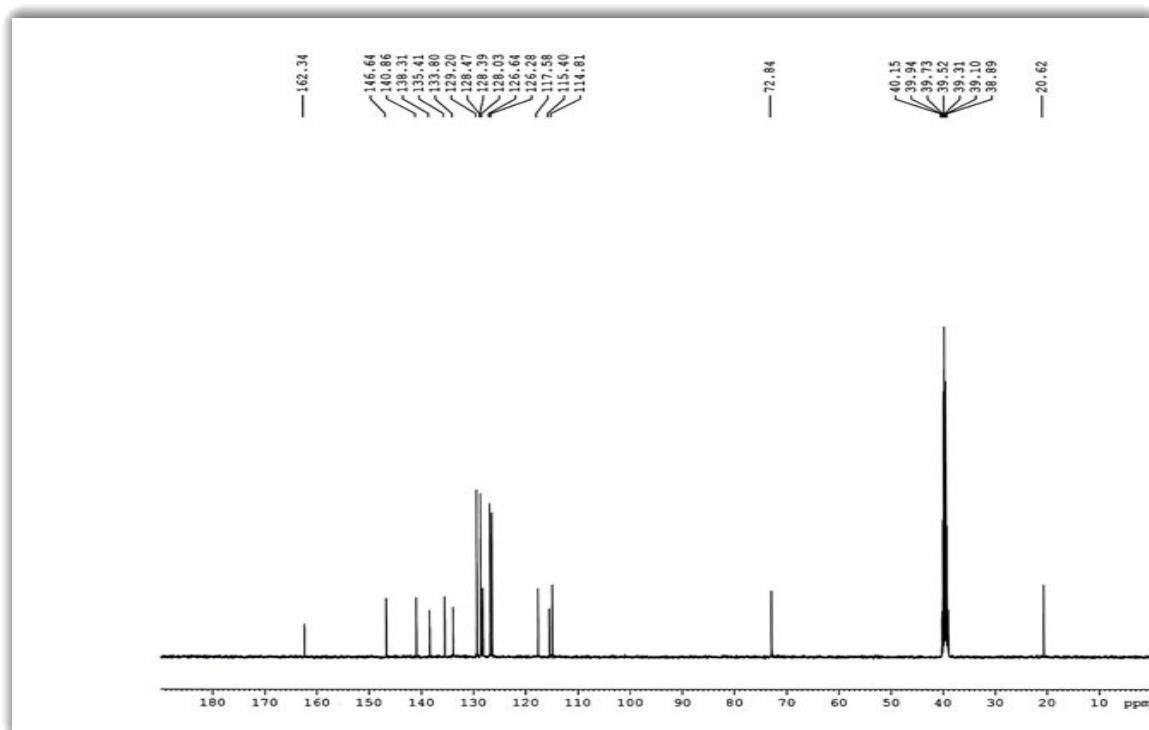
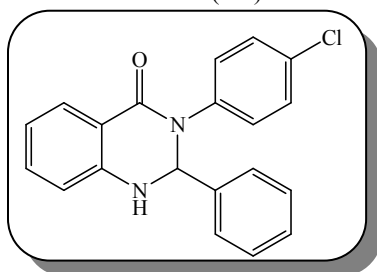


Figure 3m-C: ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) of 3-(4-Methylphenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3m).



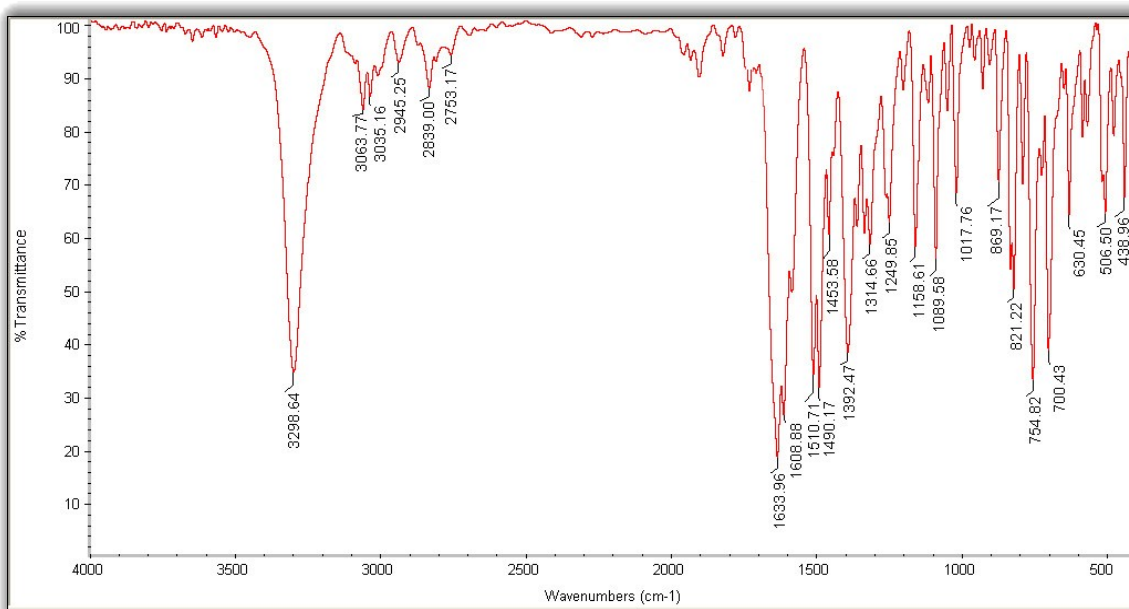


Figure 3n-A: FT-IR (KBr) of 3-(4-Chlorophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3n).

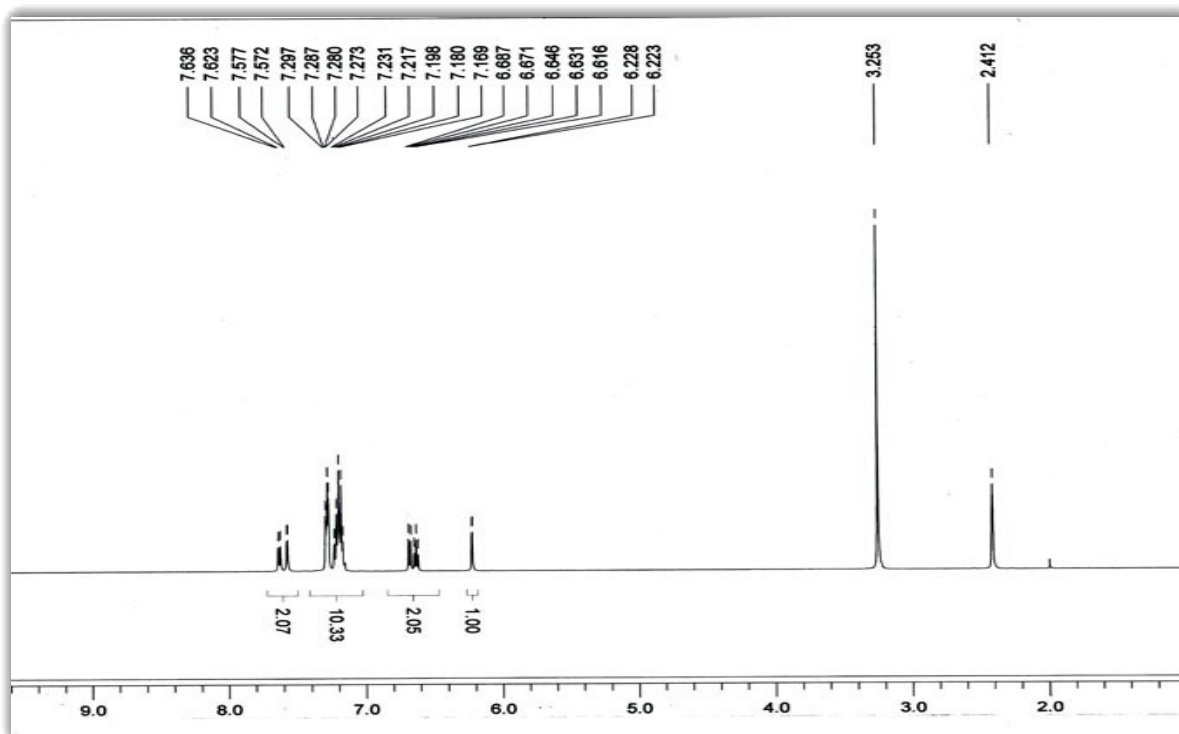


Figure 3n-B: ¹H NMR (500 MHz, DMSO-*d*₆) of 3-(4-Chlorophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3n).

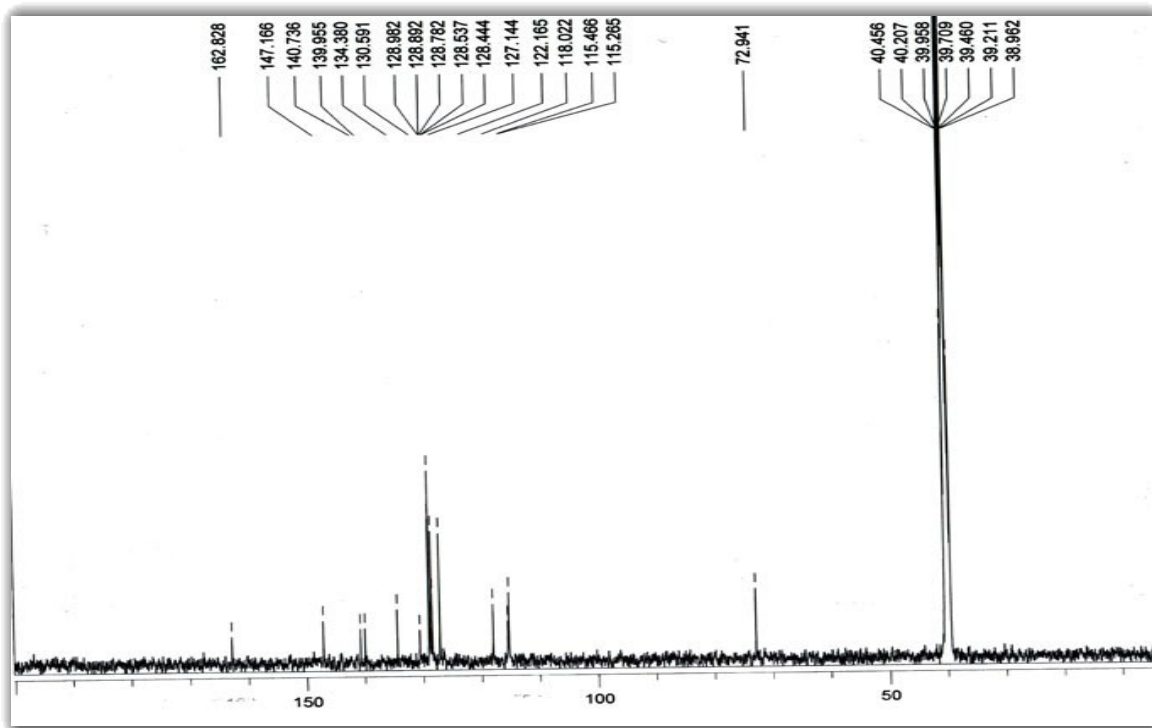


Figure 3n-C: ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of 3-(4-Chlorophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3n).

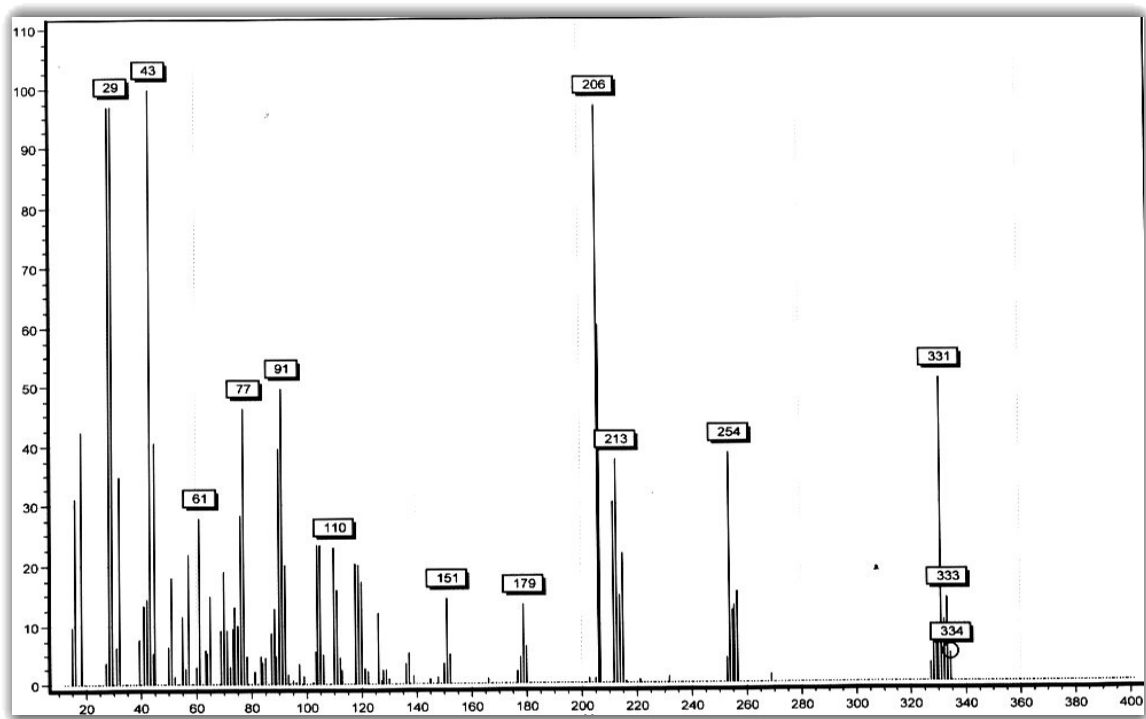


Figure 3n-D: Mass spectrum of 3-(4-Chlorophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3n).

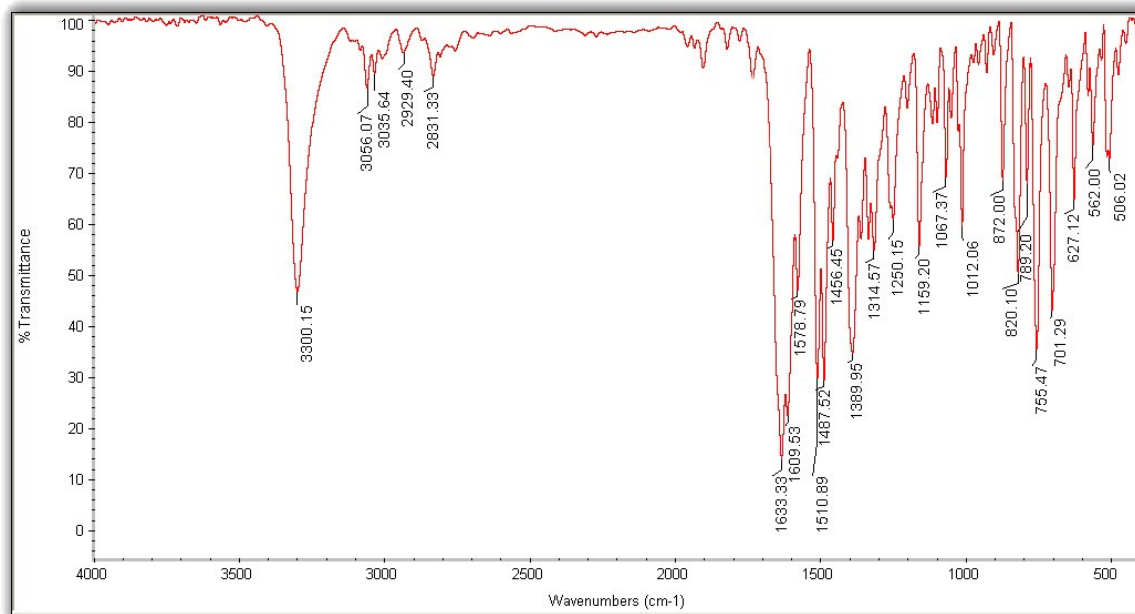
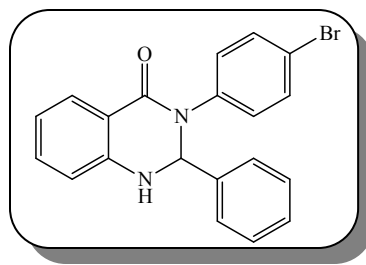


Figure 3o-A: FT-IR (KBr) of 3-(4-Bromophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3o).

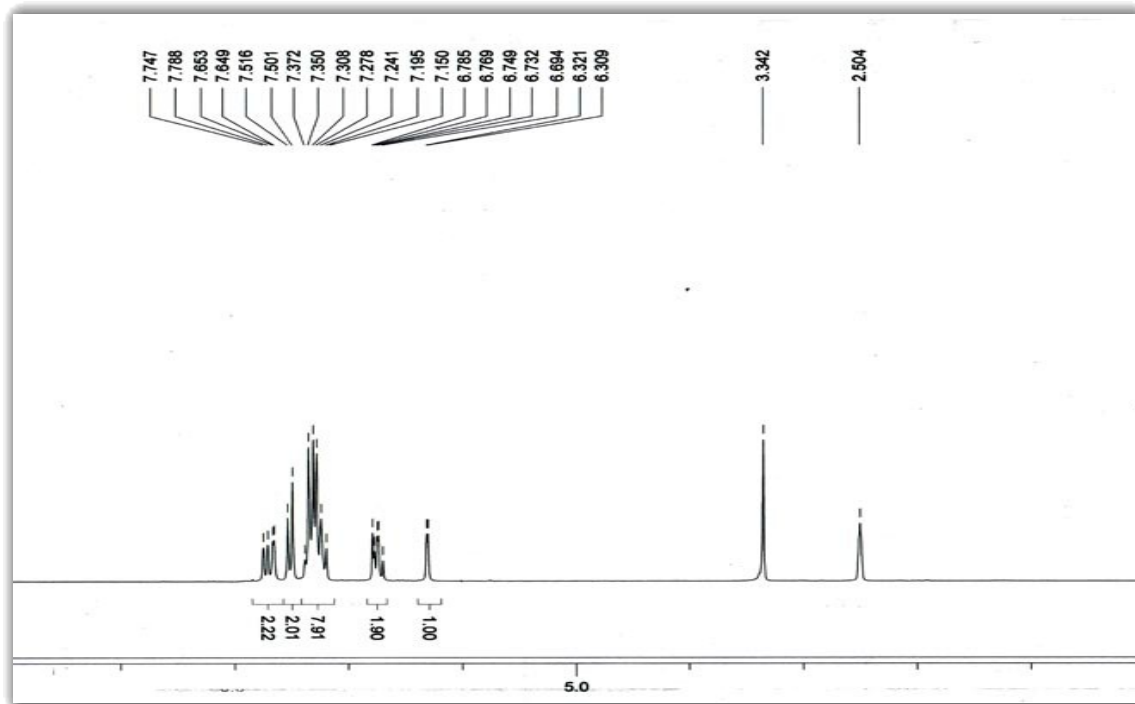


Figure 3o-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 3-(4-Bromophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3o).

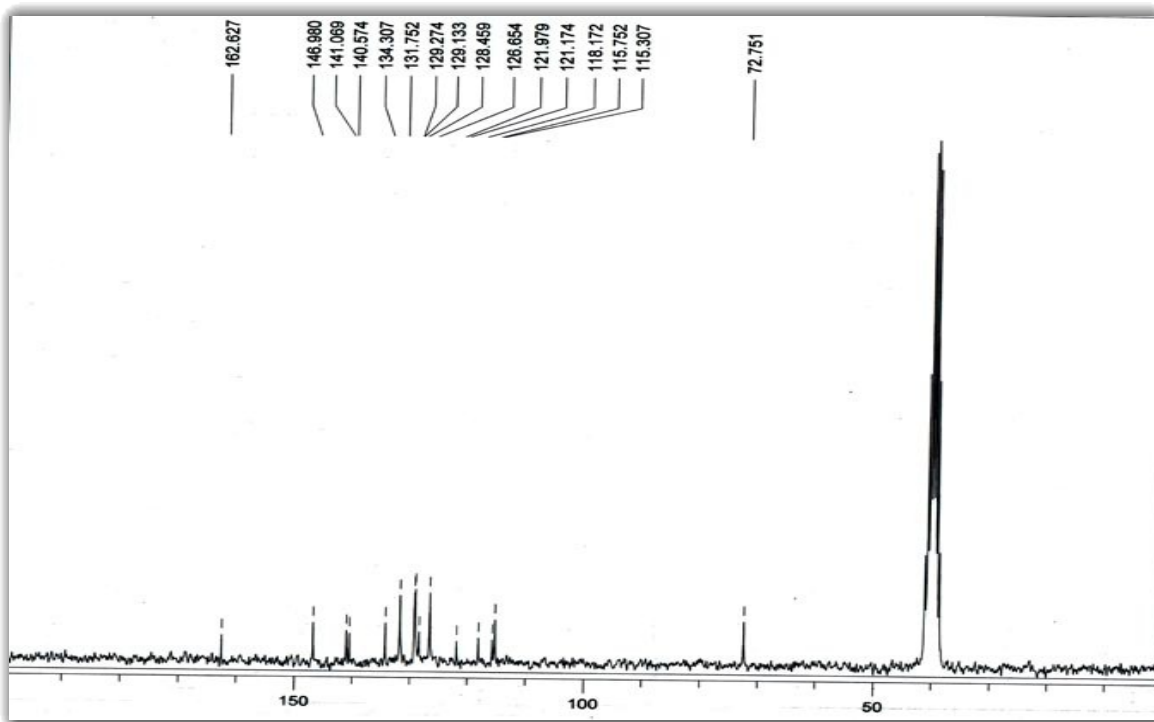


Figure 3o-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 3-(4-Bromophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3o).

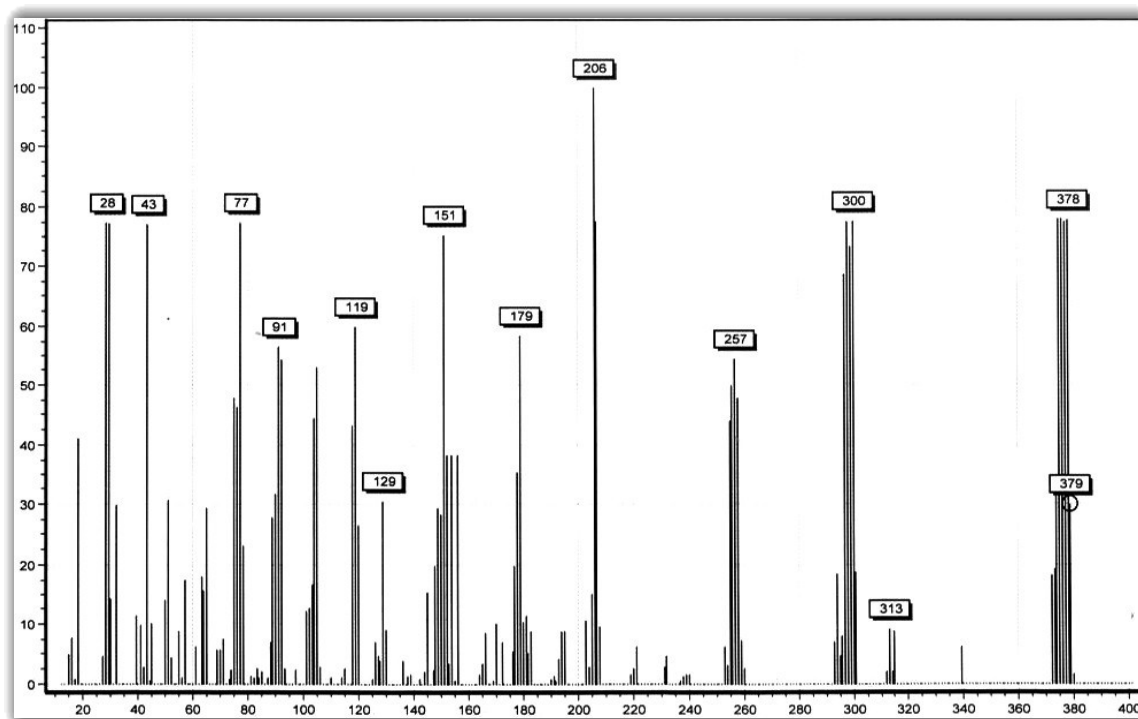


Figure 3o-D: Mass spectrum of 3-(4-Bromophenyl)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3o).

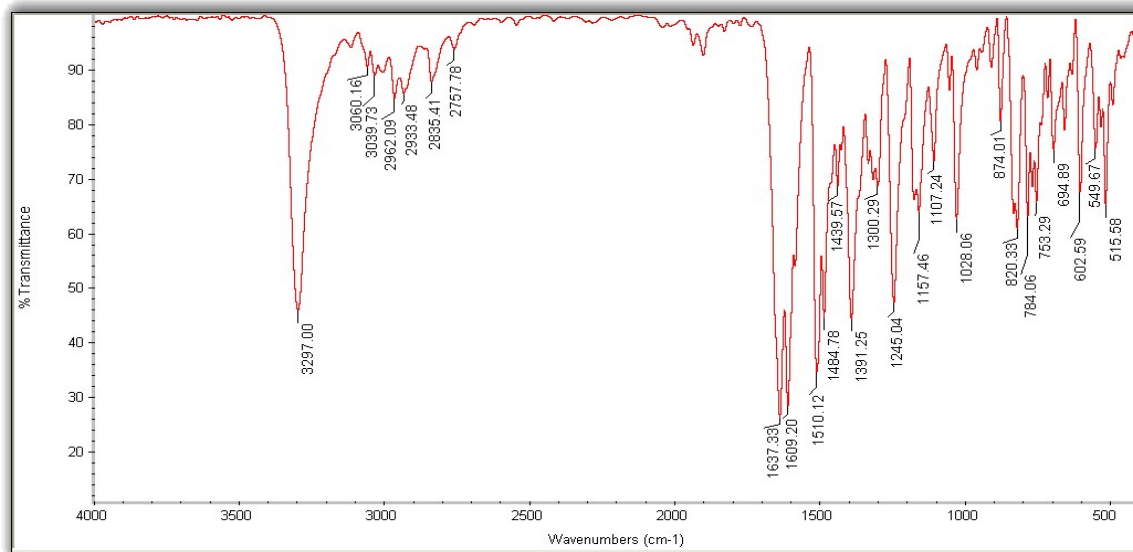
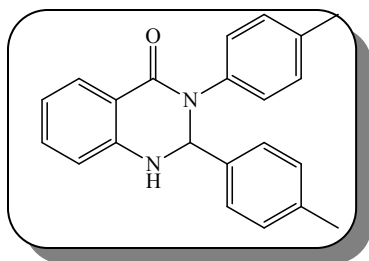


Figure 3p-A: FT-IR (KBr) of 2,3-Di(4-methylphenyl)-2,3-dihydro-quinazolin-4(1H)-one (3p).

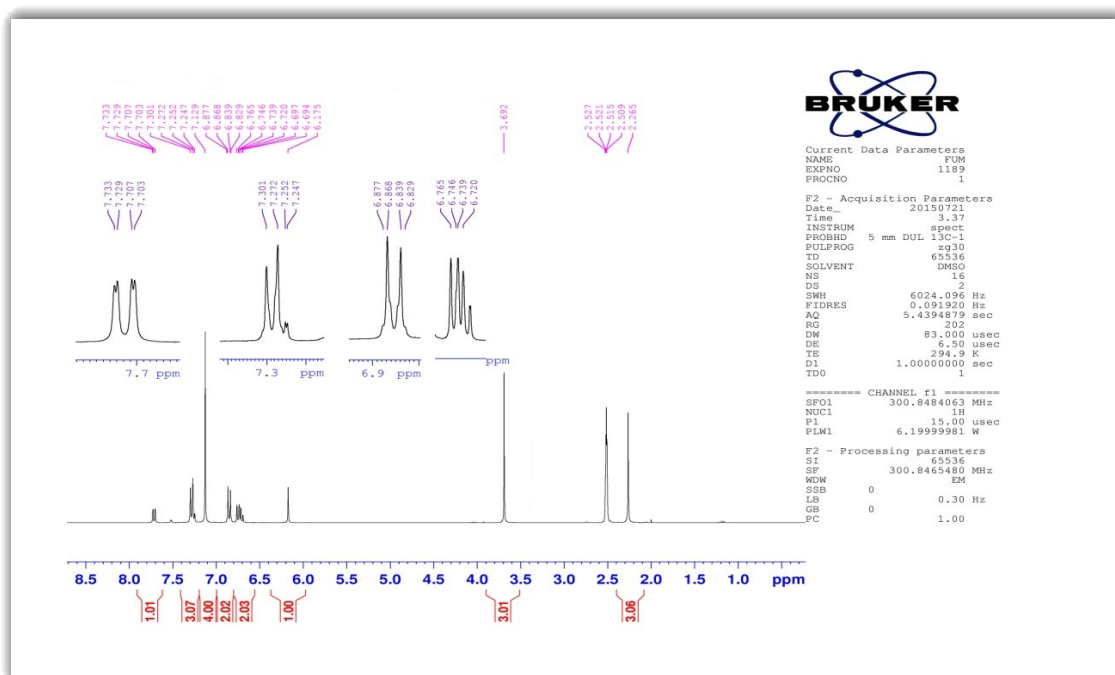


Figure 3p-B: ¹H NMR (300 MHz, DMSO-d₆) of 2,3-Di(4-methylphenyl)-2,3-dihydro-quinazolin-4(1H)-one (3p).

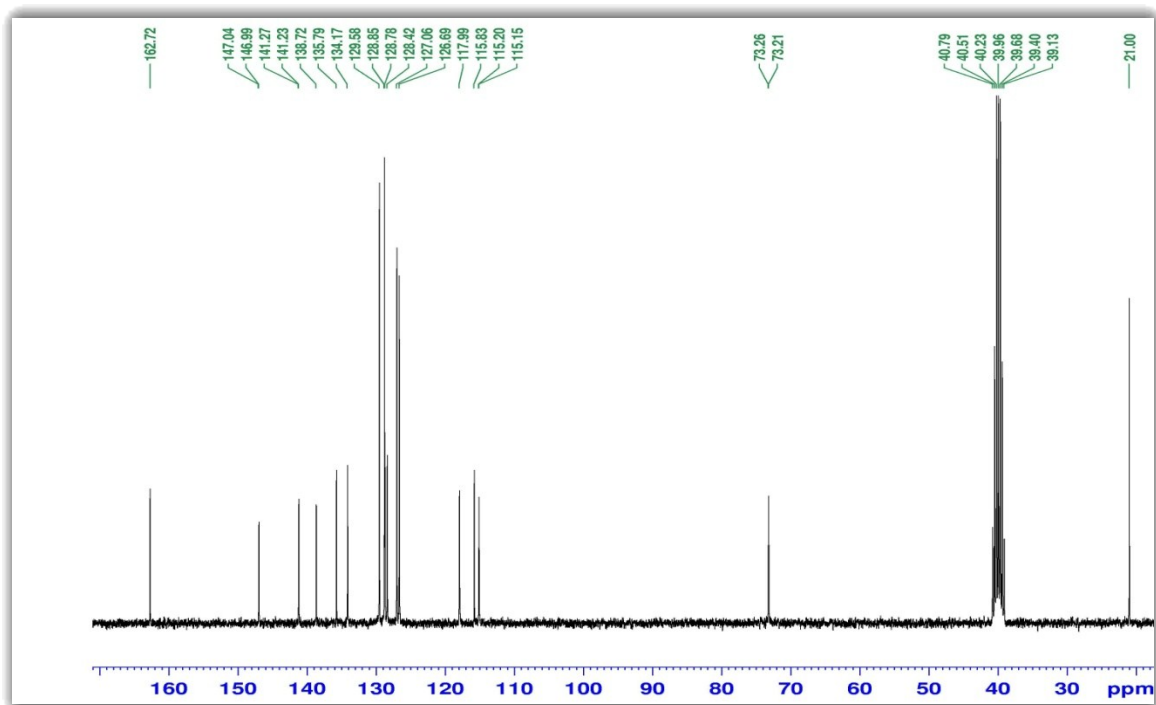


Figure 3p-C: ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) of 2,3-Di(4-methylphenyl)-2,3-dihydro-quinazolin-4(1*H*)-one (3p).

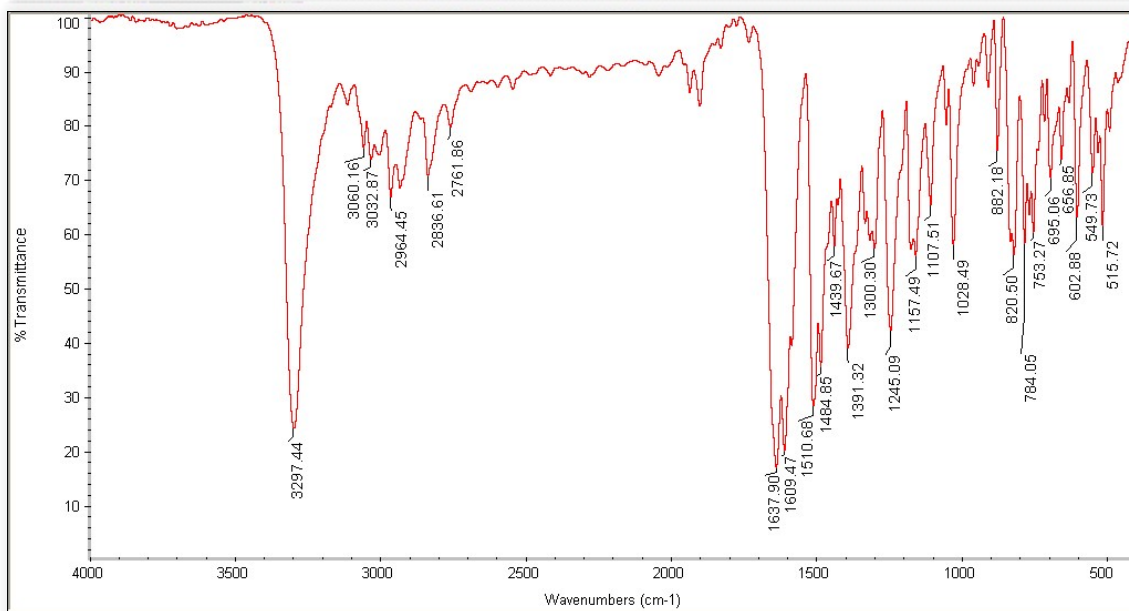
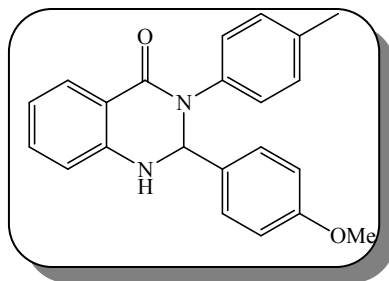


Figure 3q-A: FT-IR (KBr) of 2-(4-Methoxyphenyl)-3-(*p*-tolyl)-2,3-dihydroquinazolin-4(*1H*)-one (3q).

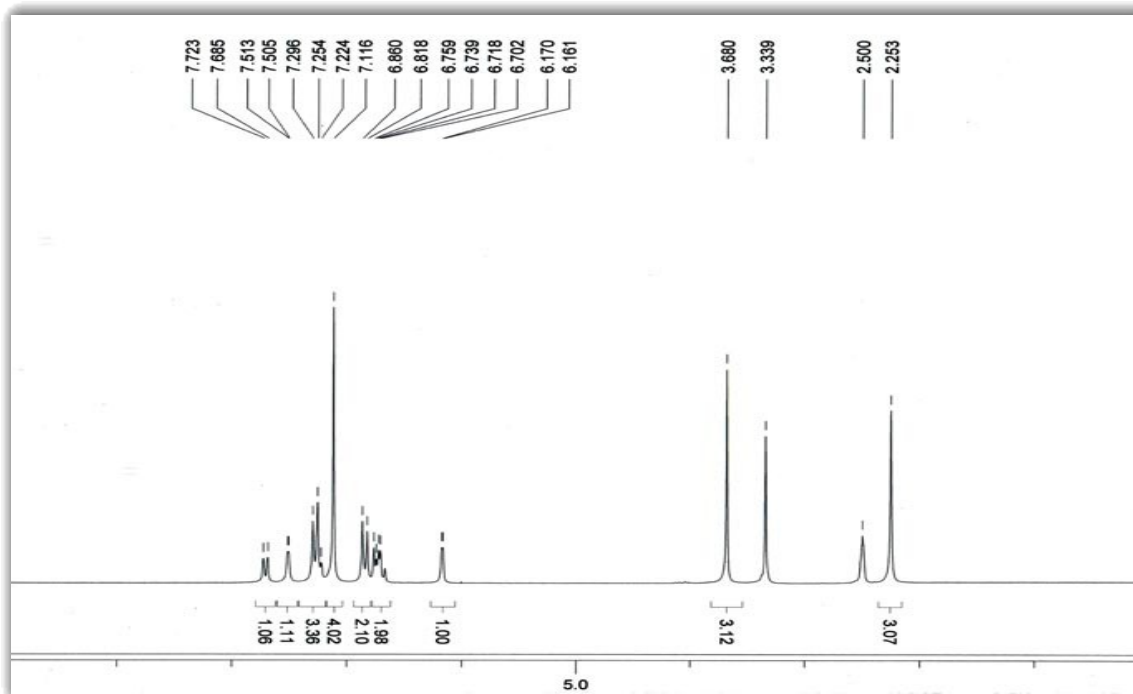


Figure 3q-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(4-Methoxyphenyl)-3-(*p*-tolyl)-2,3-dihydroquinazolin-4(*1H*)-one (3q).

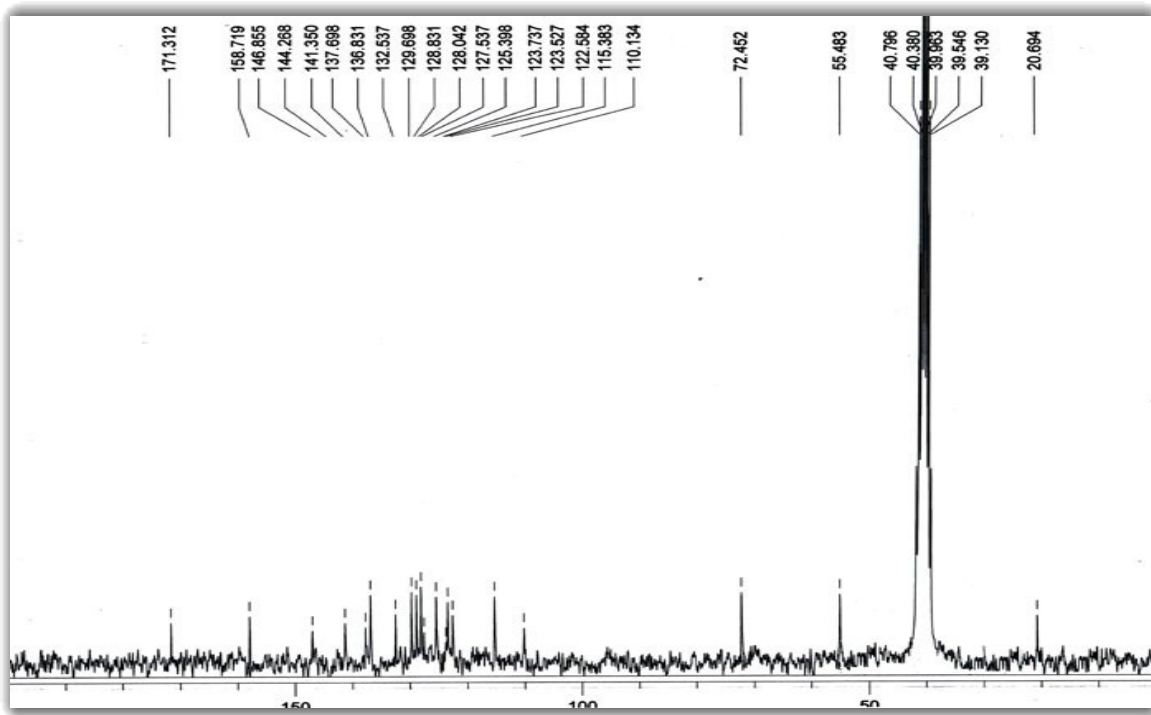


Figure 3q-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(4-Methoxyphenyl)-3-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3q).

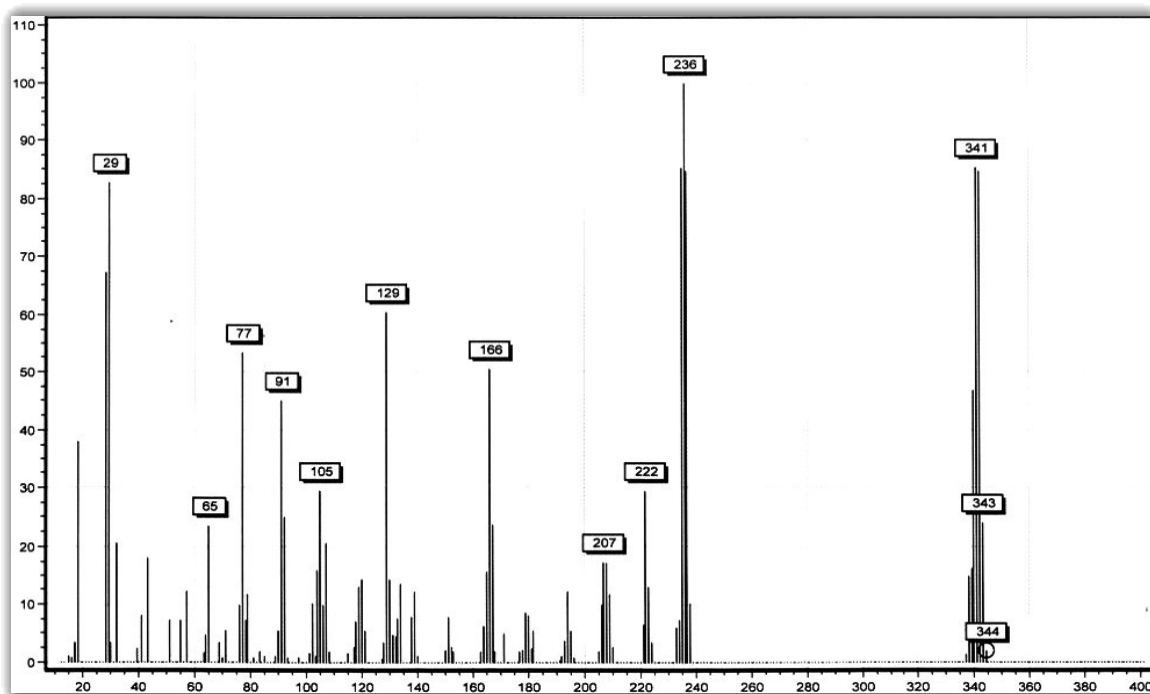


Figure 3q-D: Mass spectrum of 2-(4-Methoxyphenyl)-3-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3q).

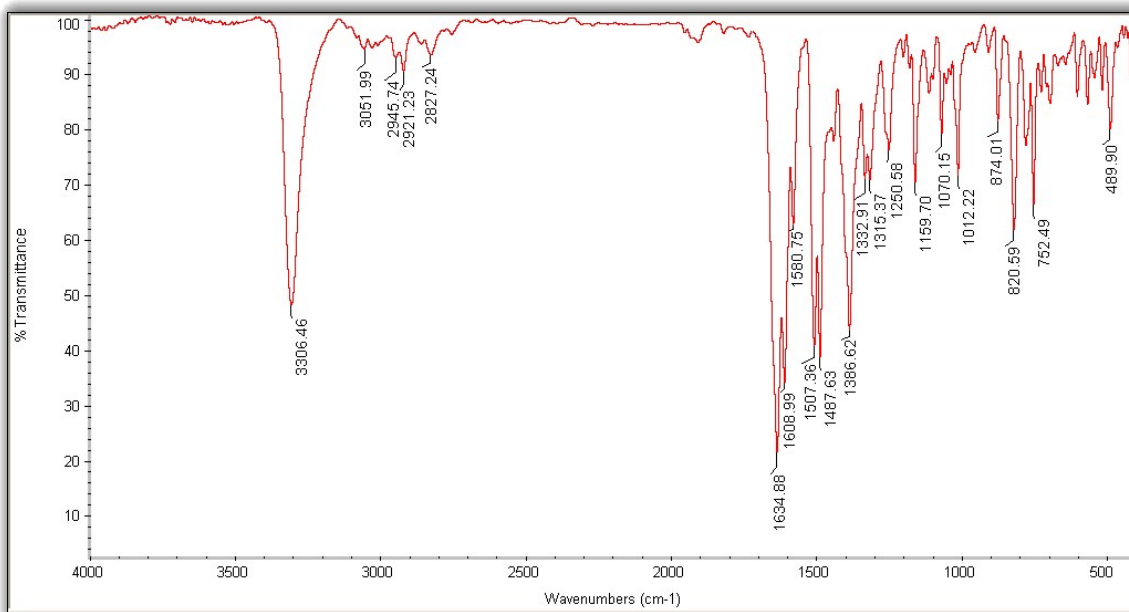
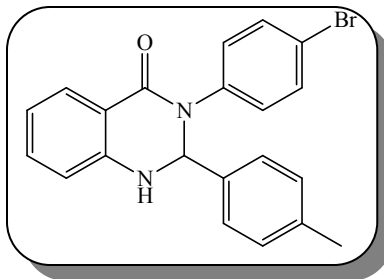


Figure 3r-A: FT-IR (KBr) of 3-(4-Bromophenyl)-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3r).

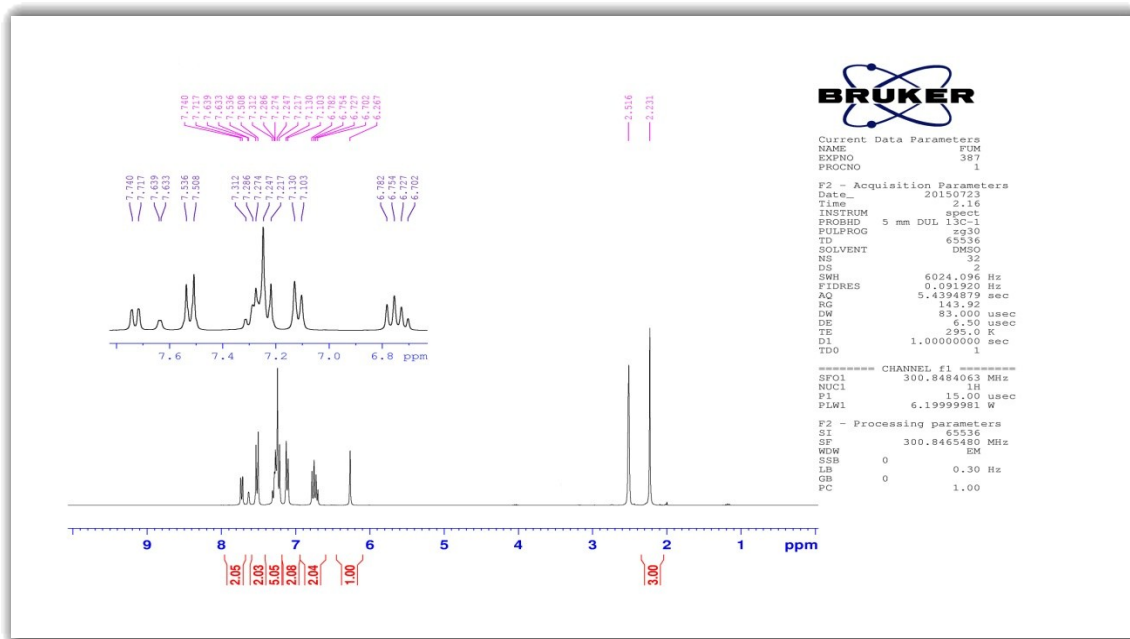


Figure 3r-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 3-(4-Bromophenyl)-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3r).

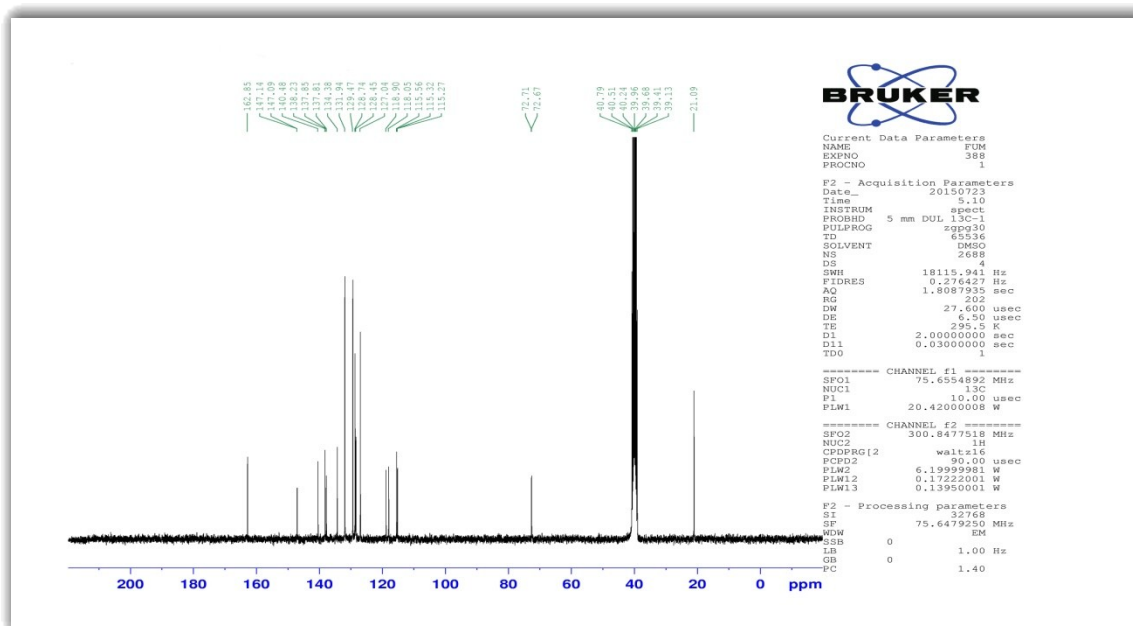


Figure 3r-C1: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 3-(4-Bromophenyl)-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3r).

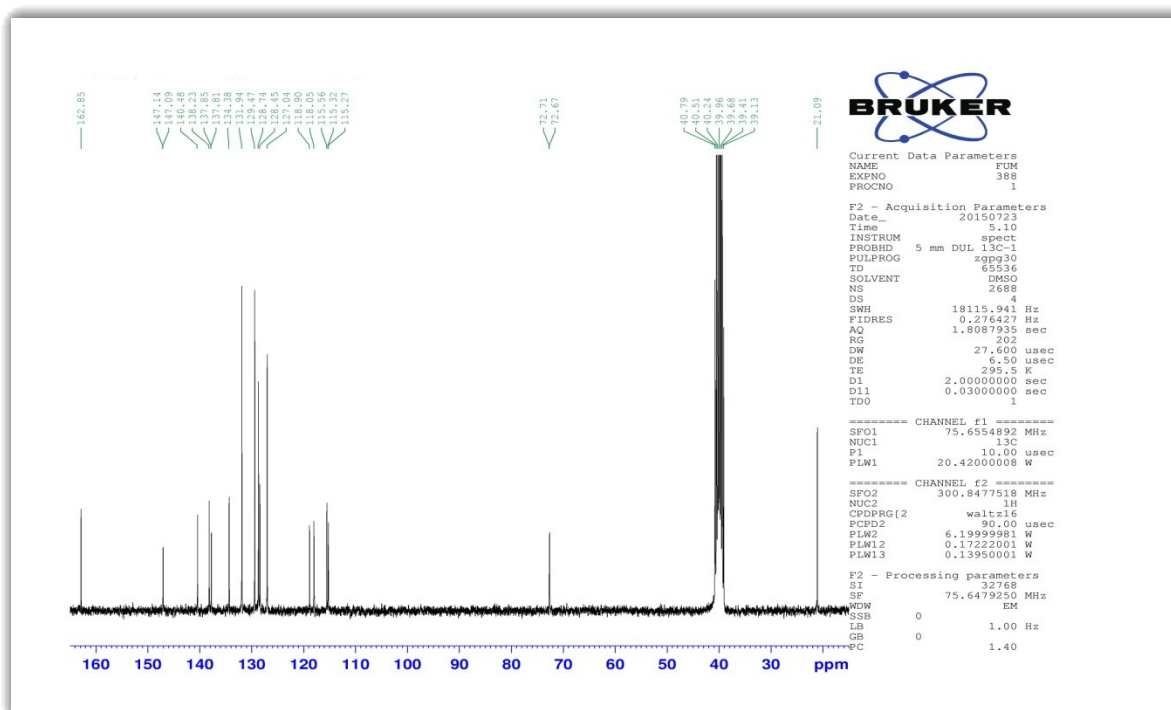


Figure 3r-C2: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 3-(4-Bromophenyl)-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3r) expanded.

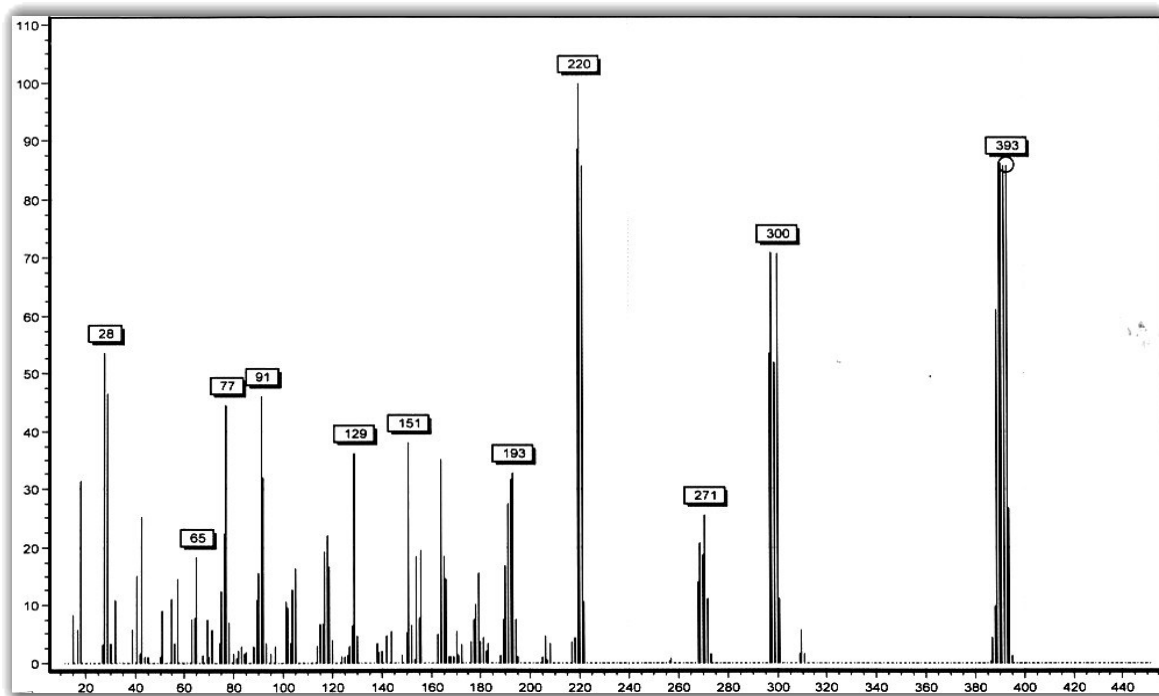


Figure 3r-D: Mass spectrum of 3-(4-Bromophenyl)-2-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3r).

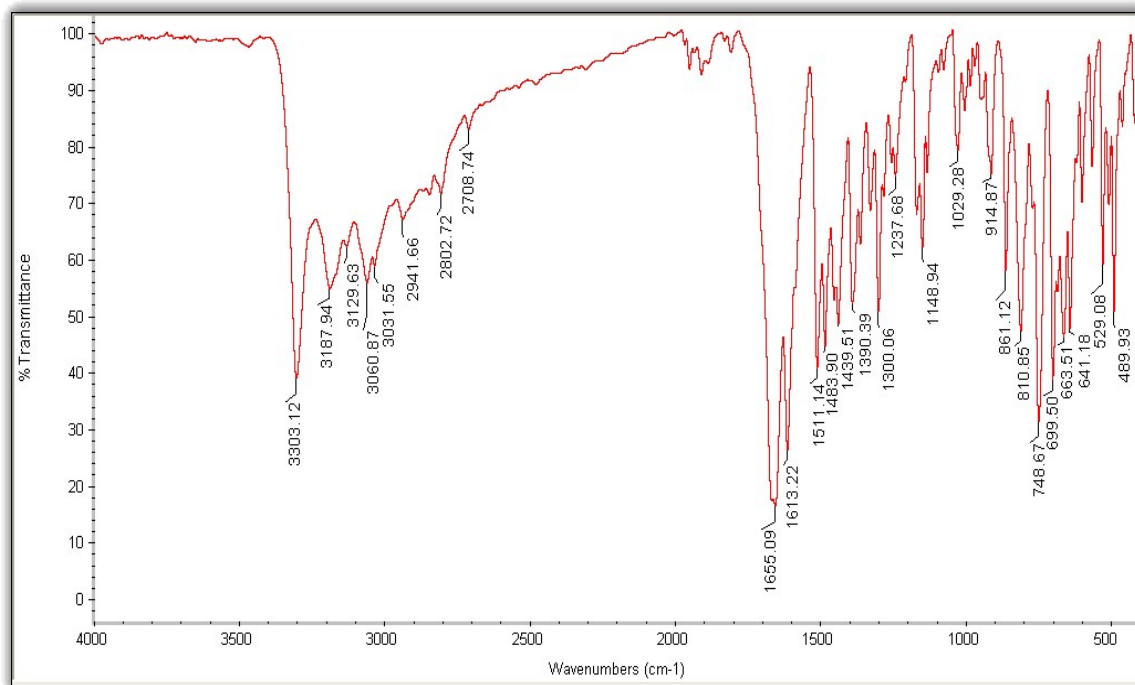
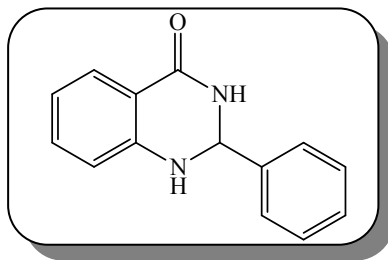


Figure 4a-A: FT-IR (KBr) of 2-Phenyl-2,3-dihydroquinazolin-4(1H)-one (4a).

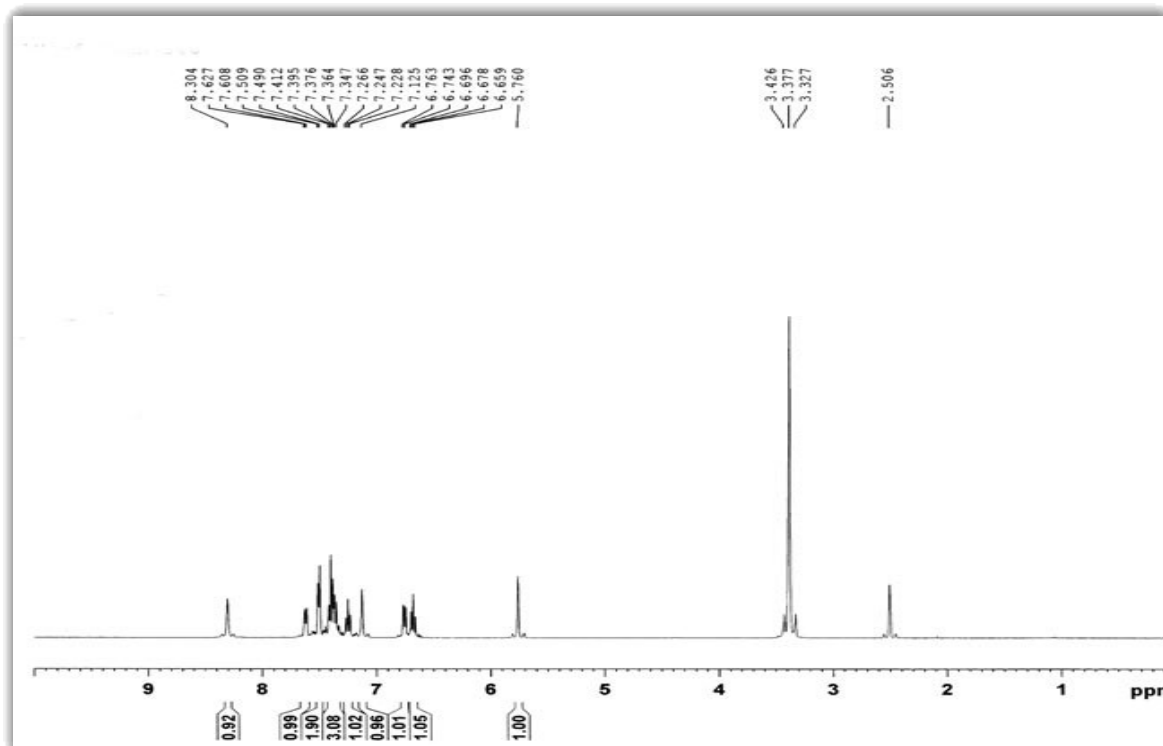


Figure 4a-B: ¹H NMR (400 MHz, DMSO-*d*₆) of 2-Phenyl-2,3-dihydroquinazolin-4(1H)-one (4a).

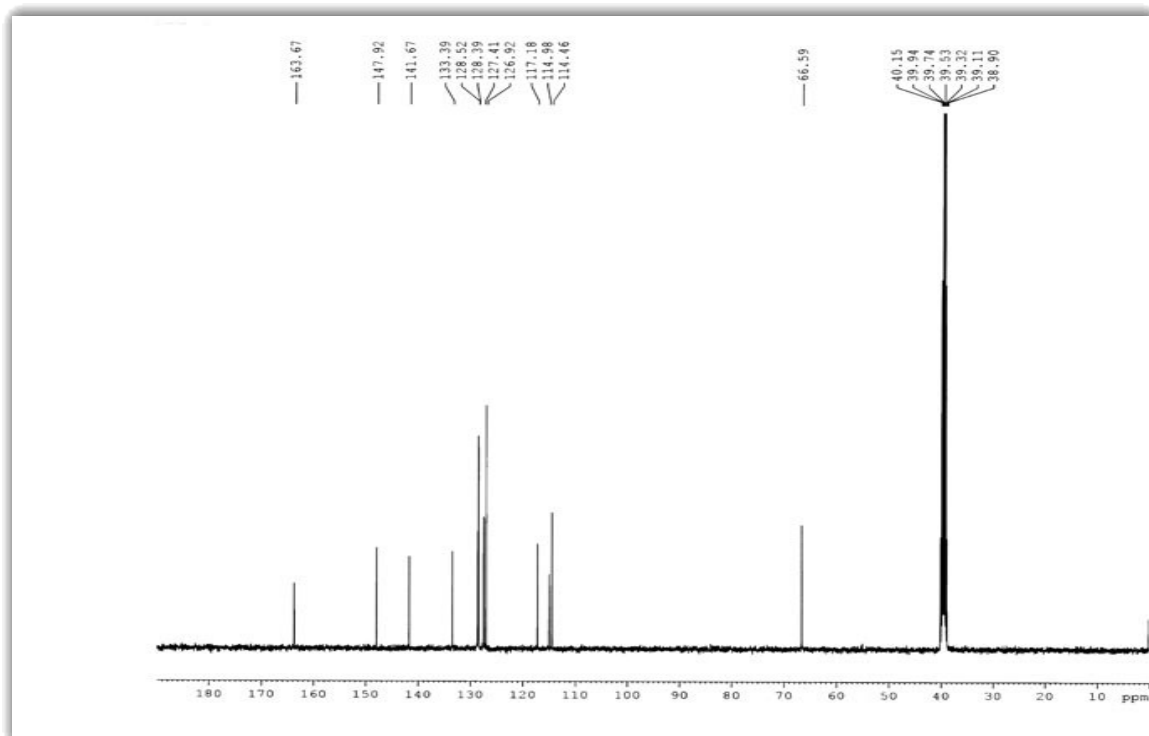


Figure 4a-C: ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of 2-Phenyl-2,3-dihydroquinazolin-4(1H)-one (4a).

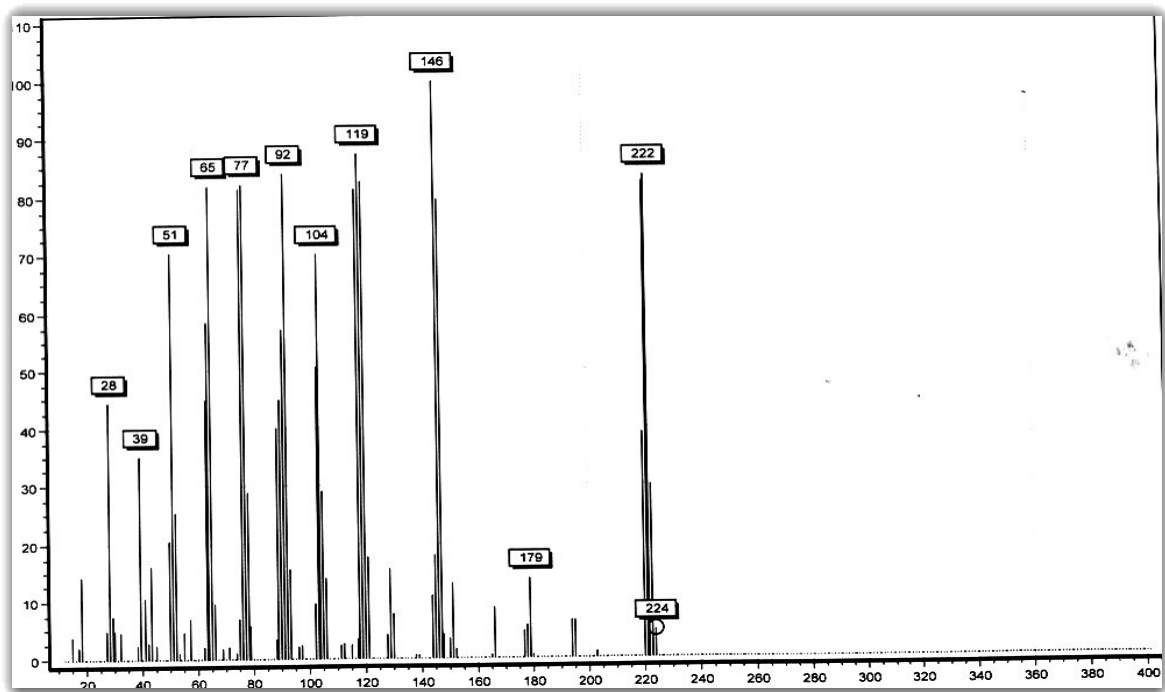


Figure 4a-D: Mass spectrum of 2-Phenyl-2,3-dihydroquinazolin-4(1H)-one (4a).

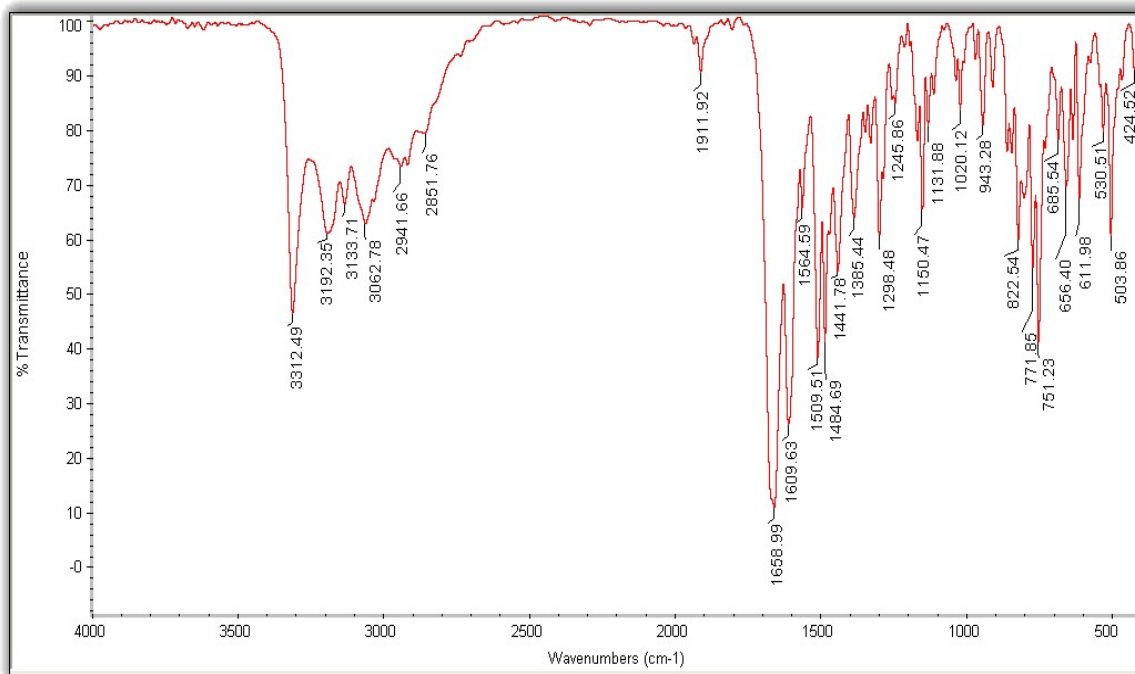
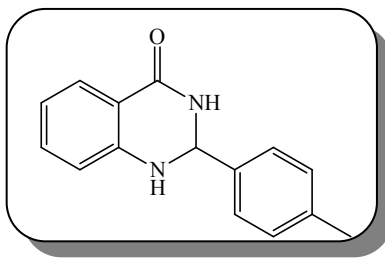


Figure 4b-A: FT-IR (KBr) of 2-(*p*-Tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4b).

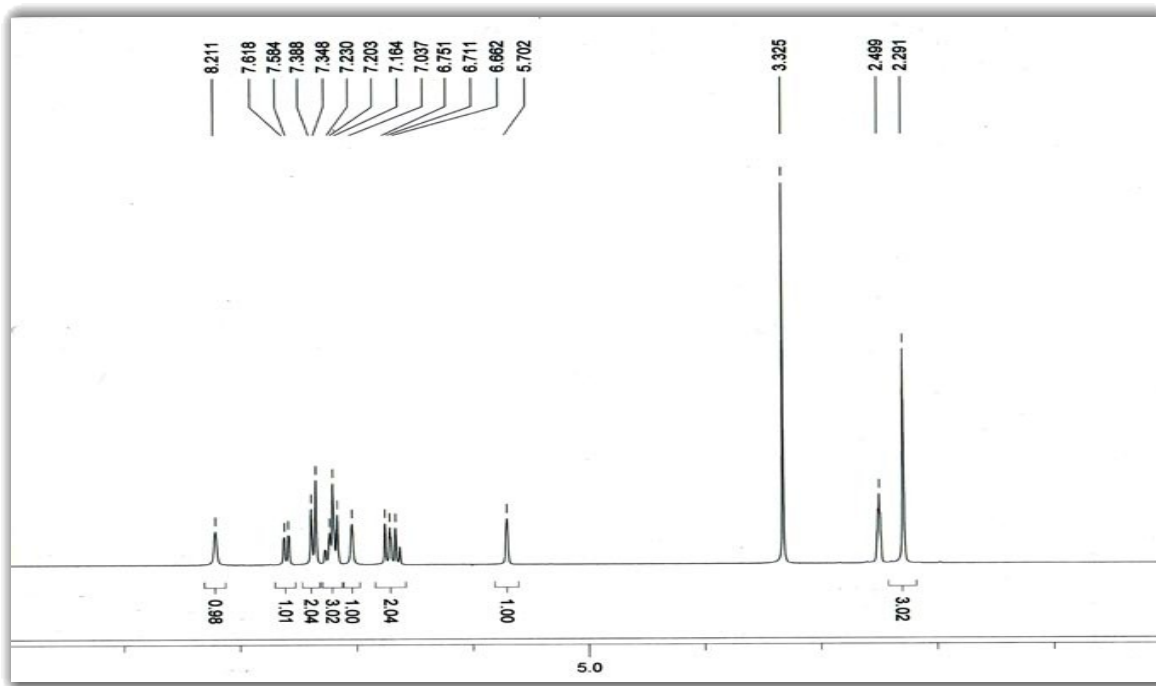


Figure 4b-B: ¹H NMR (300 MHz, DMSO-*d*₆) of 2-(*p*-Tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4b).

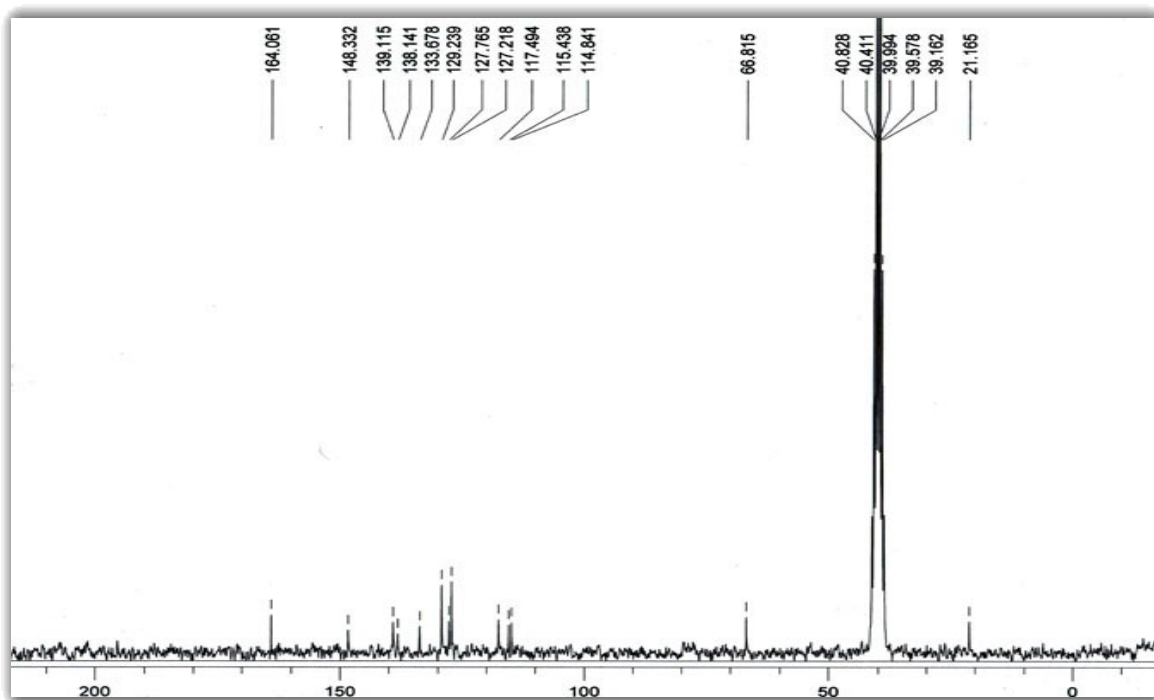


Figure 4b-C: ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) of 2-(*p*-Tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4b).

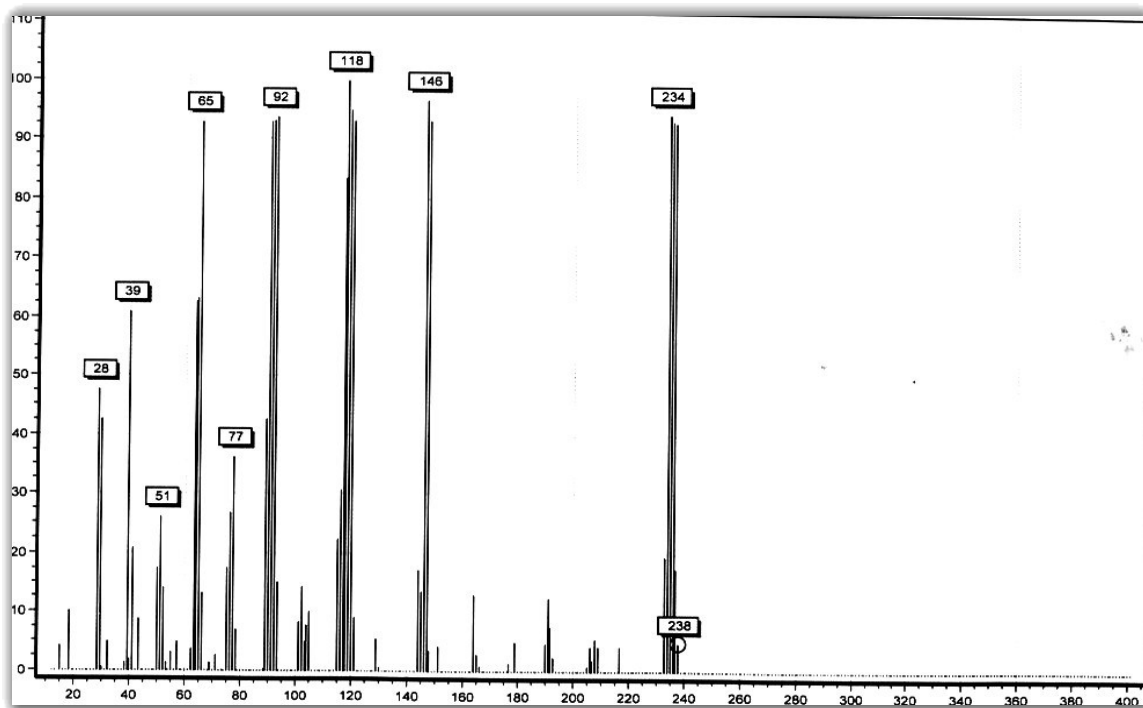


Figure 4b-D: Mass spectrum of 2-(*p*-Tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (4b).

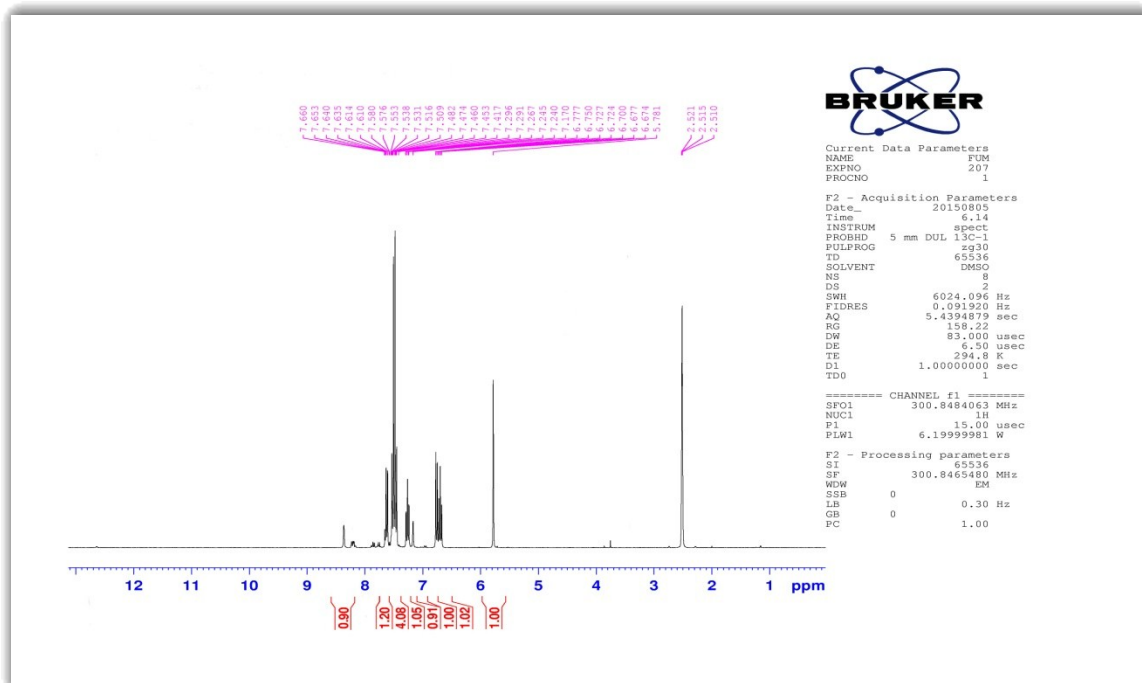
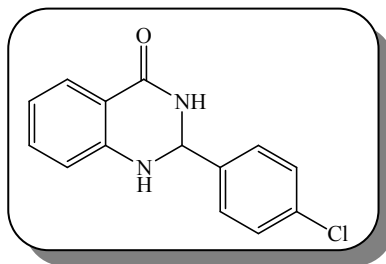


Figure 4c-B1: ^1H NMR (300 MHz, $\text{DMSO}-d_6$) of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (4c).

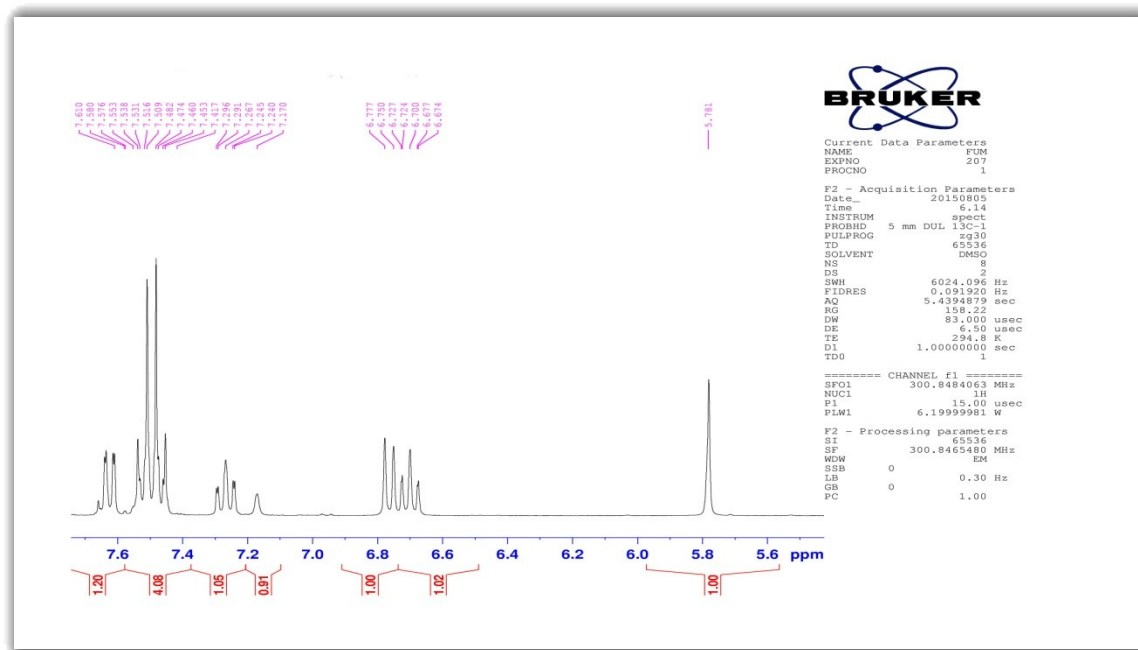


Figure 4c-B2: ^1H NMR (300 MHz, $\text{DMSO}-d_6$) of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (4c) expanded.

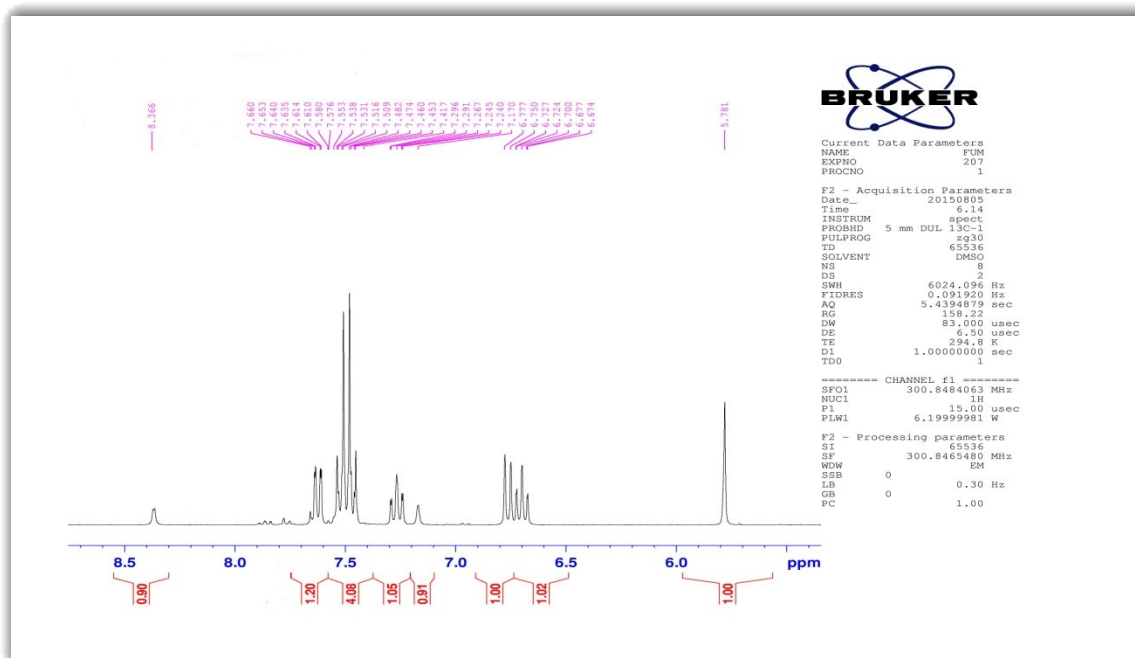


Figure 4c-B3: ^1H NMR (300 MHz, $\text{DMSO-}d_6$) of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4c) expanded.

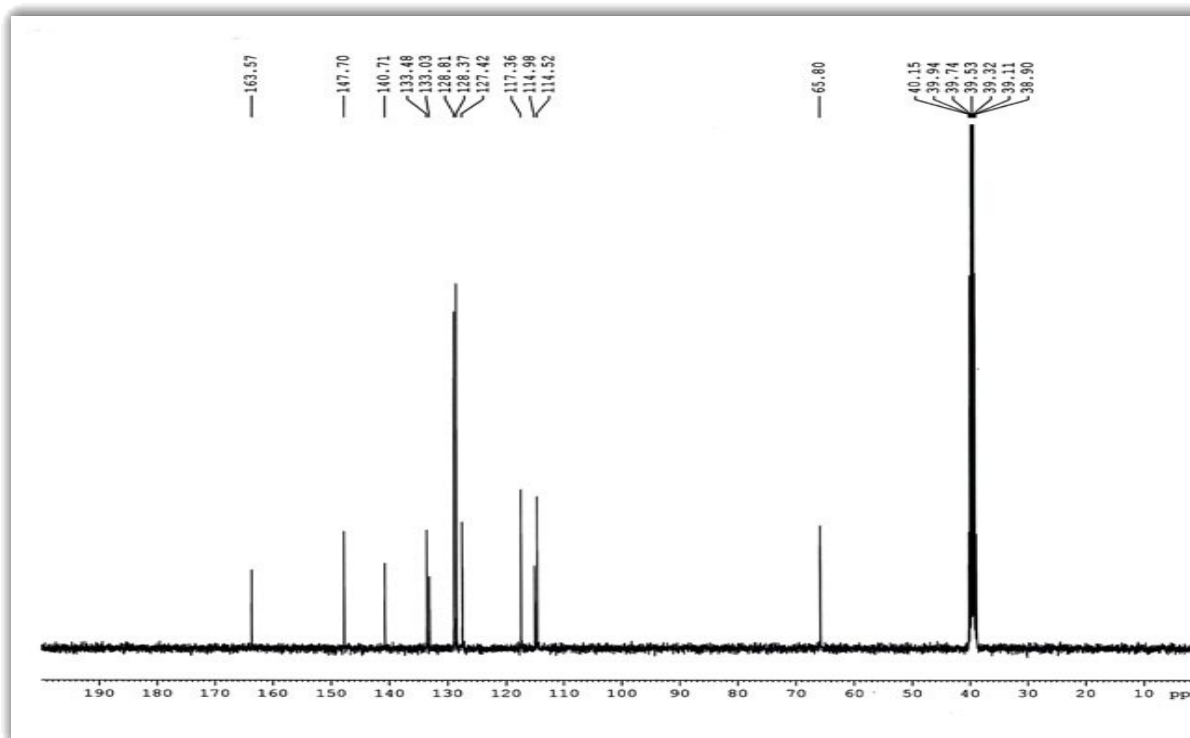


Figure 4c-C: ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4c).

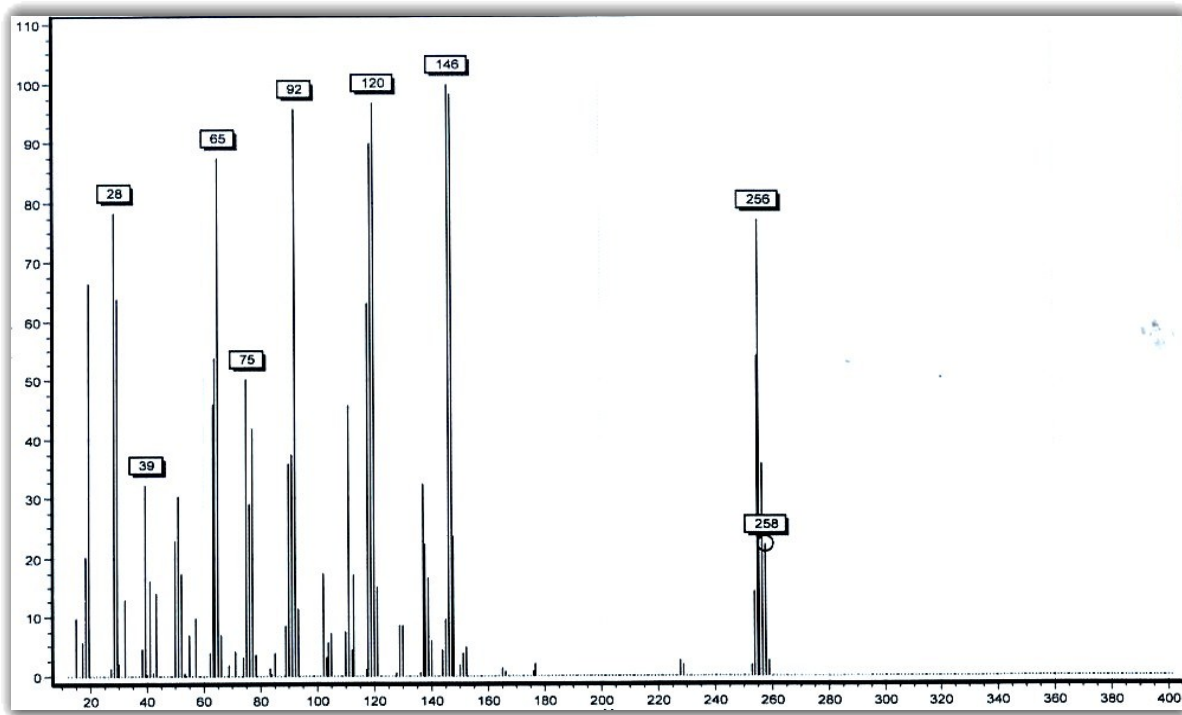


Figure 4c-D: Mass spectrum of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4c).