Chapter 8

Synthesis of 2-substituted Pyrano tetrahydroquinoline derivatives via Imino Diels-Alder reaction using Phosphotungstic acid as a catalyst
8.1 Introduction

The products containing pyrano and furanoquinoline moieties are widely distributed in nature and found to be associated with a wide range of biological activities. Pyrano tetrahydroquinolines are found in several alkaloids such as veprisine, flinderesine and oricine. These alkaloids possess important biological activities such as anti-allergic, psychrotopic, anti-inflammatory and estrogenic activities. The alkaloids skimimianine and baldflouridine which contain furanoquinoline moieties also show biological activity, which has led to the synthesis of pyrano and furanoquinoline derivatives over the years. Therefore, it is not surprising that many synthetic methods have been developed for these types of compounds. Amongst them, the Lewis acid catalyzed aza Diels–Alder reaction between $N$-benzylideneanilines and nucleophilic olefins is one of the most powerful synthetic tools for constructing nitrogen-containing six-membered heterocyclic compounds. However, an in situ generated diene is preferred over a preformed heterodiene, leading to a one-pot procedure, which is especially useful when the diene is unstable, sensitive to moisture and difficult to purify by column chromatography or distillation. Recently, $\text{KHSO}_4$ and iodine have also been used as efficient catalysts for the one-pot synthesis of the pyranoquinoline moiety. However, most of these methods involve expensive reagents and more than stoichiometric amounts of Lewis acid catalysts are needed due to strong coordination with the heterodiene, coupled with longer reaction times and strongly acidic conditions. Hence, a milder and better method is desirable.

8.2 Methods for the synthesis of pyrano quinoline derivatives

M. Z. Hoemann et al., reported 2-(1H-indol-3-yl)tetrahydroquinoline derivatives as novel anti-bacterial agents and they found to be effective in-vitro (<1.0 mg/mL) activity versus methicillin resistant S. aureus (MRSA).
C. J. Li et al., using a domino reaction of aromatic amines and cyclic enol ethers or 2-hydroxy cyclic ether catalyzed by indium chloride in water, various tetrahydroquinoline derivatives was synthesized efficiently.

J. S. Yadav et al., reported a novel and highly efficient method for the synthesis of pyranoquinoline derivatives from aryl amines and 2 equiv. of cyclic enol ether using a catalytic amount of indium trichloride. The notable features of this procedure are mild reaction conditions, greater selectivity, improved yields, cleaner reaction profiles, enhanced rates and operational simplicity which make it a useful and attractive process for the synthesis of fused pyran[3,2-c]quinolines of biological importance.
L. Chen et al.,\textsuperscript{13} reported an efficient method for the synthesis of 1,2,3,4-tetrahydroquinoline derivatives by using a domino reaction of aromatic amines with 3,4-dihydro-2\(H\)-pyran over cation-exchange resin (H form) catalysts in water is described.

\[ \text{NH}_2 + \text{OCH}_3 \text{CH}_3 \text{Cl, Br, F, CN, N}_2\text{O} \]

Z. Li et al.,\textsuperscript{14} have demonstrated a domino reaction of aromatic amines with various cyclic hemiacetals catalyzed by indium chloride in water, tetrahydroquinoline derivatives were synthesized efficiently.

D.A. Powell et al.,\textsuperscript{15} showed Ln(OTf)\textsubscript{3} catalyzed formal aza Diels–Alder (or Povarov) reaction of cyclopentadiene with in situ generated \(N\)-arylimines containing enolizable protons was described.
J. S. Yadav et al.\textsuperscript{16} have described a simple, convenient, and efficient approach for the synthesis of hexahydropyrrrolo[3,2-c]quinolines and octahydrobenzo[h][1,6]-naphthyridine derivatives in a one-pot operation by a 2:1 coupling of ene-carbamates and aryl amines using montmorillonite KSF clay as an inexpensive and environmentally benign catalyst.

A. Kamal et al.\textsuperscript{17} reported a highly efficient method that produces more of the cis product for the synthesis of 1,2,3,4-tetrahydroquinolines from aryl azides and 3,4- dihydro-2H-pyran using the FeCl\textsubscript{3}–NaI reagent system.

J. S. Yadav et al.\textsuperscript{18} studied the reaction of D-Glycals readily undergo cyclization with aryl amines in the presence of CeCl\textsubscript{3}·7H\textsubscript{2}O–NaI under mild and neutral conditions to afford a novel sugar derived tetrahydroquinoline derivatives in good yields with high stereoselectivity.
R.R. Nagawade et al.,\textsuperscript{19} reported a highly efficient domino reaction of aromatic amines with cyclic enol ether in water catalysed by zirconyl chloride to provide new 1, 2, 3, 4-tetrahydroquinoline derivatives using zirconyl chloride as a catalyst.

X. Xing et al.,\textsuperscript{20} established the microwave reaction conditions for the CF$_3$CO$_2$H-catalyzed three-component aza-Diels–Alder reactions involving 2-aminophenols as the amine building blocks.

X.F. Lin et al.,\textsuperscript{21} developed a highly efficient domino reaction of anilines with cyclic enol ether using a catalytic amount of molecular iodine to provide 1,2,3,4-tetrahydroquinoline derivatives.
G. Maiti et al., synthesized a new and effective methodology for synthesis of tetrahydropyranoquinolines and furanoquinolines in one-pot by using a catalytic amount of antimony trichloride.

A. Kamal et al., showed a highly efficient method for the synthesis of 1,2,3,4-tetrahydroquinolines from aryl azides and cyclic enol ethers using TMSCl–NaI reagent system.

E. Rafiee et al., developed an efficient, clean, and simple method for the synthesis of tetrahydroquinoline derivatives from aryl amines and glucal, using K₅CoW₁₂O₄₀·3H₂O as a reusable and non-toxic catalyst.

K.M. Mahadevan et al., reported a facile synthesis of substituted pyrano and furanoquinolines using cheap, water-stable catalyst and the domino reaction of anilines with cyclic enol ethers.
A. Srinivasa et al.,\textsuperscript{26} reported a very interesting and a facile synthesis of substituted pyrano- and furanoquinolines using cheaper, water stable, and water soluble 4-nitrophthalic acid catalyzed imino Diels-Alder reaction of \textit{N}-benzylideneanilines with cyclic enol ethers and the domino reaction of anilines with cyclic enol ethers are described.

J.L. Rogers et al.,\textsuperscript{27} synthesized a range of substituted tetrahydroquinoline derivatives via a three component coupling reaction between substituted anilines and enol ethers using bismuth bromide catalyst.

A. Kumar et al.,\textsuperscript{28} introduce a natural supramolecular carbohydrate scaffold-catalyzed synthesis of tetrahydroquinoline derivatives by the reaction of aromatic amine and cyclic enol ether in excellent yield with high diastereoselectivity has been developed.
G. Jin et al.,\textsuperscript{29} have prepared a series of 2-pentafluorophenyl pyrano [3,2-c] and furo [3,2-c]-tetrahydroquinolines (112) by the reaction of pentafluorobenzylidene aniline with DHP or DHF using I\textsubscript{2} as the catalyst in CF\textsubscript{3}CH\textsubscript{2}OH at room temperature.

V.T. Kamble et al.,\textsuperscript{30} reported the synthesis of tetrahydroquinoline derivatives via three component coupling reactions of aldehydes and anilines with various dienophiles in the presence of a catalytic amount of perchloric acid adsorbed on silica gel (HClO\textsubscript{4}-SiO\textsubscript{2}) under mild reaction conditions.
8.3 Present work

In the present work, we have interested in catalytic reaction to synthesize pyranoquinoline derivatives by using Schiff’s bases and 3,4-dihydro-2H-pyran (DHP). The research work carried out during the present investigation has been described in Scheme-1. The targeted compounds are synthesized by the reaction of Schiff’s bases and 3,4-dihydro-2H-pyran in presence of Phosphotungstic acid (PTA) as a catalyst with stirring in acetonitrile solvent at room temperature, for appropriate time (Table 1). After completion of reaction as indicated by TLC, the reaction mixture was quenched with saturated aqueous NaHCO₃ solution and extracted with ethyl acetate. The combined organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure.

Scheme-1

8.4 Materials and methods

The melting points of the products were determined by open capillaries on a Buchi apparatus and are uncorrected. The IR spectra were recorded on a Nicolet Impact-5700 FT-IR Spectrophotometer using KBr pellets. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker Avance-400F 400 MHz spectrometer in CDCl₃ using TMS as an internal standard with ¹H resonant frequency of 400 MHz and ¹³C resonant frequency of 100 MHz. D₂O exchange was applied to confirm the assignment of the signals of NH protons. The Mass spectra were recorded on a Shimadzu GC-2010. The elemental analysis was carried out by using HERAUS CHN rapid analyzer. The homogeneity of the compounds was described by TLC detected by UV light and iodine vapors. All chemical reagents were obtained from Fluka, sd fine and Merck chemical companies and were used without purification.
8.5 Experimental procedure

Synthesis of 2-substituted pyrano tetrahydroquinoline derivatives

An equimolar (3 mmol) mixture of aryl amine and p-chloro benzaldehyde was dissolved in acetonitrile (20 mL) and stirred at room temperature. To this stirred solution, 3,4-dihydro-2H-pyran (4.5 mmol), and 10 mol% of PTA were added and stirring was continued for the time period of 1h to afford pyranoquinolines derivatives THQ(29-38). After completion of the reaction, as indicated by TLC, reaction mixture was quenched by saturated solution of NaHCO₃ and extracted with ethyl acetate (2X20 mL). The combined organic layer was dried over anhydrous Na₂SO₄, concentrated and purified by column chromatography on SiO₂ with an ethyl acetate and petroleum ether mixture as eluent to afford the corresponding tetrahydroquinolines THQ(29-38). After extraction, the water layer containing the catalyst could be evaporated under reduced pressure to give a catalyst back with light yellow colored solid. The recovered catalyst was washed with ether, dried at 85 °C for 2 h under high-pressure prior to use in the further reaction.

8.6 Results and discussion

Our primary investigation was focused on the use of PTA as the catalyst in the imino Diels-Alder reaction of 4-chloro-N-[((E)-(4-chlorophenyl)methylidene] (1), and 3,4-dihydro-2H-pyran (2) stirred at room temperature (Scheme 1) in acetonitrile solvent in presence of 10 % of PTA catalyst. Similarly, several substituted Schiff’s bases reacted with 3,4-dihydro-2H-pyran (2), to give corresponding tetrahydroquinolines THQ(29-38) in good yield in the presence of 10 mol% of PTA using acetonitrile at room temperature (Scheme-1). Their structural elucidations are based on IR, ¹H NMR, ¹³C NMR and mass spectral data of the column-purified products.

In IR, the NH in all derivatives is observed around 3304-3410 cm⁻¹. In ¹H NMR, the methyl protons of pyran and 2-methyl are observed at respective regions when compared to the literature values. It was observed that the pyran ring was cis-fused in the tetrahydroquinoline moiety and the stereochemistry of the products was established based on the coupling constant of C₂-H (J₃,₂ = 4.2-
6.5 Hz) indicating the cis relationship between C3-H and C2-H, whereas ($J_{3,2} = 10.08-11.2\text{Hz}$) the coupling indicated trans. In all cases, $J_{3,4}$ was found to be 2.6–3.2Hz indicating a cis ring junction between the quinoline and pyran rings which is in accordance with literature values. From these results, the reaction undergoes the possible mechanism as in the literature.

All the newly synthesized compounds described in this chapter were screened for their in vitro anti-microbial, DNA cleavage and in vivo pharmacological activities. Results are included in Chapter 9. The X-ray analysis of the compound(s) is under progress.

**5-(4-chlorophenyl)-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ29)**

![THQ29](image)

Colorless crystalline solid: mp: 115–117°C (90%); IR (KBr): $v$ (cm$^{-1}$): 3304(NH), 2929(CH), 816(C-C1); $^1$H NMR (400 MHz, DMSO, $\delta$ ppm): 1.23-1.44(m, 2H); 1.61-1.892(m, 2H), 3.29-3.57(m, 1H), 4.24(m, 2H), 4.495(d, $J = 2.6\text{Hz}$, 1H), 4.524(s, NH, 1H), 5.196(d, $J = 5.6\text{ Hz}$, 1H), 6.182-686(m, 4H, Ar-H), 6.989-7.056(m, 4H, Ar-H); $^{13}$C NMR (100 MHz, DMSO, $\delta$ ppm): 23.55, 26.29, 46.0, 57.12, 67.08, 73.36, 113.70, 118.72, 119.70, 127.34, 128.24, 128.60, 128.67, 129.55, 130.34, 131.30, 131.77, 145.77; GC-MS: 299 [M$^+$]; Anal.Calcd. for C$_{18}$H$_{16}$ClNO: C, 72.11; H, 6.05; N, 4.67 %. Found: C, 72.07; H, 6.02; N, 4.64 %.

**9-chloro-5-(4-chlorophenyl)-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ30)**

![THQ30](image)

Colorless crystalline solid: mp 120-122°C (93%); IR (KBr): $v$ (cm$^{-1}$): 3342(NH), 2934(CH), 813(C-C1); $^1$H NMR (400 MHz, DMSO, $\delta$ ppm): 1.21-1.45(m, 2H); 1.60-1.896(m, 2H), 3.30-3.58 (m, 1H), 4.269(m, 2H), 4.498(d, $J = 2.6\text{Hz}$, 1H), 4.523(s, NH, 1H), 5.199(d, $J = 5.6\text{ Hz}$, 1H), 6.181(m, 1H, Ar-H), 6.587(m, 1H, Ar-H), 6.684(s, 1H, Ar-H), 6.989-7.056(m, 4H, Ar-H); $^{13}$C NMR (100 MHz, DMSO, $\delta$ ppm): 23.37, 25.02, 45.60, 59.85, 67.03, 71.25, 114.97, 120.67, 121.12, 125.83, 128.39, 189
128.66, 128.90, 129.51, 131.44, 131.90, 139.91, 144.17; GC-MS: 333 [M^+], 334 [M^+1], 335 [M^+2]; Anal. Calcd. for C_{18}H_{17}Cl_{2}NO: C, 64.68; H, 5.13; N, 4.19 %. Found: C, 64.65; H, 5.10; N, 4.17 %.

5-(4-chlorophenyl)-9-nitro-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline

(THQ31): Colorless crystalline solid: mp: 116-118 °C (90%); IR (KBr): v (cm^{-1}): 3323(NH), 2931(CH), 819(C-C); \textsuperscript{1}H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45 (m, 2H); 1.60-1.896 (m, 2H), 3.30-3.58 (m, 1H), 4.269 (m, 2H); 4.498 (d, J = 2.6 Hz, 1H), 4.523 (s, NH, 1H), 5.199 (d, J = 5.6 Hz, 1H), 6.188 (m, 1H, Ar-H), 6.614 (m, 1H, Ar-H), 6.710 (s, 1H, Ar-H), 6.995-7.079 (m, 4H, Ar-H); \textsuperscript{13}C NMR (100 MHz, DMSO, δ ppm): 23.33, 26.25, 46.0, 58.4, 66.8, 74.5, 114.2, 119.09, 120.7, 124.2, 128.24, 129.55, 130.34, 131.30, 136.77, 152.02; GC-MS: 344 [M^+]; Anal. Calcd. for C_{18}H_{17}Cl_{2}NO: C, 62.52; H, 5.25; N, 8.10 %. Found: C, 62.48; H, 5.23; N, 8.07 %.

5-(4-chlorophenyl)-9-methyl-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline

(THQ32): Pale yellow crystalline solid: mp: 120-122 °C (92%); IR (KBr): v (cm^{-1}): 3387(NH), 2926(CH), 811(C-Cl); \textsuperscript{1}H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45 (m, 2H); 1.60-1.896 (m, 2H), 2.35 (s, 3H, CH_{3}), 3.30-3.58 (m, 1H), 4.269 (m, 2H), 4.498 (d, J = 2.6 Hz, 1H), 4.523 (s, NH, 1H), 5.199 (d, J = 5.6 Hz, 1H), 6.181 (m, 1H, Ar-H), 6.587 (m, 1H, Ar-H), 6.684 (s, 1H, Ar-H), 6.989-7.056 (m, 4H, Ar-H); \textsuperscript{13}C NMR (100 MHz, DMSO, δ ppm): 23.55, 24.8, 26.31, 46.0, 58.42, 67.08, 78.01, 113.02, 118.72, 126.6, 127.34, 128.60, 129.55, 130.34, 131.30, 131.77, 142.77; GC-MS: 313 [M^+]; Anal. Calcd. for C_{19}H_{20}ClNO: C, 72.72; H, 6.42; N, 4.46 %. Found: C, 72.69; H, 6.39; N, 4.43 %.
5-(4-chlorophenyl)-9-methoxy-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ33): Colorless crystalline solid: mp: 118-120 °C (90%); IR (KBr): ν (cm⁻¹): 3321(NH), 2927(CH), 813.3(C-Cl); ¹H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45(m, 2H); 1.60-1.896(m, 2H), 3.30-3.58 (m, 1H), 3.72(s, 3H, CH₃), 4.269(m, 2H), 4.443(d, J = 2.6Hz, 1H), 4.5(s, NH, 1H), 5.12(d, J = 5.6 Hz, 1H), 6.15(m, 1H, Ar-H), 6.571(m, 1H, Ar-H), 6.684(s, 1H, Ar-H), 6.989-7.014(m, 4H, Ar-H); ¹³C NMR (100 MHz, DMSO, δ ppm): 23.3, 26.2, 46.0, 55.9, 58.4, 67.08, 76.7, 113.0, 114.3, 114.8, 121.8, 128.24, 128.60, 128.67, 129.55, 137.5, 137.9, 138.6; GC-MS: 329 [M⁺]; Anal.Calcd. for C₁₉H₂₀ClNO₂: C, 69.19; H, 6.11; N, 4.25 %. Found: C, 69. 16; H, 6.09; N, 4.22 %.

5-(4-chlorophenyl)-9-fluoro-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ34): Colorless crystalline solid: mp: 116-118 °C (91%); IR (KBr): ν (cm⁻¹): 3403(NH), 2926(CH), 812(C-Cl); ¹H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45(m, 2H); 1.60-1.88(m, 2H), 3.30-3.56 (m, 1H), 4.269(m, 2H), 4.47(d, J = 2.6Hz, 1H), 4.54(s, NH, 1H), 5.196(d, J = 5.6 Hz, 1H), 6.184(m, 1H, Ar-H), 6.589(m, 1H, Ar-H), 6.687(s, 1H, Ar-H), 6.989-7.058(m, 4H, Ar-H); ¹³C NMR (100 MHz, DMSO, δ ppm): 23.55, 26.29, 46.0, 57.12, 67.08, 73.36, 113.70, 114.9, 115.1, 116.0, 121.4, 128.67, 129.55, 137.5, 138.6, 145.3; GC-MS: 317 [M⁺]; Anal.Calcd. for C₁₉H₁₇ClFNO: C, 68.03; H, 5.39; N, 4.41 %. Found: C, 68. 00; H, 5.37; N, 4.38 %.

5-(4-chlorophenyl)-8-fluoro-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ35): Colorless crystalline solid: mp: 123-125 °C (91%); IR (KBr): ν (cm⁻¹): 3410(NH), 2928(CH), 823(C-Cl); ¹H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45(m, 2H); 1.60-
1.88(m, 2H), 3.30-3.56 (m, 1H), 4.269(m, 2H), 4.47(d, J = 2.6Hz, 1H), 4.54(s, NH, 1H), 5.196(d, J = 5.6 Hz, 1H), 6.184(m, 1H, Ar-H), 6.589(m, 1H, Ar-H), 6.688(s, 1H, Ar-H), 6.989-7.058(m, 4H, Ar-H); $^{13}$C NMR (100 MHz, DMSO, δ ppm): 23.55, 26.29, 46.0, 57.12, 67.08, 73.36, 101.70, 103.7, 115.4, 118.72, 119.70, 127.34, 128.24, 128.67, 129.55, 130.34, 138.77, 162.03; GC-MS: 317 [M$^+$]; Anal.Calcd. for C$_{18}$H$_{17}$ClFNO: C, 68.03; H, 5.39; N, 4.41 %. Found: C, 68.00; H, 5.37; N, 4.38 %.

5-(4-chlorophenyl)-7-fluoro-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ36): Colorless crystalline solid: mp: 1137-139 °C (92%); IR (KBr): ν (cm$^{-1}$): 3408(NH), 2930(CH), 817(C-C1); $^1$H NMR (400 MHz, DMSO, δ ppm): $^1$H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45(m, 2H); 1.60-1.88(m, 2H), 3.30-3.56 (m, 1H), 4.27(m, 2H), 4.47(d, J = 2.6Hz, 1H), 4.524(s, NH, 1H), 6.184(m, 1H, Ar-H), 6.589(m, 1H, Ar-H), 6.687(s, 1H, Ar-H), 6.989-7.034(m, 4H, Ar-H); $^{13}$C NMR (100 MHz, DMSO, δ ppm): 23.55, 26.29, 46.0, 57.12, 67.08, 73.36, 113.70, 118.72, 119.70, 121.4, 124.6, 127.34, 128.24, 128.60, 128.67, 129.55, 130.34, 131.30, 131.77, 154.7; GC-MS: 317 [M$^+$]; Anal.Calcd. for C$_{18}$H$_{17}$ClFNO: C, 68.03; H, 5.39; N, 4.41 %. Found: C, 68.00; H, 5.37; N, 4.38 %.

5-(4-chlorophenyl)-7,9-difluoro-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ37): Light yellow crystalline solid: mp: 141-143 °C (92%); IR (KBr): ν (cm$^{-1}$): 3343(NH), 2929(CH), 814.9(C-C1); $^1$H NMR (400 MHz, DMSO, δ ppm): 1.21-1.45(m, 2H); 1.61-1.88(m, 2H), 3.30-3.56 (m, 1H), 4.259(m, 2H), 4.48(d, J = 2.6Hz, 1H), 4.532(s, NH, 1H), 5.179(d, J = 5.6 Hz, 1H), 6.210(m, 1H, Ar-H), 6.634(m, 1H, Ar-H), 6.992-7.120(m, 4H, Ar-H); $^{13}$C NMR (100 MHz, DMSO, δ ppm): 23.55, 26.29, 46.0, 57.12, 67.08, 73.36, 102.7, 113.70, 123.34, 128.24, 128.60, 128.67, 129.55,
130.34, 136.7, 149.3, 158.02; GC-MS: 335 [M⁺]; Anal. Calcd. for C₁₈H₁₆ClF₂NO: C, 64.39; H, 4.80; N, 4.17 %. Found: C, 64.37; H, 4.77; N, 4.16 %.

5-(4-chlorophenyl)-7,10-difluoro-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinoline (THQ38): Light yellow crystalline solid: mp: 122-124 °C (93%); IR (KBr): ν (cm⁻¹): 3358(NH), 2930(CH), 818(C-C); ¹H NMR (400 MHz, DMSO, δ ppm): 1.23-1.48(m, 2H); 1.62-1.876(m, 2H), 3.30-3.556 (m, 1H), 4.321(m, 2H), 4.478(d, J = 2.6 Hz, 1H), 4.55(s, NH, 1H), 5.219(d, J = 5.6 Hz, 1H), 6.198(m, 1H, Ar-H), 6.64(m, 1H, Ar-H), 6.992-7.211(m, 4H, Ar-H); ¹³C NMR (100 MHz, DMSO, δ ppm): 23.55, 26.29, 46.0, 57.12, 67.08, 73.36, 102.7, 113.70, 123.34, 128.24, 128.60, 128.67, 129.55, 130.34, 136.7, 150.3, 157.02; GC-MS: 335 [M⁺]; C₁₈H₁₆ClF₂NO: C, 64.39; H, 4.80; N, 4.17 %. Found: C, 64.37; H, 4.77; N, 4.16 %.
Spectrum 1: IR Spectrum of compound THQ30
Spectrum 2: $^1$H NMR Spectrum of compound THQ30 in DMSO
Spectrum 3: $^{13}$C NMR Spectrum of compound THQ30 in DMSO
Spectrum 4: GC-MS Spectrum of compound THQ30
References