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Synthesis and Characterization of Some New 1,3-Oxazepine from"Schiff Bases Contain 1,4-Dihydropyridine

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ABSTRACT
"This study focuses on the synthesis and the development of new Schiff bases and heterocyclic compounds (oxazepine) derived from the starting material 2,6-dimethyl-1,4-dihydropyridine by traditional reflux and green microwave methods."The synthesis of Schiff bases " "using "microwave irradiation" has proven to be significantly easier, faster, reduced solvent, lowering costs and high yield compared to conventional heating methods. Various physical and spectroscopic techniques "FT-IR, ^{1}H-NMR, ^{13}C-NMR and"TLC"were used to"characterize the prepared compounds. Given the documented biological activity of related compounds in the scientific literature, it is expected that these newly synthesized compounds will display similar properties against micro-bacterial.

Keywords: 1,4-dihydropyridine, Schiff Bases, 1,3-oxazepine Derivatives, Heterocyclic Compounds.

1. INTRODUCTION

"Chemists have long encountered "unique challenges in heterocyclic chemistry due to its" extensive knowledge base and diversity [1]. Nonetheless, heterocyclic chemistry and synthesis techniques remain central to contemporary medicinal and pharmaceutical research [2]. Heterocyclic compounds are ring-like structures containing atoms such as oxygen, sulfur, or nitrogen. Typically found in nature, they are essential in many fields, including as industry and medicine. Proteins, nucleic acids, enzymes, carbohydrates, and their derivatives are all synthesized using these substances [3] & [4]. Oxazepine and its variants are among the most common heterocyclic compounds. They consist of a seven-membered ring with an oxygen "atom at position 1 and a nitrogen atom at position"2, 3, or 4 within the heptane ring. These compounds may also contain double bonds and carbonyl groups, which would render them unsaturated and non-aromatic [5].

Over time, extensive research and documentation have been done on the synthesis of oxazepine. [6]. Green chemical methods can be used to make it. [7] & [8] together with the cyclization addition of succinic, phthalic, and maleic anhydrides to Schiff base or hydrazone [9] & [10]. Numerous oxazepine compounds exhibit a variety of biological actions, including hypnotic, antifungal, antagonistic, antibacterial, and muscle relaxant properties [11], and anti-inflammatory effects [12] and [13].

In our research, we aim to synthesize 1,2-oxazepine-3,6-dicarbonyl ring derivatives through the cycloaddition reaction between Schiff bases and anhydrides. Additionally, we will characterize the resulting products using various techniques.

2. MATERIAL AND METHODS

All chemicals used were of commercial analytical grade and supplied by Aldrich, Fluka, BDH, CDH, Scharlau, or Thomas Baker. All solvents and other chemicals were dried and purified as necessary. For examining the synthesized Schiff base compounds and their heterocyclic oxazepine derivatives a Bruker 400 MHz Ultra shield NMR spectrometer was employed to collect ^{1}H-NMR and ^{13}C-NMR spectra. Samples were dissolved in deuterated dimethyl sulfoxide (DMSO) at room temperature (298 K), with tetramethyl silane (TMS) acting as the internal standard and measured at University of Basra, Iraq. FT-IR spectra were recorded using a Bruker spectrophotometer in the range 400 to 4000 cm^{-1}, employing directly without using KBr disc method at"the University of Mosul, College of Science." The melting points of the products were determined using a Stuard-SMP30 device and were not corrected at University of Mosul, College of Science.

Synthesis of 3,5-diacetyl-2,6-dimethyl-1,4-dihyropyridine (M1) [14]
A mixture of paraformaldehyde (4.8 g, 0.16 mol), acetylacetone (32 g, 0.32 mol), ammonium acetate (18.5 g, 0.24 mol), and 25 ml of water were placed in a dried 250 ml round-bottom flask with a magnetic stirrer bar. The flask was sealed with a calcium chloride tube, and the reaction mixture was stirred at 80°C for 15 minutes. After the reaction time, the crude product was isolated by adding ice-cold water and scratching. The precipitate "was filtered, washed with cold water, and recrystallized from methanol to yield""2,6-dimethyl-3,5-diacetyl-1,4-dihydropyridine" (M1) as a yellow powder (32.2 g, 52%), with a melting point of 215-216°C, as shown in Scheme (1).

Scheme 1: Synthesis of Started Material M1

Synthesis of Schiff Base Compounds (M2-M7)
Method 1: Synthesis of Schiff Base Compounds (M2-M7) [15]
A mixture was prepared by combining 0.002 mol of M1 with 0.004 mol of a substituted aniline (as 4-nitroaniline, 4-aminobenzoic acid, 4-bromoaniline, 3-nitroaniline, 4-chloroaniline, or 3-chloro-4-methylaniline). To this mixture, 10 drops of absolute ethanol and 4-5 drops of glacial acetic acid were added as solvents and catalysts. The combined mixture was thoroughly mixed in a beaker and subsequently irradiated in a microwave oven at 300W for several minutes."The progress of the reaction was monitored using thin-layer chromatography (TLC). Once the reaction was complete, the mixture was poured into" either cold water or diethyl ether. After that, the crystals were filtered, cleaned, dried, and put through the recrystallization process. Scheme (2) shows the general reactions of the produced compounds.

Scheme 2: "Synthesis of Schiff Base"Compounds

Method 2: "Synthesis of Schiff Base" Compounds (M2 & M3) [16]
In 20 milliliters of pure ethanol, a solution containing 0.002 moles of M1 was made. Four or five drops of glacial acetic acid were added to this solution, along with 0.004 moles of 4-nitroaniline or 4-aminobenzoic acid. The mixture was then heated for 15 or 18 hours, depending on the particular reactant utilized, under reflux in a water bath. Using thin-layer chromatography (TLC) and a solvent system made up of hexane and ethyl acetate in a 4:6 ratio, the reaction's progress was tracked. The mixture was refluxed and "then allowed to cool to room temperature. The resulting-colored precipitate was filtered" and washed with water, following the procedure outlined in Scheme (3). Table 2 illustrate some physical properties and figure (1) graphical procedure for synthesis of Schiff base compounds.

Scheme 3: Synthesis of Schiff Base Compounds

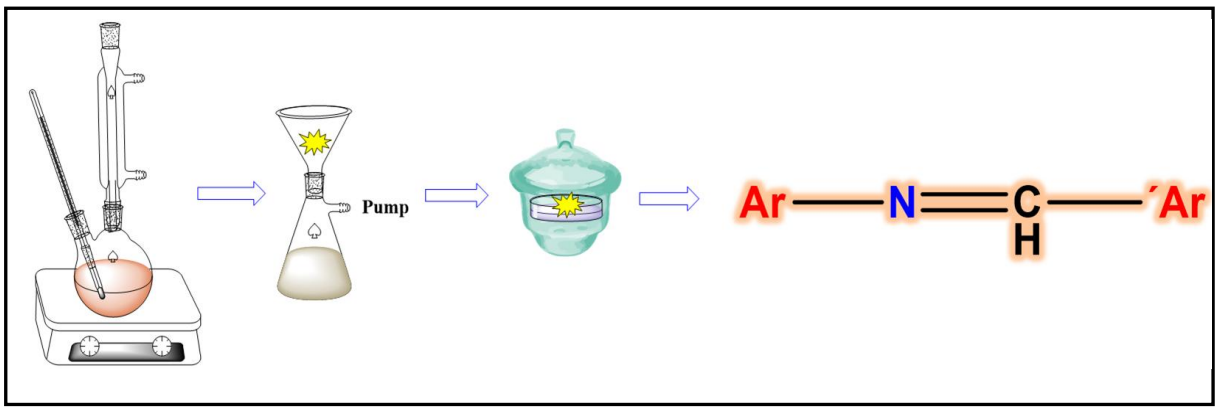


Fig. 1: Graphical "procedure for synthesis of Schiff base compounds".

Synthesis of 1,3-Oxazepine Derivatives (A1-A6) [13]

A mixture comprising 0.001 mol of Schiff base compounds (M2-M4) and 0.002 mol of maleic or phthalic anhydride in 30 mL of dry benzene was placed in a 100 Ml"round-bottom flask equipped with a double-surface condenser, an anhydrous calcium chloride guard tube, and"a magnetic stirring"bar. The reaction mixture was refluxed for 10 hours, then allowed to cool to room temperature and stirred overnight. The resulting solid product was filtered, dried, and recrystallized from ethanol. The synthetic pathway for producing the desired 1,3-oxazepine derivatives (A1-A6) is illustrated in Scheme (4).

Scheme 4: General Reaction of Preparation of 1,3-Oxazepine Derivatives.

3. RESULT AND DISCUSSIONS

The "compound 3,5-diacetyl-2), (6-dimethyl-1), (4"-dihydropyridine) (M1)-was synthesized through a three-

component reaction using paraformaldehyde, acetylacetone, and ammonium acetate as starting materials. Subsequently, Schiff base compounds (M2-M7) were produced from (M1) as the ketone and various substituted anilines (such as 4-nitroaniline, 4-aminobenzoic acid, 4-bromoaniline, 3-nitroaniline, 4-chloroaniline, or 3-chloro-4-methylaniline) using both traditional and green methods. Finally, these compounds were cyclized with maleic or phthalic anhydride to yield the final heterocyclic oxazepine compounds (A1-A6), as illustrated in Scheme (5). The prepared compounds were identified based on spectroscopic methods as FTIR, ^{1}H-NMR, ^{13}C-NMR, TLC and their physical properties. Table 1 offers a detailed summary of the physical characteristics of these synthesized compounds, including melting points, color, metal content, and other relevant attributes. This provides a deeper understanding of the properties of these compounds.

Table 1: The Physical Properties of Prepared Schiff Base Compounds.

Comp. No.	Comp. Name	Color	M.p ºC	Yield %
M1	3,5-diacetyl-2,6-dimethyl-1,4-dihyropyridine	Yellow	215-217	82
M2	1,1'-"(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(N-(4-nitrophenyl)ethan-1-imine)"	Brown	126-128	81
M3	1,1'-"(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(N-(4-carboxyphenyl)ethan-1-imine)"	Deep Brown	137-139	75
M4	1,1'-"(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(N-(4-bromophenyl)ethan-1-imine)"	Green	197-199	78
M5	1,1'-"(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(N-(3-nitrophenyl)ethan-1-imine)"	Brown	115-117	80
M6	1,1'-"(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(N-(4-chlorophenyl)ethan-1-imine)"	Deep Brown	164-166	60
M7	1,1'-"(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(N-(3-chloro-4-methylphenyl)ethan-1-imine)"	Light Brown	143-145	67
A1	"2,2'-(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis(2-(methyl))-3-(4-(carboxyphenyl)-2,3-(dihydro-1,3-oxazepine-4),(7-dione)"	Deep Brown	219-217	72
A2	"2,2'-(2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis,(2-methyl-3-((4-nitrophenyl))-2,3,-dihydro-1,3-,oxazepine-4, 7-,dione)"	Light Brown	198-196	68
A3	3,3'-("2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)"bis"(3-methyl-4-(4-carboxyphenyl)-3,4-dihydrobenzo[e][1,3]oxazepine-1,5-dione)"	Off White	250-252	83
A4	3,3'-("2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)"bis"(3-methyl-4-(4-nitrophenyl)-3,4-dihydrobenzo[e][1,3]oxazepine-1,5-dione)"	Black	201-203	70
A5	2,2'-("2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)bis"(3-(4-bromophenyl)-2-methyl-2,3-dihydro-1,3-oxazepine-4,7-dione)	Black	>300	65
A6	3,3'-("2,6-dimethyl-1,4-dihydropyridine-3,5-diyl)"bis"(4-(4-bromophenyl)-3-methyl-3,4-dihydrobenzo[e][1,3]oxazepine-1,5-dione)"	Deep Brown	261-263	76

Scheme 5: General scheme of synthesis of heterocyclic compounds

3,5-diacetyl-2,6-dimethyl-1,4-dihyropyridine DHP (M1)

The compound (M1) was readily prepared using the classical Hantzsch method by heating a mixture of paraformaldehyde, acetylacetone, and ammonium acetate in an aqueous medium. The reaction yielded 52%, with a melting point of 215-217°C, compared to the published melting point of 213-215°C, [14] and [17].

The prepared 3,5-diacetyl-2,6-dimethyl-1,4-dihydropyridine was identified based on spectral data from FT-IR, as well as by measuring its melting point and comparing it with the published value. FT-IR spectrum displayed the most significant bands (3380, 1668 and 1642)"cm^{-1} which corresponding to the stretching vibration of (N-H, C=O and C=C)"groups respectively, as shown in figure (2).

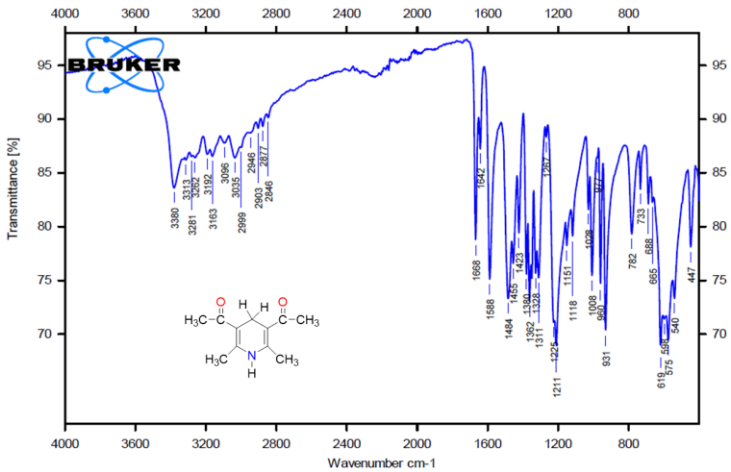


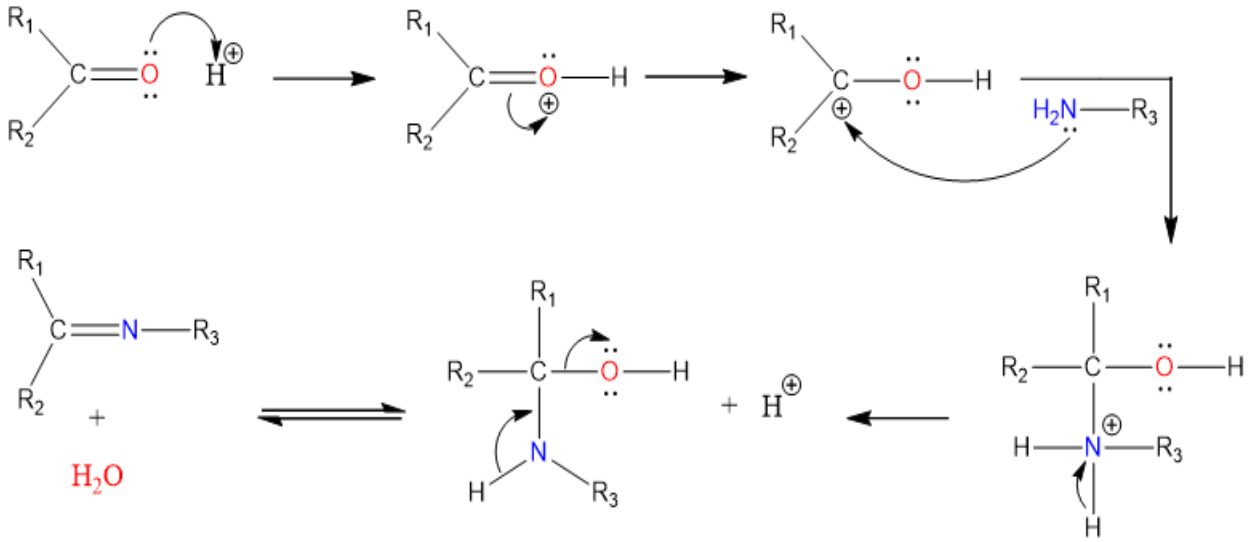
Fig. 2: FT-IR of compound (M1)

"Synthesis of Schiff Base Compounds"(M2-M7)

The new Schiff bases were synthesized using two methods: a green method involving microwave irradiation at 300W and a traditional method involving reflux, [16] & [15]**.**

The synthesis of Schiff bases using microwave irradiation has been discovered to be significantly easier and faster compared to conventional heating methods. Utilizing microwave irradiation in solvent-free or lower solvent conditions offers an effective means to reduce pollution, lower costs, increase product yield, and simplify processing and handling (Mahmood, 2022) and (Shntaif & Rashid, 2016).

The Mechanism of this reaction was summarized in scheme (6)."When synthesizing Schiff bases, nucleophilic amines attack electrophilic carbonyl compounds via nucleophilic addition, forming" a hemiaminal group. This hemiaminal group then undergoes dehydration to produce imine compounds. Initially, "the amine reacts with the aldehyde or ketone to" form the unstable addition product, carbinolamine. Carbinolamine undergoes dehydration, catalyzed by either acid or base. Since carbinolamine is an alcohol, it dehydrates when exposed to an acid catalyst. "The formation of a Schiff base from aldehydes or ketones" often involves reversible acid or base catalysis or heating. The reaction is driven to completion when the product is isolated, water is evaporated, or both (Berski & Ciunik, 2015).



Scheme 6: Mechanism of Schiff Base Formation (M2-M7)

The route of the reaction was achieved by examining certain physical properties, such as the melting point and comparing it to the reactants, as well as observing the color changes of the resulting compounds."The structure of synthesized"compounds has been characterized based on their spectral"methods including FT-IR, ^{1}H-NMR and ^{13}C-NMR". Figure (3-6) designate the disappearance of absorption peak at (3350-3480) cm^{-1} of amino group $\upsilon(NH_2)$ [18] and at (1668) cm^{-1} of carbonyl group of υ(C=O) in started material. In same time, new absorption peak manifested at the range (1626-1672) cm^{-1} which was assigned to υ(C=N), other bands illustrated in table (2).

Table 2: FT-IR bands of the prepared Schiff base compounds (M2-M7) in cm^{-1}

Comp. No.	*υ* N-H	*υ* C-H arom.	*υ* C-H aliph.	*υ* C=N	*υ* C=C Conj.	*υ* C-C arom.	Others
M2	3355	3108	2910, 2842	1628	1585	1532	1504 asymm. N-O 1293 symm. N-O
M3	3353	3226	2965, 2820	1626	1595	1521	3461 O-H,1662 C=O,1285 C-O
M4	3381	3036	2909, 2877	1686	1642	1588	618 C-Br
M5	3301	3005	2926, 2848	1677	1657	1575	1478 asymm. N-O 1216 symm. N-O
M6	3381	3192	2971, 2877	1672	1672	1581	741 C-Cl
M7	3254	3105	2923, 2847	1645	1599	1535	824 C-Cl

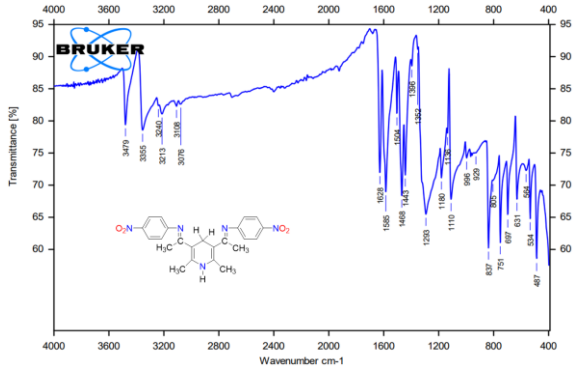


Fig. 3. FT-IR of compound (M2)

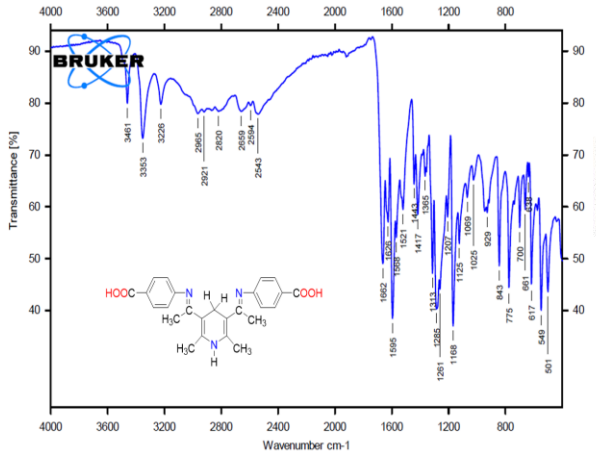


Fig. 4. FT-IR of compound (M3)

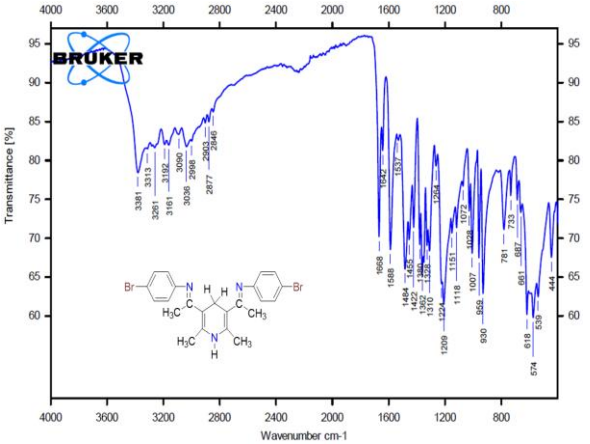


Fig. 5. FT-IR of compound (M4)

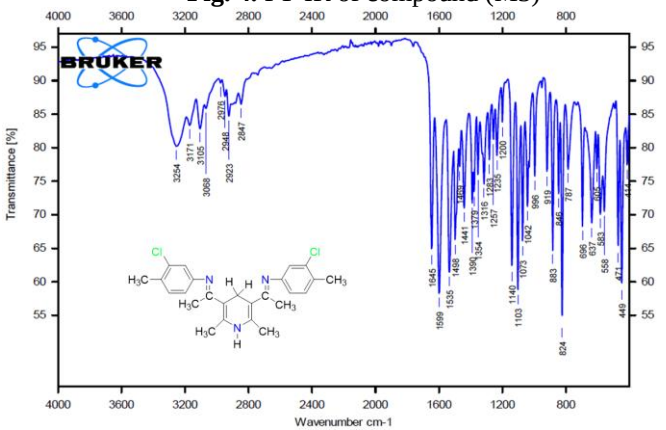


Fig. 6: FT-IR of compound (M7)

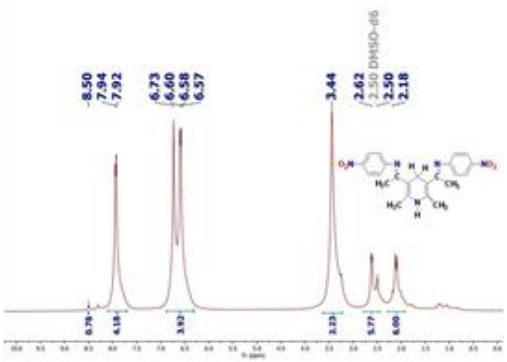


Fig. 7: ^{1}H-NMR spectrum of compound (M2)

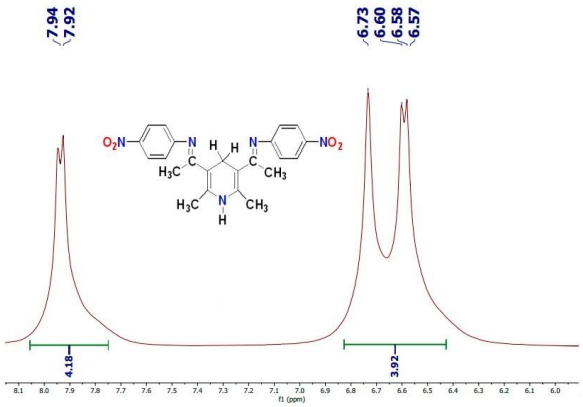


Fig. 8: Expansion ^{1}H-NMR of compound (M2)

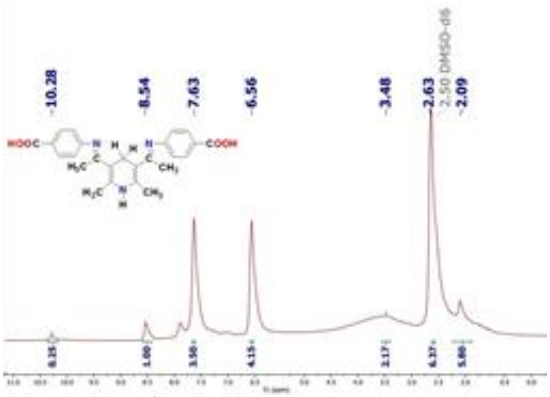


Fig. 9: ^{1}H-NMR spectrum of compound (M3)

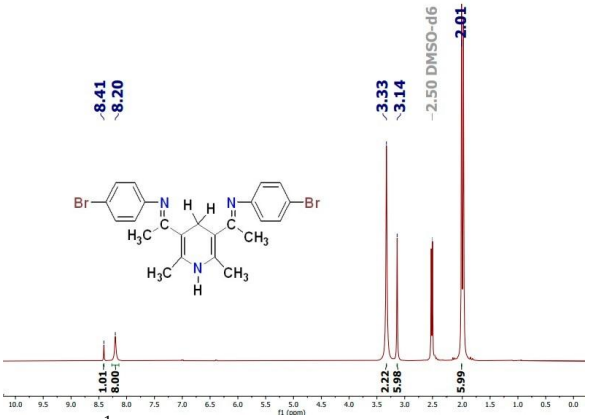


Fig. 10: ^{1}H-NMR spectrum of compound (M4)

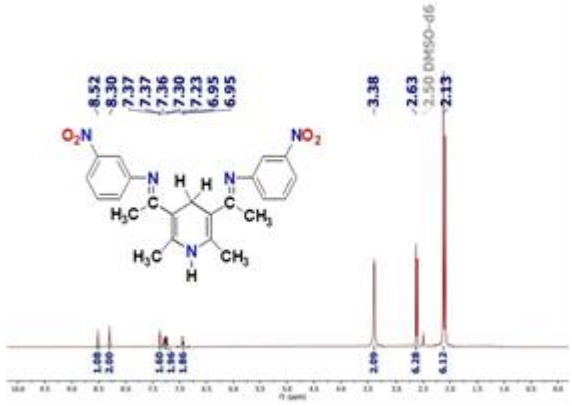


Fig. 11: ^{1}H-NMR spectrum of compound (M5)

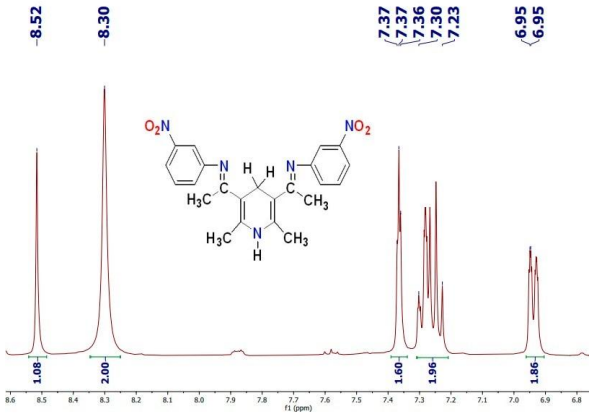


Fig. 12: Expansion ^{1}H-NMR of compound (M5)

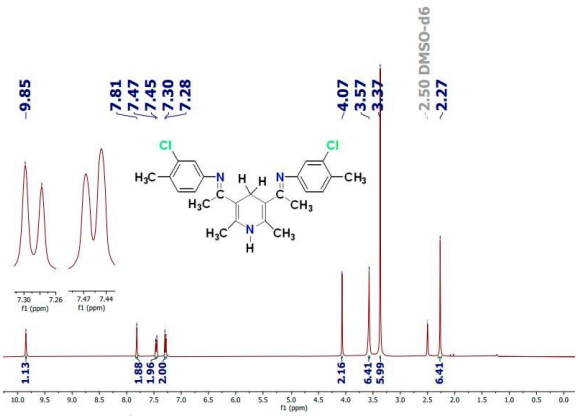


Fig. 13: ^{1}H-NMR spectrum of compound (M7)

The NMR technique, operating at 400 MHz, was utilized to determine the structure of the synthesized compounds."The samples were dissolved in deuterated dimethyl sulfoxide (DMSO-d6) at room temperature.""In the ^{1}H-NMR spectra of the" prepared Schiff base and their heterocyclic compounds, a signal observed at 2.5 ppm indicates the presence of DMSO as the solvent.

The ^{1}H-NMR spectra of Schiff base compounds (M2-M7), shown in figures (7-13), display a singlet signal between (8.52-9.85) ppm, corresponding to one proton of the (N-H) group. Multiple peaks observed between (6.57-8.30) ppm is likely attributed to the eight aromatic protons. Additionally, a signal in the range of (3.33-4.07) ppm is associated with two protons of the pyridine ring, while peaks around (2.01-2.27) and (2.62-3.37) ppm correspond to twelve protons of the methyl groups, with the first set attached to imine and the second to pyridine.

The ^{13}C-NMR operating at (100 MHz) using DMSO solvent were listed in table (4) and the signal at 40 ppm belong to the solvent DMSO in all spectra as shown in figures (14-18). The chemical structures of the Schiff base and related heterocyclic compounds can be understood in large part thanks to the ^{1}H- and ^{13}C-NMR data. The chemical makeup, atomic connection, and environmental context of the atoms within the compounds can all be thoroughly examined thanks to these spectroscopic investigations. In general, the integrated examination of

^{1}H-NMR and ^{13}C-NMR spectra provides a thorough comprehension of the chemical configurations of the ligands and their compounds, which is crucial for additional investigation into their characteristics and possible uses.

Synthesis of 1,3-Oxazepine Derivatives (A1-A6)

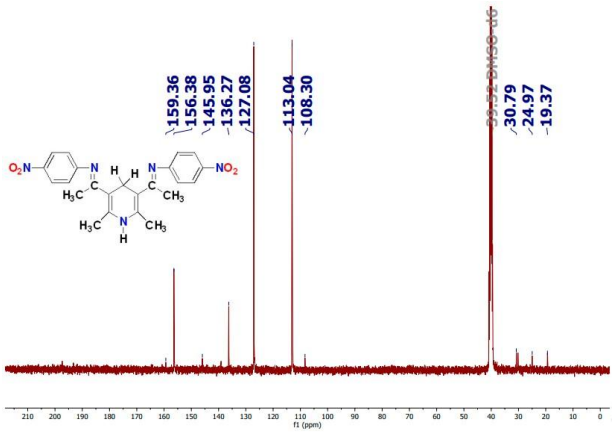


Fig. 14. ^{13}C-NMR spectrum of compound (M2)

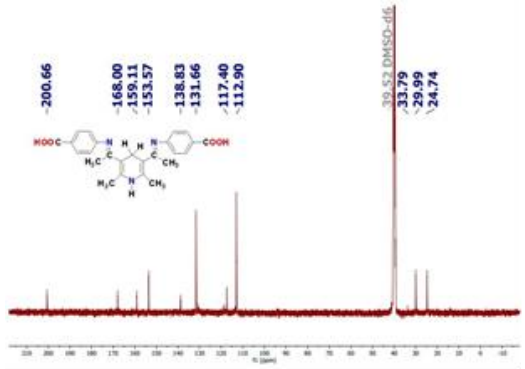


Fig. 15. ^{13}C-NMR spectrum of compound (M3)

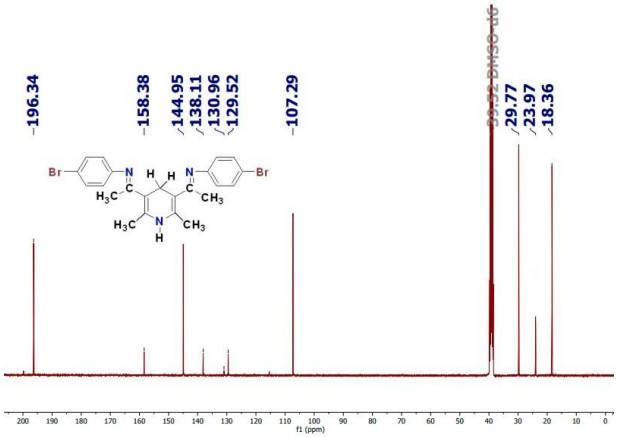


Fig. 16. ^{13}C-NMR spectrum of compound (M4)

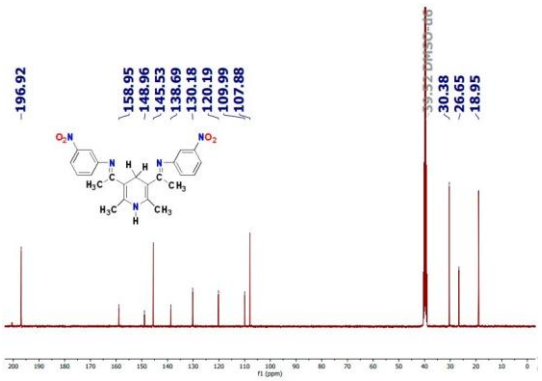


Fig. 17. ^{13}C-NMR spectrum of compound (M5)

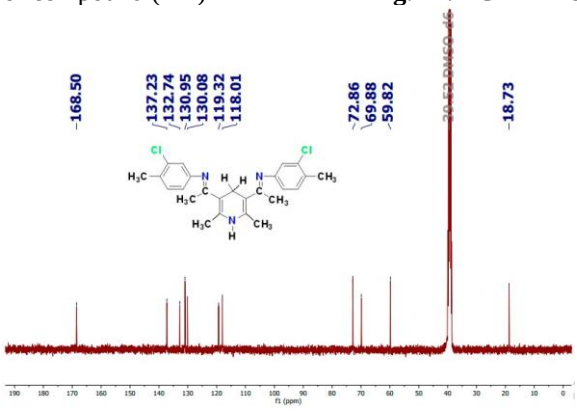
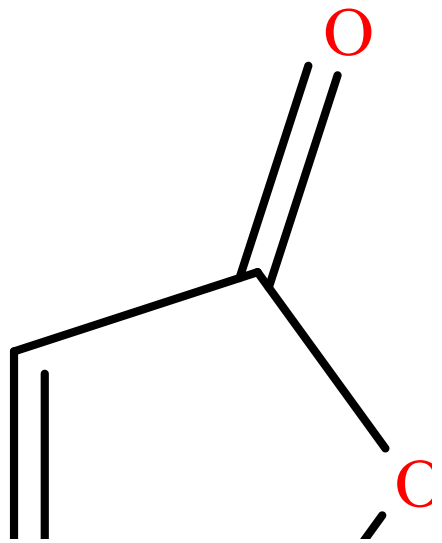


Fig. 18: ^{13}C-NMR spectrum of compound (M7)

One equivalent mole of Schiff base compounds (M2-M4) was cycled with two equivalent moles of maleic or phthalic anhydride in dry benzene under reflux for ten hours to create the compounds (A1-A6), [13].

It is suggested that the reaction will proceed by means of a nucleophilic attack on the electrophilic carbonyl group of the cyclic anhydride by the lone pair of electrons in the slightly nucleophilic imino group. A dipolar intermediate [I] is formed as a result of this interaction, and it can either collapse to produce intermediate [II] or generate intermediate [II] directly. The target molecule is then created by internal cyclization of intermediate [II] [13] and [19]. Scheme (7) provides an illustration of the conceivable process by which 1,3-oxazepine derivatives are formed.



Scheme 7: The mechanism that is suggested to create derivatives of oxazepane

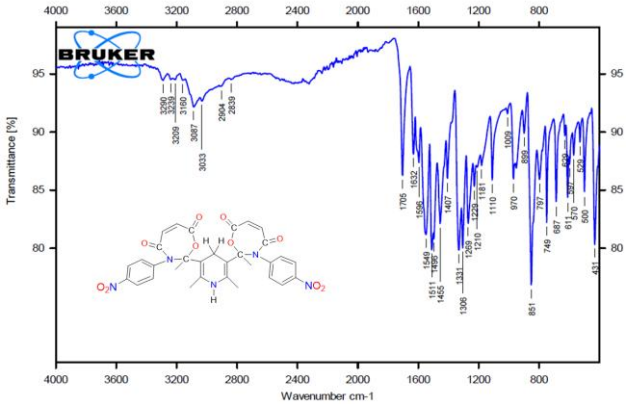


Fig. 19: FT-IR of compound (A2)

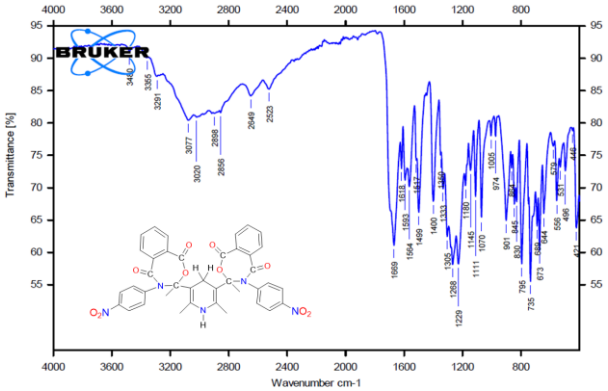


Fig. 20: FT-IR of compound (A4)

The reactions' progress was monitored through physical parameters like melting points and changing the color, distinguishing them from the raw materials. Additionally, TLC was utilized to determine the reaction's endpoint and the purity of the resulting compounds,"using a solvent mixture of n-hexane and ethyl acetate in a 4:6 ratio. The TLC was conducted on silica gel 60 F254 aluminum sheets, with ultraviolet light and a permanganate

solution used to visualize the spots of the synthesized compounds". The spectral methods including FTIR, ^{1}H-NMR and ^{13}C-NMR spectroscopy were utilizing to predict the structure of the prepared oxazepine compounds, in addition to examining their physical properties.

The main infrared absorption bands for the oxazepine compounds have been documented in table (3) and correlate very well with the proposed structures as shown in figures (19 & 20). The bands at the range (3212-3346) cm^{-1} corresponds to υ(N-H) and shift to a lower frequency compared to the Schiff base, indicating the cyclization of the compounds. In addition, the stretching bands observed at the range (1692-1886) cm^{-1} attributed to the υ(C=O) lactone, while the bands (1623-1682) cm^{-1} corresponding to υ(C=O) lactam. These bands offer strong evidence for the cyclization of maleic or phthalic anhydride with the Schiff base.

Table 3: FT-IR bands of the prepared 1,3-Oxazepine Derivatives (A1-A6) cm^{-1}

Comp. No.	***υ*N-H**	***υ*C-H** arom.	***υ*C-H** aliph.	***υ*C=O** lactone	***υ*C=O** lactam	***υ*C=C** Conj.	***υ*C-C** arom.	***υ*C-N**	***υ*C-O**	others
A1	3212	3051	2995, 2880	1886	1623	1598	1575	1173	1117	3312 OH, 1682 C=O
A2	3239	3087	2904, 2839	1705	1632	1596	1549	1181	1110	1511 N-O asymm. 1269 N-O symm.
A3	3290	3100	2990, 2891	1692	1647	1592	1531	1177	1118	3400 OH 1685 C=O
A4	3291	3077	2898, 2856	1685	1669	1618	1593	1180	1111	1499 N-O asymm. 1333 N-O symm.
A5	3346	3105	2920, 2891	1695	1680	1622	1556	1169	1070	555 C-Br
A6	3310	3015	2999, 2892	1700	1682	1596	1576	1161	1073	621 C-Br

The ^{1}H-NMR spectrum (400 MHz, DMSO) of compound (A2) shows a singlet signal at (10.95) ppm, attributed to the proton of the N-H group, which shifts downfield compared to its Schiff base, indicating the formation of oxazepine compounds. Additionally, multiplate peaks observed in the range of (7.85-8.24) ppm corresponding to aromatic protons, while singlet signals between (6.34-6.53) ppm are assigned to the four protons of the methylene group in maleic anhydride. The peak around (3.46) ppm appeared singlet which related to two protons of the pyridine ring, and the singlet signals in the range of (2.08-3.16) ppm are associated with twelve protons of the methyl groups, with the first set attached to the imine and the second to the pyridine. At the same time, the ^{1}H-NMR spectrum (400 MHz, DMSO) of compound (A3) shows a signal at (8.52) ppm, attributed to the proton of the N-H group, and a peak at (10.69) ppm corresponding to the proton of the COOH group. Additionally, a singlet peak at (13.12) ppm might indicate hydrogen bonding. The multiplate signals in the (7.56-8.10) ppm range are associated with aromatic protons, whereas the singlet signal around (3.79) ppm corresponds to two protons of the pyridine ring, as depicted in figures (21-23).

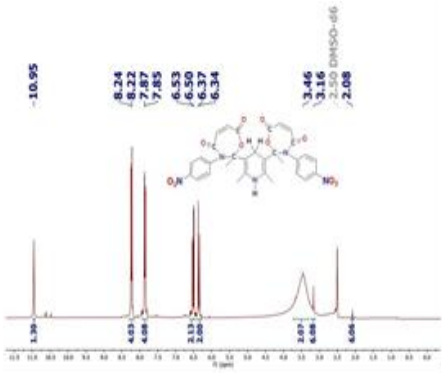


Fig. 21. ^{1}H-NMR spectrum of the compound (A2)

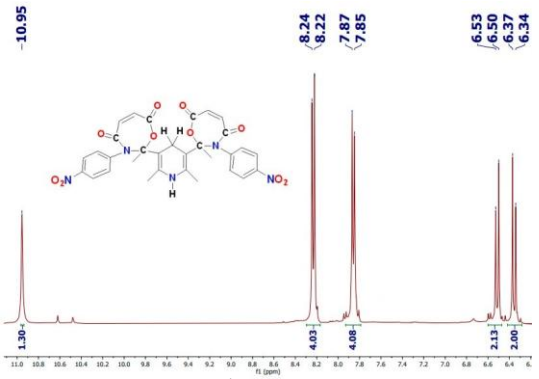


Fig. 22: Expansion ^{1}H-NMR of the compound (A2)

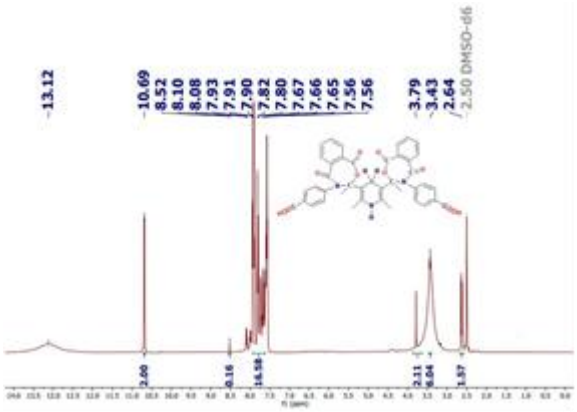


Fig. 23: ^{1}H-NMR spectrum of the compound (A3)

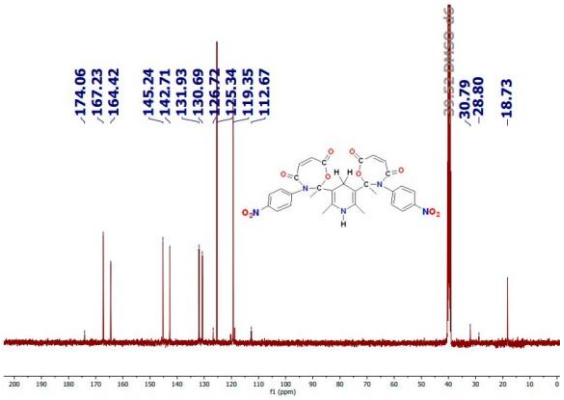


Fig. 24: ^{13}C-NMR spectrum of the compound (A2).

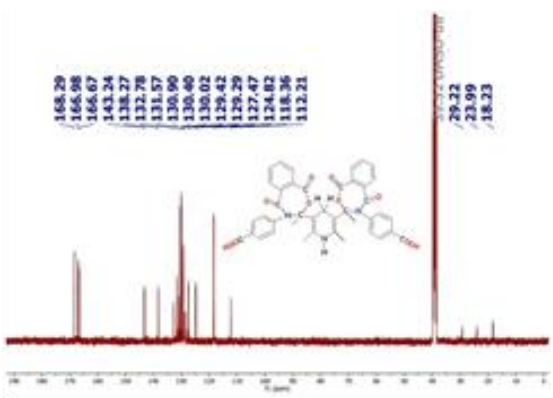


Fig. 25: ^{13}C-NMR spectrum of the compound (A3).

The ^{13}C-NMR operating at (100 MHz) using DMSO solvent were listed in table (4) and the signal at 40 ppm belong to the solvent DMSO in all spectra as shown in figures (24 & 25).

Table 4: ^{13}C-NMR data of the prepared compounds

Comp. NO.	Comp. Structure	^{13}C-NMR (100 MHz, DMSO) ppm
M2		C_{imine} = 159.36, $C_{arom.}$ = (156.38-127.08), $C_{pyridine}$ =(113.04 & 108.30), C_{CH2} = 30.76, $C_{CH3\text{-}pyridine}$ = 24.79, $C_{CH3\text{-}imine}$ = 19.37.
M3		$C_{carbonyl}$ = 200.66, C_{imine} =168, $C_{arom.}$ = (1159.11-131.66), $C_{pyridine}$ = (117.40 & 112.90), C_{CH2} = 33.79, $C_{CH3\text{-}pyridine}$ = 29.99, $C_{CH3\text{-}imine}$ = 24.74.
M4		C_{imine} = 196.34, $C_{arom.}$ = (158.38-130.96), $C_{pyridine}$ =(129.52 & 107.29), C_{CH2} = 29.77, $C_{CH3\text{-}pyridine}$ = 23.97, $C_{CH3\text{-}imine}$ = 18.36.
M5		C_{imine} = 196.92, $C_{arom.}$ = (158.95-120.19), $C_{pyridine}$ = (109.99 & 107.88), C_{CH2} = 30.38, $C_{CH3\text{-}pyridine}$ = 26.65, $C_{CH3\text{-}imine}$ = 18.95.

M7		C_{imine} = 168.50, $C_{arom.}$ = (137.23-130.08), $C_{pyridine}$ = (119.32 & 118.01), C_{CH2} = 72.86, $C_{CH3\text{-}pyridine}$ = 69.88, $C_{CH3\text{-}imine}$ = 59.82, $C_{CH3\text{-}ph}$ =18.73.
A2		$C_{O\text{-}C=O}$ = 174.06, $C_{N\text{-}C=O}$ = 167.23, C_{arom} = (164.42, 145.24,131.93 |& 126.72), $C_{pyridine}$ = (130.69 & 119.35), $C_{Oxazepine}$ = (142.71 & 125.34), $C_{N\text{-}C\text{-}O}$= 112.67, C_{CH3} = (30.79 & 28.80), C_{CH2}= 18.73.
A3		$C_{carboxcylic}$ = 168.29, $C_{O\text{-}C=O}$ = 166.98, $C_{N\text{-}C=O}$= 166.67, $C_{pyridine}$= (129.42 & 118.36), $C_{arom.}$= (143.24-124.82), C_{CH3}= (29.22 & 23.99), C_{CH2}= 18.23

4. CONCLUSION

In this study,"a series of Schiff bases and 1,3-oxazepine derivatives were"successfully synthesized, starting from 2,6-dimethyl-1,4-dihydropyridine. Using both conventional and green methods, Schiff bases were first formed. These Schiff bases were then cyclized with maleic or phthalic anhydride to yield 1,3-oxazepine derivatives. Such a synthetic process involved multiple steps.

A variety of"spectroscopic methods, including FT-IR, ^{1}H-NMR", and ^{13}C-NMR, as well as physical property studies, were employed to characterize the synthesized compounds. These methods confirmed the structures of the compounds and provided insights into their chemical properties. The"melting points, colors, and yields of the compounds"were also documented, indicating successful synthesis.

Given the known biological activities of related compounds, these newly synthesized Schiff bases and oxazepine derivatives are expected to exhibit significant micro-bacterial properties, making them potential candidates for further biological evaluation and possible pharmaceutical applications. The study's findings contribute valuable knowledge to the field of heterocyclic chemistry, particularly"in the development of compounds with potential therapeutic"benefits.

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