Adıyaman University Journal of Science
https://dergipark.org.tr/en/pub/adyujsci
DergiPark AKADEMİK
ISSN 2147-1630
e-ISSN 2146-586X

Development and Comprehensive Analysis of New Schiff Base Compounds Originating from Methylpiperazine

Yıldız UYGUN CEBECİ[1,*]

[1]*Kırklareli University, Faculty of Science, Department of Chemistry, Kırklareli, Türkiye*
y.uyguncebeci@klu.edu.tr; ORCID: 0000-0001-7949-0329

Received: 02.05.2025 **Accepted:** 05.12.2025 **Published:** 31.12.2025

Abstract

A novel series of Schiff base derivatives was synthesized starting from methylpiperazine through a multistep reaction sequence involving esterification, hydrazide formation, and condensation with various aromatic aldehydes. The resulting compounds (4a–g) were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, and EI-MS spectroscopy, which confirmed the successful formation of the imine (C=N) linkage and the incorporation of functional groups such as methoxy, hydroxyl, halogen, and heteroaryl moieties. Spectral data revealed characteristic azomethine proton signals (7.19–8.93 ppm) and imine carbon stretches (1603–1623 cm^{-1}), consistent with Schiff base formation. Mass spectrometry further supported the molecular structures with well-defined molecular ion peaks and expected fragmentation patterns. The synthetic strategy afforded high product yields (81–93%) under mild conditions, demonstrating the efficiency of the condensation approach. The structural diversity and ease of modification suggest that these Schiff bases represent valuable scaffolds for further biological evaluation and materials research.

***Keywords*:** Schiff bases, Methylpiperazine condensation, NMR, IR spectroscopy, Characterization.

*Corresponding Author DOI: 10.37094/adyujsci.1689333

Metilpiperazinden Türeyen Yeni Schiff Bazı Bileşiklerinin Sentezlenmesi ve Kapsamlı Analizi

Öz

Metilpiperazinden başlanarak çok basamaklı bir reaksiyon dizisiyle (esterleşme, hidrazid oluşumu ve çeşitli aromatik aldehitlerle kondenzasyon) yeni bir Schiff bazı türevleri serisi sentezlenmiştir. Elde edilen bileşikler (4a–g), FT-IR, ^{1}H NMR, ^{13}C NMR ve EI-MS spektroskopisi ile karakterize edilmiş ve bu analizler, imin (C=N) bağının başarılı bir şekilde oluştuğunu ve metoksi, hidroksil, halojen ve heteroaril gibi fonksiyonel grupların bileşiklere dahil edildiğini doğrulamıştır. Spektral veriler, Schiff bazı oluşumuyla uyumlu olarak karakteristik azometin proton sinyallerini (7.19–8.93 ppm) ve imin karbon gerilme bantlarını (1603–1623 cm^{-1}) ortaya koymuştur. Kütle spektrometrisi, belirgin moleküler iyon pikleri ve beklenen parçalanma desenleriyle moleküler yapıları desteklemiştir. Sentez stratejisi, ılımlı koşullar altında yüksek ürün verimleri (%81–93) sağlamış ve kondenzasyon yaklaşımının etkinliğini göstermiştir. Yapısal çeşitlilik ve modifikasyon kolaylığı, bu Schiff bazlarının biyolojik değerlendirme ve malzeme araştırmaları için değerli iskeletler olduğunu göstermektedir.

Anahtar Kelimeler: Schiff bazları, Metilpiperazin kondenzasyonu, NMR, IR spektroskopisi, karakterizasyon.

1. Introduction

Schiff bases are a highly versatile and significant class of organic compounds with a broad range of applications in medicinal chemistry, organic synthesis, and industrial chemistry. The term "Schiff base" originates from the work of Hugo Schiff, who in 1864 first described these compounds as the products of the condensation reaction between primary amines and carbonyl compounds (such as aldehydes or ketones), resulting in the substitution of the carbonyl group by an imine or azomethine group (–C=N–) [1, 2]. This fundamental reaction forms the basis for the synthesis of various Schiff bases, which are characterized by the general formula RHC=N–R1, where R and R1 can be alkyl, aryl, cycloalkyl, or heterocyclic groups, contributing to a wide diversity of chemical structures and properties [3, 4]. The nitrogen analogs of aldehydes and ketones, Schiff bases play an integral role in organic chemistry, particularly due to their ability to act as versatile intermediates for the synthesis of more complex molecules. They exhibit remarkable reactivity because of the electron-rich nitrogen atom and the conjugated double bond system, which allows for various chemical transformations [5]. This reactivity has been extensively harnessed in fields such as medicinal chemistry, where Schiff bases are frequently

utilized in the design of bioactive compounds, as well as in materials science for the development of functional materials like polymers and dyes [6].

Schiff bases are widely recognized for their diverse biological activities, which include anti-inflammatory, analgesic, antibacterial, antifungal, antiviral, antimalarial, and antipyretic properties [7, 8]. These biological effects are largely attributed to the presence of the imine group, which plays a critical role in their mode of action by enabling Schiff bases to interact with biological macromolecules such as enzymes and receptors. The azomethine linkage serves as an essential pharmacophore that facilitates the binding to active sites of enzymes or targets in living organisms, thereby influencing various biological pathways [9, 10]. Additionally, Schiff bases and their metal complexes have shown potent antiproliferative effects against various cancer cell lines, making them promising candidates in the development of new anticancer agents [11, 12]. The metal coordination ability of Schiff bases allows for the formation of stable complexes with transition metals, which can enhance their biological activity by increasing the lipophilicity and facilitating cellular uptake [13, 14].

The versatility of Schiff bases extends to their potential as enzyme inhibitors and their role in the treatment of neurodegenerative diseases. For instance, Schiff bases derived from natural aldehydes, such as cinnamaldehyde, have shown promising results as cholinesterase inhibitors, which are crucial in the management of Alzheimer's disease [15, 16]. Furthermore, Schiff bases with antioxidant properties have been explored for their neuroprotective effects in the treatment of diseases such as Parkinson’s and Huntington’s [17].

In addition to their biological significance, Schiff bases have substantial industrial applications. Their ability to form complexes with metal ions is extensively exploited in coordination chemistry for the development of homogeneous and heterogeneous catalysts [18, 19]. These metal-Schiff base complexes are particularly useful in various catalytic processes, including oxidation, hydrogenation, and polymerization reactions [20]. The catalytic activity is often enhanced by the presence of the imine group, which facilitates electron transfer processes, thus making Schiff base-metal complexes valuable in industrial chemical synthesis [21].

Schiff bases are also employed in material science for the synthesis of dyes and pigments due to their chromophoric properties. The azomethine linkage can stabilize the dye molecules and improve their lightfastness, making them suitable for various textile and industrial applications [22, 23]. In polymer chemistry, Schiff bases are used as curing agents and stabilizers due to their ability to form cross-linked networks with epoxy resins and other polymerizable materials [24]. Their utility as corrosion inhibitors is another noteworthy application, particularly in metal

surface treatments, where Schiff bases form protective films that prevent oxidation and degradation [25].

The structural diversity of Schiff bases can be attributed to the wide range of amine and carbonyl compounds available for their synthesis, leading to derivatives with varying degrees of saturation, aromaticity, and functional group substitutions. Such structural diversity facilitates the fine-tuning of their physicochemical and biological properties, enabling the design of Schiff bases tailored for specific applications [26]. The introduction of heteroatoms (e.g., sulfur or oxygen) and functional groups into Schiff base structures can further enhance their reactivity and coordination potential [27]. The incorporation of heterocyclic moieties, such as imidazole, pyridine, or quinoline, into Schiff base frameworks has been shown to improve their bioactivity by increasing target specificity and binding affinity [28].

The development of green synthetic methodologies for Schiff base synthesis is an area of growing interest, aiming to reduce the environmental impact of chemical processes. Recent advancements in solvent-free synthesis, microwave-assisted synthesis, and the use of renewable resources have significantly improved the sustainability of Schiff base production [29, 30]. These methods not only reduce the use of hazardous solvents but also improve reaction efficiency and yield.

In summary, Schiff bases are a crucial class of compounds in chemistry due to their extensive range of applications in medicinal, industrial, and synthetic chemistry. Their ability to act as ligands in coordination chemistry, bioactive agents in drug development, and versatile intermediates in organic synthesis highlights their importance. Future research will likely focus on the development of novel Schiff base derivatives with enhanced biological activity, improved synthetic methodologies, and new applications in emerging fields such as nanotechnology and materials science.

2. Materials and Methods

2.1. Experimental

All chemicals were obtained from Fluka Chemie AG, Buchs, Switzerland, and used as received without further purification. Melting points were determined in open capillaries using a Büchi B-540 melting point apparatus and are reported uncorrected. Reaction monitoring was conducted via thin-layer chromatography (TLC) on aluminum silica gel 60 F254 plates, with a mobile phase consisting of a 1:1 mixture of ethyl acetate and diethyl ether, and detection achieved under UV light. FT-IR spectra were recorded from potassium bromide pellets using a Perkin

Elmer 1600 series FTIR spectrometer. For NMR analysis, both ^{1}H and ^{13}C NMR spectra were acquired in DMSO-d6 on a Bruker Avance II 400 MHz spectrometer (operating at 400.13 MHz for ^{1}H and 100.62 MHz for ^{13}C NMR. Chemical shifts are given in parts per million (ppm) relative to tetramethylsilane (TMS), with coupling constants (J values) reported in hertz. Mass spectra were obtained using a Quattro EI-MS spectrometer at 70 eV.

Methyl (4-methylpiperazin-1-yl)acetate (2)

To a stirred solution of compound 1 (10 mmol) in tetrahydrofuran, triethylamine (20 mmol) was added slowly under ambient conditions. The mixture was stirred for an initial period to ensure thorough mixing. Following this, ethyl bromoacetate (10 mmol) was introduced dropwise to the reaction mixture over a span of several minutes, allowing for controlled addition. The reaction was then maintained at room temperature with continuous stirring for 24 hours to ensure complete conversion. After this period, the formation of a white precipitate was observed. The solid was separated by filtration, and the filtrate was concentrated by evaporating the solvent to yield the crude product.

Yie1d: % 89, m.p: 85-87°C. FT IR (υmax, cm^{-1}): 1734 (C=O). ^{1}H NMR (DMSO-*d6*, δ ppm): 1.1 7- 1.20 (3H, m, CH_3), 1.99 (4H, s, $2CH_2$), 2.14 (2H, s, CH_2), 2.30 (2H, s, CH_2), 3. 17 (2H, s, CH_2), 3.39 (2H, s, CH_2), 4.06-4.10 (3H, m, CH_3). ^{13}CNMR (DMSO-d6, δ ppm): l4.57 (CH_3), 46.17 (CH_3), 53.24 (CH_2), 55.06 (CH_2), 58.98 (CH_2), 60.20 (CH_2), 63.93 (CH_2), 170.36 (C=O). EI MS m/z (%):173.25 ($[M+1]^+$, 100), 195.40 ($[M+Na]^+$, 70).

2-(4-methylpiperazin-1-yl)acetohydrazide (3)

Hydrazine hydrate (25 mmol) was added to a solution of compound 2 (10 mmol) in ethanol, and the mixture was heated under reflux for 15 hours. After cooling, the reaction mixture was stored overnight at low temperature, resulting in the formation of a white solid. The precipitate was collected by filtration, and the crude product was further purified by recrystallization from 2:1 ethanol/water mixture.

Yield: % 85, m.p: 134-136°C. FTIR (υmax, cm^{-1}): 1734 (C=O). ^{1}HNMR (DMSO-*d6*, δ ppm): 2.14 (3H, s, CH_3), 2.30 (2H, s, CH_2), 2.40 (4H, s, $2CH_2$),0 2.88 (4H, s, $2CH_2$), 3.75 (2H, brs, NH_2), 8.84 (1H, s, NH). ^{13}C NMR (DMSO-d6, δ ppm): 46.20 (CH_3), 53.21 ($2CH_2$), 55.01 ($2CH_2$), 60.37 (CH_2), 168.69 (C=O). EI MS m/z (%): 173.89 ($[M+1]^+$, l00), 195.75 ($[M+Na]^+$,75).

General method for the synthesis of compounds 4a–g

Compound 2 (10 mmol) and a suitable aldehyde (10 mmol) were mixed in absolute ethanol and refluxed for 3 hours with continuous stirring. After cooling to room temperature, a white solid formed. The crude product was collected by filtration and purified through recrystallization using a 1:2 mixture of dimethyl sulfoxide and water. The final product was obtained by filtering, washing, and drying the recrystallized solid.

***N*'-[(1*Z*)-(4-methoxyphenyl)methylene]-2-(4-methylpiperazin-1-yl)aceto hydrazide (4a)**

FT IR (υmax, cm^{-1}): 3089 (aromatic CH), 3215 (NH), 2943 (azomethine C-H) 1711 (C=O), 1603 (C=N), 1141 (-OCH_3). ^{1}H NMR (DMSO-*d6*, δ ppm): 2.19 (3H, s, CH_3), 2.21 (3H, d, *J*= 4.0 Hz, CH_3), 2.45 (2H, s, CH_2),2.61 (2H, s, CH_2), 2.91 (2H, s, CH_2),3.07 (2H, s, CH_2), 3.52 (2H, s, CH_2),7.79 (1H, s, Ar-H), 7.81 (1H, s, Ar-H), 7.93 (1H, s, Ar-H), 8.28 (1H, s, Ar-H), 8.62 (1H, s, CH), 11.21 (1H, s, NH). ^{13}C NMR (DMSO-d6, δ ppm): 14.50 (CH_3), 47.85 (CH_2), 49.41 (CH_3), 50.10 (CH_2), 51.27 (CH_2), 53.78 (CH_2), 56.70 (CH_2), 110.51 (CH), ArC: [112.74 (CH), 126.85 (CH), 127.89 (CH), 129.90 (CH), 133.45 (C), 140.41 (C)], 170.12 (C=O). EI MS m/z (%): 291.45 ($[M+1]^+$, 100), 188.45 (85), 179.33 (71), 125.10 (55).

***N*'-[(1*Z*)-(4-fluorophenyl)methylene]-2-(4-methylpiperazin-1-yl)aceto hydrazide (4b)**

FT IR (υmax, cm^{-1}): 3077 (aromatic CH), 3218 (NH), 2955 (azomethine C-H), 1722 (C=O), 1607 (C=N). ^{1}H NMR (DMSO-d6, δ ppm): 2.15 (3H, s, CH_3), 2.41 (2H, s, CH_2), 3.11 (2H, s, CH_2), 3.34 (2H, s, CH_2), 3.60 (2H, s, CH_2), 5.07 (2H, s, CH_2), 6.77 (2H, d, *J*= 8.0 Hz, Ar-H), 6.90 (2H, d, *J*= 8.0 Hz, Ar-H), 7.19 (1H, s, CH), 7.96 (1H, s, NH). ^{13}C NMR (DMSO-d6, δ ppm): 15.10 (CH_3), 48.62 (CH_2), 49.11 (CH_2), 50.78 (CH_2), 51.21 (CH_2), 52.55 (CH_2), 112.21 (CH), ArC: [113.78 (CH), 114.52 (CH), 115.06 (CH), 116.89 (CH), 128.52 (C), 131.70 (C)], 175.89 (C=O). EI MS m/z (%): 279.58 ($[M+1]^+$, 100), 210.11 (85), 191.25 (71), 142.52 (51).

N'-[(1*Z*)-1*H*-indol-3-ylmethylene]-2-(4-methylpiperazin-1-yl)acetohydrazide (4c)

FT IR (υmax, cm^{-1}): 3081 (aromatic CH), 3215 (NH), 2978 (azomethine C-H), 1703 (C=O), 1621 (C=N). ^{1}H NMR (DMSO-*d6*, δ ppm): 2.19 (3H, s, CH_3), 2.91 (2H, s, CH_2), 3.07 (2H, s, CH2), 3.46 (4H, s, $2CH_2$), 3.62 (2H, s, CH_2), 7.49 (2H, d, *J*= 8.0 Hz, Ar-H), 8.37 (2H, d, *J*= 8.0 Hz, Ar-H), 8.93 (1H, s, CH), 10.82 (1H, s, NH), 11.71 (1H, s, NH). ^{13}C NMR (DMSO-d6, δ ppm): 17.44 (CH_3), 47.21 (CH_2), 48.44 (CH_2), 49.70 (CH_2), 50.51 (CH_2), 51.47 (CH_2), 109.41 (CH), 111.20 (CH), ArC: [113.47 (CH), 115.51 (CH), 116.78 (CH), 120.14 (CH), 125.47 (C), 129.56 (C)], 173.41 (C=O). EI MS m/z (%): 300.78 ($[M+1]^+$, 100), 273.52 (79), 198.76 (52), 103.47 (33).

N'-[(1*Z*)-(2-hydroxyphenyl)methylene]-2-(4-methylpiperazin-1-yl)acetohydrazide (4d)

FT IR (υmax, cm^{-1}): 3411 (OH), 3065 (aromatic CH), 3209 (NH), 2966 (azomethine C-H), 1721 (C=O), 1516 (C=N). ^{1}H NMR (DMSO-*d6*, δ ppm): 2.08 (3H, s, CH_3), 2.27 (4H, s, $2CH_2$), 3.12 (2H, s, CH_2), 3.41 (4H, s, $2CH_2$), 6.95 (2H, m, Ar-H), 7.68-7.71 (2H, m, Ar-H), 8.52 (1H, s, CH), 9.00 (1H, s, NH), 11.34 (1H, s, OH). ^{13}C NMR (DMSO-d*6*,δ ppm): 15.12 (CH_3), 46.52 (CH_2), 47.41 (CH_2), 48.79 (CH_2), 50.51 (CH_2), 51.79 (CH_2), 106.45 (CH), ArC: [112.87 (CH), 118.09 (CH), 121.45 (CH), 136.47 (C), 137.82 (C)], 177.52 (C=O). EI MS m/z (%): 277.59 ([M+1]+, 100), 214.89 (89), 191.03 (71), 155.40 (49).

N'-[(*E*)-(4-chlorophenyl)methylidene]-2-(4-methylpiperazin-1-yl)aceto hydrazide (4e)

FT IR (υmax, cm^{-1}): 3039 (aromatic CH), 3209 (NH), 2981 (azomethine C-H), 1718 (C=O), 1519 (C=N), 861 (-C-Cl). ^{1}H NMR (DMSO-*d6*, δ ppm): 2.33 (3H, s, CH_3), 2.50 (2H, s, CH_2), 2.54 (2H, s, CH_2), 2.66 (2H, s, CH_2), 2.68 (2H, s, CH_2), 3.21 (2H, s, CH_2), 7.25 (2H, s, Ar-H), 7.44 (2H, s, Ar-H), 7.59 (1H, s, CH), 8.73 (1H, s, NH). ^{13}C NMR (DMSO-*d6*, δ ppm): 18.25 (CH_3), 49.02 (CH_2), 49.78 (CH_2), 50.08 (CH_2), 50.97 (CH_2), 52.63 (CH_2), 110.74 (CH), ArC: [112.70 (CH), 113.40 (CH), 114.96 (CH), 119.56 (CH), 130.02 (C), 132.89 (C)], 172.88 (C=O). EI MS m/z (%): 295.78 ($[M+1]^+$, 100), 210.11 (78), 172.02 (42).

N'-[(*E*)-(5-methylfuran-2-yl)methylidene]-2-(4-methylpiperazin-1-yl)aceto hydrazide (4f)

FT-IR (υmax, cm^{-1}): 3289 (furan CH), 3178 (NH), 2973 (azomethine C-H), 1709 (C=O), 1610 (C=N). ^{1}H NMR (DMSO-*d6*, δ ppm): 2.14 (3H, s, CH_3), 2.34 (3H, s, CH_3), 2.52 (2H, s, CH_2), 2.54 (2H, s, CH_2), 2.68 (2H, s, CH_2), 2.74 (2H, s, CH_2), 3.17 (2H, s, CH_2), 6.36 (1H, s, furan-H), 6.50 (1H, s, furan-H), 7.97 (1H, s, CH), 8.13 (1H, s, NH). ^{13}C NMR (DMSO-*d6*, δ ppm): 19.56 (CH_3), 30.45 (CH_3), 47.41 (CH_2), 48.63 (CH_2), 49.55 (CH_2), 50.08 (CH_2), 51.78 (CH_2), 111.03 (CH), ArC: [118.42 (CH), 119.07 (CH), 132.78 (C), 135.44 (C)], 171.10 (C=O). EI MS m/z (%): 265.89 ($[M+1]^+$, 100), 188.10 (89), 112.25 (56).

2-(4-methylpiperazin-1-yl)-N'-[(1*E*)-2-phenylethylidene]acetohydrazide (4g)

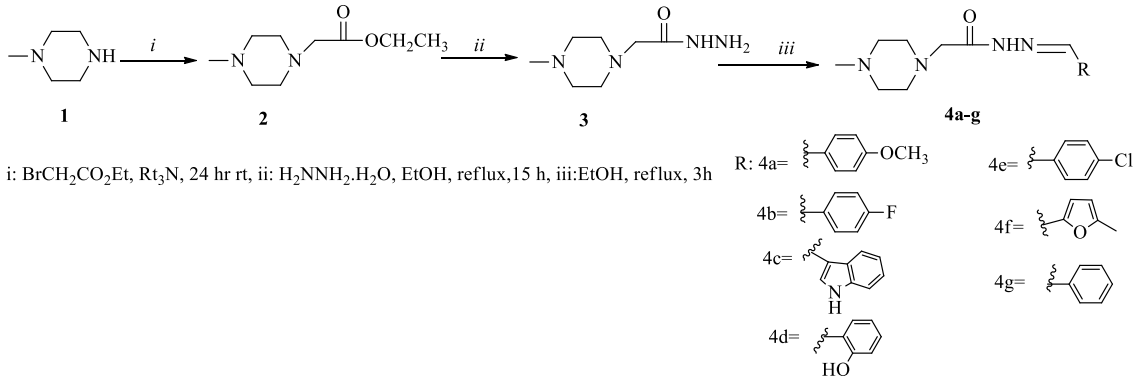
FT IR (υmax, cm-1): 3041 (aromatic CH), 3209 (NH), 2989 (azomethine C-H), 1785 (C=O), 1623 (C=N). ^{1}H NMR (DMSO-*d6*, δppm): 2.31 (3H, s, CH_3), 2.45 (2H, s, CH_2), 2.53 (2H, s, CH_2), 2.65 (2H, s, CH_2), 2.67 (2H, s, CH_2), 3.24 (2H, s, CH_2), 3.59 (2H, s, CH_2), 7.26 (2H, s, Ar-H), 7.39 (3H, s, Ar-H), 7.46 (1H, s, CH), 9.21 (1H, s, NH). ^{13}C NMR (DMSO-*d6*, δ ppm):

20.03 (CH_3), 30.90 (CH_2), 48.78 (CH_2), 49.09 (CH_2), 49.89 (CH_2), 50.60 (CH_2), 51.44 (CH_2), 112.52 (CH), ArC: [118.90 (CH), 120.52 (CH), 122.70 (CH), 123.03 (CH), 129.36 (CH), 134.70 (C)], 173.88 (C=O). EI MS m/z (%):275.78 ($[M+1]^+$, 100), 200.06 (80), 187.36 (55).

3. Results and Discussion

In this study, we aimed to synthesize a series of novel Schiff base compounds, starting from the precursor methylpiperazine. The synthetic pathway was designed to introduce specific functional groups through sequential reactions, leading to the formation of the desired imine structures. The characterization and confirmation of the chemical structures of the final products were carried out using a combination of spectroscopic techniques. The ^{1}H NMR and ^{13}C NMR spectra provided detailed information on the chemical environment and connectivity of the hydrogen and carbon atoms in the molecules. FT-IR spectroscopy was employed to identify the characteristic functional groups, including the imine (C=N) stretch, which is a key feature of Schiff bases. Additionally, electron impact mass spectrometry (EI-MS) was utilized to determine the molecular weights and fragmentation patterns, further confirming the structures of the synthesized compounds.

The synthetic routes undertaken, including the starting materials, reaction conditions, and the formation of intermediate and final products, are outlined in Scheme 1, which illustrates the stepwise synthesis of the target Schiff base compounds. This approach allowed for systematic modification and optimization of the reaction steps to achieve the desired molecular architecture.



Scheme 1: Scheme of the preparation of Schiff's bases from Methylpiperazine

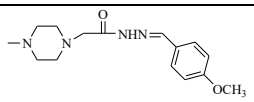
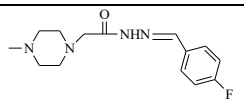
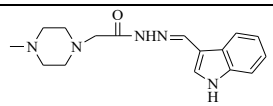
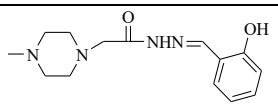
In this study, a series of Schiff bases (4a-g) were synthesized through the refluxing of methylpiperazine with various aromatic aldehydes in ethanol as the solvent. The reactions were carried out under controlled conditions to ensure complete condensation between the amine and aldehyde, forming the characteristic imine (C=N) linkage of Schiff bases. The process yielded

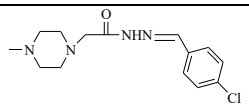
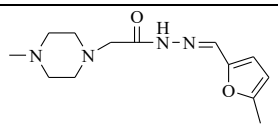
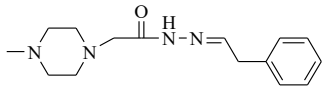
high-efficiency results, with isolated product yields ranging from 81% to 93%, demonstrating the effectiveness of the synthetic approach employed [31].

The structural characterization of the synthesized compounds was performed using multiple spectroscopic techniques to confirm their identity and purity. ^{1}H NMR and ^{13}C NMR spectroscopy provided detailed information on the chemical shifts and coupling patterns of the hydrogen and carbon atoms, indicating the presence of the expected functional groups and confirming the formation of the imine bond. Infrared (IR) spectroscopy further corroborated the presence of key functional groups, such as the C=N stretch characteristic of Schiff bases, along with other absorption bands associated with aromatic rings and methyl groups. Additionally, mass spectrometry (EI-MS) was employed to determine the molecular weight and fragmentation patterns of each compound, providing further evidence for the successful synthesis of the target molecules. The spectroscopic data indicated that not only the Schiff bases (4a-g) but also the intermediate compounds (2 and 3) were synthesized with high efficiency and in accordance with the expected structures. These findings were consistent across all analytical techniques, confirming the integrity of the synthetic process.

Table 1 presents a comprehensive summary of the physical properties, such as melting points, and analytical data, including elemental analysis, for the Schiff bases (4a-g), highlighting the consistency and reproducibility of the synthesized products. This information provides a thorough understanding of the compounds' characteristics and supports the successful synthesis of the desired Schiff bases.

Table 1: New Schiff base compounds (4a-g)

Compound no	Molecular Formula	Melting Point (^{0}C)	Yield (%)
4a		79-81	81
4b		110-112	89
4c		115-117	84
4d		93-95	88

4e		105-107	80
4f		77-79	90
4g		122-124	93

The infrared (IR) spectroscopy analysis of the synthesized Schiff bases revealed characteristic absorption peaks that provided valuable insights into the functional groups present in the compounds. Key absorption bands were observed in the IR spectra at approximately 3020, 2960, 1620, 1480, and 1330 cm^{-1} which were indicative of specific chemical bonds. The bands at around 3020 and 2960 cm^{-1} corresponded to the stretching vibrations of aromatic C–H bonds, confirming the presence of aromatic rings within the molecular structure [32]. The absorption peak at 1620 cm-1 was assigned to the azomethine (C=N) stretch, which is a defining feature of Schiff bases, indicating successful formation of the imine linkage during the condensation reaction. Additionally, bands at 1480 and 1330 cm^{-1} were associated with other aromatic and imine vibrations, further validating the structure of the synthesized compounds.

The stretching frequency of the aromatic C–H group contributed to the absorption bands located between 3039 and 3089 cm-1, showing minor variations across different Schiff base derivatives, likely due to the electronic effects of various substituents on the aromatic ring. In the case of compound 4a, a strong absorption band was detected at approximately 1141 cm^{-1} which was attributed to the stretching vibration of the methoxy (CH_3O–) group, confirming its presence as a substituent on the aromatic system.

Compound 4d exhibited a significant broad absorption band at 3411 cm^{-1}, which was due to the O–H stretching vibration, indicating the presence of a hydroxyl group in the structure. This strong and broad band confirmed the characteristic stretching frequency associated with the hydroxyl functionality, distinguishing compound 4d from other derivatives.

For compound 4e, a distinct absorption peak was observed at around 861 cm^{-1}, which corresponded to the C–Cl stretching vibration, confirming the incorporation of a chloro substituent in the molecule. This band was prominent and fell within the expected range for alkyl halide stretching vibrations, supporting the successful introduction of the chlorine atom as part of the Schiff base structure. Overall, the IR spectroscopic data for all synthesized Schiff bases

matched the expected range for the functional groups present in the molecules, thereby confirming the successful synthesis of the target compounds. A detailed summary of the IR absorption bands and their corresponding functional groups is provided in Table 2, illustrating the consistency of the spectroscopic findings with the predicted molecular structures.

Table 2: IR spectral data (cm^{-1})

Compound no	Aromatic CH	Azomethine C-H	C=N
4a	3089	2943	1603
4b	3077	2955	1607
4c	3081	2978	1621
4d	3065	2966	1616
4e	3039	2981	1619
4g	3041	2989	1623

The ^{1}H NMR spectroscopic analysis of the synthesized Schiff bases provided further confirmation of their chemical structures, with characteristic signals corresponding to the various functional groups. A key feature observed in the ^{1}H NMR spectra was a singlet appearing in the range of 7.19–8.93 ppm, which had an integration intensity corresponding to a single proton. This signal was attributed to the azomethine proton (–CH=N–), confirming the presence of the imine linkage that is central to the structure of Schiff bases [33]. The chemical shift of the azomethine proton varied slightly among different Schiff base derivatives, likely due to the electronic effects exerted by substituents on the aromatic rings or other functional groups in the vicinity, which can influence the deshielding of the imine proton.

The aromatic protons appeared as multiple peaks distributed between 6.67 and 8.37 ppm, indicating the presence of different aromatic environments within the molecules. These multiplet signals were consistent with the protons attached to the benzene ring or substituted aromatic systems. The exact chemical shifts of the aromatic proton signals varied depending on the nature and position of substituents on the ring, which can affect the electron density and result in slight upfield or downfield shifts. The complex pattern of these peaks reflected the various coupling interactions between neighboring protons, providing insights into the aromatic substitution pattern and confirming the structural features of each Schiff base derivative.

The synthesized Schiff bases (4a–g) can theoretically exist as *E* or *Z* isomers with respect to the C=N double bond. The stereochemistry of the imine bond was assigned based on spectroscopic data and literature precedents. In general, the *E* configuration is favored due to steric repulsion minimization between the azomethine hydrogen and the substituents on the

aromatic ring. In some cases, intramolecular hydrogen bonding (e.g., between –NH and –OH groups in compound 4d, or between –NH and heteroatoms in 4c and 4f) stabilizes the *Z* isomer, which is reflected in the downfield shift of the azomethine proton in the ^{1}H NMR spectra. Therefore, the observed isomerism of compounds 4a–g has been designated as *E* or *Z* according to the relative stability supported by the spectral evidence and substituent effects.

Additionally, the methyl protons of the methylpiperazine moiety (N-CH_3) were clearly identified in the ^{1}H NMR spectra, appearing as distinct peaks in the range of 2.08–2.33 ppm. These signals were relatively sharp, reflecting the protons attached to the nitrogen atom in the piperazine ring. The presence of these peaks in the specified region was consistent across all Schiff base derivatives, indicating the successful incorporation of the methylpiperazine unit into the molecular framework.

Overall, the ^{1}H NMR spectral data provided strong evidence supporting the successful synthesis and structural integrity of the Schiff bases. The characteristic signals for the azomethine, aromatic, and methylpiperazine protons matched the expected chemical shift ranges, thus confirming the identity of the synthesized compounds.

4. Conclusion

This research demonstrates the successful and efficient synthesis of a series of novel Schiff base compounds, achieved through the condensation of methylpiperazine with various aromatic aldehydes. The synthesized compounds were thoroughly characterized using multiple spectroscopic techniques to confirm their chemical structures and establish their purity. The structural elucidation was performed using infrared (IR) spectroscopy, ^{1}H NMR and ^{13}C NMR nuclear magnetic resonance (NMR) spectroscopy, as well as mass spectrometry, each providing complementary information that confirmed the identity and composition of the new compounds.

IR spectroscopy was employed to identify key functional groups present in the molecules, with characteristic absorption bands corresponding to the azomethine (C=N) stretch, aromatic C–H stretching vibrations, and other functional groups such as methoxy, hydroxyl, or halide substituents. These absorption peaks were in line with the expected spectral features of Schiff bases and indicated successful formation of the imine linkage. The ^{1}H NMR spectra provided further insights, with distinct singlets corresponding to the azomethine protons observed between 7.19 and 8.93 ppm, confirming the formation of the imine bond in each compound. The aromatic

protons appeared as multiple signals across the 6.67–8.37 ppm range, reflecting the complex aromatic environments present in the Schiff bases.

Additionally, the methylpiperazine protons were detected in the 2.08–2.33 ppm range, supporting the inclusion of the piperazine moiety in the structure. ^{13}C NMR spectra complemented these findings by revealing the carbon environments, including signals for the azomethine carbon and aromatic carbons, further verifying the molecular framework of the synthesized compounds.

Mass spectrometry was utilized to determine the molecular weights and fragmentation patterns of the Schiff bases, providing additional confirmation of the molecular composition. The molecular ion peaks observed in the spectra matched the calculated molecular weights of the compounds, supporting the accuracy of the synthesized structures. Fragmentation patterns were consistent with the expected breakdown of the molecular structure, giving further evidence for the formation of the intended Schiff bases.

All the spectroscopic data, including ^{1}H NMR and ^{13}C NMR spectra, have been compiled and presented as supplementary information, providing a detailed overview of the spectral characteristics and ensuring the reproducibility of the results. This supplementary data serves as a comprehensive reference for the synthesized Schiff base compounds, offering valuable insights into their structural features and confirming the success of the synthetic methodology used in this study.

Acknowledgements

The author has no received any financial support for the research, authorship or publication of this study.

References

[1] Schiff, H., *Mittheilungen aus dem Universitätslaboratorium in Pisa: Eine neue Reihe organischer Basen*, Justus Liebigs Annalen der Chemie, 131(1), 118-119, 1864.

[2] Ali, M.A., Mirza, A.H., *Schiff bases and their coordination chemistry*, Coordination Chemistry Reviews, 23, 329-345, 1977.

[3] Araujo, E. L., Barbosa, H. F. G., Dockal, E. R., & Cavalheiro, É. T. G. Synthesis, characterization and biological activity of Cu (II), Ni (II) and Zn (II) complexes of biopolymeric Schiff bases of salicylaldehydes and chitosan. International journal of biological macromolecules, 95, 168-176, 2017

[4] Singh, K., Barwa, M.S., Tyagi, P., *Synthesis, characterization and biological activity of Schiff bases and their transition metal complexes: a review*, Journal of Scientific & Industrial Research, 66, 180-190, 2007.

[5] Harikrishnan, P., Kamaraj, P., *Schiff base metal complexes as versatile catalysts in organic synthesis*, Journal of Organometallic Chemistry, 754, 1-14, 2014.

[6] Mishra, A.P., Gupta, S., Bhatt, I.D., *Role of Schiff bases in organic chemistry: synthesis and applications,* Current Organic Chemistry, 20(6), 669-677, 2016.

[7] Shukla, P., Singh, H., *Schiff bases and their metal complexes as anti-inflammatory agents*, International Journal of Chemical and Pharmaceutical Sciences, 4(1), 1-9, 2013.

[8] Kumar, M., Kumar, A., *Synthesis of Schiff base derivatives and their biological applications: a review*, International Journal of Chemical Studies, 4(2), 29-33, 2016.

[9] Ramachandran, E., Janarthanan, S., *Review on imine metal complexes: synthesis and applications*, International Journal of Chemical Technology Research, 3(2), 812-817, 2011.

[10] Dhar, D.N., Taploo, C.L., *Schiff bases and their applications*, Journal of Scientific & Industrial Research, 41, 501-506, 1982.

[11] Zaki, M.E.A., Hashish, N.E., Killa, H.M., *Antimicrobial activity of Schiff bases derived from some drugs*, Il Farmaco, 61(1), 739-747, 2006.

[12] Ali, H., Rizvi, S.A.A., *Biological screening of Schiff bases of indole derivatives*, Acta Poloniae Pharmaceutica - Drug Research, 67(5), 539-546, 2010.

[13] Gupta, K.C., Sutar, A.K., *Catalytic activities of Schiff base transition metal complexes*, Coordination Chemistry Reviews, 252(12-14), 1420-1450, 2008.

[14] Patel, R.N., Patel, P.H., *Schiff bases: applications in organic chemistry and metal complex formation*, International Journal of Organic Chemistry, 1(2), 67-72, 2011.

[15] How, F.N.F., Heng, W.W*., Schiff bases as cholinesterase inhibitors: a review*, Journal of Enzyme Inhibition and Medicinal Chemistry, 34(1), 1334-1345, 2019.

[16] Sobolewski, M., Skibinski, R., *Schiff bases in the development of neuroprotective agents*, Current Medicinal Chemistry, 22(25), 2985-3006, 2015.

[17] Chevalier, A., Amara, S., *Antioxidant properties of Schiff bases: potential therapeutic implications in neurodegenerative disorders,* Bioorganic & Medicinal Chemistry Letters, 27(4), 816-821, 2017.

[18] Al Zoubi, W. and Ko, Y. G. *Organometallic complexes of Schiff bases: Recent progress in oxidation catalysis*, Journal of Organometallic Chemistry, 822, 173-188, 2016.

[19] Kabeer, T.K.A., Khan, S., *Schiff base complexes: versatile catalysts for various organic reactions*, Current Catalysis, 6(1), 33-53, 2017.

[20] Taghizadeh, S., Valiollahzadeh, S., *Schiff base-metal complexes as catalysts in organic synthesis*, RSC Advances, 8, 24610-24627, 2018.

[21] Jahromi, H.R., Majidnia, Z., *Applications of Schiff bases in the synthesis of pharmaceuticals*, Journal of Chemical Research, 39(5), 257-265, 2015.

[22] Çetinkaya, E., Zengin, A., *Synthesis and application of azo-Schiff base dyes*, Dyes and Pigments, 54(2), 115-123, 2002.

[23] Mathur, A., Mathur, P., *Dyes based on Schiff bases*, Coloration Technology, 117(6), 324-330, 2001.

[24] Diallo, K., Lecomte, P., *Schiff base polymers and materials: a review*, Polymer Chemistry, 7(13), 2341-2361, 2016.

[25] Popoola, L.T., Fayomi, O.S.I., *Schiff bases as corrosion inhibitors for metals in acidic media: a review*, International Journal of Electrochemical Science, 10, 1747-1770, 2015.

[26] Thakuria, H., Nath, R., *Synthetic strategies and biological activities of Schiff bases*, Asian Journal of Chemistry, 26(12), 3607-3620, 2014.

[27] Sousa, G.F., Magalhães, A.J., *Recent developments in the synthesis and applications of sulfur-containing Schiff bases*, Journal of Sulfur Chemistry, 33(3), 271-279, 2012.

[28] Mente, S.R., Pratap, R., *Schiff bases containing heterocycles as biologically important motifs,* Mini-Reviews in Medicinal Chemistry, 15(10), 813-827, 2015.

[29] Varma, R.S., Dahiya, R., *Microwave-assisted green synthesis of Schiff bases*, Green Chemistry, 4(1), 41-43, 2002.

[30] Khurana, J.M., Mehta, S., *Solvent-free synthesis of Schiff bases*, Synthetic Communications, 39(6), 1041-1050, 2009.

[31] Rao, R.V.K., Reddy, S.S., Krishna, B.S., Naidu, K.R.M., Raju, C.N., Ghosh, S.K., *Synthesis of Schiff's bases in aqueous medium: a green alternative approach with effective mass yield and high reaction rates*, Green Chemistry Letters and Reviews, 3(3), 217-223, 2010.

[32] Salonen, L.M., Ellermann, M., Diederich, F., *Aromatic rings in chemical and biological recognition: energetics and structures*, Angewandte Chemie International Edition, 50(21), 4808-4842, 2011.

[33] Moanta, A., *Classification, synthesis, isomerism, and spectral characterization of Schiff bases*, Mini-Reviews in Organic Chemistry, 2025.