Synthesis and Spectral Characterization of a Novel Indole-Pyrazole-Based Schiff Base

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Abstract

In order to integrate two biologically relevant heterocycles—indole and pyrazole—a novel Schiff base, (E)-N-(2-(1H-indol-3-yl) ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl) methanimine (IPM), was synthesized and thoroughly characterized. 1-(4-chlorophenyl)-1H-pyrazole-4-carbaldehyde and 2-(1H-indol-3-yl)ethan-1-amine underwent a condensation reaction to accomplish the synthesis, which produced IPM with 83% efficiency. The structure and purity of the compound have been confirmed through elemental analysis, mass spectrometry, FT-IR, UV-Vis, and NMR spectroscopy. The ^{1}H NMR spectrum revealed characteristic signals for the indole N–H, imine (C=N), aromatic protons, and ethyl linker. FT-IR analysis confirmed the presence of the azomethine linkage and characteristic vibrational modes of the aromatic systems. Indicative of prolonged conjugation between the indole, pyrazole, and imine units, UV-Vis spectroscopy revealed absorption bands corresponding to π-π* and n-π* transitions. The suggested molecular formula was supported by the ESI-MS spectrum, which showed a molecular ion peak at m/z 348.11 in addition to an isotopic pattern characteristic to chlorine. The successful synthesis and detailed characterization of IPM set the groundwork for future investigations into its potential applications in drug discovery and catalysis.
Keywords- *Schiff, Methanimine, Imine, Fragmentation*

1. Introduction

Schiff bases are a diverse class of molecules with a wide range of uses in coordination chemistry, organic synthesis, and medical research. They are distinguished by the presence of an azomethine (-C=N-) functional group (Manvatkar et al., 2023; More et al., 2019). Their structural diversity, ease of synthesis, and capability to form stable complexes along with metal ions have made them a subject of extensive investigation (Murugavel et al., 2008; Yuan et al., 2018). Of particular interest are Schiff bases that incorporate heterocyclic scaffolds, as these often exhibit enhanced biological and physicochemical properties. Indole and pyrazole, two pharmacologically significant heterocycles, are well-documented for their contributions to the biological activity of many natural and synthetic compounds (Mallappa et al., 2024; Mustafa et al., 2022).

Indole, a bicyclic system containing a benzene ring fused to a pyrrole, is a privileged pharmacophore found in a variety of bioactive molecules (Mustafa et al., 2022). Because of its ability to engage in hydrogen bonding, π-π stacking interactions, and cation-π interactions, which enable strong binding to biological targets, it is essential to drug development (Mahadevi et al., 2013; Zhou et al., 2025). Pyrazole, a five-membered heterocyclic ring having two nitrogen atoms, is equally important, especially when substituted with electron-withdrawing groups such as 4-chlorophenyl (Singh et al., 2020; Faisal et al., 2019). These substitutions enhance the electronic properties and bioactivity of the pyrazole framework, making it a valuable component in designing drug candidates with diverse pharmacological profiles (Yuan et al., 2018; Mahadevi et al., 2013; Faisal et al., 2019; Murugavel et al., 2008).

1-(1H-indol-3-yl) ethyl (E)-N-(2-)-1H-pyrazol-4-yl (1-(4-chlorophenyl)-1). These two important heterocyclic motifs are combined in the new Schiff base methanimine. This compound was designed to explore the synergistic effects of indole and pyrazole on the compound's structural, electronic, and potential biological properties. The indole part contributes to the molecule's capability to engage in key non-covalent contacts, while the pyrazole ring, with its electron-withdrawing chlorophenyl group, enhances stability and furnishes a favorable electronic environment (Yuan et al., 2018; Mahadevi et al., 2013; Faisal et al., 2019; Citarella et al., 2023). These characteristics make the compound an excellent

candidate for further investigation in drug discovery and catalysis (Manvatkar et al., 2023; More et al., 2019; Murugavel et al., 2008; Yuan et al., 2018; Mahadevi et al., 2013; Faisal et al., 2019; Citarella et al., 2023; Wang et al., 2024).

A comprehensive characterization has been completed using analytical approaches to better understand this Schiff base's molecular geometry and properties. Mass spectrometry furnished insights into the molecular weight and fragmentation patterns of the compound, demonstrating its structural integrity. Nuclear magnetic resonance (NMR) spectroscopyelucidates the connectivity and electronic environment of the atoms within the molecule. IR (Infrared) spectroscopy has been executed to identify functional groups and confirm the presence of the characteristic azomethine (-C=N-) bond, while UV-Vis (ultraviolet-visible) spectroscopy enabled the evaluation of the compound's electronic transitions and chromophoric behavior. Elemental analysis complemented these techniques by verifying the compound's purity and stoichiometry.

The combination of various characterization methods promoted a careful examination of the electrical and structural characteristics of the chemical. In addition to providing a basic grasp of (E)-N-(2-(1H-indol-3-yl)ethyl),-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine, but also establishes the framework for examining its possible uses.. Future studies may focus on leveraging its structural properties in developing novel therapeutic agents, catalysts, or materials with specialized functionalities.

2. Methods and Materials

2.1. Methods

A Perkin-Elmer FT-IR spectrometer was used to investigate the FT-IR spectra of (E)-N-(2-(1H-indol-3-yl)ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM) at 25 °C in order to determine the functional groups and vibrational modes present in the molecule.The structural details of the carbon and hydrogen atoms were examined using 1H NMR spectroscopy on a Bruker AVANCE-III spectrometer. With a 1 nm bandwidth and a spectral range of 200 to 600 nm, UV-Vis spectroscopy using a Perkin-Elmer Lambda 35 spectrometer revealed information about the compound's electronic absorption properties. A WATERS Q-ToF Premier Mass Spectrometer was used for mass spectrometric analysis using electrospray ionization (ESI-MS), which made it easier to determine the molecular ion and fragmentation behavior. Furthermore, a Perkin-Elmer 2400 Series II CHNS/O Analyzer verified the compound's elemental composition, guaranteeing that it matched theoretical values.

2.2 Materials

Every reagent utilized in the production of (E)The ethyl (N-(2-(1H-indol-3-yl))Sigma-Aldrich provided the -1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM), which was used straight into the reaction without going through any further purification procedures.

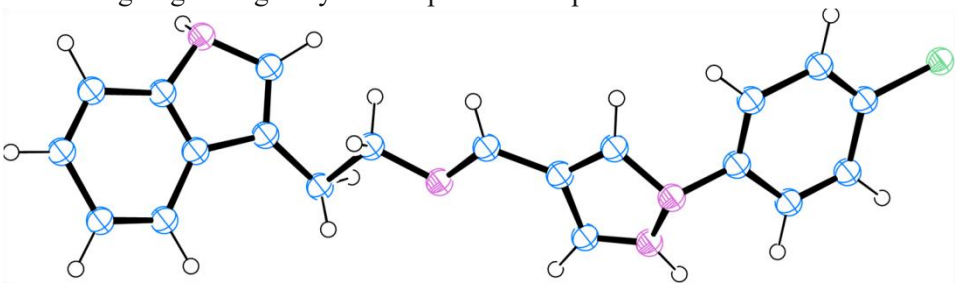

Fig. 1 Structure of (E)-N-(2-(1H-indol-3-yl)ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM)

3. Results and discussion

3.1 Synthesis of (E)-N-(2-(1H-indol-3-yl)ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM)

As shown in Fig. 1.1, 1-(4-chlorophenyl)-1H-pyrazole-4-carbaldehyde (1) and 2-(1H-indol-3-

yl)ethan-1-amine (2) were reacted to create IPM. First, 20 mL of methanol was used to dissolve 0.50 g (3.12 mmol) of 2-(1H-indol-3-yl)ethan-1-amine. 0.64 g (3.09 mmol) of 1-(4-chlorophenyl)-1H-pyrazole-4-carbaldehyde was added to this mixture. A pale yellow precipitate appeared when the volume of the solution dropped to 10 mL during the five hours while the reaction mixture was refluxed. After filtering off the precipitate, it was successively cleaned with 10 mL of hexane and 5 mL of cold methanol (Jamal et al., 2024; Jamal et al., 2025).

After being recrystallized from methanol, the solid product was vacuum-dried. The final IPM product, which weighed.95 g and had an 83% yield, was a yellow solid. The elemental analysis of IPM revealed the following results: C, 68.86%; H, 4.91%; Cl, 10.16%; N, 16.06% were the calculated values, while C, 68.76%; H, 4.81%; Cl, 10.11%; N, 16.01% were the experimental (found) values. Nonetheless, Fig. 1 illustrates the IPM structure.

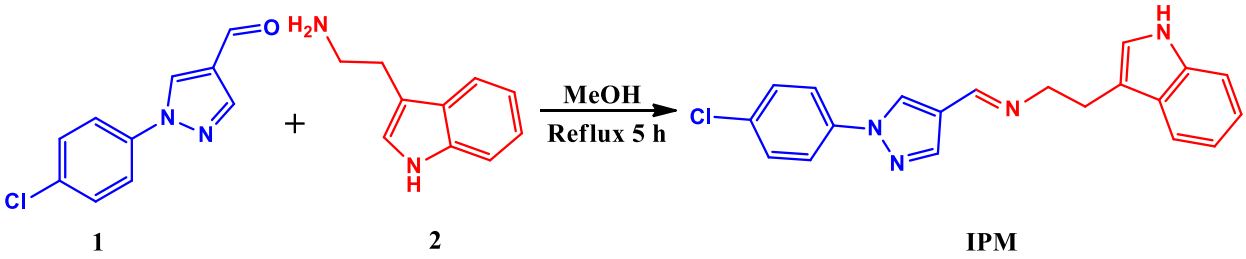

Fig. 1.1 1-(4-chlorophenyl)-1H-pyrazole-4-carbaldehyde (1) and 2-(1H-indol-3-yl)ethan-1-amine (2) rection

3.2 ^{1}H NMR study

The ^{1}H NMR spectrum (Fig. 2) of (E)-N-(2-(1H-indol-3-yl) ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl) methanimine (IPM), recorded in DMSO-d_6, displayed characteristic signals confirming the proposed structure. A singlet observed at δ 10.0 ppm was assigned to the N–H proton of the indole moiety (Pavia et al., 2015). Two distinct signals appearing in the range δ 9.0–8.0 ppm were attributed to the imine proton (–CH=N–) and the proton attached to the pyrazole ring (Pretsch et al., 2013;Jamal et al., 2024; Pretsch et al., 2000). A broad and intense multiplet spanning δ 8.0–7.0 ppm was observed, which corresponds to the aromatic protons of the indole, pyrazole, and chlorophenyl groups. The broadness and overlap in this region are consistent with the presence of multiple aromatic environments. A multiplet in the region δ 3.0–2.0 ppm was assigned to the methylene protons (–CH_2–) directly attached to the nitrogen atom of the indole side chain (Pavia et al., 2015; Pretsch et al., 2013; Pretsch et al., 2000).

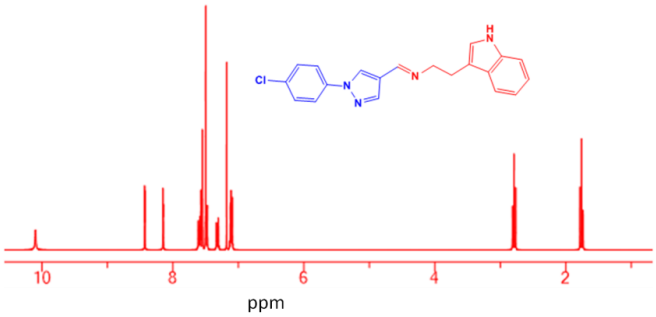

Fig. 2 1H NMR spectra for IPM

Another multiplet observed between δ 2.0–1.0 ppm was attributed to the second set of methylene protons of the ethyl linker (Pavia et al., 2015; Pretsch et al., 2013). The presence of the imine linkage, aromatic systems, and the ethyl chain connecting the indole moiety is confirmed by the chemical shift values and the splitting patterns, which are in good accord with the anticipated structure of IPM. The absence of significant contaminants and the purity of the produced substance were demonstrated by the spectrum's lack of unexpected signals.

3.3 FT-IR study

Fig. 3 shows the FT-IR spectra of (E). The ethyl (N-(2-(1H-indol-3-yl))A wide absorption band at 3600 cm^{-1} was seen in -1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM), which corresponded to the N–H stretching vibration of the indole molecule. A small peak at 2372 cm^{-1} can be the result of overtone or combination bands, but the band at 3053 cm^{-1} is ascribed to aromatic C–H stretching (Pavia et al., 2015; Jamal et al., 2025; Socrates, 2004). The imine group's C=N stretching vibration is represented by a significant absorption at 1667 cm^{-1}. The aromatic and pyrazole rings' C=C stretching vibrations are attributed to the bands at 1584 and 1538 cm^{-1}. C–C stretching and C–H bending vibrations are responsible for the absorptions at 1485 and 1448 cm^{-1}, whereas C–N stretching is responsible for the band at 1399 cm^{-1} (Pretsch et al., Jamal et al., 2024; 2013; Socrates, 2004). The pyrazole ring's N–N stretching vibration is visible at 1331 cm^{-1}. C–N stretching and C–H bending vibrations are attributed to the peaks at 1214 and 1178 cm^{-1}, respectively. The C–Cl stretching is represented by the absorption at 1073 cm^{-1}. Additional bands at 1009 and 957 cm^{-1} are attributed to C–H in-plane and out-of-plane bending, respectively(Pavia et al., 2015; Socrates, 2004). The band at 831 cm^{-1} indicates aromatic C–H out-of-plane bending vibrations, particularly for a para-substituted benzene ring. Peaks at 755 and 645 cm^{-1} are also due to C–Cl stretching and aromatic C–H out-of-plane bending. Finally, bands at 491 and 457 cm^{-1} are associated with skeletal vibrations involving the aromatic and pyrazole rings(Pavia et al., 2015; Pavia et al., 2015; Socrates, 2004).

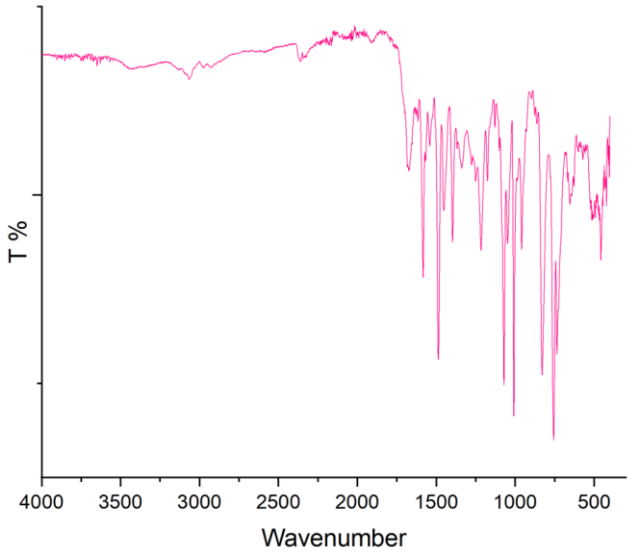

Fig. 3 IR spectra for IPM

3.4 UV-Visstudy

The UV-Vis spectrum of the (E)-N-(2-(1H-indol-3-yl)ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine displayed distinct absorption features, furnishing an understanding of its electronic structure. The spectrum demonstrated a prominent absorption band around 300 nm, which is characteristic of the π-π* transition of the conjugated aromatic systems in the indole and pyrazole rings(Pavia et al., 2015; Pretsch et al., 2013). This absorption signifies the existence of conjugation between the heterocyclic rings and the imine group, which enables electronic transitions. The n-π* transition, which is commonly seen in compounds having imine groups, like the azomethine bond in the structure, is represented by another prominent absorption peak that emerges at about 350 nm (Pavia et al., 2015; Pretsch et al., 2013; Pretsch et al., 2000). The electrical interaction between the imine group and the conjugated aromatic groups is further supported by the absorption in this area.

The absorption maxima in the 200–400 nm range are consistent with the conjugated nature of the molecule, as the extended conjugation system allows for the absorption of ultraviolet light (Pavia et al., 2015; Pretsch et al., 2013). The compound’s absorption profile indicates a strong interaction between the aromatic and heterocyclic components of the molecule, which is the feature of numerous organic

compounds with extended conjugation(Pavia et al., 2015). These UV-Vis characteristics align with the expected electronic transitions in the structure, providing confirmation of the compound's conjugated system and functional groups. Overall, the UV-Vis spectrum supports the proposed molecular structure, with key absorptions reflecting the presence of conjugated systems involving both aromatic and heteroaromatic rings, as well as the imine functionality.

3.5 Mass Spectrum

The electrospray ionization mass spectrum (ESI-MS) of (E)-N-(2-(1H-indol-3-yl)ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM) confirmed the molecular structure through the observation of characteristic peaks. A prominent molecular ion peak was detected at m/z 348.11 ($[M + H]^+$) with 100% relative intensity, corresponding to the protonated molecular ion (Smith, 2004; McLafferty et al.,1993; DeHoffmann et al., 2007). Additional peaks were observed at m/z 349.12 (21.8%), m/z 350.11 (32.3%), m/z 351.11 (7.4%), m/z 350.12 (2.3%), and m/z 349.11 (1.5%), which are consistent with the expected isotopic pattern due to the existence of a chlorine atom in the molecule. The more abundant ^{35}Cl isotope (about 75.77%) is responsible for the peaks at m/z 348.11 and 350.11 (Pavia et al., 2015; McLafferty et al.,1993; DeHoffmann et al., 2007), whereas the ^{37}Cl isotope (approximately 24.23%) is responsible for the peaks at m/z 350.11 and 352.11 (NIST; Smith, 2004; McLafferty et al.,1993) . The intensity ratios and observed isotopic distribution match the theoretical values for a mono-chlorinated species quite well. The ESI-MS spectral data, along with the characteristic isotopic pattern, intensely support the successful synthesis of the targeted compound (IPM) and further validate its molecular formula. No additional significant peaks corresponding to impurities or fragmentation were detected, indicating the high purity of the synthesized IPM.

4. Conclusion

An 83% yield was obtained in the effective synthesis of (E)-N-(2-(1H-indol-3-yl)ethyl)-1-(1-(4-chlorophenyl)-1H-pyrazol-4-yl)methanimine (IPM), a new Schiff base. Its structure and purity were validated by thorough characterization using elemental analysis, FT-IR, UV-Vis, NMR, and ESI-MS. While FT-IR identified the crucial azomethine link, the ^1H NMR spectra confirmed the existence of indole, imine, and aromatic moieties. π-π^* and n-π^* transitions were detected by UV-Vis analysis, which is consistent with extended conjugation. The molecular formula was confirmed by mass spectrometry, which showed a chlorine-specific isotopic signature and a molecular ion signal at m/z 348.11. Every analytical result showed good purity and matched theoretical expectations. These results make IPM a viable option for upcoming catalysis and drug discovery research.

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