



Synthesis and Characterization of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine

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Abstract

The synthesis and characterization of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) are presented. CIA was synthesized by reacting 1-methylindole-3-carboxaldehyde with (3-cyclopentylpropyl)amine, yielding a yellow solid with 89% efficiency. The compound was characterized using ¹H and ¹³C NMR, which confirmed the structure, including the cyclopentyl group, indole moiety, and Schiff base (C=N) linkage. FT-IR spectroscopy revealed key functional groups, such as aromatic C-H, C=N, and C-N stretches. The UV-Vis spectrum showed characteristic electronic transitions associated with the conjugated aromatic rings and imine group. The mass spectrum confirmed the molecular weight of 268.19 g/mol, with isotopic peaks at m/z 269.20 and 270.20, corresponding to [M+1]⁺ and [M+2]⁺ ions. These results verify the successful synthesis and structural features of CIA, offering insight into its electronic properties.

Keywords- Cyclopentyl, Schiff, Aromatic, Mass

1 Introduction

The development of novel organic compounds with potential therapeutic applications has been a central focus in medicinal chemistry [1, 2]. Schiff bases, which are synthesized via the condensation of one-degree amines with carbonyl compounds, convey an effective class of compounds with diverse biological activities, including antibacterial, antifungal, anticancer, and anti-inflammatory properties [3-6]. These properties make Schiff bases valuable candidates for drug discovery. Among these, (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) has emerged as a promising compound due to its unique structural features and potential pharmacological effects. CIA contains a cyclopentyl group, which introduces rigidity and stability into the molecule, and an indole moiety, a well-known pharmacophore that

enhances its biological potential [7-9]. The (Z)-configuration of the imine bond plays a pivotal role in controlling the reactivity and electronic geometry of the novel molecule [10-12]. The existence of the amine group in the propan-1-amine chain is expected to enhance interaction with biological targets, constructing CIA as a good agent for further exploration [13, 14]. Various characterization methods are used to confirm the structure as well as purity of the CIA. NMR spectroscopy furnishes detailed information about the molecular structure, including the configuration of atoms and functional groups. UV-Vis (Ultraviolet-visible) examination enables the study for the compound's electronic transitions, providing insight into its electronic properties and stability. Fourier-transform infrared (FT-IR) spectroscopy is used to identify the functional groups present in CIA, aiding in the confirmation of the Schiff base formation and the presence of specific bonds. MS (Mass spectrometry) permits determining the molecular weight and confirms the presence of the desired molecular fragments, ensuring the purity of the compound. Given its unique structural features and the wealth of characterization data obtained through NMR, UV-Vis, FT-IR, and mass spectrometry, CIA represents an intriguing compound for further study. Its synthesis, structural elucidation, and potential biological properties provide a promising foundation for future investigations aimed at developing therapeutic agents.

2. Methods and Materials

2.1. Methods

The compound (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) was characterized by FT-IR (Perkin-Elmer) for functional groups, ^1H and ^{13}C NMR (Bruker AVANCE-III) for structural analysis, and UV-Vis (Perkin-Elmer Lambda 35) for electronic transitions. ESI-MS (WATERS Q-ToF Premier) confirmed the molecular ion and fragmentation, while elemental composition was verified using a Perkin-Elmer 2400 Series II CHNS/O analyzer.

2.2 Materials

All starting chemicals for the preparation of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) were sourced from Sigma-Aldrich and employed in the synthesis without any prior purification or modification.

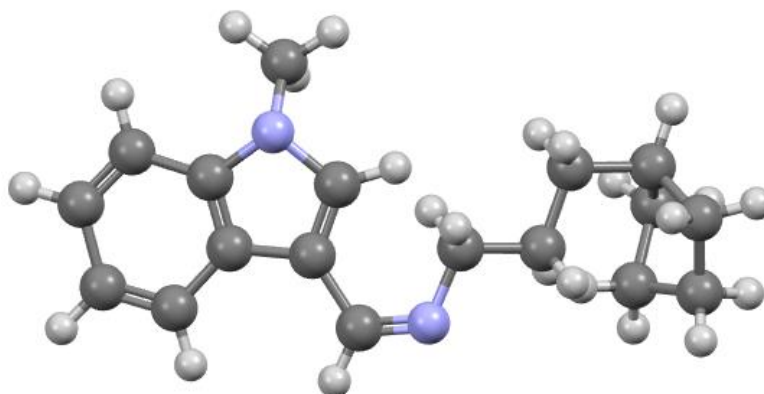
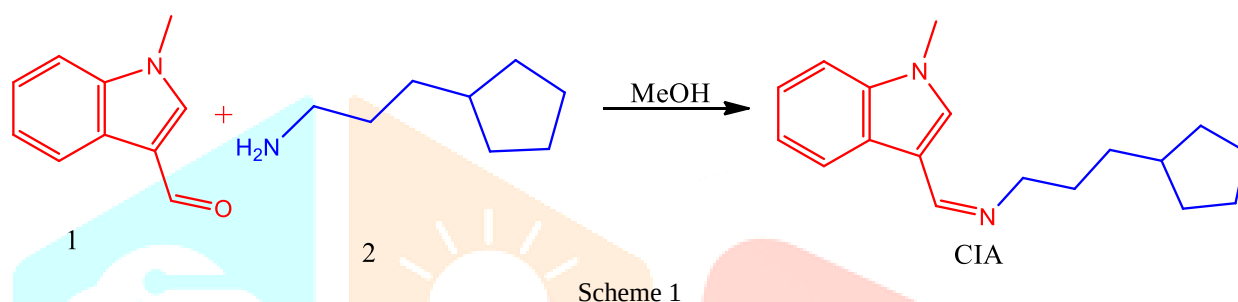


Figure 1 Structure of CIA

3. Results and discussion

3.1 Synthesis of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA)

The synthesis of CIA was carried out by reacting 1-Methylindole-3-carboxaldehyde (1) with (3-Cyclopentylpropyl)amine (2), as described in Scheme 1. To begin, 0.50 g (3.14 mmol) of (3-Cyclopentylpropyl)amine was dissolved in 20 mL of methanol, followed by the addition of 0.39 g (3.06 mmol) of 1-Methylindole-3-carboxaldehyde. The mixture was then heated under reflux for 10 hours, during which a pale yellow precipitate formed as the solvent evaporated, reducing the solution volume to 10 mL. The precipitate was collected by filtration and purified by washing with cold methanol (10 mL) and hexane (15 mL). The solid was recrystallized from methanol and dried under vacuum, resulting in 0.80 g of the CIA product (89% yield), which appeared as a yellow solid. However, the structure of the CIA is given in Figure 1.



3.2 NMR

The ^{13}C NMR and ^1H NMR spectra of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) provide essential information for confirming the molecular structure and the arrangement of atoms within the compound.

In the ^{13}C NMR spectrum, the signals are observed for various carbon atoms present in the structure. The cyclopentyl ring typically shows a set of signals in the range of 20–40 ppm, corresponding to the five carbon atoms in the ring. The carbon atoms of the methylene group ($-\text{CH}_2-$) in the propan-1-amine chain resonate around 45–55 ppm, while the carbon attached to the imine ($-\text{CH}=\text{N}$) bond appears around 135–145 ppm [15, 16]. The indole ring contributes several signals, with the carbons at positions 2, 4, and 5 typically appearing in the range of 120–135 ppm. The methyl group attached to the nitrogen atom in the indole moiety ($-\text{CH}_3$) appears around 10–15 ppm [15, 17].

In the ^1H NMR spectrum, the cyclopentyl group shows a set of multiplets in the range of 1.5–2.5 ppm, corresponding to the hydrogen atoms in the ring. The methylene group ($-\text{CH}_2-$) adjacent to the amine group typically appears as a quartet around 3.0–3.5 ppm, with the chemical shift influenced by the electron-donating amine group. The imine proton ($-\text{CH}=\text{N}$) resonates as a singlet around 8.0–8.5 ppm, characteristic of the (Z)-configuration of the imine bond [15–17]. The aromatic protons of the indole ring resonate in the region of 6.5–8.5 ppm, with signals corresponding to the protons at positions 2, 3, and 5 of the indole ring. The methyl group attached to the nitrogen in the indole ring appears as a singlet around 2.5–3.0 ppm [16, 17].

Together, the ^1H and ^{13}C NMR spectra confirm the structure of CIA, providing crucial information regarding the proton and carbon environments, which support the proposed molecular framework.

3.3 FT-IR

The FT-IR spectrum of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) reveals key functional group characteristics that confirm the compound's structure. The absorption bands around 3050–3100 cm^{-1} correspond to the aromatic C-H stretches of the indole ring, while the 2920–2850 cm^{-1} region indicates the aliphatic C-H stretches from the cyclopentyl and methylene groups [15, 18]. The C=N stretch of the Schiff base imine bond appears around 1650–1600 cm^{-1} , confirming its formation [15, 17, 18]. Additionally, the 1500–1600 cm^{-1} region displays aromatic C=C stretching vibrations, and the C-N stretching of the amine group is observed around 1250–1350 cm^{-1} [18, 15]. A weak N-H bending absorption around 1600 cm^{-1} and a small peak around 1450 cm^{-1} for the methyl group attached to nitrogen [17, 18] further support the presence of the indole moiety and the amine functionality, thereby confirming the key structural features of CIA.

3.4 UV-Vis

The UV-Vis spectrum of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) provides insights into the electronic transitions of the compound, particularly those related to its conjugated systems. In the spectrum, the $\pi \rightarrow \pi^*$ transitions of the aromatic rings, particularly from the indole and cyclopentyl groups, are expected to appear as strong absorbances in the 250–350 nm range [15, 17]. The indole moiety, being conjugated, will likely contribute a distinct absorption band in this region, corresponding to the electronic transitions of the conjugated π -electrons. Additionally, a $n \rightarrow \pi^*$ transition* involving the imine group (C=N) might result in an absorption band around 400–450 nm, indicative of the electron-withdrawing nature of the imine group [15-17]. These absorptions, in combination with any additional bands arising from the conjugation between the indole and methylene groups, provide critical information about the electronic structure of CIA, revealing the compound's ability to absorb light in the UV-visible region and giving further insight into its potential electronic properties.

3.5 Mass spectrum

The mass spectrum of (Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) exhibits distinct peaks that confirm its molecular identity and isotopic distribution. The molecular ion peak at m/z 268.19 (100.0%) corresponds to the intact molecular ion, $[M]^+$, of CIA, with a molecular weight of 268.19 g/mol. The peaks at m/z 269.20 (19.7%) and m/z 270.20 (1.8%) are the isotopic variants of the molecular ion, corresponding to the $[M+1]^+$ and $[M+2]^+$ ions, respectively. The peak at m/z 269.20 results from the natural isotopic distribution of carbon (^{13}C), while the peak at m/z 270.20 arises from the incorporation of a heavier isotope (e.g., ^{13}C or ^{15}N). These isotopic peaks are typical for organic molecules containing elements like carbon and nitrogen and confirm the molecular composition of CIA. The dominance of the $[M]^+$ peak in the spectrum indicates that CIA is relatively stable in the mass spectrometer, with minimal fragmentation observed under the experimental conditions.

4. Conclusion

(Z)-3-cyclopentyl-N-((1-methyl-1H-indol-3-yl)methylene)propan-1-amine (CIA) was successfully synthesized via a condensation reaction between 1-methylindole-3-carboxaldehyde and (3-cyclopentylpropyl)amine, yielding a high-purity product with excellent yield. Comprehensive characterization using spectroscopic techniques, including NMR, FT-IR, UV-Vis, and mass spectrometry, confirmed the molecular structure and purity of the compound. The NMR data validated the chemical environments of protons and carbons consistent with the proposed structure. FT-IR analysis identified key functional groups such as C=N and C-N, while UV-Vis spectroscopy revealed the $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions associated with the conjugated indole-imine system. Mass spectrometry further confirmed the molecular weight and isotopic distribution. These consequences establish the successful synthesis and structural elucidation of CIA, furnishing a strong foundation for additional study into its electronic and potential biological characteristics.

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