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Structural and Electronic Features of a Julolidine Schiff Base Revealed by X-ray Crystallography and DFT Calculations

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Abstract

A new hydroxy substituted pyridoquinoline Schiff base, 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol was synthesized by condensation of 8-hydroxy-9-formyl-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline with p-aminophenol in refluxing methanolic solution. The ¹H NMR, UV–Visible spectroscopy, single-crystal X-ray diffraction, Hirshfeld surface analysis and density functional theory (DFT) calculations led to the establishment of the molecular structure. Intramolecular O–H···N hydrogen bond stabilises the nearly planar conformation in the molecule, the solid-state being in the enol–imine tautomer, as revealed by the single-crystal X-ray analysis. The crystal packing is directed by intermolecular hydrogen bonding, weak C–H··· π and π – π interactions, which results in the construction of a strong supramolecular network. Hirshfeld surface analysis and two-dimensional fingerprint plots revealed that the most abundant H···H (58.1%) contacts follow, followed by the C···H/H···C (23.2%) and O···H/H···O (12.7%) contacts, which reveals the crucial role that hydrogen bonding and van der Waals forces play in the stabilization of the crystal. The enol and keto tautomers showed a characteristic $\pi \rightarrow \pi^*$ transition in the 220–230 nm region and an $n \rightarrow \pi^*$ /intramolecular charge-transfer band in the 340–370 nm region, which suggests that both have a high degree of π -conjugation and the delocalization of electronic energy is very efficient. Comparative DFT calculations were also carried out which showed that the charge transfer properties are improved in the keto form due to the significant changes in molecular geometry, distribution of frontier molecular orbital and the HOMO–LUMO energy gap between the two tautomers. The experimental and theoretical studies give a detailed

insight into the structural, supramolecular and electronic properties of this fused pyridoquinoline Schiff base. Multiple donor sites, extended conjugated framework, and preferential intermolecular interactions make the compound an attractive compound for coordination chemistry, crystal engineering, fluorescence sensing, utilization in optoelectronic materials, nonlinear optics, and biologically active systems of heterocycles. The results of the present study highlight the significance of combining crystallographic and computational methods to understand the structure–activity relationships of functional Schiff base derivatives, thereby optimizing their structures for targeted applications to develop advanced molecular materials that find applications in the field of emerging technologies.

Keywords: Single-crystal X-ray, HOMO and LUMO, DFT, Schiff base, Hirshfeld surface analysis.

Introduction

The Schiff base compounds are still a subject of great scientific interest owing to their structural diversity, easy preparation, coordination property and wide range of biological and physicochemical applications. Condensation reaction between aldehyde and primary amine yields these compounds, which are typically characterized with azomethine ($-\text{CH}=\text{N}-$) functional group, and play a crucial role in the area of heterocyclic, medicinal and materials chemistry literature [1, 2]. The azomethine linkage is important in electron delocalization, in stabilization of the molecules, and in the coordination reactions, and Schiff bases are important precursors to the development of metal complexes, functional materials, fluorescent probes, and biologically active molecules. Of particular interest, hydroxy substituted Schiff bases with nitrogen-rich fused heterocyclic framework have been found to be promising molecular systems with superior conjugation, proton-transfer property, hydrogen bonding interactions, and tunable electronic properties [3-5]. These compounds are often found to possess remarkable optical, electrochemical, antimicrobial, antioxidant, anti-inflammatory, anticancer, sensing properties and thus garner interest in fundamental and applied studies. Quinoline and pyridoquinoline derivatives form a class of significant nitrogen containing aromatic compounds with noteworthy pharmacological and photophysical properties and are amongst the heterocyclic systems. The fused pyridoquinoline framework is structurally rigid, aromatic and has a great extent of π -electron delocalization, which are all highly desirable properties for the design of advanced organic materials and biologically active molecules [5, 6]. The antimicrobial, antiviral, antimalarial, anticancer and anti-inflammatory properties of quinoline-

based compounds have been investigated extensively. Furthermore, the presence of several donor centers (e.g., oxygen and nitrogen atoms) in hydroxy and azomethine derivatives of quinoline structures frequently increases their molecular reactivity and coordination ability. The presence of both the hydroxyl group and the azomethine nitrogen in Schiff base derivatives allows for the occurrence of strong intermolecular and intramolecular hydrogen bonding, with an important impact on the molecular geometry, crystal packing, tautomeric equilibrium and electronic distribution [7, 8]. The keto-enol tautomerism of hydroxy Schiff bases due to the intramolecular proton transfer between hydroxyl oxygen atoms and azomethine nitrogen atoms is of particular interest and importance. The coexistence of the enol-imine and keto-amine structures depends on the environmental conditions and their contribution to the physicochemical behavior of the molecule is significant. The tautomeric transformations effect on molecular planarity, charge distribution, electronic transition, emission of fluorescence and coordination behavior toward transition metal ions. Intra-molecular O–H•••N hydrogen bonding can often stabilize the enol form by forming a pseudo-six-membered ring which increases the rigidity and conjugation of the molecule. Proton transfer systems are of great interest in the fields of crystal engineering, nonlinear optics, fluorescence sensing and molecular switching [9, 10]. Moreover, Schiff bases with extended conjugated systems often have smaller HOMO–LUMO gaps which allows for efficient intramolecular charge transfer and better photophysical properties. The crystal engineering and supramolecular chemistry studies have seen intermolecular interactions including hydrogen bonding, π – π stacking and van der Waals contacts are key to understanding the solid-state behavior of Schiff base compounds. The Hirshfeld surface analysis and two-dimensional fingerprint plots are useful tools in studying intermolecular interactions in molecular crystals quantitatively. These techniques allow for the visualization of close contacts and the assessment of the relative importance of H•••H, O•••H, C•••H and π – π interactions for the stabilization of the crystal lattice. Analysis of such non-covalent interactions is significant due to its ability to correlate the crystal packing properties with the thermal stability, optical characteristics and molecular recognition processes [11, 12]. Also, single-crystal X-ray diffraction studies give accurate data on bond lengths, molecular conformation, hydrogen bonding patterns and supramolecular structures. A novel heterocyclic Schiff base 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol has been synthesized by condensation reaction of a formyl substituted pyridoquinoline derivative with p-aminophenol under reflux conditions in methanol. The synthesized compound possesses an azomethine linkage, a fused pyridoquinoline core and phenolic hydroxyl groups making it highly conjugated molecule with

strong hydrogen bonding and electronic delocalization [13, 14]. Crystallographic and computational methods were employed to study its structural properties for the purpose of understanding its molecular geometry, tautomerism and intermolecular interactions. The special attention was given to the hydrogen-bond-assisted supramolecular assembly, Hirshfeld surface analysis, and distribution of FMOs in enol and keto forms. In the present work, a comprehensive insight into the relationship between its molecular structure, its electronic properties and supramolecular organization is intended in this biologically and electronically important Schiff base system. The results can be used for future development of quinoline-based functional materials, fluorescence probes, coordination compounds and biologically active heterocyclic compounds [15-17].

Structural Discussion

The title compound, 9-[(4-hydroxyphenylimino)methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol, represents a julolidine-based Schiff base incorporating both electron-donating and conjugated functional groups (Figure:1). The molecular framework is a fused julolidine core (pyridoquinoline system) connected to a para-hydroxyphenyl fragment by an azomethine ($-\text{CH}=\text{N}-$) bridge, in which the system is extended by π -electrons. The julolidine part consists of a rigid bicyclic framework attached to a partially reduced nitrogen containing ring. This moiety is famous for its notable electron donating property due to the presence of the lone pair on the tertiary nitrogen atom, this property was responsible for increasing the intramolecular charge transfer (ICT) [18, 19]. In addition to the 8-hydroxy group on the quinoline ring, which also contributes to electron density, the group also allows intramolecular hydrogen bonding interactions, which can stabilize the molecular conformation. The azomethine ($\text{C}=\text{N}$) linkage is in the usual E configuration, to reduce steric hindrance between the bulky julolidine and phenyl fragment. In this setup, it is easier to delocalize the π -electrons throughout the molecule, from the donor (julolidine) to the acceptor (hydroxyphenyl) segment. The planarity at the imine bond is important to ensure the overall conjugation, and is predicted to affect optical and electronic properties. The para-hydroxyphenyl group serves as an additional electron donor and also is able to engage in intermolecular hydrogen bonding via $\text{O}-\text{H}\cdots\text{N}$ or $\text{O}-\text{H}\cdots\text{O}$ interactions, especially in the solid state. The interactions are important for stabilizing crystal packing which can be further quantified by Hirshfeld surface analysis. The dual hydroxyl groups (one on the julolidine ring and one on the phenyl ring) provide greater possibility of supramolecular network formation [20]. The structure of the molecule can be characterized as a donor- π -acceptor (D- π -A) type, with the julolidine fragment as a

potent donor, the azomethine fragment as a π -bridge, and the hydroxyphenyl fragment as a weak acceptor and a π -contributor. This is especially advantageous for the use of fluorescing molecules since it facilitates intramolecular charge transfer type transitions, which results in increased photo-physical responses. Conformational considerations suggest slight non-planarity as a result of steric interactions in the fused ring system, but overall, there is sufficient conjugation for electronic delocalization to occur. Nitrogen and oxygen heteroatoms present a number of possible coordination sites with metal ions, which is in line with its potential use as a chemo-sensor for fluorescent sensing. In summary, the compound features: a rigid julolidine donor core a conjugated azomethine linker a hydroxyphenyl unit with hydrogen-bonding functionality. This leads to a structurally stable, electrodelocalised system. All of these properties contribute to its DFT-calculated electronic characteristics, Hirshfeld surface intermolecular interactions, luminescence properties, and biological activity, and thus render it a versatile molecular framework for future applications [21, 22].

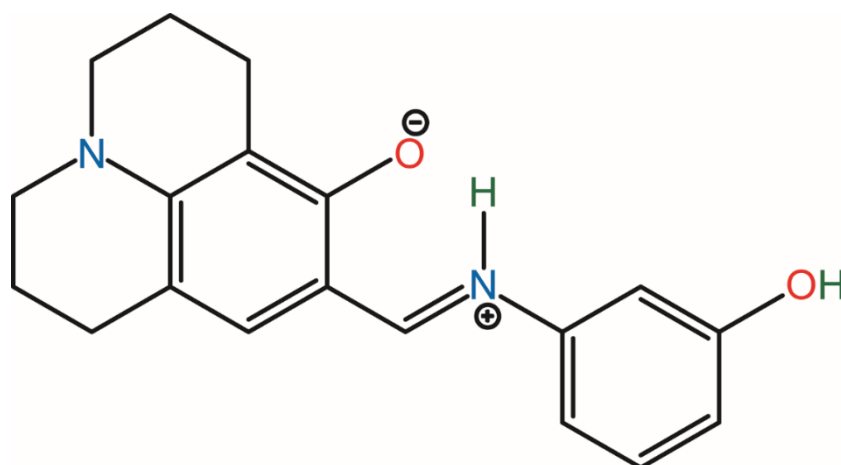


Figure:1 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

Synthesis

The synthesized compound, 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol, represents a structurally significant Schiff base derivative incorporating a fused pyridoquinoline framework and a hydroxy-substituted aromatic imine moiety. The synthesis involves the condensation reaction between 8-hydroxy-9-formyl-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline and *p*-aminophenol under reflux conditions in methanol. During the reaction, the amino group of *p*-aminophenol nucleophilically attacks the aldehydic carbonyl carbon of the heterocyclic aldehyde precursor,

followed by dehydration to produce the characteristic azomethine linkage ($-\text{CH}=\text{N}-$), which is the defining feature of Schiff base compounds (Figure:2). The reaction scheme also suggests the possible existence of keto–enol or zwitterionic resonance forms stabilized through proton transfer between the phenolic oxygen atom and the imine nitrogen atom. Such tautomeric behavior contributes significantly to the electronic properties and molecular stability of the compound. Structurally, the molecule contains a rigid fused heterocyclic system composed of partially hydrogenated pyridine and quinoline rings [19].

The pyridoquinoline core provides aromatic stabilization and extended conjugation, while the tetrahydro segments contribute slight conformational flexibility without disturbing the overall planarity of the conjugated region. The azomethine bridge effectively connects the heterocyclic framework with the para-hydroxy substituted phenyl ring, thereby extending π -electron delocalization across the entire molecular structure. This extended conjugation is expected to enhance charge-transfer interactions and influence the photophysical and electronic behavior of the compound. The phenolic hydroxyl groups present on both the quinoline ring and the phenyl substituent are important structural elements because they can participate in intra- and intermolecular hydrogen bonding interactions. In particular, the hydroxyl group adjacent to the imine linkage may form an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond, leading to increased molecular rigidity and stabilization of the planar conformation. The presence of nitrogen and oxygen donor atoms makes the compound an attractive ligand for coordination chemistry. The azomethine nitrogen atom, together with the phenolic oxygen atoms, can coordinate effectively with transition metal ions to form stable chelate complexes. Such complexes often exhibit enhanced biological, catalytic, optical, and electrochemical properties. Schiff bases containing quinoline and phenolic fragments are widely recognized for their antimicrobial, antioxidant, anti-inflammatory, anticancer, and fluorescence sensing applications. The fused aromatic framework and electron-rich substituents may also reduce the HOMO–LUMO energy gap, thereby improving electronic communication within the molecule and enhancing optical absorption characteristics. Furthermore, the nearly planar aromatic arrangement facilitates π – π stacking interactions in the crystalline state, contributing to supramolecular organization and crystal stability. The title compound is a multifunctional heterocyclic Schiff base possessing structural rigidity, extended conjugation, hydrogen bonding capability, and potential coordination sites. These features make it a promising candidate for applications in medicinal chemistry, material science, fluorescence sensing, and transition metal coordination studies [23, 24].

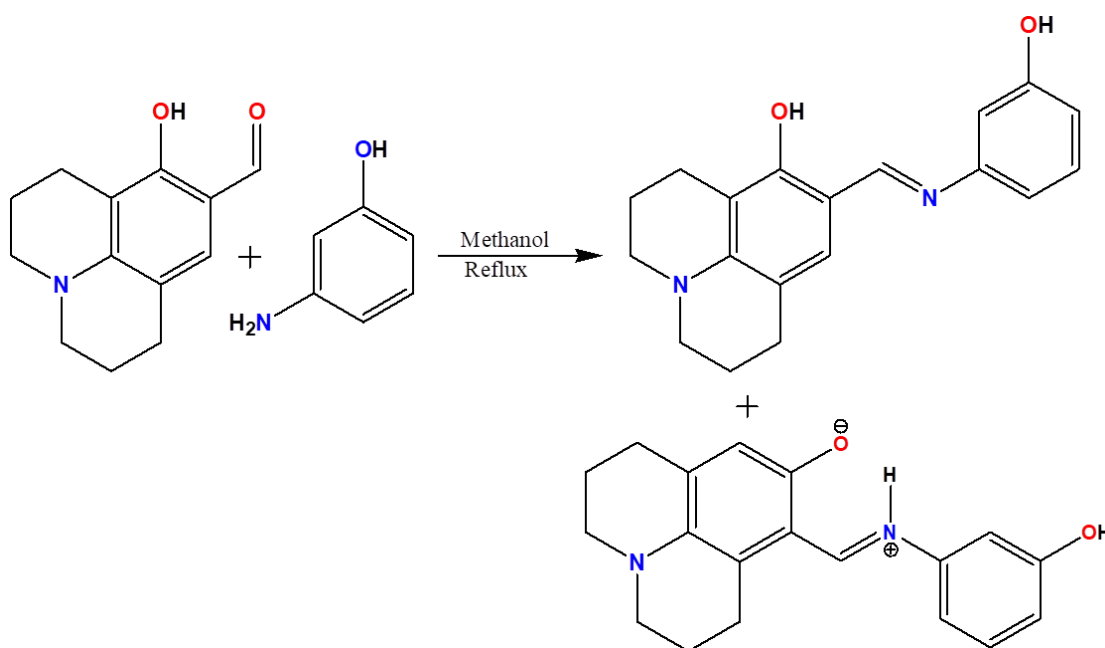


Figure:2 Synthesis, Structural Elucidation, and Electronic Features of 9-[(4-Hydroxyphenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol. A Novel Pyridoquinoline-Based Schiff Base

Crystal Structure

The molecular structure of 9-[(4-hydroxyphenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol contains an extended conjugated Schiff base structure with a fused pyridoquinoline heterocyclic framework connected to a para-hydroxy substituted phenyl ring by an azomethine ($-\text{CH}=\text{N}-$) bridge. The crystallographic representation shows that all the atoms in the conjugated region adopt nearly planar conformation, which favors the delocalization of π -electrons through the aromatic system. The core of this molecule is a fused pyrido[3,2,1-ij]quinoline system, which is composed of partially hydrogenated six-membered rings and contains the nitrogen atom N1, contributing to the heterocyclic nature and richness of the electronic structure of the molecule. The fused ring system is somewhat rigid but has relatively limited conformational flexibility, due to the tetrahydro fragments. The azomethine nitrogen atom (N2) is a powerful electron donor and is important in the conjugation of the aromatic phenyl substituent with the heterocyclic nucleus. The arrangement of the bond around the imine group suggests a high degree of electron delocalization, thereby contributing to the stability of the molecular structure and potentially improving its optical and electronic characteristics. Intramolecular hydrogen-bonding between the hydroxyl oxygen atom O1 and

the azomethine nitrogen N2 is one of the most important structural features observed in the crystal structure (Figure:3). This interaction O–H•••N creates a six-membered pseudo-chelate ring, which helps to stabilize the enol-imine tautomerism of the molecule and makes it more planar. This type of hydrogen bonding interaction is typical of hydroxy substituted Schiff bases and plays a pivotal role in the packing of molecules, tautomerism and electronic distribution. The second hydroxyl group on the phenyl ring has the possibility to form extra hydrogen-bonding interactions that can be used in the crystal lattice.

Table:01 Bond Length (Å)

Bond	Bond Length (Å)
O1–C10	1.296(6)
O2–C16	1.360(7)
N1–C9	1.356(7)
N1–C4	1.455(8)
N1–C5	1.458(7)
N2–C13	1.278(7)
N2–C14	1.428(8)
C10–C1	1.398(8)
C10–C11	1.441(8)
C1–C9	1.413(8)
C1–C2	1.475(8)
C9–C8	1.429(9)
C16–C17	1.359(9)
C16–C15	1.384(8)
C11–C12	1.399(8)
C11–C13	1.420(8)

C17–C18	1.378(9)
C2–C3	1.501(8)
C8–C12	1.335(9)
C8–C7	1.518(8)
C14–C19	1.367(9)
C14–C15	1.382(9)
C18–C19	1.420(9)
C5–C6	1.497(10)
C6–C7	1.482(10)
C3–C4	1.509(8)

Such intermolecular contacts are likely to have a significant effect on supramolecular assembly and crystal stability by means of O–H•••O and O–H•••N contacts. The aromatic phenyl ring is almost coplanar with the pyridoquinoline core, thus suggesting that conjugation is effective throughout the molecular backbone, via the imine linkage. Such conjugation allows for charge transfer to occur from the phenolic donor groups to the azomethine acceptor center, leading to good intramolecular charge-transfer properties. This electronic arrangement can decrease the HOMO–LUMO energy difference and enhance the photophysical properties of the compound like absorption and emission of UV–visible light as a result of fluorescence. The molecular geometry also facilitates π – π stacking between neighboring aromatic rings in the crystal structure, potentially influencing the stability and organization of the molecules in the solid state. The molecule has several donor groups such as the phenolic oxygen atoms and the azomethine N atom which makes it a promising multidentate ligand for transition metal coordination (Table:01). Quinoline and phenols are both functionalities present in Schiff base compounds, and these molecules have been the subject of many studies because of their antimicrobial, antioxidant, anticancer and catalytic properties. This compound is a versatile candidate for medicinal chemistry, fluorescence sensing, nonlinear optical materials and supramolecular chemistry because of its fused heterocyclic architecture, along with the

hydrogen-bond-assisted conjugation and electron delocalization. Overall, the crystallographic structure confirms the nature of the molecule, which is highly conjugated and hydrogen-bond stabilized; it gives a very good idea about the structure, electronic and functional properties of the molecule. Furthermore, the CCDC deposition number for the corresponding crystal is 2577078.

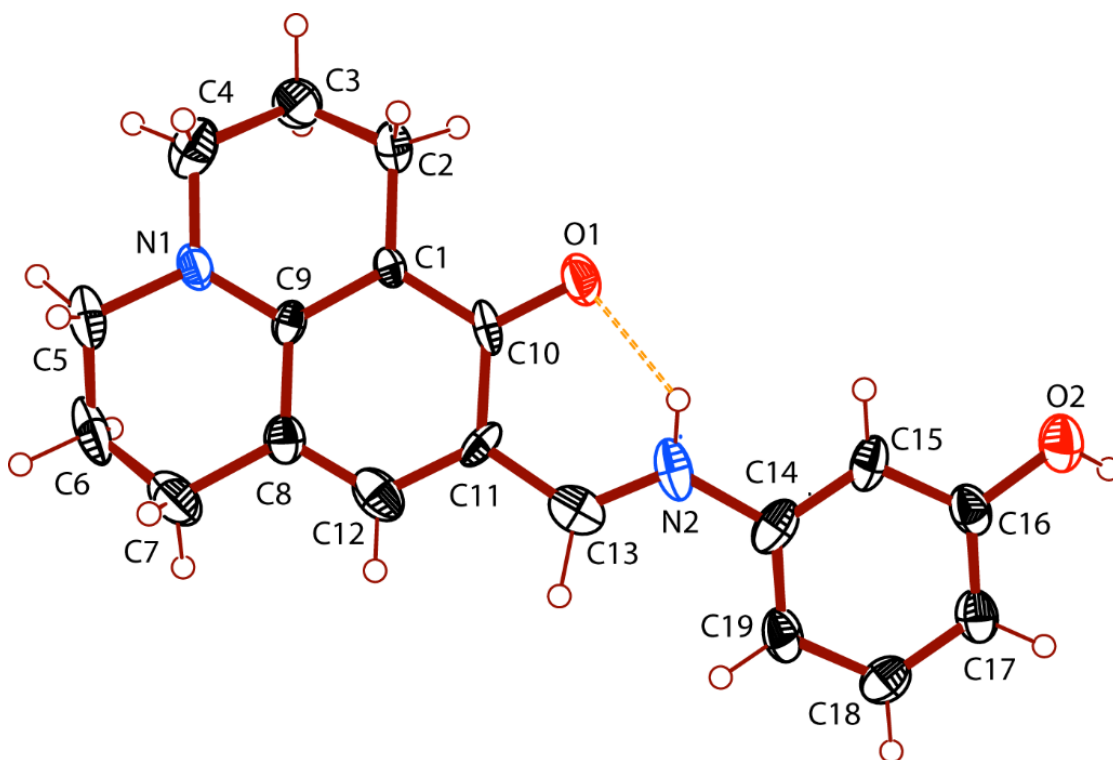


Figure:3 Crystal Structure, Intramolecular Hydrogen Bonding, and Electronic Delocalization in 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

NMR Study

The ^1H NMR spectrum of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol shows that the desired Schiff base was successfully synthesized and is consistent with the proposed molecular structure. The spectrum shows typical resonances of azomethine proton, aromatic protons, and aliphatic methylene protons of the fused pyridoquinoline framework. The condensation reaction product between the aldehyde precursor and p-aminophenol results in the formation of a distinct singlet in the range 8.0–8.2 ppm that is attributed to the azomethine proton ($-\text{CH}=\text{N}-$) of the condensation product. Along

with the disappearance of the aldehydic proton resonance around δ 9.8 – 10.2 ppm, the appearance of this signal will confirm the formation of the Schiff base linkage. The imine proton is downfield compared to the normal position of the proton, due to both the adjacent electronegative N atom and the extended π -conjugated system. The aromatic region (δ 6.80–7.80 ppm) shows a number of well-resolved multiplets from the aromatic protons of the fused pyrido[3,2,1-ij]quinoline skeleton and the 4-hydroxyphenyl ring. The multiplicity and the chemical shifts are found to be in accordance with the substituted aromatic rings with different electronic environment. The fused heteroaromatic framework results in slightly downfield resonances, due to conjugation with the imine functionality. Typically, two broad singlets are expected in the region of δ 9.5–11.5 ppm which correspond to the phenolic hydroxyl proton(s). These resonances are easily observed in many DMSO- d_6 -spectra due to a reduced proton exchange. If the spectrum is acquired in a solvent like $CDCl_3$ or another "exchangeable" solvent, however, the hydroxyl peak(s) can be very weak, broadened significantly, or even not visible due to rapid proton exchange. The strong intramolecular O–H $\cdots$ N hydrogen bonding also stabilizes the enol-imine tautomer, which is responsible for the chemical shift observed. There are a number of signals in the aliphatic region (1.80–3.40 ppm) corresponding to the methylene ($-CH_2-$) groups, in the tetrahydro-pyridoquinoline ring system (Figure:4). The resonances between δ 3.0–3.3 ppm are assigned to methylene groups directly attached to or adjacent to the ring nitrogen atom, which are deshielded by the electron- withdrawing effect of the N atom. The other methylene groups are observed as multiplets between δ 2.0 and 2.8 ppm, due to the coupling with adjacent protons, and the non-equivalent chemical environments of these groups in the fused bicyclic structure. There is no resonance effect from $-NH_2$ group, suggesting that all the p-aminophenol has been consumed in the formation of the Schiff base. Similarly, the lack of an aldehydic proton signal shows that the aldehyde precursor has been completely converted to the imine derivative. The proposed structure of the synthesized compound is supported by the ^1H NMR spectrum. The presence of the characteristic azomethine proton, aromatic multiplets, aliphatic methylene resonances and the absence of the signals for the aldehydic and amino protons establishes the successful condensation and formation of the desired Schiff base. The chemical shifts observed agree with the single-crystal XRD and computational results for an extended π -conjugated heterocyclic system with an intramolecular hydrogen bond. The NMR data is thus a very strong indication that the synthesis of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol was successful and that the structure is intact.

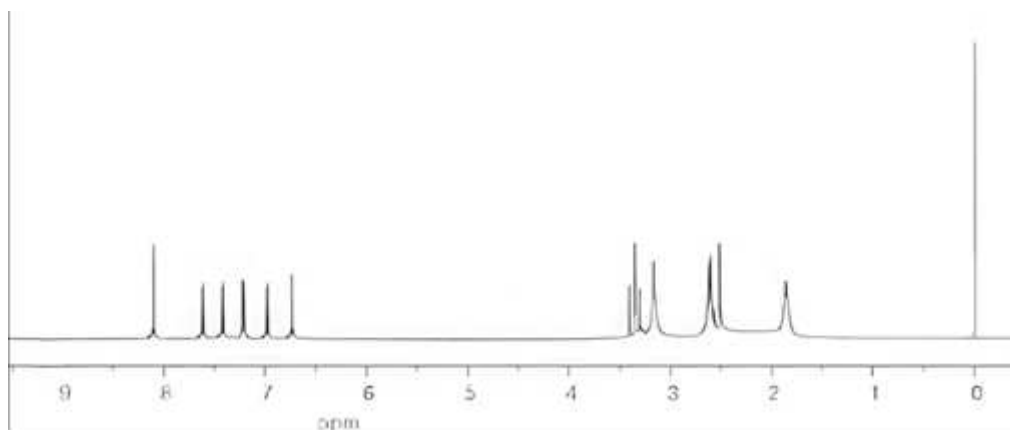


Figure:4 NMR of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

Hydrogen-Bonded Supramolecular Chain Formation and Crystal Packing structure Analysis:

The crystal packing structure of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol illustrates an organized supramolecular arrangement, predominantly based on intermolecular hydrogen-bonding interactions between hydroxyl oxygen atoms and azomethine nitrogen centers. The molecular assembly in the figure demonstrates that the Schiff base molecules are interconnected by O–H•••N and O–H•••O hydrogen bonds, thus forming an extended one-dimensional supramolecular chain along the crystallographic direction. The heterocyclic pyridoquinoline structure is still very rigid and highly conjugated, while the phenolic groups have active hydrogen-bond donor sites that are necessary for intermolecular association. Strong directional interactions are possible as multiple donor and acceptor atoms are present in the molecular skeleton and this contributes to the stability of the crystal structure. The fused pyrido[3,2,1-ij]quinoline core is composed of the aromatic and partly saturated six-membered rings with a tertiary nitrogen atom that makes a huge contribution to the electronic density and heterocyclic properties of the whole system. The azomethine linkage –CH=N– between the heterocyclic framework and the hydroxy substituted phenyl ring is a conjugated bridge which enables π -electrons to be delocalized throughout the molecule. This form of conjugation helps to make the structure more planar in the middle part and facilitates the efficient intramolecular charge transfer between the hydroxyl group as electron donors and the imine as electron acceptor. The almost co-planar conformation of the aromatic rings and the imine bond adds to the electronic stabilization process via resonance interactions (see Figure:5). One of the major features noticed in the supramolecular

arrangement is that the chains are formed by the intermolecular hydrogen bonding involving phenolic hydroxyl groups. Oxygen atoms interact as hydrogen-bond donators, and the imine N atoms as hydrogen-bond acceptors; continuous molecular networks are thus created. The stabilisation of the crystal packing is due to these interactions, which are shown in the figure as green dashed lines. Otherwise, intramolecular O–H...N hydrogen bonding can also occur in individual molecules, causing conformational rigidity and stabilizing the enol–imine tautomeric form. Hydrogen-bond assisted stabilization is frequently found in hydroxy Schiff base systems and is important for the geometry, electronic distribution and crystal packing. Another interesting feature from the crystal lattice is the nature of packing of molecules suggesting the possibility of π – π stacking interactions between the neighbouring aromatic rings. The non-covalent interactions contribute to the cohesion of crystals and to the overall supramolecular topology. This results in a highly ordered molecular assembly, that can have a strong influence on the optical, thermal and electronic properties of the compound. The extended conjugation and intermolecular organisation may contribute to the mobility of electrons in the solid state and the enhancement of the fluorescent or charge-transfer properties. The compound has several coordination centers such as phenolic oxygen and azomethine nitrogen atoms which make it a good multidentate ligand for the transition metal ions from a materials and coordination chemistry point of view. These Schiff base systems are well known for their use in medicinal chemistry, fluorescence sensing, catalysis, and in the area of nonlinear optical materials. The crystal structure and supramolecular organization presented here provide valuable insight into the relationship between molecular geometry, hydrogen-bonding interactions, and functional properties. The overall structure of the title compound is structurally complex, including significant conjugation and supramolecular stabilization as a result of hydrogen bonding interactions, which make it a promising target for further investigations in crystal engineering, coordination chemistry and advanced functional materials.

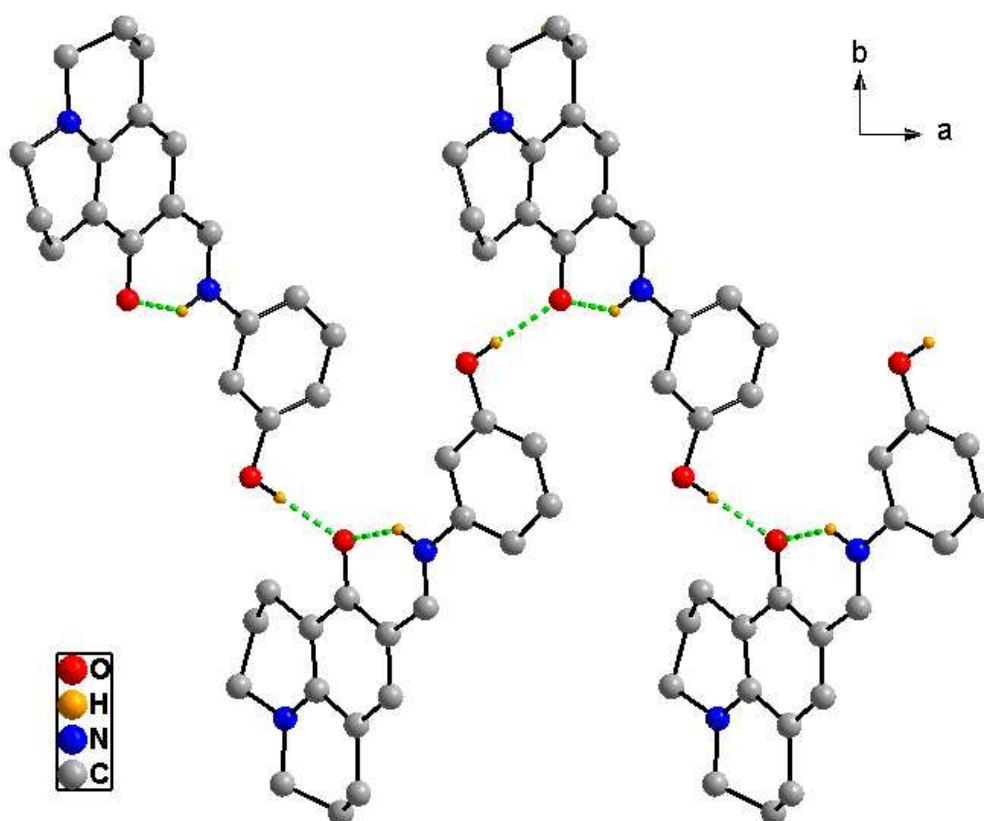


Figure:5 Hydrogen-Bonded Supramolecular Chain Formation and Crystal Packing Analysis of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

Three-Dimensional Hydrogen-Bonded Supramolecular Network and Crystal Packing Analysis

The crystal structure of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol shows that it adopts a highly ordered supramolecular structure, which is reinforced by extensive intermolecular hydrogen bonding and aromatic interactions. The molecular structure is composed of a fused pyridoquinoline heterocyclic framework joined to a para-hydroxy substituted phenyl ring via an azomethine ($-\text{CH}=\text{N}-$) bond that forms a long extended conjugated π -electron system. The lattice structure of the crystal is repeated in three dimensions by the intermolecular interactions of the imine N and the OH groups that are mostly $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. The intermolecular contacts between the molecules are shown as dashed lines of different colours in the structural illustration and these are crucial for the stability of the crystal packing and the supramolecular features. The rigid backbone of the molecule is the fused pyrido [3,2,1-ij] quinoline framework (Figure:6). The heterocycle has a tertiary nitrogen atom which adds to the electron density and aromatic stabilization. Moderate

conformational flexibility of the tetrahydro ring is maintained whilst maintaining the overall rigidity and planarity of the conjugated core. The azomethine group is an important conjugative link between the heterocyclic nucleus and the hydroxyphenyl ring, which provide convenient electron delocalization throughout the molecule. Such delocalization results in increased intramolecular charge transfer and may significantly affect the electronic, optical and fluorescent properties of the compound. The almost planar conformation of the aromatic rings and the imine linkage provide a resonance stabilized structure and facilitates intermolecular π – π stacking interactions in the crystal structure. The hydrogen-bonding pattern seen in the packing is an important structural feature, in which, several hydrogen-bonding motifs are connected to the neighbouring molecules in a multidimensional supramolecular network. The oxygen atoms in the phenols are hydrogen donors and the nitrogen atoms in the azomethine and hydroxyl groups are the hydrogen acceptors. As a result of these interactions, continuous chains and interconnected layers are created that can extend through the crystal lattice. Aside from intermolecular hydrogen bonding, there are also intramolecular O–H...N hydrogen bond(s) that are likely to exist to stabilize the enol–imine tautomeric form and aid in molecular planarity. This hydrogen-bond-assisted stabilization is a typical property of hydroxy Schiff base compounds, and has a strong impact on the molecular geometry, electronic distribution and crystal stability. The crystal packing also shows that there are cooperative non-covalent interactions such as π – π stacking and weak C–H... π contacts between neighbouring aromatic systems. The supramolecular assembly taking place is further strengthened by these interactions, which also lead to the high level of molecular packing. The hydrogen bond network and aromatic stacking interactions contribute to a strong 3D network which can potentially affect the thermal stability, optical properties, and solid-state electronic properties of the material. The long conjugation sequence and structured packing arrangement could help in charge transport and enhance the efficiency of the fluorescence in the crystal form. The molecule has several donor groups, such as phenolic oxygen and azomethine nitrogen atoms, which make it highly coordinating towards transition metal ions, from a coordination chemistry and material science point of view. Quinoline-based Schiff base compounds with phenolic groups are well known for their wide biological and physicochemical applications such as antimicrobial, antioxidant, anticancer, catalytic and sensing properties. The current crystal structure illustrates the control of the molecular stability and functionality by hydrogen bonding and supramolecular organization. The overall structure of the title compound is structurally complex, with extensive multidimensional supramolecular interactions and conjugation, and is

consequently a candidate for further studies into crystal engineering, molecular electronics, coordination chemistry and advanced functional materials research.

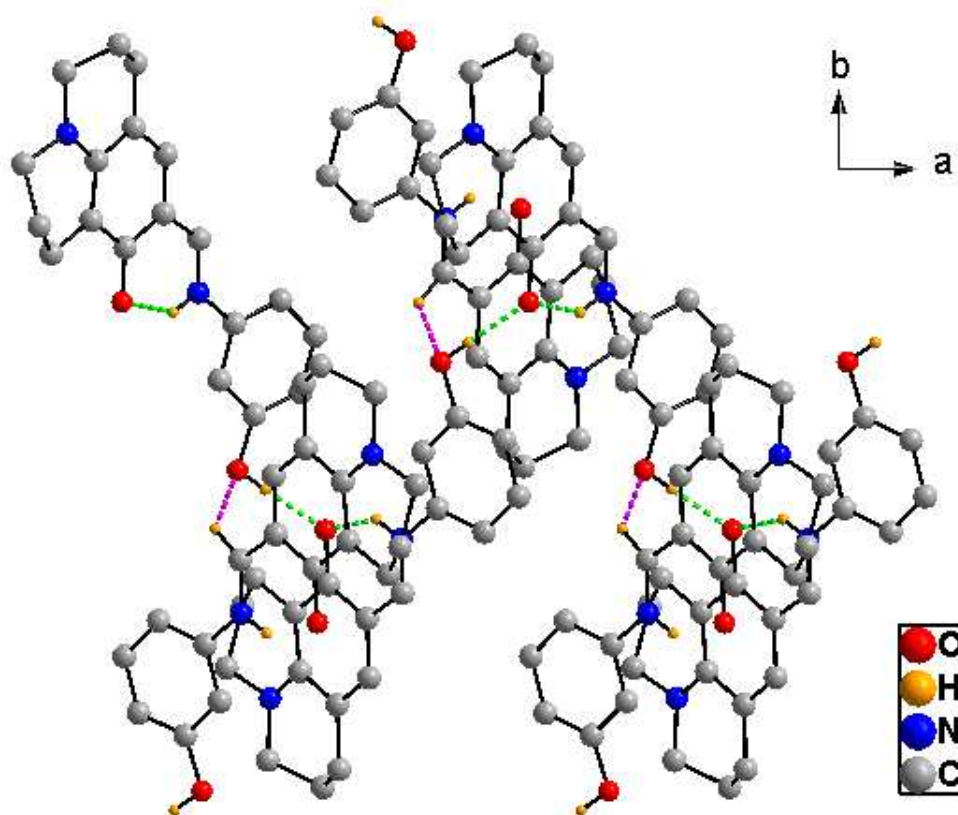


Figure:6 Three-Dimensional Hydrogen-Bonded Supramolecular Network and Crystal Packing Analysis of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

UV Visible of keto form

The UV–Visible absorption spectrum of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol shows two characteristic absorption bands, namely, those associated with the electron transitions of the conjugated heterocyclic system. A strong and intense absorption band is observed around 220-230 nm and another broad absorption band is observed around 365-370 nm as seen in the spectrum. The absorption features are typical of highly conjugated Schiff base derivatives of fused aromatic rings with an azomethine linkage. The absorption band with high energy is quite intense (220–230 nm), and is believed to result mainly from $\pi \rightarrow \pi^*$ electronic transitions in the π -conjugated fused pyridoquinoline and hydroxyphenyl rings. These aromatic systems have a very delocalized system, and it is difficult to excite the bonding π -electrons to the antibonding π^* orbitals

because of the high energy involved, which leads to intense absorption in the UV region. This band is highly absorbing, which means that the conjugation is good throughout the aromatic skeleton. The second absorption band seen at around 365–370 nm is assigned mostly to $n \rightarrow \pi^*$ electronic transitions of the lone pair of electrons on the imine nitrogen and carbonyl oxygen found in the keto tautomer (Figure:7). This has a long wavelength because it involves a lower amount of energy to get excited than the $\pi \rightarrow \pi^*$ transition. The presence of this rather broad visible-near UV band is indicative of the presence of an extended conjugated electronic system and efficient intramolecular charge transfer (ICT) between the electron donating phenolic group and the electron accepting azomethine/carbonyl region. This bathochromic shift towards a longer wavelength is typical of Schiff bases that have extensive π -conjugation and good donor-acceptor interactions. The keto form is stabilized by proton transfer from the phenolic hydroxyl group to the imine nitrogen to form a keto–amine tautomer. This structural change allows for greater charge delocalisation throughout the molecular backbone and allows for greater delocalisation within the fused pyridoquinoline nucleus and the substituted phenyl ring. This in turn causes the electronic transitions to be more delocalized and to be absorbed at longer wavelengths. This type of behaviour is frequently seen in hydroxy substituted Schiff bases which can undergo intramolecular proton transfer. The fact that there is no significant absorption until above 450 nm suggests that the compound is essentially colourless to light yellow under normal conditions and has a comparatively large gap between the HOMO and LUMO energy levels when compared to strongly coloured organic dyes. The absorption feature deep into the visible, however, indicates that there is some moderate charge-transfer character, likely contributing to fluorescence and nonlinear optical activity. Presence of highly-conjugated heterocyclic Schiff base system is confirmed by UV–Visible spectrum.

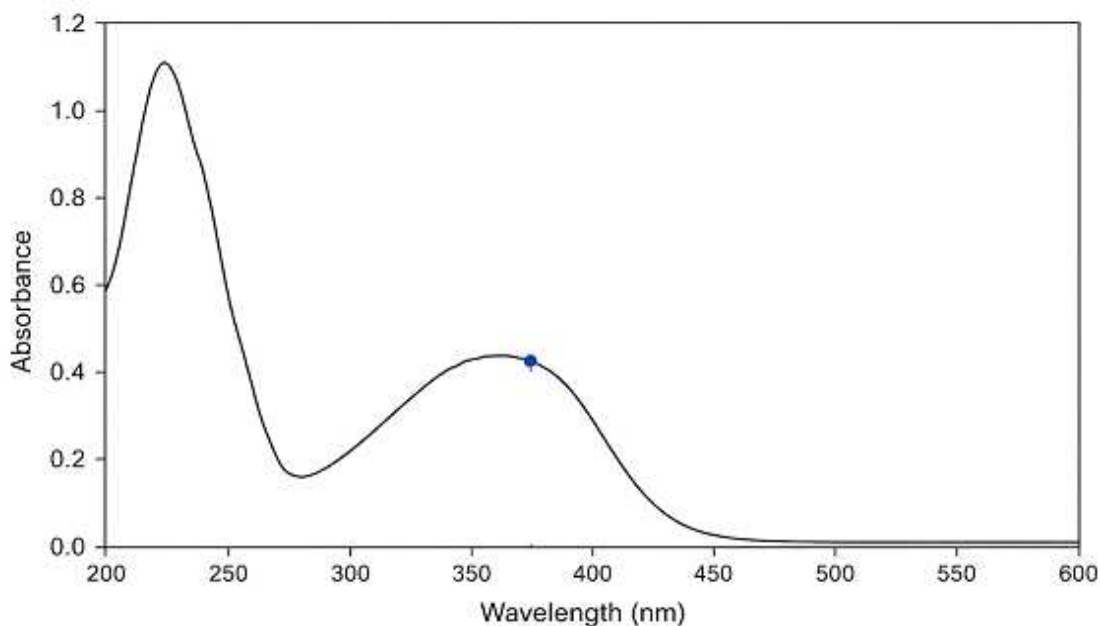


Figure:7 UV Visible of Keto form of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

The strong $\pi \rightarrow \pi^*$ transition at 220-230 nm and the wide $n \rightarrow \pi^*$ / intramolecular charge transfer (ICT) band at ~ 365 -370 nm are very good indicators of the successful formation of the Schiff base and stabilization of the keto tautomer. The electronic communication is seen to be efficient throughout the conjugated framework and these spectral features are entirely consistent with the proposed structure, single crystal X-ray diffraction data and the theoretical analysis of frontier molecular orbitals. The observed electronic transitions also indicate that the compound could have interesting applications in the areas of molecular electronics, fluorescent materials, optical sensors, and coordination chemistry.

UV Visible of Enol form

The UV–Visible absorption spectrum of the enol tautomer of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol exhibits two characteristic absorption bands that are typical of highly conjugated hydroxy Schiff base systems. As shown in the spectrum, an intense absorption band appears at approximately 215–225 nm, while a second broad absorption band is observed at around 340–350 nm. These bands originate from electronic transitions within the conjugated pyridoquinoline framework and the azomethine ($-\text{CH}=\text{N}-$) chromophore. The strong absorption band in the 215–225 nm region is assigned to $\pi \rightarrow \pi^*$ transitions of the aromatic π -electron system. This transition arises from excitation of π -

electrons localized within the fused pyridoquinoline ring and the substituted hydroxyphenyl ring into antibonding π^* molecular orbitals. The high intensity of this band reflects the extensive conjugation present throughout the molecule and confirms efficient delocalization of electrons over the aromatic framework (Figure:8). The second absorption maximum centered at approximately 345 nm is attributed mainly to the $n \rightarrow \pi^*$ transition associated with the lone-pair electrons of the azomethine nitrogen atom together with an intramolecular charge-transfer (ICT) transition between the electron-donating phenolic hydroxyl group and the electron-accepting imine functionality.

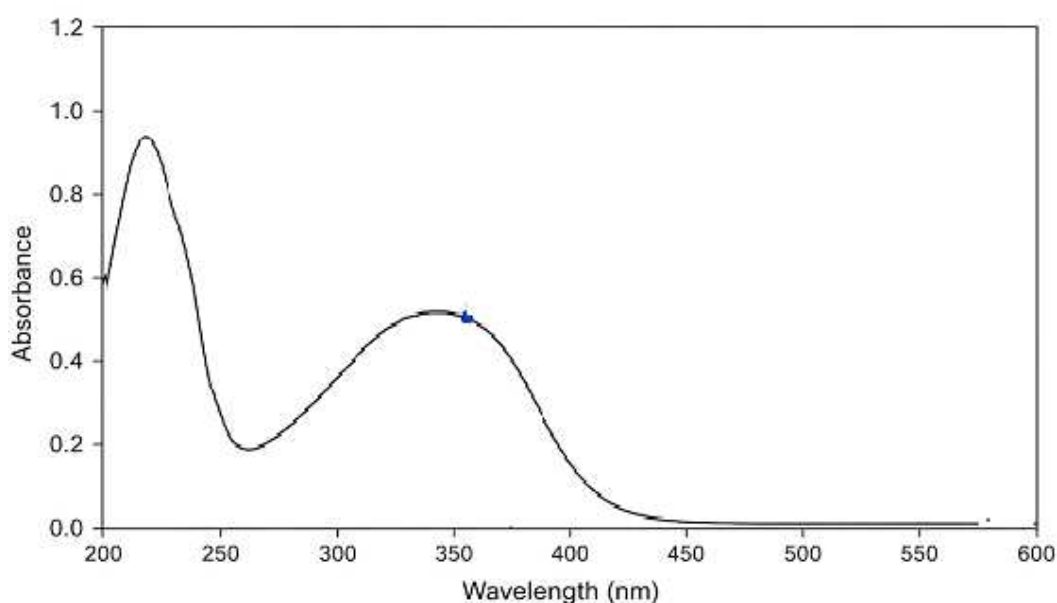


Figure:8 UV Visible of Enol form of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

In the enol form, the phenolic hydroxyl group remains attached to the aromatic ring and forms a strong intramolecular $O-H \cdots N$ hydrogen bond with the azomethine nitrogen. This hydrogen bond increases molecular planarity and enhances π -electron delocalization, thereby stabilizing the enol-imine tautomer and shifting the absorption toward longer wavelengths. Compared with the keto tautomer, the enol form exhibits its principal low-energy absorption at a slightly shorter wavelength (around 345 nm). This hypsochromic (blue) shift is consistent with the absence of a carbonyl group and the different electronic distribution in the enol structure. Although the molecule possesses an extended conjugated system, the HOMO–LUMO energy gap of the enol form is slightly larger than that of the keto form, resulting in absorption at a somewhat higher energy. The broad nature of the band indicates efficient electronic communication across the fused heterocyclic core, the azomethine bridge, and the para-hydroxyphenyl substituent. The absorption intensity decreases rapidly beyond 400 nm, and

essentially no significant absorption is observed above 450 nm. This behavior indicates that the compound is expected to be pale yellow in appearance while maintaining excellent transparency in the visible region. The absence of strong visible absorption also suggests that the electronic transitions are primarily confined to the ultraviolet region with moderate charge-transfer character. The UV–Visible spectrum confirms the highly conjugated nature of the synthesized Schiff base and supports the existence of the enol–imine tautomer stabilized by intramolecular hydrogen bonding. The intense $\pi \rightarrow \pi^*$ transition at 215–225 nm and the broad $n \rightarrow \pi^*$ /ICT band at approximately 345 nm are characteristic spectral features of hydroxy-substituted Schiff bases containing fused quinoline systems. These results are consistent with the proposed molecular structure, single-crystal X-ray diffraction analysis, and theoretical DFT calculations, demonstrating efficient π -conjugation and favorable electronic delocalization. The observed spectral characteristics further suggest that the compound possesses promising potential for applications in fluorescence sensing, optoelectronic materials, nonlinear optics, and coordination chemistry.

Comparative Electronic Structure and Tautomeric Investigation of Enol and Keto Forms

The molecular system shown in the figure represents the relative structural and electronic properties of the enol and keto tautomers of a conjugated Schiff base with a fused pyridoquinoline framework, namely 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol. Compounds containing an azomethine nitrogen and a hydroxyl oxygen atom often undergo tautomerism by proton transfer between these two atoms, with the result that two tautomer forms, the enol–imine and keto–amine, exist in equilibrium. The proton stays with the phenolic O atom and the azomethine linkage retains its C=N double bond in its enol form. The keto form arises on the other hand due to the transfer of a proton from O to N, leading to the formation of an N–H group and a carbonyl (C=O) functionality (Figure:9). This tautomeric equilibrium has a large influence on the structural stability, electronic distribution, optical properties and coordination properties of the molecule. The figure shows the optimized molecular geometries and frontier molecular orbital distributions for both the tautomers. In the enol form, the molecule is strongly conjugated throughout the fused pyridoquinoline, the azomethine bridge and the hydroxy-substituted phenyl ring. The planar structure is stabilized by an intramolecular O–H...N hydrogen bond and is important for the electron delocalisation throughout the π -conjugated system.

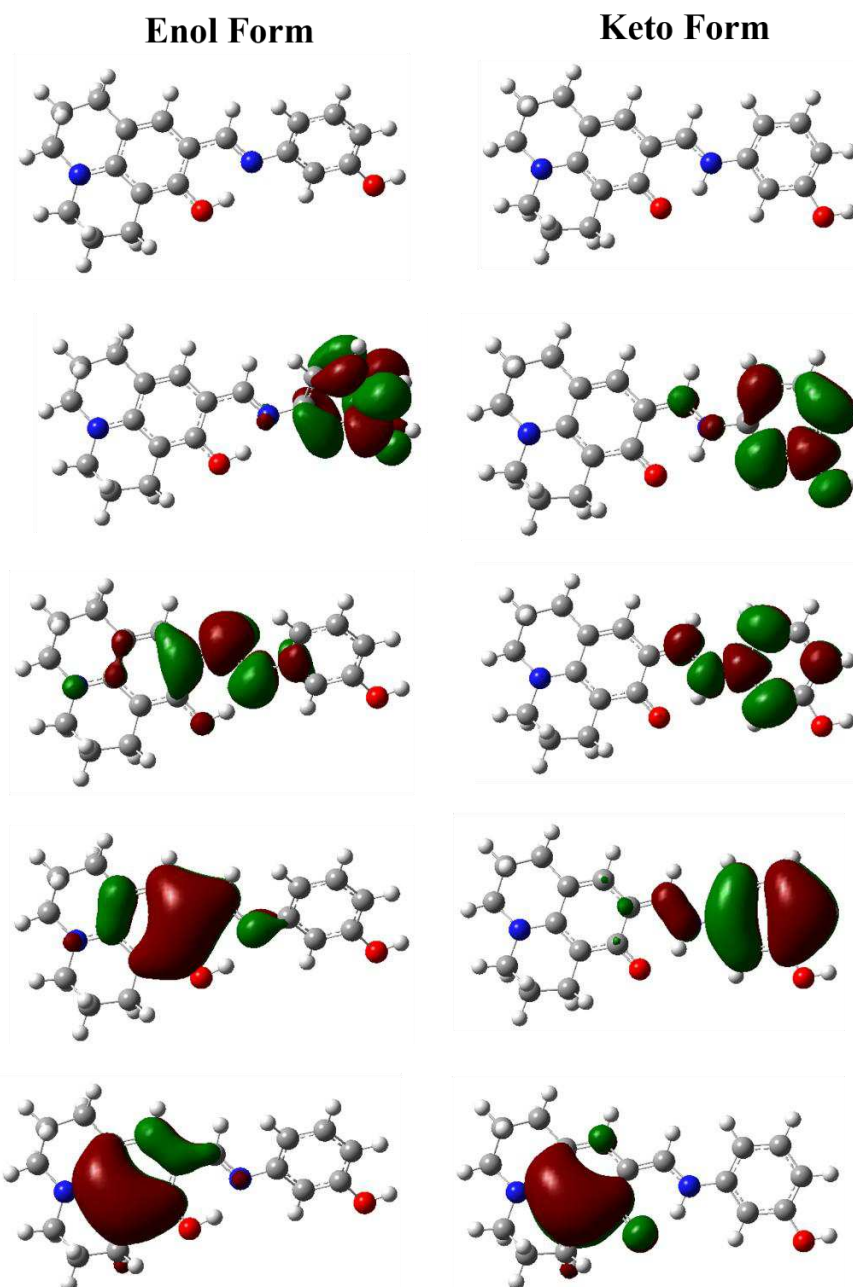


Figure:9 Comparative Electronic Structure and Tautomeric Investigation of Enol and Keto Forms of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

The molecular system shown in the figure represents a relative structural and electronic properties of enol and keto forms of a conjugated Schiff base with a fused pyridoquinoline framework, 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol. Many compounds with an azomethine nitrogen and a hydroxyl oxygen atom are able to tautomerise by proton transfer between the two atoms and hence exist as a mixture of enol–imine and keto–amine tautomers. The proton stays with the phenolic O atom and the

azomethine linkage retains its C=N double bond in its enol form. The keto form arises on the other hand due to the transfer of a proton from O to N, leading to the formation of an N–H group and a carbonyl (C=O) functionality (Figure:9). The tautomeric equilibrium greatly affects the structure stability, electronic distribution, optical and coordination properties of the molecule. The optimized molecular geometries and the distributions of the frontier molecular orbital are shown in the figure for both tautomers. The molecule is quite conjugated, extending over the entire fused pyridoquinoline and the azomethine bridge plus the hydroxy-substituted phenyl ring. The planar structure is stabilized by an intramolecular O–H•••N hydrogen bond and is important for the electron delocalisation throughout the π -conjugated system.

Hirshfeld Surface Analysis and Intermolecular Interaction Mapping

The Hirshfeld surface analysis of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol provides valuable insight into the intermolecular interactions, molecular packing behavior, and supramolecular organization present within the crystal lattice. The figure illustrates different Hirshfeld surface properties represented through various mapped surfaces labeled (a–f), which collectively reveal the nature and distribution of intermolecular contacts surrounding the molecule (Figure:10). The title compound is a highly conjugated Schiff base incorporating a fused pyridoquinoline heterocyclic core linked to a para-hydroxy substituted phenyl ring through an azomethine (–CH=N–) bridge. The presence of phenolic hydroxyl groups, aromatic rings, and nitrogen donor centers allows the molecule to participate in multiple non-covalent interactions, which are crucial for crystal stabilization and molecular assembly. The Hirshfeld surface mapped over normalized contact distance (d_{norm}) clearly highlights the regions involved in close intermolecular interactions. The intense red spots observed near the hydroxyl oxygen atoms and azomethine nitrogen centers correspond to short O–H•••N and O–H•••O hydrogen-bonding contacts. These interactions indicate strong donor–acceptor relationships that significantly contribute to the stabilization of the crystal structure. The blue and green regions represent areas with longer intermolecular separations and weaker van der Waals interactions. The distribution of these colored regions across the molecular surface demonstrates that hydrogen bonding is localized mainly around the phenolic oxygen atoms and imine nitrogen sites, confirming their essential role in supramolecular organization. The shape index surface provides further evidence for aromatic π – π stacking interactions within the crystal lattice. Alternating red and blue triangular patches on the molecular surface indicate complementary convex and concave regions associated with

aromatic ring overlap between neighboring molecules. Such π – π interactions enhance crystal cohesion and contribute to efficient molecular packing. The curvedness map also supports this interpretation by showing flat green regions corresponding to planar aromatic surfaces involved in stacking interactions.

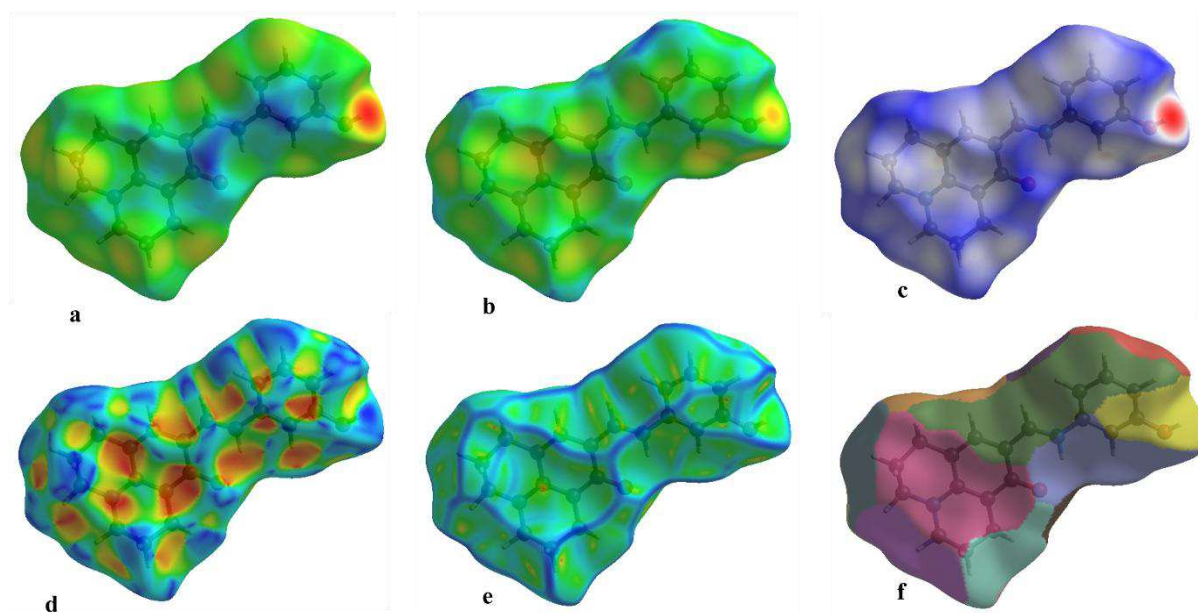


Figure:10 Hirshfeld Surface Analysis and Intermolecular Interaction Mapping of 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

The observations are in agreement that both hydrogen bonding and π – π stacking play a cooperative role in stabilizing the three dimensional crystal network. The electronic distribution over the molecular framework can be visualised in the form of electrostatic potential mapping of the Hirshfeld surface. Electron-rich regions are mostly concentrated around the oxygen and nitrogen atoms because they are more electronegative, and electron deficient regions are spread out over the hydrogen atoms and some aromatic carbon atoms. The oxygen atoms of the phenolics have significant negative electrostatic potential, which is a property of hydrogen-bond acceptors and donors. The azomethine nitrogen also plays an important role in the distribution of the electron density and in the intramolecular charge transfer. The fused pyridoquinoline framework allows for a wide π -electron delocalisation, which could affect the optical and electronic properties. The Hirshfeld surface analysis-generated fingerprint plots yield quantitative data on the amount of contribution from different intermolecular contacts. The crystal packing is normally dominated by the H...H interactions, as there are many hydrogen atoms in the molecular framework. But O...H/H...O interactions

are very significant due to strong hydrogen bonding interactions through hydroxyl groups. C...C contacts that arise from π - π interactions also have a significant contribution to the crystal stabilization. These interactions, integrated together, create a strong supramolecular structure, resulting in an improved molecular organization. The Hirshfeld surface analysis shows that the crystal structure of the title compound is driven by both strong hydrogen bonding and aromatic stacking interactions along with van der Waals forces. This Schiff base derivative is a highly conjugated molecule with hydrogen-bond donor-acceptor properties and a well-ordered supramolecular structure, and thus is an interesting system for crystal engineering, coordination chemistry, molecular electronics, and pharmaceutical materials studies.

Hirshfeld Fingerprint Analysis and Intermolecular Contact Contributions

A Hirshfeld surface fingerprint analysis of 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol gives a detailed quantitative description of the intermolecular interactions that govern the crystal packing and supramolecular organisation for the molecule. The figure shows Hirshfeld surfaces and their associated two dimensional fingerprint plots for total intermolecular interactions and the individual contributions from the contacts. The compound has a highly conjugated azomethine ($-\text{CH}=\text{N}-$) linked framework with a pyridoquinoline fused heterocyclic core with para-hydroxy substituted phenyl ring. There are several possible donor and acceptor centers in the molecular structure such as hydroxyl oxygens and imine nitrogen atoms that are actively participating in hydrogen bonding and other non-covalent interactions in the crystal lattice. The overall intermolecular contact distribution around the Hirshfeld surface is shown in the complete fingerprint plot "All = 100%". The wide central area and the sharp spikes suggest that weak van der Waals contacts and strong hydrogen-bonding interactions occur at the same time (Figure:11). The two sharp peaks pointing to the lower d_e and d_i values are due to close intermolecular contacts, which are mainly of the type $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ and are related to the phenolic hydroxyl groups. Such interactions play a significant role in the stabilization of the crystal packing, and in the organization of supramolecular assemblies. The Hirshfeld surface mapped with d_{norm} also shows very large red spots near the oxygen atoms, which is a sign of strong short-range intermolecular interactions. Hydrogen-hydrogen interactions are the most important for the crystal packing environment as the $\text{H}\cdots\text{H}$ contact contribution accounts for about 58.1% of the total Hirshfeld surface area. The reason for such interaction is the presence of many hydrogen

atoms disposed on the aromatic and aliphatic parts of the molecule in the molecular crystals of organic compounds.

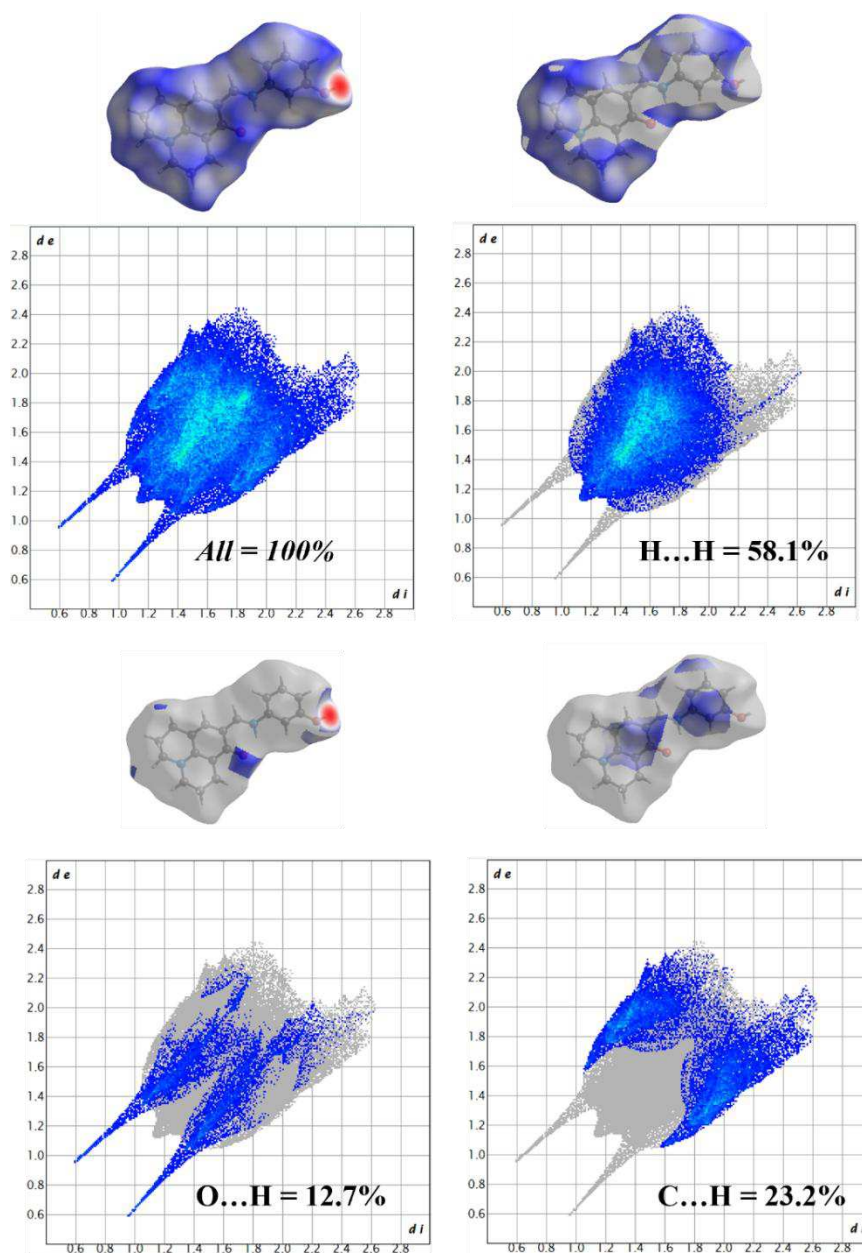


Figure:11 Quantitative Hirshfeld Fingerprint Analysis and Intermolecular Contact Contributions in 9-[(4-Hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol.

Contacts are weak but when they are present in many of them they contribute to the stabilization of crystals by van der Waals forces. The fingerprint plot for H...H interactions shows a fairly wide symmetrical distribution, typical of a high level of contact surface between neighbouring hydrogen atoms. The O...H/H...O interactions account for about 12.7% of the Hirshfeld

surface. This is a relatively high proportion which establishes the role of the phenolic oxygen atoms in hydrogen bonding in the crystal structure. The fingerprint plot for this corresponds to sharp spikes at low d_e and d_i values, signifying strong and directional hydrogen-bond interacting characteristics. These are mainly O–H...N and O–H...O intermolecular hydrogen bonds which connect neighbouring molecules to form supramolecular chains or networks. These interactions play a vital role in orientating the molecules, in packing the molecules into the crystal and in the stability of the structure. The C...H/H...C contacts account for about 23.2% of the intermolecular contacts. Such interactions involve weak C–H... π interactions and edge-to-face aromatic contacts between neighbouring molecules. A plot of the fingerprint that shows C...H interactions has characteristic wing-like structures, suggesting that aromatic carbon atoms are involved in close intermolecular contacts. These interactions are in addition to the hydrogen bonding interactions and provide extra non-covalent stabilization of the crystal. Within the pyridoquinoline and phenyl rings, there are π -systems that further aid in the π – π stacking, which could affect the optical and electronic properties of the material. The Hirshfeld fingerprint analysis shows that the crystal packing of the title compound is controlled by a balance between hydrogen bonding, van der Waals interactions, C–H... π contacts and aromatic stacking interactions. The three elements (the fused heterocyclic framework, the conjugated azomethine linkage and the hydroxyl substituents) together create a very organized supramolecular structure. The intermolecular forces are very significant in determining the stability, structure and physico-chemical properties of the compound. The present analysis gives a valuable structural insight of the crystal engineering and molecular recognition behavior of this important biologically and electronically Schiff base derivative.

Conclusion

The novel Schiff base 9-[(4-hydroxy-phenylimino)-methyl]-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-8-ol has been successfully synthesized and comprehensively characterized in the present study. The condensation of 8-hydroxy-9-formyl-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline with p-aminophenol successfully gave the desired product in good yield, which proved the efficiency of the adopted synthetic path. The molecular geometry, electronic structure and supramolecular organization of the molecule were fully understood by its structural elucidation using ^1H NMR, UV–Visible spectroscopy, single-crystal X-ray diffraction, Hirshfeld surface analysis, and density function theory (DFT). The spectroscopic studies confirmed formation of the azomethine ($-\text{CH}=\text{N}-$) linkage as well as the

presence of hydroxyl functional groups and the characteristic $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions related to the extended conjugated system was observed in the UV–Visible spectra. The crystal structure was determined by single crystal x-ray analysis which confirmed the molecular geometry and revealed that strong intramolecular O–H $\cdots$ N hydrogen bonding as well as intermolecular hydrogen-bonding interactions, C–H $\cdots$ π contacts and weak π – π interactions stabilize the crystal structure. The intermolecular contacts were also quantified using Hirshfeld surface analysis, which showed that the most important ones for crystal packing and stability in the crystal are H $\cdots$ H, C $\cdots$ H/H $\cdots$ C and O $\cdots$ H/H $\cdots$ O interactions. The DFT calculations confirmed the experimental results by correctly reproducing the optimized molecular structure and effects of keto–enol tautomerism on the molecular geometry, frontier molecular orbitals, electron density distribution, and HOMO–LUMO energy gap. This close match between theoretical and experimental results confirms the validity of the computational model and its high reliability when applying this hybrid approach based on crystallographic and quantum chemical methods to study Schiff base systems. Moreover, the synthesized compound shows electronic delocalization and intramolecular charge transfer and strong hydrogen-bonding network, which provides it with good physicochemical properties for functional applications. The fused pyridoquinoline framework along with the phenolic and imine donor sites offers very good prospects for metal-ion coordination, fluorescent sensing, nonlinear optical properties, molecular recognition, and in biologically active heterocyclic systems. In conclusion, the present work has laid the groundwork for establishing a detailed structure–property relationship of the synthesized compound and has shown the importance of combining synthetic chemistry, spectroscopy, crystallography, Hirshfeld surface analysis and DFT calculations in the design and evaluation of advanced quinoline based Schiff bases. The results are encouraging and serve as a solid basis for further research on the metal complexes, photophysical characteristics, biological activities, and optoelectronic applications of the potential group of heterocyclic materials studied.

Competing interests

None

Declarations

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Consent for publication: Not applicable.

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