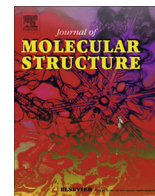




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Synthesis, biological activity, DNA binding and anion sensors, molecular structure and quantum chemical studies of a novel bidentate Schiff base derived from 3,5-bis(trifluoromethyl)aniline and salicylaldehyde



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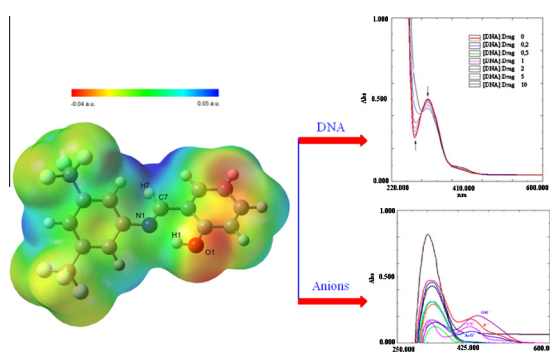
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HIGHLIGHTS

- The molecular structure of the compound in the ground state was studied.
- The potential binding ability of Schiff base to CT-DNA was characterized.
- The antimicrobial activities of the compound were investigated.
- The colorimetric response of the Schiff base receptors in DMSO was investigated.
- ¹H NMR titrations were carried out in DMSO-d₆.

GRAPHICAL ABSTRACT



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ABSTRACT

Synthesis, biological activity, spectroscopic and crystallographic characterization and density functional theory (DFT) studies of the Schiff base 3,5-bis(trifluoromethyl)aniline and salicylaldehyde are reported. It crystallizes as a monoclinic space group $P2_1/c$ with $a = 7.7814(3)$ Å, $b = 26.8674(9)$ Å, $c = 7.4520(2)$ Å, $V = 1379.98(8)$, $Z = 4$, $D_c = 1.6038$ g cm⁻³, and $\mu = 0.156$ mm⁻¹. The molecular structure obtained from X-ray single-crystal analysis of the investigated compound in the ground state was compared using Hartree-Fock (HF) and density functional theory (DFT) with the functionals B3LYP and B1B95 using the 6-311++G(d,p) basis set. The antimicrobial activities of the compound were investigated for its minimum inhibitory concentration (MIC). The interaction of the Schiff base with calf thymus DNA was investigated using UV-visible spectra. The colorimetric response of the Schiff base receptors in DMSO was investigated before and after the addition of an equivalent amount of each anion to evaluate the anion recognition properties.

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Introduction

Schiff bases have been reported for their biological properties, such as antibacterial, antifungal, antiinflammatory, analgesic,

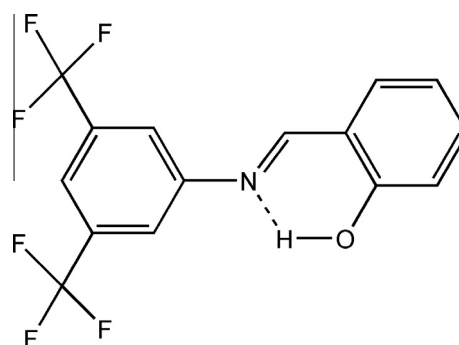
anticonvulsant, antitubercular, anticancer, antioxidant and anti-helminthic activities [1–26]. Schiff base metal complexes have applications in the areas from material science to biological sciences. They have been widely studied because they have anticancer and herbicidal applications [20,21]. Schiff base complexes show greater biological activity than free ligands [3,6,22–26]. The DNA binding, cytotoxicity and apoptosis induction activity were studied for Schiff base copper(II) complexes [27–29]. A rather commonly used technique regards the development of fluorescent chemosensor quenching of fluorescence by interaction with anions. The sensors can provide fast and visible color changes from yellow to red in the presence of strong basic anions. Over the past 10 years, several excellent chemosensors have been reported for recognition and sensing of anions with high selectivity and sensitivity [30–37]. Tautomerism in Schiff bases with an OH group in ortho position to the imino group both in solution and in solid state were investigated using spectroscopy and X-ray crystallography techniques [4,5,38–44]. Schiff bases with OH group in ortho position to the imino group are of interest mainly due to the existence of either O—H···N or O···H—N type hydrogen bonds and tautomerism between enol-imine and keto-amine form. In some instances the hydrogen from the OH group is completely transferred to the imine nitrogen. In other words, enol-imine \rightleftharpoons keto-amine equilibrium shifts predominantly to the keto-amine side. The keto-amine form is always observed when the Schiff base is derived from 2-hydroxy-1-naphthaldehyde and aromatic amine. In Schiff bases derived from salicylaldehyde and aromatic amines, the keto-amine form is not observed in solution and solid state.

In this study, a novel bidentate Schiff base has been synthesized by the reaction of 3,5-bis(trifluoromethyl)aniline with 2-hydroxy-1-benzaldehyde. The structure of the synthesized Schiff base was investigated using data obtained from elementary analysis, FT-IR, UV-visible, ^1H NMR and ^{13}C NMR techniques. The solid state structure of the Schiff base (*E*)-2-[(3,5-bis(trifluoromethyl)phenylimino)methyl]phenol (Scheme 1) was also determined crystallographically. The minimal inhibitory concentration (MIC) of the compound was screened in vitro against bacteria and yeast cultures using broth micro dilution tests [45–48]. DNA binding of the Schiff base was investigated. Also, anion sensing ability of the Schiff base was observed colorimetrically in DMSO for F^- , Br^- , I^- , CN^- , SCN^- , ClO_4^- , HSO_4^- , CH_3COO^- , H_2PO_4^- , N_3^- and OH^- anions. The molecular structure, atomic charges, molecular electrostatic potential (MEP), nonlinear optical (NLO) effects and thermodynamic properties of the compound were investigated by DFT. The result of theoretical calculations was compared with crystallographic data. Additionally, we theoretically investigated the geometric structure and energy contents of both enol-imine and keto-amine tautomers of the compound.

Experimental

Reagents and techniques

The ^1H and ^{13}C NMR spectra were recorded on a Bruker AVANCE-500 spectrometer operating at 400 and 101.6 MHz. Infrared absorption spectra were obtained from a Perkin Elmer BX II spectrometer in KBr discs and were reported in cm^{-1} units. The UV-Vis spectra were measured using a SHIMADZU 1800 series spectrometer. Elementary analyses were performed on a Vario EL III CHNS elemental analyzer. Melting points were measured with an Electro Thermal IA 9100 apparatus using a capillary tube. 3,5-Bis(trifluoromethyl)aniline, salicylaldehyde, EtOH, Ethidium bromide (EB), calf thymus DNA (CT-DNA), $(\text{Bu})_4\text{NF}$, $(\text{Bu})_4\text{NBr}$, $(\text{Bu})_4\text{NI}$, $(\text{Bu})_4\text{NCN}$, $(\text{Bu})_4\text{NSCN}$, $(\text{Bu})_4\text{NClO}_4$, $(\text{Bu})_4\text{NH}_2\text{SO}_4$, $(\text{Bu})_4\text{NCH}_3\text{COO}$, $(\text{Bu})_4\text{NH}_2\text{PO}_4$, $(\text{Bu})_4\text{NN}_3$, $(\text{Bu})_4\text{NOH}$ and DMSO were purchased from Aldrich. The Tris-HCl buffer solution was



Scheme 1. The chemical formula of the title compound.

prepared with triple-distilled water. CT-DNA stock solution was prepared by diluting DNA to Tris-HCl/NaCl buffer (5 mM Tris-HCl, 50 mM NaCl, pH 7.2), and kept at 4 °C for no longer than two days.

Synthesis of (*E*)-2-[(3,5-bis(trifluoromethyl)phenylimino)methyl]phenol

3,5-Bis(trifluoromethyl)aniline (0.50 g, 2.18×10^{-3} mol) was added to EtOH (100 mL) solution of salicylaldehyde (0.265 g, 2.18×10^{-3} mol) [44]. The mixture was stirred and refluxed for 1 h. Compound (**1**) was obtained from the evaporation of EtOH. It was crystallized from CHCl_3 : n-hexane (3:2) as a yellow crystal, mp 86 °C, 0.57 g (85%) yield. Found: C, 54.05; H, 2.72; 4.20. Calc. For $\text{C}_{15}\text{H}_9\text{F}_6\text{NO}$; C, 54.07; H, 2.70; N, 4.20%. IR(KBr, cm^{-1}); $\nu_{\text{O-H}}$; 3434 m, $\nu_{\text{Ar-H}}$; 3098 w, $\nu_{\text{C=N}}$; 1629 s, $\nu_{\text{C=C}}$; 1616–1602, 1582s, $\nu_{\text{C-N}}$; 1497 m, $\nu_{\text{C-O}}$; 1361 m. ^1H NMR (DMSO); δ ppm, 12.25 (s, 1H, Ar—OH); 9.07 (s, 1H, Ar—CH=N—); 8.10–6.97 (m, 7H, Ar—H). ^{13}C NMR (DMSO); δ ppm, 119.89 (s, 1C, C—CH=N); 160.23 (s, 1C, C—OH); 116.73 (s, 1C, CH—C—OH); 132.71 (s, 1C, CH—CH—C—OH); 122.07 (s, 1C, CH—CH—C—CH=N); 131.48 (s, 1C, CH—C—CH=N); 166.57 (s, 1C, —CH=N); 150.62 (s, 1C, C—N=CH); 124.24 (s, 2C, CH—C—N=CH); 134.15 (s, 2C, C—CF₃); 122.48 (s, 1C, CH—C—CF₃); 131.21 (s, 2C, CF₃).

Crystallography

Crystallographic data were recorded on a Bruker Kappa APEXII CCD area-detector diffractometer using Mo K α radiation ($\lambda = 0.71073$ Å) at $T = 100$ K. Data collection, reduction and corrections for absorption and crystal decomposition for the compound were achieved by using X-AREA, X-RED software [49] and the structure was solved by SHELXS-97 and refined with SHELXL-97 [50,51]. The positions of the H atoms bonded to C atoms were calculated (C—H distance 0.96 Å), and refined using a riding model, but the H1 atom of the O1 was found in a difference electron-density map at the end of the refinement process as a small positive electron density. All atoms (except hydrogen) were located from a difference Fourier map and refined anisotropically. The atoms of $\text{C}(10)\text{F}_3$ group are disordered over two positions. For F1, F2 and F3 atoms the site occupancy factor is 0.65 and for F1A, F2A, and F3A atoms the site occupancy factor is 0.35. The details of the X-ray data collection, structure solution and structure refinements are given in Table S1. The bond distances, bond and torsion angles are listed in Table S2. The molecular structure with the atom-numbering Scheme is shown in Fig. 1 [52]. Crystallographic data (excluding structure factors) for the structures reported in this paper has been deposited with the Cambridge Crystallographic

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