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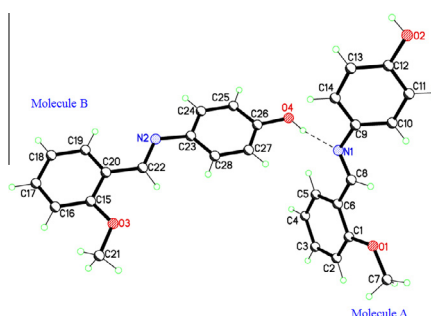
Anticancer, photoluminescence and electrochemical properties of structurally characterized two imine derivatives

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HIGHLIGHTS

- Anticancer.
- Photoluminescence.
- Imine derivatives.
- X-ray crystallography.

GRAPHICAL ABSTRACT

Molecular structure of the compound L¹ with atom numbering. Intra-molecular hydrogen bonding (OH...N) is shown as dashed lines.

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ABSTRACT

Two imine compounds, 4-[(E)-(2-methoxybenzylidene)amino]phenol (L¹) and 4-[(E)-(3,4-dimethoxybenzylidene)amino]phenol (L²) were synthesized and characterized by the analytical and spectroscopic methods. The electrochemical and photoluminescence properties of the imine compounds L¹ and L² were investigated in different solvents. The compounds L¹ and L² show different redox processes at some potentials. The molecular structures of two Schiff base compounds are broadly similar, differing principally in the position, the number of methoxy (–OCH₃) groups and dihedral angles between aromatic rings. While the compound L¹ has only one methoxy group located on the *o*-position with respect to the imine bond (C=N), the L² contains two methoxy groups on the *p*-*m*-positions with respect to the imine bond. The imine compounds show two or three emission bands in the 619–832 nm range in organic solvents. In the 1.0 × 10^{−3} M concentration, the compounds have the highest excitation and emission bands. The imine compounds L¹ and L² were screened for their *in vitro* cytotoxicity on HeLa cell lines using the xCELLigence system (Real Time Cell Analyzer).

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Introduction

Imine compounds (called also Schiff bases) are synthesized from the reaction of aliphatic or aromatic primary amines with

aldehydes or ketones. They are nitrogen analog of an aldehyde or a ketone in which the carbonyl group (CO) has been replaced by an imine (azomethine –C=N–) group. Schiff bases form an important class of the most widely used as organic compounds and has a wide variety of applications in many fields, e.g., biological, inorganic and analytical chemistry. Some of them are the basic units in certain dyes and are also used as liquid crystals. Schiff bases

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appear to be important intermediates in a number of enzymatic reactions involving interaction of an enzyme with an amino or a carbonyl group of a substrate [1].

Imine compounds, obtained frequently from various of the heterocyclic primary amines, were reported to possess a broad spectrum of pharmacological activities with a wide range of biological properties, development of a new chemotherapeutic imine compounds is now attracting the attention of medicinal chemists [2]. They are known to exhibit a wide variety of potent activities. The pharmacologically useful activities include antibacterial, anti-convulsant, anti-inflammatory, anticancer, anti-hypertensive, anti-fungal, antipyretic, antimicrobial, anti-HIV, cytotoxic activity, hypnotic and herbicidal activities [3].

Our research group reported a series of imine compounds and their transition metal complexes as biocidal against bacteria and fungi species [4–10]. The biological effects of these compounds were found to be dose dependent. In our other research, the polydentate Schiff base ligands and their Cu(II) and Cd(II) complexes were synthesized [11]. In this research, the Schiff base complexes of cadmium were found to inhibit the intense chemiluminescence reaction in dimethylsulfoxide (DMSO) solution between luminol and dioxygen in the presence of a strong base. This effect is significantly correlated with the stability constants K_{CDL} of the complexes and the protonation constants K_{OH} of the ligands; it also has no significant association with antibacterial activity. We investigated the antioxidant and anticancer properties of the sterically hindered Schiff base compounds [12–14]. Higher absorbance of the reaction mixture indicated greater reducing power of the Schiff base ligands.

In this study, two imine compounds from the reaction of the 2-methoxy benzaldehyde or 3,4-dimethoxy benzaldehyde with 4-aminophenol in the ethanolic solution were prepared and characterized by the analytical and spectroscopic methods. The compounds were structurally characterized by X-ray diffraction studies. Additionally, electrochemical, luminescence, antioxidant and anticancer properties of the compounds were investigated. The electrochemical and photoluminescence properties of the imine compounds were investigated in different solvents and concentrations.

Experimental

Materials and measurements

All reagents and solvents were of reagent-grade quality and obtained from commercial suppliers (Aldrich or Merck). Elemental analyses (C, H, N) were performed using a LECO CHNS 932. Infrared spectra were obtained using KBr disc ($4000\text{--}400\text{ cm}^{-1}$) on a Perkin Elmer Spectrum 100 FT-IR. The electronic spectra in the $200\text{--}900\text{ nm}$ range were obtained on a Perkin Elmer Lambda 45 spectrophotometer. Mass spectra of the ligands were recorded on a LC/MS APCI AGILENT 1100 MSD spectrophotometer. ^1H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz instrument and TMS was used as an internal standard and DMSO- d_6 as solvent. The thermal studies of the compounds were performed on a Perkin Elmer STA 6000 simultaneous Thermal Analyzer under nitrogen atmosphere at a heating rate of $10\text{ }^\circ\text{C}/\text{min}$.

The single-photon fluorescence spectra of the Schiff base compounds L^1 and L^2 were collected on a Perkin Elmer LS55 luminescence spectrometer. All samples were prepared in spectrophotometric grade solvents and analyzed in a 1 cm optical path quartz cuvette. The solutions of ligands ($1.0 \times 10^{-3}\text{--}1.0 \times 10^{-7}\text{ mol L}^{-1}$) were prepared in DMF solvent. To investigate the solvent effect on the photoluminescence spectra of the ligands, the DMF,

Table 1
UV-vis absorption spectral data of the imine compounds L^1 and L^2 in the different solvents.

	$\lambda_{\text{max}} (\epsilon_{\text{max}})$									
	Methanol	Ethanol	CHCl_3	DMSO	DMF	n-Hexane	n-Heptane	Cyclohexane	Toluene	Dichloromethane
L^1	242(1.10×10^4) 272(1.00×10^4) 345(1.06×10^4)	240(0.98×10^4) 273(0.50×10^4) 342(0.72×10^4)	265(0.95×10^4) 350(1.10×10^4)	236(1.66×10^4) 343(0.66×10^4)	235(2.30×10^4) 335(1.25×10^4)	212(3.80×10^4) 250(1.40×10^4) 278(1.25×10^4) 415(1.40×10^4)	209(2.90×10^4) 256(0.80×10^4) 357(0.60×10^4)	210(3.10×10^4) 255(1.00×10^4) 358(0.80×10^4)	240(2.55×10^4) 350(2.00×10^4)	208(2.60×10^4) 256(1.30×10^4) 345(2.50×10^4)
L^2	223(2.25×10^4) 265(1.66×10^4) 291(1.70×10^4) 315(1.90×10^4)	234(1.00×10^4) 267(1.30×10^4) 322(1.50×10^4)	220(1.95×10^4) 266(1.33×10^4) 319(1.70×10^4)	275(0.75×10^4) 310(0.90×10^4)	277(0.30×10^4) 317(0.25×10^4)	219(3.50×10^4) 283(1.20×10^4) 350(1.00×10^4)	214(2.95×10^4) 289(0.95×10^4) 370(0.50×10^4)	229(1.30×10^4) 292(0.30×10^4) 355(0.10×10^4)	227(1.75×10^4) 300(0.65×10^4) 375(0.30×10^4)	225(1.55×10^4) 289(0.40×10^4) 380(0.10×10^4)

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