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Article

Structural and Theoretical Investigations, Hirshfeld Surface Analyses, and Cytotoxicity of a Naphthalene-Based Chiral Compound

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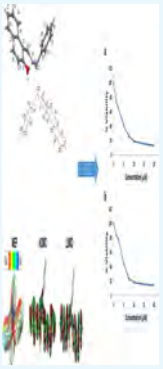
ABSTRACT: A novel Schiff base compound derived from the condensation of 2-hydroxy-1-naphthaldehyde with (1*S*,2*S*)-(−)-1,2-diphenylethylenediamine in 2:1 M ratio was reported and investigated by elemental analyses, Fourier transform infrared and NMR spectroscopic studies, and single-crystal X-ray crystallography. Hirshfeld surface analyses were also carried out to measure the various intermolecular contacts controlling the supramolecular topology, suggesting the H···O (7.6%) contacts to be the most significant interactions, whereas the H···H (48.9%) and C···H (40.2%) interactions are less-significant. The data obtained from the energy calculations revealed the structure observed experimentally to be the most stable isomer and its energy being lower by 18.0441 kcal/mol than the less stable one. Density functional theory calculations were also carried out to analyze the natural charges, reactivity descriptors, and different intramolecular charge transfer interactions. The *in vitro* anticancer activity of the compound was evaluated by MTT assays against human colorectal cancer cells, HT-29 and SW620. The results showed that the compound has potential anticancer activity against these cells lines.



INTRODUCTION

Despite the significant advances, cancer, which is caused by the unregulated proliferation of abnormal cells, remains one of the leading causes of death worldwide.[1,2] Over the years, the clinical success of cisplatin and its second-generation analogues encouraged researchers to discover new drugs with minimal side effects and maximal curative potential.[3,4] However, the use of cisplatin is limited because of severe toxic side effects including nephrotoxicity, neurotoxicity, and ototoxicity. Low water solubility, instinct, and acquired resistance exhibited in various types of cancers are also valid problems prohibiting the usage of cisplatin.[3−5] For these reasons, the development of new potential chemotherapeutic drugs with high efficacy and low toxicity is a great challenge in modern cancer research.[6]

Over the years, Schiff bases have received enormous significance in medicinal chemistry because of their biological, pharmacological, and antitumor properties, chelating behavior, preparative accessibilities, structural varieties, and varied denticities.[7−9] It is shown that the presence of the >C═N functional group is supposed to be responsible for medicinal properties exhibited by Schiff bases.[10] Furthermore, there are several reports that Schiff bases have the capability of stabilizing oxidation states of various metal ions and therefore play an extensive role in various catalytic reactions.[11] However, the geometry of Schiff bases largely depends on the diamine structural unit, nature of the ancillary ligand, and central metal ion.[12]

We are reporting here a novel Schiff base compound derived from 2-hydroxy-1-naphthaldehyde and (1*S*,2*S*)-(−)-1,2-diphenylethylenediamine in 2:1 M ratio. There are several reports published on the synthesis of the studied compound in the literature.[13−16] In our work, we discuss the never previously reported crystal structure of the compound, enriched by elemental analyses and spectroscopic studies [Fourier transform infrared (FT-IR) and NMR]. However, we used the methods of quantum crystallography [density functional theory (DFT) calculations and Hirshfeld surface analyses] to provide even better insights into the properties of the structure. We conclude our investigation with an analysis of potential anticancer activity against the colorectal cancer cells HT-29 and SW620. Results suggest potential activity against both types of the studied cancer cells.

RESULTS AND DISCUSSION

All atoms of the studied Schiff base compound [Figure 1] occupy general positions, but the 2-fold rotation axis going through the midpoint of the ethylenediamine C−C bond causes one molecule to be located in two asymmetric units.

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