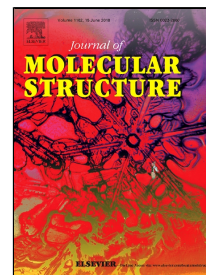


# Accepted Manuscript

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# Different Chemical Behaviors and Antioxidant Activity of Three Novel Schiff bases Containing Hydroxyl Groups. X-ray structure of $\text{CH}_2\{\text{cyclo-C}_6\text{H}_{10}\text{-NH=CH-(2-O-naphth)}\}_2\cdot\text{H}_2\text{O}$

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**Dedicated to Prof Dr. K. C. Kumara Swamy in honor of his 60<sup>th</sup> birthday.**

The antioxidant activities of three new Schiff base compounds, **1** – **3**, were studied through their direct scavenging ability to eliminate free radicals using DPPH and ABTS methods and also through their indirect antioxidant activity as measured using the ferric thiocyanate (FTC) method. The number of OH groups in the compounds and their positions play a role in the activity. The crystal structure of  $\text{CH}_2\{\text{cyclo-C}_6\text{H}_{10}\text{-NH=CH-(2-O-naphth)}\}_2\cdot\text{H}_2\text{O}$  (**1**), has been determined and proves the existence of intramolecular hydrogen-bonds and hydrogen-bonded water molecules and reveals the keto-amine ( $\text{N-H}\cdots\text{O}$ ) tautomer of this compound. One *cyclo*-hexyl ring was found to be disordered, and was resolved in two orientations. Hydrogen atoms of the  $\text{NH=CH}$  groups were located in difference maps and were refined freely. Compounds **2** and **3** exhibit the enol-imine form. The UV-vis spectra of the three compounds have been studied in organic solvents of different polarity, and in basic and acidic media, and were found helpful in understanding the tautomeric forms in these compounds; the polarity was modified by adding ( $\text{CF}_3\text{COOH}$ ) or  $[(\text{C}_2\text{H}_5)_3\text{N}]$  to the solvent. All three compounds have been characterized by elemental analysis, UV-vis, FTIR, NMR and MS.

**Keywords:** UV-vis, crystal structure; hydroxyl Schiff bases; intramolecular H-bonding and tautomers; antioxidant activities; DPPH, ABTS and FTC methods.

## Introduction

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