

Synthesis, Physical Characterization, Antibacterial and Antifungal Activities of 2-((*E*)-1-(2-((*E*)-1-(2-Hydroxyphenyl)ethylideneamino) phenylamino) ethyl) phenol

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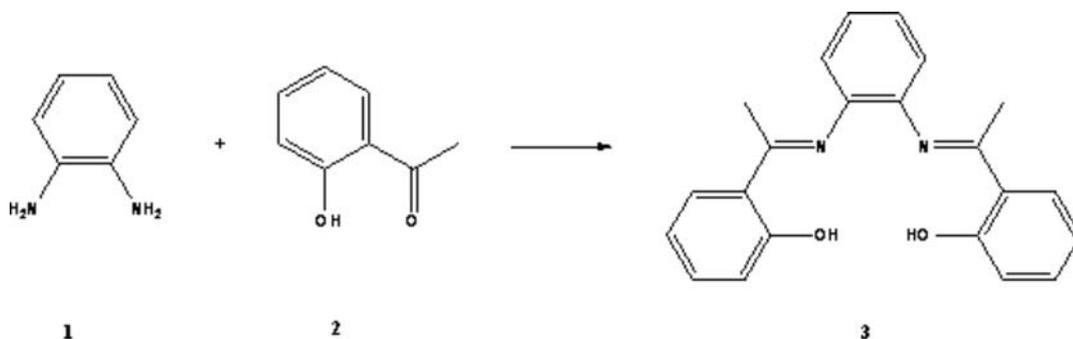
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Abstract:

In this paper we report the synthesis of 2-((*E*)-1-(2-((*E*)-1-(2-hydroxyphenyl)ethylideneamino) phenylamino) ethyl) phenol. In addition to its synthesis we present AM1 and B3LYP/6-31G* calculations to characterize the physical properties of this molecule. Finally, the antifungal and antibacterial activities of this derivative have been evaluated.

Introduction

Schiff bases are an important class of ligands, such ligands and their metal complexes have a variety of applications including biological, clinical, analytical and industrial in addition to their important roles in catalysis and organic synthesis [1]. Those that having multidentate coordination sites are known to form complexes with transition metal ions readily [2]. Such complexes play an important role in bioinorganic chemistry and redox enzyme systems [3] and may provide the basis of models for active sites of biological systems [4] or act as catalysts [5]. Schiff base compounds are of increasing interest because such dinuclear systems are known to act as a paramagnetic building block for multidimensional expanded structures as well as for their important roles in biological systems, e.g., in many metalloenzymes, redox and nonredox proteins and also as a catalyst in olefin epoxidation [6]. Ardakani and his coworkers have reported a selective nitrate PVC membrane electrode from 2-hydroxyacetophenone [7]. Synthesis and metal ion uptake studies of chelating resins by use of 2-hydroxyacetophenone have been reported by Samal [8].



Results and Discussion:

1, 2- phenylenediamine **1** (1.08g, 10mmol) and 2-Hydroxyacetophenone **2** (2.71 g, 20 mmol) were dissolved in 25 ml of warm ethanol. The reaction mixture was refluxed for 7h at 85 °C, and allowed to stand. The solid crystals were filtered off and washed with ethanol. The pure Schiff base **3** was isolated as

S	$42.38515 \cdot \ln(t) + 1150.64098 \cdot t + 29.96975 \cdot t^2/2 - 367.20075 \cdot t^3/3 + 723.17337/(2 \cdot t^2) + 162.84889$	432.48	703.25	1444.07
ΔH	$133.5428 \cdot t + 1417.88899 \cdot t^2/2 - 523.88367 \cdot t^3/3 - 52.55339 \cdot t^4/4 + 0.2264/t - 563.55851$	10.32	63.16	526.8

Table 1. Thermodynamic properties of the molecules in Figure 1-2 (A-B), calculated at the AM1 level and B3LYP/6-31G* level of theory, where C_p is the heat capacity in $\text{J mol}^{-1} \text{K}^{-1}$, S is the entropy in $\text{J mol}^{-1} \text{K}^{-1}$, and ΔH is the standard enthalpy kJ mol^{-1} . These were fitted to the Shomate equations which are implemented by the JANAF tables of the NIST databases. These equations converged to an R^2 value of 0.999 on average.

Antibacterial and antifungal activity tests

Derivative **3** was evaluated for its *in vitro* biological properties against human pathogens [15]. This compound was found to possess no antifungal activities against *S. cerevisiae* (ATCC 28383) and no antibacterial activities against Gram-positive and Gram-negative bacteria have been noticed (Table 2).

Sample CIP	Antimicrobial activity (MIC), $\mu\text{g/mL}$			
	<i>S. cerevisiae</i> (ATCC 28383)	<i>S. aureus</i> (4.83)	<i>C. albicans</i> (1180-79)	<i>E. Coli</i> (54127)
3	>50	>50	>50	>50

Table 2. Antimicrobial activity of Schiff base **3**

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