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## Quinazolinone derivative: Model compound for determination of dipole moment, solvatochromism and metal ion sensing

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### ABSTRACT

A dihydroquinazolinone derivative 2-(2,4-Dimethoxy-phenyl)-2,3-dihydro-1H-quinazolin-4-one (**1**) was synthesized and characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR and FT-IR and its spectral, photophysical, intramolecular charge transfer characteristics were studied by absorption and emission spectroscopy. The compound exhibits significant changes in their photophysical properties depending on the solvent polarity. The observed bathochromic emission band and difference in Stokes shift on changing the polarity of the solvents clearly demonstrate the highly polar character of the excited state, which is also supported by the enhancement of dipole moment of the molecule upon photoexcitation. Solvatochromic shift methods based on Lippert–Mataga, Bakhshiev–Kawski and Reichardt's correlations were applied to calculate the ground, excited and change in dipole moments. The effect of solute–solvent interactions on compound **1** was studied using multi-parameter solvent polarity scales proposed by Kamlet–Taft and Catalan. The interactions of various metal ions on compound **1** were also studied using steady state fluorescence measurements. The emission profile reveals that it acts as on-off type fluorescent chemosensor for selective and sensitive detection of Hg<sup>2+</sup> ions. Complexation stoichiometry and mechanism of quenching were determined from Benesi–Hildebrand and Stern–Volmer plot.

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### 1. Introduction

Quinazolinones and their derivatives symbolizes an important class of N-heterocyclic organic molecules endowed with diverse biological activities such as antitumour, antibiotic, antidiarrhoeal, antipyretic, analgesic, diuretic, antihistamine, antidepressant and vasodilating behavior [1–4]. Apart from their biological point of view, derivatives of quinazolin-4-one are lesser known for their luminescent properties and their photophysical phenomena are only minimally studied [5,6]. Owing to their interesting features in their electronic spectra, quinazolinone derivatives display excellent fluorescence in solutions depending on the solvents and exhibit the phenomenon called excited state intramolecular proton transfer and intramolecular charge transfer (ICT) that have attracted great interest due to good photophysical properties such as intense luminescence, large Stokes shifts and significant photostability [7–9].

The polarity of solvents effects on the electronic absorption and emission spectra of  $\pi$ -conjugated donor-acceptor kind of molecules gives an insight into the photophysics of their excited states [10,11]. The spectral details can be used to extract important information as the environment of the solvent largely regulates the changes in the electro-optical properties of the probe molecule [12]. The spectral behavior of the solute

molecule largely depends on the strength of the intermolecular forces between the substituent groups of the solute molecule and physical properties of the surrounding solvent molecules such as polarity, polarizability and dielectric constant. Correlation of absorption and emission spectra with the solvent parameters attract much attention because of their application as suitable probes for the determination of solvent polarity, dipole moment and potential applications for pH sensors [13].

There has been an excessive deal of attention in the growth of numerous probes for the selective detection of transition metal ions owing to their essential role in industrial and biochemical processes. Although metals are essential for the metabolic activity of living organism, elevated levels of metal will be toxic and therefore causes severe damage to organs and wide variety of diseases [14]. For instance, copper is the third most abundant metal in the human body and considered as one of the vital nutrients for plants and animals, but prolonged exposure of copper can lead to diseases like vomiting, headaches, stomach-aches, dizziness, and even cause brain damage [15–17]. Conversely, Fe<sup>3+</sup> ion is an essential element and serves as a carrier of oxygen to tissues from the lungs by hemoglobin as a transport medium but it may cause eye disorders in some cases at higher concentration [18,19]. Owing to these significant importance, it is extremely preferred to spot them in the related systems.

Design and synthesis of fluorescent chemosensors based on fluorescence intensity modulation upon binding to transition metal ions species has formed the basis for the construction of many reported

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fluorescence sensors [20,21]. Development of chemosensors for the selective and efficient detection of chemically and biologically important ionic species has drawn considerable attention since years [22]. Mostly, conjugation of a well-established and efficient binding site with a suitable signaling moiety is the most rewarding approach for sensitive and selective detection of the target guest. Due to the concern over the toxic effect of mercury on the environment and human health, the design of molecules that can induce prominent spectroscopic changes upon selective binding of  $\text{Hg}^{2+}$  ions is highly desirable for ease of quantifications and signal transductions. The present stratagem aims toward the photophysical studies of dihydro quinazolinone derivative using selected traditional solvent polarity functions and empirical scales of solvent polarity to describe the solvatochromism and unravels the potential as a sensor for polarity and turn off fluorescence chemosensor for  $\text{Hg}^{2+}$  ion by applying steady state absorption and emission spectroscopy.

## 2. Experimental

### 2.1. Materials

Spectroscopic grade solvents used in this work were obtained from Sigma–Aldrich and used without further purification. The solvents were found free from impurities and appeared transparent in the spectral region of interest and verified by recording the emission spectra in the studied spectral region. 2-Aminobenzamide was purchased from BDH organics and 2,4 dimethoxy benzaldehyde from Aldrich chemicals. The solvents used in this work were, Toluene, Acetonitrile, DMF, Chloroform, THF, Ethyl acetate, Ethylene glycol, Propanol, Methanol, and water. Stock solution the title compound was prepared and dilutions of this were prepared for UV–visible and fluorescent study at different concentrations. Stock solutions of the salts of  $\text{Ag}^{1+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Hg}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Sr}^{2+}$  and  $\text{Pb}^{2+}$  were prepared in ethanol and test solutions for metal ion detection were prepared by diluting appropriate aliquot of each metal ion stock and compound stock solution to desired concentration.

### 2.2. Spectral measurements

Melting points were determined using a Gallenkamp melting point apparatus; about 1 mg of the compound was taken into melting point capillary tube by gently tapping the base of the capillary tube and then carefully placed into the apparatus. Slowly heated the sample and the reading was taken when the first bit of liquid was observed. Infrared (IR) spectra were recorded on Shimadzu FT-IR 8400S infrared spectrophotometer using the KBr pellets. The NMR ( $^1\text{H}$  and  $^{13}\text{C}$ ) spectra were recorded on a Bruker DPX-600 at 600 MHz and 150 MHz, respectively, using TMS as the internal standard. The chemical shift values are documented on  $\delta$  scale and coupling constants (J) in Hertz; Splitting patterns were

entitled as follows: s: singlet; d: doublet; m: multiplet. UV–Vis electronic absorption spectra was recorded on a Shimadzu UV-160A spectrophotometer, and the steady-state fluorescence spectra were measured using Varain Cary Eclipse spectrofluorophotometer using a rectangular quartz cell of dimensions 0.2 cm  $\times$  1 cm. The emission was monitored at right angle. The fluorescence quantum yield ( $\phi_f$ ) in different solvents were measured using a comparative method where quinine sulfate [9] was used as the reference and calculated using Eq. (1):

$$\phi_u = \phi_s \times \frac{I_u}{I_s} \times \frac{A_s}{A_u} \times \frac{n_u^2}{n_s^2} \quad (1)$$

where  $\phi_u$ ,  $\phi_s$  are the fluorescence quantum yields of the unknown and standard, respectively,  $I$  denote the integrated emission intensity;  $A$  is the absorbance at excitation wavelength, and  $n$  denote the refractive index of the solvent. The subscript  $u$  and  $s$  stand for the unknown and standard, respectively.

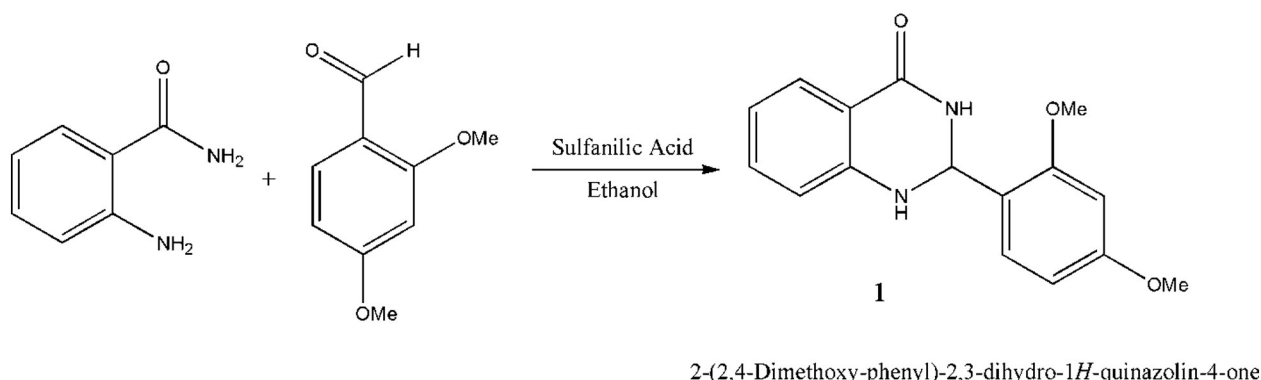
Synthetic procedure for 2-(2,4-Dimethoxy-phenyl)-2,3-dihydro-1H-quinazolin-4-one (**1**).

The title compound was synthesized by the sulfanilic acid catalyzed reaction between 2-amino benzamide and 2, 4-dimethoxy benzaldehyde in aqueous ethanol [23]. A mixture of 2-amino benzamide (10 mmol), 2,4-dimethoxy benzaldehyde (10 mmol) and sulfanilic acid (1 mmol) in 50% aq ethanol (25 mL) was stirred at 70 °C and the reaction progress was monitored by TLC. The obtained product was collected by simple filtration and washed with 50% aq ethanol and purified by crystallization using aq ethanol to get the product as white solid. The structure of the compound was confirmed by IR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR. Melting point 174–176 °C;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  = 5.75 (s, 1H), 6.65–6.90 (dt, 1H,  $J$  = 0.8 and 7.8 Hz, Ar–H), 6.69–6.72 (dd, 1H,  $J$  = 0.4 and 7.6 Hz, Ar–H), 7.08 (s, 1H), 8.24 (s, 1H), 7.22–7.26 (m, 1H, Ar–H), 7.34–7.41 (m, 3H, Ar–H), 7.48–7.50 (m, 2H, Ar–H), 7.60–7.62 (dd, 1H,  $J$  = 1.6 and 8.0 Hz, Ar–H) 3.34–3.38 (s, 6H, Ar-OMe);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  = 67.2, 80.4, 112.4, 114.9, 118.1, 128.8, 128.3, 128.6, 128.4133.3, 141.6, 147.8, 173.6; IR (KBr): 3027, 1569, 1492, 1417, 1360, 1153, 803, 707, 636. IR (KBr): 3227, 1669, 1492, 1417, 1360, 1153, 803, 707, 636.

## 3. Results and discussion

### 3.1. Chemistry

Dihydro quinazolinone derivative 2-(2,4-Dimethoxy-phenyl)-2,3-dihydro-1H-quinazolin-4-one (**1**) having intramolecular charge transfer characteristics have been synthesized and characterized. Lippert–Mattaga and Reichardt's correlations were applied to calculate the change in dipole moments of these molecules. Solvents having different polarity have been used to investigate the solvent effect on the absorption and emission spectra in detail. The structures of compounds were confirmed by IR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR and Scheme 1 outlines the



Scheme 1. Synthetic route of Compound 1.

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