

# A Multifunctional Probe For Selective And Sensitive Detection of Tryptamine And Fions Based on A Novel 5-Bromoindolehydrazone Anchored Diiodo Salicylaldehyde Derivative

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## Abstract

2-((5-bromo-1H-indol-2-yl) methylene) hydrazone) methyl)-4, 6-diiodophenol (BHDL), a novel indole-based chemosensor, has been created for the selective and sensitive detection of biogenic tryptamine and F ions. UV-visible/fluorescence spectroscopy was used to examine the binding affinity of probe BHDL for F/tryptamine (TryptA). Probe showed a substantial elevation in an emission band at 433 nm in the presence of TryptA, while the band at 555 nm suffered a blue shift with a decrease in intensity due to suppression of Excited State Intramolecular Proton Transfer (ESIPT) on BHDL. Due to the inhibition of ESIPT and deprotonation process began by the hydrogen bonding complex formation, complexation with F ions also causes an increase in a fluorescence band at 430 nm with the simultaneous disappearance of the emission band at 555 nm. Furthermore, Density Functional Theoretical (DFT) calculations were done to support the mechanism that worked on the probe BHDL when TryptA/F was present.

**Keywords:** Chemosensor; BHDL; ESIPT; Tryptamine; Fluoride ion

## Introduction

Because of its potential application in pharmacology, physiology, and environmental production, fluorescent detection of biological and environmentally relevant species has become a recent emphasis. Because of the preferential binding ability of metal ions in water, various fluorescence sensors were initially created solely for the detection of metal ions [1]. Because of its potential application in pharmacology, physiology, and environmental production, fluorescent detection of biological and environmentally relevant species has become a recent emphasis. Because of the preferential binding ability of metal ions in water, various fluorescence sensors were initially created solely for the detection of metal ions. Fluoride, as a strong electronegative element, can interfere with a variety of enzyme systems, and hence functions as an enzyme inhibitor. It can be found in biological fluids and tissues, particularly bone and tooth [2]. The link between high fluoride levels in drinking water and skeletal fluorosis has been widely recognized.

Fluoride, on the other hand, can benefit human health by treating osteoporosis and safeguarding tooth health. As a result, detecting F<sup>-</sup> is critical in order to reduce its direct effects on human health. Nitrogenous organic bases or deaminated derivatives of amino acids are biogenic amines. Grapes, food, and beverages are natural sources of biogenic amines, which can be produced through fermentation or microbial decarboxylation of amino acids. Biogenic amines are a key component in the creation of hormones, alkaloids, nucleic acids, and proteins [3]. Tryptamine (TryptA), a natural product of biogenic amines, can affect a variety of activities in the central nervous system, including sleep, cognition, memory, temperature regulation, and behaviour. As a result, the detection and quantification of TryptA is critical since it has a substantial pharmacological effect. Because of their simplicity, excellent selectivity, sensitivity, and versatility, fluorescence sensor detection stands out among classic analytical approaches for exploring ions and neutral substances. Furthermore, combining many targets with a single receptor would allow for faster analytical processing and cost savings. As a result, developing a sensor that recognises both TryptA and F<sup>-</sup> above other competing anions/biogenic amines using multiple optical modes is extremely desirable. Because of their important function in biological activity, indoles have gained a lot of attention from scientists. They are the core structure of a

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lot of inhibitor and therapeutic compounds

The fact that the majority of indole derivatives are fluorescent has led to the development of indole-based receptors for selective chemosensing of metal ions and anions. We have used a simple condensation approach to manufacture a novel indole-based dual mode chemosensor BHDL, which has been used for the selective and sensitive detection of TryptA and F<sup>-</sup> in DMSO/H<sub>2</sub>O (9:1, v/v) medium [4].

### The Effect of BHDL on Biogenic Amines Was Studied Using Uv-Vis and Fluorescence

In order to develop a bifunctional chemosensor, we also tested the sensitivity of the probe BHDL to biogenic amines in the presence of other important aliphatic, aromatic, and biogenic amines such as azane, methylamine, dimethylamine, trimethylamine, phenylethylamine, spermidine, spermine, tyramine, cadaverine, serotonin, histamine, L-tryptophan. We can deduce from these findings that both components are in equilibrium and display noticeable colour shifts in this state. In addition, the fluorescence sensing potential of BHDL towards amines in a DMSO/H<sub>2</sub>O (9:1, v/v) mixture was investigated. In contrast, when competing biogenic amines were added to the probe BHDL, there was no difference in fluorescence intensity, with the exception of TryptA [5].

### BHDL DFT Investigations Using TryptA/F Ions

DFT simulations were also performed to aid the fluorescence amplification of probe BHDL binds with TryptA/F<sup>-</sup>. Using the DFT/B3LYP6-311G/LANL2DZ basis set, the ground state optimal geometry of probe BHDL and BHDLTryptA and BHDL-F<sup>-</sup> complexes was discovered. The HOMO-LUMO energy gap was reduced when BHDL complexed with TryptA/F<sup>-</sup> ion, according to these findings. The HOMO and LUMO are delocalized over the diiodo moiety in probe BHDL, but the LUMO is diffused over the indole unit. HOMO is diffused over the diiodo moiety alone when complexed with TryptA, whereas the LUMO is localised in the TryptA moiety alone. When BHDL interacts with F<sup>-</sup>, it inhibits ES IPT and deprotonates -OH proton processes, resulting in ratiometric responses in absorption bands at 372 nm and 492 nm, as well as an increase in fluorescence band at 430 nm and a decrease in emission band at 555 nm [6].

The goal of the current work is the amalgamation of 1,2,3-triazole subordinates and assessment of their movement as consumption inhibitor for carbon steel in destructive conditions.

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