

# Union and Optical Properties of Pentamethine Cyanine Dyes with Carboxylic Acid Moieties

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## ABSTRACT

Cyanine colors having carboxylic corrosive gatherings have been utilized in a wide range of fields of study. The corrosive gatherings can go about as handles for bioconjugation or as metal chelators. A few pentamethine cyanine colors with propionic corrosive handles were combined and their optical properties were concentrated to decide their convenience as fluorescent tests. The optical properties thinks about performed incorporate the absorbance and discharge maxima values and in addition the estimation of quantum yield and sub-atomic splendor levels. Sub-atomic models were likewise computed to help examine the colors' conduct and were contrasted and comparative colors with changing alkyl chain lengths supplanting the corrosive moieties.

**Keywords :** Carboxylic Acid, Pentamethine, Cyanine, Optical Properties

## I. INTRODUCTION

Since the disclosure of a blue carbocyanine compound in 1856,<sup>1</sup> the cyanine class has been contemplated widely for different applications, for example, in vivo imaging,<sup>2-6</sup> ex vivo imaging (pH detecting and DNA stains),<sup>7,8</sup> blood scatter analysis,<sup>9</sup> and sun powered vitality conversion.<sup>10</sup> The enthusiasm for the utilization of these colors for the treatment and imaging of malignancy and different maladies has expanded in the previous couple of decades. Colors, and specifically polymethine cyanine colors, can be depended on amid tumor location of numerous malignancies with methods, for example, attractive reverberation imaging (MRI) and positron emanation tomography (PET), and intraoperatively continuously. Progressively, there is an enthusiasm for utilizing close infrared (NIR) colors for imaging carcinomas because of the numerous particular properties of the cyanine color family. A cyanine color atom comprises of 2 nitrogen-containing heterocycles associated by a

prolonged, unsaturated carbon chain. The carbon tie adds to the general state of the atom being straight. The length of this chain decides the wavelength at which the colors ingest and fluoresce light. On the off chance that the length of the polymethine connect is reached out by 1 twofold bond, the absorbance and fluorescence maxima red move by around 100 nm.<sup>5</sup> This places the wavelengths of the colors in what is known as the NIR window. The NIR window lies between around 650 and 900 nm, and it is a critical paradigm to configuration colors inside this wavelength go for in vivo imaging. Body tissue will autofluoresce light at wavelengths lower than 650 nm, while water ingests light over 1000 nm; the area between these 2 limits is exceptionally important for tissue imaging.

The cyanine color class is likewise profoundly modifiable, with precedents of substitution on each position existing in the literature.<sup>2</sup> Another advantageous property of cyanine colors is their

moderately restricted excitation band from S0 to S1.14 Cyanine colors highlighting alkyl carboxylic acids have been already investigated widely for both color sharpened sun based cells and conjugation of different gatherings onto the dye.15– 19 Researchers have exploited a few key properties of the corrosive group(s) joined onto the chromophore: (1) the watersoluble idea of the corrosive gatherings, as this takes into consideration the investigation of bigger, bulkier gatherings somewhere else on the color and for fluid in vivo studies20; (2) the pH affectability of the corrosive groups21; (3) the metal-restricting capacity of the corrosive gatherings, or, in other words color sharpened sun powered cells to grapple the color onto a metal surface; and (4) the capacity of the corrosive gatherings to be functionalized as a connection to other focusing on ligands. Even however colors containing alkyl acids exist and have been utilized for fluctuating applications, there is an extraordinary absence of distributed material accessible with regards to the optical proficiency of these colors. The present writing has not yet addressed whether the carboxylic corrosive gatherings influence the state of the color or the by and large optical properties of the colors on the off chance that they are outside the conjugated framework.

Besides, lead chromophores that use the COOH handle for further ligand conjugation have been totally overlooked when considering their optical properties. Thus, an arrangement of 6 cyanine tests was blended and their optical effectiveness was considered. To accomplish this errand, the absorbance and fluorescence spectra were gotten. From these informational indexes, the molar absorptivity ( $\epsilon$ ), quantum yield esteems ( $\phi$ ), and sub-atomic brilliance esteems are inferred. These qualities are significant for the execution of the colors as they demonstrate the general effectiveness and value of the lead tests. The atomic splendor is, for this situation, the result of the 2. By setting a lower-end adequate edge for these 3 optical properties, potential compound contender

for in vivo studies can be viably separated from unsuitable particles.

## II. EXPERIMENTAL

### *Instrumentation*

Absorbance spectra were estimated utilizing a Cary 50 spectrophotometer (Varian, Palo Alto, CA, USA) interfaced to a PC, with an unearthly transmission capacity of 2 nm. Fluorescence spectra for the pentamethine cyanine colors were acquired utilizing a Shimadzu RF-1501 Spectrofluorophotometer (Shimadzu Scientific Instruments, Columbia, MD, USA) interfaced to a PC, with the phantom data transmissions for both excitation and emanation set to 10 nm and the affectability set to high.

### *Stock solutions*

Stock arrangements of the colors were set up by gauging the strong on a 5-digit scientific equalization straightforwardly into a dark colored glass vial and including dimethyl sulfoxide (DMSO) (99.9% for spectroscopy; Acros Organics, Bridgewater, NJ, USA) through a class A volumetric pipette (Kimble/Kontes, Vineland, NJ, USA). The substance of the vial were vortexed for 20 seconds and afterward sonicated for 5 minutes to guarantee finish disintegration. The stock arrangements were shielded from light and put away in the cooler when not being used.

### *Method for determining molar absorptivity*

Stock arrangements were utilized to get ready sequential weakenings in ethanol or phosphate-supported saline (PBS) running from 0.8 to 16  $\mu$ M. Tests were set up in 5.00 ( $\pm$ 0.02) and 10.00 ( $\pm$ 0.02) mL volumetric jars utilizing a 5-to 50- $\mu$ L Micropipette 821 and a 200-to 1000- $\mu$ L Pipetman (P1000) micropipette (Gilson, Inc., Middleton, WI, USA). The absorbance range of each example was estimated utilizing the Cary 50 spectrophotometer (Varian, Palo Alto, CA, USA), and the absorbance at the wavelength of greatest absorbance ( $\lambda_{max}$  AB) was

resolved. The absorbance esteems ( $A_n$ ) of each example at  $\lambda_{max}$  AB were plotted as an element of color fixation (C), and the direct relapse condition utilizing Excel was registered.

### III. COMPUTATIONAL METHODS

The structure of each compound was first optimized using the Hartree-Fock Density Functional Theory (HF-DFT) method with the hybrid exchange-correlation functional B3LYP/6-31G\* basis set using Spartan '14 (Irvine, CA, USA). The torsional angles from the quaternary nitrogen to the  $\alpha$ -carbon on the alternate heterocycle were restricted to obtain the calculated absorbance values and highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The electrostatic potential maps and the calculated HOMO and LUMO orbitals were obtained using a restricted hybrid HF-DFT self-consistent field in vacuum performed with B3LYP/6-31G\* basis set.

#### *Optical properties and molecular modelling*

The optical properties of compounds 4a-f (Scheme 1) were measured separately in either an ethanol solution or a phosphate buffer, pH 7.4, and the collected data. A stock solution of 1 mM was made by weighing 2.0 mg of each dye which then was dissolved with the necessary amount of DMSO depending on the molecular weight of the compound. From the stock solution, dilutions with either ethanol or PBS to achieve working samples of 16, 14, 12, 10, 8 and 6  $\mu$ M were tested. The absorption values and excitation and emission profiles from 400 to 800 nm of each sample were obtained. To obtain the fluorescence spectra, a 10-times dilution from the absorption sample was performed so as to not flood the detector.

### IV. CONCLUSIONS

The optical properties of cyanine colors highlighting carboxylic acids stay unstudied and unpublished. In

this investigation, 6 cyanine mixes, 4a-f, were blended and their optical properties were broke down to take in more about the impacts that carboxylic corrosive gatherings would have on the general atom structure. The proficiency of the colors was broke down in 2 distinct solvents, one natural and one fluid, to watch the dissolvable impacts. When taking a gander at the patterns for the indolenine colors, the molar absorptivities of the colors 4a-c diminished with expanding hydrophobicity managed from expanding halogen measure on the extension.

Generally, the atomic splendor estimations of the colors don't really make these colors reasonable for in vivo representation of tissues. In any case, future in vivo studies could be performed to decide the inalienable take-up and biodistribution of these colors. Different perceptions through atomic demonstrating were seen and used to think of a speculation of how the structure influences the optical properties of the colors. In examination with alkyl chain (methyl or butyl) substituted indolenine mixes, there was noteworthy puckering of the atom that changes the bearing in which the hydrogens and substituents on the unsaturated scaffold point. The puckering might be because of the intramolecular dimerization of the carboxylic corrosive gatherings.

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