Analysis of fluorescence quenching of newly synthesized Coumarin-triazol derivative

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Abstract: Around the world, the number of cases of diabetes has been rising rapidly in recent decades, and one of the most exciting fields of research is the search for small chemicals with strong anti-diabetic properties. Diabetes mellitus (DM) is a chronic metabolic condition characterized by an increase in blood glucose levels due to an imbalance in glucose homeostasis [1, 2]. Two relatively prevalent risk factors that contribute to both neurological diseases and cardiovascular disease are type 2 diabetes and hypertension [3]. With decades of history and potential for growth, heterocyclic chemistry has dominated the field and is essential to the synthesis of new medications. Among the heterocycles, triazoles and coumarins received the most attention due to their significant biological activity and natural occurrence. Coumarins are prepared via Pechmann condensation, catalytic annulation phenolic acetates with acrylates [4], $ZnBr_2$ catalyzed reaction of salicylaldehyde with ynamides [5], Amberlyst-15 catalyzed reaction of 1,3-dihydroXybenzene and ethyl acetoacetate under micro- wave irradiation in a solvent free conditions [6] etc. Naturally occurring coumarins in the glycoside forms are useful in medicine [7], and coumarins shows antimicrobial [8], anti-HIV [9], radical scavenging [10], and anti-viral [11] properties.

Key Words: AMTCC, Fluorescence quenching, Diffusion Coefficient, Activation Energy

I. Introduction

The compound known as coumarin traizole derivatives has attracted significant attention in the field of medicinal chemistry due to its biological significance and use in the pharmaceutical sectors. According to a recent review [12], they display a variety of biological actions, including antibacterial, analgesic, anti-inflammatory, antipyretic, antihypertensive, and anticancer properties. Fluorescence quenching is a phenomenon that results in a decrease in the lifetime and intensity of fluorescence molecules, resulting in spontaneous emission. In general, it is a process where in the electronic excitation energy of an excited molecule is transferred to a quencher molecule through a variety of methods, including charge transfer and diffusion, resulting in the quencher molecule's non-fluorescent emission [13]. The Stern-Volmer relation is used to study the fluorescence quenching of 3-(4-Amino-5-mercapto-4H-1,2,4-triazol-3-yl)-chloro-2H-6chromen-2-one (AMTCC) molecules by aniline [14]. It is given by

$$\frac{F_0}{F} = 1 + K_{SV}[Q] \qquad (1)$$

where F_0 and F represent the fluorescence intensities, respectively, in the absence quencher and quencher conditions. Ksv represents the S-V constant, τ_0 denotes the solute lifespan without quencher, and [Q] indicates the quencher concentration.

II. Materials and Methods

The coumarin-triazole derivative are produced a suspension of the potassium salt of coumarin thiocarbazinate in water (5 mL) was dissolved with 10 mmol of hydrazine hydrate. In a water bath, the mixture reacted for eighteen to twenty hours. After the reaction was carried out until a homogenous reaction mixture was obtained, a color shift associated with the release of H_2S was noticed. Subsequently, the solution was lowered in temperature and diluted using 20 milliliters of cold water. It was then neutralized using diluted hydrochloric acid to extract the desired chemicals, which were then separated from ethyl alcohol 3-(4-Amino-5-mercapto-4H-1,2,4-triazol-3-yl)-chloro-2H-6chromen-2-one (AMTCC) molecule is Obtained as pale yellow solid in 61% yield with R=H, R'=H and R''= Cl as shown in fig.1.The spectroscopic grade solvents methanol, ethanol, proponal, heptanol, and ethyl acetate were purchased from S.D Fine Chemicals Ltd. in India. Before usage, the quencher aniline passed a double distilled and a purity test. All five solvents having solutions prepared with the solute with concentration is fixed at 1×10^{-5} M and the quencher concentration ranging from 0.00 to 0.10 M
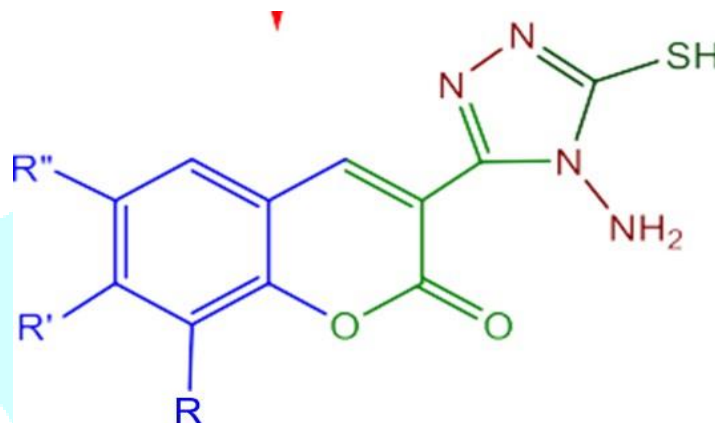

Fig.1.Molecular structure of AMTCC

III. Results and Discussion

At room temperature, the fluorescence spectra of the 3-(4-Amino-5-mercapto-4H-1,2,4-triazol-3-yl)-chloro-2H-6chromen-2-one (AMTCC) molecule are recorded for five different solvents at various quencher concentrations as shown in fig.2.
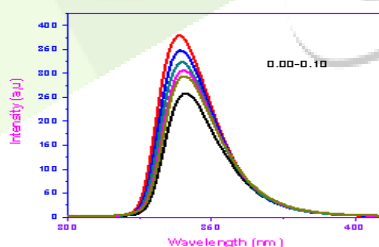

Fig.2. Emission spectra of AMTCC with varying quencher concentration

The Stoke's Einstein equation (2) can be used to estimate the diffusion coefficients of the solute D_S and the quencher D_Q [15].and Table 1 displays these results.

$$D = \frac{KT}{a\pi\eta R} \qquad (2)$$

where "a" is the Stoke's Einstein number, which is equal to a = 6 for a solute and a = 3 for a quencher. K, T, and η represent for the Boltzmann constant, temperature, and solvent viscosity, respectively.

$$k_d = 4\pi N' DR\left[1 + \frac{R}{(2D\tau_0)^{1/2}}\right] \qquad (3)$$

The Avogadro's number is N'. The Edward method [16] is used to estimate the sum of the radii of the quencher and solute. Equation (3) is used to estimate the diffusion rate parameter kd,

$$p = \frac{k_q}{k_d} \qquad (4)$$

Additionally, equation (4) was used to determine the probability of quenching each encounter p the results are displayed in Table 1. Equation (5) is used to estimate the activation energy of quenching,

$$E_a = E_d + RT \ln\left(\frac{1}{p} - 1\right) \qquad (5)$$

Table.1: The various quenching rate parameters of for AMTCC molecule.

IV.

Solvent	$k_q X10^9$ $(M^{-1}s^{-1})$	$k_d X10^9$ $(M^{-1}s^{-1})$	$DX 10^{-5}$ $(cm^{-1}s^{-1})$	p	E_d (kcal/M)	E_a (kcal/M)
Methanol	1.59	200.46	3.69	0.0079	3.05	14.68
Ethanol	0.61	139.02	2.12	0.0043	3.02	14.70
Proponal	1.20	55.01	1.02	0.0218	3.58	21.76
Heptanol	2.10	315	1.05	0.0066	3.76	22.08
Ethyl acetate	2.18	324	4.98	0.0067	2.60	5.02

Conclusion

In summary, the AMTCC molecule undergoes fluorescence quenching by aniline in five different solvents at room temperature. The value of p is calculated and also the values of E_a are greater than E_d in all five solvents studied. It is in referred that the fluorescence quenching reactions in AMTCC molecule are more significantly affected by activation energy.

REFERENCES:

[1].S. Odeyemi, J. Dewar, In vitro antidiabetic activity affecting glucose uptake in hepg2 cells following their exposure to extracts of Lauridia tetragona (L.f.) R.H. Archer, Processes 8 (2020) 33.

[2]. N. Holman, B. Young, R. Gadsby, Current prevalence of Type 1 and Type 2 diabetes in adults and children in the UK, Diab. Med. 32 (2015) 1119–1120.

[3].J.R. Petrie, T.J. Guzik, R.M. Touyz, Diabetes, hypertension, and cardiovascular disease: clinical insights and vascular mechanisms, Can. J. Cardiol. 34 (2018) 575–584.

[4].H.J.Yoo.Catalysed one part synthesis of Coumarins.Org.letter 21(2019),3422-3426.

[5].M. Tasior, Y.M. Poronik, O. Vakuliuk, B. Sadowski, M. Karczewski, D.T. Gryko, V-Shaped bis-coumarins: synthesis and optical properties, J. Org. Chem. 79 (2014) 8723–8732.

[6].J.Amarao.Coumarin derivative solvent.J.lumisence (2017),2072.

[7].K. Ostrowska, Coumarin-piperazine derivatives as biologically active compounds, Saudi Pharmaceut. J. 28 (2020) 220–232

[8]. N.Renuka. Synthesis and biological evaluation bearing coumarin moiety as potent antimicrobial agents, Philip. J. Sci. 144 (2015) 91–96.

[9]. X.-M. Peng, G.L.V. Damu, C. He Zhou, Current developments of coumarin compounds in medicinal chemistry, Curr. Pharmaceut. Des. 19 (2013) 3884–3930

[10].P.Gurunanjappa.Synthesis ofCoumarin derivative1,3-oXazines as potent antimicrobial and antioXidant agents, Pharm. Chem. J. 51 (2017) 582–589.

[11].J.R. Hwu, S.-Y. Lin, S.-C. Tsay, E. De Clercq, P. Leyssen, J. Neyts, Coumarin Purine ribofuranoside conjugates as new agents against Hepatitis C Virus, J. Med. Chem. 54 (2011) 2114–2126.

[12]. S. Dubey, P.A.Bhosle. Med. *Chem. Res.* DOI 10.1007/s00044-015-1398-5 (2015).

[13]. J.R. Lackowicz. Principles of Fluorescence Spectroscopy New York (1983).

[14]. M. Basanagouda, M. V. Kulkarni. *Synthetic Communications*. **41,** 2569 (2011).

[15]. A. Einstein. Investigations on the Theory of Brownian movement, New York (1956).

[16]. J. T. Edward, *Chem. Edu.* **47** (1970).